SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
INTERNATIONAL VIRTUAL CONFERENCE

SOUTHERN
BRAZILIAN
JOURNAL OF CHEMISTRY

ESTABLISHED IN 1993

FROM 1993-2022

PROCEEDINGS OF THE 2021 INTERNATIONAL VIRTUAL CONFERENCE

SOUTHERN
JOURNAL OF SCIENCES

ESTABLISHED IN 1993

2022 – FORWARD

2022

ISBN 978-65-996490-0-4

Southern Journal of Sciences [recurso eletrônico] :
S727 Southern brazilian journal of chemistry 2021 international virtual conference. / comissão organizadora Luis Alcides Brandini De Boni; Walter José Peláez... [et al.]. – Nova Prata - RS, 2022.
VI, 410 f. : il. ; 29 cm.

ISBN 978-65-996490-0-4

1. Química. 2. Ciências médicas. 3. Engenharia. 4. Medicina veterinária. 5. Educação. I. Southern Brazilian Journal of Chemistry 2021 International Virtual Conference. II. De Boni, Luis Alcides Brandini. III. Peláez, Walter José.

CDD 23. ed. 500
600

ISBN: 978-65-996490-0-4
9 786599 649004

Open Access and Copyright Information

All articles published by the Southern Brazilian Journal of Chemistry (Southern Journal of Sciences) are made immediately available worldwide under an open-access license, Creative Commons Attribution License (CC BY 4.0). This means:

- everyone has free and unlimited access to the full text of all articles published in the Southern Brazilian Journal of Chemistry (Southern Journal of Sciences);
- everyone is free to reuse the published material if proper accreditation/citation of the original publication is given;
- Open access publication is supported by the authors' institutes or research funding agencies by payment of an Article Processing Charge (APC) for accepted articles.

Open Access journals are no different from traditional subscription-based journals; they undergo the same peer-review and quality control as any other scholarly journal. Moreover, Open Access allows for maximum visibility, uptake, and use of the published material.

Why Open Access?

- Quick discoverability: With open access, researchers can read and build on the findings of others without restriction.
- Public enrichment: Much scientific and medical research is paid for with public funds. Open access allows taxpayers to see the results of their investments.
- Research exchange: Open access means that teachers and their students access the latest research findings throughout the world.

Permissions

No special permission is required to reuse all or part of an article published by the Southern Brazilian Journal of Chemistry (Southern Journal of Sciences), including figures and tables. For articles published under an open access Creative Common CC BY license, any part of the article may be reused without permission, provided that the original article is clearly cited. Reuse of an article does not imply endorsement by the authors or the Southern Brazilian Journal of Chemistry.

Copyright Information

Authors who publish with this journal agree to the following terms:

- The authors retain the copyrights and grant the journal right of first publication with the work simultaneously licensed under a Creative Commons Attribution License (CC BY 4.0), which permits use, sharing, adaptation, distribution, and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made. The images or other third-party material in this article are included in the article's Creative Commons license unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons license and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder.
- The authors can enter into separate, additional contractual arrangements for the non-exclusive distribution of the journal's published version of the work (e.g., post it to an institutional repository or publish it in a book), with an acknowledgment of its initial publication in this journal.
- Authors are permitted and encouraged to post their work online (e.g., in institutional repositories or on their website) prior to and during the submission process, as it can lead to productive exchanges, as well as earlier and greater citation of published work (Effect of Open Access).

Book organizer

- Luis Alcides Brandini De Boni, Ph.D., Brazil, TQG. *Co-Chair of the conference. Event Treasurer*.

Editorial comission

- Eduardo Goldani, Ph.D., Brazil, TQG. *Chair of the conference*.
- Walter José Peláez, PhD, Argentina, UNC. *General Secretary*
- Oana Maria Popa, Ph.D., Romania, Eurofins Romania.
- Teresa M. Roseiro Maria Estronca, PhD., Portugal, UC.
- Ketevan Kupatadze, PhD., Georgia, ISU.
- Shaima R. Banoon, MsC., Iraq, University of Misan.
- Francisco José Santos Lima, Ph.D., Brazil, UFRN.
- Carlos Eduardo Cardoso, Ph.D., Brazil, Universidade de Vassouras.
- Sérgio Machado Corrêa, Ph.D., Brazil, UERJ.
- Andrian Saputra, Ph.D., Indonesia, University of Lampung.
- Marcos Antônio Klunk, Ph.D., Brazil, UNISINOS.
- Andrey Vladimirovich Sevbitov, Ph.D., Russian Federation, Sechenov University.
- Olga D. Polezhaeva, Ph.D., Russian Federation, Russian Presidential Academy of National Economy and Public Administration.
- Daniel Ricardo Arsand, Ph.D., Brazil, IFSul.
- Élcio J. de Oliveira, Ph.D., Sweden, Luleå Tekniska Universitet.
- Rafael Rodrigues de Oliveira, PhD., Brazil, Neoprospecta.
- Masurquede de Azevedo Coimbra, M.Sc., Brazil, LACEN-RS.
- Gerzon E. Delgado, Ph.D. Venezuela, Universidad de los Andes.
- Paulo Sergio Souza, Ph.D., Brazil, Fundação Osorio.
- Danyelle Medeiros de Araújo Moura, Ph.D., Brazil, UFRN.
- Isaac Newton Lima da Silva, Ph.D., Brazil, PUCRS.
- Denise Alves Fungaro, Ph.D., Brazil, IPEN.
- Jorge Fernando Silva de Menezes, Ph.D., Brazil, UFRB.
- Cristián Andrés Quintero, Ph.D., Argentina, Universidad Juan Agustín Maza

PREFACE

This book is the product of a conference organized to celebrate the 30 years of the Southern Brazilian Journal of Chemistry. It was the first time in the history of the journal that such a dynamic project was put in motion. This new form of interaction between the journal and the Universities, authors, and speakers was very positive, and the journal team considered repeating it in collaboration with it's partners.

The journal and the Conference organizing committee are extremely grateful to the supporting institutions, from Brazil the Vassouras University; IFSul; UERJ; UFRN; IPEN; AEB; IFRJ; UFRB; ABQRS; ITA; and CRQ-V. From Georgia ISU. From Kazakhstan Satbayev University. From Argentina University of Cordoba and INFIQC. From South Korea INNOSPACE. From Venezuela ULA. From Colombia UDFJC. From Nigeria, the University Of Ilorin. From Russia I.M. SECHENOV FMSMU. From Ecuador UTA. We hope to keep counting on your trust in the years to come.

The readers of this book may note that two dates are present in the conference date. This is because there was a change in the conference schedule, and we decided not to bother the authors with these details since, at present, we have bigger things to concern ourselves about, such as a virus with unknown origins and a horrible war where brother has turned against brother. Let God have mercy on us.

Please scan the QR-Code below the image to remember the opening ceremony and the announcements done during the conference.

SCAN ME

Please visit the journal's new website at https://sjofsciences.com/.

BEST POSTERS SELECTED BY THE PARTICIPATING AUTHORS

1. **TITLE**: SELF-ASSEMBLED MULTILAYERS OF WATER-SOLUBLE MODIFIED-CHITOSAN AND GLUCOSE OXIDASE FOR DETECTION OF GLUCOSE IN MILK SAMPLES. **AUTHORS**: PICCOLI, María Belén, VICO, Raquel Viviana, FERREYRA, Nancy Fabiana. **COUNTRY**: Argentina.

2. **TITLE**: AUTHORS: SANTOS, Maricel del Valle, *VELEZ, Alexis Rafael*, MAGARIO, Ivana Maria. **COUNTRY**: Argentina

3. **TITLE**: OPTIMIZATION OF BIODIESEL PRODUCTION FROM WASTE VEGETABLE OIL USING Zr- OXIDE CATALYST ANCHORED ON CARBONIZED MATERIAL **AUTHORS**: BABATUNDE, Esther Olubunmi, ADERIBIGBE, Fatai Alade, ADEKUNLE, Joseph Isaac, ARE, Comfort Temitope, OLUWATOBI, Paul-lasisi Joshua. **COUNTRY**: Nigeria

HONORABLE MENTIONS

- **TITLE**: MYO-INOSITOL AS A POTENTIAL LOCALLY SUPPRESSING ANTI-SEIZURE THERAPEUTIC AGENT. **AUTHORS**: KANDASHVILI, Manana, GAMKRELIDZE, Giorgi, LORDKIPANIDZE, Tamar, NANOBASHVILI, Zaqaria, SOLOMONIA, Revaz. **COUNTRY**: Georgia

- **TITLE**: THE EVOLUTION OF CATARACT IN A DOG WITH TYPE I DIABETES - CASE REPORT. **AUTHORS**: SAMAN, Thiago Abreu , RODRIGUES, Isabelle Medeiros, FILHO, Mário dos Santos. **COUNTRY**: BRAZIL

PERIÓDICO

Journal of Law, Public Policies and Human Sciences
Established in 2020

SOUTHERN
JOURNAL OF SCIENCES
ESTABLISHED IN 1993

TITLE INDEX

AUTHOR INDEX

SPEAKERS INDEX

www.21scon.org

LIST OF ABSTRACTS

ABSTRACT TITLE: ACTIVE METHODOLOGIES: CONSTRUCTION OF EDUCATIONAL EXPERIENCES THROUGH CONTINUOUS TRAINING OF TEACHERS

Authors: RICCI, Maria Fernanda Caravana de Castro Moraes, MEDEIROS, Maria Luiza Delgado de, CRAHIM, Suely Cristina de Souza Fernandes, AMORIM, Suzana Medeiros Batista, SOUZA, Therezinha Coelho de

Abstract: Education has undergone major changes in these pandemic times. Educational technologies are a reality in educational practice, and even if a “new normal” is established, new teaching practices must remain and be re-signified. Even before the occurrence of COVID-19, the regulatory bodies of higher education already signaled in the national directives of higher education courses the emergence of the adoption of active methodologies in teaching practices. This is an announced change, but what has to be changed is the conception of the educational activity. One that builds a profile of student training aligned with the professional profiles required by the market, increasingly demanding teaching and learning methodologies that meet the process of building an entrepreneurial spirit, autonomy, a look at multidimensional processes, which take into account the pillars of knowledge: learning to know, learning to do, learning to live together and learning to be highly demanded in our society with more plural and complex relationships.

Country: Brazil

Language: Portuguese/English

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.26_abstract_RICCI.pdf.

ABSTRACT TITLE: ACTIVITY-BASED KINETIC MODELLING OF LIPASE CATALYSED SYNTHESIS OF PEROCTANOIC ACID

Authors: BRANDOLÍN, Salvador Eduardo, SCILIPOTI, José, MAGARIO, Ivana,

Abstract: Carboxylic peroxy acids are organic oxidants of relevance in the cosmetic, food, and agrochemical industries. However, they are traditionally used as intermediaries in a process known as Prileschajew epoxidation and synthesized using sulfuric acid as a catalyst, promoting undesirable reactions on the final epoxides. Therefore, the study of selective catalysts such as enzymes is a topic of interest. In this work, peroctanoic acid synthesis was carried out using n-hexane as the solvent and an immobilized Candida Antarctica Lipase B commercial preparation as the catalyst. On the other hand, the oxidant, hydrogen peroxide was supplied as an aqueous solution, comprising the disperse phase of the reacting system. The reaction progression was quantified by iodometric and cerimetric titration of the peroctanoic acid concentration in the hexane phase. Four different initial amounts of octanoic acid were tested (0.74, 1.57, 10, and 20 millimoles). Substrate inhibition by octanoic acid was observed having at 1.57 millimoles the maximum initial reaction rate. The experimental data were fitted to a ping-pong bi-bi enzymatic kinetic model to estimate the initial reaction rate. Since this system constituted a liquid-liquid (organic-aqueous) two-phase system, the model was evaluated employing the thermodynamic activities of all species involved, assuming phase equilibria with time. The activities of all species were estimated using UNIFAC. As a result, the model was able to reproduce the trend of the initial rate with the change of the initial amount of octanoic acid.

Country: Argentina

Language: English

Institution: Universidad Nacional de Córdoba

DOI: 10.48141/SBJCHEM.21scon.12_abstract_BRANDOLIN.pdf.
ABSTRACT TITLE: ADSORPTION STUDIES OF ZINC, COPPER, AND LEAD IONS FROM PHARMACEUTICAL WASTEWATER ONTO SILVER MODIFIED CLAY ADSORBENT

Authors: AJALA, Mary Adejoke, ADEYEMI, Ayomide Samuel, TIJANI, Jimoh Oladejo, KOVO, Abdulsalami Sanni, ABDULKAREEM, Ambali Saka,

Abstract: Clay-supported silver nanoparticles were green synthesized using the aqueous leaf extract of Parkia biglobosa. The phytochemical analysis and FTIR results of the Parkia biglobosa showed that the leaf contains phenol, tanning, and flavonoids, which act as reducing, capping, and stabilizing agents required for the synthesis of the silver nanoparticles. The prepared adsorbent has good morphology, is rich in silica, and contains functional groups suitable for heavy metal binding. The adsorptions of Zn, Cu, and Pb from pharmaceutical wastewater onto the silver-modified clay were studied as an adsorbent dosage and contact time. From the percentage removal results obtained, the adsorbent had up to 99.96%, 99.5%, and 99.44% removal efficiency for Zn, Pb, and Cu, respectively. The present work shows that the synthesized silver nanoparticles supported on local clay can be used as a potentially low-cost adsorbent to remove heavy metal ions from industrial wastewater. v

Country: Nigeria

Language: English

Institution: University of Ilorin

DOI: 10.48141/SBJCHEM.21scon.10_abstract_AJALA.pdf.

ABSTRACT TITLE: ANALYSIS OF FALSE-POSITIVE RESULTS AND THE REAL EFFECTIVENESS OF LUMINOL IN THE DETECTION OF BLOOD SPOTS.

Authors: ZILIOTTO, Luis Henrique Carra, DA SILVA, Isaac Newton Lima

Abstract: Forensic investigators have widely used luminol for more than 90 years in the identification of blood in life crime scenes. When mixed with an alkaline solution and sprayed on a catalyst (iron present in blood hemoglobin), it reproduces a chemiluminescent reaction with a bluish color. As it is a presumptive blood test, the present study sought to demonstrate that only the photons emission is not a prerogative to attest that the result is indeed human blood. In this perspective, 24 samples of both liquid and solid substances that can easily be found in residences and potentially used by criminals to impair the interpretation of the investigator at the crime scene were prepared. Out of the total of the analyzed samples, there was a chemical reaction with sodium hypochlorite and wood varnish, proving the known understanding that some samples may cause interference in the examination with luminol.

Country: Brazil

Language: Portuguese

Institution: PUCRS

DOI: 10.48141/SBJCHEM.21scon.28_abstract_ZILIOTTO.pdf.

ABSTRACT TITLE: ANALYSIS OF THE SEXUAL BEHAVIOR OF BULLS OF THE TABAPUÃ BREED

Authors: LOREDO NETO, Francisco Antonio , FREITAS, Gabriela Santos, SERAPIÃO, Raquel Varella, GOMES, Leticia Patrão, MARQUES, Thiago Luiz Pereira,

Abstract: Beef cattle is one of the main sectors that drive the national economy, given the great generation of employment, presence in the consumer market, and exports. Among the various services generated, technical assistance to producers stands out, who work in several areas and, especially reproduction, which is a great ally to bovine production, because through it it is possible to monetize the creation with the use of reproducers with high fertility potential boosting livestock productivity. Therefore, the andrological evaluation in the sires is an important factor in selecting superior animals, seeking to improve the fertility of the herd. The present study aimed to analyze the sexual behavior of bulls of the Tabapuã breed, through the libido test, as part of the andrological examination. Ten young bulls of the Tabapuã breed were used, aged between 24-43 months, with an average weight of 375kg, without sexual experience. The libido test was performed from the contact of males with females in estrus and out of estrus to assess sexual interest. It was observed that half of the animals were classified with low libido (50%) and the other part with medium (30%) and high (20%) libido. In addition, it was observed that the most frequent sexual events were the identification of estrus. Finally, given the results of animals classified with low libido, it is suggested that sexual inexperience is correlated, and it is recommended to insert these cattle with high libido bulls so that they can observe the behaviors and gain experience.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.43_abstract_LOREDO.pdf.

ABSTRACT TITLE: ASSESSMENT OF SERUM SCLEROSTIN LEVEL AS A BIOMARKER ASSOCIATED WITH BONE DISORDERS IN B-THALASSEMIA PATIENTS IN AL- NAJAF CITY, IRAQ

Authors: SHARBA, Intisar Razzaq, AL-DUJAILI, Arshad Noori

Abstract: Aim of the study: To assess serum sclerostin in female patients with beta-thalassemia and compare with the healthy controls and to predict its complication associated with the bone pathophysiology, for designed improvement the lifestyle goodliness for these patients. Material and methods: Sixty-nine female beta-thalassemia (βT) patients (54 βT major and 15 βT Intermedia), aged 8-40 years who dependent on transfused blood, and 20 healthy controls were evaluated serum sclerostin, and was examined the relationship with hematological parameters RBC, Hb, PCV, WBC, PLT, BMI, splenic status, iron, and ferritin levels. The information of beta-thalassemia patients was collected and recorded by the questioner. Results: A significantly increased serum sclerostin level (mean 26.80±0.91) pg/ml was shown in βT patients compared with the healthy controls (10.03±0.68, p smaller than 0.001) pg/ml. Furthermore, a significant decrease (p smaller than 0.05) of the sclerostin level was observed in β-thalassemia major compared to intermedia β-thalassemia patients. Serum sclerostin level revealed a significant increase in progress age; it is highest in the age group (30-40) year as compared with age group (8-18) and (19-29) year respectively. Sclerostin showed no associations with the RBC, Hb, PCV, and significantly positively correlated (p smaller than 0.05) with serum iron, ferritin levels, WBC, and PLT count. Significantly higher sclerostin levels in splenectomized and underweight groups were observed compared to unsplenectomized and normal-weight groups (p smaller than 0.05) of βT patients. Conclusion: Sclerostin plays an important role in beta-thalassemia patients and can serve as a biomarker associated with the bone pathophysiology and indicator to prevent the continuation of such serious diseases caused by iron overload in these patients.

Country: Iraq

Language: English

Institution: University of Kufa, Faculty of Science, Department of Biology

DOI: 10.48141/SBJCHEM.21scon.05_abstract_SHARBA.pdf.

ABSTRACT TITLE: BIOPOLYMERS AS DOSIMETERS - A PROPOSAL

Authors: GENNARI, Roseli Fernandes, GOVEIA, Gilson, CHUBACI, José Fernando Diniz,

Abstract: The radiation study has led to advances in various areas of our everyday lives despite that several events had occurred, causing health damage to several researchers. Thus, if somebody wants to study irradiation effects on materials must use equipment that quantifies the radiation received. Dosimeters do this quantification of ionizing radiation. There are numerous applications for ionizing radiation so far, and many materials can be used for dosimetric purposes. Despite that, there is always a constant search for new materials, focusing on more efficient processes or less environmental impact. For dosimetric purposes, the material has to be radiation sensitive. Many materials have been the subject of research recently, aiming to be environment friendly: among them, we can mention biopolymers that have the great advantage of being biodegradable. A commercial solid-state dosimeter uses silver-activated phosphate glass for radiophotoluminescence (RPL) purposes. This dosimeter has an enormous advantage since it does not lose the dose information after dose reading. It can be reread many times until annealing is done to reset the exposure condition. It can be reused several times. This dosimeter is commercially available as “GD-450” (Chiyoda Technol Corporation). Our research group successfully proposed using silicate glass instead of phosphate glass as RPL dosimeters. Face to the need for a high-temperature furnace for glass sintering, and it was decided to test biopolymers as RPL dosimeters. Once our goal was to have a regenerative dosimeter, we used silver as a sensible radiation element. This work it was synthesized two biopolymers with and without adding silver to them. The biopolymers synthesized used starch and collagen as polymer base material. The biopolymers analysis was done by microscopy and by optical spectrometry (UV-Vis-NIR). We observed irradiation effects on absorption bands from biopolymer of collagen doped with silver.

Country: Brazil

Language: Portuguese

Institution: USP

DOI: 10.48141/SBJCHEM.21scon.42_abstract_GENNARI.pdf.

ABSTRACT TITLE: BONDS, PRACTICE, AND CHEMISTRY: EXPERIENCE REPORT AND REFLECTIONS ON POTENTIALITIES OF TEACHING-LEARNING PROCESS OF CHEMICAL TECHNICIANS IN MIDST OF THE COVID-19 PANDEMIC

Authors: MESQUITA, Iago Santos, PAZ, Miguel Pedro Alves da

Abstract: This work aims to report the experience of teaching a course with practical contents in chemistry in the distance modality due to the period of isolation by the COVID-19 pandemic. The target of the course was students of the Federal Institute of Education, Science, and Technology of Rio de Janeiro (Duque de Caxias campus), who study to be technicians in the field of Chemistry. In order to do so, the importance of experimentation in professional learning is discussed, as well as the difficulty of distance learning in practical training is analyzed. Following the course format and the resources used to overcome the limitations of distance learning and help the students keep the contents in mind are introduced. Student participation was an important component in choosing some themes for the course modules. Realizing the importance

of construction that understands them as active subjects in the teaching-learning process, it was possible to offer modules that touched the students reality and expanded their knowledge through comprehensive training. The themes and approaches were proposed to help them define or rethink their career through contact with different realities of the work of a technician in the field of chemistry. The report ends by analyzing how a transdisciplinary education could help students connect knowledge acquired separately and aggregate it to see reality more broadly and completely. The difficulties arising from the COVID-19 pandemic made it possible to discuss a teaching way that would lead students to participate more actively in their training and, dialectically, strengthen pedagogical praxis.

Country: Brazil

Language: English

Institution: Instituto Federal de Educação, Ciência e Tecnologia do Rio de Janeiro

DOI: 10.48141/SBJCHEM.21scon.18_abstract_MESQUITA.pdf.

ABSTRACT TITLE: CHARACTERISTICS OF WOOD SAWDUST-DERIVED BIOCHAR: POTENTIAL AS ADSORBENT MATERIAL

Authors: LIMA, Daniele de Andrade Villarim, REZENDE, Fabiana Abreu, FUNGARO, Denise Alves,

Abstract: Biochar is a potential additive for agricultural soil and can be used as an eco-friendly and economical adsorbent material. Biochar properties are affected by several technological parameters, mainly pyrolysis temperature and feedstock, which differentiation can lead to products with a wide range of characteristics. The biochar sample was produced from wood sawdust at 450˚C via slow pyrolysis and was characterized. Parameters characterized to include: physical properties (bulk density, porosity), chemical properties (composition, pH, conductivity, cation exchange capacity), hydraulic property (water holding capacity), proximate analysis, X-ray diffractometry to obtain information on the mineralogical composition, among others. The analysis of biochar properties is important for determining the biochar application.

Country: Brazil

Language: Portuguese/English

Institution: IPEN - Nuclear and Energy Research Institute

DOI: 10.48141/SBJCHEM.21scon.11_abstract_LIMA_IPEN.pdf.

ABSTRACT TITLE: CHILD DEPRESSION IN BRAZIL - A LITERATURE REVIEW

Authors: ERTHAL, Luísa Canto, SILVA, Guilherme Felipe Dutra, QUEIROZ, Aline Trovão,

Abstract: Childhood depression is a very prevalent mental health condition in today s society. Its debate began to become relevant in the 1960s and, although there is no doubt about its existence, the subject is still little discussed. This paper aims to demonstrate the relevance of the subject due to its high prevalence and underdiagnosis. A literature review on Childhood Depression in Brazil was carried out based on research in Pubmed, Scielo, and Google Scholar databases, between 1989 and 2020, in Portuguese and English, using the descriptors: “child depression”, “symptoms of depression” and “treatment of childhood depression” combined. Textbooks, data from Ministério da saúde, the World Health Organization (WHO), and key articles selected from citations in other articles were used to compose the paper. From the data analysis, twenty-two titles that are directly related to the current work were selected. In Brazil, girls and children between thirteen and fourteen years old are the most affected by the disease. The DSM does not

differentiate it from adult depression, despite the atypical manifestations of its symptoms in children. Families still have great difficulty on identifying this disorder the biggest obstacle is understanding and accepting that behavioral changes can be part of a depressive condition. Normalizing the discussion of the topic is important so that there is more information about the disease and, consequently, more knowledge is disseminated both to the medical community and the families of affected children. This way, it will be possible to prevent its appearance and, when present, facilitate its detection, improving life quality of those involved and avoiding negative outcomes such as child suicide.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.44_abstract_ERTHAL.pdf.

ABSTRACT TITLE: COMPARATIVE STUDY OF DEATHS FROM ILL-DEFINED AND UNKNOWN CAUSES BEFORE AND DURING THE SARSCOV-2 PANDEMIC

Authors: SOUZA, Andreza Rozendo, SANTOS, Marcus Asevedo, QUEIROZ, Aline Trovão,

Abstract: Documenting the cause of death is important to know the health situation of the population. After the beginning of the pandemic caused by the new coronavirus, institutional protocols were created to minimize the spread of the virus, including changes in the handling of bodies. The main objective of this study was to identify whether there was a change in the number of deaths from unknown to ill-defined causes comparing two years before the pandemic and two years during the pandemic in Brazil and the state of Rio de Janeiro and to determine the main epidemiological characteristics. A documentary, retrospective, and historical study were carried out based on data collection in the mortality information system from 2018 to 2021. The period was divided into two phases to make comparisons, two years before and two during the pandemic. Mortality rate, sex, color, and age data were included. Before the pandemic, there was a lower mortality rate from an ill-defined or unknown cause in Brazil and the State of Rio de Janeiro. In addition to the problems faced before, the changes caused by the pandemic may have influenced the rise in death notifications from this cause. The age group most affected in the two biennia analyzed was over 80. During the pandemic, men were more affected than women, browns in Brazil and whites in Rio de Janeiro had the highest number of notifications. In general, during the pandemic, it was shown that there was an increase in the number of people who died from unknown or poorly defined causes, especially the elderly. Additional studies need to be performed for definitive elucidation. In addition, it is necessary to identify better the conditions that caused the increase in the number of deaths from unknown or poorly defined causes.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.19_abstract_SOUZA.pdf.

ABSTRACT TITLE: COMPARISON OF TWO STAINING METHODS FOR ANODIZING IN ALLOY 6063 ALUMINUM PROFILES

Authors: PESSUTTO, Ana Carla, JONKO, Eliena

Abstract: Aluminum stands out for being a light, corrosion-resistant, and recyclable metal, achieving wide coverage in the market. When incorporated into alloying elements, it is possible to acquire other desirable characteristics. Alloy 6063, intended for architectural purposes, has

aesthetic, structural, and strength functions. This study aims to compare two different staining methods on the surface of anodized profiles of aluminum alloy 6063. Anodized finishing is performed through an electrolytic process using sulfuric acid as an electrolyte to change the surface layer of the material, ensuring a more resistant aluminum oxide film than that formed naturally. For decorative purposes, the anodic film coloration can be performed by several methodologies, including, in this case, the coloration by organic adsorption, with the use of aniline, and the electrolytic coloration, composed of tin sulfate salts, both for obtaining the black color. To compare, neutral saline mist tests, scanning electron microscopy analysis, determination of the anodic layer thickness, and immersion tests with 3.5 percent sodium chloride for 1000 hours. The results obtained highlight that both were shown to be resistant to corrosion due to the fact that they do not present corrosion points when exposed to the neutral saline mist test for 600 hours. In the immersion tests, both remained resistant to sodium chloride. Because both methodologies present satisfactory results in all tests, the quality of the applied stains is ensured, and it is found that they are equivalent when the parameters discussed are used.

Country: Brasil

Language: Portuguese/English

Institution: Universidade de Caxias do Sul, Engenharia Química

DOI: 10.48141/SBJCHEM.21scon.03_abstract_Pessutto.pdf.

ABSTRACT TITLE: CROHN S DISEASE: THE IMPACTS AND HOW TO MAINTAIN A GOOD QUALITY OF LIFE FOR PATIENTS

Authors: SILVA, Guilherme Felipe Dutra, ERTHAL, Luisa Canto, QUEIROZ, Aline Trovão,

Abstract: Crohn s disease (CD) can affect any portion of the gastrointestinal tract, characterized a chronic inflammation. It is most prevalent among patients in more productive phases, which correspond to periods that are more active in their work and with reproductive possibilities. Its treatment aims at the regression of the exacerbation phases and the healing of injuries, involving pharmacological and surgical possibilities. The objective of this paper was to delve into the issues surrounding the impacts on the quality of life of patients with Crohn s disease from diagnosis to treatment. This paper is a cross-sectional, descriptive study of a systematic literature review. The articles were searched in several databases (PUBMED, SCIELO, MEDLINE, LILACS), between the years 2000 and 2022. The inclusion criteria were: first publications that determined the direct impacts of coexistence and management on the patient s life carrier, exposing the presentations and possible complications of the natural course of the disease, and second the written language (Portuguese and English). The CD shows great clinical importance because it is a prolonged condition with huge repercussions on the patient s quality of life, whether due to possible complications of the underlying condition or even the treatment itself. Nutritional deficiencies, weight loss, sexual dysfunction, mood swings, low self-esteem, depression, and anxiety, have been shown to reflect the worsening quality of life associated or not with the natural course of the disease. It was observed that including multi-professional care in the treatment of the patient aiming at a biopsychosocial model can demonstrate a greater permanence in the remission phase, as well as provide an improvement in the quality of life indexes.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.48_abstract_DUTRA.pdf.

ABSTRACT TITLE: DIABETES IN PREGNANCY AND FETAL CARDIAC RISK: LITERATURE REVIEW

Authors: TAVARES, Lívia Hygino, MOURA, Bruno

Abstract: Gestational diabetes mellitus (MGD) is associated with poor cardiac malformation in the fetus. It is related to changes in the clinical course of the disease and pre-gestational periods. The prevalence and incidence of MGD have been increasing worldwide. Early screening, diagnosis, and lifestyle change, such as physical exercise and healthy eating, provide better outcomes for children s health. This study aims to analyze the data concerning gestational diabetes and fetal malformations and to group the various protocols for diagnosis, highlighting the risk factors associated with MGD and their prevention. A systematic review of the literature was conducted with the PubMed, Scielo, Medline databases with English, Portuguese, and Spanish articles. The studies gathered clinical trials, randomized clinical trials, and original articles. In 12 articles analyzed maternal alterations, while 11 articles analyzed fetal alterations, and 9 articles analyzed how to diagnose cardiac changes in the fetus. The patient with MGD should be inserted in multidisciplinary activities seeking the change of lifestyle, physical exercises, and food reeducation, intending to give the fetus the appropriate nutrients and optimize the drug treatment; cardiac malformations are among the most severe and recurrent complications. However, they can be avoided with the control of pre-gestational diabetes (stricter follow-up from the moment the patient feels the desire to become pregnant) and the diagnosis and treatment of early gestational diabetes, as strict control of maternal blood glucose during pregnancy reduces morbidities and mortality. The study showed that hyperglycemic status during pregnancy is related to increased mortality and morbidity, even if it is asymptomatic. Therefore, it is necessary to guide the diabetic woman to plan her pregnancy in a euglycemic period because only this control can guarantee health to the fetus. The diagnosis of pregnant women with gestational diabetes needs to be early to optimize treatment.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.45_abstract_TAVARES.pdf.

ABSTRACT TITLE: EFFECT OF MOLAR WEIGHT OF CARBOXYLIC ACIDS ON THE ENZYMATIC ESTERIFICATION OF GLYCEROL

Authors: SANTOS, Maricel del Valle, VELEZ, Alexis Rafael, MAGARIO, Ivana Maria,

Abstract: Glycerol is a by-product in biodiesel synthesis, and its current market condition allows the possibility to transform into value-added compounds. In this work, the enzymatic esterification between glycerol and carboxylic acids of different molar weights was studied to obtain glycerides of industrial relevance. Therefore, eight different carboxylic acids were evaluated: formic, acetic, levulinic, caprylic, capric, lauric, stearic, and oleic. Immobilized lipase from Candida Antarctica was employed as a catalyst. Solvent-free reactions were carried out at 65 °C, 450 rpm, at a molar ratio of glycerol: carboxylic acid of 1:1 and a 1,6% enzyme concentration (based on reagents weight). Conversion of carboxylic acids was followed with time by titration. Under these conditions, acids from octanoic to oleic, which initially formed biphasic systems with glycerol, showed high conversions (68%-80%) and initial reaction rates in the same magnitude order. On the other hand, no enzymatic catalysis was observed with formic, acetic, and levulinic acids. Formic acid exhibited a higher rate and 58% of conversion without catalyst. However, for acetic and levulinic acids, conversion was low in uncatalyzed reactions. Then, for these acids, toluene was added as a reaction solvent. As a result, conversions and initial rates increased for these lighter acids, indicating the need for a non-polar media or a biphasic character to activate the enzyme.

Country: Argentina

Language: English

Institution: Universidad Nacional de Córdoba.

DOI: 10.48141/SBJCHEM.21scon.13_abstract_SANTOS.pdf.

ABSTRACT TITLE: EFFECTS OF UTERINE LAVAGE FRACTIONS ON EMBRYO RECOVERY RATE IN MANGALARGA MARCHADOR MARES

Authors: PASSOS, Raiza Argon, ROIER, Erica Cristina Rocha, GOMES, Letícia Patrão de Macedo, SERAPIÃO, Raquel Varella, GOMES, Gustavo Mendes,

Abstract: Since 1986, the use of embryo transfer has gained prominence in the equine industry, allowing the increase in the number of descendants of genetically superior donors, competition mares, foals, and mares considered subfertile. The success of an embryo transfer program is directly related to the rate of embryonic recovery by mare, which is characterized by the percentage of embryos collected by uterine lavage. However, the recovery rate can be influenced by several factors, type of donor used, age, day of collection, and physical activity. Considering the advancement of biotechnology and the growing need for research in the area of equine embryo transfer, the present work aimed to study in Mangalarga marchador animals the effects of uterine lavage fractions on embryo recovery rates. The present study included 35 mares aged between 3 and 15 years, used as donors of clinically healthy embryos from an equestrian property in the southern region of Rio de Janeiro. Thus, 67 uterine washes were performed, where 67% of the embryos were recovered through different volumes of ringer s solution with sodium lactate. The embryo crops and transfers period was from September 2021 to January 2022. For statistical analysis of the data, the simple logistic regression test was used, where no significant difference (p less than0.05) was observed in the embryo indices recovered on total crops (67) regarding fractions (F) 1 (43.2%), (F) 2 (14.9%) and (F) 3 (5.97%). Thefore, it can be concluded that there was no significant difference between the lavage fractions, however, more studies are needed with a larger sample of uterine washing.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.32_abstract_ARGON.pdf.

ABSTRACT TITLE: ELECTROCHEMICAL CHARACTERIZATION OF GLASSY CARBON ELECTRODES MODIFIED WITH SWCNT FUNCTIONALIZED WITH DIAZONIUM SALT

Authors: PICCOLI, María Belén, VICO, Raquel Viviana, FERREYRA, Nancy Fabiana,

Abstract: Although carbon nanotubes have unique properties, one of the biggest drawbacks in practice is the difficulty in forming dispersions of individual nanotubes in a given solvent. Covalent functionalization of carbon nanotubes allows the incorporation of chemical groups at the nanotube surface that, according to its polarity, facilitates the dispersibility in different solvents. In this work, singled-wall carbon nanotubes were functionalized by spontaneous grafting with a diazonium salt obtained from the 4-aminobenzoic acid to obtain SWCNT-pB. The nanomaterial obtained was characterized by several methodologies that the covalent incorporation of the functional groups. SWCNT-pB were dispersed in ethanol/water 50% V/V under ultrasonic treatment, and the exfoliation degree was evaluated by UV-Vis spectrophotometry. under optimal conditions, SWCNT-pB dispersion was stable for more than 45 days. Glassy carbon electrodes (GCE) modified with the nanomaterial show significant increases in their capacitive current and a faradaic process due to redox species confined on the surface of SWCNT-pB whose anodic peak currents depend linearly with the scan rate. The modified electrodes also show a catalytic response towards ascorbic acid (AA) and notorious increments in the oxidation and reduction

currents of H2O2. The stability of the dispersions and the excellent electrochemical responses obtained make this nanomaterial very interesting for its application in electrochemical detection.

Country: Argentina

Language: English

Institution: Instituto de Investigaciones en Fisicoquímica de Córdoba, Universidad Nacional de Córdoba.

DOI: 10.48141/SBJCHEM.21scon.08_abstract_FERREYRA.pdf.

ABSTRACT TITLE: EQUINE (Equus caballus) INFUNDIBULAR DISEASE: CASE REPORT

Authors: NONATO, Manuelly Rufino, MORAES, Renata Fernandes Ferreira, ÁVILA, Leticia Meirelles, VIEIRA, Ana Cláudia Tavares , ROIER, Erica Cristina Rocha ,

Abstract: Raising horses has become increasingly important over the years, generating great income for breeders and contributing to the economy of the entire country. Dental care with these animals occurs less frequently than necessary, which causes weakness and loss of performance in them. Infundibular disease is a dental disorder, defined as a necrotizing bacteriosis characterized by destroying the inorganic material of the dental tissues, affecting mainly the premolar and molar teeth. This pathology may predispose to other alterations such as colic syndrome, gingivitis, difficulty in feeding, and consequent weight loss, besides resistance in the adaptation to mouth movements, which cause significant losses to the breeders. Its diagnosis is made through anamnesis, general and specific clinical examination of the oral cavity, and complementary exams, such as x-ray. This paper reports the case of a 13-year-old horse weighing about 400 kg of live weight, whose chosen treatment was the extraction of the affected tooth. The study aimed to review predisposing factors, diagnosis, the effects that this clinical change can cause on the animal's organism, and infundibular disease treatment, describing the therapy used and its results.

Country: Brazil

Language: Portuguese/English

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.16_abstract_NONATO.pdf.

ABSTRACT TITLE: EVALUATION OF THE EFFECTIVENESS OF TREATMENT OF THE ORAL MUCOSA WITH PHYTO-OINTMENT BASED ON PHYTOECDYSTEROIDS

Authors: TIMOSHIN, Anton, DOROFEEV, Aleksei, ERSHOV, Kirill, PUSTOKHINA, Inna, EMELINA, Elena,

Abstract: An indicator of the health of the human body in the state of the oral mucosa. Mechanical and chemical factors constantly influence it. At the first stage of the study, a comparative analysis of the frequency of various forms of traumatic injuries of the oral mucosa was carried out. The distribution of patients into groups was also carried out, depending on the medicinal product used. Then clinical examinations were carried out. After that, the therapy of traumatic erosive and ulcerative lesions of the oral mucosa began. The developed method for treating traumatic lesions of the oral mucosa with medicine based on phytoecdysteroids provides for the elimination of the traumatic factor, applying ointment based on phytoecdysteroids to the dried out focus twice a day. The use of phyto-ointment leads to complete repair of traumatic erosive and ulcerative lesions of the oral mucosa on average by the eighth day from the start of treatment; a similar effect with the use of "Solcoseryl dental adhesive paste" is achieved by the tenth day, and the gel "Cholisal Dental" - at a later date, which is confirmed in this study. The most significant positive effect on

the level of quality of life associated with the effectiveness of treatment of traumatic erosive and ulcerative lesions of the oral mucosa in comparison with the dental “Solcoseryl dental adhesive paste” and the gel “Cholisal Dental” is exerted by phyto-ointment, where a decrease in the total points was recorded. When conducting routine examinations of patients, it is necessary to pay attention to the oral mucosa damage. Moreover, in treating traumatic injuries of the oral mucosa, it is recommended to use phytoointment, which contains phytoecdysteroids.

Country: Russia

Language: English

Institution: I.M. Sechenov First Moscow State Medical University (Sechenov University)

DOI: 10.48141/SBJCHEM.21scon.09_abstract_TIMOSHIN.pdf.

ABSTRACT TITLE: EVALUATION OF THE IMPORTANCE OF HOUSEHOLD ENVIRONMENTAL CHARACTERISTICS IN THE DEVELOPMENT OF CANINE VISCERAL LEISHMANIASIS

Authors: BELEGOTE, Amanda Alfeld, FERREIRA, Lucas Leal, SILVA, Laís Freire, DA SILVA, Stephanie Esteves Sant’ana, OLIVEIRA, Glenda Ribeiro de,

Abstract: Visceral leishmaniasis is a zoonosis of great importance due to its incidence and high lethality, and the dog as its main reservoir in urban centers. Furthermore, environmental characteristics such as soil with abundant organic matter can predispose local ecosystems to the development of the vector Lutzomyia longipalpis. This study aimed to carry out a data collection in partnership with the Health Department of the municipality of Vassouras, determining environmental characteristics and favorable means for the dissemination of the sand fly, in an area of 150 meters from a confirmed human case of leishmaniasis in the Itakamosi neighborhood. During the months of October and November 2021, an environmental study was carried out in 7 homes, where a total of 14 dogs lived. Through questionnaires, data were collected regarding the environmental conditions of these homes. It was observed that 100% of the animals lived in households close to the forest and vegetation. Of the 7 households analyzed (6/7), 85,71% had banana trees in their surroundings, followed by the presence of fruit trees, which corresponds to (5/7) 71,42% of households. In contrast, in (3/7), 42,83% and (2/7) 28,57% represent the number of houses with the presence of chicken coops and kennels, respectively. In contrast, in (1/7) 14,28% of the households, there was the presence of organic matter debris, aiding in the sand fly cycle. The animals residing in these houses were tested for leishmaniasis and showed a negative result, but the possibility of future infection of these animals cannot be ruled out, given that these factors corroborate the easy adaptation of the sandfly exploiting the accumulation of organic matter in areas of socioeconomic vulnerability.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.31_abstract_BELEGOTE.pdf.

ABSTRACT TITLE: EXPERIMENTAL STUDY OF THE INFLUENCE OF TEMPERATURE ON PASTEURIZATION OF PÊRA RIO IN NATURA ORANGE JUICE

Authors: GALIASSI, Gabriela Regina Rosa, RAMIREZ, Maribel Valverde

Abstract: Heat treatment is one of the most used methods to preserve food, such as orange juices, which are an excellent source of ascorbic acid. To avoid vitamin C degradation and reduce loss, fast heating is recommended. This work aimed to determine the vitamin C content using the

iodometric method and the convective heat transfer coefficient using the method of dimensionless numbers and the experimental method. Time and temperature were controlled throughout the experiment. In pasteurization, the solution was heated to 80 °C, heating lasted 50 minutes and cooling for 42 minutes. The convective heat transfer coefficient was evaluated in two regions of the cylindrical container: near the wall and in the central region. The graphic profile of the curve follows the same trend of the literature. The convective heat transfer coefficient is higher in the region near the wall. As time passes and temperature decreases, the central region tends to equilibrium, and the coefficient becomes more constant. The vitamin C content remained constant before and after pasteurization, so it was observed that the pasteurization did not cause ascorbic acid degradation since the heating step was fast in the heat treatment. As a result of the study, it was noted that studying the thermal behavior in the cooling of orange juice is extremely important to ensure its quality. It is pertinent to mention that in order to avoid this degradation and reduce its loss, it is necessary that in thermal treatments, fast heating is carried out and that the juice has low exposure to air and heat at the time of its preparation.

Country: Brasil

Language: English

Institution: Universidade Federal de Mato Grosso, Faculdade de Engenharia

DOI: 10.48141/SBJCHEM.21scon.02_GALIASSI.pdf.

ABSTRACT TITLE: EXTRACTION, PURIFICATION, AND COMBINATION OF LAPACHOL IN NOVEL EUROPIUM COMPLEX

Authors: SILVA, Andrei Marcelino Sá Pires, MENEZES, Jorge Fernando Silva de, ALMEIDA, Edna Aparecida Faria de,

Abstract: Lapachol belongs to the group of 1,4-naphthoquinones, with the addition of a hydroxide group attached to carbon 2 and a branched alkene nomenclature 3-methyl-2-butenyl attached to carbon 3, with final nomenclature 2-hydroxy-3 -(3-methyl-2-butenyl)-1,4-naphthoquinone. As a chromophore, it exhibits near-ultraviolet absorption, one of the important characteristics in the process of choosing ligands to integrate photoluminescent lanthanide complexes. Photoluminescent materials are currently widely used in the market for making plates, paints, plates, tapes, pigments, and other luminescent equipment. The use of what are called DMCLs (Molecular Light Converting Devices) is increasing in Photovoltaic Cells, Optical Luminescent Tracers, Forensic Chemistry, Fluoroimmunoassays, and more. Knowing the great demand for these devices, it is feasible to study and characterize new compounds that have favorable emission characteristics and that allow their use in the aforementioned categories. For this, the use of lanthanides is a great proposal, and the application of a chromophore ligand, such as Lapachol, aims to provide an increase in the emission of the final product. In the present work, the extraction, a new purification process of Lapachol from its natural source, the Ipê Roxo wood, is reported, as well as the characterizations that attest to the feasibility of the new process, in addition to the use of the material as a binder in lanthanide complexes.

Country: Brazil

Language: Portuguese

Institution: UFRB

DOI: 10.48141/SBJCHEM.21scon.38_abstract_SILVA.pdf.

ABSTRACT TITLE: GRAPHICAL METHOD FOR DETERMINATION OF MQ-SERIES GAS SENSOR CIRCUIT PARAMETERS FOR A STANDALONE GAS ALARM SYSTEM

Authors: AJIBOYE, Aye Taiwo, OPADIJI, Jaye Femi, AJAYI, Adebimpe Ruth,

Abstract: MQ-series gas sensors belong to the metal oxide semiconductor (MOS) family of sensors that can sense the presence of many gases. These sensors find their application in gas alarm systems as key components. While necessary sensor circuit output voltage value for alarm point in a standalone gas alarm system is desirable, but what exact combination of the sensor circuit parameters is required? Hitherto, the determination of these circuit parameters has not been much attention in the research community. This study explores a structured graphical approach of determining MQ series gas sensor circuit parameters for a standalone gas alarm system that yields the desired sensor circuit output voltage value for the alarm point. Model equations were developed for the sensor dynamics, and based on these model equations, graphs for the determination of required sensor parameters were plotted for a case of MQ-4 gas sensor response to liquefied petroleum gas (LPG). A structured graphical approach for determining MQ-series gas sensor circuit parameters for alarm points in a standalone gas alarm system showed that using MQ-4 gas sensor and LPG as the target gas. For a sensor circuit output voltage of 2 V for alarm point at 1000 ppm of LPG, the corresponding value of RO, RS, and RL obtained were 20 kΩ, 30 kΩ, and 20 kΩ, respectively. Hence, the developed structured graphical approach is suitable for determining MQ series gas sensor circuit parameters for a standalone gas alarm system under the influence of its associated gases.

Country: Nigeria

Language: English

Institution: University of Ilorin

DOI: 10.48141/SBJCHEM.21scon.20_abstract_AJIBOYE.pdf.

ABSTRACT TITLE: IDENTIFICATION OF HUB GENES IN CROHN S AND CELIAC DISEASES: A BIOINFORMATIC PERSPECTIVE

Authors: KOZALAK, Gül, ATCEKEN, Nazente

Abstract: Chronic inflammatory diseases are the repetitive response of the organism to any stimulus. Crohn s and Celiac diseases are among chronic inflammatory diseases, and both cause chronic inflammation in the intestines. Both diseases are thought to be caused by genetic and environmental factors. Although the relationship between the two diseases is frequently mentioned in the literature, very few studies, have been conducted to elucidate their common mechanisms. From a bioinformatics perspective, this study aimed to determine the genes whose expression alters in both Crohn s and celiac diseases. For this purpose, NCBI-GEO datasets were downloaded, and advanced statistical analyzes were performed. Statistical analyzes revealed 54 DEGs in both Crohn s and celiac diseases. As a result of bioinformatics analysis, it was determined that 13 of these differentiated genes were hub genes. It has been defined that 11 of these genes are involved in similar biological processes employing GeneCards, Gene ontology, and Kyoto encyclopedia of genes and genomes pathway. GZMB, GZMA, GZMH, CD160, CXCR1, CXCR2, ANPEP, FPR2, GAB2, PI3, and NCF4 genes are located in a connected pathway. Contrary, CTSL, and KAT6A genes are on different pathways. Common biological processes that antigen presentation by MHC class molecules, cell death pathways mediated by immune cells and ROS, maintain the continuity of gut epithelial cells have been suggested. Given the increasing prevalence of both Crohn s and celiac diseases in the population, it is clear that more studies are needed on the collective mechanisms of these diseases.

Country: Turkey

Language: English

Institution: Aksaray University

DOI: 10.48141/SBJCHEM.21scon.25_abstract_KOZALAK.pdf.

ABSTRACT TITLE: IMPACTS CAUSED BY THE COVID-19 PANDEMIC ON PEOPLE WITH AUTISM SPECTRUM DISORDER

Authors: PEREIRA, Carlla Alessandra Silva,

Abstract: COVID-19, first identified in Wuhan, China in 2019, has the SARS-CoV-2 virus as its etiological agent, spread rapidly around the world, became a pandemic and directly impacted the lives of individuals. Due to the advance of the pandemic the means for control was social isolation. Since individuals with autism spectrum disorder have difficulties in social interaction due to cognitive impairment, interpersonal development tends to be more impaired with the beginning of restrictive measures. This study aims to analyze the changes in the routine of individuals with autism spectrum disorder during social isolation. The search was conducted in the PubMed and BVS databases, using the following descriptors from the DECS database: autism spectrum disorder, covid pandemic and anxiety, using the Boolean indicator AND between words in the search fields. The inclusion criterium for the texts were: English, Portuguese and Spanish languages, from 2017 to 2022. As exclusion criterium, articles that did not address the topic were excluded. The study showed that with the closure of schools and migration to remote education, several students developed a regression in social interaction and triggered new psychiatric symptoms due to the change in routine. In compliance with safety protocols, cognitive-behavioral therapies, migrated to the digital medium and were also rejected at first, but were instrumental in controlling the creation and worsening of symptoms. Due to physical and social distancing requirements, individuals with autism spectrum disorder tend to have greater difficulties with social interaction after the COVID-19 pandemic. The change in routine contributes to the worsening of symptoms such as anxiety, aggressiveness, and irritability and can worsen the mental health of parents.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.24_abstract_PEREIRA.pdf.

ABSTRACT TITLE: INFLUENCE OF EDGE TREATMENT BY POLISHING WITH ABRASIVE BRUSH BRUSHES ON THE LIFE OF THE TOOL FOR THE MILLING PROCESS

Authors: BOGO, Ricardo, ZEILMANN, Rodrigo Panosso

Abstract: Machining is a process in constant evolution, the search for greater productivity, reliability, and quality of machined materials is fundamental for the constant evolution of the process. The condition of the tool edge is of great importance for the tool performance in machining, the edge of a tool after the manufacturing or re-sharpening process has defects such as: microcracks, irregularities, and an extremely sharp edge. The cutting edge treatment is used to remove these defects, which originate from the tool manufacturing and re-sharpening processes. In view of these listed points, this work aims to understand and evaluate the effects of cutting edge treatment by abrasive bristle brushes, taking into account the evolution of wear on the edge and tool life in the end milling process. The abrasive brushes covered in this work are technical brushes from the 3M brand, these brushes have different grain sizes and two different abrasives, silicon carbide (SiC) and aluminum oxide (Al2O3), their bristles are made of nylon of two different thicknesses. Based on the literature and to evaluate the performance of these brushes, points such as roughness and edge contour were addressed in this step, and as a result, the fine bristle brush with a SiC particle size of 1 micron had the best performance, these brushes produced a radius of 0.06 mm on the tool edges. The polishing process treated two tools,

these tools went through the milling process in AISI P20 steel. As a result, the treated tools had a superior performance by 15,30% compared to untreated tools. In addition to increasing the useful life, the cutting edge treatment provided linear flank wear, delaying the presence of wear such as adhesion, microcracks, and microchips. The polishing edge treatment with abrasive bristle brushes proves to be an effective and reliable process for improving the performance of machining tools.

Country: Brazil

Language: Portuguese/English

Institution: Universidade de Caxias do Sul, Engenharia Química.

DOI: 10.48141/SBJCHEM.21scon.17_abstract_BOGO.pdf.

ABSTRACT TITLE: IVORY CHARACTERIZATION USING PORTABLE VIBRATIONAL SPECTROMETRY

Authors: ENGEL, Wanda, GENNARI, Roseli Fernandes, FERREIRA, Cauê, RIZZUTTO, Marcia

Abstract: Ivory was commonly used in the manufacture of numerous objects. It refers to the tusk and teeth of animals. Almost all ivory pieces, in the past, found on the market were authentic; however, nowadays, ivory extraction is an illegal practice. Thus, official government and animal protection entities have been fighting intensely against this criminal practice, but the production and sale continue. There are numerous difficulties in identifying the illegal extraction and use of ivory, and the correct characterization is certainly a great challenge. A proper ivory characterization is an important tool in the fight against ivory extraction once it is possible to trace the piece to the animal and sometimes even to its origin. It is also useful for museums and art collectors to verify the authenticity of the piece. Ivory, also known as the inorganic gemstone, is composed of calcium phosphate, collagen, elastin, and lipids. Different tests can differentiate ivory from bones or celluloid; however, some can damage the piece. Because of that, analytical techniques are preferred. However, the method to be used must have the capability of differencing small differences once the chemical elements present in ivory, bone, or even celluloid are the same. In this work, three analytical methodologies were used to check the possibility of having an alternative test applied on supposed ivory samples. All three methods used, X-Ray Fluorescence (XRF) and vibrational spectrometry techniques (FT-IR and Raman), are portable equipment to facilitate the analysis in situ. FT-IR and Raman spectra obtained had shown differences between bone and ivory samples, indicating the art collector samples are probably ivory. These differences allied with the portability of the analysis can be used as an additional test to be done in ivory and bone-based materials.

Country: Brazil

Language: Portuguese

Institution: USP

DOI: 10.48141/SBJCHEM.21scon.40_abstract_ENGEL.pdf.

ABSTRACT TITLE: MOLECULAR MODELING, REACTIVITY PARAMETERS AND SPECTROCHEMIC STUDIES OF ε-CAPROLACTAM AND o-PHENANTROLINE

Authors: Francisco José Santos Lima, Maria José de Oliveira Pessoa, Lucas da Silva Araújo, Ademir Oliveira da Silva, Francisco Claudece Pereira,

Abstract: In this work, molecular models were obtained, and the reactivity parameters of ε-caprolactam and o-phenanthroline were calculated to evaluate the interaction in the formation of complex molecular compounds. It was observed that the main electron donor atoms, in the

formation of the metal-ligand bond, are centered mainly on the oxygen and nitrogen atoms, respectively, which are sterically more favorable in these species. Conductance measurements in an aqueous solution were obtained to observe the electrolytic behavior of these compounds. Infrared spectra were also recorded to characterize vibrational transitions in identifying these species when present in complex systems. Molecular spectra of absorption in the UV-visible region were recorded to evaluate the spectrochemical properties of these individual ligands and further verify their influence on the formation of complex molecular systems. The parameters evaluated include the molar absorptivity ε, integrated absorption coefficient, oscillator force, and transition dipole moment. It was observed that the ε parameter indicates molecular transitions in the 190 – 300 nm region and the near-infrared, and the oscillator strength is typical of molecules used as dyes and sensitizers for optical light-emitting systems or light-to-electricity converters.

Country: Brazil

Language: Português/Inglês

Institution: Universidade Federal do Rio Grande do Norte, Centro de Ciências Exatas, Instituto de Química, Brazil

DOI: 10.48141/SBJCHEM.21scon.01_lima.pdf.

ABSTRACT TITLE: MYO-INOSITOL AS A POTENTIAL LOCALLY SUPPRESSING ANTI-SEIZURE THERAPEUTIC AGENT

Authors: KANDASHVILI, Manana, GAMKRELIDZE, Giorgi, LORDKIPANIDZE, Tamar, NANOBASHVILI, Zaqaria, SOLOMONIA, Revaz,

Abstract: Required for all manuscripts in which the epilepsy belongs to several neurological diseases whose treatment is currently symptomatic, and some patients are resistant to anticonvulsant drugs. Thus, it is essential to create and discover antiepileptic medications. Myo-inositol (MI) is considered to be a future cure agent for epilepsy. In this study, using an electrophysiological method, we revealed that MI has a time and concentration-dependent anticonvulsant effect. During the experiment, two bipolar electrodes were inserted into the dorsal hippocampal structure along with a cannula. MI and saline were injected, and the subsequent duration of electrical stimulation-induced after discharge were recorded from the same location in the hippocampus. 5 minutes after 1 M of MI infusion, the duration of the afterdischarge was significantly reduced compared with the duration of the pre-injection after discharge in the same animals and the duration of the pre-injection afterdischarges in animals administered saline or MI in the contralateral hippocampus. In addition, 0.055 M myo-inositol significantly decreased the afterdischarge duration at 5 minutes after injection as compared to 40 minutes post-injection. It should be noted that after the injection of different MI concentrations (1.0 M and 0.055 M), the afterdischarge duration was restored to its initial value (pre-injection afterdischarge duration) 40 minutes after the MI injection. For the first time it was demonstrated that myo-inositol has time and concentration-dependent effects on the evoked seizure afterdischarges. Based on the results obtained from previous laboratory studies and current data, it was concluded that MI has a local suppressive effect on seizures and is therefore considered a promising therapeutic agent for treating patients with epilepsy.

Country: Georgia

Language: English

Institution: Ilia State University

DOI: 10.48141/SBJCHEM.21scon.47_abstract_MANANA.pdf.

ABSTRACT TITLE: NOSOLOGICAL CHARACTERISTICS OF DOGS SUBMITTED TO TPLO BY AN ORTHOPEDIC SERVICE IN THE STATE OF RJ, BRAZIL

Authors: ROCHA, Amanda da Silva, MOTTA, Lucas Baptista, COSTA, Andrei Ferreira Nicolau, MOTTA, Pedro Paulo de Assis, DE CARVALHO, Eduardo Butturini,

Abstract: Cranial cruciate ligament rupture in dogs causes knee instability. It is one of the main causes of pelvic limb lameness in this species. There are several techniques for surgical treatment, and TPLO – tibial plateau leveling osteotomy aims to change the biomechanics of the knees in an attempt to better distribute the forces and generate dynamic stability in the joint. Still, little epidemiological data about dogs submitted to TPLO has been published. This retrospective study investigated nosological and epidemiological characteristics of 76 dogs submitted to this technique performed by a private orthopedic service in two cities in the state of Rio de Janeiro over fourteen months. The mean time between diagnosis and surgery was 23 days (median nine days). The mean age of the dogs was 73±43 months, and there were no differences between males and females. Approximately 10,5% of dogs had contralateral ligament rupture. Most animals were spayed or neutered (66,66% vs. 33,33%, p=0,02). There were no transpiratory complications in 89,6% of patients, and 79,2% had no postoperative complications. Exploratory arthrotomy was the most performed associated surgery technique (61% of patients). It is believed that studies like this allow a better understanding of this rupture and its treatment options, providing a better quality of life for affected dogs.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.39_abstract_ROCHA.pdf.

ABSTRACT TITLE: OPTIMIZATION OF BIODIESEL PRODUCTION FROM WASTE VEGETABLE OIL USING Zr- OXIDE CATALYST ANCHORED ON CARBONIZED MATERIAL

Authors: BABATUNDE, Esther Olubunmi, ADERIBIGBE, Fatai Alade, ADEKUNLE, Joseph Isaac , ARE, Comfort Temitope, OLUWATOBI, Paul-lasisi Joshua,

Abstract: The current investigation emphasizes preparing low-cost carbon-based zirconium impregnated heterogeneous catalysts from wood dust to produce biodiesel from waste vegetable oil (WVO). Response Surface Methodology via Central Composite Design (RSM-CCD) optimized the biodiesel production process. The physico-chemical properties of waste vegetable methyl ester were determined following the American Standard Testing of Materials (ASTM). The optimum conditions were observed to be 8:1 methanol/oil ratio, 5 wt% catalyst loading, 55°C temperature, and 3 h reaction time. The corresponding response was observed to be 98.39%. The catalyst morphology and elemental composition were determined using Scanning Electron Microscopy (SEM) and Energy-Dispersive X-ray (EDX), respectively. The experimental analysis confirmed that the synthesized catalyst from wood dust under optimized conditions can transesterify WVO into biodiesel.

Country: Nigeria

Language: English

Institution: University of Ilorin

DOI: 10.48141/SBJCHEM.21scon.37_abstract_BABATUNDE.pdf.

ABSTRACT TITLE: OSTEOMYELITIS OF THE FIRST PHALANX IN A HORSE ATHLETE: CASE REPORT

Authors: ÁVILA, Letícia Meirelles, GOMES, Letícia Patrão de Macedo, GOMES, Gustavo Mendes, ABREU, Ana Paula Martinez de, ROIER, Erica Cristina Rocha,

Abstract: Equinoculture is an activity of great importance in Brazil, moving millions of reais annually. For many years these animals were used only as a means of transport; however, currently, horses have assumed coverage in other areas of activity, such as leisure, sports, and even therapies, without escaping their main work functions in agricultural activities. Due to the significant requirement of the locomotor system, the affections of this system are quite common in this species. Therefore, these conditions must be diagnosed and treated early to completely restore the animal s functions. Intense exercises and very demanding tests subject these animals to limb injuries. They are fast-reacting animals and, sometimes, they can generate injuries due to the shock on surfaces and objects. These skin continuity solutions can act as a door of entry for infectious agents. Osteomyelitis is an infectious process that is accompanied by bone destruction, mainly caused by gram-positive bacteria. The prognosis of animals affected by this pathology is directly influenced by the speed of correct diagnosis and the beginning of appropriate treatment. It can put the sporting purpose of the animal and life at risk if it occurs late. The present report aims to describe the case of an adult female athlete, used for polo, presenting a lesion in the right forelimb and claudication grade 4/5. The diagnosis was obtained through clinical examination and radiographic study, finding radiographic changes compatible with osteomyelitis, and established treatment.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.22_abstract_AVILA.pdf.

ABSTRACT TITLE: POISONING BY HOUSEHOLD CHEMICALS IN CHILDREN

Authors: SOUZA, Maria Cristina Almeida de , PINHEIRO, Cristina Fidalgo Affonso , FERNANDES, Renan Lopes ,

Abstract: Children are the main victims of intoxication, considering that, with child development, especially between one and four years of age, they learn to walk and acquire agility, reaching objects and bringing them to the mouth. The objective of this study was to review the literature on exogenous intoxications by chemical products used in households in children in Brazil. Household cleaning products are the second leading cause of poisoning in domestic environments, preceded only by the accidental ingestion of medication. From 2017 to 2021, 128,794 exogenous intoxications resulting from exposure to toxic agents were recorded in the age group from zero to 14 years in Brazil. Among this total of exogenous intoxications, 18,733 reports of poisoning by household products were registered, representing 14.54% of the total of exogenous intoxications. Intoxication records in Brazil increased by up to 23%, from January to April 2021, compared to the same period in 2019. This is because the world is facing the COVID-19 pandemic, in which hygiene products are being commercialized for cleaning and antisepsis of domestic environments, which led to an intensification of accidents caused by these chemical materials. Therefore, it is concluded that the rate of exogenous intoxication by domestic chemical products is high in children, especially in the age group of zero to five years. It is also worth mentioning that with the COVID-19 pandemic, there was a greater consumption of chemical products for domestic use and, consequently, an increase in the number of poisonings by these products in children. Therefore, it is evident the need to adopt actions to avoid these accidents to reduce the poisoning rate by these toxic agents.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.36_abstract_FERNANDES.pdf.
ABSTRACT TITLE: PREVENTION OF CANDIDIASIS IN PATIENTS USING REMOVABLE DENTURES

Authors: SEVBITOV, Andrey, DOROFEEV, Aleksey, MIRONOV, Sergey, AL-KHOURY, Samer, TIMOSHIN, Anton,

Abstract: Despite innovations in orthopedic dentistry, removable dentures belong to the most popular orthopedic care category. Removable dentures are combined stimuli that affect the mucous membrane and neuro-receptor apparatus. Acrylic plastic prostheses, widely used in prosthetic dentistry, have a negative side mechanical, chemical-toxic, sensitizing, and thermal insulating effect on oral tissue and prosthetic impression area. This is often complicated by a violation of the biocenosis of the oral cavity, the growth of pathogenic microflora that releases toxins, especially an increase in the number of yeast colonies that irritate the oral mucosa and prosthetic stomatitis. It was observed 100 patients with oral candidiasis of various age groups from 45 to 65 years. Of these, 60 patients with removable plate prostheses; 40 patients with partially removable prostheses. Chronic forms of candidiasis were diagnosed in 40 patients and with exacerbation of chronic forms of candidiasis in 60 people. The number of untreated carious cavities and poor hygienic condition of the oral cavity directly affects the severity of candidiasis. Acute forms of candidiasis were observed mainly in patients with high DMF and PMA indices. The severity of candidiasis depends on the degree and duration of wearing dentures and hygienic conditions - the most severe forms of invasive candidiasis were observed in the presence of removable plate prostheses, the complete absence of teeth, and the use of a prosthesis for more than 10-15 years. A combined lesion of the oral mucosa and the red border of the lips was observed mainly in patients older than 60 years. The presence of candidiasis in the oral cavity in patients with removable plate prostheses leads to a statistically significant change in the indicators of local immunity of the oral cavity: an increase in the concentration of serum IgG and IgA and the values of the coefficient of the balance of local immunity factors.

Country: Russia

Language: English

Institution: I.M. Sechenov First Moscow State Medical University (Sechenov University)

DOI: 10.48141/SBJCHEM.21scon.04_abstract_SEVBITOV.pdf.

ABSTRACT TITLE: PRL-R ISOFORMS LONG / SHORT RATIO IS INCREASED IN SYSTEMIC LUPUS ERYTHEMATOSUS BLOOD MONONUCLEAR CELLS

Authors: MORENO-SOSA María Tamara, GARCIA Daiana Sthefania, HEREDIA Rocío, BITTAR-RIVERO-PEDROSA, Victor, MACKERN-OBERTI, Juan Pablo,

Abstract: Prolactin (PRL) displays several functions in the whole body by binding its receptor (PRL-R). Two main PRL-R isoforms are reported that differ in their capacity to trigger signaling pathways, PRL-R long isoform is the activation receptor, and the short isoform is the inhibitory oner. Although many autoimmune diseases display hyperprolactinemia, the role of each PRL-R isoform expression in autoimmunity remains unknown. This work aimed to correlate PRL-R isoforms expression in human peripheral blood mononuclear cells (PBMCs) of female Systemic Lupus Erythematosus patients and healthy controls. To this end, PBMCs from lupus patients (n=9) and healthy controls (n=5) were enriched by the ficoll-hypaque method. Then, RNA extraction, cDNA synthesis, and real-time PCR were performed to determine mRNA expression. We found that PRL-R long and short isoforms expression from lupus patients display similar expression to healthy controls. However, the PRL-RL/PRL-RS ratio is higher than healthy controls (P-value two-tailed smaller than 0,05). Additionally, PRL-RL isoform expression correlates with

the short isoform in lupus patients (Spearman r 0,8945; 95% confidence interval 0,6834 to 0,9676; P-value two-tailed smaller than 0,0001). However, the expression of neither long and short isoforms correlates with active disease nor disease duration. Similarly, lupus patients display similar PRL-R isoforms expression than healthy controls. Although much work must be done, our data indicate that similar mechanisms may regulate the expression of both PRL-R isoforms in immune cells, and “their expression goes hand by hand”.

Country: Argentina

Language: English

Institution: IMBECU-UNCuyo

DOI: 10.48141/SBJCHEM.21scon.21_abstract_MACKERN.pdf.

ABSTRACT TITLE: PYROLYSIS OF SOYBEAN WASTE: A ROUTE TO ACTIVATED CARBON FOR FUNGICIDE CHLOROTHALONIL CAPTURE

Authors: CEBALLOS, Noelia Marcela, RIMONDINO, Guido Noé, MALANCA, Fabio, PELÁEZ, Walter José

Abstract: Soybean residues were transformed through static pyrolysis carried out at temperatures between 250 °C and 350 °C. The gaseous fraction analysis showed that the gases emanated in the pyrolysis are mainly CO2 and CO. Furthermore, it was proved that this methodology constitutes a simple way to obtain useful carbons for the capture of pesticides present in an aqueous matrix. For example, the concentration of Chlorothalonil in a 7:3 water: acetonitrile solution decreases by 76-77 % through adsorption on the carbons obtained.

Country: Argentina

Language: English

Institution: Instituto de Investigaciones en Fisicoquímica de Córdoba, Universidad Nacional de Córdoba.

DOI: 10.48141/SBJCHEM.21scon.35_abstract_CEBALLOS.pdf.

ABSTRACT TITLE: RELEASE PROFILE OF BISPHENOL-A FROM DENTAL RESINS IN WATER ASSESSED BY LC-MS/MS

Authors: SILVA, Bruno Pereira da, RÜBENSAM, Gabriel, SAAFELD, Claudiela Wachholz, WEBER, João Batista Blessmann

Abstract: Dental resins have been designed to replace amalgam restorations due to their more favorable physical, chemical, and biological properties. However, depending on its composition, the efficiency of its polymerization, and the degradation of the polymer matrix, Bisphenol-A can be present and therefore released from this material to the human body. It has been reported that residues of additives and minority by-products of polymer reactions, such as Bisphenol-A, can be released from plastics into aqueous media through polymer hydration, water-polymer diffusion, residue dissolution, and equilibrium between dissolved residues in water and polymer. Over time, this could lead to a polymer material with an external layer practically free of Bisphenol-A. However, the newly formed layer could be removed by brushing during oral cleaning, similar to toothbrushing, exposing the new layer containing Bisphenol-A to the aqueous media. Due to the toxic effects of this compound, an increasing number of plastics labeled as BPA-free have been introduced to the dental market, including tooth coating, dental sealants, and resins. Nevertheless, more specific studies on analytical chemistry have revealed a trace of Bisphenol-A in dental resins labeled as BPA-free and pointed out the need for even more sensitive and accurate detection methods to help manufacturers evaluate the presence of background

contaminations in their products and to avoid false-negative results. In this way, liquid chromatography-tandem mass spectrometry has been considered one of the most suitable methods for confirming Bisphenol-A even at low concentrations, in high complex matrices, due to its high select sensitivity. In the present work, we developed a sensitive, reliable, and efficient approach to trace the release profile of Bisphenol-A by LC-MS/MS in dental resin samples purchased in the Brazilian dental market. With the analysis of five different brands of resin composites performed in eight days of exposition to water, four of them released Bisphenol-A from 3.4 pg/mm2 to 10.1 ng/mm2. The brand labeled as BPA-free released BPA at concentrations of 1.1 ng/mm2. However, one sample reached the maximum of released BPA in only 3 days, one in 4 days, and two virtually did not reach a maximum of BPA released into the water in the window time assessed. Limits of detection and quantification of the LC-MS/MS method were 40 pg/mm2 and 100 pg/mm2, respectively, and allowed the quantification of BPA released from a composite labeled as BPA-free. For future analysis, we will conduct a more comprehensive study on the release profile of BPA from resin composites into the water using a tooth brushing simulator to determine if the obtained profiles might have clinical implications

Country: Brazil

Language: English

Institution: PUCRS

DOI: 10.48141/SBJCHEM.21scon.23_abstract_RUBENSAN.pdf.

ABSTRACT TITLE: RELEVANCE OF THE HEALTH CONDITION AND CLINICAL CHARACTERISTICS OF SPOROTRICHOSIS

Authors: ROCHA, Sofia Marques, PEREIRA, Bruna Hudson Neves , OLIVEIRA, Emanuelle Silva, JUNQUEIRA, Letícia Santos , OLIVEIRA, Glenda Ribeiro,

Abstract: Feline sporotrichosis is a zoonosis caused by S. brasiliensis, and it presents a degree of great underreporting due to its contamination. Caused by inoculation directly into the skin, in most cases through scratches or bites by infected animals. With its first diagnosis in 1907 among naturally infected mice. The study presents information on the health of the animal, composed of 24 felines of both sexes, obtaining information through questionnaires about food along with vaccination, deworming, and ectoparasites control. In addition to depicting the types of injuries and body parts such as head, limbs, and trunk. Seeking to provide important information about animal health, along with the follow-up of a Veterinary Doctor. General care that meets the health of no animal meets all care. The disease may present some systemic symptoms such as secretions, anorexia, apathy, difficulty breathing, fever, ulcers, and abscesses. In the study, 4% of the cats had a respiratory clinical picture. Regarding the lesions, it was mostly noted that 96% of the felines had multiple lesions and 4% had single lesions in the areas of the body, being 67% of secretion with pure bloody characteristics and 33% had no secretions, with the main sites of involvement being 58% in the head region, 36% in the limbs and 6% in the trunk. Factors related to feline immunocompromise may result in more severe cases of sporotrichosis as observed in the study animals. All information obtained was evaluated using basic descriptive statistics. Relative frequency values and percentage values were assigned to the variables observed in the research.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.41_abstract_ROCHA.pdf.

ABSTRACT TITLE: SELF-ASSEMBLED MULTILAYERS OF WATER-SOLUBLE MODIFIED-CHITOSAN AND GLUCOSE OXIDASE FOR DETECTION OF GLUCOSE IN MILK SAMPLES

Authors: GULOTTA, Florencia A., MONTENEGRO, Mariana, DIAZ VERGARA, Ladislao, FERREYRA Nancy F., PAZ ZANINI, Verónica I.,

Abstract: Multilayer films made of glucose-functionalized chitosan (G-Chit) and glucose oxidase (GOx) were built by layer-by-layer self-assembly technique onto carbon paste electrodes (CPE). The obtained bioelectrodes were characterized by cyclic voltammetry and chronoamperometry. Results indicated that catalytic response increases with the number of bilayers G-Chit/GOx and the enzyme concentration obtaining the best responses for 3 bilayers and 2 mg ml-1, respectively. The effect of pH on the bioelectrode response was also investigated, it was found that the optimal working value is 7.0. Under optimized experimental conditions, the biosensor exhibits a sensitivity of (0.81 ± 0.03) μA mM-1 in a glucose concentration range 0.18 to 1.75 mM. The analytical response of the biosensor was tested in milk samples with negligible matrix effects. Results show that G-Chti appears promising for the immobilization of enzymes.

Country: Argentina

Language: English

Institution: Instituto de Investigaciones en Fisicoquímica de Córdoba, Universidad Nacional de Córdoba.

DOI: 10.48141/SBJCHEM.21scon.07_abstract_FERREYRA.pdf.

ABSTRACT TITLE: SEROPREVALENCE AND CLINICAL MANIFESTATIONS OF DOMICILED DOGS (CANIS LUPUS FAMILIARIS) CLOSE TO A HUMAN CASE OF VISCERAL LEISHMANIASIS

Authors: FERREIRA, Lucas Leal, BELEGOTE, Amanda Alfeld, SILVA, Laís Freire , CABRAL, Steffany Souza , DOS SANTOS Priscilla Nunes ,

Abstract: Canine visceral leishmaniasis (CVL) is a disease with a great impact on public health in Brazil due to its zoonotic potential. One of the biggest challenges in controlling the disease is the fact that its main reservoir in urban areas is the domestic dog, and thus, it is a source of infection that lives very close to the human being. This study aimed to determine the seroprevalence of L. chagasi and the symptoms of CVL present in dogs living near a human case confirmed by the Municipal Health Department of the municipality of Vassouras. Blood samples were collected from the cephalic vein of 14 resident dogs within a radius of 150 meters from a confirmed human case. This collected material was submitted to the DPP screening test, and the positive samples were submitted to the ELISA confirmatory test. Information was also obtained through questionnaires about the presence of the disease s clinical signs. Of the 14 animals tested in the DPP, only 4 were positive in the screening test, and all presented negative results in the ELISA confirmatory test. Of the 14 dogs, 4 had symptoms. Of these, 2 presented skin lesions, and 1 animal showed cough, while the last one exhibited vomiting. It is concluded that the DPP screening test for CVL is a practical and easy to handle method, although it requires attention due to the possibility of cross-reaction with other etiological agents in dogs. The human case is probably a result of a non-autochtone infection. Therefore, asymptomatic dogs should be under disease surveillance since these hosts also act as a source of infection for vector insects.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.30_abstract_FERREIRA.pdf.

ABSTRACT TITLE: “SIX THINKING CARDS”: A GAME FOCUSED ON DEVELOPING ARGUMENTATIVE SKILLS IN THE CHEMISTRY CLASSROOM

Authors: DE ALMEIDA, Luciana Pereira, DE OLIVEIRA, Victória Beatriz dos Santos, PASSINATO, Cristiana de Barcellos,

Abstract: Considering the increasing need to develop the argumentation and communication skills of the students, teaching practice has to consider how to do this concerning individual needs and preferences. Meaningful Learning proposes that education should consider the already acquired knowledge of the students in the process of building new learning. Therefore, when applied to the learning process, argumentation is a way to express acquired knowledge to other participants of this process. The Six Thinking Cards game permits students to explore their thinking in focused stages that are represented by the colors proposed in the Six Thinking Hats strategy by Edward De Bono, thus creating an environment where students have time and space to study and think about scientific concepts in a throughway. It is expected that the game also helps students develop soft skills that are considered essential for 21st century learning, such as empathy, communication, problem-solving, and teamwork. The game also adds Libras (Brazilian Sign Language) and Braille (tactile writing system) elements for accessibility purposes towards the objective of building an inclusive classroom. This game should be able to be applied in the chemistry classroom once Covid-19 hard restrictions and quarantine are over and in-person studies are permitted, allowing the authors to do qualitative and quantitative research of this proposal’s reach and relevance for beyond of the projection of this proposal. Interviews with both teachers and students are to understand better how students’ metacognitive skills improve as they engage in cooperative learning and express their ideas.

Country: Brazil

Language: English

Institution: UFRJ

DOI: 10.48141/SBJCHEM.21scon.29_abstract_ALMEIDA.pdf.

ABSTRACT TITLE: THE EFFECTS OF PARTICLE SIZE, COMPACTION PRESSURE, AND TORREFACTION ON QUALITY AND THERMAL PROPERTIES OF PELLETIZED CORNCOB RESIDUES

Authors: SAIDU, Nurudeen Sabi, ALADODO, Muhammad Alamin, AJIMOTOKAN, Habeeb Adewale,

Abstract: Torrefaction and biomass pelletization into pellets for solid fuel development are considered sustainable energy solutions to mitigate fossil fuel dependency and environmental challenges. This study investigated the effect of particle size, compaction pressure, and torrefaction on the quality and thermal properties of pelletized corncob residues. The corncob samples were collected, sorted, and pulverized before the torrefaction pretreatment. The torrefaction was achieved by placing the corncob in a furnace at a temperature and residence time of 280 °C and 30 minutes, respectively. The inert atmosphere was attained and maintained by initially purging a nitrogen gas into the torrefying chamber and passing it at 100mL/min during the processes. The raw and torrefied corncob fines were screened to 0.3 mm, 0.5 mm, and 1.0 mm grain sizes. Using starch as a binder (5% wt), pellets were produced employing their respective raw and torrefied fines at compaction pressures of 50 MPa, 75 MPa, and 100 MPa. Though all pellet samples exhibited good quality and thermal properties, the pellets from torrefied corncob are better. Also, the effects of particle size and compaction pressure are significant on the produced pellets. The compressed density varied from 760 to 1,250 kg/m3 and 637 to 920

kg/m3 for raw and torrefied corncob pellets. A maximum heating value of 25.8 MJ/kg was obtained from the torrefied pellet sample of 1.0 mm, rendering improvements of 37.2% when compared with 18.8 MJ/kg of raw corncob of the same particle size. The energy values obtained for torrefied corncob for all particle sizes compared favorably with the value obtained in coal. Investigation of particle size, compaction pressure, and torrefaction on quality and thermal properties of pelletized corncob residue proved that it can replace coal and hence could be used for energy applications.

Country: Nigeria

Language: English

Institution: University of Ilorin

DOI: 10.48141/SBJCHEM.21scon.14_abstract_SAIDU.pdf.

ABSTRACT TITLE: THE EVOLUTION OF CATARACT IN A DOG WITH TYPE I DIABETES - CASE REPORT

Authors: SAMAN, Thiago Abreu , RODRIGUES, Isabelle Medeiros, FILHO, Mário dos Santos,

Abstract: Diabetes Mellitus is one of the endocrine diseases that most affect dogs in Brazil and worldwide. It is characterized by a chronic metabolic disorder, where the ability to respond or produce the hormone insulin is impaired, resulting in the abnormal activity of carbohydrate metabolism, coursing with hyperglycemia and glucosuria. The signs of 4P s (polyuria, polyphagia, polydipsia, and weight loss) are classic in this disease. As Diabetes Mellitus progresses, complications such as cataracts, retinopathy, and metabolic ketoacidosis may occur. Cataract is one of the most frequent complications in diabetic and early-onset dogs. It has a rapid development, as the lens has high permeability to glucose, converting it into fructose and sorbitol, which, as they are sugars with osmotic potential, can attract water, causing lens edema. The definitive treatment for cataract is surgical, with phacoemulsification being the most used technique. A canine male, Shih-tzu, weighing 5 kg, 06 months old, and not neutered, was treated at the private veterinary clinic in the city of Nilópolis. The patient had polyuria, polydipsia, polyphagia, weight loss and was prostrate most of the time. The diagnosis of diabetes mellitus was confirmed and a protocol was started with the use of Insulin NPH for human use. In addition, a diet was performed with the consumption of food for weight control, glycemic, and drug treatment. After six months of DM treatment, the dog presented bilateral lens opacity (crystalline), confirming a diagnosis of cataract secondary to diabetes, and underwent phacoemulsification surgery on the left eye. With the good post-surgical evolution, the doses of the prescribed medications were gradually reduced until the animal recovered completely. The present work aims to report the clinical case, atypical, of a young dog, with type I DM, with cataract manifestation after six months of diagnosis.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.46_abstract_SAMAN.pdf.

ABSTRACT TITLE: THE IMPACT OF THE LACK OF KNOWLEDGE OF THE FEMALE AUTISTIC PROFILE IN THE QUALITY OF LIFE OF AUTISTIC WOMEN

Authors: SILVA, Sophia dos Santos Tavares Freitas da, LASNEAU, Larissa Primo Pereira

Abstract: In this work, the literature reviewed points out significant differences between the presentation of autism spectrum disorder in men and women, including variations in the behavior pattern, given the distinct process of socialization of the genders. However, these gender

differences in the autistic phenotype were poorly studied, analyzed, and disseminated, making the female profile of autism not as well known as the male profile. Furthermore, the little attention given to the presentation of autism in girls led to the creation of diagnostic tools that were less efficient in recognizing them, causing difficulties related to late, missed, or incorrect diagnoses. These types of occurrences make it difficult for autistic women to access the support they need, in addition to being able to trigger or worsen identity crises related to their autistic traits and their self-perception in society. This abstract aims to highlight the importance of understanding the gender differences present in autism spectrum disorder and how their non-recognition can negatively affect the mental health of undiagnosed autistic women.

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.49_abstract_SILVA.pdf.

ABSTRACT TITLE: TOTAL CONTENT OF CALCIUM AND PHOSPHORUS IN SERUM OF WISTAR RATS BY AN OPTIMIZED METHOD OF ICP-MS

Authors: RUBENSAM, Gabriel, KOTH, Valesca, BARREIRO, Bernardo Ottoni Braga , STEIN, Thaynã Spencer, CHERUBINI, Karen,

Abstract: In the Odontology field, the modeling process of alveolar bone has been a topic of investigation for the last years since the lost bone after tooth extraction can preclude aesthetic and function. In this practice, the volume of the tissue to be modeled depends on, among other factors, the serum levels of calcium and phosphorus, and it is of interest to monitor these elements to better understand the mechanism of tissue regeneration. These elements are routinely analyzed for clinical purposes, as serum constituents, by UV-VIS spectrophotometry after chromogenic reactions for each metal with different reagents. Depending on the analytical demands and work objectives, it is necessary to have methods based on technologies that allow multi-element quantification in a single experiment. In this context, ICP-MS has been considered a powerful tool for rapid multi-element analysis due to its high selectivity and sensitivity. However, it has been reported that samples with high content of salts and proteins, such as serum samples, cause matrix-induced interferences due to weak sample preparation and the presence of polyatomic ions. The present study aimed to identify and mitigate matrix effects in rat serum samples during the simultaneous quantification of calcium and phosphate using ICP-MS and evaluate its capability of differentiating element levels from Wistar rats subjected to tooth extraction with and without alveolar bone grafting. In addition, the optimized method can be used for more comprehensive mineralomics studies related to the bone modeling process in future studies.
KOTH, Valesca

Country: Brazil

Language: English

Institution: PUCRS

DOI: 10.48141/SBJCHEM.21scon.27_abstract_KOTH.pdf.

ABSTRACT TITLE: TRANSCRANIAL DIRECT STIMULATION IN THE NEUROMODULATION OF CONTROLLING MAIN SYMPTOMS OF PARKINSON'S DISEASE: A CASE STUDY

Authors: SOUZA, Alice Medeiros de, AMADEU, Lilian Campos, VOSNIADOU, Eleni, CORRÊA, Fernanda Ishida, DALL'AGNOL, Letizzia,

Abstract: Parkinson's disease (PD) is a central nervous system neurodegenerative disorder that primarily affects the motor system, decreasing motor coordination, balance and generating tremors, and a progressive loss of everyday mobility, including walking. This study was conducted to verify the effects of Transcranial Direct Current Stimulation (tDCS) on balance, motor control, and the quality of life in Parkinson's disease patients. The patient received three treatments consisting of 10 sessions of 20 minutes each and a one-week interval between treatments. Active stimulation was applied on the primary motor cortex (M1), the dorsolateral prefrontal cortex (DLPFC), and the dorsolateral prefrontal cortex (D Sham-tDCS. DLPFC stimulation produced the best improvements in terms of motor control, balance, gait, and overall PD symptoms, as evaluated by different scales and questionnaires. As a result, active stimulation of the DLPFC produced superior outcomes and may contribute to treating Parkinson's disease.

Country: Brazil

Language: English

Institution: Universidade Nove de Julho, Faculdade de Fisioterapia

DOI: 10.48141/SBJCHEM.21scon.06_abstract_ISHIDA.pdf.

ABSTRACT TITLE: UNILATERAL HYDRONEPHROSIS DUE TO URETER OBSTRUCTION AFTER OVARIO-HYSTERECTOMY IN A FELINE - CASE REPORT

Authors: RODRIGUES, Isabelle Medeiros, TOLEDO, João Francisco Bianchini de, SAMAN, Thiago Abreu, FILHO, Mário dos Santos

Abstract: Hydronephrosis is characterized by the renal pelvis and calyces distension resulting from total or partial urinary outflow obstruction. Ureter injuries are recognized complications of abdominal surgeries, especially sterilization, due to the frequency which they are performed in cats and dogs and the proximity between the ureter and the uterine stump. Some injuries may be acute or chronic, uni or bilaterally, affecting the urinary tract segment parts. Therefore, diagnosis is very important, especially early on, since it makes immediate management easier and may result in a better prognosis, especially when the disease course gets interrupted or its progression gets slowed. Furthermore, the importance of performing sporadic exams, even without previous clinical history for feline patients, is notorious since the nature of the species to hide clinical signs is well known. To certify the success of the surgery and integrity of the organs, it is very important to perform post sterilization exams. It is also crucial to state the importance of computed tomography for the diagnosis since some obstruction causes, such as blood clot, may not be shown in the ultrasound. Computed tomography is also necessary to differentiate hydronephrosis from many injuries that may affect the kidneys and ureters, like ectopic ureter, obstruction by calculi, and surgical ligature. The present study has the objective of reporting and discussing the laboratory, imaging findings, and clinical state of a patient with unilateral hydronephrosis, with asymptomatic evolution of iatrogenic origin due to obstruction by ureter obliteration after ovariohysterectomy (OVH).

Country: Brazil

Language: Portuguese

Institution: Universidade de Vassouras

DOI: 10.48141/SBJCHEM.21scon.34_abstract_RODRIGUES.pdf.

ABSTRACT TITLE: UTILIZAÇÃO DEBANANA PRATA (MUSASAPIENTUM) E BANANA OURO (MUSAACUMINATA) NO CONTROLE DE NEMATÓIDES GASTROINTESTINAIS DE BEZERROS

Authors: ÁVILA, Letícia Meirelles, CHAGAS, Jônathan David Ribas, MARQUES, Thiago Luiz Pereira, MORAES, Renata Fernandes Ferreira, ROIER, Erica Cristina Rocha,

Abstract: Cattle, both beef and dairy, are of great importance for Brazil, as it moves a good part of the country economy. But gastrointestinal infections caused by nematodes cause significant damage to cattle due to weight loss of animals, decreased production index, increased mortality rate, and increased expenses by producers. This work aims to demonstrate the elimination of gastrointestinal nematodes through the use of the leaves of two different banana species in calves and to verify if there are differences in the effectiveness of both. For the study, 30 calves were selected, aged between 3 and 8 months, of both sexes and already fed on pasture. These were divided into three groups. Group A was treated with banana leaves of the Musa sapientum species; Group B – was treated with banana leaves of the Musa acuminata species; Group C – control group, in which no substance was found administered. The feces collection was performed at intervals of 7 days, totaling 3 collections. The samples were taken directly from the animals rectum, stored in a plastic bag, and placed in a styrofoam container with ice, and then the material was taken to the laboratory for the eggs per gram (eggs/g)examination. It can be concluded that the use of banana leaf proved to be effective in reducing the parasitic load of intestinal nematodes in calves, proving that the use of Musa acuminata was more efficient than the result of the use of Musa sapientum when compared.

Country: Brazil

Language: Portuguese/English

Institution: Universidade Federal Rural do Rio de Janeiro

DOI: 10.48141/SBJCHEM.21scon.15_abstract_AVILA.pdf.

ABSTRACT TITLE: VALIDATION OF A GC-FID METHODOLOGY FOR THE DETERMINATION OF 2,5-HEXANEDIONE IN URINE

Authors: BORGES, Henrique Bordin Lucena, RÜBENSAM, Gabriel

Abstract: 2,5-hexanedione is the main metabolite of hexane and methyl butyl ketone excreted into urine and is currently used to estimate the human exposure levels to these solvents in professional environments. In Brazil, occupational exposure is regulated by a national control program (PCMSO) and applied to public and private organizations that hire your employees according to the actual Brazilian legislation. In the present work, we validated a methodology based on a gas chromatography−flame ionization detector (GC-FID) for the quantification of 2,5-hexanedione in urine to attend the new occupational limit of urinary 2,5-hexanedione, established by a recent revision of the Brazilian legislation, which reduced this limit from 5.0 to 0.5 mg/L. Before GC-FID analysis, sample treatment was based on a simple liquid-liquid extraction with dichloromethane. Considering that there is no specific validation guide for occupational purposes, the adopted validation process was performed using a “fit-for-purpose” approach based on different guides, including FDA bioanalytical method validation, European Commission Decision 2002-657-EC, and ANVISA Guidelines RDC 166/2017. After method optimization, the performance characteristics determined by the present validation study were considered satisfactory and demonstrate the method suitability for the routine analysis in the Brazilian PCMSO, including CCα and CCβ values, which are used to avoid the presentation of false-positive and false-negative results. Intra and interday reproducibility were below 2.66, and 4.08 % and analyte recoveries were above 95.4% for three evaluated levels. The limits of detection and quantification were 0.05 and 0.17, respectively. To our knowledge, this is the first application of CCα and CCβ approaches in an analytical method intended for occupational purposes, which are important to know when a sample is out or following the legislation. Then real samples were analyzed herein, and none presented 2,5-hexanedione above the required limits.

Country: Brazil

Language: Portuguese

Institution: PUCRS

DOI: 10.48141/SBJCHEM.21scon.33_abstract_BORGES.pdf.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

METODOLOGIAS ATIVAS: CONSTRUÇÃO DE VIVÊNCIAS EDUCACIONAIS ATRAVÉS DE CAPACITAÇÃO CONTINUADA DE DOCENTES

RICCI, Maria Fernanda Caravana de Castro Moraes[1]*; MEDEIROS, Maria Luiza Delgado de[1]; CRAHIM, Suely Cristina de Souza Fernandes[1]; AMORIM, Suzana Medeiros Batista[1]; SOUZA, Therezinha Coelho de[1]

[1] Universidade de Vassouras, Curso de Pedagogia, Brasil

** Correspondence author*
e-mail: mariafernanda.ricci@gmail.com

Received 10 February 2022; received in revised form 19 February 2022; accepted 21 February 2022

ABSTRACT

Education has undergone major changes in these pandemic times. Educational technologies are a reality in educational practice, and even if a "new normal" is established, new teaching practices must remain and be re-signified. Even before the occurrence of COVID-19, the regulatory bodies of higher education already signaled in the national directives of higher education courses the emergence of the adoption of active methodologies in teaching practices. This is an announced change, but what has to be changed is the conception of the educational activity. One that builds a profile of student training aligned with the professional profiles required by the market, increasingly demanding teaching and learning methodologies that meet the process of building an entrepreneurial spirit, autonomy, a look at multidimensional processes, which take into account the pillars of knowledge: learning to know, learning to do, learning to live together and learning to be highly demanded in our society with more plural and complex relationships.

Keywords: *Active Methodologies; Teacher training; Learning; Education.*

1. INTRODUÇÃO

A primordialidade da reflexão sobre modelos formativos que atendam a construção de atos de currículo que, inspirados pela insurgência da mediação pedagógica ubíqua, mediados por tecnologia de informação e comunicação (TIC), aproximem experiências de simulação, apresentou um caminho novo cujo percurso é irretornável. Para além disso, já desde 2002, quando o Conselho Nacional de Educação (CNE) sinaliza a necessidade de formação por competências, aponta que o profissional do futuro demanda uma visão sistêmica, holística, norteada pela inovação.

Nesse sentido, o desenvolvimento de uma atitude empreendedora, o foco da resolução de problemas e no trabalho cooperativo, como também de habilidades socioemocionais, são fundantes, já que "empreendedorismo e a educação são duas oportunidades que devem ser alavancadas e interligadas para desenvolver o capital humano necessário para construir as sociedades do futuro" (Wilson *et al*., 2009), uma vez que o empreendedorismo é o motor que sustenta a inovação, a geração de emprego e o crescimento econômico e social. Todo esse processo assume um aspecto mais direto com a Resolução CNE/CES nº 02/2019 (Brasil, 2019) que, de pronto, estabelece a necessidade de melhores parâmetros de implantação e de formação acadêmica em que os docentes adotem a avaliação por competência, bem como apresenta indicação de quais seriam os diferentes níveis desejados de proficiência em cada uma delas, tudo isso amparado em um diálogo com os setores produtivos e na emergência da indústria 4.0, visando, desta feita, articular o perfil de formação às demandas do mercado, sem, contudo, olvidar da responsabilidade social e do desenvolvimento sustentável.

Nesse cenário, as novas Diretrizes Curriculares Nacionais (DCNs) de diversos cursos de graduação preconizam, de forma recorrente, a adoção de práticas formativas baseadas em metodologias ativas. Reforçam esse conceito

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.26_abstract_RICCI.pdf

valorizando a orientação para atividades práticas, uso de tecnologia de simulação de produtos e processos, automação e realidade virtual, que permitem aos discentes a realização, de forma efetiva, de experiências de aprendizagem mais autônomas, seguras e auto monitoradas, o que promove, ao fim e a cabo, uma ancoragem eficiente desse conhecimento às reflexões teóricas já constituídas. Este mesmo referente desafia os Institutos formadores a integrar esses saberes construídos, não apenas em um sentido transversal, mas em rede, buscando um olhar para habilidades humanísticas, técnicas e tecnológicas de uma sociedade em movimento.

A primeira etapa de apropriação desses novos modelos de docência é uma que rompa com uma postura tradicional, vinculada à educação bancária e mais próxima de um modelo humanista, cognitivista e sociocultural. Da imbricação desses modelos surgem as metodologias ativas, como situações didáticas alternativas em que se propõe que os discentes façam mais que ouvir. Assim, a aplicação das metodologias ativas em sala de aulas pode desenvolver habilidades e competências nesse futuro profissional, sejam elas técnicas ou não técnicas (Morán, 2015).

Ao se falar de metodologias ativas, há de se considerar que existem várias delas, todas aplicáveis nos afazeres docentes. Umas mais disruptivas, outras com uma proposta de modificação sustentada, em que os processos de transformação da prática docente se constituam por modelos mais próximos das práticas instaladas, mas com aspectos inovadores frente aos papéis e funções dos agentes no paradigma de escolarização formal. A literatura apresenta algumas opções como mais recorrentes no oferecimento de formação docente continuada para Metodologias Ativas. Entre elas, tem especial destaque a Sala Invertida, *Problem Based Learning* (PBL), Simulação, Estudo de Caso e Gamificação. Nelas há uma característica comum: o docente arquiteta a estrutura do desafio e conduz o discente para, pelos fazeres associados, encontrar um desfecho possível ao desafio apresentado. Então, o aluno se põe ativo, engajado e de forma investigativa, o que desperta maior interesse e dedicação. A aprendizagem baseada em problemas, do inglês *Problem Based Learning* (PBL) (Munhoz, 2016), e a aprendizagem por estudo de caso (*Case-Based Learning*) são métodos bastante próximos. Diferem no fato de que, neste, o problema se apresenta preciso, vinculado a uma situação prévia objetiva coerente com ocorrência comumente apresentável no mundo do trabalho, podendo haver uma integração de disciplinas ou não para sua resolução. Já o PBL, por conceito, embarca muitos conteúdos, e o discente tem que promover a integração entre eles para a resolução da questão proposta. Nelas, há a intenção de obtenção de uma solução, não necessariamente de um produto. Outra metodologia bastante recorrente tem sido a sala de aula invertida (Schell, 2018), que propõe que o conteúdo didático seja disponibilizado antecipadamente aos discentes, preferencialmente em mídias distintas, para que se potencialize, dessa forma, o momento de encontro com o docente, posto que esse prévio contato estabeleceria de pronto os conceitos fundantes a serem explorados, ficando o momento consequente destinado à aplicação desses conceitos ou ao esclarecimento de dúvidas. Também a Gamificação, como uma metodologia que estimula o engajamento, tem ganhado força no ensino universitário. A apropriação de conceitos associados a criação de jogos é baseada na tríade metas, regras, sistema de feedback instantâneos, que garantem o conhecimento do processo de aprendizagem e a sinalização e, caso haja necessidade, o reposicionamento de estratégias para a conquista almejada, para além de ludicidade própria do jogar.

A utilização dessas metodologias almeja fortalecer a aprendizagem e incrementar o engajamento e protagonismo dos estudantes. Elas podem ser mais facilmente implantadas em sistemas com pouca flexibilidade curricular ou com docentes ainda neófitos em metodologias inovadoras. Todas essas metodologias, mais ou menos disruptivas, constituem o discente como agente de sua formação e se norteiam com o perfil do profissional ético, socialmente responsável, gestor de pessoas, processos e soluções técnicas arrojadas.

O uso de Metodologias Ativas no processo de formação docente é tendência nas Universidades Brasileiras, principalmente no nível superior. No entanto, a construção de um ecossistema de inovação não se dá apenas pelo embarque de tecnologia. É imperioso que o docente alinhe seus fazeres a esse paradigma, que é diverso daquele que ele próprio significou na sua formação profissional.

As diretrizes também nos desafiam a repensar os processos de avaliação da aprendizagem, agora focadas em observar um tripé composto por habilidade, atitude e conhecimento, que darão substância ao processo formativo do estudante. Isso impõe uma mudança

na cultura pedagógica, tanto do docente como do discente, pois desfoca do conteúdo para a habilidade, do produto para o processo, da formação episódica para a formação permanente, e do isolamento para o coletivo. Novamente, apresenta-se um fazer novo, demandante de formação em serviço, já que, por princípio, o docente universitário, como comum nos cursos de formação técnica, não tem, durante seu percurso formativo, o viés formal da preparação para a docência, o pensar-se como professor. Por normal, o que há é um espelhamento de práticas exitosas experienciadas.

Ocorre que o acadêmico que se foi está afastado daquele que está hoje nos bancos universitários. O mercado demanda da universidade a formação de um novo profissional, e metodologias ativas, tecnologia educacional, práticas avaliativas sistêmicas e auto monitoradas devem ser incorporadas no cotidiano docente.

O presente trabalho relata uma pesquisa-ação desenhada como formação em serviço, objetivando promover formação continuada dos professores dos cursos de graduação da Universidade de Vassouras para o uso de metodologias ativas na docência.

2. DESENVOLVIMENTO:

A pesquisa propôs acompanhar a formação continuada de docentes da Universidade de Vassouras, em Vassouras, Rio de Janeiro, Brasil, a partir do Projeto de Capacitação Contínua Docente, desenvolvido no segundo semestre de 2021. O acompanhamento de todo o processo formativo foi realizado, nos encontros presenciais, pelo preenchimento de formulários diagnósticos pelo Google Forms, objetivando mapear o conhecimento formal dos docentes acerca das metodologias propostas e sua efetiva utilização em sua prática pedagógica. Durante a capacitação, o acompanhamento se deu pelos dados gerados no Ambiente Virtual de Aprendizagem (AVA) de forma individualizada, referente a cada uma das unidades de aprendizagem que compunham o processo formativo.

Primeiramente, foi oferecido um conjunto de palestras aos professores objetivando discussão dos temas abordados na formação, a saber, metodologias ativas utilizadas na docência do ensino superior. Nelas foram apresentadas situações didáticas de aplicação de metodologias ativas realizadas por docentes da Instituição de Ensino Superior. Em seguida, os participantes realizaram um curso EaD institucional para formação na utilização de práticas docentes alinhadas a esse novo fazer.

3. RESULTADOS E DISCUSSÕES:

Como produto dessa formação, o docente participante da capacitação planejou, para mais tarde executar, pelo menos, um ato de currículo referente a um conteúdo didático de uma trilha de aprendizagem sob sua responsabilidade, considerando uma das metodologias ativas por ele experienciadas. O resultado dessa prática foi postado em uma atividade no AVA.

Como política de formação permanente, todos os materiais da formação foram disponibilizados no AVA da IES, onde também foi criado um espaço de compartilhamento de boas práticas, em que se socializam experiências exitosas na prática docente amparada por metodologias ativas. Tais experiências foram postadas como tarefa final da capacitação através de vídeos, portifólios, ou apresentações das práticas efetivadas. Para além disso, em um encontro mediado por ferramenta de streaming, os docentes foram instados, de forma voluntária, a compartilhar essas práticas e relatar suas impressões sobre sua aplicabilidade. Ao final desse processo, foram convidados a avaliar, em formulário do Google Forms, voluntária e anonimamente, o processo formativo como um todo.

4. CONCLUSÃO:

Mediante as observações e análise de dados qualitativos oriundos dos registros ocorridos durante a capacitação e com base nos conceitos explicitados é importante salientar que o estudo possibilitou entender que o bom uso das Metodologias Ativas no ensino superior e aplicabilidades das mesmas contribuem com a produção educacional.

A capacitação para os docentes universitários no tema discutido favorece à aplicabilidade das metodologias ativas nas aulas de modo a desenvolver e fortalecer a construção do conhecimento do universitário efetivamente.

5. AGRADECIMENTOS:

Agradecemos à Universidade de Vassouras e a todas as outras instituições de ensino responsável pelo *Southern brazilian jornal of chemistry 2021 virtual conference* o ensejo de

refletir sobre uma temática de relevância educacional.

6. REFERÊNCIAS:

1. Wilson, K. E., Vyakarnam, S., Volkmann, C., Mariotti, S., & Rabuzzi, D. (2009, April). Educating the next wave of entrepreneurs: Unlocking entrepreneurial capabilities to meet the global challenges of the 21st century. In *World Economic Forum: A Report of the Global Education Initiative*.
2. Brasil, Conselho Nacional de Educação, (2002). *Parecer CNE/CES n.1/2002*. Recuperado em 10 dezembro, 2021, de https://www.in.gov.br/web/dou/-/resolu%C3%87%C3%83o-
3. Morán, J. (2015). Mudando a educação com metodologias ativas. *Coleção mídias contemporâneas. Convergências midiáticas, educação e cidadania: aproximações jovens*, *2*(1), 15-33.
4. MUNHOZ, A. S. (2016). ABP–Aprendizagem baseada em problemas.
5. Schell, J. (2018). *Mitos sobre a Sala de Aula Invertida, desmitificados*. Recuperado em 10 dezembro, 2021, de https://blog. peerinstruction. net/7-mitos-sobre-a-salade-aula-invertida-desmitificados/.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

METODOLOGIAS ATIVAS: CONSTRUÇÃO DE VIVÊNCIAS EDUCACIONAIS ATRAVÉS DE CAPACITAÇÃO CONTINUADA DE DOCENTES

Maria Fernanda Caravana de Castro Moraes Ricci*
Universidade de Vassouras, Curso de Pedagogia, Brasil.

Maria Luiza Delgado de Medeiros
Universidade de Vassouras, Curso de Pedagogia, Brasil

Suely Cristina de Souza Fernandes Crahim
Universidade de Vassouras, Curso de Pedagogia, Brasil

Suzana Medeiros Batista Amorim
Universidade de Vassouras, Curso de Pedagogia, Brasil

Therezinha Coelho de Souza
Universidade de Vassouras, Curso de Pedagogia, Brasil

December/2021

SUMMARY

SBJChem Conference 2021

INTRODUCTION

SBJChem Conference 2021

- Modelos formativos que atendam a construção de atos de currículo;
- Insurgência da mediação pedagógica ubíqua, amparados por tecnologia de informação e comunicação (TIC);
- As novas Diretrizes Curriculares Nacionais (DCNs) de diversos cursos de graduação preconizam, de forma recorrente, à adoção de práticas formativas baseadas em metodologias ativas;

BACKGROUND

SBJChem Conference 2021

- A Resolução CNE/CES nº 02/2019 (Brasil, 2019) que, de pronto, estabelece a necessidade de melhores parâmetros de implantação e de formação acadêmica em que os docentes adotem à avaliação por competência;
- Destaque Sala Invertida, *Problem Based Learning* (PBL), Simulação, Estudo de Caso e Gamificação;

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

Promover formação continuada dos professores dos cursos de graduação das IES mantidas pela

FUSVE para o uso de metodologias ativas na docência

5

METHODOLOGY

SBJChem Conference 2021

A pesquisa propôs acompanhar a formação continuada de docentes das IES mantidas pela FUSVE, Vassouras, Rio de Janeiro, Brasil, a partir do Projeto de Capacitação Contínua Docente, desenvolvido no segundo semestre de 2021.

Tratou-se de uma pesquisa-ação, desenhada como formação em serviço.

Primeiramente, foi oferecido um conjunto de palestras aos professores objetivando discussão do tema.

Nelas foram apresentadas situações didáticas de aplicação de metodologias ativas realizadas por docentes da Instituição de Ensino Superior.

Em seguida, os participantes realizaram um curso EaD institucional para formação na utilização de práticas docentes alinhadas à esse novo fazer.

6

RESULTS AND DISCUSSION

SBJChem Conference 2021

- O docente participante da capacitação planejou, para mais tarde executar, pelo menos um ato de currículo referente à um conteúdo didático de uma trilha de aprendizagem sob sua responsabilidade, considerando uma das metodologias ativas por ele experienciadas.
- Como política de formação permanente, todos os materiais da formação foram disponibilizados no AVA da IES, onde também foi criado um espaço de compartilhamento de boas práticas, em que se socializam experiências exitosas na prática docente amparada por metodologias ativas.

7

CONCLUSIONS

SBJChem Conference 2021

- Uso das Metodologias Ativas no ensino superior;
- Aplicabilidades das Metodologias Ativas contribuem com a produção educacional.
- A capacitação para os docentes universitários;
- A construção do conhecimento do universitário efetivamente.

8

ACKNOWLEDGEMENTS

SBJChem Conference 2021

- Universidade de Vassouras, Vassouras – RJ- Brasil;
- Todas as outras instituições de ensino responsáveis pelo *Southern brazilian jornal of chemistry 2021 virtual conference*;

REFERENCES

SBJChem Conference 2021

1. Wilson, K. E., Vyakarnam, S., Volkmann, C., Mariotti, S., & Rabuzzi, D. (2009, April). Educating the next wave of entrepreneurs: Unlocking entrepreneurial capabilities to meet the global challenges of the 21st century. In *World Economic Forum: A Report of the Global Education Initiative*.
2. Brasil, Conselho Nacional de Educação, (2002). *Parecer CNE/CES n.1/2002*. Recuperado em 10 dezembro, 2021, de https://www.in.gov.br/web/dou/-/resolu%C3%87%C3%83o-
3. Morán, J. (2015). Mudando a educação com metodologias ativas. *Coleção mídias contemporâneas. Convergências midiáticas, educação e cidadania: aproximações jovens*, *2*(1), 15-33.
4. MUNHOZ, A. S. (2016). ABP–Aprendizagem baseada em problemas.
5. Schell, J. (2018). *Mitos sobre a Sala de Aula Invertida, desmitificados*. Recuperado em 10 dezembro, 2021, de https://blog. peerinstruction. net/7-mitos-sobre-a-salade-aula-invertida-desmitificados/.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ACTIVITY-BASED KINETIC MODELLING OF LIPASE CATALYSED SYNTHESIS OF PEROCTANOIC ACID

BRANDOLÍN, Salvador Eduardo[1*]; SCILIPOTI, José[1]; MAGARIO, Ivana[1]

[1] Instituto de Investigación y Desarrollo en Ingeniería de Procesos y Química Aplicada (IPQA), Universidad Nacional de Córdoba, Facultad de Ciencias Exactas, Físicas y Naturales.

** Correspondence author*
e-mail: salvadorebrandolin@mi.unc.edu.ar

Received 10 December 2021; received in revised form 10 January 2021; accepted 28 January 2022

ABSTRACT

Carboxylic peroxy acids are organic oxidants of relevance in the cosmetic, food, and agrochemical industries. However, they are traditionally used as intermediaries in a process known as Prileschajew epoxidation and synthesized using sulfuric acid as a catalyst, promoting undesirable reactions on the final epoxides. Therefore, the study of selective catalysts such as enzymes is a topic of interest. In this work, peroctanoic acid synthesis was carried out using n-hexane as the solvent and an immobilized *Candida Antarctica* Lipase B commercial preparation as the catalyst. On the other hand, the oxidant, hydrogen peroxide was supplied as an aqueous solution, comprising the disperse phase of the reacting system. The reaction progression was quantified by iodometric and cerimetric titration of the peroctanoic acid concentration in the hexane phase. Four different initial amounts of octanoic acid were tested (0.74, 1.57, 10, and 20 millimoles). Substrate inhibition by octanoic acid was observed having at 1.57 millimoles the maximum initial reaction rate. The experimental data were fitted to a ping-pong bi-bi enzymatic kinetic model to estimate the initial reaction rate. Since this system constituted a liquid-liquid (organic-aqueous) two-phase system, the model was evaluated employing the thermodynamic activities of all species involved, assuming phase equilibria with time. The activities of all species were estimated using UNIFAC. As a result, the model was able to reproduce the trend of the initial rate with the change of the initial amount of octanoic acid.

Keywords: *Kinetic modeling, Candida Antarctica Lipase B, UNIFAC, Heterogeneous catalysis.*

1. INTRODUCTION

Carboxylic peroxy acids are organic oxidants of relevance in the cosmetic, food, and agrochemical industries. On the other hand, they are used as intermediates in the Baeyer-Villiger reaction and the Prileschajew epoxidation. The peroxy acids synthesis consists of the reversible reaction of a carboxylic acid and hydrogen peroxide to give a peroxy acid and water as in Equation 1:

$$\mathrm{R-CO_2H + H_2O_2 \leftrightarrow R-CO_3H + H_2O} \qquad \text{(Eq. 1)}$$

In the Prileschajew epoxidation, the formed peroxy acid reacts with an unsaturated organic substrate to produce an epoxide. Traditionally, sulfuric acid was the catalyst used in the peroxy acid synthesis despite being abrasive, difficult to handle at industrial scale, and unselective, thus promoting oxirane ring-opening of final epoxides. Therefore, the study of alternative environmentally friendly catalysts as lipases is a topic of interest. Particularly, the immobilized lipases, as heterogeneous catalysts, have the advantage that they are not required to be separated from the final reaction products, allowing them to be reused in multiple batches. The widely widespread technical Candida Antarctica Lipase B (CALB) was proved to be active in this reaction, known as a promiscuous lipase activity (Ortiz, 2019). This reaction was initially proposed by Björkling (Björkling, 1990). The mechanism proposed for peroxidation consists of a strict order entrance and outlet of substrates and products known as ping-pong bi-bi. First, the carboxylic acid must enter the CALB's active site pocket and be esterified with

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.12_abstract_BRANDOLIN.pdf

the alcohol group of Ser105, liberating a water molecule in the process. Then, hydrogen peroxide can perhydrolyze the Ser105-Carboxylic acid ester leaving a peroxy acid as a product (Warwel, 2000). This system is conformed by two liquid phases: a continuous organic phase, containing the substrates of epoxidation, and a disperse phase of aqueous nature, which contains hydrogen peroxide. Some authors postulated that this reaction occurs in the organic phase by H_2O_2 molecules transferred from the aqueous droplets. (Orellana-Coca, 2005). However, reaction at the organic-aqueous double layer interface was also postulated (Schmid, 1998; Verger, 1997; Silvestrini, 2020).

2. MATERIALS AND METHODS

2.1. Materials

Candida Antarctica Lipase B IMMCALB-T1-350 from ChiralVision (Den Hoorn, The Netherlands) (particle size: 0.35 mm, activity: 11000 PLU/g) was used as the catalyst. The solvent utilized was n-hexane from Cicarelli (Santa Fe, Argentina). Hydrogen peroxide 30% w/w analytical grade solution (Taurus, Argentina) and octanoic acid p.a (Tetrahedron, India) were used as reagents. Potassium iodide, ammonium cerium (IV) nitrate, sodium thiosulfate, sulfuric acid 95-98%, and potassium hydroxide of analytical grade were used for the analytical procedure.

2.2. Methods

The experimental setup consisted of a 4.6 cm of i.d glass reactor, not baffled, with a maximum capacity of 100 ml. The reactor was submerged in a thermostatic bath to maintain the temperature at a constant value of 30 ± 1 °C. The system was mechanically agitated at 600 rpm with a helix-type agitator with 2.5 cm of diameter.

Peroctanoic acid synthesis runs were carried with 1.799 g of hydrogen peroxide aqueous solution 25% w/w (0.01323 moles of hydrogen peroxide). The amounts of octanoic acid fed to the reactor were 0.1073, 0.2267, 1.4421, and 2.8842 g (0.74, 1.57, 10, and 20 millimoles, respectively). The amount of n-hexane loaded on each essay was 52.245, 52.113, 50.768, and 49.173 ml, respectively, to produce a total reaction volume of 54 ml. For all experimental runs, 0.5 g of catalyst were used.

The sampling methodology consisted of stopping the mechanic agitation for 30 seconds to allow the complete separation of the liquid phases. Then, 0.5 ml of the upper phase (organic) were sampled. The amount of peroctanoic acid produced was quantified by iodometric and cerimetric titration (Bhattacharya, 2011).

The Nelder-Mead algorithm of the function fminsearch in the software Matlab 8.4.0 was used to fit the kinetic parameters to the experimental data. First, the initial reaction rate was calculated from an order 2 polynomial fit of the initial condition of the system and the first 2 measurements of the reaction progress. The polynomial was derived concerning time and evaluated in time zero.

3. RESULTS AND DISCUSSION

3.1. Synthesis runs

Figure 1 shows the production of peroctanoic acid with time for each run.

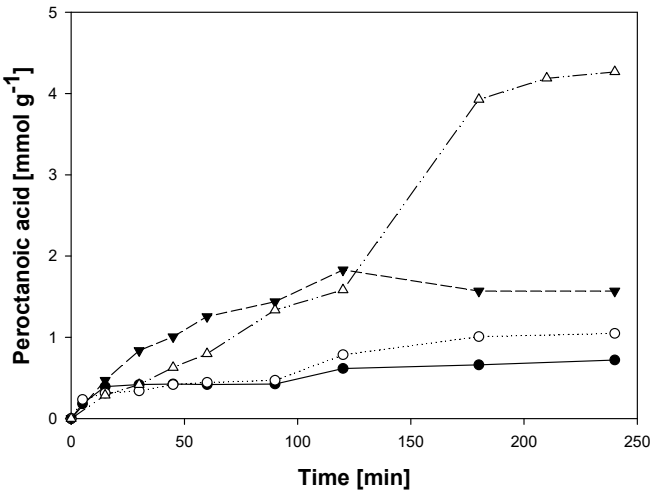


***Figure 1**. mmoles of peroctanoic per gram of catalyst produced for each octanoic acid initial load. ●: 0.74 mmol; ○: 1.57 mmol; ▼:10 mmol; △: 20 mmol.*

The increase of the initial load of octanoic acid from 10 mmoles produced a decrease in the initial reaction rate. Therefore, the system exhibited an inhibitory effect by the octanoic acid. The initial reaction rate at 20 mmoles loading was the lowest, with a value of 0.0244 mmol g^{-1} min^{-1}. At the 120 min of the reaction, the value of the reaction rate raised to 0.033 mmol g^{-1} min^{-1} despite the consumption of the substrate, showing that the octanoic acid initial amount is a critical parameter to calibrate. In a dynamic system where the peroxy carboxylic acid is used as an intermediary for an epoxidation series reaction, its consumption will turn the peroxy acid synthesis back to an initial rate condition. Therefore, the maximization of the initial rate for peracidation rather than the chemical equilibrium will probably increase the productivity

of the epoxidation.

3.2. Kinetic-thermodynamic model

A Michaelis-Menten ping-pong bibi mechanism with an octanoic acid reversible inhibition term was proposed to fit the initial rate of reaction (Eq. 2).

$$V_0 = \frac{k_r\, a_A\, a_B}{K_{M,B}\, a_A \left(1+\frac{a_A}{K_{i,A}}\right) + K_{M,A}\, a_B + a_A\, a_B} \qquad (Eq.2)$$

Where a_A is the initial activity of octanoic acid, a_B is the initial activity of hydrogen peroxide, $K_{M,B}$ is the Michaelis-Menten constant of hydrogen peroxide, $K_{M,A}$ is the Michaelis-Menten constant of octanoic acid, $K_{i,A}$ is the inhibitory constant of octanoic acid and k_r is the main kinetic constant.

The kinetic law is evaluated in the initial thermodynamic activities of the reaction substrates. This methodology is known as TABEK (thermodynamic activity-based enzyme kinetic), which was used to fit kinetic data of lipase-catalyzed esterifications (Castillo, 2016; Sandoval, 2002). In order to use this procedure is required to assume that interfacial diffusional resistances do not affect the reaction rate and that all species in both liquid phases are in thermodynamic equilibrium. However, considering this is not necessary to assume in which liquid phase or interface the reaction is taking place because the activity has the same value in both liquid phases.

Table 1 shows the value of the initial thermodynamics activities of the substrates for each run.

Table 1. *Initial activities of the reaction substrates on each essay - UNIFAC 30 °C*

Oc. Acid initial load (mmol)	a_{acid}	a_{H2O2}	a_{water}
0.74	0.0073	0.1325	0.8438
1.57	0.0152	0.1326	0.8438
10	0.0847	0.1326	0.8435
20	0.1471	0.1329	0.8430

The thermodynamic model UNIFAC was used for the phase stability analysis and the calculation of the initial activities (Fredenslund, 1975). In Table 2 are summarized the activity coefficients of the reagents on each octanoic acid loading condition. These UNIFAC predictions indicate the deviation of the ideal behavior. As the activity coefficient becomes higher than 1, more non-ideal is the system.

Since hydrogen peroxide is added as an aqueous solution to the system, water activity is different from zero at the initial time. However, since no peroctanoic acid is present, the backward reaction can be neglected at time zero. As shown, the initial activities of water and hydrogen peroxide were maintained practically constant, and the octanoic acid activity increases according to the increased feeding from run to run. As the initial activity of water is constant, any effect that it may have on the initial reaction rate can be neglected in the kinetic model (Sandoval, 2001).

Table 2*. Initial activity coefficients on each phase of the reagents – UNIFAC 30 °C*

	Aqueous phase		Organic phase	
Oc. Acid initial load (mmol)	γ Oc. Acid	γ H_2O_2	γ Oc. Acid	γ H_2O_2
0.74	270.6	0.891	3.791	8240
1.57	270.2	0.891	3.740	7667
10	266.3	0.890	3.280	4007
20	262.5	0.890	2.848	2139

Figure 2 shows the initial experimental velocities and the model estimation as a function of the initial activity of octanoic acid. These experiments were utilized to obtain the kinetic parameters (Table 3).

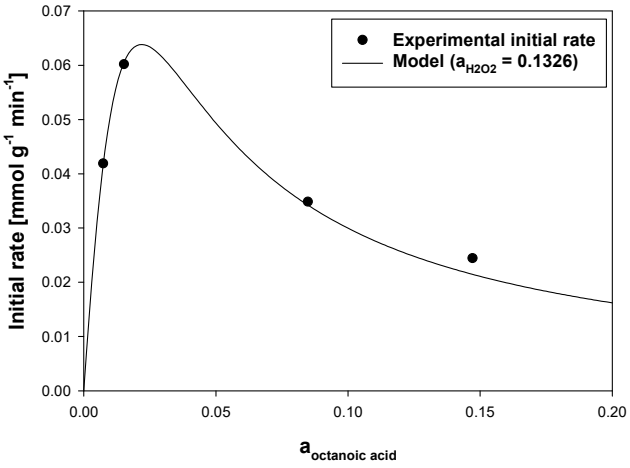


Figure 2. *Experimental and model estimation of initial reaction rate vs. octanoic acid activity.*

Table 3*. Kinetic parameters*

k_r (mmol g^{-1} min^{-1})	$K_{M,A}$	$K_{M,B}$	$K_{i,A}$
0.9561	0.1324	0.2466	0.0067

The inhibitory effect of butyric acid was reported previously in the literature (Dutta Banik, 2016). However, it is an uncommon behavior and apparently occurs around certain concentrations

of carboxylic acids. Therefore, the inhibition mechanism of carboxylic acids is not specified. Considering the reaction mechanism proposed, where the octanoic acid is the first substrate that interacts with the active site, the inhibitory effect should not be due to octanoic acid interfering with the normal functionality of the active site amino acids. It is assumed that the inhibitory mechanism could be that octanoic acid interacts with another structure of the enzyme, minimizing its catalytic activity. The other possibility is that the large amounts of octanoic acid are competing to enter the active site leading to a steric problem. This behavior indicates the existence of an optimum initial octanoic acid activity for each initial hydrogen peroxide activity, and it can be evaluated with equation 3.

$$a_A = \sqrt{\frac{K_{iA} K_{mA} a_B}{K_{mB}}} \qquad (Eq.3)$$

This equation is obtained deriving the initial velocity concerning the octanoic acid activity, with constant hydrogen peroxide activity and equating to zero.

For the particular initial hydrogen peroxide activity used in this work, the optimal initial activity of the octanoic acid, obtained from equation 2, is 0.02184, which corresponds with an initial load of 2,2024 mmole (0.3176 g).

4. CONCLUSIONS

The TABEK methodology results in a satisfactory tool to fit the experimental data of the initial peroctanoic synthesis rate considering its inhibitory effect in the reaction. The mechanism of the inhibitory effect of the carboxylic acid is still undetermined and needs more deep investigation in further works.

6. REFERENCES:

1 Ortiz, C., Ferreira, M.L., Barbosa, O., Santos, J., Rodrigues, R., Berenguer-Murcia, A., Briand, L., Fernandez-Lafuente, R. *Catal. Sci. Technol.*, **2019**, *9*, 2380

2 Björkling, F., Godtfredsen, S. E. Kirk, O. *J. Chem. Soc. Chem. Commun*, **1990**, 19, 1301.

3 Warwel, S., Klaas, M. R. gen. in *Peroxide Chemistry*, **2000**, 234, 209

4 Orellana-Coca, C., Camocho, S., Adlercreutz, D., Mattiasson, B. Hatti-Kaul, R. *Eur. J. Lipid Sci. Technol,* **2005***,* 107, 864

5 Schmid, R. D., Verger, R. *Angew. Chemie - Int. Ed.*, **1998**, *37*, 1608

6 Verger, R. *Trends Biotechnol.*, **1997**, *15*, 32

7 Silvestrini, L. Cianci, M. *Int. J. Biol. Macromol.*, **2020**,158, 358

8 Bhattacharya, S. *P.H.D.Thesis- Universitat Berlin*, **2011**.

9 Castillo, E. Casas-Godoy, L., Sandoval, G. *Biocatalysis*, **2016**, *1*, 178

10 Sandoval, G., Condoret, J. S., Monsan, P. Marty, A. *Biotechnol. Bioeng., **2002**, 78*, 313

11 Fredenslund, A., Jones, R. L., Prausnitz, J. M. *AIChE J.*, **1975**, *21*, 1086

12 Sandoval, G. C., Marty, A., Condoret, J. S. *AIChE J.*, **2001**, 47, 718

13 Dutta Banik, S., Nordblad, M., Woodley, J. M., Peters, G. H. *ACS Catal.*, **2016**, *6*, 6350

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THERMODYNAMIC AND KINETIC APPROACH TO ENZYMATIC SYNTHESIS OF PEROCTANOIC ACID

Salvador Eduardo Brandolín; José Scilipoti; Ivana Magario

Universidad Nacional de Córdoba

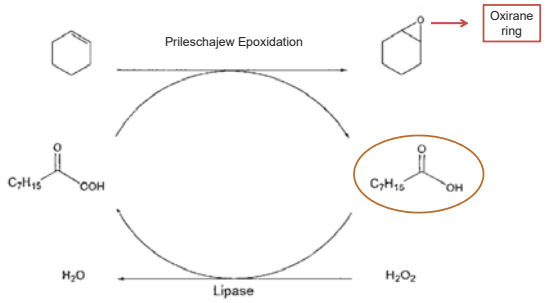
Instituto de Investigación y Desarrollo en Ingeniería de Procesos y Química Aplicada (IPQA) - Argentina

IPQA

March/2022

INTRODUCTION

SBJChem Conference 2021



Candida Antarctica Lipase B (CalB)

Peracidation

2

INTRODUCTION

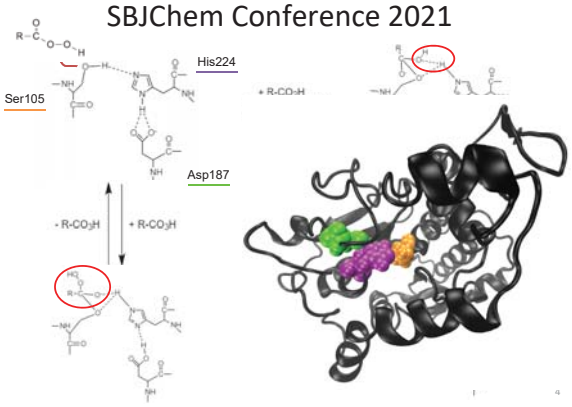
SBJChem Conference 2021

Aqueous phase	Organic phase
H_2O	$R-COOH$
H_2O_2	$R-COOOH$
	Epoxidation Substrate

3

INTRODUCTION

SBJChem Conference 2021



4

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

The purpose of this work Is to study the influence of the initial load of octanoic acid in the peroctanoic acid synthesis and propose a kinetic law that fits the experimental initial reaction rate

5

METHODOLOGY

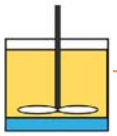
SBJChem Conference 2021

1.799 g hydrogen peroxide 25% solution (0.01323 mole H_2O_2)
0.5 g catalyst (IMMCALB-T1-350)

Thermostatic bath 30 ± 1 °C – 600 rpm (helix agitator)

- Oc. acid: 0.74 mmol, Hexane: 52.245 ml
- Oc. acid: 1.57 mmol, Hexane: 52.113 ml
- Oc. acid: 10.0 mmol, Hexane: 50.768 ml
- Oc. acid: 20.0 mmol, Hexane: 49.173 ml

Total volume 54 ml



Stop mechanical agitation for 30 s

0.5 ml sample of the upper liquid phase (organic)

Titrate peroctanoic acid by cerimetry and iodometry

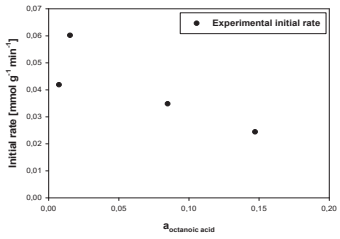
6

RESULTS AND DISCUSSION

SBJChem Conference 2021

Oc. Acid initial load [mmol]	a_{acid}	a_{H2O2}	a_{water}
0.74	0.0073	0.1325	0.8438
1.57	0.0152	0.1326	0.8438
10	0.0847	0.1326	0.8435
20	0.1471	0.1329	0.8430

UNIFAC



7

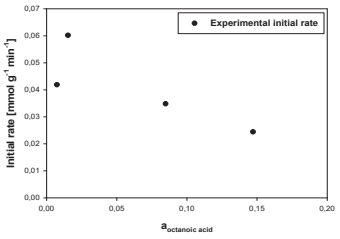
RESULTS AND DISCUSSION

SBJChem Conference 2021

$$V_0 = \frac{k_r\, a_A\, a_B}{K_{M,B}\, a_A \left(1 + \frac{a_A}{K_{I,A}}\right) + K_{M,A}\, a_B + a_A\, a_B} \qquad (Eq.1)$$

k_r [mmol g⁻¹ min⁻¹]	$K_{M,B}$	$K_{M,A}$	$K_{I,A}$
0.9561	0.1324	0.2466	0.0067

Subscript A: octanoic acid
Subscript B: hydrogen peroxide



8

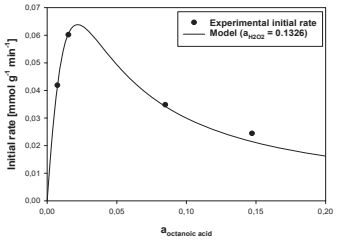
RESULTS AND DISCUSSION

SBJChem Conference 2021

$$V_0 = \frac{k_r\, a_A\, a_B}{K_{M,B}\, a_A \left(1 + \frac{a_A}{K_{i,A}}\right) + K_{M,A}\, a_B + a_A\, a_B} \qquad (Eq.\ 1)$$

k_r [mmol g^{-1} min^{-1}]	$K_{M,A}$	$K_{M,B}$	$K_{i,A}$
0.9561	0.1324	0.2466	0.0067

Subscript A: octanoic acid
Subscript B: hydrogen peroxide



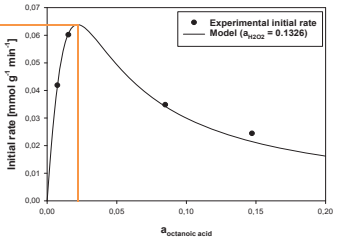
RESULTS AND DISCUSSION

SBJChem Conference 2021

$$a_A^{\ optimum} = \sqrt{\frac{K_{iA} K_{mA} a_B}{K_{mB}}} = 0.02184$$

2.2024 mmole initial load of octanoic acid

0.06381 mmol / (g min)



CONCLUSIONS

SBJChem Conference 2021

- The TABEK methodology results a satisfactory tool to fit the experimental data of initial peroctanoic synthesis rate considering the inhibitory effect of octanoic acid in the reaction.

- The mechanism of the inhibitory effect of the carboxylic acid still undetermined and needs more deep investigation in further works.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

Pelaez, Walter José; Group: Química Teórica-Experimental de moléculas de interés ambiental; Universidad Nacional de Córdoba

REFERENCES

SBJChem Conference 2021

1. Warwel S, Klaas MR gen. New Peroxycarboxylic Acids by Lipase Catalysis: Preparation and Oxidation Properties. In: *Peroxide Chemistry*. Vol 234. Wiley; 2000:209-231. doi:10.1002/3527600396.ch10
2. Björkling F, Godtfredsen SE, Kirk O. Lipase-mediated formation of peroxycarboxylic acids used in catalytic epoxidation of alkenes. *J Chem Soc Chem Commun*. 1990;(19):1301-1303. doi:10.1039/C39900001301
3. Bhattacharya S. Solvent-free chemo-enzymatic epoxidation: Experimental and kinetic modelling studies. Published online 2011:175.
4. Castillo E, Casas-Godoy L, Sandoval G. Medium-engineering: a useful tool for modulating lipase activity and selectivity. *Biocatalysis*. 2016;1(1):178-188. doi:10.1515/boca-2015-0013
5. Sandoval G, Condoret JS, Monsan P, Marty A. Esterification by immobilized lipase in solvent-free media: Kinetic and thermodynamic arguments. *Biotechnol Bioeng*. 2002;78(3):313-320. doi:10.1002/bit.10224
6. Fredenslund A, Jones RL, Prausnitz JM. Group contribution estimation of activity coefficients in nonideal liquid mixtures. *AIChE J*. 1975;21(6):1086-1099. doi:10.1002/aic.690210607
7. Sandoval GC, Marty A, Condoret JS. Thermodynamic Activity-Based Enzyme Kinetics: Efficient Tool for Nonaqueous Enzymology. *AIChE J*. 2001;47(3):718-726. doi:10.1002/aic.690470318
8. Dutta Banik S, Nordblad M, Woodley JM, Peters GH. A Correlation between the Activity of Candida antarctica Lipase B and Differences in Binding Free Energies of Organic Solvent and Substrate. *ACS Catal*. 2016;6(10):6350-6361. doi:10.1021/acscatal.6b02073

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

Salvador Eduardo Brandolín; José Scilipoti; Ivana Magario

Universidad Nacional de Córdoba

Instituto de Investigación y Desarrollo en Ingeniería de Procesos y Química Aplicada (IPQA) - Argentina

IPQA

Contact email: salvadorebrandolin@mi.unc.edu.ar

Institute's web: https://ipqa.unc.edu.ar/

December/2021

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ADSORPTION STUDIES OF ZINC, COPPER, AND LEAD IONS FROM PHARMACEUTICAL WASTEWATER ONTO SILVER MODIFIED CLAY ADSORBENT

AJALA, Mary Adejoke[1,2,4*]; ABDULKAREEM, Ambali Saka[2,4]; KOVO, Abdulsalami Sanni[2,4.]; TIJANI, Jimoh Oladejo[3,4]; ADEYEMI, Ayomide Samuel[1]

[1] Department of Chemical Engineering, University of Ilorin, Ilorin, Kwara State, Nigeria.

[2] Department of Chemical Engineering, Federal University of Technology, Minna
.

[3] Department of Chemistry, Federal University of Technology, Minna, Niger State, Nigeria.

[4] Nanotechnology Research Group, Centre for Genetic Engineering and Biotechnology (CGEB), Federal University of Technology, P.M.B 65, Bosso, Minna, Niger State, Nigeria.

**Corresponding author*
email: ajala.ma@unilorin.edu.ng

Received 15 October 2021; received in revised form 06 January 2022; accepted 24 January 2022

ABSTRACT

Clay-supported silver nanoparticles were green synthesized using the aqueous leaf extract of *Parkia biglobosa*. The phytochemical analysis and FTIR results of the *Parkia biglobosa* showed that the leaf contains phenol, tanning, and flavonoids, which act as reducing, capping, and stabilizing agents required for the synthesis of the silver nanoparticles. The prepared adsorbent has good morphology, is rich in silica, and contains functional groups suitable for heavy metal binding. The adsorptions of Zn, Cu, and Pb from pharmaceutical wastewater onto the silver-modified clay were studied as an adsorbent dosage and contact time. From the percentage removal results obtained, the adsorbent had up to 99.96%, 99.5%, and 99.44% removal efficiency for Zn, Pb, and Cu, respectively. The present work shows that the synthesized silver nanoparticles supported on local clay can be used as a potentially low-cost adsorbent to remove heavy metal ions from industrial wastewater.

Keywords: *Green synthesis, Parkia biglobosa, Silver oxide, Nanoadsorbent, heavy metals.*

1. INTRODUCTION

The pharmaceutical industry is a major producer of wastewater effluents containing pollutants such as heavy metals (zinc (Zn), copper (Cu) and lead (Pb)), microbes (bacteria), and dyes (yellow). The pollutants reduce the photosynthetic activity of aquatic life and could poison certain forms of aquatic life (Gardare *et al*., 2014). Therefore, Zn, Cu, and Pb in pharmaceutical wastewater are hazardous and harmful to human health. Although Zn is an essential element in human beings because it could serve food supplements, its excess is extremely dangerous as it may cause paralysis and neurological problems. Excess Zn may also lead to a state of depression and other unwanted effects such as dizziness, breathing problems, and chest pain (Kaur and Sharma, 2017). The WHO guidelines gave the maximum admissible concentration of Zn in an aqueous solution as 5.0 mg/l (WHO, 2008). Also, Cu has been reported to have adverse effects on human health. These include mental disorders, anemia, arthritis/rheumatoid arthritis, hypertension, and liver enlargement (Lakherwal, 2014).

Furthermore, the WHO gave the maximum admissible concentration of Cu in an aqueous solution as 0.05 mg/l (Bankole *et al*., 2019). On the other hand, lead is responsible for lung dysfunction, liver damage, reduced pulmonary function, and cardiovascular dysfunction (Balali-mood *et al*., 2021). Hence, Zn, Cu, and Pb removal from pharmaceutical wastewater are essential for human and aquatic survival.

Several conventional techniques such as photocatalytic oxidation, chemical coagulants, bioremediation, ion-exchange resins, reverse osmosis, membrane filtration, solvent extraction, and electrolysis have been reported for the removal of various heavy metals from wastewater

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.10_abstract_AJALA.pdf

(Dave and Chopda, 2014). However, they are inadequate with some challenges and drawbacks, such as cost-effectiveness, disposal after use, efficiency, and lack of eco-friendliness of the technological processes (Dutta *et al*., 2021). Therefore the need for more research on some other methods such as adsorption.

Adsorption technique is advancing to remove heavy metals, colors, and microbes from wastewater. Since the process is highly efficient, adsorbate-specific, cost-effective, easy to handle, and eco-friendliness (Dutta *et al*., 2021). Adebayo *et al*. (2020), however, justified the use of nanomaterials as good adsorbents for the removal of heavy metals. Furthermore, it was reported that nanomaterials have appropriate adsorption surfaces that possess unique characteristics vis-à-vis a very high surface-area-to-volume ratio. All of these advantages give a tremendous driving force for diffusion, especially at high temperatures [9].

Several nanomaterials have been used for the removal of heavy metals from wastewater. For example, Mustapha *et al*. (2019) utilized modified kaolinite clay to remove Zn and Cr from tannery wastewater [10]. Bankole *et al*. (2019) also eliminate Zn and Cu from electroplating wastewater using nanoadsorbent (Bankole *et al*., 2019). Kariim *et al*. (2020) used nanoadsorbent to treat pharmaceutical wastewater [11].

Therefore, this study investigated the development of Ag Nps/clay adsorbent to remove Zn, Cu, and Pb from pharmaceutical wastewater.

2. MATERIALS AND METHODS

2.1. Preparation procedures

2.1.1 Beneficiation of clay

The ball clay collected from Akerebiata, Ilorin, Kwara state was soaked in water for 48 h to allow the clustered clay to dissolve. It was then sieved to ease the removal of the sand particles and later allowed to sediment to get the fine particles of the clay. The fine particles obtained were sun-dried, oven-dried at 100℃, pulverized, and then sieved with a sieve mesh of < 0.2μm.

2.1.2 Preparation of leaf extract

Fresh leaves of *Parkia biglobosa* were washed with clean water and air-dried for two weeks at room temperature to prevent the destruction of the thermolabile constituents present in the plant by direct sun rays. The room dried leaves were then pulverized, and the phytochemical analysis for the plants was carried out. Next, 100 mL of deionized water was added to 5g of the pulverized leaf. The solution was then boiled at 60℃ for 30min to extract the reducing and stabilizing agents. Finally, the aqueous extract was filtered using a muslin cloth and filter paper (Whatman no.1). The filtrate was kept in a refrigerator for the biosynthesis of silver nanoparticles.

2.1.3 Green synthesis of silver nanoparticles

The adopted plant was pulverized. 5g of the pulverized plant was added to 100 mL of deionized water, boiled at 60℃, and stirred continuously for 30 min using a magnetic stirrer to extract the reducing and stabilizing agents. The solution was filtered using a muslin cloth and filter paper (Whatman no.1). The varied volume of leaf extract was added to a varied volume of 1mM $AgNO_3$ solution following the data gotten from the factorial design of the Design Expert. The solution was allowed to stand for 20 minutes. The pH of the resultant solution was adjusted between pH 4 and pH 10 with either 2 M NaOH or HCl. The color change from green to brown indicates the formation of nanoparticles. The solutions were characterized using a UV-Visible spectrophotometer.

2.1.4 Silver/Clay loading procedure

Forty grams (40 g) of the beneficiated clay was weighed on an analytical balance and added to a flask containing 400 mL of 1 mM $AgNO_3$. The flask was sealed and shaken at room temperature for 24 hours in a thermostatic water batch shaker (SHA-C); the suspension was filtered using a filter paper (Whatman no.1) and gradually dried at 50℃ for 24 h. Based on the result obtained, the silver ions present in the silver-synthesized clay were reduced by adding 20 mL of the leaf extract of Parkia biglobosa under continuous stirring for a few minutes. After reduction, the solution was filtered using a filter paper (Whatman no.1) and washed several times with deionized water to remove residual Ag^+ ions.

2.2 Adsorption Studies

The investigations were carried out in batches of adsorbent dosage and contact time to check the proclivity of the adsorption process. After undergoing the required experimental procedures, 100 – 1000 mg/L concentration was adopted. In each 100 mL measuring flasks, 25 mL of the wastewater of known concentrations was poured having a known amount of adsorbent. The mixture was shaken for 60 min, the supernatant was filtered through Whatman Filter Paper No. 1, and the wastewater was analyzed.

3. RESULTS AND DISCUSSION

3.1 Characterization result

3.1.1 FTIR of Parkia Biglobosa, Clay and Ag-clay

The structural exposition and macromolecules of *Parkia biglobosa* were evaluated using FTIR technique (Figure 1). The FTIR spectra showed characteristic peaks of hydrogen-bonded O-H stretch at 3533.71, 3417.98, 3363.97, and 3271.38 cm^{-1}. The peak at 3055.35 cm^{-1} indicates C=C-H asymmetric stretch. The peaks at 3417.98, 3363.97, 3271.38, and 3055.35 cm^{-1} indicate N-H stretch. Peaks of H-C-H asymmetric and symmetric stretch were shown at 2924.18 and 2862.46 cm^{-1}, while 2746.73 cm^{-1} indicates C-H stretch off C=O; the peak at 2345.52 cm^{-1} is as a result of C≡N stretch. The peaks at 1728.28 and 1627.97 cm^{-1} indicate C=O stretch; 1535.39 and 1442.80 cm^{-1} are due to H-C-H bend and C-C=C asymmetric stretch. The peaks at 1373.36, 1327.07, and 1026.16 cm^{-1} indicate the C-O stretch. The presence of the O-H stretch, which is related to phenol, serves as a reducing and stabilizing agent in the formation of the silver nanoparticles.

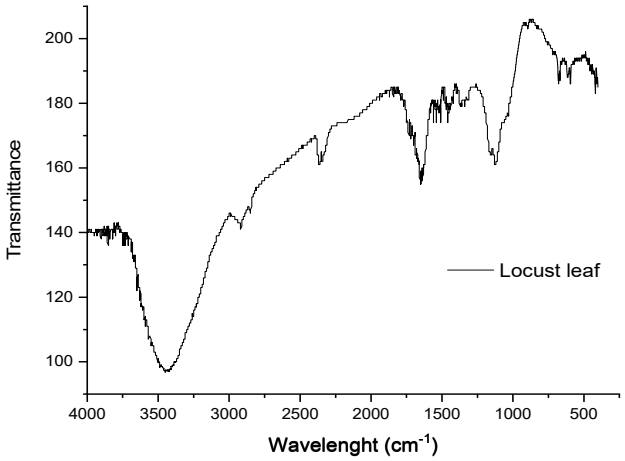


Figure 1: FTIR spectrum of Parkia biglobosa

The Fourier transform infrared (FTIR) spectroscopy of the clay was evaluated in Figure 2a. The characteristic peaks at 3701.70 and 3615.89 cm^{-1} represent the O-H stretch of alcohols, and phenolic group, the peak at 1111.01cm^{-1} represents the C-O stretch of esters, while the C-O stretching peak at 1004.77cm^{-1} is of ethers. The peaks at 914.87, 792.28, and 706.47cm^{-1} are attributed to the Si-O-Si and Al-O-Si bonds of silicate clay. The FTIR spectra of the silver-clay in Figure 2b shows several peaks indicating the functional groups embedded in the adsorbent. The characteristic peak of the hydrogen-bonded O-H stretch, at 3305.86 cm^{-1}, is the phenolic and alcohol group. Bonded O-H of carboxylic acids is observed at 2928 cm^{-1}. The peaks at 1621 and 1600 are attributed to the C=O stretch of carbonyl and ketones. Other peaks at 1298 cm^{-1}, 1251 cm^{-1}, and 1186 cm^{-1} depict C-O stretch attributed to esters and ethers, indicating a shift from the previously observed in unmodified clay likely due to the chemical modification (Dhand *et al*., 2016). Si-O-Si and Al-O-Si bonds of silicate clay are at 910 cm^{-1}, 800.24 cm^{-1}, and 700 cm^{-1}. New peaks, which deviated entirely from those on the clay spectral, are observed at 534.78 cm-1, 462.34 cm-1, and 432.66 cm-1 attributed to Ag loading, which is similar to the findings of Krishnan and Mahalingam (2017).

