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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

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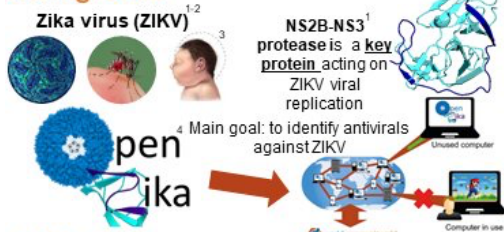
OpenZika: an open science collaboration project enables the discovery of a potent NS3 protease inhibitor as new antiviral candidate against Zika Virus



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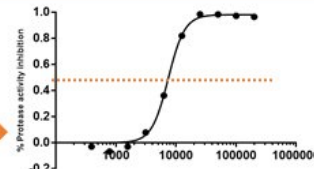
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Background

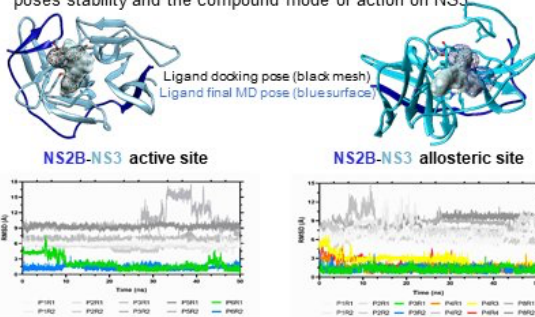
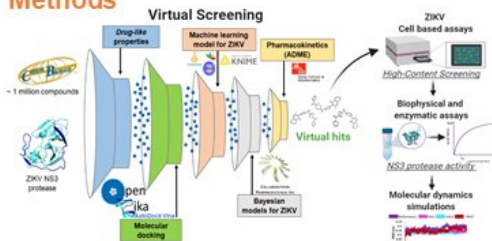


Results

- ✓ 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 ± 0.3 μ M, EC_{50} 6.68 μ M and low cytotoxicity.
- ✓ Molecular dynamics (MD) simulations investigated docking poses stability and the compound mode of action on NS3



Methods



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 being performed to investigate the compound mechanism of inhibition.

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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

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Universidade Federal de Pernambuco (UFPE)



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

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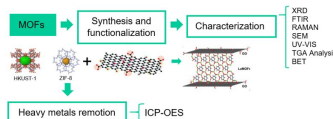
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INTRODUÇÃO

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.

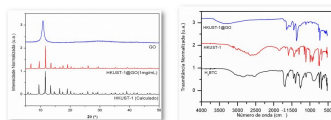
Neste trabalho sintetizamos uma nova rede metal-orgânica HKUST-1@GO para uso de suas propriedades de adsorção na área ambiental através da remoção de Pb(II) da água.

MATERIAL E MÉTODOS



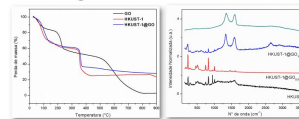
RESULTADOS E DISCUSSÃO

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



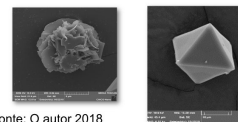
Fonte: O autor, 2018

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 determinouse 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 solvotermal com uma estrutura bem definida e com alta capacidade de adsorção de Pb²⁺.

REFERÊNCIAS

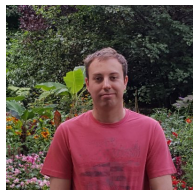
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#LatinXChemEd ED-32

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

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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.

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 ammoniacal 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 and Industrial Revolutions; plant 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 interdisciplinarity teaching. As a result, interdisciplinarity cannot be solved alone, but we believe it provides an interesting reflection of its need and possibility.

Sodium carbonate production in Europe in the XVIII. century

Innovations: Lead chamber Limestone use thanks to Deforestation French Revolution Urbanization Maritime Blocking created Troubled diplomatic relations Industrial Revolution provided Foreigner dependence which had Competition with natural Na_2CO_3 ; *Salicornia, Sarcosium*, kelp led to Demand for artificial Na_2CO_3 reflected in the industries to supply Industries: Soap Glass Paper Textile integrating a Industrial complex

Leblanc process led to Demand for artificial Na_2CO_3

represented by $2 \text{NaCl} + \text{H}_2\text{SO}_4 = \text{Na}_2\text{SO}_4 + 2 \text{HCl}$
 $\text{Na}_2\text{SO}_4 + \text{CaCO}_3 + 2 \text{C} = \text{Na}_2\text{CO}_3 + \text{CaS} + 2 \text{CO}_2$

produced in Na_2CO_3 factories created HCl environmental problems CO_2 production Sulfur contamination Harmful by-products: inhabitants, plantations and cattle

