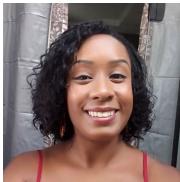


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#LatinXChemBio BIO-163

OpenZika: An Open Science Collaboration Project Enables the Discovery of Potent NS3 Protease Inhibitors as New Antiviral Candidates Against Zika Virus

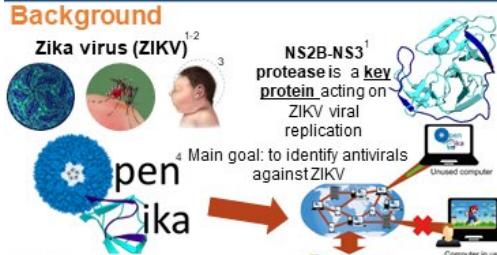
Bruna Katiele de Paula Sousa, PhD Student Universidade Federal de Goiás (UFG)

OpenZika: an open science collaboration project enables the discovery of a potent NS3 protease inhibitor as new antiviral candidate against Zika Virus

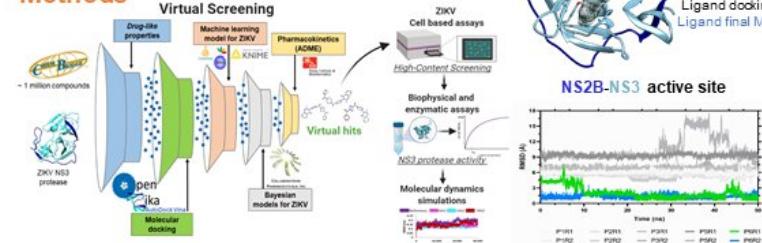


Bruna K. P. Sousa¹; Melina Mottin¹; Jean Bernatchez²; Nathalya C. M. R. Mesquita³; Zhe Zhu²; Jeremy Rich²; Alex E. Clark²; Kimberly M. Zorn⁴; Daniel Foil⁴; Geraldo R. Sartori⁵; Aline O. Albuquerque⁶; João H. M. Silvati⁷; Bruno J. Neves⁸; Eugene Muratov⁹; Alexander Perryman¹⁰; Glaciúis Oliva¹¹; Jair Siqueira-Neto¹²; Sean Ekins¹³; Carolina Horta Andrade¹⁴
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Background

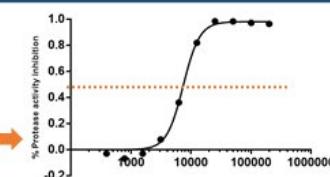
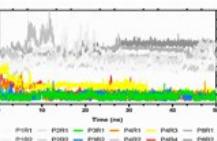


Methods



Results

- VS based on docking and machine learning models prioritized 59 virtual hits;
- 16 compounds had presented good potency against ZIKV in cell-based assays(Glioblastoma Stem Cells) and low cytotoxicity;
- One compound inhibited ZIKV NS3 protease with $IC_{50} = 7.4 \pm 0.3 \mu\text{M}$, $EC_{50} = 6.68 \mu\text{M}$ and low cytotoxicity.
- Molecular dynamics (MD) simulations investigated docking poses stability and the compound mode of action on NS3



Conclusions

The OpenZika project enabled the identification of promising virtual hits and an experimental potent inhibitor against ZIKV NS2B-NS3 protease. Kinetics assays are currently been performed to investigate the compound mechanism of inhibition.

References

1. Molin, M. et al. *Drug Discov. Today* (2018); 2. Cao-Lormeau, V. M. et al. *Lancet* (2016); 3. Cugia, F. R. et al. *Nature* (2016); 4. Ekins, S. et al. *PLOS Negl. Trop. Dis.* (2016)

Acknowledgments



Carlos A. L. Filgueiras

Origens da Química no Brasil



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#LatinXChemNanoMat NANO-111

Uso de Redes Metalorgânicas (MOF's) como um Eficiente Adsorvente de Chumbo na Água

Ivonne Valenzuela Jaramillo, PhD Student
Universidade Federal de Pernambuco (UFPE)



USO DE REDES METALORGÂNICAS (MOFs) COMO UM EFICIENTE ADSORVENTE DE CHUMBO NA ÁGUA

Valenzuela I. E.¹ e Paim A. P.²

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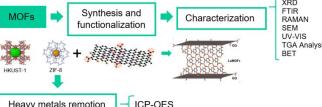
² Universidade Federal de Pernambuco, Recife/Pernambuco

INTRODUÇÃO

A superabundância de metais pesados em muitos processos industriais gera graves problemas de saúde e riscos para os seres humanos e outras formas de vida através da bioacumulação ao longo das cadeias alimentares.