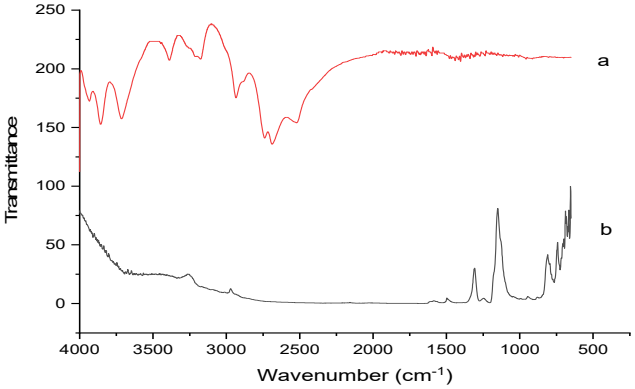


Figure 2: FTIR spectrum of (a) Clay and (b) Ag supported on clay Adsorbent

3.2 Morphology and Structure

The Scanning Electron Microscope was used to examine the surface morphology of the prepared adsorbent. Figure 3 reveals an evenly distributed arrangement of spherical nanocomposites. The flat-lying stacks are pseudo-hexagonal in a structure having curved edges, which are the characteristics of kaolinite clays. The even arrangement implies polydispersity and intercalation of the silver nanoparticles into the clay structure. The EDS result presented in Figure 4 shows that the clay is truly rich in silica of 13.97%, bonded oxygen is up to 42.27% of the entire weight, titanium and iron have low weight percent of 0.29 and 1.77%, respectively.

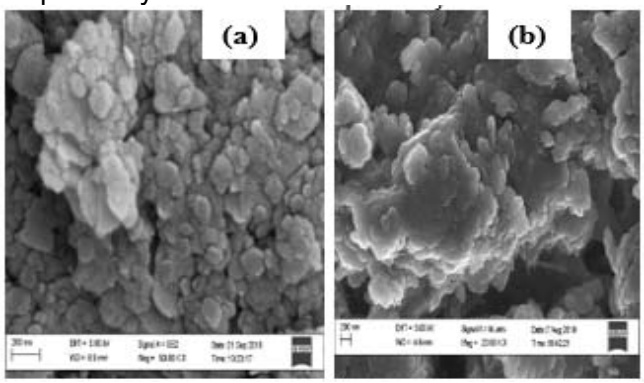


Figure 3: SEM Image of (a) Clay (b) Silver-Clay Adsorbent

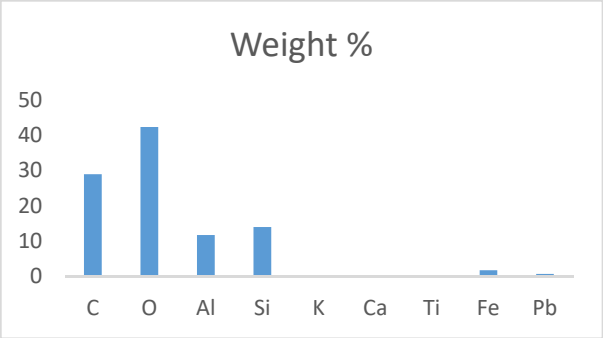


Figure 4: EDS of the Silver-Clay Adsorbent

3.2 Adsorption studies

3.2.1 Effect of adsorbent dose on the removal of the heavy metals

As adsorbent dosage increases from 0.1 g to 0.3 g, the percentage removal of Zn^{2+}, Pb^{2+} and Cu^{2+} increases and then begins to decline as adsorbent dosage increases beyond 0.3 g, as shown in Figure 5. This is because at lower adsorbent concentration number of active sites is higher. In addition, with the increase in adsorbent dosage, aggregation of particles occurs due to the low volume of solution. As a result, removal efficiency and adsorption of Zn^{2+}, $Pb^{2+,}$ and Cu^{2+} decreases.

3.2.2 Effect of contact time on the removal of the heavy metals

Figure 6 shows the effect of time on adsorption. As the adsorption time was changed from 30 to 240 minutes, efficiency for Zn^{2+}, $Pb^{2+,}$ and Cu^{2+} increased from 92.3%, 81.2%, and 80.1% at 30minutes to 97.82%, 85.83%, and 85.39% at 90minutes respectively, and remained constant afterward. As time progresses, the surface coverage of the adsorbent is high, and further, no adsorption takes place.

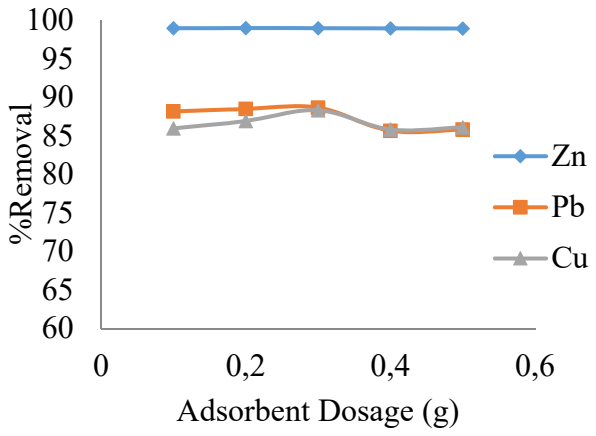


Figure 5: Effect of adsorbent dosage on % removal

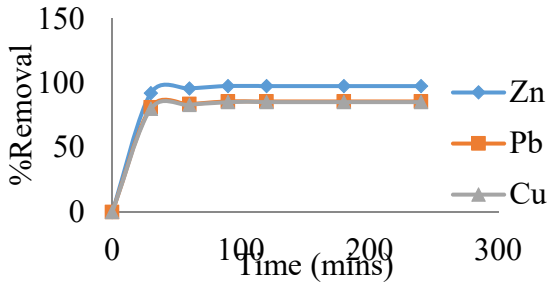


Figure 6: Effect of contact time on % removal

4. CONCLUSIONS

A new adsorbent was synthesized using local clay from Akerebiata, Ilorin modified with silver nanoparticles. The synthesis of Ag nanoparticles in a green process confirms the suitability of *Parkia biglobosa* leaf extract as a reducing, capping, and stabilizing agent. The local clay was also confirmed kaolinite in nature, rich in silica, and contains functional groups capable of binding metal ions to themselves. The adsorption of three heavy metal ions such as Zn^{2+}, $Pb^{2+,}$ and Cu^{2+} onto the silver-modified clay was feasible, spontaneous, and exothermic in nature in the order $Zn^{2+}>Pb^{2+}>Cu^{2+}$. Therefore, the silver-clay adsorbent is suitable and efficient for removing heavy metal ions from an aqueous solution.

5. REFERENCES

1. Adebayo, G. B., Adegoke, H. I., and Fauzeeyat, S. *Applied Water Science*, **2020,** *10*(9), 1.
2. Balali-mood, M., Naseri, K., Tahergorabi, Z., and Khazdair, M. R. *Frontiers in Pharmacology*, **2021**, 12(April), 1.
3. Bankole, M. T., Abdulkareem, A. S., Mohammed, I. A., Shaibu, S., Tijani, J. O., and Abubakre, O. K. *Scientific Report*, **2019**. May 2018, 1.
4. Dave, P. N., and Chopda, L. V. *Journal of Nanotechnology*, **2014**, 14.
5. Dutta, D., Borah, J. P., and Puzari, A. *Adsorption Science and Technology*, **2021**, 1.
6. Gardare, V. N., Yadav, S., Avhad, D. N., and Rathod, V. K. *Desalination and Water Treatment*, **2014**, *December*, 37.
7. Kariim, I., Abdulkareem, A. S., and Abubakre, O. K. *Scientific African*, **2020**, 7.
8. Kaur, A., and Sharma, S. *Indian Journal of Science and Technology*, **2017** *10*(34), 1.
9. Lakherwal, D. *International Journal of Environmental Research and Development*, **2014**. *4*(1), 41.
10. Mustapha, S., Ndamitso, M. M., Abdulkareem, A. S., Tijani, J. O., and Mohammed, A. K. *Heliyon*, **2019** *5*(October), 1.
11. World Health Organization (WHO). (2008). *Guidelines for Drinking-water Quality*. *Third Edit*, Third Edition Incorporating First and Second Adden.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ADSORPTION STUDIES OF ZINC, COPPER, AND LEAD IONS FROM PHARMACEUTICAL WASTEWATER ONTO SILVER MODIFIED CLAY ADSORBENT

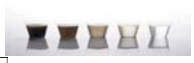
Mary Adejoke Ajala
University of Ilorin, Ilorin. Faculty of Engineering And Technology, Department of Chemical Engineering, Kwara State, Nigeria.
Ambali Saka Abdulkareem
Federal University of Technology, Minna. Faculty of Engineering And Technology, Department of Chemical Engineering, Niger State, Nigeria.
Abdulsalami Sanni Kovo
Federal University of Technology, Minna. Faculty of Engineering And Technology, Department of Chemical Engineering, Niger State, Nigeria.
Jimoh Oladejo Tijani
Federal University of Technology, Minna. Faculty of Engineering And Technology, Department of Chemical Engineering, Niger State, Nigeria.
Ayomide Samuel Adeyemi
University of Ilorin, Ilorin. Faculty of Engineering And Technology, Department of Chemical Engineering, Kwara State, Nigeria.

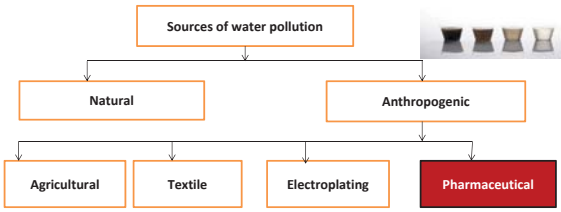
March/2022

INTRODUCTION

SBJChem Conference 2021

- Water Pollution
- Wastewater
- Pollutants and Heavy Metals



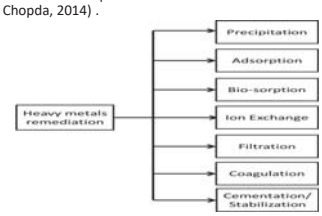


BACKGROUND

SBJChem Conference 2021

• Consumptions of heavy metal in water is very dangerous responsible for renal failure, reproduction problem, cancer and death (Balaali-mood et al., 2021).

•Several techniques are used for its remediation but are with attendant challenges(Dave & Chopda, 2014) .



Adsorption techniques is preferred over others because of its flexibility, low initial cost, ease of operation, and effectiveness towards wide range of pollutants (Bankole et al., 2019).

AIM/OBJECTIVE/PURPOSE

SBJChem Conference 2021

The main goal of this study is to develop AgNps/clay composites for the removal of Zn(II), Cu(II) and Pb(II) ions from pharmaceutical wastewater.

JUSTIFICATION

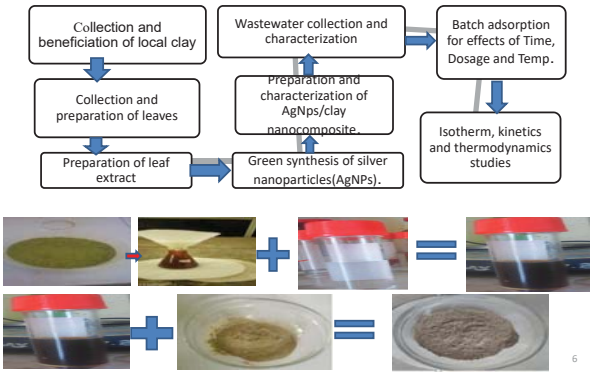
SBJChem Conference 2021

❑Several materials such as sand, gravels, activated carbon, and biomass char had been used as adsorbents to remove pollutants (Adebayo et al., 2020). In this research work, metallic nanoparticles (silver oxide composite) was used to remove selected heavy metals in pharmaceutical wastewater. These were employed due to their large specific surface area, ability to adsorb wide range of contaminants and fast kinetics.

❑ Nanoparticles (NPs) tends to aggregate when used as individual components to treat wastewater, which results in release of NPs into the environment. Therefore, clay was used as a support for silver oxide nanoparticles. The combination was considered as a promising sequester of heavy metals from industrial wastewater.

METHODOLOGY

SBJChem Conference 2021



RESULTS AND DISCUSSION

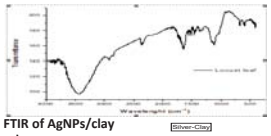
SBJChem Conference 2021

Physical Characterization of Silver-clay Nanoparticles (AgNPs/clay)

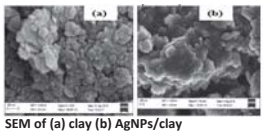
❑X-ray diffractionXRD, SEM, EDS analysis

•The XRD analysis successfully unfolded the crystalline nature of the synthesized AgNPs/Clay composite.

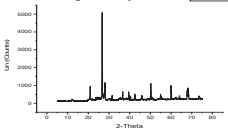
•The SEM particle size distribution has average particle size of 42.90nm.



FTIR of AgNPs/clay



SEM of (a) clay (b) AgNPs/clay



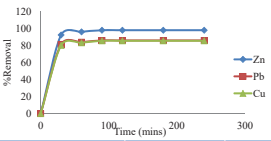
XRD of AgNPs/clay

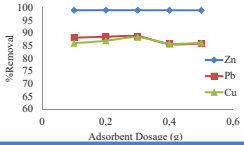
EDS of AgNPs/clay

RESULTS AND DISCUSSION (Cont'd)

SBJChem Conference 2021

Adsorption Effects





Results of Adsorption kinetics

Model	Parameter	Metal ion		
		Zn^{2+}	Pb^{2+}	Cu^{2+}
	$q_{m,exp}$ (mg/g)	97.8	97	96.4
Pseudo first-order	k_1 (min^{-1})	0.003	0.003	0.002
	$q_{e,calc}$ (mg/g)	0.360	0.375	0.286
	R^2	0.022	0.284	0.766
Pseudo second-order	k_2 (min^{-1})	0	0.0058	0.0058
	$q_{e,calc}$(mg/g)	100	90.9	90.9
	R^2	1.000	0.999	0.999

CONCLUSION

SBJChem Conference 2021

- ❖ FTIR result of *Parkia biglobosa* leaf extract confirms that the leaf can be used as a reducing, capping and stabilizing agent.
- ❖ The local clay was also confirmed kaolinite in nature, rich in silica and contains functional groups capable of binding metal ions to themselves.
- ❖ The results of the batch experiments indicated that the adsorption process was affected by adsorbent dose, contact time, and temperature.
- ❖ The kinetic study indicated adsorption was governed and better represented by the Pseudo-second-order kinetics for the adsorbent.

•The adsorption of three heavy metal ions such as Zn^{2+}, Pb^{2+} and Cu^{2+} onto the silver modified clay was feasible, spontaneous, and exothermic in nature in the order Zn^{2+}>Pb^{2+}>Cu^{2+}

•The silver-clay adsorbent is therefore suitable and efficient for removal of heavy metal ions from aqueous solution.

REFERENCES

SBJChem Conference 2021

1. Adebayo, G. B., Adegoke, H. I., & Fauzeeyat, S. (2020). Adsorption of Cr (VI) ions onto goethite , activated carbon and their composite : kinetic and thermodynamic studies. *Applied Water Science*, *10*(9), 1–18. https://doi.org/10.1007/s13201-020-01295-z
2. Balali-mood, M., Naseri, K., Tahergorabi, Z., & Khazdair, M. R. (2021). *Toxic Mechanisms of Five Heavy Metals : Mercury , Lead , Chromium , Cadmium , and Arsenic*. *12*(April), 1–19. https://doi.org/10.3389/fphar.2021.643972
3. Bankole, M. T., Abdulkareem, A. S., Mohammed, I. A., Shaibu, S., Tijani, J. O., & Abubakre, O. K. (2019). *Selected Heavy Metals Removal From Electroplating Wastewater by Purified and Polyhydroxylbutyrate Functionalized Carbon Nanotubes Adsorbents*. *May 2018*, 1–19. https://doi.org/10.1038/s41598-018-37899-4
4. Dave, P. N., & Chopda, L. V. (2014). Application of Iron Oxide Nanomaterials for the Removal of Heavy Metals. *Journal of Nanotechnology*, *2014*, 14. https://doi.org/10.1155/2014/398569

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ANALYSIS OF FALSE-POSITIVE RESULTS AND THE REAL EFFECTIVENESS OF LUMINOL IN THE DETECTION OF BLOOD SPOTS.

ZILIOTTO, Luis Henrique Carra[1]*; DA SILVA, Isaac Newton Lima[1];

[1] Pontifícia Universidade Católica do Rio Grande do Sul, Faculdade de Engenharia Mecânica. Brasil.

** Autor correspondente*
e-mail: luisziliotto@gmail.com

Received 20 January 2022; received in revised form 20 February 2022; accepted 23 February 2022

ABSTRACT

Forensic investigators have widely used luminol for more than 90 years in the identification of blood in life crime scenes. When mixed with an alkaline solution and sprayed on a catalyst (iron present in blood hemoglobin), it reproduces a chemiluminescent reaction with a bluish color. As it is a presumptive blood test, the present study sought to demonstrate that only the photons emission is not a prerogative to attest that the result is indeed human blood. In this perspective, 24 samples of both liquid and solid substances that can easily be found in residences and potentially used by criminals to impair the interpretation of the investigator at the crime scene were prepared. Out of the total of the analyzed samples, there was a chemical reaction with sodium hypochlorite and wood varnish, proving the known understanding that some samples may cause interference in the examination with luminol.

Keywords: *Luminol, false positive, false negative, chemiluminescence, blood.*

1. INTRODUÇÃO

A crescente onda de crimes contra a vida sempre assolou a população que vive nos maiores centros urbanos. É conhecimento comum que, muitas vezes, quem está praticando o ato delituoso possui armamento tecnológico superior ao dos próprios órgãos de segurança, não somente de poderio balístico, mas também de técnicas e métodos que dificultam a identificação da autoria do crime. Por consequência, o número de assassinatos sem solução também é crescente, segundo dados retirados do Atlas da Violência de 2018, o número de crimes violentos intencionais no ano de 2016 foi de 62.517, desses, a taxa de resolução varia de 5% a 8%.

A área das ciências forenses vem desempenhando um papel de extrema importância aumentando a taxa de crimes solucionados. Mesmo que diversas evidências físicas sejam facilmente notadas e encontradas na cena de um assassinato, muitas passam desapercebidas por não serem visíveis a olho nu, como: impressões digitais, fibras, saliva, sêmen e sangue. Essa última pode ser detectada por meio de uma reação quimioluminescente entre os íons férricos presentes na hemoglobina e a solução de luminol. Dos métodos para detecção de sangue, o exame com luminol é o que apresenta maior facilidade de uso e agilidade de detecção, sendo o mais utilizado por investigadores forenses.

A ampla utilização do luminol no meio forense se dá pela facilidade de utilização e agilidade na obtenção dos resultados, uma vez que basta borrifar o composto sobre a região em que há a suspeita de sangue. Por mais que a cena do crime tenha sido limpa e o sangue não esteja visível, o contato do composto com um catalisador faz com que as moléculas atinjam um estado eletronicamente excitado e liberem parte de sua energia por meio de fótons, para alcançarem seu estado fundamental.

Para que ocorra a reação quimioluminescente é necessário que o reagente luminol entre em contato com uma solução alcalina (geralmente utiliza-se peróxido de hidrogênio) e um catalisador suave. Ao utilizar o luminol em um ambiente com suspeita de um crime contra a vida, os investigadores forenses buscam no átomo de ferro presente na hemoglobina do sangue, já oxidado em sua forma

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.28_abstract_ZILIOTTO.pdf

Fe^{+3}, o catalisador necessário para gerar a reação quimioluminescente e assim liberar a luz azulada visível, se essa se manifestar pode ser que haja sangue no local.

Pelo fato da aplicação com o Luminol ser um teste presuntivo para sangue, muitos investigadores forenses cometem o equívoco de atestar que somente a quimioluminescência é o suficiente para afirmar que a luz emitida é de fato sangue humano. Nessa perspectiva, o presente trabalho tem por finalidade demonstrar que podem haver falhas no teste com o reagente, isso é, o luminol também pode causar o efeito de emissão de fótons quando em contato com outros catalisadores suaves e não somente com o íon férrico (Fe^{+3}) presente no sangue. Essas interferências são conhecidas como falso–positivo e falso–negativo para sangue.

Os resultados denominados como falso–positivos, são aqueles em que a mistura luminol associada à solução alcalina reage com o catalisador, mas esse não é o ferro da hemoglobina do sangue. Em contra partida, podem ocorrer resultados falso–negativos, quando uma determinada substância posta sobre o sangue acaba inibindo a reação quimioluminescente com o luminol.

Para identificar e comprovar a existência dessas interferências, foram testadas 24 amostras de diversos produtos líquidos e sólidos. A escolha das amostras foi embasada na facilidade de encontrar os respectivos produtos no dia a dia e, consequentemente, na predisposição de serem utilizadas propositalmente (ou não) para prejudicarem a investigação de uma cena de crime.

2. MATERIAIS E MÉTODOS

O luminol (5-amino-2,3-dihidroftalazina-1,4-diona) é um sólido cristalino de coloração branco-amarelada, composto por átomos de carbono, hidrogênio, oxigênio e nitrogênio ($C_8H_7O_2N_3$). Pode ser considerado insolúvel em água (<0,1g/100mL), possui temperatura de fusão entre 319 ºC e 320 ºC e massa molar de 177,16 g/mol. Suas propriedades gerais são: estável a temperatura ambiente, sensível à luz e combustível. Apresenta incompatibilidade com fortes agentes oxidantes, ácidos, básicos e redutores (Barni, Lewis, Berti, Miskelly, and Lago, 2007).

O exame para a obtenção da quimioluminescência consiste na preparação das amostras e do local em que o composto químico luminol será aplicado. Os testes visam a identificação e confirmação da manifestação de resultados falso–positivos de amostras previamente investigadas por outros pesquisadores e de outras sem registros de análises prévios.

As amostras utilizadas seguem representadas na Tabela 1:

Tabela 1. *Amostras utilizadas*

Nº	Amostra
1	Hipoclorito de sódio
2	Limpador Multiuso
3	Sabão em pó
4	Diluente Aguarrás
5	Vinagre branco de álcool
6	Detergente para uso geral
7	Saponáceo Líquido
8	Cera incolor antiderrapante
9	Detergente Automotivo com cera
10	Desengraxante extraforte
11	Tinta automotiva oxidada
12	Verniz
13	Limão
14	Laranja
15	Bergamota
16	Maracujá
17	Aveia
18	Semente de moranga
19	Brócolis
20	Beterraba
21	Espinafre
22	Leite de coco
23	Suplemento Alimentar Infantil (diluído em água)
24	Suplemento Alimentar Infantil (em pó)

Todas as amostras selecionadas foram armazenadas separadamente em recipientes próprios de 70 mililitros, fabricados em polímero termoplástico politereftalato de etileno (Figura 1). As amostras líquidas e sólidas foram aplicadas e sobrepostas em discos de algodão hidrófilo, posicionados sobre 6 blocos de uma chapa de madeira de MDP (Medium Density Particleboard), com largura de 8 cm, comprimento de 30 cm e espessura de 0,9 cm.

Figura 1. *Recipientes e blocos utilizados nos exames*

As amostras preestabelecidas para o teste são substâncias que podem ser facilmente encontradas no dia a dia, usualmente empregadas para limpeza, alimentação e serviços gerais (Tabela 1). Por serem fáceis de obter, podem ser utilizadas para mascarar a cena do delito, seja de maneira proposital ou não.

O kit de luminol utilizado nos testes foi fornecido e preparado pela Divisão de Genética Forense/DPL/IGP-RS. Sua formulação é bastante similar a aquela pesquisada por Weber (1996).

O conjunto é composto pelos seguintes itens: um frasco com 50 mL de NaOH (hidróxido de sódio), um frasco com 50 mL de solução estoque de luminol, um frasco com 50 mL de H_2O_2 (peróxido de hidrogênio), um frasco borrifador com 350 mL de água ultrapura.

A preparação do reagente consiste em misturar o luminol, o hidróxido de sódio e o peróxido de hidrogênio dentro do borrifador com água ultrapura. É recomendado que após o composto estar formado não se agite severamente o borrifador e que o líquido seja utilizado em no máximo 24 horas. As soluções antes e após serem misturadas devem ser mantidas refrigeradas.

Os registros fotográficos foram realizados antes e após a aplicação do reagente luminol nas amostras, primeiramente com as luzes acesas e na sequência com o ambiente escurecido, o mesmo procedimento foi repetido para todas as amostras utilizadas. Para melhorar a visualização dos resultados, os exames foram realizados à noite.

Os registros foram captados com uma câmera fotográfica digital, da marca Nikon, modelo D5300. Com o ambiente iluminado, fixou-se a câmera no tripé, direcionando-a para a cena a ser fotografada, selecionou-se o modo automático de foco para enquadramento, após modificou-se o foco para manual para evitar reajuste intuitivo do mesmo no escuro. Os parâmetros de configuração utilizados foram: flash inicial fraco e sem retorno estroboscópico, tempo de exposição 1/60 segundos, diafragma com abertura máxima, distância focal de 48 mm e velocidade ISO 1600.

A fim de melhorar a visualização e identificação das amostras após a aplicação do luminol, aumentou-se o contraste da imagem em 100% e reduziu-se o brilho em 100%.

3. RESULTADOS E DISCUSSÃO:

Esse projeto propôs analisar a efetividade do reagente luminol, frente a diversas substâncias líquidas e sólidas que possam interferir no exame de detecção de sangue em locais de crimes contra a vida. As amostras testadas foram divididas em 4 grupos, sendo eles: produtos de limpeza, materiais de pintura, alimentação e suplemento alimentar infantil. No total foram analisadas 24 amostras.

A reação quimioluminescente ocorreu nitidamente nas amostras de hipoclorito de sódio e verniz para madeira. A amostra de número 1 apresentou brilho bastante característico, que se manteve por um longo período. Já na amostra de número 12, a reação ocorreu em locais pontuais do disco de algodão, sendo mais fácil de ser observada *in loco* que por meio dos registros fotográficos. Restou comprovado que os compostos hipoclorito de sódio e verniz para madeira, apresentam resultados falsos positivos para o reagente luminol.

A amostra de sabão em pó apresentou indicativo de reação, todavia, pelo produto ser de coloração azulada pode ter ocorrido interferência na análise visual e fotográfica, sendo o resultado considerado inconclusivo, neste trabalho.

As amostras de números 23 e 24 (suplemento alimentar) foram escolhidas porque o composto apresenta em sua composição sulfato ferroso ($FeSO_4$), que possui o íon Fe^{+2}. Em ambos os casos a reação com luminol não foi evidenciada, o que pode ser explicado pela ausência de oxidação do íon ferro para Fe^{+3}. Os estudos realizados apontam que se essa oxidação tivesse ocorrido, o suplemento alimentar poderia ter reagido positivamente com o luminol, gerando mais um resultado falso positivo.

Na Figura 2 constam os resultados falsos positivos das amostras de hipoclorito de sódio e verniz para madeira e a amostra suspeita de sabão em pó. As imagens da linha superior foram obtidas com ambiente iluminado e as da linha inferior após aplicação do luminol, em ambiente

escurecido.

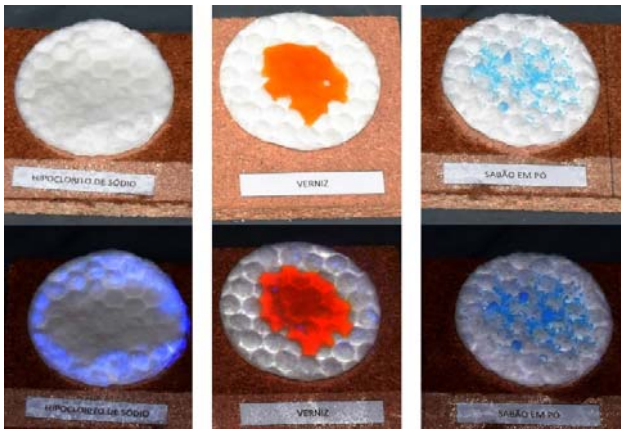


Figura 2. *Da esquerda para a direita: hipoclorito de sódio, verniz para madeira e sabão em pó.*

Os demais elementos testados não apresentaram reação química evidente com o luminol. É interessante destacar que, ao contrário dos estudos realizados por Creamer *et al*. (2003) e Nilsson (2006), no exame realizado o limpador multiúso, o removedor de manchas (diluente aguarrás) e a ferrugem (tinta automotiva oxidada) apresentaram resultados negativos. Também, investigadores forenses experientes alertaram sobre a possível reação falso positiva com a amostra de beterraba, embora neste estudo não tenha manifestado quimioluminescência.

4. CONCLUSÃO:

O sítio de um acidente deve ser investigado cuidadosamente, principalmente quando se trata de um crime contra a vida, em que resoluções inadequadas podem atribuir a responsabilidade do ato delituoso a quem não cometeu a ação, incorrendo em injustiças que podem devastar vidas.

O principal objetivo do trabalho foi munir o investigador forense com o conhecimento de quais elementos encontrados no local do crime podem ter sido utilizados pelo criminoso para mascarar a real cronologia dos eventos. Também, para demonstrar que somente o fato de ocorrer a reação quimioluminescente não é prerrogativa para atestar que se trata de sangue humano.

Foram analisadas 24 amostras, divididas em 4 grupos, sendo eles: produtos de limpeza, materiais de pintura, alimentação e suplemento alimentar infantil. Desse montante de amostras, 2 apresentaram resultado falso positivo (hipoclorito de sódio e verniz para madeira) e 1 teve resultado inconclusivo (sabão em pó), conforme já exposto. Isso é, a mistura luminol associada à solução alcalina reagiu com um catalisador, que não foi o ferro da hemoglobina do sangue, ou seja, o teste foi positivo para a quimioluminescência, mas negativo para a presença de sangue humano.

Além dessas amostras, os estudos realizados por Nilsson (2006) apontaram que os seguintes produtos geraram resultados falsos positivos com o luminol, sendo eles: salsinha, nabo, rabanete, agente de limpeza com hipoclorito de sódio (NaClO), ferrugem da placa de ferro, verniz para parquet e dáfnia. Já Cavalcanti e Barros (2016) relataram que chá-verde, chá-preto e vinho branco podem inibir a reação quimioluminescente, causando interferência com o reagente luminol.

Os resultados obtidos dos testes experimentais foram de acordo com o embasamento teórico estudado, que seja: o exame com luminol é apenas um teste presuntivo para sangue, sendo necessária a coleta da amostra suspeita e sua análise em laboratório para concluir que se trata de sangue humano.

5. REFERÊNCIAS:

1. Barni, F., Lewis, S. W., Berti, A., Miskelly, G. M., and Lago, G. (15 de Maio de 2007). Forensic application of the luminol reaction as a presumptive test for latent blood detection. *Talanta*, 896-913.
2. Cavalcanti, D. R., and Barros, R. M. (2016). Escondendo Manchas de Sangue em Locais de Crime. *Brazilian Journal of Forensic Sciences, Medical Law and Bioethics*, 1-14.
3. Creamer, J., Quickenden, T., Apanah, M., Kerr, K., and Robertson, P. (2003). A comprehensive experimental study of industrial, domestic, and environmental interferences with the forensic luminol test for blood. *Wiley InterSciece*, 193-198.
4. Nilsson, A. (2006). *The forensic luminol test for blood: unwanted interference and the effect on subsequent analysis.* Linköping.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ANÁLISE DE RESULTADOS FALSO-POSITIVOS E DA REAL EFETIVIDADE DO LUMINOL NA DETECÇÃO DE MANCHAS DE SANGUE

Luis Henrique Carra Ziliotto
Pontifícia Universidade Católica do Rio Grande do Sul, Faculdade de Engenharia Mecânica. Brasil

Isaac Newton Lima da Silva
Pontifícia Universidade Católica do Rio Grande do Sul, Faculdade de Engenharia Mecânica. Brasil

Fevereiro/2022

INTRODUCTION

SBJChem Conference 2021

O uso de luminol é amplamente empregado por investigadores forenses há mais de 90 anos na identificação de sangue em cenas de crime à vida. Ao ser misturado com uma solução alcalina e borrifado sobre um catalisador (ferro presente na hemoglobina do sangue), produz uma reação quimioluminiscente de coloração azulada. Por se tratar de um teste presuntivo para sangue, buscou-se no presente trabalho demonstrar que apenas a emissão de fótons não é prerrogativa para atestar que se trata de sangue humano, uma vez que podem se manifestar resultados falso-positivo e falso-negativos.

BACKGROUND

SBJChem Conference 2021

Pelo fato da aplicação com o Luminol ser um teste presuntivo para sangue, muitos investigadores forenses cometem o equívoco de atestar que somente a quimioluminescencia é o suficiente para afirmar que a luz emitida é de fato sangue humano. Nessa perspectiva, o presente trabalho tem por finalidade demonstrar que podem haver falhas no teste com o reagente, isso é, o luminol também pode causar o efeito de emissão de fótons quando em contato com outros catalisadores suaves e não somente com o íon férrico (Fe+3) presente no sangue. Essas interferências são conhecidas como falso–positivo e falso–negativo para sangue.

- Falso–positivos: O teste é positivo para a quimioluminescência, mas negativo para a presença de sangue.

- Falso–negativos: O teste foi negativo para a quimioluminescência e falso para a presença de sangue, mesmo que no local houvesse moléculas de sangue.

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

O principal objetivo do trabalho é munir o investigador forense com o conhecimento de quais elementos encontrados no local do crime podem ter sido utilizados pelo criminoso para mascarar a real cronologia dos eventos. Também, para demonstrar que somente o fato de ocorrer a reação quimioluminescente não é prerrogativa para atestar que se trata de sangue humano.

Para identificar e comprovar a existência dessas interferências, foram testadas 24 amostras de diversos produtos líquidos e sólidos. A escolha das amostras foi embasada na facilidade de encontrar os respectivos produtos no dia-a-dia e, consequentemente, na predisposição de serem utilizadas propositalmente (ou não) para prejudicarem a investigação de uma cena de crime.

METHODOLOGY

SBJChem Conference 2021

5

METHODOLOGY

SBJChem Conference 2021

Todas as amostras selecionadas foram armazenadas separadamente em recipientes próprios de 70 mililitros, fabricados em polímero termoplástico politereftalato de etileno (PET). As amostras líquidas e sólidas foram aplicadas e sobrepostas em discos de algodão hidrófilo, posicionados sobre 6 blocos de uma chapa de madeira de MDP (Medium Density Particleboard), com largura de 8 cm, comprimento de 30 cm e espessura de 0,9 cm. Foi demarcada uma distância de 5 cm entre os discos para evitar o contato entre as amostras

6

METHODOLOGY

SBJChem Conference 2021

Amostras utilizadas:

7

METHODOLOGY

SBJChem Conference 2021

Amostras utilizadas:

8

RESULTS AND DISCUSSION

SBJChem Conference 2021

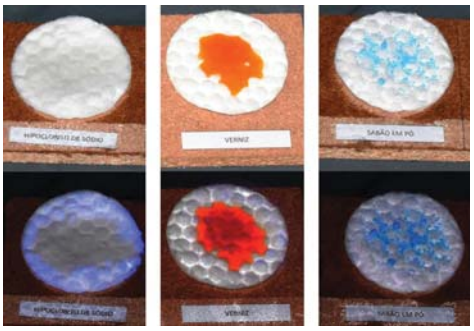
A reação quimioluminescente ocorreu nitidamente nas amostras de hipoclorito de sódio e verniz para madeira.

A amostra de Hipoclorito de Sódio apresentou brilho bastante característico, que se manteve por um longo período. Já na amostra de Verniz, a reação ocorreu em locais pontuais do disco de algodão, sendo mais fácil de ser observada in loco que por meio dos registros fotográficos.

Restou comprovado que os compostos hipoclorito de sódio e verniz para madeira, estudados por Nilsson (A., 2006) apresentam resultados falso-positivos para o reagente luminol.

RESULTS AND DISCUSSION

SBJChem Conference 2021



RESULTS AND DISCUSSION

SBJChem Conference 2021

Os demais elementos testados não apresentaram reação quimíca evidente com o luminol.

É interessante destacar que, ao contrário dos estudos realizados por Creamer et al. (2003) e Nilsson (2006), no exame realizado o limpador multiuso, o removedor de manchas (diluente aguarrás) e a ferrugem (tinta automotiva oxidada) apresentaram resultados negativos.

Também, investigadores forenses experientes alertaram sobre a possível reação falso-positiva com a amostra de beterraba, embora neste estudo não tenha manifestado quimioluminescência.

CONCLUSIONS

SBJChem Conference 2021

Foram analisadas 24 amostras, divididas em 4 grupos, sendo eles: produtos de limpeza, materiais de pintura, alimentação e suplemento alimentar infantil. Desse montante de amostras, 2 apresentaram resultado falso-positivo (hipoclorito de sódio e verniz para madeira) e 1 teve resultado inconclusivo (sabão em pó), conforme já exposto. Isso é, a mistura luminol associada à solução alcalina reagiu com um catalisador, que não foi o ferro da hemoglobina do sangue, ou seja, o teste foi positivo para a quimioluminescencia, mas negativo para a presença de sangue humano.

- Luminol é apenas um teste presuntivo para detector sangue;
- Podem ocorrer resultados falso-positivos e falso-negativos;
- Hipoclorito de Sódio e Verniz são exemplos de resultados falso-positivos
- A amostra que reagir com o Luminol deve ser coletada e analisada em laboratório.

REFERENCES

SBJChem Conference 2021

1. Barni, F., Lewis, S. W., Berti, A., Miskelly, G. M., & Lago, G. (15 de Maio de 2007). Forensic application of the luminol reaction as a presumptive test for latent blood detection. *Talanta*, 896-913.

2. Cavalcanti, D. R., & Barros, R. M. (2016). Escondendo Manchas de Sangue em Locais de Crime: Análise da Ação Antioxidante dos Chás Verde e Preto Sobre o Luminol. *Brazilian Journal of Forensic Sciences, Medical Law and Bioethics*, 1-14.

3. Creamer, J., Quickenden, T., Apanah, M., Kerr, K., & Robertson, P. (2003). A comprehensive experimental study of industrial, domestic and environmental interferences with the forensic luminol test for blood. *Wiley InterSciece*, 193-198.

4. Nilsson, A. (2006). *The forensic luminol test for blood: unwanted interference and the effect on subsequent analysis.* Linköping University, Faculty of Health Sciences, Linköping.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2022 VIRTUAL CONFERENCE

ANALYSIS OF THE SEXUAL BEHAVIOR OF BULLS OF THE TABAPUÃ BREED

LOREDO NETO, Francisco Antonio[1*]; FREITAS, Gabriela Santos[1]; SERAPIÃO, Raquel Varella[1]; GOMES, Leticia Patrão[1]; MARQUES, Thiago Luiz Pereira[1];

[1] Universidade de Vassouras, Instituto de Medicina Veterinária, Centro de desenvolvimento de genética bovina.

** Autor correspondente*
E-mail: loredocontato@gmail.com

Received 20 February 2022; received in revised form 02 March 2022; accepted 07 March 2022

ABSTRACT

Beef cattle is one of the main sectors that drive the national economy, given the great generation of employment, presence in the consumer market, and exports. Among the various services generated, technical assistance to producers stands out, who work in several areas and, especially reproduction, which is a great ally to bovine production, because through it it is possible to monetize the creation with the use of reproducers with high fertility potential boosting livestock productivity. Therefore, the andrological evaluation in the sires is an important factor in selecting superior animals, seeking to improve the fertility of the herd. The present study aimed to analyze the sexual behavior of bulls of the Tabapuã breed, through the libido test, as part of the andrological examination. Ten young bulls of the Tabapuã breed were used, aged between 24-43 months, with an average weight of 375kg, without sexual experience. The libido test was performed from the contact of males with females in estrus and out of estrus to assess sexual interest. It was observed that half of the animals were classified with low libido (50%) and the other part with medium (30%) and high (20%) libido. In addition, it was observed that the most frequent sexual events were the identification of estrus. Finally, given the results of animals classified with low libido, it is suggested that sexual inexperience is correlated, and it is recommended to insert these cattle with high libido bulls so that they can observe the behaviors and gain experience.

Keywords: *andrology, bovine, reproduction.*

1. INTRODUÇÃO

Em 2020, a Associação Brasileira das Indústrias Exportadoras de Carnes (ABIEC) divulgou que o Brasil possui 213,68 milhões de cabeças de gado, ocupando o primeiro lugar no ranking mundial de exportação de carne bovina. Considerando que a melhoria na eficiência reprodutiva pode impactar positivamente na lucratividade do rebanho, o uso de reprodutores com alto potencial para fertilidade é relevante no cenário produtivo e econômico da bovinocultura (Fonseca *et al*., 2019).

Além da fertilidade é necessário que o animal apresente um comportamento sexual adequado, que é uma interação sócio-sexual, podendo ser influenciada por diversos fatores, como: genéticos, ambientais, nutricionais, hormonais, frequência de acasalamentos, receptividade do heterossexo, acuidade sensorial, idade, experiência prévia do indivíduo e ordem de dominância social (Bascunan *et al.,* 2008; Lopes *et al.,*2009). Nessa perspectiva, os métodos desenvolvidos para avaliar esses eventos do touro enfatizam testes cuja finalidade compreende a quantificação e qualificação do interesse e da capacidade sexual na tentativa de identificar os melhores reprodutores (Lopes, 2009). Além disso, também como critério de seleção, deve-se atentar às ações do macho relacionado à detecção do estro e à capacidade de cópula com uma fêmea, que envolve basicamente, libido e a capacidade de serviço (Chenoweth, 1983).

Entendendo a metodologia e o perfil desses animais é possível realizar a seleção de touros de elevada eficiência reprodutiva que, consequentemente apresentarão grande importância econômica. O resultado dessa escolha é a possibilidade de incluir uma maior quantidade de vacas por touro ao que tem sido rotineiramente empregado na pecuária brasileira (Franco *et al*., 2006).

ISSN 2674-6891. 2022. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.43_abstract_LOREDO.pdf

O presente trabalho tem como objetivo realizar a análise do comportamento sexual dos touros, uma vez que o teste possibilita a identificação dos machos que apresentam alterações na libido.

2. MATERIAIS E MÉTODOS

Foram utilizados 10 touros jovens da raça Tabapuã, com idade entre 24-43 meses, desprovidos de experiência sexual, provenientes de uma propriedade rural localizada na cidade de Paraíba do Sul, no estado do Rio de Janeiro. O projeto foi submetido a Comissão de Ética no Uso de Animais (CEUA), sendo registrado e aprovado sob o protocolo n° 007/2021.

Os bovinos, com peso médio de 375 Kg obtidos por balança manual e foram identificados por meio da numeração de registro contida no membro posterior direito na região da coxa através de marcação por ferro quente. Os machos foram submetidos a uma relação touro:vaca de 1:20, sendo incluídas no estudo somente vacas que apresentavam intervalo entre partos de 12 meses. Antes de realizar o exame da libido as fêmeas utilizadas nesse estudo foram submetidas a uma avaliação ginecológica. Em seguida, foi realizado um protocolo hormonal composto pela administração da prostaglandina sintética com o intuito de induzir o cio.

Segundo o Manual de Exame Andrológico e Avaliação de Sêmen Animal do Colégio Brasileiro de Reprodução Animal (CBRA, 2013), a análise do comportamento sexual pode ser através da observação do animal em atividade sexual, de modo que, seja um teste simples, rápido, com elevada repetibilidade e predictabilidade do desempenho reprodutivo dos machos. Mas para realizar a avaliação de um touro é necessário que tenha um bom conhecimento dos comportamentos expressos pela espécie e pela raça.

Os touros jovens da raça Tabapuã foram submetidos ao teste da libido com o enfoque de avaliação o comportamento sexual, conforme o método recomendado pelo autor Vale Filho *et al.* (1994). Esse método consiste em uma análise da libido na presença de um agrupamento de 20 fêmeas, composto por vacas no estro e outras que se encontram fora do estro. Ao longo do teste as vacas foram substituídas a cada dois serviços completos, para que não ocorra rejeição de novas montas.

Os touros foram inseridos num piquete próximo do lote das fêmeas, para que esses animais possam identificar as fêmeas no estro, em que permaneceram por 15 minutos para que ocorra uma estimulação de maneira coletiva. Posteriormente, apenas um macho foi colocado em um piquete ao lado do piquete das fêmeas, com o intuito de realizar uma estimulação de forma individual. Por fim, o animal foi posto junto a todas as vacas em um piquete, com o propósito de observar o comportamento sexual durante os 15 minutos do teste proposto.

Foram atribuídos valores de zero a 10 (Tabela 1) para os principais comportamentos sexuais dos touros em relação as fêmeas para observar no decorrer da avaliação.

Desse modo, a cada atitude dos touros na presença das vacas, atribuiu-se um ponto logo após ao encerramento do teste da libido, consequentemente, os touros foram classificados em três categorias (Tabela 2).

Tabela 2. *Classificação dos touros em categorias de acordo com a libido.*

Categorias	Pontuação
Baixa	0,1,2,3
Média	4,5,6
Alta	7,8,9,10

3. RESULTOS E DISCUSSÃO:

Durante a avaliação notou-se que dentro do lote utilizado no estudo metade dos animais apresentaram uma baixa reação ao teste (Tabela 3), em contrapartida, a outra metade dos animais foi classificada com média ou alta libido (Tabela 4). Já no trabalho realizado por Dias *et al.* (2020), foram utilizados 24 touros jovens da raça Guzerá, no qual esses animais foram submetidos ao teste da libido em piquete ao longo de 15 minutos. As frequências desses animais foram classificadas, também, em alta, média e baixa libido e os resultados foram 0,0; 25,0 e 75%, respectivamente. Sendo que, esses animais não tinham experiência sexual.

Tabela 3. *Classificação dos touros em categorias de acordo com a libido.*

Identificação	Pontuação	Libido
01	5	Média
02	8	Alta
03	3	Baixa
04	3	Baixa

05	4	Média
06	2	Baixa
07	3	Baixa
08	4	Média
09	2	Baixa
10	8	Alta

Tabela 4. *Frequência da classificação dos animais em alta, média e baixa libido.*

Libido	Frequência (%)
Baixa	50%
Média	30%
Alta	20%

Ao longo do teste foi possível observar que os animais se acanharam e consequentemente não demonstraram os comportamentos sexuais de identificação e interesse, sendo assim, evidencia que essa ausência de expressão está correlacionada a baixa idade e juntamente a inaptidão sexual, ocasionando um resultado classificado em baixa libido.

Foi possível observar, no decorrer do teste, que todos os animais expressaram com mais frequência os comportamentos de identificação, principalmente os eventos de reflexo de Flehmen e de cheirar e lamber a região perineal. Dessa forma, notou-se que essas expressões demonstradas pelos touros jovens da raça Tabapuã, mesmo ausência de experiência sexual, evidenciam que os machos podem apresentar interesse pelas fêmeas no cio. Essa mesma ocorrência foi relatada pelos autores Oliveira *et al.* (2007), e Salvador *et al.,* (2008).

Durante a execução dos testes da libido, a utilização de fêmeas no estro juntamente com as fora do estro teve grande importância, como uma forma de atestar que os machos foram atraídos às fêmeas em estro, condensando os eventos comportamentais sexuais, sobre estas. Sendo assim, assemelha-se no que foi retratado na literatura para avaliação de zebuínos de Salvador *et al.* (2008). Além disso, mostrando que o estado reprodutivo da fêmea foi a causa do estímulo ao comportamento sexual dos touros no momento do teste (Salvador *et al.,* 2019).

4. CONCLUSÃO:

Diante dos resultados dos animais classificados em baixa libido, sugere-se ter relação com as suas inexperiências sexuais e recomenda-se inserir esses bovinos com os touros de alta libido para que possam observar os comportamentos e adquirirem experiência. Além disso, o teste da libido pode atestar a eficiência em detectar o perfil do interesse sexual e de analisar o comportamento sexual dos machos jovens da raça Tabapuã, quando estão em contato com as fêmeas no cio.

5. REFERÊNCIAS:

1. Associação Brasileira das Indústrias Exportadoras de Carnes (ABIEC). *Beef Report: Perfil da Pecuária no Brasil.* São Paulo, **2020.**
2. Bascunan, D.S.R., Jorge, A.M., Rocha, G. P., Weschler, F.S., Andrighetto, C. Comportamento sexual de touros Zebuínos e Angus em central de coleta e processamento de sêmen. *Revista Brasileira de Zootecnia,* **2008**, 37, 254-260.
3. Chenoweth, P.J. Sexual behavior of the bull: a review. *Journal of Dairy Science*, **1983**, 66, 173-179.
4. Colégio Brasileiro de Reprodução Animal. *Manual para exame andrológico e avaliação de sêmen animal*, 3ªed. Belo Horizonte, **2013**, 28-29.
5. Dias, J.C., Emerick, L.L., Martins, J.A.M., Andrade, V.J., Vale Filho, V.R. Comportamento sexual de touros jovens Gúzera em teste da libido em curral e piquete. *Revista de Ciências Agrárias*, **2020**, 43, 124-132.
6. Fonseca, V.O., Souza, C.F., Azevedo, N.A., Oliveira, L.Z., Monteiro, G.A., Cavalcanti, L.F.L., Molina, L.R. Parâmetros reprodutivos de touros Nelore (Bos taurus indicus) criados a pasto de diferentes faixas etárias. *Arquivo Brasileiro de Medicina Veterinária e Zootecnia*, **2019**, 71, 385-392.
7. Franco, C.S., Fonseca, V.O., Gaste, L. Potencial reprodutivo de touros Nelore acasalados coletivamente na proporção de um touro para 100 vacas. *Arquivo Brasileiro de Medicina Veterinária e Zootecnia*, **2006**, 58, 1154-1161.
8. Lopes, F.G., Guimarães, J.D., Costa, E.P., Carvalho, G.R., Neto, T.M. Avaliação Andrológica por pontos e

comportamento sexual em touros da raça Nelore. *Revista Brasileira de Zootecnia*, **2009**, 38, 1018-1025.
9. Oliveira, C.B., Guimarães, J.D., Costa, E.P., Siqueira, J.B., Torres, C.A.A., Carvalho, G.R., Guimarães, S.E.F. Avaliação do comportamento sexual de touros Nelore: comparação entre os testes da libido em curral e do comportamento sexual a campo. *Revista Brasileira de Zootecnia*, **2007**, 36, 32-42.
10. Salvador, D.F., Andrade, V.J., Nogueira, L.A.G., Vale Filho, V. Avaliação dos eventos sexuais de touros Nelore adultos em teste de libido realizado em curral. *Revista Brasileira de Ciências Veterinária*, **2008**, 15, 15-20.
11. Salvador, D.F., Nogueira, L.A.G., Andrade, V.J. Potencial de fecundação diária de touros Nelore na monta a campo selecionados por avaliações andrológicas e comportamento sexual. *Pubvet*, **2019**, 13, 1-11.
12. Santos, M.D., Torres, C.A.A., Ruas, J.R.M., Silva Filho, J.M., Costa, E.P., Pereira, J. C. Teste da libido e atividade de monta em touros da raça Nelore. *Arquivo Brasileiro de Medicina Veterinária e Zootecnia*, **2004**, 56. 504-510.
13. Vale Filho, V.R., Bergmann, J.A.G., Andrade, V.J., Mendonça, R.M.A., Reis, S.R., Ferreira, M.B.D. Classificação andrológica por pontos (CAP), versus libido, na eficiência para fecundação de touros Nelore de 2 e 3 anos de idade, usados em estação de monta bem definida. *In: Anais do XIV Encontro de Pesquisa da Escola de veterinária da UFMG*, Belo Horizonte, MG, Brasil, UFMG, **1994**, 88.

Tabela 1. *Pontuação atribuída em relação ao comportamento dos touros em relação as fêmeas.*

Pontuação	Comportamento
0	Ausência de atração sexual.
1	Apresentação de único interesse (ex.: cheirar e lamber a região perineal).
2	Atração em duas ou mais vezes (ex.: reflexo de Flehmen).
3	Frequente perseguição com constante interesse (ex.: impulso de monta).
4	Única monta ou tentativa, porém sem realização de serviço.
5	Dois eventos de monta ou tentativas, entretanto nenhum serviço.
6	Acima de duas montas ou tentativas, ainda assim nenhum serviço.
7	Um serviço (cópula) acompanhado por desinteresse sexual.
8	Um serviço com posterior interesse sexual, incluindo montas ou tentativas.
9	Duas cópulas com consequente desinteresse sexual.
10	Dois serviços ou mais, acompanhados por interesse sexual, incluindo montas ou tentativas e serviços.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2022 VIRTUAL CONFERENCE

ANALYSIS OF THE SEXUAL BEHAVIOR OF BULLS OF THE TABAPUÃ BREED

Francisco Antonio Loredo Neto
Universidade de Vassouras, Veterinary Medicine - Brazil

Gabriela Santos Freitas
Universidade de Vassouras, Veterinary Medicine - Brazil

Raquel Varella Serapião
Universidade de Vassouras, Veterinary Medicine - Brazil

Letícia Patrão Gomes
Universidade de Vassouras, Veterinary Medicine - Brazil

Thiago Luiz Pereira Marques
Universidade de Vassouras, Veterinary Medicine - Brazil

March/2022

INTRODUCTION

SBJChem Conference 2021

- The importance of Brazilian cattle farming;
- Improvement in reproductive efficiency;
- Use of bulls with high fertility potential;
- Positive impact on herd profitability;

INTRODUCTION

SBJChem Conference 2021

- Sexual behavior;
- Libido test;
- Identify the best breeders
- Estrus detection;

AIM

SBJChem Conference 2021

Analyze the sexual behavior of bulls of the Tabapuã breed, through the libido test, as part of the andrological examination.

METHODOLOGY

SBJChem Conference 2021

- 10 young Tabapuã bulls (*Bos taurus*)
- Age: 24-43 months;
- Without sexual experience;
- Committee on Ethics in the Use of Animals (CEUA).
- Location: Paraíba do Sul- RJ;

Source: Personal archive

METHODOLOGY

SBJChem Conference 2021

- Libido test (Vale Filho et al. 1994)
- Lot of 20 cows composed of cows in estrus and out of estrus;
- The bull stays in the cow lot for 15 minutes;
- Classification according to the table;

Score	Libido
0,1,2,3	Low
4,5,6	Medium
7,8,9,10	High

METHODOLOGY

SBJChem Conference 2021

Score	Behavior
0	Absence of sexual attraction.
1	Single interest presentation
2	Attraction in two or more times
3	Frequent pursuit with constant interest
4	Single mount or attempt, but no service.
5	Two mount events or attempts, but no service.
6	Above two mounts or attempts, still no service.
7	One service accompanied by sexual disinterest.
8	One service with further sexual interest, including mounts or attempts.
9	Two copulations with consequent lack of sexual interest.
10	Two services or more, accompanied by sexual interest, including mounts or attempts and services.

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Half of the animals did not demonstrate the sexual behaviors of estrus identification and interest.

Libido	Frequency (%)
Low	50%
Medium	30%
Alta	20%

- Dias et al. (2020) - 24 young Guzerá bulls.
- High (0%), Medium (25%); Low (75%).

CONCLUSIONS

SBJChem Conference 2021

- The results of animals classified as low libido show sexual inexperience;
- It is recommended to place these animals with high libido bulls to observe behaviors and gain experience.
- It is important to associate the libido test with the andrological exam for the selection of good bulls.

REFERENCES

SBJChem Conference 2021

1. ABIEC – Associação Brasileira das Indústrias Exportadoras de Carnes. (2020). *Beef Report: Perfil da Pecuária no Brasil.* São Paulo.
2. Colégio Brasileiro de Reprodução Animal (2013). Manual para exame andrológico e avaliação de sêmen animal, 3ªed. Belo Horizonte, CBRA, 28-29.
3. Dias, J. C., Emerick, L. L., Martins, J. A. M., Andrade, V. J., Vale Filho, V. R. (2020). Comportamento sexual de touros jovens Gúzera em teste da libido em curral e piquete. *Revista de Ciências Agrárias*, 43(1): 124-132.
- Vale Filho, V. R., Bergmann, J. A. G., Andrade, V. J., Mendonça, R. M. A., Reis, S. R., Ferreira, M. B. D. (1994). Classificação andrológica por pontos (CAP), versus libido, na eficiência para fecundação de touros Nelore de 2 e 3 anos de idade, usados em estação de monta bem definida. In: *Anais do XIV Encontro de Pesquisa da Escola de veterinária da UFMG*, Belo Horizonte, MG, Brasil, UFMG, 88.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ASSESSMENT OF SERUM SCLEROSTIN LEVEL AS A BIOMARKER ASSOCIATED WITH BONE DISORDERS IN B-THALASSEMIA PATIENTS IN AL- NAJAF CITY, IRAQ

SHARBA, Intisar Razzaq [1*]; AL-DUJAILI, Arshad Noori [1];

[1] University of Kufa, Faculty of Science, Department of Biology, Iraq.

** Correspondence author*
e-mail: intisar.sharba@uokufa.edu.iq

Received 09 September 2021; received in revised form 30 November 2021; accepted 02 December 2021

ABSTRACT

Aim of the study: To assess serum sclerostin in female patients with beta-thalassemia and compare with the healthy controls and to predict its complication associated with the bone pathophysiology, for designed improvement the lifestyle goodliness for these patients. Material and methods: Sixty-nine female beta-thalassemia (βT) patients (54 βT major and 15 βT Intermedia), aged 8-40 years who dependent on transfused blood, and 20 healthy controls were evaluated serum sclerostin, and was examined the relationship with hematological parameters RBC, Hb, PCV, WBC, PLT, BMI, splenic status, iron, and ferritin levels. The information of beta-thalassemia patients was collected and recorded by the questioner. Results: A significantly increased serum sclerostin level (mean 26.80±0.91) pg/ml was shown in βT patients compared with the healthy controls (10.03±0.68, $p < 0.001$) pg/ml. Furthermore, a significant decrease ($p<0.05$) of the sclerostin level was observed in β-thalassemia major compared to intermedia β-thalassemia patients. Serum sclerostin level revealed a significant increase in progress age; it is highest in the age group (30-40) year as compared with age group (8-18) and (19-29) year respectively. Sclerostin showed no associations with the RBC, Hb, PCV, and significantly positively correlated ($p<0.05$) with serum iron, ferritin levels, WBC, and PLT count. Significantly higher sclerostin levels in splenectomized and underweight groups were observed compared to unsplenectomized and normal-weight groups ($p<0.05$) of βT patients. Conclusion: Sclerostin plays an important role in beta-thalassemia patients and can serve as a biomarker associated with the bone pathophysiology and indicator to prevent the continuation of such serious diseases caused by iron overload in these patients.

Keywords: *Sclerostin, β-thalassemia, BMD, iron overload, ferritin, and biochemical analysis of blood*.

1. INTRODUCTION

Beta-thalassemia (βT) is a hereditary hemopathy, and significant clinical symptoms of these patients are ineffective erythropoiesis, with extramedullary involvement, hemolysis, and severe anemia (Almousawi, and Sharba, 2019; Thein, 2013). Bone abnormalities play an important role in β-thalassemia patients, which arises from the hematological disorder and its complications with hypertransfusion, iron overload, treatment and iron chelation, nutritional deficits, and sedentarism (Sapunarova *et al.*, 2020).

Sclerostin is a member of the Wnt signaling pathway inhibitor. It is a glycoprotein expressed predominantly by mature osteocytes under physiological and pathological conditions released into circulation and binding with the cell membrane receptors of osteoblasts (Drake *et al.,* 2010; Wijenayaka *et al*., 2011). The major role of Sclerostin in β Thalassemia patients is related to the reduced bone mineral density and the development of osteoporosis (Voskaridou *et al.*, 2012). However, the research about the role of sclerostin in female patients with beta-thalassemia is still rather inadequate, and it required further investigations; for this causes, the current study aimed to assess serum sclerostin in female patients with beta-thalassemia and comparison with the healthy controls, the relationship between sclerostin levels with the hematological parameters, age, BMI and splenic status, to predict of its complication that associated with bone pathophysiology such as osteoporosis, for designed improvement the lifestyle goodliness for these patients.

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.05_abstract_SHARBA.pdf

2. MATERIALS AND METHODS

2.1. Study design

Sixty-nine females with β-thalassemia (54 major βT and 15 intermedia βT), the aged range from (8–40) year. Patients were enrolled at The Thalassemia Center in Al–Zahraa Teaching Hospital in Al–Najaf province, Iraq. They were frequently blood transfused and treated every two or three weeks to maintain a Hb level of more than 10 g/dl and regulate iron-chelating therapy. Twenty participate of healthy females with matched age served as a control group; β-thalassemia patients were classified into many divisions according to types of β-thalassemia into two groups Major and Intermedia β-Thalassemia, three aged groups Group 1 (8 –18 years), Group 2 (19–29 year), and Group 3 (30–40 year), Splenic situation divided into Splenectomized and unsplenectomized patients (Sharba and Al-Dujaili, 2020). Also, according to Body Mass Index (BMI), patients were divided into two groups: normal weight and underweight the normal range (5th – 85th) % for (≤ 20) years of age, and (18.5 – 25) kg/m^2 for (>20) years of age.

2.2. Methods

An electronic balance and height unit carried out the BMI measurement to measure weight (kg) divided on the height square (m^2), according to Equation 1. Both patients and healthy were withdrawn 5 ml of venue blood for hematological criteria were conducted on EDTA anticoagulated blood by using a completely automated hematology analyzer Mythic 18 (RINGELSAN CO., Turkey) for estimated complete blood count (CBC), which included RBC, PCV, Hb, WBC, and PLT. Estimation of biomarkers by using ELISA technique using the bioelisa ELx 80000 reader (biokit, USA). According to the Manufacturing Firm, the Human Accu Bind Ferritin ELISA Kit (Monobind Inc., USA, code number 2825-300). (Anderson and Kelly, 1981). The assay Human Sclerostin (SOST) ELISA Kit was conducted according to the manufacturing company (CUSABIO BIOTECH Co., Ltd., PRC, code number CSB-E13146h). Serum iron concentration was measured by iron (using the chromogen ferrozine method) kit (bt 35i, Turkey).

BMI= weight (kg) / height square (m^2) (Eq. 1)

3. RESULTS AND DISCUSSION:

3.1. The general characteristics of the studied groups

The β-thalassemia patients and healthy controls are shown in Table 1.

3.2. Sclerostin level effects by study categories (Thalassemia types, age, BMI, and splenectomy status)

Figure 1 describes the ROC curves of sclerostin for β-thalassemia patients, and Figure 2 summarizes several comparisons of Sclerostin levels in the studied groups of βT control groups.

3.3. Relationship of Sclerostin level with the hematological Parameters in beta-thalassemia patients

It is described in Table 2 the correlation coefficient of sclerostin with other variables in β-thalassemia patients

4. CONCLUSIONS:

Sclerostin plays an important role in beta-thalassemia patients and can serve as a biomarker associated with the bone pathophysiology and indicator to prevent the continuation of such serious diseases caused by iron overload in these patients.

6. REFERENCES:

1. **Almousawi,** A. S., and Sharba, I. R. (2019). Erythroferrone Hormone, a Novel Biomarker, is associated with Anemia and Iron Overload in Beta-Thalassemia Patients. Journal of Physics: Conference Series, 1294, 062045.
2. **Drake** MT, Srinivasan B, Modder UI, Peterson JM, McCready LK, Riggs BL, Dwyer D, Stolina M, Kostenuik P, and Khosla S. (2010). Effects of parathyroid hormone treatment on circulating sclerostin levels in postmenopausal women. J Clin Endocrinol Metab. 95(11):5056-5062
3. **Sapunarova,** K., Goranova-Marinova, V., Georgiev, P., Deneva, T., Tsvetkova, S., & Grudeva-Popova, Z. (2020). Associations of serum sclerostin with bone mineral density, markers of bone metabolism, and thalassemia characteristics in adult patients with transfusion-dependent beta-thalassemia. Annals of medicine, 52(3-4),

94–108.
4. **Sharba,** I. R., and Al-Dujaili, A. N. (2020). E-SELECTIN AS A BIOMARKER IN FEMALE PATIENTS WITH B-THALASSEMIA IN AL-NAJAF PROVENCE, IRAQ. SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY, 28(29), 66–73.
5. **Thein** SL. (2013). Molecular basis of β-thalassemia. Cold Spring Harb Perspect Med. 3(5): a011700.
6. **Voskaridou** E, Christoulas D, Plata E, Bratengeier C, Anastasilakis AD, Komninaka V, Kaliontzi D, Gkotzamanidou M, Polyzos SA, Dimopoulou M, and Terpos E. (2012). High circulating levels of sclerostin correlate with bone mineral density in patients with thalassemia and osteoporosis: the role of the Wnt signaling in the pathogenesis of bone loss in thalassemia. Horm Metab Res. 44(12):909-13.
7. **Wijenayaka** AR, Kogawa M, Lim HP, Bonewald LF, Findlay DM, and Atkins GJ. (2011). Sclerostin Stimulates Osteocyte Support of Osteoclast Activity by a RANKL-Dependent Pathway. PLoS One 6:e25900.

Table 1. *Demographic of the clinical characteristics between female patients with β-thalassemia and the healthy controls*

Clinical characteristics	Patients n= 69	Healthy Controls n= 20	P- Value
Age (year)	16.62 ± 0.96	20.75 ± 1.86	
Group (8 – 18) n (%)	51(74%)		0.612
Group (19 – 29) n (%)	12(17.4%)		
Group (30 – 40) n (%)	6(8.7%)		
Major βT n (%)	54(78.2%)	0	NA
Intermedia n (%)	15(21.8%)	0	
Hb (mg/dl)	7.7 ± 0.14 *	12.01 ± 0.19	0.027
RBC (10^6/ml)	3.13 ± 0.07 *	4.36 ± 0.07	0.038
WBC (10^3/ml)	11.05 ± 0.26 *	7.59 ± 0.33	0.036
PCV %	23 ± 0.41 *	36.34± 0.52	0.036
PLT (10^3/ml)	361.86 ± 13.92 *	244 ± 14.23	0.034
BMI (kg/m^2)	17.59 ± 0.43 *	22.15 ± 0.36/	
Underweight, n (%)	13.09±0.52, 40(58%)	0	0.001
Normal weight, n (%)	23.7±2.04, 29(42%)	20(100%)	
Iron (µg/ml)	172.2 ± 4.4 *	29.86 ± 2.32	0.0001
Ferritin (ng /ml)	5156.5 ± 438.7 *	99.15 ± 8.95	0.0001
Splenectomized n (%)	29 (42%)	0	NA
Unsplenectomized n (%)	40(58%)	0	NA

* Statistically significant at p< 0.05; NA: not application; RBC: red blood corpuscles; Hb: hemoglobin; PCV: pact corpuscular volume; WBC: White Blood Cells. BMI: body max index; PLT: platelets. Data represented as mean± standard division.

Table 2: *Correlation coefficient of sclerostin with other variables in* β*-thalassemia patients*

Variables	**Sclerostin (pg/ml)**	
	P-value	R
RBC (106/ml)	0.440	0.094
PCV %	0.751	0.031
PLT (103/ml)	0.030	0.260 *
Hb (mg/dl)	0.661	0.054
WBC (103/ml)	0.001	0.770 **
Iron (µg/ml)	0.0006	0.513 **
Ferritin (µg/ml)	0.0005	0.522 **

Significant difference * p-value <0.05. ** p-value <0.01

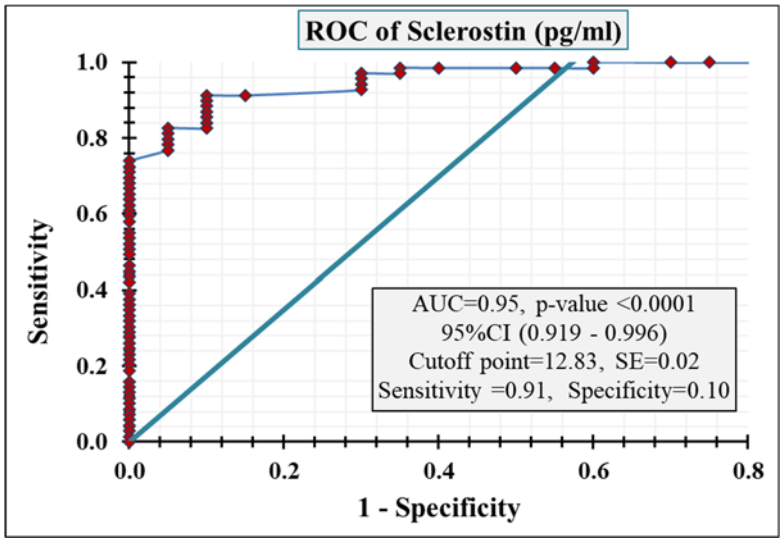


Figure 1. *ROC curves of sclerostin for β-thalassemia patients. ROC: receiver operating characteristic; AUC: area under the curve*

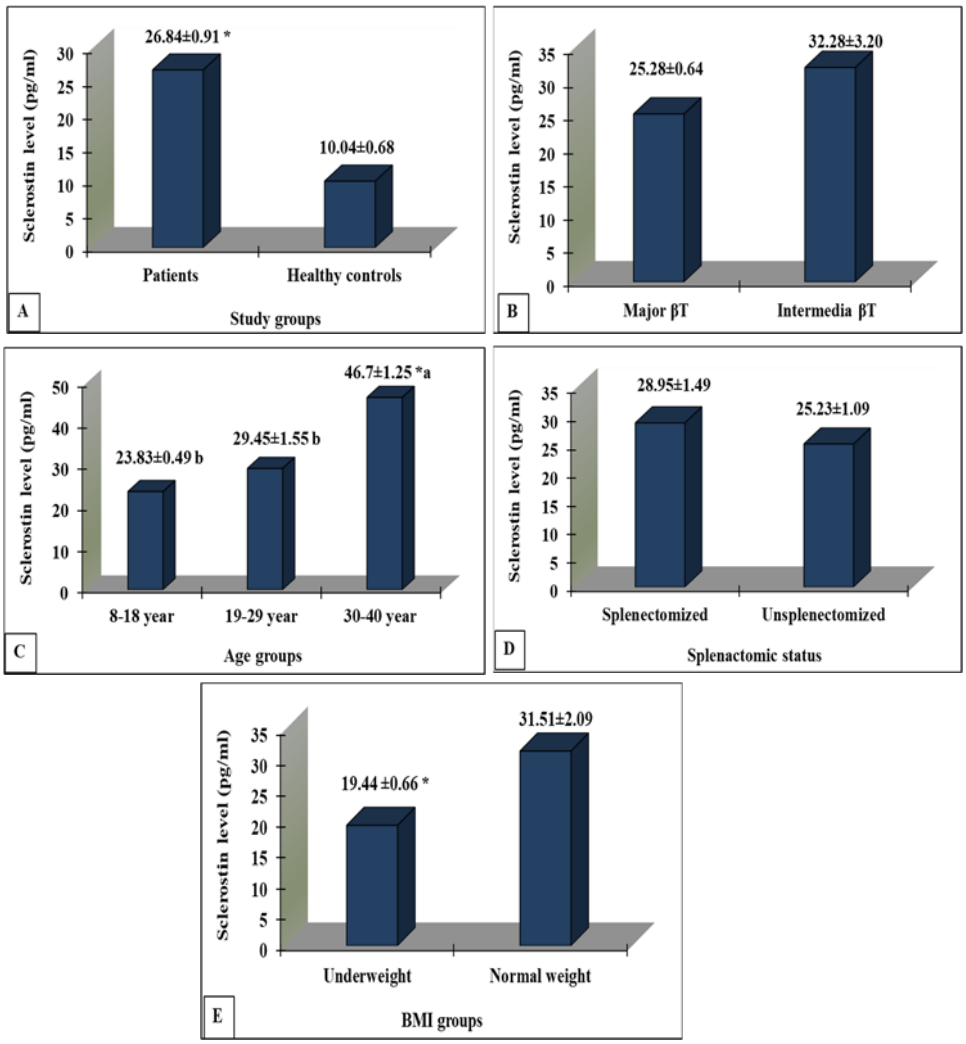


Figure 2. A: Comparison of Sclerostin levels in studied groups βT patients and healthy control groups. B: Effects of thalassemia types on Sclerostin levels in patients with βT major and βT intermedia. C: Effects of Age on Sclerostin levels among age groups. D: Effects of splenectomy status on Sclerostin levels in splenectomized and un splenectomized groups. E: Effects of BMI on Sclerostin levels in underweight and normal-weight groups. * and deferent litters significant $p<0.05$. data represented as mean ±SD.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ASSESSMENT OF SERUM SCLEROSTIN LEVEL AS A BIOMARKER ASSOCIATED WITH BONE DISORDERS IN B-THALASSEMIA PATIENTS IN AL- NAJAF CITY, IRAQ

Intisar Razzaq Sharba
University of Kufa, Faculty of Science, Department of Biology – Iraq.

Arshad Noori Al-Dujaili
University of Kufa, Faculty of Science, Department of Biology – Iraq.

March/2022

INTRODUCTION

SBJChem Conference 2021

- Beta-thalassemia (βT) is a hereditary defect in the beta-globin chain.
- Ineffective erythropoiesis, Hemolysis, and Severe anemia .
- Diminished bone mineral density (BMD). in β-thalassemia patients.
- Sclerostin is a member of the Wnt signaling pathway inhibitor.

BACKGROUND

SBJChem Conference 2021

- Sclerostin is a glycoprotein expressed predominantly by mature osteocytes and binding with the cell membrane receptors of osteoblasts.
- Osteoclast precursors can secrete sclerostin in bone marrow and reductions in the development of their maturation.
- Several clinical states such as inflammatory, sclereostosis, fracture risk spinal injury, multiple myeloma, ankylosing chronic kidney disease, type-II diabetes and another disease .
- Sclerostin in β Thalassemia patients related to the reduced bone mineral density and the development of osteoporosis.

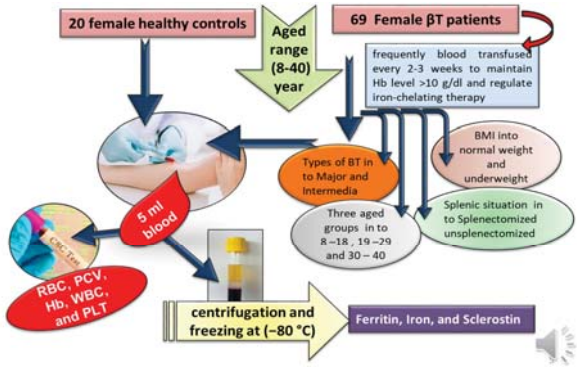
AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

The aimed to assess serum sclerostin in female patients with beta-thalassemia and comparison with the healthy controls, the relationship between sclerostin levels with the hematological parameters, age, BMI and splenic status, to predict of its complication that associated with bone pathophysiology such as osteoporosis, for designed improvement the lifestyle goodliness for these patients.

METHODOLOGY

SBJChem Conference 2021



RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 1: Demographic of the clinical characteristics between female patients with β-thalassemia and the healthy controls

Clinical characteristics	Patients n= 69	Healthy Controls n= 20	P-Value
Age (year)	16.62 ± 0.96	20.75 ± 1.86	
Group (8 – 18) n (%)	51(74%)		0.612
Group (19 – 29) n (%)	12(17.4%)		
Group (30 – 40) n (%)	6(8.7%)		
Major βT n (%)	54(78.2%)	0	NA
Intermedia n (%)	15(21.8%)	0	
Hb (mg/dl)	7.7 ± 0.14 *	12.01 ± 0.19	0.027
RBC (10^6/ml)	3.13 ± 0.07 *	4.36 ± 0.07	0.038
WBC (10^3/ml)	11.05 ± 0.26 *	7.59 ± 0.33	0.036
PCV %	23 ± 0.41 *	36.34± 0.52	0.036
PLT (10^3/ml)	361.86 ± 13.92 *	244 ± 14.23	0.034
BMI (kg/m^2)	17.59 ± 0.43 *	22.15 ± 0.36/	
Underweight, n (%)	13.09±0.52, 40(58%)	0	0.001
Normal weight, n (%)	23.7±2.04, 29(42%)	20(100%)	
Iron (µg/ml)	172.2 ± 4.4 *	29.86 ± 2.32	0.0001
Ferritin (ng /ml)	5156.5 ± 438.7 *	99.15 ± 8.95	0.0001
Splenectomized n (%)	29 (42%)	0	NA
Unsplenectomized n (%)	40(58%)	0	NA

** statistically significant at p< 0.05; NA: not application; RBC: red blood corpuscles; Hb: hemoglobin; PCV: pact corpuscular volume; WBC: White Blood Cells. BMI: body max index; PLT: platelets. Data represented as mean± standard division.*

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 2: Correlation coefficient of sclerostin with other variables in beta thalassemia patients.

Variables	Sclerostin (pg/ml)	
	P-value	R
RBC (10^6/ml)	0.440	0.094
PCV %	0.751	0.031
PLT (10^3/ml)	0.030	0.260 *
Hb (mg/dl)	0.661	0.054
WBC (10^3/ml)	0.001	0.770 **
Iron (µg/ml)	0.0006	0.513 **
Ferritin (µg/ml)	0.0005	0.522 **

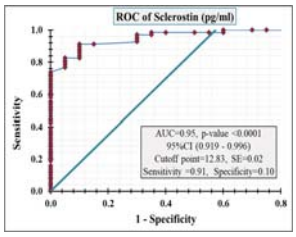


***Figure 1**: ROC curves of sclerostin for beta thalassemia patients. ROC: receiver operating characteristic; AUC: area under the curve*

RESULTS AND DISCUSSION

SBJChem Conference 2021

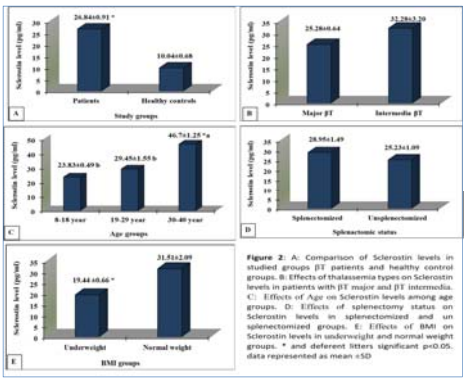


Figure 2: A: Comparison of Sclerostin levels in studied groups βT patients and healthy control groups. B: Effects of thalassemia types on Sclerostin levels in patients with βT major and βT intermedia. C: Effects of Age on Sclerostin levels among age groups. D: Effects of splenectomy status on Sclerostin levels in splenectomized and un splenectomized groups. E: Effects of BMI on Sclerostin levels in underweight and normal weight groups. * and deferent litters significant p<0.05. data represented as mean ±SD

CONCLUSIONS

SBJChem Conference 2021

- Sclerostin positively correlated with WBC and PLT. These are indicated to Inflammation influence of bone cells activity in beta thalassemia then increased sclerostin.
- Sclerostin a positive significance correlated with Serum Iron and Ferritin levels.
- Sclerostin plays an important role in beta-thalassemia patients and can serve as a biomarker associated with the bone pathophysiology and indicator to prevent the continuation of such serious diseases caused by iron overload in these patients.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

- Acknowledgement for university of kufa, faculty of science, biology department. Iraq.
- Acknowledgement Proudly offer my thanks and appreciation to all Thalassemia patients, without them, this study will not be completed
- Acknowledgement for all staff of hematology diseases center in Al–Zahraa Educational Hospital in Al–Najaf province, Iraq. for their cooperation during this study.

REFERENCES

SBJChem Conference 2021

- Galanello, R., and Origa, R. (2010). Beta-thalassemia. Orphanet journal of rare diseases, 5(1), 1-15.
- Almousawi, A. S., and Sharba, I. R. (2019). Erythroferrone Hormone, a Novel Biomarker, is associated with Anemia and Iron Overload in Beta-Thalassemia Patients. Journal of Physics: Conference Series, 1294, 062045.
- Delgado-Calle, J., Sato, A. Y., and Bellido, T. (2017). Role and mechanism of action of sclerostin in bone. Bone, 96, 29-37.
- Sapunarova, K., Goranova-Marinova, V., Georgiev, P., Deneva, T., Tsvetkova, S., & Grudeva-Popova, Z. (2020). Associations of serum sclerostin with bone mineral density, markers of bone metabolism, and thalassaemia characteristics in adult patients with transfusion-dependent beta-thalassaemia. Annals of medicine, 52(3-4), 94–108.
- Wehmeyer, C., Frank, S., Beckmann, D., Böttcher, M., Cromme, C., König, U., Fennen, M; Held, A; Paruze, P; Hartmann, C; Stratis, A... & Dankbar, B. (2016). Sclerostin inhibition promotes TNF-dependent inflammatory joint destruction. Science translational medicine, 8(330), 330ra35-330ra35.
- Amrein K, Amrein S, Drexler C, Dimai HP, Dobnig H, Pfeifer K, Tomaschitz A, Pieber TR, and Fahrleitner-Pammer A. (2012).Sclerostin and its association with physical activity, age, gender, body composition, and bone mineral content in healthy adults. J Clin Endocrinol Metab. 97(1):148–154.

REFERENCES

SBJChem Conference 2021

- Ardawi MS, Rouzi AA, Al-Sibiani SA, Al-Senani NS, Qari MH, and Mousa SA. (2012). High serum sclerostin predicts the occurrence of osteoporotic fractures in postmenopausal women: The Center of Excellence for Osteoporosis Research Study. J Bone Miner Res. 27(12):2592–2602.
- Arshad B, Iqbal T, Jami A and Hasan IJ. (2014). Hematological and Biochemical Changes in Male Patients with Thalassemia Major. Pak. j. life soc. Sci. 12(1): 31-35.
- Baldini M, Forti S, Marcon A, Ulivieri FM, Orsatti A, Tampieri B, Airaghi L, Zanaboni L, and Cappellini MD. (2010). Endocrine and bone disease in appropriately treated adult patients with beta-thalassemia major. Annals of Hematology.89(12):1207-1213.
- Bellido T, Saini V, and Pajevic PD. (2013). Effects of PTH on osteocyte function. Bone 54 (2): 250–7.
- Center for Disease Control (CDC). (2014). Body Mass Index: BMI for Children and Teens.
- Chen D, Li Y, Zhou Z, Wu C, Xing Y, Zou Y, and Tian W. (2013). HIF-1α Inhibits Wnt Signaling Pathway by Activating Sost Expression in Osteoblasts. PLoS ONE. 8(6): e65940.
- Easa ZO. (2009). Complications of High Serum Ferritin Level after Splenectomy in â Thalassemic Patients. Kufa Med. Journal. 12(1):243-250.
- Eissa DS and El-Gamal RA. (2014). Iron overload in transfusion-dependent β-thalassemia patients: defining parameters of comorbidities. Egypt J Haematol. 39(3):164-70.
- Garnero P, Sornay-Rendu E, Munoz F, Borel O, and Chapurlat RD. (2013). Association of serum sclerostin with bone mineral density, bone turnover, steroid, and parathyroid hormones, and fracture risk in postmenopausal women: the OFELY study. Osteoporos Int. 24(2):489–494
- Ginzburg Y. and Rivella S. (2012). β-thalassemia: a model for elucidating the dynamic regulation of ineffective erythropoiesis and iron metabolism. Blood. 118 (16): 4321-4330.


SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

BIOPOLYMERS AS DOSIMETERS - A PROPOSAL

GENNARI, Roseli Fernandes; GOVEIA, Gilson; CHUBACI, José Fernando Diniz*;

Universidade De São Paulo (USP) , Instituto de Física, Departamento de Física Nuclear

** Correspondence author*
e-mail: rgennari@if.usp.br

Received 30 January 2022; received in revised form 28 February 2022; accepted 08 March 2022

ABSTRACT

The radiation study has led to advances in various areas of our everyday lives despite that several events had occurred, causing health damage to several researchers. Thus, if somebody wants to study irradiation effects on materials must use equipment that quantifies the radiation received. Dosimeters do this quantification of ionizing radiation. There are numerous applications for ionizing radiation so far, and many materials can be used for dosimetric purposes. Despite that, there is always a constant search for new materials, focusing on more efficient processes or less environmental impact. For dosimetric purposes, the material has to be radiation sensitive. Many materials have been the subject of research recently, aiming to be environment friendly: among them, we can mention biopolymers that have the great advantage of being biodegradable. A commercial solid-state dosimeter uses silver-activated phosphate glass for radiophotoluminescence (RPL) purposes. This dosimeter has an enormous advantage since it does not lose the dose information after dose reading. It can be reread many times until annealing is done to reset the exposure condition. It can be reused several times. This dosimeter is commercially available as “GD-450” (Chiyoda Technol Corporation). Our research group successfully proposed using silicate glass instead of phosphate glass as RPL dosimeters. Face to the need for a high-temperature furnace for glass sintering, and it was decided to test biopolymers as RPL dosimeters. Once our goal was to have a regenerative dosimeter, we used silver as a sensible radiation element. This work it was synthesized two biopolymers with and without adding silver to them. The biopolymers synthesized used starch and collagen as polymer base material. The biopolymers analysis was done by microscopy and by optical spectrometry (UV-Vis-NIR). We observed irradiation effects on absorption bands from biopolymer of collagen doped with silver.

Keywords *Biopolymer, Dosimeter, Radiophotoluminescence (RPL), Silver*.

1. INTRODUCTION

The discovery of X-rays in the 19th century by Roentgen can be considered as the beginning of a new era in science (Tubiana, M., 1996). The radiation study has led to advances in various areas of our everyday life, mainly in medicine, where diagnosis and treatment have become viable.

Ionizing radiation studies are certainly responsible for very important discoveries. However, these discoveries several times have been combined with many episodes that have caused health damage to several researchers. Furthermore, it is known that inadequate exposure to ionizing radiation causes irreversible somatic and genetic damage in living beings. Thus, it is of fundamental importance to quantify the radiation received to be used safely by the operator and, later, by the user. Dosimeters do the quantification of ionizing radiation.

The dosimeter indicates the absorbed radiation dose that the operator, user, or material was subjected to in a certain period. Once there are numerous applications for ionizing radiation so far, there are also a large number of materials that can be used for dosimetric purposes. Despite the expressive number of these materials, there is always a constant search for new materials, focusing on more efficient processes or less

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.42_abstract_GENNARI.pdf

environmental impact. The environmental impact is directly related to the disposal of any material submitted to radiation, and this practice is not always trivial.

Many materials have been the subject of research recently, aiming to be environment friendly; among them are biopolymers that have the great advantage of being biodegradable. These polymers are produced by living beings or obtained from raw materials from renewable sources. In terms of the manufacture of plastic packaging, their use allows the replacement of polymers derived from petroleum. Biopolymers have been used in several applications, for instance, in drug delivery (Oh, J. K.; Lee D. I.; Park, J. M., 2009), in tissue engineering (Weinstein-Oppenheimer, C. R et al. l, 2017), and as coatings (Nathanael, A. J., Oh, T. H., 2020).

As pointed out above, the material must be radiation-sensitive and ideally with very low environmental impact for dosimetric purposes. With this purpose, Yamamoto (Yamamoto T. et al., 2011) proposed using silver-activated phosphate glass as a radiophotoluminescence (RPL) solid-state detector. This dosimeter has an enormous advantage once it can be regenerated by annealing, so it can be used several times. This dosimeter is commercially available as “GD-450” (Chiyoda Technol Corporation).

Our research group has successfully proposed using silicate glass instead of phosphate glass as these RPL dosimeters (Chubaci, J. F. D.; 2017). However, the need for a high-temperature furnace for glass sintering was decided to test biopolymers as RPL dosimeters. Once our goal was to have a regenerative dosimeter, we used silver as a sensible radiation element.

In this work, it was synthesized two biopolymers with and without adding silver to them. The biopolymers synthesized used starch and collagen as polymer base material. The biopolymers analyses were done by microscopy and by optical spectrometry (UV-Vis-NIR). In addition, UV and β irradiation effects were evaluated on the biopolymer.

2. MATERIALS AND METHODS

The biopolymers were prepared on a hot plate. First, we mix the reagents described below. Then, after the solution boiled for around fifteen minutes, it was poured on Petri dishes. Later, the samples were cured at 100^0 C for one hour in a furnace.

2.1. Reagents

The following reagents were used: a) for starch biopol: 1.5 g of commercial culinary starch, b) for collagen biopol: 1.5 g of hydrolyzed collagen from Sanofi. In both preparations, it was also added also 10 ml of a 5 $\%_{(v/v)}$ solution of acetic acid (P.A. ACS, Vetec), 40 ml of purified water (Mili Q System), and the desired amount of silver nitrate (P.A. ACS, Sigma Aldrich). It is important to mention silver nitrate was first dissolved on acetic acid before adding to the polymer base material.

2.2. Instrument

In the microscopy analysis, it was used a binocular petrographic microscope ZEISS-JENA (Jenapol model).

The spectrometric analyses were done in an optical spectrometer (Cary 7000, Agilent).

UV irradiation was done with a Xe lamp (Oriel - 450 W, energy applied 8000 mJ, distance sample to lamp 85 cm).

Beta irradiation was done on a β irradiator system (model 733 - ELSEC - Oxford, UK).

3. RESULTS AND DISCUSSION:

One can easily note a clear difference in the biopolymer appearance in microscope images. There was also a difference in the mechanical resistance. The starch biopolymer synthesized is more fragile despite being cured at 100^0 C for one hour. The same heat treatment was done in collagen biopolymer also.

The NIR region spectra are quite similar to the ones from Sekar (Sekar, S. K. V., Mora A. D., Taroni, P., Ruggeri, A., 2017) and Pant (Pant B. R., Jeon Hye-Jin, Song H. H., 2011),. It shows we had success on both biopolymers syntheses.

Shortly we will analyze the biopolymers by vibrational techniques to better identify them.

In the UV-Vis region, it is possible to observe that the starch spectrum has broadband around 400 nm. This band does not appear on the collagen spectrum. Due to starch fragility, we first decided to do silver addition first in a collagen matrix. We added 0.5 $\%_{(w/w)}$ and 1.0 $\%_{(w/w)}$ of silver. We also exposed the three

biopolymers (C01 without any silver, C11 with 0.5 $\%_{(w/w),}$ and C21 with 1.0 $\%_{(w/w)}$ to a Xe lamp for 60 minutes after the heat treatment mentioned before.

It was possible to observe on UV-Vis spectra range that silver presence had affected the polymer behavior once an absorption peak appeared around 300 nm. The broadband, around 400 nm, on the pure collagen biopolymer disappeared with UV irradiation.

Without UV irradiation, replicates of C01 and C11 samples were β irradiated for 10 minutes. In this case, β irradiation has originated an absorption band around 500 nm.

In the future, we will be able to make a biopolymer-dosimeter. First, however, additional irradiation tests must be done, including to verify the possibility of using it several times.

4. CONCLUSIONS:

The collagen biopolymer synthesized has shown to be radiation-sensitive (UV and β). However, the synthesized starch biopolymer was very fragile, so irradiation tests could not be done. Alternative synthesis tests will be done. A factorial design plan will be used on it.

5. ACKNOWLEDGMENTS:

The authors want to acknowledge CNPq, FAPESP, and CAPES for supporting us on equipment purchase.

One of the authors (Gilson Goveia) wants to acknowledge USP for his grant.

6. REFERENCES

1. Tubiana, M., (1996) Wilhelm Conrad Röntgen and the discovery of X-rays, Bulletin de L'Académie Nationale de Médecine, 180(1), 97-108.
2. Oh, J. K.; Lee D. I.; Park, J. M., (2009) Biopolymer-based microgels/nanogels for drug delivery applications, Progress in Polymer Science 34, 1261–1282.
3. Weinstein-Oppenheimer, C. R., Brown D., Coloma, R., Morales, P., Reyna-Jeldesa, M., Díaz J. M., Sánchez, E., Acevedo, C. A., (2017), Design of a hybrid biomaterial for tissue engineering: Biopolymer-scaffold integrated with an autologous hydrogel carrying mesenchymal stem-cells, Materials Science and Engineering: C 79(1), 821-830.
4. Nathanael, A. J., Oh, T. H., (2020) Biopolymer Coatings for Biomedical Applications, Polymers, 12, 3061.
5. Yamamoto, T., Maki, D., Sato, F., Miyamoto Y., Nanto, H., Lida T., (2011), The recent investigations of radiophotoluminescence and its application, Radiation Measurements 46, (12), 1554-1559.
6. Chubaci, J. F. D.; Gonzales, C. D., Silva-Carrera, B. N., Zanardo, E., Miyamoto, M., Watanabe, S., (2017), RPL Dosimetry Application in Nuclear Medicine. In 13th International Workshop on Ionizing Radiation Monitoring (IWIMIR-12), Oarai, Ibaraki-ken, Abstracts. Tokyo, Japan: Chiyoda Technology Corporation, 20-20.
7. Sekar, S. K. V., Mora A. D., Taroni, P., Ruggeri, A., (2017) Diffuse optical characterization of collagen absorption from 500 to 1700 nm, Journal of Biomedical Optics 22(1), 015006.

Pant B. R., Jeon Hye-Jin, Song H. H., (2011), Radiation Cross-linked Carboxymethylated Starch and Iron RemovalCapacity in Aqueous Solution, Macromolecular Research, 19(3), 307-312.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

BIOPOLYMERS AS DOSIMETERS - A PROPOSAL

Roseli Fernandes Gennari
Universidade De São Paulo (USP) , Instituto de Física, Departamento de Física Nuclear - Brazil

Gilson Goveia
Universidade De São Paulo (USP) , Instituto de Física, Departamento de Física Nuclear - Brazil

José Fernando Diniz Chubaci
Universidade De São Paulo (USP) , Instituto de Física, Departamento de Física Nuclear - Brazil

March/2022

INTRODUCTION

SBJChem Conference 2021

- The radiation study has led to several advances in various areas of our everyday life;
- Inadequate exposure to ionizing radiation causes irreversible somatic and genetic damage in living beings;
- There are numerous applications for ionizing radiation, so far there are several materials can be used for dosimetric purposes;
- The search for new dosimetric materials is constant and, recently it focus on more efficient processes or less environmental impact.

BACKGROUND

SBJChem Conference 2021

- Biopolymers are environment friendly and are used in medical applications;
- Yamamoto (2011) had propose using silver-activated phosphate glass as radiophotoluminescence (RPL) solid-state detector. This dosimeter has an enormous advantage, once it can be used several times;
- Our research group (2017) had proposed using silicate glass instead of phosphate glass as RPL dosimeters.

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

- We have decided to test biopolymers as RPL dosimeter.
- Our goal is to have a regenerative dosimeter using silver as radiation sensible element.
- The biopolymer synthesis should be without using high-temperature furnace.

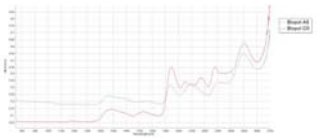
METHODOLOGY

SBJChem Conference 2021

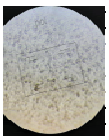
- The biopolymers were prepared on a hot plate. First we mix the reagents described below. Then after the solution boiled for around fifteen minutes it was poured on Petri dishes. Later the samples were cured at 100^0 C for one hour in a furnace. We used the following reagents: a) for starch biopolymer: 1.5 g of commercial culinary starch, b) for collagen biopolymer : 1.5 g of hydrolyzed collagen from Sanofi. In both preparations we added also 10 ml of a 5 %(v/v) solution of acetic acid (P.A. ACS, Vetec), 40 ml of a purified water (Mili Q System) and the desired amount of silver nitrate (P.A. ACS, Sigma Aldrich).
- In the microscopy analysis, it was used a binocular petrographic microscope ZEISS-JENA, (Jenapol model).
- For spectrometric analyses it was used a optical spectrometer (Cary 7000, Agilent).
- UV irradiation were done with a Xe lamp (Oriel - 450 W, energy applied 8000 mJ, distance sample to lamp 85 cm).
- Beta irradiation was done on a β irradiator system (model 733 - ELSEC - Oxford, UK).

RESULTS AND DISCUSSION

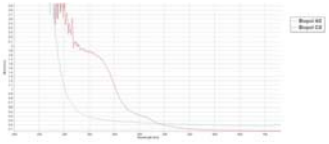
SBJChem Conference 2021



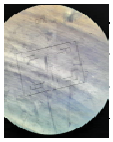
Biopolymers Spectra (NIR region)



Starch Biopolymer Microscope Image (200 x magnification)



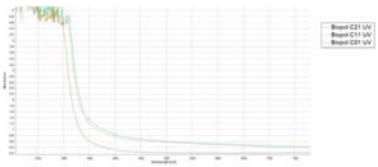
Biopolymers Spectra (UV-Vis region)



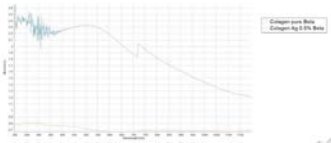
Collagen Biopolymer Microscope Image (200 x magnification)

RESULTS AND DISCUSSION

SBJChem Conference 2021



Collagen + Ag Biopolymers Spectra (UV irradiated)



Collagen + Ag Spectra (β irradiated)

CONCLUSIONS

SBJChem Conference 2021

- We had success on both biopolymers syntheses. However, starch biopolymer was very fragile so, irradiation tests could not be done;
- The collagen biopolymer synthesized has shown is radiation sensible (UV and β).

ACKNOWLEDGEMENTS

SBJChem Conference 2021

- The authors want to acknowledge CNPq, FAPESP and CAPES for supporting us on equipment purchase.
- One of us (Gilson Goveia) wants to acknowledge USP for his grant.

REFERENCES

SBJChem Conference 2021

1. Oh , J. K., Lee D. I., Park, J. M., (2009), Biopolymer-based microgels/nanogels for drug delivery applications, Progress in Polymer Science 34 1261–1282.
2. Weinstein-Oppenheimer, C. R., Brown D., Coloma, R., Morales, P., Reyna-Jeldesa, M., Díaz J. M., Sánchez, E., Acevedo, C. A., (2017), Design of a hybrid biomaterial for tissue engineering: Biopolymer-scaffold integrated with an autologous hydrogel carrying mesenchymal stem-cells, Materials Science and Engineering: C Volume 79, 1 Pages 821-830.
3. Nathanael, A. J., Oh, T. H., (2020), Biopolymer Coatings for Biomedical Applications, Polymers, 12, 3061.
4. Yamamoto T., Maki, D., Sato, F., Miyamoto Y. , Nanto H., Iida T., (2011), The recent investigations of radiophotoluminescence and its application, Radiation Measurements Volume 46, Issue 12, Pages 1554-1559.
5. Chubaci, J. F. D.; Gonzales, C. D., Silva-Carrera, B. N., Zanardo, E., Miyamoto, M., Watanabe, S., (2017), RPL Dosimetry Application in Nuclear Medicine. In 13th International Workshop on Ionizing Radiation Monitoring (IWIMIR-12), Oarai, Ibaraki-ken, Abstracts. Tokyo, Japan: Chiyoda Technology Corporation, p. 20-20.
6. Sekar, S. K. V., Mora A. D., Taroni, P., Ruggeri, A., (2017) Diffuse optical characterization of collagen absorption from 500 to 1700 nm, Journal of Biomedical Optics 22(1), 015006.
7. Pant B. R., Jeon Hye-Jin, Song H. H., (2011), Radiation Cross-linked Carboxymethylated Starch and Iron Removal Capacity in Aqueous Solution, Macromolecular Research, Vol. 19, No. 3, pp 307-312.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

BONDS, PRACTICE, AND CHEMISTRY: EXPERIENCE REPORT AND REFLECTIONS ON POTENTIALITIES OF TEACHING-LEARNING PROCESS OF CHEMICAL TECHNICIANS IN MIDST OF THE COVID-19 PANDEMIC

MESQUITA, Iago Santos[1*]; PAZ, Miguel Pedro Alves da[1]

[1] Instituto Federal de Educação, Ciência e Tecnologia do Rio de Janeiro, Coordenação de Segurança e Administração de Ambientes Tecnológicos

** Correspondence author*
e-mail: iago.mesquita@ifrj.edu.br

Received 15 October 2021; received in revised form 20 January 2022; accepted 05 February 2022

ABSTRACT

This work aims to report the experience of teaching a course with practical contents in chemistry in the distance modality due to the period of isolation by the COVID-19 pandemic. The target of the course was students of the Federal Institute of Education, Science, and Technology of Rio de Janeiro (Duque de Caxias *campus*), who study to be technicians in the field of Chemistry. In order to do so, the importance of experimentation in professional learning is discussed, as well as the difficulty of distance learning in practical training is analyzed. Following the course format and the resources used to overcome the limitations of distance learning and help the students keep the contents in mind are introduced. Student participation was an important component in choosing some themes for the course modules. Realizing the importance of construction that understands them as active subjects in the teaching-learning process, it was possible to offer modules that touched the students reality and expanded their knowledge through comprehensive training. The themes and approaches were proposed to help them define or rethink their career through contact with different realities of the work of a technician in the field of chemistry. The report ends by analyzing how a transdisciplinary education could help students connect knowledge acquired separately and aggregate it to see reality more broadly and completely. The difficulties arising from the COVID-19 pandemic made it possible to discuss a teaching way that would lead students to participate more actively in their training and, dialectically, strengthen pedagogical praxis.

Keywords: *Distance learning, Pandemic, Education in Science, Experimental Education, Active Teaching Methodologies*

1. INTRODUCTION

Theoretical activity exists only from and in relation to practice; there is no thinking outside of human action. Consciousness and conceptions are formulated through the movement of thought, which focuses on the "world of actions" and the relationships they generate. Even if theoretical activity reframes conceptions, it transforms representations, produces theories, in none of these cases transforms reality alone. Ideas need to be transformed into actions (Kuenzer, 2017).

In this sense, Saviani (1983) highlights that education acts on the practice subjects in an indirect and mediated way. This author view distances itself from the conception that the teaching and learning process occurs first in a theoretical way so that, finally, it is developed - a perspective often reinforced by the traditional formatting. In this context, it is appropriate to quote Dewey that *"Education is a life process; no preparation for the future life*" (Dewey, 1940, p. 6). Dewey (1940), in the conception of Experimental Education, understands that the student must be subjected to real problems. Therefore, the educational process would consist of analyzing the mechanisms of the problem, in the creation of hypotheses about the problem, and in the reflection on the solution alternatives: in the re-signification of their experiences, in short.

The principles of Experimental Education and theory-practice articulation are very clear in the training of professionals in the field of

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.18_abstract_MESQUITA.pdf

chemistry. Moreover, these subjective ideas are even frequently performed in objects: the curricular contents are represented in practices, and theories, in glassware, reagents, and other laboratory utensils.

However, in 2020, the COVID-19 pandemic posed unthinkable challenges to humanity as a whole, mainly to education. How to think about the training process of technicians in the field of chemistry, professionals so linked to laboratory practice, in a context of *lockdown*? How to mitigate the effects of distance learning in the training of these professionals? More than that, and perhaps more essential: how to keep these students motivated? How to maintain the bonds between academic community members?

This work does not intend to exhaust these issues, which are so deep and delicate for the teaching-learning process nowadays, but rather to provide alternatives. This text is intended to be an experience report on an extracurricular course of continuous training given by the Technological Environments Safety and Administration Coordination (CoSAAT) of the Federal Institute of Education, Science, and Technology of Rio de Janeiro (Duque de Caxias *campus*) in 2021. From this report, reflections on potentialities flourish on concrete challenges of these times.

2. MATERIALS AND METHODS

With the impossibility of conducting the course in face-to-face mode, the course was offered in distance learning through synchronous meetings on the *Google Meet* platform.

During planning, topics such as reagent compatibility, laboratory safety, and waste management remained on the course menu, but with activities designed directly for the modality of training offered.

In addition, other topics were proposed aimed at specific professional fields, which could break new ground in their careers, such as chemical products inspection and control, first aid in the laboratory, the pharmacy chemical industry, among others.

2.1 Resources Examples

In the presential course, the chemical compatibility module had an activity using cards and the laboratory board to favor active teaching methodologies. This theme was approached with an interactive activity in a 3D virtual Chemical Storage Room using *Paint 3D* software (Figure 1). Every time a reagent was placed with an incompatible one, the “technician” suffered an injury, like in a hangman game. Therefore, the target was to complete the arrangement of the stock without the technician dying. At the end of the activity, students knew the necessary conditions for safe storage.

Figure 1. *Chemical Storage Room*

The online laboratory safety training, with expanded time, enabled the presentation of different safety equipment and the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). After topic explanation through images, videos and discussions were proposed activities to keep in mind the contents. The activities were offered within the presentation itself and through free external resources such as *wordwall.net* (Figure 2).

Figure 2. *Quiz of Lab Safety Module*

In addition to these, other online resources such as electronic spreadsheets with remote access and screen mirroring of specific programs and websites enabled students to observe and even use some of these programs.

3. RESULTS AND DISCUSSION:

Fifteen modules were offered during 10 months, as shown in Table 1:

Table 1. *Modules and Duration*

Module	Duration (h)
Chemical Compatibility	1,5
Excel applied to the field of chemistry*	1,5
Solid characterization techniques and data treatment by the Origin software	1,5
English applied to in the field of chemistry*	1,5
Laboratory Safety I and II	3
Waste Management	1,5
Chemsketch software*	1,5
Chemicals Control	1,5
Laboratory First Aid	1,5
Laboratory Equipment*	1,5
Industrial Equipment*	1,5
Experimental Planning and Data Analysis I and II	3
Creating Charts Using Spreadsheets	1,5
Organic Compounds Industrial Production	1,5
Technical Sales and Laboratory Accreditation	1,5

** Suggested by the students*

The students behaved as subjects of the teaching-learning process: they participated in the course of their own volition and, without any summative assessment tool, they remained in it. Moreover, the theme of many of the modules was a suggestion by the participating students themselves. By participating in the course, they gradually take on the lead in this course: they raise doubts and possible deficiencies in their regular course, suggest topics that can help them in college entrance exams, the labor market, or even in their daily lives. Therefore, they begin to have autonomy in their formative process.

The construction of this autonomy is linked to a less conservative and more humane education proposal. By collectivizing the curricular decision – and here it is remembered that curriculum is an instrument of power – it is understood that a formative process is distinct from that in which knowledge is organized for the individual, but that the individual empowers himself to organize his knowledge. From the theoretical perspective of Rogers (1997), the motivation for this process would be a self-fulfilling tendency of the individual to become who he is.

It is noteworthy then that the disruptions caused by the COVID-19 pandemic led to an unlikely scenario in education. In this scenario, many control tools dissociated, liquefied; time became spatialized, and the notion of the place was resignified. In this strange place, new ways of conducting the teaching-learning process abound. It is believed that here through this report, one can think of some of them.

One of the concerns was to guarantee in this process the teacher-student interaction and among the students themselves. However, it is believed that the methodology of active learning, such as the proposition of games, allowed this engagement. In many moments, a student was noticed participating in the colleague response, discussing together, even with all the limitations that a remote class can have.

It should be noted that in the group discussion, students can exchange knowledge, argue, and build something together, and, often, they can find a locus of speech to talk to their doubts and concerns. In this argument, analytical capacities and interconnections between subjects are present: in this otherness, in the encounter with the thought of others, that apprentices can actively discern their cognitive processes (Lévinas, 1993).

Another concern was the maintenance of bonds between students and with the symbolic place of school. However, the bonds maintained by the regularity of the course led to contradictions about the practices – and the thinking about practices – of the notion of space. Perrenoud (2000) clarifies that the antagonism between non-spaces and physical or symbolic spaces transcends the perception of mobility restrictions. They also become a dynamo of contradictions and constructions between the political, economic, and cultural forces that subject themselves to a territory. That is, the digital did not necessarily subtract territorialities but essentially make them

more fluid.

What kind of links are built from the perspective of the physical place? It was realized that in the course, with discussions about careers, about living the pandemic, about deciding on its formation, they became much more powerful tools in constructing these bonds with a symbolic place than with the physical place itself.

Moreover, finally, the different types of knowledge worked together with the students stand out. Some graduates reported that contents were covered later, at the beginning of their undergraduate course. Content of chemistry, such as safety, compatibility, analytical tools, and knowledge in human health, computer languages, and industry, were addressed. That is, the proposition of a curriculum is not only collectively thought out but transdisciplinary. Many of the themes from other areas were suggested by the students themselves.

This strengthens the hypothesis that when taking autonomy in building his career, the subject perceives the need to draw connections between different types of knowledge. Decompartmentalization, facing real problems and experience as a focus naturally led to a transdisciplinary approach. Thus, a chemical technician is not formed only on chemical bonds but on the bridges he builds with different knowledge permeating his work.

Therefore, it is believed that the contradictions arising from teaching in times of pandemic paths could be rethought. All the contradictions raised by the challenges imposed on the pandemic can be seen as an opportunity to think about pedagogical practice. That is a dialectical path of strengthening the *praxis* in difficult times for humanity.

4. CONCLUSIONS:

Under the adversities of the imposition of abruptly remote teaching, a training course was designed to mitigate the damages in the training of technicians in the chemistry area of the IFRJ – Duque de Caxias *campus*. However, especially in the training of these professionals, whose work is directly linked to work in laboratories, the losses could be even more worrying.

With the intention of attenuating such effects, during a liquid scenario, new paths could be thought. The contradictions imposed on this path gave rise to a dialectical process by questioning the perspectives of bonds, syllabus, transdisciplinarity, and theoretical-practical articulation. The search for answers to these questions led to fruitful reflections for both the face-to-face and virtual teaching-learning process – that is, dialectically they fostered praxis.

5. ACKNOWLEDGMENTS:

For all students of IFRJ, who, in the process of building themselves, made it possible to rethink and rebuild our educational practices.

6. REFERENCES:

1. Dewey, J. My pedagogic creed. In: Education today. New York: G.P. Putnam's Sons, 1940.
2. Kuenzer, A. Z. Trabalho e escola: a flexibilização do ensino médio no contexto do regime de acumulação flexível. Educação & Sociedade, Campinas, 2017.
3. Lévinas, E. Humanismo do outro homem. Trad. de Pergentino S.Pivatto. Petrópolis: Vozes, 1993.
4. Perrenoud, P. Dez novas competências para ensinar. Porto Alegre: Artmed, 2000.
5. Rogers, C. R. Tornar-se Pessoa. 5 a ed. São Paulo: Martins Fontes, 1997
6. Saviani, D. Escola e Democracia. São Paulo, Cortez/Autores Associados, 1983.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

BONDS, PRACTICE AND CHEMISTRY: EXPERIENCE REPORT AND REFLECTIONS ON POTENTIALITIES OF TEACHING-LEARNING PROCESS OF CHEMICAL TECHNICIANS IN MIDST OF THE COVID-19 PANDEMIC

Iago Santos Mesquita
Instituto Federal de Educação, Ciência e Tecnologia do Rio de Janeiro - Brazil

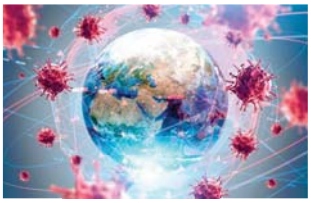
Miguel Pedro Alves da Paz
Instituto Federal de Educação, Ciência e Tecnologia do Rio de Janeiro – Brazil

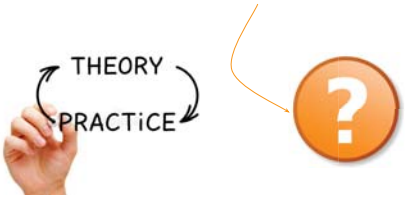
March/2022

INTRODUCTION

SBJChem Conference 2021

- Experimental education in midst of COVID-19 pandemic;
- How to think the training process of technicians in the field of chemistry?





AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

This study proposes to be an experience report, accompanied by its intrinsic theoretical reflections on the pedagogical *praxis*, about an extracurricular training course for technicians in the field of chemistry during a COVID-19 pandemic.

METHODOLOGY

SBJChem Conference 2021

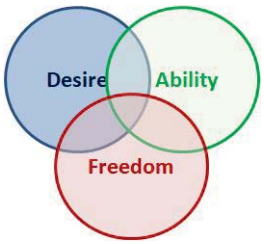
Active methodologies

Flexible syllabus

RESULTS AND DISCUSSION

SBJChem Conference 2021

Module	Duration
Chemical Compatibility	1,5
Excel to the technician in the field of chemistry*	1,5
Solid characterization techniques and data treatment by the "Origin" software	1,5
English applied to the daily life of the technician in the field of chemistry*	1,5
Laboratory Safety I and II	3
Waste Management	1,5
The use of "Chemsketch" software*	1,5
Chemicals Control	1,5
Laboratory First Aid	1,5
Laboratory Equipment*	1,5
Industrial Equipment*	1,5
Experimental Planning and Data Analysis I and II	3
Creating Charts Using Excel	1,5
Organic Compounds Industrial Production: *	1,5
Technical Sales and Laboratory Accreditation	1,5

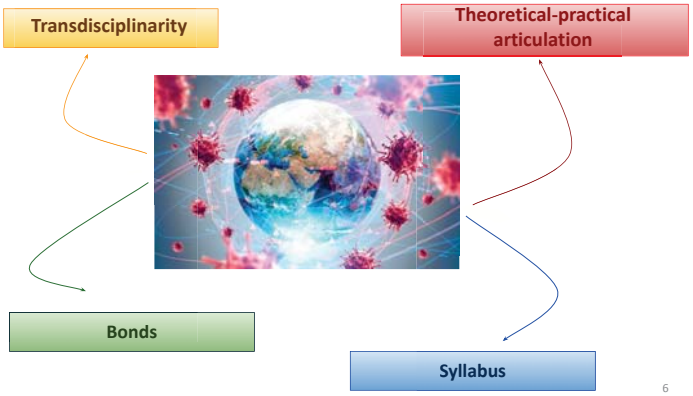


- Bonds;
- Transdisciplinarity;

5

CONCLUSIONS

SBJChem Conference 2021



6

REFERENCES

SBJChem Conference 2021

1. Dewey, J. My pedagogic creed. In: Education today. New York: G.P. Putnam's Sons, 1940.
2. Kuenzer, A. Z. Trabalho e escola: a flexibilização do ensino médio no contexto do regime de acumulação flexível. Educação & Sociedade, Campinas, v. 38, n. 139, p. 331- 354, 2017.
3. Lévinas, E. Humanismo do outro homem. Trad. de Pergentino S.Pivatto. Petrópolis: Vozes, 1993.
4. Perrenoud, P. Dez novas competências para ensinar. Porto Alegre: Artmed, 2000.
5. Rogers, C. R. Tornar-se Pessoa. 5 a ed. São Paulo: Martins Fontes, 1997.
6. Saviani, D. Escola e Democracia. São Paulo, Cortez/Autores Associados, 1983.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

CHARACTERISTICS OF WOOD SAWDUST-DERIVED BIOCHAR: POTENTIAL AS ADSORBENT MATERIAL

LIMA, Daniele de Andrade Villarim[1]; REZENDE, Fabiana Abreu[2]; FUNGARO, Denise Alves[1*]

[1] Instituto de Pesquisas Energéticas e Nucleares, IPEN–CNEN/SP, São Paulo, SP, Brazil

[2] Embrapa Agrossilvipastoril, Sinop,MT, Brazil

** Correspondence author*
e-mail: dfungaro@ipen.br

Received 20 October 2021; received in revised form 28 December 2021; accepted 24 January 2022

ABSTRACT

Biochar is a potential additive for agricultural soil and can be used as an eco-friendly and economical adsorbent material. Biochar properties are affected by several technological parameters, mainly pyrolysis temperature and feedstock, which differentiation can lead to products with a wide range of characteristics. The biochar sample was produced from wood sawdust at 450˚C via slow pyrolysis and was characterized. Parameters characterized to include: physical properties (bulk density, porosity), chemical properties (composition, pH, conductivity, cation exchange capacity), hydraulic property (water holding capacity), proximate analysis, X-ray diffractometry to obtain information on the mineralogical composition, among others. The analysis of biochar properties is important for determining the biochar application.

Keywords*: biochar, characteristics, wood sawdust, slow pyrolysis, physicochemical properties*

1. INTRODUCTION

Biochar is a carbonaceous material generated from biomass pyrolysis under limited oxygen and temperature (<700 °C). Biomass derived from agroindustrial wastes stands out because it is an inexpensive, abundant, renewable, and biodegradable material. However, it becomes an environmental problem when inadequately disposed (Wang *et al.*, 2020).

Depending on the production conditions and feedstock, biochars' physical and chemical characteristics can vary widely, resulting in biochars with different types and quantities of surface functional groups, surface area, pH, and chemical composition (Tomczyk *et al*., 2020).

Due to their surface characteristics, including a porous structure, high surface area, and carbonized and non-carbonized domains, biochar can adsorb heavy metals and various organic pollutants in the aqueous phase (Yaashikaa *et al*., 2020).

This work aims to investigate the properties of wood sawdust-derived biochar to evaluate its suitability as an adsorbent material.

2. MATERIALS AND METHODS

2.1. Biochar production

Biochar (BC) was obtained from native forest species from timber management. To obtain the BC, sawdust was processed in a slow pyrolysis reactor (vertical furnace), with 25 min residence time, at 450°C.

2.2. Biochar characterization

All solutions were prepared using ultrapure water (18.2 MΩ cm resistivity, TOC 10.0 mg L^{-1}) and analytical grade reagents unless otherwise stated. Proximate analysis (moisture content, volatile matter, fixed carbon, and ash content) was determined according to EBC recommended methods (EBC, 2012). Dry bulk density, water holding capacity, air-filled porosity, and saturated bulk density of biochar were determined by methods described in the literature (Duong *et al.*, 2017; CAO *et al*., 2014; EBC, 2012). Electrical conductivity and pH were measured in a sample/deionized water ratio of 1:10 (w/v) (Singh *et al.*, 2017). BC was saturated with sodium acetate and ammonium acetate solutions for the

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.11_abstract_LIMA_IPEN.pdf

cation exchange capacity (CEC). Na^+ concentration of the resulting solution was determined by ICP-OES (Spedtroflame — M120). For the Point of Zero Charge (PCZ) determination, 0.1 g of BC was mixed with 50.0 mL of 0.1 mol L^{-1} $NaNO_3$ under different conditions of initial pH (pH_i), adjusted from 2.0 to 12.0 by the addition of HCl or NaOH solution. The final pH values (pH_f) were recorded in the remaining suspensions after 24 h contact time at 120 rpm. The difference between pH_i and pH_f (ΔpH) was plotted against pH_i values. The pH at PZC corresponded to the point of intersection in the resulting curve. The mineralogical composition was determined by X-ray diffraction analyses (XRD) with an automated Rigaku Miniflex 2 diffractometer with Cu anode using Co Kα radiation at 40 kV and 20 mA over the range (2θ) of 5–80° with a scan time of 0.5 °/min. Chemical composition was determined by X-ray fluorescence (XRF) spectrometry in Malvern Panalytical, model Zetium.

3. RESULTS AND DISCUSSION:

3.1. Proximate analysis

Proximate analysis is a measure of total biomass components in terms of moisture content, ash content, volatile solids, and fixed carbon of the solid fuel (Qian *et al*., 2013). The proximate analyses of biochar are shown in Table 1.

Table 1. *Proximate analysis of biochar*

Parameter	Values
moisture (%)	1,003 ± 0,05078
ash content (%)	14,0 ± 0,655
volatile matter (%)	28,4 ± 1,41
fixed carbon (%)	56,5 ± 2,05

It can be seen that the moisture content still presented in the biochar was not zero, even when pyrolyzed at a high temperature.

BC had ash and volatile matter contents relatively low. Ash content is attributable to the different concentrations of ash-forming elements, such as calcium carbonate, potassium silicates, iron, and other metals (Lewandowski and Kicherer, 1997).

In contrast to ash content, volatile solids retention was primarily affected by the pyrolysis temperature. Biomass typically consists of three components: hemicellulose, cellulose, and lignin (Yang *et al*., 2006). Generally, hemicellulose is the most volatile, cellulose is less volatile, and lignin is the most difficult to volatilize.

Fixed carbon is an important information of biomass quality since it is the most resistant portion that remains in biochar after pyrolysis. It is organized in aromatic chains and is inversely related to volatile materials and ash content (Amonette and Joseph, 2009).

3.2. Physical-chemical and hydraulic properties

Physical and chemical characteristics and hydraulic properties (water holding capacity) of the biochar are shown in Table 2.

Table 2. *Physical-chemical and hydraulic properties of biochar*

Property	Value
dry bulk density (kg/l)	0.2622 ± 0.0076
water-holding capacity (%)	317.9 ± 48.54
air-filled porosity (%)	10 ± 0.35
saturated bulk density (%)	2.84 ± 0.02
pH	4.10
conductivity (μS cm^{-1})	18.8 ± 0.350
CEC (meq $100g^{-1}$)	3.08 ± 0.0495

The dry bulk density of biochars derived from different types of wood processed in different types of traditional ovens ranged from 0.30 kg/L to 0.43 kg/L (Pastor-Villegas *et al.*, 2006). The value of the biochar in the present study is close to the minimum value of this range. The water holding capacity of biochars could improve soil water retention capacity, reduce water leaching, and increase water availability in the root zone of crops. The ability of biochar to retain water is strongly related to the surface area and its porosity. Therefore, the smaller the BC particles, the greater the water retention capacity.

Biochars with low ash content, such as those produced using woody feedstocks, generally have lower pH values than biochars with higher ash content (Singh *et al*., 2017). The biochar sample in the present study has a low ash content, and the low pH value indicates that acidic functional groups were not degraded during pyrolysis. Furthermore, cellulose and hemicelluloses decompose around 200–300 °C, yielding organic acids and phenolic substances that lower the pH of the biochar (Yu *et al.*, 2014).

The relatively low conductivity value is also related to the low ash content, which probably decreases the dissolution of water-soluble salts. Biochar presented a CEC value close to that of another biochar obtained with pyrolyzed sawdust at 350 °C (Santos *et al*., 2019). CEC is influenced

by the groups of carboxylic and phenolic compounds present in the biomass that originated the biochar.

3.2. Chemical composition

Table 3 presents the major inorganic elements in biochar identified by XRF. The major inorganic elements identified in BC came from the plant biomass that are present naturally (Saleem *et al.*, 2020). It can be observed that the major constituents are SiO_2, Al_2O_3, and Fe_2O_3.

Table 3. *Chemical composition of the major elements in BC*

Oxides	Value
SiO_2 (wt. %)	5.20
Al_2O_3 (wt. %)	3.05
Fe_2O_3 (wt. %)	1.34
others (wt. %)	< 0.40
loss of ignition (%)	89.6

3.3. Mineralogical composition

The X-ray diffractogram of biochar shows a typical band of predominantly amorphous material with a maximum of around 2θ = 20º (Figure 1). The occurrence of this band indicates that the cellulose, which is the only crystalline material present in the sawdust, was destroyed in the pyrolysis process (Chowdhury *et al.*, 2016). On the other hand, hemicellulose and lignin, which are also part of the composition of sawdust, are both amorphous in nature.

The pronounced peak at 2θ = 26.75º is attributed to the presence of SiO2. Silicon is a mineral element that, after being absorbed by plants, polymerizes and accumulates in the cell wall of the epidermis, acting to increase their defenses (Gomes *et al.*, 2005). The peak at ~2θ = 55º is attributed to impurities present in the sample or in the pyrolysis process.

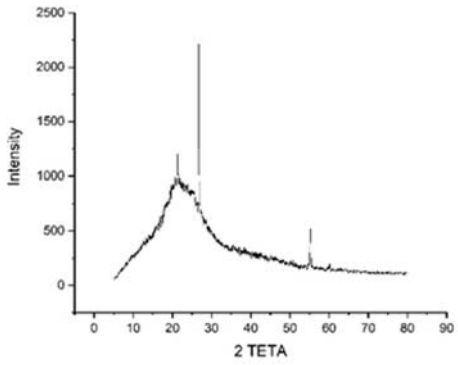


Figure 1. *X-ray diffractogram of biochar*

3.4. Point of zero charge

As seen in Figure 2, biochar had a pHPCZ value equal to 5.2. At a pH lower than this value, the surface charge of biochar will be positive and there will be a preference for adsorbing anions through the electrostatic attraction mechanism. After pHPCZ, the charge will be negative and the attraction of cations to the biosorbent surface will predominate.

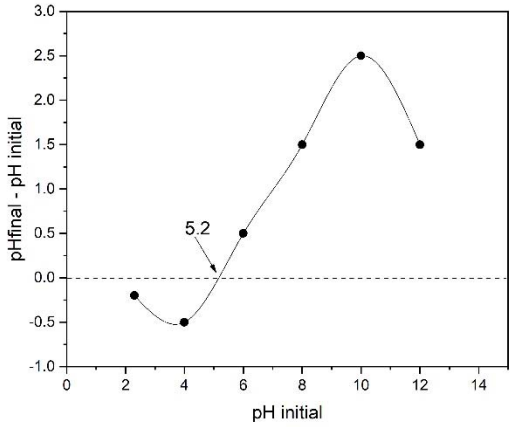


Figure 2. *Point Zero Charge for biochar*

4. CONCLUSIONS:

This study characterized the physical, chemical and hydraulic properties of waste wood-derived biochar (BC) produced by slow pyrolysis. BC presented ash and volatile matter contents relatively low. The pH value in water was low, suggesting that BC may be suitable for improving alkaline soils. The dry bulk density and CEC values are typical of wood-derived biochar. The results of this study may guide the preparation of sawdust biochar and the utilization of this product as adsorbent material.

5. ACKNOWLEDGMENTS:

The authors are grateful to Prof. F.A. Rezende, a researcher at Embrapa Agrossilvipastoril, Sinop, MT, for providing biochar samples.

6. REFERENCES:

1. Wang, X., Guo, Z., Hu, Z.,Zhang, J. Recent advances in biochar application for water and wastewater treatment: a review, **2020**, PeerJ8:e9164http.
2. Tomczyk, A., Sokołowska, Z., Boguta, P. Biochar physicochemical properties: pyrolysis temperature and feedstock kind effects. Rev Environ Sci Biotechnol 19, **2020**, 191–215.
3. Yaashikaa, P.R., Kumar, S. P., Sunita, V., Saravanan, A. A critical review on the biochar production techniques, characterization, stability and applications for circular bioeconomy, Biotechnology Reports, **2020**, 28:1-15.
4. EBC, **2012**, 'European Biochar Certificate - Guidelines for a Sustainable Production of Biochar.' European Biochar Foundation (EBC), Arbaz, Switzerland.
5. Duong, V. K., Nguyen, N., Nguyen, P., Tan, D. X. Impact of biochar on the water holding capacity and moisture of basalt and grey soil. Journal of Science Ho Chi Minh City Open University, **2017**, 7. 36-43.
6. Cao, C. T., Farrell, C., Kristiansen, P. E., Rayner, J. P. Biochar makes green roof soils lighter and improves water supply to plants. Ecol. Eng, **2014**, 71, 368–374.
7. Singh, B., Dolk, M. M., Shen, Q., Camps-Arbestain, M. Biochar pH, electrical conductivity and liming potential. Biochar: A Guide to Analytical Methods, **2017**, 23.
8. Qian, K., Kumar, A., Patil, K., Bellmer, D., Wang, D., Yuan, W., Huhnke, R. L. Effects of biomass feedstocks and gasification conditions on the physiochemical properties of char. Energies, **2013**, 6, 3972–3986.
9. Lewandowski, I., Kicherer, A. Combustion quality of biomass: Practical relevance and experiments to modify the biomass quality of Miscanthus × giganteus. Eur. J. Agron, **1997**, 6, 163–177.
10. Yang, H., Yan, R., Chen, H., Zheng, C., Lee, D. H., Liang, D. T. In-depth investigation of biomass pyrolysis based on three major components: Hemicellulose, cellulose and lignin. Energy Fuels, **2006**, 20, 388–393.
11. Amonette, J. E., Joseph, S. Characteristics of biochar: microchemical properties. In: LEHMANN, J.; JOSEPH, S. (Ed.). Biochar for environmental management science and technology. London: Earthscan, **2009**, p. 34.
12. Pastor-Villegas, J., Pastor-Valle, J. F., Meneses Rodríguez, J. M., García, M. 'Study of commercial wood charcoals for the preparation of carbon adsorbents', Journal of Analytical and Applied Pyrolysis, **2006**, vol 76, pp103–108.
13. Yu, H., Zhang, Z., Li, Z., Chen, D. Characteristic of tar formation during cellulose, hemicellulose and lignin gasification. Fuel, **2014**, 118:25–256.
14. Santos, S. R., Filho, J. F. L., Vergütz, L., Melo, L. C. A. Biochar association with phosphate fertilizer and its influence on phosphorus use efficiency by maize. Ciência e Agrotecnologia, **2019**, 43:e025718.
15. Saleem, M.H., Ali, S., Rehman, M., Hasanuzzaman, M., Rizwan, M., Irshad, S., Shafiq, F., Iqbal, M., Alharbi, B.M., Alnusaire, T.S., Qari, S.H. Jute. A Potential Candidate for Phytoremediation of Metals—A Review. Plants, **2020**, 9, 258.
16. Chowdhury, Z. Z., Karim, Md. Z., Ashraf, M. A., Khalid, K. Influence of Carbonization Temperature on Physicochemical Properties of Biochar derived from Slow Pyrolysis of Durian Wood (Durio zibethinus) Sawdust. BioResources, **2016**, 11(2), pp. 3356 - 3372.
17. Gomes, F. B., Moraes, J. C., Santos, C. D., Goussain, M. M. Resistance induction in wheat plants by silicon and aphids. Scientia Agricola, Piracicaba, **2005**, v. 62, n. 6, p. 547-551.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

CHARACTERISTICS OF WOOD SAWDUST-DERIVED BIOCHAR: POTENTIAL AS ADSORBENT MATERIAL

Daniele de Andrade Villarim Lima
Instituto de Pesquisas Energéticas e Nucleares, IPEN–CNEN/SP, São Paulo, SP, Brazil .

Fabiana Abreu Rezende
Embrapa Agrossilvipastoril, Sinop, MT, Brazil

Denise Alves Fungaro
Instituto de Pesquisas Energéticas e Nucleares, IPEN–CNEN/SP, São Paulo, SP, Brazil .

March/2022

SUMMARY

SBJChem Conference 2021

INTRODUCTION

SBJChem Conference 2021

Biochar (BC) is a carbonaceous material generated from biomass pyrolysis under conditions of limited oxygen and temperature (< 700 °C);

Physical and chemical characteristics may vary depending on the biomass;

The biochar can adsorb heavy metals and a variety of organic pollutants in the aqueous phase.

Figure 1. Biochar Cycle

Fonte: https://www.sciencedirect.com/science/article/abs/pii/S0045653514015008

OBJETIVE

SBJChem Conference 2021

The aim of this work is to investigate the properties of wood sawdust-derived biochar to evaluate its suitability as adsorbent material.

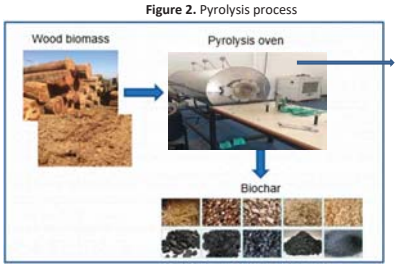
METHODOLOGY

SBJChem Conference 2021

1. Biochar production

Material: native forest species were obtained from timber management.

Figure 2. Pyrolysis process



Sawdust was processed in a **slow pyrolysis reactor** (vertical furnace), with 25 min residence time, at 450°C

Fonte: Rezende et al.In book: Embrapa Agrossilvipastoril Primeiras contribuições para o desenvolvimento de uma Agropecuária Sustentável. Chapter 1. 2019

METHODOLOGY

SBJChem Conference 2021

2. Biochar characterization

- Proximate analysis
- Physical-chemical and hydraulic properties
- Mineralogical composition
- Point of zero charge

RESULTS AND DISCUSSION

SBJChem Conference 2021

1. Proximate analysis

Table 1. Proximate analysis of biochar

Parameter	Values
moisture (%)	1.003 ± 0.05078
ash content (%)	14.0 ± 0.655
volatile matter (%)	28.4 ± 1.41
fixed carbon (%)	56.5 ± 2.05

- The moisture content still present in the biochar was not zero
- Ash and volatile matter contents are relatively low
- Fixed carbon content is relatively high

RESULTS AND DISCUSSION

SBJChem Conference 2021

2. Physical-chemical and hydraulic properties

Table 2. *Physical-chemical and hydraulic properties of biochar*

Property	Value
dry bulk density (kg/L)	0.2622 ± 0.0076
water holding capacity (%)	317.9 ± 48.54
air-filled porosity (%)	10 ± 0.35
saturated bulk density (%)	2.84 ± 0.02
pH	4.10
conductivity (µS cm^{-1})	18.8 ± 0.350
CEC (meq $100g^{-1}$)	3.08 ± 0.0495

- Dry bulk density and CEC values are close to others sawdust-based biochar
- Conductivity value is relatively low
- pH is acidic

RESULTS AND DISCUSSION

SBJChem Conference 2021

3. Chemical composition

Table 3. Chemical composition of the major elements in BC

Oxides	Value
SiO_2 (wt. %)	5.20
Al_2O_3 (wt. %)	3.05
Fe_2O_3 (wt. %)	1.34
others (wt. %)	< 0.40
loss of ignition (%)	89.6

The major inorganic elements identified came from the plant biomass that are present naturally

RESULTS AND DISCUSSION

SBJChem Conference 2021

4. Mineralogical composition

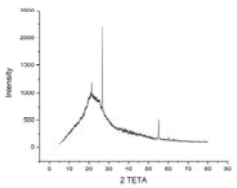


Figure 3. X-ray diffractogram of biochar

- BC is predominantly amorphous material with a maximum around 2θ = 20°
- The pronounced peak at 2θ = 26.75° is attributed to the presence of SiO_2

5. pH of Point of Zero Charge

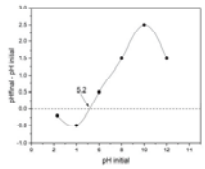


Figure 4. Point Zero Charge for biochar

BC had a pHPCZ value equal to 5.2

CONCLUSIONS

SBJChem Conference 2021

In this study, physical, chemical and hydraulic properties of waste wood-derived biochar (BC) produced by slow pyrolysis were characterized;

BC presented ash and volatile matter contents relatively low;

The value of pH in water was low suggesting that use of BC may be suitable for improving alkaline soils;

The dry bulk density and CEC values have typical value of wood-derived biochar;

The results of this study may provide guidance in the preparation of sawdust biochar and in the utilization of this product as adsorbent material.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

❖ The authors are grateful to Prof. F.A. Rezende, researcher at Embrapa Agrossilvipastoril, Sinop, MT, for providing biochar sample.

REFERENCES

SBJChem Conference 2021

1. Wang, X., Guo, Z., Hu, Z.,Zhang, J. (2020). Recent advances in biochar application for water and wastewater treatment: a review, PeerJ8:e9164http.
2. Tomczyk, A., Sokołowska, Z., Boguta, P. (2020). Biochar physicochemical properties: pyrolysis temperature and feedstock kind effects. Rev Environ Sci Biotechnol 19, 191–215.
3. Yaashikaa, P.R., Kumar, S. P., Sunita, V., Saravanan, A. (2020). A critical review on the biochar production techniques, characterization, stability and applications for circular bioeconomy, Biotechnology Reports, 28:1-15.
4. EBC (2012) 'European Biochar Certificate - Guidelines for a Sustainable Production of Biochar.' European Biochar Foundation (EBC), Arbaz, Switzerland.
5. Duong, V. K., Nguyen, N., Nguyen, P., Tan, D. X. (2017). Impact of biochar on the water holding capacity and moisture of basalt and grey soil. Journal of Science Ho Chi Minh City Open University, 7. 36-43.
6. Cao, C. T., Farrell, C., Kristiansen, P. E., Rayner, J. P. (2014). Biochar makes green roof soils lighter and improves water supply to plants. Ecol. Eng, 71, 368–374.
7. Singh, B., Dolk, M. M., Shen, Q., Camps-Arbestain, M. (2017). Biochar pH, electrical conductivity and liming potential. Biochar: A Guide to Analytical Methods, 23.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

CHILD DEPRESSION IN BRAZIL - A LITERATURE REVIEW

ERTHAL, Luísa Canto[1*]; SILVA, Guilherme Felipe Dutra[1]; QUEIROZ, Aline Trovão[1];

[1] Universidade de Vassouras, Pró-reitoria de Ciências médicas, Faculdade de Medicina. Brasil.

** Autor correspondente*
e-mail:lcantoerthal@hotmail.com

Received 20 January 2022; received in revised form 28 February 2022; accepted 08 March 2022

ABSTRACT

Childhood depression is a very prevalent mental health condition in today's society. Its debate began to become relevant in the 1960s and, although there is no doubt about its existence, the subject is still little discussed. This paper aims to demonstrate the relevance of the subject due to its high prevalence and underdiagnosis. A literature review on Childhood Depression in Brazil was carried out based on research in Pubmed, Scielo, and Google Scholar databases, between 1989 and 2020, in Portuguese and English, using the descriptors: “child depression”, “symptoms of depression” and “treatment of childhood depression” combined. Textbooks, data from *Ministério da saúde*, the World Health Organization (WHO), and key articles selected from citations in other articles were used to compose the paper. From the data analysis, twenty-two titles that are directly related to the current work were selected. In Brazil, girls and children between thirteen and fourteen years old are the most affected by the disease. The DSM does not differentiate it from adult depression, despite the atypical manifestations of its symptoms in children. Families still have great difficulty on identifying this disorder the biggest obstacle is understanding and accepting that behavioral changes can be part of a depressive condition. Normalizing the discussion of the topic is important so that there is more information about the disease and, consequently, more knowledge is disseminated both to the medical community and the families of affected children. This way, it will be possible to prevent its appearance and, when present, facilitate its detection, improving life quality of those involved and avoiding negative outcomes such as child suicide.

Keywords: *Childhood depression; Mood disorder in childhood; Child psychiatry*.

1. INTRODUÇÃO

Depressão é definida como um transtorno de humor caracterizado por tristeza contínua e perda de interesse em realizar atividades que antes eram consideradas prazerosas, junto a uma impossibilidade de realizar atividades diárias por, pelo menos, duas semanas (Organização Mundial da Saúde, 2007).

A Depressão Infantil começou a ser discutida no campo da psiquiatria a partir da década de 60. Antes disso, acreditava-se que ela não existia ou até, que seria extremamente rara na população. Atualmente não há mais dúvida quanto a sua ocorrência (White, 1998; Bandim, Sougey e Carvalho, 1995; Cruvinel e Boruchovitch, 2003).

De acordo com o Manual Diagnóstico e Estatístico de Transtornos Mentais V (DSM, 2014), a depressão na criança se manifesta de maneira semelhante à depressão no adulto, podendo apresentar algumas alterações como, por exemplo, humor irritável ao invés de tristeza ou queda de rendimento acadêmico devido ao prejuízo da capacidade de pensar e se concentrar.

O objetivo do presente artigo é ressaltar a importância quanto à discussão da Depressão Infantil no Brasil, por ser uma doença que engloba fatores sociais, psicológicos e familiares, sendo sua discussão de extrema relevância para a melhor compreensão do ser humano em seu contexto biopsicossocial, além de esclarecer dúvidas que ainda possam existir sobre o assunto.

2. MATERIAIS E METODOS

O presente trabalho apresenta uma revisão da literatura a respeito da Depressão Infantil no Brasil. A busca foi realizada nas bases de dados Pubmed, Scielo e Google Acadêmico, entre os anos de 1989 e 2020, em português e

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.44_abstract_ERTHAL.pdf

inglês, por meio dos seguintes descritores: “depressão infantil”, “sintomas de depressão” e “tratamento da depressão infantil” combinados entre si.

Foram utilizados também livros-textos, considerando o valor informativo do material, dados do Ministério da Saúde e Organização Mundial da Saúde (OMS) além de artigos-chave selecionados a partir de citações em outros artigos.

A partir da análise dos dados encontrados, foram selecionados vinte e dois títulos que apresentam relação direta com o atual trabalho. Para essa seleção foram levados em conta trabalhos desde o início dos estudos sobre o tema até os dias atuais devido à relevância de seu entendimento por ser um assunto ainda tão pouco explorado. Outros artigos encontrados a partir dos descritores foram excluídos por abordarem assuntos isolados ou muito específicos que fogem ao foco do artigo em questão.

3. RESULTADOS E DISCUSSÃO:

Table 1. *Resultados da pesquisa*

	Bases de dados (número de títulos)		
Palavra- chave			
“Depressão infantil”	04	76.400	139
“Sintomas da depressão infantil”	12	176.000	1.286
“Tratamento da depressão infantil”	0	56.000	14

Table 2. *Critérios de seleção da pesquisa*

Trabalhos encontrados (total)	**Trabalhos descartados**	**Trabalhos selecionados**
309.850	309.828	22

Dentre os artigos, dois foram selecionados na base de dados Pubmed, oito no Google Acadêmico e cinco no Scielo. Além desses, foram selecionados quatro livros-textos, um material eletrônico disponível na internet e dois dados de autoria corporativa. Em caráter de suas relevâncias acerca do assunto, foram selecionados e incluídos como referência do atual artigo.

No Brasil ainda existem poucos estudos a respeito da Depressão Infantil. Uma pesquisa realizada por Hallak (2001) com 602 escolares na faixa etária de sete a doze anos de uma escola pública em Ribeirão Preto – SP revelou que 6% das crianças apresentavam depressão quando avaliadas pelo Inventário de Depressão Infantil (CDI) e 3% quando utilizada a Escala de Sintomatologia Depressiva para professores (ESDM). Independentemente da idade, a prevalência da doença foi significativamente maior em meninas.

Em comparação, um estudo realizado na Paraíba por Barbosa e Gaião (2001) evidenciou que 22% das 807 crianças na faixa etária de sete a dezessete anos avaliadas apresentavam sintomas depressivos, principalmente entre treze e catorze anos. Ainda a fim de analisar as características psicométricas da escala para avaliação de depressão em crianças (CDRS-R), os mesmos autores observaram 344 crianças entre onze e treze anos, em que foi registrado uma prevalência de 0,9% de depressão maior e 3,2% de distimia.

Apesar de não haver diferenciação no diagnóstico de depressão infantil e depressão do adulto de acordo com o DSM (2014), é preciso ficar atento quanto às manifestações atípicas dos sintomas na criança. Isso ocorre devido a variações de idade e de fase do desenvolvimento em que cada uma se encontra. Dessa forma, alguns autores sugerem o uso do termo “depressão mascarada” para caracterizar a doença quando se apresenta em crianças, ou seja, ela existe, mas é mascarada por outros problemas comportamentais (DSM, 2014; Dilillo, *et al.*, 2015).

A depressão infantil pode se apresentar com sintomas de melancolia, baixa autoestima, pessimismo, isolamento social, sentimento de rejeição, baixa energia para realizar atividades físicas e de lazer, cansaço, dificuldade para iniciar tarefas, atenção e concentração reduzidas, irritabilidade ou agressividade, medo inexplicado, transtornos alimentares, transtornos de sono, dor de cabeça, indigestão, ideação ou tentativas suicidas (White, 1989; Seligman, 1992).

A taxa de suicídio infantil ainda é pequena quando comparada à idade adulta (Reynolds & Mazza, 1994). É mais prevalente em meninos até os doze anos e, a partir desta idade, se torna

mais frequente em meninas (Dilillo, *et al.*, 2015; Rossi e Medeiros, 2020).

A grande questão a cerca da depressão infantil está no fato de que as famílias ainda têm muita dificuldade em identificar o distúrbio na criança, principalmente devido a sua apresentação muitas vezes atípica. Estudos revelam que o maior obstáculo está em entender que as mudanças comportamentais demonstradas pela criança possam fazer parte de um quadro depressivo e aceitar que as mesmas podem ficar deprimidas (Nakamura e Santos, 2007).

Muitas vezes a doença só é percebida pelos familiares quando as atitudes e comportamentos dessas crianças já se destacam o suficiente para que chamem atenção dos adultos, dessa forma, seu diagnóstico precoce é atrasado, dificultando a resolução do caso (Nakamura e Santos, 2007).

Após o diagnóstico é importante que rapidamente a criança seja avaliada e o tipo de tratamento adequado seja definido. Inicialmente é necessário definir a origem da depressão, o porquê dela estar ocorrendo (Lima, 2004).

Para a escolha do tratamento correto é importante realizar o exame do estado mental da criança e ainda levar em conta a idade, duração do transtorno, sua gravidade, cronicidade, questões contextuais e grau de comprometimento psicossocial (Maj e Sartorius, 2005).

Na maior parte das vezes o tratamento mais indicado para o transtorno é psicoterapia que envolva tanto a família como a escola. Nos casos de maior gravidade, em que seja necessário um resultado mais imediato e os que não são resolvidos com psicoterapia deve ser empregado o uso de terapia medicamentosa (Sigolo, 2008; Miranda, *et al.*, 2013).