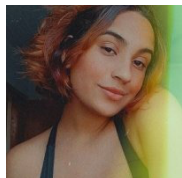
generating the need and opportunity to use the by-products in other factories, integrating a true

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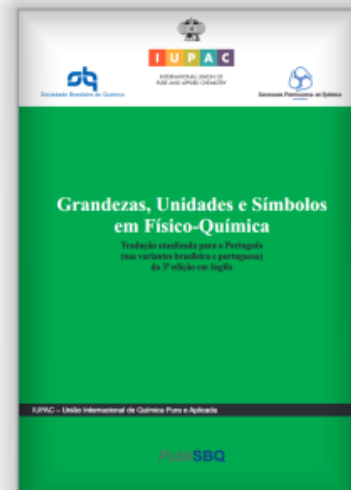
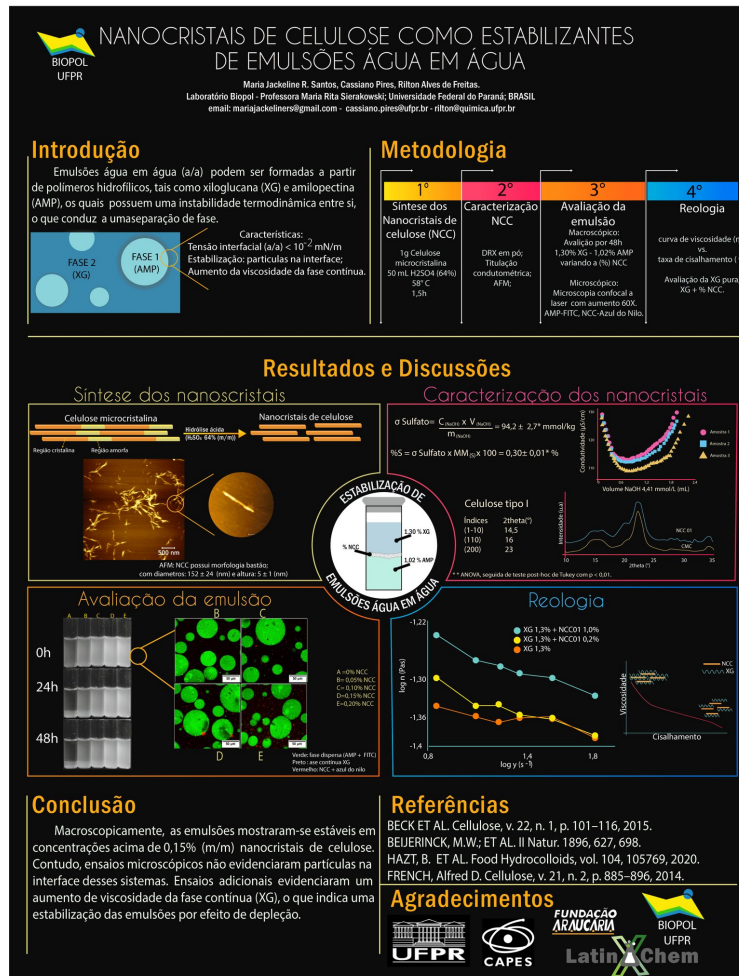
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#LatinXChemPhys PHYS-05