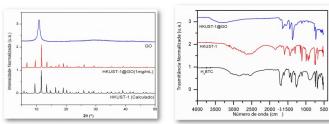
Neste trabalho sintetizamos uma nova rede metal-orgânica HKUST-1@GO para uso de suas propriedades de adsorção na área ambiental através da remoção de Pb(II) da água.

MATERIAL E MÉTODOS



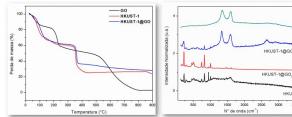
RESULTADOS E DISCUSSÃO

Figure 01: DRX e FTIR do HKUST-1@GO



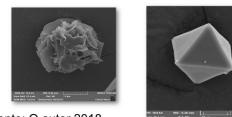
Fonte: O autor, 2018

Figura 02: Análise Termogravimétrica e Ramam do HKUST-1@GO



Fonte: O autor, 2018

Figura 03: MEV do HKUST-1 e HKUST-1@GO



Fonte: O autor 2018

Utilizando a técnica de ICP-OES determinou-se a porcentagem de remoção, em uma solução de 5 mg/L de Pb²⁺ e 10 mg de composto em pH: 5 durante 5h, resultando uma remediação de 93% do metal.

CONCLUSÃO

A rede metal-Orgânica HKUST-1@GO foi obtida pelo método solvothermal com uma estrutura bem definida e com alta capacidade de adsorção de Pb²⁺.

REFERÊNCIAS

- Kuen Song Ling, et al. ELSEVIER, International Journal of Hydrogen Energy, Volume 37, Issue 18, September 2012.
- Paulina A Kobielak, et al. ELSEVIER, Coordination Chemistry Reviews 358 (2018), Pages 92-107.
- LIN, K.; HSIEH, YT. Copper-based organic metal structure (MOF), HKUST-1, as an efficient adsorbent to remove p-nitrophenol from water. Journal of the Taiwan Institute of Chemical Engineers, v. 50, p. 223- 228, 2015.

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#LatinXChemEd ED-32

The Case of Sodium Carbonate Production in Europe as a Dialogue between History and Philosophy of Science and Interdisciplinarity in Science Education

Ivo Freitas, PhD Student, University of Campinas (UNICAMP)

The case of sodium carbonate production in Europe as a dialogue between History and Philosophy of Science and Interdisciplinarity in Science Education

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Background

Approaches of History and Philosophy of Science (HPS) in Science Education (SE) aim to present Science as a human and socially constructed activity.

Besides, we propose HPS to reveal the broad network of scientific knowledge, in which a given episode of Science is inserted, seeking to contribute to a more connected form of knowledge, one of the main criticism of theorists who advocate for interdisciplinarity in SE.

Through a hybrid research between the theoretical background of HPS, SE, and interdisciplinarity, using secondary sources of research, we analyzed the historical episode of sodium carbonate production in Europe, trying to reveal that historical episodes go beyond disciplinary boundaries and represent good options for interdisciplinarity in school education.

Aims

We aim to discuss how HPS can support thinking about interdisciplinarity through a given historical episode. We do not intend to present a work proposal for the classroom, but rather seek to point out that a historical episode of Science can only be understood in its complexity by approaching various disciplines for a more critical and more elaborate comprehension, without the typical fragmentation of school knowledge. From a less limited view of Science, we seek to discuss the potential of HPS to select, organize, and communicate scientific knowledge. This reflection can open possibilities to think SE in an interdisciplinary way.

Sodium carbonate production in Europe in the XVIII. century

Interdisciplinarity dialogues

Episode	Context	Dimensions	Disciplines	Concepts
Sodium carbonate production	Demand for artificial Na_2CO_3 ; French and Industrial Revolutions; deforestation; British blockade; pollution of rivers and lakes by ammonical waters from the lighting gas industries.	Scientific, technological, environmental, social, political and economic	Chemistry, Physics, Biology, History and Geography.	Interaction between matter and energy; separation and characterization of substances; environment pollution; carbon cycle and greenhouse effect; heat exchanges; polarization between British and French interests; French physiology; urbanization and demographic growth.