4. CONCLUSÃO:

A partir dos dados analisados, verifica-se a extrema importância de existir o debate sobre o assunto de forma preventiva. A cada ano estudos mostram aumento no número de diagnósticos de depressão infantil e tentativas de suicídio entre crianças.

Doenças que ainda são tratadas como “tabu” pela sociedade, como a depressão infantil, envolvem desinformação e desconhecimento, dificultando dessa forma a detecção do diagnóstico, procura de tratamento e, inclusive, aderência ao mesmo.

Normalizar esse tipo de discussão amplia o acesso a informações a cerca da doença, possibilitando a identificação dos acometidos e, consequentemente, melhorando a qualidade de vida tanto da criança como de seus familiares. Além disso, ainda permite a redução do número de casos com desfecho negativo, sendo o suicídio o mais grave.

6. REFERÊNCIAS:

1. *AMERICAN PSYCHIATRIC ASSOCIATION DSM-5 ®*. (2014). http://www.niip.com.br/wp-content/uploads/2018/06/Manual-Diagnosico-e-Estatistico-de-Transtornos-Mentais-DSM-5-1-pdf.pdf

2. Bandim, J. M., Sougey, E. B., and Carvalho, T. F. R. de. (1995). Depressão em crianças: características demográficas e sintomatologia. [Review of *Depressão em crianças: características demográficas e sintomatologia.*]. *Jornal Brasileiro de Psiquiatria*, *1*(44), 27–32. Index Psicologia - Periódicos.

3. Barbosa G.A., Gaião A. A. (2001). *Apontamentos em Psicopatologia infantil*. *João Pessoa: Ideia*.

4. Cruvinel, M., and Boruchovitch, E. (2003). Depressão infantil: uma contribuição para a prática educacional. *Psicologia Escolar E Educacional*, *7*(1), 77–84. https://doi.org/10.1590/s1413-85572003000100008

5. Dilillo, D., Mauri, S., Mantegazza, C., Fabiano, V., Mameli, C., and Zuccotti, G. V. (2015). Suicide in pediatrics: epidemiology, risk factors, warning signs and the role of the pediatrician in detecting them. *Italian journal of pediatrics*, *41*(1), 1-8.

6. Hallak, L. R. L. (2001). *Estimativa da prevalência de sintomas depressivos em escolares da rede pública de Ribeirão Preto*. Dissertação de Mestrado, Faculdade de Medicina de Ribeirão Preto da Universidade de São Paulo.

7. Lima, D. (2004). Depressão e doença bipolar na infância e adolescência. *Jornal de Pediatria*, *80*(2), 11-20.

8. Maj, M., Sartorius, N (2005). *Transtornos depressivos*. Porto Alegre Artmed.

9. Miranda, M. V., Firmo, W. D. C. A., de Castro, N. G., Alves, L. P. L., Dias, C. N., Rêgo, M. M., e Dias, R. S. (2013). Depressão infantil: aspectos gerais, diagnóstico e tratamento. *Cadernos de Pesquisa*, *20*(3), 101-111.

10. Nakamura, E., Santos, J. Q. D. (2007). Depressão infantil: abordagem antropológica. *Revista de saúde pública*, *41*, 53-60.

11. Organização Mundial da Saúde (2007). *Depressão: o que você precisa saber.* Recuperado em 09 de fevereiro de 2022, de https://www.paho.org/pt/topicos/depressao

12. Reynolds WM, Mazza JJ (1994). *Suicide and Suicidal Behaviors in Children and Adolescents In: Reynolds WM. Handbook of Depression in Children and Adolescents. New York: Plenum Pres.*

13. Rossi, C., Medeiros, I. S. (2020). SUICÍDIO INFANTIL: QUANDO A BRINCADEIRA É FATAL. *Revista Inova Saúde*, *10*(1), 56-69.

14. Seligman, M. E. P. (1992). *Aprenda a ser otimista*. Record.

15. SIGOLO A. M. (2008). Depressão infantil. Monografia [Especialização em Psicopedagogia) - Universidade Tuiuti do Paraná.

16. White, J. L. (1989). *The troubled adolescent*. Pergamon Press.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

DEPRESSÃO INFANTIL NO BRASIL – UMA REVISÃO DA LITERATURA

Luísa Canto Erthal
Universidade de Vassouras, Pró-reitoria de ciências médicas , Faculdade de Medicina – Brasil.

Guilherme Felipe Dutra Silva
Universidade de Vassouras, Pró-reitoria de ciências médicas , Faculdade de Medicina – Brasil.

Aline Trovão Queiroz
Universidade de Vassouras, Pró-reitoria de ciências médicas , Faculdade de Medicina – Brasil.

Fevereiro/2022

INTRODUÇÃO

SBJChem Conference 2021

A depressão infantil é um transtorno de humor muito prevalente na sociedade atual. Seu debate começou a se tornar relevante a partir dos anos 60 e, apesar de não haver dúvidas quanto a sua existência, o assunto ainda é muito pouco discutido.

- Tristeza contínua e perda de interesse em realizar atividades que antes eram consideradas prazerosas junto a uma impossibilidade de realizar atividades diárias por, pelo menos, duas semanas.
- 3ª maior causa de incapacidade
- Humor irritável, queda de rendimento acadêmico devido ao prejuízo da capacidade de pensar e se concentrar.
- Melhor diagnóstico através de adaptações dos critérios de Depressão do adulto.

OBJETIVOS

SBJChem Conference 2021

Demonstrar a relevância da discussão sobre Depressão Infantil no Brasil, por ser uma doença cada vez mais prevalente na sociedade que engloba fatores sociais, psicológicos e familiares. Possibilitar uma melhor compreensão do ser humano em seu contexto biopsicossocial para que o diagnóstico seja feito de maneira correta e evitar desfechos negativos como o suicídio.

METODOLOGIA

SBJChem Conference 2021

Foi realizada uma revisão da literatura a respeito da Depressão Infantil no Brasil. A busca foi feita nas bases de dados Pubmed, Scielo e Google Acadêmico, entre os anos de 1989 e 2020, em português e inglês, por meio dos seguintes descritores: “depressão infantil”, “sintomas de depressão” e “tratamento da depressão infantil” combinados entre si.

Foram utilizados também livros-textos, considerando o valor informativo do material, dados do Ministério da Saúde e Organização Mundial da Saúde (OMS) além de artigos-chave selecionados a partir de citações em outros artigos.

A partir da análise dos dados encontrados, foram selecionados vinte e dois títulos que apresentam relação direta com o atual trabalho. Para essa seleção foram levados em conta trabalhos desde o início dos estudos sobre o tema até os dias atuais devido à relevância de seu entendimento por ser um assunto ainda tão pouco explorado. Outros artigos encontrados a partir dos descritores foram excluídos por abordarem assuntos isolados ou muito específicos que fogem ao foco do artigo em questão.

RESULTADOS E DISCUSSÃO

SBJChem Conference 2021

- No Brasil meninas e crianças entre 13 e 14anos são as mais acometidas pela doença;
- A depressão infantil pode se apresentar com sintomas de melancolia, baixa autoestima, pessimismo, isolamento social, sentimento de rejeição, baixa energia para realizar atividades físicas e de lazer, cansaço, dificuldade para iniciar tarefas, atenção e concentração reduzidas, irritabilidade ou agressividade, medo inexplicado, transtornos alimentares, transtornos de sono, dor de cabeça, indigestão, ideação ou tentativas suicidas;
- Tentativas de suicídio são mais prevalente em meninos até os doze anos e, a partir desta idade, se torna mais frequente em meninas;
- As famílias ainda apresentam grande dificuldade em identificar o distúrbio na criança, sendo o maior obstáculo entender e aceitar que as mudanças comportamentais possam fazer parte de um quadro depressivo.
- A escolha do tratamento correto deve levar em conta a idade, duração do transtorno, sua gravidade, cronicidade, questões contextuais e grau de comprometimento psicossocial.

CONCLUSÃO

SBJChem Conference 2021

- O debate sobre depressão infantil é uma forma de prevenção.
- Doenças que ainda são tratadas como “tabu” pela sociedade, como a depressão infantil, envolvem desinformação e desconhecimento, dificultando seu diagnóstico, procura de tratamento e, inclusive, aderência ao mesmo.
- Normalizar esse tipo de discussão amplia o acesso a informações a cerca da doença, possibilitando a identificação dos acometidos e, consequentemente, melhorando a qualidade de vida tanto da criança como de seus familiares.
- A discussão leva a redução do número de casos com desfecho negativo, sendo o suicídio o mais grave.

REFERÊNCIAS

SBJChem Conference 2021

1. AMERICAN PSYCHIATRIC ASSOCIATION DSM-5 ®. (2014). http://www.niip.com.br/wp-content/uploads/2018/06/Manual-Diagnosico-e-Estatistico-de-Transtornos-Mentais-DSM-5-1-pdf.pdf
2. Bandim, J. M., Sougey, E. B., & Carvalho, T. F. R. de. (1995). Depressão em crianças: características demográficas e sintomatologia. [Review of *Depressão em crianças: características demográficas e sintomatologia.*]. *Jornal Brasileiro de Psiquiatria*, *1*(44), 27–32. Index Psicologia - Periódicos.
3. Cruvinel M, Boruchovitch, E (2009). *Sintomas de depressão infantil e ambiente familiar. Rev Psicol em Pesq*, 3(1): 87-100.
4. Miranda, M. V., Firmo, W. D. C. A., de Castro, N. G., Alves, L. P. L., Dias, C. N., Rêgo, M. M., ... & Dias, R. S. (2013). Depressão infantil: aspectos gerais, diagnóstico e tratamento. *Cadernos de Pesquisa*, *20*(3), 101-111.
5. Nakamura, E., & Santos, J. Q. D. (2007). Depressão infantil: abordagem antropológica. *Revista de saúde pública*, *41*, 53-60.
6. Weersing, V. R., Jeffreys, M., Do, M.-C. T., Schwartz, K. T. G., & Bolano, C. (2017). Evidence Base Update of Psychosocial Treatments for Child and Adolescent Depression. *Journal of Clinical Child and Adolescent Psychology : The Official Journal for the Society of Clinical Child and Adolescent Psychology, American Psychological Association, Division 53*, *46*(1), 11–43. https://doi.org/10.1080/15374416.2016.1220310

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

COMPARATIVE STUDY OF DEATHS FROM ILL-DEFINED AND UNKNOWN CAUSES BEFORE AND DURING THE SARSCOV-2 PANDEMIC

SOUZA, Andreza Rozendo[1*]; SANTOS, Marcus Asevedo[1]; QUEIROZ, Aline Trovão[1];

[1] Universidade de Vassouras, Pró-reitoria de Ciências médicas, Faculdade de Medicina. Brasil.

** Autor correspondente*
e-mail:rozendo.andrezal@gmail.com

Received 12 January 2022; received in revised form 30 January 2022; accepted 08 February 2022

ABSTRACT

Documenting the cause of death is important to know the health situation of the population. After the beginning of the pandemic caused by the new coronavirus, institutional protocols were created to minimize the spread of the virus, including changes in the handling of bodies. The main objective of this study was to identify whether there was a change in the number of deaths from unknown to ill-defined causes comparing two years before the pandemic and two years during the pandemic in Brazil and the state of Rio de Janeiro and to determine the main epidemiological characteristics. A documentary, retrospective, and historical study were carried out based on data collection in the mortality information system from 2018 to 2021. The period was divided into two phases to make comparisons, two years before and two during the pandemic. Mortality rate, sex, color, and age data were included. Before the pandemic, there was a lower mortality rate from an ill-defined or unknown cause in Brazil and the State of Rio de Janeiro. In addition to the problems faced before, the changes caused by the pandemic may have influenced the rise in death notifications from this cause. The age group most affected in the two biennia analyzed was over 80. During the pandemic, men were more affected than women, browns in Brazil and whites in Rio de Janeiro had the highest number of notifications. In general, during the pandemic, it was shown that there was an increase in the number of people who died from unknown or poorly defined causes, especially the elderly. Additional studies need to be performed for definitive elucidation. In addition, it is necessary to identify better the conditions that caused the increase in the number of deaths from unknown or poorly defined causes.

Keywords: *Mortality, new coronavirus, cause of death*

1. INTRODUÇÃO

A determinação da causa de morte é importante instrumento utilizado para conhecer a situação de saúde da população e com isso determiner ações visando a melhoria das condições de saúde pública. Para tanto, as declarações de óbitos devem ser adequadamente preenchidas e com informações precisas. (Ministério da Saúde, 2006). Além disso é instrumento legal e parte integrante da assintencia médica (Conselho Federal de Medicina, 2005).

Após o início da pandemia da doença causada pelo novo coronavírus, declarada pela organização mundial de saúde em 11 de março de 2020 (Organização Mundial de Saúde, 2020) diversos protocolos e fluxos foram adotados pelas instituições de saúde para salvarguardar a saúde da população e dos profissionais de saúde. (Agência nacional de vigilância sanitária, 2021). Incluindo mudança no manejo de corpos, impactanto nos serviços de verificações de óbitos e institutos médicos legais do país (Ministério da saúde, 2020).

Neste contexto é de se inferir que que haja mudanças nos perfis de causa de óbitos que podem impactar na análise de dados referente a saúde populacional e consequente tomada de decisão quanto a políticas de saúde pública. Nesse sentido este trabalho visa determinar se houve alteração no número de mortes por causa mal definida e desconhecida durante a pandemia comparando os dois anos antecedentes da pandemia (2018 e 1019) e nos dois anos de pandemia (2020 e 2021) no estado do Rio de janeiro. Além de identificar as principais características epidemiológicas dos pacientes que morreram por esta causa.

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.19_abstract_SOUZA.pdf

2. MATERIAIS E METODOS

Foi realizado um estudo documental, retrospectivo e histórico, apartir da coleta de dados de causas de mortalidade no período de 2018 a 2021, sendo os dois últimos anos durante a pandemia do novo coronavirus. Os dados epidemiológicos foram obtidos a partir do Sistema de informações sobre mortalidade, do painel de monitoramento de mortalidade, que é extraído da declaração de óbito, documento preenchido por pelo médico assitente, pelo serviço de verificação de óbito ou mesmo pelo médico legista do instituto médico legal dependendo da causa da morte.

O período foi dividido em duas fases de análise para que fosse possível realizar comparações entre os subperíodos temporais, dois anos antes da pandemia e nos dois anos durante a pandemia. Os seguimentos foram denominados como “biênio pré-pandemia” representando os anos de 2018 e 2019 e “biênio durante a pandemia” representando os anos de 2020 e 2021.

Foram incluídos dados referentes a taxa de mortalidade de causa mal definida e desconhecida, sexo, raça/cor e grupo etário ocorridos no Brasil e na unidade federativa do Rio de Janeiro. E o local de registro selecionado foi óbitos por ocorrência.

3. RESULTADOS E DISCUSSÃO:

No presente estudo constata-se tanto no brasil como no Estado do Rio de Janeiro que houve um aumento significativo do número de notificação de óbitos por causa mal definida e desconhecida (Tabela 1). Além dos problemas ja enfredados anteriormente a pandemia como a falta de capacitação de vários profissionais de saúde, o não conhecimento da importância destas informações, troca frequente dos técnicos municipais responsáveis pelos sistemas, preenchimento inadequado e/ou incompleto dos campos, dentre outros (Minto *et al*, 2017) as mudanças acarretadas pela pandemia, além da pouca informação a cerca da doença podem ter sido influencia para a alta das notificações de morte por esta causa.

Tanto no Brasil quanto no Rio de Janeiro, mais homens morreram por causa desconhecida ou mal determinanda tanto no período pré-pandemia quanto no período durante a pandemia, guardando uma proporção semelhante aproximadademente 40 % de mulheres e 59 % de homens (Tabela 2). Tal proporção é semelhante, mas não igual ao total de mortes geral que no Brasil é de 44,5% para as mulheres e 55,5 para os homens e no Estado do Rio é de 48,1% para o sexo feminino e 51,7% para o masculino (secretaria de vigilância em Saúde, 2022).

No que diz respeito a faixa etária, a mais atingida por causa desconhecida ou mal definida são os idosos, sobre tudo os maiores de 80 anos, com aumento durante a pandemia. No Brasil houveram 34.519 no biênio pré-pandemia e 47.105 durante a pandemia, enquando no Rio de janeiro houve 5.200 pré-pandemia e 7.285 durante (Tabela 3).

Em idades avançadas nenhuma causa de morte pode parecer óbvia, especialmente quando várias doenças de longa duração estão presentes na pessoa idosa, além do fenômeno progressivo de declínio das funções fisiológicas, especialmente nessa fase da vida. O verdadeiro motivo do óbito, em parte considerável da população idosa, seria o próprio envelhecimento, velhice, senilidade ou demência senil, senescência, todos esses termos aceitos e incluídos como senilidade no código internacional de doenças (Mathias *et al*., 2005).

4. CONCLUSÕES:

Os dados epidemiológicos dos períodos analizados demonstram que em geral, durante a pandemia, houve um crescimento do número de pessoas que morreram por causas desconhecidas ou mal definidas, sobre tudo os idosos. Investigar e diminuir o número de óbitos por esta causa é vital para se traçar politicas públicas que melhorem a saúde da população. A medida que conhecemos as causas de óbito, conseguimos previnir e tartar antes que culminem na morte.

Considerando os resultados que demonstraram uma maior ocorrencia durante a pandemia sugere-se que investimentos nas áreas de investigação epidemiológica e atenção a saúde necessitam ser imediantos, visto que ainda estamos na vigência da pandemia. Além, da testagem em massa da população, pois parte das mortes podem ter ocorrido pela COVID-19 e possivelmente não foi identificada.

Estudos adicionais precisam ser realizados para uma elucidação definitiva, pois os os números coletados dos anos de 2020 e 2021 são preliminpares. Além de ser preciso identificar melhor o perfil epidemiológico e as condições que causaram o aumento do número de óbitos por causa desconhecida ou mal definida.

6. REFERENCIAS:

1. Brasil. Agencia nacional de vigilância Sanitária (2021) Nota técnica gvims/ggtes/anvisa nº 04/2020 Orientações para serviços de saúde: medidas de prevenção e controle que devem ser adotadas durante a assistência aos casos suspeitos ou confirmados de infecção pelo novo coronavírus (sars-cov-2) – atualizada em 09/09/2021. Brasília, DF. Recuperado em 01 de dezembro de 2021 de:
2. Brasil. Ministério da Saúde (2006). Declaração de óbito : documento necessário e importante. Recuperado em 01 de dezembro de 2021 de https://bvsms.saude.gov.br/bvs/publicacoes/declaracao_de_obito_final.pdf
3. Brasil, Ministério da Saúde (2020) Manejo de corpos no contexto da doença causada pelo coronavírus Sars-CoV-2 Covid-19. Brasília, DF. Recuperado em 3 de janeiro de 2022 de: https://www.gov.br/saude/pt-br/coronavirus/publicacoes-tecnicas/recomendacoes/manejo-de-corpos-no-contexto-da-covid-19#:~:text=Durante%20os%20cuidados%20com%20corpos,no%20item%2010%20desta%20publica%C3%A7%C3%A3o.
4. Brasil. Ministério da Saúde. Secretaria de Vigilância em Saúde (2022). Boletim Epidemiológico Especial. Recuperado em 8 de janeiro de 2022 de: https://www.gov.br/saude/pt-br/centrais-de-conteudo/publicacoes/boletins/boletins-epidemiologicos/covid-19/2022/boletim-epidemiologico-no-95-boletim-coe-coronavirus.pdf.
5. Conselho Federal de medicina (2005). RESOLUÇÃO CFM nº 1.779/2005. Recuperado em 21 de janeiro de 2022 de https://sistemas.cfm.org.br/normas/visualizar/resolucoes/BR/2005/1779.
6. Mathias, T. A. F., Jorge, M. H. P M., Laurenti, R., Aidar, T., (2005). Considerações sobre a qualidade de informações de mortalidade na população idosa residente no Município de Maringá, Estado do Paraná, Brasil, no período de 1979 a 1998. *Epidemiologia e Serviços de Saúde*, *14*(3), 159-169. https://dx.doi.org/10.5123/S1679-49742005000300004
7. Minto, C. M., Villela E. F. M., Paula, R. A. C., (2021) Desafios de Vigilância de Eventos Vitais no Estado de Saõ Paulo Durante a pandemia de COVID-19. Boletim Epidemiológico Paulista 18(208). Recuperado em 8 de janeiro de 2022 de : https://pesquisa.bvsalud.org/controlecancer/resource/pt/biblio-1248184?src=similardocs.
8. Organização Mundial da Saúde (2020) Coronavirus disease 2019 (COVID-19) Situation Report – 51. Recuperado em 15 de dezembro de 2021 de https://apps.who.int/iris/handle/10665/331475.

Tabela 1. *Número total de mortes por causa mal definida e desconhecida.*

Período	Brasil	Rio de janeiro
Biênio pré-pandemia	118.040	19.447
Biênio durante a pandemia	154.071	25.715

Referencia: Painel de Monitoramento da Mortalidade. **Secretaria de Vigilânci em Saúde em 23 de janeiro de 2022**

Tabela 2. *Número de mortes por causa mal definida e desconhecida de acordo com sexo*

Variável	Biênio pré-pandemia	Biênio durante pandemia
Brasil		
Sexo feminino	47.436	62.269
Sexo masculino	70.383	91.548
Rio de Janeiro		
Sexo feminino	8.599	11.584
Sexo masculino	10.790	14023

Referencia: Painel de Monitoramento da Mortalidade. **Secretaria de Vigilânci em Saúde em 23 de janeiro de 2022**

Tabela 3. *Número de mortes por causa mal definida e desconhecida de acordo com a faixa etaria*

Variável	Biênio pré-pandemia	Biênio durante a pandemia
Brasil		
<1 ano	1.561	1.405
1 a 4	595	466
5 a 9	270	219
10 a 14	343	353
15 a 19	1.322	1.327
20 a 29	4.104	4.952
30 a 39	6.559	8.015
40 a 49	10.086	13.422
50 a 59	15.715	20.293
60 a 69	20.303	26.761
70 a 79	21.710	28.738
>80	34.519	47.105
Rio de Janeiro		
<1 ano	114	82
1 a 4	46	33
5 a 9	23	13
10 a 14	28	32
15 a 19	175	176
20 a 29	549	702
30 a 39	757	979
40 a 49	1.343	1837
50 a 59	2.741	3.527
60 a 69	4.054	5.305
70 a 79	4.133	5.378
>80	5.200	7.285

Referencia: Painel de Monitoramento da Mortalidade. **Secretaria de Vigilância em Saúde em 23 de janeiro de 2022**

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ESTUDO COMPARATIVO DE MORTES POR CAUSA MAL DEFINIDA E DESCONHECIDA ANTES E DURANTE A PANDEMIA CAUSADA POR SARSCOV-2

Andreza Rozendo de Souza
Universidade de Vassouras, Pró-reitoria de ciências médicas , Faculdade de Medicina – Brasil.

Marcus Asevedo dos Santos
Universidade de Vassouras, Pró-reitoria de ciências médicas , Faculdade de Medicina – Brasil.

Aline Trovão Queiroz
Universidade de Vassouras, Pró-reitoria de ciências médicas , Faculdade de Medicina – Brasil.

Janeiro/2022

INTRODUÇÃO

SBJChem Conference 2021

Documentar a causa de morte é importante para conhecer a situação de saúde da população. Após o início da pandemia causada pelo novo coronavírus protocolos institucionais foram criados para minimizar a disseminação do vírus, incluindo mudança no manejo de corpos.

- Todos os pacientes contaminados são potencias transmissores;
- Intervenções como distanciamento social são efetivos;
- Criação de protocolos para conter a disseminação do vírus;
- Mudança no manejo de corpos;

OBJETIVOS

SBJChem Conference 2021

O principal objetivo deste estudo foi identificar se houve alteração no número de mortes de causa desconhecida ao mal definida comparando dois anos antes da pandemia e dois anos durante a pandemia no Brasil e do estado do Rio de Janeiro e determiner principais características epidemiológicas.

METODOLOGIA

SBJChem Conference 2021

Foi realizado um estudo documental, retrospectivo e histórico, apartir da coleta de dados no sistema de informações sobre mortalidde no período de 2018 a 2021. O período foi dividido em duas fases para realizar comparações, dois anos antes e dois durante a pandemia. Foram incluídos dados de taxa de mortalidade, sexo, cor e idade

- Fonte de Dados foi o Sistema de informações sobre mortalide, extraido do Painel de Monitoramento de mortalidade

RESULTADOS E DISCUSSÃO

SBJChem Conference 2021

- Maior mortalidade por causa mal definida ou desconhecida no Brasil e no Estado do Rio de Janeiro durante a pandemia

Além dos problemas já enfrentados antes, as mudanças acarretadas pela pandemia podem ter influenciado a alta das notificações de morte por esta causa.

- A faixa etária mais acometida nos dois biênios analisados foi maior de 80 anos, com aumento durante a pandemia
- Mulheres foram mais afetadas que homens, os pardos no Brasil e os brancos no Rio de Janeiro teve maior número de notificações.

Período	Brasil	Rio de janeiro
Biênio pré-pandemia	118.040	19.447
Biênio durante a pandemia	154.071	25.715

CONCLUSÃO

SBJChem Conference 2021

Foi demonstrado em geral, durante a pandemia, que houve um crescimento do número de pessoas que morreram por causas desconhecidas ou mal definidas, sobre tudo os idosos. Estudos adicionais precisam ser realizados para elucidação definitiva. Além de ser preciso identificar melhor as condições que causaram o aumento do número de óbitos por causa desconhecida ou mal definida.

REFERÊNCIAS

SBJChem Conference 2021

1. Brasil. Agencia nacional de vigilância Sanitária (2021) Nota técnica gvims/ggtes/anvisa nº 04/2020 Orientações para serviços de saúde: medidas de prevenção e controle que devem ser adotadas durante a assistência aos casos suspeitos ou confirmados de infecção pelo novo coronavírus (sars-cov-2) – atualizada em 09/09/2021. Brasília, DF. Recuperado em 01 de dezembro de 2021 de www.gov.br/anvisa/pt-br/centraisdeconteudo/publicacoes/servicosdesaude/notas-tecnicas/nota-tecnica-gvims_ggtes_anvisa-04_2020-25-02-para-o-site.pdf.

2. Brasil, Ministério da Saúde (2020) Manejo de corpos no contexto da doença causada pelo coronavírus Sars-CoV-2 Covid-19. Brasília, DF. Recuperado em 3 de janeiro de 2022 de: https://www.gov.br/saude/pt-br/coronavirus/publicacoes-tecnicas/recomendacoes/manejo-de-corpos-no-contexto-da-covid-19#:~:text=Durante%20os%20cuidados%20com%20corpos,no%20item%2010%20desta%20publica%C3%A7%C3%A3o.
3. Brasil. Ministério da Saúde. Secretaria de Vigilância em Saúde (2022). Boletim Epidemiológico Especial. Recuperado em 8 de janeiro de 2022 de: https://www.gov.br/saude/pt-br/centrais-de-conteudo/publicacoes/boletins/boletins-epidemiologicos/covid-19/2022/boletim-epidemiologico-no-95-boletim-coe-coronavirus.pdf.
4. Brasil. Ministério da Saúde. Secretaria de Vigilância em Saúde (2022). Boletim Epidemiológico Especial. Recuperado em 8 de janeiro de 2022 de: https://www.gov.br/saude/pt-br/centrais-de-conteudo/publicacoes/boletins/boletins-epidemiologicos/covid-19/2022/boletim-epidemiologico-no-95-boletim-coe-coronavirus.pdf.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

COMPARISON OF TWO STAINING METHODS FOR ANODIZING IN ALLOY 6063 ALUMINUM PROFILES

PESSUTTO, Ana Carla [1*]; JONKO, Eliena [2];

[1]Universidade de Caxias do Sul, Engenharia Química

[2] Universidade de Caxias do Sul, Laboratório de Corrosão e Proteção Superficial

** Correspondence author*
e-mail: acpessutto1@gmail.com

Received 02 October 2021; received in revised form 5 November 2021; accepted 14 November 2021

ABSTRACT

Aluminum stands out for being a light, corrosion-resistant, and recyclable metal, achieving wide coverage in the market. When incorporated into alloying elements, it is possible to acquire other desirable characteristics. Alloy 6063, intended for architectural purposes, has aesthetic, structural, and strength functions. This study aims to compare two different staining methods on the surface of anodized profiles of aluminum alloy 6063. Anodized finishing is performed through an electrolytic process using sulfuric acid as an electrolyte to change the surface layer of the material, ensuring a more resistant aluminum oxide film than that formed naturally. For decorative purposes, the anodic film coloration can be performed by several methodologies, including, in this case, the coloration by organic adsorption, with the use of aniline, and the electrolytic coloration, composed of tin sulfate salts, both for obtaining the black color. To compare, neutral saline mist tests, scanning electron microscopy analysis, determination of the anodic layer thickness, and immersion tests with 3.5 percent sodium chloride for 1000 hours. The results obtained highlight that both were shown to be resistant to corrosion due to the fact that they do not present corrosion points when exposed to the neutral saline mist test for 600 hours. In the immersion tests, both remained resistant to sodium chloride. Because both methodologies present satisfactory results in all tests, the quality of the applied stains is ensured, and it is found that they are equivalent when the parameters discussed are used.

Keywords: *Aluminium alloys. Anodizing. Corrosion resistance. Coloring.*

1. INTRODUÇÃO

O mercado do alumínio (Al) em escala industrial no Brasil, de acordo com informações da Revista Alumínio (2019), registrou aumento no consumo de produtos fabricados de Al em cerca de 10 % do ano de 2017 para o ano de 2018, sendo este oriundo de matéria-prima virgem e de reciclagem, com tonelagem de 1 milhão e 383 mil.

Levando-se em consideração as questões ambientais, em alta no atual cenário mundial, é de suma importância avaliar os impactos causados durante a produção e a utilização dos metais. Dentre estes, o Al tem destaque por ser um metal leve e versátil, além de resistente à corrosão e reciclável, obtendo ampla aplicação no mercado.

Em busca de materiais com durabilidade, resistência à corrosão e de embelezamento da superfície, podem ser realizados, embasado na engenharia de superfície, tratamentos que envolvem as mudanças das propriedades visando obter estas características.

A anodização é um dos tipos tratamentos de superfície mais aplicados sobre peças de Al. O processo é realizado com o intuito de formar uma fina camada de óxido de alumínio (Al_2O_3) que possibilita o aumento da vida útil do material, principalmente pelo fato de formar um filme cristalino, com poros de maior espessura, resistente à abrasão e à corrosão, proporcionando maior durabilidade aos meios que ficará exposto.

Devido à camada de óxido ser bastante porosa, a mesma pode vir a ser base para a aplicação de cores, quando o material for utilizado para fins decorativos. Há diferentes metodologias que podem propiciar cor ao material, sendo as mais frequentes a pôr imersão, através da adsorção de substâncias orgânicas com o uso de

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.03_abstract_Pessutto.pdf.

anilinas ou outros componentes; e a pôr coloração eletrolítica, com o auxílio de eletrólitos e de sais metálicos, havendo entre estes processos diferenciações na aparência e na durabilidade.

Com isso, verifica-se a necessidade de comparar estes dois métodos para colorir a camada anódica sobre perfis da liga de alumínio 6063, avaliando-se o desempenho da resistência que o material possui contra a corrosão em meios neutros e em meios agressivos, além da resistência às intempéries enquadrados em cada processo.

2. MATERIAIS E METOOS

2.1. Materiais

Os corpos de prova utilizados foram perfis extrudados de liga de Al 6063, com tratamento térmico de solubilização, têmpera e envelhecimento (T6), amplamente utilizado para perfis destinados à construção civil.

A primeira etapa do processo foi a coleta de perfis de 6 m de comprimento e a realização do jateamento mecânico com pequenas esferas de aço inox. O objetivo do jateamento, neste caso, remete à homogeneização da superfície, eliminando possíveis manchas e riscos.

Após, realizou-se o corte, com 20 cm de comprimento, e furos nas extremidades dos corpos de prova. Posteriormente foram enganchados com pequenos ganchos de alumínio, em bases de Al de liga 6063, para que o material pudesse receber a passagem de corrente elétrica durante o processo de anodização.

Os corpos de prova, tanto para a coloração eletrolítica, quando para a coloração por imersão passaram pelas etapas de limpeza, conforme apresentado no Quadro 1.

Quadro 1. *Etapas de limpeza*

Banho	Produto químico	Concentração (g/L)	Tempo (min)	Temperatura (ºC)
Desengraxe	Ácido sulfúrico	147	10	20
Fosqueamento	Hidróxido de sódio	65,33	5	5
	Alumínio	101,7		
Neutralizante	Ácido sulfúrico	147	10	30

Fonte: Os Autores

Na etapa seguinte, foi realizada a anodização para formar uma espessura de 20 µm, submetida as condições descritas no Quadro 2.

Quadro 2. *Condições do banho de anodização*

Produto químico	Concentração (g/L)	Tempo (min)	Temperatura (ºC)	Densidade de corrente (A/dm²)
Ácido sulfúrico	197,96	30	21	1,5
Alumínio	11,16			

Fonte: Os Autores

Neste tanque são necessários contatos de cobre na base superior, o que possibilita a condução da corrente elétrica ao material. Também estava composto por eletrodos da liga de Al 6063 nas laterais do tanque, posicionados verticalmente. Após todas as etapas apresentaddas, os corpos de prova passaram por enxagues.

A etapa seguinte tem por função colorir a camada anódica formada. Os estágios foram realizados de maneiras diferentes para os dois métodos de coloração aplicados.

Para a coloração eletrolítica, os corpos de prova foram submetidos as condições de acordo com o Quadro 3, para a obtenção da cor preta.

Quadro 3. *Características do banho de coloração eletrolítica*

Produto químico	Concentração (g/L)	Tempo (min)	Temperatura (ºC)	Densidade de corrente (A/dm²)
Ácido sulfúrico	20	12	24	0,8
Sulfato de estanho	10,81			

Fonte: Os Autores

Neste estágio, assim como no banho de anodização, contava-se com a presença de contatos de cobre, além de eletrodos de aço inox 316 posicionados na lateral do tanque. Para obter-se a coloração preta, o retificador possuia um programa com diferentes correntes, tempos e amplitudes de onda, para o depósito de estanho (Sn) na base do poro.

Em seguida, os corpos de prova foram direcionados para a selagem, conforme Quadro 4.

Quadro 4. *Caracterísiticas do banho de selagem a frio para coloração eletrolítica*

Produto químico	Concentração (ppm)	Tempo (min)	Temperatura (ºC)	pH
Níquel	1467,75	20	30	6,80
Flúor	700			

Fonte: Os Autores

Em paralelo, foi realizada a coloração por adsorção orgânica. Nesta, os corpos de prova

foram imersos em uma solução contendo anilina na cor preta, conforme Quadro 5.

Quadro 5. *Características banho de coloração por adsorção orgânica*

Produto químico	Marca	Concetração (g/L)	Tempo (min)	Temp. (ºC)	pH
Sanodal Preto Escuro H-BL	Clariant	10	30	57	5,6

Fonte: Os Autores

A anilina utilizada se destaca pela resistência à luz e ao calor, possuindo características para a exposição em áreas externas, direcionadas à fins arquitetônicos. Em seguida, passou-se para a selagem, abordada no Quadro 6.

Quadro 6. *Características selagem a frio para coloração por adsorção orgânica*

Produto químico	Concentração (ppm)	Tempo (min)	Temperatura (ºC)	pH
Níquel	1800	20	18	7,12
Flúor	300			

Fonte: Os Autores

Os corpos de prova de ambas as metodologias foram enxaguados e direcionados para uma estufa durante 30 min, a 75 ºC, com queima por GLP para a secagem do material.

2.2. Métodos

Os métodos de análise foram realizados a fim de obter-se um padrão comparativo entre as metodologias de coloração do filme anódico.

2.1.1. Microscopia eletrônica de varredura por emissão de campo (MEV/FEG)

Para a visualização da superfície a nível microscópico e a medição da espessura da camada anódica, foi realizado um ensaio através de um microscópio eletrônico de varredura por emissão de campo (MEV/FEG), realizado no Laboratório Central de Microscopia (LCMIC), da Universidade de Caxias do Sul.

2.1.2. Névoa Salina Neutra

O método consiste em manter os corpos de prova em uma câmara fechada que simula a atmosfera marinha, por base na norma ASTM B117 (2018), por meio de uma solução de cloreto de sódio (NaCl P.A.) a 5 %, com pH mantido em uma faixa de 6,5 a 7,2 e temperatura de 35 ºC (PERTILE; BEUX; BIRRIEL, 2018). O ensaio foi realizado no Laboratório de Corrosão e Proteção Superficial (LCOR), da UCS.

2.1.3. Ensaio de Imersão

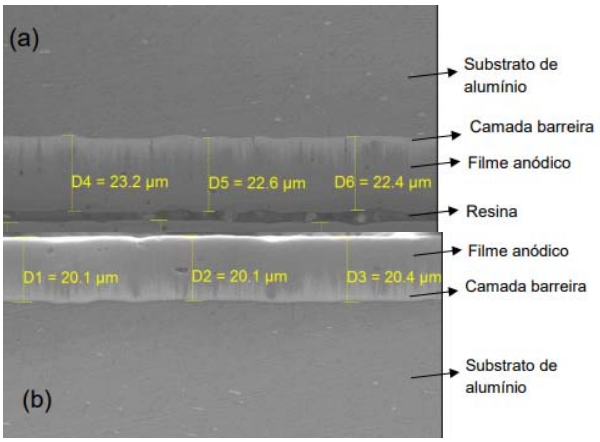
O ensaio de imersão foi baseado na norma ASTM G31-12a, com uma solução de NaOH 0,1 M, pelo período de 1.000 horas, em triplicata. Os principais efeitos que podem ser analisados a olho nu são a descoloração, mudança de brilho e pontos de corrosão. Também foi realizado um corte em forma de X em cada corpo de prova.

3. RESULTADOS E DISCUSSÕES:

3.1. Microscopia eletrônica de varredura por emissão de campo (MEV/FEG)

No corpo de prova para coloração por adsorsão orgânica, a média obtida da espessura do filme anódico é de 22,7 µm, conforme (a), na Figura 1. Já na coloração eletrolítica, a média de espessura é 20,2 µm, conforme (b), na Figura 1.

Figura 1. *Camada anódica obtida na coloração por adsorção orgânica*



Nota: Magnificação de 2.000x.
Fonte: A Autora (2020).

Observa-se, numericamente, que a camada anódica possui espessura uniforme em ambos os corpos de prova. Ressalta-se que há a presença de alguns picos e vales, que são formados devido à presença destes na própria camada do substrato do metal, tendo em vista que o filme Al_2O_3 se forma sobre esta superfície (COURROL; PRETO, 2011). Esta uniformidade se dá por diversos fatores do processo, dentre eles, a escolha do eletrólito, a temperatura e o tempo de imersão na solução eletrolítica.

3.2. *Névoa Salina Neutra*

Nos corpos de prova de coloração por adsorção orgânica, após 192 horas (h) de exposição, observou-se o surgimento de pequenas manchas em várias regiões da superfície. Posteriormente, a 504 horas, manchas maiores foram observadas sobre quase a totalidade da superfície dos corpos de prova.

Já para o ensaio com os corpos de prova de coloração eletrolítica, apenas no período de 192 horas foram visualizadas pequenas manchas sobre a superfície e mais nenhuma alteração foi visualizada a olho nu.

Ambas metodologias foram finalizados em 600 h de exposição e não houveram alterações após o exposto acima. De acordo com a QUALANOD (2020), para ensaios de névoa salina neutra mantem-se os corpos de prova pelo tempo máximo de 336 h e como resultado, não deve apresentar quaisquer pontos de corrosão. Sendo assim, os corpos de prova apresentaram resultados positivos, pois apenas foram visualizadas pequenas manchas, demonstrando que os óxidos formados na anodização foram protetivos contra a corrosão.

3.3. Ensaio de Imersão

Os corpos de prova foram observados em 48 h, 240 h, 408 h, 552 h e 1.000 h de imersão.

Para a coloração por adsorção orgânica, no tempo de imersão de 408 h, visualizou-se alguns pontos de corrosão na interseção realizada. Em 552 h estes pontos de corrosão aumentaram de tamanho, sendo visíveis apenas na interseção, estando a área superficial com aparência igual ao corpo de prova padrão. Em 1.000 h, o corpo de prova apresentou pontos de corrosão ainda mais sobressalentes. No restante da área superficial, nenhum ponto de corrosão foi visualizado a olho nu. Também não foram notadas alterações de cor e nem perda de brilho.

Na coloração eletrolítica, no período de 408 h visualizaram-se alguns pontos de corrosão na interseção. Após 552 h de imersão, estes pontos de corrosão aumentaram de tamanho. Ressalta-se que o restante da área superficial se manteve com aparência igual ao corpo de prova padrão não sendo notada nenhuma alteração de cor e nem de brilho. Em 1.000 h, os corpos de prova apresentaram pontos de corrosão ainda mais sobressalentes. No restante da área, não são visualizados pontos de corrosão, tampouco alteração de cor e perda de brilho.

O Al e suas ligas têm sua passividade destruída quando em contato com íons cloretos (Cl^-), sendo a corrosão mais frequente por pites, que ocorre em pontos ou áreas localizadas (GENTIL, 2017). É possível constatar que a área onde não houve interseção, não ocorreram pontos de corrosão, demonstrando a resistência do filme.

4. CONCLUSÔES:

A partir dos resultados obtidos, conclui-se:

a) Pode-se observar que os corpos de prova apresentaram filmes homogêneos;

b) Para o ensaio de névoa salina neutra, ambas as metodologias apresentaram resultados satisfatórios, o que não era esperado pela literatura;

c) Nos ensaios de imersão em solução de NaCl, não houve perda de coloração e a corrosão foi visível posteriormente a 336 h.

Verifica-se que a metodologia de coloração eletrolítica possui resistência à corrosão, se mantendo com coloração uniforme e boa aparência após ensaios realizados. A coloração por adsorção orgânica também apresentou as mesmas características, se atribuindo estes resultados à anilina testada, que possui modificação estrutural, fazendo com que a mesma resista aos ensaios, sem perder as propriedades. Desta forma, pode-se concluir que é possível equivaler as metodologias para coloração de acordo com os parâmetros testados.

5. REFERENCIAS:

1. REVISTA ALUMÍNIO. **Consumo de alumínio no Brasil cresce em 10% em 2018**. 25 abr. 2019. Disponível em: https://revistaaluminio.com.br/consumo-de-aluminio-no-brasil-cresce-10-em-2018/. Acesso em: 30 mar. 2020.
2. PERTILE, T. S.; BEUX, T. D.; BIRRIEL, E. J. In: INTERCORR. 38., São Paulo, 2018. **Anais** [...]. São Paulo: ABRACO. 2018. 9 p.
3. COURROL, L. C.; PRETO, A. O. **Óptica geométrica** [online]. 1. ed. São Paulo: Editora Unifesp, 2011. 168 p.
4. GENTIL, V. **Corrosão**. 6. ed. Rio de Janeiro: LTC, 2017. 360 p.
5. QUALANOD. **Diretivas para a Marca de Qualidade QUALANOD para Anodização do Alumínio Baseada em Ácido Sulfúrico**. Zurique, 2020.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

COMPARISON OF TWO STAINING METHODS FOR ANODIZATION IN ALLOY 6063 ALUMINIUM PROFILES

Ana Carla Pessutto
Universidade de Caxias do Sul, Chemical Engineering - Brazil.

Eliena Jonko
Universidade de Caxias do Sul, Corrosion Laboratory – Brazil.

March/2022

INTRODUCTION

SBJChem Conference 2021

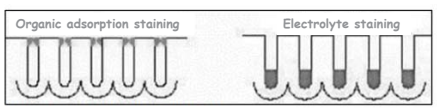
- Search for stronger and more durable materials based on surface treatment;
- Surface beautification through coloring;
- Compare electrolytic and organic adsorption staining.

BACKGROUND

SBJChem Conference 2021

- Accorging to the literature, organic adsorption staining tends to be less resistant when compared to electrolyte staining (AHMADI; NOROUZI; GANJALI, 2006; ASSOCIAÇÃO BRASILEIRA DA INDÚSTRIA QUÍMICA, 2011 apud VELOSO, 2012).

Figure 1 – Methods for coloring anodic film



Source: Adapted from Gazapo and Gea (1994).

AIM/OBJETIVE/PURPOSE

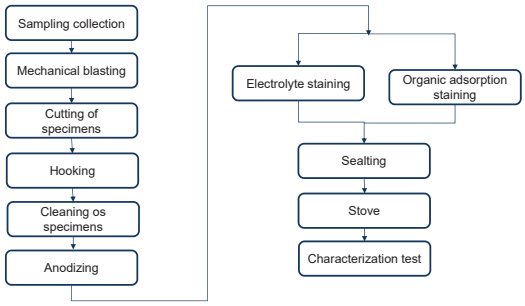
SBJChem Conference 2021

Main Goal

Compare performance with respect to corrosion resistance using two diferente methods of coloring anodic films on aluminum alloy 6063 specimens.

METHODOLOGY

SBJChem Conference 2021



METHODOLOGY

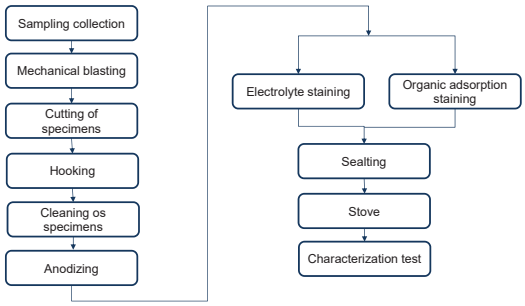
SBJChem Conference 2021

Figure 2 – Hooked parts to start anodizing process

Source: The authors (2020).

METHODOLOGY

SBJChem Conference 2021

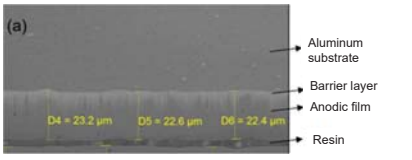


RESULTS AND DISCUSSION

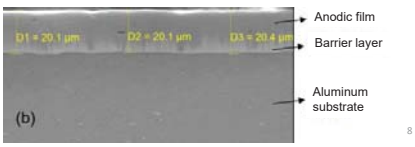
SBJChem Conference 2021

1. Field Emission Scanning Electron Microscopy

Organic adsorption staining



Electrolyte staining

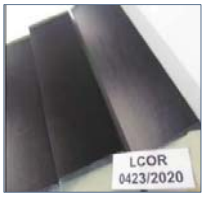


RESULTS AND DISCUSSION

SBJChem Conference 2021

2. Neutral Saline Mist

Organic adsorption staining



Note: referring to 504 hours of exposure.
Source: LCOR | UCS (2020).

Electrolyte staining

Note: After 192 hours of exposure.
Source: LCOR | UCS (2020).

RESULTS AND DISCUSSION

SBJChem Conference 2021

3. Immersion Test

Organic adsorption staining

Electrolyte staining

CONCLUSIONS

SBJChem Conference 2021

- The specimens were maintained with uniform and homogeneous anodic films between the points measured in each methodology;
- For the neutral salt mist test, both methodologies showed satisfactory results, which was not expected in the literature;
- In the immersion tests in neutral solution, there was no loss of color and corrosion was visible after 408 hours of exposure in both methodologies.

REFERENCES

SBJChem Conference 2021

1. AHMADI, A.; NOROUZI, P.; GANJALI, M. R. Study of corrosion resistance of colored anodized aluminum with Quinizarin using cyclic voltammetry and impedance measurement methods. *Progress in Organic Coatings*, [S.l.], n. 56, p. 227-233.
2. GAZAPO, J. L.; GEA, J. Anodizing of aluminium. *TALAT Lecture* 5203. EEA (European Aluminium Association): 1994. 27 p.
3. SUKIMAN, N. L. et al. Durability and corrosion of aluminium and its alloys: overview, property space, techniques and developments. *InthechOpen*, Dec. 2012.
4. VELOSO, L. A. Corantes e pigmentos. Dossiê técnico. *Instituito de tecnologia do Paraná*. Serviço Brasileiro de Nomas Técnicas (SBNT), Fev. 2012.


SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

CROHN'S DISEASE: THE IMPACTS AND HOW TO MAINTAIN A GOOD QUALITY OF LIFE FOR PATIENTS

SILVA, Guilherme Felipe Dutra[1*]; ERTHAL, Luisa Canto[1]; QUEIROZ, Aline Trovão[1]

[1] Universidade de Vassouras, Pró-reitoria de Ciências médicas, Faculdade de Medicina. Brasil.

** Autor correspondente*
e-mail:guilherme_dutras@hotmail.com

Received 12 February 2022; received in revised form 25 February 2022; accepted 08 March 2022

ABSTRACT

Crohn's disease (CD) can affect any portion of the gastrointestinal tract, characterized a chronic inflammation. It is most prevalent among patients in more productive phases, which correspond to periods that are more active in their work and with reproductive possibilities. Its treatment aims at the regression of the exacerbation phases and the healing of injuries, involving pharmacological and surgical possibilities. The objective of this paper was to delve into the issues surrounding the impacts on the quality of life of patients with Crohn's disease from diagnosis to treatment. This paper is a cross-sectional, descriptive study of a systematic literature review. The articles were searched in several databases (PUBMED, SCIELO, MEDLINE, LILACS), between the years 2000 and 2022. The inclusion criteria were: first publications that determined the direct impacts of coexistence and management on the patient's life carrier, exposing the presentations and possible complications of the natural course of the disease, and second the written language (Portuguese and English). The CD shows great clinical importance because it is a prolonged condition with huge repercussions on the patient's quality of life, whether due to possible complications of the underlying condition or even the treatment itself. Nutritional deficiencies, weight loss, sexual dysfunction, mood swings, low self-esteem, depression, and anxiety, have been shown to reflect the worsening quality of life associated or not with the natural course of the disease. It was observed that including multi-professional care in the treatment of the patient aiming at a biopsychosocial model can demonstrate a greater permanence in the remission phase, as well as provide an improvement in the quality of life indexes.

Keywords: *Crohn's disease; maintaining quality of life; biopsychosocial model*

1. INTRODUÇÃO

A doença de Crohn (DC) enquadra-se em um grupo de doenças crônicas e recidivantes caracterizadas por processo inflamatório do trato gastrointestinal que transcorre entre períodos de remissão e exacerbação. Seu acometimento é marcado por apresentação transmural e descontinua englobando o trato digestório alto e baixo. Tem-se que sua provável origem seja multifatorial, envolvendo predisposição genética, microbiota, fatores ambientais e resposta imunitária. Ainda não é bem esclarecido se decorre de uma resposta apropriada a um patógeno não reconhecido ou de uma resposta inadequada a um estímulo inócuo (Roda *et al.*, 2020).

Frequentemente, a doença de Crohn manifesta-se com sinais e sintomas tais como diarreia, constipação, febre e emagrecimento associado a uma síndrome disabsortiva (Papacosta, Nunes, Pacheco, Cardoso, e Guedes, 2017). Estudos demonstraram que sua maior incidência está presente em indivíduos de faixa etária inferior aos 30 anos. Sabe-se que a condição crônica e progressiva da DC reflete negativamente nas atividades sociais, educacionais, profissionais e familiares de seus portadores, devido ao seu caráter debilitante. Na pratica clínica, é evidente a necessidade do médico ampliar a percepção do seu paciente sobre sua condição de saúde assim como os efeitos de seu tratamento (Roda *et al.*, 2020).

O presente trabalho disserta sobre os impactos diretos do curso natural e do manejo da doença de Crohn dentro de um âmbito biopsicossocial, levando em consideração a tentativa de manutenção da boa qualidade de vida.

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.48_abstract_DUTRA.pdf

2. MATERIAIS E METODOS

Este trabalho constitui-se de um estudo transversal, descritivo, de uma revisão sistemática da literatura. Os artigos foram pesquisados em várias bases de dados (PUBMED, SCIELO, MEDLINE, LILACS) com os descritores “doença de Crohn”, “manejo da doença de Crohn”, “depressão e ansiedade na doença de Crohn” e “nutrição e doença de Crohn”, entre os anos de 2000 e 2022.

Os artigos selecionados foram analisados e comparados para a realização de revisão bibliográfica, os critérios de inclusão foram: primeiro, publicações que determinavam os impactos diretos do convívio e do manejo na vida do paciente portador, expondo as apresentações e possíveis intercorrências do curso natural da doença e segundo, a língua escrita (português e inglês).

Demais artigos encontrados, mas excluídos, não foram selecionados pelo fato de que abordavam assuntos isolados não se atentando aos impactos globais e abrangentes da doença, que trata-se do objetivo principal dessa revisão bibliográfica. Outro critério de exclusão aplicado foi de artigos em que a data de publicação ultrapassasse o limite dos últimos 20 anos. A partir dessa pesquisa foram colhidos dados importantes para agregar o presente estudo.

3. RESULTADOS E DISCUSSÃO:

Tabela 1. *Resultados da pesquisa*

Descritores	Pubmed	Scielo	Medline	Lilacs
“Doença de Crohn”	55	285	37024	806
“Manejo da doença de Crohn”	0	18	121	144
“Depressão e ansiedade na doença de Crohn”	0	5	8	5
“Nutrição e doença de crohn”	1	6	461	14

Tabela 2. *Critérios de seleção da pesquisa*

Trabalhos encontrados (total)	Trabalhos descartados	Trabalhos selecionados
38.953	38.935	18

Sarlo, Barreto e Domingues (2008), em seu estudo, constatou que existem duas fases da doença de Crohn, denominadas de ativa e silenciosa. A primeira, corresponde a um período em que os portadores tendem a ter uma alimentação mais restrita, com redução progressiva das calorias ingeridas diariamente devido a prevalência de náuseas, cólicas e distensão abdominal. Além do mais, pode cursar com fístulas, diarreia e fadiga, prejudicando pontualmente as atividades de vida diária do portador. Em contrapartida, na segunda, que corresponde a fase silenciosa, trata-se da doença em remissão ou estabilizada por via farmacológica, sendo essa essencial para manutenção do estado de saúde do paciente (Sarlo, Barreto e Domingues, 2008).

Em um estudo prospectivo e quantitativo com 104 portadores de DC, utilizando como instrumento o Questionário Sociodemográfico (QSD), a Escala de Bem-Estar Psicológico (EBEP), a Escala dos Pilares da Resiliência (EPR), Inventário das Estratégias de Coping de Folkman e Lazarus (Coping) e o Índice de Atividade da Doença de Crohn (IADC) Acciari, Leal, Coy e Dias (2019), evidenciaram que os aspectos clínicos influenciaram menos o bem-estar psicológico, resiliência e o coping quando comparado aos aspectos sociodemográficos. Constatou, portanto, que variáveis como escolaridade, situação ocupacional, renda e atividades complementares ao tratamento clínico estão mais fortemente interligadas com a melhora do quadro psicológico do paciente do que o próprio estágio de evolução da doença em que o mesmo se encontra (Acciari, Leal, Coy e Dias, 2019).

A grande parte dos pacientes portadores de doença de Crohn são acometidos durante as fases mais produtivas de suas vidas, que correspondem a períodos em que estão mais ativos em seus trabalhos e com possibilidades reprodutivas (Roda *et al.*, 2020). Sendo assim, distúrbios psiquiátricos como ansiedade e depressão, podem ser desencadeados ou intensificados após o diagnóstico do Crohn. Como uma reação em cadeia, sabe-se que o descontrole dessas situações clinicas, concomitantes, podem

interferir pontualmente no potencial de remissão da DC (Graff, Walker e Bernstein, 2009).

Quadros que envolvem reoperação das apresentações graves, muitas vezes mutilantes, não são isentos de repercussões psicológicas haja vista que o paciente passa a ter uma percepção de perda da imagem corporal tendo que conviver com os impactos visuais e as limitações da capacidade anatômico-funcional do órgão operado(Leite *et al.*, 2020; Araújo, 2016).

Para uma melhor abordagem dos impactos globais da DC na qualidade de vida do paciente portador, estudos utilizam como norte o Questionário da Doença inflamatória intestinal (Bowel Disease Questionnaire – IBDQ) criado nos Estados Unidos 1988. Através desse questionário, demonstraram uma prevalência maior dos sintomas de ansiedade em detrimento da depressão no processo de quantificação do bem estar pleno do paciente com doença de Crohn (Tomazoni e Benvegnú, 2018; Lima *et al.*, 2012).

4. CONCLUSÕES:

Após revisão bibliográfica criteriosa e análises dos artigos selecionados pode-se dizer que a doença de Crohn, em todo seu curso, expõe o paciente a diversas manifestações que englobam desde danos estruturais até emocionais e comportamentais. Por se tratar de uma doença incurável, impões mudanças drásticas na percepção do indivíduo sobre sua situação de saúde e até mesmo sobre seu próprio corpo..

As terapias clínicas e cirúrgicas, quando iniciadas no tempo correto interferem drasticamente na redução da morbidade e expansão da doença, além de melhorar o padrão qualidade de vida relacionada à saúde. Sintomas, como depressão e ansiedade, acompanham boa parte dos portadores, podendo ser iniciados com o diagnóstico ou intensificados após o mesmo. Dessa forma, é sugerível que, dentro de um contexto biopsicossocial de abordagem, a psicoterapia deva ser inserida.

Para mais, pode-se inferir o valor indispensável da avaliação nutricional haja vista que essa é capaz de identificar uma desnutrição precoce e ao mesmo tempo triar os pacientes de maior risco. Além do mais, o suporte alimentar pode melhorar os parâmetros relacionados a aparecia física e estimular um acréscimo da autoestima que está interligada aos parâmetros de bem estar e até mesmo qualidade de vida sexual.

6. REFERENCIAS:

1. Acciari, A. S., Leal, R. F., Coy, C. S. R., Dias, C. C., and Ayrizono, M. D. L. S. (2019). Relationship among psychological well-being, resilience and coping with social and clinical features in Crohn's disease patients. Arquivos de Gastroenterologia, 56, 131-140:

2. Graff, L. A., Walker, J. R., and Bernstein, C. N. (2009). Depression and anxiety in inflammatory bowel disease: a review of comorbidity and management. Inflammatory bowel diseases, 15(7), 1105-1118.

3. Leite, V. M., Lopes, C. M., Vilela, M. D. G. A., Cardoso, M. G., Carvalho, S. O., da Silva, V. A. P., e Faria, B. B. (2020). Impacto dos aspectos psicológicos em portadores de doença inflamatória intestinal. Brazilian Journal of Health Review, 3(2), 1363-1367.

4. Papacosta, N. G., Nunes, G. M., Pacheco, R. J., Cardoso, M. V., e Guedes, V. R. (2017). Doença de crohn. Revista de patologia do Tocantins, 4(2), 25-35.

5. Roda, G., Chien Ng, S., Kotze, P. G., Argollo, M., Panaccione, R., Spinelli, A., Kaser, A., Peyrin-Biroulet, L., and Danese, S. (2020). Crohn's disease. Nature reviews. Disease primers, 6(1), 22. https://doi.org/10.1038/s41572-020-0156-2.

6. Sarlo, R. S., Barreto, C. R., and Domingues, T. A. M. (2008). Understanding the experience of patients who have Crohn's disease. Acta Paulista de Enfermagem, 21(4), 629-635.

7. TOMAZONI, E. I., e BENVEGNÚ, D. M. (2018). Sintomas de ansiedade e depressão, e a qualidade de vida de pacientes com doença de Crohn. Arquivos de Gastroenterologia, 55(2), 148-153.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

DOENÇA DE CROHN: OS IMPACTOS E AS TENTATIVAS DE MANUTENÇÃO DE UMA BOA QUALIDADE DE VIDA AO PORTADOR.

Guilherme Felipe Dutra Silva
Universidade de Vassouras, Pró-reitoria de ciências médicas , Faculdade de Medicina – Brasil.

Luisa Canto Erthal
Universidade de Vassouras, Pró-reitoria de ciências médicas , Faculdade de Medicina – Brasil.

Aline Trovão Queiroz
Universidade de Vassouras, Pró-reitoria de ciências médicas , Faculdade de Medicina – Brasil.

Março/2022

INTRODUÇÃO

SBJChem Conference 2021

A doença de Crohn (DC) enquadra-se em um grupo de doenças crônicas e recidivantes caracterizadas por processo inflamatório do trato gastrointestinal que transcorre entre períodos de remissão e exacerbação.

- Manifestações iniciais;
- Faixa etária de incidência;

(Roda et al., 2020)

OBJETIVOS

SBJChem Conference 2021

O presente trabalho disserta sobre os impactos diretos do curso natural e do manejo da doença de Crohn dentro de um âmbito biopsicossocial, levando em consideração a tentativa de manutenção da boa qualidade de vida.

METODOLOGIA

SBJChem Conference 2021

O trabalho constitui-se de um estudo transversal, descritivo, de uma revisão sistemática da literatura. Os artigos foram pesquisados em várias bases de dados (PUBMED, SCIELO, MEDLINE, LILACS) com os descritores "doença de Crohn", "manejo da doença de Crohn", "depressão e ansiedade na doença de Crohn" e "nutrição e doença de Crohn", entre os anos de 2000 e 2022.

- Critérios de inclusão x Critérios de exclusão

RESULTADOS E DISCUSSÃO

SBJChem Conference 2021

- Fase ativa x Silenciosa (Sarlo, Barreto e Domingues 2008).
- Melhora do quadro psicológico: escolaridade, situação ocupacional, renda e atividades complementares ao tratamento x estágio de evolução da doença (Acciari, Leal, Coy & Dias, 2019).
- Nutrição inadequada: fragilidade e baixa autoestima (inconstância do estado de saúde / composição corporal e emagrecimento) (Leite et al., 2020).
- Manejo - Clinico x Cirurgico:

1. Natalizumabe: melhorias em âmbitos de funcionalidade física, dor corporal, vitalidade e funcionamento social (Dudley-Brown et al., 2009).
2. Cirurgia e as possibilidades de ostomias: agravantes da instabilidade emocional do paciente (Casellas, López-Vivancos, Badia, Vilaseca & Malagelada, 2000).
3. Índice de qualidade de vida: Remissão por via cirúrgica x Remissão por terapia medicamentosa (Casellas et al., 2000)

RESULTADOS E DISCUSSÃO

SBJChem Conference 2021

- Distúrbios psiquiátricos (ansiedade e depressão) (Graff, Walker & Bernstein, 2009);
- Apresentações graves – Cirurgias mutilantes - perda da imagem corporal x impactos visuais e as limitações anatômico-funcional (Leite et al., 2020; Araújo, 2016);
- Necessidade de inclusão ao manejo:

1. Aspectos físicos, emocionais e sociais
2. Saúde sexual (desejo, satisfação, disfunção sexual) (Roseira et al., 2020);

CONCLUSÃO

SBJChem Conference 2021

A doença de Crohn, em todo seu curso, expõe o paciente a diversas manifestações que englobam desde danos estruturais até emocionais e comportamentais. Por se tratar de uma doença incurável, impões mudanças drásticas na percepção do indivíduo sobre sua situação de saúde e até mesmo sobre seu próprio corpo;

1. Acompanhamento global multiprofissional;
2. Terapias clínicas e cirúrgicas iniciadas no tempo correto
3. Avaliação nutricional x suporte alimentar x qualidade de vida (até mesmo sexual);

REFERÊNCIAS

SBJChem Conference 2021

1. Roda, G., Chien Ng, S., Kotze, P. G., Argollo, M., Panaccione, R., Spinelli, A., Kaser, A., Peyrin-Biroulet, L., & Danese, S. (2020). Crohn's disease. Nature reviews. Disease primers, 6(1), 22. https://doi.org/10.1038/s41572-020-0156-2.
2. Sarlo, R. S., Barreto, C. R., & Domingues, T. A. M. (2008). Understanding the experience of patients who have Crohn's disease. Acta Paulista de Enfermagem, 21(4), 629-635.Brasil. Ministério da Saúde. Secretaria de Vigilância em Saúde (2022). Boletim Epidemiológico Especial. Recuperado em 8 de janeiro de 2022 de: https://www.gov.br/saude/pt-br/centrais-de-conteudo/publicacoes/boletins/boletins-epidemiologicos/covid-19/2022/boletim-epidemiologico-no-95-boletim-coe-coronavirus.pdf.
3. Acciari, A. S., Leal, R. F., Coy, C. S. R., Dias, C. C., & Ayrizono, M. D. L. S. (2019). Relationship among psychological well-being, resilience and coping with social and clinical features in Crohn's disease patients. Arquivos de Gastroenterologia, 56, 131-140.
4. Dudley-Brown, S., Nag, A., Cullinan, C., Ayers, M., Hass, S., & Panjabi, S. (2009). Health-related quality-of-life evaluation of Crohn disease patients after receiving natalizumab therapy. Gastroenterology Nursing, 32(5), 327-339
5. Leite V.M, Lopes C.M, Vilela M.D.G.A, Cardoso M.G, Carvalho S.O, da Silva V.A, et al (2020). Impact of psychological aspects in patients with inflammatory bowel disease. Braz J Hea Rev, 3(2):1363-1367
6. Casellas, F., López-Vivancos, J., Badia, X., Vilaseca, J., & Malagelada, J. R. (2000). Impact of surgery for Crohn's disease on health-related quality of life. The American journal of gastroenterology, 95(1), 177-182
7. Graff, L. A., Walker, J. R., & Bernstein, C. N. (2009). Depression and anxiety in inflammatory bowel disease: a review of comorbidity and management. Inflammatory bowel diseases, 15(7), 1105-1118.

REFERÊNCIAS

SBJChem Conference 2021

8. Roseira, J., Magro, F., Fernandes, S., Simões, C., Portela, F., Vieira, A. I., Patita, M., Leal, C., Lago, P., Caldeira, P., Gago, T., Currais, P., Dias, C. C., Santiago, M., Dias, S., & Tavares de Sousa, H. (2020). Sexual Quality of Life in Inflammatory Bowel Disease: A Multicenter, National-Level Study. Inflammatory bowel diseases, 26(5), 746–755. https://doi.org/10.1093/ibd/izz185

9. TOMAZONI, E. I., & BENVEGNÚ, D. M. (2018). Sintomas de ansiedade e depressão, e a qualidade de vida de pacientes com doença de Crohn. Arquivos de Gastroenterologia, 55(2), 148-153.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

DIABETES IN PREGNANCY AND FETAL CARDIAC RISK: LITERATURE REVIEW

TAVARES, Lívia Hygino[1*]; MOURA, Bruno[1]

[1] Universidade de Vassouras, Pró-reitoria de Ciências médicas, Faculdade de medicina. Brasil.

** Autor Correspondente*
e-mail: liviatmello@gmail.com

Received 12 February 2022; received in revised form 03 March 2022; accepted 11 March 2022

ABSTRACT

Gestational diabetes mellitus (MGD) is associated with poor cardiac malformation in the fetus. It is related to changes in the clinical course of the disease and pre-gestational periods. The prevalence and incidence of MGD have been increasing worldwide. Early screening, diagnosis, and lifestyle change, such as physical exercise and healthy eating, provide better outcomes for children's health. This study aims to analyze the data concerning gestational diabetes and fetal malformations and to group the various protocols for diagnosis, highlighting the risk factors associated with MGD and their prevention. A systematic review of the literature was conducted with the PubMed, Scielo, Medline databases with English, Portuguese, and Spanish articles. The studies gathered clinical trials, randomized clinical trials, and original articles. In 12 articles analyzed maternal alterations, while 11 articles analyzed fetal alterations, and 9 articles analyzed how to diagnose cardiac changes in the fetus. The patient with MGD should be inserted in multidisciplinary activities seeking the change of lifestyle, physical exercises, and food reeducation, intending to give the fetus the appropriate nutrients and optimize the drug treatment; cardiac malformations are among the most severe and recurrent complications. However, they can be avoided with the control of pre-gestational diabetes (stricter follow-up from the moment the patient feels the desire to become pregnant) and the diagnosis and treatment of early gestational diabetes, as strict control of maternal blood glucose during pregnancy reduces morbidities and mortality. The study showed that hyperglycemic status during pregnancy is related to increased mortality and morbidity, even if it is asymptomatic. Therefore, it is necessary to guide the diabetic woman to plan her pregnancy in a euglycemic period because only this control can guarantee health to the fetus. The diagnosis of pregnant women with gestational diabetes needs to be early to optimize treatment.

Keywords: *Gestational diabetes; Obstetric history, Fetal doppler echo; Congenital heart defects; Pregnancy in people with diabetes*.

1. INTRODUÇÃO

A diabetes mellitus gestacional (DMG) é uma alteração no metabolismo dos carboidratos exibida pela hiperglicemia. É a alteração metabólica mais comum durante a gestação. O diagnóstico é condicional a gravidez, e a doença geralmente desaparece no pós-parto (Weinert, 2011).

A fisiopatologia tem alguns determinantes, como o aumento dos hormônios contra reguladores da insulina, lactogênio placentário, cortisol e estrogênio (Brody, 2003).

A incidência de DMG é de 3% a 7%, variando de acordo com a população estudada e com os critérios diagnósticos utilizados.(Brody, 2003) As gestantes geralmente têm de 21 a 30 anos de idade, e o diagnóstico é feito entre 21 a 36 semanas de gestação. Por ser de origem multifatorial, alguns fatores de risco podem ser observados, tais como: idade superior a 25 anos, obesidade ou ganho de peso excessivo durante a gravidez, acúmulo de gordura centrípeta, história familiar de primeiro grau de diabetes mellitus, e baixa estatura (Mocarzel, 2021).

Nas consultas de pré-natal o rastreamento é sempre realizado com o objetivo de detectar a DMG em uma fase precoce da gravidez (Zielinsky *et al*., 2004).

É importante distinguir o diabetes pré gestacional e o diabetes gestacional. Pois eles têm efeitos diferentes na gravidez, e no desenvolvimento fetal. O diabetes pré gestacional pode causar complicações graves, pois seus

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.45_abstract_TAVARES.pdf

efeitos começam desde a fertilização e implantação, atuando na organogênese (Brody, 2003). A diabetes gestacional, e as mães previamente diabéticas precisam de um controle adequado da glicemia, pois a hiperglicemia e a hiperinsulinemia decorrente do estimulo da glicose, está relacionada com as comorbidades fetais. Para realizar este controle, é preciso fazer o diagnóstico e tratamento precoce (Owens *et al*., 2012).

Durante o primeiro trimestre deve ser realizado o ultrassom para avaliar a idade gestacional e a translucência nucal, para estimar o risco de malformação fetal. No segundo trimestre, realiza-se a US morfológico, para avaliar as mal formações (24-26 semanas), o ecocardiograma fetal é feito a partir das 24-28 semanas em caso de diabetes preexistentes, e a partir da 24ª semana, caso seja confirmado, é necessário a realização do US mensal, para avaliar o crescimento fetal e polidramnia. No terceiro trimestre, realiza-se US mensal até o parto, também o doppler das artérias umbilicais, e contagem dos movimentos fetais a partir da 28 semana (Davies *et al*., 2003).

As malformações cardíacas estão entre as complicações mais severas e recorrentes. Por isso é necessário o diagnóstico precoce, para minimizar os efeitos da hiperglicemia. Além disso, o acompanhamento contínuo durante todo o pré-natal de forma individualizada, é alteamente recomendável para se ter resultados satisfatórios (Weinert *et al*., 2011).

2. MATERIAIS E MÉTODOS

Foi realizada uma pesquisa eletrônica da literatura nas bases de dadosMedline, PubMed e Scielo, nos idiomas português e inglês. Utilizando-se os seguintes termos de procura: gestational diabetes, obstetric history, fetal doppler echo, congenital heart defects, pregnancy in diabetics

Os critérios de inclusão foram artigos com populações intrauterinas e recém-nascidos, metanálise, revisões sistemáticas, publicados entre 1996 e 2020, em ingles e portugues, que avaliassem aspectos epidemiológicos, diagnósticos e terapêuticos de filhos cardiopatas de mães diabéticas.

2. RESULTADOS E DISCUSSÃO:

A Tabela 1 contém os resultados do número de artigos encontrados em cada plataforma, sendo que o número de resultados utilizados como base para construção deste artigo é exclusivamente referente aos temas citados, apesar de encontramos uma variedade expressiva de publicações, nem todas abordam especificamente o assunto chave.

Tabela 1. *Resultados das buscas nos bancos de dados.*

TERMOS	PUBMED	SCIELO	MEDLINE
Gestational diabetes	26.488	168	193
Fetal doppler echo	132	ZERO	50
Congenital heart defects	168.857	400	4.718
Pregnancy in diabetics	13.813	14	1.762
Total Results	209.290	582	6.723
Used results	23	12	13
Resultados descartados	209.267	570	6.710

A diabetes materna pode causar alteração cardíaca no feto tanto estruturalmente como funcionalmente, neste caso a estrutura cardíaca está preservada, porém a função cardíaca está comprometida (Reis *et al*., 2010). Esta alteração está relacionada com a alteração metabólica da paciente no início da gestação (Alves *et al*., 2020). Por isso o rastreamento da diabetes gestacional é universal. As cardiopatias fetais podem ser classificadas com comprometimento fetal precoce e tardio. As mal formações tardias não apresentam disfunção intrauterina, e não tem sofrimento cardíaco no período neonatal, um exemplo desta classificação é a tetralogia de Fallot e a estenose pulmonar não critica.20 Já as doenças de acometimento precoce são as cardiopatias com circulação pulmonar dependente do canal arterial, como a atresia pulmonar com septo integro, atresia pulmonar com comunicação interventricular (Silveira *et al*., 2021).

As cardiopatias fetais podem ser dividas em ativas, passivas e progressivas. As passivas têm repercussão apenas no período neonatal com o fechamento do canal arterial, pois não apresentam alteração da hemodinâmica no pré-natal. O grupo das cardiopatias fetais ativas inclui

todas as alterações do sistema cardiovascular fetal que provocam alterações na hemodinâmica na vida intrauterina, entre elas estão as arritmias cárdicas, as cardiopatias estruturais com regurgitação valvar (Reis *et al*., 2010).

O período da embriogênese ocorre até a décima segunda semana, neste momento é necessário o aporte nutricional adequado ao feto (Dervisoglu *et al*., 2018).

As frutosaminas são cetoamidas formadas pela interação de proteínas com a glicose. Seu valor de referência sanguíneo é 2, 68 mMol/L. Estão aumentadas na presença de hiperglicemia persistente. É útil para avaliar o controle glicêmico na gestação, principalmente a curto prazo. A American Diabetes Association (ADA) reconhece a frutosamina um exame útil em que a hemoglobina glicada não está disponível, ou para ser usada associada a ela na monitorização das gestantes diabéticas (Silveira *et al*., 2022).

No início da gestação, a hiperglicemia tem um efeito teratogênico comprometendo a cardiogênese primária. E o acometimento no final da gestação tem relação com a cardiomiopatia hipertrófica. (Owens *et al*., 2018). O ecocardiograma fetal com doppler tem sido essencial para obter o prognostico da doença, pois analisa as modificações do fluxo cardiovascular dos fetos em questão. O exame cardíaco fetal consiste de um estudo cuidadoso do situs atrial e das conexões veno-atrial, atrioventricular e ventrículo-arterial. Este exame tem grande importância, pois a partir do momento em que é identificado arritmias e cardiopatias (Alves *et al*., 2020).

A miocardiopatia hipertrófica é a anormalidade mais prevalente no diabetes gestacional, evidenciando cerca de 35% dos bebes. Está associada com o hiperinsulinemismo principalmente nas últimas semanas de gestação. Esta condição acarreta no aumento das células do miocárdio, e por isso as células tem aumento de tamanho, levando a rigidez da parede do ventrículo (Owens *et al*., 2018).

A taxa de mal formação cardíaca, vem aumentando em todo o mundo, visto que muitas mulheres são reféns a diabetes gestacional, muitas vezes desenvolvida pelo o estilo de vida. Ficou claro que a atividade física e o acompanhamento multidisciplinar da gestante teve efeitos essenciais para o controle da glicemia e para minimizar os efeitos deletérios no feto (Zielinsky *et al*., 2003).

Alguns estudos mostraram que a hipertrofia cardíaca é a alteração mais comumente mostrada (Nold, 2004). O aumento do fluxo pelo ducto venoso começa a ser percebido, a partir do momento que o coração se torna hipertrofiado, visto que há uma menos área para circulação e armazenamento do fluxo sanguíneo, tanto na sístole como na diástole (Codazzi, *et al*., 2021).

4. CONCLUSÃO:

O estudo evidenciou que o estado hiperglicêmico durante a gestação, mesmo que seja assintomático, está relacionada a um aumento de mortalidade e de morbidade. Por isso é necessário orientar a mulher diabética para que a mesma planeje sua gestação em um período euglicêmico, pois apenas este controle é capaz de garantir saúde ao feto. O diagnóstico da gestante com diabetes gestacional precisa ser precoce, para assim otimizar o tratamento. A doença muitas vezes é silenciosa, dificultando o diagnóstico. Dessa forma a detecção da mesma, e o tratamento adequado trazem a mãe e ao feto um período gestacional mais saudável e tranquilo.

REFERÊNCIA:

1- Weinert, L. S., Silveiro, S. P., Oppermann, M. L., Salazar, C. C., Simionato, B. M., Siebeneichler, A., and Reichelt, A. J. (2011). Gestational diabetes management: a multidisciplinary treatment algorithm. Arquivos Brasileiros de Endocrinologia and Metabologia, 55(7), 435–445. https://doi.org/10.1590/S0004-27302011000700002

2- Surita, F. G., Nascimento, S. L. do, and Silva, J. L. P. e. (2014). Exercício físico e gestação. Revista Brasileira de Ginecologia E Obstetrícia, 36(12), 531–534. https://doi.org/10.1590/so100-720320140005176

3- Brody, S. (2003). Screening for gestational diabetes: a summary of the evidence for the U.S. Preventive Services Task Force. Obstetrics and Gynecology, 101(2), 380–392. https://doi.org/10.1016/s0029-7844(02)03057-0

4- Mocarzel, C. (2021, September 5). Recomendações da ADA 2021 para manejo diabetes gestacional. PEBMED. https://pebmed.com.br/recomendacoes-da-ada-2021-para-manejo-diabetes-gestacional/

5- Zielinsky, P., Satler, F., Luchese, S., Nicoloso, L. H., Piccoli Jr, A. L., Gus, E. I., Manica, J. L.,

Scheid, M., Marcantonio, S., and Hatem, D. (2004). Estudo do encurtamento global do átrio esquerdo em fetos de mães diabéticas. Arquivos Brasileiros de Cardiologia, 83, 470–472. https://doi.org/10.1590/S0066-782X2004001800005

6- Davies, G. A. L., Wolfe, L. A., Mottola, M. F., MacKinnon, C., and Society of Obstetricians and gynecologists of Canada, SOGC Clinical Practice Obstetrics Committee. (2003). Joint SOGC/CSEP clinical practice guideline: exercise in pregnancy and the postpartum period. Canadian Journal of Applied Physiology = Revue Canadienne de Physiologie Appliquee, 28(3), 330–341. https://pubmed.ncbi.nlm.nih.gov/12955862/

7- Owens, L. A., Avalos, G., Kirwan, B., Carmody, L., and Dunne, F. (2012). ATLANTIC DIP: Closing the Loop: A change in clinical practice can improve outcomes for women with pregestational diabetes. Diabetes Care, 35(8), 1669–1671. https://doi.org/10.2337/dc12-0120

8- Alves, P., Malheiro, M. F., Gomes, J. C., Ferraz, T., and Montenegro, N. (2020). Risks of Maternal Obesity in Pregnancy: A Case-control Study in a Portuguese Obstetrical Population. Revista Brasileira de Ginecologia E Obstetrícia, 41, 682–687. https://doi.org/10.1055/s-0039-3400455

9- Alves, P., Malheiro, M. F., Gomes, J. C., Ferraz, T., and Montenegro, N. (2020). Risks of Maternal Obesity in Pregnancy: A Case-control Study in a Portuguese Obstetrical Population. Revista Brasileira de Ginecologia E Obstetrícia, 41, 682–687. https://doi.org/10.1055/s-0039-3400455

10- Zielinsky, P., Piccoli Jr, A. L., Teixeira, L., Gus, E. I., Mânica, J. L., Satler, F., Vaz, H., Nicoloso, L. H., Luchese, S., Sheid, M., Marcantonio, S., and Hatém, D. (2003). Pulsatilidade venosa pulmonar em fetos de mães diabéticas: estudo doppler-ecocardiográfico pré-natal. Arquivos Brasileiros de Cardiologia, 81, 604–607. https://doi.org/10.1590/S0066-782X2003001400007

11- Brody, S. (2003). Screening for gestational diabetes: a summary of the evidence for the U.S. Preventive Services Task Force. Obstetrics and Gynecology, 101(2), 380–392. https://doi.org/10.1016/s0029-7844(02)03057-0

12- Satler, F., Luchese, S., Piccoli, A., Manica, J. L., Gus, E. I., Vaz, H. A., Nicoloso, L. H. S., Marcantônio, S., Scheid, M. M., Teixeira, L. P., Hatem, D. M., and Zielinsky, P. (2002). Estudo do encurtamento global do átrio esquerdo na avaliação da função diastólica em fetos de mães diabéticas. Www.lume.ufrgs.br. https://www.lume.ufrgs.br/handle/10183/6035 9

13- Yamila, D., Lay, C., Marcos, S., Salcedo, L., José, M., and Alvarez Rodríguez. (2014). Algunas variables epidemiológicas en pacientes con diabetes mellitus gestacional Some epidemiological variables in gestational diabetes mellitus patients. Revista Cubana de Ginecología Y Obstetricia, 40(1), 2–12. http://scielo.sld.cu/pdf/gin/v40n1/gin02114.pdf

14- Reis, Z. S. N., Miranda, A. P. B., Rezende, C. de A. L., Detofol, R. B., Costa, C. R., and Cabral, A. C. V. (2010). Rastreamento de cardiopatias congênitas associadas ao diabetes mellitus por meio da concentração plasmática materna de frutosamina. Revista Brasileira de Ginecologia E Obstetrícia, 32, 66–71. https://doi.org/10.1590/S0100-72032010000200003

15- Macklon, N., Hop, N., and Wladimiroff, J. (1998). Fetal cardiac function and septal thickness in diabetic pregnancy: a controlled observational and reproducibility study. British Journal of Obstetrics and Gynaecology, 105, 661–666. https://pure.eur.nl/en/publications/fetal-cardiac-function-and-septal-thickness-in-diabetic-pregnancy

16- Zielinsky, P., da Costa, M. H., Oliveira, L. T., Bonow, F. P., da Silva, N. I., and Hagemann, L. L. (1997). [Natural history of myocardial hypertrophy and its association with hyperinsulinism in infants of diabetic mothers]. Arquivos Brasileiros de Cardiologia, 69(6), 389–394. https://doi.org/10.1590/s0066-782x1997001200005

17- Zielinsky, P., da Costa, M. H., Oliveira, L. T., Bonow, F. P., da Silva, N. I., and Hagemann, L. L. (1997). [Natural history of myocardial hypertrophy and its association with hyperinsulinism in infants of diabetic mothers]. Arquivos Brasileiros de Cardiologia, 69(6), 389–394. https://doi.org/10.1590/s0066-782x1997001200005

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

DIABETES NA GRAVIDEZ E O RISCO CARDÍACO FETAL: REVISÃO DE LITERATURA

Lívia Hygino Tavares
Universidade de Vassouras, Brazil

Bruno Moura
Universidade de Vassouras, Brazil

Janeiro/2021

INTRODUÇÃO

O QUE É?

- A Diabetes Mielitus Gestacional (DMG) é caracterizada pela hiperglicemia em gestantes diagnosticadas na gravidez.
- Esta condição aumenta o risco de eventos adversos e compromete a saúde da mãe e do feto a curto e longo prazo.

INTRODUÇÃO

COMO RASTREAR?

- O programa de educação em diabetes deve ser sempre fornecido na primeira consulta do pré natal.
- O diagnóstico é feito entre 21 e 36 semanas de gestação, através da glicemia de jejum.
- O rastreamento é realizado precocemente para impedir as alterações cardíacas nos fetos de mães diabéticas.

INTRODUÇÃO

COMPLICAÇÕES CARDÍACAS

- O período da embriogênese ocorre até a décima segunda semana, o estado hiperosmolar causado pela hiperglicemia pode levar à hipóxia fetal e alterações cardíacas.
- As más formações cardíacas estão entre as complicações mais severas e recorrentes.
- Podem ser divididas em estruturais e funcionais. Tal distribuição está relacionada com a idade gestacional, idade materna e o nível de alteração metabólica.

OBJETIVO

- Abordar os principais aspectos relacionados as más-formações cardíacas de fetos de mães diabéticas e seu diagnóstico.

5

METODOLOGIA

Pesquisa eletrônica da literatura usando os dados do Medline, PubMed e Scielo, na língua portuguesa e inglesa. Utilizou-se os seguintes termos de procura: gestational diabetes, obstetric history, fetal doppler echo, congenital heart defects, pregnancy in diabetics.

Os critérios de inclusão foram artigos com populações intrauterinas e recém nascidos, metanálise, revisões sistemáticas, publicadas entre 1996 e 2021, nas línguas inglesa e portuguesa, que avaliassem aspectos epidemiológicos, diagnósticos e terapêuticos de filhos cardiopatas de mães diabéticas.

Ao pesquisar o termo diabetes materna gestacional no PubMed foram encontrado 552 títulos, no Scielo 465 títulos, e 1046 no Medline. Já a palavra ecodoppler fetal foi encontrada em 6 títulos do PubMed, 5 títulos no Scielo e 2 MedLine. Já o termo diagnóstico diabetes gestacional, foi encontrato 144 vezes no Scielo, 18 vezes no PubMed, e 62 vezes no MedLine.

6

RESULTADOS E DISCUSSÃO

7

- As cardiopatias podem ser classificadas com comprometimento fetal precoce e tardio
  - As doenças de acometimento precoce pela hiperglicemia são as cardiopatias de circulação pulmonar, como atresia pulmonar.
  - As mal formações de acometimento tardio, são a tetralogia de Fallot e estenose pulmonar não critica.

RESULTADOS E DISCUSSÃO

8

- São divididas em ativas, passivas e progressivas.
  - As passivas tem repercussão apenas no período neonatal, com o fechamento do canal arterial.
  - As cardiopatias ativas inclui toda alteração no sistema cardiovascular fetal que leva a alterações na hemodinâmica da vida intrauterina, ou seja no período pré natal. Entre elas estão as arritmias cardíacas, regurgitação valvar, e cardiopatias estruturais.

RESULTADOS E DISCUSSÃO

9

- A american Diabetes Association (ADA) reconhece a frutosamina um exame útil para monitorização das gestantes diabéticas.
- Pacientes com níveis elevados de frutosamina apresentavam alteração ecocardiográfica fetal.
- No início da gestação, a hiperglicemia tem efeito teratogênico comprometendo a cardiogênese primária.

RESULTADOS E DISCUSSÃO

10

- O ecocardiograma fetal com doppler avalia o prognóstico da doença.
- No período pré natal, e neonatal, uma minoria de pacientes apresentava alterações clínicas, e apresentavam alterações ecocardiográficas. Por isso este exame tem uma grande importância
- Pois a partir do momento que é identificado arritmias, e cardiopatias, o tratamento já pode ser estabelecido, intrautero ou no pós parto imediato.

RESULTADOS E DISCUSSÃO

11

- A miocardiopatia hipertrófica é a anormalidade mais prevalente.
- A condição de resistência insulínica, com hiperglicemia, aumentam as células do miocárdio, levando a rigidez da parede do ventrículo.
- Levam a diminuição da complacência cardíaca, com diminuição do débito cardíaco.
  - Se a doença não for controlada, e a com o comprometimento da diástole, o feto pode entrar em hipóxia.
  - Outro estado de hipóxia é a hiperglicemia propriamente dita, pois a proliferação do endotélio vascular.

RESULTADOS E DISCUSSÃO

12

- Diagnóstico da miocardiopatia hipertrófica:
  - Como parâmetro para avaliar a hipertrofia cardíaca, tem-se a pulsatilidade do fluxo do ducto venoso.
  - As ondas E da válvula mitral e tricúspide aumentam a pulsatilidade, a partir do momento que o coração se torna hipertrofiado.

CONCLUSÃO

- O estudo evidenciou que o estado hiperglicêmico, mesmo que assintomático, leva ao aumento de mortalidade e morbidade. É necessário que a mulher diabética planeje sua gestação em um período euglicêmico.
- As alterações cardíacas mais comuns são: Miocardiopatia hipertrófica; Regurgitação valvar e Arritmias cardíacas
  - São consequentes ao aumento do fluxo sanguíneo pelo ducto venoso.
- A doença é silenciosa, por isso o rastreamento, o diagnóstico precoce, e o tratamento adequado e individualizado são essenciais para o período gestacional ser mais saudável e sem intercorrências.

REFERÊNCIAS BIBLIOGRÁFICAS

1. Schwerz Weinert L, Pinho Silveiro S, Lúcia Oppermann M, Caetano Salazar C, Marina Simonato B, Siebeneichler A, et al. Diabetes gestacional: um algoritmo de tratamento multidisciplinar Gestational diabetes management: a multidisciplinary treatment algorithm. Vol. 55, Arq Bras Endocrinol Metab. 2011.
2. Surita FG, Lira S, Pinto E Silva JL. Exercício físico e gestação Physical exercise during pregnancy.
3. Brody SC, Harris R, Lohr K. Screening for gestational diabetes: a summary of the evidence for the U.S. Preventive Services Task Force. Obstet Gynecol. 2003;101:380-92.
4. Diabetes na gestação: recomendações para o preparo e o acompanhamento da mulher com diabetes durante a gravidez [Internet]. Available from: https://www.diabetes.org.br/profissionais/diabetes-gestacional/92-diabetes-na-gestacao-recomendacoes-para-o-preparo-e-o-acompanhamento-da-mulher-com-diabetes-durante-a-gravidez
5. Zielinsky P, Satler F, Lucchese S, Henrique Nicoloso L, Piccoli Jr AL, Gus Ei, et al. Estudo do Encurtamento Global do Átrio Esquerdo em Fetos de Mães Diabéticas. Vol. 83, Arquivos Brasileiros de Cardiologia. 2004.
6. Davies GA, Wolfe LA, Mottola MF, MacKinnon C, Arsenault MY, Bartellas E et al. Society of Obstetricians and Gynecologists of Canada Clinical Practice Obstetrics Committee, Canadian Society for Exercise Physiology Board of Directors. Exercise in pregnancy and the postpartum period. J Obstet Gynecol Can. 2003;25:516-29.
7. Matthew C R et. a. Standars of Medical Care in Diabetes 2020 ADA. Am Diabetes Assoc [Internet]. 2020;42(479):960–1010. Available from: https://care.diabetesjournals.org/content/diacare/suppl/2019/12/20/43.Supplement_1.DC1/Standards_of_Care_2020.pdf
8. Owens LA, Avalos G, Kirwan B, Carmody L, Dunne F. ATLANTIC DIP: closing the loop: a change in clinical practice can improve outcomes for women with pregestational diabetes. Diabetes Care. 2012 Aug;35(8):1669-71
9. SILVEIRA LO, MARQUEZ, D S. Diabetes Gestacional: Consequências para a mãe e o recém-nascido. Rev Científica online da Fac Atenas. 2013;1–18.
10. ADA Reports. Position of the American Dietetic Association: Use of nutritive and nonnutritive sweeteners. J Am Diet Assoc. 2004;255-75.
11. Diabetes na gestação: recomendações para o preparo e o acompanhamento da mulher com diabetes durante a gravidez [Internet]. Available from: https://www.diabetes.org.br/profissionais/diabetes-gestacional/92-diabetes-na-gestacao-recomendacoes-para-o-preparo-e-o-acompanhamento-da-mulher-com-diabetes-durante-a-gravidez
12. Zielinsky P, Piccoli AL, Teixeira L, Gus Ei, Mânica JL, Satler F, et al. Zielinsky e cols Pulsatilidade venosa pulmonar em fetos de mães diabéticas Arq Bras Cardiol 2003; 81: 600-3
13. Surita FG, Lira S, Pinto E Silva JL. Exercício físico e gestação Physical exercise during pregnancy.
14. Brody SC, Harris R, Lohr K. Screening for gestational diabetes: a summary of the evidence for the U.S. Preventive Services Task Force. Obstet Gynecol. 2003;101:380-92.
15. Zielinsky P, Satler F, Lucchese S, Henrique Nicoloso L, Piccoli Jr AL, Gus Ei, et al. Estudo do Encurtamento Global do Átrio Esquerdo em Fetos de Mães Diabéticas. Vol. 83, Arquivos Brasileiros de Cardiologia. 2004.
16. Lay Y, Salcedo M, Rodriguez J. Algunas variables epidemiológicas en pacientes con diabetes mellitus gestacional. Rev Cuba Obstet y Ginecol. 2014 Mar 1;40:2–12

REFERÊNCIAS BIBLIOGRÁFICAS

17. Nold JL, Georgieff MK. Infants of diabetic mothers. Pediatr Clin North Am. 2004; 51:619-37
18. Aberg A, Westbom L, Källén B. Congenital malformations among infants whose mothers had gestational diabetes or preexisting diabetes. Early Hum Dev. 2001;61(2):85-95.
19. Cléfia R., Diniz C. UNIVERSIDADE FEDERAL DE MINAS GERAIS PROGRAMA DE PÓS-GRADUAÇÃO EM CIÊNCIAS DA SAÚDE ÁREA DE CONCENTRAÇÃO EM SAÚDE DA CRIANÇA E DO ADOLESCENTE.
20. Keywords FE, Objetivo FE, Fetal M. Rastreamento de cardiopatias congênitas associadas ao diabetes mellitus por meio da concentração plasmática materna de frutosamina.
21. Silveira J, Reis N, Brum Miranda P. Congenital cardiopathies screening associated with diabetes mellitus using maternal fructosamine plasma concentration.
22. Szyld NA, Segre CA de M, Machado MV. Diabetes e gestação: análise das gestantes submetidas à ecocardiografia fetal em um período de dez anos. Einstein (São Paulo). 2008;6(1):42-50
23. Dervisoglu P, Kosecik M, Kumbasar S. Effects of gestational and pregestational diabetes mellitus on the foetal heart: a cross-sectional study. J Obstet Gynaecol (Lahore) [Internet]. 2018 Apr 3 [cited 2020 Aug 25];38(3):408–12. Available from: https://pubmed.ncbi.nlm.nih.gov/29355062/.
24. Hernandez-Andrade E, Figueroa-Diesel H, Kottman C, Illanes S, Arrattoa J, Acosta-Rojas R, et al. Gestational-age-adjusted reference values for the modified myocardial performance index for evaluation of fetal left cardiac function. Ultrasound Obstet Gynecol [Internet]. 2007 [cited 2020 Aug 19];29(3):321–5. Available from: https://pubmed.ncbi.nlm.nih.gov/17354122/
25. Palmieri CR, Sindeo MA, Silva JC, Santos AD Dos, Silva MRE, Ferreira B. Prevalence of Hypertrophic Cardiomyopathy in Fetuses of Mothers with Gestational Diabetes before Initiating Treatment. Rev Bras Ginecol Obstet [Internet]. 2017 Jan 1 [cited 2020 Aug 26];39(1):9–12. Available from: http://www.thieme-connect.de/DOI/DOI?10.1055/s-0037-1598602
26. Luisi A. Recém-nascido de mãe diabética. Aspectos anatomo-patológicos. Matern Infanc (Sao Paulo) [Internet]. 1967 Jul [cited 2020 Aug 25];26(3):241–9. Available from: https://pubmed.ncbi.nlm.nih.gov/5829034/
27. Macklon NS, Hop WCJ, Wladimiroff JW. Fetal cardiac function and septal thickness in diabetic pregnancy: a controlled observational and reproducibility study. BJOG An Int J Obstet Gynaecol [Internet]. 1998 Jun 1 [cited 2020 Aug 19];105(6):661–6. Available from: http://doi.wiley.com/10.1111/j.1471-0528.1998.tb10182.x
28. Zielinsky P, Scheid MM, Nicoloso LH, Frajndlich R, Piccoli Jr AL, Mânica JL, et al. Comportamento do fluxo pelo Forame Oval em Fetos de Mães Diabéticas com Hipertrofia Miocárdica Behavior of the Foramen Ovale Flow in Fetuses of Diabetic Mothers and Myocardial Hypertrophy A r t i g o O r i g i n a l.
29. Hod M, Dye TD. Perinatal complications following gestational diabetes mellitus – How sweet is it ? Acta Obstet Gynecol Scand 1996; 75: 809-15.
30. Zielinsky P, Costa M, Oliveira L, Telles M, Hagemann L. Estudo da história natural da hipertrofia miocárdica e sua associação com hiperinsulinismo em filhos de mães diabéticas. Arq Bras Cardiol 1997; 69: 389-94
31. Diretrizes P. Diabetes Mellitus Gestacional Autoria: Sociedade Brasileira de Endocrinologia e Metabologia.
32. Matthew C R et. a. Standars of Medical Care in Diabetes 2020 ADA. Am Diabetes Assoc [Internet]. 2020;42(479):960–1010. Available from: https://care.diabetesjournals.org/content/diacare/suppl/2019/12/20/43.Supplement_1.DC1/Standards_of_Care_2020.pdf

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EFFECT OF MOLAR WEIGHT OF CARBOXYLIC ACIDS ON THE ENZYMATIC ESTERIFICATION OF GLYCEROL

SANTOS, Maricel del Valle[*1]; VELEZ, Alexis Rafael[1]; MAGARIO, Ivana Maria[1]

[1] Instituto de Investigación y Desarrollo en Ingeniería de Procesos y Química Aplicada (IPQA), CONICET, Universidad Nacional de Córdoba

** Correspondence author*
e-mail: maricel.santos@mi.unc.edu.ar

Received 10 December 2021; received in revised form 10 January 2021; accepted 28 January 2022

ABSTRACT

Glycerol is a by-product in biodiesel synthesis, and its current market condition allows the possibility to transform into value-added compounds. In this work, the enzymatic esterification between glycerol and carboxylic acids of different molar weights was studied to obtain glycerides of industrial relevance. Therefore, eight different carboxylic acids were evaluated: formic, acetic, levulinic, caprylic, capric, lauric, stearic, and oleic. Immobilized lipase from *Candida Antarctica* was employed as a catalyst. Solvent-free reactions were carried out at 65 °C, 450 rpm, at a molar ratio of glycerol: carboxylic acid of 1:1 and a 1,6% enzyme concentration (based on reagents weight). Conversion of carboxylic acids was followed with time by titration. Under these conditions, acids from octanoic to oleic, which initially formed biphasic systems with glycerol, showed high conversions (68%-80%) and initial reaction rates in the same magnitude order. On the other hand, no enzymatic catalysis was observed with formic, acetic, and levulinic acids. Formic acid exhibited a higher rate and 58% of conversion without catalyst. However, for acetic and levulinic acids, conversion was low in uncatalyzed reactions. Then, for these acids, toluene was added as a reaction solvent. As a result, conversions and initial rates increased for these lighter acids, indicating the need for a non-polar media or a biphasic character to activate the enzyme.

Keywords: *Glycerol, Glycerides, Lipase, Direct Esterification.*

1. INTRODUCTION

In the last years, ecological requirements produced an accelerated growth of the biofuel industry. The biodiesel industry produces glycerol as a by-product representing 10% of the total mass. Thus, it is generated in large amounts. This causes a low price of glycerol and a favorable scenery to propose its transformation in higher-value compounds (Zheng, 2008).

One option is the direct esterification between glycerol (GLY) and carboxylic acids (CA) to produce glycerides. This reaction generates mono, di, and triglycerides with different applications such as emulsifiers, surfactants, plasticizers, among others. Currently, they are obtained through triglyceride glycerolysis. However, one advantage of direct esterification lies in selecting type and number of carboxylic acid units to achieve specific applications.

This reaction can be biocatalyzed by lipases with the advantages of mild temperature conditions (Stergiou, 2013) and versatility in front of many substrates and media reactions. Most enzymatic syntheses are performed in the presence of organic non-polar solvents, although solvent-free systems are technically feasible (Freitas, 2007). Furthermore, reactions in aqueous and low-water media are described (Silvestini and Cianci, 2020). The lipase source and the solvent influence were widely studied on glycerol esterification, especially with fatty acids (Kristensen *et al.*, 2005; Dutta Banik *et al.*, 2016). Jassen *et al*. (1993) studied the effect of molecular weight in the thermodynamic equilibrium of esterification of glycerol and carboxylic acids in

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.13_abstract_SANTOS.pdf

range C6-C18 with a Lipase from *Chrombacterium viscosum.* They found that equilibrium constants are similar in all cases.

In this work, eight different carboxylic acids were used to evaluate the influence of molar weight and unsaturations in equilibrium conversion and initial rate values. A lipase B from *Candida antarctica* (CaLB1) absorbed on dry hydrophobic acrylic beads was used as a biocatalyst. The acids used were: formic (C1), acetic (C2), levulinic (C5), caprylic (C8), capric (C10), lauric (C12), stearic (C18), and oleic (C18).

2. MATERIALS AND METHODS

2.1. Materials

The enzyme used was a Lipase from *Candida antarctica* (lipase B adsorbed on acrylic beads. Activity: 10000 PLU / g. IMMCALB-T1-350) supplied by ChiralVision (the Netherlands). All chemicals were of analytical grade; levulinic acid, caprylic acid, capric acid (>98% purity, Sigma-Aldrich, USA), anhydrous glycerol 98%, formic acid 85%, ethyl ether, toluene, KOH (Cicarelli, Argentina), lauric acid 99% (Serquim, Argentina), stearic acid 65%, oleic acid 77% (Pura Química, Argentina) and acetic acid (Biopack, Argentina).

2.2. Esterification Reaction

Reactions were carried out in a three-necked glass reactor immersed in a thermostatic bath. Agitation was provided through a mechanical stirrer at 450 rpm. The temperature was registered using a “K” type thermocouple submerged in the liquid system, and a lateral position was kept free for sampling. Experiments were carried out at a 1:1 glycerol:acid molar ratio, and the initial reaction volume was 30 mL. The mixture was incubated at 65 ºC for 4 hours. The lipase concentration was 1,6% of the reagent weight. When solvent was used, 15 mL of reagents were prepared with the same molar ratio and lipase concentration, and 15 mL of toluene was added.

In order to measure the carboxylic acid conversion, samples were taken in time intervals with an automatic pipette. These aliquots were diluted in 15 mL of an ethanol/ethyl ether 50:50 (v/v) mixture and titrated with KOH solution in ethanol using phenolphthalein as the endpoint indicator.

To calculate the initial reaction rate, the conversion was plotted against time; then, a non-linear regression was used to fit the curve and the derivative at time zero was determined. Finally, the rate was expressed as a function of the enzyme weight and the initial concentration of acid.

3. RESULTS AND DISCUSSION:

Figure 1. shows the results for the conversion of the eight acids. Under these conditions, the upper molecular weight acids (from C8 to C18:1) reached equilibrium due to the activity of the enzyme. In previous work, reactions with the same molar ratio and without catalysis at 100 °C did not extend conversion above 20%, except for C1 and C2 (***Table 1***). Therefore, blank reactions were carried out for C1 and C2 at 65 °C to verify the lipase activity in these cases, and the blank curves were similar to reaction curves (***Figure 2.)***

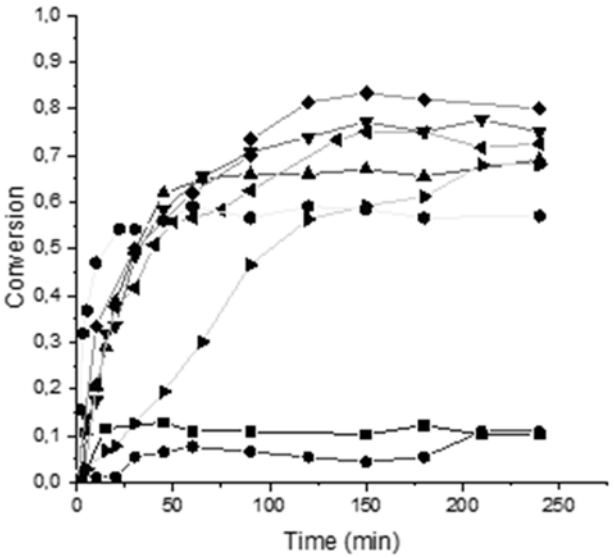


Figure 1. Acid conversion vs. time. C_1(⬢) C_2 (■) C_5 (●) C_8 (▲) C_{10}(▼) C_{12}(◆) C_{18}(◄) $C_{18:1}$(►)

Table 1. *Acid conversion for enzymatic and blank reactions at 65°C and 100°C after 4 h.*

Acid	$X_{1,6\%\ CaLB\ -\ 65°C}$	$X_{Blank-100°C}$	$X_{Blank-65°C}$
C1	0,59	0,55	0,59
C2	0,10	0,60	0,10
C5	0,11	0,16	
C8	0,69	0,11	
C10	0,75	0,20	
C12	0,80	0,18	
C18	0,73	-	
C18:1	0,68	-	

These results indicate that the enzyme did not catalyze reactions with acids from C1 to C5. This behavior corresponds to the number of phases at the beginning of the reaction. The

systems were biphasic when increasing the molecular weight of the acids due to the increment of the hydrophobicity, starting from C8. Therefore, the enzyme showed high activity in two-phase systems with non-polar substrates, but the activity was low or negligible in polar systems, probably due to the hydrophobicity of the natural lipase substrates. Smaller acids had a polar behavior and higher acidity, negatively affecting the enzyme activity. Furthermore, some authors compared different solvents concluding that less polar media increases lipase activity whereas hydrophilic solvents interfere with the interactions between the substrate and the active site of the enzyme (Dutta Banik *et al.*, 2016; Li *et al.,* 2010). The reactions with C2 and C5 were carried out to test these hypotheses, adding toluene as a non-polar solvent. ***Figure 3.*** shows that conversion increased from 11% to 34% for C5 and from 10% to 24% for C2.

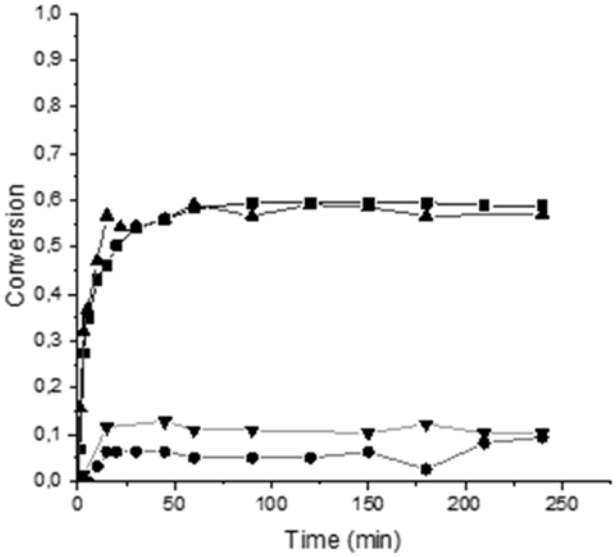


Figure 2. Effect of enzyme catalysis in light acid conversion at 65°C

C_1 blank (■) C_2 blank(●) C_1 (▲) C_2(▼)

For the analysis three groups of acids could be identified: light acids: C1, C2, and C5; medium acids: C8, C10, and C12; and heavy acids: C18 and C18:1. ***Figure 4.*** shows the initial reaction rate of all of them.

C1 exhibited the highest initial rate, but the enzyme did not affect the reaction, as mentioned before. Then, in this case, the rate is the effect of its higher reactivity as a reagent and not as a substrate of the enzyme. C2 showed the same initial rate with and without solvent, and C8 only exceeded it. However, the conversion was much lower than the rest of the acids. The initial reaction rate with toluene was higher for C5 than without solvent. Nevertheless, it was the lowest except for the unsaturated acid. C5 is the only acid with a second functional group; this keto group may interact with the active site causing an inhibition (Dutta Banik *et al.*, 2016).

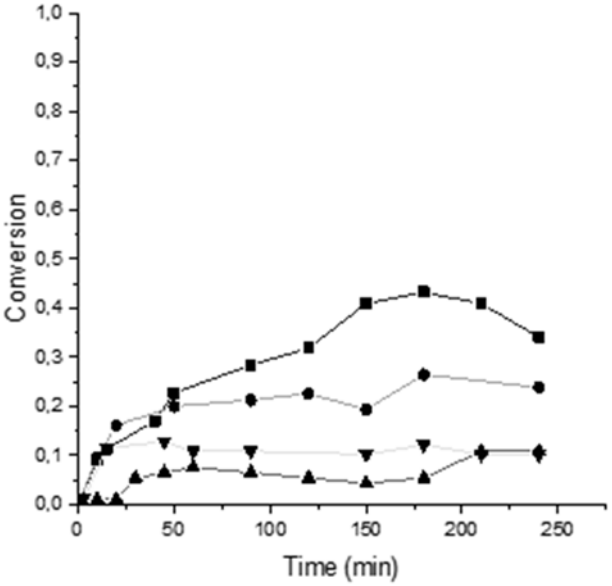


Figure 3. Influence of solvent in acid conversion

C_5 toluene (■) C_2 toluene(●) C_5 (▲) C_2(▼)

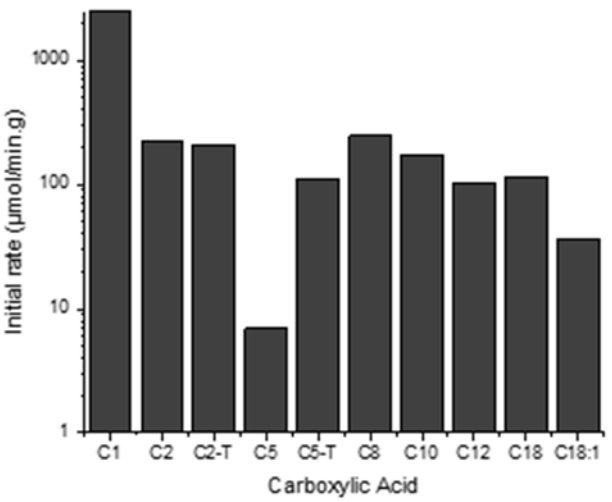


Figure 4. Initial rate in enzyme catalysis reaction. C2-T and C5-T reactions with toluene.

In the medium acids group, it was observed that the higher the molecular weight, the lower the reaction rate, but the final conversion values showed the opposite behavior (***Table 1***). C18 disrupted this tendency because it exhibited a higher rate and lower conversion in comparison to C12. Nevertheless, the conversion was near to the latter. Regarding the enzyme activity over saturated and unsaturated acids, it was observed that the presence of a double bond reduces the

initial rate, probably due to steric hindrance.

4. CONCLUSIONS:

A better understanding of the performance of enzymatic esterification reactions between different carboxylic acids and glycerol was achieved. Systems without solvent were used for acids from C1 to C18:1. The enzymatic catalysis did not work in single-phase systems with high polarity. However, this behavior changed when a non-polar solvent increased the conversion and reaction rate for C1, C2, and C5 acids. On the other hand, the less polar acids which initially form biphasic systems with glycerol showed acceptable conversions and similar reaction rates. These results indicate the need for a non-polar media or a biphasic character to activate the enzyme at the reaction conditions studied in this work.

5. REFERENCES:

1. Dutta Banik, S., Nordblad, M., Woodley, J. M., Peters, G. H., *ACS Catalysis*, **2016**, 6(10), pp. 6350–6361.

2. Freitas, L., Perez, V. H., Santos, J. C., de Castro, H. F., *Journal of the Brazilian Chemical Society*, **2007**, 18(7), pp. 1360–1366.

3. Janssen, A. E. M., Van der Padt, A. and Riet, K. V. t, *Biotechnology and Bioengineering*, **1993**, 42(8), pp. 953–962.

4. Kristensen, J. B., Xu, X. and Mu, H., *JAOCS,* **2005**, 82(5), pp. 329–334.

5. Li, C. Tan, T., Zhang, H., Feng, W. and, *Journal of Biological Chemistry*, **2010**, 285(37), pp. 28434–28441.

6. Silvestrini, L., Cianci, M., *International Journal of Biological Macromolecules*. Elsevier B.V., **2020**, 158, pp. 358–363.

7. Stergiou, P. Y., Foukis, A., Filippou, M., Koukouritak, M., Parapouli, M., Theodorou, L. G., Hatziloukas, E., Afendra, A., Pandey, A., Papamichael, E. M., *Biotechnology Advances*, **2013**, 31(8), pp. 1846–1859.

8. Zheng, Y., Chen, X., Shen, Y., *Chemical Reviews*, **2008**, 110(3), p. 1807.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

Effect of molar weight of carboxylic acids on the enzymatic esterification of glycerol

Maricel Santos; Alexis Velez; Ivana Magario
Universidad Nacional de Córdoba, Instituto de Investigación y Desarrollo en Ingeniería de Procesos y Química Aplicada

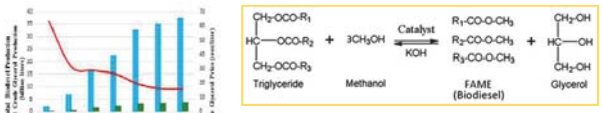
IPQA

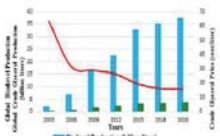
December/2021

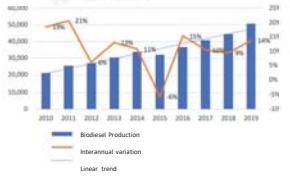
INTRODUCTION

SBJChem Conference 2021

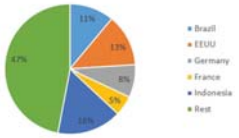
Biodiesel synthesis





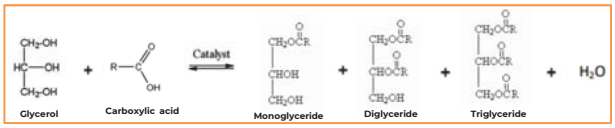


World Production



BACKGROUND AND OBJECTIVE

SBJChem Conference 2021



- Can be catalysed by lipases (Stergiou, 2013)
- Solvent-free systems are feasible (Freitas, 2007)
- Lipase source and the solvent influence were studied (Kristensen *et al.*, 2005 ;Dutta Banik *et al.*, 2016)

OBJECTIVE

SBJChem Conference 2021

Eight different carboxylic acids were used to evaluate the influence of molar weight and unsaturations in equilibrium conversion and initial reaction rate using a immobilized lipase B from *Candida antarctica*

Formic - C1
Acetic - C2
Levulinic - C5
Caprylic - C8
Capric - C10
Lauric - C12
Stearic - C18
Oleic -C18:1

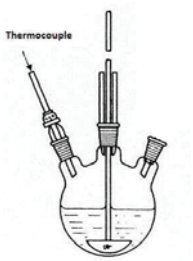
METHODOLOGY

SBJChem Conference 2021

Reaction parameters
T = 65 °C
Agitation= 450 rpm
GLY:AC = 1:1
Enzyme = 1,6% w/w
Solvent* = Toluene
*When was used

Carboxylic acid conversion

Conventional acid titration



5

RESULTS AND DISCUSSION

SBJChem Conference 2021

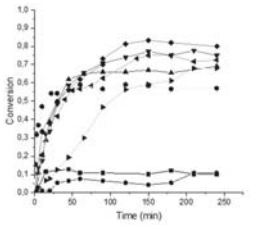


Figure 1. Acid Conversions ● C1 —■— C1 —●— C5 —▲— C8 —▼— C10 —◆— C12 —◀— C18 —▶— C18:1

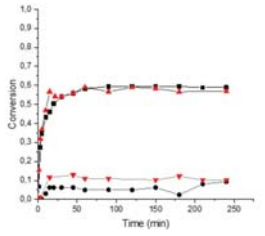


Figure 2. Effect of enzyme catalysis in light acid conversion —■— C1 (Blank) —▲— C1 —●— C2 (Blank) —▼— C2

6

RESULTS AND DISCUSSION

SBJChem Conference 2021

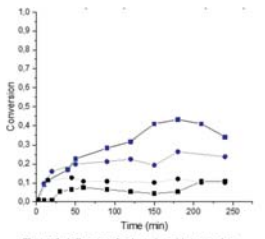


Figure 3. Influence of solvent in acid conversion —■— C5 (Toluene) —■— C5 —●— C2 (Toluene) ● C2

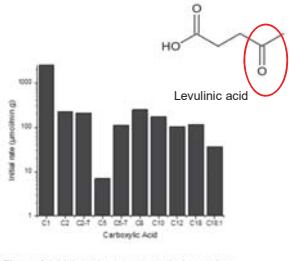


Figure 4. Initial rate in enzyme catalysis reaction. C2-T and C5-T reactions with toluene.

7

CONCLUSIONS

SBJChem Conference 2021

SYSTEMS WITHOUT SOLVENT FOR ACIDS FROM C1 TO C18:1

One phase polar system
C1-C2-C5

Two phase system
C8-C10-C12-C18-C18:1

Toluene added as solvent C2-C5

8

REFERENCES

SBJChem Conference 2021

- Dutta Banik, S. *et al.* (2016) 'A Correlation between the Activity of Candida antarctica Lipase B and Differences in Binding Free Energies of Organic Solvent and Substrate', *ACS Catalysis*, 6(10), pp. 6350–6361. doi: 10.1021/acscatal.6b02073.
- Freitas, L. *et al.* (2007) 'Enzymatic synthesis of glyceride esters in solvent-free system: Influence of the molar ratio, lipase source and functional activating agent of the support', *Journal of the Brazilian Chemical Society*, 18(7), pp. 1360–1366. doi: 10.1590/S0103-50532007000700011.
- Janssen, A. E. M., Van der Padt, A. and Riet, K. V. t. (1993) 'Solvent effects on lipase-catalyzed esterification of glycerol and fatty acids', *Biotechnology and Bioengineering*, 42(8), pp. 953–962. doi: 10.1002/bit.260420806.
- Kristensen, J. B., Xu, X. and Mu, H. (2005) 'Diacylglycerol synthesis by enzymatic glycerolysis: Screening of commercially available lipases', *JAOCS, Journal of the American Oil Chemists' Society*, 82(5), pp. 329–334. doi: 10.1007/s11746-005-1074-5.
- Li, C. *et al.* (2010) 'Analysis of the conformational stability and activity of Candida antarctica lipase B in organic solvents: Insight from molecular dynamics and quantum mechanics/simulations', *Journal of Biological Chemistry*, 285(37), pp. 28434–28441. doi: 10.1074/jbc.M110.136200.
- Silvestrini, L. and Cianci, M. (2020) 'Principles of lipid–enzyme interactions in the limbus region of the catalytic site of Candida antarctica Lipase B', *International Journal of Biological Macromolecules*. Elsevier B.V., 158, pp. 358–363. doi: 10.1016/j.ijbiomac.2020.04.061.
- Stergiou, P. Y. *et al.* (2013) 'Advances in lipase-catalyzed esterification reactions', *Biotechnology Advances*, 31(8), pp. 1846–1859. doi: 10.1016/j.biotechadv.2013.08.006.
- Zheng, Y., Chen, X. and Shen, Y. (2010) 'Erratum: Commodity chemicals derived from glycerol, an important biorefinery feedstock (Chemical Reviews (2008) 108 (5253))', *Chemical Reviews*, 110(3), p. 1807. doi: 10.1021/cr100058u.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EFFECTS OF UTERINE LAVAGE FRACTIONS ON EMBRYO RECOVERY RATE IN MANGALARGA MARCHADOR MARES.

PASSOS, Raiza Argon[1]*; ROIER, Erica Cristina Rocha[1]; GOMES, Letícia Patrão de Macedo[1]; SERAPIÃO, Raquel Varella[1]; GOMES, Gustavo Mendes[1].

[1] Universidade de Vassouras

** Correspondence author*
e-mail: raiza_argon@hotmail.com

Received 20 January 2022; received in revised form 20 February 2022; accepted 26 February 2022

ABSTRACT

Since 1986, the use of embryo transfer has gained prominence in the equine industry, allowing the increase in the number of descendants of genetically superior donors, competition mares, foals, and mares considered subfertile. The success of an embryo transfer program is directly related to the rate of embryonic recovery by mare, which is characterized by the percentage of embryos collected by uterine lavage. However, the recovery rate can be influenced by several factors, type of donor used, age, day of collection, and physical activity. Considering the advancement of biotechnology and the growing need for research in the area of equine embryo transfer, the present work aimed to study in *Mangalarga marchador* animals the effects of uterine lavage fractions on embryo recovery rates. The present study included 35 mares aged between 3 and 15 years, used as donors of clinically healthy embryos from an equestrian property in the southern region of Rio de Janeiro. Thus, 67 uterine washes were performed, where 67% of the embryos were recovered through different volumes of ringer's solution with sodium lactate. The embryo crops and transfers period was from September 2021 to January 2022. For statistical analysis of the data, the simple logistic regression test was used, where no significant difference ($p<0.05$) was observed in the embryo indices recovered on total crops (67) regarding fractions (F) 1 (43.2%), (F) 2 (14.9%) and (F) 3 (5.97%). Thefore, it can be concluded that there was no significant difference between the lavage fractions, however, more studies are needed with a larger sample of uterine washing.

Keywords: *Biotechnologies. Equine. Uterine lavation. Embryonic recovery. Reproduction.*

1. INTRODUÇÃO

Desde 1986 o uso da transferência de embrião tem ganhado destaque na indústria equina, possibilitando o aumento de número de descendentes de doadoras zootecnicamente superiores, de éguas de competição, de potrancas e de éguas consideradas subférteis. Porém, assim como qualquer outra biotecnologia, a TE apresenta algumas limitações. As principais dizem respeito a dificuldade em induzir a superovulação de éguas, elevado percentual de doadoras idosas e manipulação inadequada do sémen (Alvarenga *et al*., 2017).

O sucesso de um programa desta biotecnologia está diretamente relacionado com a taxa de recuperação embrionária por égua, caracterizada pela percentagem de embriões coletados por lavado uterino. Entretanto, a taxa de recuperação pode ser influenciada por vários fatores, como: tipo de doadora utilizada, idade, dia da coleta, atividade física. (Jacob *et al*., 2019).

Segundo Fleury *et al*. (2001) e Imel *et al*. (1981), há diferenças significativas na taxa de recuperação embrionária entre as frações das colheitas, e que o maior número de embriões são recuperados na primeira fração da lavagem.

Considerando o avanço da biotecnologia e a necessidade crescente de pesquisas na área de transferência de embrião em equinos, o trabalho tem por objetivo avaliar o efeito das frações do lavado uterino utilizando de um a três litros de soro ringer com lactato sobre os índices de recuperação de embriões.

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.32_abstract_ARGON.pdf

2. MATERIAIS E MÉTODOS

Foram utilizados 35 equinos, fêmeas, com idades entre 3 e 15 anos, da raça Mangalarga Marchador, utilizadas como doadoras de embriões, clinicamente saudáveis, provenientes de uma propriedade equestre da região Sul Fluminense do estado do Rio de Janeiro.

O período de colheitas e transferências dos embriões foi de setembro de 2021 a janeiro de 2022. As 35 doadoras foram monitoradas através da palpação retal e ultrassonografia. Neste período foram realizados 67 lavados uterinos para realização da recuperação embrionária. As recuperações embrionárias ocorreram no oitavo dia após a ovulação, de forma não cirúrgica, realizando os lavados uterinos em três frações de um litro cada da solução de ringer com lactato de sódio previamente aquecida de 37 a 40 ºC (Alvarenga *et al*., 1993).

Com a égua contida no tronco, foi realizada a lavagem da região perineal com detergente suave e água abundante, seguida da secagem. Desta forma, foi então utilizado um cateter bivona 32 FR, onde o mesmo foi introduzido pela cérvix até o corpo uterino. Este cateter possui um balão na porção anterior, que quando inflado, impede que o meio de lavagem reflua através da cérvix para a vagina. Após bem posicionado o cateter, procedeu-se à introdução do meio de lavagem e sua posterior recolha (Braga *et al*., 2017).

Ao termino de cada fração, o filtro foi desconectado do cateter, desta forma, foram transferidos 20 a 30 ml do meio de lavagem para placas de Petri estéreis. O embrião foi então procurado nas referidas placas, através do rastreamento minucioso, utilizando uma lupa estereoscópica. Os lavados uterinos em que o embrião foi recuperado, foram considerados positivos e aqueles que não foram recuperados, foram considerados negativos (Nogueira *et al*., 2011). No final do procedimento de lavagem do embrião, a égua doadora recebeu prostaglandina-F2α a fim de desencadear a luteólise e induzir um novo estro. (Lopes *et al*., 2013).

A análise estatística dos dados foi realizada por meio do teste de regressão logística simples.

3. RESULTADOS E DISCUSSÃO:

O estudo contou com 35 éguas, realizando 67 lavados, sendo que em 43 (64,18%) deles ocorreu a recuperação de embriões através de diferentes volumes. Foi observado que 29 lavados (43,2%) tiveram seus embriões recuperados no primeiro litro, enquanto 10 lavados (14,9%) no segundo litro e 4 no terceiro litro (5,97%). Não foi possível recuperar os embriões de 24 lavados (35,82%) independentemente do volume utilizado (Tabela 1).

Tabela 1 – Análise do número de embriões recuperados de acordo com o volume em litros (L) de lavado uterino.

Prenhez/volume do lavado	1 L	2 L	3 L
	n (%)	n (%)	n (%)
Lavado positivo (+)	29 (43,2%)	10 (14,9%)	4 (5,97%)
Lavado negativo (-)	24 (35,8%)	24 (35,8%)	24 (35,8%)

Legenda: (+) = prenhez positiva; (-) = prenhez negativa. n = número

A tabela 2 mostra a regressão logística simples das éguas prenhas em relação ao volume de lavado utilizado para recuperação do embrião. Não foi observada diferença estatística entre a recuperação do embrião e a quantidade de vezes em que foi feito o lavado.

Tabela 2 – Regressão logística simples da recuperação de embriões pelo volume de lavado uterino.

Variáveis	Coeficiente de regressão (Coeficiente ± erro padrão)	p-valor
1L x lavado (+)	11.7 ± 30.5	0.70
2L x lavado (+)	10.8 ± 51,9	0.83
3L x lavado (+)	10.7 ± 82.1	0.89

Legenda: (+) = prenhez positiva; (-) = prenhez negativa. L = litros

Analise estatística: Regressão logística simples ($p<0.05$).

Fleury *et al*., (2001), relatou em seu estudo 27% dos embriões recuperados na primeira

fração da lavagem, 15% na segunda e 18% na terceira, assim como Imel *et al*., (1981), que encontraram 52% na primeira, 34% na segunda e 14% na terceira. Ambos apresentaram diferenças significativas nos índices de recuperação embrionária entre as frações das colheitas, diferindo do presente estudo, onde não foram observadas diferenças significativas. No entanto, é preciso levar em consideração o número de lavados realizados, sendo o do presente estudo inferior.

Outro ponto importante, é que apesar de não haver diferença significativa, os três experimentos apresentaram resultados semelhantes, confirmando que a maioria dos embriões são recuperados na 1ª fração da lavagem.

4. CONCLUSÃO:

Conclui-se que não houve diferença significativa entre as frações da lavagem, entretanto, é necessário um estudo com uma amostragem maior de lavado uterino.

5. REFERÊNCIAS:

1. Alvarenga, M. A., and Tongu, E. A. O. Estratégias para melhorar a eficiência reprodutiva em programas de transferência de embrião de equinos. Revista Brasileira de Reprodução Animal, **2017,** 41, 19-24.
2. Jacob, J. C. F., Guerson, Y. B., and Ferraz, P. J. Como melhorar os índices reprodutivos em um programa de transferência de embrião equino. Revista Brasileira de Reprodução Animal, **2019**, 43, 222-228.
3. Fleury, J. J., Pinto, A. J., Marques, A., and Lima, C. G. Fatores que afetam a recuperação embrionária e os índices de prenhez após transferência transcervical em equinos da raça Mangalarga. Brazilian Journal of Veterinary Research and Animal Science, **2001**, 38, 29-33.
4. Imel, K. J., Squires, E. L., Elsden, R. P., and Shideler, R. K. Collection and transfer of equine embryos. Journal of Animal Veterinary Medical Association, **1981**, 179, 987-991.
5. Alvarenga, M. A., Landim e Alvarenga, F. C., and Meira, C. Modification in the technique used to recovered equine embryos. Equine Veterinary Journal, Suppl, **1993**, 15, 111-112.
6. Braga, R. L., and Crusco, S. E. Transferência embrionária em equinos: Método não cirúrgico baseado na técnica ultrassonográfica de injeção ultra uterina. PUBVET, **2017**, 11, 143-148.
7. Nogueira, I. V., Gomes, L. P. M., Athayde, F. P., Dornelas, G. N., and Gomes, G. M. Influência do Clima na Recuperação Embrionária em Éguas da Raça Mangalarga Marchador no Município de Vassouras- RJ. Revista de Saúde, **2011**, 2, 27-34.
8. Lopes, E. P., Pinho, R. O., Siqueira, J. B., Rocha, A. N., Pereira, J. V. T. N., Martins, L. F., Freitas, B. W., and Guimarães, J. D. Correlação dos fatores que interferem na eficiência reprodutiva de éguas mangalarga marchador em programas de transferência de embriões. Revista Brasileira de Medicina Veterinária, **2013**, 35, 69-75.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EFFECTS OF UTERINE LAVAGEM FRACTIONS ON THE EMBRYONIC RECOVERY RATE IN MANGALARGA MARCHADOR MARES.

Raiza Argon Passos
University of Vassouras, Brazil.

Erica Cristina Rocha Roier
University of Vassouras, Brazil.

Letícia Patrão de Macedo Gomes
University of Vassouras, Brazil.

Raquel Varella Serapião
University of Vassouras, Brazil.

Gustavo Mendes Gomes
University of Vassouras, Brazil.

December/2021

INTRODUCTION

SBJChem Conference 2021

EMBRYO TRANSFER

- Highlight of embryo transfer in the equine industry;
- Factors that affect the success of this biotechnology;
- Growing need for research in the area;

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

The study aims to evaluate the effect of uterine lavage fractions using one to three liters of ringer serum with sodium lactate on embryo recovery rates.

METHODOLOGY

SBJChem Conference 2021

- Animals used;
- Period of embryo collections and transfers;
- Preparation of mares;
- Uterine washed;
- Embryo tracking;
- Statistical analysis of the data;

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 1 – analysis of the number of embryos recovered according to the volume in liters (L) of uterine lavage.

Pregnancy/volume of the wash	1 L	2 L	3 L
	n (%)	n (%)	n (%)
Positive washed (+)	29 (43,2%)	10 (14,9%)	4 (5,97%)
Negative washed (-)	24 (35,8%)	24 (35,8%)	24 (35,8%)
Legend: (+) = positive pregnancy; (-) = negative pregnancy. n = number.			

Table 2 – simple logistic regression of embryo recovery for uterine lavagem volume.

Variables	Regression coefficient (Coefficient ± standard error)	p-value
1L x wahsed (+)	11.7 ± 30.5	0.70
2L x washed(+)	10.8 ± 51,9	0.83
3L x washed (+)	10.7 ± 82.1	0.89
Legend: (+) = positive pregnancy; (-) = negative pregnancy. L = liters		
Statistical analysis: simple logistic regression (p<0.05).		

- Fleury et al;
- Imel et al.

CONCLUSIONS

SBJChem Conference 2021

- There was no significant difference between the wash fractions;
- Funther studies with a larger sample of uterine lavage are needed;

6

REFERENCES

SBJChem Conference 2021

1. ALVARENGA, M. A.; et al (2017). Strategies to improve reproductive efficiency in horse embryo transfer programs. *Brazilian Journal of Animal Reproduction, 1* (41): 19-24.
2. JACOB, J. C. F.; et al (2019). How to improve reproductive indices in a program of equine embryo transfer. *Brazilian Journal of Animal Reproduction, 2* (43): 222-228.
3. FLEURY, J. J.; et al (2011). Factors that affect embryo recovery and pregnancy rates after transcervical transfer in Mangalarga Marchador. *Brazilian Journal of Veterinary Research and Animal Science, 1* (38): 29-33.
4. IMEL, K. J.; et al (1981). Collection and transfer of equine embryos. *Journal of Animal Veterinary Medical Association, 10* (179): 987-991.
5. ALVARENGA, M. A.; et al (1993). Modification in the technique used to recovered equine embryos. *Equine Veterinary Journal, Suppl*, (15): 111-112.
6. BRAGA, R. L.; et al (2017). Embryonic transfer in horses: non-surgical method based on the ultrasound technique of ultrauterine injection. *PUBVET, 2* (11): 143-148.
7. NOGUEIRA, I. V.; et al (2011). Influence of climate on embryonic recovery in Mangalarga Marchador mares in the municipality of Vassouras – RJ. *Health Magazine, 1* (2): 27-34.
8. LOPES, E. P.; et al (2013). Correlation of factors that interfere with the reproductive efficiency of Mangalarga Marchador mares in embryo transfer programs. *Brazilian Journal of Veterinary Medicine, 1* (35): 69-75.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ELECTROCHEMICAL CHARACTERIZATION OF GLASSY CARBON ELECTRODES MODIFIED WITH SWCNT FUNCTIONALIZED WITH DIAZONIUM SALT

PICCOLI, María Belén[1], VICO, Raquel Viviana[2], FERREYRA, Nancy Fabiana[1*]

[1] INFIQC, CONICET. Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Fisicoquímica.

[2] INFIQC, CONICET. Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Química Orgánica.

** Correspondence author*
** e-mail: nfferreyra@unc.edu.ar*

Received 20 December 2021; received in revised form 03 January 2022; accepted 14 January 2022

ABSTRACT

Although carbon nanotubes have unique properties, one of the biggest drawbacks in practice is the difficulty in forming dispersions of individual nanotubes in a given solvent. Covalent functionalization of carbon nanotubes allows the incorporation of chemical groups at the nanotube surface that, according to its polarity, facilitates the dispersibility in different solvents. In this work, singled-wall carbon nanotubes were functionalized by spontaneous grafting with a diazonium salt obtained from the 4-aminobenzoic acid to obtain SWCNT-pB. The nanomaterial obtained was characterized by several methodologies that the covalent incorporation of the functional groups. SWCNT-pB were dispersed in ethanol/water 50% V/V under ultrasonic treatment, and the exfoliation degree was evaluated by UV-Vis spectrophotometry. under optimal conditions, SWCNT-pB dispersion was stable for more than 45 days. Glassy carbon electrodes (GCE) modified with the nanomaterial show significant increases in their capacitive current and a faradaic process due to redox species confined on the surface of SWCNT-pB whose anodic peak currents depend linearly with the scan rate. The modified electrodes also show a catalytic response towards ascorbic acid (AA) and notorious increments in the oxidation and reduction currents of H_2O_2. The stability of the dispersions and the excellent electrochemical responses obtained make this nanomaterial very interesting for its application in electrochemical detection.

Keywords: *Single-walled carbon nanotubes, diazonium salt, electrochemistry.*

1. INTRODUCTION

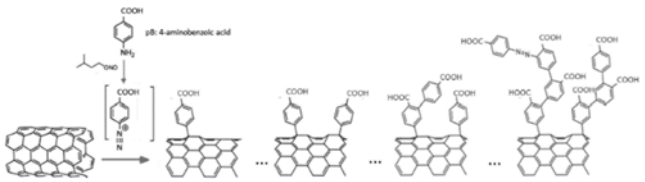
Although carbon nanotubes (CNT) have unique properties, one of the biggest drawbacks in practice is the difficulty in forming dispersions of individual nanotubes in a given solvent. Their hydrophobicity and large surface area make them poorly dispersible. Therefore, different methods have been developed to modify the surface properties of CNT and improve their dispersibility (Bollella & Katz, 2020). Covalent functionalization of CNT includes the chemical modification of the surface by oxidation of C with strong acids, reduction by alkali metals, and incorporating aryldiazonium salts (DS) (Pilan, 2021). The advantage of these methods lies in the better dispersibility and stability of functionalized nanomaterials in different solvents provided by the polarity of the functional groups attached. In addition, the functionalization of CNT with DS makes it possible to achieve a high degree of functionalization by spontaneous grafting of the nanotubes. DS can be obtained from arylamines either in an acid medium or in isopentyl nitrite.

In this work, single-wall carbon nanotubes (SWCNT) were functionalized with the DS obtained from the 4-aminobenzoic acid, as shown in scheme 1. The nanomaterial obtained, SWCNT-pB, was characterized by several methodologies and applied to modify GCE. In addition, the electrochemical responses of different redox probes were analyzed at the modified electrodes to evaluate the possible application of these surfaces as electrochemical transductors for

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com

DOI: 10.48141/SBJCHEM.21scon.08_abstract_FERREYRA.pdf

developing electrochemical enzymatic (bio)sensors.



Scheme 1: *SWCNT functionalization reaction.*

2. MATERIALS AND METHODS

2.1. Reactives

It was used SWCNT of chirality (7, 6) containing more than 77% of nanotubes with (0.7 to 1.1) nm of diameter (Sigma-Aldrich, 704121-16). 4-aminobenzoic acid (pB), anhydrous N,N-dimethylformamide (DMF), acetonitrile, and isopentyl nitrite were also provided by Sigma-Aldrich. All the other reactives were of analytical degree. All solutions were prepared with ultrapure water (18 MΩ cm).

2.2 Functionalization of SWCNT

200.7 mg de SWCNT (16.725 mmol) were dispersed in 50 mL of DMF in an ultrasonic bath for 1 h and then with an ultrasonic probe for 30 min using cycles of 30 s with an amplitude of 60% in an ice bath. 2.7455 g (20.02 mmol) of pB were dissolved in 50 mL of deoxygenated DMF and added to the dispersion of SWCNTs under N_2 flow. To produce de DS, 2 mL of isopentyl nitrite were added. The reaction proceeded for 17 h at 60 °C under stirring. The reaction product was washed exhaustively with DMF and dimethyl ether, filtered under vacuum and dried in an oven to constant weight.

2.3 Equipment

During the syntheses, a Heischer model UP400S probe was used. In addition, a VCX 130W probe from Sonics and Materials with a 3 mm diameter titanium alloy micro-tip was employed to obtain the dispersions. Spectrophotometric determinations were carried out with a Shimadzu UV2600 spectrophotometer and a 0.1 cm optical path quartz cuvette. Raman spectra were obtained with a Horiba Jobin Yvon Model HR 800 UV Raman microscope with a LASER of 632.8 nm. A 100X objective lens (0.7 NA) focused the laser beam and collected the scattered Raman signal. The laser power used 0.48 mW and the acquisition time was 5 seconds for an average of 5 spectra per sample. Cyclic voltammetry (CV) was performed with an Autolab PGSTAT128N potentiostat, and glassy carbon disk electrodes (GCE) of 3 mm diameter (Model CHI104, CH Instruments) were used as substrates. In all experiments, platinum wire and Ag/AgCl,3M NaCl electrodes (Model RE-5B, BAS) were used as counter and reference electrodes, respectively. All reported potentials are referred to this reference electrode.

2.4 Surface modification

GCE was cleaned before each experiment by polishing with alumina powder 0.05 ⌈m for 2 min, followed by sonication in deionized water for 30 s. The electrodes were electrochemically treated by CV applying fifteen consecutive cycles between -0.30 V and 0.80 V at 0.100 Vs^{-1} in 0.10 M, pH 7.0 phosphate buffer (PBS). The electrodes were modified by drop coating with 10 ⌈L of the SWCNT-pB dispersion. The solvent was allowed to evaporate.

3. RESULTS AND DISCUSSION:

Raman spectroscopy was used to characterize SWCNTs and to verify the chemical modification. Figure 1 shows the Raman spectra before (A) and after (B) functionalization. For the analysis, the spectra were adjusted using Lorentzian and Breit-Wigner-Fano (BWF) functions according to previous reports (Ojha *et al*., 2019). From the analysis, a ratio of intensities between the D and G band (I_D /I_G) of (0.042±0.003) and (0.45±0.09) was determined for the SWCNT and SWCNT-pB, respectively. These values indicate an increase in the density of defects due to chemical functionalization. The FTIR spectra of SWCNTs-pB showed the bands corresponding to the symmetric and asymmetric stretching, 1384 and 1657 cm^{-1} respectively, of the deprotonated carboxylic groups bound at the surface of the nanomaterial, confirming the presence of the chemical groups. From thermogravimetric analysis, a degree of functionalization of 21.3% was determined. SWCNTs-pB colloidal dispersions were prepared with 0.50 mg of the modified nanomaterial per mL of solvent (ethanol/water 50/50 V/V) applying ultrasonic treatment for different times, followed by ultracentrifugation at 15000 rpm to decanted the impurities and agglomerated nanotubes. To analyze the effectiveness of the method and select the optimal conditions, the absorbance at 254 nm of 1/10 dilutions of the colloidal dispersions was measured, Figure 2.

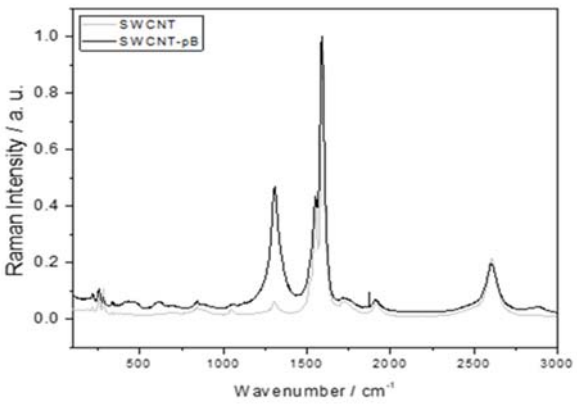


Figure 1: *Normalized Raman spectrum of (A) SWCNT and (B) SWCNT-pB obtained with a 632 nm laser.*

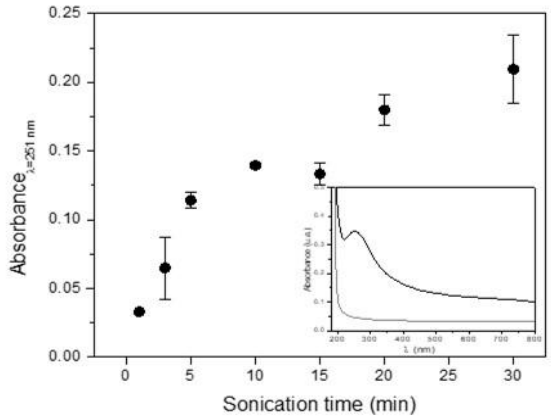


Figure 2: *Variation of Absorbance at 251 nm vs. ultrasound treatment time and pictures of the 1/10 dilutions of the supernatants obtained. The inset graph shows the UV-Vis absorption spectrum of the SWCNT-pB dispersion obtained with 20 min of treatment. Optical path 0.1 cm.*

At short times of ultrasonic treatment, the absorbance is lower due to the fact that the SWCNTs-pB are agglomerated and decant during the centrifugation. Therefore, its concentration in the supernatant is lower. As the sonication time increases, the nanotubes exfoliated in the supernatant increments and absorbance accordingly. From these results 20 min of ultrasonic treatment was selected as the optimal time. The optimized colloidal dispersions were stable for at least 45 days.

The electrochemical response of GCE modified with the optimized dispersion was analyzed by CV. Figure 3 shows the voltammograms obtained at GCE/SWCNT-pB in H_2SO_4 0.5 M at different scan rates. The CVs exhibit a notorious increment of the capacitive current and several anodic and cathodic peaks between 0.0 and 0.8 V. The peak currents at 0.440 V were found to vary linearly with the scan rate, indicating that the redox process was due to redox species confined on the surface of SWCNT-pB. The anodic (E_{pa}) and cathodic (E_{pc}) peak potentials of this process negatively shifted with increasing pH. The peak position depended linearly on the pH range between 2.0 and 10.0, according to the equation E_p = (0.51±0.01) V - (0.060±0.001) pH. The slope value is very close to the theoretical one at 25 °C (0.059 V pH^{-1}) and indicates that the redox process involves the same number of protons as electrons transferred. The peaks observed at GCE/SWCNT-pB electrodes might correspond to a redox process of carboxylic acid groups present at the nanotube surface. The -COOH groups are reduced to -CH_2OH in a four proton/four-electron process. However, the redox processes of quinoid and pyrone groups can not be discarded, and further characterizations should be done for a deeper analysis of the nature of the functional groups at the SWCNT surface.