Nanocristais de Celulose como Estabilizantes de Emulsões Água em Água

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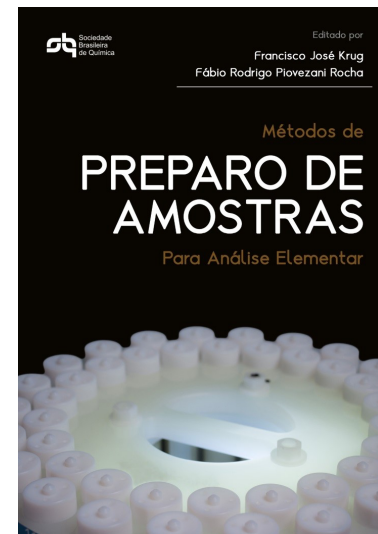
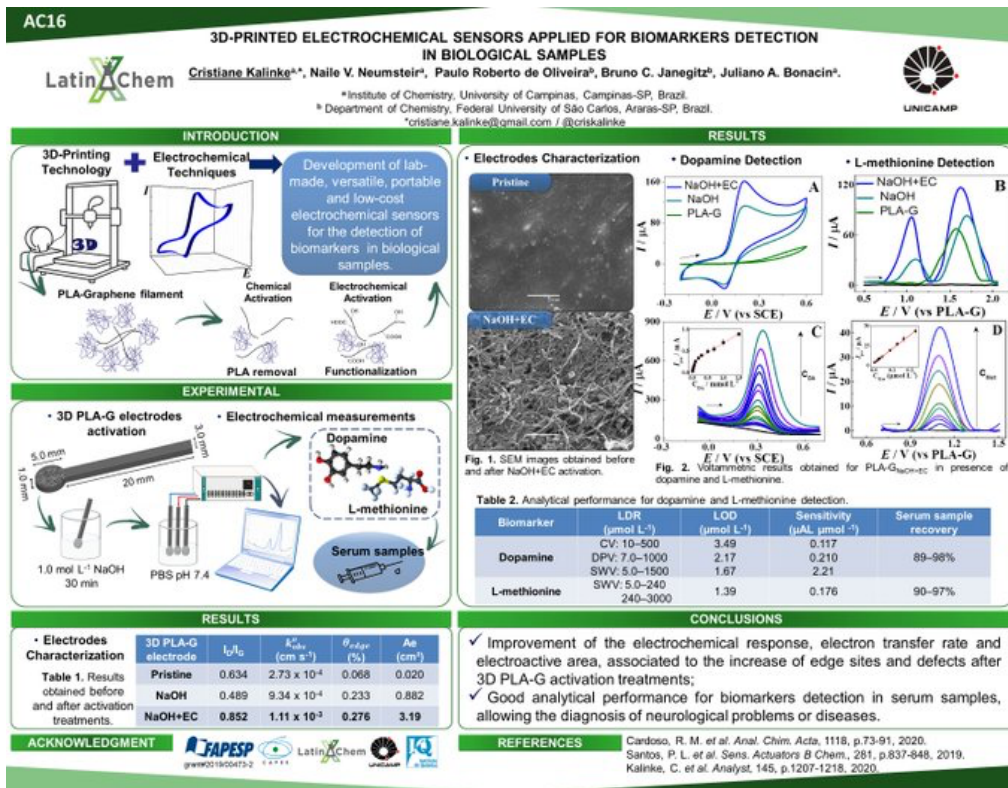


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#LatinXChemAnalytical AC-16

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

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



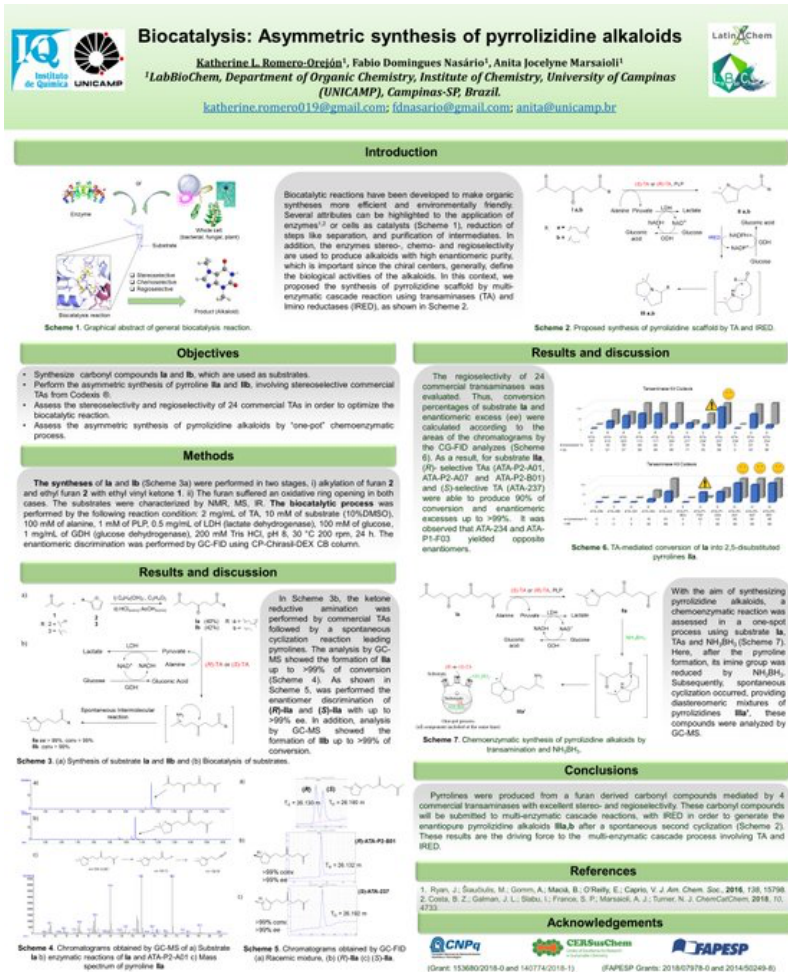
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#LatinXChemOrg OC-19

Biocatalysis: Asymmetric Synthesis of Pyrroline Alkaloids

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Métodos de

PREPARO DE AMOSTRAS

Para Análise Elementar