Conclusions

We believe that working with historical episodes of Science has the potential to encourage students to understand Science as a human and socially constructed activity, which is immersed in a network of complex contexts and interrelated dimensions that are found in a network of meanings, contributing to a less fragmented view of knowledge production and socialization. We tried to point out that a historical episode highlights scientific knowledge in a network. This fact can bring new perspectives to think about interdisciplinary teaching. As a result, interdisciplinarity cannot be solved alone, but we believe it provides an interesting reflection of its need and possibility.

References

Boltran, M.H.R. and Trindade, L.S.P. (2017). *História da Ciência e Ensino: Abordagens Interdisciplinares*. São Paulo: Editora Lítraria da Física.

Bonsaude-Vincent, B. and Stengers, I. (1996). *História da Química*. Lisboa: Instituto Pláget.

Thiesen, J.S. (2007). A interdisciplinaridade como um movimento de articulação no processo ensino-aprendizagem. *PerCurso*, 8 (1), 87-102.

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#LatinXChemPhys PHYS-05

Nanocristais de Celulose como Estabilizantes de Emulsões Água em Água

Maria Jackeline Rodrigues dos Santos,
Undergraduate, Universidade Federal do Paraná (UFPR)

NANOCRISTais DE CELULOSE COMO ESTABILIZANTES DE EMULSÕES ÁGUA EM ÁGUA

Maria Jackeline R. Santos, Cassiano Pires, Rilton Alves de Freitas.
Laboratório Biopol - Professora Maria Rita Sierakowski; Universidade Federal do Paraná; BRASIL
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Introdução

Emulsões água em água (a/a) podem ser formadas a partir de polímeros hidrofílicos, tais como xiloglucana (XG) e amilopectina (AMP), os quais possuem uma instabilidade termodinâmica entre si, o que conduz a umasseparação de fases.

Características:
Tensão interfacial (α/α) $< 10^{-2}$ mN/m
Estabilização: partículas na interface;
Aumento da viscosidade da fase contínua.

Metodologia

1º	2º	3º	4º
Síntese dos Nanocristais de celulose (NCC)	Caracterização NCC	Avaliação da emulsão	Reologia
1g Celulose microcristalina 50 mL de H ₂ O (0%) 88°C 1,5h	DRX em pó: Titulação condutivimétrica; ATM	Microscópico: Microscopia confocal à laser com aumento 60X; AMP-FTC, NCC-Acel do NiO. Avaliação por 48h 1,30% XG + 1,02% AMP variando a (%) NCC	curva de viscosidade (η) vs. taxa de círculoamento ($\dot{\gamma}$). Avaliação da XG pura; XG + NCC.

Resultados e Discussões

Síntese dos nanocristais

Celulose microcristalina → Hidrólise ácida → Nanocristais de celulose

Caracterização dos nanocristais

$\sigma_{\text{Sulfato}} = \frac{C_{\text{Sulfato}} \times V_{\text{NaOH}}}{m_{\text{NCC}}} = 94.2 \pm 2.7 \text{ mmol/kg}$
 $\%S = \text{Sulfato mm.} / 100 = 0.30 \pm 0.01 \%$

ESTABILIZAÇÃO DE EMULSÕES ÁGUA EM ÁGUA

Avaliação da emulsão

0h, 24h, 48h

Reologia

$\eta = 1.22 \text{ Pa.s}$ (NCC 0%)
 $\eta = 1.30 \text{ Pa.s}$ (AMP 1,02%)
 $\eta = 1.36 \text{ Pa.s}$ (AMP 1,30%)
 $\eta = 1.40 \text{ Pa.s}$ (NCC 1,02%)
 $\eta = 1.42 \text{ Pa.s}$ (NCC 1,30%)

Conclusão

Macroscopicamente, as emulsões mostraram-se estáveis em concentrações acima de 0,15% (m/m) nanocristais de celulose. Contudo, ensaios microscópicos não evidenciaram partículas na interface desses sistemas. Ensaios adicionais evidenciaram um aumento de viscosidade da fase contínua (XG), o que indica uma estabilização das emulsões por efeito de depleção.