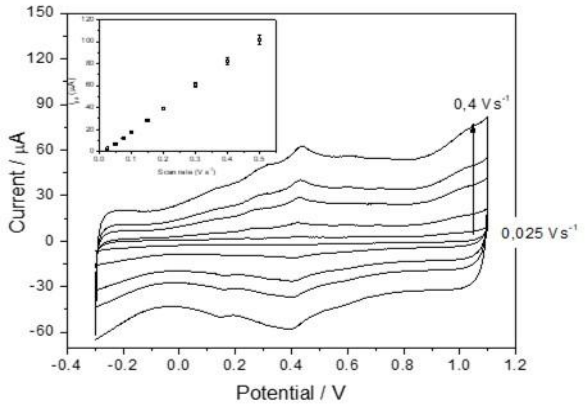


Figure 3: *Cyclic Voltammograms obtained at GCE/SWCNT-pB in H_2SO_4 0.5 M at different scan rates. The inset shows the variation of the peak current at 0.440 V vs. v.*

Ascorbic acid (AA) and H_2O_2 are widely used to evaluate the electrochemical response at CNT-modified electrodes. Figure 4 shows the CVs of AA obtained at GCE/SWCNT-pB with the colloidal dispersion prepared with different sonication times. Compared with bare GCE, the electrooxidation of AA exhibits a decrease of the peak potential as increase the sonication time, In addition, an increment of both capacitive current and peak current of AA is observed due to the increase in the amount of SWCNT-pB deposited on the electrode's surface. The remarkable diminution of the oxidation potential for AA is due

to the catalytic effect of the nanotubes, as it was described by another author(Eguílaz *et al*., 2016).

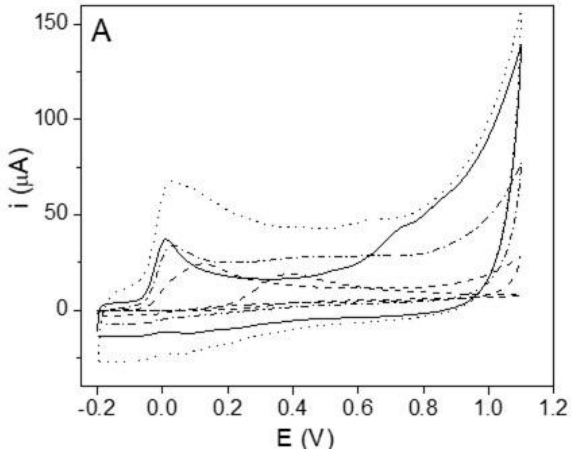


Figure 4: A) *Cyclic Voltammograms of ascorbic acid 1 x 10^{-3} M in phosphate buffer 0.1M pH 7.0 at GCE/SWCNT-pB, v: 100 mVs^{-1}.*

In the field of enzymatic biosensors, the detection of H_2O_2 is very important since this molecule is the by-product of reactions catalyzed by oxidase enzymes.

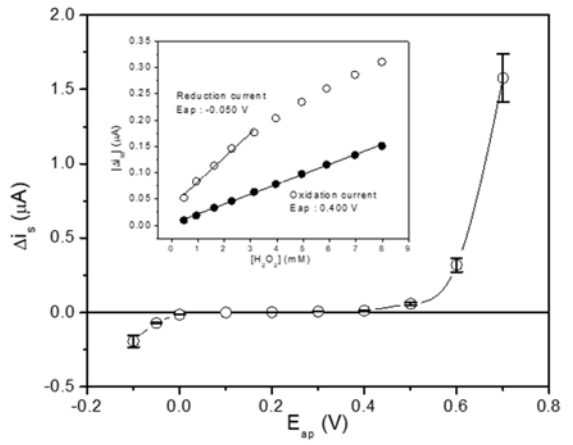


Figure 5: *Hydrodynamic voltammogram of 5.0 x10^{-4} M H_2O_2 at GCE/SWCNT-pB. Inset: Calibration plot at -0.050 V (open symbol) and +0.400 V (full symbol). Supporting electrolyte phosphate buffer 0.1M pH 7.0*

Figure 5 shows the hydrodynamic voltammogram and calibration plots for H_2O_2. The notorious reduction and oxidation currents are associated with the increment of the electroactive area of the electrode, while the decrease of oxidation potential to the presence of carboxylic groups of the functionalized nanotubes.

4. CONCLUSIONS:

SWCNTs were functionalized by spontaneous grafting of the DS from 4-aminobenzoic acid. Raman and thermogravimetry demonstrated the functionalization. FTIR evidenced the presence of carboxylic groups at the SWCNT surface. The dispersion of the SWCNT-pB was optimized in ethanol/water 50% V/V, selecting 20 min of sonication treatment for further studies. The dispersion was stable for more than 45 days. The modified electrodes show significant increases in their capacity, catalytic response towards AA, and notorious increments in the oxidation and reduction currents for H_2O_2.

The electrochemical responses obtained, the stability of the dispersions, and the reproducibility of the system are promising for the immobilization of redox enzymes to develop enzyme biosensors.

5. ACKNOWLEDGMENTS:

The authors thank SECyT-UNC, and Agencia Nacional de Promoción Científica y Tecnológica (ANPCYT) [grant number PICT-2015-0479] for the financial support. M. B. Piccoli, thanks CONICET for the fellowship.

6. REFERENCES:

1. Bollella, P., Katz, E. Methods in Enzymology 1st ed., 2020, 630, 215.
2. Pilan, L. Bioelectrochem., 2021,138, 107697.
3. Eguilaz, M. Gutierrez A, Gutierrez F., Gonzalez-Domínguez J. M. Anson-Casaos A.,Hernandez-Ferrer J. Ferreyra, N. F., Martínez M. T. , Rivas G. (2016), 909, 25, 51.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

ELECTROCHEMICAL CHARACTERIZATION OF GLASSY CARBON ELECTRODES MODIFIED WITH SWCNT FUNCTIONALIZED WITH DIAZONIUM SALT

María Belén Piccoli
Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Fisicoquímica, Instituto de Investigaciones en Fisicoquímica de Córdoba (INFIQC-CONICET)- Argentina.

Raquel Viviana Vico
Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Fisicoquímica, Instituto de Investigaciones en Fisicoquímica de Córdoba (INFIQC-CONICET)- Argentina.

Nancy Ferreyra
Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Departamento de Química Orgánica, Instituto de Investigaciones en Fisicoquímica de Córdoba (INFIQC-CONICET)- Argentina.

CONICET UNC Universidad Nacional de Córdoba
I N F I Q C

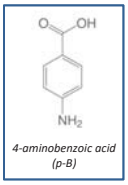
December/2021

INTRODUCTION
SBJChem Conference 2021

- Carbon nanotubes (CNT) have unique properties, but van der Waals interactions make them poorly dispersible in most of the commonly used solvents.
- Grafting of CNT with aryldiazonium salts (DS) makes possible to achieve a high degree of functionalization to improve its dispersibility in various solvents.
- Chemical modification of CNT makes them suitable materials to immobilize enzymes applicable in electroanalysis.

OBJECTIVE
SBJChem Conference 2021

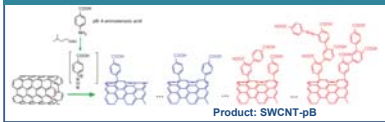
- ★ Functionalize single-walled carbon nanotubes (SWCNT) with the diazonium salt of 4-aminobenzoic acid (p-B).
- ★ Characterize and apply the nanomaterial obtained in the modification of glassy carbon electrodes.
- ★ Analyze the electrochemical responses of different redox probes.



4-aminobenzoic acid (p-B)

METHODOLOGY
SBJChem Conference 2021

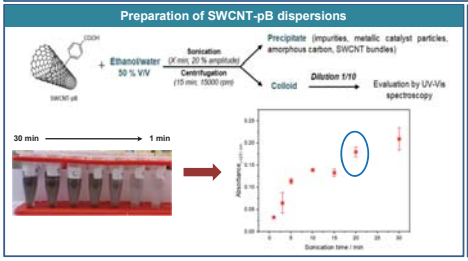
Functionalization of SWCNT with DS from 4-aminobenzoic acid



- ✔ SWCNT was dispersed in DMF.
- ✔ Ratio arylamine/SWCNT: 1.2.
- ✔ Reaction time: 17 h.
- ✔ Temperature: 60 ºC.

Product: SWCNT-pB

Preparation of SWCNT-pB dispersions



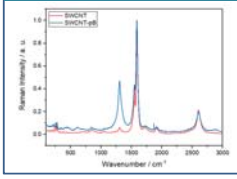
Electrochemical characterization of GCE/SWCNT-pB by CV

- ✔ 0.1 M H_2SO_4.
- ✔ 1 mM ascorbic acid (AA).
- ✔ 0.01 M H_2O_2.
- ✔ Supporting electrolyte: phosphate buffer 0.1 M, pH 7.0.

RESULTS AND DISCUSSION

SBJChem Conference 2021

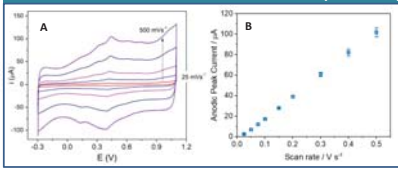
Raman Spectroscopy of SWCNT and SWCNT-pB



Normalized Raman spectrum of (A) SWCNT and (B) SWCNT-pB obtained with a 632 nm laser.

I_D/I_G (SWCNT) = (0.042 ± 0.003)
I_D/I_G (SWCNT-pB) = (0.45 ± 0.09)

Electrochemical response in H_2SO_4



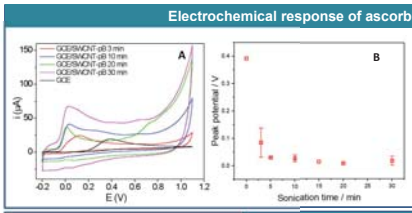
A) CVs at GCE/SWCNT-pB in H_2SO_4 0.1 M.

B) Peak current at 0.440 V vs v.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Electrochemical response of ascorbic acid

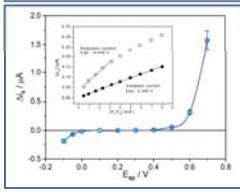


A) CVs of ascorbic acid 1 x 10^{-3} M at GCE/SWCNT-pB. Obtained with different sonication time (st).

B) E_{pa} vs st.

Supporting electrolyte phosphate buffer 0.1M pH 7.0 , v 100 mVs^{-1}.

Electrochemical response of H_2O_2



Hydrodynamic voltammogram of H_2O_2 5.0 x10^{-4} M on GCE/SWCNT-pB.

Inset: Calibration plot for H_2O_2 at -0.050 V (open symbol) and +0.400 V (full symbol).

CONCLUSIONS

SBJChem Conference 2021

- SWCNTs were functionalized by spontaneous grafting with DS from 4-aminobenzoic acid to obtain SWCNT-pB.
- The functionalization was evidenced by Raman, thermogravimetry and FTIR.
- SWCNT-pB were well dispersed in ethanol/water 50% V/V with 20 min of sonication treatment and the dispersion was stable for more than 45 days.
- GC/SWCNT-pB electrodes show high capacitive current, catalytic response towards AA and notorious increments in the oxidation/reduction currents of H_2O_2.
- The electrochemical responses obtained, the stability of the dispersions and the reproducibility of the system are promising characteristics for its application in electroanalytical detection and for the immobilization of redox enzymes.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

- SECyT-UNC.
- Agencia Nacional de Promoción Científica y Tecnológica (ANPCYT) [PICT-2015-0479].
- M. B. Piccoli, thanks CONICET for the fellowship.
- SBJChem organizing committee.

UNC Universidad Nacional de Córdoba

AGENCIA NACIONAL DE PROMOCION CIENTIFICA Y TECNOLOGICA

CONICET

REFERENCES

SBJChem Conference 2021

1. Bollella, P., Katz, E. *Methods in Enzymology* (2020). 1st ed., 2020, 630, 215.
1. Pilan, L. *Bioelectrochemisry*, 2021,138, 107697.
1. Schirowski, M., Hauke, F., & Hirsch, A. (2019) *Chem. Eur. J.* 2019, 25, 12761.
1. Eguilaz, M. Gutierrez A, Gutierrez F., Gonzalez-Domínguez J. M. Anson-Casaos A.,Hernandez-Ferrer J. Ferreyra, N. F., Martínez M. T. , Rivas G. (2016), 909, 25, 51.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EQUINE (*Equus caballus*) INFUNDIBULAR DISEASE: CASE REPORT

NONATO, Manuelly Rufino[1], MORAES, Renata Fernandes Ferreira[2]; ÁVILA, Leticia Meirelles[3]; VIEIRA, Ana Cláudia Tavares[4]; ROIER, Erica Cristina Rocha [2*]

[1] Médica Veterinária autônoma, Vassouras, RJ, Brasil

[2] Universidade de Vassouras, Docente do Mestrado Profissional em Diagnóstico em Medicina Veterinária

[3] Universidade Federal Rural do Rio de Janeiro, Discente do Mestrado em Ciências Veterinárias

[4] Universidade de Vassouras, Discente do Mestrado Profissional em Diagnóstico em Medicina Veterinária

** Correspondence author*
e-mail: roier.erica@gmail.com

Received 10 January 2022; received in revised form 20 January 2022; accepted 03 February 2022

ABSTRACT

Raising horses has become increasingly important over the years, generating great income for breeders and contributing to the economy of the entire country. Dental care with these animals occurs less frequently than necessary, which causes weakness and loss of performance in them. Infundibular disease is a dental disorder, defined as a necrotizing bacteriosis characterized by destroying the inorganic material of the dental tissues, affecting mainly the premolar and molar teeth. This pathology may predispose to other alterations such as colic syndrome, gingivitis, difficulty in feeding, and consequent weight loss, besides resistance in the adaptation to mouth movements, which cause significant losses to the breeders. Its diagnosis is made through anamnesis, general and specific clinical examination of the oral cavity, and complementary exams, such as x-ray. This paper reports the case of a 13-year-old horse weighing about 400 kg of live weight, whose chosen treatment was the extraction of the affected tooth. The study aimed to review predisposing factors, diagnosis, the effects that this clinical change can cause on the animal's organism, and infundibular disease treatment, describing the therapy used and its results.

Keywords: *odontology, surgical treatment, horses, sedatives*

1. INTRODUÇÃO

Os equinos são mamíferos domésticos de dentição heterodonte, isto é, possuem quatro tipos de dentes divididos de acordo com sua função: os incisivos, responsáveis por cortar o alimento; os caninos, que servem para a defesa, caso necessário; e os pré-molares e molares, com a função de esmagar e triturar o alimento. Esses animais também são classificados como difiodontes, ou seja, possuem duas dentições, sendo a primeira chamada decídua, popularmente conhecida como "dente de leite", composta por 24 dentes, e a segunda denominada dentição permanente, com 36 a 44 dentes. Além dessas duas classificações esses animais são ainda denominados hipsodontes, possuem um grande desenvolvimento de coroa e erupção contínua ao longo de sua vida.

Os dentes pré-molares e molares dos equinos possuem invaginações do esmalte, chamadas de infundíbulos, que são preenchidas por cemento e com a função de aumentar a superfície de contato e o atrito, a fim de potencializar a eficiência mastigatória.

A doença infundibular é uma infecção necrosante, conhecida popularmente como "cárie", que afeta os dentes pré-molares e molares, principalmente, de cavalos mais idosos. É caracterizada pela destruição do material inorgânico dos tecidos dentários através da ação de ácidos provenientes da fermentação microbiana de um substrato, normalmente carboidratos, podendo predispor à ocorrência de

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.16_abstract_NONATO.pdf

fraturas dentárias, além de pulpite e doença periapical.

Os sinais clínicos observados incluem dificuldades na alimentação e na adaptação à embocadura, emagrecimento progressivo, acúmulo de alimentos que podem predispor à gengivite e, em casos mais graves, fístulas maxilares ou mandibulares.

O diagnóstico da doença infundibular inclui anamnese, sinais clínicos gerais e específicos e uma minuciosa inspeção da cavidade oral, associada a exames radiográficos. O tratamento para esta enfermidade é a extração dentária ou tratamento prostético, porém, este último, apenas nos casos com menor gravidade, em que o infundíbulo não foi profundamente afetado.

O presente trabalho teve por objetivo relatar o caso de um equino diagnosticado com doença infundibular, cujo tratamento escolhido foi a cirurgia para extração do elemento dentário acometido.

2. DESENVOLVIMENTO

2.1. Anamnese e exame clínico

Equino, macho, sem raça definida, de 13 anos de idade, pesando cerca de 400 kg, alojado na região de Itaguaí, município do estado do Rio de Janeiro.

Na anamnese foi relatado emagrecimento progressivo do animal e dificuldade na mastigação, com frequente extravasamento do alimento da boca para o cocho de alimentação, além de uma ferida que não cicatrizava no lado esquerdo da mandíbula.

Figura 1. Imagem demonstrando fístula no lado esquerdo da mandíbula do equino. Fonte: Autores.

No exame clínico geral o animal apresentava baixo escore corporal (2/5) e foi possível confirmar a presença da fístula na mandíbula (Figura 1), que drenava material purulento. Os demais parâmetros clínicos se encontravam dentro da normalidade para a espécie equina.

Para o exame clínico específico da cavidade oral o animal foi submetido a sedação com Cloridrato de Detomidina (Dormium V®) na dose de 0,04 mg/kg administrado por via intravenosa. Aproximadamente 5 minutos após a administração do α-2 agonista foi realizada a colocação do espéculo oral modelo “Open Light”, com o animal devidamente contido em tronco próprio para a espécie.

A inspeção da cavidade oral constatou alteração no elemento dentário 308 (Figura 2) compatível com fratura, indicando possível comprometimento ósseo, além de Pontas Excessivas de Esmalte Dentário (PEED) na borda vestibular da arcada superior.

Baseado nos dados obtidos no exame clínico da cavidade oral foi solicitado exame radiográfico realizado nas posições látero-lateral direita e esquerda.

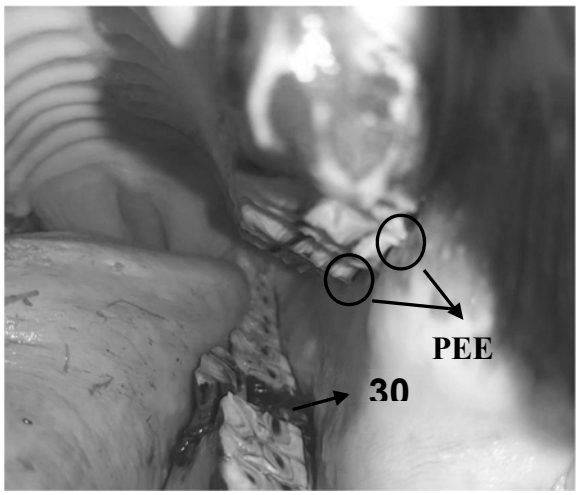


Figura 2. Cavidade oral demonstrando fratura do elemento dentário 308 e PEED. Fonte: Autores

Na análise das imagens radiográficas (Figura 3) foi possível detectar fratura de linha sagital até o limite da raiz dentária no terceiro pré-molar (308); reação periosteal na raiz dentária do terceiro pré-molar (308); área de absorção com remodelação óssea no osso mandibular na subárea dos dentes pré-molares; partes moles e seios nasais sem alterações dignas de nota.

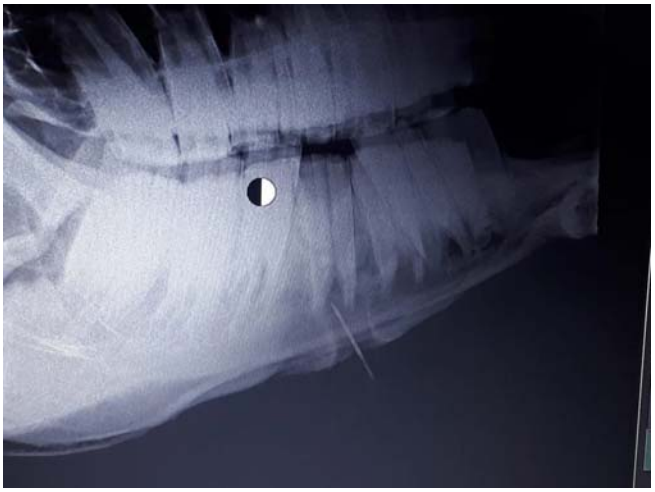


Figura 3. Radiografia látero-lateral esquerda, evidenciando o caminho da fístula. Fonte: Autores.

Com os dados obtidos na anamnese, no exame clínico específico da cavidade oral e nas imagens radiográficas foi possível estabelecer o diagnóstico de doença infundibular. O tratamento proposto para este caso foi a exodontia intraoral do elemento 308 e curetagem do alvéolo e tecidos adjacentes.

Para o procedimento o animal foi submetido a sedação com Cloridrato de Detomidina (Dormium V®) na dose de 0,04 mg/kg administrada por via intravenosa e analgesia com Butorfanol (Butorfin 1%®) na dose de 0,1 mg/kg via intravenosa. Para o bloqueio local do nervo mandibular foram utilizados 20 mL de Cloridrato de Lidocaína (Lidovet®). Após colocação do espéculo oral o procedimento foi realizado com a utilização fórcepses extratores, sondas odontológicas e alavancas apicais para o rompimento dos ligamentos periodontais e posterior retirada do fragmento dentário, seguida pela curetagem do alvéolo. A região foi coberta com curativo de silicone de modelagem protética.

No pós operatório foi administrado 2,0 mg/kg de Ceftiofur Sódico (Excenel®), por via intramuscular, SID, durante sete dias; 25 mg/kg de Metronidazol (Flagyl®), via intravenosa, BID durante cinco dias e Meloxicam (Maxican® Injetável) na dose de 0,6 mg/kg via intravenosa, SID, durante cinco dias.

A troca do curativo de silicone foi realizada incialmente a cada 3 dias durante os quinze primeiros dias após o procedimento e semanalmente nas 3 semanas posteriores, totalizando oito substituições. A completa cicatrização do alvéolo e alta do paciente ocorreu após oito semanas da realização da extração.

3. DISCUSSÃO:

A odontologia equina vem crescendo e demonstrando ser uma importante ferramenta para melhorar a performance e qualidade de vida desses animais. A fim de evitar o desenvolvimento de doenças mais graves são necessárias avaliações periódicas semestrais (Botelho *et al*., 2007), entretanto muitos proprietários e/ou tratadores somente buscam atendimento especializado quando o animal já está bastante debilitado e necessitando de uma intervenção mais séria, como relatado neste trabalho.

Segundo Alencar-Araripe *et al*. (2013) perda de peso, dificuldade de mastigação e emagrecimento são os principais sinais verificados nas odonpatias em geral, inclusive na doença infundibular. No animal relatado esses sinais estavam presentes além da fístula drenante, ocasionada pelo agravamento da enfermidade, o que confirma a longa evolução do processo.

A doença infundibular é diagnosticada mais frequentemente em cavalos idosos e, alimentados com concentrados (Jacques *et al*., 2017). O equino do nosso relato, com 13 anos de idade já se encaixa nessa categoria e de acordo com Pizzigatti *et al.,* (2014), existe uma relação entre a idade desses animais e o aparecimento dessa condição, pois existe uma diminuição no potencial de erupção e mudanças na angulação dos dentes molares e redução da força mastigatória.

O diagnóstico precoce possibilita a adoção de tratamentos conservativos, como Jacques *et al.,* (2017) que relataram o caso de um equino de 15 anos de idade diagnosticado com cárie infundibular durante atendimento médico veterinário de rotina, cujo tratamento proposto foi a restauração do elemento dentário, mantendo assim as características anatômicas e funcionais do mesmo a fim de evitar a proliferação da cárie. No nosso relato o diagnóstico foi realizado após uma longa evolução do caso, sendo o tratamento proposto a extração dentária pela técnica intraoral. Lima *et al*. 2019 relatam este tratamento como bastante comum, podendo ser realizado por meio da trepanação óssea, bucotomia lateral ou exodontia intraoral, sendo esta última a mais utilizada por ser menos invasiva, de menor custo e gerar menos complicações no pós-operatório.

O protocolo de sedação e analgesia utilizado foi bastante satisfatório, possibilitando a realização do procedimento. Este mesmo protocolo é frequentemente usados por outros

autores, como Leandro (2014).

De acordo com Alencar-Araripe *et al*. (2013), é recomendado o uso de antibiótico de largo espectro e anti-inflamatório, reforçando o tratamento proposto pelo médico veterinário deste relato feito com Ceftiofur, Metronidazol e Meloxicam

4. CONCLUSÃO:

Após avaliação rigorosa e diagnóstico correto de doença infundibular, a técnica de exodontia intraoral realizada corretamente por profissional capacitado e com materiais adequados resulta quadro pós-cirúrgico satisfatório, evitando maiores complicações ao paciente. Nota-se também a importância da rotina de avaliação odontológica semestral, que possibilita o diagnóstico precoce de problemas da cavidade oral, antes de seu agravamento e a adoção de tratamentos mais conservativos.

6. REFERÊNCIAS:

1. Alencar-Araripe, M. G., Costa, A. C. H., Costa, B. O., Castelo-Branco, D. S. C. M., Nunes-Pinheiro, D. C. S. **(2013)** *Rev Bras Hig San An,* 7: 288-300.
2. Botelho, D. L. M., Cesar, J. A. W., Filadelpho, A. L. **(2007)** *Rev Cient Med Vet, ano IV, n.8.*
3. Jacques, T. S., Dietrich, L. O., Raupp, S. M. M. **(2017)** *Rev Acad Ci An*, 5: 363-364.
4. Leandro, E. E. S., Goulart, L. T., Dantas, F. T. D., Costa, M. S., Pinto, F. A., Tinôco, A. A. C., Brandão, D. C. **(2014)** *Rev Ed Cont Med Vet Zoot. CRMV-SP*, 13: 74-74.
5. Lima, G. R. F., Filho, N. M. P., Silva, A. T. S., Mendes, A. B. S., Araripe, M. G. A. **(2019)** *Ci An*, 29: 37-40.
6. Pizzigati, D., Martins, C. F., Curcio, B., Nogueira, C. E. W., Esteves, R. S. P., Batista, F. A., Muller, T. R. **(2014)** *J Vet Dent,* 31(3): 178-182.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EQUINE (*Equus caballus*) INFUNDIBULAR DISEASE: CASE REPORT

Manuelly Rufino Nonato
Veterinary Doctor, Vassouras, Brazil

Renata Fernandes Ferreira de Moraes
Universidade de Vassouras, Professional Master's in Diagnosis in Veterinary Medicine, Brazil

Leticia Meirelles Ávila
Universidade Federal Rural do Rio de Janeiro, Master's student in Veterinary Science, Brazil

Ana Cláudia Tavares Vieira
Universidade de Vassouras, Professional Master's in Diagnosis in Veterinary Medicine, Brazil

Erica Cristina Rocha Roier
Universidade de Vassouras, Professional Master's in Diagnosis in Veterinary Medicine, Brazil

March, 2022

INTRODUCTION and BACKGROUND

SBJChem Conference 2021

- Infundibular disease
- Periapical disease, pulpite and dental fractures
- Clinical signs
- Diagnosis
- Treatment: prosthetic or dental extraction

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

- ✓ Horse diagnosed with infundibular disease
- Anamnesis
- General and specific clinical examination
- Image exam
- Treatment
- Result

DEVELOPMENT

SBJChem Conference 2021

- Equine, male, SRD, 13 years old
- General clinical examination
- Low body score (2/5)
- Fistula in the mandible that drained purulent material.
- The other clinical parameters were within the normal range for the equine species.

Source: Authors

DEVELOPMENT

SBJChem Conference 2021

- Examination of the oral cavity change in tooth 308 compatible with fracture, Excessive Enamel Tips (PEED) on the buccal edge of the upper arch

Source: Authors

5

DEVELOPMENT

SBJChem Conference 2021

X-ray - right and left side-to-side positions

Source: Authors

6

RESULTS AND DISCUSSION

SBJChem Conference 2021

Sedation:

- Detomidine Hydrochloride (Dormium V®) 0.04 mg/kg IV
- Butorphanol (Butorfin 1%®) 0.1 mg/kg IV
- Local block of the mandibular nerve - 20 mL of Lidocaine Hydrochloride (Lidovet®).

Procedure

Post operative

- Ceftiofur Sodium (Excenel®) 2.0 mg/kg, IM, SID, 7 days
- Metronidazole (Flagyl®) 25 mg/kg, IV, BID 5
- Meloxicam (Maxican® Injectable) 0.6 mg/kg IV, SID, 5 days

7

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Silicone dressing change: 3/3 days for 15 days and 7/7 days for 21 days
- Discharge: 8 weeks after the extraction

Source: Authors

8

CONCLUSIONS

SBJChem Conference 2021

- Accurate assessment and diagnosis
- Intraoral extraction
- Importance of the semiannual dental evaluation routine

REFERENCES

SBJChem Conference 2021

1. Alencar-Araripe, M. G., Costa, A. C. H., Costa, B. O., Castelo-Branco, D. S. C. M., Nunes-Pinheiro, D. C. S. **(2013)** *Revista Brasileira de Higiene e Sanidade Animal,* 7: 288-300.
2. Botelho, D. L. M., Cesar, J. A. W., Filadelpho, A. L. **(2007)** *Revista Científica Eletrônica de Medicina Veterinária, ano IV, n.8.*
3. Jacques, T. S., Dietrich, L. O., Raupp, S. M. M. **(2017)** *Revista Acadêmica de Ciência Animal*, 5: 363-364.
4. Leandro, E. E. S., Goulart, L. T., Dantas, F. T. D., Costa, M. S., Pinto, F. A., Tinôco, A. A. C., Brandão, D. C. **(2014)** *Revista de Educação Continuada em Medicina Veterinária e Zootecnia do CRMV-SP*, 13: 74-74.
5. Lima, G. R. F., Filho, N. M. P., Silva, A. T. S., Mendes, A. B. S., Araripe, M. G. A. **(2019)** *Ciência Animal*, 29: 37-40.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EVALUATION OF THE EFFECTIVENESS OF TREATMENT OF THE ORAL MUCOSA WITH PHYTO-OINTMENT BASED ON PHYTOECDYSTEROIDS

TIMOSHIN, Anton*; DOROFEEV, Aleksei; ERSHOV, Kirill;; PUSTOKHINA, Inna; EMELINA, Elena

I.M. Sechenov First Moscow State Medical University (Sechenov University), E.V. Borovsky Institute of dentistry, Department of propaedeutics of dental diseases

** Correspondence author*
e-mail:anton-timoshin007@yandex.ru

Received 06 October 2021; received in revised form 15 December 2021; accepted 18 January 2022

ABSTRACT

An indicator of the health of the human body in the state of the oral mucosa. Mechanical and chemical factors constantly influence it. At the first stage of the study, a comparative analysis of the frequency of various forms of traumatic injuries of the oral mucosa was carried out. The distribution of patients into groups was also carried out, depending on the medicinal product used. Then clinical examinations were carried out. After that, the therapy of traumatic erosive and ulcerative lesions of the oral mucosa began. The developed method for treating traumatic lesions of the oral mucosa with medicine based on phytoecdysteroids provides for the elimination of the traumatic factor, applying ointment based on phytoecdysteroids to the dried out focus twice a day. The use of phyto-ointment leads to complete repair of traumatic erosive and ulcerative lesions of the oral mucosa on average by the eighth day from the start of treatment; a similar effect with the use of "Solcoseryl dental adhesive paste" is achieved by the tenth day, and the gel "Cholisal Dental" - at a later date, which is confirmed in this study. The most significant positive effect on the level of quality of life associated with the effectiveness of treatment of traumatic erosive and ulcerative lesions of the oral mucosa in comparison with the dental “Solcoseryl dental adhesive paste” and the gel “Cholisal Dental” is exerted by phyto-ointment, where a decrease in the total points was recorded. When conducting routine examinations of patients, it is necessary to pay attention to the oral mucosa damage. Moreover, in treating traumatic injuries of the oral mucosa, it is recommended to use phyto-ointment, which contains phytoecdysteroids.

Keywords: *oral mucosa, phytoecdysteroids, erosive and ulcerative lesions, trauma to the oral mucosa.*

1. INTRODUCTION

The condition of the oral mucosa is an indicator of the health of the human body. This is because the mucous membrane of the mouth is often constantly exposed to various influences beyond physiological parameters (Utyuzh *et al*., 2020).

The mucous membrane of the mouth is continuously exposed to various stimuli. Therefore, factors such as mechanical and chemical affect the mucous membrane even when eating. However, due to the enormous strength of immunity: local and general, these factors do not exert much harm since the mucous membrane has good regenerative and protective properties (Ajayi *et al*., 2019, Bokov *et al*., 2020).

In connection with the above, the search for a new modern method of treating traumatic erosive and ulcerative mucous membrane lesions is an important area of therapeutic dentistry and orthodontics.

This study aims to increase the effectiveness of the treatment of erosive and ulcerative lesions of the oral mucosa.

2. MATERIALS AND METHODS

The study involved 110 patients with erosive and ulcerative lesions of the oral mucosa. The local ethics committee (protocol № 05-16) approved the study of Sechenov University. All patients signed voluntary informed consent for the study before the study. The distribution of patients

into groups was carried out depending on the type of drug used (Table 1).

Table 1. *Principle of group formation in the study*

No of group	Medicine name	Number of observations
1	Phyto-ointment	38
2	“Cholisal Dental”	35
3	“Solcoseryl dental adhesive paste”	37

After a clinical examination, photographing the lesion, and cytological examination, therapy of traumatic erosive and ulcerative lesions of the oral mucosa were carried out.

For treatment, phyto-ointment with phytoecdysteroids (group 1), gel “Cholisal Dental” (Jelfa SA, Poland) with a predominant analgesic effect (group 2), and dental paste “Solcoseryl dental adhesive paste”, (Legacy Pharmaceuticals Switzerland, GmbH), mainly with an effect that stimulates regeneration (group 3).

Phyto-ointment was developed jointly by the teams of the Department of Pharmacognosy with the course of botany at the Ryazan State Medical University and the Department of Propedeutics of Dental Diseases of the Sechenov University. The developed phytopreparation has the following composition: 40% alcohol (1: 5) tincture of resinous herbs and rhizomes with roots of leuzea, marigold flowers (calendula), meadowsweet herb taken in mass parts (3: 1: 1) respectively - 30 ml; petrolatum, anhydrous lanolin taken in parts by weight (3: 2) respectively - 68.0 g; essential clove oil - 1.0 g; eucalyptus essential oil - 1.0 g.

"Cholisal Dental" - a medicine for treating ulcerative necrotic and trophic lesions of the oral mucosa. It has a pronounced anti-inflammatory and analgesic effect at the site of application.

“Solcoseryl dental adhesive paste” represents such drugs that stimulate regeneration and have a cytoprotective, membrane-stabilizing, wound-healing effect. However, Solcoseryl dental adhesive paste may cause partial taste changes and swelling in the application area.

After the elimination of the traumatic factor, local application of these medicines was carried out. First, the erosive and ulcerative areas were dried with a cotton swab, on which the medicinal preparation was applied 2 times a day until the complete epithelialization of the traumatic injury.

The distribution of acute and chronic traumatic injuries by observation groups is presented in Table 2.

Table 2. *Distribution of the frequency of acute and chronic erosive and ulcerative lesions of the oral mucosa by observation groups*

No of group	Medicine name	Number of observations	
		Acute	Chronic
1	Phyto-ointment	34	4
2	“Cholisal Dental”	33	2
3	“Solcoseryl dental adhesive paste”	34	3
TOTAL		101	9

Control examinations of patients were carried out at least once every 2-3 days. Cases with severe pain symptoms were observed daily. The treatment was discontinued when complete healing of traumatic erosive and ulcerative lesions of the oral mucosa was established, that is, on the 8-10th day.

All patients were surveyed using a special questionnaire, “Oral Health Impact Profile” (OHIP-14), before and after traumatic injury treatment. The questioning was used to determine the level of quality of life before and after treatment (Sevbitov *et al*., 2020).

The obtained results were processed in the IBMSPSS program, version 21.0.

3. RESULTS AND DISCUSSION:

The degree of edema and hyperemia of the wound surface in patients decreased with time at different rates, depending on the applied therapeutic agent.

The intensity of hyperemia evidenced the disappearance of signs. For example, in group 1 - by the 6th day of observation, group 2 - by the 10th day, and group 3 - by the 8th day. The final disappearance of edema signs in group 1 was on the 8th day of observation and in 2 and 3 - on day 10.

Simultaneously, the statistical significance

($p \leq 0.05$) of the difference between similar average intensity indicators in groups 2 and 3 relatives to the corresponding values in group 1 was recorded starting from the fourth day of observation and further.

The highest rates of decrease in the average point indicators of the intensity of hyperemia and edema were noted in group 1, the lowest - in group 2. Intermediate values of the corresponding indicators were recorded in group 3.

Thus, the three considered medications, signs of hyperemia, and edema in the zone of erosive-ulcerative traumatic lesions of the oral mucosa are most effective and quickly eliminate ointment with phytoecdysteroids.

Compared to the initial data, the most pronounced indicators of the quality of life associated with dental health following the treatment results were stated in the scale "Problems in eating".

Similar but slightly less pronounced changes were recorded following the treatment results in the "Problems of everyday life" scale.

The sum of average points on this scale in group 1 before treatment was 18.0 points, in group 2 - 18.2, and in group 3 - 17.6. However, as a result of treatment, the corresponding indicators in group 1 were determined at the level of 10.4 points, in group 2 - 14.3, and group 3 - 12.8. Thus, as a result, the sum of the average points characterizing the scale "Problems of everyday life" at the end of treatment decreased.

Changes in the indicators of the quality of life associated with dental health determined by the treatment results in the scale "Communication problems" are recorded in the minimum range. The initial sum of mean points on this scale in group 1 before treatment was 4.7 points and in group 2 and 3 - 4.8. However, at the end of treatment, the corresponding indicators in group 1 were determined at the level of 4.3 points, in group 2 - 4.7, and in group 3 - 4.4. Thus, the sum of the mean points characterizing the scale "Communication problems" at the end of treatment decreased compared to the initial indicator.

4. CONCLUSIONS:

It was concluded that the healing time of erosive and ulcerative lesions of the oral mucosa is faster when using phyto-ointment based on phytoecdysteroids than when using “Cholisal Dental” and “Solcoseryl dental adhesive paste” ($p < 0.05$)

An insignificant dependence of changes in the quality of life indicators in relation to treatment methods and outcome, traumatic erosive and ulcerative lesions of the oral mucosa were established.

Changes in the quality of life indicators associated with dental health, determined by the treatment results, in comparison and the initial values were found most pronounced in group 1, where a decrease in the total score from 35.6 to 20.2 (by 43, 3%).

5. REFERENCES:

1. Ajayi TO, Srivedavyasasri R, Nyong EE, Odeniyi MA, Moody JO, Ross SA. Two new phytoecdysteroids from sphenocentrum jollyanum pierre root. *Steroids*. **2019**;150
2. Bokov DO, Sidorova YS, Mazo VK, Bessonov VV. Prospects for the use of spinach (spinacia oleracea L.) containing phytoecdysteroids and polyphenols. *Pharmacogn J*. **2020**;12(2):246-50.
3. Sevbitov A, Davidyants A, Balykin R, Timoshin A, Kuznetsova M. Analysis of the effectiveness of immunotherapy using an autologous complex of immunopeptides in the surgical treatment of periodontitis. *Per Tche Quim*. **2020**;17(35):381-90.
4. Utyuzh AS, Yumashev AV, Isakov EI, Makarov AL, Matveeva EA. Diagnosis and treatment of inflammatory periodontal diseases. *Per Tche Quim*. **2020**;17(34):343-51.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EVALUATION OF THE EFFECTIVENESS OF TREATMENT OF THE ORAL MUCOSA WITH PHYTO-OINTMENT BASED ON PHYTOECDYSTEROIDS

TIMOSHIN, Anton
I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

DOROFEEV, Aleksey
I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

ERSHOV, Kirill
I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

PUSTOKHINA, Inna
I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

EMELINA, Elena
I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

March/2022

BACKGROUND

SBJChem Conference 2021

- An indicator of the health of the human body in the state of the oral mucosa. Mechanical and chemical factors constantly influence it. At the first stage of the study, a comparative analysis of the frequency of various forms of traumatic injuries of the oral mucosa was carried out. The distribution of patients into groups was also carried out, depending on the medicinal product used. Then clinical examinations were carried out. After that, the therapy of traumatic erosive and ulcerative lesions of the oral mucosa began. The developed method for treating traumatic lesions of the oral mucosa with medicine based on phytoecdysteroids provides for the elimination of the traumatic factor, applying ointment based on phytoecdysteroids to the dried out focus twice a day. The use of phyto-ointment leads to complete repair of traumatic erosive and ulcerative lesions of the oral mucosa on average by the eighth day from the start of treatment; a similar effect with the use of "Solcoseryl dental adhesive paste" is achieved by the tenth day, and the gel "Cholisal Dental" - at a later date, which is confirmed in this study.

BACKGROUND

SBJChem Conference 2021

- The most significant positive effect on the level of quality of life associated with the effectiveness of treatment of traumatic erosive and ulcerative lesions of the oral mucosa in comparison with the dental “Solcoseryl dental adhesive paste” and the gel “Cholisal Dental” is exerted by phyto-ointment, where a decrease in the total points was recorded. When conducting routine examinations of patients, it is necessary to pay attention to the oral mucosa damage. Moreover, in treating traumatic injuries of the oral mucosa, it is recommended to use phyto-ointment, which contains phytoecdysteroids.;

METHODOLOGY

SBJChem Conference 2021

The study involved 110 patients with erosive and ulcerative lesions of the oral mucosa. The local ethics committee (protocol № 05-16) approved the study of Sechenov University. All patients signed voluntary informed consent for the study before the study. The distribution of patients into groups was carried out depending on the type of drug used.
Therapy of traumatic erosive and ulcerative lesions of the oral mucosa was carried out after a clinical examination, photographing the lesion, and cytological examination.
For treatment, phyto-ointment with phytoecdysteroids (group 1), gel “Cholisal Dental” (Jelfa S.A., Poland) with a predominant analgesic effect (group 2), and dental paste “Solcoseryl dental adhesive paste”, (Legacy Pharmaceuticals Switzerland, GmbH), mainly with an effect that stimulates regeneration (group 3).
Phyto-ointment was developed jointly by the teams of the Department of Pharmacognosy with the course of botany at the Ryazan State Medical University and the Department of Propedeutics of Dental Diseases of the Sechenov University. The developed phytopreparation has the following composition: 40% alcohol (1: 5) tincture of resinous herbs and rhizomes with roots of leuzea, marigold flowers (calendula), meadowsweet herb taken in mass parts (3: 1: 1) respectively - 30 ml; petrolatum, anhydrous lanolin taken in parts by weight (3: 2) respectively - 68.0 g; essential clove oil - 1.0 g; eucalyptus essential oil - 1.0 g.

METHODOLOGY

SBJChem Conference 2021

"Cholisal Dental" - a medicine for treating ulcerative necrotic and trophic lesions of the oral mucosa. It has a pronounced anti-inflammatory and analgesic effect at the site of application.

“Solcoseryl dental adhesive paste” is a representative of such drugs that stimulate regeneration, have a cytoprotective, membrane-stabilizing, wound-healing effect. Solcoseryl dental adhesive paste in the area of application may cause partial taste changes and swelling.

After elimination of the traumatic factor, local application of these medicines was carried out. The erosive and ulcerative areas were dried with a cotton swab, on which the medicinal preparation was applied 2 times a day until the complete epithelialization of the traumatic injury.

The distribution of acute and chronic traumatic injuries by observation groups.

Control examinations of patients were carried out at least once every 2-3 days. Cases with severe pain symptoms were observed daily. The treatment was discontinued when complete healing of traumatic erosive and ulcerative lesions of the oral mucosa was established, that is, on the 8-10th day.

All patients were surveyed using a special questionnaire “Oral Health Impact Profile” (OHIP-14) before and after traumatic injury treatment. The questioning was used to determine the level of quality of life before and after treatment (Sevbitov *et al.*, 2020).

The obtained results were processed in the IBMSPSS program, version 21.0.

RESULTS AND DISCUSSION

SBJChem Conference 2021

The degree of edema and hyperemia of the wound surface in patients decreased with time at different rates, depending on the applied therapeutic agent.

The disappearance of signs was evidenced by the indicator of the intensity of hyperemia. In group 1 - by the 6th day of observation, in group 2 - by the 10th day, and in group 3 - by the 8th day. The final disappearance of edema signs in group 1 was on the 8th day of observation, and in 2 and 3 - on day 10.

Simultaneously, the statistical significance ($p \leq 0.05$) of the difference between similar average intensity indicators in groups 2 and 3 relatives to the corresponding values in group 1 was recorded starting from the 4th day of observation and further.

The highest rates of decrease in the average point indicators of the intensity of hyperemia and edema were noted in group 1, the lowest - in group 2. Intermediate values of the corresponding indicators were recorded in group 3.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Thus, of the three considered medications, signs of hyperemia and edema in the zone of erosive-ulcerative traumatic lesions of the oral mucosa are most effective and quickly eliminates ointment with phytoecdysteroids.

Compared to the initial data, the most pronounced changes in the indicators of the quality of life associated with dental health following the results of the treatment were stated in the scale "Problems in eating".

Similar, but slightly less pronounced changes were recorded following the results of treatment in the scale "Problems of everyday life".

The sum of average points on this scale in group 1 before treatment was 18.0 points, in group 2 - 18.2, and in group 3 - 17.6. As a result of treatment, the corresponding indicators in group 1 were determined at the level of 10.4 points, in group 2 - 14.3, and in group 3 - 12.8. Thus, as a result, the sum of the average points characterizing the scale "Problems of everyday life" at the end of treatment decreased.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Changes in the indicators of the level of quality of life associated with dental health determined by the results of the treatment in the scale "Communication problems" are recorded in the minimum range. The initial sum of mean points on this scale in group 1 before treatment was 4.7 points, and in group 2 and 3 - 4.8. At the end of treatment, the corresponding indicators in group 1 were determined at the level of 4.3 points, in group 2 - 4.7, and in group 3 - 4.4. Thus, the sum of the mean points characterizing the scale "Communication problems" at the end of treatment decreased compared to the initial indicator.

CONCLUSIONS

SBJChem Conference 2021

It was concluded that the healing time of erosive and ulcerative lesions of the oral mucosa is faster when using phyto-ointment based on phytoecdysteroids than when using “Cholisal Dental” and “Solcoseryl dental adhesive paste” ($p < 0.05$)

An insignificant dependence of changes in the quality of life indicators in relation to the methods and outcome of treatment, traumatic erosive and ulcerative lesions of the oral mucosa was established. Changes in the indicators of the quality of life associated with dental health, determined by the treatment results, in comparison and the initial values were found most pronounced in group 1, where a decrease in the total score from 35.6 to 20.2 (by 43, 3%).

ACKNOWLEDGEMENTS

SBJChem Conference 2021

This work was completed at Sechenov University and supported by the “Russian Strategic Academic Leadership Program”.

REFERENCES

SBJChem Conference 2021

1. Ajayi T.O., Srivedavyasasri R., Nyong E.E., Odeniyi M.A., Moody J.O., Ross S.A. Two new phytoecdysteroids from sphenocentrum jollyanum pierre root. Steroids. 2019;150
2. Bokov D.O., Sidorova Y.S., Mazo V.K., Bessonov V.V. Prospects for the use of spinach (spinacia oleracea L.) containing phytoecdysteroids and polyphenols. Pharmacogn J. 2020;12(2):246-50.
3. Dikhit P.S., Srivastava A., Boyena K.K. Injury to the oral mucosa by organophosphates without systemic toxicity: A rare case. Br J Oral Maxillofac Surg. 2018;56(8):755-7.
4. Dinan L., Balducci C., Guibout L., Lafont R. Small-scale analysis of phytoecdysteroids in seeds by HPLC-DAD-MS for the identification and quantification of specific analogues, dereplication and chemotaxonomy. Phytochem Anal. 2020;31(5):643-61.
5. Gafurovich V.U., Kilichevna K.M. The use of various techniques in the treatment of traumatic injuries of the oral mucosa in children. Eur J Mol Clin Med. 2020;7(3):3743-8.
6. Jurenka R., Russell K., O'Neal M. Phytoecdysteroids as antifeedants towards several beetles that include polyphagous and monophagous feeding guilds. Pest Manage Sci. 2017;73(8):1633-7.
7. Kaçar S.D., Özuğuz P., Ulu Ş., Karaca Ş., Tokyol Ç. Lymphangioma of oral mucosa after chronic trauma: A case report. Turk Dermatoloji Derg. 2013;7(3):158-60.
8. Kharazmi M., Carlsson A-., Hallberg P., Modig M., Björnstad L., Hirsch J-. Surgical approach to snus-induced injury of the oral mucosa. J Oral Sci. 2014;56(1):91-4.
9. Kim S-., Kim Y-., Koh K-, Youn Y-., Suh G-., Cho E-., Leem D-, Baek J-., Shin H-., Ko S-. Activation of NF-κB pathway in oral buccal mucosa during small intestinal ischemia-reperfusion injury. J Surg Res. 2013;179(1):99-105.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EVALUATION OF THE IMPORTANCE OF HOUSEHOLD ENVIRONMENTAL CHARACTERISTICS IN THE DEVELOPMENT OF CANINE VISCERAL LEISHMANIASIS

BELEGOTE, Amanda Alfeld[1*]; FERREIRA, Lucas Leal[1]; SILVA, Laís Freire[1]; DA SILVA, Stephanie Esteves Sant'ana[1]; OLIVEIRA, Glenda Ribeiro de[1.]

[1] Universidade de Vassouras

** Correspondence author*
e-mail: a.abelegote@gmail.com

Received 01 February 2022; received in revised form 30 February 2022; accepted 14 February 2022

ABSTRACT

Visceral leishmaniasis is a zoonosis of great importance due to its incidence and high lethality, and the dog as its main reservoir in urban centers. Furthermore, environmental characteristics such as soil with abundant organic matter can predispose local ecosystems to the development of the vector Lutzomyia longipalpis. This study aimed to carry out a data collection in partnership with the Health Department of the municipality of Vassouras, determining environmental characteristics and favorable means for the dissemination of the sand fly, in an area of 150 meters from a confirmed human case of leishmaniasis in the Itakamosi neighborhood. During the months of October and November 2021, an environmental study was carried out in 7 homes, where a total of 14 dogs lived. Through questionnaires, data were collected regarding the environmental conditions of these homes. It was observed that 100% of the animals lived in households close to the forest and vegetation. Of the 7 households analyzed (6/7), 85,71% had banana trees in their surroundings, followed by the presence of fruit trees, which corresponds to (5/7) 71,42% of households. In contrast, in (3/7), 42,83% and (2/7) 28,57% represent the number of houses with the presence of chicken coops and kennels, respectively. In contrast, in (1/7) 14,28% of the households, there was the presence of organic matter debris, aiding in the sand fly cycle. The animals residing in these houses were tested for leishmaniasis and showed a negative result, but the possibility of future infection of these animals cannot be ruled out, given that these factors corroborate the easy adaptation of the sandfly exploiting the accumulation of organic matter in areas of socioeconomic vulnerability.

Keywords: dogs, phlebotomine, organic matter, environment.

1. INTRODUÇÃO:

A Leishmaniose é uma doença de caráter zoonótico, provocada pelo protozoário *Leishmania chagasi*, e vem se expandindo em larga escala pelo Brasil nos últimos anos, tendo grande prevalência no estado do Rio de Janeiro (SESRJ - Boletim Epidemiológico de Leishmanioses, 2019). De acordo com o Boletim Epidemiológico de Leishmanioses, publicado pela Secretaria de Estado de Saúde do Rio de Janeiro (2019) a maior ocorrência de Leishmaniose Visceral do estado se concentra na região Sul Fluminense (com casos positivos em Barra Mansa, Barra do Piraí e Vassouras). Entre o período de 01/01/2018 e 13/08/2019, houve um caso confirmado, com consequente óbito por Leishmaniose Visceral no município de Vassouras, além da confirmação de 6 cães diagnosticados com a doença durante o mesmo período no município (Contreras, 2019).

O cão (*Canis familiaris*) representa uma importante fonte de infecção para o vetor, uma vez que precede a maioria dos casos nos seres humanos, promovendo a dispersão da doença para áreas não endêmicas (Ministério da Saúde, 2014). O vetor *Lutzomyia longipalpis* se desenvolve em solos ricos em material orgânico e se adapta facilmente ao meio urbano, vivendo em volta ou dentro dos domicílios ou em abrigos animais, como galinheiros, estábulos e pocilgas

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.31_abstract_BELEGOTE.pdf.

(SESRJ - Boletim Epidemiológico de Leishmanioses, 2019). Cães infectados, mesmo quando assintomáticos ou com poucos sintomas, são eficazes na transmissão do parasito ao flebotomíneo e são considerados hospedeiros domésticos (Ministério da Saúde, 2014). Sendo assim, a realização de inquéritos sorológicos em cães é de suma importância por possibilitarem a detecção de reservatórios caninos nas áreas. Além disso, também permitem que sejam detectados focos silenciosos da doença, e viabilizam a delimitação de regiões e locais de maiores casuísticas onde se faz necessário a realização de medidas de controle (Julião FS *et al.*, 2007).

O presente estudo teve o objetivo de avaliar as características ambientais de domicílios de cães testados sorologicamente para leishmaniose visceral**.**

2. MATERIAL E MÉTODOS:

O estudo ocorreu nos meses de outubro à novembro de 2021 no bairro Itakamosi, do município de Vassouras, Rio de Janeiro. O estudo foi realizado em conjunto com a Secretaria Municipal de Saúde do município de Vassouras. Devido à ocorrência de confirmação de um caso positivo para leishmaniose em espécime humano, foi realizado um estudo ambiental em 7 domicílios, com um total de 14 cães previamente testados para LVC em um raio de até 150 metros do caso humano notificado.

Por meio de questionários foram obtidas informações acerca do ambiente em que os animais residiam, contendo dados como a respeito do destino do esgoto (fossas, céu aberto ou rede pública), vegetação ao entorno (Mata, campo, pasto ou plantação) e presença de ambiente favorável ao vetor *Lutzomyia longipalpis* (bananeiras, árvores frutíferas, galinheiro, canil e entulho). Durante a análise dos dados coletados no estudo, utilizou-se o método de avaliação descritiva básica, determinando-se os valores de frequência relativa e os percentuais dos resultados obtidos nas fichas ambientais de cada residência.

3. RESULTADOS E DISCUSSÃO:

Em relação à vegetação no entorno das residências (4/7) 57,14 % das 7 moradias avaliadas estavam próximas a pastos, (3/7) 42,85% próximas à mata, (2/7) 28,57% ao campo e (1/7) 14,28% a plantações. Em relação ao destino do esgoto, as fossas representavam o destino de (4/7) 57,14% das residências, enquanto (3/7) 42,85% tinham como destino a rede pública de esgoto e (1/7) 14, 28% possuíam esgoto a céu aberto. Dentre as características que tornam o ambiente favorável ao vetor, a principal foi a presença de bananeiras representando ¨(6/7) 85,71%, seguido da presença de árvores frutíferas , que corresponde a (5/7) 71,42% dos domicílios , enquanto que (3/7) 42,83% das casas possuíam galinheiro, (2/7) 28,57% possuíam canis e (1/7) 14,28% correspondiam às residências com a presença de entulhos (Figura 1). Árvores e plantações no peridomicílio têm sido tratadas como fatores de risco para surgimento das leishmanioses, por servirem de alimento e abrigo para os flebotomíneos. Estes fatores influenciam a presença desta doença emergente em áreas urbanas, uma vez que o flebotomíneo adapta-se facilmente às condições peridomiciliares em áreas pobres, explorando o acúmulo de matéria orgânica em decomposição. (Moura *et al.*, 2014). A matéria orgânica fornecida pelas bananeiras, árvores frutíferas, galinheiros, canis e entulhos auxilia no ciclo do flebotomíneo (Ministério da Saúde, 2014).

De acordo com o estudo, 100% dos animais avaliados eram domiciliados próximos á mata ou vegetação, o que corroborou para a suspeita, Figura 2. Pesquisas demonstram que a proximidade da moradia dos cães com a mata e vegetação abundante são fatores de risco para a infecção por *Leishmania sp*. (Silva *et al.*, 2005).

Os animais domiciliados nas residências avaliadas neste estudo não estavam infectados por *L. chagasi*, porém não se pode descartar a possibilidade de que os animais desta área não possam eventualmente ser infectados pelo protozoário. Deve-se também levar em consideração o trânsito da população entre a cidade de Vassouras e áreas endêmicas da região do Médio Paraíba e Sul Fluminense, podendo representar alguns casos positivos para LV em humanos (SESRJ-Boletim Epidemiológico Leishmanioses, 2019). Novos estudos de uma área de abrangência maior, a inclusão mais ampla da população, devem ser elaborados para o controle efetivo da leishmaniose no município de Vassouras.

4. CONCLUSÕES:

Tendo em vista gravidade da leishmaniose visceral em animais e seres humanos, percebe-se a importância da vigilância ambiental, pois

existem características ambientais propícias para o desenvolvimento do vetor no município de Vassouras. Considerando que já ocorreram casos prévios de leishmaniose no município, a detecção de potenciais criadouros do flebotomíneo e estímulo políticas públicas que visem eliminá-los são muito importantes para o controle da doença.

5. AGRADECIMENTOS:

Os autores agradecem a Secretaria Municipal de Saúde do Município de Vassouras pelo apoio material e logístico.

6. REFERÊNCIAS:

1. Contreras, I.K., Machado, M.A., Rocha, C.O.J.M., Oliveira, G.R., Carvalho, F.F.G. Sinais clínicos apresentados por cães positivos para leishmaniose visceral no município de Vassouras, Rio de Janeiro. PUBVET, **2019**, 13, 1-6.
2. Julião, F.S., Souza, B.M.P.S., Freitas, D.S., Oliveira, L.S., Larangeira, D.F., Dias-Lima, A.G., Souza, V.M.M., Barrouin-Melo, S.M., Moreira Jr, E.D., Paule, B.J.A., Franke, C.R. Investigation of risk areas as complemental methodology for the control of canine visceral leishmaniasis. Pesquisa Veterinária Brasileira, **2007**, 27, 319-324.
3. MOURA, L. M. A.; MONTE, N. D. P.; SOUSA, R. L. T. Nível dos Conhecimentos Sobre as Leishmanioses Visceral e Tegumentar pela População de Alguns Bairros de Teresina, Piauí, Brasil. Journal of Health Sciences, 2015, 17, 21-30.
4. Silva A.V.M., Paula A.A., Cabrera M.A.A., Carreira J.C.A. Leishmaniose em cães domésticos: aspectos epidemiológicos. Caderno de Saúde Pública, **2005**, 21, 324-328.
5. Pimentel, M. I. F. Cenário Epidemiológico: Leishmanioses em humanos no estado do RJ. SES-RJ -Boletim Epidemiológico Leishmanioses. RJ. Nº 001. GERÊNCIA DE DOENÇAS TRANSMITIDAS POR VETORES E ZOONOSES – GDTVZ, **2019**.
6. Ministério da Saúde. Manual de Vigilância e Controle da Leishmaniose Visceral. Ministério da Saúde, **2014**, 1ª Edição.

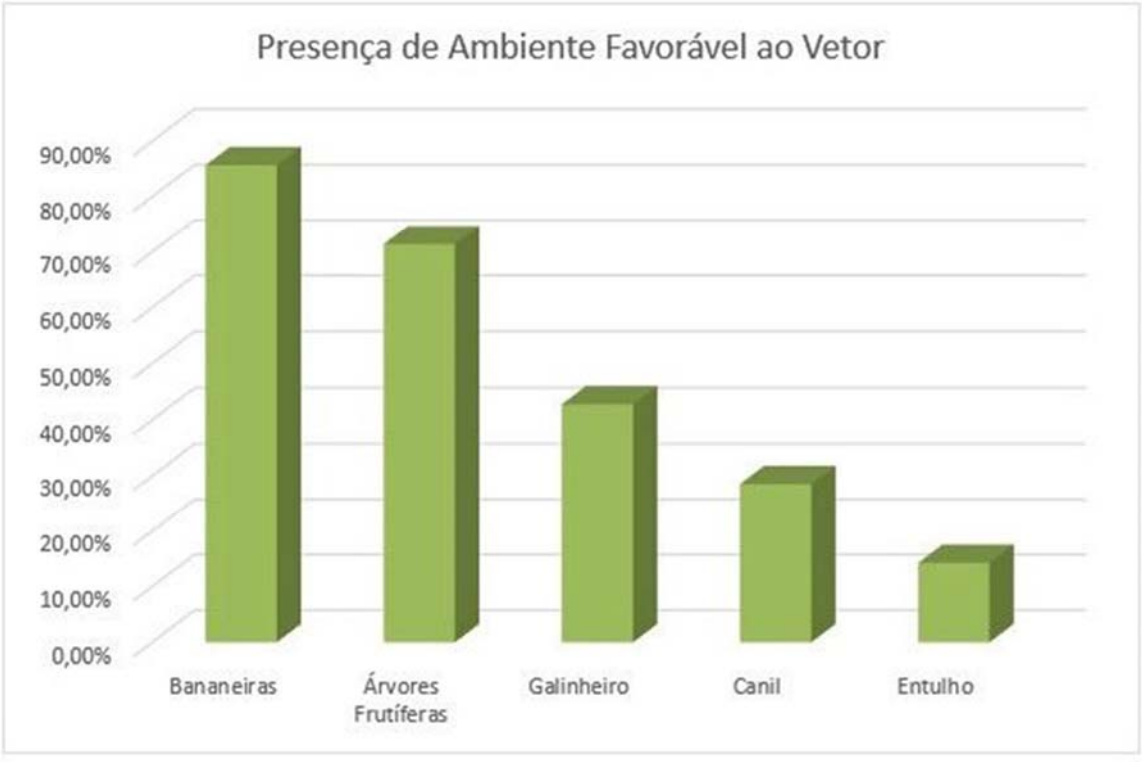


Figure 1. *Dados relacionados a presença do ambiente favorável ao vetor obtidos no segundo semestre de 2021.*

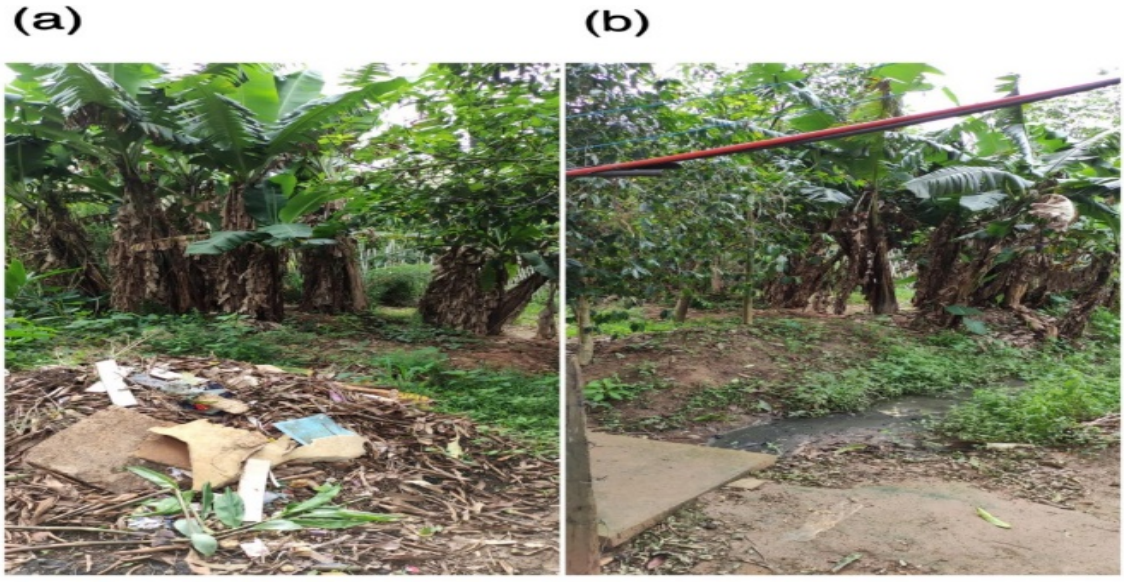


Figure 2. *Ambientes adequados para os flebotomíneos. (a) Foto retirada na avaliação ambiental da área com entulho. (b) Habitat propício para os flebotomíneos com presença de bananeiras, árvores frutíferas e fossa.*

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EVALUATION OF THE IMPORTANCE OF HOUSEHOLD ENVIRONMENTAL CHARACTERISTICS IN THE DEVELOPMENT OF CANINE VISCERAL LEISHMANIASIS

Amanda Alfeld Belegote
Universidade de Vassouras, Veterinary Medicine - Brazil.

Lucas Leal Ferreira
Universidade de Vassouras, Veterinary Medicine - Brazil.

Laís Freire e Silva
Universidade de Vassouras, Veterinary Medicine - Brazil.

Stephanie Esteves Sant'Ana da Silva
Universidade de Vassouras, Veterinary Medicine - Brazil.

Glenda Ribeiro de Oliveira
Universidade de Vassouras, Veterinary Medicine - Brazil.

March/2022

INTRODUCTION

SBJChem Conference 2021

- Canine Visceral Leishmaniasis (CVL)
- Constantly growing zoonotic disease in Brazil
- Adaptation of the vector to the urban environment

Source: MINISTÉRIO DA SAÚDE, 2014.

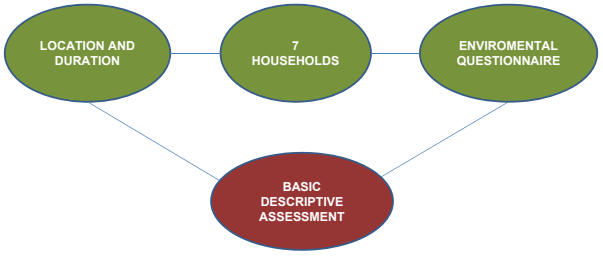
AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

Evaluation of the home environmental characteristics of dogs serologically tested for canine visceral leishmaniasis (CVL).

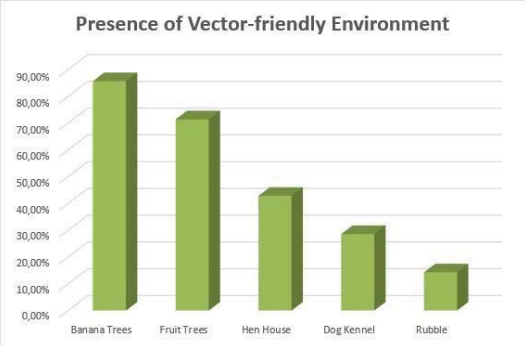
METHODOLOGY

SBJChem Conference 2021



RESULTS AND DISCUSSION

SBJChem Conference 2021



5

RESULTS AND DISCUSSION

SBJChem Conference 2021

Houses near to:	Percentage (%)
Pastures	57,14
Woods	42,85
Field	28,57
Plantations	14,28
Sewage destination in:	
Cesspol	57,14
Public service	42,85
Open sewage	14,28

6

RESULTS AND DISCUSSION

SBJChem Conference 2021

Source: PERSONAL FILE.

7

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Vegetation in the peridomicile are risk factors
- Traffic of the population in different cities in the southern region of Rio de Janeiro
- Negative animals

8

CONCLUSIONS

SBJChem Conference 2021

- Importance of environmental surveillance
- Environments conducive to vector development
- Need for public policies

9

ACKNOWLEDGEMENTS

SBJChem Conference 2021

We thank the Municipal Health Department of the municipality of Vassouras for logistical support to obtain the information.

10

REFERENCES

SBJChem Conference 2021

1. CONTRERAS, IRIS KRAUSE *ET AL.* (2019). **Sinais clínicos apresentados por cães positivos para leishmaniose visceral no município de Vassouras, Rio de Janeiro.** PUBVET, V.13, N.4, A302, P.1-6.
2. Moura LMA. (2014). Nível dos Conhecimentos Sobre as Leishmanioses Visceral e Tegumentar pela População de Alguns Bairros de Teresina, Piauí, Brasil. Universidade Estadual do Piauí, Núcleo de Pesquisa em Zoologia e Biologia Parasitária, Programa de Pós-Graduação em Ciência Animal,PI,Brasil.
3. Silva AVM, Paula AA, Cabrera MAA, Carreira JCA. (2005). Leishmaniose em cães domésticos: aspectos epidemiológicos. Caderno de Saúde Pública 21:324-328.
4. PIMENTEL, M. I. F. (2019). Cenário Epidemiológico: Leishmanioses em humanos no estado do RJ. Boletim Epidemiológico Leishmanioses. RJ. Nº 001. GERÊNCIA DE DOENÇAS TRANSMITIDAS POR VETORES E ZOONOSES – GDTVZ.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EXPERIMENTAL STUDY OF THE INFLUENCE OF TEMPERATURE ON PASTEURIZATION OF *PÊRA RIO IN NATURA* ORANGE JUICE

GALIASSI, Gabriela Regina Rosa [1*]; RAMIREZ, Maribel Valverde [1]

[1,2] Universidade Federal de Mato Grosso, Faculdade de Engenharia

**Correspondence author*
e-mail: gabigaliassi@gmail.com

Received 19 October 2021; received in revised form 10 November 2021; accepted 15 November 2021

ABSTRACT

Heat treatment is one of the most used methods to preserve food, such as orange juices, which are an excellent source of ascorbic acid. To avoid vitamin C degradation and reduce loss, fast heating is recommended. This work aimed to determine the vitamin C content using the iodometric method and the convective heat transfer coefficient using the method of dimensionless numbers and the experimental method. Time and temperature were controlled throughout the experiment. In pasteurization, the solution was heated to 80 °C, heating lasted 50 minutes and cooling for 42 minutes. The convective heat transfer coefficient was evaluated in two regions of the cylindrical container: near the wall and in the central region. The graphic profile of the curve follows the same trend of the literature. The convective heat transfer coefficient is higher in the region near the wall. As time passes and temperature decreases, the central region tends to equilibrium, and the coefficient becomes more constant. The vitamin C content remained constant before and after pasteurization, so it was observed that the pasteurization did not cause ascorbic acid degradation since the heating step was fast in the heat treatment. As a result of the study, it was noted that studying the thermal behavior in the cooling of orange juice is extremely important to ensure its quality. It is pertinent to mention that in order to avoid this degradation and reduce its loss, it is necessary that in thermal treatments, fast heating is carried out and that the juice has low exposure to air and heat at the time of its preparation.

Keywords: *Heat Transfer. Pasteurization. Orange Juice. Convective Coefficient.*

1. INTRODUCTION

The citrus industry is an extremely important sector for the Brazilian economy, as the country is responsible for 34% of the fruits and 56% of the juice produced in the world. Furthermore, the orange is the most consumed fruit by the Brazilian population, and among the different cultivars is the Pêra Rio orange (Citrus sinensis L. Osbeck) (Leonello *et al.,* 2019).

Heat treatment is one of the most used methods to preserve food, such as orange juice, increasing its shelf life. However, little is known about the temperature and speed profiles during heat treatment of liquid food in commercial packaging (Ghani *et al.*, 2001).

Pasteurization is a process used in foods when the aim is to destroy pathogenic microorganisms and denature low heat resistance enzymes present in foods. In addition, another goal is to increase the shelf life of the food. The process consists of heating the food to a certain temperature and time and subsequently cooling it to a temperature lower than the previous one (Potter; Hotchikiss, 1995). The literature presents three types of pasteurization, and for orange juice, HTST (High Temperature and Short Time) is used (Jing *et al.*, 2013).

Orange juice is an excellent source of ascorbic acid, commonly known as Vitamin C, and belongs to the water-soluble vitamins. The quality of the juice can be influenced when it is exposed to oxygen and light, which can reduce the Vitamin C content and sensorially modify the product. To avoid vitamin C degradation and reduce loss, fast heating and low exposure to air are recommended when preparing the juice. Proper storage of the juice, which should be at low temperatures, helps preserve vitamin C and does not darken the juice. If the juice is kept between 15 ºC and 25 ºC, there will be a significant loss of Ascorbic Acid (Cozzolino, 2012; Teixeira; Monteiro, 2006).

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.02_GALIASSI.pdf

It is possible to find in the literature studies about heat transfer during pasteurization and about food cooling. Teruel *et al.* (2003), experimentally studied the cooling of *valência* oranges with forced air and water. In the chilled water system, cooling occurred uniformly and lasted about 57 minutes. Jing *et al.* (2013) carried out a theoretical study of temperature distribution through pasteurization for orange juice in a cylindrical container based on 3D CFD simulation. Pasteurization for orange juice was simulated at three different temperatures, and the temperature field in each was obtained. Data were compared, and an optimal computational model was obtained for this case.

Also, Maharramov (2021) studied the thermal conductivity of orange and tangerine juices in a non-steady state. The author states that all known experimental installations measure the thermal conductivity of liquids in a steady-state, even if in the production and processing of liquid food products, as a rule, the main substance is in a mobile state.

This work aims to determine the vitamin C content using iodometric method and the convective heat transfer coefficient using the method of dimensionless numbers and the experimental method in the pasteurization of orange juice.

2. MATERIALS AND METHODS

The juice was prepared and placed in a 200 mL cylindrical glass container, sealed. To control the temperature during the experiment, thermometers (Brax Tecnologia, model -10 + 110 ºC) and a stopwatch were used. The vitamin C content was analyzed before and after the pasteurization using iodometric method.

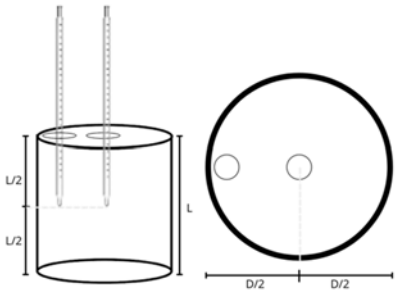


Figure 1. *Representation of the system used to control temperature and analysis regions*

The juice was heated in a water bath, and the temperature was recorded every 2 minutes.

The water bath was already heated to 80 ºC when the juice was placed in the bath. When the central region of the container with orange juice reached 74 ºC, heating was stopped.

Then, cooling was performed, where the sample was placed inside a stainless steel pan with ice. The variation in juice temperature was monitored using thermometers, which were already installed in the cylindrical container, and this was measured every 2 minutes. When the center of the juice container reached 6 °C, cooling was stopped. Next, the bath was cooled to 0 °C.

3. RESULTS AND DISCUSSION:

3.1. Temperature Profile in pasteurization

In this study, pasteurization lasted 92 minutes, where heating lasted 50 minutes and cooling 42 minutes.

It is possible to observe in Figure 2 that the two regions presented practically the same temperature variation. In the literature of Bhuvaneswari (2014) and Priest; Stewart (2006), the profile of the curve follows the same trend.

3.2. Convective Heat Transfer coefficient in pasteurization

In this research, heat transfer was analyzed in the cooling stage. Under these conditions, the concentrated capacity method is applied. In the wall region, heat transfer via conduction in a transient regime was used, where the concentrated capacity method was applied, given that the number of Biot was less than 0.1. In the central region of the container, Newton's theory of cooling was used. In both regions, the convective heat transfer coefficients were determined.

To determine the convective coefficient in the wall region, the thermophysical properties used in the calculations were those of glass. To determine the convective coefficient in the central region, the thermophysical properties of the fluid were used, in this case, the orange juice.

It is possible to observe in Figure 3 that the convective heat transfer coefficient is higher in the region near the wall, and there is a sharp drop in the convective coefficient curve in the wall region. This is because the temperature is very high at this moment, as it is the period when cooling starts, so the value is lower. As time passes and temperature decreases, the central region tends to equilibrium, and the coefficient becomes more constant. The standard deviation for the convective coefficient in the central region and in the wall region were 3.99 and 16.74, respectively.

Regarding the vitamin C content, it remained constant before and after pasteurization.

4. CONCLUSIONS:

It was possible to observe that both the region of the center of the container and the region of the wall have similar temperature variations, which agree with the profiles found in the literature. The convective heat transfer coefficient is higher in the wall region and tends to equilibrium over time.

It was observed that the pasteurization did not cause ascorbic acid degradation since the heating step was fast in the heat treatment. In order to avoid this degradation and reduce its loss, it is necessary that in thermal treatments, fast heating is carried out and that the juice has low exposure to air and heat at the time of its preparation. Therefore, studying the thermal behavior in the cooling of orange juice is extremely important to guarantee its quality.

5. REFERENCES:

1. Bhuvaneswari, E.; Anandharamakrishnan, C.; *Innov Food Sci Emerg Technol.*, **2014**, *23*, 162.
2. Cozzolino, S.M.F.; *Biodisponibilidade de nutrientes*, 4th ed; Manole: São Paulo, Brazil, 2012.
3. Ghani, A.G.A.; Farid, M.M.; Chen, X.D.; Richards, P.; *Journal of Food Engineering*, **2001**, *48*, 147-156.
4. Jing, X.; Yong-yan, L.; Jin-feng, W.; Yi, T.; Chen, M.; *Advanced Materials Research*, **2013**, *740*, 245.
5. Leonello, E.C.; Esperancini, M. S. T.; Guerra, S.P.S.; *Citrus Res. Technol.*, **2019**, *40*, e1043.
6. Maharramov, M.A.; *E3S Web of Conferences*, **2021**, *254*.
7. Potter, N.N.; Hotchikiss, J.H.; *Food Science*, 5th ed; Chapman and Hall: New York, USA, 1995.
8. Priest, F. G., & Stewart, G. G.; *Handbook of Brewing*, 2nd ed; CRC Taylor and Francis Group: Boca Raton, USA, 2006.
9. Teixeira, M.; Monteiro M.; *Alimentos e Nutrição*; Araraquara, Brazil, 2006, ch.14.
10. Teruel, B.; Cortez, L.; Neves Filho, L.; *Ciênc. Tecnol. Aliment.*, **2003**, *23(2)*, 174-178.

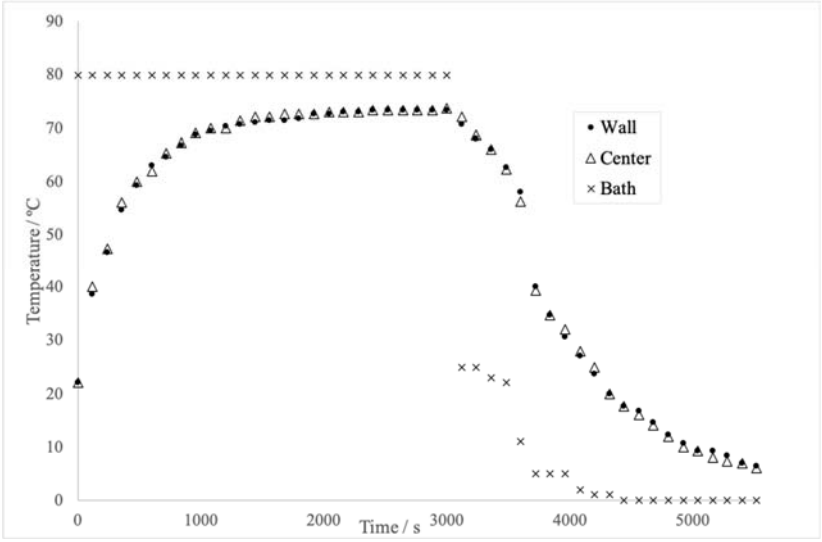


Figure 2. *Time-temperature behavior during pasteurization*

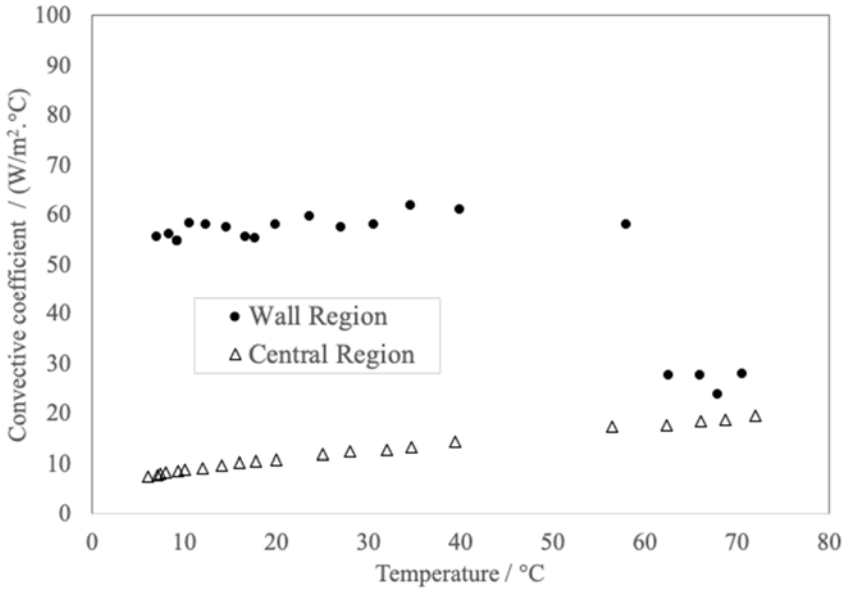


Figure 3. *Convective heat transfer coefficient in the cooling stage*

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EXPERIMENTAL STUDY OF THE INFLUENCE OF TEMPERATURE ON PASTEURIZATION OF *PÊRA RIO IN NATURA* ORANGE JUICE

Gabriela Regina Rosa Galiassi
Universidade Federal de Mato Grosso, Faculdade de Engenharia - Brazil.

Maribel Valverde Ramirez
Universidade Federal de Mato Grosso, Faculdade de Engenharia - Brazil.

March/2021

INTRODUCTION

SBJChem Conference 2021

- Citrus Industry: extremely important sector for Brazil (responsible for 34% of the fruits and 56% of the juice produced in the world;
- Heat treatment is one of the most used methods to preserve food: increase its shelf life;
- Little is known about the temperature and speed profiles during heat treatment of liquid food in commercial packaging;
- Pasteurization: HTST;
- Orange juices are an excellent source of ascorbic acid: To avoid vitamin C degradation and reduce loss, fast heating and low exposure to air are recommended when preparing the juice.

BACKGROUND

SBJChem Conference 2021

Literature: other studies about heat transfer during pasteurization and about food cooling:

- Teruel *et. al.* (2003);
- Jing *et. al.* (2013);
- Maharramov (2021).

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

This work aims to determine the vitamin C content using iodimetric method and the convective heat transfer coefficient using the method of dimensionless numbers and the experimental method in the pasteurization of orange juice.

METHODOLOGY

SBJChem Conference 2021

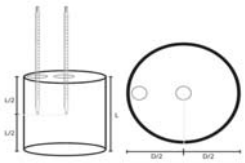


Figure 1. *Representation of the system used to control temperature and analysis regions*

- Temperature: monitored every 2 minutes.
- Water bath: already heated to 80 ºC;
- Central region reached 74 ºC, stop heating;
- Cooling: center reached 6 °C, stop cooling;
- Bath was cooled to 0 ºC.
- 200 mL cylindrical glass container, sealed;
- Thermometers (Brax Tecnologia, model -10 + 110 ºC);
- Stopwatch;
- Vitamin C content analized before and after the pasteurization: iodimetric method.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Temperature Profile in pasteurization

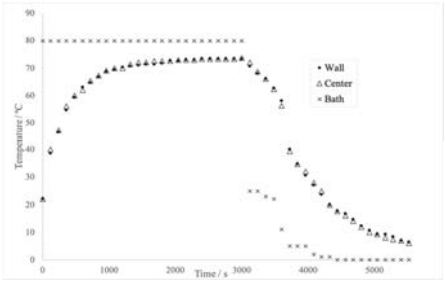


Figure 2. *Time-temperature behavior during pasteurization*

RESULTS AND DISCUSSION

SBJChem Conference 2021

Convective Heat Transfer coefficient in pasteurization

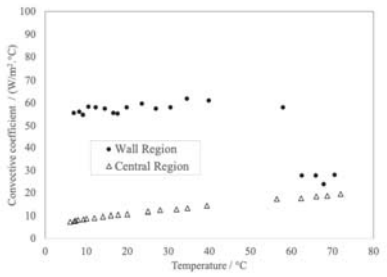


Figure 3. *Convective heat transfer coefficient in the cooling stage*

RESULTS AND DISCUSSION

SBJChem Conference 2021

Vitamin C content: remained constant before and after pasteurization.

CONCLUSIONS

SBJChem Conference 2021

- The region of the center of the container and of the wall have similar temperature variations, corresponding to the profiles found in the literature;
- Convective heat transfer coefficient is higher in the wall region and tends to equilibrium over time;
- The pasteurization did not cause ascorbic acid degradation;
- Studying the thermal behavior in the cooling of orange juice is extremely important to guarantee its quality.

REFERENCES

SBJChem Conference 2021

1. Bhuvaneswari, E.; Anandharamakrishnan, C. (2014). Heat transfer analysis of pasteurization of bottled beer in a tunnel pasteurizer using computational fluid dynamics. *Innov Food Sci Emerg Technol.*, *23*, 162.
2. Cozzolino, S.M.F. (2012). Biodisponibilidade de nutrientes, 4th ed; Manole: São Paulo, Brazil.
3. Ghani, A.G.A.; Farid, M.M.; Chen, X.D.; Richards, P. (2001).Thermal sterilization of canned food in a 3-D pouch using computational fluid dynamics. *Journal of Food Engineering*, *48*, 147-156.
4. Jing, X.; Yong-yan, L.; Jin-feng, W.; Yi, T.; Chen, M. (2013). Theoretical Study of Temperature Distribution though Pasteurization for Orange Juice Based on 3D CFD Simulation. *Advanced Materials Research*, *740*, 245.
5. Leonello, E.C.; Esperancini, M.S.T.; Guerra, S.P.S. (2019). Rentabilidade da produção familiar de laranja Valência: estudo de caso no município de Mogi Guaçu – SP. *Citrus Res. Technol*., *40*, e1043.
6. Maharramov, M.A. (2021). Investigation of thermal conductivity of orange and tangerine juices in non-stationary state. *E3S Web of Conferences*, *254*.
7. Potter, N.N.; Hotchikiss, J.H. (1995). *Food Science*, 5th ed; Chapman & Hall: New York, USA.
8. Priest, F. G., & Stewart, G. G. (2006). *Handbook of Brewing*, 2nd ed; CRC Taylor and Francis Group: Boca Raton, USA.
9. Teixeira, M.; Monteiro M. (2006). Degradação da vitamina C em suco de fruta. *Alimentos e Nutrição*; Araraquara, Brazil, ch.14.
10. Teruel, B.; Cortez, L.; Neves Filho, L. (2003). Estudo comparativo do resfriamento de laranja valência com ar forçado e com água. *Ciênc. Tecnol. Aliment*., *23(2)*, 174-178.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EXTRACTION, PURIFICATION, AND COMBINATION OF LAPACHOL IN NOVEL EUROPIUM COMPLEX

SILVA, Andrei Marcelino Sá Pires[1*]; MENEZES, Jorge Fernando Silva de[1]; ALMEIDA, Edna Aparecida Faria de[2];

[1] Universidade Federal do Recôncavo da Bahia, Centro de Formação de Professores, Curso de Lic. Em Química, Brasil

[2] Escola Técnica Estadual Júlio de Mesquita, Brasil

** Autor correspondente*
e-mail: and123rei@gmail.com

Received 12 February 2022; received in revised form 26 February 2022; accepted 03 March 2022

ABSTRACT

Lapachol belongs to the group of 1,4-naphthoquinones, with the addition of a hydroxide group attached to carbon 2 and a branched alkene nomenclature 3-methyl-2-butenyl attached to carbon 3, with final nomenclature 2-hydroxy-3 -(3-methyl-2-butenyl)-1,4-naphthoquinone. As a chromophore, it exhibits near-ultraviolet absorption, one of the important characteristics in the process of choosing ligands to integrate photoluminescent lanthanide complexes. Photoluminescent materials are currently widely used in the market for making plates, paints, plates, tapes, pigments, and other luminescent equipment. The use of what are called DMCLs (Molecular Light Converting Devices) is increasing in Photovoltaic Cells, Optical Luminescent Tracers, Forensic Chemistry, Fluoroimmunoassays, and more. Knowing the great demand for these devices, it is feasible to study and characterize new compounds that have favorable emission characteristics and that allow their use in the aforementioned categories. For this, the use of lanthanides is a great proposal, and the application of a chromophore ligand, such as Lapachol, aims to provide an increase in the emission of the final product. In the present work, the extraction, a new purification process of Lapachol from its natural source, the Ipê Roxo wood, is reported, as well as the characterizations that attest to the feasibility of the new process, in addition to the use of the material as a binder in lanthanide complexes.

Keywords: *Lapachol, Naphtoquinone, Lanthanide, Complex, Coordination Compounds*.

1. INTRODUÇÃO

O lapachol, de nomenclatura IUPAC 2-hidroxi-3-(3-metil-2-butenil)-1,4-naftoquinona, é um composto orgânico natural pertencente ao grupo das naftoquinonas. Está presente no cerne de árvores da família *Bignoniaceae*, gênero *Tabebuia* (S; P; RAGHAVENDRA, 2011), entre as quais pode-se citar Pau d'Arco, Peúva e outras, além de outros ipês, sendo que em sua maioria atualmente são admitidos como pertencentes ao gênero *Handroanthus*, mas foram antes pertencentes ao gênero *Tabebuia*. As árvores desses grupos possuem características muito singulares, como a coloração de suas folhas, como ipê roxo e ipê amarelo, porém algo em comum é a coloração da madeira, que pode ser considerada marrom-avermelhado ou roxo (CAMPÊLO DA FONSECA FILHO *et al.,* 2017). São arvores típicas da Amazônia, mas que podem ser encontradas em áreas de Cerrado, com exemplo da Bahia.

Para este trabalho, o complexo proposto apresenta um ligante orgânico (Lapachol) com elevada absortividade molar (ε ~ 18 000 M^{-1} cm^{-1}) e um lantanídeo (Európio) com baixa absortividade molar (ε < 1 M^{-1} cm^{-1}) (MOORE; SAMUEL; RAYMOND, 2009). Dessa maneira, o ligante pode atuar como sensibilizador de luminescência, possibilitando a absorção e transferência eficiente de energia para o Centro Emissor (CE). Isso potencializa o rendimento quântico de emissão desde que os níveis energéticos do ligante orgânico sejam superiores ao do Centro Metálico. Este processo é conhecido

como Efeito Antena (MOORE; SAMUEL; RAYMOND, 2009). Tais moléculas são altamente estáveis devido a formação de quelatos já que as naftoquinonas possuem mais de um sítio de ligação, sendo eles as carboxilas (os lantanídeos são oxifílicos), produzindo-se assim complexos com alta estabilidade química (KAI; PAULO, 2009; SANTOS, 2008).

Deste modo, o objetivo do presente trabalho é a extração do Lapachol a partir da serragem da madeira de Pau d'Arco, sua purificação via novo método elaborado e sua combinação com o sistema $Eu(DBM)_3$, formando assim um novo complexo, que será posteriormente aplicado como biomarcador químico.

2. MATERIAIS E MÉTODOS

2.1.1 Extração Do Lapachol

Dissolveu-se cerca de 200g de serragem de Pau d'Arco em 1L de solução saturada de bicarbonato de sódio, até a formação de uma solução vermelho intensa. Agitou-se por 45 minutos, e filtrou-se a solução descartando o sólido. Adicionou-se ao líquido cerca de 50mL de ácido clorídrico gota a gota, até a solução vermelha tornar-se amarela com precipitado. Filtrou-se a vácuo e descartou-se o líquido. Nesta etapa, obteve-se o lapachol ainda com impurezas oriundas da serragem.

2.1.2 Purificação Do Lapachol

Dissolveu-se o Lapachol impuro em Acetato de Etila, fez-se a filtração simples e colocou-se a solução resultante em Placa de Petri para evaporação do solvente, formando os cristais de Lapachol puro na superfície da vidraria

2.2 Síntese Do Complexo

2.2.1 Síntese de Cloretos de Eu^{3+}

Pesou-se aproximadamente cerca de 1g de óxido de Eu^{3+} e dissolveu-se em 200mL de água destilada, em bequer de 400mL, colocou-se o sistema sobre agitação magnética e aquecimento em uma temperatura de 100 °C em uma chapa aquecedora/agitadora. Em seguida adicionou-se ao sistema 2 mL de ácido clorídrico, gotejando-se lentamente até que restasse apenas uma pequena quantidade de óxido no fundo do béquer. Verificou-se o pH do sistema com fitas indicadoras, e ao constatar que o mesmo estava entre 5-6 cessou-se a agitação e o aquecimento e submeteu-se a uma filtração simples. Recolheu-se a fase líquida límpida e submeteu-se ao aquecimento evaporando a água até obtenção de um sólido branco.

2.2.2 Síntese dos complexos $Eu(DBM)_3.2H_2O$

Dissolveu-se o HDBM (0,03 mols) em 75mL de etanol 95%, adicionou-se à solução alcoólica 30ml (0,03 mols) de hidróxido de amônio 1M até a solução atingir pH= 7,0. Adicionou-se à solução 0,01 mol de $EuCl_3.6H_2O$ dissolvido previamente em 120mL de água destilada. Deixou-se a mistura em repouso sob agitação magnética por cerca de 2 horas, até a formação de um óleo, que posteriormente tornou-se um sólido. Filtrou-se o sólido, lavou-se com água destilada e secou-se em estufa. Fez-se a recristalização do composto com Acetona. Secou-se, lavou-se com pentano e secou-se novamente.

2.2.3 Síntese do complexo $Eu(DBM)_3.LAP$

Dissolve-se cerca de 0,0002 mols de $Eu(DBM)_3.2H_2O$ em aproximadamente 30 mL de etanol, bem como 0,0004 mol de Lapachol. Após a dissolução do sal e do ligante misturou-se os mesmos e iniciou-se uma agitação. Armazenou-se a suspensão por um período de dez dias. Partes do sobrenadante passam a ser retirados e os cristais agrupam-se de forma bem definida. Fez-se a lavagem usando o mesmo solvente utilizado como meio reacional.

3. RESULTADOS E DISCUSSÃO:

3.1 Lapachol

O material extraído e purificado apresenta-se na forma de cristais amarelos. A medida de Ponto de Fusão foi feita na amostra purificada e obteve-se o resultado no intervalo de 141°C – 143°C, que é um dado positivo, considerando os valores da literatura em 139,5°C – 140,2°C (ARAÚJO; ALENCAR; NETO, 2002; PEREIRA BARBOSA; HERMES; NETO, 2013), o que indica pureza do material.

3.2 Complexo $Eu(DBM)_3.LAP$

O complexo $Eu(DBM)_3.LAP$ apresenta-se na forma de um pó roxo escuro, o que revela a presença da naftoquinona na forma de íon

lapacholato. O complexo mostrou-se solúvel em solventes orgânicos, como acetato de etila, hexano, etanol, e pouco solúvel em água, devido à presença de muitos ligantes orgânicos na primeira esfera de coordenação do metal. O ponto de fusão do material foi aferido e excede 300°C, que é a temperatura máxima do aparelho utilizado.

3.3 Infravermelho

O espectro Infravermelho do complexo contendo o Lapachol purificado pelo novo método apresenta banda intensa e larga referente ao grupamento O–H, com máximo em 3427,84 cm^{-1}, enquanto que o espectro do lapachol puro apresenta banda estreita nesse intervalo, o que pode significar a presença de OH livre no complexo, pois segundo a literatura a faixa de 3500 cm^{-1} a 3100 cm^{-1} possui registros de bandas de ligação de hidrogênio e O–H livre. Os registros na região 3100-2700 cm^{-1} são características de deformações simétricas e assimétricas de C – H sp2 e sp3, com relação à ramificação e ao anel benzênico da estrutura da naftoquinona. Houve um deslocamento no registro das ligações C=O de 1640 cm^{-1} para 1621 cm^{-1}, referente à complexação com o centro metálico via Oxigênios das Cetonas. Analisando o espectro na região de 1400 abaixo percebe-se que houve supressão em alguns registros comuns em cadeias carbônicas com metil terminal como no caso do metil-propeno presente na molécula do lapachol. Esse resultado indica a formação de uma nova espécie química, por meio da complexação do ligante ao centro metálico, dado que bandas características do ligante livre apresentam-se deslocadas, principalmente as cetonas, que são apontadas como os pontos de coordenação, além de outras bandas que foram suprimidas.

3.4 UV-Vis

Os principais picos de absorção das curvas UV-Vis dos materiais estão dispostos na tabela 1.

Na curva do Lapachol, observa-se que os picos mais intensos se encontram na região entre 200 e 250 nm, intervalo característico das transições - *, correspondente ao grande número de ligações C=C observadas na estrutura da molécula, desde o anel aromático bicíclico da naftoquinona ao radical insaturado, enquanto os picos menos intensos, de 250 a 277 nm correspondem às transições n- *, oriundas dos elétrons livres nas ligações C=O das cetonas.

O Dibenzoilmetano apresenta pico mais intenso em 350nm, referente às transições n- * dos elétrons livres nas ligações C=O das cetonas, característica das β-dicetonas. Ademais, apresenta picos com intensidades próximas em 211 e 253, referentes às transições - * dos anéis benzênicos terminais.

Na curva do $Eu(DBM)_3$.LAP pode-se observar picos em comprimentos de onda equivalentes aos dos ligantes componentes, o que indica dependência desses ligantes para absortividade do complexo, e esse dado corrobora com as informações obtidas na literatura (MOORE; SAMUEL; RAYMOND, 2009). Entre os dois ligantes, o complexo apresenta maior dependência do Dibenzoilmetano, dado à sua afinidade por moléculas do grupo das β-dicetonas (MENEZES, 1999; PEARSON; BUSCH, 1963), e devido à sua maior proporção na estrutura do complexo (1:3:1, respectivamente Eu^{3+}, DBM^- e LAP). Esses dados endossam os resultados obtidos no Infravermelho, revelando que há uma combinação dos ligantes com o Lantanídeo.

4. CONCLUSÕES:

O Lapachol extraído e purificado por novo método elaborado mostrou características positivas quando comparado ao material obtido pelo método padrão previsto na literatura, o que endossa a eficácia do novo método para purificação. O complexo $Eu(DBM)_3$.LAP apresentou cor diferente de seus componentes, além de singularidades espectrais, observadas nos espectros de Infravermelho e UV-vis. Os dados obtidos apontam para a combinação efetiva dos ligantes com o centro metálico, o que possibilita a aplicação do novo material em estudos como biomarcador, devido ao potencial farmacológico oriundo dos ligantes constituintes.

5. AGRADECIMENTOS:

Nossos reconhecimentos/agradecimentos vão aos órgãos CNPq e INCT-Energia & Ambiente pelo fomento à pesquisa; à USP, na pessoa do Dr. Brenno Espósito, pela obtenção dos espectros de Infravermelho.

6. REFERÊNCIAS:

1. ARAÚJO, E. L.; ALENCAR, J. R. B.; NETO, P. J. R. Lapachol: segurança e eficácia na terapêutica. **Revista Brasileira de Farmacognosia**, v. 12, p. 57–59, 2002.
2. CAMPÊLO DA FONSECA FILHO, I. et al. Pau-d'arco-roxo (HandroantHus impetiginosus (Mart. ex dc.) Mattos): conheciMento e uso Madeireiro eM coMunidades rurais do nordeste do Brasil. v. 11, n. 2, p. 57–70, 2017.
3. KAI, J.; PAULO, S. **Desenvolvimento de sistemas luminescentes à base dos polímeros PHB e PMMA dopados com complexos de terras raras**. São Paulo: [s.n.].
4. MOORE, E. G.; SAMUEL, A. P. S.; RAYMOND, K. N. From antenna to assay: lessons learned in lanthanide luminescence. **Accounts of Chemical Research**, v. 42, n. 4, p. 542–552, 21 abr. 2009.
5. PEREIRA BARBOSA, T.; HERMES, E.; NETO, D. **PREPARAÇÃO DE DERIVADOS DO LAPACHOL EM MEIO ÁCIDO E EM MEIO BÁSICO: UMA PROPOSTA DE EXPERIMENTOS PARA A DISCIPLINA DE QUÍMICA ORGÂNICA EXPERIMENTALQuim. Nova**. [s.l: s.n.]. Disponível em: <http://quimicanova.sbq.org.br,>.
6. S, S. T.; P, C. C.; RAGHAVENDRA, V. B. Antimicrobial and antioxidant activities of endophytes from Tabebuia argentea and identification of anticancer agent (lapachol). **Journal of Medicinal Plants Research**, v. 5, n. 16, p. 3643–3652, 2011.
7. MENEZES, J. F. S. DE. **Estudo Fotoluminescente de Tristenoiltrifluoroacetonatos de Lantanídeos com Sulfóxidos**. São Paulo: [s.n.], 1999.
8. PEARSON, R. G.; BUSCH, D. H. **Hard and Soft Acids and Bases**, 1963.

Tabela 1: Picos de Absorção no Espectro de UV-vis (comprimento de onda e intensidade, entre parênteses)

$Eu(DBM)_3$.LAP	**Lapachol**	**Dibenzoilmetano**
211 (0,89)	**208 (3,347)**	*211 (1,036)*
250 (1,205)	250 (2,205)	253 (1,424)
352 (1,43)	*277 (1,661)*	**352 (2,423)**

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

EXTRACTION, PURIFICATION AND COMBINATION OF LAPACHOL IN NOVEL EUROPIUM COMPLEX

Andrei Marcelino Sá Pires Silva
Universidade Federal do Recôncavo da Bahia, Centro de Formação de Professores - Brazil.

Jorge Fernando Silva de Menezes
Universidade Federal do Recôncavo da Bahia, Centro de Formação de Professores - Brazil.

Edna Aparecida Faria de Almeida
Escola Técnica Estadual Júlio de Mesquita - Brazil

February/2022

SUMMARY

List of contents. All presentations should include mainly, but not necessarily, the following topics **(this slide may be deleted for the final version. It is just a guide to orientate the authors about the topics they should include):**

INTRODUCTION

SBJChem Conference 2021

- The Lapachol can be combined with Europium complex as ligand
- Lapachol can be obtained from Sawdust of Pau d'Arco

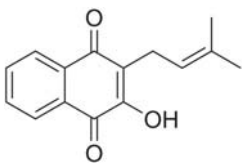


Figure 1: Lapachol Structure


Figure 2: Pau d'Arco Sawdust

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

In the present work, the extraction, a new purification process of Lapachol from its natural source, the Ipê Roxo wood, is reported, as well as the characterizations that attest to the feasibility of the new process, in addition to the use of the material as a binder in europium complexes.

METHODOLOGY

SBJChem Conference 2021

- Lapachol was extracted and purified by the new method.
- Lapachol was combined with the first complex, resulting on the final complex $Eu(DBM)_3.LAP$

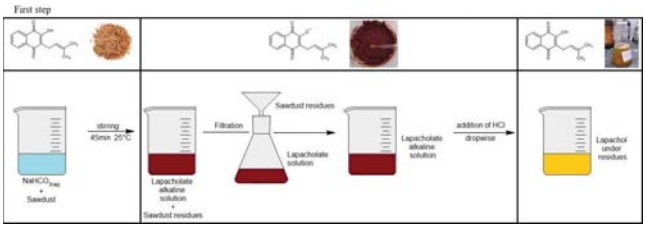


Figure 3: Extraction process

METHODOLOGY

SBJChem Conference 2021

- Lapachol was extracted and purified by the new method.
- Lapachol was combined with the first complex, resulting on the final complex $Eu(DBM)_3.LAP$

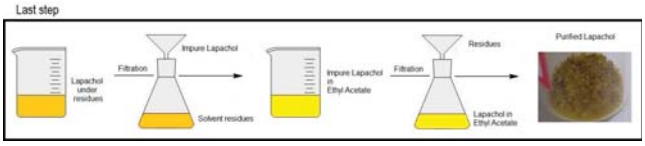


Figure 4: Purification process

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Lapachol and Novel Purification Process;
- $Eu(DBM)_3.LAP$
- IR Spectra
- UV-Vis Spectra

Figure 5: Purified Lapachol

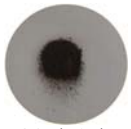


Figure 6: Synthesized complex

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Lapachol and Novel Purification Process;
- $Eu(DBM)_3.LAP$
- IR Spectra
- UV-Vis Spectra

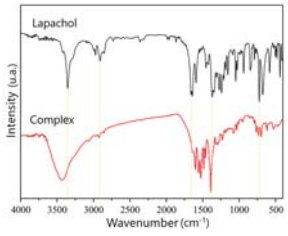


Figure 7: IV Spectra

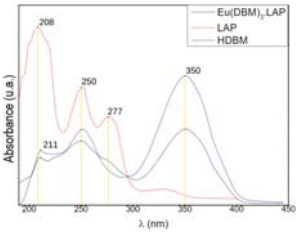


Figure 8: UV-Vis Spectra

CONCLUSIONS

SBJChem Conference 2021

- The new method of purification was effective.
- The complex have been formed with success.
- The complex will be used in further researches as biomarker of superfungus.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

- CNPq;
- INCT-Energia & Ambiente;
- USP – Dr. Brenno Espósito;

REFERENCES

SBJChem Conference 2021

1. ARAÚJO, E. L.; ALENCAR, J. R. B.; NETO, P. J. R. Lapachol: segurança e eficácia na terapêutica. **Revista Brasileira de Farmacognosia**, v. 12, p. 57–59, 2002.
2. CAMPÊLO DA FONSECA FILHO, I. et al. Pau-d'arco-roxo (HandroantHus impetiginosus (Mart. ex dc.) Mattos): conheciMento e uso Madeireiro eM coMunidades rurais do nordeste do Brasil. v. 11, n. 2, p. 57–70, 2017.
3. KAI, J.; PAULO, S. **Desenvolvimento de sistemas luminescentes à base dos polímeros PHB e PMMA dopados com complexos de terras raras**. São Paulo: [s.n.].
4. MOORE, E. G.; SAMUEL, A. P. S.; RAYMOND, K. N. From antenna to assay: lessons learned in lanthanide luminescence. **Accounts of Chemical Research**, v. 42, n. 4, p. 542–552, 21 abr. 2009.
5. PEREIRA BARBOSA, T.; HERMES, E.; NETO, D. **PREPARAÇÃO DE DERIVADOS DO LAPACHOL EM MEIO ÁCIDO E EM MEIO BÁSICO: UMA PROPOSTA DE EXPERIMENTOS PARA A DISCIPLINA DE QUÍMICA ORGÂNICA EXPERIMENTALQuim. Nova**. [s.l: s.n.]. Disponível em: <http://quimicanova.sbq.org.br,>.
6. S, S. T.; P, C. C.; RAGHAVENDRA, V. B. Antimicrobial and antioxidant activities of endophytes from Tabebuia argentea and identification of anticancer agent (lapachol). **Journal of Medicinal Plants Research**, v. 5, n. 16, p. 3643–3652, 2011.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

GRAPHICAL METHOD FOR DETERMINATION OF MQ-SERIES GAS SENSOR CIRCUIT PARAMETERS FOR A STANDALONE GAS ALARM SYSTEM

AJIBOYE, Aye Taiwo[1*]; OPADIJI, Jaye Femi[1]; AJAYI, Adebimpe Ruth[1]

[1] University of Ilorin, Faculty of Engineering and Technology, Department of Computer Engineering. Nigeria.

** Correspondence author*
e-mail: ajiboye.at@unilorin.edu.ng

Received 12 October 2021; received in revised form 30 January 2022; accepted 18 February 2022

ABSTRACT

MQ-series gas sensors belong to the metal oxide semiconductor (MOS) family of sensors that can sense the presence of many gases. These sensors find their application in gas alarm systems as key components. While necessary sensor circuit output voltage value for alarm point in a standalone gas alarm system is desirable, but what exact combination of the sensor circuit parameters is required? Hitherto, the determination of these circuit parameters has not been much attention in the research community. This study explores a structured graphical approach of determining MQ series gas sensor circuit parameters for a standalone gas alarm system that yields the desired sensor circuit output voltage value for the alarm point. Model equations were developed for the sensor dynamics, and based on these model equations, graphs for the determination of required sensor parameters were plotted for a case of MQ-4 gas sensor response to liquefied petroleum gas (LPG). A structured graphical approach for determining MQ-series gas sensor circuit parameters for alarm points in a standalone gas alarm system showed that using MQ-4 gas sensor and LPG as the target gas. For a sensor circuit output voltage of 2 V for alarm point at 1000 ppm of LPG, the corresponding value of R_O, R_S, and R_L obtained were 20 kΩ, 30 kΩ, and 20 kΩ, respectively. Hence, the developed structured graphical approach is suitable for determining MQ series gas sensor circuit parameters for a standalone gas alarm system under the influence of its associated gases.

Keywords: *alarm point, base gas, calibration-concentration, gas concentration, gas sensor resistance*

1. INTRODUCTION

MQ-series gas sensors belong to the family of metal oxide semiconductor (MOS) gas sensors that can detect the presence of some volatile, oxidizable, or reducible gases in an oxygenated environment (Gómez, Pelegri-Sebastia and Lajara, 2020). MQ-series gas sensors are commonly used for gases detection owned to their high sensitivity, stability, and long-life characteristics in this regard (Örnek and Karlik, 2012). Furthermore, when connected as one of the basic components in the sensor circuit, a certain voltage that depends on the type and concentration of the gas can be measured at the circuit output (Nayyar, Puri, and Le, 2016; Ponzoni *et al*., 2017).

The MQ-series gas sensors form the major component in many gas alarm systems due to their cost and sensitivity advantages. Developed by (Ahmed *et al*., 2018) is a microcontroller-based gas alarm system that triggers a buzzer and LED indicator when the alarm set point for the MQ-9 gas sensor was 37,000 ppm of Methane gas. Designed by (Kumar and Kumari, 2019) is an Arduino-based system with MQ2, MQ4, and MQ135 gas sensors capable of monitoring the concentration of gases and giving an alarm when the concentration of the various types of gases in the atmosphere is above the threshold value. Also developed by (Ibrahim, 2018) is a microcontroller-based carbon monoxide and carbon dioxide detector using MQ-7 and MQ-135 for carbon monoxide and air quality sensing, respectively. The gas concentration was displayed in ppm on LCD. The alarm is triggered when the threshold for the safe gas concentration is reached. However, determining the sensor circuit parameters to achieve the required sensor circuit output voltage for a given alarm point has not been well researched. Therefore, this study presents a structured graphical method for determining the sensor circuit parameter that yielded the needed sensor circuit output voltage for the alarm point.

To achieve the aim of this study, the

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.20_abstract_AJIBOYE.pdf

mathematical model equations that relate the: (i) sensor resistance (R_S) with the gas concentration (x) and the sensor resistance at standard calibration concentration of the sensor base gas in the clean air (R_O) and (ii) sensor circuit output voltage (V_{RL}), load resistance (R_L) and sensor resistance (R_S) were developed. The graphs that relate the parameters together were plotted based on these model equations.

Using these graphs for a particular case of an MQ-4 gas sensor under the influence of LPG, the parameters that yielded the desired sensor circuit output voltage of 2V for 1000 ppm of LPG alarm point were determined.

2. MATERIALS AND METHODS

The model Equations 1 and 2 were derived (Ajiboye *et al*., 2021a, b, c) to establish the relationship among the:

i. R_S, x and R_O
ii. V_{RL}, R_L and R_S

$$R_S = 10^{\wedge(mlog_{10}x+log_{10}c+log_{10}R_O)} \quad \text{(Eq.1)}$$

$$V_{RL} = \frac{R_L V_{CC}}{(10^{(mlog_{10}x+log_{10}c+log_{10}R_O)} + R_L)} \quad \text{(Eq. 2)}$$

These equations were used to plot the graphs to determine the circuit parameters value for a particular case of an MQ-4 gas sensor under the influence of LPG.

2.1. Determination of Ro

To determine R_O, the mesh plot of Figure 1 was carried out using Equation 1.

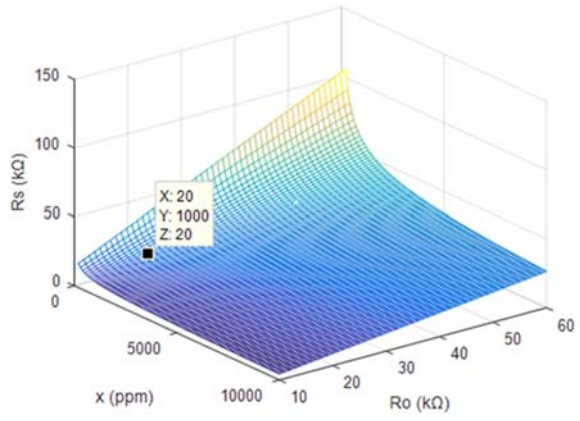


Figure 1. *Mesh plot of R_S versus x and R_O for MQ-4 gas sensor in the CH_4*

The value of R_O was determined at 1000 ppm of CH_4, since R_S = R_O at this concentration and the value of R_S under this condition is always given in the sensor data sheet (Ajiboye *et al*., 2021a)

2.2. Determination of Rs in the gas under investigation

To determine R_S for the sensor in LPG, the mesh of Figure 2 was plotted using Equation 1.

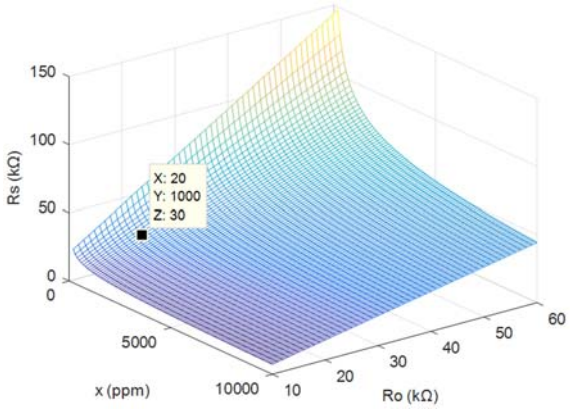


Figure 2. *Mesh plot of R_S versus x and R_o for MQ-4 gas sensor in LPG*

Using Figure 2, the value of R_S can be determined for the given versus of x and R_o.

2.3. Determination of the sensor circuit R_L for alarm point determination of Ro

To determine the sensor circuit load resistance, R_L for alarm point, the mesh plot of Figure 3 was plotted using Equation (2).

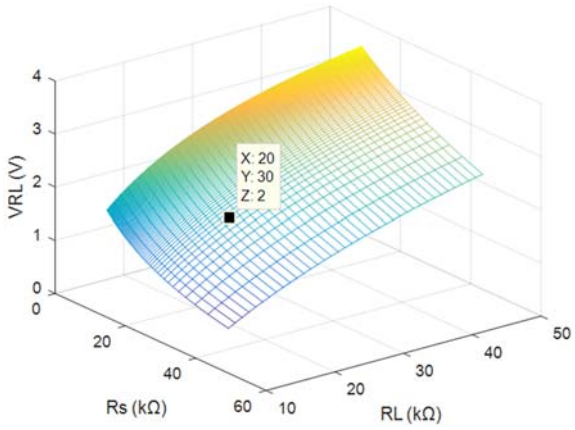


Figure 3. *Mesh plot of V_{RL} versus R_S and R_L for MQ-4 gas sensor in LPG*

Using Figure 3, the value of R_L can be determined for known values of $V_{RL}$and R_S.

2.4. Experimental setup

The system was calibrated using simulation and emulation data. Simulation and emulation were achieved using Equation 3 and the experimental setup of Figure 4, respectively (Ajiboye *et al*., 2021b, c).

$$x = 10^{\left(\frac{log_{10}\left(\frac{R_L V_{CC}}{V_{RL}} - R_L\right) - log_{10} c - log_{10} R_O}{m}\right)} \quad \text{(Eq. 3)}$$

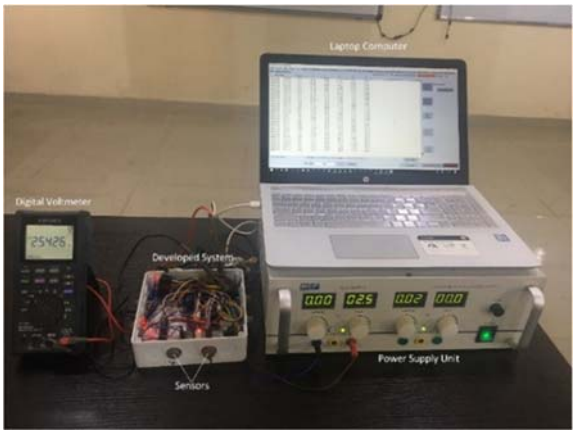


Figure 4. *System emulation experimental setup* (Ajiboye *et al*., 2021b, c)

The experimental emulation setup of Figure 4 consists:

i. a digital multi-meter for monitoring the sensor circuit emulated voltage,

ii. the developed system,

iii. variable dc power supply unit for supplying of the sensor circuit emulated voltage and

iv. a laptop PC to monitor and store system output (emulated concentration).

To mimic the sensor circuit output voltage, the power supply was connected to the input pin of the microcontroller. Then the voltage from the power supply was varied within 1.545 V and 3.455 V. This is because the expected minimum and maximum sensor circuit output voltage range when LPG concentration was in the range of 200 to 10000 ppm is between 1.545 and 3.455 V. The system output (emulated LPG concentration level) was logged into the laptop PC. Finally, the simulated data were plotted against emulated data to obtain the system calibration graph.

3. RESULTS AND DISCUSSION:

From Figure 1, $\mathrm{R_O}$ and $\mathrm{R_S}$ was $20\ k\Omega$ each at calibration concentration of 1000 ppm for $\mathrm{CH_4}$ in clean air (Ajiboye *et al*., 2021a). When $\mathrm{R_O} = 20\ k\Omega$ with the sensor in 1000 ppm of LPG the corresponding value of $\mathrm{R_S}$ is $30\ k\Omega$ as can be seen in Figure 2. As revealed in Figure 3, for a required sensor circuit output voltage value of 2 V at an alarm point of 1000 ppm for LPG, the corresponding value of $\mathrm{R_L}$ is $20\ k\Omega$.

The system calibration graph of Figure 5 was obtained by plotting the simulated against emulated LPG concentration data.

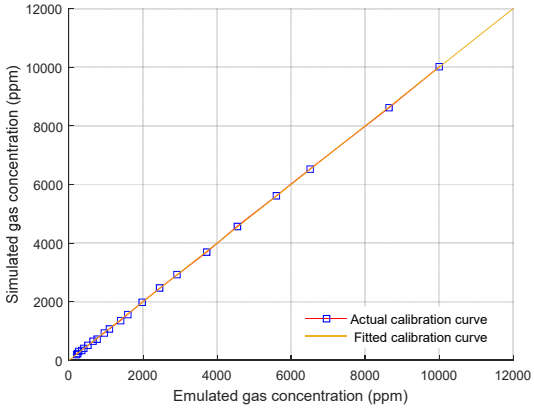


Figure 5. system calibration curve

Since the plot yielded a straight-line graph, the data were fitted linearly. The resulting system calibration equation is shown in Equation 4.

$$y = x + 8.6 \quad \text{(Eq. 4)}$$

where y and x are the predicted and emulated LPG concentration in ppm, respectively

4. CONCLUSIONS:

A structured graphical method was developed for determining MQ-series gas sensor circuit parameters for alarm points. The method was demonstrated using an MQ-4 gas sensor and LPG as the target gas. The developed method is concise, straightforward forward, and time-saving. The method is less prone to analytical errors since all that is required is the proper visual reading of the parameter value from the graph. For a particular case of expected sensor circuit output voltage of 2 V for alarm point at 1000 ppm of LPG, the corresponding value of R_O ,$\mathrm{R_S}$ and $\mathrm{R_L}$ obtained were $20\ k\Omega$, $30\ k\Omega$, and $20\ k\Omega$ respectively. Using simulation and emulation LPG concentration data, an Arduino-based standalone gas-alarm system was developed and calibrated.

The method can be applied to any type of MQ-series gas sensor under the influence of its associated gases.

5. REFERENCES:

1. Ahmed, N. B., Tahsin, K. N., Khan, S., Hoq, M. and Alam, D. (2018). Design and implementation of a microcontroller-based flammable gas detector and automatic alarm

system to ensure the industrial and domestic safety. Asian Journal of Science and Technology, 9(1), 7425-7429.
2. Ajiboye, A., Opadiji, J., Yusuf, A. and Popoola, J. (2021a). Analytical determination of load resistance value for MQ-series gas sensors: MQ-6 as case study.Telkomnika, 19(2), 575-582.
3. Ajiboye, A.T., Opadiji, J.F., Popoola, J.O. and Ajayi, A.R. (2021b). Liquefied Petroleum Gas Concentration Monitoring System with Alarm and Cloud-based Logging. Nigerian Research Journal of Engineering and Environmental Sciences, 6(2), 1-9.
4. Ajiboye, A.T., Opadiji, J.F. and Ajayi, A.R. (2021c). Graphical Method for Determination of MQ-Series Gas Sensor Circuit Parameters for a Standalone Gas Alarm System. Southern Brazilian Journal of Chemistry, 29(31), 632-641.
5. Gómez, J.C., Pelegri-Sebastia, J., and Lajara, R. (2020). Circuit Topologies for MOS-Type Gas Sensor. Electronics, 9(3), 525.
6. Ibrahim, A. A. (2018) Carbon Dioxide and Carbon Monoxide Level Detector. 21st International Conference of Computer and Information Technology (ICCIT), 1-5.
7. Kumar, P. N. S. and Kumari, A. K. (2019). Design of Gas Detection and Monitoring System using IoT. International Journal of Engineering Research and Technology (IJERT), 8, 463 - 468.
8. Nayyar, A., Puri, V. and Le, D.-N. (2016). A comprehensive review of semiconductor-type gas sensors for environmental monitoring. Review of Computer Engineering Research, 3(3), 55-64.
9. Örnek, Ö., and Karlik, B. (2012). An overview of metal oxide semiconducting sensors in electronic nose applications. In Proc. of the 3rd International Symposium on Sustainable Development, 2, 506-515.
10. Ponzoni, A., Baratto, C., Cattabiani, N., Falasconi, M., Galstyan, V. and Nunez-Carmona, E., (2017) Metal oxide gas sensors, a survey of selectivity issues addressed at the SENSOR Lab, Brescia (Italy). Sensors,17(4), 714.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

GRAPHICAL METHOD FOR DETERMINATION OF MQ-SERIES GAS SENSOR CIRCUIT PARAMETERS FOR A STANDALONE GAS ALARM SYSTEM

AJIBOYE Aye Taiwo
University of Ilorin, Faculty of Engineering and Technology, Department of Computer Engineering. Nigeria.

OPADIJI Jaye Femi
University of Ilorin, Faculty of Engineering and Technology, Department of Computer Engineering. Nigeria.

AJAYI Adebimpe Ruth
University of Ilorin, Faculty of Engineering and Technology, Department of Computer Engineering. Nigeria.

December/2021

INTRODUCTION

SBJChem Conference 2021

- MQ-series gas sensors belong to the metal oxide semiconductor (MOS) family ;
- It can sense the presence of many gases (Gómez, Pelegri-Sebastia and Lajara, 2020);
- These sensors find their application in gas alarm systems as key components;
- The determination of exact sensor circuit parameters value for optimal output in a standalone gas alarm system has not been given much attention in the research community.

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

The aim of this study is to explore structured graphical approach for determination of MQ series gas sensor circuit parameters value that yields desired sensor circuit output voltage for the alarm point in a standalone gas alarm system.

METHODOLOGY

SBJChem Conference 2021

- The model Equations (1) and (2) (Ajiboye *et al*., 2021) were derived to established the relationship among the:
  i. sensor resistance (R_S), gas concentration (x) and sensor resistance at standard calibration concentration of the sensor base gas in the clean air (R_O)
  ii. sensor circuit output voltage (V_{RL}), load resistance (R_L) and sensor resistance (R_S)

$$R_S = 10^{\wedge(m\log_{10}x+\log_{10}c+\log_{10}R_O)} \quad \text{(Eq.1)}$$

$$V_{RL} = \frac{R_L V_{CC}}{(10^{(m\log_{10}x+\log_{10}c+\log_{10}R_O)}+R_L)} \quad \text{(Eq. 2)}$$

- These equations were used for plotting the graphs for the determination of the circuit parameters value for a particular case of an MQ-4 gas sensor under the influence of LPG.

METHODOLOGY

SBJChem Conference 2021

Determination of sensor circuit parameters value:

- For determination of Ro, the mesh plot of Figure 1 was carried out using Equation (1)

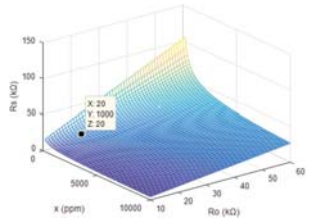


***Figure* 1.** Mesh plot of R_S versus x and R_O for MQ-4 gas sensor in the CH_4

METHODOLOGY

SBJChem Conference 2021

- To determine R_S for the sensor in LPG the mesh of Figure 2 was plotted using Equation (1)

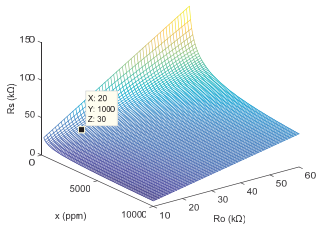


Figure 2. Mesh plot of R_S versus x and R_S for MQ-4 gas sensor in LPG

METHODOLOGY

SBJChem Conference 2021

- To determination the sensor circuit load resistance, R_L for alarm point, the mesh plot of Figure 3 was plotted using Equation (2).

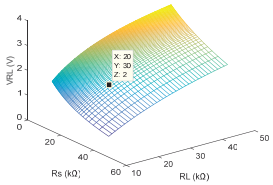


Figure 3. Mesh plot of V_{RL} versus R_S and R_L for MQ-4 gas sensor in LPG

METHODOLOGY

SBJChem Conference 2021

System calibration:

- The system was calibrated using simulated and emulated data.
- Simulation and emulation was achieved using Equation (3) and Experimental Set up of Figure 4 respectively.

$$x = 10^{\left(\frac{\left(log_{10}\left(\frac{R_L V_{CC}}{V_{RL}} - R_L\right) - log_{10}c - log_{10}R_O\right)}{m}\right)} \quad \text{(Eq. 3)}$$

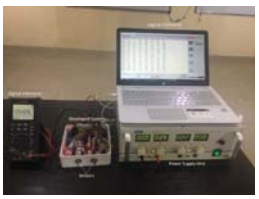


Figure 4. System emulation experimental set up

METHODOLOGY

SBJChem Conference 2021

- The emulation experimental set up consists of:
  i. a digital multi-meter for monitoring the sensor circuit emulated gas concentration equivalent voltage,
  ii. the developed system,
  iii. variable dc power supply unit for supplying of the sensor circuit emulated gas concentration equivalent voltage and
  iv. a laptop PC for monitoring and storage of system output (emulated concentration).

METHODOLOGY

SBJChem Conference 2021

- To mimic the sensor circuit output voltage the power supply was connected to input pin of the microcontroller
- Then the voltage from the power supply was varied within 1.545 V and 3.455 V ,
- The system output (emulated LPG concentration level) was logged into the laptop PC
- To obtain the system calibration graph, the simulated data was plotted against emulated data

RESULTS AND DISCUSSION

SBJChem Conference 2021

- From Figure 1, R_O and R_S was $20\ k\Omega$ each at calibration concentration of 1000 ppm for CH_4 in clean air (Ajiboye *et al*., 2021)
- When $R_O = 20\ k\Omega$ with the sensor in 1000 ppm of LPG the corresponding value of R_S is $30\ k\Omega$ as can be seen Figure 2
- As revealed in Figure 3, for a required sensor circuit output voltage value of 2 V at alarm point of 1000 ppm for LPG the corresponding value of R_L is $20\ k\Omega$
- The system calibration graph of Figure 5 was obtained by plotting the simulated against emulated LPG concentration data

RESULTS AND DISCUSSION

SBJChem Conference 2021

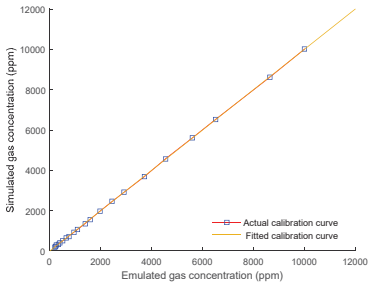


Figure 5. system calibration curve

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Since the plot yielded a straight-line graph, the data were fitted linearly
- The resulting system calibration equation is shown in Equation (4)

$$y = x + 8.6 \quad \text{(Eq. 4)}$$

- where y and x are the predicted and emulated LPG concentration in ppm respectively

CONCLUSIONS

SBJChem Conference 2021

- A structured graphical method for determining MQ-series gas sensor circuit parameters for alarm points was developed ;
- The developed method is concise, straightforward, timesaving and can be applied to any MQ-series gas sensor;
- For a particular case of expected sensor circuit output voltage of 2 V for alarm point at 1000 ppm of LPG, the corresponding value of R_O ,R_S and R_L obtained were $20\ k\Omega$, $30\ k\Omega$, and $20\ k\Omega$ respectively;

REFERENCES

SBJChem Conference 2021

1. Ajiboye, A., Opadiji, J., Yusuf, A. and Popoola, J. (2021). Analytical determination of load resistance value for MQ-series gas sensors: MQ-6 as case study. *Telkomnika, 19*(2), 575-582.
2. Gómez, J.C., Pelegri-Sebastia, J., and Lajara, R. (2020). Circuit Topologies for MOS-Type Gas Sensor. *Electronics,* 9(3), 525.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

IDENTIFICATION OF HUB GENES IN CROHN'S AND CELIAC DISEASES: A BIOINFORMATIC PERSPECTIVE

KOZALAK, Gül[1*]; ATCEKEN, Nazente[1]

[1] Aksaray University, Graduate School of Natural and Applied Sciences, Department of Biology, Molecular Biology Division (Ph.D.).

** Correspondence author*
e-mail: gulkozalak@gmail.com

Received 02 January 2022; received in revised form 16 February 2022; accepted 21 February 2022

ABSTRACT

Chronic inflammatory diseases are the repetitive response of the organism to any stimulus. Crohn's and Celiac diseases are among chronic inflammatory diseases, and both cause chronic inflammation in the intestines. Both diseases are thought to be caused by genetic and environmental factors. Although the relationship between the two diseases is frequently mentioned in the literature, very few studies, have been conducted to elucidate their common mechanisms. From a bioinformatics perspective, this study aimed to determine the genes whose expression alters in both Crohn's and celiac diseases. For this purpose, NCBI-GEO datasets were downloaded, and advanced statistical analyzes were performed. Statistical analyzes revealed 54 DEGs in both Crohn's and celiac diseases. As a result of bioinformatics analysis, it was determined that 13 of these differentiated genes were hub genes. It has been defined that 11 of these genes are involved in similar biological processes employing GeneCards, Gene ontology, and Kyoto encyclopedia of genes and genomes pathway. GZMB, GZMA, GZMH, CD160, CXCR1, CXCR2, ANPEP, FPR2, GAB2, PI3, and NCF4 genes are located in a connected pathway. Contrary, CTSL, and KAT6A genes are on different pathways. Common biological processes that antigen presentation by MHC class molecules, cell death pathways mediated by immune cells and ROS, maintain the continuity of gut epithelial cells have been suggested. Given the increasing prevalence of both Crohn's and celiac diseases in the population, it is clear that more studies are needed on the collective mechanisms of these diseases.

Keywords: *bioinformatics, celiac disease, Crohn's disease, hub genes, inflammation*.

1. INTRODUCTION

Chronic inflammatory diseases arise due to the interaction of hereditary, genetic predisposition, environmental, and lifestyle factors (Furman *et al.* 2019; Heap and van Heel 2009). These diseases continue throughout life, reducing the patient's quality of life and increasing the social burden of disease and mortality (Furman *et al.*, 2019). Chronic inflammatory diseases are the chronic response of the immune system to endogenous-exogenous stimuli. Celiac and Crohn's diseases are chronic inflammatory diseases with complex etiology (Heap and van Heel 2009). The etiology and immunopathogenesis of these diseases, which share the intestine as the target organ, are unclear. However, both celiac and Crohn's diseases are characterized by chronic inflammation of the innate and adaptive immune systems.

Celiac disease is an intestinal disease in which immune cells damage the villi due to the intake of gluten-containing foods such as wheat, rye, and barley (Kagnoff 2007). The malabsorption of nutrients causes complaints such as vomiting, diarrhea, abdominal pain, abdominal distension, loss of appetite, and anemia in patients. Celiac disease can be genetically inherited with HLA-DQ2 and HLA-DQ8, but environmental factors are also effective in the emergence of the disease (Fasano and Catassi 2012).

Crohn's disease is an intestinal disease of unknown cause, which can occur under the influence of genetic and environmental factors. The disease is manifested by inflammation in one region of the digestive system (mouth-anus) or in more than one region at the same time. In addition, it is affected by changes in the gut microbiome,

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon. 25_abstract_KOZALAK.pdf.

causing immune cells to attack and damage the mucosa (Petagna *et al.*, 2020). Crohn's and ulcerative colitis diseases together form the inflammatory bowel disease group, so they are often evaluated and confused together. Generic symptoms of Crohn's disease include diarrhea, abdominal pain, rectal bleeding, fever, weight loss, and fatigue (Lichtenstein *et al.*, 2018).

Celiac and Crohn's diseases are both diseases due to gut inflammation. Abdominal pain and diarrhea are common symptoms in both. It is known that the activation of immune cells causes a disease to become chronic by perpetuating it. Therefore, one is likely to trigger the other. According to a study, celiac disease also has a high prevalence in patients with Crohn's disease (Tursi *et al.*, 2005). Conversely, a patient with celiac disease was later found to have Crohn's disease (Lail *et al.*, 2016). The relationship of these two complex diseases has been mentioned in the literature. Still, until now, very few studies have been done on their collective mechanisms (Festen *et al.*, 2011). Therefore, it is necessary to study the differentially expressed genes that are mutual in both diseases for all these reasons.

2. MATERIALS AND METHODS

Datasets GSE11501 and GSE3365 in NCBI GEO (National Center for Biotechnology Information-Gene Expression Omnibus) were downloaded and analyzed in GEO2R for celiac and Crohn's diseases, respectively. The downloaded data were imported to excel, and the genes with $p < 0.05$ were defined. In each dataset, genes whose expression was up or down-regulated according to logFC were determined separately. Candidate genes whose expression differentiated according to logFC and $p < 0.05$ were identified. Differentiating genes for protein-protein interaction (PPI) network was performed with STRING online tool. GeneCards, Gene ontology (GO), and Kyoto encyclopedia of genes and genomes (KEGG) pathway enrichment analyses were used.

3. RESULTS AND DISCUSSION:

Datasets were downloaded and analyzed in GEO2R for celiac and Crohn's diseases. The analysis file was transferred to excel for further statistical processing. To eliminate the differences of the platforms used in the datasets, the logFC rates specific to each dataset were defined ($|\log FC| \geq 0.05$ in GSE3365 and $|\log FC| \geq 0.02$ in GSE11501) (Maouche *et al.* 2008). There were 147 up and 87 down-regulated genes in celiac disease, while 1506 up to and 1343 down-regulated genes in Crohn's disease. Multiple List Comparator online tools were detected 54 DEGs in both diseases (Figure 1).

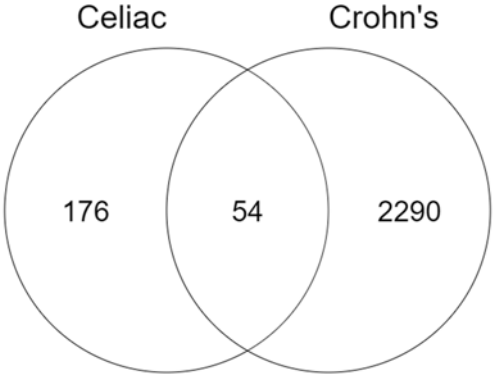


Figure 1. *Differentially expressed genes in Crohn's and celiac diseases.*

Possible functional pathways between proteins emerged via PPI networks. 28 edges detected between 54 nodes with STRING default settings. Analysis results for generated PPI network were PPI enrichment p-value: $2.98e^{-05}$ and average local clustering coefficient: 0.407. Then, the file was imported to Cytoscape 3.9.1 and analyzed with its plugin CytoHubba. It predicts key nodes in the PPI network using various algorithms using shortest paths and centrality. The top 15 hub genes were calculated according to a degree. Network Analyzer plugin was performed to calculate the clustering coefficient (0.311). As a result of the analysis, it was defined that 13 of these genes were hub genes (Table 1). GeneCards, Gene ontology (GO), and Kyoto encyclopedia of genes and genomes (KEGG) pathway enrichment analyses have been used to describe the functions of proteins identified as hub genes and the signaling pathways they are involved in.

Table 1. *Hub genes in celiac and Crohn's diseases.*

Degree	Gene
7.0	GZMB
4.0	CXCR2
4.0	ANPEP
4.0	CXCR1
3.0	GAB2
3.0	GZMA
2.0	FPR2
2.0	NCF4
2.0	KAT6A
2.0	CTSL
2.0	PI3
2.0	CD160
2.0	GZMH

This study identified DEGs with a bioinformatics approach in both celiac and Crohn's diseases with datasets obtained from NCBI-GEO. Particular attention was paid to both celiac and Crohn's datasets being blood samples. In this way, mutual inflammation pathways in celiac and Crohn's diseases, which are chronic inflammatory diseases, were determined. Bioinformatics analysis results among the identified hub genes, GZMB is in the center position in the mutual pathway and has the most connections. GZMB, GZMA, GZMH, CD160, CXCR1, CXCR2, ANPEP, FPR2, GAB2, PI3, and NCF4 genes are located in the same interconnected pathway. On the other hand, CTSL and KAT6A genes are independently on separate pathways.

Granzymes are serine protease granules secreted by CTL and NK to induce cell death (Bots and Medema 2006). NK, CTL express CD160 antigen, and Intestinal intraepithelial lymphocytes, leading to cell activation and differentiation (Agrawal *et al.* 1999). This branch demonstrates the similarity of immune regulation between antigen-presenting cells (APC)-lymphocytes involved in both diseases. This similarity is immune cells that induce apoptosis in intestinal cells via MHC class I molecules and granzymes.

CXCR1/2 chemokine receptors belong to the G-coupled-protein-receptor family and are expressed by endothelial cells (Bergin *et al.*, 2010). ANPEP can increase presentation to T cells by cleavage of peptides bound to MHC II molecules in antigen-presenting cells (Dong *et al.*, 2000). FPR2 activates the phosphatidylinositol-calcium secondary messenger via the G-protein and directs phagocytosis (Polakis, Uhing, and Snyderman 1988). This branch is associated with the presentation of endogenous or exogenous stimuli in both diseases via MHC class II molecules. This loop, IL-8-mediated phagocytosis, and ROS-induced oxidative damage occur in intestinal epithelia.

GAB2 plays a role in mast cell-related inflammation with PI3K activation (Simister and Feller 2012). PI3 prevents the proteolysis of the epithelial tissue and ensures its persistence (Correnti *et al.*, 2018). NCF4 is involved in generating ROS products in cell defense and has a role in PI3K signaling (Wientjes *et al.* 1993). While this branch supports cell death due to inflammation, it also increases cell proliferation and protects intestinal cells.

CTSL is a lysosomal cysteine protease that can induce apoptosis in inflammation (Gomes *et al.* 2020). In addition, it regulates the degradation of the extracellular matrix by accumulating around APCs. CTSL's down expression in both diseases suggests that the inflammation has begun to resolve.

KAT6A is an acetyltransferase involved in chromatin remodeling. In this way, it plays an important role in developing hematopoietic stem cells (Yang and Ullah 2007). Furthermore, upregulation of KAT6A in both diseases suggests that cell proliferation is induced via stem cells.

4. CONCLUSIONS:

As a result of the bioinformatic analyzes performed in this study, common DEGs in inflammation in Crohn's and celiac diseases were identified. While the expression alters of these genes have been mentioned separately in celiac and Crohn's diseases, it has been revealed for the first time that they may be involved in two disease inflammation mechanisms with our study. Further studies are needed on the underlying mechanisms of these two chronic inflammatory diseases.

5. REFERENCES:

1. Agrawal, S., Marquet, J., Freeman, G. J., Tawab, A., Bouteiller, P. L., Roth, P., Bolton, W., Ogg, G., Boumsell, L., Bensussan, A. J. Immunol, **1999**, 162: 1223-6.
2. Bergin, D. A., Reeves, E. P., Meleady, P., Henry, M., McElvaney, O. J., Carroll, T. P., Condron, C., Chotirmall, S. H., Clynes, M., O'Neill, S. J., McElvaney, N. G. J. Clin. Invest, **2010**, 120: 4236-50.
3. Bots, M., Medema, J. P. J. Cell Sci, **2006**,

119: 5011-14.
4. Correnti, C. E., Gewe, M. M., Mehlin, C., Bandaranayake, A. D., Johnsen, W. A., Rupert, P. B., Brusniak, M. Y., Clarke, M., Burke, S. E., De Van Der Schueren, W., Pilat, K., Turnbaugh, S. M., May, D., Watson, A., Chan, M. K., Bahl, C. D., Olson, J. M., Strong, R. K. Nat. Struct. Mol. Biol, **2018**, 25: 270-78.
5. Dong, X., An, B., Salvucci Kierstead, L., Storkus, W. J., Amoscato, A. A., Salter, R. D. J. Immunol, **2000**, 164: 129-35.
6. Fasano, A., Catassi, C. N. Engl. J. Med, **2012**, 367: 2419-26.
7. Festen, E. A. M., Goyette, P., Green, T., Boucher, G., Beauchamp, C., Trynka, G., Dubois, P. C., Lagacé, C., Stokkers, P. C. F., Hommes, D. W., Barisani, D., Palmieri, O., Annese, V., van Heel, D. A., Weersma, R. K., Daly, M. J., Wijmenga, C., Rioux, J. D. PLOS Genetics, **2011**, 7: e1001283.
8. Furman, D., Campisi, J., Verdin, E., Carrera-Bastos, P., Targ, S., Franceschi, C., Ferrucci, L., Gilroy, D. W., Fasano, A., Miller, G. W., Miller, A. H., Mantovani, A., Weyand, C. M., Barzilai, N., Goronzy, J. J., Rando, T. A., Effros, R. B., Lucia, A., Kleinstreuer, N., Slavich, G. M. Nat. Med, **2019**, 25: 1822-32.
9. Gomes, C. P., Fernandes, D. E., Casimiro, F., da Mata, G. F., Passos, M. T., Varela, P., Mastroianni-Kirsztajn, G., Pesquero, J. B. Front. Cell. Infect. Microbiol, **2020**, 10.
10. Heap, G. A., van Heel, D. A. Hum. Mol. Genet, **2009**, 18: R101-R06.
11. Kagnoff, M. F. J. Clin. Invest, **2007**, 117: 41-9.
12. Lail, G., Tasneem, A. A., Butt, M. O., Luck, N. H., Laeq, S. M., Abbas, Z., Mubarak, M. J. Coll. Physicians Surg. Pak, **2016**, 26: 536-8.
13. Lichtenstein, G. R., Loftus, E. V., Isaacs, K. L., Regueiro, M. D., Gerson, L. B., Sands, B. E. Am. J. Gastroenterol, **2018**, 113: 481-517.
14. Maouche, S., Poirier, O., Godefroy, T., Olaso, R., Gut, I., Collet, J. P., Montalescot, G., Cambien, F. BMC Genomics, **2008**, 9: 302.
15. Petagna, L., Antonelli, A., Ganini, C., Bellato, V., Campanelli, M., Divizia, A., Efrati, C., Franceschilli, M., Guida, A. M., Ingallinella, S., Montagnese, F., Sensi, B., Siragusa, L., Sica, G. S. Biology Direct, **2020**, 15: 23.
16. Polakis, P. G., Uhing, R. J., Snyderman, R. J. Biol. Chem, **1988**, 263: 4969-76.
17. Simister, P. C., Feller, S. M. Molecular BioSystems, **2012**, 8: 33-46.
18. Tursi, A., Giorgetti, G. M., Brandimarte, G., Elisei, W. Inflamm. Bowel. Dis, **2005**, 11: 662-6.
19. Wientjes, F. B., Hsuan, J. J., Totty, N. F., Segal, A. W. Biochem. J, **1993**, 296 (Pt 3): 557-61.
20. Yang, X. J., Ullah, M. Oncogene, **2007**, 26: 5408-19.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

IDENTIFICATION OF HUB GENES IN CROHN'S AND CELIAC DISEASES: A BIOINFORMATIC PERSPECTIVE

KOZALAK, Gül[1*]; ATCEKEN, Nazente[2]
[1,2] Aksaray University, Graduate School of Natural and Applied Sciences, Department of Biology, Molecular Biology Division (PhD), Aksaray, Turkey.

***Gül KOZALAK**
Aksaray University, Graduate School of Natural and Applied Sciences, Department of Biology, Molecular Biology Division (PhD), Aksaray, Turkey.

Nazente ATCEKEN
Aksaray University, Graduate School of Natural and Applied Sciences, Department of Biology, Molecular Biology Division (PhD), Aksaray, Turkey.

March/2022

INTRODUCTION

SBJChem Conference 2021

Chronic inflammatory diseases arise as a result of the interaction of hereditary, genetic predisposition, environmental and lifestyle factors (Furman et al. 2019; Heap and van Heel 2009). These diseases continue throughout life, reducing the patient's quality of life and increasing the social burden of disease and mortality (Furman et al. 2019). Celiac and Crohn's diseases are among the chronic inflammatory diseases with complex etiology (Heap and van Heel 2009). The etiology and immunopathogenesis of these diseases, which share the intestine as the target organ, are not clear.

BACKGROUND

SBJChem Conference 2021

Celiac disease is an intestinal disease in which immune cells damage the villi due to the intake of gluten-containing foods such as wheat, rye and barley (Kagnoff 2007). The malabsorption of nutrients causes complaints such as vomiting, diarrhea, abdominal pain, abdominal distension, loss of appetite and anaemia in patient. Celiac disease can be genetically inherited with HLA-DQ2 and HLA-DQ8, but environmental factors are also effective in the emergence of the disease (Fasano and Catassi 2012).