Referências

BECK ET AL. Cellulose, v. 22, n. 1, p. 101–116, 2015.
BEIJERINCK, M.W.; ET AL. II Natur. 1896, 627, 698.
HAZI, B.; ET AL. Food Hydrocolloids, vol. 104, 105769, 2020.
FRENCH, Alfred D. Cellulose, v. 21, n. 2, p. 885–896, 2014.

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#LatinXChemAnalytical AC-16

3D-printed Electrochemical Sensors Applied for Biomarkers Detection in Biological Samples

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Cristiane Kalinke, Postdoctoral Researcher, University of Campinas (UNICAMP), Brazil

AC16

3D-PRINTED ELECTROCHEMICAL SENSORS APPLIED FOR BIOMARKERS DETECTION IN BIOLOGICAL SAMPLES

Cristiane Kalinke^a, Naile V. Neumstein^a, Paulo Roberto de Oliveira^b, Bruno C. Janegitz^b, Juliano A. Bonacini^a.

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^b Department of Chemistry, Federal University of São Carlos, Araras-SP, Brazil.
**cristiane.kalinka@gmail.com / @cristinkalinka*

INTRODUCTION

3D-Printing Technology + Electrochemical Techniques → Development of lab-made, versatile, portable and low-cost electrochemical sensors for the detection of biomarkers in biological samples.

PLA-Graphene filament → Chemical Activation → PLA removal → Functionalization → Electrochemical Activation

EXPERIMENTAL

- 3D PLA-G electrodes activation
- Electrochemical measurements

Dopamine
L-methionine
Serum samples

1.0 mol L⁻¹ NaOH 30 min
PBS pH 7.4

RESULTS

Electrodes Characterization

Pristine
NaOH+EC

Dopamine Detection

A: CV of NaOH+EC, NaOH, PLA-G in presence of dopamine. B: Amperometric response of dopamine at NaOH+EC, NaOH, PLA-G.

L-methionine Detection

C: CV of NaOH+EC, NaOH, PLA-G in presence of L-methionine. D: Amperometric response of L-methionine at NaOH+EC, NaOH, PLA-G.

Fig. 1. SEM images obtained before and after NaOH+EC activation.

Fig. 2. Voltammetric results obtained for PLA-G_{NaOH+EC} in presence of dopamine and L-methionine.

Table 1. Results obtained before and after activation treatments.

	3D PLA-G electrode	I _p /I _c	k _{ads} (cm s ⁻¹)	θ _{edge} (%)	Ae (cm ²)
Pristine	0.634	2.73 × 10 ⁻⁴	0.068	0.020	
NaOH	0.489	9.34 × 10 ⁻⁴	0.233	0.882	
NaOH+EC	0.852	1.11 × 10 ⁻³	0.276	3.19	

RESULTS

Electrodes Characterization

3D PLA-G electrode → I_p/I_c → k_{ads} (cm s⁻¹) → θ_{edge} (%) → Ae (cm²)

CONCLUSIONS

- ✓ Improvement of the electrochemical response, electron transfer rate and electroactive area, associated to the increase of edge sites and defects after 3D PLA-G activation treatments;
- ✓ Good analytical performance for biomarkers detection in serum samples, allowing the diagnosis of neurological problems or diseases.

ACKNOWLEDGMENT

JAPESP grant 2018/00473-2

REFERENCES

Cardoso, R. M. et al. *Anal. Chim. Acta*, 1118, p.73-91, 2020.
Santos, P. L. et al. *Sens. Actuators B Chem.*, 281, p.837-848, 2019.
Kalinka, C. et al. *Analyst*, 145, p.1207-1218, 2020.

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Fábio Rodrigo Piovezani Rocha

Métodos de
PREPARO DE AMOSTRAS
Para Análise Elementar



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#LatinXChemOrg OC-19

Biocatalysis: Asymmetric Synthesis of Pyrrolidine Alkaloids

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(UNICAMP)

Biocatalysis: Asymmetric synthesis of pyrrolizidine alkaloids

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Introduction

Biocatalytic reactions have been developed to make organic synthesis more efficient and environment friendly. Several authors have highlighted the application of enzymes^{1,2} or cells as catalysts (Scheme 1), reduction of steps like separation, and purification of intermediates. In addition, enzymes, stereoselectivity, and regioselectivity are used to produce products with high enantiomeric purity, which is important since the chiral centers, generally, define the biological activities of the alkaloids. In this context, we proposed the synthesis of pyrrolidine scaffolds by multi-enzymatic cascade reaction using transaminases (TA) and amino reductases (IRED), as shown in Scheme 2.