BACKGROUND

SBJChem Conference 2021

Crohn's disease is an intestinal disease of unknown cause, which can occur under the influence of genetic and environmental factors. It is affected by changes in the gut microbiome, causing immune cells to attack and damage the mucosa (Petagna et al. 2020). Generic symptoms of crohn's disease include diarrhea, abdominal pain, rectal bleeding, fever, weight loss, and fatigue (Lichtenstein et al. 2018).

BACKGROUND

SBJChem Conference 2021

Celiac and Crohn's diseases are both diseases due to inflammation of the gut. Abdominal pain and diarrhea are common symptoms in both. It is known that the activation of immune cells causes a disease to become chronic by perpetuating it. Therefore, one is likely to trigger the other. In the literature, the relationship of these two complex diseases has been mentioned, but until now, very few studies have been done on their collective mechanisms (Festen et al. 2011). For all these reasons, it is necessary to study the similarities in chronic inflammation which are mutual in both diseases.

AIM/OBJETIVE/PURPOSE

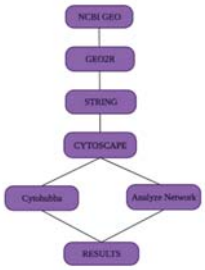
SBJChem Conference 2021

In this study, we aimed to define differentially expressed genes in chronic inflammation of Crohn's and Celiac diseases that occur in the same tissue.

METHODOLOGY

SBJChem Conference 2021

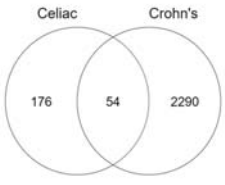
Dataset	Platform	Healthy	Crohn's	Celiac	Total
GSE11501	GPL6104	22	0	110	132
GSE3365	GPL96	42	59	0	101



RESULTS AND DISCUSSION

SBJChem Conference 2021

Multiple List Comparator online tool was detected 54 DEGs in both diseases.



RESULTS AND DISCUSSION

SBJChem Conference 2021

Degree	Gene
7.0	GZMB
4.0	CXCR2
4.0	ANPEP
4.0	CXCR1
3.0	GAB2
3.0	GZMA
2.0	FPR2
2.0	NCF4
2.0	KAT6A
2.0	CTSL
2.0	PI3
2.0	CD160
2.0	GZMH

RESULTS AND DISCUSSION

SBJChem Conference 2021

CONCLUSIONS

SBJChem Conference 2021

As a result of the bioinformatic analyzes performed in this study, common DEGs in inflammation in crohn's and celiac diseases were identified. While the expression alters of these genes have been mentioned separately in celiac and crohn's diseases, it has been revealed for the first time that they may be involved in two disease inflammation mechanisms with our study. Further studies are needed on the underlying mechanisms of these two chronic inflammatory diseases.

REFERENCES

SBJChem Conference 2021

1. Fasano, A., Catassi, C. N. Engl. J. Med, 2012, 367: 2419-26.
2. Festen, E. A. M., Goyette, P., Green, T., Boucher, G., Beauchamp, C., Trynka, G., Dubois, P. C., Lagacé, C., Stokkers, P. C. F., Hommes, D. W., Barisani, D., Palmieri, O., Annese, V., van Heel, D. A., Weersma, R. K., Daly, M. J., Wijmenga, C., Rioux, J. D. PLOS Genetics, 2011, 7: e1001283.
3. Furman, D., Campisi, J., Verdin, E., Carrera-Bastos, P., Targ, S., Franceschi, C., Ferrucci, L., Gilroy, D. W., Fasano, A., Miller, G. W., Miller, A. H., Mantovani, A., Weyand, C. M., Barzilai, N., Goronzy, J. J., Rando, T. A., Effros, R. B., Lucia, A., Kleinstreuer, N., Slavich, G. M. Nat. Med, 2019, 25: 1822-32.
4. Heap, G. A., van Heel, D. A. Hum. Mol. Genet, 2009, 18: R101-R06.
5. Kagnoff, M. F. J. Clin. Invest, 2007, 117: 41-9.
6. Lichtenstein, G. R., Loftus, E. V., Isaacs, K. L., Regueiro, M. D., Gerson, L. B., Sands, B. E. Am. J. Gastroenterol, 2018, 113: 481-517.
7. Petagna, L., Antonelli, A., Ganini, C., Bellato, V., Campanelli, M., Divizia, A., Efrati, C., Franceschilli, M., Guida, A. M., Ingallinella, S., Montagnese, F., Sensi, B., Siragusa, L., Sica, G. S. Biology Direct, 2020, 15: 23.


SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

IMPACTS CAUSED BY THE COVID-19 PANDEMIC ON PEOPLE WITH AUTISM SPECTRUM DISORDER

PEREIRA, Carlla Alessandra Silva *

Universidade de Vassouras

** Correspondence author*
e-mail: carllaalessandrasp@gmail.com

Received 15 January 2022; received in revised form 10 February 2022; accepted 20 February 2022

ABSTRACT

COVID-19, first identified in Wuhan, China in 2019, has the SARS-CoV-2 virus as its etiological agent, spread rapidly around the world, became a pandemic and directly impacted the lives of individuals. Due to the advance of the pandemic the means for control was social isolation. Since individuals with autism spectrum disorder have difficulties in social interaction due to cognitive impairment, interpersonal development tends to be more impaired with the beginning of restrictive measures. This study aims to analyze the changes in the routine of individuals with autism spectrum disorder during social isolation. The search was conducted in the PubMed and BVS databases, using the following descriptors from the DECS database: autism spectrum disorder, covid pandemic and anxiety, using the Boolean indicator AND between words in the search fields. The inclusion criterium for the texts were: English, Portuguese and Spanish languages, from 2017 to 2022. As exclusion criterium, articles that did not address the topic were excluded. The study showed that with the closure of schools and migration to remote education, several students developed a regression in social interaction and triggered new psychiatric symptoms due to the change in routine. In compliance with safety protocols, cognitive-behavioral therapies, migrated to the digital medium and were also rejected at first, but were instrumental in controlling the creation and worsening of symptoms. Due to physical and social distancing requirements, individuals with autism spectrum disorder tend to have greater difficulties with social interaction after the COVID-19 pandemic. The change in routine contributes to the worsening of symptoms such as anxiety, aggressiveness, and irritability and can worsen the mental health of parents.

Keywords: *Autism, Anxiety, Social interaction*.

1. INTRODUÇÃO

A COVID-19, identificada pela primeira vez em Wuhan, na China em 2019, tem como agente etiológico o vírus SARS-CoV-2, disseminada rapidamente pelo mundo, tornou-se uma pandemia e impactou diretamente na vida de todos os indivíduos, tanto socialmente, economicante, psiciologicamente, quanto na saúde física. O meio para controle da pandemia foi o isolamento social, pois o vírus se propaga por meio de gotículas de muco ou saliva no ar, ao espirrar ou tossir e é transmitido de pessoa para pessoa.

O transtorno do espectro autista (TEA) é uma condição com variabilidade individual no funcionamento cognitivo, apresenta comportamentos repetitivos e dificuldades de comunicação social (Charman *et al*., 2011).

No entanto, o presente estudo tem por objetivo a análise da mudança que houve na vida e na rotina de indivíduos com transtorno do espectro autista durante o isolamento social. Crianças, adolescentes e adultos podem ter sintomas exacerbados devido a alteração de suas atividades habituais, pois indíviduos com TEA são altamente vinculados às rotinas diárias, como ir a escola ou educação especial (Mutluer *et al*., 2020). Esses sintomas são relacionados à ansiedade, alteração do sono, transtornos comportamentais, irritabilidade e agressividade (Amorin *et al*, 2020).

Essas alterações comportamentais dos individuos com TEA refletem em aumento dos índices de ansiedade em seus cuidadores (Mutluer *et al*., 2020).

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.24_abstract_PEREIRA.pdf

2. METODOLOGIA

A busca foi realizada nas bases de dados: PubMed e BVS, utilizando os seguintes descritores retirados da base do DECS: autism spectrum disorder, covid pandemic e anxiety, utilizando o indicador booleano AND entre as palavras nos campos de busca. Foram adotados como critérios para a inclusão nos textos: idiomas inglês, português e espanhol, no período de 2017 a 2022. Como critério de exclusão, foram excluídos os artigos que não abordassem o tema. Foram encontrados 48 artigos e após a aplicação dos critérios foram selecionados 15 artigos.

3. DESCOBERTAS:

A Tabela 1 sumariza os resultados da pesquisa realizada na base de dados PubMed.

Tabela 1. *Resultados da pesquisa em PubMed*.

Base de dados	PubMed
Resultados utilizados	12
Resultados descartados	32
Total de resultados	44

A pandemia do COVID-19 é recente, mas já impactou fortemente a vida de pessoas com transtorno do espectro autista. Devido ao avanço do vírus, foi decretado o fechamento de todos os serviços, exceto serviços essenciais, com isso as escolas paralisaram suas atividades. Visto que o meio escolar é de grande importância para o desenvolvimento social dos individuos com TEA, é necessário um período de adaptação para que isso faça parte de sua rotina, também há o apoio de profissionais capacitados para auxiliarem esses alunos que demandam de atenção especial. Com o fechamento das escolas, houve a migração para aulas remotas, diversos alunos com TEA não se adaptaram ao novo desafio, além disso não tinham mais a ajuda de mediadores que antes os auxiliavam. Para isso, médicos orietaram frequentar as aulas em períodos que gradativamente fossem aumentados, pois ajudaria na adaptação, outro método também foi intercalar os dias de aula com outra atividade realizada pelos pais (Kalvin *et al*., 2020).

Entretando, uma pesquisa feita com alunos com TEA rotulados com autismo de alto funcionamento (HFA), constatou que muitas crianças preferem o ensino remoto, pois estes relatam ter ansiedade pela demanda de sociabilidade que lhe é imposta pela escola (Reicher *et al*., 2020).

Outra maneira de estimular o desenvolvimento de individuos com TEA são terapias cognitivo-comportamentais, estas também foram adequadas a forma remota, a telessaúde, para garantir que os protocolos de segurança fossem cumpridos. A continuidade do tratamento durante o isolamento foi necessária, pois a alteração na rotina influenciou no agravamento de sintomas como: ansiedade, depressão, agressividade, irritabilidade, além disso, individuos que não apresentavam sintomas psiquiátricos comecaram a desenvolver durante a pandemia. Um estudo realizado com 257 crianças e adolescentes mostrou que 64% das criancas tinham condição psiquiátrica prévia, das quais 41% experimetaram um agravamento desses sintomas e 53% da amostra desenvolveu novos sintomas, dos quais 29% não tinham problemas psquiátricos prévios. Os novos sintomas mais comuns foram irritabilidade, sono e ansiedade (Vasa *et al*., 2021).

Alguns estudos relataram que a compreensão da COVID-19 e o impacto da COVID-19 na família podem ser fatores de risco para problemas psiquiátricos infantis. O diálogo dos cuidadores deveria ser cauteloso para não desencadear mais ansiedade acerca do problema mundial. Alguns indivíduos podem ser incapazes de se adequar as medidas de distanciamento, uso de máscaras e realização de alguns procedimentos médicos devido a aversões de estimualação sensorial. Para isso, foram desenvolvidas medidas visuais para alertar os passos que seriam seguidos durante o protocolo de cuidado nos hospitais durante o tratamento em caso de adoecimento (Goh *et al*., 2020).

As mudanças na rotina de indivíduos com TEA refletem na saúde mental de seus pais e cuidadores, estes possuem maior resposta de cortisol ao estresse psicossocial (Pattini *et al*., 2019) podendo resultar em maior estresse e ansiedade durante a pandemia do COVID-19.

4. CONCLUSÕES:

Devido aos requisitos de distanciamento físico e social, pode ser que criancas com TEA tenham maiores dificuldades com interação social após a pandemia do COVID-19 (Cardy *et al*, 2021). O aumento do tempo por uso de telas pode influenciar, visto que alguns individuos

preferem o meio digital do que a convívio social, embora alguns não tenham se adaptado as aulas remotas, os jogos e vídeos atraem essas crianças e geram resultados negativos na saúde física, como sedentarismo e obesidade.

A mudança na rotina aumenta os sintomas como ansiedade, agressividade, irritabilidade e como consequência pode agravar a saúde mental dos pais.

5. REFERÊNCIAS

1. Amorim, R; Catarino, S; Miragaia, P; Ferreras, C; Viana, V; Guardiano, M. (2020). Impacto de la COVID-19 en niños con trastorno del espectro autista. *Revista de neurología*, https://doi.org/10.33588/rn.7108.202038.

2. Cardy, R. E; Dupuis, A; Anagnostou, E; Ziolkowski, J; Biddiss, E. A; Monga, S; Brain J; Penner, M; Kushki, A. (2021). Characterizing Changes in Screen Time During the COVID-19 Pandemic School Closures in Canada and Its Perceived Impact on Children With Autism Spectrum Disorder. *Frontiers in Psychiatry*, 10.3389/fpsyt.2021.702774.

3. Charman, T; Picles, A; Simonoff, E; Chandler, S; Loucas, T; Baird, G. (2011). IQ in children with autism spectrum disorders: data from the Special Needs and Autism Project (SNAP). *Psychological Medicine*, 10.1017/S0033291710000991.

4. Goh, T. J; Lim, T; Foo, M; Ong, S. K. A; Aishworiya, R; Nair, T; Kang, Y. Q; Agarwal, P. K; Sung, M. (2020). Supporting individuals with Autism Spectrum Disorder in medical setting during COVID-19. *Asian Journal of Psychiatry*, 10.1016/j.ajp.2020.102441.

5. Kalvin, C. B; Jordan, R. P; Rowley, S. N; Weis, A; Wood, K. S; Wood, J. J; Ibrahim, K; Sukhodolsky, D. G. (2020). Conducting CBT for Anxiety in Children with Autism Spectrum Disorder During COVID-19 Pandemic. *Journal of Autism and Developmental Disorders*, https://doi.org/10.1007/s10803-020-04845-1.

6. Mutluer, T; Doenyas, C; Genc, H. A. (2020). Behavioral Implications of the COVID-19 Process for Autism Spectrum Disorder, and Individuals Comprehension of and Reactions to the Pandemic Conditions. *Frontiers in Psychiatry,* 10.3389/fpsyt.2020.561882.

7. Pattini, E. Carnevali, L; Troisi, A; Matrella, G; Rollo, D; Fornari, M. (2019). Psychological characteristics and physiological reactivity to acute stress in mothers of children with autism spectrum disorder. *Stress Health*, 10.1002/smi.2870.

8. Reicher, D. (2020). Debate: Remote learning during COVID-19 for children with high functioning autism spectrum disorder. *Child and Adolescent Mental Health*, 10.1111/camh.12425.

9. Vasa, R. A; Singh, V; Holingue, C; Kalb, L. G; Jang, Y; Keefer, A. (2021). Psychiatric problems during the COVID-19 pandemic in children with autism spectrum disorder. Autism Research, 10.1002/aur.2574.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

IMPACTS CAUSED BY THE COVID-19 PANDEMIC ON PEOPLE WITH AUTISM SPECTRUM DISORDER

Carlla Alessandra Silva Pereira
Universidade de Vassouras

December/2021

INTRODUCTION

SBJChem Conference 2021

A pandemia da COVID-19 impactou diretamente toda a população mundial, alterando a rotina dos indivíduos, em especial, as pessoas com transtorno do espectro austista.

- Isolamento social
- Rotina
- Alterações comportamentais

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

Analisar a mudança que houve na vida e na rotina de indivíduos com transtorno do espectro autista durante o isolamento social, em decorrência da pandemia da COVID-19.

METHODOLOGY

SBJChem Conference 2021

A busca foi realizada nas bases de dados: PubMed e BVS, utilizando os seguintes descritores retirados da base do DECS: autism spectrum disorder, covid pandemic e anxiety, utilizando o indicador booleano AND entre as palavras nos campos de busca. Foram adotados como critérios para a inclusão nos textos: idiomas inglês, português e espanhol, no período de 2017 a 2022. Como critério de exclusão, foram excluídos os artigos que não abordassem o tema. Foram encontrados 48 artigos e após a aplicação dos critérios foram selecionados 15 artigos

RESULTS AND DISCUSSION

SBJChem Conference 2021

- O dualismo do ensino remoto
- Terapias cognitivo-comportamentais
- Adequação à pandemia da COVID-19
- Saúde mental dos cuidadores

CONCLUSIONS

SBJChem Conference 2021

- Dificuldade de interação social
- Influência de meios digitais
- Exacerbação de sintomas

REFERENCES

SBJChem Conference 2021

1. Amorim, R; Catarino, S; Miragaia, P; Ferreras, C; Viana, V; Guardiano, M. (2020). Impacto de la COVID-19 en niños con trastorno del espectro autista. *Revista de neurología*, https://doi.org/10.33588/rn.7108.202038.
2. Cardy, R. E; Dupuis, A; Anagnostou, E; Ziolkowski, J; Biddiss, E. A; Monga, S; Brain J; Penner, M; Kushki, A. (2021). Characterizing Changes in Screen Time During the COVID-19 Pandemic School Closures in Canada and Its Perceived Impact on Children With Autism Spectrum Disorder. *Frontiers in Psychiatry*, 10.3389/fpsyt.2021.702774.
3. Charman, T; Picles, A; Simonoff, E; Chandler, S; Loucas, T; Baird, G. (2011). IQ in children with autism spectrum disorders: data from the Special Needs and Autism Project (SNAP). *Psychological Medicine*, 10.1017/S0033291710000991.
4. Goh, T. J; Lim, T; Foo, M; Ong, S. K. A; Aishworiya, R; Nair, T; Kang, Y. Q; Agarwal, P. K; Sung, M. (2020). Supporting individuals with Autism Spectrum Disorder in medical setting during COVID-19. *Asian Journal of Psychiatry*, 10.1016/j.ajp.2020.102441.

REFERENCES

SBJChem Conference 2021

5. Kalvin, C. B; Jordan, R. P; Rowley, S. N; Weis, A; Wood, K. S; Wood, J. J; Ibrahim, K; Sukhodolsky, D. G. (2020). Conducting CBT for Anxiety in Children with Autism Spectrum Disorder During COVID-19 Pandemic. *Journal of Autism and Developmental Disorders*, https://doi.org/10.1007/s10803-020-04845-1.
6. Mutluer, T; Doenyas, C; Genc, H. A. (2020). Behavioral Implications of the COVID-19 Process for Autism Spectrum Disorder, and Individuals Comprehension of and Reactions to the Pandemic Conditions. *Frontiers in Psychiatry,* 10.3389/fpsyt.2020.561882.
7. Pattini, E. Carnevali, L; Troisi, A; Matrella, G; Rollo, D; Fornari, M. (2019). Psychological characteristics and physiological reactivity to acute stress in mothers of children with autism spectrum disorder. *Stress Health*, 10.1002/smi.2870.
8. Reicher, D. (2020). Debate: Remote learning during COVID-19 for children with high functioning autism spectrum disorder. *Child and Adolescent Mental Health*, 10.1111/camh.12425.
9. Vasa, R. A; Singh, V; Holingue, C; Kalb, L. G; Jang, Y; Keefer, A. (2021). Psychiatric problems during the COVID-19 pandemic in children with autism spectrum disorder. Autism Research, 10.1002/aur.2574.


SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

INFLUENCE OF EDGE TREATMENT BY POLISHING WITH ABRASIVE BRUSH BRUSHES ON THE LIFE OF THE TOOL FOR THE MILLING PROCESS

BOGO, Ricardo[1*]; ZEILMANN, Rodrigo Panosso[2]

[1]Universidade de Caxias do Sul, Engenharia de Materiais

[2] Universidade de Caxias do Sul, Laboratório de Usinagem e Centro Técnico

** Corresponding author*
e-mail: rbogo6@yahoo.com.br

Received 05 January 2022; received in revised form 30 January 2022; accepted 03 February 2022

ABSTRACT

Machining is a process in constant evolution, the search for greater productivity, reliability, and quality of machined materials is fundamental for the constant evolution of the process. The condition of the tool edge is of great importance for the tool performance in machining, the edge of a tool after the manufacturing or re-sharpening process has defects such as: microcracks, irregularities, and an extremely sharp edge. The cutting edge treatment is used to remove these defects, which originate from the tool manufacturing and re-sharpening processes. In view of these listed points, this work aims to understand and evaluate the effects of cutting edge treatment by abrasive bristle brushes, taking into account the evolution of wear on the edge and tool life in the end milling process. The abrasive brushes covered in this work are technical brushes from the 3M brand, these brushes have different grain sizes and two different abrasives, silicon carbide (SiC) and aluminum oxide (Al_2O_3), their bristles are made of nylon of two different thicknesses. Based on the literature and to evaluate the performance of these brushes, points such as roughness and edge contour were addressed in this step, and as a result, the fine bristle brush with a SiC particle size of 1 micron had the best performance, these brushes produced a radius of 0.06 mm on the tool edges. The polishing process treated two tools, these tools went through the milling process in AISI P20 steel. As a result, the treated tools had a superior performance by 15,30% compared to untreated tools. In addition to increasing the useful life, the cutting edge treatment provided linear flank wear, delaying the presence of wear such as adhesion, microcracks, and microchips. The polishing edge treatment with abrasive bristle brushes proves to be an effective and reliable process for improving the performance of machining tools.

Keywords: *Straight end Milling, Polishing, Brushes with abrasive bristles, Wear, Tool life.*

1. INTRODUÇÃO:

Na fabricação de ferramentas de usinagem existem defeitos típicos na região do gume, defeitos recorrentes do processo de produção, como rebarbas, micro trincas e irregularidades. O processo de preparação de gume após a ferramenta pronta, surge para contornar estes problemas recorrente do processo de fabricação, eliminando defeitos e irregularidades, sendo uma região primordial para a vida útil da ferramenta, assim criando uma geometria mais bem definida e favorável para sua finalidade (RODRIGUEZ, 2009).

Um dos processos mais promissores para a preparação de gume é o por escovas com cerdas abrasivas. Com isso, verifica-se a necessidade de comparar algumas escovas disponíveis no mercado, com diferentes granulometrias e tipos de grãos abrasivos, para um melhor entendimento da técnica e suas variáveis.

2. MATERIAIS E METODOS:

2.1. Materiais

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.17_abstract_BOGO.pdf

As escovas em análise foram da marca 3M, da linha Bristle, com cerdas de nylon finas (diâmetro de 1 mm) e grossas (diâmetro de 5 mm), grãos abrasivos 80, 120 e 1 mícron, o fabricante diferencia as escovas por cores. Os grãos abrasivos seguem a Norma ANSI (*American National Standards Institute*) para os tamanhos de partícula.

Para o teste selecionou-se uma fresa reafiada, a ferramenta possui 4 gumes, referência do fabricante: Seco Tools, de código 91060 da linha Jabro.

Como corpo de prova para a usinagem foi utilizado o aço AISI P20. O corpo de prova teve suas faces retificadas, para garantir melhor fixação, diminuir a vibração e garantir uma entrada da ferramenta uniforme. As dimensões são 252 mm x 80 mm x 60 mm com dureza média de 38 HRc.

2.2. Métodos

Os métodos de análise foram realizados a fim de obter-se um padrão comparativo entre as escovas e o desempenho da melhor opção no processo de fresamento.

2.2.1. Tratamento de gume

O procedimento de tratamento de gume foi realizado nas dependências da UCS, as escovas foram fixadas em uma haste de metal que proporcionou garantias que as escovas girassem com excentricidade no eixo. Para que a escova gire usa-se uma mini retifica manual e pneumática da marca Campbell Hausfeld, com velocidade de 10.000 rpm, operando com pressão de 4 bar.

Para garantir a movimentação do gume helicoidal da fresa junto à escova foi utilizado um comando de rosqueamento. O deslocamento realizado pela ferramenta foi de 3,75 mm, no eixo z, percorrendo cada gume um total de 32 vezes. O tempo de polimento foi de aproximadamente 1 minuto por gume.

2.2.2. Contorno do gume

Para analisar o arredondamento, o contorno do gume, fez-se uso do equipamento Formtracer Avant S-3000 CR da Mitutoyo, equipamento analisa o contorno do gume, como resposta temos o raio do gume, a velocidade de apalpamento utilizada foi de 0,05 mm/s e o ponto medido foi 5 mm da quina da ferramenta.

2.2.3 Rugosidade do gume

Medições de rugosidade no gume foram medidas e comparas entre as escovas e o estado original da ferramenta. Para o parâmetro da avaliação de rugosidade, foi utilizado o critério de Ra, mensurado em 5 pontos do gume. As rugosidades foram obtidas pelo rugosímetro portátil da marca Mitutoyo, modelo SJ-301.

2.2.3. Fresamento

Para realização da usinagem o equipamento usado foi um centro de usinagem da marca Hartford (modelo LG-500). Possui uma potência máxima de 10 kW e rotação máxima de 10.000 rpm. A velocidade de corte (v_c) e o avanço (f_z) utilizados foram de 180 m/min e 0,06 mm/gume, respectivamente.

Os ensaios de fresamento foram realizados com passes de 252 mm de comprimento, com profundidade axial (a_p) e profundidade lateral (a_e) fixos, respectivamente de 0,5 mm e de 0,2 mm. A estratégia de usinagem utilizada em todo ensaio é concordante, sem uso de fluido lubrirrefrigerante, fresamento a seco.

2.2.4. Desgastes e vida útil

Com relação ao desgaste, o parâmetro que foi utilizado para o fim de vida da ferramenta foi o desgaste de flanco máximo (VB_{max}) de 0,2 mm ou lascamento da ferramenta.

3. RESULTADOS E DISCUSSÕES:

3.1. Tratamento de gume

Na Figura 1 observa-se imagens do flanco da ferramenta, geradas pelo estereoscópio trinocular de medição universal, imagens com 45 vezes de ampliação. Nota-se diferenças visuais no acabamento do flanco, em todos os tratamentos, com destaque maior para 1-B e 1-D. A ferramenta no seu estado inicial possui um acabamento homogêneo no sentido horizontal, acabamento proporcionado pela retifica, responsável pela fabricação e reafiação da

ferramenta, este acabamento pode ser visto em 1-A. O maior brilho nas imagens é devido a ação do grão abrasivo impregnado nas escovas, é visível o acabamento na direção contrária do acabamento da retifica, no sentido vertical da ferramenta. Nota-se também na imagem 1-B e 1-D que a agressividade é muito superior, devido a maior rigidez das cerdas grossas, essa agressividade pode ser demasiada no gume, produzindo raios que afetem negativamente o desempenho da ferramenta.

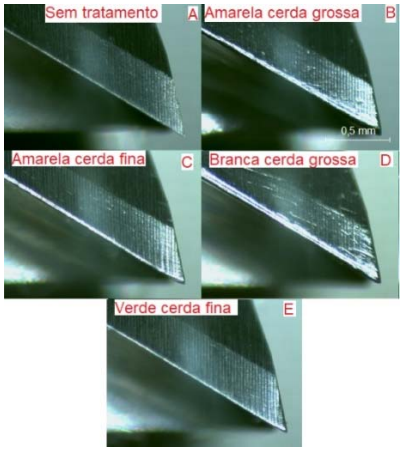


Figura 1. *Análise do flanco dos gumes antes e depois do tratamento*

3.2. Contorno do gume

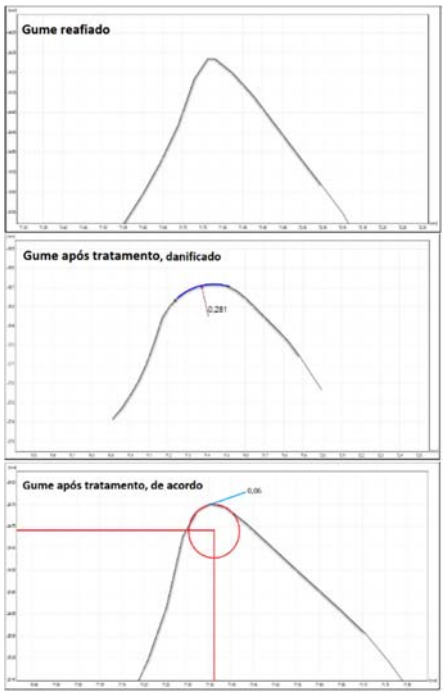


Figura 2. *Comparação entre raios gerados nos gumes da ferramenta*

A Figura 2 contém a comparação de imagens do gume da ferramenta sem tratamento, tratada com o gume danificado e tratada com o gume de acordo com o objetivo do trabalho. As análises da fresa tratada obteve como resultados no gume 1, 2 e 3 um arredondamento do gume capturado pelo software do equipamento, raios entre 0,250 e 0,282 mm, este arredondamento segundo a literatura é demasiado, podendo assim danificar o gume da ferramenta.

O gume 4 modicou o contorno, mas devido as limitações do equipamento não foi informado o raio, sendo assim o equipamento apenas gerou o perfil, porém com um cálculo manual utilizando a equação reduzida da circunferência estima-se um raio na casa de 0,06 mm aproximadamente, este valor fica dentro de um arredondamento aceitável para um gume tratado.

3.3. Rugosidade do gume

A rugosidade obtida nos gumes foram: Reafiada, 0,37 Ra; Gume 1, 0,56 Ra; Gume 2, 0,44 Ra; Gume 3, 0,51 Ra; Gume 4, 0,55 Ra. Quando a ferramenta é submetida ao tratamento com as escovas sua rugosidade é alterada, atestando que o grão abrasivo agiu na superfície da ferramenta. Segundo (DE PELLEGRIN; STACHOWIAK, 2001) as partículas de SiC mesmo em tamanhos menores possuem uma alta área de penetração.

3.3. Fresamento

O Fresamento se deu conforme o estipulado no item 2.2.3 deste trabalho. Foram submetidas 2 fresas reafiadas em estado original sem tratamento (O6-S/TRA), e 2 fresas que foram submetidas ao tratamento de gume com a escova de cerda abrasiva de 1 mícron (O6-TRA).

3.4. Desgastes e vida útil

No Gráfico 1 estão apresentadas as curvas de comportamento de desgastes. Em laranja estão representadas as curvas de comportamento do desgaste para duas fresas sem tratamento (O6-S/TRA), representada pela média de desgastes ao longo do comprimento usinado (ocorreu a cada 5040 mm usinados). Em azul, segue as mesmas premissas, mas para as fresas que foram tratadas com o polimento com escovas de cerdas abrasivas neste trabalho (O6-TRA).

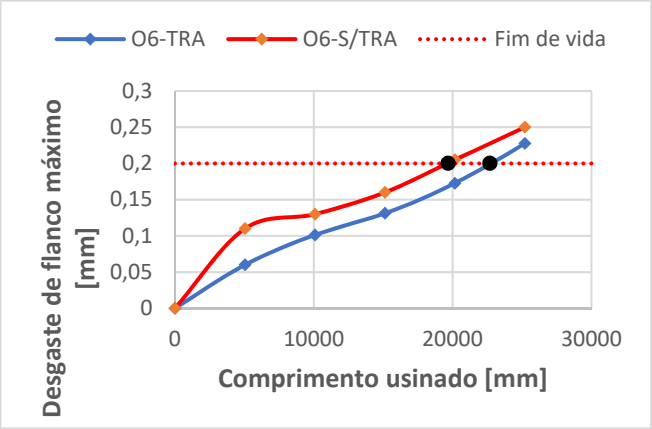


Gráfico 1. *Curvas de desgaste*

Comparando as curvas de desgaste no Gráfico 2, as fresas tratadas tiveram um comportamento de desgaste linear desde o início da usinagem, pode-se assim dizer que o tratamento amenizou os desgastes do Estágio I, neste estágio a ferramenta sofre um desgaste acelerado, natural ao sistema tribológico envolvido segundo (MACHADO *et al.*, 2015). As ferramentas ao chegarem ao $VB_{máx}$ de 0,20 mm tiveram os seguintes resultados: para uma fresa sem tratamento o final de sua vida se deve a 19681 milímetros, já as fresas tratadas tiveram sua vida útil aumentada para 22692 milímetros, aumentando sua vida útil em 15,30 %.

O desgaste linear está relacionado com o processo de tratamento de gume, segundo estudo realizado por (WANG *et al*., 2020) o desgaste linear prolonga consideravelmente a vida útil da ferramenta, contribui para uma melhor distribuição dos esforços mecânicos sofridos no processo de usinagem.

4. CONCLUSÕES:

A partir dos resultados obtidos, conclui-se:

a) O tratamento de gume por cerdas abrasivas é eficaz.

b) Grãos de carbeto de silício na granulometria de mícron se mostraram eficazes para gerar a geometria favorável para o gume.

c) Ferramentas tratadas tiveram um desempenho superior de 15,30 % em vida útil, em comparação a ferramentas não tratadas.

d) Desgaste linear, mais confiabilidade na usinagem.

5. REFERENCIAS

1. WANG, W; Saifullah, K. M.; Aßmuth, R.; Biermann, D.; Arif, A. F. M. Effect of edge preparation technologies on cutting edge properties and tool performance. **International Journal of Advanced Manufacturing Technology**, v. 106, n. 5–6, 2020.
2. MACHADO, Álisson Rocha; ABRÃO, Alexandre Mendes; COELHO, Reginaldo Teixeira. **Teoria da usinagem dos materiais.** 3. ed. São Paulo. Editora Edgard Blücher Ltda, 2015.
3. RODRÍGUEZ, C. **Cutting edge preparation of precision cutting tools by applying micro-abrasive jet machining and brushing**. [s.l: s.n.].
4. DE PELLEGRIN, D. V.; STACHOWIAK, G. W. **Abrasiveness of particles measured by Cone-Fit Analysis (CFA)**. Tribology Series. **Anais**...2001
5. AURICH, J. C.; EFFGEN, C.; KIRSCH, B. Cutting edge preparation with elastic bonded superabrasive grinding wheels. **CIRP Annals - Manufacturing Technology**, v. 65, n. 1, 2016.
6. UHLMANN, E. Oberschmidt, D.; Kuche, Y.; Löwenstein, A.; Winker, I. **Effects of Different Cutting Edge Preparation Methods on Micro Milling Performance**. Procedia CIRP. **Anais**...2016
7. OVERHOLSER, R. W.; STANGO, R. J.; FOURNELLE, R. A. Morphology of metal surface generated by nylon/abrasive filament brush. **International Journal of Machine Tools and Manufacture**, v. 43, n. 2, 2003.
8. SHATHER SAAD KARIEM, M. A. A. A. Influence Of silicon carbide (SIC) abrasive on surface roughness and metal removal rate during magnetic abrasive finishing **Global Journal of Engineering Science and R esearch Management.** v. 6, n. 1, p. 8–20, 2019.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

INFLUENCE OF EDGE TREATMENT BY POLISHING WITH ABRASIVE BRUSH BRUSHES ON THE LIFE OF THE TOOL FOR THE MILLING PROCESS

Ricardo Bogo
Universidade de Caxias do Sul, Materials Engineer- Brazil.

Dr. Rodrigo Panosso Zeilmann
Universidade de Caxias do Sul, Mechanical Technical Center - Brazil.

March/2022

INTRODUCTION

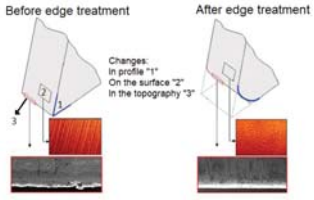
SBJChem Conference 2021

- Improve the performance of machining tools through the edge treatment method
- Understand the behavior of SiC and Al_2O_3 abrasives in the treatment
- Evaluate the performance of tools after treatment

BACKGROUND

SBJChem Conference 2021

The cutting edge preparation process after the tool is ready, appears to circumvent the recurring defects of the production process, eliminating defects and irregularities, being a primordial region for the useful life of the tool, thus creating a better defined and favorable geometry for its purpose. (RODRIGUEZ, 2009).



Source: Adapted from RODRIGUEZ (2009).

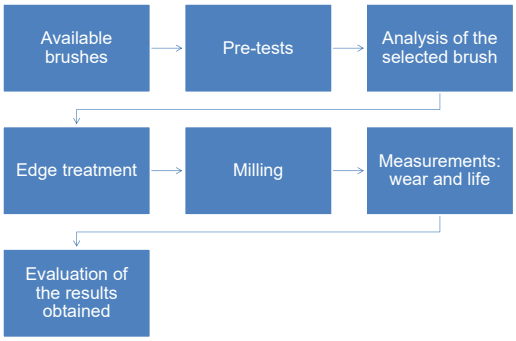
AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

The main objective of this work was to understand and evaluate the effects of cutting edge treatment by abrasive bristle brushes, taking into account the evolution of wear and tool life in the end milling process.

METHODOLOGY

SBJChem Conference 2021



METHODOLOGY

SBJChem Conference 2021

Milling cutters	• Seco Tools, code 91060 from the Jabro range, 4 cutting edges and 6 mm diameter, untreated and without corner radius;
Proof bodies	• AISI P20, 252 mm x 80 mm x 60 mm with an average hardness of 38 HRc;
Machining	• Hartford brand machining center (model LG-500);
Edge roughness	• Mitutoyo laptop, model SJ-301;
Measurement of wear	• Entex TNE-10B Trinocular Stereoscope;

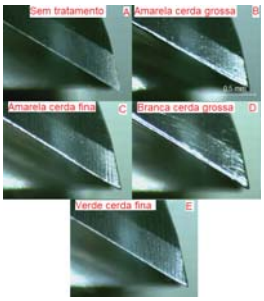
METHODOLOGY

SBJChem Conference 2021

Brush	Grain	Edge	Abrasive component
Yellow thick bristle	80	1	Aluminum oxide
Yellow fine bristle	80	2	Aluminum oxide
White thick bristle	120	3	Aluminum oxide
Green fine bristle	1 micron	4	Silicon carbide

RESULTS AND DISCUSSION

SBJChem Conference 2021

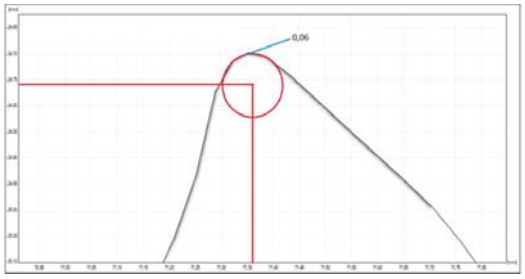


- Thick bristles with high abrasiveness (B and D);
- SiC with good interaction at the edge (E).

Source: The authors (2020).

RESULTS AND DISCUSSION

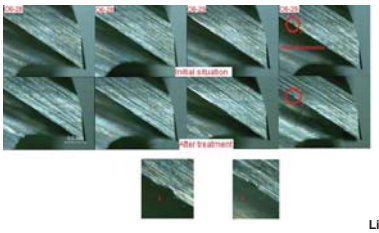
SBJChem Conference 2021



Edge after treatment with green brush fine bristle with silicon carbide grain, 1 micron

RESULTS AND DISCUSSION

SBJChem Conference 2021



Micro chipping
Initial:

- **0,14 mm long and 0,03 mm deep (1)**

After treatment:

- **0,07 mm long and 0,01 mm deep (2)**

Lifespan:
O6-S/TRA = 19681 mm
O6-TRA = 22692 mm

useful life + 15.30%

CONCLUSIONS

SBJChem Conference 2021

- Abrasive bristle brushes proved to be effective for the edge treatment process;
- Easily adaptable to companies in the industry;
- Practical and reliable process;
- Fine grains in the micron range, fine bristles, malleable. Better performance;
- Longer tool life;
- Higher productivity.

REFERENCES

SBJChem Conference 2021

1. WANG, W. et al. Effect of edge preparation technologies on cutting edge properties and tool performance. **International Journal of Advanced Manufacturing Technology**, v. 106, n. 5–6, 2020.
2. MACHADO, Álisson Rocha; ABRÃO, Alexandre Mendes; COELHO, Reginaldo Teixeira. **Teoria da usinagem dos materiais.** 3. ed. São Paulo. Editora Edgard Blücher Ltda, 2015.
3. RODRÍGUEZ, C. **Cutting edge preparation of precision cutting tools by applying micro-abrasive jet machining and brushing**. [s.l: s.n.].
4. DE PELLEGRIN, D. V.; STACHOWIAK, G. W. **Abrasiveness of particles measured by Cone-Fit Analysis (CFA)**. Tribology Series. **Anais**...2001
5. AURICH, J. C.; EFFGEN, C.; KIRSCH, B. Cutting edge preparation with elastic bonded superabrasive grinding wheels. **CIRP Annals - Manufacturing Technology**, v. 65, n. 1, 2016.

REFERENCES

SBJChem Conference 2021

6. UHLMANN, E. et al. **Effects of Different Cutting Edge Preparation Methods on Micro Milling Performance**. Procedia CIRP. **Anais**...2016
7. OVERHOLSER, R. W.; STANGO, R. J.; FOURNELLE, R. A. Morphology of metal surface generated by nylon/abrasive filament brush. **International Journal of Machine Tools and Manufacture**, v. 43, n. 2, 2003.
8. SHATHER SAAD KARIEM, M. A. A. A. Influence Of silicon carbide (SIC) abrasive on surface roughness and metal removal rate during magnetic abrasive finishing **Global Journal of Engineering Science and R esearch Management.** v. 6, n. 1, p. 8–20, 2019.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

IVORY CHARACTERIZATION USING PORTABLE VIBRATIONAL SPECTROMETRY

ENGEL, Wanda; GENNARI, Roseli Fernandes; FERREIRA, Cauê,RIZZUTTO, Marcia*;

Instituto de Fisica da Universidade de São Paulo, Departamento Física Nuclear, Brazil.

** Corresponding author*
e-mail: rizzutto@usp.br

Received 30 January 2022; received in revised form 26 February 2022; accepted 04 March 2022

ABSTRACT

Ivory was commonly used in the manufacture of numerous objects. It refers to the tusk and teeth of animals. Almost all ivory pieces, in the past, found on the market were authentic; however, nowadays, ivory extraction is an illegal practice. Thus, official government and animal protection entities have been fighting intensely against this criminal practice, but the production and sale continue. There are numerous difficulties in identifying the illegal extraction and use of ivory, and the correct characterization is certainly a great challenge. A proper ivory characterization is an important tool in the fight against ivory extraction once it is possible to trace the piece to the animal and sometimes even to its origin. It is also useful for museums and art collectors to verify the authenticity of the piece. Ivory, also known as the inorganic gemstone, is composed of calcium phosphate, collagen, elastin, and lipids. Different tests can differentiate ivory from bones or celluloid; however, some can damage the piece. Because of that, analytical techniques are preferred. However, the method to be used must have the capability of differencing small differences once the chemical elements present in ivory, bone, or even celluloid are the same. In this work, three analytical methodologies were used to check the possibility of having an alternative test applied on supposed ivory samples. All three methods used, X-Ray Fluorescence (XRF) and vibrational spectrometry techniques (FT-IR and Raman), are portable equipment to facilitate the analysis in situ. FT-IR and Raman spectra obtained had shown differences between bone and ivory samples, indicating the art collector samples are probably ivory. These differences allied with the portability of the analysis can be used as an additional test to be done in ivory and bone-based materials.

Keywords: *Ivory, Vibrational Spectrometry, FTIR, Raman, In situ analysis*.

1. INTRODUCTION

Ivory is a term used to describe a variety of animal tusk and teeth. It is the raw material for numerous objects such as sculptures, jewelry, and furniture. In general, the most used are canine teeth from elephants and mammoths; however, one can also use teeth from walrus, wild boar, hippopotamus, or narwhal. Despite the variety of animals, ivory origin also influences the material's characteristics. For example, the ivory teeth of elephants from Asia were whiter than the African ones, less closed in texture, but not susceptible to polishing. On the other hand, the most refined and beautiful type came from the Pagani region of the east coast of Africa (Tripati, S., Godfrey, I., 2007).

Ivory, also known as inorganic gemstone, is chemically composed of approximately 70% of inorganic material as calcium phosphate [$Ca_{10}(PO_4)CO_3$ H_2O] and around 30% organic material, essentially collagen, elastin, and lipids, and the ratio of organic and inorganic material vary from animal to animal (Baker, B., Jacobs, R., Mann, M., Espinoza, E., Grein, G., 2020).

Almost all ivory pieces, in the past, found on the market were authentic. However, nowadays, ivory extraction is an illegal practice however the production and sale of ivory still occur. The illegality is related to the unrestrained killing of animals. Thus, official government and animal protection entities have intensely fought against the ivory trade. This struggle is one of the reasons for the high price of ivory pieces and, consequently, responsible for the increase in ivory forgery.

Ivory forgery is a common practice

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.40_abstract_ENGEL.pdf

(Cutler, A., 2011) and is made with bone and celluloid. Different tests can differentiate ivory from bones or even from celluloid. For instance, in the visual observations, if you find parallel lines, called as Haversian System, it is probably bone that generally has also black dots. A cross pattern, the Schreger lines are characteristic from ivory. In the transverse grooves of polished elephant and mammoth ivory, the dentin shows Schreger lines, commonly referred to as growth rings. The intersections of lines range from angles less than 90 to 100 degrees in mammoth ivory. In contrast, lines between 100 and 115 degrees are evident in African/Asian elephant ivory (Tripati, S., Godfrey, I., 2007). The flame test also does not cause any damage only in ivory. However, sometimes forgery can not be noticed so easily, so the flame test is not always useful. In these cases is fundamental to have strategies to differentiate ivory from bone also from synthetic materials. A pure, simple chemical analysis does not solve the doubt once the chemical composition of animal teeth and bones are quite similar. A proper ivory characterization is an important tool in the fight against ivory extraction once it is possible to trace the piece to the animal and sometimes even to its origin. It is also useful for museums and art collectors. Because of that, it requires an association of several analytical techniques to be feasible ivory differentiation from similar materials (mainly bones and synthetic materials).

In this work, we used three analytical methodologies to check the possibility of an alternative forgery test to be applied on supposed ivory samples. All three methods used, X-Ray Fluorescence (XRF) and vibrational spectrometry techniques (FT-IR and Raman) used, are portable equipment to facilitate the analysis in situ. The decision to use vibrational techniques is based on the fact that they are commonly used in organic compound analysis.

2. MATERIALS AND METHODS

2.1. Analytical Equipment

The X-Ray Fluorescence spectrometer used is an energy dispersion system consisting of an X-ray tube, silver anode (Ag), and a Si-Drift fast semiconductor detector (SDD), both from Amptek®. During measurements, the equipment is positioned close to the object without touching it not to cause any damage to it. The experimental conditions for all measurements were voltage of 30 kV, current of 5 uA, and measurement time of 100 seconds. At the output of the X-Ray source, a 2 mm collimator was used.

Raman spectrometer is a Dual EZ Raman-N (Enwave Optronics) equipped with a 785 nm laser and 20-30 mW. The measurement range of 100 at 2200 cm^{-1} with a spatial resolution of 6 cm^{-1} was selected for each acquired spectra.

The Fourier transform infrared spectrometer (FT-IR) is from Bruker® (Alfa model). The reflectance module was used as a sampling device. The spectra shown here are an average of 32 scans in a spectral range from 4000 to 400 cm^{-1} with 4 cm^{-1} resolution and under controlled environmental conditions (temperature and humidity).

2.2. Samples

It was tested the analytical methodologies pointed out above on three samples one brooch belonging to a colleague (Nobuko) and one knife (identified here as 861-1), and one “fork” (identified here as 862-2) from a private art collector, who does not want to be identified. Nobuko’s piece has its authenticity known, but the art collector was in doubt.

2.3. Quality Control

All samples were analyzed at various points to ensure reproducibility. It is important to note that the region with the same color was always chosen once the art collector pieces had colored carvings.

The Bone Meal (Certified Reference Material, SRM 1486, NIST) was analyzed by three spectrometric methods despite its certificate referring only to elemental concentration. In addition, a hydroxyapatite reagent was also analyzed.

3. RESULTS AND DISCUSSION:

3.1. X-Ray Analysis

The obtained results on XRF analyses are concordant, which ones expected to ivory based on materials. Furthermore, the similarity of the results of both samples indicates a probability of being from the same material composition.

3.2. FT-IR Analysis

FT-IR spectra of analyzed samples were obtained, and they were compared with the FT-IR spectrum of Bone Meal. We also decided to compare Nobuko's pieces with the ones from the art collector to verify the differences or similarities between them.

In FT-IR spectra, one can easily notice there is a difference, in the range of 1200-1000 cm^{-1}, between the samples and CRM Bone Meal (pasted powder material). In samples (Nobuko's brooch, 861-1 and 862-2) appears one high-intensity peak near 1200 cm^{-1}. In CRM, the high-intensity peak appears near 1000 cm^{-1}. Sample measurements probably suffered stray light interference because we used the Kubelka-Munk function to better interpret the spectra. It probably happened because the samples are not so flat, and this can affect the measurements when the reflectance module is used as a sampling device. This is not valid for the CRM, which was analyzed as pasted powder. This region (1200 – 800 cm^{-1}) is the one characteristic for phosphate (Álvarez-Lloret P., Rodríguez-Navarro A.B., Romanek Ch.S., Gaines K.F, Congdon Y J., 2006) and through XRF analysis, it is possible to affirm there is a huge Ca and P concentration. The amide I and II region is important to differentiate ivory from bone (Álvarez-Lloret P., Rodríguez-Navarro A.B., Romanek Ch. S., Gaines K.F, Congdon Y J., 2006, Melanie M. Beasley, Eric J. Bartelink, Lacy Taylor, Randy M. Miller 2014, O'Connor S., Edwards H. G. M. 2011. Chadefaux C., Hô Anne-Solenn Le, Bellot-Gurlet L., Reiche I., 2009, Morris M. D., Mandair G. S., 2011).

We expanded the FT-IR spectra obtained, allowing us to observe of amide I and II region better. So, it became evident a difference in the FT-IR spectrum from Bone Meal from FT-IR spectra of remaining samples. This difference is indicative all analyzed samples have a high probability of being ivory.

In order to prove the adequability of using Bone Meal as reference control for vibrational analysis, we analyzed hydroxyapatite also. As a result, the FT-IR spectrum of SRM Bone Meal has a strong similarity with the FT-IR hydroxyapatite spectrum, evidencing the applicability of these materials as control ones.

3.3. Raman Analysis

Raman Spectra for the samples were also obtained.

In Raman analyses, measured pieces (861-1 and 862-2) show similarities with the Ivory Nobuko piece (brooch) and differ from the bone material (SRM Bone Meal).

The Raman vibrational mode, occurring in 1290 cm^{-1}, is characteristic of the bone material (Morris M. D., Mandair G. S., 2011), and it was not observed in either analyzed sample.

The vibrational bands identified (Amide I and II, carbonate, phosphate, protein) by both techniques are concordant with the ones presented in the literature (Edwards H.G.M., Farwell D, W., 1995).

4. CONCLUSIONS:

All the spectra presented here evidence the applicability of both vibrational techniques as a tool for characterization and forgery identification on ivory material. The equipment used is portable ones, and their response was quite similar to the bench equipment.

5. ACKNOWLEDGMENTS:

The author wants to acknowledge our colleague, Nobuko Ueta, for letting us analyze her brooch. In addition, the authors acknowledge CNPq, FAPESP, and CAPES for supporting us on equipment purchase.

One of us (Cauê Ferreira) wants to acknowledge for his grant received.

6. REFERENCES:

1. Tripati, S., Godfrey, I. (2007). Studies on elephant tusks and hippopotamus teeth collected from the early 17th century Portuguese shipwreck off Goa, west coast of India: Evidence of maritime trade between Goa, Portugal, and African countries. Current Science, 92(3), 332–339.
2. Baker, B., Jacobs, R., Mann, M., Espinoza, E., Grein, G. (2020). CITES Identification Guide for Ivory and Ivory Substitutes (4th Edition, Allan, C. (ed.)), World Wildlife Fund Inc., Washington DC.

Commissioned by CITES Secretariat, Geneva, Switzerland.
3. Cutler, A., (2011), Carving, Recarving, and Forgery: Working Ivory in the Tenth and Twentieth Centuries, West 86th: A Journal of Decorative Arts, Design History, and Material Culture 18:2, 182-195.
4. Álvarez-Lloret P., Rodríguez-Navarro A.B., Romanek Ch. S., Gaines K.F, Congdon Y J., (2006), Quantitative Analysis of Bone Mineral Using FTIR, MACLA 6 XXVI Reunion (SEM) / XX Reunion (SEA), 45-47.
5. Melanie M. Beasley, Eric J. Bartelink, Lacy Taylor, Randy M. Miller (2014), Comparison of transmission FTIR, ATR, and DRIFT spectra: Implications for assessment of bone bioapatite diagenesis, Journal of Archaeological Science 46(1), 16-20.
6. O'Connor S., Edwards H. G. M. (2011) An Interim Investigation of the Potential of Vibrational Spectroscopy for the Dating of Cultural Objects in Ivory", ArcheoSciences /1 (n° 35), 159-65.
7. Chadefaux C., Hô Anne-Solenn Le, Bellot-Gurlet L., Reiche I., (2009) Curve-fitting MICRO-ATR-FTIR studies of the Amide I and II bands of type I COLLAGEN in archaeological bone materials, e-PS, 6, 129-137.
8. Morris M. D., Mandair G. S., (2011) "Raman Assessment of Bone Quality", Clinical Orthopaedics and Related Research 469(8), 2160-9.
9. Edwards H.G.M., Farwell D, W., (1995) Ivory and simulated ivory artifacts: Fourier transform Raman diagnostic study, Spectrochimica Acta Part A, (51), 2073-2081.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

IVORY CHARACTERIZATION USING PORTABLE VIBRATIONAL SPECTROMETRY

Wanda Engel
USP, Instituto de Física - Brazil

Roseli Fernandes Gennari
USP, Instituto de Física - Brazil

Cauê Ferreira
USP, Instituto de Física - Brazil

Márcia Rizzutto
USP, Instituto de Física - Brazil

March/2022

INTRODUCTION

SBJChem Conference 2021

- Ivory, also known as inorganic gemstone, is chemically composed of approximately 70% of calcium phosphate [$Ca_{10}(PO_4)CO_3.H_2O$] and around 30% collagen, elastin, and lipids.
- Ivory forgery is a common practice so it is important to verify the authenticity of the "ivory" piece;
- Vibrational techniques are useful tool on materials characterization;
- Non destructive analysis is fundamental to historical patrimony issues.

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

The aim of this work is to propose the use of portables equipment on the investigation on the ivory authenticity .

METHODOLOGY

SBJChem Conference 2021

Samples

•Three samples were studied: one brooch belonging to a colleague (Nobuko), one knife (identified here as 861-1) and one "fork" (identified here as 862-2) from a private art collector, whom does not want to be identified. None sample preparation was done.

Analytical Equipment

•XRF is an energy dispersion system, consisting an X-ray tube, silver anode (Ag) and a Si-Drift fast semiconductor detector (SDD), both from Amptek®.

•FT-IR is from Bruker® (Alfa model). The reflectance module was used as sampling device.

•Raman spectrometer is a Dual EZ Raman-N (Enwave Optronics) equipped with a 785 nm laser, and 20-30 mW.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 1. Peak Area Obtained through XRF Analysis

Element	Knife (861-1)	Fork (862-2)
P	4490 (67)	3338 (58)
S	742 (27)	1057 (33)
K	892 (30)	1290 (36)
Ca	65478 (256)	57548 (240)
Fe	976 (31)	536 (23)
Zn	351 (19)	468 (22)
Sr	711 (27)	554 (24)
Ca/P	14.58 (0.22)	17.24 (0.31)

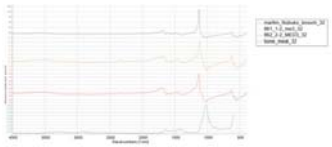


Figure 1. FT-IR Spectra of Analyzed Samples

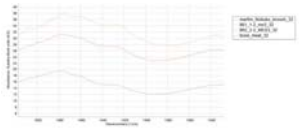


Figure 2. Expanded FT-IR Spectra of Amide Region for "ivory" samples

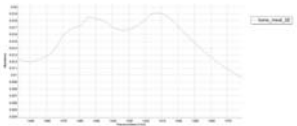


Figure 3. Expanded FT-IR Spectra of Amide Region for Bone sample

RESULTS AND DISCUSSION

SBJChem Conference 2021

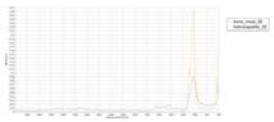


Figure 4. FT-IR Spectra of Control Samples

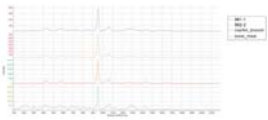


Figure 5b. Raman Spectra of Analyzed Samples (mode stack)

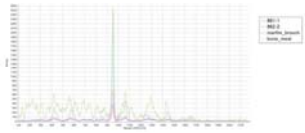


Figure 5a. Raman Spectra of Analyzed Samples (mode overlay)

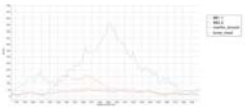


Figure 6. Expanded Raman Spectra of Analyzed Samples

CONCLUSIONS

SBJChem Conference 2021

- With the XRF analysis it is possible to affirm there is huge Ca and P concentration;
- The amide I and II region is used to differentiate ivory from bone, according several authors [4 to 7]. The behavior observed in Figs 2 and 3 is an indicative all analyzed samples have a high probability of being ivory;
- In FT-IR and Raman analyses, measured pieces show similarities with the Ivory piece (Nobuko's brooch), and differs from the bone material (SRM Bone Meal) ;
- The bone peak characteristic (1290 cm^{-1}) appeared only in bone spectrum.
- Portables equipment can be used on ivory and bone differentiation.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

- The authors wants to acknowledge our colleague Nobuko for letting us to analyze her brooch. We want also to acknowledge CNPq, FAPESP and CAPES for supporting us on equipment purchase.

REFERENCES

SBJChem Conference 2021

1. U.S. Fish & Wildlife Service – Forensics Laboratory - https://www.fws.gov/lab/ivory_natural.php
2. Baker, B., Jacobs, R., Mann, M., Espinoza, E., Grein, G. (2020). CITES Identification Guide for Ivory and Ivory Substitutes (4th Edition, Allan, C. (ed.)), World Wildlife Fund Inc., Washington DC. Commissioned by CITES Secretariat, Geneva, Switzerland.
3. PennState, Art history professor looks into the big business of ivory carving forgery https://www.psu.edu/news/arts-and-entertainment/story/art-history-professor-looks-big-business-ivory-carving-forgery/ accessed in February 02, 2022.
4. Álvarez-Lloret P., Rodríguez-Navarro A.B., Romanek Ch.S.,. Gaines K.F, Congdon Y J., (2006), Quantitative Analysis of Bone Mineral Using FTIR, MACLA 6 XXVI Reunion (SEM) / XX Reunion (SEA), pag 45-47.
5. O'Connor S., Edwards H. G. M. (2011), An Interim Investigation of the Potential of Vibrational Spectroscopy for the Dating of Cultural Objects in Ivory", ArcheoSciences , 1 (n° 35), pages 159 to 165.
6. Chadefaux C., Hô Anne-Solenn Le, Bellot-Gurlet L., Reiche I., (2009), Curve-fitting MICRO-ATR-FTIR studies of the Amide I and II bands of type I COLLAGEN in archaeological bone materials, e-PS, , 6, 129-137.
7. Morris M. D., Mandair G. S., (2011), Raman Assessment of Bone Quality, Clin Orthop Relat Res. Aug; 469(8): 2160–2169

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

MOLECULAR MODELING, REACTIVITY PARAMETERS AND SPECTROCHEMIC STUDIES OF ε-CAPROLACTAM AND o-PHENANTROLINE

LIMA, Francisco José Santos*; PESSOA, Maria José de Oliveira; ARAÚJO, Lucas da Silva; SILVA, Ademir Oliveira da, and PEREIRA, Francisco Claudece.

Universidade Federal do Rio Grande do Norte, Centro de Ciências Exatas, Instituto de Química, Brazil

** Corresponding author*
e-mail: limafjs@yahoo.com

Received 12 September 2021; received in revised form 30 September 2021; accepted 15 October 2021

ABSTRACT

In this work, molecular models were obtained, and the reactivity parameters of ε-caprolactam and o-phenanthroline were calculated to evaluate the interaction in the formation of complex molecular compounds. It was observed that the main electron donor atoms, in the formation of the metal-ligand bond, are centered mainly on the oxygen and nitrogen atoms, respectively, which are sterically more favorable in these species. Conductance measurements in an aqueous solution were obtained to observe the electrolytic behavior of these compounds. Infrared spectra were also recorded to characterize vibrational transitions in identifying these species when present in complex systems. Molecular spectra of absorption in the UV-visible region were recorded to evaluate the spectrochemical properties of these individual ligands and further verify their influence on the formation of complex molecular systems. The parameters evaluated include the molar absorptivity ε, integrated absorption coefficient, oscillator force, and transition dipole moment. It was observed that the ε parameter indicates molecular transitions in the 190 – 300 nm region and the near-infrared, and the oscillator strength is typical of molecules used as dyes and sensitizers for optical light-emitting systems or light-to-electricity converters.

Keywords: *oscillator strength, transition dipole moment, spectrochemical properties*.

1. INTRODUCTION

The ε-caprolactam is a cyclic chain amine with molecular formula $C_6H_{11}NO$, molar mass 113.16 g / mol, soluble in water (50 mg / mL), which in aqueous solution has a pH between 7.0 - 8.5 (333 g/L). In the chemical industry, it has been widely used as a precursor of polymers called nylon 6. More recently, it has been applied in the synthesis of polymeric polyamide compounds (Gong and Yang, 2010), in photochemical-photovoltaic-thermochemical systems (CP-PV-T) for the use of high-efficiency full-spectrum solar energy (Fang *et al,*, 2010), as well as its derivatives, (N-methyl-ε-caprolactam) in the synthesis of light-emitting compounds (Borges *et al*., 2016).

O-phenanthroline is a solid, white, organic heterocyclic compound with the molecular formula $C_{12}H_8N_2$, molar mass 180.21 g/mol, and has a solubility of 3.3 g/L (25 ^oC) in monohydrate form. Although 1,10-phenanthroline is widely used for fast, flexible, and reliable analysis with a high scientific reputation in research, other applications are found, such as; uses cathodic protective buffer layers as a conventional binder to improve the efficiency of organic solar cells (Sun *et al*., 2014), in the study of efficacy in the Luminol chemiluminescence system in Fenton reactions (Mitsuhiro *et al*., 2014), in complex systems with Cu(I) using mixed ligands to amplify luminescent radiative emissions by electron transfer with a high quantum efficiency (Li *et al*., 2012).

This work developed molecular modeling, calculated the reactivity parameters, obtained molar conductivity measurements, recorded infrared and UV-visible spectra, and calculated the spectrochemical properties related to the oscillator strength and induced dipole moment.

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.01_lima.pdf

2. MATERIALS AND METHODS

2.1 Molecular Modeling and Reactivity Parameters

Molecular modeling, theoretical reactivity parameters, electrostatic potential cloud, bonding distances, bonding angles, and partial charges were obtained from the WebLab ViewerPro© program. The parameters were calculated using the following expression (Lima *et al*, 2020):

$$\Re = \frac{\int q_i \, d\tau}{\sum_{i=1}^{n} \left| \int q_i \, d\tau \right|}$$

Eq. 01

2.2 Conductance, Conductivity and Molar Conductivity

Molar conductivity measurements were performed for aqueous solutions of millimolar concentration, using a QUIMIS Q-405 conductivity meter, at a temperature of 25.0 ± 1 °C, after calibration of the cell constant with freshly prepared standard solutions millimolar of NaCl and KCl. The molar conductivity was calculated using the expression below:

$$\Lambda_M = \frac{(L_{sol} - L_{solv}).Kc.10^3}{M} = \frac{(k_{sol} - k_{solv}).10^3}{M},$$

Eq. 02

2.3 Spectroscopy in the Infrared Region

The infrared spectra of the two samples were recorded in a PERKIN ELMER FRONTIER equipment, in KBr pellets, in the range of 700 – 4000 cm^{-1} and resolution 4 cm^{-1}.

:

2.4 Spectroscopy in the UV-Visible Region

The UV-vis spectra were recorded in a SHIMADZU UV model spectrophotometer in the range of 200 - 1000 nm, quartz cuvette with 1 cm optical path for aqueous ε-caprolactam solutions ($1.18x10^{-2}$ mol L^{-1}), aqueous o-Phenatroline ($1.15x10^{-2}$ mol L^{-1}) and ethanolic o-Phenatroline ($1.01x10^{-2}$ mol L^{-1}). Samples needed to be diluted. The oscillator force f was calculated by Drago's and Figgs method and described methodologies (Lima *et al*., 2020) according to the expressions:

DRAGO: $f = 4{,}6x10^{-9} \int \varepsilon_{(\sigma)} d\sigma$ Eq. 03

FIGGS: $f = 4{,}32x10^{-9} \int \varepsilon_{(\sigma)} d\sigma$ Eq. 04

Area under the absorption band =

$$\int A_{(\sigma)} d\sigma = A_{máx.}(1/\lambda_1 - 1/\lambda_2)$$ Eq. 05

The transition dipole moment was obtained by the following equation:

$$\mu_{if} = 8{,}422x10^{-22} (m\, s^{-1/2} C) . \sqrt{\frac{f}{\nu}} \quad (C\, m)$$

Eq. 06

3. RESULTS AND DISCUSSION:

3.1 Molecular modeling, obtaining structural data and reactivity parameters.

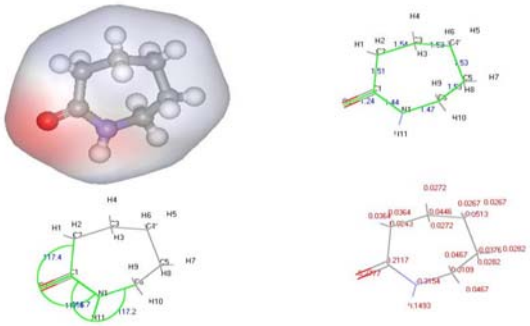


Figure 01 - Modeling obtained for ε-Caprolactam, $C_6H_{11}NO$, using the WebLab ViewerPro program©.

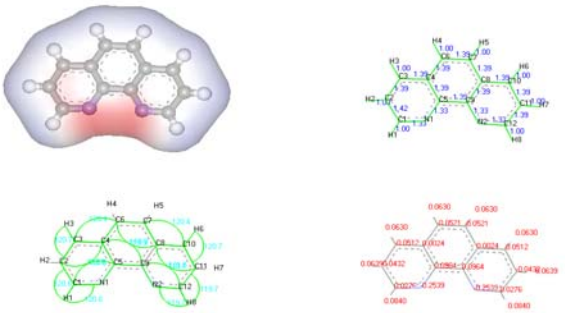


Figure 02 - Modeling obtained for o-Phenanthroline, $C_{12}H_8N_2$, using the WebLab ViewerPro program©.

Table 01 - Partial charges and PRM for ε-Caprolactam, $C_6H_{11}NO$.(main atoms)

Atoms	*Partial charges*		PRM	
	δ^-	δ^+	$\Re^-$	$\Re^+$
O_1	-0,2777		-0,3822	
C_1		0,2117		0,2913
H_1		0,0364		0,0501
H_{10}		0,0467		0,0643
N_1	-0,3154		-0,4341	
H_{11}		0,1493		0,2054

PRM - Molecular Reactivity Parameters

Table 02 - Partial charges and PRM for o-Phenanthroline, $C_{12}H_8N_2$. (main atoms)

	Partial charges		PRM	
Atoms	δ^-	δ^+	$\Re^-$	$\Re^+$
C_1		0,0276		0,0345
C_{12}		0,0276		0,0345
C_5		0,0964		0,1204
C_9		0,0964		0,1204
N_1	-0,2539		-0,3171	
N_2	-0,2539		-0,3171	

PRM - Molecular Reactivity Parameters

3.2 Conductivity measurements and the associated electrolyte type.

Table 03 – Conductivities obtained for millimolar aqueous solutions at 25.0 ± 1 ºC.

	k x10^{-6}	M Mol/L	Λ_M	Type of electrolyte
H_2O	17,6	55,5	31,7x10^{-5}	n-electrol
NaCl	121	0,001	103,4	1:1
KCl	150	0,001	132,4	1:1
ε-capro	34,4	0,001	16,8	n-electrol
o-fen	33,0	0,001	15,4	n-electrol

Units: k (S cm^{-1}); Λ_M (S cm^2 mol^{-1})

3.3 Spectra in the infrared region.

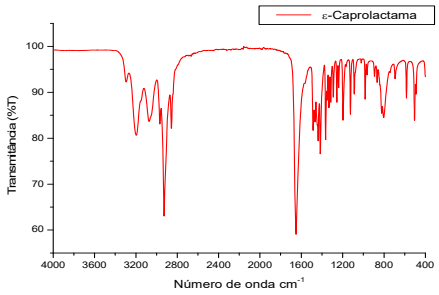


Figure 03 - Infrared spectrum of ε-Caprolactam

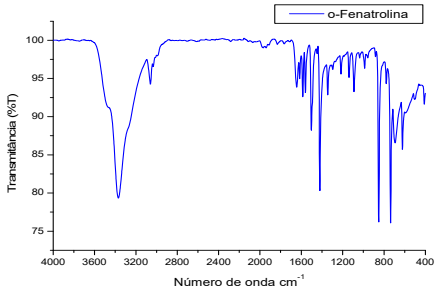


Figure 04 - Infrared spectrum of o-Phenanthroline

Table 04 - Vibrational transition assignments for ε-Caprolactam (main)

vib. modes	Silverstein 2007	Pavia 2010	Cardoso *et al* 2017	Exper
N-H	3350 3180	3300 3100		3294 w 3197 m 3073 m
C=O	1720 1706	1680 1630	1663	1652 s
C-N C-N		 1400	1461	1467 m 1417 m

w (weak); m (medium); s (strong)

Table 05 - Vibrational transition assignments for o-Phenanthroline (main)

vib. modes	Smith, 1961	Martins 2010	Maciel 2015	Exper
νC=N ν_{sim}C=C	1616		1600	1616 m
νC=N	1585 1558			1586 w 1561 m
νCC	1508	1501		1503 s
νC=C νCN	1418	1419		1421 s
C-N_{arom}	1340			1345 w
δ C=N		621		622 m

w (weak); m (medium); s (strong)

3.4 Spectra in the UV-Visible region in aqueous and ethanolic solution.

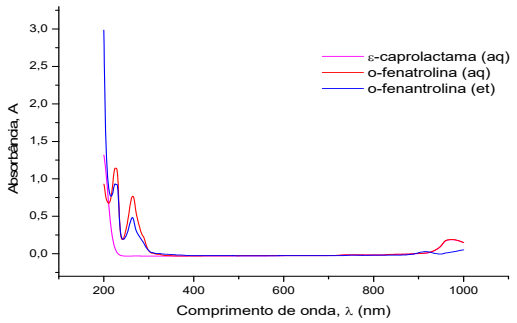


Figure 05 - UV-vis spectrum of ε-caprolactam and o-phenanthroline.

Table 07 - Oscillator strength and ligand transition dipole moment.

Ligand	Range Spectral (nm)	*f* (x10^{-3}) (adim)		μif x10^{-30} (C m) (Debye)	
		D	F	D	F
ε-cap (aq)	948–999	3,9	3,68	3,0 (0,90)	2,91 (0,872)
o-phe (aq)	948-1000	42	39,2	9,8 (2,9)	9,50 (2,85)
o-phe (et)	900-930	4,5	4,22	3,1 (0,93)	3,22 (0,905)

D – Drago; F – Figgs; 1 Debye = 3,336x10^{-30} C m (aq) aqueous solution, (et) ethanolic solution.

4. CONCLUSIONS

Through molecular modeling and reactivity parameters, elements with higher negative densities corroborate that these species function as a Lewis base and act as electron pumpers in certain systems. Conductivity revealed non-electrolyte characteristics. Infrared spectra identified the main vibrational transitions that are identified in the formation of bonds of these species in complex systems. UV-vis spectra show that they do not absorb into the visible, which may be interesting for better use of energy absorption and conversion phenomena, and that the oscillator strength and transition dipole moment reveal that more energetic transitions confirm that they can acting as optical pumps and those of lower energy show that their outermost electrons can be delocalized with some ease, and these properties and these ligands can be used in the optimization of light-emitting or electron-transfer systems in light-to-electricity converters.

5. ACKNOWLEDGMENTS

The authors are grateful to the analysis laboratories of IQ UFRN.

6. REFERENCES

1. Borges, A. S., Caliman, E. V., Dutra, J. D. L., Silva, J. G. DA, and Araújo, M. H. - *Journal of Luminescence,* V. 170, Part 2, **2016**, 654-662.
2. Cardoso, M. C. C.; Belarmino, L. D.; Zukerman-Schpector, J., - *Trabalho apresentado no XLVII Congresso Brasileiro de Química 17 a 21 de setembro.* Disponível em: http://www.abq.org.br/cbq/2007/trabalhos/2/2-303-504.htm, **2007**.
3. Fang, J., Wu, H., Liu, T., Zheng, Z., Lei, J., Liu, Q., Jin, H. - *Applied Energy*, **2020,** Volume 279.
4. Gong, Y., Liu A. Yang, G. - Composites Part A: Applied Science and Manufacturing Volume 41, (8), 1006-1011, **2010**.
5. Pavia, D. L., Lampman, G. M., Kriz, G. S., Vyvyan, J. R. – *Introdução a Espectroscopia,* **2010**, Cengage Learning Ed., Ltda.
6. Li, X. L., Ai, Y. B., Yang, B., Chen, J., Tan., M., Xin, X. L., Shi, Y. H. - Polyhedron, **2012,** 35 (1), 47-54**.**
7. Lima, S. G. M.; Cruz, T. J. T.;.Pereira, F. C.; Silva, A. O.; Lima, F. J. S. - *Periódico Tche Química*, **2020**, vol. 17(35), 203-215.
8. Maciel, J. W O., Vilela-Filho, N. C. - 55º Congresso Brasileiro de Química, 02 a 06 novembro, Goiânia, GO, **2015.**
9. Martins, E. P. S., - *Dissertação de Mestrado, UFPB*, João Pessoa - PB – Brasil, **2010.**
10. Mitsuhiro W., Hiroaki K., Rie I., Talal A. A., Suleiman M. A, Naotaka K., and Kenichiro N. – *Luminescence,* **2014**, 29: 955–958.
11. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J. - *Identificação Espectrométrica de Compostos Orgânicos*. 7. ed. Rio de Janeiro: Lct, **2007**.
12. Smith, R. C. - *Retrospective Theses and Dissertations*., **1961,** 2419 **-** https://lib.dr.iastate.edu/rtd/2419
13. Sun, C., Wu, Y., Zhang W., Jiang, N., Jiu T., and Fang J. - *ACS Appl. Mater. Interfaces*, **2014**, 6, 2, 739–744.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY 2021 VIRTUAL CONFERENCE

MOLECULAR MODELING, REACTIVITY PARAMETERS AND SPECTROCHEMIC STUDIES OF ε-CAPROLACTAM AND ORTOPHENANTROLINE

Francisco José Santos Lima
Universidade Federal do Rio Grande do Norte - Brazil

Maria José de Oliveira Pessoa
Universidade Federal do Rio Grande do Norte - Brazil

Lucas da Silva Araújo
Universidade Federal do Rio Grande do Norte – Brazil

Ademir Oliveira da Silva.
Universidade Federal do Rio Grande do Norte – Brazil

Francisco Claudece Pereira.
Universidade Federal do Rio Grande do Norte – Brazil

March/2022

INTRODUCTION

SBJChem Conference 2021

- ε-caprolactam is a cyclic chain amine with the formula $C_6H_{11}NO$, molar mass 113.16 g / mol, soluble in water (50 mg / mL), has a pH between 7.0 - 8.5 in water (333 g / L). In industry, it has been widely used as a precursor of polymers called nylon 6.
- Recently, it has been applied in the synthesis of polymeric polyamide compounds (Gong and Yang, 2010), in high-efficiency photochemical-photovoltaic-thermochemical (CP-PV-T) systems (Fang, *et al,* 2010), and their derivatives, in synthesis of light-emitting compounds (Borges, *et al.,* 2016).
- O-phenanthroline is a white solid compound with formula $C_{12}H_8N_2$, molar mass 180.21 g/mol and solubility of 3.3 g / L (25 °C) in monohydrate form. It is widely used for fast, flexible and reliable research analysis.
- Recent applications have been observed as uses in protective cathodic buffer layers to improve the efficiency of organic solar cells (Sun *et al.,* 2014), in the study of efficacy in the Luminol chemiluminescence system (Mitsuhiro *et al.,* 2014), in complex systems with Cu(I) using mixed ligands to amplify luminescent radiative emissions of high quantum efficiency (Li, *et al.,* 2012).

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

•- Obtain molecular modeling and reactivity parameters for ε-caprolactam and o-phenanthroline, to verify their ability to act as Lewis bases in electron transfer in photo-reactive systems.

•- Evaluate the molar conductivity of these ligands to observe the influence on the form of coordination and electron transfer in molecular systems.

•- Characterize the main vibrational transitions to attribute the formation of chemical bonds and recognize in these molecules the participation in complex systems.

•- Calculate the spectrochemical parameters, molar absorptivity ε, oscillator strength f and transition dipole moment μ, by recording the uv-vis spectra of these ligands.

•- These properties are fundamental to assess the potential of these species to be used in the synthesis of complex systems that can act as light emitters or in light-to-electricity converting devices.

METHODOLOGY

SBJChem Conference 2021

- Molecular modeling, theoretical reactivity parameters, electrostatic potential cloud, bonding distances, bonding angles and partial charges were obtained from the WebLab ViewerPro® program. The parameters were calculated using the following expression (Lima *et al,* 2020)

$$\Re = \frac{\int qi \; d\tau}{\sum_{i=1}^{n} |\int qi \; d\tau|} \qquad \text{Eq. 01}$$

- Molar conductivity measurements were performed for aqueous solutions of millimolar concentration, using a QUIMIS Q-405 conductivity meter, at a temperature of 25.0 ± 1 °C, after calibration of the cell constant with freshly prepared standard solutions millimolar of NaCl and KCl. The molar conductivity was calculated using the expression below:

$$\Lambda_M = \frac{(L_{sol} - L_{solv}).Kc.10^3}{M} = \frac{(k_{sol} - k_{solv}).10^3}{M} \qquad \text{Eq 02}$$

METHODOLOGY

SBJChem Conference 2021

- The infrared spectra of the two samples were recorded in a PERKIN ELMER FRONTIER equipment, in KBr pellets, in the range of 700 – 4000 cm^{-1} and resolution 4 cm^{-1}.

- The uv-vis spectra were recorded in a SHIMADZU UV model spectrophotometer in the range of 200 - 1000 nm, quartz cuvette with 1 cm optical path for aqueous ε-caprolactam solutions ($1.18x10^{-2}$ mol L^{-1}), aqueous o-phenanthroline ($1.15x10^{-2}$ mol L^{-1}) and ethanolic o-phenanthroline ($1.01x10^{-2}$ mol L^{-1}). Samples needed to be diluted. The oscillator force f was calculated by Drago's and Figgs method and described methodologies (Lima *et. al.*, 2020), according to the expressions:

DRAGO: $f = 4{,}6x10^{-9} \int \varepsilon_{(\sigma)} d\sigma$ Eq. 03

FIGGS: $f = 4{,}32x10^{-9} \int \varepsilon_{(\sigma)} d\sigma$ Eq. 04

- The transition dipole moment was obtained by the following equation:

$$\mu_{if} = 8{,}422x10^{-22} (m\, s^{-1/2} C) \sqrt{\frac{f}{\nu}} \quad (C\, m) \qquad \text{Eq. 05}$$

RESULTS AND DISCUSSION

SBJChem Conference 2021

Molecular modeling, obtaining structural data and reactivity parameters.

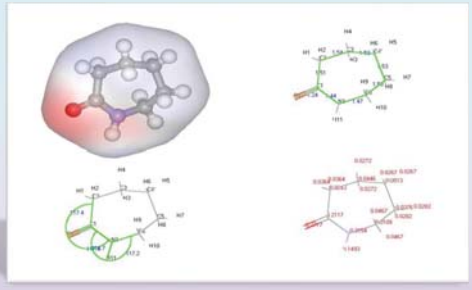


Figure 01 - Modeling obtained for ε-Caprolactam, $C_6H_{11}NO$, using the WebLab ViewerPro program©.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Molecular modeling, obtaining structural data and reactivity parameters.

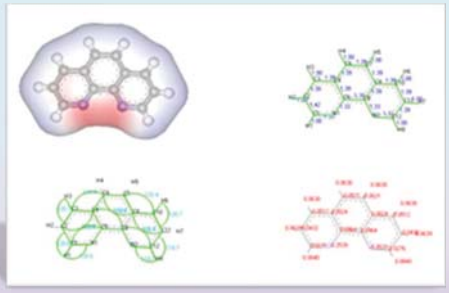


Figure 02 - Modeling obtained for o-Phenanthroline, $C_{12}H_8N_2$, using the WebLab ViewerPro program©.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Molecular modeling, obtaining structural data and reactivity parameters.

Table 01 - Partial charges and PRM for ε-caprolactam, $C_6H_{11}NO$.(main atoms)

Atoms	Partial charges		PRM	
	δ^-	δ^+	$\Re^-$	$\Re^+$
O_1	-0,2777		-0,3822	
C_1		0,2117		0,2913
H_1		0,0364		0,0501
H_{10}		0,0467		0,0643
N_1	-0,3154		-0,4341	
H_{11}		0,1493		0,2054

PRM - Molecular Reactivity Parameters

RESULTS AND DISCUSSION

SBJChem Conference 2021

Molecular modeling, obtaining structural data and reactivity parameters.

Table 02 - Partial charges and PRM for o-phenanthroline, $C_{12}H_8N_2$. (main atoms)

Atoms	Partial charges		PRM	
	δ^-	δ^+	$\Re^-$	$\Re^+$
C_1		0,0276		0,0345
C_{12}		0,0276		0,0345
C_5		0,0964		0,1204
C_9		0,0964		0,1204
N_1	-0,2539		-0,3171	
N_2	-0,2539		-0,3171	

PRM - Molecular Reactivity Parameters

RESULTS AND DISCUSSION

SBJChem Conference 2021

Conductivity measurements and the associated electrolyte type.

Table 03 – Conductivities obtained for millimolar aqueous solutions at 25.0 ± 1 °C

	k x10^{-6}	M Mol/L	Λ_M	Type of electrolyte
H_2O	17,6	55,5	31,7x10^{-5}	n-electrolyte
NaCl	121	0,001	103,4	1:1
KCl	150	0,001	132,4	1:1
ε-capro	34,4	0,001	16,8	n-electrolyte
o-fen	33,0	0,001	15,4	n-electrolyte

Units: k (S cm^{-1}); Λ_M (S cm^2 mol^{-1})

RESULTS AND DISCUSSION

SBJChem Conference 2021

Spectra in the infrared region.

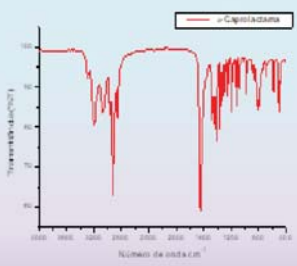


Figure 03 - Infrared spectrum of ε-Caprolactam

Table 04 - Vibrational transition assignments for ε-Caprolactam (main)

Vib. modes	Silverstein 2007	Pavia 2010	Cardoso et al 2017	Exper
N-H	3350 3180	3300 3100		3294 w 3197 m 3073 m
C=O	1720 1706	1680 1630	1663	1652 s
C-N C-N		 1400	1461	1467 m 1417 m

w (weak); m (medium); s (strong)

RESULTS AND DISCUSSION

SBJChem Conference 2021

Spectra in the infrared region.

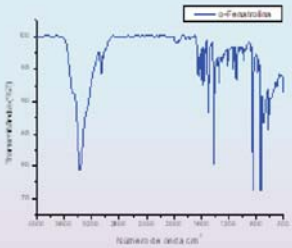


Figure 03 - Infrared spectrum of o-Phenanthroline

Table 04 - Vibrational transition assignments for o-Phenanthroline (main)

Vib. modes	Smith, 1961	Martins 2010	Maciel 2015	Exper
νC=N ν_{sim}C=C	1616		1600	1616 m
νC=N	1585			1586 w
	1558			1561 m
νCC	1508	1501		1503 s
νC=C	1418			
νCN		1419		1421 s
C-N_{arom}	1340			1345 w
δ C=N		621		622 m

w (weak); m (medium); s (strong)

RESULTS AND DISCUSSION

SBJChem Conference 2021

Spectra in the UV-Visible region in aqueous and ethanolic solution.

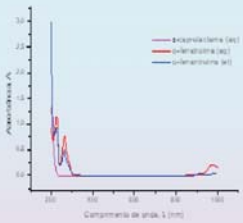


Figure 05 - UV-vis spectrum of ε-caprolactam and o-phenanthroline.

Table 07 - Oscillator strength and ligand transition dipole moment.

Ligand	Range Spectral (nm)	f ($x10^{-3}$) (adim)		μ_{if} $x10^{-30}$ (C m) (Debye)	
		D	F	D	F
ε-cap (aq)	948–999	3,9	3,68	3,0 (0,90)	2,91 (0,872)
o-phe (aq)	948-1000	42	39,2	9,8 (2,9)	9,50 (2,85)
o-phe (et)	900-930	4,5	4,22	3,1 (0,93)	3,22 (0,905)

D – Drago; F – Figgs; 1 Debye = $3,336x10^{-30}$ C m (aq) aqueous solution, (et) ethanolic solution.

CONCLUSIONS

SBJChem Conference 2021

- Through molecular modeling and reactivity parameters, elements with higher negative densities corroborate that these species function as Lewis base and act as electron pumpers in certain systems.
- Conductivity revealed non-electrolyte characteristics.
- Infrared spectra identified the main vibrational transitions that are identified in the formation of bonds of these species in complex systems.
- UV-vis spectra show that they do not absorb into the visible, which may be interesting for better use of energy absorption and conversion phenomena.
- Oscillator strength and transition dipole moment reveal that more energetic transitions confirm that they can acting as optical pumps and those of lower energy show that their outermost electrons can be delocalized with some ease.
- The properties these ligands can be used in the optimization of light-emitting or electron-transfer systems in light-to-electricity converters.

14

ACKNOWLEDGEMENTS

SBJChem Conference 2021

• The authors are grateful to the analysis laboratories of IQ UFRN.

•To the volunteer research students who made no effort to carry out the experiments in this work.

•To the organizers of the SBJC 2021 virtual conference for the opportunity and I wish everyone a great congress!

15

REFERENCES

SBJChem Conference 2021

1. Borges, A. S., Caliman, E. V., Dutra, J. D. L., Silva, J. G. DA, and Araújo, M. H. (2016) - *Journal of Luminescence,* V. 170, Part 2,, 654-662.
2. Cardoso, M. C. C.; Belarmino, L. D.; Zukerman-Schpector, J., (2007) - *Trabalho apresentado no XLVII Congresso Brasileiro de Química 17 a 21 de setembro.* Disponível em: http://www.abq.org.br/cbq/2007/trabalhos/2/2-303-504.htm.
3. Fang, J., Wu, H., Liu, T., Zheng, Z., Lei, J., Liu, Q., Jin, H., (2020) - *Applied Energy*, Volume 279.
4. Gong, Y., Liu A. Yang, G., (2010) - Composites Part A: Applied Science and Manufacturing Volume 41, (8), 1006-1011.
5. Pavia, D. L., Lampman, G. M., Kriz, G. S., Vyvyan, J. R., (2010) – *Introdução a Espectroscopia,*, Cengage Learning Ed., Ltda.
6. Li, X. L., Ai, Y. B., Yang, B., Chen, J., Tan., M., Xin, X. L., Shi, Y. H., (2012) - Polyhedron, 35(1),47-54.
7. Lima, S. G. M.; Cruz, T. J. T.;.Pereira, F. C.; Silva, A. O.; Lima, F. J. S. (2020) - *Periódico Tche Química*,, vol. 17(35), 203-215.
8. Maciel, J. W O., Vilela-Filho, N. C., (2015) - 55º Congresso Brasileiro de Química, 02 a 06 novembro, Goiânia, GO.
9. Martins, E. P. S., (2010) - *Dissertação de Mestrado, UFPB*, João Pessoa - PB – Brasil.
10. Mitsuhiro W., Hiroaki K., Rie I., Talal A. A., Suleiman M. A, Naotaka K., and Kenichiro N. (2014) - *Luminescence*, 29: 955–958.
11. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J., (2007) - *Identificação Espectrométrica de Compostos Orgânicos*. 7. ed. Rio de Janeiro: Lct,.
12. Smith, R. C.(1961) - *Retrospective Theses and Dissertations*, 2419 -https://lib.dr.iastate.edu/rtd/2419
13. Sun, C., Wu, Y., Zhang W., Jiang, N., Jiu T., and Fang J., (2014) - *ACS Appl. Mater. Interfaces*,, 6, 2, 739–744.


SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

MYO-INOSITOL AS A POTENTIAL LOCALLY SUPPRESSING ANTI-SEIZURE THERAPEUTIC AGENT

KANDASHVILI, Manana[1]; GAMKRELIDZE, Giorgi[1]; LORDKIPANIDZE, Tamar[1,2]; NANOBASHVILI, Zaqaria[2]; SOLOMONIA, Revaz[1,2*]

[1] Institute of Chemical Biology, Ilia State University, Tbilisi, Georgia

[2] I. Beritashvili Center of Experimental Biomedicine, Tbilisi, Georgia

** Correspondence author*
e-mail: revaz_solomonia@iliauni.edu.ge

Received 20 October 2022; received in revised form 30 November 2022; accepted 20 December 2022

ABSTRACT

Required for all manuscripts in which the epilepsy belongs to several neurological diseases whose treatment is currently symptomatic, and some patients are resistant to anticonvulsant drugs. Thus, it is essential to create and discover antiepileptic medications. Myo-inositol (MI) is considered to be a future cure agent for epilepsy. In this study, using an electrophysiological method, we revealed that MI has a time and concentration-dependent anticonvulsant effect. During the experiment, two bipolar electrodes were inserted into the dorsal hippocampal structure along with a cannula. MI and saline were injected, and the subsequent duration of electrical stimulation-induced after discharge were recorded from the same location in the hippocampus. 5 minutes after 1 M of MI infusion, the duration of the afterdischarge was significantly reduced compared with the duration of the pre-injection after discharge in the same animals and the duration of the pre-injection afterdischarges in animals administered saline or MI in the contralateral hippocampus. In addition, 0.055 M myo-inositol significantly decreased the afterdischarge duration at 5 minutes after injection as compared to 40 minutes post-injection. It should be noted that after the injection of different MI concentrations (1.0 M and 0.055 M), the afterdischarge duration was restored to its initial value (pre-injection afterdischarge duration) 40 minutes after the MI injection. For the first time it was demonstrated that myo-inositol has time and concentration-dependent effects on the evoked seizure afterdischarges. Based on the results obtained from previous laboratory studies and current data, it was concluded that MI has a local suppressive effect on seizures and is therefore considered a promising therapeutic agent for treating patients with epilepsy.

Keywords: *epilepsy, myo-inositol, anti-seizure drugs, afterdischarge, electroencephalography (EEG).*

1. INTRODUCTION

Epilepsy is one of the neurological diseases that is accompanied by spontaneous recurrent seizures (Duncan and Shinkareva, 2005). The current medical treatment directed against epilepsy is only symptomatic. At the same time, the process of epileptogenesis has not been finally identified, and therefore, the treatment against epilepsy it is not perfect (Löscher, 2012). It is, therefore, necessary to find remedies that will prevent or cure epilepsy. Based on experimental data, myo-inositol (MI) is considered an antiepileptic agent (Nozadze *et al*., 2011). MI is the most common of its isomers. It is synthesized and abundantly present in the tissues of the central nervous system and is an important osmolite (Fisher *et al*., 2002). Previous experimental studies conducted in the Chemical Biology laboratory of the Ilia State University have shown that pre-administration of MI in rats inhibits *status epilepticus* induced by kainic acid (KA). It is also important to notice that daily administration of MI for four weeks after status epilepticus (SE) prevents many biochemical changes triggered by SE (Nozadze *et al*., 2011; R. Solomonia *et al*., 2007; Revaz Solomonia *et al*., 2013). In addition, systemic administration of MI in the early stages of epileptogenesis inhibits the apoptotic process in the brain of rats (Tsverava *et al*., 2016). Also, recent studies have shown that daily

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.47_abstract_MANANA.pdf

administration of MI after KA-induced SE in rats causes a reduction in the frequency and duration of behavioral seizures, even four weeks after MI injection termination. (Tsverava *et al*., 2019). It is also important to determine whether MI has a local seizure suppressant effect or acts on the entire, widely extended epileptic network. In addition, it is also important to test the effect of MI on seizures that chemical agents do not induce to exclude the interaction of MI with them. In this study, we injected in the dorsal hippocampus MI and tested its anticonvulsive effects on the electrical stimulation-induced seizures to address these questions.

2. MATERIALS AND METHODS

The experiment was conducted in compliance with the norms of animal bioethics based on I. Beritashvili Center of Experimental Biomedicine.

2.1. Animal surgery

Cranial surgery was done within 3.5–4 hours. Two steel bipolar electrodes (Plastics One, Roanoke, Virginia, USA) and a cannula were implanted into the same dorsal hippocampus stereotaxically under ketamine anesthesia using coordinates from a rat brain atlas (Palkovits, 1983). One electrode was used for stimulation while another recorded electroencephalogram (EEG) activity. Following coordinates were used for the placement of the electrodes in the right hippocampus: the stimulating electrode–3.8 mm caudally from the bregma, 3.0 mm laterally from the sagittal line, 3.5 mm ventrally from the skull surface; the recording electrode–4.8 mm caudally from the bregma, 4.0 mm laterally from the sagittal line, 3.5 mm ventrally from the skull surface. The cannula was placed 5.3 mm caudally from the bregma, 4.0 mm laterally from the sagittal line, 3.5 mm ventrally from the skull surface. In some control experiments, the electrodes were placed in the right hippocampus, whereas the cannula was placed in the contralateral hippocampus with the same coordinates. The interval between the surgery and experiments was 1 week. At the beginning of every experiment, a threshold intensity of the electrical stimulation current for AD generation was determined with a stimulator (MCS GmbH, STG 4002, Reutlingen, Germany). Following stimulation protocol was used: 15-second trains of 1 ms monophasic rectangular current pulses with 40 Hz was applied with 15 minutes interval. To identify AD induction threshold, the current intensity was increased from 3 to 50 μA with 0.5 μA steps. Before MI or saline solution was administered in the hippocampus, three stable ADs were elicited with 15-minute intervals. Solutions (MI or saline) were injected within 1 minute after the last evoked AD. The stimulations were then applied at 5, 15, and 40 minutes post-injection. Stimulation intervals immediately post-injection were made shorter to increase the time resolution of detection of MI effect on evoked AD.

The last stimulus in this series was applied with a 25-minute interval to detect possible AD duration recovery to the pre-injection values with a single test stimulation. For the experiment, MI concentrations were following: 1.0 M, 0.055 M, and 0.020 M, and the injection volume for each concentration was 2 μl. A Hamilton syringe was used to inject MI and saline into the Hippocampus (Sigma-Aldrich, St. Louis, Missouri, USA). The concentrations of MI used for the experiment were selected because its physiological basis in the brain cells is 0.06M and in the CSF is 0.002M equals (Fisher et al., 2002). Amplified hippocampal EEG activity passed through a low-pass filter at 50 Hz and was recorded on an ink chart recorder (EEG 16 S; Medicor, Budapest, Hungary). The average AD duration before the injection of the solutions was determined as a mean of three ADs just preceding the injection and then averaged across different animals (n = 5). After the injection, AD durations were averaged across different animals at corresponding time intervals.

2.2. Statistical analyses

Two fixed factors (post-injection time and MI concentrations) are used for statistical analysis and a post-hoc Tukey test for data comparison. All statistical tests are two-tailed, and all data are presented as mean ± SEM.

3. RESULTS AND DISCUSSION:

AD duration was significantly reduced 5 and 15 minutes after injection of 1.0 M MI, compared to 40 minutes after injection mean level (Figure 1). Similar to the previous result, the duration of AD was significantly reduced at 5 minutes after 0.055 M MI injection compared to at 40 minutes after injection mean level. Importantly, using both concentrations of MI (1.0 M, 0.055M), the duration of AD was restored to its pre-injection value 40 minutes after MI infusion. It should be noted that the injection of 0.020 M of MI has no statistically significant effect on the duration of AD.

It follows that injected MI reduces AD duration, which is a time- and concentration-dependent outcome. Control animals were treated with saline injection instead of MI and recorded no statistically significant differences of AD duration before and after saline injection, compared to any time point (5, 15, 40 minutes) data. It should also be noted that 5 minutes after injection of 1.0 M and 0.055M of MI AD duration was statistically significantly reduced compared to the saline injection at the same 5 minute time point ($P < 0.01$ and $P < 0.05$, respectively, post hoc Tukey test). Thus, all data shows that MI mechanism of action is concentration and time-dependent effect.

4. CONCLUSIONS:

The data obtained support the hypothesis that MI is an endogenous anticonvulsant agent in the central nervous system and can locally suppress or attenuate electrical stimulation-induced seizures, which is manifested reducing the duration of AD. All data highlight the possible use of MI in the clinic for the treatment of epilepsy. Further studies are needed.

5. ACKNOWLEDGMENTS:

The experimental work supported by the Ilia State University, Georgia.

6. REFERENCES:

1. Duncan, J. R., and Shinkareva, O. (2005). Review article. *Human Resource Development International*, *8*(2), 265–271. https://doi.org/10.1080/13678860500100764
2. Fisher, S. K., Novak, J. E., and Agranoff, B. W. (2002). Inositol and higher inositol phosphates in neural tissues: Homeostasis, metabolism and functional significance. *Journal of Neurochemistry*, *82*(4), 736–754. https://doi.org/10.1046/j.1471-4159.2002.01041.x
3. Gamkrelidze, G. N., Nanobashvili, Z. I., Bilanishvili, I. G., Lordkipanidze, T., Kandashvili, M., Kokaia, M., and Solomonia, R. O. (2019). Concentration- and time-dependent effects of myo-inositol on evoked epileptic afterdischarge in the hippocampus in vivo. *NeuroReport*, *30*(16). https://doi.org/10.1097/WNR.0000000000001341
4. Löscher, W. (2012). Strategies for antiepileptogenesis: Antiepileptic drugs versus novel approaches evaluated in post-status epilepticus models of temporal lobe epilepsy. *Jasper's Basic Mechanisms of the Epilepsies*, *Md*, 1–18. http://www.ncbi.nlm.nih.gov/pubmed/22787664
5. Nozadze, M., Mikautadze, E., Lepsveridze, E., Mikeladze, E., Kuchiashvili, N., Kiguradze, T., Kikvidze, M., and Solomonia, R. (2011). Anticonvulsant activities of myo-inositol and scyllo-inositol on pentylenetetrazol induced seizures. *Seizure*, *20*(2), 173–176. https://doi.org/10.1016/j.seizure.2010.10.008
6. Palkovits, M. (1983). The rat brain in stereotaxic coordinates. *Neuropeptides*, *3*(4), 319. https://doi.org/10.1016/0143-4179(83)90049-5
7. Solomonia, R., Nozadze, M., Kuchiashvili, N., Bolkvadze, T., Kiladze, M., Zhvania, M., Kigyradze, T., and Pkhakadze, V. (2007). Effect of myo-inositol on convulsions induced by pentylenetetrazole and kainic acid in rats. *Bulletin of Experimental Biology and Medicine*, *143*(1), 58–60. https://doi.org/10.1007/s10517-007-0016-z
8. Solomonia, Revaz, Gogichaishvili, N., Nozadze, M., Lepsveridze, E., Dzneladze, D., and Kiguradze, T. (2013). Myo-inositol treatment and GABA-A receptor subunit changes after kainate-induced status epilepticus. *Cellular and Molecular Neurobiology*, *33*(1), 119–127. https://doi.org/10.1007/s10571-012-9877-4
9. Tsverava, L., Kandashvili, M., Margvelani, G., Lortkipanidze, T., Gamkrelidze, G., Lepsveridze, E., Kokaia, M., and Solomonia, R. (2019). Long-term effects of myoinositol on behavioural seizures and biochemical changes evoked by kainic acid induced epileptogenesis. *BioMed Research International*, *2019*. https://doi.org/10.1155/2019/4518160
10. Tsverava, L., Lordkipanidze, T., Lepsveridze, E., Nozadze, M., Kikvidze, M., and Solomonia, R. (2016). Myoinositol Attenuates the Cell Loss and Biochemical Changes Induced by Kainic Acid Status Epilepticus. *BioMed Research International*, *2016*. https://doi.org/10.1155/2016/2794096

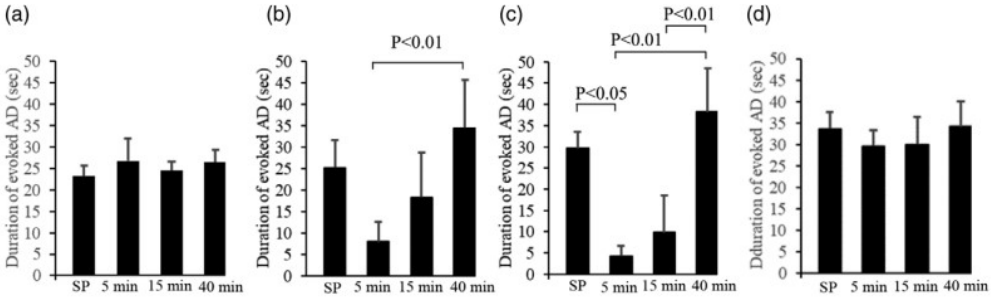


Figure 1. *Average duration of evoked ADs before and after (a) 0.020 M (b) 0.055 M and (c) 1.0 M concentration MI and (d) saline infusion into the hippocampus. Error bars represent standard errors of the means.*

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

Myo-inositol as a potential locally suppressing anti-seizure therapeutic agent

Manana Kandashvili(a), Georgi N. Gamkrelidze(a) , Zaqaria I. Nanobashvili(b) , Irina G. Bilanishvili(b), Tamar Lordkipanidze(a,b), Merab Kokaia(c) and Revaz O. Solomonia(a,b)

a. Institute of Chemical Biology, Ilia State University-Tbilisi, Georgia
b. I.Beritashvili Center of Experimental Biomedicine-Tbilisi, Georgia
c. Department of Clinical Sciences, Epilepsy Centre, Lund University Hospital-Lund, Sweden

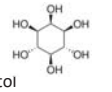
March/2022

INTRODUCTION

SBJChem Conference 2021

- Epilepsy is one of the most common neurological diseases characterized by recurrent, spontaneous seizures. Its treatment is only symptomatic (Löscher, 2012) and in many cases treatment of epileptic patients are resistant to the anti-seizure drugs.
- Recently, myo-inositol has been identified as a promising antiepileptic compound.

Empirical Formula: $C_6H_{12}O_6$



Myo-inositol

Aquilegia Vulgaris

INTRODUCTION

SBJChem Conference 2021

- In the present study, using electrophysiological method we examined for the first time the effect of myo-inositol on the generation of epileptic afterdischarges in the hippocampus evoked by **a local electrical stimulation**.
- Myo-inositol has a concentration and time dependent local seizure-suppressant effect

MATERIALS AND METHODS

SBJChem Conference 2021

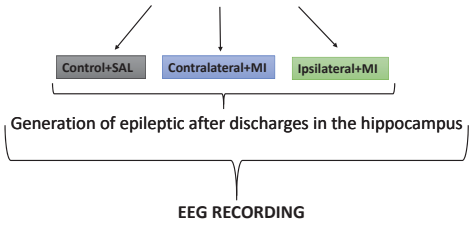
- Adult male Wistar rats at an age of about 5-6 weeks (130-135 gr)
- Canula and two seel bipolar electrodes implantation in the dorsal hippocampus stereotaxiclly and contralaterally
- Hamilton needle for Myo-inositol and Saline injection

- Brain atlas is used for the correct implantation of electrodes and cannula in the structure of the dorsal hippocampus (Paxinos et.al., 1998)
- Used myo-inositol concentrations: 0.02M, 0.055M, 1.0M

MATERIALS AND METHODS

SBJChem Conference 2021

Experimental animal groups (wistar rat)



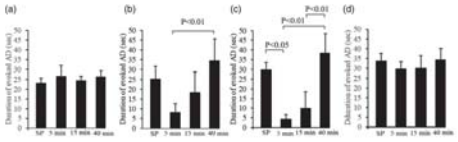
The research purpose

SBJChem Conference 2021

- Investigate the effect of mio-inositol on seizures evoked without any chemical agents to exclude interaction with other drugs
- Study the effect of myo-inositol on the duration of seizure episodes induced by electrical stimulation

RESULTS AND DISCUSSION

SBJChem Conference 2021



Average duration of evoked ADs before and after (a) 0.020 M (b) 0.055 M and (c) 1.0 M concentration MI and (d) saline infusion into the hippocampus.

five minutes after 1 M of MI infusion, the duration of the afterdischarge was significantly reduced compared with the duration of the pre-injection after discharge in the same animals and the duration of the pre-injection afterdischarges in animals administered saline or MI in the contralateral hippocampus. In addition, 0.055 M myo-inositol significantly decreased the afterdischarge duration at 5 minutes after injection as compared to 40 minutes post-injection. It should be noted that after the injection of different MI concentrations (1.0 M and 0.055 M), the afterdischarge duration was restored to its initial value (pre-injection afterdischarge duration) 40 minutes after the MI injection.

CONCLUSIONS

SBJChem Conference 2021

Based on the data obtained, support the hypothesis [6] that MI, among other functions, is an endogenous anticonvulsant agent of the central nervous system and has a suppressant effect on locally evoked seizures and can be considered and used as a potential candidate for the prevention and treatment of epilepsy.

ACKNOWLEDGEMENTS
SBJChem Conference 2021

The experimental work supported by the Ilia State University, Georgia

Ilia State University-Tbilisi, Georgia

REFERENCES
SBJChem Conference 2021

1. Löscher, W. (2012). Strategies for antiepileptogenesis: Antiepileptic drugs versus novel approaches evaluated in post-status epilepticus models of temporal lobe epilepsy. *Jasper's Basic Mechanisms of the Epilepsies*, *Md*, 1–18. http://www.ncbi.nlm.nih.gov/pubmed/22787664

2. Nozadze, M., Mikautadze, E., Lepsveridze, E., Mikeladze, E., Kuchiashvili, N., Kiguradze, T., Kikvidze, M., & Solomonia, R. (2011). Anticonvulsant activities of myo-inositol and scyllo-inositol on pentylenetetrazol induced seizures. *Seizure*, *20*(2), 173–176. https://doi.org/10.1016/j.seizure.2010.10.008

3. Palkovits, M. (1983). The rat brain in stereotaxic coordinates. *Neuropeptides*, *3*(4), 319. https://doi.org/10.1016/0143-4179(83)90049-5

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2022 VIRTUAL CONFERENCE

NOSOLOGICAL CHARACTERISTICS OF DOGS SUBMITTED TO TPLO BY AN ORTHOPEDIC SERVICE IN THE STATE OF RJ, BRAZIL

ROCHA, Amanda da Silva[1]; MOTTA, Lucas Baptista[1]; COSTA, Andrei Ferreira Nicolau[1], MOTTA, Pedro Paulo de Assis[1]; DE CARVALHO, Eduardo Butturini[1*];

[1] Universidade de Vassouras, graduação em Medicina Veterinária – Vassouras, RJ – Brasil

[4] COVET – Cirurgia e Ortopedia Veterinária – Friburgo, RJ - Brasil

** Correspondence author*
e-mail: butturini@gmail.com

Received 30 January 2022; received in revised form 26 February 2022; accepted 03 March 2022

ABSTRACT

Cranial cruciate ligament rupture in dogs causes knee instability. It is one of the main causes of pelvic limb lameness in this species. There are several techniques for surgical treatment, and TPLO – tibial plateau leveling osteotomy aims to change the biomechanics of the knees in an attempt to better distribute the forces and generate dynamic stability in the joint. Still, little epidemiological data about dogs submitted to TPLO has been published. This retrospective study investigated nosological and epidemiological characteristics of 76 dogs submitted to this technique performed by a private orthopedic service in two cities in the state of Rio de Janeiro over fourteen months. The mean time between diagnosis and surgery was 23 days (median nine days). The mean age of the dogs was 73±43 months, and there were no differences between males and females. Approximately 10,5% of dogs had contralateral ligament rupture. Most animals were spayed or neutered (66,66% vs. 33,33%, p=0,02). There were no transpiratory complications in 89,6% of patients, and 79,2% had no postoperative complications. Exploratory arthrotomy was the most performed associated surgery technique (61% of patients). It is believed that studies like this allow a better understanding of this rupture and its treatment options, providing a better quality of life for affected dogs.

Keywords: *orthopedic surgery, osteotomy, dogs, veterinary*

1. INTRODUÇÃO

Atualmente a ruptura de ligamento cruzado cranial (RLCCr) é o problema ortopédico mais prevalente em cães, podendo afetar animais de qualquer idade, sexo ou raça (Harasen, 2003). As lesões que ocorrem no ligamento cruzado cranial (LCCr) são rupturas completas ou parciais do ligamento, ou avulsões ósseas da sua origem ou inserção.

A insuficiência no LCCr pode ter causas degenerativas e traumáticas (Fossum e Schulz, 2014). Quando ocorre a ruptura parcial do LCCr, o animal apresenta claudicação, com a detecção de uma pequena instabilidade no joelho e na radiografia pode-se visualizar sinais progressivos de osteoartrite, progredindo com o tempo para a ruptura completa do ligamento (Fossum e Schulz, 2014).

Para diagnóstico da lesão é feito um teste de gaveta cranial ou teste de compressão tibial, avaliando a instabilidade craniocaudal da articulação do joelho, portanto, esses testes não podem servir para mostrar a causa da instabilidade do joelho associada ao ligamento cruzado cranial, caudal e ruptura total do ligamento cruzado. Logo, se torna necessária a radiografia com visualizações planas (posição anatômica) e de estresse (flexão) (Lee e Jeong, 2014).

O tratamento cirúrgico da RLCCr pode ser conservador ou cirúrgico, existindo mais de 60 variações de procedimentos cirúrgicos relatados para o tratamento da doença do ligamento cruzado cranial (DLCCr) (Bergh *et al*., 2014). Os

ISSN 2674-6891. 2022. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.39_abstract_ROCHA.pdf

principais fatores que predispõem a ruptura do ligamento cruzado (RLCCr) são divididos em dois grupos: biológicos e fatores biomecânicos. Os fatores biológicos incluem raça, sexo, idade e genética, enquanto fatores biomecânicos incluem conformação da articulação do joelho, força muscular e o alinhamento dos segmentos ósseos (Baker e Muir, 2018).

Esse trabalho tem como objetivo descrever as características nosológicas e epidemiológicas de cães submetidos a cirurgias para correção de RLCCr pela técnica de TPLO realizadas nos municípios do Rio de Janeiro e Nova Friburgo no período de maio de 2019 a julho de 2021.

2. MATERIAIS E MÉTODOS

Os dados foram coletados a partir do registro no sistema do serviço de ortopedia e contemplaram atendimentos entre os meses de maio de 2019 a julho de 2021 em duas clínicas localizadas no estado do Rio de Janeiro (nas cidades Rio de Janeiro e Nova Friburgo). A análise estatística foi realizada pelo software GraphPad Prism v9.0 com nível de significância de 0,05 e teste de chi-quadrado bicaudado.

3. RESULTADOS E DISCUSSÃO:

Entre maio de 2019 e julho de 2021 foram realizadas 77 cirurgias de correção de RLCCr em 76 cães atendidos em um serviço de ortopedia nos municípios do Rio de Janeiro e Nova Friburgo. Apenas um cão apresentou lesões bilaterais e necessitou ser submetido a duas cirurgias.

A média de idade dos cães (Figura 1) submetidos à TPLO foi de (73,04 ± 42,88 meses), mediana (71 meses, mín-máx: 10-166 meses) (percentis 25%: 36 meses; 75%: 114 meses). Udomsinprasert *et al*. (2018) apontam que a lesão do LCCr é comum entre 2 e 10 anos de idade.

Não houve diferença estatística para o sexo dos pacientes, sendo 31 machos e 45 fêmeas (respectivamente, 40,8% e 59,2%, p=0,087). Oito animais (10,53%) apresentavam histórico de ruptura do LCCr contralateral, 2 (2,64% de displasia coxofemoral, 5 (6,57%) de cirurgias prévias no membro a ser operado, 4 (5,26%) de luxação de patela e apenas um de desvio angular do fêmur. Dois animais apresentaram obesidade, porém o médico veterinário responsável relata de forma anedótica que certamente esta comorbidade foi subnotificada nos registros, tratando-se de uma doença mais prevalente nesses indivíduos, como descrito por Adams *et al*., 2011.

A maior parte dos animais eram castrados (66,66% contra 33,33% de inteiros), sendo a diferença estatisticamente significativa (p=0,02). Resultado semelhante foi demonstrado por McKee e Cook, 2006; Vasseur, 2003; Witsberger *et al*.,2008; Pećin, *et al*. 2017.

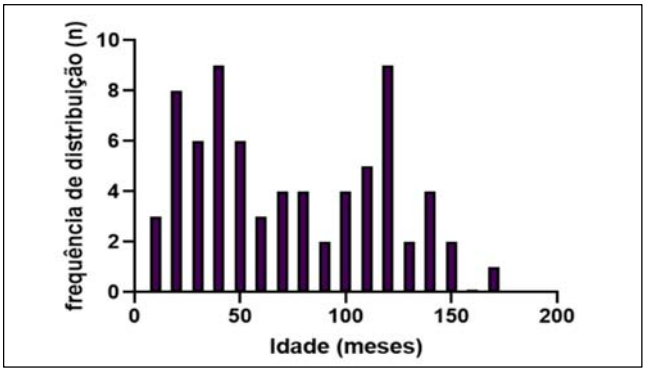


Gráfico 1. Frequência da distribuição da faixa etária dos pacientes atendidos.

Dentre os pacientes atendidos, 31,57% (n=21) eram cães sem raça definida e os 52 restantes (68,43%) eram representados pelas seguintes raças: American Bully e Pitbull (5 de cada), Buldogue Americano, Chow Chow, Labrador, Rottweiler, Spitz Alemão, Starffordshire Bull Terrier e Yorkshire Terrier (3 de cada), Boxer, Buldogue inglês, Daschund, Dogue Alemão, Poodle e Cane Corso (2 de cada), Boiadeiro Australiano, Chihuahua, Dogo Argentino, Husky Siberiano, Lhasa Apso, Pastor Alemão, Pequinês, Shi-Tzu, Weimaraner (1 de cada). Estudos relatam que as raças com maior predisposição também apresentam anomalias que podem contribuir para o enfraquecimento e ruptura do ligamento cruzado, como, por exemplo, a posição hiperextendida da pelve nos membros com ângulos articulares altamente abertos (Slocum, B. e Slocum, T. D. ,1993). Essa hiperextensão é frequentemente associada à displasia coxofemoral, que é registrada em uma alta porcentagem de cães com ruptura de LCCr (Necas, A. *et al*., 2000). No presente estudo, 2 cães apresentaram tal comorbidade associada a RLCCr.

Não houve diferença quanto aos membros afetados, sendo 48% do membro posterior esquerdo e 52% do membro posterior direito (p=0,732). Não houve complicações transoperatórias na técnica cirúrgica em 89,6% dos casos e 79,2% dos pacientes não apresentaram complicações pós-operatórias. A

complicação transoperatória mais frequente foi invasão do parafuso na articulação, acometendo três animais (3,9%), seguida de falha no bloqueio dos parafusos (2 casos, 2,6%) e de um caso de cada uma das seguintes: laceração de poplítea, falha na instalação de parafusos P1 e P4. Em relação à complicação pós-operatória na revisão de 10 a 14 dias, claudicação no membro operado foi observada em 11 casos (14,3%). Outras complicações ocorreram cada uma em um paciente: edema, seroma, deiscência de sutura, impotência funcional do membro operado e prostração. Na revisão de 8 a 10 semanas, as complicações mais frequentes foram: crepitação ao estresse varo/valgo do joelho (dois casos, 2,6%) e claudicação no membro operado (cinco casos, 6,5%). Não foram observadas complicações após 8 a 10 semanas em 70 casos (90,9%).

A técnica de artrotomia exploratória foi realizada em 47 casos (61% dos casos) e a meniscectomia em 8 casos (10,4%). Outras técnicas associadas foram: capsulectomia (n=4, 5,2%), imbricação da fáscia lata (n=3, 3,9%), sulcoplastia (n=2, 2,6%), osteotomia corretiva de fêmur (n=2, 2,6%) e osteotomia tibial p/ correção de valgo tibial simultâneo (n==1, 1,3%).

Quanto ao tempo entre o diagnóstico e a realização da cirurgia de TPLO, o estudo evidenciou que decorreram em média 23 dias, com mediana de (9 dias), (mín- máx) (1 dia-139 dias).

A antibioticoterapia profilática transoperatória foi realizada em todos os casos com ceftriaxona 25 mg/kg aplicada por via intravenosa aproximadamente uma hora antes do início da intervenção. Todos os pacientes receberam amoxicilina com clavulanato na dose de 12,5 mg/kg por via oral a cada 12 horas por 10 dias para a antibioticoterapia pós-operatória. Dos 77 casos, 74 receberam meloxicam na dose de 0,05 mg/kg, uma vez por dia, por 6 dias como parte do protocolo de analgesia pós-operatória. Um paciente recebeu robenacoxib e 71 receberam dipirona na dose de 25 mg/kg a cada 8 horas conforme necessidade de resgate analgésico. O cloridrato de tramadol foi prescrito para apenas cinco pacientes.

4. CONCLUSÃO:

Os resultados encontrados permitem concluir que, na população estudada, não houve predileção de sexo ou lado da lesão (membro direito ou esquerdo), além de uma distribuição ampla de idade (10 a 166 meses). Observou-se ainda que animais castrados foram mais frequentemente submetidos à TPLO que aqueles não castrados, fortalecendo a hipótese demonstrada por outros autores de que a castração possa ser um fator predisponente para a ruptura do ligamento cruzado cranial. Em 61% das cirurgias de TPLO, realizou-se também a artrotomia exploratória, apesar de meniscectomias só terem sido realizadas em pouco mais de 10% dos casos. Conclui-se, por fim, que a técnica realizada pelo serviço avaliado demonstrou-se segura, não havendo complicações em quase 90% das cirurgias e 80% dos pós-operatórios. Apesar de não se poder afirmar, a precocidade da intervenção (mediana de 9 dias) pode estar associada à baixa taxa de complicações, sugerindo-se que estudos investiguem essa relação.

5. REFERÊNCIAS:

1. Baker, L. A. e Muir, P. Epidemiologia da ruptura do ligamento cruzado. Em Advances in the Canine Cranial Cruciate Ligament, 2ª ed.; Muir, P., Ed.; Wiley-Blackwell, 2018, 109-114.
2. Bergh, M. S., Sullivan, C., Ferrell, C. L., Troy, J. e Budsberg, S. C. Systematic review of surgical treatments for cranial cruciate ligament disease in dogs. J. Am. Anim. Hosp. Assoc, 2014, 50, 315– 321.
3. Fossum, T. W. e Kurt S. Schulz. Princípios e técnicas gerais. In: Fossum, T. W. Cirurgia de Pequenos Animais. 4ª edição. Rio de Janeiro: Elsevier, 2014, 34, 3781-3837.
4. Haransen, Greg. Canine cranial cruciate ligament rupture in profile. Can Vet J, 2003, 44 (10): 845–846.
5. Lee, Jung-há e Jeong, Soon-wuk. Feasibility of utilizing the patellar ligament anglefor assessing cranial cruciate ligament rupture in dogs. Journal of Veterinary Science, 2014.
6. McKee, W. M. e Cook, J. L. The stifle. In Manual of Canine and Feline Musculoskeletal Disorders, 1st ed.; Houlton, J.E.F., Cook, J.L., Innes, J.F., Langley-Hobbs, S.J., Brown, G., Eds.; British Small Animal Veterinary Association, 2006, 350–366.
7. Necas, A., Zatloukal, J., Kecová, H., Dvorák, M. Predisposition of dog breeds to rupture of the cranial cruciate ligament. Acta Vet. Brno, 2000, 69, 305–310.

8. Pećin, M., Lipar, M., Kos, J., Smolec, O., Kreszinger, M., Stejskal, M. Breed, gender, age, and reproductive status in relation to the predisposition for cranial cruciate ligament rupture in 117 dogs treated by a single surgeon (2010 - 2015) - a short communication. Veterinarski Arhiv, 2017, 87 (6), 783- 789.
9. Slocum, B.; Slocum, T. D. Tibial plateau leveling osteotomy for repair of cranial cruciate ligament rupture in the canine. Veterinary Clinics of orth America: Small Animal Practice, 1993, 23, 777- 795.
10. Vasseur, P. B. Stifle Joint. In Textbook of Small Animal Surgery, 3rd ed.; Slatter, D., Ed.; Elsevier Science Saunders, 2003, 2, pp. 2090–2116.
11. Witsberger T. H., Villamil J. A., Schultz L. G. Hahn, A. W., and Cook, J. L.,. Prevalence of and risk factors for hip dysplasia and cranial cruciate ligament deficiency in dogs. J Am Vet Med Assoc, 2008, 232(12):1818–24. 2.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2022 VIRTUAL CONFERENCE

NOSOLOGICAL CHARACTERISTICS OF DOGS SUBMITTED TO TPLO BY AN ORTHOPEDIC SERVICE IN THE STATE OF RJ, BRAZIL

Amanda da Silva Rocha
Andrei Ferreira Nicolau Costa
Lucas Baptista Motta
Eduardo Butturini de Carvalho
University of Vassouras - Brazil.

Pedro Paulo de Assis Motta
COVET – Cirurgia e Ortopedia Veterinária - Brazil.

March/2022

INTRODUCTION

- CrCL insufficiency can have degenerative and traumatic causes;
- The treatment of RLCCr can be conservative or surgical (Bergh et al., 2014).
- For lesion diagnosis ⟹ cranial drawer test or tibial compression test (Assessing craniocaudal instability of the knee joint) (Lee & Jeong, 2014);
- The main factors that predispose to rupture of the cruciate ligament (RLCCr) are divided into two groups: biological and biomechanical factors (Baker & Muir, 2018).

OBJETIVE

To analyze and understand the nosological and epidemiological characteristics of dogs that underwent surgery to correct RLCCr using the TPLO technique.

METHODOLOGY

Study design:

• Retrospective descriptive and analytical study on the nosological and epidemiological characteristics of dogs submitted to RLCCr correction surgeries using TPLO techniques.

Study period and data source:

• May 2019 to July 2021.

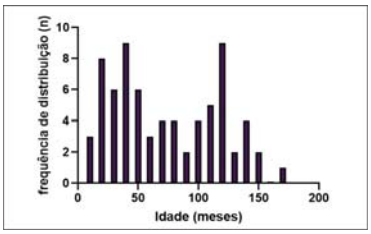
• Database of a private veterinary orthopedics service in Rio de Janeiro and Nova Friburgo.

METHODOLOGY

- Sample: 76 dogs that underwent this surgical intervention;

ANALYZED VARIABLES	
Time between diagnosis and surgery	Surgical technique used
Age	Intraoperative complications
Breed	Antibiotic prescribed preoperatively
Sex	Antibiotic prescribed for the postoperative period
Whole or neutered	Analgesic prescribed for the postoperative period
Comorbidities	Postoperative complications (10-14 days)
Affected member	Postoperative complications (8 to 10 weeks)

RESULTS AND DISCUSSION



RESULTS AND DISCUSSION

SEX → **DRLCCr had a higher incidence in females;**

ENTIRE OR CASTRATED → **Castration is directly linked to the incidence of the disease in these animals and makes this variable an important nosological characteristic of DRLCCr;**

Variable with significant statistical significance (p=0.02);

AGE → **DRLCCr had a higher incidence in dogs older than 60 months. (> 5 years old);**

BREED → **Higher incidence of RLCCr in large breed dogs (American Bully, Pitbull, Rottweiler, Chow Chow, American Bulldog and Labrador);**

RESULTS AND DISCUSSION

AFFECTED MEMBER → **There was no statistical significance, as in the other studies evaluated;**

COMPLICATION RATE → **Low postoperative complication rates were observed (10-14 days and 8-10 weeks after the surgical procedure);**

Research limitations: Underreporting of obesity and weight comorbidity in the animals' medical records, which made it impossible to assess this variable, which was widely pointed out in previous studies;

CONCLUSIONS

- One of the most common orthopedic diseases in veterinary medicine;
- sex, age, castration and breed may increase the incidence of RLCCr;
- The castrated condition of the animal was identified as the most significant factor for the development of RLCCr in this study (P = 0.02);

CONCLUSIONS

- LCCr rupture is a very common condition in large dogs;
- The performance of the TPLO surgical technique by exploratory arthrotomy combined with the adopted drug protocols proved to be extremely effective;
- It is believed that studies like this allow a better understanding of RLCCr and its treatment options, providing better care and quality of life for dogs affected with this disease.

REFERENCES

SBJChem Conference 2022

1. Haransen, G. (2002). Diagnosing rupture of the cranial cruciate ligament. *Can Vet J Volume 43*. DOI: https://pubmed.ncbi.nlm.nih.gov/12058576/.
2. Lee, J. & Jeong, S. (2014). Feasibility of utilizing the patelas ligament anglefor assessing cranial cruciate ligament rupture in dogs. *Journal of Veterinary Science*. DOI: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4269600/.
3. Durana, J. N. (2009) Characterization of the surgical clinic of cranial cruciate ligament rupture in canids. Thesis (Integrated Master's) – Faculty of Veterinary Medicine, Technical University of Lisbon. Lisbon, p. 94. DOI: https://www.repository.utl.pt/bitstream/10400.5/1593/1/Caracteriza%c3%a7%c3%a3o%20da%20Cl%c3%adnica%20Cir%c3%bargica%20da%20Ruptura%20do%20Ligamento%20Cruzado.pdf.
4. Baker, L. A. & Muir, P. (2018). Epidemiology of cruciate ligament rupture. ed .; Muir, P., Ed .; *Wiley-Blackwell*. 109-114. Doi: Em Advances in the Canine Cranial Cruciate Ligament, 2ª https://onlinelibrary.wiley.com/doi/abs/10.1002/9781119261728.ch14.


SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

OPTIMIZATION OF BIODIESEL PRODUCTION FROM WASTE VEGETABLE OIL USING Zr- OXIDE CATALYST ANCHORED ON CARBONIZED MATERIAL

BABATUNDE, Esther Olubunmi[1*]; ADERIBIGBE, Fatai Alade[1]; ADEKUNLE, Joseph Isaac [1]; ARE, Comfort Temitope[2]; OLUWATOBI, Paul-lasisi Joshua[1]

[1] Chemical Engineering Department, University of Ilorin, Ilorin, Kwara State, Nigeria

[2] Prince Abubakar Audu University, Chemistry Department Anyigba, Kogi State, Nigeria.

**Correspondence author*
e-mail: babatunde.eo@unilorin.edu.ng

Received 02 February 2022; received in revised form 26 February 2022; accepted 02 March 2022

ABSTRACT

The current investigation emphasizes preparing low-cost carbon-based zirconium impregnated heterogeneous catalysts from wood dust to produce biodiesel from waste vegetable oil (WVO). Response Surface Methodology via Central Composite Design (RSM-CCD) optimized the biodiesel production process. The physico-chemical properties of waste vegetable methyl ester were determined following the American Standard Testing of Materials (ASTM). The optimum conditions were observed to be 8:1 methanol/oil ratio, 5 wt% catalyst loading, 55°C temperature, and 3 h reaction time. The corresponding response was observed to be 98.39%. The catalyst morphology and elemental composition were determined using Scanning Electron Microscopy (SEM) and Energy-Dispersive X-ray (EDX), respectively. The experimental analysis confirmed that the synthesized catalyst from wood dust under optimized conditions can transesterify WVO into biodiesel.

Keywords: *Optimization, Waste Vegetable Oil, Zirconium, Carbonized material, Transesterification*

1. INTRODUCTION

The prospect of a fossil fuel shortage (Olutoye and Hameed, 2011; Adepoju *et al*., 2020) and the pollution that comes with it prompted researchers to search for alternatives to petroleum derivatives. The discovery from the research gave rise to "biodiesel" as an alternative fuel. Biodiesel is a biofuel that is similar to fossil diesel (Gashaw and Teshita, 2014). Vegetable oil, animal oil/fats, tallow, and waste cooking oil can produce biodiesel. Transesterification is the chemical reaction used to convert these oils into biodiesel (Yildiz *et al*., 2015; Babatunde *et al*., 2020a). Oil crops such as rapeseed, palm, and soybean provide the largest possible source of suitable vegetable oil (Yildiz *et al*., 2015; Dhawane *et al.,* 2017). In the UK, rapeseed provides the highest potential for biodiesel production. Most biodiesel synthesis comes from waste vegetable oil supplied from restaurants, chip shops, and industrial food processing. Although oil directly from the agricultural industry has the greatest potential, biodiesel has not been commercialized because of the high cost of raw materials. (Yildiz *et al*., 2015: Dhawane *et al.,* 2018, Chaveanghong *et al*., 2018).

Biodiesel is one of several alternative fuels designed to extend the life and cleanliness of diesel engines with the following advantages; low exhaust emissions, renewability, non-toxic, biodegradable, and sustainability—reduced reliance on foreign oil and economic development. (Sumit et *al*., 2016; Kamakar *et al.,* 2020, babatunde et *al*., 2020a;). Research into biofuel production is currently on in Nigeria, but there are challenges such as competition between edible vegetable oil consumption and biofuel production, long-term sustainability to meet industry demands and the high cost of virgin vegetable oil, and environmental contamination from the indiscriminate discharge of used alkali catalyst (Ramachandra *et al*., 2013; Erum *et al.,* 2014; Shaaban *et al.* 2015). Therefore, in this paper, wood dust which poses environmental pollution, was utilized to synthesize heterogeneous catalysts to produce biodiesel.

2. MATERIALS AND METHODS

2.1 Materials

Wood dust abundantly found in Tanke Iledu,

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.37_abstract_BABATUNDE.pdf

Ilorin, Kwara State, Nigeria, was chosen as a precursor for preparing catalyst support. The waste vegetable oil (WVO) was obtained from Oke-odo frying fish sellers Ilorin, Kwara State, Nigeria. Methanol, potassium hydroxide (KOH), Petroleum ether, and zirconium oxide are all analytical grades obtained from Central Research Laboratory, Ilorin, Kwara State, Nigeria.

2.2 Method

2.1 Determination of Physicochemical Properties

The physicochemical properties of the waste Vegetable oil and produced biodiesel were analyzed according to ASTM D6751-02 (Babatunde *et al*., 2020b).

2.2 Catalyst preparation

Wood dust was pretreated by washing, oven-dried at a temperature of 120 °C for 24 hours, and sieved. Next, the catalyst support was prepared by carbonizing the pretreated wood dust at a temperature of 500 °C for one hour to obtain activated carbon. The zirconium oxide was later anchored on the surface of the activated carbon by the wet impregnation method. After that, the mixture was calcined at 500 ℃ and kept in a desiccator to avoid moisture.

2.3 Catalyst Characterization

The catalyst was characterized by Scanning Electron Microscopy (SEM), used to view the surface morphology of the catalysts, Energy Dispersive Spectroscopy (EDS) used to determine the elemental analysis of the sample and the quantitative composition of the catalyst, X-ray diffraction analysis (XRD) equipped with Kά and Cu radiation source, Fourier transform infrared spectroscopy (FTIR), used to confirm the presence of the functional group. Brunauer-Emmett-Teller (BET) isothermal sorption (QUANTACHROME, 1 KE), used to determine the surface area of the catalyst through N_2-adsorption.

2.4 Design of Experiment using Central Composite Design of Response Surface Methodology

The design of the experimental conditions was carried out via the application of Central Composite Design (CCD) in Design-Expert software (version 10.0.1). Table 1 shows the process input parameters viz. methanol to oil ratio (6:1–9:1), reaction temperature (50-70 ℃), reaction time (1-4 h), and catalyst loading level (0.5–2.0 wt%) investigated for maximum yield. The CCD was used to produce 30 experimental runs. The terms of the quadratic polynomial models of the variables were fitted through multiple regressions. The model was established through various statistical analyses such as ANOVA and significance test at a 95% confidence level. Equation (2) describes the fitted second-order mathematical regression model. (Babatunde *et al.,* 2020a; Betiku *et al.,* 2019; Joseph, 2014).

Table 1: Independent variables and levels used for RSM

Symbols	Variables	Levels		
		-1	0	1
A	Methanol/oil ratio(v/v)	6:01	7.5:1	9:01
B	Temperature (°C)	50	60	70
C	Time (h)	1	2	3
D	Catalyst loading (w%)	0.5	1.25	2

2.5 Transesterification of Waste Vegetable Oil

The transesterification reaction was carried out in 100 mL conical flasks on magnetic stirrers. 10 g of waste vegetable oil was measured into the conical flasks. A calculated amount of methanol was added to a known amount of catalyst (0.5, 1.25, 2.00, and 2.75 per weight of oil) to ease miscibility and speed up the reaction rate. The mixture of methanol to oil ratios of 6:1, 7.5:1, and 9:1) was stirred vigorously at constant agitation speed, reaction temperature (50 °C, 55 °C, 60 °C, and 65 °C) and reaction time (1, 2, 3 and 4 h). The effects of alcohol-oil ratio, reaction time, reaction temperature, catalysts concentration were investigated according to the experimental runs in Table 2. At the end of the transesterification reaction, 30 ml of distilled water was added to the products; biodiesel and glycerol gave rise to two distinct phases separated using a separating funnel through a filter paper to prevent catalyst loss. The glycerol was dispersed in the water phase (lower layer) while the biodiesel was above (upper layer). The biodiesel yield was calculated using Equation 1.

$$\text{Biodiesel Yield } (\%) = \frac{\text{Mass of biodiesel}}{\text{Mass of WVO}} \times 100 \quad \text{(Eq. 1)}$$

3. RESULTS AND DISCUSSION:

3.1 Determination of Physicochemical properties of Waste Vegetable Oil

The physicochemical properties of the waste vegetable oil and produced biodiesel are presented in Table 2.

3.2 Characterization of Synthesized Catalyst

3.2.1 Morphology Elemental Analysis

The SEM images are shown in Figure 1:

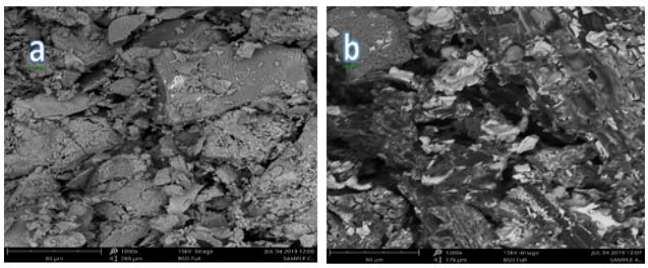


Figure 1: SEM images of (a) carbonized wood-dust and (b) synthesized catalyst

The morphological features of the wood –dust were studied using SEM. Micrographs (a and b) in Figure 1 depict the SEM images for carbonized wood dust and (b) synthesized catalyst. It can be seen that Figure 1a shows an irregular porous morphology while SEM image obtained in Figure 1b illustrates the spongy and porous nature of the particles, which are characterized by increased particles agglomeration. Furthermore, the calcination of the wood-dust sample led to smaller aggregates of the particles with high fibrous and mesoporous nature. Hence, zirconium was successfully adsorbed on the support, which also confirmed the result of Energy Dispersive Spectroscopy.

3.2.2 Elemental Analysis

Energy Dispersive Spectroscopy (EDS) analysis was used to carry out quantitative chemical analysis (elemental composition) on the catalyst preparation. Figure 2 shows that zirconium (66.06 %) is the major element, followed by calcium (16.83 %). In contrast, others such as S, Mg, Al, Si, Fe, Na, Cr, and Ti are traces in the material. The 66.06 % zirconium shows the highest composition, confirming its successful incorporation into the support (wood-dust).

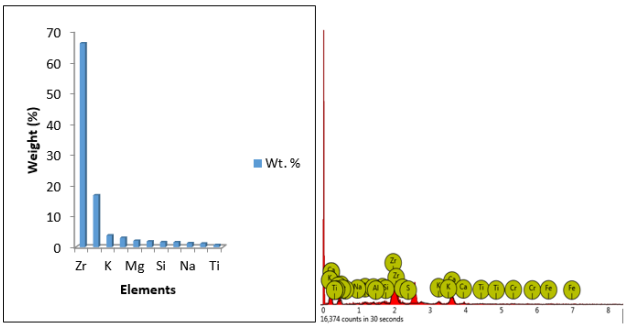


Figure 2: Energy Dispersive Spectroscopy (EDS) pattern of the synthesized catalyst

4. CONCLUSIONS:

The impregnation method of synthesizing catalysts is fast and suitable for synthesizing a low-cost carbon-based catalyst. Characterization of the synthesized catalyst by SEM and EDS confirmed the presence of zirconium in the synthesized catalyst. It was uniformly dispersed on the support material (carbonized wood-dust) synthesized by the impregnation method. The synthesized catalyst was suitable for producing biodiesel with a maximum yield of 98.39 % at methanol to oil ratio of 9:1, 5% catalyst concentration concerning the weight of oil, reaction temperature of 55 °C, and reaction time of 3 h. The physicochemical properties of the waste vegetable oil biodiesel showed that it meets the ASTM standards. The GC-MS FAME profile further confirmed the quality of the biodiesel.

6. REFERENCES:

1. Babatunde E. O., Saka H. B., Olutoye M. A., Akpan U.G. and M. Auta. Synthesis of fatty acid methyl esters from used vegetable oil using activated anthill as catalyst. *Nigerian Journal of Technology (NIJOTECH), 39,* (1), (2020a), 140-147.
2. Babatunde. E.O., Bisheswar K., Olutoye M.A., Akpan U.G., Manase A. and Gopinath H. Parametric optimization by Taguchi L9 approach towards biodiesel production from restaurant waste oil using Fe-supported anthill catalyst. *Journal of Environmental Chemical Engineering,* 8(5), (2020b)
3. 3 Betiku, E., Omilakin, O.R and Ajala, S.O. Mathematical modelling and process parameters optimization studies by artificial neural network and response surface methodology: A case of non-edible neem (*Azadirachta indica*) seed oil biodiesel synthesis. *Energy*, *72*, 2014, 266-273.
4. 4 Chaveanghong, S., Smith, S. M., Smith, C. B., 5 Luengnaruemitchai, A., and Boonyuen, S. Simultaneous transesterification and esterification of acidic oil feedstocks catalyzed by heterogeneous tungsten loaded bovine bone under mild conditions. *Renewable Energy*, *126*, 2018, 156–162. https://doi.org/10.1016/j.renene.2018.03.036
5. Dhawane, S.H., Bora, A.P., Kumar, T and Halder, G. Parametric optimization of biodiesel synthesis from rubber seed oil using iron-doped carbon catalyst by Taguchi approach. *Renewable Energy*, *105*, 2017, 616-624.
6. Dhawane, S. H., Karmakar, B., Ghosh, S., and Halder, G. Parametric optimization of biodiesel synthesis from waste cooking oil via Taguchi approach. *Journal of Environmental Chemical Engineering*, *6,*(4), 2018,3971–3980. https://doi.org/10.1016/j.jece.2018.05.053

Table 2: Physicochemical Properties of Waste Vegetable Oil and produced Biodiesel

Fuel properties (units)	WVO	Waste Vegetable oil Biodiesel	ASTM standard for biodiesel	ASTM Method
Density at 15ºC (g/cm^3)	0.937	0.887	0.860 to 0.900	ASTM D1298
Flash point (ºC)	224	173	≥130	ASTM D92
Acid value (mg KOH/g)	3.366	0.435	≤0.80	ASTM D664
Cloud point (ºC)	21	-2	-3 to -12	ASTM D2500
FFA	1.683	0.218	-	-
Viscosity @ 40 °C/(mm^2/s)	20.50	4.52	-	-
Saponification Value	185.32	165	-	-

Table 3: CCD Experimental design and biodiesel yield

Run	Methanol/oil ratio	Temperature (˚C)	Catalyst loading (w%)	Time (h)	Yield (%)
1	9.00	60.00	1.25	2.00	66.40
2	8.00	65.00	0.50	3.00	84.10
3	7.00	60.00	1.25	4.00	91.23
4	8.00	55.00	2.00	1.00	53.60
5	8.00	55.00	0.50	3.00	98.39
6	6.00	55.00	2.00	3.00	88.70
7	6.00	55.00	0.50	3.00	87.41
8	8.00	65.00	0.50	1.00	66.22
9	7.00	60.00	1.25	2.00	68.88
10	7.00	60.00	1.25	1.00	53.20
11	6.00	65.00	0.50	3.00	76.65
12	7.00	60.00	2.75	2.00	74.82
13	6.00	55.00	2.00	1.00	68.29
14	7.00	60.00	1.25	2.00	68.88
15	6.00	55.00	0.50	1.00	86.92
16	8.00	55.00	0.50	1.00	79.87
17	6.00	65.00	2.00	3.00	83.12
18	7.00	50.00	1.25	2.00	57.09
19	7.00	60.00	1.25	2.00	68.88
20	6.00	65.00	0.50	1.00	74.31
21	7.00	60.00	1.25	2.00	68.88
22	7.00	60.00	1.25	2.00	68.88
23	7.00	60.00	1.25	2.00	68.88
24	8.00	55.00	2.00	3.00	81.05
25	8.00	65.00	2.00	3.00	81.23
26	6.00	65.00	2.00	1.00	75.35
27	7.00	70.00	1.25	2.00	82.31
28	5.00	60.00	1.25	2.00	67.35
29	7.00	60.00	0.25	2.00	63.54
30	8.00	65.00	2.00	1.00	71.35

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

OPTIMIZATION OF BIODIESEL PRODUCTION FROM WASTE VEGETABLE OIL USING Zr- OXIDE CATALYST ANCHORED ON CARBONIZED MATERIAL

Babatunde, Esther Olubunmi[1*]; Aderibigbe, Fatai Alade[1]; Joseph Isaac Adekunle[1]; Are, Comfort Temitope[2]; Paul-lasisi Joshua Oluwatobi

[1]Chemical Engineering Department, University of Ilorin, Ilorin, Kwara State, Nigeria
[2]Prince Abubakar Audu University, Chemistry Department Anyigba, Kogi state, Nigeria.
*Email: babatunde.eo@unilorin.edu.ng

March/2022

INTRODUCTION

SBJChem Conference 2021

- The prospect of a fossil fuel shortage (Olutoye and Hameed, 2011; Adepoju *et al*., 2020), as well as the pollution that comes with it, prompted researchers to search for alternatives to petroleum derivatives. The discovery from the research gave rise to "biodiesel" as an alternative fuel. Biodiesel is a biofuel that is similar to fossil diesel (Gashaw and Teshita, 2014).
- Sources of Biodiesel (Yildiz *et al*., 2015; Babatunde *et al*., 2020a)
  - Vegetable oil
  - Animal oil/fats
  - Tallow
  - Waste cooking oil
- Transesterification is the process of converting these oils into biodiesel (Yildiz *et al*., 2015; Babatunde *et al*., 2020a).

BACKGROUND

SBJChem Conference 2021

- Advantages of biodiesel (Sumit et *al*., 2016; Kamakar *et al*., 2020, babatunde et *al*., 2020a)
  - Low exhaust emissions
  - renewability
  - non-toxic
  - biodegradable and sustainable
  - reduced reliance on foreign oil
  - and economic development.

BACKGROUND

SBJChem Conference 2021

- Challenges facing biodiesel production in Nigeria
  (Ramachandra *et al*., 2013; Erum *et al*., 2014; Shaaban *et al*. 2015).
  - Competition between edible vegetable oil consumption and biofuel production
  - Long-term sustainability to meet industry demands
  - High cost of virgin vegetable oil
  - Environmental contamination from indiscriminate discharge of used alkali catalyst
- In this study, wood-dust which poses environmental pollution was utilized to synthesis heterogeneous catalyst for the production of biodiesel.

METHODOLOGY

SBJChem Conference 2021

Determination of Physicochemical Properties of WVO

Catalyst Preparation:

- ✓ Wood-dust Washing
- ✓ oven dried at 120°C 24 hours and sieved
- ✓ Carbonization of the pretreated wood-dust at 500 °C for one hour to obtain activated carbon.
- ✓ wet impregnation of ZrO on activated carbon
- ✓ calcined at 500 ℃ and kept in a desiccator to avoid moisture

Catalyst Characterization

- ✓ Scanning Electron Microscopy (SEM)
- ✓ Energy Dispersive Spectroscopy (EDS)

METHODOLOGY

SBJChem Conference 2021

Transesterification of Waste Vegetable Oil Via CCD:

- ✓ Catalyst loading
- ✓ Methanol/oil ratio
- ✓ Reaction Time
- ✓ Reaction Temperature

Separation using a separating funnel through a filter paper in order to prevent catalyst lost

Determination of Physicochemical Properties of Biodiesel

$$\text{Biodiesel Yield}\ (\%) = \frac{\text{Mass of } biodiesel}{\text{Mass of } WVO} \times 100 \qquad (1)$$

METHODOLOGY

SBJChem Conference 2021

Table 1: Independent variables and levels used for RSM

Symbols	Variables	Levels -1	0	+1
A	Methanol/oil ratio(v/v)	6:1	7.5:1	9:1
B	Temperature (°C)	50	60	70
C	Time (h)	1	2	3
D	Catalyst loading (w%)	0.5	1.25	2

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 1: Physicochemical Properties of Waste Vegetable Oil and produced Biodiesel

Fuel properties (units)	WVO	Waste Vegetable oil Biodiesel	ASTM standard for Biodiesel	ASTM Method
Density at 15°C (g/cm^3)	0.937	0.887	0.860 to 0.900	ASTM D1298
Flash point (°C)	224	173	≥130	ASTM D92
Acid value (mg KOH/g)	3.366	0.435	≤0.80	ASTM D664
Cloud point (°C)	21	-2	-3 to -12	ASTM D2500
FFA	1.683	0.218	-	-
Viscosity @ 40 °C/(mm^2/s)	20.50	4.52	-	-
Saponification Value	185.32	165	-	-

RESULTS AND DISCUSSION

SBJChem Conference 2021

Characterization of Synthesized Catalyst

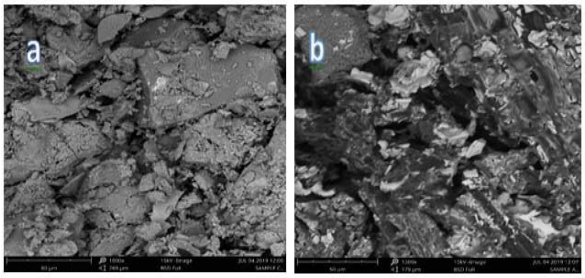


Figure 1: SEM images of (a) carbonized wood-dust and (b) synthesized catalyst

RESULTS AND DISCUSSION

SBJChem Conference 2021

Elemental Analysis

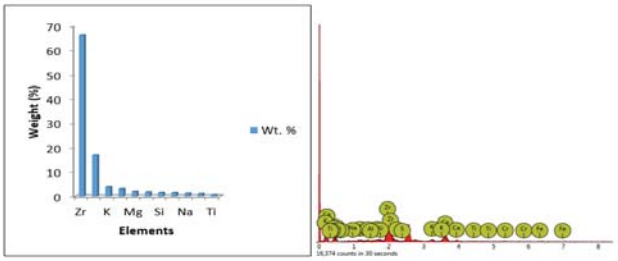


Figure 2: Energy Dispersive Spectroscopy (EDS) pattern of synthesized catalyst

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 2: Independent variables and levels used for RSM

Symbols	Variables	Levels		
		-1	0	+1
A	Methanol/oil ratio(v/v)	6:1	7.5:1	9:1
B	Temperature (°C)	50	60	70
C	Time (h)	1	2	3
D	Catalyst loading (w%)	0.5	1.25	2

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 3: CCD Experimental design and biodiesel yield

Run	Methanol/oil ratio	Temperature (°C)	Catalyst loading (w%)	Time (h)	Yield (%)
1	9.00	60.00	1.25	2.00	66.40
2	8.00	65.00	0.50	3.00	84.10
3	7.00	60.00	1.25	4.00	91.23
4	8.00	55.00	2.00	1.00	53.60
5	8.00	55.00	0.50	3.00	98.39
6	6.00	55.00	2.00	3.00	88.70
7	6.00	55.00	0.50	3.00	87.41
8	8.00	65.00	0.50	1.00	66.22
9	7.00	60.00	1.25	2.00	68.88
10	7.00	60.00	1.25	1.00	53.20
11	6.00	65.00	0.50	3.00	76.65
12	7.00	60.00	2.75	2.00	74.82
13	6.00	55.00	2.00	1.00	68.29
14	7.00	60.00	1.25	2.00	68.88
15	6.00	55.00	0.50	1.00	86.92
16	8.00	55.00	0.50	1.00	79.87
17	6.00	65.00	2.00	3.00	83.12
18	7.00	50.00	1.25	2.00	57.09
19	7.00	60.00	1.25	2.00	68.88
20	6.00	65.00	0.50	1.00	74.31
21	7.00	60.00	1.25	2.00	68.88
22	7.00	60.00	1.25	2.00	68.88
23	7.00	60.00	1.25	2.00	68.88
24	8.00	55.00	2.00	3.00	81.05
25	8.00	65.00	2.00	3.00	81.23
26	6.00	65.00	2.00	1.00	75.35
27	7.00	70.00	1.25	2.00	82.31
28	5.00	60.00	1.25	2.00	67.35
29	7.00	60.00	0.25	2.00	63.54
30	8.00	65.00	2.00	1.00	71.35

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 4: Analysis of variance (ANOVA)

-Source	Sum of Squares	Df	Mean Square	F Value	p-value Prob > F
Model	2274.27	14	162.45	2.06	0.0387
A-MeOH: Oil	30.02	1	30.02	0.38	0.0565
B-Temp.	14.32	1	14.32	0.18	0.0261
C-Time	34.13	1	34.13	0.43	0.0056
D-Cat. Conc.	1362.03	1	1362.03	17.27	0.0008
AB	8.82	1	8.82	0.11	0.7427
AC	62.09	1	62.09	0.79	0.3889
AD	114.06	1	114.06	1.45	0.2478
BC	312.58	1	312.58	3.96	0.0330
BD	52.56	1	52.56	0.67	0.4271
CD	43.16	1	43.16	0.55	0.4709
A^2	27.75	1	27.75	0.35	0.5619
B^2	80.40	1	80.40	1.02	0.3287
C^2	68.65	1	68.65	0.87	0.3656
D^2	150.29	1	150.29	1.91	0.0187
Residual	1183.07	15	78.87		
Lack of Fit	1183.07	10	118.31		
Pure Error	18.60	5	9.96		
Cor Total	3457.35	29			

RESULTS AND DISCUSSION

SBJChem Conference 2021

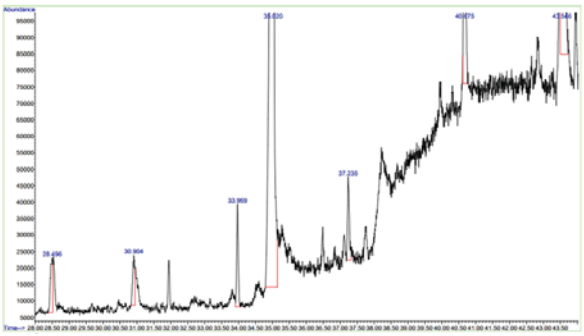


Figure 3: GC-MS of the waste vegetable oil biodiesel

14

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 6: Methyl esters composition of waste vegetable oil Biodiesel from GC-MS Analysis

Peak No.	Retention time	Methyl esters	Composition (%)
1	30.904	Tetradecanoic acid	2.08
2	33.969	Methyl palmitate	3.21
3	35.020	n-Hexadecanoic acid	54.19
4	37.235	7-Octadecanoic acid 6-Octadecanoic acid	2.93
5	40.675	Hexadecanedioic acid	12.66
6	43.546	Dimethylmalonic acid	22.32

15

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 7: Comparison of biodiesel yield for fresh and reused catalyst

		Yield (%)		
Fresh catalyst	First reuse	2nd reuse	3rd reuse	4th reuse
98.39	96.04	95.36	93.66	90.62

16

CONCLUSIONS

SBJChem Conference 2021

- Impregnation method of synthesizing catalysts is fast and suitable for the synthesis of a low-cost carbon-based catalyst.
- Characterization of the synthesized catalyst by SEM and EDS confirmed the presence of zirconium in the synthesized catalyst. It was uniformly dispersed on the support material (carbonized wood-dust) synthesized by impregnation method.
- The synthesized catalyst was suitable for the production of biodiesel with a maximum yield of 98.39 % at a methanol to oil ratio of 9:1, 5% catalyst concentration with respect to the weight of oil, reaction temperature of 55 ^{o}C and reaction time of 3 h.
- The physicochemical properties of the waste vegetable oil biodiesel showed that it meets the ASTM standards. The GC-MS FAME profile further confirmed the quality of the biodiesel.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

The authors' acknowledgement goes to the management of University of Ilorin, Ilorin, Kwara State, Nigeria for making it possible for us to attend SBJChem Conference 2021.

REFERENCES

SBJChem Conference 2021

1. Babatunde E. O., Saka H. B., Olutoye M. A., Akpan U.G. and M. Auta. (2020a). Synthesis of fatty acid methyl esters from used vegetable oil using activated anthill as catalyst. *Nigerian Journal of Technology (NIJOTECH), 39,* (1),140-147.
2. Babatunde. E.O., Bisheswar K., Olutoye M.A., Akpan U.G., Manase A. and Gopinath H. (2020b): Parametric optimization by Taguchi L9 approach towards biodiesel production from restaurant waste oil using Fe-supported anthill catalyst. *Journal of Environmental Chemical Engineering*, 8(5):104288.
3. Betiku, E., Omilakin, O.R and Ajala, S.O. (2014). Mathematical modelling and process parameters optimization studies by artificial neural network and response surface methodology: A case of non-edible neem (*Azadirachta indica*) seed oil biodiesel synthesis. *Energy*, *72*, 266-273.
4. Chaveanghong, S., Smith, S. M., Smith, C. B., Luengnaruemitchai, A., and Boonyuen, S. (2018). Simultaneous transesterification and esterification of acidic oil feedstocks catalyzed by heterogeneous tungsten loaded bovine bone under mild conditions. *Renewable Energy*, *126*, 156–162. https://doi.org/10.1016/j.renene.2018.03.036
5. Dhawane, S.H., Bora, A.P., Kumar, T and Halder, G. (2017). Parametric optimization of biodiesel synthesis from rubber seed oil using iron doped carbon catalyst by Taguchi approach. *Renewable Energy*, *105*, 616-624.
6. Dhawane, S. H., Karmakar, B., Ghosh, S., and Halder, G. (2018). Parametric optimisation of biodiesel synthesis from waste cooking oil via Taguchi approach. *Journal of Environmental Chemical Engineering*, *6*,(4), 3971–3980. https://doi.org/10.1016/j.jece.2018.05.053
7. Erum, Z., Rehana, S., Mehwish, A. H., and Anjum, Y. (2014). Study of physicochemical properties of edible oil and evaluation of frying oil quality by Fourier Transform-Infrared (FT-IR) Spectroscopy. *Arabian Journal of Chemistry*, 3870–3876. https://doi.org/10.1016/j.arabjc.2014.05.0251

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

OSTEOMYELITIS OF THE FIRST PHALANX IN A HORSE ATHLETE: CASE REPORT

ÁVILA, Letícia Meirelles[1*]; GOMES, Letícia Patrão de Macedo[2]; GOMES, Gustavo Mendes[2]; ABREU, Ana Paula Martinez de[2]; ROIER, Erica Cristina Rocha[2];

[1,2] Mestranda do Programa de Pós Graduação em Ciências Veterinárias da Universidade Federal Rural do Rio de Janeiro

[2] Professor adjunto do curso de Medicina Veterinária da Universidade de Vassouras

** Correspondenceauthor*
e-mail: leticiameirellesavila@gmail.com

Received 01 February 2022; received in revised form 17 February 2022; accepted 19 February 2022

ABSTRACT

Equinoculture is an activity of great importance in Brazil, moving millions of reais annually. For many years these animals were used only as a means of transport; however, currently, horses have assumed coverage in other areas of activity, such as leisure, sports, and even therapies, without escaping their main work functions in agricultural activities. Due to the significant requirement of the locomotor system, the affections of this system are quite common in this species. Therefore, these conditions must be diagnosed and treated early to completely restore the animal's functions. Intense exercises and very demanding tests subject these animals to limb injuries. They are fast-reacting animals and, sometimes, they can generate injuries due to the shock on surfaces and objects. These skin continuity solutions can act as a door of entry for infectious agents. Osteomyelitis is an infectious process that is accompanied by bone destruction, mainly caused by gram-positive bacteria. The prognosis of animals affected by this pathology is directly influenced by the speed of correct diagnosis and the beginning of appropriate treatment. It can put the sporting purpose of the animal and life at risk if it occurs late. The present report aims to describe the case of an adult female athlete, used for polo, presenting a lesion in the right forelimb and claudication grade 4/5. The diagnosis was obtained through clinical examination and radiographic study, finding radiographic changes compatible with osteomyelitis, and established treatment.

Keywords: *lameness, equine, locomotor, osteomyelitis, regional perfusion*

1. INTRODUÇÃO

A osteomielite é uma infecção que se inicia na cavidade medular do osso, sendo o processo acompanhado por uma grave destruição óssea provocada principalmente por agentes bacterianos (PIEREZAN, 2009). Esta patologia pode ter sua origem de três maneiras: hematógena – comum em neonatos e animais jovens; resultante de ferida perfurante ou fratura exposta; e resultante de fixação interna de fratura não exposta na qual houve falha na técnica de assepsia cirúrgica (STASHAK, 1994). Possui rápida evolução e prognóstico favorável quando tratada em sua fase inicial, porém em casos onde há demora no diagnóstico e tratamento, a osteomielite pode causar a inutilização de um animal atleta e até mesmo levá-lo a óbito (BEZERRA FILHO, 2018).

Os sinais clínicos variam conforme a duração e severidade da infecção, mas geralmente observa-se claudicação, dor à palpação, tumefação, edema generalizado de tecidos moles adjacentes e presença de secreção purulenta no local (PIEREZAN, 2009) e radiograficamente, se-

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.22_abstract_AVILA.pdf

questro necrótico com perda da densidade óssea, seguida por proliferação óssea (BEZERRA FILHO, 2018). Para a obtenção de um diagnóstico preciso é necessária realização de uma avaliação radiográfica associada a um exame físico minucioso (PIEREZAN, 2009).

As bactérias gram-negativas e gram-positivas são os principais microrganismos responsáveis pela osteomielite (BEZERRA FILHO, 2018), entretanto fungos e microbactérias também podem desencadear a afecção. É muito importante adotar um protocolo de tratamento assertivo, com antibioticoterapia, se necessário debridamento e drenagem cirúrgica (BOTTON *et al*., 2016). Para aumentar as chances de sucesso, outra abordagem terapêutica que pode ser utilizada é a técnica de perfusão regional do membro(PRM) com agentes antimicrobianos (SCHADE *et al*., 2019).

O objetivo do presente trabalho foi relatar um caso clínico de osteomielite em um equino atleta, fêmea, de 10 anos de idade.

2. RELATO DE CASO:

No dia 30 de junho de 2020 foi solicitado atendimento veterinário para um equino atleta que, de acordo com o proprietário, apresentava edema e claudicação do membro anterior direito. Este animal, utilizado para jogos de polo, uma fêmea, mestiça de PSI com 10 anos de idade estava alojada numa propriedade no município de Seropédica-RJ.

Na avaliação clínica foi possível identificar edema no membro anterior direito (Figura 1) e claudicação grave grau 4/5 (OBEL, 1948). Além disso, observou-se a existência de uma pequena fístula drenando secreção purulenta, edema, dor e calor na região do boleto.

O animal era mantido em regime extensivo e não foi possível determinar a causa exata, entretanto foi possível identificar uma fístula que pode ter atuado como porta de entrada dos agentes infecciosos, após algum acidente. Para avaliar e identificar a extensão da lesão foram solicitados exames radiográficos.

Figura 1. Membro anterior direito do equino apresentando-se edemaciado desde região da coroa do casco até a articulação radiocárpica.

De acordo comas imagens radiográficas (Figura 2) pode-se observar presença de intensa reação periosteal dorsal e palmar (Seta azul) com remodelação óssea em região peri cortical e central do endósteo, sendo sugestiva de processo inflamatório e infeccioso, além de edema na região. Estas alterações são compatíveis com osteomielite, e a partir do diagnóstico foi prescrito o tratamento.

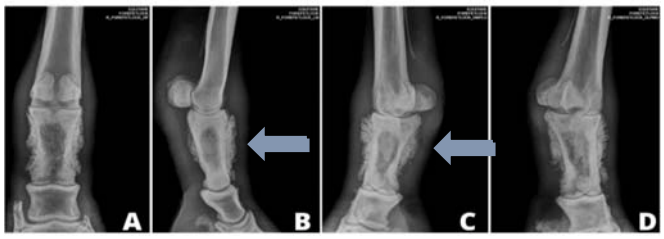


Figura 2. Imagens Radiográficas. A) Incidência dorso palmar. B) Incidência látero-medial. C) Incidência dorsomedial-plantarolateral oblíqua. D) Incidência dorsolateral-plantaromedial oblíqua.

O tratamento instituído foi à utilização de anti-inflamatórios não esteroidais (AINES), antibioticoterapia sistêmica associada com a técnica de PRM com antimicrobianos (150mg diluído em 10ml de soro NaCl 0,9%). De acordo com Rafael *et al*. (2014), a perfusão regional com antimicrobianos é uma opção terapêutica no tratamento das infecções dos membros alcançando altos níveis teciduais do fármaco nos locais afetados, em comparação com a terapia

sistêmica, a perfusão regional utiliza os mesmos fármacos em baixas doses, porém aumenta a eficácia deles e minimiza o risco de toxicidade.Para o controle do processo inflamatório foi empregado dimetilsulfóxido (Dimesol®) devido a suas características anti-inflamatórias inauditas (LEITE *et al*., 2019), na dose de 1g/kg de PV diluído em solução glicosada 5%, na concentração 10%, por via endovenosa lenta, SID, durante 3 dias consecutivos. Para antibioticoterapia parenteral optou-se pelo uso de uma cefalosporina de terceira geração (Ceftiofur)na dose 4,4mg/kg de PV, SID, por via intramuscular durante 10 dias. A escolha desta base ocorreu devida sua excelente ação antimicrobiana sobre bactérias gram negativas e gram positivas (RODRIGUES *et al*., 2004).

Após 4 meses do início do tratamento foi realizada uma nova avaliação radiográfica (Figura 3) onde foi possível observar presença de proliferação periosteal dorsal e reação proliferativa moderada em região palmar e em região peri cortical e central do endósteo (Seta verde) sendo sugestiva de processo cicatricial pós processo infeccioso. Devido à proliferação periosteal optou-se pelo emprego de contra irritantes para o controle da mesma, neste caso, o irritante de superfície utilizado foi 5-Day Blister® (POSTYME PRODUCTS, INC.) que foi aplicado sobre a pele da região acometida após tricotomia ampla. Esta técnica foi realizada durante 3 dias consecutivos, no total de três tratamentos com intervalo de 20 dias entre cada tratamento.

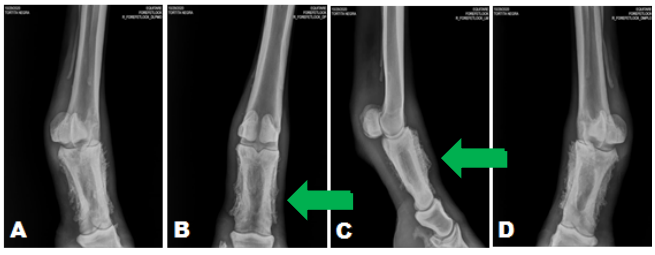


Figura 3. Imagens Radiográficas. A) Incidência DorsoLateral-PlantaroMedial Oblíqua. B) Incidência dorso palmar. C) Incidência látero-medial. D) Incidência DorsoMedial-PlantaroMedial Oblíqua.

3. RESULTADOS E DISCUSSÃO:

Embora a osteomielite tenha uma rápida evolução, a mesma tem um prognóstico favorável quando tratada em sua fase inicial, conforme observado no presente relato. Porém em casos onde há demora no diagnóstico e tratamento o animal pode vir a óbito (PYLES *et al*., 2005). No presente relato apesar de não se conhecer o início exato do processo, o diagnóstico e o tratamento foram realizados rapidamente após a identificação do caso, o que favoreceu o restabelecimento do animal o seu retorno as atividades esportivas.

4. CONCLUSÃO:

Baseando-se nos dados de literatura e nos resultados do presente relato, a osteomielite é uma enfermidade que deve ser tratada como emergência, na maioria das vezes secundária a lesões ou traumas, podendo levar a perda de desempenho do animal, e complicações que incluem o óbito. O diagnóstico e tratamento precoces e assertivos foram indispensáveis para a completa recuperação do animal.

6. REFERENCIAS

1. Bezerra Filho, J. (2018). Avulsão de casco associado a osteíte infecciosa e osteomielite em equino: relato de caso. Centro de Ciências Agrárias, Curso de Bacharelado em Medicina Veterinária. Areia, PB. 66p.
2. Botton, L. R. Bernardi, M. M. Bolze, C. D. G. Serafini, O. A. (2016). Urgências em ortopedia. Acta méd. (Porto Alegre), p 8-8.
3. Leite, N. M. Rocha, M. V. Souza, M. K. Vago, P. B. (2019). Linfangite ulcerativa em equino: relato de caso. Pubvet, v. 13, p. 150.
4. Obel, N. (1948). Estudos sobre a histopatologia da laminite aguda. Estudos sobre a histopatologia da laminite aguda.
5. Pierezan, F. (2009). Prevalência das doenças de equinos no Rio Grande do Sul. Universidade Federal de Santa Maria, Centro de Ciências Rurais, Programa de Pós-graduação em Medicina Veterinária. Santa Maria, RS. Dissertação de Mestrado, 163p.
6. Pyles, M. D. Bento, M. A. F. Mendes, R. M. Alvim, N. C. (2005). Osteomielite por ferida penetrante em equino. Revista Científica Eletrônica de Medicina Veterinária, v. 5, p. 1-5.
7. Rafael, L. A. Rodrigues, C. A. Evangelista, F. C. Neto, C. R. Rodrigues,

M. Pizzigatti, D. Perri, S. H. V. Hussni, C. A. (2014). Avaliação do efeito trombogênico da perfusão regional intravenosa com gentamicina em equinos. Arquivo Brasileiro de Medicina Veterinária e Zootecnia, v. 66, n. 5, p. 1449-1456.

8. Rodrigues, C. A. Nogueira, G. M. Loureiro, M. G. Anhesini, C. R. Wienen, L. P. Aguiar, A. J. A. Milhazes, A. S. C. Cury, L. J. Ferreira, A. M. R. (2004). Estudo comparativo entre a antibiose intravenosa regional com ceftiofur e gentamicina em bovinos acometidos de enfermidades podais. Brazilian Journal of Veterinary Research and Animal Science, v. 41, p. 306-307.
9. Rodrigues, K. A. (2014). Farmacocinética da gentamicina administrada pela via intravenosa regional em equinos com a utilização de modelos de torniquetes.Dissertação (mestrado) – Universidade Estadual Paulista, Faculdade de Medicina Veterinária e Zootecnia, Botucatu.
10. Schade, J. Curti, J. M. Gonçalves, G. R. Silva, T. P. Appolonio, E. V. P. (2019). Perfusão regional do membro com antimicrobianos em equinos. Revista de Ciências Agroveterinárias. Lages, SC, v. 18, n. 2, p. 281-291.
11. Stashak, T. S. (1994). Claudicação em equinos segundo Adams. São Paulo, ed. Rocca.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

OSTEOMYELITIS OF THE FIRST PHALANX IN A HORSE ATHLETE: CASE REPORT

Letícia Meirelles Ávila
Universidade Federal Rural do Rio de Janeiro - Brazil

Letícia Patrão de Macedo Gomes
Universidade de Vassouras – Brazil

Gustavo Mendes Gomes
Universidade de Vassouras – Brazil

Ana Paula Martinez de Abreu
Universidade de Vassouras – Brazil

Erica Cristina Rocha Roier
Universidade de Vassouras – Brazil

February/2022

SUMMARY

SBJChem Conference 2021

INTRODUCTION

SBJChem Conference 2021

- Osteomyelitis is an infection;
- Begins in the medullary cavity of the bone > Severe bone destruction;
- Mainly caused by bacterial agents;
- It has a rapid evolution and favorable prognosis when treated in its initial phase.
- Delay in diagnosis and treatment, osteomyelitis can disable an athlete animal and even lead to death.

INTRODUCTION

SBJChem Conference 2021

- Clinical signs vary according to the duration and severity of the infection, but lameness, tenderness, swelling, generalized swelling of adjacent soft tissues, and the presence of purulent discharge are usually observed at the site;
- And radiographically, necrotic sequestration with loss of bone density, followed by bone proliferation;

OBJETIVE

SBJChem Conference 2021

The objective of the present study is to report a clinical case of osteomyelitis in athlete horse, female, 10-year-old.

5

CASE REPORT

SBJChem Conference 2021

- It was possible to identify edema in the right anterior limb and severe claudication grade 4/5. In addition, there was a small fistula draining purulent secretion, edema, pain and heat in the fetlock region.
- Radiographic examinations were requested.

6

CASE REPORT

SBJChem Conference 2021

- Presence of intense periosteal reaction (blue arrow) with bone remodeling, which is suggestive of an inflammatory and infectious process, and edema in the region.
- Changes are compatible with osteomyelitis.

7

CASE REPORT

SBJChem Conference 2021

- **Treatment:**
- To control the inflammatory process, dimethylsulfoxide was used. > 1g/kg diluted in 5% glucose solution, at 10% concentration, by slow intravenous route, SID, for 3 consecutive days.
- For parenteral antibiotic therapy, we chose to use Ceftiofur at a dose of 4.4mg/kg of PV, SID, intramuscularly for 10 days.
- regional limb perfusion technique with 150mg of Gentamicin diluted in 10ml of 0.9% NaCl serum, repeated three times every other day

8

CASE REPORT

SBJChem Conference 2021

- Anew radiographic evaluation was performed where it is possible to observe the presence of periosteal proliferation, suggestive of a post-infectious healing process. And it was decided to use counter-irritants to control the same.

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Although osteomyelitis has a rapid evolution, it has a favorable prognosis when treated in its initial phase.
- In the present report, although the exact beginning of the process is not known, the diagnosis and treatment were performed as soon as possible after the identification of the case, which favored the restoration of the animal and its return to sports activities.

CONCLUSIONS

SBJChem Conference 2021

- Osteomyelitis is a disease that must be treated as an emergency, most of the time secondary to injuries or trauma, which can lead to loss of animal performance, and complications that include death. In this report, early and assertive diagnosis and treatment were essential for the complete recovery of the animal.

REFERENCES

SBJChem Conference 2021

1. Bezerra Filho, J. (2018). Avulsão de casco associado a osteíte infecciosa e osteomielite em equino: relato de caso. Centro de Ciências Agrárias, Curso de Bacharelado em Medicina Veterinária. Areia, PB. 66p.
2. Botton, L. R. Bernardi, M. M. Bolze, C. D. G. Serafini, O. A. (2016). Urgências em ortopedia. Acta méd. (Porto Alegre), p 8-8.
3. Leite, N. M. Rocha, M. V. Souza, M. K. Vago, P. B. (2019). Linfangite ulcerativa em equino: relato de caso. Pubvet, v. 13, p. 150.
4. Obel, N. (1948). Estudos sobre a histopatologia da laminite aguda. Estudos sobre a histopatologia da laminite aguda.
5. Pierezan, F. (2009). Prevalência das doenças de equinos no Rio Grande do Sul. Universidade Federal de Santa Maria, Centro de Ciências Rurais, Programa de Pós-graduação em Medicina Veterinária. Santa Maria, RS. Dissertação de Mestrado, 163p.
6. Pyles, M. D. Bento, M. A. F. Mendes, R. M. Alvim, N. C. (2005). Osteomielite por ferida penetrante em equino. Revista Científica Eletrônica de Medicina Veterinária, v. 5, p. 1-5.
7. Rafael, L. A. Rodrigues, C. A. Evangelista, F. C. Neto, C. R. Rodrigues, M. Pizzigatti, D. Perri, S. H. V. Hussni, C. A. (2014). Avaliação do efeito trombogênico da perfusão regional intravenosa com gentamicina em equinos. Arquivo Brasileiro de Medicina Veterinária e Zootecnia, v. 66, n. 5, p. 1449-1456.
8. Rodrigues, C. A. Nogueira, G. M. Loureiro, M. G. Anhesini, C. R. Wienen, L. P. Aguiar, A. J. A. Milhazes, A. S. C. Cury, L. J. Ferreira, A. M. R. (2004). Estudo comparativo entre a antibiose intravenosa regional com ceftiofur e gentamicina em bovinos acometidos de enfermidades podais. Brazilian Journal of Veterinary Research and Animal Science, v. 41, p. 306-307.
9. Rodrigues, K. A. (2014). Farmacocinética da gentamicina asministrada pela via intravensa regional em equinos com a utilização de modelos de torniques. Dissertação (mestrado) – Universidade Estadual Paulista, Faculdade de Medicina Veterinária e Zootecnia, Botucatu.
10. Schade, J. Curti, J. M. Gonçalves, G. R. Silva, T. P. Appolonio, E. V. P. (2019). Perfusão regional do membro com antimicrobianos em equinos. Revista de Ciências Agroveterinárias. Lages, SC, v. 18, n. 2, p. 281-291.
11. Stashak, T. S. (1994). Claudicação em equinos segundo Adams. São Paulo, ed. Rocca.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THANKS!

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

POISONING BY HOUSEHOLD CHEMICALS IN CHILDREN

FERNANDES, Renan Lopes [1*] ; PINHEIRO, Cristina Fidalgo Affonso [1] ; SOUZA, Maria Cristina Almeida de [1];

[1] Universidade de Vassouras, Pró-Reitoria de Pesquisa e Pós-graduação, Mestrado Profissional em Ciências Aplicadas em Saúde

** Correspondence author*
e-mail: renan.lopes1206@gmail.com

Received 02 February 2022; received in revised form 22 February 2022; accepted 01 March 2022

ABSTRACT

Children are the main victims of intoxication, considering that, with child development, especially between one and four years of age, they learn to walk and acquire agility, reaching objects and bringing them to the mouth. The objective of this study was to review the literature on exogenous intoxications by chemical products used in households in children in Brazil. Household cleaning products are the second leading cause of poisoning in domestic environments, preceded only by the accidental ingestion of medication. From 2017 to 2021, 128,794 exogenous intoxications resulting from exposure to toxic agents were recorded in the age group from zero to 14 years in Brazil. Among this total of exogenous intoxications, 18,733 reports of poisoning by household products were registered, representing 14.54% of the total of exogenous intoxications. Intoxication records in Brazil increased by up to 23%, from January to April 2021, compared to the same period in 2019. This is because the world is facing the COVID-19 pandemic, in which hygiene products are being commercialized for cleaning and antisepsis of domestic environments, which led to an intensification of accidents caused by these chemical materials. Therefore, it is concluded that the rate of exogenous intoxication by domestic chemical products is high in children, especially in the age group of zero to five years. It is also worth mentioning that with the COVID-19 pandemic, there was a greater consumption of chemical products for domestic use and, consequently, an increase in the number of poisonings by these products in children. Therefore, it is evident the need to adopt actions to avoid these accidents to reduce the poisoning rate by these toxic agents.

Keywords: *accidents, household cleaning, Covid-19, childhood*

1. INTRODUÇÃO

As intoxicações são um conjunto de sinais e sintomas tóxicos produzidos pela ingestão acidental - ou não - de substâncias químicas, ou quando estas entram em contato com a pele, olhos e mucosas, desencadeando efeitos nocivos ao organismo dos seres vivos (GONÇALVES *et al*., 2015).

As crianças são as principais vítimas de intoxicação, tendo em vista que, com o desenvolvimento infantil, especialmente na faixa etária de um a quatro anos de idade, aprendem a andar e adquirem agilidade, sendo capazes de alcançar os objetos e conduzi-los à boca. Adicionalmente, tornam-se naturalmente mais curiosas. São nos momentos de descoberta e entretenimento que ocorrem os acidentes domésticos relacionados à intoxicação, pois têm habilidade para abrir a maioria das embalagens, muitas vezes armazenadas em espaços inadequados ou sem a devida segurança (PRESGRAVE *et al*., 2008).

Quando expostas acidentalmente ao produto químico, as crianças os manuseiam ou os deglutem, podendo sofrer sérias consequências, uma vez que têm metabolismo rápido e organismo imaturo para lidar com agressão provocada por toxinas químicas (LOURENÇO *et al*., 2008)

Segundo dados do Sistema de Informação de Agravos de Notificação – SINAN, as intoxicações mais frequentes em crianças ocorridas no Brasil são causadas por

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.36_abstract_FERNANDES.pdf.

medicamentos e produtos de uso doméstico, como sabões, alvejantes, amaciantes, detergentes, entre outros (BRASIL, 2022).

Assim, para evitar intoxicações decorrentes de acidentes pelo acesso inadvertido a produtos químicos, recomenda-se manter todos os produtos tóxicos distantes do campo de visão das crianças, armazená-los em locais altos, a fim de diminuir o contato delas com esses agentes tóxicos (SILVA *et al*., 2017).

Objetivou-se neste estudo, realizar uma revisão de literatura sobre intoxicações exógenas causadas principalmente por acidentes envolvendo produtos químicos de uso doméstico em crianças no Brasil.

2. MATERIAIS E MÉTODOS

Para o estudo, foram utilizadas as bases de dados SciELO e Google Scholar com os descritores “intoxication” e “children”. Utilizaram-se como critérios de inclusão artigos em inglês e português, publicados entre 2006 e 2020, e que possuíam disponibilidade completa e gratuita. Além disso, foram utilizados para a pesquisa, artigos do Repositório Institucional - Arca do Instituto de Comunicação e Informação Científica e Tecnológica em Saúde (Icict/Fiocruz), com os descritores “intoxicação” e “produtos de limpeza”. Ademais, realizou-se uma consulta na base de dados do Departamento de Informática do Sistema Único de Saúde – DATASUS, referente às notificações por intoxicações exógenas no período de 2017-2021 e uma pesquisa na plataforma da Secretaria de Estado da Saúde do Governo de Goiás a respeito do risco de intoxicações e acidentes domésticos. Após a leitura dos artigos e do uso dos critérios foram encontrados, no total 14 referências para a presente revisão de literatura.

3. RESULTADOS E DISCUSSÃO

Após aplicar os critérios de inclusão apresentados na metodologia foram encontrados 15.576 artigos, sendo 76 na base de dados Sciello e 15.500 na base Google Scholar (Tabela 1). Ao aplicar os critérios de exclusão em ambas as plataformas, dos 15.576 artigos encontrados, 11 foram selecionados e 15.565 descartados pois tratavam-se de intoxicações por medicamentos, metais, produtos químicos que não eram de uso doméstico, alimentos e outras drogas (Tabela 2). Além disso, outras plataformas de pesquisa foram utilizadas como supracitado na metodologia para a complementação do estudo.

Tabela 1. *Resultados da Pesquisa*

	BASES DE DADOS (NÚMERO DE TÍTULOS)	
Palavra-chave	SciELO (n)	Google Scholar (n)
“intoxication” e “children”	76	15500

Tabela 2. *Critérios de seleção da pesquisa*

Trabalhos encontrados (total)	**Trabalhos descartados (n)**	**Trabalhos selecionados (n)**
15576	15565	11

Lourenço *et al*. (2008) constataram em uma unidade de emergência pediátrica em Recife (PE), no período de abril a setembro de 2006, que os produtos de limpeza são a segunda maior causa de intoxicação em ambientes domésticos, precedidos apenas pela ingestão acidental de medicamentos. Isso se deve, principalmente, à natureza da criança, curiosa com os objetos ao redor, de querer imitar o que os adultos fazem, além desses produtos estarem muitas vezes guardados em locais de fácil acesso. Ademais, dois terços de todos os acidentes com crianças ocorreram dentro de casa e a maioria poderia ser evitada, desde que algumas medidas preventivas fossem adotadas, como embalagens de segurança nos remédios e nos domissanitários.

Dados do DATASUS demonstram que, no período de 2017 a 2021, foram registradas na faixa etária de zero a 14 anos, 128.794 intoxicações exógenas decorrentes à exposição por agentes tóxicos (medicamentos, produtos de uso domiciliar, alimentos e bebidas, agrotóxicos, dentre outros). Desse total de intoxicações exógenas, foram registradas 18.733 notificações de intoxicação por produtos de uso domiciliar (detergentes, alvejantes, amaciantes, sabões, entre outros), o que representa 14,54% do total de intoxicações exógenas. Na Tabela 3 estão dados relatados.

Tabela 3. *Intoxicações exógenas ocorridas na faixa etária de 0-14 anos no período de 2017-2021, no Brasil.*

	CASOS NOTIFICADOS	**%**
TOTAL	128.794	100%
PRODUTOS DE USO DOMICILIAR	18.733	14,54%

Referência: Departamento de Informática do SUS – DATASUS- **Intoxicação Exógena - Notificações registradas no Sinan Net entre 2017 a 2021.**

O estudo de Vilança *et al*. (2020) analisou as fichas de atendimento de todos os pacientes de 0-19 anos atendidos pelo Serviço de Toxicologia do Hospital João XXIII, localizado em Belo Horizonte-MG, envolvendo intoxicação exógena acidental. Identificou-se 353 casos de intoxicação exógena acidental em crianças e adolescentes, das quais os medicamentos foram os maiores causadores, seguidos pelos produtos químicos/limpeza e pesticidas. Dos produtos químicos, o hipoclorito de sódio (cloro e água sanitária) e o hidróxido de sódio (soda cáustica) foram os maiores causadores de intoxicação. Ressalta-se que, como são domissanitários, estes muitas vezes são armazenados em locais baixos, como debaixo de pias, já que são bastante utilizados no decorrer do dia para limpeza. Por isso, as crianças, ao verem esses materiais que muitas vezes são chamativos e atraentes, acabam se acidentando.

A pesquisa realizada por Werneck *e* Hasselmann, (2009) analisaram fichas de atendimento de emergência de oito hospitais localizados na região metropolitana do Rio de Janeiro, no período de abril de 2001 até março de 2004. Foram registrados 1.574 casos de intoxicação envolvendo crianças de até cinco anos de idade. Dessas intoxicações, cerca de 40% foram por produtos químicos de uso doméstico, 35% por medicamentos e 15% por algum pesticida. Esses dados refletem a alta taxa de acidentes por produtos químicos em crianças, mostrando que medidas preventivas devem ser realizadas para diminuir esses indicadores. Um exemplo seria a adoção da Embalagem Especial de Proteção à Criança (EEPC), que tem como objetivo evitar que crianças com menos de 5 anos consigam abrir os produtos químicos contidos dentro dessas embalagens de proteção. O projeto de lei 4841/1994 elaborou a criação da EEPC no Brasil tendo sido apresentado no Congresso Nacional, contudo encontra-se arquivado.

De acordo com dados do Centro de Informação e de Assistência Toxicológica (Ciatox), divulgados pela Secretaria de Estado da Saúde de Goiás, os registros de intoxicação no Brasil aumentaram até 23%, de janeiro a abril de 2021, em relação ao mesmo período em 2019. Isso se deve ao fato do mundo estar enfrentando a pandemia da COVID-19, em que produtos de higiene estão sendo cada vez mais comercializados para a limpeza e antissepsia dos ambientes domiciliares, o que levou a uma intensificação dos acidentes por esses materiais químicos.

Outrossim, dados relatados no relatório de Chang *et al*. (2020) demonstram que, entre janeiro e março de 2020, os centros de envenenamento dos Estados Unidos receberam 45.550 chamadas de exposição relacionadas a produtos químicos de uso doméstico, representando, respectivamente, aumento de 20,4% e 16,4% em relação ao mesmo período em 2019 e 2018, o que estabelece uma relação direta entre o aumento do consumo de produtos de limpeza na pandemia com o aumento das taxas de acidentes por esses produtos. Por isso, esses resultados ajudam a reafirmar a influência da pandemia no aumento de intoxicações exógenas que acontece não somente no Brasil, mas em outros países como os EUA.

Atrelado a isso, o parecer técnico-científico de Salomon *et al.* 2021, “Intoxicações por desinfetantes e produtos de limpeza usados na higienização geral contra COVID 19” divulgado pelo Programa de Evidências para Políticas e Tecnologias de Saúde (PEPTS), mostra que a partir das evidências disponíveis até o momento, houve um aumento de casos de intoxicação por produtos de uso doméstico, como desinfetantes, em crianças menores de 5 anos de idade, durante a pandemia da COVID-19.

Por fim, como descrito por Martins *et al*. (2006) o fácil acesso das crianças a esses produtos químicos levam às intoxicações na maioria das vezes. Assim, algumas medidas devem ser tomadas pelos responsáveis das crianças, para que não aconteçam acidentes por intoxicações por esses agentes tóxicos. Dentre elas, podemos citar: implantação de lacres de segurança, o armazenamento desses materiais em locais altos para que as crianças não

consigam ver e pegá-los, a manutenção dos produtos nas embalagens originais para que não aconteça de confundir acidentalmente, a não utilização dessas embalagens como brinquedos para as crianças, dentre outras medidas.

4. CONCLUSÕES

A taxa de intoxicação exógena por produtos químicos domésticos é alta nas crianças, principalmente na faixa etária de zero a cinco anos, já que estas encontram numa fase marcada pela curiosidade e pelo desenvolvimento motor, que permitem que elas entrem em contato com esses materiais químicos, que são muitas vezes armazenados em locais inapropriados. Vale ressaltar também que com a pandemia da COVID-19, houve um consumo maior de produtos químicos de uso doméstico e, consequentemente, um aumento do número de intoxicações por esses domissanitários em crianças. Por isso, ações para evitar a ocorrência desses acidentes devem ser realizadas a fim de reduzir a taxa de intoxicação por esses agentes tóxicos.

5. AGRADECIMENTOS

Aos professores do Mestrado em Ciências Aplicadas em Saúde da Universidade de Vassouras pelo apoio e incentivo ao estudo e ao nosso desenvolvimento científico.

6. REFERÊNCIAS

1. Blank D, Waksman, RD. A importância das injúrias por acidentes domésticos em tempos de COVID-19. *Residência Pediátrica*. 2020;10(2):99-102.
2. Brasil. Ministério da Saúde. Departamento de Informática do SUS. TabNet Win32 3.0: Intoxicação Exógena - Notificações registradas no Sinan Net – Brasil [internet]. 2017-2021 [acesso em 2022 janeiro 26]. Disponível em: http://tabnet.datasus.gov.br/cgi/deftohtm.exe?sinannet/cnv/Intoxbr.def
3. Chang A, Schnall AH, Law R. Cleaning and Disinfectant Chemical Exposures and Temporal Associations with COVID-19 — National Poison Data System, United States, January 1, 2020–March 31, 2020. *MMWR Morb Mortal Wkly Rep* 2020;69:496–498.
4. Domingos SM *et al*. Internações por intoxicação de crianças de zero a 14 anos em hospital de ensino no Sul do Brasil, 2006-2011. *Epidemiol. Serv. Saúde.* 2016; 25(2):343-50.
5. Gonçalves PF, Sousa MTC, Souza JM, Carvalho PMG. Intoxicações domésticas. *Anais do IV Pesquisar*. out. 2015;4(1):1-3.
6. Lourenço J, Furtado BMA, Bonfim C. Exogenic poisoning in children assisted in a pediatric emergency unit. *Acta paul. enferm.* 2008; 21(2): 282-86.
7. Martins CBG, Andrade SM, Paiva PAB. Envenenamentos acidentais entre menores de 15 anos em município da Região Sul do Brasil. *Cad saúde pública*. 2006; 22(2):407-14
8. Mata JS, Rodrigues VR. Intoxicação exógena em uma cidade do oeste baiano. *Anais do 17º Congresso de Iniciação Científica da FASB*. 2019; 14(1):1-5.
9. Presgrave RF, Camacho LAB, Villas Boas MHS. A profile of unintentional poisoning caused by household cleaning products, disinfectants, and pesticides. *Cad. Saúde Pública.* 2008; 24 (12): 2901-08
10. Salomon FC, Ribeiro E, Silva FT. Intoxicações por desinfetantes e produtos de limpeza usados na higienização geral contra COVID-19. *Brasília: Fiocruz Brasília,* 2021. Disponível em <https://www.arca.fiocruz.br/handle/icict/46056>Acesso em 26 de janeiro de 2022.
11. Secretaria Estadual de Goiás. Cruz ER. Saúde alerta para risco de intoxicações e acidentes domésticos. 2020. Disponível em. <https://www.saude.go.gov.br/noticias/11039-ses-alerta-para-risco-de-intoxicacoes-e-acidentes-domesticos> Acesso em 26 de janeiro de 2022.
12. Silva MF, Fontinele DRS, Oliveira AVS; Bezerra MR; Rocha SS. Determining factors of domestic accidents in early childhood**.** *J. Hum. Growth* Dez.2017; 27(1):10-18.
13. Vilaça L, Volpea FM, Ladeira RM. Intoxicações exógenas acidentais em crianças e adolescentes atendidos em um serviço de toxicologia de referência de um hospital de emergência brasileiro. *Rev Paul Pediatr.* 2020;38:e2018096.
14. Werneck GL, Hasselmann MH. Intoxicações exógenas em crianças menores de seis anos atendidas em hospitais da região metropolitana do Rio de Janeiro-RJ. *R Rev Assoc Med Bras*. 2009; 55(3): 302-7.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

POISONING BY HOUSEHOLD CHEMICALS IN CHILDREN

Renan Lopes Fernandes
University of Vassouras - Brazil

Cristina Fidalgo Affonso Pinheiro
University of Vassouras - Brazil

Maria Cristina Almeida de Souza
University of Vassouras - Brazil

February/2022

INTRODUCTION

SBJChem Conference 2021

- Poisoning is a set of toxic signs and symptoms produced by the accidental or non-ingestive ingestion of chemical substances (GONÇALVES et al., 2015).
- Children are the main victims of poisoning (PRESGRAVE et al., 2008).
- The most frequent intoxications in children that occur in Brazil are caused by drugs and household products (BRASIL, 2022).
- It is recommended that you keep all toxic products away from children's field of vision, in addition to storing them in high places, in order to reduce children's contact with these toxic agents (SILVA et al., 2017).

OBJETIVE

SBJChem Conference 2021

- The objective of the present study was to carry out a literature review on exogenous intoxications caused mainly by accidents involving chemical products for domestic use in children in Brazil.

METHODOLOGY

SBJChem Conference 2021

- The following platforms were used for the study:

✓ SciELO and Google Scholar with the descriptors “intoxication” and “children”.
✓ Institutional repository-Arca of the Institute for Communication and Scientific and Technological Information in Health (Icict/Fiocruz), with the descriptors “intoxicação” and “produtos de limpeza”.
✓ Department of Informatics of the SUS -DATASUS, referring to notifications for exogenous intoxications in the period 2017-2021.
✓ Secretary of State for Health of the Government of Goiás regarding the risk of poisoning and domestic accidents.

- Articles in English and Portuguese, published between 2006 and 2020 and which had full and free availability.
- After reading the articles and using the criteria, a total of 14 references were found for this literature review.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Werneck et al. (2009)

There were 1574 cases of poisoning involving children up to five years old. Of these poisonings, about 40% were caused by household chemicals, 35% by drugs and 15% by some pesticide.

Vilança et al. (2020)

Of the chemical products, sodium hypochlorite (chlorine and bleach) and sodium hydroxide (caustic soda) were the main causes of intoxication.

Toxicological Information and Assistance Center (Ciatox)

Poisoning records in Brazil increased by up to 23% from January to April 2021 compared to the same period in 2019

Martins et al. (2006)

- Installation of security seals
- Storage of chemicals in high places
- Keeping products in their original packaging

RESULTS AND DISCUSSION

SBJChem Conference 2021

Table 1 . Exogenous intoxications occurred in the age group of 0-14 years in the period 2017-2021 in Brazil.

	NOTIFIED CASES	%
TOTAL	128794	100%
HOUSEHOLD USE PRODUCTS	18733	14,54%

Reference: Department of Informatics of SUS – DATASUS- **Exogenous Poisoning - Notifications registered on Sinan Net between 2017 and 2021**.

CONCLUSIONS

SBJChem Conference 2021

- The rate of exogenous poisoning by household chemicals is high in children.
- With the COVID-19 pandemic, there was a greater consumption of chemical products for domestic use and, consequently, an increase in the number of poisonings by these household cleaning products in children.
- Actions to prevent the occurrence of these accidents must be carried out in order to reduce the rate of intoxication by these toxic agents.

REFERENCES

SBJChem Conference 2021

1. Blank D, Waksman, RD. A importância das injúrias por acidentes domésticos em tempos de COVID-19. *Residência Pediátrica*. 2020;10(2):99-102.
2. Brasil. Ministério da Saúde. Departamento de Informática do SUS. TabNet Win32 3.0: Intoxicação Exógena - Notificações registradas no Sinan Net – Brasil [internet]. 2017-2021 [acesso em 2022 janeiro 26]. Disponível em: http://tabnet.datasus.gov.br/cgi/deftohtm.exe?sinannet/cnv/Intoxbr.def
3. Chang A, Schnall AH, Law R, et al. Cleaning and Disinfectant Chemical Exposures and Temporal Associations with COVID-19 — National Poison Data System, United States, January 1, 2020–March 31, 2020. *MMWR Morb Mortal Wkly Rep* 2020;69:496–498.
4. Domingos SM et al. Internações por intoxicação de crianças de zero a 14 anos em hospital de ensino no Sul do Brasil, 2006-2011. *Epidemiol. Serv. Saúde.* 2016; 25(2):343-50.
5. Gonçalves PF, Sousa MTC, Souza JM, Carvalho PMG. Intoxicações domésticas. *Anais do IV Pesquisar*. out. 2015;4(1):1-3.
6. Lourenço J, Furtado BMA, Bonfim C. Exogenic poisoning in children assisted in a pediatric emergency unit. *Acta paul. enferm.* 2008; 21(2): 282-86.
7. Martins CBG, Andrade SM, Paiva PAB. Envenenamentos acidentais entre menores de 15 anos em município da Região Sul do Brasil. *Cad saúde pública*. 2006; 22(2):407-14
8. Mata JS, Rodrigues VR. Intoxicação exógena em uma cidade do oeste baiano. *Anais do 17º Congresso de Iniciação Científica da FASB*. 2019; 14(1):1-5.

REFERENCES

SBJChem Conference 2021

9. Presgrave RF, Camacho LAB, Villas Boas MHS. A profile of unintentional poisoning caused by household cleaning products, disinfectants and pesticides. *Cad. Saúde Pública.* 2008; 24 (12): 2901-08
10. Salomon FC, Ribeiro E, Silva FT. Intoxicações por desinfetantes e produtos de limpeza usados na higienização geral contra COVID-19. *Brasília: Fiocruz Brasília,* 2021. Disponível em <https://www.arca.fiocruz.br/handle/icict/46056>Acesso em 26 de janeiro de 2022.
11. Secretaria Estadual de Goiás. Cruz ER. Saúde alerta para risco de intoxicações e acidentes domésticos. 2020. Disponível em. <https://www.saude.go.gov.br/noticias/11039-ses-alerta-para-risco-de-intoxicacoes-e-acidentes-domesticos> Acesso em 26 de janeiro de 2022.
12. Silva MF, Fontinele DRS, Oliveira AVS; Bezerra MR; Rocha SS. Determining factors of domestic accidents in early childhood**.** *J. Hum. Growth* Dez.2017; 27(1):10-18.
13. Vilaça L, Volpea FM, Ladeira RM. Intoxicações exógenas acidentais em crianças e adolescentes atendidos em um serviço de toxicologia de referência de um hospital de emergência brasileiro. *Rev Paul Pediatr.* 2020;38:e2018096.
14. Werneck GL, Hasselmann MH. Intoxicações exógenas em crianças menores de seis anos atendidas em hospitais da região metropolitana do Rio de Janeiro-RJ. *R Rev Assoc Med Bras*. 2009; 55(3): 302-7.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

PREVENTION OF CANDIDIASIS IN PATIENTS USING REMOVABLE DENTURES

SEVBITOV, Andrey[1]; DOROFEEV, Aleksey[1]; MIRONOV, Sergey[1]; AL-KHOURY, Samer[2]; TIMOSHIN, Anton[1]

[1] I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

[2] Dental clinic "Good Crocodile". Russia.

** Correspondence author*
e-mail: avsevbitov@mail.ru

Received 11 September 2021; received in revised form 15 November 2021; accepted 27 November 2021

ABSTRACT

Despite innovations in orthopedic dentistry, removable dentures belong to the most popular orthopedic care category. Removable dentures are combined stimuli that affect the mucous membrane and neuro-receptor apparatus. Acrylic plastic prostheses, widely used in prosthetic dentistry, have a negative side mechanical, chemical-toxic, sensitizing, and thermal insulating effect on oral tissue and prosthetic impression area. This is often complicated by a violation of the biocenosis of the oral cavity, the growth of pathogenic microflora that releases toxins, especially an increase in the number of yeast colonies that irritate the oral mucosa and prosthetic stomatitis. It was observed 100 patients with oral candidiasis of various age groups from 45 to 65 years. Of these, 60 patients with removable plate prostheses; 40 patients with partially removable prostheses. Chronic forms of candidiasis were diagnosed in 40 patients and with exacerbation of chronic forms of candidiasis in 60 people. The number of untreated carious cavities and poor hygienic condition of the oral cavity directly affects the severity of candidiasis. Acute forms of candidiasis were observed mainly in patients with high DMF and PMA indices. The severity of candidiasis depends on the degree and duration of wearing dentures and hygienic conditions - the most severe forms of invasive candidiasis were observed in the presence of removable plate prostheses, the complete absence of teeth, and the use of a prosthesis for more than 10-15 years. A combined lesion of the oral mucosa and the red border of the lips was observed mainly in patients older than 60 years. The presence of candidiasis in the oral cavity in patients with removable plate prostheses leads to a statistically significant change in the indicators of local immunity of the oral cavity: an increase in the concentration of serum IgG and IgA and the values of the coefficient of the balance of local immunity factors.

Keywords: *Candidiasis, prosthesis, inflammation, prosthetic dentistry, biochemistry.*

1. INTRODUCTION

Despite innovations in orthopedic dentistry, the manufacture of removable dentures belongs to the category of the most popular types of orthopedic care. Removable dentures are combined stimuli that affect the mucous membrane and neuro-receptor apparatus. It is known that in 52% of cases, dentures are not fixed when chewing. Moreover, in 65% of patients using dentures, various diseases of the prosthetic impression area mucous membrane and pathological processes in supporting tissues develop (Sevbitov *et al*., 2019; 2020).

According to the WHO (2020), one-fifth of the world's population suffers or has at least once suffered various forms of candidiasis (Sevbitov, Ershov, *et al*., 2020). The worldwide increase in the incidence of the disease is primarily related to the fact that this infection is opportunistic, more than half of the world's population is a carrier of fungi of this kind, i.e., in most cases, it is an endogenous infection, which makes candidiasis different from other opportunistic mycoses (Enina *et al*., 2019; Turgaeva *et al*., 2020).

2. MATERIALS AND METHODS

2.1 Materials

It was observed 100 patients with oral

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.04_abstract_SEVBITOV.pdf

candidiasis of various age groups from 45 to 65 years. Of these, 60 patients with removable plate prostheses; 40 patients with partially removable prostheses. Chronic forms of candidiasis were diagnosed in 40 patients and with exacerbation of chronic forms of candidiasis-60 people.

2.2 Methods

At the stage of clinical examination, all patients had their life history and diseases analyzed by examining the oral cavity of the patients. To identify carious cavities, general (examination, probing) and additional (X-ray, radiology) methods were used, and the localization of carious cavities, fillings, and extracted teeth was recorded. We paid attention to the nature of the existing injuries during a visual examination of the oral mucosa. To indicate changes in the mucous membrane color, moisture content, the severity of the vascular pattern, the presence of pathological elements, including primary and secondary, signs of keratinization, and inflammation. The intensity of dental caries damage was determined by calculating the DMF indices. The hygienic condition of the oral cavity was assessed by the Green-Vermillion index (1964). The prevalence of gum inflammation was determined using the PMA index in the Parma modification (1976), which is indicated in% and bleeding according to the Muleman method (1971).

The diagnosis of oral mucosal candidiasis is detected and confirmed based on clinical and laboratory signs.

The criterion for diagnosing oral candidiasis was the detection of 10–15 or more yeast cells insight.

2.2.1 Laboratory research

All patients with oral candidiasis underwent the following laboratory tests:

Microscopy of the direst smear from the mucous membrane of the oral cavity to confirm the diagnosis of oral candidiasis. Yeast cells of a round or oval shape with characteristic daughter budding cells, as well as the accumulation of long filaments of the *pseudomycelium*, allow making a preliminary diagnosis (Araviyski R.A., Gorshkova G.A., 1995).

Cultural diagnostics of scraping from the affected areas of the oral mucosa to identify the pathogen and determine the sensitivity to antifungal preparations were carried out on the micro panel "Fungi test", USA. The serial microdilution method investigated yeast sensitivity to amphotericin B, ketoconazole, itraconazole, and fluconazole, nystatin clotrimazole in two concentrations (maximum and minimum), which allowed us to differentiate the fungi according to their sensitivity.

Assessment of parameters of local immunity of the oral cavity - secretory immunoglobulins (A, G).

3. RESULTS AND DISCUSSION

3.1 Results

The diagnosis of chronic atrophic candidiasis was made in 26 patients (26 %). Exacerbation of chronic atrophic candidiasis was diagnosed in 43 patients (43 %). The diagnosis of chronic hyperplastic candidiasis of the oral cavity was made to 13 (13 %) patients; 17 (13.3 %) patients who applied were diagnosed with exacerbation of chronic hyperplastic candidiasis. Pseudomembranous candidiasis of the oral cavity was diagnosed in 1 (1 %) patients.

The severity of candidiasis depends on the degree and duration of wearing dentures and hygienic conditions - the most severe forms of invasive candidiasis were observed in the presence of removable plate prostheses, the complete absence of teeth, and the use of a prosthesis for more than 10-15 years.

It should be noted that the combined lesion of the oral mucosa and the red border of the lips was observed mainly in patients older than 60 years.

The number of untreated carious cavities and poor hygienic condition of the oral cavity directly affects the severity of candidiasis. Acute forms of candidiasis were observed mainly in patients with high DMF and PMA indices.

As a result of the conducted enzyme immunoassay of the blood of patients with chronic forms of candidiasis, 80.5 % of patients have an increased content of immunoglobulins G in the blood serum, 9.4 % - a reduced content of immunoglobulins G, 7.7 % - a negative value of immunoglobulins G, 11.2 % - the content of immunoglobulins corresponded to normal values. In the examined patients with exacerbations of chronic forms of candidiasis, the results were obtained: 13.8 % - a reduced content of immunoglobulins G in the blood serum, 84.2 % - an increased content of immunoglobulins G, 8.6 % - the content of immunoglobulins corresponded to normal values. Most of the treated patients diagnosed with chronic oral candidiasis have an increased content of immunoglobulin G.

3.2 Discussions

All patients with various forms of candidiasis of the oral mucosa are recommended to carry out the following treatment and follow the recommendations.

It is necessary to correct the pathological processes of the mucous membrane of the prosthetic impression area in the shortest possible time, detected at various stages of orthopedic treatment by applying physiotherapeutic methods (laser therapy, ozone therapy).

To accelerate the regeneration of prosthetic impression area tissues, the use of antioxidant and epithelial agents (TYCVEOLUM, thymol mixture with milk thistle oil, wikasol) is recommended; with long-term non-healing lesions, the use of plasma therapy (plasma lifting), immune correction (galavit, gepon) are recommended.

To stimulate the adaptation processes of prosthetic impression area tissues, it is necessary to consider the patient's general self-health and emotional attitude in complex dental treatment so that visits to the dentist are not perceived by stress, "hellish pain," or aversion.

Oral hygiene using soda rinses and toothpaste containing bicarbonate (blend-a-honey bicarbonate) or active oxygen (oxidizing).

The hygienic condition of removable laminar dentures is achieved by daily cleaning the denture with a gel paste and using tablets for cleaning. For a professional cleaning of removable denturesshould use a special device in the clinic of the type "Microcline" (if necessary, every two weeks).

Diets with limited intake of flour products from white flour, starchy foods, sweets, and fizzy drinks.

4. CONCLUSIONS:

1. Removable plate prostheses have a negative effect on the oral mucosa, cause a decrease in its protective properties, which contributes to an increase in the intensity of candidiasis: 60% of patients with removable plate prostheses in the oral cavity had the maximum intensity of candidiasis.

2. The presence of candidiasis in the oral cavity in patients with removable plate prostheses leads to a statistically significant change in the indicators of local immunity of the oral cavity: an increase in the concentration of serum IgG and IgA and the values of the coefficient of the balance of local immunity factors.

3. The quality of orthopedic treatment of patients with partial and complete edentulous and quality of removable dentures depends on many factors, as follows: tissue conditions of the prosthetic impression area;- level of health (psycho-emotional disorders, pathology of internal organs and systems);- design features of a removable denture;- materials used;- side effects of the prosthesis on the tissue of the prosthetic impression area;- oral hygiene of the patient and dentures;- aesthetic effect.

5. ACKNOWLEDGMENTS

This work was completed at Sechenov University and supported by the “Russian Strategic Academic Leadership Program”.

6. REFERENCES

1. Evstratenko, V., Sevbitov, A., Platonova, V., Selifanova, E., Dorofeev, A. The characteristics of crystallization of mixed saliva in patients using heroin and methadone. *Klin. Lab. Diagn*, **2018**, *63(4)*, 223.
2. Mazzeo, M., Linares, J., López, M. Analysis of saliva samples from oncological patients treated with 5-fluorouracil and leucovorin calcium by scanning electron microscopy with energy dispersive system. *J. Oral Pathol. Med*, **2013**, *42(10)*, 788.
3. Silva, P., Santos, B., Soares, G. Anti-Candida albicans activity of the association of citronelal with anfotericin B or with cetoconazole. *Periodico Tche Química*, **2019**, *16(31)*, 223.
4. Dukić, W., Dobrijević, T., Katunarić, M. Caries prevalence in chronic alcoholics and the relationship to salivary flow rate and pH. *Cent. Eur. J. Public Health*, **2013**, *21(1)*, 43.
5. Vehkalahti, M., Nikula-Sarakorpi, E., Paunio, I. Evaluation of salivary tests and dental status in the prediction of caries increment in caries-susceptible teenagers. *Caries Res*, **1996**, *30(1)*, 22.
6. Girardin, F., Hearmon, N., Negro, F. Increasing hepatitis C virus screening in people who inject drugs in Switzerland using rapid antibody saliva and dried blood spot testing: A cost-effectiveness analysis. *J. Viral Hepat*, **2019**, *26(2)*, 236.
7. Kolodkina, V., Arutyunov, A., Sirak, S., Andriutsa, N., Tsymbalov, O. Cytological characteristics of oral cavity tissues of experimental animals when using photo

polymeric material. *Med. News North Cauc,* **2018**, *13(4)*, 637.
8. Gozha, L., Talalai, T., Arunov, T. Functional disorders of saliva in toxic-chemical stomatitis caused by metal prostheses. Dentistry for all, **2010**, 3, 53.
9. Zholudev, S., Zhmakin, I. Treatment and prevention of prosthetic stomatitis in persons older than 55 years, that use removable plate prostheses. *Dentist*, **2004**, *9*, 21.
10. Zholudev, S. Ways to improve the adaptation in people with problems of tolerability of removable denture materials. *Maes. Dent*, **2005**, *19*, 5.
11. Kasatkina, E. Iodine deficiency diseases in children and adolescents. *Eligible Doctor*, **2010**, *10*, 14.
12. Kalyvradzhiyan, E., Podoprigora, A., Komarova, Yu. Clinical and experimental substantiation of the use of modified adhesive composition based on polysaccharides to improve the period of adaptation to removable denture plate prosthesis. *Modern Orthop. Dentistry*, **2010**, *13*, 31.
13. Lepilin, A., Rubin, V., Proshin, N. The effect of removable plate prostheses made of acrylic plastics on the structural and functional properties of the cellular membranes of the oral mucosa. Stomatology, **2003**, *1*, 51.
14. Nartikova, V., Oglobina, O. Modern methods in biochemistry, M. **1977**.
15. Paschina, T., Egorova, G. Modern methods in biochemistry, M. **1968**.
16. Kuznetsova, M., Nevdakh, A., Platonova, V., Sevbitov, A., Dorofeev, A. Evaluation of effectiveness of a preparation on the basis of phytoecdysteroids for treatment of traumatic injuries of oral mucosa in orthodontic patients. *Int. J. Green Pharm*, **2018**, *12(S1)*, 297.
17. Mamedov, A., Morozova, N., Yumashev, A., Dybov, A., Nikolenko, D. Criteria for provisional restorations used in preparation for comprehensive orthodontic and orthopedic rehabilitation. *Periodico Tche Quimica*, **2019**, *16(32)*, 647.
18. Yumashev, A., Semenycheva, I., Rakhadilov, B. Development of biocompatible coatings for dental implants based on transition metal nitrides. *J. Global Pharma Technol*, **2019**, *11(5)*, 22.
19. Yumashev, A., Koneva, E., Borodina, M. Electronic apps in assessing risk and monitoring of patients with arterial hypertension. *Prensa Medica Argentina*, **2019**, *105(4)*, 235.
20. Saxena, N., Habelitz, S., Marshall, G. Remineralization of demineralized dentin using a dual analog system. *Orthodon. Craniofac. Res*, **2019**, *22(S1)*, 76.
21. Rech-Ortega, C., Fernández-Estevan, L., Solá-Ruíz, M. Comparative in vitro study of the accuracy of impression techniques for dental implants: Direct technique with an elastomeric impression material versus intraoral scanner. *Med. Oral Patol. Oral Cir. Bucal*, **2019**, *24(1)*, 89.
22. Utyuzh, A., Nikolenko, D., Yumashev, A., Volchkova, I., Samusenkov, V. Adhesion of periodontal pathogens to materials used for long-term temporary crowns. *Periodico Tche Quimica*, **2019**, *16(33)*, 60.
23. Sevbitov, A., Kuznetsova, M., Dorofeev, A., Borisov, V., Mironov, S., Iusupova, I. Dental anomalies in people living in radionuclide-contaminated regions. *J. Environ. Radioact*, **2020**, *216*, 106190.
24. Sevbitov, A., Dorofeev, A., Kuznetsova, M., Timoshin, A., Ershov, K. Comparative characteristics of the crystallogram of the oral fluid in patients who use heroin and methadone. *Periodico Tche Quimica*, **2019**, *16(33)*, 94.
25. Sevbitov, A., Timoshin, A., Dorofeev, A., Davidyants, A., Ershov, K., Kuznetsova, M. Comparative characteristics of the state of hard dental tissues in drug-dependent patients who use heroin, and methadone as replacement therapy. *Periodico Tche Quimica*, **2020**, *17(34)*, 135.
26. Turgaeva, A., Kashirskaya, L., Zurnadzhyants, Yu., Latysheva, O., Pustokhina, I., Sevbitov, A. Assessment of the financial security of insurance companies in the organization of internal control. *Ent. Sust Issues*, **2020**, *7(3)*, 2243.
27. Sevbitov, A. Dental characteristics of clinical manifestations of delayed effects of radiation exposure. Abstract of the dissertation for the degree of doctor of medicine. *Central research Institute of dentistry of the Ministry of health of the Russian Federation*. Moscow, **2005**.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY 2021 VIRTUAL CONFERENCE

PREVENTION OF CANDIDIASIS IN PATIENTS USING REMOVABLE DENTURES

SEVBITOV, Andrey
I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

DOROFEEV, Aleksey
I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

MIRONOV, Sergey
I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

AL-KHOURY, Samer
Dental clinic "Good Crocodile". Russia.

TIMOSHIN, Anton
I.M. Sechenov First Moscow State Medical University (Sechenov University). Russia.

March/2022

BACKGROUND

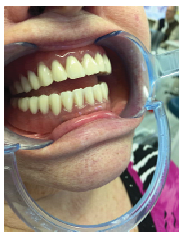
SBJChem Conference 2021

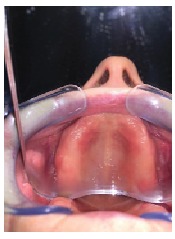
- Despite innovations in orthopedic dentistry, the manufacture of removable dentures belongs to the most popular orthopedic care category. Removable dentures are combined stimuli that affect the mucous membrane and neuro-receptor apparatus. Acrylic plastic prostheses, widely used in prosthetic dentistry, have a negative side mechanical, chemical-toxic, sensitizing, and thermal insulating effect on oral tissue and prosthetic impression area. This is often complicated by a violation of the biocenosis of the oral cavity, the growth of pathogenic microflora that releases toxins, especially an increase in the number of yeast colonies that irritate the oral mucosa and prosthetic stomatitis. ;
- **Methods:** It was observed 100 patients with oral candidiasis of various age groups from 45 to 65 years. Of these, 60 patients with removable plate prostheses; 40 patients with partially removable prostheses;

BACKGROUND

SBJChem Conference 2021

- ***Figure 1.*** *Patient with removable dentures*





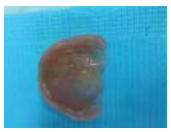


Figure 3. *Removable upper jaw plate prosthesis*

- ***Figure 2.*** *Lesion of the hard palate mucosa during adaptation to removable prostheses*

METHODOLOGY

SBJChem Conference 2021

It was observed 100 patients with oral candidiasis of various age groups from 45 to 65 years. Of these, 60 patients with removable plate prostheses; 40 patients with partially removable prostheses. Chronic forms of candidiasis were diagnosed in 40 patients and with exacerbation of chronic forms of candidiasis-60 people.

At the stage of clinical examination, all patients had their life history and diseases analyzed by examining the patients oral cavity. To identify carious cavities, general (examination, probing) and additional (X-ray, radiology) methods were used and the localization of carious cavities, fillings and extracted teeth was recorded. We paid attention to the nature of the existing injuries during a visual examination of the oral mucosa. To indicate changes in the color of the mucous membrane, moisture content, the severity of the vascular pattern, the presence of pathological elements, including primary and secondary, signs of keratinization and inflammation. The intensity of dental caries damage was determined by calculating the DMF indices. The hygienic condition of the oral cavity was assessed by the Green-Vermillion index (1964). The prevalence of gum inflammation was determined using the PMA index in the Parma modification (1976), which is indicated in%, and bleeding according to the Muleman method (1971).

The diagnosis of oral mucosal candidiasis is detected and confirmed based on clinical and laboratory signs.

The criterion for the diagnosis of oral candidiasis was the detection of 10–15 or more yeast cells insight.

METHODOLOGY

SBJChem Conference 2021

All patients with oral candidiasis underwent the following laboratory tests:
Microscopy of the direst smear from the mucous membrane of the oral cavity in order to confirm the diagnosis of oral candidiasis. Yeast cells of a round or oval shape with characteristic daughter budding cells, as well as the accumulation of long filaments of the pseudomycelium, allow making a preliminary diagnosis (Araviyski R.A., Gorshkova G.A., 1995).
Cultural diagnostics of scraping from the affected areas of the oral mucosa to identify the pathogen and determine the sensitivity to antifungal preparations were carried out on the micro panel "Fungi test", USA. The serial microdilution method investigated yeast sensitivity to amphotericin B, ketoconazole, itraconazole, and fluconazole, nystatin clotrimazole in two concentrations (maximum and minimum), which allowed us to differentiate the fungi according to their sensitivity.
Assessment of parameters of local immunity of the oral cavity - secretory immunoglobulins (A, G).

RESULTS AND DISCUSSION

SBJChem Conference 2021

The diagnosis of chronic atrophic candidiasis was made in 26 patients (26 %). Exacerbation of chronic atrophic candidiasis was diagnosed in 43 patients (43 %). The diagnosis of chronic hyperplastic candidiasis of the oral cavity was made to 13 (13 %) patients; 17 (13.3 %) patients who applied were diagnosed with exacerbation of chronic hyperplastic candidiasis. Pseudomembranous candidiasis of the oral cavity was diagnosed in 1 (1 %) patients.
The severity of candidiasis depends on the degree and duration of wearing dentures and hygienic conditions - the most severe forms of invasive candidiasis were observed in the presence of removable plate prostheses, complete absence of teeth and the use of a prosthesis for more than 10-15 years.
It should be noted that the combined lesion of the oral mucosa and the red border of the lips was observed mainly in patients older than 60 years.
The number of untreated carious cavities and poor hygienic condition of the oral cavity directly affects the severity of candidiasis. Acute forms of candidiasis were observed mainly in patients with high DMF and PMA indices.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Figure 4. *Acute pseudomembranous candidiasis*

Figure 9. *Candida angular cheilitis*

Figure 5. *Acute atrophic candidiasis*

RESULTS AND DISCUSSION

SBJChem Conference 2021

As a result of the conducted enzyme immunoassay of the blood of patients with chronic forms of candidiasis, 80.5 % of patients have an increased content of immunoglobulins G in the blood serum, 9.4 % - a reduced content of immunoglobulins G, 7.7 % - a negative value of immunoglobulins G, 11.2 % - the content of immunoglobulins corresponded to normal values. In the examined patients with exacerbations of chronic forms of candidiasis, the results were obtained: 13.8 % - a reduced content of immunoglobulins G in the blood serum, 84.2 % - an increased content of immunoglobulins G, 8.6 % - the content of immunoglobulins corresponded to normal values. Most of the treated patients with a diagnosis of chronic oral candidiasis have an increased content of immunoglobulin G.

RESULTS AND DISCUSSION

SBJChem Conference 2021

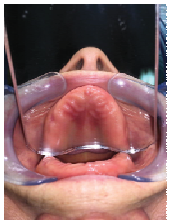


Figure 7. *Chronic hyperplastic candidiasis*

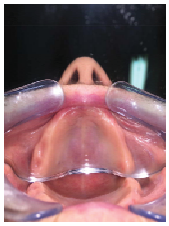


Figure 8. *Chronic atrophic candidiasis*

Figure 10. *Patient N, 62 years old, Candidomycosis of the oral mucosa*

RESULTS AND DISCUSSION

SBJChem Conference 2021

All patients with various forms of candidiasis of the oral mucosa are recommended to carry out the following treatment and follow the recommendations.

It is necessary to correct the pathological processes of the mucous membrane of the prosthetic impression area in the shortest possible time, detected at various stages of orthopedic treatment by applying physiotherapeutic methods (laser therapy, ozone therapy).

To accelerate the regeneration of prosthetic impression area tissues, the use of antioxidant and epithelial agents (TYCVEOLUM, thymol mixture with milk thistle oil, wikasol) is recommended; with long-term non-healing lesions, the use of plasma therapy (plasma lifting), immune correction (galavit, gepon) are recommended.

To stimulate the adaptation processes of prosthetic impression area tissues, it is necessary to consider the patient's general self-health and emotional attitude in complex dental treatment so that visits to the dentist are not perceived by stress, "hellish pain," or aversion.

Oral hygiene using soda rinses and toothpaste containing bicarbonate (blend-a-honey bicarbonate) or active oxygen (oxidizing).

The hygienic condition of removable laminar dentures is achieved by daily cleaning the denture with a gel paste and using tablets for cleaning. For a professional cleaning of removable denturesshould use a special device in the clinic of the type "Microcline" (if necessary, every two weeks).

Diets with limited intake of flour products from white flour, starchy foods, sweets, and fizzy drinks.

CONCLUSIONS

SBJChem Conference 2021

1. Removable plate prostheses have a negative effect on the oral mucosa, cause a decrease in its protective properties, which contributes to an increase in the intensity of candidiasis: 60% of patients with removable plate prostheses in the oral cavity had the maximum intensity of candidiasis.
2. The presence of candidiasis in the oral cavity in patients with removable plate prostheses leads to a statistically significant change in the indicators of local immunity of the oral cavity: an increase in the concentration of serum IgG and IgA and the values of the coefficient of balance of local immunity factors.
3. The quality of orthopedic treatment of patients with partial and complete edentulous and quality of removable dentures depends on many factors, as follows: tissue conditions of the prosthetic impression area;- level of health (psycho-emotional disorders, pathology of internal organs and systems);- design features of a removable denture;- materials used;- side effects of the prosthesis on the tissue of the prosthetic impression area;- oral hygiene of the patient and dentures;- aesthetic effect.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

This work was completed at Sechenov University and supported by the “Russian Strategic Academic Leadership Program”.

REFERENCES

SBJChem Conference 2021

1. Evstratenko, V., Sevbitov, A., Platonova, V., Selifanova, E., Dorofeev, A. The characteristics of crystallization of mixed saliva in patients using heroin and methadone. Klin. Lab. Diagn, 2018, 63(4), 223.
2. Mazzeo, M., Linares, J., López, M. Analysis of saliva samples from oncological patients treated with 5-fluorouracil and leucovorin calcium by scanning electron microscopy with energy dispersive system. J. Oral Pathol. Med, 2013, 42(10), 788.
3. Silva, P., Santos, B., Soares, G. Anti-Candida albicans activity of the association of citronelal with anfotericin B or with cetoconazole. Periodico Tche Química, 2019, 16(31), 223.
4. Dukić, W., Dobrijević, T., Katunarić, M. Caries prevalence in chronic alcoholics and the relationship to salivary flow rate and pH. Cent. Eur. J. Public Health, 2013, 21(1), 43.
5. Vehkalahti, M., Nikula-Sarakorpi, E., Paunio, I. Evaluation of salivary tests and dental status in the prediction of caries increment in caries-susceptible teenagers. Caries Res, 1996, 30(1), 22.
6. Girardin, F., Hearmon, N., Negro, F. Increasing hepatitis C virus screening in people who inject drugs in Switzerland using rapid antibody saliva and dried blood spot testing: A cost-effectiveness analysis. J. Viral Hepat, 2019, 26(2), 236.
7. Kolodkina, V., Arutyunov, A., Sirak, S., Andriutsa, N., Tsymbalov, O. Cytological characteristics of oral cavity tissues of experimental animals when using photo polymeric material. Med. News North Cauc, 2018, 13(4), 637.
8. Gozha, L., Talalai, T., Arunov, T. Functional disorders of saliva in toxic-chemical stomatitis caused by metal prostheses. Dentistry for all, 2010, 3, 53.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

PRL-R ISOFORMS LONG / SHORT RATIO IS INCREASED IN SYSTEMIC LUPUS ERYTHEMATOSUS BLOOD MONONUCLEAR CELLS

MORENO-SOSA María Tamara[1]; GARCIA Daiana Sthefania[1]; HEREDIA Rocío[1]; BITTAR-RIVERO-PEDROSA, Victor[2]; MACKERN-OBERTI, Juan Pablo[1,*].

[1] IMBECU-UNCuyo, Mendoza Argentina
[2] Hospital Central Mendoza, Argentina

** Correspondence author*
e-mail: jpmackern@mendoza-conicet.gob.ar

Received 13 October 2021; received in revised form 26 January 2022; accepted 18 February 2022

ABSTRACT

Prolactin (PRL) displays several functions in the whole body by binding its receptor (PRL-R). Two main PRL-R isoforms are reported that differ in their capacity to trigger signaling pathways, PRL-R long isoform is the activation receptor, and the short isoform is the inhibitory oner. Although many autoimmune diseases display hyperprolactinemia, the role of each PRL-R isoform expression in autoimmunity remains unknown. This work aimed to correlate PRL-R isoforms expression in human peripheral blood mononuclear cells (PBMCs) of female Systemic Lupus Erythematosus patients and healthy controls. To this end, PBMCs from lupus patients (n=9) and healthy controls (n=5) were enriched by the ficoll-hypaque method. Then, RNA extraction, cDNA synthesis, and real-time PCR were performed to determine mRNA expression. We found that PRL-R long and short isoforms expression from lupus patients display similar expression to healthy controls. However, the PRL-RL/PRL-RS ratio is higher than healthy controls (P-value two-tailed <0,05). Additionally, PRL-RL isoform expression correlates with the short isoform in lupus patients (Spearman r 0,8945; 95% confidence interval 0,6834 to 0,9676; P-value two-tailed <0,0001). However, the expression of neither long and short isoforms correlates with active disease nor disease duration. Similarly, lupus patients display similar PRL-R isoforms expression than healthy controls. Although much work must be done, our data indicate that similar mechanisms may regulate the expression of both PRL-R isoforms in immune cells, and “their expression goes hand by hand”.

Keywords: *autoimmunity, prolactin, expression, lupus, receptor.*

1. INTRODUCTION

For many years, numerous advances have been reported concerning the pathogenic mechanisms of autoimmune diseases. However, specific and effective therapies for systemic autoimmune disorders such as Systemic Lupus Erythematosus (SLE) or Rheumatoid Arthritis (RA) have not yet been developed (Suurmond, Zou, Kim, and Diamond, 2015). The great heterogeneity surrounding all autoimmune diseases, such as their prognosis, diagnosis, treatment, and etiology, hinders the development of new therapies (Li *et al*., 2013). Despite numerous efforts focused on searching for more effective therapies for diseases systemic autoimmune systems, most of the current therapies are based on the administration of immunosuppressive drugs leading to a generalized suppression with severe complications (Houssiau and Ginzler, 2008). Due to this, it is crucial to identify pathogenic mechanisms in the development of autoimmunity in an individualized way, thus allowing the design of personalized immunosuppressive therapies. What to protect the competence of the immune system.

In recent years, much progress has been made in understanding the modulatory role of PRL on the immune system (Ben-Jonathan, LaPensee, and LaPensee, 2008). Studies indicate that in the thymus PRL would have a role in the differentiation of T lymphocytes promoting the survival of CD4-CD8- thymocytes and their differentiation to CD4 + CD8 + 15 thymocytes. In addition, PRL participates in the activation of T lymphocytes, mainly increasing their intensity 16, 17 and increasing the proliferative response of T lymphocytes against mitogens and the production

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.21_abstract_MACKERN.pdf

of IL-2 (Xu, Lin, Lin, Huang, and Lei, 2010). Additionally, PRL has antiapoptotic effects on B lymphocytes with increased production of antibodies(M. V. Legorreta-Haquet *et al*., 2016; Maria Victoria Legorreta-Haquet *et al*., 2013).

In the case of SLE, pre-clinical studies indicate that a hyperPRL would correlate with the degree of Lupus disease activity and with high autoantibody titers (Rezaieyazdi and Hesamifard, 2006).

The actions of PRL are mediated by its receptor, which is made up of an extracellular domain, a transmembrane domain, and a highly conserved intracellular signal transducer domain between species (Bole-Feysot, Goffin, Edery, Binart, and Kelly, 1998). The PRL-R gene contains different exons that can be spliced by alternative splicing. Generate various isoforms. These isoforms have an identical extracellular domain but differ in size and sequence from the intracellular portion, which can be short or long. The short isoform of PRL-R (PRL-RC) lacks the cytoplasmic domain and therefore does not have intracellular signaling. The long isoform of PRL-R (PRL-RL) is dimerized constitutively and, after binding a single molecule of the ligand (PRL), transmits a signal through associated cytoplasmic proteins. On the other hand, heterodimers of PRL-RL and PRL-RS1b are functionally inactive and cannot conduct signal transmission. In addition to the different isoforms bound to the membrane, we can find a soluble isoform of PRL-R (PRL-RS) composed of the extracellular portion (Dagil *et al*., 2012).

It could then be speculated that due to failures in the regulation of the expression of PRL-RS short isoform, which lacks signaling, it would lead to a lesser effect on the modulation of activation mediated by PRL and PRL-RL during the activation of T lymphocytes. Thus, in susceptible individuals, these failures in regulation could favor the initiation and progression of autoimmune pathologies. On the contrary, the pharmacological induction of PRL-RS could suppress exacerbated inflammatory responses, being a potential therapeutic strategy for autoimmune diseases. Therefore, the focus of this work was to evaluate the expression of PRL-R isoforms during autoimmunity. For this, we used PBMCs from lupus patients and healthy controls to evaluate mRNA expression of PRL-RL and PRL-RS. We show these both isoforms displayed similar expression in all samples, and only PRL-RL/PRL-RS ratio from lupus samples set out differences from healthy controls.

2. MATERIALS AND METHODS

2.1. Patients

Patients For the development of the specific objectives, individuals belonging to a control group and an SLE group were recruited according to the following inclusion specifications:

Control group: composed of 5 control patients. They will be healthy female patients. With ages between 20 and 65 years. No known diseases and who are not undergoing any pharmacological treatment. Pregnant, menopausal, or lactating women were excluded. SLE group comprises 9 patients with SLE, female, who attend the rheumatology service and are enrolled by doctors belonging to the Immunology Institute of the Central Hospital of Mendoza. Inclusion criteria for SLE group:

1. Over 18 years old and under 65 years old; 2. Patients who meet the revised criteria of the American College of Rheumatology for the diagnosis of Systemic Lupus Erythematosus and Rheumatoid Arthritis; 3. Patients who, in the judgment of the treating rheumatologist, have “clinically stable” disease that makes the need for steroid dose adjustment or any initiation of a new immunosuppressive treatment during the course of the study, or both, unlikely; 4. Onset of the disease at least 6 months before inclusion in the study; 5. Active disease with SLEDAI-2k >= 6; 6. Use of hydroxychloroquine stable dose for 3 months.7; Use of stable mycophenolate or azathioprine or methotrexate; 8. In the case of women of childbearing age, the use of contraception will be consulted. Exclusion Criteria for SLE group: 1. Concomitant diagnosis of another autoimmune disease, such as Multiple Sclerosis, Type 1 Diabetes Mellitus, Scleroderma, Juvenile Idiopathic Arthritis; 2. Concomitant diagnosis of any chronic disease such as, but not exclusively, Type 2 Diabetes Mellitus, Chronic Renal Failure, Liver Cirrhosis, Acquired Immune Deficiency Syndrome, solid tumors, and hematological neoplasms, Heart Failure, Chronic Airflow Limitation; 3. Pregnancy or pregnancy intention in the year of the study; 4. Manifestations of disease that, in the opinion of the investigators, are serious and make entry into the study inappropriate. Examples: central nervous system vasculitis, lupus psychosis, active lupus nephritis, thrombocytopenia < 50,000, Hb < 8 gr/dL Leukopenia < 3000, lymphopenia < 400; 5. Life-threatening manifestations of the disease; 6. Use of prednisone doses> 30 mg daily; 7. Use of biological therapy in the 6 months prior to the

baseline visit. Cyclosporine, chlorambucil, cyclophosphamide in the previous 6 months are excluded; 8. Serious infections (use of IV antibiotics, opportunistic, latent tuberculosis, herpes zoster) six months before the baseline visit; 9. Low normal plasma immunoglobulin levels; 10. Liver tests> 3 times normal. Abnormal EKG or abnormal chest X-ray; 11. Use of anticoagulant therapy or antiphospholipid syndrome associated with SLE; 12. Have received attenuated virus vaccines during the last year; 13. Have HIV, HBV, or HCV.

2.2. Bioethics and biosafety

The patients were communicated in a simple way about the study to ensure their correct understanding. They have been informed about the use of the study data and have signed an informed consent individually. The bioethics committee approves the protocols and the informed consent document developed in this project of the Faculty of Medical Sciences of UNCuyo and the teaching and research committee of the Hospital Central Mendoza. Likewise, all sample processing mechanisms are strictly supervised by biosafety protocols.

2.3. Samples

Peripheral blood mononuclear cells (PBMC) were separated by the conventional Ficoll-Hypaque method. First, 10 ml of blood was gently poured over 3 ml of Ficoll-Hypaque previously placed in a sterile 15 ml conical tube. Next, cells are carefully aspirated using sterile 3 ml Pasteur pipettes and placed in a new 15 ml tube.

2.4. Real-time PCR

RNA was obtained using the TRIZOL reagent (Invitrogen). Subsequently, 2 micrograms of total RNA were used to synthesize DNA copy using the enzyme MMLV reverse transcriptase and oligodT as specific primers for total mRNA (poly A) according to the reaction specifications of the merchant. Real-time PCR assays were performed to quantify the mRNA of the different PRL-R isoforms. Real-time PCR assays were performed on the Corbett 6000 equipment (Quiagen, Inc) using three technical replicas for each sample tested). The abundance of mRNA expression levels was performed by the 2 (-ΔΔCt) analysis used widely for a comparison of mRNA abundance between two groups using actin as a reference gene (or housekeeping gene). The sequences used were: human ACTIN Fw AAAGACCTGTACGCCAACAC and Rv GTCATACTCCTGCTTGCTGAT; PRL-RL Fw CCTTGTCCAGGTTCGCTGCAAA and Rv AGATGAGCATCAAATCCTTTTA; PRL-R1b (short) Fw TAAATGGTCTCCACCTACCCTGAT and Rv CACCTCCAACAGATGAGCATCAAATCC. The cycles used were 3 steps using 95° 30 s- 60° 30 s - 72° 30 s in the 3 genes studied. The products generated by the PCRs were previously sequenced to corroborate their identity and correspond specifically to the PRL-R sequences. The data obtained were analyzed with the GraphPad program and Microsoft Excel.

3. RESULTS AND DISCUSSION:

The average value of the relative expression of PRL-RS1b in healthy women is 1.0630+-0.3647 and in patients with SLE 0.8630+-0.4115, this being the one with the most variability, CV = 47.69%. No statistically significant differences were observed between the means of the SLE and control groups.

The PRL-RL in the control group presents an average value of 1.063+-0.3647 in control patients and 0.8630+-0.4115 in patients with SLE and presents greater CV variability = 47.69%. No statistically significant differences were observed between the means of the SLE and control groups. The control group's PRL-RL / PRL-RS1b index presents an average value of 1.007+-0.1311 in control patients and 1.180+-0.1710 in patients with SLE and presents greater CV variability = 14.49%. Interestingly, it is observed that the SLE group presents an increase in this activation/inhibition index ($p < 0.05$ t-test) (Figure 1).

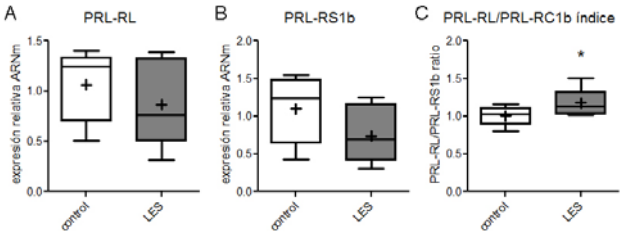
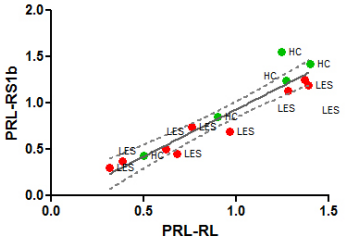


Figure 1. Relative RNA expression of PRL-R

Relative mRNA expression of PRL-RL (A), PRL-RS1b (B), and PRL-RL / PRL-RS1b (C) index in PBMC. * $p < 0.05$ "t student" test control vs SLE. +/- "T" bars show minimums and maximums. Box represents 95% confidence interval, including median represented as a line inside the box. The symbol "+" represents the mean.

Finally, intending to deepen the knowledge about the behavior of the different PRL-R isoforms, we evaluated the correlation between PRL-RL and PRL-RS1b in patient samples (Figure 2).



Spearman r	0.8945
95% confidence interval	0.6834 to 0.9676
P value (two-tailed)	P<0.0001
P value summary	***

Figure 2. PRL-RL vs PRL-RS correlation

Correlation between the mRNA expression of the two PRL-R isoforms in samples from healthy individuals and patients with SLE. The statistical test used was Spearman r, taking as a statistically significant correlation when r>0.69 and p>0.05. the expression on PRL-RL (r≈0.8945; p<0.001). These results indicate that the expression of PRL-RS1b could be regulated in a PRL-RL-dependent manner.

Surprisingly, the results showed a positive correlation of PRL-RS1b expression on PRL-RL (r≈0.8945; p<0.001). These results indicate that the expression of PRL-RS1b could be regulated in a PRL-RL-dependent manner.

4. CONCLUSIONS

To the knowledge of the authors, this is the first report where a correlation between PRL-RS1b, SLEDAI, and duration was evaluated. Similarly, the study of the expression of PRL-R isoforms in the different purified lymphocyte populations is crucial to continuing this study. In summary, the data arising from the current study do not show a significant advantage in the use of the study of the different isoforms of PRL-R as a marker of SLE. However, the use of the PRL-RL/PRL-RS1b index could contribute to a future detailed classification of patients with SLE, although in this study, the authors were unable to associate this index with clinical parameters of the disease. Therefore, the study of PRL-R expression and epigenetic parameters related to the regulation of its transcription in purified leukocyte populations could be more efficient and clinically relevant.

5. ACKNOWLEDGMENTS:

CONICET funded this work.

6. REFERENCES:

1. Ben-Jonathan, N., LaPensee, C. R., and LaPensee, E. W. (2008). What Can We Learn from Rodents about Prolactin in Humans? *Endocr Rev, 29*(1), 1-41.
2. Bole-Feysot, C., Goffin, V., Edery, M., Binart, N., and Kelly, P. A. (1998). Prolactin (PRL) and Its Receptor: Actions, Signal Transduction Pathways, and Phenotypes Observed in PRL Receptor Knockout Mice. *Endocr Rev, 19*(3), 225-268.
3. Dagil, R., Knudsen, Maiken J., Olsen, Johan G., O'Shea, C., Franzmann, M., Goffin, V., *et al*. (2012). The WSXWS Motif in Cytokine Receptors Is a Molecular Switch Involved in Receptor Activation: Insight from Structures of the Prolactin Receptor. *Structure, 20*(2), 270-282.
4. Houssiau, F., and Ginzler, E. (2008). Current treatment of lupus nephritis. *Lupus, 17*(5), 426-430.
5. Legorreta-Haquet, M. V., Chávez-Rueda, K., Chávez-Sánchez, L., Cervera-Castillo, H., Zenteno-Galindo, E., Barile-Fabris, L., *et al*. (2016). Function of Treg Cells Decreased in Patients With Systemic Lupus Erythematosus Due To the Effect of Prolactin. *Medicine (Baltimore), 95*(5), e2384.
6. Legorreta-Haquet, M. V., Flores-Fernandez, R., Blanco-Favela, F., Fuentes-Panan, E. M., Chavez-Sanchez, L., Hernandez-Gonzalez, R., *et al*. (2013). Prolactin Levels Correlate with Abnormal B Cell Maturation in MRL and MRL/lpr Mouse Models of Systemic Lupus Erythematosus-Like Disease. *Clin Dev Immunol, 2013*, 11.
7. Li, P. H., Wong, W. H. S., Lee, T. L., Lau, C. S., Chan, T. M., Leung, A. M. H., *et al*. (2013). Relationship between autoantibody clustering and clinical subsets in SLE: cluster and association analyses in Hong Kong Chinese. *Rheumatology, 52*(2), 337-345.
8. Rezaieyazdi, Z., and Hesamifard, A. (2006). Correlation between serum prolactin levels and lupus activity. *Rheumatology International, 26*(11), 1036-1039.
9. Suurmond, J., Zou, Y. R., Kim, S. J., and Diamond, B. (2015). Therapeutics to block autoantibody initiation and propagation in systemic lupus erythematosus and rheumatoid arthritis. [Journal Article]. *Sci Transl Med, 7*(280), 280-285.
10. Xu, D., Lin, L., Lin, X., Huang, Z., and Lei, Z. (2010). Immunoregulation of autocrine prolactin: Suppressing the expression of costimulatory molecules and cytokines in T lymphocytes by prolactin receptor knockdown. *Cell Immunol, 263*(1), 71-78.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

PRL-R ISOFORMS LONG / SHORT RATIO IS INCREASED IN SYSTEMIC LUPUS ERYTHEMATOSUS BLOOD MONONUCLEAR CELLS

MORENO-SOSA María Tamara
IMBECU-UNCuyo, Mendoza Argentina

GARCIA Daiana Sthefania
IMBECU-UNCuyo, Mendoza Argentina

HEREDIA Rocío
IMBECU-UNCuyo, Mendoza Argentina

BITTAR, Víctor-PEDROSA, Pablo
Hospital Central Mendoza, Argentina;

MACKERN-OBERTI, Juan Pablo
IMBECU-UNCuyo, Mendoza Argentina
email: jpmackern@mendoza-conicet.gob.ar

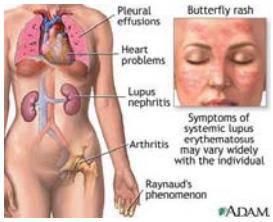
March/2022

INTRODUCTION

SBJChem Conference 2021

Systemic Lupus Erithematosus

"a complex disease"



Patients and symptoms → heterogeneous serositis, nephritis, SNC, arthritis

Therapy → Not specific. Immunosupressor drugs (methyl prednisolone, Azat, hydroxychloroq)
Antibody therapy (Belimumab)

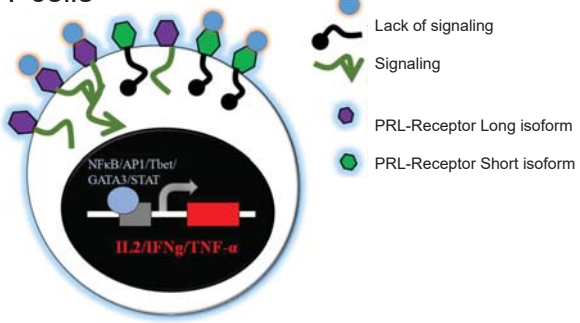
Immunological alterations → T cells (Th17, Th1, Treg)
B cells (ANA)
monocytes (clearance apoptotic cells)

Development of new therapies

BACKGROUND

SBJChem Conference 2021

T cells



AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

The focus of this work was to evaluate the expression of PRL-R isoforms during Systemic Lupus Erithematosus autoimmunity

METHODOLOGY

SBJChem Conference 2021

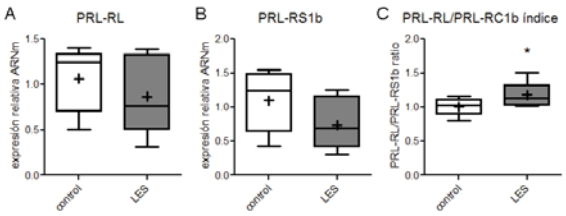
- PBMCs from lupus patients (n 9) and healthy controls (n 5) to evaluate mRNA expression of PRL-RL and PRL-RS.
- PBMC were separated by the conventional Ficoll-Hypaque method
- mRNA expression levels was performed by the 2 (-ΔΔCt) analysis between two groups using actin as a reference gene.

5

RESULTS AND DISCUSSION

SBJChem Conference 2021

Relative RNA expression of PRL-R

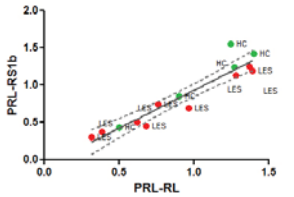


6

RESULTS AND DISCUSSION

SBJChem Conference 2021

PRL-RL vs PRL-RS correlation



Spearman r	0.8945
95% confidence interval	0.6834 to 0.9676
P value (two-tailed)	P<0.0001
P value summary	***

7

CONCLUSIONS

SBJChem Conference 2021

- the use of the PRL-RL/PRL-RS1b index could contribute to a future detailed classification of patients with SLE, and also be used a new biomarker of SLE.

- No clear association between PRL-RL/PRL-RS1b index with clinical parameters of the disease.

8

ACKNOWLEDGEMENTS

SBJChem Conference 2021

- CONICET
- ANPCYT FONCYT PICT 2015 – 1052; PICT 2018-2642; PICT-2019-1762
- PIP CONICET 0081-2015
- UNCuyo SIIP J082 (2019)

REFERENCES

SBJChem Conference 2021

❖Ben-Jonathan, N., LaPensee, C. R., & LaPensee, E. W. (2008). What Can We Learn from Rodents about Prolactin in Humans? *Endocr Rev, 29*(1), 1-41.
❖Bole-Feysot, C., Goffin, V., Edery, M., Binart, N., & Kelly, P. A. (1998). Prolactin (PRL) and Its Receptor: Actions, Signal Transduction Pathways and Phenotypes Observed in PRL Receptor Knockout Mice. *Endocr Rev, 19*(3), 225-268.
❖Dagil, R., Knudsen, Maiken J., Olsen, Johan G., O'Shea, C., Franzmann, M., Goffin, V., et al. (2012). The WSXWS Motif in Cytokine Receptors Is a Molecular Switch Involved in Receptor Activation: Insight from Structures of the Prolactin Receptor. *Structure, 20*(2), 270-282.
❖Gratz, I. K., Rosenblum, M. D., Maurano, M. M., Paw, J. S., Truong, H. A., Marshak-Rothstein, A., et al. (2014). Cutting Edge: Self-Antigen Controls the Balance between Effector and Regulatory T Cells in Peripheral Tissues. *J Immunol, 192*(4), 1351-1355.
❖Houssiau, F., & Ginzler, E. (2008). Current treatment of lupus nephritis. *Lupus, 17*(5), 426-430.
❖Jahn, G. A., Daniel, N., Jolivet, G., Belair, L., Bole-Feysot, C., Kelly, P. A., et al. (1997). In vivo study of prolactin (PRL) intracellular signalling during lactogenesis in the rat: JAK/STAT pathway is activated by PRL in the mammary gland but not in the liver. *Biol Reprod, 57*(4), 894-900.
❖Legorreta-Haquet, M. V., Chávez-Rueda, K., Chávez-Sánchez, L., Cervera-Castillo, H., Zenteno-Galindo, E., Barile-Fabris, L., et al. (2016). Function of Treg Cells Decreased in Patients With Systemic Lupus Erythematosus Due To the Effect of Prolactin. *Medicine (Baltimore), 95*(5), e2384.
❖Legorreta-Haquet, M. V., Flores-Fernandez, R., Blanco-Favela, F., Fuentes-Panan, E. M., Chavez-Sanchez, L., Hernandez-Gonzalez, R., et al. (2013). Prolactin Levels Correlate with Abnormal B Cell Maturation in MRL and MRL/lpr Mouse Models of Systemic Lupus Erythematosus-Like Disease. *Clin Dev Immunol, 2013*, 11.
❖Li, P. H., Wong, W. H. S., Lee, T. L., Lau, C. S., Chan, T. M., Leung, A. M. H., et al. (2013). Relationship between autoantibody clustering and clinical subsets in SLE: cluster and association analyses in Hong Kong Chinese. *Rheumatology, 52*(2), 337-345.
❖Orbach, H., Zandman-Goddard, G., Amital, H., Barak, V., Szekanecz, Z., Szucs, G., et al. (2007). Novel Biomarkers in Autoimmune Diseases. *Ann N Y Acad Sci, 1109*(1), 385-400.
❖Paraiba, D., Soares, C., Bartolini, P., Arthuso, F., Borba, E., Bonfa, E., et al. (2010). Lymphocytic prolactin does not contribute to systemic lupus erythematosus hyperprolactinemia. *Clin Exp Rheumatol, 28*(6), 0866-0872.
❖Rezaieyazdi, Z., & Hesamifard, A. (2006). Correlation between serum prolactin levels and lupus activity. *Rheumatology International, 26*(11), 1036-1039.
❖Suurmond, J., Zou, Y. R., Kim, S. J., & Diamond, B. (2015). Therapeutics to block autoantibody initiation and propagation in systemic lupus erythematosus and rheumatoid arthritis. [Journal Article]. *Sci Transl Med, 7*(280), 280-285.
❖Venkatesh, J., Peeva, E., Xu, X., & Diamond, B. (2006). Cutting Edge: Hormonal Milieu, Not Antigenic Specificity, Determines the Mature Phenotype of Autoreactive B Cells. *J Immunol, 176*(6), 3311-3314.
❖Xu, D., Lin, L., Lin, X., Huang, Z., & Lei, Z. (2010). Immunoregulation of autocrine prolactin: Suppressing the expression of costimulatory molecules and cytokines in T lymphocytes by prolactin receptor knockdown. *Cell Immunol, 263*(1), 71-78.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

PYROLYSIS OF SOYBEAN WASTE: A ROUTE TO ACTIVATED CARBON FOR FUNGICIDE CHLOROTHALONIL CAPTURE

CEBALLOS, Noelia Marcela[1*]; RIMONDINO, Guido Noé[1]; MALANCA, Fabio[1]; PELÁEZ, Walter José[1].

INFIQC – CONICET - Departamento de Fisicoquímica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba. Argentina. PC:5000.

**Correspondence author*
e-mail: noelia.ceballos@mi.unc.edu.ar

Received 02 February 2022; received in revised form 22 February 2022; accepted 26 February 2022

ABSTRACT

Soybean residues were transformed through static pyrolysis carried out at temperatures between 250 °C and 350 °C. The gaseous fraction analysis showed that the gases emanated in the pyrolysis are mainly CO_2 and CO. Furthermore, it was proved that this methodology constitutes a simple way to obtain useful carbons for the capture of pesticides present in an aqueous matrix. For example, the concentration of Chlorothalonil in a 7:3 water: acetonitrile solution decreases by 76-77 % through adsorption on the carbons obtained.

Keywords: *Thermal reaction, mesoporous carbons, pesticide*

1. INTRODUCTION

Many agroindustrial processes yield side-products that constitute an organic waste. Due to the high volumes of biomass produced this way, chemists have been intensively working to revalorize these residues. The techniques applied to transform the biomass are biochemical or thermochemical. The latter allows processing a greater amount of feedstock in shorter periods. In particular, biomass pyrolysis meets the conditions to generate high-energy-density bio-oil or biochar (Wang *et al.*, 2021).

The open burning of biomass undoubtedly releases carbon dioxide and other volatile organic compounds into the atmosphere. Therefore, the use of pyrolysis techniques that allow careful control of the products leaving the process is a key to minimizing the impact on the environment. To this end, static pyrolysis under vacuum conditions is presented as an advantageous technique for the study of volatile and non-volatile fractions of the pyrolysate (Pepino *et al., 2014*; Firpo *et al*.,2019)

In addition to the production of bio-oils and biochar, the transformation of biomass also produces coals that have multiple uses in the agricultural environment itself. For example, activated carbons obtained from pyrolysis can be used for industrial pollution abatement as an adsorbent for toxic pollutants in wastewater. In structure, activated carbons are highly microporous carbons with high internal surface area and porosity. Commercially, they are the most common adsorbents used to remove organic compounds from air and water streams. They are also often prepared from coal (non-renewable source) or specially dedicated biomass such as bamboo wood. However, any material with high carbon and low inorganic content can be used as a raw material for activated carbon production (Lewoyehu, 2021).

It is also an ecological issue the persistence of fungicides in the environment. For instance, the fungicide Chlorothalonil (CT) was banned in the United States and the European Union because of its permanence in humic acids and its transformation in potential toxics byproducts in groundwater (Kiefer *et al.*, 2020). But, besides this, it is still widely used in developing countries. In this way, primarily solutions involve the photochemical transformation of the pesticide into more soluble byproducts with less toxicity.

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.35_abstract_CEBALLOS.pdf

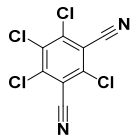


Figure 1. *Chlorothalonil structure.*

As part of our study of gaseous products emitted to the atmosphere by burning industrial biomass residues from soybean pressing, it was reported here the obtention and utilization of carbons from soybean waste static pyrolysis to retain the fungicide Clorotalonil from an aqueous matrix.

2. MATERIALS AND METHODS

The soybean residue used is the solid left-over obtained after the pressing of soybeans in the oil production process. This residue was ground to particle sizes of less than 1 mm. Subsequently, 500 mg of this material was placed in a Pyrex glass ampoule and evacuated for 2 minutes until a pressure of 10^{-2} mbar was reached. They were then sealed and subjected to static pyrolysis reactions at different times (10-60 min) and temperatures (250°C-350 °C) in an electrical furnace (ORL-T40400). The gas composition was transferred and analysed by IR spectroscopy using a Fourier transform infrared spectrometer (Bruker IFS 28) following the temporal variation of reactants and products for all the reactions performed. All spectra were recorded in the range 500−4000 cm^{-1} with a resolution of 2 cm^{-1}. The remaining solid was subjected to successive washes in a Soxhlet apparatus (3 x 120 mL ethanol, 98%) 3 hours each time. Then, the same procedure was performed but with acetonitrile (ACN, HPLC 99.5%, Sintorgan). Finally, the recovered solid was dried at atmospheric pressure until a constant weight was achieved.

The selected solids were used to perform adsorption experiments with the pesticide Chlorothalonil. The process was monitored by UV-VIS spectroscopy on an Agilent 8354 spectrophotometer (xL=3.65*10^{-2} absorbance units) using a quartz cell with an optical path of 1 cm. The Chlorothalonil was purified from a commercial sample (compressed powder 82.5% w/w) by extraction with ethyl acetate followed by purification via chromatographic column using mixtures of n-hexane and dichloromethane.

For each assay, 20 mg of the carbonaceous solid was placed in disc extraction cartridges (3M Empore - Fischer Scientific, octadecyl, 10mm/6mL). The solution passage was always performed in 2 mL aliquots using a flow rate of 2 mL every 5s. In the first stage, the carbons were washed with 20 mL (10 x 2 mL) of water: acetonitrile solution (7:3). Then, 2 mL of a solution of 1.4 mM CT in water: acetonitrile (7:3) was passed over the carbon under study.

3. RESULTS AND DISCUSSION:

3.1. Gas Analysis

In all the performed reactions, it was found that the most significant proportion of the gases corresponds to CO_2 (85 - 97 %), while CO was the second-largest gas present (2 - 9 %). In addition, it was also observed the formation of various volatile organic compounds (VOCs), whose presence and proportion depends on the temperature and time of pyrolysis: methane, propane, butane, ethylene, methanol, acetone, methyl, and ethyl acetate, among others.

It was determined that the formation of mono-carbon compounds is favored by the increase of temperature and pyrolysis time because the cracking processes were promoted and produced thermodynamically more stable compounds.

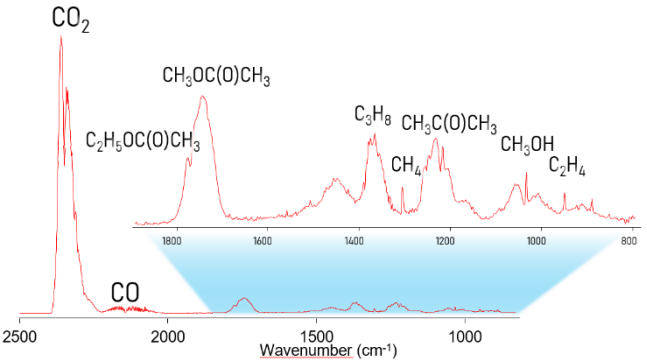
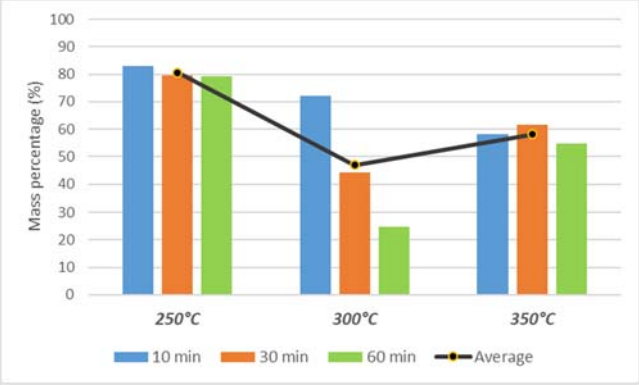


Figure 1. *Characterization of the gas fraction by IR spectrum at 350°C.*

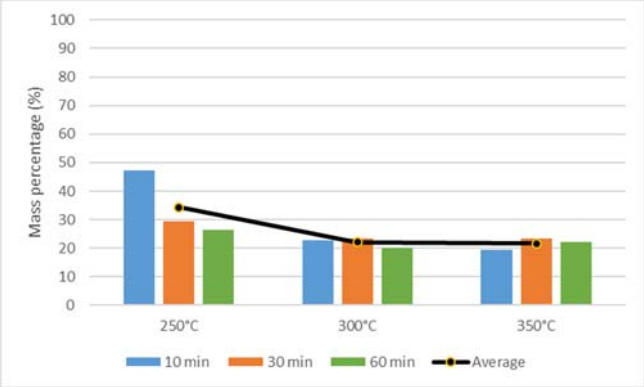
3.2. Carbon obtaining

The percentages of solid crude oil recovery at each temperature and time are shown in Graph 1. It can be seen that the mass recovered in each pyrolysis reaction (corresponding to coal and non-volatile compounds) tends to remain constant as the temperature increases (47-58%). This trend is more evident in Graph 2, where the mass percentages of carbon mass at both 300°C and 350 °C are very close. Likewise, when comparing the mass percentages of carbon at the three

reaction times studied, it is evident that this mass is independent of the reaction time. In other words, the amount of carbon initially formed in the process remains practically unchanged through the static pyrolysis of biomass.

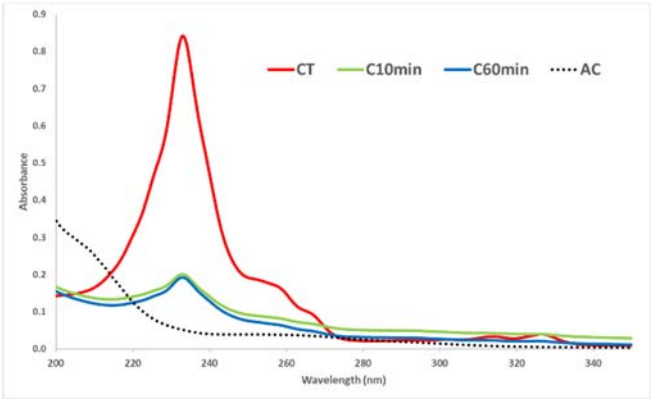


Graph 1. *Mass percentage of non-volatile fraction obtained in the static pyrolysis of soybean waste at different times and temperatures.*



Graph 2. *Mass percentage of carbon fraction obtained in the static pyrolysis of soybean waste at different times and temperatures.*

The carbons obtained at the maximum working temperature (350 °C) and at times of 10 and 60 min (labelled as C10min and C60min respectively) were selected to perform the Chlorothalonil adsorption tests. The maximum absorption wavelength of the CT is 233 nm, as can be seen in graph 3 (red line). From the analysis of the spectral curves of the solution after passage over the C10min and C60min carbons, it was found that the concentration of CT decreases by 76 and 77% (green and blue lines).



Graph 3. Spectral curves show the adsorption of CT by the carbons obtained at 350 °C at 10 min (C10min, green line) and 60 min (C60min, blue line).

When comparing the behavior of C10min and C60min with commercial activated carbon, it is evident that the latter is very efficient in adsorbing CT and produces a decrease of its concentration by 94%. However, considering that the carbons obtained in this work did not have any chemical activation, the effectiveness shown is acceptable and could be improved by further treatment.

4. CONCLUSIONS:

The production of several VOCs of potential atmospheric impact from the burning of biomass soybean residues was evidenced. In addition, it was determined that the formation of mono-carbon compounds is favored by the increase in temperature and pyrolysis time because the cracking processes are promoted.

The carbonaceous solids obtained in this work were also effective retention agents for the pesticide Chlorothalonil in an aqueous solution. It is expected that the thermal or chemical activation of the carbonaceous solids studied will further improve their compound adsorption properties. It would also be of great interest to test the carbons with aqueous matrices containing other pesticides or mixtures thereof.

5. ACKNOWLEDGMENTS:

The work at the Instituto de Investigaciones en Fisicoquímica de Córdoba (INFIQC) was supported by Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET grant number: PIP 11220170100423CO), Fondo para la Investigación Científica y Tecnológica (FONCyT grant number: PICT-2017-1555), Programa Institucional y Multidisciplinar (Primar)

en Temas Prioritarios (Primar-PT 32520170100334CB) and Secretaría de Ciencia y Tecnología (SeCyT-UNC grant number: SeCyT N°411/18).

6. REFERENCES:

1. Firpo, G.; Cooke, M. V.; Peláez, W. J.; Chans. G. M.; Argüello, G. A.; Gómez, E.; Alvarez Toledano, C. *J Phys Org Chem.* **2017**, e3789.
2. Kiefer, K.; Bader, T.; Minas, N.; Salhi, E.; Janssen, E. M.-L.; von Guten, U.; Hollender, J. *Water Research* **2020**, 183, 116066.
3. Lewoyehu, M. *J. Anal. Appl. Pyrolysis* **2021**, 159, 105279.
4. Pepino, A. J.; Peláez, W. J.; Faillace, M.; Ceballos, N. M.; Moyano, E. L.; Arguello, G. A. *RSC Advances* **2014**, 4, 60092.
5. Wang, G.; Dai, Y.; Yang, H; Qingang, X.; Wang, K.; Zhou, J.; Li, Y. Energy Fuels **2020**, 34, 12, 15557.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

PYROLYSIS OF SOYBEAN WASTE: A ROUTE TO ACTIVATED CARBON FOR FUNGICIDE CHLOROTHALONIL CAPTURE

CEBALLOS, Noelia Marcela; RIMONDINO, Guido Noé; MALANCA, Fabio; PELÁEZ, Walter José*.

INFIQC – CONICET - Departamento de Fisicoquímica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba. Argentina.

PYROLYSIS OF SOYBEAN WASTE: A ROUTE TO ACTIVATED CARBON FOR FUNGICIDE CHLOROTHALONIL CAPTURE

CEBALLOS, Noelia Marcela; RIMONDINO, Guido Noé; MALANCA, Fabio; PELÁEZ, Walter José*.

INFIQC – CONICET - Departamento de Fisicoquímica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba. Argentina.

Introduction

Corncob

Soybean paste

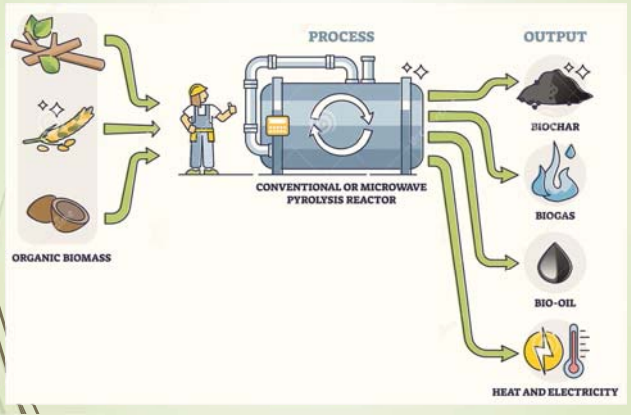
Olive pomace

Agroindustrial waste

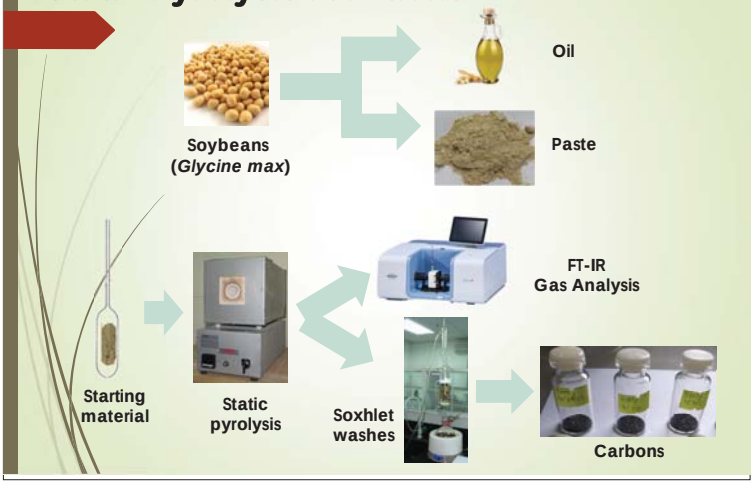
sugarcane bagasse

Biomass pyrolysis

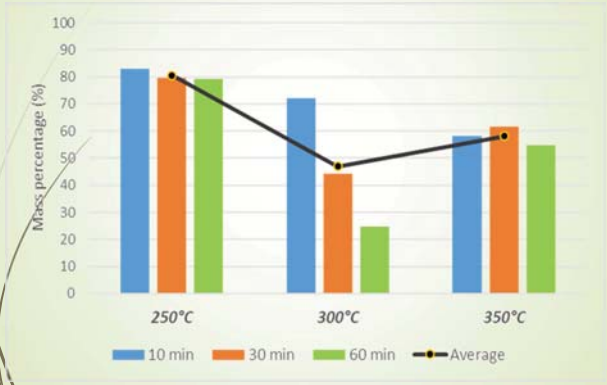
Introduction



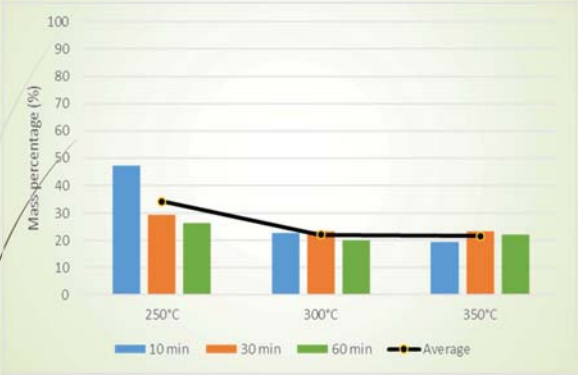
Static Pyrolysis reactions



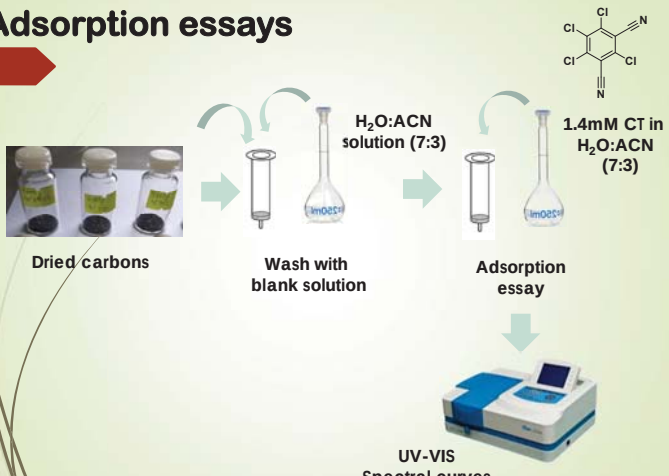
Results – Mass percentage of non-volatile fraction



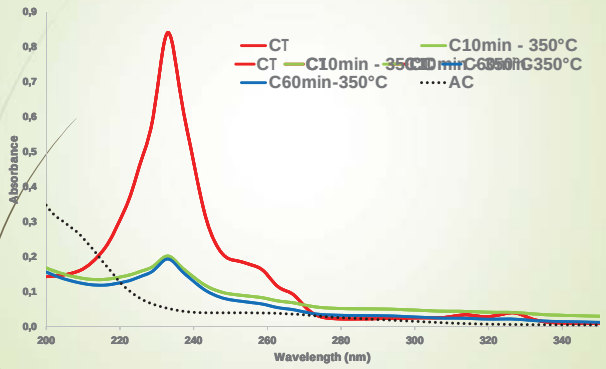
Results - Mass percentage of carbon fraction



Adsorption essays



Results – Adsorption essays



Conclusions and perspectives

Using the soybean residue we obtained effective retention agents for the pesticide Chlorothalonil in aqueous solution.

It is expected that thermal and/or chemical activation of the carbonaceous solids studied will further improve their compound adsorption properties.

It would also be of great interest to test the carbons with aqueous matrices containing other pesticides or mixtures thereof.

Química Teórica-Experimental de Moléculas de Interés Ambiental

Departamento de FISICOQUÍMICA
Facultad de Ciencias Químicas
Universidad Nacional de Córdoba

CONICET
INFIQC

Ministerio de CIENCIA Y TECNOLOGÍA
CÓRDOBA ENTRE TODOS

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

RELEASE PROFILE OF BISPHENOL-A FROM DENTAL RESINS IN WATER ASSESSED BY LC-MS/MS

SILVA, Bruno Pereira da[1*]; RÜBENSAM, Gabriel[2]; SAAFELD, Claudiela Wachholz[3]; WEBER, João Batista Blessmann[1]

[1] Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Programa de Pós-Graduação em Odontologia

[2] Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de pesquisa em Farmacologia e Toxicologia - INTOX

[3] Universidade Federal de Ciências da Saúde de Porto Alegre, Faculdade de Biomedicina
** Correspondence author*
e-mail: gabriel.rubensam@pucrs.br

Received 12 January 2022; received in revised form 30 January 2022; accepted 18 February 2022

ABSTRACT

Dental resins have been designed to replace amalgam restorations due to their more favorable physical, chemical, and biological properties. However, depending on its composition, the efficiency of its polymerization, and the degradation of the polymer matrix, Bisphenol-A can be present and therefore released from this material to the human body. It has been reported that residues of additives and minority by-products of polymer reactions, such as Bisphenol-A, can be released from plastics into aqueous media through polymer hydration, water-polymer diffusion, residue dissolution, and equilibrium between dissolved residues in water and polymer. Over time, this could lead to a polymer material with an external layer practically free of Bisphenol-A. However, the newly formed layer could be removed by brushing during oral cleaning, similar to toothbrushing, exposing the new layer containing Bisphenol-A to the aqueous media. Due to the toxic effects of this compound, an increasing number of plastics labeled as BPA-free have been introduced to the dental market, including tooth coating, dental sealants, and resins. Nevertheless, more specific studies on analytical chemistry have revealed a trace of Bisphenol-A in dental resins labeled as BPA-free and pointed out the need for even more sensitive and accurate detection methods to help manufacturers evaluate the presence of background contaminations in their products and to avoid false-negative results. In this way, liquid chromatography-tandem mass spectrometry has been considered one of the most suitable methods for confirming Bisphenol-A even at low concentrations, in high complex matrices, due to its high select sensitivity. In the present work, we developed a sensitive, reliable, and efficient approach to trace the release profile of Bisphenol-A by LC-MS/MS in dental resin samples purchased in the Brazilian dental market. With the analysis of five different brands of resin composites performed in eight days of exposition to water, four of them released Bisphenol-A from 3.4 pg/mm^2 to 10.1 ng/mm^2. The brand labeled as BPA-free released BPA at concentrations of 1.1 ng/mm^2. However, one sample reached the maximum of released BPA in only 3 days, one in 4 days, and two virtually did not reach a maximum of BPA released into the water in the window time assessed. Limits of detection and quantification of the LC-MS/MS method were 40 pg/mm^2 and 100 pg/mm^2, respectively, and allowed the quantification of BPA released from a composite labeled as BPA-free. For future analysis, we will conduct a more comprehensive study on the release profile of BPA from resin composites into the water using a tooth brushing simulator to determine if the obtained profiles might have clinical implications.

Keywords: *Dental resins, Bisphenol-A, LC-MS/MS, release profile.*

1. INTRODUCTION

Today, dental restoration is one of the basic specialties of dentistry in which the use of resinous materials has exponentially increased because of their better physical, chemical, and biological characteristics than dental amalgam (Cho et al., 2022) and, in part, due to the race against the time generated by Minamata Convention on Mercury, which considered a proposal of phase-out amalgam by 2024 (Reher *et al*., 2021). But, on the

other hand, a number of leachable and extractable chemicals from these materials have been reported, including Bisphenol-A (BPA), a well know potent endocrine disruptor (Cho *et al*., 2022; Nys *et al*., 2022).

The presence of BPA in dental resins can occur depending on the resin composition, on the efficiency of its polymerization, and on the degradation of the polymer matrix (Nys et al., 2022) and be released into an aqueous media through polymer hydration, water-polymer diffusion, residue dissolution, and equilibrium between dissolved residues in water and polymer (Asaoka *et al*., 2008). This situation could lead to a polymer material with an external layer practically free of Bisphenol-A. However, the newly formed layer could be removed by brushing during oral cleaning, similar to toothbrushing, exposing the new layer containing Bisphenol-A.

Alternative materials have been used to develop new dental resins called BPA-free. However, more specific studies on analytical chemistry have been revealed a trace of Bisphenol-A in dental resins labeled as BPA-free and pointed out the need for even more sensitive and accurate detection methods to help manufactures to evaluate the presence of background contaminations in their products and to avoid false-negative results (Tichy *et al*., 2022). In this way, liquid chromatography-tandem mass spectrometry has been considered one of the most suitable methods for confirming Bisphenol-A even at low concentrations, in high complex matrices, due to its high selectivity and sensitivity (Goeury et al., 2022).

In the present work, we developed a sensitive, reliable, and efficient approach to trace the release profile of Bisphenol-A by LC-MS/MS from dental resin samples of different brands purchased in the Brazilian dental market, including one declared as BPA-free material, to water.

2. MATERIALS AND METHODS

2.1. Chemicals

Methanol LC-MS grade (Riedel-de Haën, Germany), ammonium hydroxide 25% LiChropur (Merck, Germany), formic acid LC-MS LiChropur (Supelco, Germany), Bisphenol A 99% (Supelco, Germany), were purchased. Type 1 water was obtained by using a purifier system Milli-Q UV (Millipore, USA).

2.2. Sample Preparation

Cylinders of resin composite (8 x 6 mm) were prepared and stored according to the manufacturer. A total of five different brands of resin composites were assessed (sample 1: intermediate viscosity; sample 2: low viscosity; sample 4: high viscosity; sample 5: with nanoclusters), including one labeled as BPA-free (sample 3). Two groups for each sample composed of five pellets of finished resin composite, one without and other with burnish performed at the lower and upper extremities of the pellets (Abrasive 4000 grit, 4 microns, Agilent, USA), were gentle washed with type 1 water, and transferred into 15 mL glass falcon tubes. Type 1 water (2 mL) was added into tubes; the mixture was gently agitated for 10 s, and the samples were left to stand for 8 days at room temperature after the first collection (20 µL). All collections were carried out every 24h, and the generated aliquots were stored at -20 °C before LC-MS/MS analysis. The grinding experiment was performed using sandpaper (Abrasive 4000 grit, 4 microns, Agilent, USA). All experiments were performed in triplicate. An example of a finished sample was presented in Figure 1.

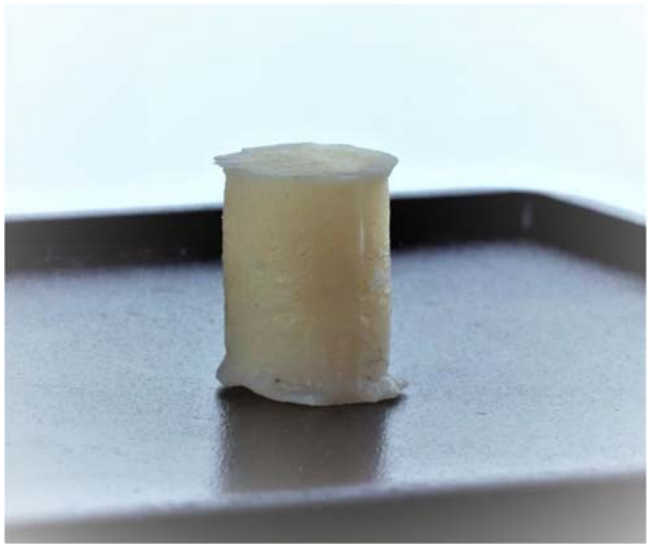


Figure 1. Example of a finished sample used to evaluate BPA release profile to water.

2.3. LC-MS/MS analysis

LC-MS/MS was used in the quantification of BPA released from resin composites. Sample aliquots were thawed at room temperature and injected (5 µL) into the liquid chromatograph

Agilent 1290 Infinity coupled to a mass spectrometer Agilent 6460 Triple Quadrupole (Agilent Technologies, USA). Chromatographic separations were performed by using a Zorbax® Extended C18 RRHD 2.1 x 50 mm 1.8-µm particle size (Agilent Technologies, USA), and mobile phase consisted of (A) ammonium formate 5 mM pH 10, and (B) methanol, in gradient mode. The gradient initiated with 5% of B, subsequently increasing to 90% in 2.5 min, remaining at this condition for one min. The initial condition was recovered and kept for 0.5 min. The flow rate was 0.4 mL/min, with a column temperature of 40 °C BPA was ionized with an electrospray (ESI) source operated in negative mode, and the mass spectrometer was optimized to monitor the transitions m/z 227>212 and 227>133, in MRM mode, for quantification and confirmatory purpose, respectively. The calibration curve was constructed in the range of 5 to 100 ng/mL, and external standardization was considered in the quantification. Results were obtained in terms of cumulative data.

3. RESULTS AND DISCUSSION:

To obtain a sensitive method for determining BPA released from dental resin composites, even in products declared as BPA-free, it was necessary to perform a more comprehensive analytical optimization. The optimal condition was reached by adding ammonia to the chromatographic mobile phase since the deprotonation of BPA is facilitated in alkaline conditions, leading to an enhancement of its ionization and analytical sensitivity (Tan *et al*., 2018). In addition, formic acid was added to pair the ionized BPA, enhancing its retention on a C18 column. An example of a chromatogram obtained with the optimized method was presented in Figure 2.

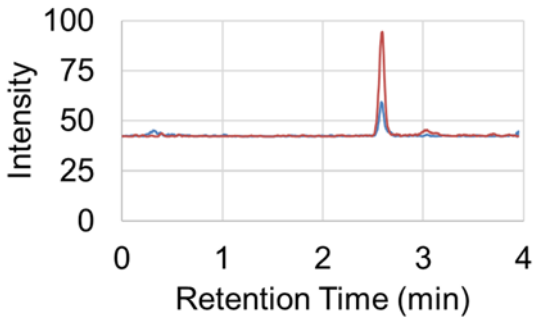


Figure 1. Representative chromatogram of a sample containing 10 ng/mL of BPA, analyzed by LC-MS/MS. Redline for the quantification transition (m/z 227>212) and blue line for the confirmatory transition (m/z 227>133).

The established conditions allowed limits of detection and quantification of 40 and 100 pg/mm^2 and the quantification of BPA released from a sample labeled as BAP-free. All samples that did not received burnish treatment released BPA at concentrations below 10 ng/mL after 8 days of exposition on water, except for the one labeled as BPA-free, which presented BPA at concentrations below the limit of quantification (data not shown). Burnished samples released BPA between the concentrations of 3.4 pg/mm2 to 10.1 ng/mm^2, except the one declared as BPA-free, which released BPA at concentrations below 1.1 ng/ mm^2. Most of them released BPA from the fourth day, while only one released BPA from the onset of exposure to water. The sample labeled as BPA-free started releasing BPA after 7 days. The release profile of the tested samples is presented in Figure 2.

It was observed two distinct behavior patterns for releasing BPA from the composite to water with the results herein presented. Both are related to the product viscosity and polymer conversion degree. Products with higher viscosity and lower conversion presented a faster water diffusion and provided more release of BPA to water. On the other hand, composites with lower viscosities and higher polymer conversions had lower release rates. A special situation was observed for a sample with low viscosity but composed of nanoclusters, which may have contributed to an increased water diffusion through the composite after sanding.

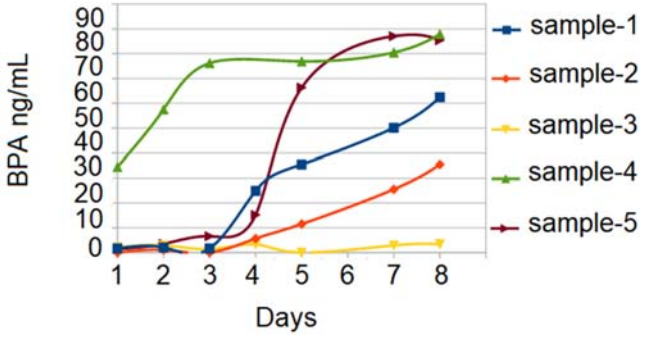


Figure 3. Release profile of BPA from the assessed composite samples to water.

The obtained results were in accordance with findings reported in the literature in terms of BPA released (Durner *et al*., 2012) and in terms of the physical properties of the composites (Schneider et al., 2012). However, more comprehensive studies involving brushing simulation must be performed to evaluate and understand the release profile of BPA in a more realistic approach and to allow more precise information for the preparation and use of the assessed resin composites.

4. CONCLUSIONS:

An LC-MS/MS method was presented as capable of determinating low BPA levels, even for resin composites labeled as BPA-free. The BPA profile released from different resin composites brands into the water after the sanding process was presented and related to their viscosity and polymer conversion degree and structure. More comprehensive testing using a tooth brushing simulator should be conducted to determine if the obtained profiles might have clinical implications.

5. REFERENCES:

1. Cho K., Rajan G., Farrar P., Prentice L., Prusty B.G. *Composites Part B*, **2022**, *230*, 109495.
2. Reher V., Reher, P., Peres K.G., Peres M.A. *Aust Dent J*, **2021**, *66*, 61-66.
3. Nys S., Duca, C.R., Vervlietd P. et. al., *J Dent*, **2022**, *116*, 103894.
4. Asaoka, K., Hirano, S., *Biomat*., **2008**, *24*, 975-979.
5. Tichy, A.; Simkova, M.; Vrbova, R.; Roubickova, A.; Duskova, M.; Bradna, P. *Polymers,* **2022**, *14*, 46.
6. Goeury K, Duy S.V., Munoz G., Prévost M., Sauvé, S. *Talanta*, **2022**, *241*, 123216.
7. Tan D., JinJ., Wang L., Zhao X., Guo C., Sun X., Dhanjai, Lu X., Chen J., *Talanta*, **2018**, *182*, 590-594.
8. Durner J., Obermaier J., Draenert M., Ilie N., *Dent mat*, **2012**, *28*, 11, 1146-1153.
9. Schneider, A.C., Mendonça, M.J., Rodrigues, R.B., Busato P.M.R., Camilotti, V. *Polímeros*, **2016**, *26*, 37-42.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

RELEASE PROFILE OF BISPHENOL-A FROM DENTAL RESINES INTO WATER ASSESSED BY LC-MS/MS

Bruno Pereira da Silva
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Programa de Pós-Graduação em Odontologia – Brazil

Gabriel Rübensam
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de pesquisa em Farmacologia e Toxicologia, INTOX - Brazil

Claudiela Wachholz Saafled
Universidade Federal de Ciências da Saúde de Porto Alegre, Faculdade de Biomedicina - Brazil

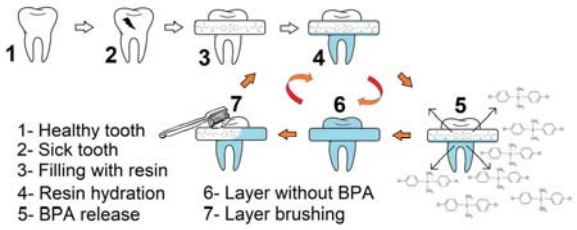
João Batista Blessmann Weber
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Programa de Pós-Graduação em Odontologia – Brazil

December/2021

INTRODUCTION

SBJChem Conference 2021

BPA release from resin composite to aqueous system.



AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

In the present work, we developed a sensitive, reliable and efficient approach to trace the release profile of BPA by LC-MS/MS in dental resin samples used for dental restoration.

METHODOLOGY

SBJChem Conference 2021

1- Finished composites were exposed to water during 8 days;

2- Sanded composites were exposed to water during 8 days.

3- A LC-MS/MS method was optimized to allow low levels of BPA by using ammonia in the chromatography

4- Results were obtained from cumulative data and expressed as ng/mm² of BPA

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Two distinct behavior patterns for release BPA from the composite to water were predominant: low and high velocity which BPA was released.
- Both are related to the product viscosity and polymeric conversion degree:

Products with higher viscosity and lower conversion presented allowed a faster water diffusion and provided more release of BPA to water. On the other hand, composites with lower viscosities and higher polymeric conversions had lower release rates.

- A special situation was observed for a sample with high viscosity, but composed by nanoclusters, which may have contributed to an increased water diffusion through the composite after sanding.

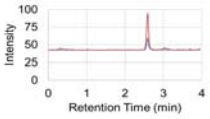


Figure 1. Representative chromatogram of a sample containing 10 ng/mm² of BPA, analyzed by LC-MS/MS. Red line for the quantification transition (m/z 227>212) and blue line for the confirmatory transition (m/z 227>133).

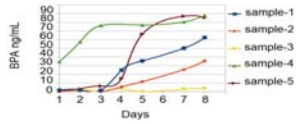


Figure 2. Release profile of BPA from the assessed composite samples to water.

CONCLUSIONS

SBJChem Conference 2021

- A LC-MS/MS method was herein presented as capable to determinate low levels of BPA, even for resin composites labeled as BPA-free.
- The profile of BPA released from different brands of resin composites into water after sanding process was presented and related to their viscosity and polymer conversion degree and structure.
- More comprehensive testing using a tooth brushing simulator should be conducted to determine if the obtained profiles might have clinical implications.

REFERENCES

SBJChem Conference 2021

1. Cho K., Rajan G., Farrar P., Prentice L., Prusty B.G. (2022). Dental resin composites: A review on materials to product realizations. *Composites Part B: Engineering, 230*(1): 109495.
2. Reher V., Reher, P., Peres K.G., Peres M.A. (2021). Fall of amalgam restoration: a 10-year analysis of an Australian university dental clinic. *Australian Dental Journal*, 66: 61-66.
3. Nys S., Duca, C.R., Vervlietd P., Covaci A., Boonen I., Elskens M., Vanoirbeek J., Godderis L, Meerbeek B.V., Landuyt K.L.V. (2022). Bisphenol A release from short-term degraded resin-based dental materials. *Journal of Dentistry, 116*: 103894.
4. Asaoka, K., Hirano, S. (2003). Diffusion coefficient of water through dental composite resin. *Biometerials, 24*(6): 975-979.
5. Tichy, A.; Simkova, M.; Vrbova, R.; Roubickova, A.; Duskova, M.; Bradna, P. (2022). Bisphenol A Release from Dental Composites and Resin-Modified Glass Ionomers under Two Polymerization Conditions. *Polymers, 14*(1): 46.
6. Goeury K, Duy S.V., Munoz G., Prévost M., Sauvé, S. (2019). Analysis of Environmental Protection Agency priority endocrine disruptor hormones and bisphenol A in tap, surface and wastewater by online concentration liquid chromatography tandem mass spectrometry. *Journal of Chromatography A, 159126*): 87-98.
7. Tan D., JinJ., Wang L., Zhao X., Guo C., Sun X., Dhanjai, Lu X., Chen J. (2018). Ammonium hydroxide enhancing electrospray response and boosting sensitivity of bisphenol A and its analogs. *Talanat, 182*: 590-594.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

RELEVANCE OF THE HEALTH CONDITION AND CLINICAL CHARACTERISTICS OF SPOROTRICHOSIS

ROCHA, Sofia Marques [1*]; PEREIRA, Bruna Hudson Neves [1]; OLIVEIRA, Emanuelle Silva [1]; JUNQUEIRA, Letícia Santos [1]; OLIVEIRA, Glenda Ribeiro [1]

[1] Universidade de Vassouras

** Correspondence author*
e-mail: sofiamarquesrocha@gmail.com

Received 10 February 2022; received in revised form 26 February 2022; accepted 05 March 2022

ABSTRACT

Feline sporotrichosis is a zoonosis caused by *S. brasiliensis*, and it presents a degree of great underreporting due to its contamination. Caused by inoculation directly into the skin, in most cases through scratches or bites by infected animals. With its first diagnosis in 1907 among naturally infected mice. The study presents information on the health of the animal, composed of 24 felines of both sexes, obtaining information through questionnaires about food along with vaccination, deworming, and ectoparasites control. In addition to depicting the types of injuries and body parts such as head, limbs, and trunk. Seeking to provide important information about animal health, along with the follow-up of a Veterinary Doctor. General care that meets the health of no animal meets all care. The disease may present some systemic symptoms such as secretions, anorexia, apathy, difficulty breathing, fever, ulcers, and abscesses. In the study, 4% of the cats had a respiratory clinical picture. Regarding the lesions, it was mostly noted that 96% of the felines had multiple lesions and 4% had single lesions in the areas of the body, being 67% of secretion with pure bloody characteristics and 33% had no secretions, with the main sites of involvement being 58% in the head region, 36% in the limbs and 6% in the trunk. Factors related to feline immunocompromise may result in more severe cases of sporotrichosis as observed in the study animals. All information obtained was evaluated using basic descriptive statistics. Relative frequency values and percentage values were assigned to the variables observed in the research.

Keywords: *Zoonosis, S. brasiliensis, Underreporting, Injury.*

1. INTRODUÇÃO

A esporotricose consiste em uma micose subcutânea, de evolução subaguda ou crônica, decorrente da infecção causada por um fungo dimórfico do gênero *Sporothrix* (Schubach *et al.,* 2004; Pereira *et al.,* 2015). O primeiro diagnóstico da doença em animais no Brasil foi no ano de 1907, entre ratos naturalmente infectados nos esgotos da cidade de São Paulo (Gremião *et al.*, 2020; Lutz, 1907). Entretanto, os primeiros casos descritos em felinos ocorreram em 1950 (Gremião *et al.*, 2020; Almeida, *et al.*, 1955).

A esporotricose felina, provocada pela inoculação de *S. brasiliensis* na pele, na maioria dos casos através de arranhaduras e/ou mordeduras por animais infectados, tem se tornado um problema crescente de saúde pública nos municípios do estado do Rio de Janeiro (Gremião *et al.*, 2020). Tal infecção apresenta um período de incubação equivalente a 14 dias, podendo chegar a seis meses após a entrada do fungo no organismo (Gremião *et al.,* 2020; Pereira, 2015). Manifesta como primeiros sinais clínicos alopecia seguida de lesões ulceradas, crostosas ou nodulares, na derme, região conjuntival, oral ou genital (Gremião *et al.*, 2020). A espécie *S. brasiliensis* pode se disseminar diretamente de um animal infectado para outros animais, através de mordidas, arranhaduras ou por contato com as lesões cutâneas apresentadas (Gremião *et al.*, 2017; Schubach *et al*., 2004).