Scheme 1: Graphical abstract of general biocatalysis reaction.

Objectives

- Synthesize carbonyl compounds **Ia** and **Ib**, which are used as substrates.
- Perform the asymmetric synthesis of pyrroline **IIa** and **IIb**, involving stereoselective commercial enzymes from 24 different companies.
- Assess the stereoselectivity and regioselectivity of 24 commercial TAs in order to optimize the biocatalytic reaction.
- Assess the asymmetric synthesis of pyrrolidine alkaloids by "one-pot" chemoenzymatic process.

Methods

The synthesis of **Ia** and **Ib** (Scheme 3a) were performed in two stages: i) reduction of furan 2 and other furan 2-ethyl vinyl ketone 1. ii) furan sulfone an oxidation step using oxygenated reagents. The substrates were characterized by NMR, MS, IR. The biocatalytic process was performed by the following reaction condition: 2 mg/ml of TA, 10 mM of substrate (10% DMSO), 100 mM of alamine, 1 mM of PLP 0.5 mg/ml, LDH (lactate dehydrogenase), 100 mM of glucose, 1 mg/ml of GDH (glucose dehydrogenase), 200 mM Tris HCl, pH = 30 °C 200 rpm, 24 h. The enantiomeric discrimination was performed by GC-FID using CP-Chirasil-DEX CB column.

Results and discussion

The regioselectivity of 24 commercial transaminases was evaluated. Thus, conversion percentages of substrate **Ia** and enantiomeric excess (ee) were calculated according to the analysis of chromatograms obtained by the GC-FID analyses (Scheme 4). As a result, for substrate **Ia** (*R*-PLP)-ATA-P-001 (ATA-P-001) and (*S*-PLP)-ATA-P-001 (ATA-P-001) and (*S*)-selective ATA (ATA-237) were able to produce 90% of conversion and enantiomeric excess. It was observed that ATA-234 and ATA-P-003 yielded opposite enantiomers.

Scheme 2: Proposed synthesis of pyrrolidine scaffolds by TA and IRED.

Scheme 3: (a) Synthesis of substrate **Ia and **Ib** and (b) Biocatalysis of substrates.**

Scheme 4: Chromatograms obtained by GC-MS of (a) Substrate **Ia (b) Enzymatic reaction of **Ia** and ATA-P-001 (c) Mass spectrum of pyrroline **IIa**.**

Scheme 5: Chromatograms obtained by GC-FID (a) Racemic mixture, (b) (*D*)-IIa** (c) (*S*)-**IIa**.**

Scheme 6: TA-mediated conversion of **Ia into 2,5-disubstituted pyrrolines **IIa**.**

Scheme 7: Chemoenzymatic synthesis of pyrrolidine alkaloids by transamination and NH₂H.

Conclusions

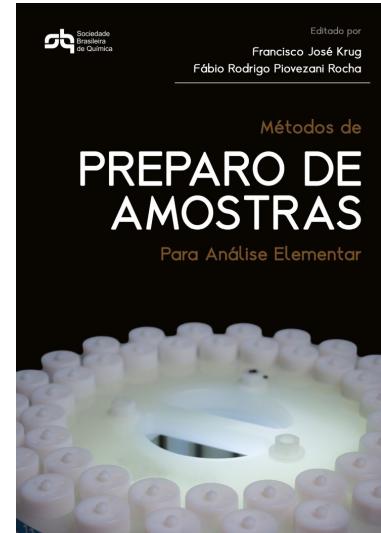
Pyrrolines were produced from a furan derived carbonyl compounds mediated by 4 commercial transaminases with excellent stereo- and regioselectivity. These carbonyl compounds will be submitted to multi-enzymatic cascade reactions, with IRED in order to generate the enantioenriched pyrrolidine alkaloids **IIIa,b** after a spontaneous second cyclization (Scheme 2). These results are the driving force to the multi-enzymatic cascade process involving TA and IRED.

References

1. Ryan, J.; Sautelius, M.; Grimm, A.; Mack, B.; O'Reilly, E.; Capri, V. *J. Am. Chem. Soc.* **2016**, *138*, 15798.
2. Costa, B. Z.; Gelman, J. L.; Silvia, I.; France, S. P.; Marsaioli, A. J.; Turner, N. J. *ChemCatChem* **2018**, *10*, 4733.

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