A doença é composta por fases e progressões distintas, sendo descritas como: fase cutânea localizada, caracterizada por lesões nodulares avermelhadas, individuais ou múltiplas na pele do animal; Fase cutânea linfática, quando a infecção progride, formando úlceras na pele e atingindo o sistema linfático; Fase cutânea

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.41_abstract_ROCHA.pdf

disseminada, se caracteriza no estágio mais avançado atingindo todo o sistema do animal, com presença de úlceras maiores, acometendo articulações, ossos e pulmões, neste estágio o animal apresenta letargia, depressão, anorexia e febre (Gremião *et al.*, 2020; Rosser *et al.*, 2006).

A forma mais comum de manifestação clínica da doença é a forma cutânea, na qual aparecem lesões profundas, majoritariamente purulentas, que não cicatrizam e evoluem rapidamente, localizadas na maioria das vezes na região da cabeça e principalmente na mucosa nasal. A enfermidade ainda pode apresentar alguns sintomas sistêmicos tais como, secreções, anorexia, apatia, dificuldade de respirar, febre, úlceras e abcessos (Gremião *et al.,* 2020; Schubach *et al*., 2004).

2. MATERIAIS E MÉTODOS

O estudo foi submetido ao Comitê de Ética em Pesquisa da Universidade de Vassouras e aprovado sob o número de protocolo 3.622.655. O estudo foi realizado nos meses de outubro e novembro de 2021, no município de Vassouras, RJ em parceria com a Secretaria Municipal de Saúde. A pesquisa foi composta por 24 felinos SRD de ambos os sexos que foram diagnosticados previamente pelo veterinário responsável da Secretaria Municipal de Saúde.

Foram obtidas informações sobre os felinos por meio de entrevista com os tutores e os dados foram anotados em questionários que continham perguntas à respeito da saúde geral dos felinos em relação à vacinação, vermifugação, controle de ectoparasitas e o tipo de alimentação fornecida. Também foram colhidas informações a respeito da apresentação clínica das lesões cutâneas dos animais, se eram lesões únicas ou múltiplas, com presença de secreção purosanguinolenta ou não, e se havia complicações com quadro respiratório. Além de pesquisa sobre as regiões mais acometidas pelas lesões nos animais, incluindo cabeça, membros e tronco.

Todas as informações obtidas foram avaliadas por meio de estatística descritiva básica. Valores de frequência relativa e valores percentuais foram atribuídos às variáveis observadas (VIEIRA, 2011).

3. RESULTADOS E DISCUSSÃO:

Dos 24 felinos, nenhum dos animais avaliados havia sido vacinado, vermifugado ou submetido a controle de ectoparasitas e todos recebiam outro tipo de alimentação ao invés de ração.

Larsson *et al.* (2011) diz que animais com a saúde debilitada são mais propensos a ter agravos no quadro de esporotricose devido a falhas na imunidade celular, podendo estar associada até mesmo a retroviroses.

A respeito dos tipos de lesões, dos 24 animais em avaliados, 96% (23/24) apresentaram lesões múltiplas e 4% (1/24) apresentaram lesões únicas (Figuras, 1, 2 e 3).

Figura 1: Gráfico do tipo de lesão encontrada.

Figura 2: Gato com esporotricose manifestando lesão única cutânea.

Figura 3: Gato com esporotricose manifestando lesões múltiplas cutâneas.

São encontradas mais lesões múltiplas que lesões únicas nos animais acometidos com esporotricose, o que sugere extensão e o agravamento da doença nesses animais, o que pode ser ainda maior caso eles apresentem a saúde geral debilitada ou algum fator que cause imunocomprometimento (SANTOS *et al*., 2020).

Em relação a característica das lesões, 67% (16/24) apresentavam lesões com secreção purosanguinolenta, em 33% (8/24) as lesões não apresentavam essa característica (Figuras 4, 5 e 6).

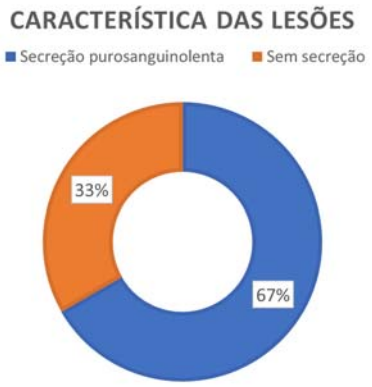


Figura 4 : Gráfico das características das lesões.

Figura 5: Gato com esporotricose manifestando lesão com secreção purosanguinolenta.

Figura 6: Gato com esporotricose manifestando lesão sem secreção.

De acordo com Gremiao *et al.* (2020) lesões com secreção representam um agravamento dos sinomas pois estão relacionadas a fase cutânea disseminada da doença.

Apenas 4% (1/24) dos animais apresentaram quadro clínico com comprometimento respiratório.

Segundo Schubach *et al*. (2004) e Crothers *et al*. (2009) é comum a presença de sintomatologia respiratória (Figura 7).

Figura 7: Gráfico da relação de quadro respiratório entre os animais.

No que diz respeito à localização das lesões, a maioria foi encontrada em região de cabeça, sendo visualizada em 58% de animais (21/24), as lesões nos membros foram encontradas em 36% animais (13/24), e apenas 6% dos animais (5/24) apresentou lesões no tronco . Considerando que a maioria dos animais apresentavam lesões múltiplas, a maioria dos animais apresentava lesões em mais de uma localização (Figuras 8, 9 e 10).

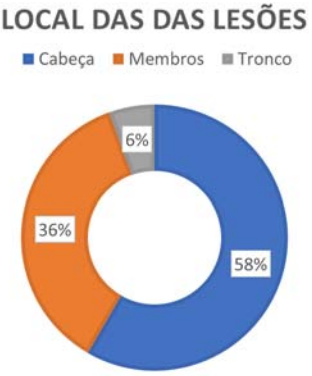


Figura 8 : Gráfico da localização das lesões.

Figura 9: Gato com esporotricose manifestando lesões na cabeça e nos membros.

Figura 10: Gato com esporotricose manifestando lesões na cabeça.

Segundo Santos *et al*. (2020) e Bazzi *et al*. (2016), as lesões são majoritariamente encontradas na região da cabeça e nos membros torácicos, semelhante ao que foi visto nos animais avaliados no estudo.

4. CONCLUSÕES

Foi observada uma predominância de lesões purosanguinolentas e múltiplas, principalmente nas regiões de cabeça e membros. Estas múltiplas lesões indicavam um acometimento mais extenso da doença, que geralmente está associado às condições de saúde dos felinos.

5. REFERÊNCIAS

1. BAZZI, T., DE MELO S. M. P., FIGHERA R. A., KOMMERS G. D. Clinical, epidemiological, histomorphological and histochemical characteristics of the feline sporotrichosis. Pesq Vet Bras. **2016**, 36, 303-311.
2. CROTHERS S. L., WHITE S. D., IHRKE P. J., AFFOLTER V K. Sporotrichosis: a retrospective evaluation of 23 cases seen in Northern California (1987-2007). Vet Dermatol. **2009**, 20, 249-259.
3. DE ALMEIDA F., SAMPAIO S. A., LACAZ C. da S., FERNANDES J. de C. Dados estatísticos sobre a esporotricose; análise de 344 casos. An Bras Derm Sifilogr. **1955**, 30, 9-12.
4. GREMIÃO I. D. F., DA ROCHA E. M. da S., MONTENEGRO H., CARNEIRO A. J. B., XAVIER M. O., DE FARIAS M. R., MONTI F., MANSHO W., PEREIRA R. H. de M. A., PEREIRA S. A., LOPES-BEZERRA L. M. Guideline for the management of feline sporotrichosis caused by *Sporothrix brasiliensis* and literature revision. Braz J Microbiol. **2021**, 52, 107-124.
5. LARSSON E. C. Sporotrichosis. Braz J of Vet Res and Anim. **2011**, 48, 250-259.
6. LUTZ A., SPLENDORE A. Sobre uma micose observada em homens e ratos: contribuição para o conhecimento das assim chamadas esporotricoses. Rev Med. **1907**, 21, 443-450.
7. PEREIRA S. A., GREMIÃO I. D. F., MENEZES R. C. Sporotrichosis in animals: zoonotic transmission. Spring Lin. **2015**, 83-102.
8. ROSSER E. J., DUNSTAN R W. Infectious diseases of the dog and cat. Saund Else. **2006**, 608-612.
9. SANTOS, A. F. Esporotricose felina: distribuição das lesões e caracterização anatomopatológica utilizando diversos métodos de diagnóstico. Dissertação (Mestrado) - Programa de Pós-Graduação em Ciência Animal, Escola de Veterinária, Universidade Federal de Minas Gerais, Belo Horizonte. **2020**, 53f.
10. SCHUBACH, T. M. P., SCHUBACH A., OKAMOTO T., BARROS M. B. L., FIGUEIREDO F. B., CUZZI T., FIALHO-MONTEIRO P. C., REIS R. S., PEREZ M. A., WANKE B. Evaluation of an epidemic of sporotrichosis in cats: 347 cases (1998-2001). J Am Vet Med Assoc. **2004**, 224, 1623-1629.
11. VIEIRA, S. Introdução à bioestatística. Elsevier. **2011**. 345.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

RELEVANCE OF FELINE HEALTH AND CLINICAL CHARACTERISTICS OF SPOROTRICOSIS

Sofia Marques Rocha
Universidade de Vassouras, veterinary medicine, Brazil.

Bruna Hudson Neves Pereira
Universidade de Vassouras, veterinary medicine, Brazil.

Emanuelle Silva de Oliveira
Universidade de Vassouras, veterinary medicine, Brazil.

Letícia dos Santos Junqueira
Universidade de Vassouras, veterinary medicine, Brazil.

Glenda Ribeiro de Oliveira
Universidade de Vassouras, veterinary medicine, Brazil.

March/2022

INTRODUCTION

SBJChem Conference 2021

Zoonosis

Mycosis → *Sporothrix* complex → *Sporothrix brasiliensis*

Infection

→ Licks, scratches, bites or contact with lesions

BACKGROUND

SBJChem Conference 2021

Cutaneous injuries:

- Localized cutaneous
- Lymphatic cutaneous
- Disseminated cutaneous

Figure 1: Nodular lesion in a cat foot. Source: Personal collection, 2021.

Figure 2: Ulcerated lesion in a cat nose. Source: Personal collection, 2021.

Figure 3: Ulcerated and serosanguineous lesion in a cat neck. Source: Personal collection, 2021.

OBJETIVE

SBJChem Conference 2021

Correlate the conditions of general health and feline management from different neighborhoods of Vassouras – RJ, with disease's presence and severety.

METHODOLOGY

SBJChem Conference 2021

The study happened from october to november in Vassouras - RJ, in association with Universidade de Vassouras and Secretaria Municipal de Saúde.

24 felines previously diagnosed with sporotrichosis.

Sudents make home visits to collect information for a questionnaire.

General health

Lesions

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Vaccine
- Vermifuge
- Ectoparasite control
- Portion (Cat food)

Poor health
(Larsson *et al., 2011)*

RESULTS AND DISCUSSION

SBJChem Conference 2021

Figure 4: Graphic of injury type.

Figure 5: Cat with single lesion. Source: Personal collection, 2021.

Figure 6: Cat with multiple lesions. Source: Personal collection, 2021.

More common to find multiple lesions.
(Santos *et al., 2020)*

RESULTS AND DISCUSSION

SBJChem Conference 2021

Figure 7: Graphic of characteristics of the lesions.

Figure 8: Serosanguineous lesion in a cat. Source: Personal collection, 2021.

Figure 9: Lesion without secretion in a cat. Source: Personal collection, 2021.

Lesions with secretion are associated with the severity of symptoms.
(Gremiao *et al., 2020)*

RESULTS AND DISCUSSION

SBJChem Conference 2021

Figure 10: Graphic of respiratory symptoms.

Video 1: Video showing cat with respiratory symptoms. Source: Personal collection, 2021.

Is common to find respiratory symptoms. (Schubach *et al., 2004*; Crothers *et al., 2009)*

RESULTS AND DISCUSSION

SBJChem Conference 2021

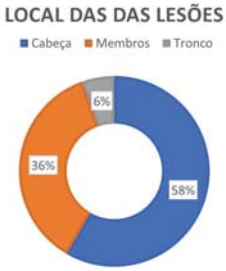


Figure 11: Graphic of lesions localization.

Figure 12: Cat with head and limb injuries.

Figure 13: Cat with head injuries.

Lesions are mostly found in the head. (Santos *et al., 2020*; Bazzi *et al., 2016)*

CONCLUSIONS

SBJChem Conference 2021

Characteristics of lesions

+

Severety of symptoms

→ General health

↓

Development of sporotrichosis

REFERENCES

SBJChem Conference 2021

1. BAZZI, Talissa *et al*. Características clínico-epidemiológicas, histomorfológicas e histoquímicas da esporotricose felina. **Pesq. Vet. Bras.** v. 3, p. 4, fev. 2016.
2. Crothers, Samantha L et al. "Sporotrichosis: a retrospective evaluation of 23 cases seen in northern California (1987-2007)." *Veterinary dermatology* vol. 20,4 (2009): 249-59. doi:10.1111/j.1365-3164.2009.00763.x
3. Gremião, I.D.F. *et al.* Guideline for the management of feline sporotrichosis caused by *Sporothrix brasiliensis* and literature revision. *Braz J Microbiol* **52,** 107–124 (2021). https://doi.org/10.1007/s42770-020-00365-3
4. Larsson, C. E. Esporotricose. **Braz. J. Vet. Res. Anim. Sci.** São Paulo, v. 48, n. 3, p. 250–259, 2011.
5. Lutz A., Splendore A. Sobre uma micose observada em homens e ratos. **Rev Med**, São Paulo, v. 21, p. 433–450, 1907.
6. SANTOS, Ágna Ferreira. **Esporotricose felina: distribuição das lesões e caracterização anatomopatológica utilizando diversos métodos de diagnóstico**. 2020. 53 f. Dissertação (Mestrado) - Programa de Pós-Graduação em Ciência Animal, Escola de Veterinária, Universidade Federal de Minas Gerais, Belo Horizonte, 2020.
7. Schubach, Tânia M P et al. "Evaluation of an epidemic of sporotrichosis in cats: 347 cases (1998-2001)." *Journal of the American Veterinary Medical Association* vol. 224,10 (2004): 1623-9. doi:10.2460/javma.2004.224.1623.


SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

SELF-ASSEMBLED MULTILAYERS OF WATER-SOLUBLE MODIFIED-CHITOSAN AND GLUCOSE OXIDASE FOR DETECTION OF GLUCOSE IN MILK SAMPLES

GULOTTA, Florencia A.[1]; DIAZ VERGARA, Ladislao[2]; MONTENEGRO, Mariana[2]; FERREYRA Nancy F.[3*], PAZ ZANINI, Verónica I.[1*]

[1] Instituto de Bionanotecnología del NOA (INBIONATEC), CONICET, Universidad Nacional de Santiago del Estero (UNSE), Argentina.

[2] Centro de Investigaciones y Transferencia de Villa María (CIT-VM), Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Universidad Nacional de Villa María (UNVM), Argentina.

[3] Instituto de Investigaciones en Fisicoquímica de Córdoba (INFIQC-UNC-CONICET), Departamento de Fisicoquímica, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba, Argentina.

** Correspondence author*
e-mail: nfferreyra@unc.edu.ar

Received 20 December 2021; received in revised form 03 January 2022; accepted 14 January 2022

ABSTRACT

Multilayer films made of glucose-functionalized chitosan (G-Chit) and glucose oxidase (GOx) were built by layer-by-layer self-assembly technique onto carbon paste electrodes (CPE). The obtained bioelectrodes were characterized by cyclic voltammetry and chronoamperometry. Results indicated that catalytic response increases with the number of bilayers G-Chit/GOx and the enzyme concentration obtaining the best responses for 3 bilayers and 2 mg ml^{-1}, respectively. The effect of pH on the bioelectrode response was also investigated, it was found that the optimal working value is 7.0. Under optimized experimental conditions, the biosensor exhibits a sensitivity of (0.81 ± 0.03) μA mM^{-1} in a glucose concentration range 0.18 to 1.75 mM. The analytical response of the biosensor was tested in milk samples with negligible matrix effects. Results show that G-Chti appears promising for the immobilization of enzymes.

Keywords: *Glucose biosensor, glucose-functionalized chitosan, carbon paste electrode*

1. INTRODUCTION

Glucose quantification is of significant importance in the chemical and biological industries, in clinical analysis, as well as in food processing and fermentation (Yusan *et al.*, 2018). In the food industry, the glucose content is associated with storage time, fermentation process, and final quality control (Paz Zanini *et al.*, 2016). For those reasons, accurate glucose quantification with a quick and simple method has driven the search for new testing devices and procedures. Various methods have been reported for GOx immobilization, such as covalent cross-linking, electrochemical polymerization, sol-gel encapsulating, and layer-by-layer (LBL) self–assembly based on the electrostatic interaction with polyelectrolytes of opposite charge (Bracamonte *et al.*, 2014). This last method has attracted great interest due to its simplicity, wide variety of materials that can be used, and the precise control of composition and thickness of the layer on the molecular level. Among other polymers, the natural polycation chitosan (Chit), a copolymer composed of randomly distributed units of N-acetyl-D-glucosamine and D-glucosamine linked by β(1→4) bonds, has been employed to immobilize enzymes. The biocompatibility, biodegradability, non-toxicity, and bioactivity of

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.07_abstract_FERREYRA.pdf

Chit associated with desirable physical and mechanical properties have made this polymer interesting and promising in biosensors development. However, Chit applications are limited because of its poor solubility at neutral or basic pH. Several studies have been carried out to obtain Chit derivatives soluble in an aqueous medium at physiologic pH, one of them involves the Maillard reaction (MR) between the amino group of Chit and the carbonyl group of reducing sugar (Badano *et al.*, 2019).

In this work, we used Chit modified with glucose residues (G-Chit) synthesized through MR reaction to immobilize GOx by the LBL self–assembly technique at carbon paste electrodes (CPE). This material has advantages: low cost of fabrication, renewable or disposable electrochemical interface, and low background current (Donmez *et al.*, 2017). The electrochemical properties of the bioelectrode have been characterized by chronoamperometry (CA) and cyclic voltammetry (CV). Furthermore, the electroanalytical performance of the biosensor was evaluated for the determination of glucose in standard solutions and also in milk samples. The presented results confirmed the suitability of this supramolecularly assembled bioelectrode for the fast quantification of glucose.

2. MATERIALS AND METHODS

2.1. Reagents and materials

Glucose Oxidase (GOx, EC 1.1.3.4 from Aspergillus Niger type II) lyophilized powder containing 17300 units g^{-1} solid. Reagent grade D-(+)-glucose and ferrocene methanol (FcMe) were purchased from Sigma-Aldrich SA (Buenos Aires, Argentina). Reagent grade buffer phosphate potassium salts KH_2PO_4 and K_2HPO_4 were obtained from Cicarelli. Solutions were prepared with ultrapure water. G-Chit was synthesized by Dr. M. Montenegro (Badano *et al.*, 2019).

2.1.1 Electrochemical measurements

Cyclic Voltammetry (CV) and chronoamperometry (CA) studies were carried out with a potentiostat /galvanostat (Teq4, Buenos Aires, Argentina). The experiments were performed in a three-compartment electrochemical cell. A large-area platinum wire and an Ag/AgCl/3 M NaCl electrode (Model RE-5B, BAS) were used as counter and reference electrodes, respectively. The reported potentials are referred to this reference electrode. All experiments were performed at room temperature. A 0.10 M phosphate buffer solution (PBS) at pH 7.0 was used as a background electrolyte, with 2.0 x 10^{-4} M FcMe as an artificial mediator of the enzymatic reaction. Solutions were deoxygenated by controlled N_2-bubbling for 20 min preceding the measurements, and the gas flow was kept over the solution during the experiments. CA experiments were performed at 0.350 V under convective conditions using magnetic stirring. The current response was registered as a function of time after sequential addition of glucose aliquots of chosen concentrations.

2.1.1.1 Preparation of composite multilayer films

Previous to the preparation of the composite multilayer film, the surface of the CPE was activated by applying an anodic potential of 1.20 V in Na_2CO_3 saturated solution for 5 min to expose negative charges. Next, the LbL film was prepared by alternating immersions of the electrode in solutions containing G-Chit (0.5 mg mL^{-1} aqueous solution, pH 5) and GOx (2 mg mL^{-1} in PBS pH 7.0). The adsorption time was 30 min for both polyelectrolytes, G-Chit and GOx.

3. RESULTS AND DISCUSSION:

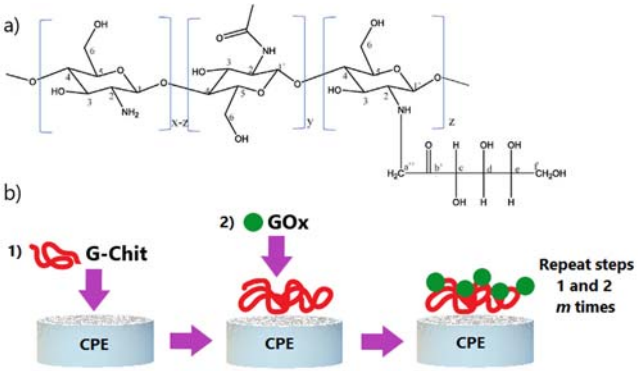


Figure 1. *G-Chit structure and construction of the self-assembled structure*

Figure 1 shows the chemical structure of the polycation and the self-assembled procedure. In an aqueous solution, the polymer has a zeta potential of (89±7) mV that allows the construction of the multilayer structure with GOx negatively charged at the pH of the assembly (the isoelectric point of the enzyme is 4.2). The enzymatic response at the CPE modified electrode was analyzed by CV. Figure 2 shows cyclic voltammograms of CPE/(G-Chit/GOx)$_m$, where m correspond to the number of bilayers (m=1,2,3,4) in N_2-saturated solution. In the absence of glucose, reversible redox waves of FcMe are observed. After the addition of 0.050 M glucose, a

well-defined sigmoidal voltammetric profile is noticed due to the GOx catalytic reaction at the bioelectrode according to the following scheme:

$$FcMe_{red} \rightleftharpoons FcMe_{ox} + e$$

$$GOx(FAD) + G \rightleftharpoons GOx(FADH_2) + GL$$
$$GOx(FADH_2) + 2FcMe_{ox} \rightarrow GOx(FAD) + 2FcMe_{red}$$

$$G = Glucose;\ GL = Gluconolactone$$

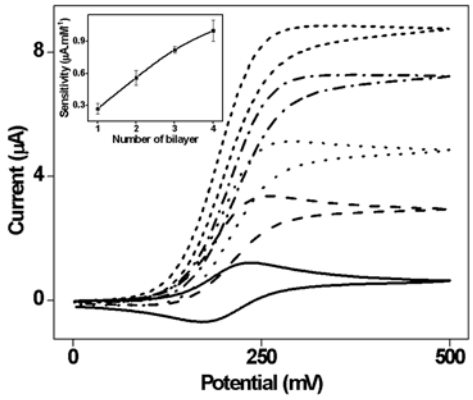


Figure 2. *CV at CPE/(G-Chit-GOx)$_m$ in 0.10 M phosphate buffer solution pH 7.0* + 2 x 10^{-4} M *FcMe in absence (solid line) and presence of 0.050 M of glucose. Scan rate 5 mV s^{-1}.*

This result suggested that the enzyme has successfully assembled on the electrode surface and remains active. Moreover, the catalytic current, i_{cat}, increases proportionally with the number of G-Chit/GOx bilayers in the range evaluated up to m=4.

The influence of enzyme concentration used in the construction of CPE/(G-Chit-GOx)$_3$ was evaluated by analyzing the sensitivity obtained in CA experiments. The values obtained are (0.44 ± 0.06), (0.82 ± 0.03) and (0.8 ± 0.1) μA mM^{-1} for 1, 2 and 5 mg·mL^{-1} of the enzyme, respectively. The sensitivity value duplicates when the concentration of enzyme increases from 1 to 2 mgmL^{-1} and then remains unchanged, indicating that the maximal amount of enzyme adsorbed is reached under this condition.

The ionization state of the amino acids in the active site can affect enzyme activity. Thus, pH has a significant function in maintaining the proper conformation of the active site in the enzyme. The pH effect on the biosensor response was evaluated by CV in the range from 5.0 to 9.0, adding 0.050 M glucose to the cell. The ratio between the i_{cat}, and the current in the absence of glucose, i_b, were calculated. The maximum response, i_{ca}/i_b, was obtained at pH 7.0 (Fig. 3), and hence it was chosen as optimum pH for further studies. The results are an average of five measurements.

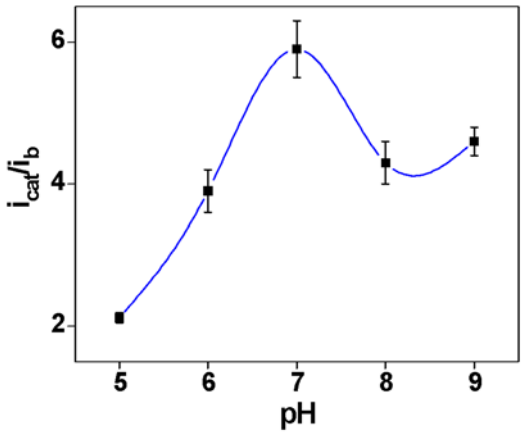


Figure 3. *Effect of pH on the response of the CPE/(G-Chit-GOx)$_1$ at 0.486 V in 0.10 M phosphate buffer at different pH* + 2 x 10^{-4} M *FcMe and 0.050 M of glucose.*

The electroanalytical properties of the bioelectrode immediately after preparation for the optimized experimental conditions: m=3, GOx 2mg mL^{-1}, and pH 7.0 were analyzed. The detection limit (LOD) and LOQ were calculated using the criterion of *3 x SD/s* or 10 *x SD/s, respectively,* where *SD* is the standard deviation of the background current and *s* the sensitivity (Paz Zanini et al. 2016). The linear range of operation is (0.18-1.55) mM. At the same time, LOD, LOQ, and Sensitivity are values obtained are 60 μM, 180 μM, and (0.81 ± 0.03) μA mM^{-1}, respectively.

The bioelectrode was tested in real samples of commercial milk La Serenisima®. The obtained value for the seven consecutive determinations was (2.2 ± 0.2) g·L^{-1}. According to a t-test at a 95% confidence level, these values agree with the manufacturer reported value, e.g., 2 g·L^{-1}. In addition, in order to check possible matrix effects, the percentage of relative recovery

(RA%) of the current signal produced by an aliquot of 0.25 mmol l^{-1} glucose before and after the addition of 10 µL of the sample was measured, Fig. 4, and calculated by the following equation:

$$RA(\%) = \frac{i_2}{i_1}\, x\, 100\%$$

where i_1 and i_2 are the amperometric signals before and after adding the sample. The sample volume used produced %RA values ranging 62-85%.

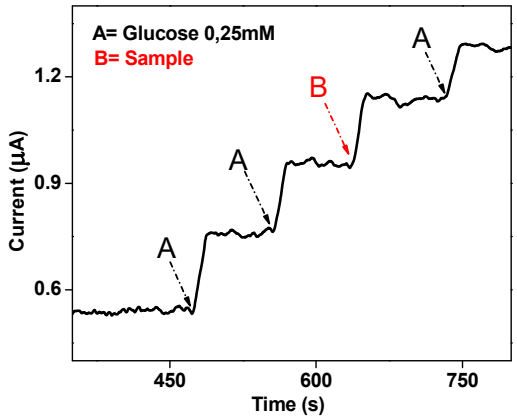


Figure 4. *Amperometric response at 0.35 V on the selected bioelectrode for successive additions of (A) Glucose 2.5 x 10^{-4} M and (B) milk sample. Supporting electrolyte: 0.10 M phosphate buffer solution containing 2.0 x 10^{-4} FcMe.*

4. CONCLUSIONS:

Multilayer films made of G-Chit and GOx were successfully built onto CPE. The best responses were obtained with 2 mg ml^{-1} of enzyme, 3 bilayers of polyelectrolytes, and working at pH 7.0. Under optimized experimental conditions, the biosensor exhibits a sensitivity of (0.81 ± 0.03) µA mM^{-1} and a linear range of (0.18 to 1.75) mmol·L^{-1}. In addition, the analytical response of the biosensor was tested in milk samples with negligible matrix effects. Results show that G-Chit appears promising for the immobilization of enzymes.

5. ACKNOWLEDGMENTS:

The authors thank SECyT-UNC, and Agencia Nacional de Promoción Científica y Tecnológica (ANPCYT) [grant number PICT-2015-0479] and CICyT-UNSE [grant number 23/A260] for the financial support. F.A. Gulotta, thanks CONICET for the fellowship.

6. REFERENCES:

1. Badano, J. A., Braber Vanden, N., Rossi, Y., Díaz Vergara, L., Bohl, L., Porporatto, C., Falcone, R. D., Montenegro, M. *Carbohydr Polym*, **2019**, *224*.

2. Bracamonte, M. V., Yañez, C., Bollo, S., Rivas, G. A., Ferreyra, N. F. *J. Electroanal. Chem.*, **2014**, *712*, 124–131.

3. Donmez, S., Arslan, F., Sarı, N., Hasanoğlu Özkan, E., Arslan, H. *Biotechnol Appl Biochem*, **2017** *64*(5), 745–753.

4. Paz Zanini, V. I., Gavilán, M., López De Mishima, B. A., Martino, D. M., Borsarelli, C. D. *Talanta*, **2016**, *150*, 646–654.

5. Yusan, S., Rahman, M. M., Mohamad, N., Arrif, T. M., Latif, A. Z. A., Mohd Aznan, M. A., Wan Nik, W. S. B. *J Anal Methods Chem*, **2018**, *2018*.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

SELF-ASSEMBLED MULTILAYERS OF WATER SOLUBLE MODIFIED-CHITOSAN AND GLUCOSE OXIDASE FOR DETECTION OF GLUCOSE IN MILK SAMPLES

Florencia Alejandra Gulotta
Universidad Nacional de Santiago del Estero, Facultad de Agronomía y Agroindustrias, Instituto de Bionanotecnología del NOA (INBIONATEC), CONICET - Argentina.

Ladislao Diaz Vergara
Universidad Nacional de Villa María, Centro de Investigaciones y Transferencia de Villa María (CIT-VM), CONICET- Argentina

Mariana Montenegro
Universidad Nacional de Villa María, Centro de Investigaciones y Transferencia de Villa María (CIT-VM), CONICET- Argentina

Nancy Fabiana Ferreyra
Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, Instituto de Investigaciones en Fisicoquímica de Córdoba (INFIQC), CONICET - Argentina

Verónica Irene Paz Zanini
Universidad Nacional de Santiago del Estero, Facultad de Agronomía y Agroindustrias, Instituto de Bionanotecnología del NOA (INBIONATEC), CONICET - Argentina.

December/2021

INTRODUCTION

SBJChem Conference 2021

- Chitosan (Chit) polymer have demonstrated to be an interesting element to develop biosensors.
- Chit applications are limited because of its poor solubility at neutral or basic pH.
- To improve the solubility, Chit has been chemically modified by different methodologies.
- Maillard Reaction (MR) between amino groups of Chit and the carbonyl groups (–C=O) of carbohydrates like glucose can be used to obtain water soluble Chit (G-Chi).
- The polycation, G-Chit, can be electrostatically self assembled with polyelectrolytes of opposite charge, like glucose oxidase (GOx) enzyme.

OBJECTIVE

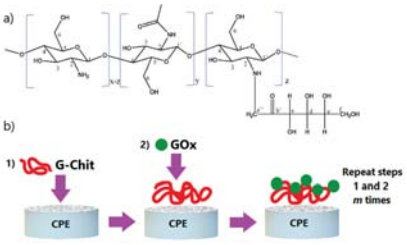
SBJChem Conference 2021

- Immobilize the enzyme glucose oxidase on carbon paste electrodes by electrostatic assembly with modified-chitosan.
- Apply the bioelectrode in detection of glucose in milk samples.

METHODOLOGY

SBJChem Conference 2021

Preparation of the working electrode



Electrochemical measurements
✔ Cyclic Voltammetry (CV)
✔ Chronoamperometry (CA)

CPE: graphite/mineral oil (70/30 %w/w).

Activation of CPE: 1.20 V in Na_2CO_3 saturated solution, 5 min

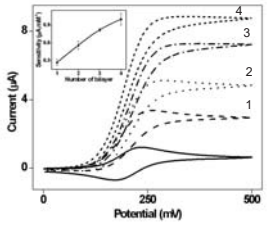
1) 0.5 mg ml^{-1} G-Chit aqueous solution. Time =30 min

2) 2.0 mg mL^{-1} GOx in 0.10 M PBS pH 7.0. Time =30 min

RESULTS AND DISCUSSION

SBJChem Conference 2021

Catalytic current of CPE/(G-Chit/GOx)$_m$



$FcMe_{red} \rightleftharpoons FcMe_{ox}+e$

$GOxFAD+G \rightleftharpoons GOx(FADH_2)+GL$

$GOx(FADH_2)+ 2FcMe_{ox} \rightarrow GOxFAD+2FcMe_{red}$

G=Glucose; GL=Gluconolactone

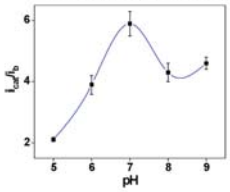


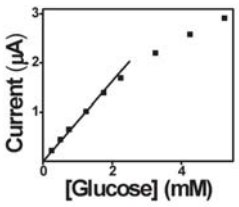
Figure 1. *CV at CPE/(G-Chit-GOx)$_m$ with m=1,2,3,4 in 0.10 M PBS pH 7.0 + 2 x 10^{-4} M FcMe in absence (solid line) and presence of 0.050 M of glucose. Scan rate 5 mV s^{-1}.*

Figure 2. *Effect of pH on the response of the CPE/(G-Chit-GOx)$_1$ at 0.486 V in 0.10 M PBS at different pH + 2 x 10^{-4} M FcMe + 0.050 M of glucose.*

RESULTS AND DISCUSSION

SBJChem Conference 2021

Calibration plot at CPE/(G-Chit-GOx)$_3$



Determination of glucose in milk samples

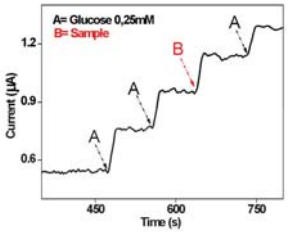


Figure 3. *A) Calibration plot. B) CA response at 0.35 V on the selected bioelectrode, for successive additions of (A) Glucose 2.5 x 10^{-4} M and (B) milk sample. Supporting electrolyte: 0.10 M PBS + 2.0 x 10^{-4} MFcMe.*

CONCLUSIONS

SBJChem Conference 2021

✔ G-Chit obtained by MR is soluble a pH compatibles with the enzyme reaction.

✔ The positive charges of G-Chit allowed to immobilize GOx by the LBL electrostatic self–assembly at CPE.

✔ The bioelectrode with best responses was obtained with 2.0 mg ml^{-1} of GOx, 3 bilayers of (G-Chit-GOx) and working at pH 7.0.

✔ Under optimized experimental conditions, the biosensor exhibits a sensitivity of (0.81 ± 0.03) μA mM^{-1}, LOQ (18 ± 6) 10^{-5} M and a linear range of (180 to 1750) μM.

✔ The analytical response of the biosensor was tested in milk samples with negligible matrix effects.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

- SECyT-UNC.
- Agencia Nacional de Promoción Científica y Tecnológica (ANPCYT) [PICT-2015-0479].
- F. A. Gulotta thanks CONICET for the fellowship.
- SBJChem organizing committee.

UNC Universidad Nacional de Córdoba

AGENCIA NACIONAL DE PROMOCION CIENTIFICA Y TECNOLOGICA

CONICET

REFERENCES

SBJChem Conference 2021

1. Badano, J. A., Braber Vanden, N., Rossi, Y., Díaz Vergara, L., Bohl, L., Porporatto, C., Falcone, R. D., Montenegro, M. (2019). Physicochemical, in vitro antioxidant and cytotoxic properties of water-soluble chitosan-lactose derivatives. *Carbohydrate Polymers.*, (224). doi:10.1016/j.carbpol.2019.115158

1. Bracamonte, M. V., Yañez, C., Bollo, S., Rivas, G. A., Ferreyra, N. F. (2014). Physico-chemical characterization of ferrocenyl-modified hyperbranched poly(ethylenimine) self-assembled multilayers. *Journal of Electroanalytical Chemistry,* (712): 124–131. doi: 10.1016/j.jelechem.2013.11.018.

1. Donmez, S., Arslan, F., Sarı, N., Hasanoğlu Özkan, E., Arslan, H. (2017). Glucose biosensor based on immobilization of glucose oxidase on a carbon paste electrode modified with microsphere-attached l-glycine. *Biotechnology and Applied Biochemistry, 64*(5): 745–753. doi: 10.1002/bab.1533.

1. Paz Zanini, V. I., Gavilán, M., López De Mishima, B. A., Martino, D. M., Borsarelli, C. D. (2016). A highly sensitive and stable glucose biosensor using thymine-based polycations into laponite hydrogel films.*Talanta*, (150): 646–654. doi: 10.1016/j.talanta.2015.12.046.

1. Yusan, S., Rahman, M. M., Mohamad, N., Arrif, T. M., Latif, A. Z. A., Mohd Aznan, M. A., Wan Nik, W. S. B. (2018). Development of an Amperometric Glucose Biosensor Based on the Immobilization of Glucose Oxidase on the Se-MCM-41 Mesoporous Composite. *Journal of Analytical Methods in Chemistry*, (2018). doi: 10.1155/2018/2687341.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

SEROPREVALENCE AND CLINICAL MANIFESTATIONS OF DOMICILED DOGS (CANIS LUPUS FAMILIARIS) CLOSE TO A HUMAN CASE OF VISCERAL LEISHMANIASIS

FERREIRA, Lucas Leal [1*]; BELEGOTE, Amanda Alfeld [1]; SILVA, Laís Freire [1]; CABRAL, Steffany Souza [1]; DOS SANTOS Priscilla Nunes [1]

[1]Universidade de Vassouras, Medicina Veterinária

** Correspondence author*
e-mail: lucaslferreira98@gmail.com

Received 02 February 2022; received in revised form 16 February 2022; accepted 24 February 2022

ABSTRACT

Canine visceral leishmaniasis (CVL) is a disease with a great impact on public health in Brazil due to its zoonotic potential. One of the biggest challenges in controlling the disease is the fact that its main reservoir in urban areas is the domestic dog, and thus, it is a source of infection that lives very close to the human being. This study aimed to determine the seroprevalence of *L. chagasi* and the symptoms of CVL present in dogs living near a human case confirmed by the Municipal Health Department of the municipality of Vassouras. Blood samples were collected from the cephalic vein of 14 resident dogs within a radius of 150 meters from a confirmed human case. This collected material was submitted to the DPP screening test, and the positive samples were submitted to the ELISA confirmatory test. Information was also obtained through questionnaires about the presence of the disease's clinical signs. Of the 14 animals tested in the DPP, only 4 were positive in the screening test, and all presented negative results in the ELISA confirmatory test. Of the 14 dogs, 4 had symptoms. Of these, 2 presented skin lesions, and 1 animal showed cough, while the last one exhibited vomiting. It is concluded that the DPP screening test for CVL is a practical and easy to handle method, although it requires attention due to the possibility of cross-reaction with other etiological agents in dogs. The human case is probably a result of a non-autochtone infection. Therefore, asymptomatic dogs should be under disease surveillance since these hosts also act as a source of infection for vector insects.

Keywords: *Leishmania chagasi. DPP. Seroprevalence*.

1. INTRODUÇÃO

A leishmaniose visceral canina (LVC) é uma zoonose de grande importância na saúde pública. No Brasil, seu principal agente etiológico é o protozoário *Leishmania chagasi*, transmitido principalmente através da picada do flebotomíneo *Lutzomyia longipalpis* (Ministério da Saúde, 2014). Na área urbana, o cão doméstico (*Canis familiaris*) é o principal reservatório animal (Romero; Boelaert, 2010) e principal fonte de infecção por estar em contato direto com o ser humano, tornando-se assim, presente entre as seis endemias de prioridade mundial (Ministério da Saúde, 2014). Animais infectados podem ser classificados de acordo com os sinais clínicos, como: assintomáticos, oligossintomáticos e sintomáticos. Os sintomas da LVC são variados e inespecíficos, porém, os mais característicos quando plenamente apresentados são: alterações cutâneas, onicogrifose, emagrecimento, ceratoconjuntivite e paresia dos membros posteriores (Ministério da Saúde, 2014). Já foi demonstrado que cães infectados por *L. chagasi*, ainda que assintomáticos, são fontes de infecção para os flebotomíneos, tendo papel ativo no ciclo de *Leishmania* (Gontijo; Melo, 2004), ressaltando a importância da testagem e identificação destes animais infectados, para o controle da doença.

De acordo com o Ministério da Saúde (2011), o protocolo de testagem se dá pelo Teste rápido de triagem *Dual Path Platform* (TR-DPP®-Bio-Manguinhos) e o ELISA – (*Enzyme Linked Immunosorbent Assay*-Bio-Manguinhos) como teste confirmatório.

O objetivo do presente estudo, foi realizar uma avaliação da soroprevalência de *L. chagasi* e

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.30_abstract_FERREIRA.pdf

avaliar a presença de sintomas de LVC em cães domiciliados em uma área de 150 metros a partir de um caso humano confirmado no município de Vassouras, Rio de Janeiro.

2. MATERIAIS E MÉTODOS

O estudo ocorreu nos meses de outubro e novembro de 2021 no bairro Itakamosi, no município de Vassouras, RJ em conjunto com a Secretaria Municipal de Saúde. Devido à ocorrência de confirmação de um caso positivo para leishmaniose em um ser humano, foram realizadas coletas de sangue e testes sorológicos de 14 cães domiciliados em um raio de até 150 metros do caso humano notificado.

Para a coleta de sangue, foram utilizados escalpes 21G e 23G ou agulhas 25x7 mm, acoplados a seringas descartáveis de 5mL com prévia antissepsia, utilizando algodão embebido em álcool etílico 70% para acessar a veia cefálica. A partir do sangue coletado, uma pequena amostra foi utilizada no teste rápido de triagem *Dual Path Platform* (TR-DPP®-Bio-Manguinhos), enquanto o restante foi reservado em um tubo de coleta com ativador de coágulo para posterior centrifugação e obtenção de soro. Nos casos positivos para o teste rápido, as respectivas amostras de soro foram encaminhadas para a FIOCRUZ, onde foram submetidas ao teste sorológico confirmatório ELISA (*Enzyme Linked Immuno Sorbent Assay*-Bio-Manguinhos).

Foram coletadas informações dos animais testados a partir de questionários, a respeito da presença de manifestações clínicas. Utilizou-se a estatística descritiva básica, para a avaliação de resultados dos testes sorológicos e dos dados obtidos por meio dos questionários, determinando-se as frequências relativas e os percentuais de cada variável.

3. RESULTADOS E DISCUSSÃO

No inquérito sorológico foram testados 14 animais, sendo que 28,50% (4/14) obtiveram resultado positivo (Figura 1), e 71,4% (10/14) dos animais apresentaram resultado negativo.

Figura 1. *Resultado positivo, obtido através do teste rápido (DPP). A linha representada pela letra "C" indica o controle, e a linha representada pela letra "T", a amostra teste (que ao aparecer representa um resultado positivo).*

Os animais que apresentaram resultado positivo para a doença no teste de triagem (DPP) e foram submetidos ao teste confirmatório ELISA (*Enzyme Linked Immuno Sorbent Assay*-Bio-Manguinhos), apresentaram um resultado negativo para leishmaniose visceral canina em 100% (4/4) dosanimais (Figura 2).

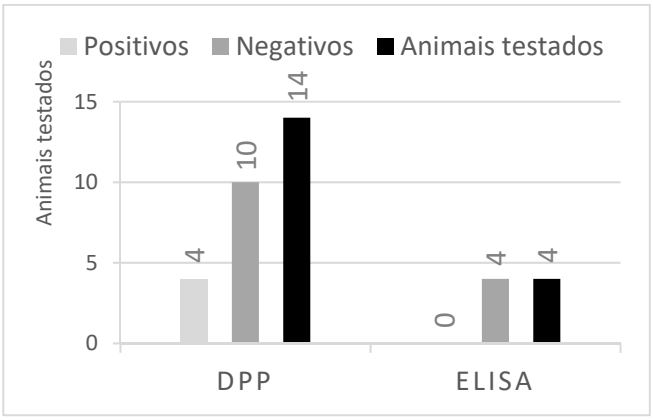


Figura 2. *Resultados obtidos no teste rápido (DPP), e no teste sorológico confirmatório (ELISA).*

Embora o teste DPP tenha vantagens como fácil manipulação, transporte, resultado rápido e uma pequena quantidade de amostra requerida, ele apresenta uma baixa especificidade em comparação aos testes sorológicos convencionais, ocorrendo reações cruzadas com agentes como *Babesia canis, Ehrlichia canis, Anaplasma spp*. e produzindo um resultado falso-positivo para LVC (Lima *et al*.,2010; Maia;

Campino, 2008). Considerando que todos os animais do presente estudo apresentaram resultados negativos no teste confirmatório, pode-se afirmar que todos os resultados positivos no DPP se configuravam como resultados falsos-positivos, possivelmente em decorrência de uma reação cruzada com hemoparasitos. Os resultados negativos encontrados em cães, apesar do caso humano positivo previamente notificado, indicam que a infecção no ser humano não foi autóctone, pois em regra geral os casos em cães são mais prevalentes e precedem a ocorrência de casos em humanos (Dantas-Torres, 2007).

Dos 14 animais testados, apenas 28,50% (4/14) apresentaram sintomas. Observou-se que 2 destes 4 animais, apresentaram lesões de pele. Também foi observado que outros 2 apresentaram sintomas inespecíficos, com a manifestação de tosse em um animal e vômito no outro. Um animal infectado pode manifestar sinais clínicos graves ou permanecer assintomático por muito tempo (Brandonisio *et al*., 1992; Dantas-Torres *et al* 2006; Lanotte *et al*., 1979). A manifestação de sinais clínicos pode ser variada, dentre eles os mais comuns que correspondem a linfadenomegalia, alopecia, atrofia muscular, anorexia, alterações oftalmológicas e neurológicas (Contreras, *et al*., 2019). Os sinais clínicos no cão são variáveis, dependendo do órgão que for atingido. Um dos principais sinais clínicos são apatia, anorexia, emagrecimento, lesões cutâneas (especialmente no focinho e nas orelhas), crescimento exacerbado das unhas (onicogrifose), linfadenomegalia e febre (Crivellenti, 2015). Outros sintomas e sinais são hepatite, epistaxe, anemia não-regenerativa, diarreia, hepatoesplenomegalia, problemas articulares, conjuntivite, lesões oculares e lesões dermatológicas (Dantas-Torres *et al*., 2012; Feitosa *et al*., 2000; Wilson *et al*., 2012). Houve uma predominância de animais assintomáticos, representando 71% (10/14) dos animais avaliados. Embora neste estudo os animais fossem negativos, animais assintomáticos também representam potenciais reservatórios da doença (Michalsky *et al*., 2007). Em áreas endêmicas a LVC gera problemas no âmbito de saúde pública, devido principalmente ao alto percentual (até 85%) de animais assintomáticos (Dantas, *et al*., 2006). Os animais assintomáticos, assim como os sintomáticos, podem servir como reservatórios para a transmissão vetorial de Leishmania spp. para animais e humanos suscetíveis (Michalsky *et al*., 2007; Molina *et al*., 1994). Solano-Galego *et al*. (2009) observaram em seu estudo que 50% dos animais não apresentavam sintomas clássicos ou comuns da doença e, portanto, é de suma importância instituir inquéritos sorológicos em animais que não tenham apresentado sintomas. Desta maneira, a identificação precoce dos reservatórios (cães) é crucial para qualquer estratégia de controle bem-sucedida da doença. (Otranto *et al*., 2009).

4. CONCLUSÃO:

Conclui-se que, o teste de triagem DPP é uma ferramenta de estudo valiosa a campo devido a ser um teste prático, de fácil manuseio e exigir pouco material para manipulação. Apesar disto, há a possibilidade de reação cruzada com agentes etiológicos comumente encontrados em cães. Os resultados negativos em cães apontam para a possibilidade de a infecção humana não ser autóctone. A vigilância epidemiológica e os inquéritos sorológicos são muito importantes, haja vista que cães que habitam no domicílio e peridomicílio servem como reservatórios da doença e podem apresentar-se assintomáticos, contribuindo com a dispersão da doença e trazendo mais agravos e impactos à saúde pública.

5. AGRADECIMENTOS:

Agradecemos a Secretaria Municipal de Saúde do município de Vassouras pelo apoio logístico para a obtenção das informações.

6. REFERÊNCIAS:

1. Ministério da Saúde. Manual de Vigilância e Controle da Leishmaniose Visceral*, Ministério da Saúde,* **2014,** *1ª Edição.*
2. Romero, G. A. S., Boelaert, M. Control of Visceral Leishmaniasis in Latin America-A Systematic Review. *PLoS Neglected Tropical Diseases*, **2010**, 4, e584.
3. Gontijo, C.M.F., Melo, M.N. Leishmaniose visceral no Brasil: quadro atual, desafios e perspectivas. *Revista brasileira de epidemiologia,* **2004**, 7, 338-349.
4. Lima, V.M.F, Fattori, K.R., Michelin, A.F., Net, L.S., Vasconcelos, R. Comparison between Elisa using total antigen and immunochromatography with antigen rk39 in the diagnossis of canine visceral leishmaniasis. *Veterinary parasitology*,

2010,173, 330-333.
5. Contreras, I. K., Machado, M. A., Rocha, C.O.J.M., Oliveira, G. R., Carvalho, F.C.G. Sinais clínicos apresentados por cães positivos para leishmaniose visceral no município de Vassouras, Rio de Janeiro. *PUBVE ,* **2019**, 13, 1982-1263.
6. Dantas-Torres, F., Solano-Gallego, L., Baneth, G., Ribeiro, V. M., Paiva-Cavalcanti, M. & Otranto, D. Canine leishmaniosis in the Old and New Worlds: unveiled similarities and differences. *Trends in Parasitology,* **2012**, 28, 531-538.
7. Dantas-Torres, F. & Brandão-Filho, S. P. Expansão geográfica da leishmaniose visceral no Estado de Pernambuco. *Revista da Sociedade Brasileira de Medicina Tropical*, **2006**, 39, 352-356.
8. Feitosa, M. M., Ikeda, F. A., Luvizotto, M. C. R. & Pirre, S. H. V. Clinical aspects of dogs with visceral leishmaniasis from Araçatuba-São Paulo State (Brazil). *Clínica Veterinária,* **2000**, 5, 36-44.
9. Wilson, T. M., Magalhães, L. F., Medeiros, A. A. & Furquim, M. E. C. Alterações macroscopicas em cães sororreagentes para Leishmania chagasi e sua correlação com teste parasitologico. *Veterinária Notícias Veterinary News,* **2012**,18, 20-25.
10. Solano-Gallego, L, Koutinas, A. Miro, G. Cardoso, L., Pennisi, M.G.; Ferrer, L.; Bourdeau, P., Oliva, G., Baneth, G. Directions for the diagnosis, clinical staging, treatment and prevention of canine leishmaniosis. *Veterinary parasitology***, 2009**, 65, 1-18.
11. Brandonisio, O., G. Carelli, L. Ceci, B. Consenti, A. Fasanella e V. Puccini. Leishmaniose canina no promontório de Gargano (Apúlia, sul da Itália). *EUR. J. Epidemiol*. **1992**, 8, 273-276.
12. Lanotte, G., JA Rioux, J. Periers e Y. Vollhardt. Ecologie des leishmanioses dans le sud de la France. 10. Les formes evolutives de la leishmaniose viscérale canine. *Ana Parasitol. Zumbir. Comum*. **1979**, 54, 277-295.
13. Michalsky, EM, MF Rocha, AC da Rocha Lima, JC França-Silva, MQ Pires, FS Oliveira, RS Pacheco, SL dos Santos, RA Barata, AJ Romanha, CL Fortes-Dias e ES Dias. *Infecciosidade de soropositivos.* **2007**.
14. Molina, R., C. Amela, J. Nieto, M. San-Andrés, F. González, JA Castillo, J. Lucientes e J. Alvar. Infecciosidade de cães naturalmente infectados com Leishmania infantum coloniz Phlebotomus perniciosus. *Trans. R. Soc. Tropa Med. Hyg.***1994**, 88, 491-493.
15. Otranto, D., Paradies, P., Caprariis de D., Stanneck, D., Testini, G., Grimm, F., Deplazes, P., Capelli, G. Toward diagnosing Leishmania infantum infection in asymptomatic dogs in an area where leishmaniasis is endemic. *Clinical and Vaccine Immunology*, **2009,** 16, 337-343.
16. Crivellenti. L.Z, Crivellenti, S.B.Casos de Rotina em Medicina Veterinária de Pequenos Animais**.***São Paulo-SP: editora MedVet*, **2015,** 2ª edi.166-167.
17. Dantas-Torres F. The role of dogs as reservoirs of Leishmania parasites, with emphasis on Leishmania (Leishmania) infantum and Leishmania (Viannia) braziliensis. *Vet Parasitol*. **2007**, 149, 139-146.
18. Ministério da Saúde, Departamento de Vigilância das doenças transmissíveis, Esclarecimento sobre substituição do protocolo de diagnóstico da leishmaniose visceral canina (LVC), *Ministério da Saúde*, Brasília, **2011**.
19. Maia, C; Campino, L. Methods for diagnosis of canine leishmaniasis and immune response to infection. *Veterinary parasitology*, **2008**, 158, 274-87.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

SEROPREVALENCE AND CLINICAL MANIFESTATIONS OF DOMICILED DOGS (*CANIS LUPUS FAMILIARIS*) CLOSE TO A HUMAN CASE OF VISCERAL LEISHMANIASIS

Lucas Leal Ferreira
Universidade de Vassouras, Veterinary Medicine - Brazil.

Amanda Alfeld Belegote
Universidade de Vassouras, Veterinary Medicine - Brazil.

Laís Freire e Silva
Universidade de Vassouras, Veterinary Medicine - Brazil.

Steffany Souza Cabral
Universidade de Vassouras, Veterinary Medicine - Brazil.

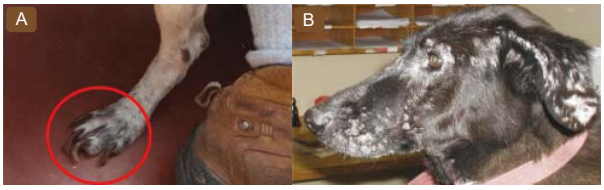
Priscilla Nunes dos Santos
Universidade de Vassouras, Veterinary Medicine - Brazil.

March/2022

INTRODUCTION

SBJChem Conference 2021

- Canine visceral leishmaniasis (CVL);
- Classification of animals according to clinical signs;



onychogryphosis
Source: Baneth (2008)

facial skin lesions
Source: Fujisawa (2021)

INTRODUCTION

SBJChem Conference 2021

- Testing protocol;

  - DPP (Dual Path Plataform®-Bio-Manguinhos)

  - ELISA (Enzyme Linked Immunosorbent Assay-Bio-Manguinhos)

Source: Fiocruz (2017)

Source: Personal archive

OBJETIVE

SBJChem Conference 2021

Evaluation of the Seroprevalence of *L. chagasi* and presence of symptoms in dogs domiciled in an area of up to 150 meters of a confirmed human case in the municipality of Vassouras.

METHODOLOGY

SBJChem Conference 2021

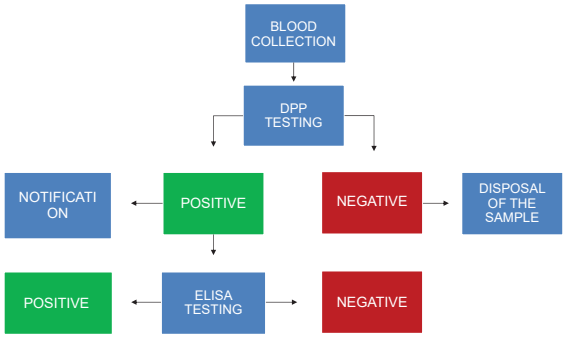
- Location and duration of the study
- 14 dogs submitted to blood collection
- Material used
- Questionnaire on clinical manifestations

5

METHODOLOGY

SBJChem Conference 2021

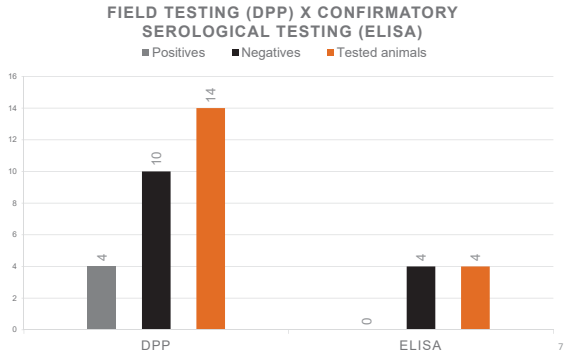
Field testing (Dpp) and confirmatory serological testing (ELISA)



6

RESULTS AND DISCUSSION

SBJChem Conference 2021

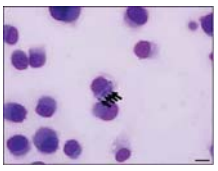


7

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Probable cross-reaction with *Ehrlichia canis, Babesia canis, Anaplasma spp* and others etiologic agents
- Non-autochthonous case

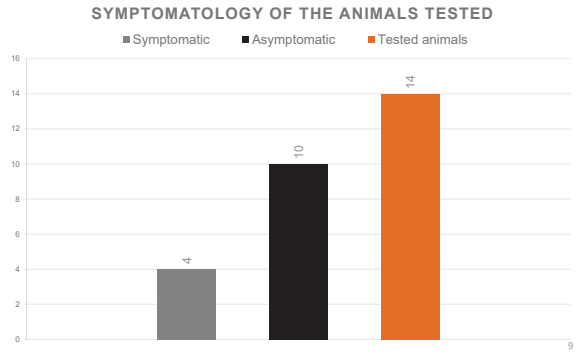


Erlichia canis
***Source:* Alves (2014)**

8

RESULTS AND DISCUSSION

SBJChem Conference 2021



RESULTS AND DISCUSSION

SBJChem Conference 2021

Importance of asymptomatic animals identification

(Gontijo; Melo, 2004)

CONCLUSIONS

SBJChem Conference 2021

- DPP x Cross reaction
- Non-autochthonous infection
- Importance of epidemiological surveillance and serological surveys

ACKNOWLEDGEMENTS

SBJChem Conference 2021

We thank the Municipal Health Department of the municipality of Vassouras for logistical support to obtain the information.

REFERENCES

SBJChem Conference 2021

1. Ministério da Saúde. (2014). Manual de Vigilância e Controle da Leishmaniose Visceral, *Ministério da Saúde, 1ª Edição.*
2. Romero, G. A. S., Boelaert, M. (2010). Control of Visceral Leishmaniasis in Latin America-A Systematic Review. *PLoS Neglected Tropical Diseases*, 4(1), e584. doi:10.1371/jornal.pntd.0000584
3. Gontijo, C.M.F., Melo, M.N. (2004). Leishmaniose visceral no Brasil: quadro atual, desafios e perspectivas. *Revista brasileira de epidemiologia,* 7*:* 338-349. doi.org/10.1590/S1415-790X2004000300011
4. Dantas-Torres, F., Solano-Gallego, L., Baneth, G., Ribeiro, V. M., Paiva-Cavalcanti, M. & Otranto, D. (2012). Canine leishmaniosis in the Old and New Worlds: unveiled similarities and differences. *Trends in Parasitology*, 28(12):531-538.
5. Lima, V.M.F, *et al*. (2010). Comparison between Elisa using total antigen and immunkchromatography with antigen rk39 in the diagnossis of canine visceral leishmaniasis. *Veterinary parasitology*, vol.173, p. 330-333.
6. Feitosa, M. M., Ikeda, F. A., Luvizotto, M. C. R. & Pirre, S. H. V. (2000). Clinical aspects of dogs with visceral leishmaniasis from Araçatuba-São Paulo State (Brazil). *Clínica Veterinária*, 5(28):36-44.
7. Fujisawa K, Silcott-Niles C, Simonson P, Lamattina D, Humeres CA, Bhattacharyya T, et al. (2021) Emergent canine visceral leishmaniasis in Argentina: Comparative diagnostics and relevance to proliferation of human disease. *PLoS Negl Trop Dis* 15(7): e0009552. https://doi.org/10.1371/journal.pntd.0009552
8. Baneth, G, et al. (2008). Canine leishmaniosis – new concepts and insights on an expanding zoonosis: part one. *Trends in Parasitology.* Vol 24, n.7. https://doi.org/10.1016/j.pt.2008.04.001
9. *Alves* R. N., et al. (2014). Isolation, in vitro propagation, genetic analysis, and immunogenic characterization of an Erlichia canis strain from southeastern Brazil. *J. Vet. Sci.* 15(2), 241-248 http://dx.doi.org/10.4142/jvs.2014.15.2.241

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

"SIX THINKING CARDS": A GAME FOCUSED ON DEVELOPING ARGUMENTATIVE SKILLS IN THE CHEMISTRY CLASSROOM

DE ALMEIDA, Luciana Pereira[1*]; DE OLIVEIRA, Victória Beatriz dos Santos[1]; PASSINATO, Cristiana de Barcellos[1]

[1] Universidade Federal do Rio de Janeiro, Instituto de Química, Setor de Acessibilidade

** Correspondence author*
e-mail: luciana.almeida@ufrj.br

Received 25 January 2022; received in revised form 19 February 2022; accepted 23 February 2022

ABSTRACT

Considering the increasing need to develop the argumentation and communication skills of the students, teaching practice has to consider how to do this concerning individual needs and preferences. Meaningful Learning proposes that education should consider the already acquired knowledge of the students in the process of building new learning. Therefore, when applied to the learning process, argumentation is a way to express acquired knowledge to other participants of this process. The Six Thinking Cards game permits students to explore their thinking in focused stages that are represented by the colors proposed in the Six Thinking Hats strategy by Edward De Bono, thus creating an environment where students have time and space to study and think about scientific concepts in a throughway. It is expected that the game also helps students develop soft skills that are considered essential for 21st century learning, such as empathy, communication, problem-solving, and teamwork. The game also adds Libras (Brazilian Sign Language) and Braille (tactile writing system) elements for accessibility purposes towards the objective of building an inclusive classroom. This game should be able to be applied in the chemistry classroom once Covid-19 hard restrictions and quarantine are over and in-person studies are permitted, allowing the authors to do qualitative and quantitative research of this proposal's reach and relevance for beyond of the projection of this proposal. Interviews with both teachers and students are to understand better how students' metacognitive skills improve as they engage in cooperative learning and express their ideas.

Keywords: *Meaningful Learning, cognition, focused thinking, Six Thinking Hats, argumentation.*

1. INTRODUCTION

The North-American psychiatrist who focused his studies on educational psychology, David Ausubel, theorized the importance of meaningful learning to the cognitive process. Conscious thought plays an important role in teaching and learning and should be at the forefront of didactic planning (Ausubel, 1976). According to Moreira (2006), the Meaningful Learning Theory is "the process through which new information acquires meaning by interaction (not association) with preexistent relevant aspects in the cognitive structure". That means that learning should consider the meaningful knowledge that students have already acquired and use it as a motivation strategy. Considering students' previous thoughts, opinions, hypotheses, and even feelings is essential for significant long-term learning.

The study also considers the effects of "mechanical learning" where students merely memorize required knowledge for a short period, as in for an exam, and discard it as soon as it isn't "needed" anymore. At first glance, learning seems effective, as students can reproduce steps learned in problem-solving to excellence and show a good amount of critical thinking skills in explaining theories during a test. However, the problem lies in long-term learning and association skills, seeing that students only memorize steps and explanations, don't reflect on cognition, and don't create personal mental structures to accommodate learning deliberately and critically.

Thinking about the increasing search for strategies that help to develop critical thinking, meaningful learning, and expression skills, the work proposed in this paper focuses on the importance of understanding chemical concepts in a real way: both in a broad sense and in a

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.29_abstract_ALMEIDA.pdf.

concentrated way. To do that, we propose a game called “Six Thinking Cards” based on Edward de Bono’s book and strategy, “Six Thinking Hats”.

The “Six Thinking Hats” method is a metacognitive strategy that organizes learning in stages of focused thought (De Bono, 1985). According to De Bono, it’s a “great technique to categorize opinion and fact” in the process of creating critical thinking. This technique is used in companies to increase productivity and solve creative divergence (Kivunja, 2015 and Lewis, 2004) and, more recently, has been used in education to promote lateral thinking and explore a problem, or concept, through different perspectives, as described by the NSW Department of Education.

De Bono proposed an approach that allows exploring various aspects of the same problem. According to him, the brain can function as a self-educating and self-organizing system, capable of effective information processing through a few basic operations, and processes in which the colors of the hats correlate to the concepts addressed. The author believes that creativity is a type of horizontal thinking that is difficult to cultivate because it violates traditional habits of logical thinking where the essence must be corrected at every step when it strays away from logical and straightforward analysis. In the “horizontal” thinking described by him, though, this direct view is not the only important process. Other aspects such as creativity, emotion, and judgment are considered just as meaningful for learning as facts, methodology, and data.

In education, this technique has been used to develop data comprehension, problem-solving and emotional response regulation skills (Lystopad, 2017), going hand in hand with Ausubel’s Meaningful Learning Theory and promoting global development of student's skills and competencies in a way that always considers them at the center of their cognitive process. The work proposed in the present paper also considers inclusion as a key to didactic planning, seeing that the game is built with both Libras (Brazilian Sign Language) and Braille (tactile writing system) elements.**2. MATERIALS AND METHODS**

The game is called “Six Thinking Cards” and it uses the idea behind the color scheme proposed by De Bono to organize learning in focused stages. The cards will all have a common back with the name of the game (Figure 1) and a front containing a color and a chemical concept (Figure 2). The color and chemical concept indicated in the card will point to the focused stage of thought that the students should express.

The cards will contain a tactile writing

Figure 1. Common back of all cards based the card created based on Six Thinking Hats by De Bono

of the card created based on Six Thinking Hats by De Bono

system so students with low sight and blind can read the cards without being told what is written in there. Seeing that colors represent the different stages of thought, there was a need for a tactile representation for them. This need was addressed by the method *see color* (Marchi, 2019). This method is a combination of tactile dashes and dots that represent colors without the need of writing their names in braille and subjecting the students to a word that might not have a concrete meaning.

Thus, the *see color* method creates a symbol for each card that will be recognizable by each student that uses braille.

The cards will also contain the image of the Libras sign for the scientific concept allowing participants that use that language to instantly understand the concept instead of using a Libras-Portuguese translator.

According to the color-associated mechanism proposed by De Bono, the colors will be organized as seen in table 1.

Table 1. *Color association*

Color	Meaning
Blue	Process
Yellow	Positivity
Red	Emotion
Black	Caution
Green	Creativity
White	Fact

Reference: De Bono's Six Thinking Hats color scheme

The game will start with the students mixing up all the cards. Then, the first student will pull out a card, read its scientific concept and color and have some time to prepare their arguments. Once they feel confident, they start their arguments which should reflect the stage of focused thought represented by the color of the card.

The other ones taking part in the game should understand which the argumentation used by the student is expressing concept and color. The objective of the game is going over all six stages of focused thought for a same concept.

3. RESULTS AND DISCUSSION:

In the development phase, this work proposes to help students improve their communicative skills through selective argumentation. Seeing that each color represents a stage of thought, it is expected that as students gain confidence and familiarity with the game, their arguments in each specific type of thought get better and more sophisticated.

According to De Bono, this type of selective thought, and subsequent argumentation, allows people to use it to develop a thorough understanding of a concept. Thus, students engaging in this type of activity should develop great argumentation and communicative skills. Another skill that this game aims to develop is emotional response control. When students are asked to direct their thinking to emotions, as in the red card, they are working on their ability to reflect upon their personal experiences and feelings associated and also on other people's emotional response to it, improving their intrapersonal and interpersonal response. Seeing that empathy, the ability to relate and try to understand others, and communication, being able to express one's ideas, are soft skills so essential in the 21st century, this game cares in helping the students develop themselves to their full potential.

Considering that the school environment needs to work on students' real-lives challenges, like the ability of communication and teamwork, this game offers a cooperative atmosphere in which students learn to work with others to achieve a common goal. This game also doesn't apply the pressure of competition on its participants, seeing that competition can act against the purpose of making the participants comfortable to think and voice their argumentations.

All things considered, the game aims to act as a tool for active learning that is sensitive to the environment and needs of each individual student as they build their knowledge by means of argumentation and exposure of opinion.

4. CONCLUSIONS

In conclusion, this game can improve students' argumentative skills and it can be applied in inclusive classrooms. With the help of the game, students are also encouraged to engage in cooperative learning environment developing 21st century essential soft skills such as communication and problem-solving.

5. ACKNOWLEDGMENTS:

We would like to thank our project supervisor, Cristiana de Barcellos Passinato, for the orientation in touching on some topics on accessibility and inclusion in the learning and teaching process.

6. REFERENCES:

1. Ausubel, D. P. Psicología educativa: Un punto de vista cognoscitivo. Ed. Trillas, 1976.
2. Capovilla, F. C., Raphael, W. D., Mauricio, A. C. L. Dicionário Enciclopédico Ilustrado Trilíngue da Língua de Sinais Brasileira (Libras) baseado em linguística e neurociências cognitivas. Rev. e Ampl. São Paulo, 2013, 1401.
3. De Bono, E. Six Thinking Hats. Boston, Back Bay Books, 1985.

4. Kivunja, C. Using de bono's six thinking hats model to teach critical thinking and problem solving skills essential for success in the 21st century economy. Creative Education, 2015, 6(03), 380.
5. Lewis, C. Being creative in the workplace. Manager, 24,.
6. Lystopad, O. A., Mardarova, I. K., Kuk, T. Forming Students' Motivation for Creativity by Means of Edward De Bono's "Six Thinking Hats" Technique, 2017.
7. Marchi, S. R. Design Universal de Código de Cores Tátil: Contribuição de Acessibilidade para Pessoas com Deficiência Visual. Universidade Federal do Paraná, 2019, 249.
8. Moreira, M. A., Masini, E. A. S. Aprendizagem Significativa: a teoria de aprendizagem de David Ausubel. Ed. Centauro, 2006.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

"SIX THINKING CARDS": A GAME FOCUSED ON DEVELOPING ARGUMENTATIVE SKILLS IN THE CHEMISTRY CLASSROOM

Luciana Pereira de Almeida
Universidade Federal do Rio de Janeiro, Instituto de Química, Setor de Acessibilidade, Brazil.

Victória Beatriz dos Santos de Oliveira
Universidade Federal do Rio de Janeiro, Instituto de Química, Setor de Acessibilidade, Brazil.

Cristiana de Barcellos Passinato
Universidade Federal do Rio de Janeiro, Instituto de Química, Setor de Acessibilidade, Brazil.

February/2022

INTRODUCTION

SBJChem Conference 2021

- The increasing need to develop students' argumentation and communication skills had led teaching practice to consider how to do this with respect to individual needs and preferences;
- Meaningful Learning Theory is "the process through which new information acquires meaning by interaction (not association) with preexistent relevant aspects in the cognitive structure";
- The "Six Thinking Hats" method is a metacognitive strategy that organizes learning in stages of focused though;

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

The game aims to act as a tool for active learning that is sensitive to the environment and needs of each individual student as they build their knowledge by means of argumentation and exposure of opinion.

METHODOLOGY

SBJChem Conference 2021

- The cards will all have a common back with the name of the game and a front containing a color and a chemical concept. The color and chemical concept indicated in the card will point to the focused stage of thought that the students should express.
- The cards will have the tactile writing system so students with low sight and blind can read the cards without being told what is written in there. It was also used a combination of dashes and dots to represent the colors associated with the focused thought.
- The cards will also contain the image of the Libras sign for the scientific concept allowing participants that use that language to instantly understand the concept instead of using a Libras-Portuguese translator.
- The first student will pull out a card, read its scientific concept and color and have some time to prepare their arguments. Once they feel confident, they start their arguments which should reflect the stage of focused thought represented by the color of the card.
- The other ones taking part on the game should be able to understand which concept and color is being expressed by the argumentation used by the student. The objective of the game is going over all six stages of focused thought for a same concept.

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Help students to improve their communicative skills by means of selective argumentation.
- The type of selective thought proposed in this game, and subsequent argumentation, allows people using it to develop a thorough understanding of a concept.
- Another skill that this game aims to develop is the emotional response control. When students are asked to direct their thinking to emotions, as in the red card, they are working on their ability to reflect upon their personal experiences and feelings associated and also on other people's emotional response to it improving their intrapersonal and interpersonal response.

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Considering the inherent school-environment need to work on students' real-life challenges, this game offers a cooperative atmosphere in which students learn to work with other with the objective of achieving a common goal.
- This game also doesn't apply the pressure of competition on its participants seeing that competition can act against the purpose of making the participants comfortable to think and voice their argumentations.

CONCLUSIONS

SBJChem Conference 2021

- The game has the potential to improve students' argumentative skills;
- It can be applied in inclusive classrooms;
- Students are encouraged to engage in cooperative learning environment developing 21st century essential soft skills such as communication and problem-solving.

ACKNOWLEDGEMENTS

SBJChem Conference 2021

We would like to thank our project supervisor, Cristiana de Barcellos Passinato for the orientation in touching some topics on accessibility and inclusion in the learning and teaching process.

REFERENCES

SBJChem Conference 2021

1. Ausubel, D. P. Psicología educativa: Un punto de vista cognoscitivo. Ed. Trillas, 1976.
2. Capovilla, F. C., Raphael, W. D., Mauricio, A. C. L. Dicionário Enciclopédico Ilustrado Trilíngue da Língua de Sinais Brasileira (Libras) baseado em linguística e neurociências cognitivas. Rev. e Ampl. São Paulo, 2013, 1401.
3. De Bono, E. Six Thinking Hats. Boston, Back Bay Books, 1985.
4. Kivunja, C. Using de bono's six thinking hats model to teach critical thinking and problem-solving skills essential for success in the 21st century economy. Creative Education, 2015, 6(03), 380.
5. Lewis, C. Being creative in the workplace. Manager, 2004, 24..
6. Lystopad, O. A., Mardarova, I. K., Kuk, T. Forming Students' Motivation for Creativity by Means of Edward De Bono's "Six Thinking Hats" Technique, 2017.
7. Marchi, S. R. Design Universal de Código de Cores Tátil: Contribuição de Acessibilidade para Pessoas com Deficiência Visual. Universidade Federal do Paraná, 2019, 249.
8. Moreira, M. A., Masini, E. A. S. Aprendizagem Significativa: a teoria de aprendizagem de David Ausubel. Ed. Centauro, 2006.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THE EFFECTS OF PARTICLE SIZE, COMPACTION PRESSURE, AND TORREFACTION ON QUALITY AND THERMAL PROPERTIES OF PELLETIZED CORNCOB RESIDUES

SAIDU, Nurudeen Sabi1*; ALADODO, Muhammad Alamin[1]; AJIMOTOKAN, Habeeb Adewale[1]

[1] University of Ilorin, Faculty of Engineering and Technology, Department of Mechanical Engineering

** Correspondence author*
e-mail: sabious33@gmail.com

Received 20 October 2021; received in revised form 10 January 2021; accepted 31 January 2022

ABSTRACT

Torrefaction and biomass pelletization into pellets for solid fuel development are considered sustainable energy solutions to mitigate fossil fuel dependency and environmental challenges. This study investigated the effect of particle size, compaction pressure, and torrefaction on the quality and thermal properties of pelletized corncob residues. The corncob samples were collected, sorted, and pulverized before the torrefaction pretreatment. The torrefaction was achieved by placing the corncob in a furnace at a temperature and residence time of 280 °C and 30 minutes, respectively. The inert atmosphere was attained and maintained by initially purging a nitrogen gas into the torrefying chamber and passing it at 100mL/min during the processes. The raw and torrefied corncob fines were screened to 0.3 mm, 0.5 mm, and 1.0 mm grain sizes. Using starch as a binder (5% wt), pellets were produced employing their respective raw and torrefied fines at compaction pressures of 50 MPa, 75 MPa, and 100 MPa. Though all pellet samples exhibited good quality and thermal properties, the pellets from torrefied corncob are better. Also, the effects of particle size and compaction pressure are significant on the produced pellets. The compressed density varied from 760 to 1,250 kg/m^3 and 637 to 920 kg/m^3 for raw and torrefied corncob pellets. A maximum heating value of 25.8 MJ/kg was obtained from the torrefied pellet sample of 1.0 mm, rendering improvements of 37.2% when compared with 18.8 MJ/kg of raw corncob of the same particle size. The energy values obtained for torrefied corncob for all particle sizes compared favorably with the value obtained in coal. Investigation of particle size, compaction pressure, and torrefaction on quality and thermal properties of pelletized corncob residue proved that it can replace coal and hence could be used for energy applications.

Keywords: *Thar coal; Torrefied pellets; Pelletised particles; Raw corncob*.

1. INTRODUCTION

Fossil fuel plays an important role as the key driver for industrialization. It has the highest percentage in overall energy consumption. However, its proportion in the world energy trend remained almost unchanged until recent years (Nwabunwanne et al., 2021; Krongkaew *et al.,* 2017). With the environmental impact, especially of global warming and the rapid depletion of fuel of this type, it is essential to seek renewable energy for sustainability (Ajimotokan *et al.,* 2019a; Parachwittawin *et al.* 2017; Tumuluru 2015). Biomass, a naturally abundant energy source, is considered a promising renewable fuel due to its renewability, greenish and global availability, and carbon-neutral balance (Ajimotokan *et al.* 2019b). Biomass includes agricultural residues from forestry activities, products, and by-products such as cobs, pods, and shells.

Corncobs are agro-residues abundant in temperate regions such as Nigeria (Anthony *et al*., 2017). In corn mills, empty corn cobs are used as a substitute fuel in convectional boilers (Krongkaew *et al.,* 2017). The thermal efficiency is low due to its poor fuel properties. Compared to low-to-medium grade fuel, corncobs have high moisture content, low fixed carbon, high volatile matter, fibrous and tenacious nature, and low energy value (Hassan *et al.,* 2016). In fact, high

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.14_abstract_SAIDU.pdf

volumes of empty cobs are needed due to their low energy density. Therefore, the Problems associated with transportation, grinding, storage, and handling become issues at a cogeneration plant (Rabiu *et al.* 2019; Krongkaew *et al.* 2017). One of the crucial steps to circumvent the above limitations is through torrefaction and pelletization. (Adeleke *et al.,* 2020; Ajimotokan *et al.* 2019b). Torrefaction is a thermo-chemical conversion method where biomass is subjected to thermal heating in an inert environment, typically in the temperature range of 200 to 300 at atmospheric pressure (Matali *et al.,* 2016). Torrefied product has a higher mass yield, and energy content is retained with incomplete removal of volatile matters (Tumuluru *et al.,* 2015). The fuel of this type is regarded as an improved version of its raw form. On the other hand, pelletization addresses low bulk density and transportation problems.

Extensive research on the effects of bio-residues pretreatment and densification processes on their quality and thermal properties for energy application has been carried out. However, only a few works are tailored to the pelletization of agro-residue, and in particular, there is no known published or near absent research on torrefied and pelletized corncob residues. For instance, Kanwal *et al.* 2019 examined the physicochemical characteristics of thar coal and torrefied corncob with five distinct torrefaction temperatures and four different residence times. The torrefied corncob was reported to be suitable as a substitute for thar coal. Ibitoye *et al.,* 2021 investigated the combustion properties of corncob biomass via torrefaction for solid fuel applications with varied torrefaction temperature and residence time. The study results revealed that torrefaction improves the thermal and combustion characteristics of the biomass residue. Thus, this study seeks to investigate the effect of particle sizes, compaction pressure, and torrefaction on the quality and thermal properties of pelletized corncob residue.

2. MATERIALS AND METHODS

2.1. Materials

The raw corncobs utilized in this study were obtained from the University of Ilorin farm and the starch from the cassava processing factory within Ilorin, Kwara State, Nigeria. The samples were stored in the University of Ilorin woodwork laboratory (latitude 8.4799 N and longitude 4.5418 E). The equipment used in this study was a set of sieves, muffle furnace, weighing balance, oven, thermometer, the crucible, Venire caliper, compression machine, stopwatch, die, and piston.

2.1.1 *Material preparation and torrefaction*

The stored samples of corncob were sorted by handpicking technique, which involved the removal of every form of dirt and foreign materials. Such as sand, stone, ashes, and plant residue. It was then dried by placing it in an oven at a temperature of 105 °C for 2 hours to minimize the interference of surface water. Torrefaction of the biomass was achieved by placing the biomass in a furnace at a temperature and residence time of 280 °C and 30 minutes, respectively. The inert atmosphere was attained and maintained by initially purging a nitrogen gas into the torrefying chamber and passing it at 100mL/min during the torrefaction processes (see Figure 1). The samples were then crushed to reduce the particle size for better workability and compactness. The sieve analyses based on BS EN 15149-2 (2010) were used for this experiment. Samples were screened into three (3) different sizes (0.3, 1.0, and 1.7 mm). The sieved samples of raw and torrefied corncob were then stored separately in a zip-locked polythene bag.

2.1.1.1 Pelletisation procedure

The pellets were produced at the Department of Civil Engineering, University of Ilorin, Nigeria. Raw and torrefied corncob samples were weighed using an electronic weighing balance. The binder at 5% of the total mass of the samples was used for the respective agglomerate samples (Ajimotokan *et al.* 2019b). The compaction was achieved using a manual hydraulic jack machine (Figure 2), model EL31 072. The aggregates were mixed manually using a manual stirrer. After thorough mixing was achieved, the feedstock was then poured into the mold. Different compaction pressures that were considered were 50, 75, and 100 MPa. After the pellets formed were removed from the molds, the weight and dimensions were taken before sun drying.

2.1.1.2 Density

The compressed density was calculated by dividing the mass of pellet bulk (m) with its volume (V), as depicted in Equation 1: The relaxed density was then determined 30 days after being sun-dried (Ajimotokan *et al.* 2019a).

$$\rho = \frac{m}{v} \qquad \text{(Eq. 1)}$$

ρ denotes the green density, m is the mass of the pellet, and v is the volume.

2.1.1.3 Calorific value

The calorific value (HHV) for the raw and torrefied samples was carried out using an oxygen bomb calorimeter following ASTM standard D-5865.

3. RESULTS AND DISCUSSION:

3.1 Density

Figure 1 shows the effect of variations in compaction pressure and particle size on the compressed density of the produced fuel pellets. The green density of the produced pellets varied from 760 to 1,250 kg/m^3 and 637 to 920 kg/m^{3}for the raw and torrefied pellets, respectively. The density of the torrefied pellets was observed to be lower than the density of the raw pellets produced under the same condition. This may be as a result of the loss of chemically bonded water and low melting point compounds (i.e., volatiles), which would have added to the binding effect during densification.

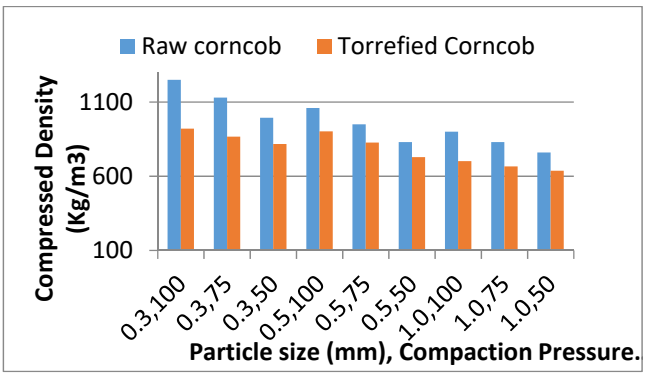


Figure 1: *Effect of particle size and compaction pressure on the compressed density of raw and torrefied corncob pellets.*

3.2 Calorific value

Figure 2 shows the calorific value profiles of raw and torrefied corncob samples. The calorific values varied from 16 to 18.8 MJ/kg and 24 to 25.8 MJ/kg for the raw and torrefied pellets. It depicted that the heating value also increases with an increase in the particle size for both the raw and torrefied corncob residues. A maximum increase was observed at 1.0mm particle size, i.e., 25.8 MJ/kg, which is almost equal to the heating value found in coal, i.e., 24.6 MJ/kg. An increase in heating value could be associated with a decrease in moisture content that resulted due to torrefaction (Kanwal *et al.*, 2014). Torrefaction pretreatment rendered an average improvement of 37.2%. These results revealed that torrefaction has an obvious impact on the rise of calorific values of the torrefied corncob residues.

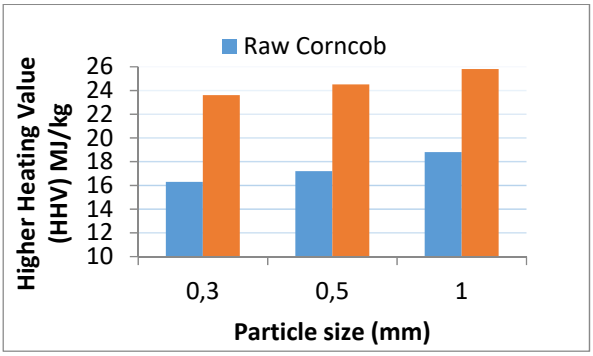


Figure 2*: Calorific values of raw and torrefied corncob samples of different particle sizes*

4. CONCLUSIONS:

The effects of particle size, compaction pressure, and torrefaction on the quality and thermal properties of pelletized corncob residues were examined. The effects of torrefaction were significant on the overall properties of the pellets produced. Particle sizes, compaction pressure, and their combined effect affect the densities and moisture uptake of the pellets produced from both the raw and torrefied corncob residues. In addition, the higher value of the calorific value of torrefied corncob samples depicts that torrefied corncob will produce greater heat of combustion during char burnout. Thus, pellets produced from all categories of particle size of torrefied corncob can be used for energy applications.

5. REFERENCES:

1. ASTM D5865-12. (2012) Standard Practice for Calorific value of Coal and Coke; ASTM International: West Conshohocken, PA, USA.
2. Adeleke A. A., Odusote J. K., Lasode O. A., Ikubanmi P. P., Malathi M. and Paswan D. (2020)," Essential *Basics on Biomass Torrefaction, Densification and Utilization"* Heliyon 5(2160)
3. Ajimotokan, H. A., Ehindero, A. O., Ajao, K. S., Adeleke, A. A., Ikubanni, P. P. and Shuaib-Babata, Y. L. (2019a), *"Combustion Characteristics of Fuel Briquettes Made from Charcoal Particles and Sawdust Agglomerates"* Scientific African, 6, 1-10.
4. Ajimotokan, H. A., Ibitoye, S. E., Odusote, J. K. and Omoniyi, P. O. (2019b), *"Physico-Mechanical Properties of composites Briquettes from Corncob and Rice Husk",* Bio-resources and Bi-products, 4(3), 159-165.
5. Anthony, I. A., Goso, P. B., Okoh O. O. and Mamphweli, S. N. (2017), "*Studies on Characterization of Corncob for Application in a Gasification Process for Energy Production" Chemistry* 7(5), 18-28.
6. Hassan, M., Jusoh, M., Abdulrahman, R., Syahrullail, S. and Latiff, Z. (2016), "*Torrefaction of palm biomass briquettes at different temperature*", Science and Engineering, 78(9-2), 61-67.
7. Ibitoye, S. E., Jen, T., Mahamood, R. M. (2021), *"Improving the Combustion Properties of Corncob Biomass via Torrefaction for Solid Fuel Applications"* Composites Science, 5(260), 1-13.
8. Kanwal S., Munir S., Chaudhry N. and Sana H (2019) *"Physicochemical Characterization of Thar Coal and Torrefied Corncob"* Energy Exploration and Exploitation. 0(0) 1-20.
9. Krongkaew Laohalidanand, Kongkaew N. and Kerdsuwan S. (2017) *"Gasification Behaviour Study of Torrefied Empty Corncobs"* Energy 138 175-180.
10. Matali, S., Rahman, N. A., Idris, S. S., Yaacob, N. and Alias, A. B. (2016), "*Lignocellulosic Biomass Solid Fuel Properties Enhancement Via Torrrefaction"* Procedia Engineering, 148, 671-678.
11. Nwabunwanne, N.; Vuyokazi, T.; Olagoke, A.; Mike, O.; Patrick, M.; Anthony, O. (2021), *Torrefaction Characteristics of Blended Ratio of Sewage Sludge and Sugarcane Bagasse for Energy Production.* Appl. Sci. 2021, 11, 2654.
12. Prachwittawin, L., Krongkaew, L. and Somrat, K. (2017), "*In-depth Study of Fuel Properties of Corn Residue (Cob, Stems/Leaves and Husk) through the Torrefaction Process",* Energy,138, 662-667.
13. Tumuluru, J. S. (2015), "*Comparison of Chemical Composition and Energy Property of Torrefied Switchgrass and Corn Stover",* Bioenergy and Biofuels3(46), 1-11.
14. Rabiu A. B., Lasode O. A., Popoola O. T., Babatunde O. P. and Ajimotokan H. A. (2019), "*Densification of Tropical Wood Residues for the Development of Solid Fuels"* Sustainability, Energy, and Environment.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THE EFFECTS OF PARTICLE SIZE, COMPACTION PRESSURE, AND TORREFACTION ON QUALITY AND THERMAL PROPERTIES OF PELLETIZED CORNCOB RESIDUES

SAIDU, Nurudeen Sabi
University of Ilorin, Faculty of Engineering and Technology, - Nigeria.

ALADODO, Muhammad Alamin
University of Ilorin, Faculty of Engineering and Technology, - Nigeria.

AJIMOTOKAN, Habeeb Adewale
University of Ilorin, Faculty of Engineering and Technology, - Nigeria.

March/2022

INTRODUCTION

SBJChem Conference 2021

- Fossil fuel plays an important role as the key driver for industrialization. It has the highest percentage in overall energy consumption, and its proportion in the world energy trend remained almost unchanged till recent years.
- With the environmental impact especially of global warming and the rapid depletion of fuel of this type, it is essential to seek renewable energy for sustainability.
- Biomass, a naturally abundant energy source is considered as promising renewable fuel due to its renewability, greenish and global availability, and carbon neutral balance.
- The thermal efficiency of biomass based fuel is low, due to its poor fuel properties. Compare to low-to- medium grade fuel, corncobs have high moisture content, low fixed carbon, high volatile matter, fibrous and tenacious nature and low energy value

BACKGROUND

SBJChem Conference 2021

- One of the crucial steps to circumvent the above limitations is through torrefaction and pelletization.
- Torrefied product has higher mass yield, energy content is retained and with incomplete removal of volatile matters. Fuel of this type is regarded as an improved version of its raw form.
- Pelletization on the other hand addresses low bulk density and transportation problems.

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

This study seeks to investigate the effect of particle sizes, compaction pressure and torrefaction on quality and thermal properties of pelletized corncob residue.

The aim of the experiment was achieved through the following objectives.

- Torrefaction and production of pellets from raw and torrefied corncobs at different particle sizes and compaction pressure;
- Determination of some selected quality properties of the produced pellet from raw and torrefied corncobs;
- Determination of some selected combustion properties such as calorific value of raw and torrefied samples of corncob.

METHODOLOGY

SBJChem Conference 2021

- The stored samples of corncob were sorted by handpicking technique, which involve the removal of every form of dirt and foreign materials. Such as sand, stone, ashes and plant residue.
- It was then dried by placing it in an oven at a temperature of 105°C for 2 hours to minimize the interference of surface water.
- Torrefaction of the biomass was achieved by placing the biomass in a furnace at a temperature and residence time of 280 °C and 30 minutes respectively.
- Inert atmosphere was attained and maintained by initially purging a nitrogen gas into the torrefying chamber and passing it at 100mL/min during the torrefaction processes.
- The pellets were produced using manual hydraulic jack machine.
- All test were carried out in accordance with the ASTM standard.

RESULTS AND DISCUSSION

SBJChem Conference 2021

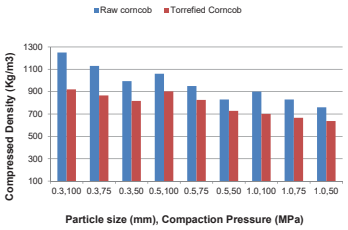


Figure 1: Effect of particle size and compaction pressure on compressed density of raw and torrefied corncob pellets.

RESULTS AND DISCUSSION

SBJChem Conference 2021

•The moisture absorption conducted on dry raw and torrefied pellets of corncob exposed to 90% humidified air at 30°C in a humidity chamber over 5 h was measured.

•For comparison, the moisture uptake for raw corncob pellets was within the range of 17.2 to 19.4wt%. The water absorption capacity of torrefied corncob pellets was however, around 2.2–3.7wt% translating to about 80% reduction in moisture absorption capacity.

•This is associated with the slight difference in the structure and composition of the torrefied pellets.

RESULTS AND DISCUSSION

SBJChem Conference 2021

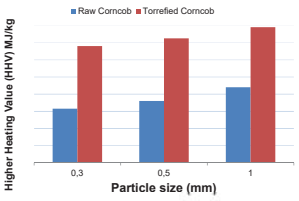


Figure 2: Calorific values of raw and torrefied corncob samples of different particle sizes

CONCLUSIONS

SBJChem Conference 2021

- The effects of torrefaction were significant on the overall properties of the pellets produced.
- Particle sizes, compaction pressure and their combined effect affect the densities and moisture uptake of the pellets produced from both the raw and torrefied corncob residues.
- The higher value of calorific value of torrefied corncob samples depict that torrefied corncob will produce greater heat of combustion during char burnout.
- Pellet produced from all category of particle size of torrefied corncob can be used for energy applications.

REFERENCES

SBJChem Conference 2021

Ajimotokan, H. A., Ibitoye, S. E., Odusote, J. K. and Omoniyi, P. O. (2019b), *"Physico-Mechanical Properties of composites Briquettes from Corncob and Rice Husk",* Bio-resources and Bi-products, 4(3), 159-165.

Ajimotokan, H. A., Ehindero, A. O., Ajao, K. S., Adeleke, A. A., Ikubanni, P. P. and Shuaib-Babata, Y. L. (2019a), *"Combustion Characteristics of Fuel Briquettes Made from Charcoal Particles and Sawdust Agglomerates"* Scientific African, 6, 1-10.

Ibitoye, S. E., Jen, T., Mahamood, R. M. (2021), *"Improving the Combustion Properties of Corncob Biomass via Torrefaction for Solid Fuel Applications"* Composites Science, 5(260), 1-13.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THE EVOLUTION OF CATARACT IN A DOG WITH TYPE I DIABETES - CASE REPORT

SAMAN, Thiago Abreu [1*]; RODRIGUES, Isabelle Medeiros[1]; FILHO, Mário dos Santos[2]

[1] Academic of Veterinary Medicine, University of Vassouras
[2] Professor of the Veterinary Medicine Course, University of Vassouras.

** Correspondence author*

e-mail: thiagosaman@hotmail.com

Received 20 February 2022; received in revised form 02 March 2022; accepted 11 March 2022

ABSTRACT

Diabetes Mellitus is one of the endocrine diseases that most affect dogs in Brazil and worldwide. It is characterized by a chronic metabolic disorder, where the ability to respond or produce the hormone insulin is impaired, resulting in the abnormal activity of carbohydrate metabolism, coursing with hyperglycemia and glucosuria. The signs of 4P's (polyuria, polyphagia, polydipsia, and weight loss) are classic in this disease. As Diabetes Mellitus progresses, complications such as cataracts, retinopathy, and metabolic ketoacidosis may occur. Cataract is one of the most frequent complications in diabetic and early-onset dogs. It has a rapid development, as the lens has high permeability to glucose, converting it into fructose and sorbitol, which, as they are sugars with osmotic potential, can attract water, causing lens edema. The definitive treatment for cataract is surgical, with phacoemulsification being the most used technique. A canine male, Shih-tzu, weighing 5 kg, 06 months old, and not neutered, was treated at the private veterinary clinic in the city of Nilópolis. The patient had polyuria, polydipsia, polyphagia, weight loss and was prostrate most of the time. The diagnosis of diabetes mellitus was confirmed and a protocol was started with the use of Insulin NPH for human use. In addition, a diet was performed with the consumption of food for weight control, glycemic, and drug treatment. After six months of DM treatment, the dog presented bilateral lens opacity (crystalline), confirming a diagnosis of cataract secondary to diabetes, and underwent phacoemulsification surgery on the left eye. With the good post-surgical evolution, the doses of the prescribed medications were gradually reduced until the animal recovered completely. The present work aims to report the clinical case, atypical, of a young dog, with type I DM, with cataract manifestation after six months of diagnosis.

Keywords: *Phacoemulsification, Intraocular lens, Opacity, Endocrinopathy, and Insulin.*

1. INTRODUÇÃO

A Diabetes mellitus (DM) é a endocrinopatia que mais acomete cães no Brasil e no mundo (AMATO, 2020). Caracteriza-se por distúrbios do metabolismo dos carboidratos, e tem como fator primário, desencadeador de suas complicações, a hiperglicemia persistente e crônica. Isso ocorre porque a secreção de insulina e/ou a ação da insulina podem estar prejudicadas (KERNER, 2014), impedindo a sua principal função que é promover a entrada de glicose para as células.

A DM tipo I, (insulinodependente) é a mais frequente encontrada em cães, sendo caracterizada pela perda ou disfunção da secreção de insulina nas células-beta do pâncreas, impossibilitando o controle glicêmico e a entrada de glicose nas células. (GILOR, 2016).

De acordo com (MILLER, 2018), a catarata é uma das complicações mais frequentes em cães diabéticos, tendo seu início precoce. Ela se desenvolve de maneira rápida, devido à alta permeabilidade do cristalino à glicose, convertendo-a em frutose e sorbitol, o que desencadeia acúmulo osmótico de água, intumescência e agregado de proteínas no cristalino, cursando com opacidade. É importante realizar exame oftalmológico completo com a avaliação da resposta ao reflexo pupilar à luz, chamado PLR (do inglês, *Pupillary Light Reflex*), reflexo de ameaça, teste lacrimal de Schirmer, mensuração da pressão intraocular

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.46_abstract_SAMAN.pdf

(PIO), exame da câmera anterior por lâmpada de fenda e oftalmoscopia direta ou indireta, após instilação de colírios midriáticos, devendo estes exames serem realizados em todos os pacientes diabéticos (GOMES, 2017).

A ultrassonografia, ou ecografia ocular, é um exame seguro, de baixo custo, não invasivo, e de fácil realização, sendo importante para complementar o exame oftálmico e avalia o corpo ciliar. O tratamento indicado para a catarata é cirúrgico, e o procedimento de eleição é a facoemulsificação. Esta técnica vem demonstrando eficácia, redução no tempo cirúrgico, além de melhor cicatrização e recuperação do paciente (GUIMARÃES, 2015).

O objetivo deste trabalho foi relatar o caso clínico de um cão com alterações endócrinas e com suspeita de associação com catarata, de forma precoce, com 1 ano de idade.

2. MATERIAIS E MÉTODOS

O presente estudo foi desenvolvido em uma clínica veterinária particular do Município de Nilópolis, com autorização do tutor do paciente para utilização da descrição do caso para fins acadêmicos e científicos, com assinatura do Termo de Consentimento Livre e Esclarecido (TCLE).

Por meio do fenômeno observado, baseou-se a metodologia do estudo na evolução e resultados de exames para a descrição do relato do caso clínico analítico e descritivo, sendo reportado em sua ordem cronológica de ocorrência de evolução dos eventos. Seus detalhes, bem como a evolução do mesmo têm como objetivo servir de base para os colegas frente a casos clínicos e fenômenos semelhantes, facilitando sua resolução a partir do reporte de experiências prévias.

Deste modo, a importância da descrição dos relatos representam evidências científicas particulares, uma vez que a condução do caso envolve a pessoalidade do profissional que o acompanha e o descreve, levando-se em conta os fatores e condução ética do caso (KIENLE & KIENE, 2011).

3. RESULTADOS E DISCUSSÃO

3.1 Descrição do caso clínicos

Foi atendido, em uma clínica veterinária particular do município de Nilópolis, no estado do RJ, um paciente canino, macho, Shih-tzu, com peso de 5 kg, 6 meses, não castrado, com queixa de poliúria, polidipsia, polifagia, perda de peso, cansaço aparente e prostrado, na maior parte do tempo. Segundo o tutor, eram observadas formigas ao redor do local onde o animal urinava. O animal possuía vacinação e vermifugação em dia, e se alimentava de ração seca Royal Canin (Shih-Tzu–Filhote). De acordo com o relatado pelo tutor, o animal não fazia uso de medicações periódicas para comorbidades.

Ao exame físico, o paciente apresentou-se com sinais vitais dentro dos parâmetros de normalidade. Verificou-se a glicemia do animal por meio do glicosímetro portátil, onde foi constatado que o mesmo estava hiperglicêmico, com 380 mg/dl (ref.: 60 a 110mg/dl). A notar, que o paciente estava em jejum, no momento da avaliação.

Após os dados obtidos por meio do exame clínico, procedeu-se a coleta de sangue, com avaliação do hemograma, bioquímica sérica renal e hepática, dosagem de glicose e urinálise. Os exames laboratoriais apresentaram algumas alterações, os quais as mais relevantes: glicemia de 428 mg/dL (ref.: 60-110 mg/dL) e urinálise com características físico-químicas de urina em coloração amarelo-claro, com aspecto límpido, cetunúria e glicosúria. Demais achados sem alterações.

Na dosagem da bioquímica sérica hepática, o paciente apresentou alteração na ALT, (156 U/L, ref.: 10-88 U/L), sem demais alterações em bioquímicas. Como forma de complementar a avaliação clínica, realizou-se a curva glicêmica (figura 2) no paciente para avaliar, durante 24 horas, a sua “flutuação” da glicemia. Após análise dos exames, foi confirmada a suspeita de diabetes mellitus juvenil.

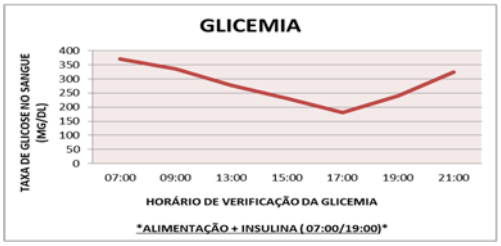


Figura 2: *Gráfico da curva glicêmica do cão. Fonte: Arquivo Pessoal, 2021.*

Diante do exposto, iniciou-se protocolo medicamentoso para o controle da DM com a utilização da Insulina NPH de uso humano, dosagem de 3 (UI), a cada 12 horas, por via subcutânea e de uso contínuo (de acordo com a resposta da aferição da curva glicêmica). Além disso, foi realizada dieta com o consumo de 60g, fracionada em 02 porções ao dia da ração (Hills® Prescrip-

tion Diet W/D Controle do Peso e Glicêmico Para Cães Filhotes Diabéticos®) e tratamento medicamentoso de suporte, onde foram instituídos: SAMe – S-Adenosil-Metionina e Ursacol – Ácido Ursodesoxicólico, Chromo Dog Tabs – Suplemento Alimentar, Hepvet – Suplemento Alimentar, e Gaviz – Omeprazol.

Após seis meses de controle e manejo adequado sobre a DM, o cão apresentou opacidade bilateral em lentes (cristalino), sendo encaminhado para um oftalmologista para melhor avaliação. Foi constatada catarata bilateral por decorrência da DM, com indicação cirúrgica. Realizou se exame clínico oftalmológico completo, através dos métodos semiológicos para a avaliação do sistema visual do animal, para determinar se os mesmos encontravam se em condições de serem operados.

Figura 1: *Paciente canino, com catarata. Fonte: HalinaMedina.*

Foram solicitados exames pré-operatórios (hemograma, bioquímica renal, hepática e glicose). Também foram solicitados exames complementares como: eletrocardiograma, eletrorretinograma e ecografia ocular.

Após a realização de todas as etapas pré-cirúrgicas, foi realizado apenas a cirurgia no olho esquerdo do animal. Para o tratamento pós-cirúrgico, foi instituído um protocolo medicamentoso de uso tópico: colírios à base de acetato de prednisolona, AINEs, Antibiótico, Midriático e Cicloplégico, todos QID. Para tratamento sistêmico, foi prescrito prednisona, SID e Antibiótico de amplo espectro BID. O animal retornou 7 dias depois para revisão, apresentando reflexos oculares e com uma opacidade na córnea, que foi melhorando ao longo do tempo com o uso do medicamento Tracolimus (Imunossupressor).

3.2. Discussão

Os sinais clínicos clássicos de cães diabéticos incluem a polidipsia, poliúria, polifagia e perda de peso (GILOR, 2016). Esses sinais foram observados pelo tutor e relatados durante a anamnese no presente caso.

De acordo com (MILLER, 2018), a catarata é uma das complicações mais frequentes em cães diabéticos e com início precoce. Esse sinal clínico foi relatado pelo tutor durante a anamnese, informando que mesmo depois de todo controle necessário sobre a DM, o animal teria ficado com opacidade ocular bilateral.

A catarata tem maior incidência em cães do que em gatos, com destaque para as raças mais predispostas como: Poodle Toy, Cocker Spaniel, Schnauzer, Pequinês, Shih-Tzu e Dachshund (FREITAS, 2008). Estas informações condizem com o caso em questão, o qual temos um paciente da raça Shih-tzu, macho e que foi diagnosticado com catarata com 1 ano de idade.

Ocorrendo a persistência da hiperglicemia, esta pode cursar com lesão em órgãos, como os olhos, onde ocorre difusão de glicose para dentro da lente, característico da catarata (KERNER, 2014). Foi constatada pelo tutor durante o exame físico com oftalmologista a evidência de catarata bilateral, que muito provavelmente ocorreu pelo edema e precipitação proteica decorrente da presença do sorbitol, remetendo-se na opacificação de lente.

Na urinálise, por meio do EAS, foi evidenciada cetunúria e glicosúria neste paciente, fatores de extrema importância para o disgnóstico da DM tipo 1, pois somente a hiperglicemia em jejum pode ter influência do estresse do exame pela contenção. Ainda, a cetonúria possui valor prognóstico que remete a um estágio de complicação da DM, a cetoacidoce diabética, uma vez que já denota a formação de corpos cetônicos decorrente do distúrbio do metabolismo dos carboidratos, por via gliconeogênica, sendo fundamental esta interpretação neste caso, para o estabelecimento da conduta médica (KERNER, 2014).

Foi observado no exame bioquímico, hiperglicemia de 428 mg/dL (ref.: 60-110 mg/dL). Alteração comum encontrada em bioquímicos de cães com diabetes não descartando a necessidade de urinálise, que neste paciente cetonúrico, corroboram valores que indicam gravidade da doença e prognóstico reservado. Ainda, a ALT, isoladamente, não sugere ligação com o DM neste caso, mas pode estar aumentado por conta da fase de crescimento do paciente, por não ser marcador

específico para algum órgão, isoladamente (KERNER, 2014).

Erros no tratamento da DM pode fazer com que os pacientes desenvolvam, como por exemplo, a cetoacidose diabética, a retinopatia e a piora no quadro da catarata. A importância no tratamento e o manejo adequado são essenciais para controle da doença. Caso não aconteça, a doença pode representar um grave risco à vida do paciente e, possivelmente levá-lo a óbito (MILLER, 2018).

Com a boa evolução pós-cirúrgica do animal, as doses das medicações prescritas no tratamento foram gradativamente diminuídas até o animal se recuperar por completo. Das diversas técnicas utilizadas na remoção da catarata, a facoemulsificação é a técnica mais utilizada nos dias atuais, com melhores resultados, menos complicações no pós-operatório e porcentagem positiva na recuperação da visão do paciente (GUIMARÃES, 2015).

4. CONCLUSÃO

O diagnóstico da DM foi possível após o entendimento dos sinais clínicos apresentados, realização e interpretação de exames laboratoriais, juntamente com apoio de exames complementares, mesmo em pacientes jovens.

A rapidez no controle da doença foi primordial, pois casos não controlados podem levar o animal a óbito, principalmente após a manifestação de cetoacidose.

O tratamento definitivo para a catarata é cirúrgico e o quanto mais precoce for realizado, maiores são as chances de resultado favorável e a possibilidade do implante da lente intraocular no paciente.

5. REFERÊNCIAS

1. AMATO, B. P.; BARROS, T.C. Diabetes mellitus em cães: buscando uma relação entre obesidade e hiperglicemia. **Pubvet**, São Paulo, n.9, v. 14, p. 1-7, mar. 2020.

2. GILOR C. et al. "O que há em um nome? Classificação do Diabetes Mellitus em Medicina Veterinária e por que é importante. " **Journal of Veterinary Internal Medicine**, vol. 30,p. 927-40, Jul/Ago. 2016.

3. GOMES et al. Aspectos e estágios da catarata em cães, **Revista Brasileira de Higiene e Sanidade Animal,** v.11, n.4, p. 456 – 471, Out/Dez. 2017.

4. GUIMARÃES, T.G. et al. FACOEMULSIFICAÇÃO COM IMPLANTAÇÃO INTRAOCULAR DE LENTE EM CÃES. **Revista Investigação Medicina Veterinária**, v. 14, p. 66-71, 2015.

5. KERNER W.; BRUCKEL J. German Diabetes Association. Definition, classification and diagnosis of diabetes mellitus. **Experimental and Clinical Endocrinology & Diabetes**, New York, v.122, p.384-386, 2014.

6. KIENLE, G.S, Kiene, H. Como escrever um relato de caso. **Arte Médica Ampliada.** Ano XXXI n.2 Inverno, 2011.

7. MILLER E.J.; BRINES C.M. Canine Diabetes Mellitus Associated Ocular Disease. **Top Companion Animal Medicine**, v.33, p.29-34, 2018.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THE EVOLUTION OF CATARACT IN A DOG WITH TYPE I DIABETES - CASE REPORT

Thiago Abreu Saman
Universidade de Vassouras, veterinary medicine, Brazil.

Isabelle Medeiros Rodrigues
Universidade de Vassouras, veterinary medicine, Brazil.

Mário dos Santos Filho
Universidade de Vassouras, veterinary medicine, Brazil.

FEBRUARY/2022

SUMMARY

SBJChem Conference 2021

INTRODUCTION

SBJChem Conference 2021

- ✓ **Diabetes Mellitus;**
- ✓ **Clinical Signs → 4P´s;**
- ✓ **Cataract;**
- ✓ **Complete Eye Examination;**
- ✓ **Treatment → Phacoemulsification;**

PANCREAS ANATOMY

SBJChem Conference 2021

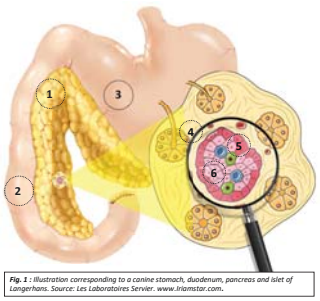


Fig. 1 : Illustration corresponding to a canine stomach, duodenum, pancreas and islet of Langerhans. Source: Les Laboratoires Servier. www.irismstar.com.

1. Pancreas
2. Duodenum
3. Stomach
4. Islet of Langerhans
5. Pancreatic Alpha Cell
6. Pancreatic Beta Cell

EYE BULB ANATOMY

SBJChem Conference 2021

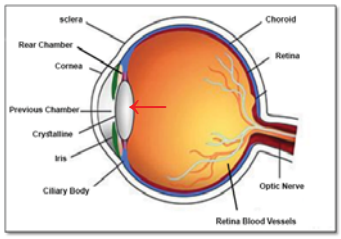


Fig. 2: Illustration corresponding to the anatomy of a canine eye. Source: Dr. Pedro Malho - ECVO Veterinary Ophthalmology.www.smart.servier.com

OPHTHALMOLOGICAL CHANGES

SBJChem Conference 2021

CATARACT

Fig. 3: Canine patient with cataract. Source: HolinaMedina. www.tudosobrecachorros.com.br.

X

CORNEAL EDEMA

Fig. 4: Canine patient with corneal edema. Source: ICBA. www.mimvet.blogspot.com/atlasdeoftalmologia.

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

To report a clinical case of a canine patient, with type I diabetes mellitus and associated with the manifestation of cataract resulting from cellular metabolic alteration.

METHODOLOGY

SBJChem Conference 2021

- ✓ The present study was developed in a private veterinary clinic in the city of Nilópolis, with authorization from the patient's tutor to use the case description for academic and scientific purposes, with the signature of the Free and Informed Consent Term (TCLE).
- ✓ Through the observed phenomenon, the study methodology was based on the evolution and results of exams for the description of the analytical and descriptive clinical case report.

RESULTS AND DISCUSSION

SBJChem Conference 2021

History and Anamnesis

Canine

Male

Shih-Tzu

06 Months

Not Neutered

Body Score of 8 (1 to 9 - According to Laflamme, 1997) and Weighing 5 kg

Vaccine, Vermifuge and Ectoparasite Control up to Date

Fig. 5: Canine patient of the present report. Source: Personal Archive, 2015.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Physical Exam

Frequency Respiratory
30 mpm
(25-40 mpm)

Temperature
38,2 ºC
(37,2-39,5ºC)

Frequency Cardiac
100 bpm
(80-120 bpm)

TPC
2 seconds
(1-3 seconds)

Sinais Clínicos:

Prostration;
Polypsia;
Polyphagia;
Polyuria;
Weight loss.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Laboratory exams

- ✓ Blood count;
- ✓ Renal and Liver Biochemistry;
- ✓ EAS;
- ✓ Glucose.

EXAMS	VALUES	REFERENCES
TOTAL PLASMA PROTEINS	7,0 g/dL	5,8 – 8,0 g/dL
UREA	37,7 mg/dL	30 – 60 mg/dL
CREATININE	0,6 mg/dL	0,5 – 1,9mg/dL
ALT (TGP)	156 U/L	10 - 88 U/L
AST (TGO)	67.1U/L	10 - 88 U/L
F.A	43 U/L	20 a 156 U/L
GGT	9,3 U/L	Até 10 U/L
GLUCOSE	428 mg/dL	60 - 100 mg/dL

Table 1: Values found in the laboratory evaluation of the patient, followed by the reference values for the species.

DEVELOPMENT

SBJChem Conference 2021

Laboratory Exams

- ✓ EAS;

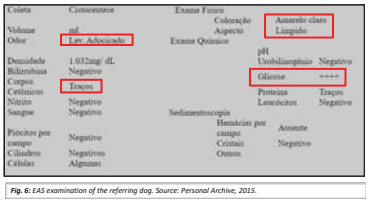


Fig. 6: EAS examination of the referring dog. Source: Personal Archive, 2015.

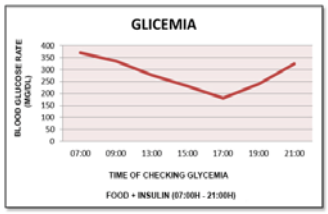
RESULTS AND DISCUSSION

SBJChem Conference 2021

Complementary Exams

Glycemic Curve:

- (07:00 as 21:00h)



Graph 1: Data from the dog's glycemic curve. Source: Personal Archive, 2021.

RESULTS AND DISCUSSION

SBJChem Conference 2021

Diabetic Cataract

After six months of control and adequate management of DM, the dog presented bilateral lens opacity (crystalline), being referred to an ophthalmologist for further evaluation. Bilateral cataract was found due to DM.

Fig. 7: Canine patient of the present report. Source: Personal Archive, 2015.

CONCLUSIONS

SBJChem Conference 2021

- ✓ The diagnosis of DM was possible after understanding the clinical signs presented, performing and interpreting laboratory tests, together with the support of complementary tests, even in young patients.
- ✓ The definitive treatment for cataract is surgical and the earlier it is performed, the greater the chances of a favorable result and the possibility of implanting the intraocular lens in the patient.

REFERENCES

SBJChem Conference 2021

1. AMATO, B. P.; BARROS, T.C. Diabetes mellitus em cães: buscando uma relação entre obesidade e hiperglicemia. **Pubvet**, São Paulo, n.9, v. 14, p. 1-7, mar. 2020.

2. GILOR C. et al. "O que há em um nome? Classificação do Diabetes Mellitus em Medicina Veterinária e por que é importante. " **Journal of Veterinary Internal Medicine**, vol. 30,p. 927-40, Jul/Ago. 2016.

3. GOMES et al. Aspectos e estágios da catarata em cães, **Revista Brasileira de Higiene e Sanidade Animal,** v.11, n.4, p. 456 – 471, Out/Dez. 2017.

4. GUIMARÃES, T.G. et al. FACOEMULSIFICAÇÃO COM IMPLANTAÇÃO INTRAOCULAR DE LENTE EM CÃES. **Revista Investigação Medicina Veterinária**, v. 14, p. 66-71, 2015.

5. KERNER W.; BRUCKEL J. German Diabetes Association. Definition, classification and diagnosis of diabetes mellitus. **Experimental and Clinical Endocrinology & Diabetes**, New York, v.122, p.384-386, 2014.

6. KIENLE, G.S, Kiene, H. Como escrever um relato de caso. **Arte Médica Ampliada.** Ano XXXI n.2 Inverno, 2011.

7. MILLER E.J.; BRINES C.M. Canine Diabetes Mellitus Associated Ocular Disease. **Top Companion Animal Medicine**, v.33, p.29-34, 2018.


SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THE IMPACT OF THE LACK OF KNOWLEDGE OF THE FEMALE AUTISTIC PROFILE IN THE QUALITY OF LIFE OF AUTISTIC WOMEN

SILVA, Sophia dos Santos Tavares Freitas da[1]*; LASNEAU, Larissa Primo Pereira[2]

[1] Universidade de Vassouras, Discente na Graduação em Psicologia

[2] Universidade de Vassouras, Docente na Graduação em Psicologia

** Correspondence author*
e-mail: sophiatavares7@gmail.com

Received 16 February 2022; received in revised form 08 March 2022; accepted 10 March 2022

ABSTRACT

In this work, the literature reviewed points out significant differences between the presentation of autism spectrum disorder in men and women, including variations in the behavior pattern, given the distinct process of socialization of the genders. However, these gender differences in the autistic phenotype were poorly studied, analyzed, and disseminated, making the female profile of autism not as well known as the male profile. Furthermore, the little attention given to the presentation of autism in girls led to the creation of diagnostic tools that were less efficient in recognizing them, causing difficulties related to late, missed, or incorrect diagnoses. These types of occurrences make it difficult for autistic women to access the support they need, in addition to being able to trigger or worsen identity crises related to their autistic traits and their self-perception in society. This abstract aims to highlight the importance of understanding the gender differences present in autism spectrum disorder and how their non-recognition can negatively affect the mental health of undiagnosed autistic women.

Keywords: *autism spectrum disorder, mental health, gender differences, diagnostic problems.*

1. INTRODUÇÃO

Desde o início, pesquisas sobre o transtorno do espectro autista (TEA) foram realizadas baseando-se em como ele se apresentava em meninos (Grove *et al*., 2017), desconsiderando as diferenças de gênero existentes (Driver e Chester, 2021). Essa propensão fez com que o perfil de meninas autistas fosse pouco estudado em comparação com o perfil masculino, consequentemente originando ferramentas de diagnóstico do TEA que fossem pouco sensíveis à sua apresentação em mulheres (Lai *et al*., 2011).

Estima-se que, aproximadamente, homens com TEA são três vezes mais diagnosticados do que mulheres (Loomes *et al*., 2017), uma vez que muitas delas passam despercebidas, ou só recebam o diagnóstico tardiamente na vida, ou que ainda, tenham sua condição confundida com outros transtornos (Driver e Chester, 2021). O diagnóstico viabiliza, primordialmente, o acesso dessas meninas aos seus direitos enquanto pessoa autista, além de auxiliá-las em seus processos de auto-aceitação e auto-conhecimento, tendo em vista os comuns relatos de se sentirem “confusas” e “sobrecarregadas” perante a sociedade (Hendrickx, 2015).

Nesse sentido, este trabalho tem como objetivo principal destacar as distinções de gênero presentes na manifestação do TEA e evidenciar a necessidade de se conhecer o fenótipo autista feminino, a fim de promover melhores condições de vida a essas mulheres.

2. MATERIAIS E MÉTODOS

Foi realizada uma pesquisa bibliográfica, através de artigos publicados e indexados na base de dados Google Acadêmico. Foram pesquisadas as palavras-chave: “autism in women”; “diagnosis of autism in women”; e “female profile of autism”. Os critérios utilizados para inclusão foram: textos publicados desde o ano de 2019, nos idiomas inglês e português. Como critério utilizado para exclusão, foram descartados os textos que não

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.49_abstract_SILVA.pdf

abordassem o tema, ou o abordassem de forma imprecisa. Foram localizados no total 32 artigos, e considerando os critérios aplicados, 12 artigos foram selecionados.

3. RESULTADOS E DISCUSSÃO:

3.1. Resultados

A Tabela 1 sumariza os resultados da pesquisa realizada na base de dados Google Acadêmico.

Tabela 1. *Resultados da pesquisa bibliográfica.*

Base de dados	Google Acadêmico
Resultados utilizados	12
Resultados descartados	22
Total de resultados	32

3.2. Discussões

Segundo Driver e Chester (2021), o transtorno do espectro autista se apresenta de forma diferenciada entre homens e mulheres. Sugere-se que, devido às pressões e expectativas típicas do processo de socialização feminina, meninas tendem a possuir mais facilidade em "camuflar" seus traços autísticos em uma maior frequência e intensidade do que meninos, ainda que o ato de camuflagem (também chamado de "masking") não seja restrito ao feminino (Lai *et al*., 2017). Essa camuflagem visa esconder, de maneira consciente ou não, características relacionadas ao TEA, com o propósito de alcançar maior aceitação social (Lai *et al*., 2017). Entretanto, por se tratar de uma tentativa de encobrimento de traços inerentes ao autista, a prática constante do masking acaba resultando em danos à saúde mental, visto que exige uma quantidade considerável de esforço emocional e cognitivo para ser realizada (Bargiela *et al*., 2016). Por conta dessa camuflagem, as dificuldades sociais e sensoriais, assim como os comportamentos repetitivos, podem aparentar serem mais sutis e, consequentemente, se tornam pouco detectáveis em um processo de diagnóstico.

Além disso, os "temas" de interesses restritos, comuns a pessoas autistas, também costumam divergir em uma comparação de gênero (Driver e Chester, 2021). Estudos apontam que meninos autistas usualmente possuem interesses restritos relacionados a física, computação, mecânica e construção, enquanto meninas autistas se interessam mais por televisivos, psicologia, política, religião, dentre outros temas de um nicho mais "social" (Nowell *et al*., 2019). Essa distinção contribui para que os interesses restritos de meninas autistas não sejam reconhecidos como um traço do TEA, dado que eles se desviam do padrão masculino geralmente utilizado para o diagnóstico (Nowell *et al*., 2019).

Nesse sentido, o despreparo profissional no reconhecimento das diferenças de gênero evidentes no TEA contribui para que muitas mulheres autistas não sejam diagnosticadas, o que, por sua vez, pode impactar negativamente na qualidade de vida delas, considerando que a ausência desse diagnóstico compromete o acesso ao suporte necessário que é de direito do autista (Driver e Chester, 2021).

4. CONCLUSÕES:

A partir da revisão realizada, conclui-se que, por motivações de viés histórico, há uma escassez de pesquisas que dizem respeito às mulheres autistas, principalmente em âmbito nacional. Essa carência de estudos afeta as ferramentas de diagnóstico do transtorno do espectro autista, e por conseguinte, também afetas os indivíduos que necessitam desse diagnóstico o mais cedo possível. É notória, portanto, a necessidade de se alterar esse cenário, através de investigações científicas e treinamento adequado, de modo que os profissionais possam aprimorar seus conhecimentos a respeito do perfil autista feminino.

5. REFERÊNCIAS:

1. Bargiela, S., Steward, R. e Mandy, W. (2016) 'The experiences of late-diagnosed women with autism spectrum conditions: An investigation of the female autism phenotype', *Journal of Autism and Developmental Disorders*, 10 (46): 3281-3294.

2. Driver, B. e Chester, V. (2021) 'The presentation, recognition, and diagnosis of autism in women and girls', *Advances in Autism*, 3 (7): 194-207.

3. Grove, R., Hoekstra, R. A., Wierda, M. e Begeer, S. (2017) 'Exploring sex differences in autistic traits: A factor analytic study of adults with autism', *autism*, 6 (21): 760-768.

4. Hendrickx, S. (2015) *'Women and Girls with Autism Spectrum Disorder'*, London: Jessica Kingsley Publishers.

5. Lai, M., Lombardo, M. V., Pasco, G., Ruigrok, A. N. V., Wheelwright, S. J., Sadek, S. A., Chakrabarti, B. e Baron-Cohen, S. (2011) 'A behavioral comparison of male and female adults with high functioning autism spectrum conditions', *PloS one*, 6 (6), e20835.
6. Lai, M., Lombardo, M. V., Ruigrok, A. N., Chakrabarti, B., Auyeung, B. e Szatmari, P. (2017) 'Quantifying and exploring camouflaging in men and women with autism', *autism: the International Journal of Research and Practice*, 21 (6), 690-702.

7. Loomes, R., Hull, L. e Mandy, W. (2017) 'What Is the Male-to-Female Ratio in Autism Spectrum Disorder? A Systematic Review and Meta-Analysis', J*ournal of the American Academy of Child and Adolescent Psychiatry*, 56 (6), 466-474.

8. Nowell, S. W., Jones, D. R. e Harrop, C. (2019) 'Circumscribed interests in autism: are there sex differences?', *Advances in Autism*, 3 (5): 187-198.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THE IMPACT OF THE LACK OF KNOWLEDGE OF THE FEMALE AUTISTIC PROFILE IN THE QUALITY OF LIFE OF AUTISTIC WOMEN

Sophia dos Santos Tavares Freitas da Silva
Universidade de Vassouras, Undergraduate student in Psychology - Brazil

Larissa Primo Pereira Lasneau
Universidade de Vassouras, Undergraduate professor in Psychology - Brazil

February/2022

INTRODUCTION

SBJChem Conference 2021

- Historically, studies of autism spectrum disorder have focused on boys;
- Gender biased diagnostic tools;
- Missed diagnosis, late diagnosis or misdiagnosis;
- Access to needed support and help with identity crises.

OBJETIVE

SBJChem Conference 2021

Highlight the gender distinctions present in the manifestation of autism spectrum disorder and the need to know the female autistic profile, in order to promote better living conditions for these women.

METHODOLOGY

SBJChem Conference 2021

- A bibliographic search was carried out in the Google Scholar database. The keywords were searched: “autism in women”; “diagnosis of autism in women” and “female profile of autism”;
- The criteria used for inclusion were: texts published since 2019, in English and Portuguese;
- As a criterion used for exclusion, texts that did not address the subject, or addressed it inaccurately, were discarded;
- A total of 32 articles were found, and considering the criteria applied, 12 articles were selected.

DISCUSSION

SBJChem Conference 2021

- Women tend to camouflage more than men, making social and sensory difficulties seem milder;
- The consequences of autistic camouflage/masking;
- Topics of Restricted Interests can differ between genders;
- Professional unpreparedness in recognizing these differences negatively affects autistic women.

5

CONCLUSION

SBJChem Conference 2021

It is evident the need to change this scenario, through scientific investigations and adequate training, so that professionals can improve their knowledge about the female autistic profile.

6

REFERENCES

SBJChem Conference 2021

1. Bargiela, S., Steward, R. and Mandy, W. (2016). The experiences of late-diagnosed women with autism spectrum conditions: An investigation of the female autism phenotype. *Journal of Autism and Developmental Disorders, 10* (46): 3281-3294.
2. Driver, B. and Chester, V. (2021). The presentation, recognition and diagnosis of autism in women and girls. *Advances in Autism, 3* (7): 194-207.
3. Grove, R., Hoekstra, R. A., Wierda, M. e Begeer, S. (2017). Exploring sex differences in autistic traits: A factor analytic study of adults with autism. *Autism, 6* (21): 760-768.
4. Hendrickx, S. (2015). *Women and Girls with Autism Spectrum Disorder*. London: Jessica Kingsley Publishers.
5. Lai, M., Lombardo, M. V., Pasco, G., Ruigrok, A. N. V., Wheelwright, S. J., Sadek, S. A., Chakrabarti, B. e Baron-Cohen, S. (2011). A behavioral comparison of male and female adults with high functioning autism spectrum conditions. *PloS one, 6* (6), e2083S.
6. Lai, M., Lombardo, M. V., Ruigrok, A. N., Chakrabarti, B., Auyeung, B. e Szatmari, P. (2017). Quantifying and exploring camouflaging in men and women with autism. *Autism: the international journal of research and practice, 21* (6), 690-702.
7. Loomes, R., Hull, L. e Mandy, W. (2017). What Is the Male-to-Female Ratio in Autism Spectrum Disorder? A Systematic Review and Meta-Analysis. *Journal of the American Academy of Child and Adolescent Psychiatry, 56* (6), 466-474.
8. Nowell, S. W., Jones, D. R. e Harrop, C. (2019). Circumscribed interests in autism: are there sex differences?. *Advances in Autism, 3* (5): 187-198.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

TOTAL CONTENT OF CALCIUM AND PHOSPHORUS IN SERUM OF WISTAR RATS BY AN OPTIMIZED METHOD OF ICP-MS

KOTH, Valesca[1*]; RUBENSAM, Gabriel[2]; BARREIRO, Bernardo Ottoni Braga[1]; STEIN, Thaynã Spencer[2]; CHERUBINI, Karen[1];

[1] Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Programa de Pós-Graduação em Odontologia

[2] Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de Pesquisa em Farmacologia e Toxicologia

** Correspondence author*
e-mail: valesca.koth@acad.pucrs.br

Received 30 January 2022; received in revised form 15 February 2022; accepted 23 February 2022

ABSTRACT

In the Odontology field, the modeling process of alveolar bone has been a topic of investigation for the last years since the lost bone after tooth extraction can preclude aesthetic and function. In this practice, the volume of the tissue to be modeled depends on, among other factors, the serum levels of calcium and phosphorus, and it is of interest to monitor these elements to better understand the mechanism of tissue regeneration. These elements are routinely analyzed for clinical purposes, as serum constituents, by UV-VIS spectrophotometry after chromogenic reactions for each metal with different reagents. Depending on the analytical demands and work objectives, it is necessary to have methods based on technologies that allow multi-element quantification in a single experiment. In this context, ICP-MS has been considered a powerful tool for rapid multi-element analysis due to its high selectivity and sensitivity. However, it has been reported that samples with high content of salts and proteins, such as serum samples, cause matrix-induced interferences due to weak sample preparation and the presence of polyatomic ions. The present study aimed to identify and mitigate matrix effects in rat serum samples during the simultaneous quantification of calcium and phosphate using ICP-MS and evaluate its capability of differentiating element levels from Wistar rats subjected to tooth extraction with and without alveolar bone grafting. In addition, the optimized method can be used for more comprehensive mineralomics studies related to the bone modeling process in future studies.

Keywords: *Bone mineralization, rat serum, sample preparation, ICP-MS*

1. INTRODUCTION

The modeling and remodeling process of alveolar bone after tooth extraction has been a topic of investigation for the last years to maintain the volume of the tissue since tooth extraction results in bone loss, which can affect aesthetic and function (Stavropoulos *et al.,* 2015; Lopes *et al.,* 2018). The use of bone grafting during the surgical procedure favors this process (Stavropoulos *et al.,* 2015). Three main types of cells are involved in bone remodeling: osteoclasts, which resorb bone; osteoblasts, which deposit new bone, and osteocytes, responsible for mechanical senses perception and stimulus of bone remodeling (Alford *et al.,* 2015). These cells are regulated by local (mechanical or cytokines) and systemic (hormones) signals (Lopes *et al.,* 2018). The bone tissue is composed of organic and inorganic matrices. Collagen fibers are the main constituents of the organic part. At the same time, hydroxyapatite - a molecule structured by calcium phosphate - is the key element of the inorganic matrix (Tobeiha *et al.,* 2020). Bone neoformation starts with the deposition of collagen fibrils by osteoblasts, forming a scaffold, which is then mineralized by the precipitation of ions of calcium and phosphate, promoting the hydroxyapatite crystals' formation. The process requires normalized levels of calcium and phosphate in the blood. Otherwise, there can be inadequate bone mineralization with an excess of non-calcified

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.27_abstract_KOTH.pdf

bone matrix (Alford *et al.,* 2015; Murshed *et al.,* 2018). Indeed, the knowledge of seric calcium and phosphorus levels is important to better understand the process of alveolar bone modeling. Therefore, using a preclinical *in vivo* model analog to the human. To study the alveolar healing after tooth extraction, rodents are the most used *in vivo* model, since they are cheaper and faster than larger animals and allow harvest of specimens to analysis, which is not possible in human studies, added to issues related to practical and safety, ethics and regulatory concerns (Stavropoulos *et al.,* 2015).

Serum levels of calcium and phosphorus are routinely quantified, for clinical purposes, by UV-VIS spectrophotometry after chromogenic reactions for each metal with different reagents (Bueno & Czepielewski, 2010). However, depending on the analytical demands and work objectives, such as the determination of free or total elements, sample type, and the number of samples, it is necessary to have methods based on technologies that allow multi-element quantification in a single experiment with good selectivity. In this context, ICP-MS has been considered a powerful tool for rapid multi-element analysis due to its high selectivity and sensitivity (Laur et al., 2020). However, it has been reported that samples with high salts and proteins, such as serum samples, struggle with suppression and enhancement of analytic signal on ICP-MS methodologies, especially due to weak sample preparation and the presence of polyatomic ions (Lu *et al.,* 2015). Some works have been published to overcome these problems presenting different sample treatments, such as digestion conditions (Lu *et al.,* 2015) and types of equipment with different configurations (Konz *et al.,* 2017). Although good results were demonstrated, some adaptations are occasionally required to reach specific analysis needs.

The present study aimed to identify and mitigate matrix effects caused by rat serum samples during the simultaneous quantification of calcium and phosphate by ICP-MS and evaluate its capability of differentiating element levels from Wistar rats submitted to tooth extraction with or without alveolar bone grafting.

2. MATERIALS AND METHODS

2.1. Chemicals

Sub-boiling distilled Nitric acid 65% EMSURE® Reagent Ph Eur, ISO (Merck, Germany); Type 1 water obtained by Milli-Q UV system (Millipore, USA), were used. In addition, multi-element standard solution XVI (Merck Darmstadt, Germany), Calcium and phosphorus TraceCert standard at 1000 mg/L in 2% nitric acid and water, respectively; ketamine and xylazine were purchased from Syntec (Syntec do Brasil LTDA, Brazil).

2.2. Animals

This study was approved by the Ethics Committee on Animals Use of the Pontifícia Universidade Católica do Rio Grande do Sul (PUCRS, protocol #9108), and performed following the guidelines for the National Council for Animal Experimentation Control (CONCEA). Ten adult female Wistar rats (±220 g) were kept in cages with temperature-controlled rooms and with food and water offered *ad libitum*. After an acclimatization period, the animals were subjected to tooth extraction of molars of the right side of the jaw under general anesthesia with a mixture of ketamine and xylazine. Five rats had the socket filled with bone grafting (group 1), and five animals did not receive grafting (group 2). The animals were euthanized after 35 days by blood exsanguination and anesthetic overdose. The collected blood was centrifuged at 3000 rpm for 10 min after the formation of the clot. The serum was stored at -20 ºC until analysis. In addition, the maxilla was collected for histological examination of the alveolar socket.

2.3. Sample Preparation

Serum samples were prepared according to described elsewhere (Lu *et al.,* 2015), with modifications. Briefly, thawed samples were transferred to 15 mL polymeric vials with a screw cap and added by sub-boiling nitric acid. The vials were heated to the water boiling point in a thermostated water bath. After digestion, all samples were added by type 1 water at a final volume of 10 mL and were injected into the ICP-MS system. To evaluate the digestion efficiency, a group of five distinct serum samples was added by standards at a final concentration of 50 mg/L and nitric acid at the sample: acid ratio of 100:308; 50:308; 33:308; 25:308; and 20:308 µL (v/v), representing the dilution factors of 1, 2, 3, 4, and 5 respectively. These factors were used to normalize the analyte signal and evaluate matrix effects. The digestion time was evaluated using another group of five serum samples added by standards and nitric acid at a ratio of 20:308 µL (v/v), which were digested at the times of 0, 15, 30, 60, 120, and 180 min. Calibration curves were constructed at concentrations of 50, 100, 250, 500,

and 750 µg/L, prepared in 2% nitric acid. All test samples were analyzed in triplicate.

The the collected jaws were fixed, decalcified, and embedded in paraffin. One section of 4 µm was cut in the middle of the alveolar socket and stained with hematoxylin and eosin (HE) for histological evaluation.

2.4. ICP-MS analysis

It was used an ICP-MS 7700 (Agilent Technologies, Tokyo, Japan) system equipped with an autosampler, 2.5mm quartz torch, Ni sampler, and skimmer cones, i.d. 1.0 and 0.4 mm. The operating conditions were 1550W plasma RF power, 1.3 L/min argon carrier gas, and 4 L/min helium collision gas flow. The isotopes monitored for calcium were ^{42}Ca and ^{44}Ca, and phosphorus was ^{31}P, with a dwell time of 0,3 s. The oxide species (CeO/Ce) level was below 1.5%, and doubly charged (Ce^{2+}/Ce) was below 3%. The quantification was performed with external calibration curves in gas (He) and no gas mode.

3. RESULTS AND DISCUSSION:

The parameters optimized for sample digestion were the digestion time and the sample: acid ratio. After optimization, the proposed method was applied to determine the total content of phosphorus and calcium in Wistar rat serum by ICP-MS. As presented in Figure 1, effective sample digestion was obtained after 60 min. Considering the amount of analyte released from the matrix. The optimal sample:acid ratio was obtained from the dilution factor of 3 (33:308 µL, v/v). However, we fixed the factor of 5 to avoid matrix effects. Matrix effects were evaluated by examining the signal suppression or enhancement after reducing the amount of sample concerning the amount of nitric acid in the digestion step and after normalizing analytes signals by the dilution factor.

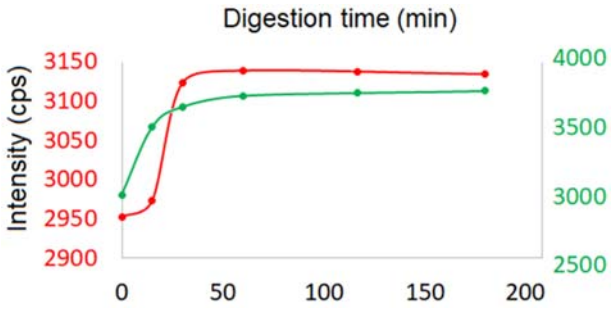


Figure 1. *Digestion efficiency due to contact time between the sample and nitric acid. Total serum calcium (average) was presented in red, and total serum phosphorus (average) was presented in red. Y-axis as signal intensity (cps).*

As presented in Figure 2, this effect was observed for sample:acid ratios of 100:308 and 50:308 µL (v/v), in which analyte signals were higher than the other ratios. We also added multi-element standards into the samples to evaluate the effects caused by polyatomic interferences over phosphorus and calcium signals.

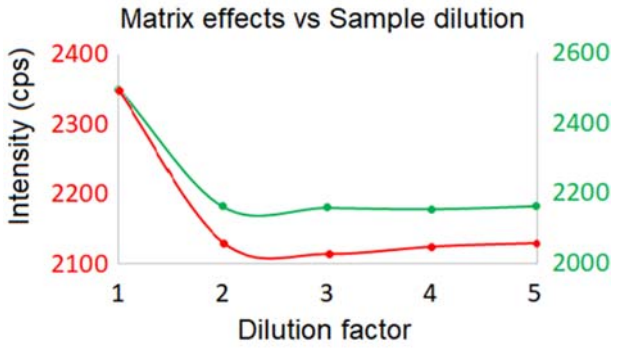


Figure 2. *Matrix effects correction with sample dilution. Total serum calcium (average) was presented in red, and total serum phosphorus (average) was presented in red. Y-axis as signal intensity (cps).*

Indeed, we observed an enhancement of calcium signal due to the presence of magnesium in the standard, which interferes with ($^{26}Mg^{16}O^{+}$ and $^{26}Mg^{18}O^{+}$) in both calcium isotopes used in the present work (^{42}Ca and ^{44}Ca). For this purpose, calibration curves were constructed with single-element standards.

We tested the capability of the optimized method to differentiate element levels from Wistar rats submitted to tooth extraction with (group 1) or without (group 2) bone grafting inside the socket. As presented in Figure 3, the group that received grafting treatment presented a lower concentration of total calcium and a higher amount of phosphorus. The calcium analysis showed a significant difference between groups ($p<0.05$, Mann Whitney test), indicating a higher mobilization of calcium to the alveolar bone. However, it is important to emphasize that the levels of this mineral remained inside normal ranges in serum of rats (Hernández-Becerra *et al.*, 2020) and, therefore, bone remodeling could happen in a standard way in both groups, which was observed in histological evaluation. Calcium is an essential mineral, and serum levels between 92 – 140 mg/L are considered normal (Mulyaningsih *et al.*, 2019). Figure 4 shows the alveolar bone of group 2.

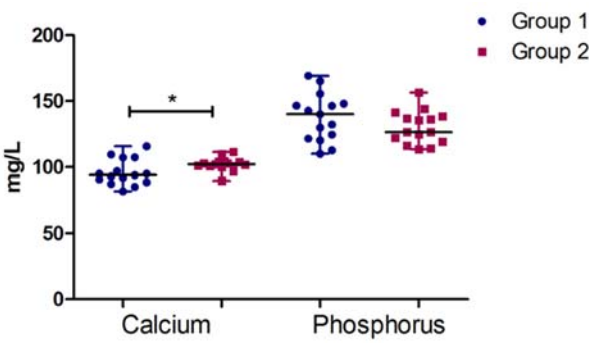


Figure 3. *Concentration of calcium and phosphorus in serum according to the groups. Data is shown as median and range*.

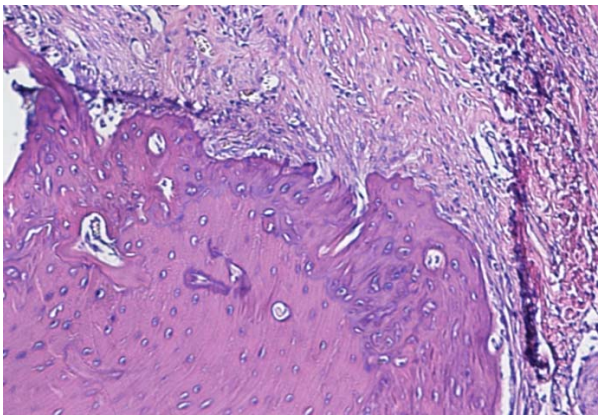


Figure 4. *Alveolar bone formed after tooth extraction in group 2*. HE stains, 100x

Considering that total calcium and phosphorus content in human and rat blood is similar (Zaksas *et al.,* 2010), the results obtained in the present work were relatively similar to the findings reported by other authors that also used ICP-MS (Konz *et al.,* 2017; Tao *et al.,* 2019, Xia *et al.,* 2021). However, total calcium levels were slightly higher than reported in the literature, probably due to magnesium in the serum, which ranged from 0.5 to 21.3 mg/L (Laur *et al*., 2020).

4. CONCLUSIONS:

A simple and effective acid digestion method was proposed here to determine the total content of calcium and phosphorus in rat serum samples with reduced matrix effects. The methodology pointed a small difference between the groups that stayed inside normal ranges of the minerals to provide normal bone remodeling. The optimized method was considered useful for monitoring calcium and phosphorus in rat serum samples and propitious for more comprehensive mineralogical studies related to the bone modeling process in future studies.

5. ACKNOWLEDGMENTS:

This study was supported by National Council for Scientific and Technological Development (CNPq, Brazil) and Coordenação de Aperfeiçoamento de Pessoal de Nivel Superior (CAPES, Brazil).

6. REFERENCES:

1. Alford, A. I., Kozloff, K. M., Hankenson, K. D. *Int. J. Biochem. Cell Biol.,* **2015**, *65*, 20.
2. Bueno, A. L. & Czepielewski, M.A. *Rev. Nutr.,* **2010**, *3*, 65-73.
3. Hernández-Becerra, E., Jímenez-Mendoza, D., Mutis-Gonzalez, N., Pineda-Gomez, P., Rojas-Molina, I., & Rodríguez-García, M. E. Calcium Deficiency in Diet Decreases the Magnesium Content in Bone and Affects Femur Physicochemical Properties in Growing Rats. *Biol. Trace Elem. Res.*, **2020**, 197(1), 224–232.
4. Konz, T., Migliavacca, E., Dayon, L., Bowman, G., Oikonomidi, A., **J. Proteome Res., 2017**, *16*, 2080–2090.
5. Laur N, Kinscherf R, Pomytkin K, Kaiser L, Knes O, Deigner HP. *PLOS ONE*, **2020**, 15
6. Lopes, D., Martins-Cruz, C., Oliveira, M. B., Mano, J. F. *Biomaterials*, **2018**, *185*, 240–275.
7. Lu, Y., Kippler, M., Harari, F., Grandér, M. Palm, B., Nordqvist, H., Vahter, M., *Clin. Biochem.,* **2015**, *48*, 140–147.
8. Mulyaningsih, N.N.; Juwono, A.; Soejoko, D.S.; Astuti, D.A.. Serum Mineral Status and Long Bone Morphometry of Ovariectomized Rats Fed a Nano-Calcium Phosphate Diet. *Pak. J. Nutr*, **2019**, 18: 1058-1067
9. Murshed, M. *Cold. Spring. Harb. Perspect. Med.*, **2020**, *3*, a031229.
10. Stavropoulos, A., Sculean, A., Bosshardt, D. D., Buser, D., Klinge, B. *Periodontol. 2000*, **2015**, *68*, 55–65.
11. Tao, Y., Huang, S., Yan, J., Li, W., Cai, B. *J. ethnopharmacol.*, **2019**, 234, 85–95
12. Tobeiha, M., Moghadasian, M. H., Amin, N., Jafarnejad, S. *BioMed. Res. Int.*, **2020,** 6910312.
13. Zaksas, N.P.; Gerasimov, V.A.; Nevinsky, G.A..*Talanta*, **2010**, *80,* 2187-2190.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

TOTAL CONTENT OF CALCIUM AND PHOSPHORUS IN SERUM OF WISTAR RATS BY AN OPTIMIZED METHOD OF ICP-MS

Valesca Koth
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde, Programa de Pós-Graduação em Odontologia

Gabriel Rubensam
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de Pesquisa em Farmacologia e Toxicologia

Bernardo Ottoni Braga Barreiro
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde, Programa de Pós-Graduação em Odontologia

Thaynã Spencer Stein
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de Pesquisa em Farmacologia e Toxicologia

Karen Cherubini
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde, Programa de Pós-Graduação em Odontologia

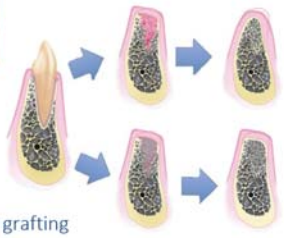
February/2022

INTRODUCTION

SBJChem Conference 2021

Aesthetic

Function

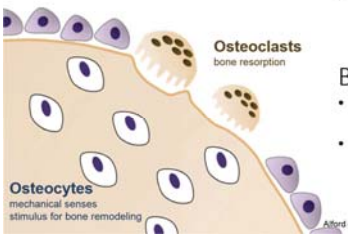


Alveolar bone grafting

Lopes et al., 2018; Pagni et al., 2021; Stavropoulos et al., 2015

BACKGROUND

SBJChem Conference 2021



Bone remodeling

- Bone cells
- Cytokines
- Mechanical forces
- Hormones

Bone tissue

- Organic
  collagen
- Inorganic
  hydroxyapatite crystals – calcium and phosphate

Alford et al., 2015; Lopes et al., 2018; Tobeiha et al., 2020; Murshed et al., 2018

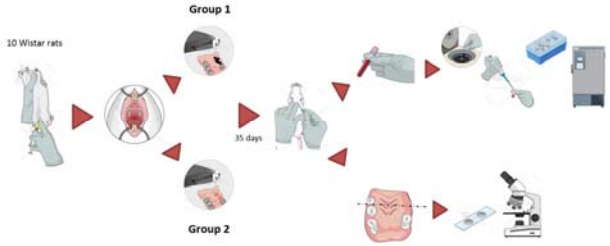
AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

The present study aimed to identify and mitigate matrix effects caused by rat serum samples during the simultaneous quantification of calcium and phosphate by ICP-MS, and evaluate its capability of differentiating element levels from Wistar rats submitted to tooth extraction with or without alveolar bone grafting.

METHODOLOGY

SBJChem Conference 2021

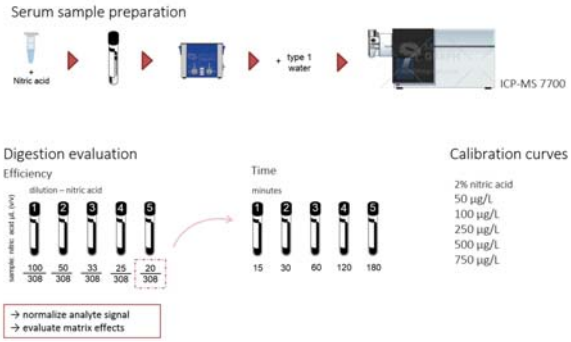


Ethics Committee on Animals Use of the PUCRS, protocol #9108

mindthegraph.com

METHODOLOGY

SBJChem Conference 2021

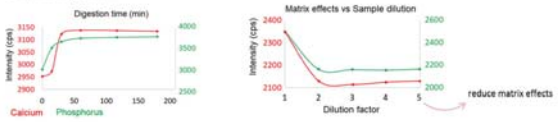


Lu, et al., 2015 ; mindthegraph.com

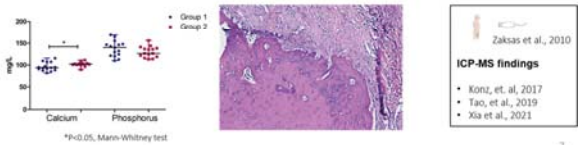
RESULTS AND DISCUSSION

SBJChem Conference 2021

Sample digestion



Differentiation of levels of calcium and phosphorus in rats after tooth extraction



7

Hernández-Becerra, et al., 2020; Mulyaningsih et al., 2019

CONCLUSIONS

SBJChem Conference 2021

- A simple and effective acid digestion method was here proposed to allow the determination of total content of calcium and phosphorus in rat serum samples, with reduced matrix effects.
- The methodology was able to point a small difference between the groups that stayed inside normal ranges of the minerals to provide normal bone remodeling.
- This method was considered useful for monitoring calcium and phosphorus in serum samples and propitious for a more comprehensive mineralomics studies related to the bone modeling process in future studies.

8

ACKNOWLEDGEMENTS

SBJChem Conference 2021

- This study was supported by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq, Brazil) and
- Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES, Brazil)

REFERENCES

SBJChem Conference 2021

1. Alford, A. I., Kozloff, K. M., Hankenson, K. D. *Int. J. Biochem. Cell Biol.,* **2015**, *65*, 20.
2. Bueno, A. L. & Czepielewski, M.A. *Rev. Nutr.,* **2010**, *3*, 65-73.
3. Hernández-Becerra, E., Jímenez-Mendoza, D., Mutis-Gonzalez, N., Pineda-Gomez, P., Rojas-Molina, I., & Rodríguez-García, M. E. Calcium Deficiency in Diet Decreases the Magnesium Content in Bone and Affects Femur Physicochemical Properties in Growing Rats. *Biol. Trace Elem. Res.*, **2020**, 197(1), 224–232.
4. Konz, T., Migliavacca, E., Dayon, L., Bowman, G., Oikonomidi, A., **J. Proteome Res., 2017**, *16*, 2080–2090.
5. Laur N, Kinscherf R, Pomytkin K, Kaiser L, Knes O, Deigner HP. *PLOS ONE*, **2020**, 15
6. Lopes, D., Martins-Cruz, C., Oliveira, M. B., Mano, J. F. *Biomaterials*, **2018**, *185*, 240–275.
7. Lu, Y., Kippler, M., Harari, F., Grandér, M. Palm, B., Nordqvist, H., Vahter, M., *Clin. Biochem.,* **2015**, *48*, 140–147.
8. Mulyaningsih, N.N.; Juwono, A.; Soejoko, D.S.; Astuti, D.A.. Serum Mineral Status and Long Bone Morphometry of Ovariectomized Rats Fed a Nano-Calcium Phosphate Diet. *Pak. J. Nutr*, **2019**, 18: 1058-1067
9. Murshed, M. *Cold. Spring. Harb. Perspect. Med.*, **2020**, *3*, a031229.
10. Stavropoulos, A., Sculean, A., Bosshardt, D. D., Buser, D., Klinge, B. *Periodontol. 2000*, **2015**, *68*, 55–65.
11. Pagni, G., Pellegrini, G., Giannobile, W. V., & Rasperini, G.. Postextraction alveolar ridge preservation: biological basis and treatments. International journal of dentistry, 2012, 151030
12. Tao, Y., Huang, S., Yan, J., Li, W., Cai, B. *J. ethnopharmacol.*, **2019**, 234, 85–95
13. Tobeiha, M., Moghadasian, M. H., Amin, N., Jafarnejad, S. *BioMed. Res. Int.*, **2020,** 6910312.
14. Zaksas, N.P.; Gerasimov, V.A.; Nevinsky, G.A..*Talanta*, **2010**, *80*, 2187-2190.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

TOTAL CONTENT OF CALCIUM AND PHOSPHORUS IN SERUM OF WISTAR RATS BY AN OPTIMIZED METHOD OF ICP-MS

Valesca Koth
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde, Programa de Pós-Graduação em Odontologia

Gabriel Rubensan
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de Pesquisa em Farmacologia e Toxicologia

Bernardo Ottoni Braga Barreiro
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde, Programa de Pós-Graduação em Odontologia

Thaynã Spencer Stein
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de Pesquisa em Farmacologia e Toxicologia

Karen Cherubini
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde, Programa de Pós-Graduação em Odontologia

February/2022

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

TRANSCRANIAL DIRECT STIMULATION IN THE NEUROMODULATION OF CONTROLLING MAIN SYMPTOMS OF PARKINSON'S DISEASE: A CASE STUDY

SOUZA, Alice Medeiros de[1]; AMADEU, Lilian Campos[1]; VOSNIADOU, Eleni[1]; CORRÊA, Fernanda Ishida[1]; DALL'AGNOL, Letizzia[1]*;

[1] Universidade Nove de Julho, Faculdade de Fisioterapia

*Letizzia Dall'Agnol
e-mail: fisioterapiador@gmail.com

Received 20 September 2021; received in revised form 30 December 2021; accepted 10 January December 2022

ABSTRACT

Parkinson's disease (PD) is a central nervous system neurodegenerative disorder that primarily affects the motor system, decreasing motor coordination, balance and generating tremors, and a progressive loss of everyday mobility, including walking. This study was conducted to verify the effects of Transcranial Direct Current Stimulation (tDCS) on balance, motor control, and the quality of life in Parkinson's disease patients. The patient received three treatments consisting of 10 sessions of 20 minutes each and a one-week interval between treatments. Active stimulation was applied on the primary motor cortex (M1), the dorsolateral prefrontal cortex (DLPFC), and the dorsolateral prefrontal cortex (D Sham-tDCS. DLPFC stimulation produced the best improvements in terms of motor control, balance, gait, and overall PD symptoms, as evaluated by different scales and questionnaires. As a result, active stimulation of the DLPFC produced superior outcomes and may contribute to treating Parkinson's disease.

Keywords: *Parkinson's disease, tDCS, Motor Control, Rest Tremor, Quality of Life*.

1. INTRODUCTION

Parkinson's disease (PD) is a progressive neurodegenerative disorder of the central nervous system that mainly affects the motor system, impairing motor coordination, balance, causing tremors with progressive loss of everyday movement, including walking (de Lau, 2006). Epidemiological studies indicate that PD currently affects about 1% of the population of the world over 60 years of age (Marttila, 1981). However, it can affect young adults and, in rare cases, individuals under 40 years of age (Darweesh, 2017). Furthermore, the incidence increases with age, and the disease symptoms appear more frequently after age 55 (Olanow, 1999).

The main characteristic of PD is the progressive loss of predominantly dopaminergic neurons found in the gray matter located in the midbrain. These neurons are part of the extrapyramidal system, which is directly related to the motor system (de Lau, 2006). Neurotransmitter dopamine acts directly on the basal nuclei to facilitate voluntary automatic movement of the body. PD becomes evident at the loss of approximately 80% of the dopaminergic neurons, and PD patients begin to present a great variety of symptoms, mainly related to a lack of motor control (Jankovic, 2020).

Brain neuromodulation therapies, such as transcranial direct current stimulation (tDCS), are known to improve symptoms associated with PD (Ferrucci, 2016; Fateme, 2021). tDCS can induce significant improvement in motor function when applied to the primary motor cortex (M1) (Elsner, 2016) and also a significant antidepressant effect when applied over the dorsolateral prefrontal cortex (DLPFC) (Dinkelbach, 2017). However, very few studies currently demonstrate the effects of tDCS on the overall improvement in motor function and quality of life in patients with PD. Therefore, we conducted a study to verify the effects of tDCS on balance, motor control, and the quality of life of patients with PD.

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM. 21scon.06_abstract_ISHIDA.pdf

2. MATERIALS AND METHODS

2.1. Participant

After signing the Informed Consent Form, the patient participating in the study, a 72-year-old male, was recruited voluntarily through the Supervised Clinical Practice in Neurology at Universidade Nove de Julho. Unfortunately, by the time the study started, the participant could not receive any sort of motor rehabilitation that may interfere with the results to be included in the research.

2.2 tDCS protocol

The participant received three treatments, consisting of 10 sessions of 20 minutes each and a one-week interval in between treatments. Treatments were randomized, resulting in the following order: (1) active tDCS over M1, (2) active tDCS over DLPFC, and (3) Sham tDCS. For both M1 and DLPFC, we used the intensity of 2mA. During the sham-tDCS treatment, the participant stayed for 20 minutes with the electrodes in the same locations as in the a-tDCS condition. However, the device was turned off after 30 seconds of active stimulation. Adverse effects of the stimulation were minor and not persistent (skin redness and tingling during active stimulation and drowsiness/sleepiness during Sham).

2.3 Outcome measures

The following scales and questionnaires were used to assess the effectiveness of the treatments: Timed up and go test (TUG), e Unified Parkinson's Disease Rating Scale (UPDRS), Scales for Outcomes in Parkinson's Disease - Motor Function (SCOPA-M), Berg Balance Scale (BBS), State-Trait Anxiety Inventory (STAI), Pittsburgh Sleep Quality Index (PSQI), Parkinson's Disease Questionnaire (PDQ-39), and Beck Depression Inventory (BDI). Before and after each treatment, all scales and questionnaires were used to analyze the participant (Table 1).

3. RESULTS AND DISCUSSION

After active tDCS stimulation over M1, the patient showed an increase in motor control, a decrease in rest tremors, a broader range of motion in the upper limbs, hands, and fingers, and considerably improved control of pinch motions as measured by the UPDRS (16%) and SCOPA (9%) scales.

Stimulation over DLPFC presented the highest motor control improvement, balance, and gait, as well as a reduction in symptoms associated with PD, according to an improvement of results in TUG (50%), BBS (20%), UPDRS (38,18%) and SCOPA (36%). On the other hand, sham intervention, in comparison to DLPFC stimulation, showed a decrease in TUG (12,5%), UPDRS (8%), and BBS (3%), thus demonstrating a worsening in the condition of the patient. (see Table 1 for results).

While analyzing the results, we found that, in regards to the quality of sleep and levels of anxiety, the patient presented worsening after active stimulation over M1 according to increased values of PSQI (71%), PDQ-39 (19%), and BDI (50%). However, it is essential to note that these results correspond with the period when the physician of the patient adjusted the prescription for Parkinson's disease (Pramipexole), which caused hallucinations and worsened sleep quality before reverting to the initial dosage of medicine. Although it was not possible to come to conclusive findings in relation to the anxiety levels of the patient, DLPFC stimulation showed the highest results, demonstrating improvement in quality of sleep, as shown on the PSQI (60%).

While not conclusive, our results suggest that active M1 and DLPFC stimulation might improve parkinsonian symptoms, such as resting tremor, loss of motor control and balance. This goes along with the review (Broeder, 2015), showing the efficacy of M1 stimulation in improving motor function and indicating that DLPFC stimulation benefited executive function. However, it is unclear which form of stimulation delivers the best results. According to (Lattari, 2016) substantial findings were obtained when comparing the influence of left DLPFC stimulation on balance and functional mobility.

Regarding the results on DLPFC stimulation, we could find significance on the TUG, UPDRS, SCOPA, BBS, and PSQI results. This corroborates with the findings of (Manenti, 2014), showing a substantial motor improvement following DLPFC stimulation compared to Sham-tDCS.

As additional information, the patient reported increasing resting tremors and rigidity during the one-week intervals in between treatments. Also, the patient had insomnia at the time he was receiving active stimulation but had hypersomnolence when receiving Sham stimulation, during and after each session, being represented by the increase of the PSQI (50%), PDG-39 (29%), and BDI (13%) scales during Sham-tDCS.

4. CONCLUSIONS

In this study, DLPFC stimulation showed the highest improvements in motor control, balance, gait, and overall PD symptoms. Additionally, improved sleep quality was observed on the PSQI scale during DLPFC stimulation and Sham-tDCS. Thus, active stimulation over DLPFC has better results than stimulation over M1 and Sham-tDCS.

One limitation of the present study was the absence of investigation of further long-lasting effects of the therapy. In addition, future research investigating cortical excitability in its relation to controlling the main symptoms of PD might provide more explanations for our findings. Finally, this study was a case study involving only one patient, and we hope studies with larger sample sizes might better explore the present study results.

5. REFERENCES

1. Broeder, S., Nackaerts, E., Heremans, E., Vervoort, G., Meesen, R., Verheyden, G., and Nieuwboer, A. (2015). Transcranial direct current stimulation in Parkinson's disease: Neurophysiological mechanisms and behavioral effects. Neuroscience and biobehavioral reviews, 57, 105–117.
2. Darweesh, S. K., Verlinden, V. J., Stricker, B. H., Hofman, A., Koudstaal, P. J., and Ikram, M. A. (2017). Trajectories of prediagnostic functioning in Parkinson's disease. Brain: a journal of neurology, 140(2), 429–441.
3. de Lau, L. M., and Breteler, M. M. (2006). Epidemiology of Parkinson's disease. The Lancet. Neurology, 5(6), 525–535.
4. Dinkelbach, L., Brambilla, M., Manenti, R., and Brem, A. K. (2017). Non-invasive brain stimulation in Parkinson's disease: Exploiting crossroads of cognition and mood. Neuroscience and biobehavioral reviews, 75, 407–418.
5. Elsner, B., Kugler, J., Pohl, M., and Mehrholz, J. (2016). Transcranial direct current stimulation for improving idiopathic Parkinson's syndrome. An abridged version of a Cochrane review. European journal of physical and rehabilitation medicine, 52(6), 902–906.
6. Ferrucci, R., Mameli, F., Ruggiero, F., and Priori, A. (2016). Transcranial direct current stimulation as treatment for Parkinson's disease and other movement disorders. Basal ganglia, 6, 53-61.
7. Jankovic, J., and Tan, E. K. (2020). Parkinson's disease: etiopathogenesis and treatment. Journal of neurology, neurosurgery, and psychiatry, 91(8), 795–808.
8. Lattari, E., Costa, S. S., Campos, C., de Oliveira, A. J., Machado, S., and Maranhao Neto, G. A. (2017). Can transcranial direct current stimulation on the dorsolateral prefrontal cortex improves balance and functional mobility in Parkinson's disease?. Neuroscience letters, 636, 165–169.
9. Manenti, R., Brambilla, M., Rosini, S., Orizio, I., Ferrari, C., Borroni, B., and Cotelli, M. (2014). Time up and go task performance improves after transcranial direct current stimulation in patients affected by Parkinson's disease. Neuroscience letters, 580, 74–77.
10. Marttila, R. J., and Rinne, U. K. (1981). Epidemiology of Parkinson's disease an overview. Journal of neural transmission, 51(1-2), 135–148.
11. Olanow, C. W., and Tatton, W. G. (1999). Etiology and pathogenesis of Parkinson's disease. Annual review of neuroscience, 22, 123–144.
12. Pol, F., Salehinejad, M. A., Baharlouei, H., and Nitsche, M. A. (2021). The effects of transcranial direct current stimulation on gait in patients with Parkinson's disease: a systematic review. Translational neurodegeneration, 10(1), 22.
13. Rizzo, G., Copetti, M., Arcuti, S., Martino, D., Fontana, A., and Logroscino, G. (2016). Accuracy of clinical diagnosis of Parkinson disease: A systematic review and meta-analysis. Neurology, 86(6), 566–576.

Table 1. *Scores for motor, balance, quality of life, and quality of sleep scales before and after each transcranial direct current stimulation (tDCS) protocol over M1, DLPFC, and sham tDCS, respectively.*

Scales	tDCS over M1			tDCS over DLPFC			Sham tDCS		
	before	after	%	before	after	%	before	after	%
TUG	3	3	0	22	33	50	32	36	12.5
UPDRS	75	63	-16	55	34	-38	37	34	-8
SCOPA	45	41	-9	33	21	-36	16	16	0
BBS	7	7	0	25	30	20	31	32	3
STAI-Y1	32	32	0	30	28	-7	29	30	3
STAI-Y2	34	33	-3	32	31	-3	27	27	0
PSQI	7	12	71	10	4	-60	4	2	-50
PDQ-39	72	86	19	95	89	-6	59	4	-29
BDI	4	6	50	7	7	0	8	7	-13

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

TRANSCRANIAL DIRECT CURRENT STIMULATION IN THE NEUROMODULATION OF CONTROLLING MAIN SYMPTOMS OF PARKINSON'S DISEASE: A CASE STUDY

Alice Medeiros de Souza
Universidade Nove de Julho - Faculdade de Fisioterapia

Lillian Campos Amadeu
Universidade Nove de Julho - Faculdade de Fisioterapia

Eleni Vosniadou
Universidade Nove de Julho - Faculdade de Fisioterapia

Fernanda Ishida Corrêa
Universidade Nove de Julho - Faculdade de Fisioterapia

Letizzia Dall'Agnol
Universidade Nove de Julho, Faculdade de Fisioterapia

December/2021

INTRODUCTION

SBJChem Conference 2021

- Parkinson's disease (PD) is a progressive neurodegenerative disorder of the central nervous system that mainly affects the motor system, impairing motor coordination, balance, causing tremors with progressive loss of everyday movement, including walking (de Lau, 2006). Brain neuromodulation therapies, such as transcranial direct current stimulation (tDCS), are known to improve symptoms associated with PD (Ferrucci, 2016; Fateme, 2021).

INTRODUCTION

SBJChem Conference 2021

- Currently there are very few studies demonstrating the effects of tDCS on the overall improvement in motor function and quality of life in patients with PD.
- tDCS can induce significant improvement in motor function when applied to the primary motor cortex (M1) (Elsner, 2016).
- Active stimulation has shown significant antidepressant effect when applied over the dorsolateral prefrontal cortex (DLPFC) (Dinkelbach, 2017).

AIM OF STUDY

SBJChem Conference 2021

This study was conducted to verify the effects of Transcranial Direct Current Stimulation (tDCS) on balance, motor control and the quality of life in Parkinson's disease patients.

METHODOLOGY

SBJChem Conference 2021

PARTICIPANT

The patient participating in the study, a 72-year-old male, was recruited voluntarily through the Supervised Clinical Practice in Neurology at Universidade Nove de Julho. After signing the Informed Consent Form.

METHODOLOGY

SBJChem Conference 2021

tDCS PROTOCOL

- The participant received 3 treatments, consisting of 10 sessions of 20 minutes each and a one-week interval in between treatments.
- Treatments were randomized resulting in the following order:
  - (1) active tDCS over M1
  - (2) active tDCS over DLPFC
  - (3) Sham tDCS.
- For both M1 and DLPFC we used the intensity of 2mA.
- During the sham-tDCS treatment, the participant stayed for 20 minutes with the electrodes in the same locations as in the a-tDCS condition, but the device was turned off after 30 seconds of active stimulation.

METHODOLOGY

SBJChem Conference 2021

RESULTS MEASURES

The following scales and questionnaires were used before and after each intervention to assess the effectiveness of the treatments:

- Timed up and go test (TUG)
- Unified Parkinson's Disease Rating Scale (UPDRS)
- Parkinson's Disease Outcome Scale
- Motor Function (SCOPA-M)
- Berg Balance Scale (BBS)
- State-Trait Anxiety Inventory (STAI)
- Pittsburgh Sleep Quality Index (PSQI)
- Parkinson's Disease Questionnaire (PDQ-39)
- Beck Depression Inventory (BDI)

RESULTS

SBJChem Conference 2021

After active tDCS stimulation over M1, the patient showed:

- An increase in motor control,
- A decrease in rest tremors,
- A broader range of motion in the upper limbs, hands, and fingers,
- Considerably improved control of pinch motions,

as measured by scales:

- UPDRS (16%)
- SCOPA (9%) scales.

RESULTS

SBJChem Conference 2021

After active tDCS stimulation over M1, the patient also presented worsening in quality of sleep and levels of anxiety according to increased values of:

PSQI (71%)

PDQ-39 (19%)

BDI (50%)

RESULTS

SBJChem Conference 2021

After active stimulation over DLPFC, the patient showed:

- Highest motor control improvement, balance and gait,
- A reduction in symptoms associated with PD,

according to an improvement of results such as:

- TUG (50%)
- BBS (20%)
- UPDRS (38,18%)
- SCOPA (36%).

RESULTS

SBJChem Conference 2021

- Although we did not come to conclusive findings in relation to the patient's anxiety levels, DLPFC stimulation showed the best results, demonstrating improvement in quality of sleep, as shown on the PSQI (60%).
- Regarding the results on DLPFC stimulation, we could find significance on the TUG, UPDRS, SCOPA, BBS and PSQI results showing a substantial motor improvement following DLPFC stimulation when compared to Sham-tDCS.

RESULTS

SBJChem Conference 2021

- Sham intervention, in comparison to DLPFC stimulation, demonstrated worsening in the patient's condition as shown in the following results (see Tab 1):
  - A decrease in TUG (12,5%)
  - A decrease in UPDRS (8%)
  - A decrease in BBS (3%)

Table 1. Scores for motor, balance, quality of life and quality of sleep scales before and after each transcranial direct current stimulation (tDCS) protocol over M1, DLPFC and sham tDCS, respectively.

Scales	tDCS over M1			tDCS over DLPFC			Sham tDCS		
	before	after	%	before	after	%	before	after	%
TUG	3	3	0	22	33	50	32	36	12.5
UPDRS	75	63	-16	55	34	-38	37	34	-8
SCOPA	45	41	-9	33	21	-36	16	16	0
BBS	7	7	0	25	30	20	31	32	3
STAI-Y1	32	32	0	30	28	-7	29	30	3
STAI-Y2	34	33	-3	32	31	-3	27	27	0
PSQI	7	12	71	10	4	-60	4	2	-50
PDQ-39	72	86	19	95	89	-6	59	4	-29
BDI	4	6	50	7	7	0	8	7	-13

13

DISCUSSION

SBJChem Conference 2021

- While not definitive, our findings imply that active M1 and DLPFC stimulation may help with parkinsonian symptoms such resting tremor, loss of motor control, and balance. This is consistent with a review made by Broeder(2015), which demonstrated the effectiveness of M1 stimulation in enhancing motor performance while simultaneously revealing that DLPFC activation helped executive function. However, it is unknown which type of stimulation produces the best outcomes. According to Lattari(2016), substantial findings were obtained when comparing the influence of left dorsolateral prefrontal cortex (DLPFC) transcranial direct current stimulation (tDCS) on balance and functional mobility.

14

DISCUSSION

SBJChem Conference 2021

- In terms of the DLPFC stimulation outcomes, we were able to detect significance on the TUG, UPDRS, SCOPA, BBS and PSQI scales results. This supports the results found by Manenti(2014), demonstrating a significant motor improvement following DLPFC stimulation as compared to Sham-tDCS.
- And while we did not reach any definitive conclusions about the patient's anxiety levels, DLPFC stimulation produced the best outcomes, demonstrating improvement in quality of sleep, as shown on the PSQI (60%).

15

CONCLUSIONS

SBJChem Conference 2021

In this study, DLPFC stimulation showed the highest results in terms of motor control, balance, gait, and overall PD symptoms. Additionally, improved sleep quality was observed on the PSQI scale during DLPFC stimulation and Sham-tDCS. Thus suggesting that active stimulation over DLPFC has better results than stimulation over M1 and Sham-tDCS.

16

CONCLUSIONS

SBJChem Conference 2021

One limitation of our study is that we did not investigate further long-lasting effects of the therapy. Future research investigating cortical excitability in its relation to controlling main symptoms of PD might provide more explanations for our findings. Finally, this study was a case study involving only one patient, and we hope studies with larger sample sizes might better explore the present study results.

REFERENCES

SBJChem Conference 2021

1. de Lau, L. M., Breteler, M. M. (2006). Epidemiology of Parkinson's disease. *The Lancet. Neurology,* 5(6): 525–535.
2. Marttila, R. J., Rinne, U. K. (1981). Epidemiology of Parkinson's disease--an overview. *Journal of neural transmission*, 51(1-2): 135–148.
3. Darweesh, S. K., Verlinden, V. J., Stricker, B. H., Hofman, A., Koudstaal, P. J., Ikram, M. A. (2017). Trajectories of prediagnostic functioning in Parkinson's disease. *Brain : a journal of neurology*, 140(2): 429–441.
4. Olanow, C. W., Tatton, W. G. (1999). Etiology and pathogenesis of Parkinson's disease. *Annual review of neuroscience*, 22:123–144.
5. Jankovic, J., Tan, E. K. (2020). Parkinson's disease: etiopathogenesis and treatment. *Journal of neurology, neurosurgery, and psychiatry*, 91(8): 795–808.
6. Pol, F., Salehinejad, M. A., Baharlouei, H., Nitsche, M. A. (2021). The effects of transcranial direct current stimulation on gait in patients with Parkinson's disease: a systematic review. *Translational neurodegeneration*, 10(1):22.
7. Ferrucci, R., Mameli, F., Ruggiero, F., Priori, A. (2016). Transcranial direct current stimulation as treatment for Parkinson's disease and other movement disorders. *Basal ganglia*, 6: 53-61.

REFERENCES

SBJChem Conference 2021

8. Elsner, B., Kugler, J., Pohl, M., Mehrholz, J. (2016). Transcranial direct current stimulation for improving idiopathic Parkinson's syndrome. An abridged version of a Cochrane review. *European journal of physical and rehabilitation medicine*, 52(6): 902–906.
9. Dinkelbach, L., Brambilla, M., Manenti, R., Brem, A. K. (2017). Non-invasive brain stimulation in Parkinson's disease: Exploiting crossroads of cognition and mood. *Neuroscience and biobehavioral reviews*, 75: 407–418.
10. Rizzo, G., Copetti, M., Arcuti, S., Martino, D., Fontana, A., Logroscino, G. (2016). Accuracy of clinical diagnosis of Parkinson disease: A systematic review and meta-analysis. *Neurology*, 86(6): 566–576.
11. Broeder, S., Nackaerts, E., Heremans, E., Vervoort, G., Meesen, R., Verheyden, G., Nieuwboer, A. (2015). Transcranial direct current stimulation in Parkinson's disease: Neurophysiological mechanisms and behavioral effects. *Neuroscience and biobehavioral reviews*, 57: 105–117.
12. Lattari, E., Costa, S. S., Campos, C., de Oliveira, A. J., Machado, S., Maranhao Neto, G. A. (2017). Can transcranial direct current stimulation on the dorsolateral prefrontal cortex improves balance and functional mobility in Parkinson's disease?. *Neuroscience letters*, 636: 165–169.
13. Manenti, R., Brambilla, M., Rosini, S., Orizio, I., Ferrari, C., Borroni, B., Cotelli, M. (2014). Time up and go task performance improves after transcranial direct current stimulation in patient affected by Parkinson's disease. *Neuroscience letters*, 580:74–77.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

UNILATERAL HYDRONEPHROSIS DUE TO URETER OBSTRUCTION AFTER OVARIO-HYSTERECTOMY IN A FELINE - CASE REPORT

RODRIGUES, Isabelle Medeiros[1*]; TOLEDO, João Francisco Bianchini de[1]; SAMAN, Thiago Abreu[1]; FILHO, Mário dos Santos[1]

[1] Academic of Veterinary Medicine, University of Vassouras

** Correspondence author*
e-mail: isabellemerod@gmail.com

Received 26 January 2022; received in revised form 20 February 2022; accepted 26 February 2022

ABSTRACT

Hydronephrosis is characterized by the renal pelvis and calyces distension resulting from total or partial urinary outflow obstruction. Ureter injuries are recognized complications of abdominal surgeries, especially sterilization, due to the frequency which they are performed in cats and dogs and the proximity between the ureter and the uterine stump. Some injuries may be acute or chronic, uni or bilaterally, affecting the urinary tract segment parts. Therefore, diagnosis is very important, especially early on, since it makes immediate management easier and may result in a better prognosis, especially when the disease course gets interrupted or its progression gets slowed. Furthermore, the importance of performing sporadic exams, even without previous clinical history for feline patients, is notorious since the nature of the species to hide clinical signs is well known. To certify the success of the surgery and integrity of the organs, it is very important to perform post sterilization exams. It is also crucial to state the importance of computed tomography for the diagnosis since some obstruction causes, such as blood clot, may not be shown in the ultrasound. Computed tomography is also necessary to differentiate hydronephrosis from many injuries that may affect the kidneys and ureters, like ectopic ureter, obstruction by calculi, and surgical ligature. The present study has the objective of reporting and discussing the laboratory, imaging findings, and clinical state of a patient with unilateral hydronephrosis, with asymptomatic evolution of iatrogenic origin due to obstruction by ureter obliteration after ovariohysterectomy (OVH).

Keywords: *Iatrogenic, Nephrectomy, Castration, Uremia.*

1. INTRODUÇÃO

As injúrias ureterais podem ter origem congênita, de baixa incidência, ou adquirida. Afecções de ureter caracterizadas como adquiridas são, geralmente, secundárias a enfermidades (Ioannidi *et al*, 2019; Litlle, 2015) ou de origem iatrogênica, comumente resultante de procedimentos cirúrgicos, como a ovariohisterectomia (OVH) (Adin, 2011), frequentemente realizada na rotina e incentivada aos tutores (Adin, 2011; santos *et al*, 2009; Plater, 2020). Embora as incidências de complicações sejam relativamente baixas, dada a frequência de realização desses procedimentos, são descritas diversas complicações (Adin, 2011; Santos *et al.*, 2009).

A hidronefrose é originada pela obstrução total ou parcial do fluxo de saída urinário, resultando na dilatação da pelve e dos cálices renais, por consequência, provocam o aumento da pressão hidrostática intraluminal e atrofia do parênquima (Little, 2015; Wajczyk, 2020). A obstrução pode cursar de modo agudo ou crônico, acometendo qualquer porção do segmento do ureter, podendo ocorrer de forma uni ou bilateral (Crivellenti, 2015). Quando acometido unilateralmente, os sinais clínicos tendem a se apresentar de modo gradual ou até mesmo não serem evidenciados, uma vez que o rim contralateral supre a função fisiológica do rim afetado (Little, 2015).

O diagnóstico precoce de doenças renais é fundamental para o manejo imediato do paciente e, especialmente, para o estadiamento do mesmo com a definição de um prognóstico, possibilitando delimitar o curso da doença, e o manejo apropriado para que se possa interromper ou retardar a evolução para estágios mais avançados (Freitas, 2014).

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.34_abstract_RODRIGUES.pdf

Os métodos de diagnóstico complementar baseiam-se no hemograma, bioquímica sérica hepática e renal, urinálise e exames de imagem. Os indicadores laboratoriais, comumente utilizados como marcadores de lesão renal, são ureia e creatinina. Contudo, seus valores somente se apresentarão elevados, no caso de comprometimento mínimo entre 66%-75% dos néfrons (Crivellenti, 2015).

Quanto ao diagnóstico por imagem, na radiologia pode-se observar aumento do órgão acometido (Crivellenti, 2015). A ultrassonografia abdominal (USG), permite uma avaliação da pelve renal, com a mensuração da morfologia e das demais estruturas (D'anjou, Bédard and Dunn, 2011). Tanto a tomografia computadorizada (TC), quanto a urografia excretora possibilitam a identificação do local obstruído, por meio da visualização da passagem do fluxo ou não nas vias urinárias, após uso de contraste (Crivellenti, 2015).

O presente projeto tem por objetivo relatar o caso clínico e discutir os achados laboratoriais e de imagens de um felino com hidronefrose unilateral iatrogênica, com evolução assintomática decorrente de obstrução de ureter pós ovariohisterectomia (OVH).

2. DESENVOLVIMENTO

O estudo foi desenvolvido em uma clínica veterinária particular do Município de Vassouras, com autorização do tutor do paciente para utilização da descrição do caso para fins acadêmicos e científicos, com assinatura do Termo de Consentimento Livre e Esclarecido (TCLE). A metodologia do estudo se baseia na evolução, nos resultados de exames e na escolha dos métodos de diagnósticos para a descrição do relato do caso clínico analítico e descritivo, por meio do fenômeno observado (Pereira et al., 2018), sendo reportado detalhadamente em ordem cronológica de ocorrência dos eventos a fim de servir de base para os colegas frente a casos clínicos e fenômenos similares, facilitando sua resolução.

2.1. Histórico e Anamnese

Foi atendido, um paciente felino, fêmea, sem raça definida, de 3 anos, castrada, com peso de 3,400 kg. O animal foi levado com o intuito de participar de uma aula prática de diagnóstico por imagem. Durante a anamnese prévia, foi relatado que o paciente já havia passado por OVH e, posterior a esterilização, já havia realizado exame USG, não apresentando sinais de alterações.

2.2. Exame Ultrassonográfico

Durante a USG, realizada na aula, foi observada dilatação da pelve renal além de perda da definição da relação cortico-medular (Figura 1).

Figura 1: *Exame ultrassonográfico evidenciando conteúdo anecoico, sem definição de contorno e arquitetura e ureter esquerdo apresentando área de dilatação próxima ao trígono vesical (seta). Fonte: Arquivo Pessoal, com autorização da M.V Bianca Affonso,2020.*

O rim direto apresentava-se sem alterações. Procederam-se, então, hemograma, bioquímica sérica hepática e renal, dosagem de fósforo e potássio. Dentre esses, foram apresentadas as seguintes alterações: ureia com 72 mg/dl (ref.: 30-60 mg/dl), proteínas plasmáticas totais 8,8 g/dl (ref.: 5,8-8,0 g/dl) e ALT 89,0 UI/l (ref.: 10-88 UI/l).

2.3. Exames Laboratoriais

A fim de elucidar o quadro, o animal foi encaminhado ao nefrologista onde foram solicitados: hemograma, bioquímica sérica renal e hepática, dosagem de fósforo e potássio, EAS, urocultura com antibiograma e USG abdominal. Os achados laboratoriais alterados foram hiperpotassemia (4,9 mEq/L, ref.:4,0-4,5) e hipofosfatemia (4,1 mg/dl, ref.:4,5-8,1.. O leucograma apresentou linfopenia (1.140 cels/µl, ref.:2.500 a 10.000), eosinopenia (60 cels/µl, ref.:100 a 1.500) e hiperproteinemia (8,6 g/dl, ref.:5,0 a 8,0). Na urinálise, evidenciou-se hematúria, proteinúria e bacteriúria. A relação proteína:creatinina urinária foi 0,12 (ref.: <0,5).

2.4. Diagnóstico por Imagem

Ao novo exame ultrassonográfico, observou-se rim esquerdo medindo 3,58cm de diâmetro, com perda de definição de contorno e arquitetura, e dilatação em pelve de 2,99cm de diâmetro e ureter de 0,25cm de diâmetro, sugerindo hidronefrose, sendo recomendada a TC,

Na TC com contraste foi evidenciado rins assimétricos, de densidade e contorno normais. O rim esquerdo apresentava-se mais alterado, sendo observado redução de volume, dilatação pélvica de aproximadamente 1,2 cm de diâmetro, ainda, apresentando retardo acentuado/ausência na excreção do meio de contraste durante o tempo do exame. Observou-se ureter proximal levemente distendido (medindo 0,4 cm de diâmetro), apresentando trajeto tortuoso, sem sinais de processos obstrutivos evidentes até a porção terminal, onde tangencia o coto uterino (imediatamente antes desta região medindo cerca de 0,2 cm). Desta forma, foi concluído que o paciente apresenta hidronefrose, associada à dilatação ureteral, sugerindo obstrução mecânica ao nível de região de coto uterino, trazendo como diagnóstico presuntivo da causa, a ligadura de ureter em porção distal. Procedeu-se, então, a retirada cirúrgica do órgão afetado.

3. DISCUSSÃO

Doenças de curso compensatório, como o descrito neste caso, são insidiosas e de difícil percepção de sinais clínicos específicos. O fato do paciente passar pela USG com os achados incidentais, reforça a importância de realização de exames esporádicos, mesmo sem histórico pregresso, para pacientes felinos, uma vez que é notória a natureza da espécie em ocultar sinais clínicos (Meric, 1997).

De acordo com Adin (2011), o diagnóstico das injúrias ureterais consiste na combinação de métodos de diagnóstico por imagem, uma vez que apenas um não supre o diagnóstico completo da doença. Alguns autores avaliam o uso da USG abdominal como eficiente na confirmação de nefropatias obstrutivas (Ioannidi *et al.*, 2019). Em contrapartida, Lemieux (2021), afirma que o diagnóstico por meio de USG, não é considerado padrão ouro para visualização de obstruções de ureter, visto que determinadas estruturas, como cálculos sanguíneos, podem ser difíceis de serem localizadas.

Segundo um estudo realizado por D'anjou, claBédard and Dunn (2011) onde foi avaliada a dilatação pélvica renal de pacientes caninos e felinos clinicamente saudáveis em comparação com pacientes portadores de afecções renais (obstrutivas e não obstrutivas), foi determinada a existência de uma dilatação fisiológica da pelve renal em pacientes saudáveis. Indivíduos saudáveis apresentaram determinada dilatação da pelve renal quando submetidos à fluidoterapia endovenosa ou administração de diuréticos. O autor afirma que, apesar dessa dilatação fisiológica não ser visualizada por USG na maioria dos casos, esta não deve ser utilizada como parâmetro de diagnóstico.

A TC permite uma avaliação minuciosa e detalhada com maior nitidez quando comparada a USG, uma vez que não evidencia-se sobreposição de outras estruturas anatômicas, com a possibilidade da visualização de estruturas de modo transversal e helicoidal, além de permitir distinguir densidade e o tipo de tecido de diferentes órgãos (Samii *et al*., 2004). Segundo um estudo realizado por Samii *et al* (2004), a TC por contraste e a urografia excretora apresentaram seus diagnósticos fidedignos quando confirmados por cirurgia ou necrópsia.

No caso em questão, a primeira suspeita de nefropatia foi a partir de um achado de imagem ultrassonográfica, onde foi notada dilatação anormal da pelve renal. Apesar deste achado não ser utilizado como ferramenta de diagnóstico conclusivo, foi sugestivo de hidronefrose, exigindo exame mais específico: a tomografia computadorizada.

Nas fêmeas a ocorrência de imperícias médicas com banalização da OVH, têm se tornado rotineiras. Aliado a isto, a anatomia particularmente sintópica dos órgãos reprodutivos com as veias e artérias renais, e ureteres, são pontos que favorecem a ligadura destas estruturas, obstruindo, assim, o fluxo da filtração glomerular ou a drenagem do filtrado até a urina, respectivamente. Ambos podem evoluir com a hidronefrose e possível afuncionalidade do órgão (Ioannidi *et al*., 2019). Infecção urinária bacteriana recorrente em trato urinário inferior é a manifestação clínica mais frequentemente descrita, e está associada à ausência de peristaltismo ureteral. Esta por sua vez, pode levar a instabilidade do músculo detrusor e consequente incontinência. Porém, isso não se aplicava a paciente, já que a mesma não apresentava infecção, e sim respostas inespecíficas do hemograma, mas já evidente aumento de ureia, proteínas plasmáticas, bem como de potássio, remetendo um quadro de possível desidratação,

embora sem alterações físicas durante o exame clínico (McLoughlin, 2008). Ressaltando que não necessariamente serão observadas alterações clínicas ou laboratoriais de injúria renal, uma vez que o rim contralateral compensa as funções do órgão afetado.

O tratamento de escolha foi a nefrectomia do órgão afetado, a fim de evitar complicações como infecção urinária (Meric, 1997). Entretanto, 30% dos felinos tratados cirurgicamente podem apresentar algum grau de incontinência, porém tal fato não ocorreu na paciente em questão (Bjorling & Christie, 1998). A média anual de castração de pacientes felinos é de aproximadamente de 20 a 30 mil indivíduos (IBGE, 2020). Isso reforça que, embora seja o procedimento mais amplamente difundido e realizado, requer especial atenção quanto aos cuidados transoperatórios, principalmente considerando o quantitativo de indivíduos expostos ao risco que o próprio procedimento origina (Espada *et al*., 2006). Diante disto, nota-se que a orientação de exames periódicos, mesmo nos pacientes assintomáticos, é um fator importante a ser repassado aos tutores que venham a castrar seus animais, uma vez que os procedimentos não são isentos de possíveis complicações que possam ficar despercebidas.

4. CONCLUSÃO

A TC foi primordial para o diagnóstico definitivo quando comparado à USG, pois a hidronefrose possui diversos diagnósticos diferenciais, como a ectopia ureteral, obstrução intraluminal ou ligadura. Tendo em vista a presente evolução do caso, recomenda-se especial atenção para os profissionais veterinários, no caso de sinais clínicos relevantes e similares, enriquecendo e trazendo à tona pontos dos cuidados nos protocolos de OVH nos pacientes felinos.

5. REFERÊNCIAS

1. Adin, C., (2011). Complications of and Orchiectomy in Companion Animals. *Veterinary Clinics of North America: Small Animal Practice*, 41(5), pp.1023-1039.
2. Christie, B. A.; Bjorling, D. E. and Slatter, D., (1998). *Manual de cirurgia de pequenos animais.* São Paulo, Manole.
3. Crivellenti, L. Z. and Crivellenti, S. B., (2015). *Casos de Rotina em Medicina Veterinária de Pequenos Animais. p.*157.
4. D'anjou, M., Bédard, A. and Dunn, M., (2011). Clinical significance of renal pelvic dilatation on ultrasound in dogs and cats. *Veterinary Radiology & Ultrasound*.
5. Espada, Y., Novellas, R. and Ruiz de Gopegui, R. (2006). Renal ultrasound in dogs and cats. *Veterinary Research Communications,* 30(1):133-137.
6. Freitas, G.; Veado, J; and Carregaro, A., (2014). Testes de avaliação de injúria renal precoce em cães e gatos. *Semina: Ciências Agrárias*, 35(1), pp.411.
7. Instituto Brasileiro de Geografia e Estatística (IBGE), 2020. site: www.ibge.gov.br. acesso em: 19/02/2022
8. Ioannidi, O., Papazoglou, L., Psalla, D., Papadopoulou, D., Tsampa, N. and Mylonakis, M., (2019). Congenital Unilateral Ureteral Stenosis With Hydronephrosis in a Kitten. *Topics in Companion Animal Medicine*, 36, p.22-24.
9. Lemieux, C., Vachon, C., Beauchamp, G. and Dunn, M., (2021). Minimal renal pelvis dilation in cats with benign ureteral obstruction by antegrade pyelography: a retrospective study of 82 cases (2012–2018). *Journal of Feline Medicine and Surgery*, 23(10), pp.892-899.
10. Little, S. E., (2015) *O gato: medicina interna.* Rio de Janeiro, Roca.
11. McLoughlin M.A. (2008). *Doenças do sistema urogenital.* Manual saunders de clínica de pequenos animais. São Paulo: Roca, p.906-907.
12. Meric, S.M. (1997). *Poliúria e polidipsia.* In: Ettinger, S.J. & Feldman, E.C. Tratado de medicina interna veterinária. 4.ed. São Paulo: Manole, p.220-226.
13. Pereira, A. S. *et al*., (2018). *Metodologia da pesquisa científica.*
14. Plater, B. and Lipscomb, V., (2020). Treatment and outcomes of ureter injuries due to complications in cats and dogs. *Journal of Small Animal Practice*, 61(3), pp.170-176.
15. Samii, V., McLoughlin, M., Mattoon, J., Drost, W., DiBartola, S. and Hoshaw-Woodard, S., (2004). Digital Fluoroscopic Excretory Urography. *Journal of Veterinary Internal Medicine*, 18(3), pp.271-281.
16. Santos, F.C. *et al*. (2009). Complicações da esterilização de fêmeas caninas e felinas. *Veterinária e Zootecnia* ,pp. 8-18.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

UNILATERAL HYDRONEPHROSIS DUE TO URETER OBSTRUCTION AFTER OVARIOHYSTERECTOMY IN A FELINE - CASE REPORT

Isabelle Medeiros Rodrigues
Universidade de Vassouras, Academic of Veterinary Medicine - Brazil

João Francisco Bianchini de Toledo
Universidade de Vassouras, Academic of Veterinary Medicine - Brazil

Thiago Abreu Saman
Universidade de Vassouras, Academic of Veterinary Medicine - Brazil

Mário dos Santos Filho
Universidade de Vassouras, Teacher of the Veterinary Medicine Course- Brazil

February/2022

INTRODUCTION AND REVIEW OF LITERATURE

SBJChem Conference 2021

• URETERAL INJURIES → CONGENITAL/ ACQUIRED/ **IATROGENIC** → **OVARIOHYSTERECTOMY** (OVH)

• HYDRONEPHROSIS → OBSTRUTION → RENAL PELVIS AND CALYCES DILATATION

• DIAGNOSIS → LABORATORY/IMAGE

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

REPORT AND DISCUSS THE LABORATORY, IMAGING FINDINGS AND CLINICAL STATE OF A FELINE PATIENT WITH UNILATERAL HYDRONEPHROSIS.

- ASYMPTOMATIC;
- IATROGENIC;
- URETER LIGATURE;
- POST OVARIOHYSTERECTOMY.

METHODOLOGY

SBJChem Conference 2021

- SPECIFIC INFORMED CONSENT DOCUMENT;
- DEVELOPED IN A PRIVATE CLINIC - CITY OF VASSOURAS;
- REPORT DESCRIPTION → CRONOLOGIC ORDER OF EVENTS;
- TO FACILITATE THE RESOLUTION OF SIMILAR CLINICAL CASES;
- FULFILL CIENTIFIC GAPS YET TO BE EXPLORED.

RESULTS AND DISCUSSION

SBJChem Conference 2021

- FELINE / FEMALE / STERELIZED / 3 YEARS / 3.400 KG / NOT RACIALLY DEFINED

11-05-2020

- DIAGNOSTIC IMAGING CLASS → ULTRASONOGRAFIC;
- PACIENT DID NOT PRESENT CLINICAL ALTERATIONS;
- RENAL PELVIC DILATATION → LEFT KIDNEY;
- LABORATORY TESTS:
  - ↑ UREA;
  - ↑ ALT;
  - ↑ TOTAL PLASMATIC PROTEINS.

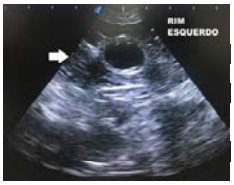


Fig 1: Ultrasonography exam showing anechoic content, without definition of contour and architecture and left ureter showing area of dilatation near the bladder trigone region (arrow). Source: Personal file, with permission from M.V. Bianca Affonso, 2020.

RESULTS AND DISCUSSION

SBJChem Conference 2021

11-25-2020 → NEPHROLOGIST

- **NO** CLINICAL SIGNS;
- LABORATORY TEST:

CBC:

- ↑ POTASSIUM;
- ↓ PHOSPHORUS;
- ↑ URINARY PROTEIN;
- ↑ URINARY CREATININE.

WBC:

- ↓ LYMPHOCYTES;
- ↓ EOSINOPHILS;
- ↑ PROTEIN.

URINE ANALYSIS:

- HAEMATURIA;
- PROTEININURIA;
- BACTEURIA.

RESULTS AND DISCUSSION

SBJChem Conference 2021

- DISEASES WITH COMPENSATORY AND INSIDIOUSNESS COURSE;
- HARD PERCEPTION OF SPECIFIC CLINICAL SIGNS;
- IMPLEMENTATION OF SPORADIC EXAMS → PATIENTS WITH OR WITHOUT PREVIOUS INFORMATION;
- URETERAL INJURY DIAGNOSIS = COMBINATION OF MANY IMAGE DIAGNOSIS METHODS;
- MALPRACTICE → OVARIOHYSTERECTOMY + SYNTOPIC ANATOMY;
- CONTRALATERAL KIDNEY COMPENSATION;
- NEPHRECTOMY.

CONCLUSIONS

SBJChem Conference 2021

- COMPUTED TOMOGRAPHY IN COMPARISON TO ULTRASONOGRAPHY;
- DIFFER HYDRONEPHROSIS FROM ECTOPIC URETER AND OBSTRUCTIONS;
- SPECIAL ATTENTION TO SIMILAR CLINICAL SIGNS.

REFERENCES

SBJChem Conference 2021

1. Adin, C., (2011). Complications of Ovariohysterectomy and Orchiectomy in Companion Animals. *Veterinary Clinics of North America: Small Animal Practice*, 41(5), pp.1023-1039.
2. Christie, B. A.; Bjorling, D. E. and Slatter, D., (1998). *Manual de cirurgia de pequenos animais.* São Paulo, Manole.
3. Clarke, D., (2018). Feline ureteral obstructions Part 1: medical management. *Journal of Small Animal Practice*, 59(6), pp.324-333.
4. Costa Neto, J. M.; Silva, A. E.; Martins Filho, E.F.; Ribeiro, L .G. R.; Gama, R. O.G.; Penha, E.M.; Toríbio, J.M.M.L. and Gomes Jr., D.C. (2011). Ectopia ureteral em cães. *Arquivos de Ciências Veterinárias e Zoologia,* 14 (1):151-156.
5. Crivellenti, L. Z. and Crivellenti, S. B., (2015). *Casos de Rotina em Medicina Veterinária de Pequenos Animais. p.*157.
6. D'anjou, M., Bédard, A. and Dunn, M., (2011). Clinical significance of renal pelvic dilatation on ultrasound in dogs and cats. *Veterinary Radiology & Ultrasound*.
7. Espada, Y., Novellas, R. and Ruiz de Gopegui, R. (2006). Renal ultrasound in dogs and cats. *Veterinary Research Communications,* 30(1):133-137.
8. Freitas, G.; Veado, J; and Carregaro, A., (2014). Testes de avaliação de injúria renal precoce em cães e gatos. *Semina: Ciências Agrárias*, 35(1), pp.411.

REFERENCES

SBJChem Conference 2021

9. Instituto Brasileiro de Geografia e Estatística (IBGE), 2020. site: www.ibge.gov.br. acesso em: 19/02/2022
10. Ioannidi, O., Papazoglou, L., Psalla, D., Papadopoulou, D., Tsampa, N. and Mylonakis, M., (2019). Congenital Unilateral Ureteral Stenosis With Hydronephrosis in a Kitten. *Topics in Companion Animal Medicine*, 36, p.22-24.
11. Kienle, G. and Kiene, H., (2011). Clinical judgement and the medical profession. *Journal of Evaluation in Clinical Practice*, 17(4), pp.621-627.
12. Lemieux, C., Vachon, C., Beauchamp, G. and Dunn, M., (2021). Minimal renal pelvis dilation in cats with benign ureteral obstruction by antegrade pyelography: a retrospective study of 82 cases (2012–2018). *Journal of Feline Medicine and Surgery*, 23(10), pp.892-899.
13. Little, S. E., (2015) *O gato: medicina interna.* Rio de Janeiro, Roca.
14. McLoughlin M.A. (2008). *Doenças do sistema urogenital.* Manual saunders de clínica de pequenos animais. São Paulo: Roca, p.906-907.
15. Meric, S.M. (1997). *Poliúria e polidipsia.* In: Ettinger, S.J. & Feldman, E.C. Tratado de medicina interna veterinária. 4.ed. São Paulo: Manole, p.220-226.
16. Pereira, A. S. *et al*., (2018). *Metodologia da pesquisa científica.*

REFERENCES

SBJChem Conference 2021

17. Plater, B. and Lipscomb, V., (2020). Treatment and outcomes of ureter injuries due to ovariohysterectomy complications in cats and dogs. *Journal of Small Animal Practice*, 61(3), pp.170-176.
18. Santos, F.C. *et al*. (2009). Complicações da esterilização cirúrgica de fêmeas caninas e felinas. *Veterinária e Zootecnia* ,pp. 8-18.
19. Wajczyk, T. *et al*., (2020). Nefrectomia associada à renomegalia direita em cão com hidronefrose. *Pubvet*, 14(10), pp.1-8.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

UTILIZAÇÃO DE BANANA PRATA (*MUSASAPIENTUM*) E BANANA OURO (*MUSAACUMINATA*) NO CONTROLE DE NEMATÓIDES GASTROINTESTINAIS DE BEZERROS

ÁVILA, Letícia Meirelles[1*]; CHAGAS, Jônathan David Ribas[2]; MARQUES, Thiago Luiz Pereira[3]; MORAES, Renata Fernandes Ferreira[3]; ROIER, Erica Cristina Rocha[3];

[1,2] Mestranda doPrograma de Pós Graduação em Ciências Veterinárias da Universidade Federal Rural do Rio de Janeiro

[2] Residente em Patologia Clínica do Programa de Residência Veterinária da Universidade Federal Rural do Rio de Janeiro

[3] Professor adjunto do curso de Medicina Veterinária da Universidade de Vassouras

** Correspondenceauthor*
e-mail: leticiameirellesavila@gmail.com

Received 06 January 2022; received in revised form 30 January 2022; accepted 02 February 2022

ABSTRACT

Cattle, both beef and dairy, are of great importance for Brazil, as it moves a good part of the country economy. But gastrointestinal infections caused by nematodes cause significant damage to cattle due to weight loss of animals, decreased production index, increased mortality rate, and increased expenses by producers. This work aims to demonstrate the elimination of gastrointestinal nematodes through the use of the leaves of two different banana species in calves and to verify if there are differences in the effectiveness of both. For the study, 30 calves were selected, aged between 3 and 8 months, of both sexes and already fed on pasture. These were divided into three groups. Group A was treated with banana leaves of the Musa sapientum species; Group B – was treated with banana leaves of the Musa acuminata species; Group C – control group, in which no substance was found administered. The feces collection was performed at intervals of 7 days, totaling 3 collections. The samples were taken directly from the animals' rectum, stored in a plastic bag, and placed in a styrofoam container with ice, and then the material was taken to the laboratory for the eggs per gram (eggs/g)examination. It can be concluded that the use of banana leaf proved to be effective in reducing the parasitic load of intestinal nematodes in calves, proving that the use of *Musa acuminata* was more efficient than the result of the use of *Musa sapientum* when compared.

Keywords: *alternative treatment, banana, worms, cattle*

1. INTRODUÇÃO

A bovinocultura, tanto de corte quanto leiteira, é uma área de grande importância para o Brasil, pois movimenta uma boa parte da economia do país. O rebanho brasileiro é considerado o maior do mundo, possuindo cerca de 214 milhões de cabeças de gado (IBGE, 2018).

Um dos problemas que o rebanho apresenta e que gera consideráveis perdas para a economia são as infestações parasitárias. As infecções gastrointestinais causadas por nematódeos causam significativo prejuízo para a bovinocultura, devido à perda de peso dos animais, diminuição do índice de produção, aumento da taxa de mortalidade e aumento de gastos pelos produtores (MOTA *et al*., 2003).

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.15_abstract_AVILA.pdf

É imprescindível que o controle correto desses parasitos seja feito. No entanto, o uso de anti-helmínticos, na maioria das vezes, é realizado de forma incorreta, podendo ocasionar resistência parasitária. Isto posto, o surgimento de métodos alternativos é bem visto para o tratamento, uma vez que eles não sofrem influência à resistência anti-helmíntica (AMARANTE, 1992; ECHEVARRIA, 1995).

Um dos métodos alternativos de controle parasitário é o uso da bananeira. Esta planta possui diversas substâncias em sua composição, como o tanino, um composto fenólico derivado do metabolismo secundário de diversas plantas (COSTA, 2008).

O objetivo deste trabalho é demonstrar a eliminação de nematóides gastrointestinais através do uso da folha de duas espécies diferentes de bananeira em bezerros, e verificar se existem diferenças na eficácia de ambas.

2. MATERIAIS E MÉTODOS:

Nesse estudo foram selecionados 30 bezerros, com idade entre 3 a 8 meses, ambos os sexos e já com alimentação a pasto. A coleta das amostras foi feita diretamente do reto dos animais, armazenadas em saco plástico e colocadas em recipiente de isopor com gelo, conforme Girão (1999). Em seguida o material foi levado ao laboratório de Análises Clínicas da Universidade de Vassouras para a realização do exame de OPG, que foi feito de acordo com a técnica de Gordon e Withlock (1939).. Após a realização do exame, os animais foram divididos em três grupos de 10 animais,ranqueados de forma homogênea e tratados da seguinte maneira: Grupo A – tratado com folha da bananeira da espécie *Musa sapientum* (banana prata); Grupo B – tratado com folha da bananeira da espécie *Musa acuminata* (banana ouro); Grupo C – grupo controle, em que não houve administração de nenhuma substância, somente alimentação normal já existente no manejo da propriedade. Ambos os tratamentos foram feitos *ad libidum*. O tratamento foi feito por dois dias seguidos e as fezes coletadas nos dias 7, 14 e 21 pós aplicação do método para obtenção da média do OPG nos grupos.

3. RESULTADOS E DISCUSSÃO:

Com os resultados obtidos dos OPG (Gráfico 1) oriundos das coletas de fezes de cada animal dos grupos A, B e C, pôde-se obter a média do D-2 (dia antes da administração das folhas de bananeira), D+7, D+14 e D+21 (após o tratamento). No dia anterior ao tratamento (D-2), para que os grupos fossem organizados e divididos sem diferenças estatísticas entre si levou-se em consideração os OPG dos animais até que fossem obtidas médias similares entre os grupos. Portanto, o Grupo A apresentou uma média de OPG de 740, o Grupo B de 733 e Grupo C uma média de 735. Posteriormente ao uso das folhas de bananeira na alimentação dos animais, no D+7 o Grupo A demonstrou média de 640, Grupo B de 160 e Grupo C de 865. Ao D+14 o Grupo A obteve média de 530, Grupo B de 125 e Grupo C de 915. No D+21, o Grupo A teve média de 380, Grupo B de 90 e Grupo C 785.

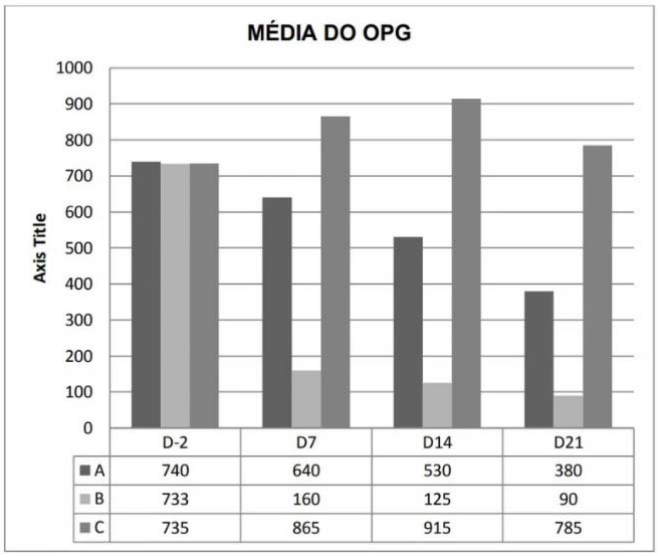


Gráfico 1. Acompanhamento das médias de OPG dos Grupos A, B e C em D-2, D+7, D+14 e D+21, demonstrando a diminuição das médias dos dois primeiros grupos.

Observa-se que a folha da banana ouro demonstrouuma eficácia maior que a folha da banana prata, de acordo com dados obtidos no teste Wilcoxon Pareado, que compara diretamente a banana prata com a banana ouro no D+21 após o tratamento. O teste mostrou que com um nível de significância de 5%, a média das diferenças é maior que 0. Isto posto, as evidências mostram que a média de OPG do

Grupo A (prata) é maior quando comparada ao grupo B (ouro).

Os resultados deste estudo demonstram significância na taxa de redução de infestações por verminoses, assim como diminuição nos valores do OPG, o que corrobora com o estudo de Girão (1998), onde os mesmos resultados em relação à infestação e queda no OPG foram vistos. Este estudo utilizou folhas de bananeira por dois dias, *ad libidum* e os resultados foram considerados significantes na comparação dos exames de OPG, o que vai de encontro com o estudo de Ribas *et al*. (2009) que utilizaram folhas e talos de bananeira (banana nanica e banana de são tomé, *Musa sinensis L.* e *Musa paradisiaca L*. respectivamente) na alimentação de caprinos e ovinos, com o objetivo de analisar a ação anti-parasitária.

O presente estudo não atingiu a porcentagem de eficácia proposta por Coles *et al*. (1992), que afirma que resultados de TRCOF (Teste de redução na contagem de ovos nas fezes) inferiores a 90% não são considerados como eficazes. Porém a banana ouro se aproximou significativamente, chegando a 88% no D+21 (Gráfico 2), indicando que a mudança no protocolo de tratamento possa atingir o número necessário para que seja considerado eficaz.

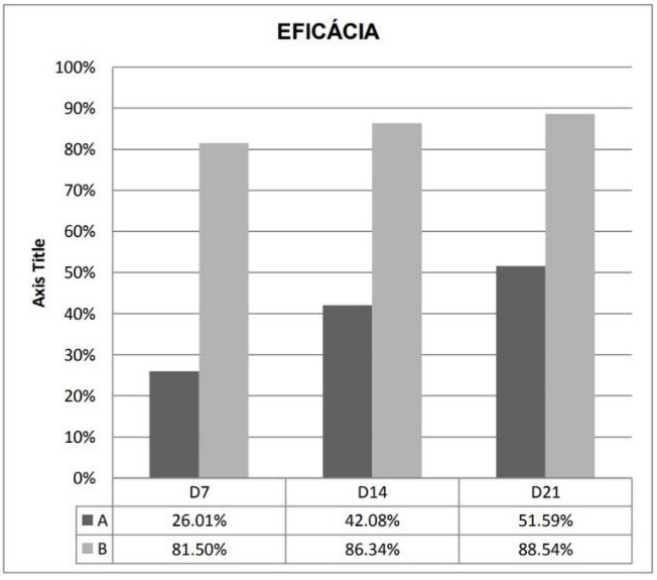


***Gráfico 2*.** Resultados do cálculo da eficácia dos Grupos A e B em D+7, D+14 e D+21 após o uso das folhas de bananeira e comprovação de maior eficiência das utilizadas no grupo B (banana ouro, Musa acuminata) que da utilizada no Grupo A (banana prata, Musa sapientum).

4. CONCLUSÃO:

O uso da folha de bananeira demonstrou-se eficaz quanto à diminuição da carga parasitária dos nematóides intestinais em bezerros, provando ainda que o uso da banana ouro (*Musa acuminata*) foi mais eficiente que o resultado do uso da banana prata (*Musa sapientum)* quando comparados. Mesmo não alcançando um número de eficácia ideal (90%), a pesquisa conseguiu chegar a 88% da eficácia com o uso da folha da banana ouro, o que mostra que protocolos podem ser criados buscando alcançar o objetivo do uso desse tratamento alternativo.

6. REFERENCIAS

1. Amarante, AFT, Barbosa, MA, de Oliveira, MAG, Carmello, MJ, and Padovani, CR (1992). Efeito da administração de oxfendazol, ivermectina e levamisol sobre os exames coproparasitológicos de ovinos. *Revista Brasileira de Pesquisa Veterinária e Zootecnia* , *29* (1), 31-38.
2. Coles, GC, Bauer, C., Borgsteede, FHM, Geerts, S., Klei, TR, Taylor, MA, and Waller, PJ (1992). Associação Mundial para o Avanço da Parasitologia Veterinária (WAAVP) métodos para a detecção de resistência anti-helmíntica em nematóides de importância veterinária. *Parasitologia veterinária* , *44* (1-2), 35-44.
3. Costa, C. T. C., Bevilaqua, C. M. L., Morais, S. M., and VIEIRA, L. D. S. (2008). Taninos e sua utilização em pequenos ruminantes. *Embrapa Caprinos e Ovinos-Artigo em periódico indexado (ALICE)*.
4. Echevarria, F. (1995). Situação da resistência de helmintos de bovinos e ovinos no Brasil. *Anais 9º Seminário Brasileiro de Parasitologia Veterinária, Campo Grande, MS*, 277-281.
5. Girão, E. S., de CARVALHO, J. H., Lopes, A. S., Medeiros, L. P., and Girão, R. N. (1998). Avaliacao de plantas medicinais com efeito anti-helmintico para caprinos. *Embrapa Meio-Norte-Séries anteriores (INFOTECA-E)*.
6. Girão, E. S., Leal, J. A., Girão, R. N., and Medeiros, L. P. (1999). Verminose bovina. *Embrapa Meio-Norte-Documentos (INFOTECA-E)*.
7. INSTITUTO BRASILEIRO DE GEOGRAFIA E ESTATISTICA (IBGE). Indicadores IBGE 2019. Disponível em: https://sidra.ibge.gov.br/tabela/3939#resultado. Acesso em: 06 de Agosto de 2020.
8. Mota, M. D. A., Campos, A. K., and Araújo, J.

V. D. (2003). Controle biológico de helmintos parasitos de animais: estágio atual e perspectivas futuras. *Pesquisa Veterinária Brasileira*, *23*(3), 93-100.

9. Ribas, J. L., RICHTER, E. M., MILCZEWSKI, V., CERDEIRO, A. P., and SCHAFHCUSER, E. (2009). Eficácia da folha de bananeira (Musa sp.) no controle de vermes gastrintestinais em pequenos ruminantes. *Cadernos de Agroecologia*, *4*(1).

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

USE OF BANANA PRATA (*MUSA SAPIENTUM*) AND BANANA OURO (*MUSA ACUMINATA*) IN THE CONTROL OF GASTROINTESTINAL NEMATOIDS IN CALVES

Letícia Meirelles Ávila
Universidade Federal Rural do Rio de Janeiro - Brazil

Jônathan David Ribas Chagas
Universidade Federal Rural do Rio de Janeiro - Brazil

Thiago Luiz Pereira Marques
Universidade de Vassouras – Brazil

Renata Fernandes Ferreira de Moraes
Universidade de Vassouras – Brazil

Erica Cristina Rocha Roier
Universidade de Vassouras – Brazil

January/2022

SUMMARY

SBJChem Conference 2021

INTRODUCTION

SBJChem Conference 2021

- Importance of cattle breeding for Brazil;
- Parasitic infestations > Considerable losses to the economy;
- Using anthelmintics incorrectly > Parasite resistance;
- Emergence of alternative methods.;

OBJETIVE

SBJChem Conference 2021

The objective of this work was to demonstrate the elimination of gastrointestinal nematodes through the use of leaves of two different banana species in calves, and to verify if there are differences in the effectiveness of both.

METHODOLOGY

SBJChem Conference 2021

METHODOLOGY

SBJChem Conference 2021

Group A

Musa sapientum
(Banana Prata)

Group B

Musa acuminata
(Banana Ouro)

Group C

Control

METHODOLOGY

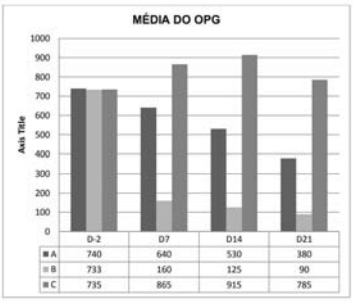
SBJChem Conference 2021

- Treatment performed for two consecutive days (Ad libitum)
- Samples collected 7, 14 and 21 days after treatment
- Conducting eggs/g to obtain the average of the groups

RESULTS AND DISCUSSION

SBJChem Conference 2021

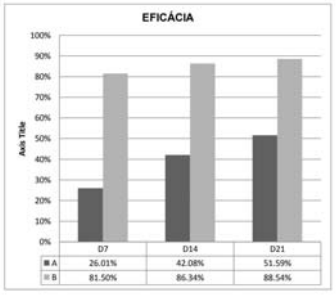
Graph I: Monitoring of the means of eggs per gram (eggs/g) of Groups A, B and C in D-2, D+7, D+14 and D+21, demonstrating the decrease of the means of the first two groups.



RESULTS AND DISCUSSION

SBJChem Conference 2021

Graph 2: Results of the calculation of the effectiveness of Groups A and B in D+7, D+14 and D+21 after the use of banana leaves and evidence of greater efficiency of those used in group B (gold banana, Musa acuminata) that used in Group A (silver banana, Musa sapientum).



RESULTS AND DISCUSSION

SBJChem Conference 2021

- The results of this study demonstrate significance in the rate of reduction of infestations by worms, as well as a decrease in the values of OPG >> Girão (1998): same results in relation to infestation and drop in eggs/g
- The present study did not reach the percentage of efficacy proposed by Coles et al. (1992): TRCOF (Faeces Egg Count Reduction Test) results of less than 90% are not considered effective

CONCLUSIONS

SBJChem Conference 2021

- Effective in decreasing the parasitic load of intestinal nematodes in calves
- Banana ouro (Musa acuminata) was more efficient than banana prata (Musa sapientum) when compared
- Even not reaching an ideal effectiveness number (90%), the research managed to reach 88% of effectiveness with the use of banana ouro leaf >> Adequacy of protocols

REFERENCES

SBJChem Conference 2021

1. Amarante, AFT, Barbosa, MA, de Oliveira, MAG, Carmello, MJ, & Padovani, CR (1992). Efeito da administração de oxfendazol, ivermectina e levamisol sobre os exames coproparasitológicos de ovinos. *Revista Brasileira de Pesquisa Veterinária e Zootecnia* , *29* (1), 31-38.
2. Coles, GC, Bauer, C., Borgsteede, FHM, Geerts, S., Klei, TR, Taylor, MA, & Waller, PJ (1992). Associação Mundial para o Avanço da Parasitologia Veterinária (WAAVP) métodos para a detecção de resistência anti-helmíntica em nematóides de importância veterinária. *Parasitologia veterinária* , *44* (1-2), 35-44.
3. Costa, C. T. C., Bevilaqua, C. M. L., Morais, S. M., & VIEIRA, L. D. S. (2008). Taninos e sua utilização em pequenos ruminantes. *Embrapa Caprinos e Ovinos-Artigo em periódico indexado (ALICE)*.
4. Echevarria, F. (1995). Situação da resistência de helmintos de bovinos e ovinos no Brasil. *Anais 9º Seminário Brasileiro de Parasitologia Veterinária, Campo Grande, MS*, 277-281.
5. Girão, E. S., de CARVALHO, J. H., Lopes, A. S., Medeiros, L. P., & Girão, R. N. (1998). Avaliacao de plantas medicinais com efeito anti-helmintico para caprinos. *Embrapa Meio-Norte-Séries anteriores (INFOTECA-E)*.
6. Girão, E. S., Leal, J. A., Girão, R. N., & Medeiros, L. P. (1999). Verminose bovina. *Embrapa Meio-Norte-Documentos (INFOTECA-E)*.
7. Mota, M. D. A., Campos, A. K., & Araújo, J. V. D. (2003). Controle biológico de helmintos parasitos de animais: estágio atual e perspectivas futuras. *Pesquisa Veterinária Brasileira*, *23*(3), 93-100.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THANKS!

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

VALIDATION OF A GC-FID METHODOLOGY FOR THE DETERMINATION OF 2,5-HEXANEDIONE IN URINE

BORGES, Henrique Bordin Lucena e RÜBENSAM, Gabriel*

Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de Pesquisa em Toxicologia e Farmacologia

** Correspondence author*
e-mail: gabriel.rubensam@pucrs.br

Received 20 January 2022; received in revised form 20 February 2022; accepted 26 February 2022

ABSTRACT

2,5-hexanedione is the main metabolite of hexane and methyl butyl ketone excreted into urine and is currently used to estimate the human exposure levels to these solvents in professional environments. In Brazil, occupational exposure is regulated by a national control program (PCMSO) and applied to public and private organizations that hire your employees according to the actual Brazilian legislation. In the present work, we validated a methodology based on a gas chromatography−flame ionization detector (GC-FID) for the quantification of 2,5-hexanedione in urine to attend the new occupational limit of urinary 2,5-hexanedione, established by a recent revision of the Brazilian legislation, which reduced this limit from 5.0 to 0.5 mg/L. Before GC-FID analysis, sample treatment was based on a simple liquid-liquid extraction with dichloromethane. Considering that there is no specific validation guide for occupational purposes, the adopted validation process was performed using a “fit-for-purpose” approach based on different guides, including FDA bioanalytical method validation, European Commission Decision 2002-657-EC, and ANVISA Guidelines RDC 166/2017. After method optimization, the performance characteristics determined by the present validation study were considered satisfactory and demonstrate the method suitability for the routine analysis in the Brazilian PCMSO, including CCα and CCβ values, which are used to avoid the presentation of false-positive and false-negative results. Intra and interday reproducibility were below 2.66, and 4.08 % and analyte recoveries were above 95.4% for three evaluated levels. The limits of detection and quantification were 0.05 and 0.17, respectively. To our knowledge, this is the first application of CCα and CCβ approaches in an analytical method intended for occupational purposes, which are important to know when a sample is out or following the legislation. Then real samples were analyzed herein, and none presented 2,5-hexanedione above the required limits.

Keywords: *Occupational toxicology, 2,5-hexanodiona, validation, gas chromatography.*

1. INTRODUÇÃO

O hexano (HEX) é um dos solventes orgânicos mais utilizados em processos industriais com liberações atmosféricas estimadas em 20.000 ton/ano (Díaz, *et al.*, 2020; ATSDR, 1999). Já a metilbutilcetona (MBK) não apresenta a mesma amplitude de uso, mas é um dos constituintes de produtos comuns em ambientes profissionias como carpetes, forros, pinturas, entre outros (Jantunen *et al.*, 1997). Em humanos, tanto o HEX quanto a MBK são metabolizados e excretados pela urina na forma de 2,5-hexanodiona livre (2,5-HD livre) e na forma de outros metabólitos conjugados (2,5-HD total), permitindo o monitoramento dos niveis de exposição (NIOSH, 2015). Entre os anos de 1980 e início dos anos 2000, o monitoramento ocupacional desses solventes em diversos países era realizado considerando o somatório da forma livre e conjugada e, atualmente, a maioria monitora somente a forma livre (NIOSH, 2015; EPA, 2009). No Brasil, o monitoramento da exposição ocupacional é realizado de acordo com a Norma Regulamentadora 7 (NR-7), que estabelece um Programa de Contole Médico de Saúde Ocupacional (PCMSO), aplicado nas organizações privadas e órgãos públicos que possuam empregados regidos pela Consolidação das Leis do Trabalho (CLT) (BRASIL, 2021; BRASIL, 2020). Desde a sua criação em 1978, essa norma vem acompanhando e implementando as atualizações propostas por

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.33_abstract_BORGES.pdf

diferentes comissões nacionais e internacionais. A atualização mais recente ocorreu em 2020, com vigência a partir de agosto de 2021, recomendando, entre outros, a redução de alguns Indicadores Biológicos de Exposição Excessiva (IBE/EE), a forma de expressão de alguns resultados (se na forma livre ou conjugada do metabólito) e a introdução do IBE/EE para exposição ao MBK (BRASIL, 2020).

Com a atualização do PCMSO, o IBE/EE da 2,5-HD urinária passou de 5 mg/g de creatinina para 0,5 mg/L. Considerando que os valores médios esperados da creatinina sejam próximos a 1 mg/mL (Sallsten *et al.,* 2021) e que agora há a recomendação para que os resultados sejam expressos como 2,5-HD livre, houve uma redução no seu limite de aproximadamente 10 vezes. Essa redução, portanto, requer metodologias analíticas mais sensíveis e confiáveis. Assim o presente trabalho objetivou a otmização e a validação de um método de GC-FID para a quantificação de 2,5-HD em urina para atendimento dos novos limites estabelecidos pela legislação brasileira vigente, incluindo uma abordagem para avaliação da sua capacidade de decisão (CCα) e detecção (CCβ) que ajudaram a identificar quando uma amostra esteve abaixo ou acima do limite regulatório com probabilidade de erro α e β, respectivamente.

2. MATERIAIS E MÉTODOS

2,5-hexanodiona, ciclohexanona, cloreto de sódio e diclorometano, foram adquiridos da Sigma (Sigma-Aldrich, USA). A água do tipo I foi obtida de sistema de purificação do tipo Milli-Q (Millipore, USA). Os padrões foram preparados em água nas concentrações de 0,1 g/L para 2,5-HD e 0,3 mL/L de ciclohexanona (padrão interno, PI). As amostras de urinas foram obtidas de voluntários, coletadas em frasco de polietileno de 50 mL, posteriormente transferidas (5 mL) para tubos de ensaio com tampa rosca para armazenamento em geladeira ou freezer. Foram consideradas amostras brancas as urinas que não apresentaram 2,5-HD ou concentrações inferiores ao limite de detecção do método.

2.1. Extração

A etapa de extração consistiu em adicionar aproximadamente 1 g de cloreto de sódio em tubos de ensaio de 12 mL com tampa rosca. Em seguida, foram adicionados 5 mL de amostra (ou controles, ou soluções da curva de calibração) e a mistura foi agitada até a dissolução do sal. A extração líquido-líquido (ELL) foi realizada após a adição de 25 uL de PI e 2mL de diclorometano, agitação orbital a 70 rpm durante 1,5 minutos. O extrato foi separado da matriz após centrifugação da mistura a 2500 rpm, a 4 oC, durante 10 minutos, e transferido (aproximadamente 1 mL) para vials de vidro, deixando-os abertos em rack de alumínio (modelo VT98, Agilent Technologies, CA, USA) aquecida a 50 oC, por aproximadamente 10 minutos para promover evaporação de uma fração do solvente. Quando o volume do extrato atingiu aproximadamente 0,5 mL, os vials foram tampados e a rack transferida para o GC-FID para injeção.

2.2 Análise por GC-FID

Os extratos foram analisados em sistema de cromatografia gasosa 7890B GC-System equipado com amostrador automático GC Sampler 80 (Agilent Technologies, CA, USA). A separação foi performada em coluna megabore DB-624 (30m x 0,53mm di, 0,25 µm) com gás de arraste sendo nitrogênio, com fluxo constante de 10 mL/min. A temperatura inicial do forno foi de 90 ºC mantida em isoterma por 5 minutos, seguida de aquecimento de 30 ºC /min até chegar em 120 oC, mantido isoterma de 0,5 min. Uma nova rampa de 50 ºC /min foi aplicada até obter 180 ºC, permanecendo nesta condição por 0,5 min e, por fim, retomando a condição inicial da análise. O injetor foi mantido à temperatura de 230 ºC e injeção foi realizada no modo *splitless*, com volume de extrato de 4 uL. A temperatura do detector FID foi mantida a 250 ºC. A quantificação foi realizada por padronização interna

2.3 Validação

Foram adotados os procedimentos de validação da U. S. Food and Drug Administration (U.S. FDA, 2001), da resolução da Comunidade Européia 2002/657/EC (E.C, 2002), RDC 166/2017 (Anvisa, 2017) utilizando a abordagem "*fit-for-purpose*" (Uvarova *et al.,* 2019). As características de performance avaliadas foram seletividade, utilizando urinas obtidas de, pelo menos, seis coletas distintas adicionadas (ou não) por candidatos a contaminantes externos, como metanol, etanol, metiletilcetona, isopropanol, acetato de etila, acetona, acetonitrila, hexano e ciclohexano, clorofórmio, tetrahidrofurano, formaldeído e metilisobutilcetona; robustez, variando os tempos e velocidades de centrifugação dos extratos, quantidade de cloreto de sódio na etapa de *salting out*, volume de solvent extractor, tipos de solvents diferentes na construção das curvas de calibração;

repetibilidade e reprodutibilidade, a partir do cálculo do desvio padrão relativo de amostras adicionadas por padrão nas concentrações de 0,25 mg/L (limite de quantificação), 0,5 mg/L (IBE/EE) e 1,5 mg/L, no mesmo dia e em dias diferentes, com técnicos diferentes, respectivamente; linearidade, realizando estudo da significância da regressão e desvio da linearidade de curvas construidas em matriz, por análise de variância ($p < 0.05$); estabilidade, trabalhando com adição em matriz e armazenamento em temperature ambiente (ambiente iluminado e não iluminado), em geladeira e em freezer por até 7 dias; limite de decisão (CCα) e capacidade de detecção (CCβ), fortificando lotes de amostras brancas com as concentrações equivalentes a 0,5, 1,0 e 1,5 vezes o IBE/EE do analito; teste do CCα contaminando 22 amostras brancas na concentração equivalente ao IBE/EE da 2,-HD; e efeito de matriz, a partir das curvas de calibração construídas em água e em matriz, observando-se os devios percentuais dos coeficientes angulares da equações de regressão lineares e utilização de volumes de injeção diferentes.

3. RESULTADOS E DISCUSSÃO

3.1 Otimização da etapa de extração

A 2,5-HD foi diretamente extraída de amostras de urina utilizando como base uma das metodologias mais simples até hoje presentes na literatura (Kawai *et al.,* 1990). Para atingir um limite de quantificação não superior a metade do IBE/EE de 2,5-HD proposto na nova legislação brasileira, foi necessária a realização de uma etapa de evaporação do extrato. A variação da concentração de 2,5-HD no extrato causada pela evaporação de solvente foi corrigida pelo padrão interno. Com o método de extração otimizado, foi possível preparar cerca de 30 extratos em menos de 40 minutos, incluindo a curva de calibração, utilizando aproximadamente 60 mL de solvente.

3.2 Validação

O método apresentou seletividade adequada, não sendo observadas coeluições de contaminantes externos. A Figura 1 ilustra os cromatogramas obtidos nae tapa de seletividade. Variações do volume de diclorometano, da quantidade de cloreto de sódio, do tempo de agitação e centrifugação do extrato não causaram alterações superiores a 3,2% no limite quantificação da 2,5-HD em urina (dados não apresentados). Os resultados da avaliação das características de performance do presente método foram compilados na Tabela 1. A precisão vista como repetibilidade e reprodutibilidade do método foram inferiores a 2,66 e 4,08 %, respectivamente. O método apresentou linearidade na faixa de concentração utilizada (de 0,25 até 1,25 mg/L de 2,5-HD) tanto com curvas construídas em água quanto em curvas contruídas em matriz, sem apresentar desvios significativos de variância, com coeficientes de correlação superiores a 0,99 e regressão significativa com interval de confiança de 95%. Não foram observados efeitos de matriz significativos (dados não apresentados), considerando que os desvios entre os coeficientes angulares das curvas de calibração construídas em água e na matriz foram inferiores àqueles obtidos na precisão (Hoff *et al.,* 2015). Os limites de detecção e de quantificação foram de 0,05 e 0,17 mg/L. CCα e CCβ foram 0,53 e 0,56 mg/L, respectivamente, e, dessa forma foi possível estimar a capacidade do método em diferenciar amostras conformes (amostras que apresentaram concentrações de 2,5-HD abaixo do IBE/EE) de amostras não conformes (amostras que apresentaram concentrações de 2,5-HD acima do IBE/EE) e reduzir a probabilidade de apresentar resultados falsos-positivos e falsos-negativos para menos de 5%, conforme recomendado no guia de validação adotado (E.C, 2012). O método foi aplicado para a análise de 10 amostras, sendo que em nove amostras os resultados foram inferiores ao limite de quantificação e, em uma amostra, o resultado foi acima do limite de detecção, mas abaixo do limite de quantificação. Frente a isto, foram realizadas simulações de análises de urinas adicionadas por 2,5-HD na concentração de IBE/EE (22 amostras), para avaliar a metodologia com relação a sua capacidade de gerar resultados falsos-positivos de acordo com a legislação ocupacional vigente. Em uma das amostras simuladas, o resultado foi de 0,55 mg/L, acima do CCα, representando menos de 5% de resultados falsos-positivos.

4. CONCLUSÕES

A presente metodologia foi considerada adequada para aplicação em rotina de análises ocupacionais para a determinação de 2,5-HD em urina considerando os resultados de desempenho obtidos da validação. De acordo com as bases de dados consultadas na literatura, o presente trabalho foi o primeiro a avaliar a capacidade analítica de um método em diferenciar resultados de quantificação em situação de conformidade e não-conformidade de amostras com a legislação vigente, na área de análises de toxicologia

ocupacional, baseados nos dados de CCα e CCβ.

6. REFERÊNCIAS:

1. Díaz C.C., Yeste M.P., Vidal H., Gatica J.M., Cadús L.E., Morales M.R., *Fuel*, V. 262, **2020**, 116564.
2. U.S. Department of health and human services – ATSDR, **1999**, disponível em: https://www.atsdr.cdc.gov/toxprofiles/tp113.pdf, acessado em 12/12/2021.
3. Jantunen M., Jaakkola J.J.K. and Krzyzanowski M., *WHO*, **1997**, No. 78.
4. NIOSH 8318, *NMAM* 5th Edition, **2015**.
5. EPA, *Env Prot Ag*, EPA/635/R-09/008F, **2009**.
6. BRASIL, Ministério do Trabalho e da Previdência, *Norma Regulamentadora No. 7 (NR-7)*, **2021**.
7. BRASIL, Ministério Da Economia, *NR 07* – **2020**.
8. Sallsten G., Barregard L., *Int. J. Environ*. 262, **2020**, 116564
9. U.S. Department of health and human services – ATSDR, **1999**.
10. U.S. FDA, U.S. *Dep. Heal. Hum. Serv. Food Drug Adm*. **2018,** 1–41.
11. E.C., 2002/657/EC - *Commission of the European Communities,* Off. J. Eur. Comm. No. L221/8, **2002**.
12. Anvisa, *Resolução da Diretoria Colegiada RDC 166* de 24 de julho de **2017**
13. Uvarova, N.E., Eremenko, N.N., Ramenskaya, G.V. *Pharm Chem J.* **2019**, *53*, 759–765.
14. Kawai T., Mizunuma K., Yasugi T., Uchida Y.& Ikeda M., *Int. Arch Occup Environ Heath*, **1990**, *62*, 403–408.
15. R.B. Hoff, G. Rübensam, L. Jank, F. Barreto, M.C.R. Peralba, T.M. Pizzolato, M. S. Díaz-Cruz, D. Barceló, *Talanta*,**2015**, *132*, 443-450.

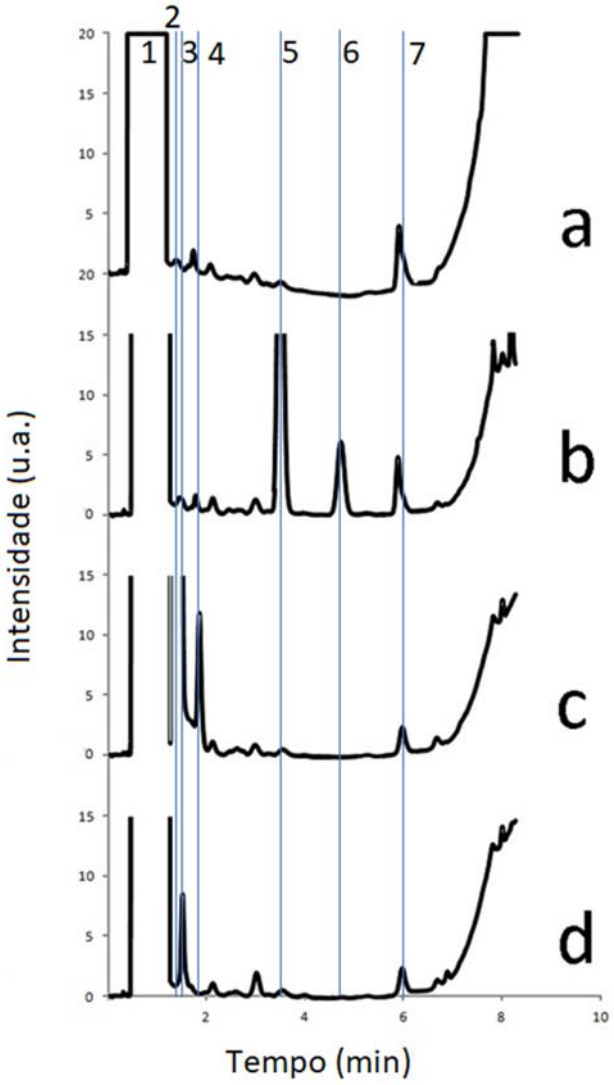


Figura 1: Cromatograma “a”, Extrato de urina sem adição de padrões; cromatograma “b”, extrato de urina com adição de 2,5-HD e padrão interno (picos 5 e 6); cromatograma “c” e “d”, extrato de urina com adição de solventes interferentes.

Tabela 1. *Tabela 1. Compilação dos resultados da etapa de validação*

	Níveis de validação utilizados									Limites[b]			
	0.5 x IBE/EE [a]			1.0 x IBE/EE [a]			1.5 x IBE/EE [a]						
2,5-HD	R (%)	Intra-dia CV (%)	Inter-dias CV (%)	R (%)	Intra-dia CV (%)	Inter-dias CV (%)	R (%)	Intra-dia CV (%)	Inter-dias CV (%)	LD	LQ	CCα	CCβ
	95.4	2.66	4.02	99.5	1.05	4.08	99.1	0.98	2.82	0.05	0.17	0.53	0.56

[a] IBE/EE: níveis de validação utilizados.

[b] Concentrações em mg L−1.

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

VALIDAÇÃO DE MÉTODO PARA DETERMINAÇÃO DE 2,5-HEXANODIONA EM URINA POR CROMATOGRAFIA GASOSA E DETECÇÃO POR IONIZAÇÃO EM CHAMA

Henrique Bordin Lucena
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de Pesquisa em Farmacologia e Toxicologia, INTOX - Brazil.

Gabriel Rübensam
Pontifícia Universidade Católica do Rio Grande do Sul, Escola de Ciências da Saúde e da Vida, Centro de Pesquisa em Farmacologia e Toxicologia, INTOX - Brazil.

December/2021

INTRODUCTION

SBJChem Conference 2021

- 2,5-Hexanodiona (2,5-HD) Metabólito de exposição ao hexano (HEX) e a metilbutilcetona (MBK).
- No Brasil Programa de Controle Médico de Saúde Ocupacional (PCMSO)
- PCMSO Norma Reguladora 07 (NR-07)
- Redução do Indicador Biológico de Exposição Excessiva (IBE/EE) Limite máximo atualmente de 0,5mg/L em urina

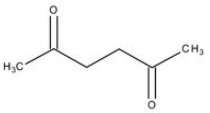


Imagem 1: estrutura química da 2,5-hexanodiona

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

O presente trabalho objetivou a otmização e a validação de um método de GC-FID para a quantificação de 2,5-HD em urina para atendimento dos limites estabelecidos pela legislação brasileira vigente.

METHODOLOGY

SBJChem Conference 2021

- 2,5-Hexanodiona, ciclohexanona (padrão interno, PI), NaCl, diclorometano, água do tipo I.
- Gás nitrogênio, gás hidrogênio e ar sintético.
- Tubos de ensaio com tampa rosca, vials de vidro, rack de alumínio (modelo VT98, Agilent Technologies, CA, USA), agitador orbital, centrífuga, GC Sampler 80 (Agilent Technologies, CA, USA), sistema de cromatografia gasosa 7890B GC-System (Agilent Technologies, CA, USA) e coluna Megabore DB-624 (30m x 0,53mm di, 0,25 µm).

Imagem 2: sistema de cromatografia gasosa 7890B GC-System (Agilent Technologies, CA, USA)

AIM/OBJETIVE/PURPOSE

SBJChem Conference 2021

- Extração líquido-líquido (LLE)
- Adição com homogeneização e agitação dos reagentes (NaCl + amostra/controle/água + PI + diclorometano)
- Centrifugação para separação das fases
- Transferência do extrato para vials de vidro
- Evaporação parcial do extrato nos vials de vidro
- Injeção no GC-FID

RESULTS AND DISCUSSION

SBJChem Conference 2021

- Utilização da abordagem *"fit-for-purpose"* a partir de guias de validação com adoção dos critérios da resolução da Anvisa 166/2017, FDA e 2002/657/EC.

- O método foi avaliado quanto a seletividade, repetibilidade, reprodutibilidade, linearidade, limite de decisão (ccα), capacidade de detecção (ccβ) e estabilidade.

Tabela 1. *Tabela 1. Compilação dos resultados da etapa de validação*

	Níveis de validação utilizados									Limites[b]			
	0.5 x IBE/EE [a]			1.0 x IBE/EE [a]			1.5 x IBE/EE [a]						
2,5-HD	R (%)	Intra-dia CV (%)	Inter-dias CV (%)	R (%)	Intra-dia CV (%)	Inter-dias CV (%)	R (%)	Intra-dia CV (%)	Inter-dias CV (%)	LD	LQ	CCα	CCβ
	95.4	2.66	4.02	99.5	1.05	4.08	99.1	0.98	2.82	0.05	0.17	0.53	0.56

[a] IBE/EE: níveis de validação utilizados.
[b] Concentrações em mg L-1.

CONCLUSIONS

SBJChem Conference 2021

A presente metodologia foi considerada adequada para aplicação em rotina de análises ocupacionais para a determinação de 2,5-HD em urina considerando os resultados de desempenho obtidos da validação. De acordo com as bases de dados consultadas na literatura, o presente trabalho foi o primeiro a avaliar a capacidade analítica de um método em diferenciar resultados de quantificação em situação de conformidade e não-conformidade de amostras com a legislação vigente, na área de análises de toxicologia ocupacional.

REFERENCES

SBJChem Conference 2021

1. J.M. Guzmán-Albores, E. Bojórquez-Velázquez, A. De León-Rodríguez, O.J. Calva-Cruz, A.P.B. Rosa, V.M. Ruíz-Valdiviezo, *Comparison of Moringa oleifera oils extracted with supercritical fluids and hexane and characterization of seed storage proteins in defatted flour*, Food Biosci, 40, **2021**, 100830.
2. U.S. Department of health and human services – ATSDR, *Toxicological profile for n-hexane*, **1999**, disponível em: https://www.atsdr.cdc.gov/toxprofiles/tp113.pdf, acessado em 12/12/2021.
3. M. Jantunen, J.J.K. Jaakkola and M. Krzyzanowski, *Assessment of exposure to indoor air pollutants*, WHO regional publications. European series, No. 78.
4. BRASIL, Ministério do Trabalho e da Previdência, *Comissão Tripartite Paritária Permanente - CTPP Norma Regulamentadora No. 7 (NR-7)*, disponível em: https://www.gov.br/trabalho-e-previdencia/pt-br/composicao/orgaos-especificos/secretaria-de-trabalho/inspecao/seguranca-e-saude-no-trabalho/ctpp-nrs/norma-regulamentadora-no-7-nr-7, acessado em: 25/11/2021.


SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

STEREOSELECTIVE SYNTHESIS AND ANTIPROLIFERATIVE ACTIVITY OF STEVIOL- AND ISOSTEVIOL-BASED BI- AND TRIFUNCTIONALIZED DITERPENOIDS

SZAKONYI, Zsolt[1*]; OZSVÁR, Dániel[1]; BAI, Dorottya[1]; NAGY, Viktória[2]; ZUPKÓ, István[2]

[1] Institute of Pharmaceutical Chemistry, University of Szeged, H-6720 Szeged, Eötvös utca 6, Hungary

[2] Department of Pharmacodynamics and Biopharmacy, University of Szeged, H-6720 Szeged, Eötvös utca 6, Hungary

** Correspondence author*
e-mail: szakonyi.zsolt@szte.hu

Received 09 February 2022; received in revised form 01 March 2022; accepted 07 March 2022

ABSTRACT

Starting from steviol and isosteviol, a series of diterpenoid 3-amino-1,2-diol and 1,3-aminoalcohol derivatives were stereoselectively synthesized. The key intermediate steviol methyl ester was prepared according to the literature procedure. Depending on the epoxidation process, both cis- and trans-epoxyalcohols were obtained. Subsequent oxirane ring-opening with primary and secondary amines afforded 3-amino-1,2-diols. The acid-catalysed hydrolysis and rearrangement of natural stevioside gave isosteviol, which was transformed to the key intermedier methyl ester. In the next step, Mannich condensation of diterpenoid ketone, paraformaldehyde, and secondary amines resulted in the formation of 1,3-aminoketones with different stereoselectivities. Alternatively, aminoalcohols were obtained via stereoselective hydroxy-formylation, followed by oxime preparation, reduction, and, finally, reductive alkylation of the obtained primary aminoalcohols. An alternative 1,3-aminoalcohol library was prepared by reductive amination of the intermedier 3-hydoxyaldehyde obtained from isosteviol in a two-step synthesis. Cytotoxic activity of compounds against human tumor cell lines (A2780, SiHa, HeLa, MCF-7, and MDA-MB-231) was investigated. It was consistently found that the *N*-benzyl substituent is an essential part within the molecule to increase the antiproliferative activity to a level comparable with that of *cisplatine*.

Keywords: *3-amino-1,2-diol, 1,3-aminoalcohol; isosteviol; steviol; diterpene; antiproliferative activity*.

1. INTRODUCTION

In the recent decade, stevia glycosides (isolated from Paraguayan shrub *Stevia rebaudiana* L.) have been proved important natural compounds in the market of artificial sweeteners because of the easy cultivation, the high diterpene glycoside content of the plant, and easy isolation of its glycoside content (Ceunen and Geuns, 2013). Furthermore, because of the huge volume isolation of glycosides, the aglycon steviol and its isomer isosteviol have come into prominence nowadays as promising starting material for the synthesis of bioactive compounds (Ukiya *et al.*, 2013; Shi *et al.*, 2011).

2. MATERIALS AND METHODS

Starting material stevioside was obtained from Molar Chemicals Ltd, Halásztelek, Hungary. Steviol and isosteviol were prepared from commercially available stevioside or a mixture of steviol glycosides in a one-step synthesis according to the literature method (Ceunen and Geuns, 2013; Ukiya *et al.*, 2013; Shi *et al.*, 2011), and their all spectroscopic data were the same as described in the literature.

Optical rotations were measured in MeOH at 20 °C with a Perkin-Elmer 341 polarimeter. Melting points were determined on a Kofler apparatus. ^{1}H-, ^{13}C-NMR and NOESY, 2D-HMBC, and 2D-HMQC spectra were recorded on Brucker Avance DRX 500 spectrometer [500 MHz (^{1}H) and 125 MHz (13C), δ = 0 (TMS)]. HRMS flow injection analysis was performed with a Thermo Scientific Q Exactive Plus hybrid quadrupole-Orbitrap mass spectrometer coupled to a Waters Acquity I-Class UPLC™.

Determination of antiproliferative effect: The growth-inhibitory effects of the steviol and

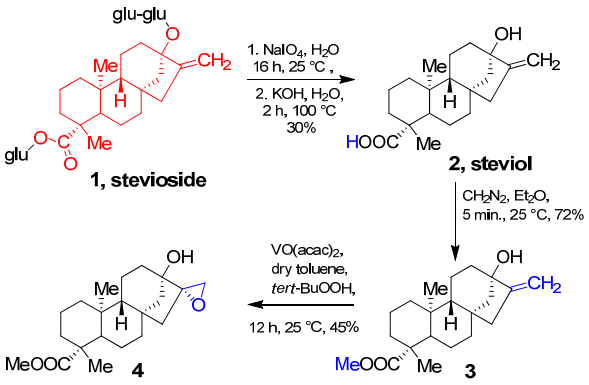
ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.s1_abstract_Zsolt.pdf

isosteviol-based aminodiols and 1,3-aminoalcohols were determined by a standard MTT assay on a panel containing five cell lines, including Hela and Siha (cervical cancers), MDA-MB-231 and MCF-7 (breast cancers), and A2780 ovarian cancer cells. All cell lines were purchased from the European Collection of Cell Cultures (Salisbury, UK) except the SiHa, obtained from the American Tissue Culture Collection (Manassas, VA, USA). The cells were maintained in minimal essential medium supplemented with 10% fetal bovine serum, 1% non-essential amino acids, and 1% penicillin-streptomycin at 37 °C in a humidified atmosphere containing 5% CO_2. All media and supplements were obtained from Lonza Ltd.

3. RESULTS AND DISCUSSION:

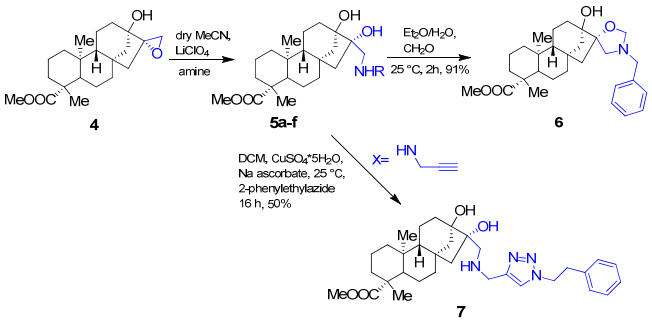
The aim of the present lecture is to give a short review on the chemical and biological applications of promising diterpenoid type compounds with 3-amino-1,2-diol and 1,3-aminoalcohol functions according to our recent results.

A library of steviol-based trifunctional chiral ligands has been developed from commercially available natural stevisoide. The key intermediate steviol methyl ester was prepared according to the literature procedure. Then, depending on the epoxidation process, both *cis*- and *trans*-epoxyalcohols were obtained (Scheme 1).



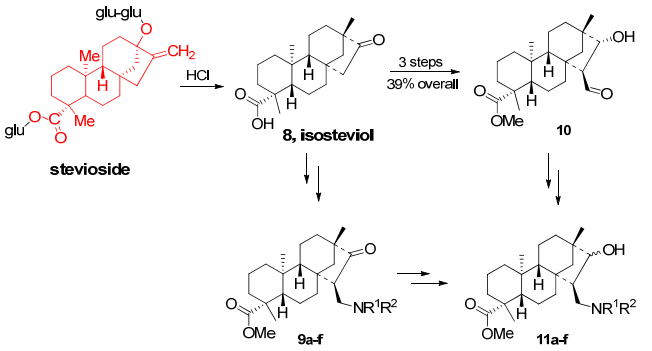
Scheme 1.

Subsequent oxirane ring-opening with primary and secondary amines afforded 3-amino-1,2-diols (Ozsvar *et al*., 2019). The ring-opening with sodium azide followed by “click” reaction with alkynes resulted in dihydroxytriazoles. The regioselective ring closure of *N*-substituted aminodiols with formaldehyde was also investigated (Scheme 2).



Scheme 2.

The acid-catalyzed hydrolysis and rearrangement of natural stevioside gave isosteviol, which was transformed to the key intermedier methyl ester. In the next step, Mannich condensation of diterpenoid ketone, paraformaldehyde, and secondary amines resulted in the formation of 1,3-aminoketones with different stereoselectivities (Scheme 3). During the Mannich condensation with dibenzylamine, an interesting *N*-benzyl → *N*-methyl substituent exchange was observed. Reduction of 1,3-aminoketones produced diastereoisomeric 1,3-aminoalcohols.



Scheme 3.

Alternatively, aminoalcohols were obtained via stereoselective hydroxy-formylation, followed by oxime preparation, reduction, and, finally, reductive alkylation of the obtained primary aminoalcohols. An alternative 1,3-aminoalcohol library was prepared by reductive amination of the intermedier 3-hydroxyaldehyde obtained from isosteviol in a two-step synthesis. The antiproliferative activities of the prepared diterpene analogs were determined employing MTT assay on a panel of human adherent cancer lines, including cells from cervical (HeLa, SiHa), breast (MDA-MB-231, MCF-7), and ovary cancers (A2780).

Primary aminoalcohols and aminodiols, and secondary amine derivatives exerted pronounced antiproliferative action. The calculated IC50 values of these compounds are comparable to or lower than those of reference

agent cisplatin. It seems clear that both the aminoalcohol/aminodiol function and the *N*-benzyl substitution, but not the aliphatic substitution are essential for the remarkable antiproliferative activity. Cervical cell lines are especially sensitive to these agents. Aminoketones are much less effective, and most of them exert only negligible activity. Aminoalcohols or aminodiols bearing tertiary amino function proved to elicit more pronounced action compared only with aminoketones, and the orientation of the newly formed alcohol function has no substantial impact on the efficacy of the product.

4. ACKNOWLEDGMENTS:

We are grateful for financial support from the Hungarian Research Foundation (NKFI K138871), UNKP-21-3-SZTE-272, and Ministry of Human Capacities, Hungary grant 20391-3/2018/FEKUSTRAT.

5. REFERENCES

1. Ceunen, S., Geuns, J.M.C. *J. Nat. Prod*. **2013**, *76*, 1201.
2. Ukiya, M., Sawada, S., Kikuchi, T., Kushi, Y.; Fukatsu, M., Akihisa, T. *Chem. Biodivers*. **2013**, *10*, 177.
3. Shi, L.-Y., Wu, J.-Q., Zhang, D.-Y., Wu, Y.-C., Hua, W.-Y., Wu, X.-M. *Synthesis*, **2011**, 3807.
4. Ozsvár, D., Nagy, V., Zupkó, I., Z. Szakonyi *Int. J. Mol. Sci*. **2019**, *21*, 184.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

OVERVIEW OF AIR MONITORING IN TBILISI (CAPITAL OF GEORGIA) ACCORDING TO 2018-2021 DATA

KUPATADZE, Ketevan

Ilia State University

** Correspondence author*
e-mail: ketevan_kupatadze@iliauni.edu.ge

Received 09 February 2022; received in revised form 01 March 2022; accepted 07 March 2022

ABSTRACT

Air pollution is one of the major environmental challenges facing modern humanity. Atmospheric air is polluted with harmful substances emitted from anthropogenic and natural sources. The presented paper provides an overview of monitoring results conducted in Tbilisi from 2018 to 2021. Results from automated air quality monitoring stations show that particulate matter (PM_{10}, $PM_{2.5}$) and nitrogen dioxide represent problematic pollutants in major cities of the country. Based on the data obtained, it can be assumed that the air in most districts of Tbilisi is moderately polluted. In some cases, the data exceeds the maximum allowable norm. There may be several reasons for this. 1. The unauthorized slashing of Green islands and massive construction of high-rise residential buildings on their place in Tbilisi. 2. Malfunctioning vehicles, the technical inspection of which has recently been made stringent. However, some vehicles still pollute the air. 3.Emissions produced by mini-factories and enterprises. Based on the research, the following recommendations can be made: Avoid parking the vehicle with the engine running; Replace the engine air filter promptly; Maintain the recommended air pressure in the tires; Do not continue to refuel after the refueling device (pistol) automatically shuts off after filling up the tank; Use cruise control as much as possible, which itself regulates the speed of movement; Moving at low engine speeds reduces fuel consumption; The gearbox should be switched to high gear as early as possible and to low gear as late as possible; When moving the traffic light in red mode, move-in approaching the traffic light using inertia; Plan the movement; Do not preheat the engine. Instead, start the car and drive for a short time at low engine speeds until the engine warms up.

Keywords: *Air monitoring, Air Pollution, Pollutant agents, Air purity Recommendations*.

1. INTRODUCTION

Air pollution is one of the significant environmental challenges facing modern humanity. Atmospheric air is polluted with harmful substances emitted from anthropogenic and natural sources.

The key sources of air pollution are transport, power-generating, industrial and agricultural sectors. Compliant to World Health Organization, 91% of the population across the globe lives in an environment where the quality of air does not meet the WHO standards. The problem of free air pollution in Georgia has been observed in the largest cities of the country, as well as in extensive industrial facilities or industrial zones (Cichowicz, 2017).

Air pollution is associated with many human health disorders, including lungs, cardiovascular and nervous system diseases. Human health effects are individual. High-risk groups such as the elderly, children, pregnant women, and people with chronic heart and lung diseases prove to be more susceptible to air pollution (Castanas, 2016).

Even though pollutants may negatively affect the skin, eyes, and other systems, they are mainly harmful to the respiratory system. The nose exhales the air, which acts as a primary filtration

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com

DOI: 10.48141/SBJCHEM.21scon.s2_abstract_KUPATADZE.pdf

system. Tiny hair, warmth, and humid environment inside the nostrils effectively filter the air and remove coarse polluting particles. Before reaching the entrance to the trachea, air passes through the larynx, esophagus, and throat. The trachea is divided into two parts, the right, and the left bronchi. Each bronchus is divided into smaller components. The smallest parts are called the bronchioles, containing millions of air bubbles called alveoli. The bronchioles and alveoli form the lungs.

Continuously inhaled polluted air may slow down the normal cleaning function and cause more particles to get into tiny parts of the lungs.

(Vallero, 2014).

2. MATERIALS AND METHODS

The presented paper provides an overview of monitoring results conducted in Tbilisi from 2018 to 2021.

Results from automated air quality monitoring stations show that particulate matter (PM_{10}, $PM_{2.5}$) and nitrogen dioxide represent problematic pollutants in major cities of the country.

The Data was taken from the National Environmental Monitoring Agency website, being displayed online (Figure 1).

Data was transmitted from the different types of sensors (https://air.gov.ge/en/ VanLoon, 2011. Williams, 2012).

Mainly, the following pollutants are investigated:

Solid particles of dust; Nitrogen dioxide; Ozone; Sulphur Dioxide; Carbon Dioxide; Benzene.

3. RESULTS AND DISCUSSION:

According to 2018 data, atmospheric air pollution was monitored at 3 stationary booths located on Kvinitadze Street, Tsereteli, and Moscow Avenues. The following 6 polluting ingredients were determined at Kvinitadze Street: dust, sulfur dioxide, carbon dioxide, nitrogen dioxide, ozone, and lead. On Moscow Avenue - carbon dioxide and nitrogen dioxide, and Tsereteli Avenue - dust, carbon dioxide, nitrogen dioxide, and lead. An automatic station also monitored air pollution in Tbilisi. The following pollutants were detected automatically: carbon dioxide, sulfur dioxide, nitrogen oxides, ozone, PM2,5, and PM10. The maximum concentrations of dust reached 2.1 mg/m^3 (4.2 zdc), carbon dioxide 22 mg/m^3 (4.4 zdc), nitrogen dioxide 0.332 mg/m^3 (1.7 zdc) and ozone - 0.398 mg/m^3 (2.5 zdc), one-time maximum concentration of sulfur dioxide - 0.22 mg/m^3 did not exceed the maximum allowable norm.

According to the data from the automatic station, the average annual concentration of all defined ingredients was within the norm, except for ozone, the average annual concentration of which slightly exceeded the maximum allowable value. As a result, in recent years the average annual concentrations of sulfur dioxide, dust, and ozone in the air of Tbilisi increased, and the concentration of carbon dioxide increased slightly. In contrast, the concentration of nitrogen dioxide decreased slightly.

Indicative measurements were performed in several stages. At the first stage, 11 indicator measurements were conducted in Tbilisi. Low indices of sulfur dioxide, ozone, and benzene were observed everywhere, and the index of nitrogen dioxide was moderate everywhere, except for one point - Tovstonogov Street, where its low index was observed.

2019 At the second stage, 11 indicators were measured in Tbilisi. Low indexes of sulfur dioxide and ozone were observed in all the areas. Nitrogen dioxide indices were both low and medium. Mainly, average indexes of nitrogen dioxide were observed at six points. The benzene index was low everywhere except at one point - Tashkent Street, where the average index was observed.

From January to October, the atmospheric air in Tbilisi was monitored by a single background automatic station located on Vashlijvari meteorological station (6 Marshal Gelovani Ave.). Concentrations of the following harmful pollutants were measured at the station in January: carbon dioxide, nitrous oxide, dioxide, NO_X, and ozone.

Ten-month average carbon dioxide concentrations, nitrous oxide, and dioxide at the Vashlijvari background automatic station were within the norm. However, the average concentration of ozone was 0.044 mg/m^3, 1.5 times higher than the corresponding maximum allowable concentration. Three automatic stations also conducted atmospheric air monitoring in Tbilisi on Tsereteli, Kazbegi Avenues, and Varketili. Concentrations of the following pollutants were measured at these stations: PM10, PM2.5,

carbon dioxide, sulfur dioxide, nitrous oxide and dioxide, NO_X, and ozone.

Average annual concentrations of sulfur dioxide, carbon dioxide, and ozone on Tsereteli Avenue were within the norm. The average annual concentration of nitrogen dioxide was 0.058 mg/m^3, 1.5 times higher than the corresponding maximum allowable concentration, and 0.085 mg $/m^3$ - 1.4 times. The average annual concentrations of nitrogen dioxide and oxide, sulfur dioxide, and carbon dioxide on Kazbegi Avenue were within the norm. In contrast, the average annual ozone concentration was 0.041 mg/m^3, 31.4 times the corresponding maximum allowable concentration. The average annual concentrations of nitrogen dioxide and oxide, sulfur dioxide, and carbon dioxide in Varketil were within the norm. However, the yearly average concentration of ozone was 0.055 mg/m^3, 1.8 times higher than the corresponding maximum allowable concentration. On Tsereteli Avenue, Kazbegi Avenue, and Varketili, the year-round PM10 content was compared to EU 27 | with the 24-hour norm set by 0.05 mg /m3 and the annual allowable concentration 0.04 mg/m3.

212-day data of PM10 on Tsereteli Avenue exceeded the norm, and its highest concentration - 0.165 mg/m^3 was recorded on January 17. It was 3.3 times higher than the allowable value. Excessive concentrations on the Kazbegi Avenue were observed for 86 days: the maximum indicator was observed on September 7, when the PM10 content reached 0.139 mg/m3, which was 2.8 times higher than the norm, while in Varketili, the excess was also observed for 85 days and reached a maximum of 18 days. 0.130 mg/m3 was 2.6 times higher than the allowable value.

As for the average annual value of PM10, it was 1.5 times on Tsereteli Avenue, slightly on Kazbegi Avenue, and in Varketili, it did not exceed the allowable norm. The content of PM2.5 was also compared with the annual allowable concentration set by the EU - 0.025 mg/m^3. Again, its content in Kazbegi Avenue and Varketili did not exceed the norm. In contrast, on Tsereteli Avenue, it was slightly exceeded.

Results of indicator measurements 110 indicator measurements were conducted in four stages in 21 points of Tbilisi city. Measurements of nitrogen dioxide - 80, sulfur dioxide - 6, ozone - 12 and benzene - 12. Low indices of sulfur dioxide and ozone were observed everywhere. The nitrogen dioxide index was low in only 15 cases, moderate in - 55 cases and high in - 10 cases. The benzene index was low in 9 cases and moderated in 3 cases.

The study also showed a relatively low rate of pollution in 2020, most likely due to a pandemic-related transport ban.

Based on the research, the following recommendations can be made:

- Avoid parking the vehicle with the engine running
- Replace the engine air filter promptly
- Maintain the recommended air pressure in the tires
- Do not continue to refuel after the refueling device (pistol) automatically shuts off after filling up the tank
- Use cruise control as much as possible, which itself regulates the speed of movement
- Moving at low engine speeds reduces fuel consumption
- The gearbox should be switched to high gear as early as possible and to low gear as late as possible.
- When moving the traffic light in red mode, move-in approaching the traffic light using inertia
- Plan the movement in advance
- Do not preheat the engine. Instead, start the car and drive for a short time at low engine speeds until the engine warms up.
- Do not drive in summer with winter tires
- Minimize the use of air conditioning
- The catalyst can be damaged if the vehicle is clogged by towing it
- Free the car from unnecessary load
- Try to place the load in the trunk of the car and not on the roof

4. CONCLUSIONS:

Based on the rusults obtained, it can be

assumed that the air in most districts of Tbilisi is moderately polluted. However, in some cases, the data exceeds the maximum allowable norm. There may be several reasons for this.

1. The unauthorized slashing of Green islands and massive construction of high-rise residential buildings on their place in Tbilisi.
2. Malfunctioning vehicles, the technical inspection of which has recently been made stringent. However, some vehicles still pollute the air.
3. Mini-factories and enterprises produce emissions.

5. REFERENCES:

1. Cichowicz, R., Wielgosiński, G. & Fetter, W. Dispersion of atmospheric air pollution in summer and winter season. *Environ Monit Assess,* ***2017,*** 189, 605.
2. Kampa, M., Castanas, E. Human Health effects of air pollution, ***2016***.
3. Vallero, D. Fundamentals of Air Pollution, ***2014***.
4. VanLoon, G.W. "Environmental Chemistry-a global perspective", ***2011***, Oxford Group.
5. Williams, J. "Environmental Chemistry". J.Wiley & Sons, ***2012***, Canada.

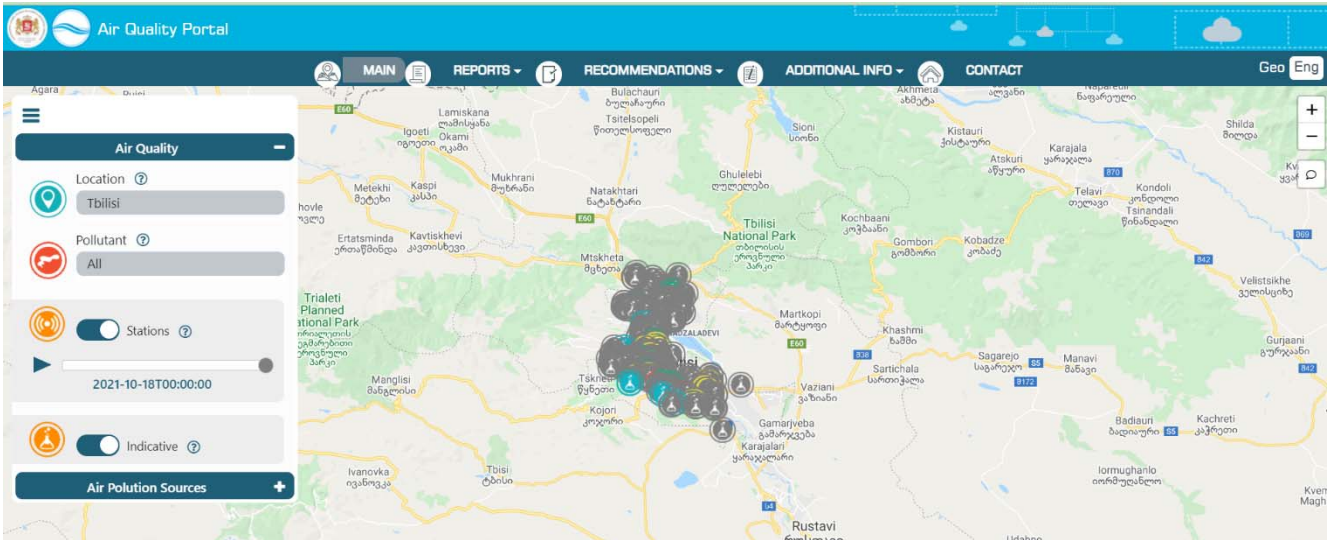


Figure 1. *Air Monitoring Portal*

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

THE PHYSICAL CHEMISTRY BEHIND GLOBAL WARMING WITH A REMEMBRANCE OF MY MENTORS, PROFS. E. H. STARICCO AND M. J. MOLINA

ARGÜELLO, Gustavo A.

Universidad Nacional de Córdoba, Facultad de Ciencias Químicas, INFIQC, Departamento de Físico Química

** Correspondence author*
e-mail: gaac.isea@gmail.com

Received 12 October 2021; received in revised form 30 November 2021; accepted 14 December 2021

ABSTRACT

The author will give a very brief resemblance of the two late persons that have most contributed to his career, namely the Nobel Prize awardee Mario J. Molina and his Ph.D. director Prof. Eduardo H. Staricco. Nobel Laureate Mario J. Molina received his degree in Chemical Engineering from the Universidad Nacional Autónoma de México; he studied at the University of Freiburg and received his PhD in Physicochemistry from the University of California, Berkeley (1972). Dr. Molina was one of the world's leading researchers in atmospheric chemistry at a very young age. In 1974 he predicted the thinning of the ozone layer as a consequence of the emission of industrial gases of massive use, the chlorofluorocarbons (CFCs), a fact that earned him a share in the 1995 Nobel Prize in Chemistry. His research led to the establishment and signing of the United Nations Montreal Protocol (1987). From 2004 until his death, he chaired the Mario Molina Research Center in Mexico City, an association that contributes to finding solutions to problems related to environmental protection. Another of the most influential personalities for Dr. Argüello was Prof. Dr. Eduardo H. Staricco, who graduated as a Biochemist in 1959 with a Gold Medal and Diploma of Honor at the National University of Córdoba. He then left Argentina to do several post-doctorates and in 1962 he returned to the Faculty of Chemical Sciences to work as Full Professor (1964-1985), Full Professor (1985- 2000), or Emeritus Professor (2000). At CONICET he reached the highest category of Senior Researcher. He was also very active in management at the Faculty of the National University of Córdoba (UNC), where he was Vice-Dean (1972-1973), Dean (1986-1988), Vice-Rector of the National University of Córdoba (1987-1992), and then Rector (1995-1998). Dr. Argüello will then introduce some of the basic concepts of physical chemistry to understand Global Warming.

Keywords: *Absorption and Emission of light; Black body radiation; Fluorinated substances*

1. INTRODUCTION

During my first year as a graduate student in Córdoba, trying to implement a new lab to study chemical lasers, it came to my hand a copy of a newsletter from the Inter American Photochemical Society with an advertisement from Mario Molina (McNeill, 2020) who was seeking a person to work in his lab in a project involving vacuum UV fluorescence. I immediately remembered two things: 1) my boss had worked with Mario during His Ph.D. in Berkeley, and 2) Mario himself had done his Ph.D. with Chemical lasers. Therefore, I needed to talk to my boss to get his permission to go and work in Mario´s lab for a year to learn as much as possible about the effective implementation of the chemical laser lab. One hour later, I had already contacted Mario.

That year with Mario produced good results because once in Córdoba, I finally put the Iodine chemical laser to work for the first time in Argentina. My boss was also happy with the results and continued encouraging me to undertake new challenges. I finished my Ph.D., continued working in the Uni to finally became a scientist for life. Since many of the research lines of the Departamento de Físico Química had to do with the kinetics and photochemistry of gaseous fluorinated substances, I could not escape from that tradition. Neither could I escape from Mario´s influence since he was becoming the most prominent scientist warning people of the ozone hole problem (Molina *et al.*, 1974).

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com

DOI: 10.48141/SBJCHEM.21scon.s3_abstract_ARGUELLO.pdf

In short, since the whole atmosphere could be considered a giant phase photochemical reactor, and the ascendancies I had from my mentors, it is not surprising that I have dug into the issue of Global Warming (GW).

Let´s begin.

2. RESULTS AND DISCUSSION:

We all know that the system Sun-Earth has maintained a *thermal balance* for millions of years (that is, roughly speaking, that even though the sun has been permanently heating the Earth, its temperature has not increased). We also know that the temperature on Earth should have been 18°C *below zero* if it were not because of the gaseous layer, called the atmosphere, that surrounds Earth.

Why has this layer helped to maintain a temperature above -18°C? Because one of the most basic properties that *all substances have*: the ability to absorb light. But not just any light. Some substances absorb UV light, some others Visible light and still others IR light (Rimondino *et al.*, 2017; Cooke *et al.,* 2020).
The ones that absorb UV light, like ozone, for example, protect us from those (hazardous for life) wavelengths from reaching the surface of the Earth.

In general, Visible radiation is not absorbed by the Gases that conform to the atmosphere, so these wavelengths reach the surface and warm up it.

How does the Earth manage to get rid of the ceaseless energy (in the form of visible light) coming from the sun to keep the temperature around the same?..... Simple, it maintains the thermal balance **emitting radiation!!!!**.... But not just any. The Earth *only emits* IR radiation

Remember, there are gaseous substances that absorb IR radiation that are spread around the atmosphere. Since ancient times, CO_2, H_2O, CH_4, and other gases have been part of the atmosphere and are responsible for the temperature being around 25°C because of the IR radiation that they have absorbed. These are the so-called GHGs (Green House Gases).
Thanks to them, we have a livable Earth.

But today, these guys have increased their concentrations (particularly after the industrial revolution and exclusively due to our excessive use of fossil fuels) to the point of becoming a serious problem. Today, we have an *exacerbated* greenhouse effect!!!.....and the temperature on Earth has been steadily increasing. And there is still more…..

If one takes a look to the spectrum of radiation that should go out of the Earth, were it not have the atmosphere (Figure 1, red line), and compares this picture to what Earth really emits (Figure 1, blue line), one can extract some conclusions: 1- different gases absorb in different regions; CO_2 mostly to the left of the figure, ozone in the middle, N_2O, CH_4 and Water mainly to the right; 2- CO_2 is by far the bad cop, with a contribution to Global Warming by itself of about 57%; 3- there are two regions where the radiation can escape as it should.

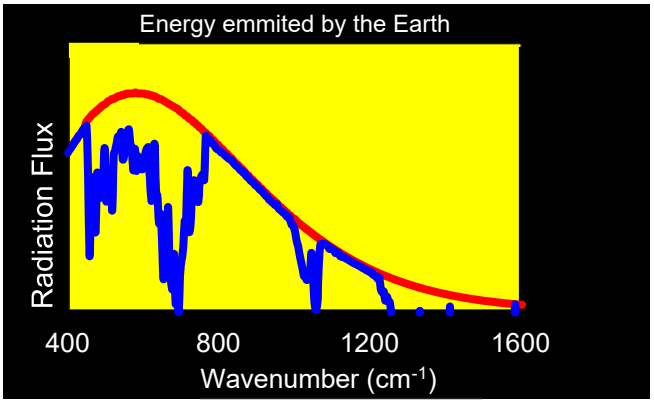


Figure 2. *Energy actually emitted (in red what it should emit)*

So important are these two regions that we call them “the atmospheric windows”……and we should keep them wide open……..but……

Not only the products of the combustion of fossil fuels (mostly CO_2) are injected into the atmosphere.

In the last century, hundreds of tons of fluorinated molecules (Chlorofluorocarbons, CFCs), used as refrigerants, were released into the atmosphere (Malanca *et al.*, 1997; Malanca *et al.*, 1998). They were such a brilliant discovery (they were inert species, harmless, they did not react with other molecules in the troposphere and therefore their lifetimes were of the order of decades or centuries….and more) that we used them extensively…..until Mario Molina studied their behavior, once having reached the stratosphere, and begun warning people of the consequences in the depletion of the ozone layer (Molina *et al.*, 1974).

Scientific Concern, Lobby, Montreal Protocol, Kyoto Protocol, and others, all helped stop (and eventually ban) the production of CFCs

as well as to decrease consumption of fossil fuels in order to keep our world livable.

After the Ozone Depletion Issue, scientists made a huge effort to develop new substances that could play the role of the CFCs, in terms of refrigerant power, without their drawbacks. They came out with a series of new molecules (in a way very similar to the CFCs) having good refrigerant properties that proved to be moderately short-lived due to their reaction with OH radicals produced by the "high" water concentration of the troposphere. Thus, these bunch of molecules received the fancy name of "CFC Replacements". Strictly speaking, they are Hydrofluorocarbons, Hydrochlorofluorocarbons, and Hydrofluoroethers; that is, they all have at least one labile hydrogen atom that reacts with an OH radical and begin the degradation of the molecule in the troposphere, thus substantially reducing the amount of molecules that enter the stratosphere and behave as ozone-depleting substances. However, not all these replacements react completely in the troposphere…… they have different lifetimes. Some of them are long enough to allow molecules to enter and remain intact into the stratosphere (remember that the stratosphere is "dry", that is, there is no water, and therefore the OH radical concentration is low) where they **now contribute to Global Warming because of their absorption properties**!!!!

What is the light they absorb to become a problem in GW?..... Of course, IR radiation, and where do they absorb?..... Unfortunately, exactly in the region where we have the atmospheric windows……That is the reason why these molecules are at the top in terms of "Global Warming Potential".

3.CONCLUSIONS:

My conclusion is that "nothing is for free". We fight to reduce the ozone problem, we are winning that fight, but at the same time, we are creating another potential issue. Fortunately, the concentration of these replacements (as well as all the remainings from CFCs) is still low to contribute much less to GW than CO_2, which remains the enemy we have to fight against and defeat to keep the rising temperatures within tolerable limits.

4. REFERENCES:

1. Molina, M. and Rowland, F. *Nature,* **1974***, 249, 8*10 – 812.
2. McNeill, V. F. *Nature,* **2020,** *587*, 193.
3. Malanca, F. E., Argüello, G. A., Staricco, E. H., Wayne, R. P., *J. Photchem. Photobiol. A: Chemistry*, **1998**, *17*, 163 – 169.
4. Malanca, F. E., Argüello, G. A., Staricco, *J. Photchem. Photobiol. A: Chemistry*, **1997**, *103*, 19 – 25.
5. Rimondino, G. N., Henao, D., Peláez, W. J., Argüello, Malanca, F. E., *J. Phys. Chem. A*, **2017**, *121*, 8577 – 8582.
6. Cooke, M. V, Chans, G. M., Argüello, G.A., Peláez, W. J., *Heliyon*, **2020**, *6*(7), e04457.

SCAN ME

SOUTHERN BRAZILIAN JOURNAL OF CHEMISTRY
2021 VIRTUAL CONFERENCE

DEVELOPMENT OF SYNTHESIS OF GRANULAR ZEOLITE NaA FROM COAL FLY ASH

FUNGARO, Denise Alves

Instituto de Pesquisas Energéticas e Nucleares, IPEN–CNEN/SP, São Paulo, SP, Brazil

* Correspondence author
e-mail: dfungaro@ipen.br

Received 12 January 2022; received in revised form 30 January 2022; accepted 14 February 2022

ABSTRACT

Pelletization of zeolitic materials is required to facilitate their practical industrial and commercial applications. The fusion method synthesized Zeolite NaA from fly ash and shaped it into spherical granules. Bentonite, kaolinite, and bentonite with kaolinite were tested as binders with different contents from 5 wt% to 10 wt%. The pellet formation was optimized. Different techniques characterized the binders, zeolite powder, and zeolite granular. The pellet obtained the best performance with 10% bentonite with mechanical strength and satisfactory water resistance

Keywords*: fly ash, zeolite, NaA, pelletization*

1. INTRODUCTION

The production of zeolites from coal fly ash by means of different hydrothermal activation methods is a well-known process. The synthesis methods include direct hydrothermal, two-step hydrothermal, fusion-assisted hydrothermal, and microwave-assisted methods (Azizi *et al.*, 2021; Zhang *et al.*, 2022; Ren *et al.*, 2020; Harja and Ciobanu, 2020; Khaleque *et al.,* 2020; Paramitha, 2020).

High purity NaA zeolite can be obtained through a two-step process consisting of a fusion of the fly ash and alkali mixture and adding an external aluminate source in the first stage. Then, the alkali melt product is processed through hydrothermal treatment in the second stage. Upon completion of the synthesis process, fly ash zeolite is obtained in the form of powder (Izidoro et al., 2019; 2013).

Depending on the application is necessary to perform a pelletization process. Because pure zeolite powder does not exhibit binding properties, an appropriate binder needs to be applied to form pellets

In the present study, fly ash-based zeolite NaA powder, bentonite, kaolinite, and bentonite with kaolinite were considered in the pelletization process. The content of NaA zeolite powder was fixed at 90% by mass (minimum) in all methods so that the greatest possible amount of material containing coal ash was used.

2. MATERIALS AND METHODS

2.1. Materials

All chemicals used for experimental studies were of analytical grade. Coal fly ash sample was collected in the Thermoelectric Complex Jorge Lacerda, located in the Santa Catarina State, Brazil. Bentonite and kaolinite used as a binder in this study were commercially produced material. Sodium hydroxide (97%) and sodium aluminate (100%) obtained from Sigma-Aldrich Pty. Ltd. (Australia) were used in the preparation of zeolite synthesis.

2.2. Preparation of NaA granules

Synthesis of NaA zeolite from fly ash in powder form (ZAP) was carried out as reported in previous studies (Izidoro et al., 2019; 2013).

To prepare the NaA granules, ZAP was mixed with a binder (bentonite, kaolinite, or bentonite + kaolinite) and homogenized. Then, deionized water, with ratio dry mixture mass:volume = 1:1, was slowly poured into a cavity in the center of the container containing the

ISSN 2674-6891. 2021. Downloaded from www.sbjchem.com
Established in 1993.
DOI: 10.48141/SBJCHEM.21scon.s4_abstract_FUNGARO.pdf

dry mixture until a paste was obtained. After homogenization, the pasty mixture was molded into spherical granules. After the molding step, the material was dried in an oven at 100 °C for 2 h and calcined in a muffle at 500 °C for 2 h. ZAP zeolite content was maintained at 90 and 95 wt.%. Bentonite, kaolinite, and a mixture of the two binders were assessed with different amounts shown in Table 1, and samples were named as ZAG1, ZAG2, ZAG3, ZAG4, ZAG5, ZAG6. Fig. 1 illustrates one of the pellet samples produced.

Table 1 *- Composition of binders used in pelleting of NaA zeolite powder*

Zeolite granular sample	Composition (wt.%)	
	Bentonite	Kaolinite
ZAG1	5	5
ZAG2	8	2
ZAG3	10	0
ZAG4	0	10
ZAG5	5	0
ZAG6	4	1

Figure 1. *Photograph of NaA granules*

Physico-chemical properties of fly ash, NaA, and other characterizations of materials have been reported in previous studies (Bertolini, 2019; Bertolini et al., 2017).

3. RESULTS AND DISCUSSION:

3.1. Evaluation of the produced granular zeolites

Important characteristics of the six granular zeolites were determined. The investigated properties included workability, drop resistance, water stability, and cation exchange capacity (Bertolini, 2019).

The structure of ZAG1, ZAG4, and ZAG6 samples collapsed.

The best results were obtained with ZAG2; ZAG3, and ZAG5 samples. These granules were the most resistant and showed similar cationic exchange capacity values to the value obtained with zeolite A in the powder form (ZAP).

The deformation and the breakage behavior of granulate samples ZAG2, ZAG3, and ZAG5 were described by force-displacement curves (not shown). The samples exhibit dominant elastic-plastic properties.

The average values of mechanical properties of granulate samples ZAG2, ZAG3, and ZAG5 were examined. The pellet prepared by 90 wt.% zeolite and 10 wt.% (ZAG3) bentonite exhibit the highest fracture strength (2.9 MPa) and breakage force (32.7 N).

3.2. Characterization of granular synthesis product ZAG3

The chemical composition of the granular zeolite ZAG3 is reported in Table 2, along with the SiO_2/Al_2O_3 ratio.

An increase of silica and alumina in the chemical composition of the zeolite after pelletization compared to powder zeolite (ZAP) was confirmed, since these are the main constituents of binding agent used in the process.

Table 1. **Chemical composition of the major elements of ZAG3**

Oxides	wt. %
SiO_2	41.5
Al_2O_3	28.3
Na_2O	15.4
Fe_2O_3	5.77
CaO	5.67
MgO	1.10
TiO_2	1.01
K_2O	0.685
SO_3	0.202
P_2O_5	0.045
MnO	0.028
ZnO	0.021
SiO_2/Al_2O_3	1.47

The X-ray patterns of synthetic zeolitic materials in powder and granular form are illustrated in Figure 2. The pelletizing process has no effect on the crystallinity of the powder zeolite, as evidenced by X-ray diffraction. In addition, no new diffraction peaks were observed, indicating no new crystalline phase formation, that is important to maintain the zeolite properties.

The reduced intensities observed for the granules in relation to the powder material result from the inclusion of the bentonite. This decrease in reflection intensity was also observed in the diffractogram of ZSM-5 zeolite granular prepared using attapulgite as a clay binder (Michels et al., 2012).

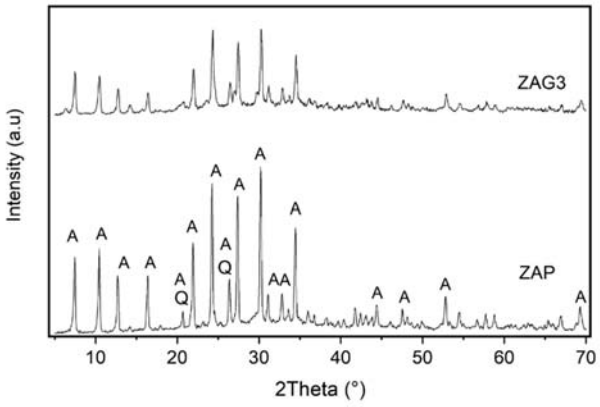


Figure 1. *The XRD patterns of powder zeolite ZAP and granular zeoliteZAG3 (Q = Quartz, A = NaA zeolite)*

4. CONCLUSIONS:

NaA zeolite granule in spherical form was successfully prepared using fly ash-based-zeolite powder and 10 w% bentonites as binder via wet granulation. Zeolite in granular form showed physico-chemical properties similar with zeolite in powder form. In addition, the NaA granules exhibit dominant elastic-plastic properties. The maximum force required to break granules was 32.7 N. It may be concluded that the selected composition may be used to prepare pelletized zeolite from coal fly ash as raw material, presenting a conception of waste management under the circular economy.

5. ACKNOWLEDGMENTS:

The authors is grateful to CNPq, CAPES for supporting this study, and Jorge Lacerda coal-fired power plant for providing coal ash sample.

6. REFERENCES:

1. Azizi, D., Ibsaine, F., Dionne, J., Pasquier,L-C., Coudert, L., Blais, J-F. Microporous and macroporous materials state-of-the-art of the technologies in zeolitization of aluminosilicate bearing residues from mining and metallurgical industries: A comprehensive review, *Microporous Mesoporous Mater.* **2021,** 318, 111029.
2. Bertolini, T. C. R., Guilhen, S. N., Fungaro, D. A. *Pellets Manufactured from Coal Fly Ash: Preparation, Characterization and Environmental Applications.* In: Parker, J. (Ed.). Fly Ash: Properties, Analysis and Performance Hauppauge, N.Y.: Nova Science Publishers. **2017,** Chapter 10, 195.
3. Bertolini, T. C. R. “Synthesis and characterization of zeolitic material granular of coal ash and evaluation in the application as adsorbent”, Thesis Doctorate, Instituto de Pesquisas Energéticas e Nucleares, São Paulo, **2019**.
4. Harja M., Ciobanu G. *Eco-friendly Nano-adsorbents for Pollutant Removal from Wastewaters.* In: Kharissova O., Martínez L., Kharisov B. (eds) Handbook of Nanomaterials and Nanocomposites for Energy and Environmental Applications. Springer, Cham, **2020,** 1.
5. Izidoro, J., D. Castanho, C. Rossati, D. Fungaro, S. Guilhen, T. Nogueira and M.D.F. Andrade. Application of high-purity zeolite A synthesized from different coal combustion by-products in carbon dioxide capture. *Int. J. Environ. Imp*. **2019**, 2, 215.
6. Izidoro, J. C., Fungaro, D. A., Abbott, J. E., Wang, S. Synthesis of zeolites X and A from fly ashes for cadmium and zinc removal from aqueous solutions in single and binary ion systems. Fuel, **2013**, 103, 827.
7. Khaleque, M. M. Alam, M. Hoque et al. Zeolite synthesis from low-cost materials and environmental applications: A review. *Environ. Adv.* (**2020**,2 100019.
8. Michels, N-L., Mitchell, S., Milina, M., Kunze, K., Krumeich, F., Marone F., Erdmann, M., Marti, N., Pérez-Ramírez, J. Hierarchically Structured Zeolite Bodies: Assembling Micro-, Meso-, and Macroporosity Levels in Complex Materials with Enhanced Properties. *Adv. Funct. Mater.*, **2012**, 22, 2509.
9. Paramitha, T. Conversion of Coal Fly Ash to Zeolite by Alkaline Fusion-Hydrothermal Method: A Review. *Adv. Eng. Res.* **2020**, 198, 407.
10. Ren, X., Qu, R., Liu, S., Zhao, H., Wu, W., Song, H., Zheng, C., Wu, X., and Gao, X. *Aerosol Air Qual. Res*. **2020**, 20, 1127.
11. Zhang, X-Y.; Li, C-Q.; Zheng, S-L.; Di, Y-

H.; Sun,Z-M. A review of the synthesis and application of zeolites from coal-based solid wastes, Int. J. Miner. Metall. Mater. **2022,** 29, 1.

LAUNCH VEHICLE DEVELOPMENT IN BRAZIL

By: M. Sc. SANTOS, Fábio.

Country: **Brazil**

PRODUCTION OF SYNTHETIC BIOFUELS

By: Dr. DE BONI, Luis, and Dr. GOLDANI, Eduardo.

Country: **Brazil**

PESQUISA APLICADA EM TEMPOS DE PANDEMIA

By: Dr. TRAJANO, Eduardo Tavares Lima.

Country: **Brazil**

TREATING CHEMICAL RESIDUES WITH POAs (CASE STUDY)

By: Dr. DE BONI, Luis

Country: **Brazil**

NON-INVASIVE DIALYSIS

By: Dr. Bhavna Ambudkarr

Country: **India**