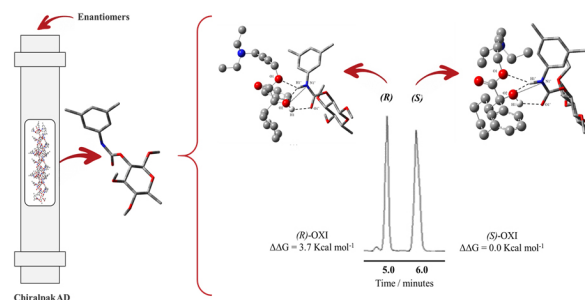


Artigos/Articles

- 263 Separação enantiosseletiva da oxibutinina: uma investigação teórica e experimental

Lilian C. Zin, Camilla F. Silva, Luciana Guimarães, Keyller B. Borges e Clebio S. Nascimento Jr.

<http://dx.doi.org/10.21577/0100-4042.20170815>



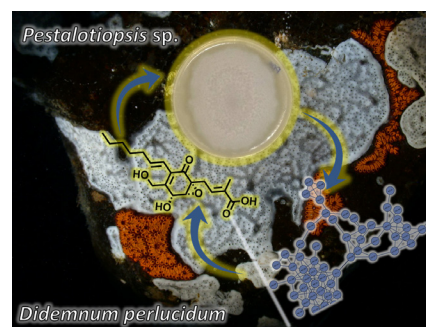
Enantioselective separation of oxybutynin studied by HPLC and DFT calculations.

- 268 Molecular networking-based dereplication of ambuic acid derivatives from the marine fungus *Pestalotiopsis* sp. 4A11

Luis C. Kellner Filho, Rhenner N. A. Assis, Aline O. dos Santos, Sabrina K. Targanski, Kátia A. Siqueira, Livia S. de Medeiros, Célio F. F. Angolini, Felipe M. A. da Silva, Marcos A. Soares, Gustavo M. Dias, Marcio L. A. Silva, Wilson R. Cunha, Patricia M. Pauletti, Hector H. F. Koolen and Ana H. Januario

<http://dx.doi.org/10.21577/0100-4042.20170819>

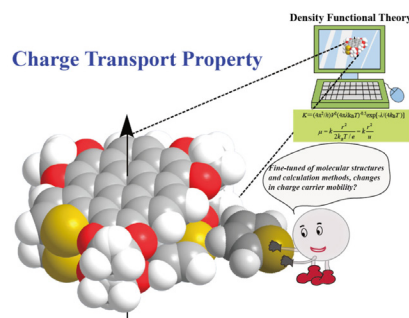
The marine fungus *Pestalotiopsis* sp. 4A11, isolated from the ascidian *Didemnum perlucidum* after cultivation in solid medium, produced ambuic acid and 10 other derivatives, which were dereplicated using LC-MS/MS-based molecular networking.



- 275 Theoretical investigation of the effect of conjugation of thiophene rings on the charge transport of thienocoronene derivatives

Ziran Chen, Yujin Zhang, Zhanrong He, Yuan Li, Meihao Xia and Wenhao Yu

<http://dx.doi.org/10.21577/0100-4042.20170820>

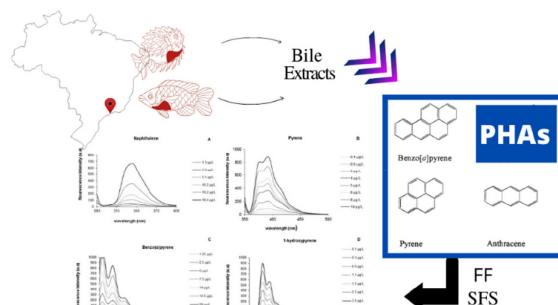


Quantum chemical calculations of the charge-transport rates were performed for five derivatives of 1,2,5,6,9,10-hexa(methoxy)coronene with varying numbers of thiophene rings, using different basis sets and hybrid functionals.

- 283 Biliary PAH metabolites in fish from the highly impacted Guanabara Bay, in southeastern Brazil, determined by fixed and synchronous fluorescence spectroscopy

Marina M. Freire, Cristina Gómez, Anabela S. Oliveira, Josino C. Moreira and Ana Rosa L. Arias

<http://dx.doi.org/10.21577/0100-4042.20170823>

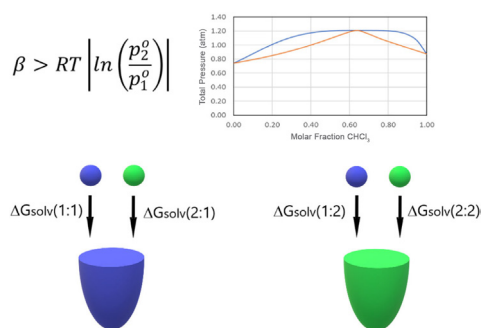


The analysis of fish bile extracts for PHA derivatives using fixed and synchronous fluorescence spectroscopy could help determine exposure to contaminated waters.

- 292 Formação de azeótropos do ponto de vista da termodinâmica de solvatação

Josefredo R. Pliego Jr.

<http://dx.doi.org/10.21577/0100-4042.20170824>

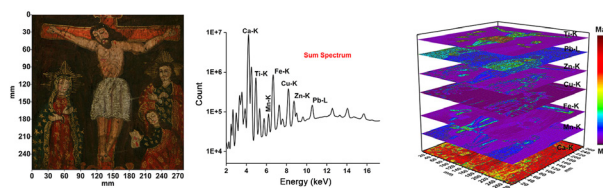


The formation of azeotrope is interpreted in terms of the relative solvation free energy in the pure liquid and its diluted solution in the other component.

- 297 Exemplificando o uso do macro mapeamento elementar por XRF (MA-XRF) na investigação forense de obras de arte

André R. Pimenta, Valter S. Felix, Daniele M. Silva, Marcelo O. Pereira, Ana L. Oliveira, Douglas S. Ferreira, Cristiano S. Carvalho, Fabricio L. Silva, Elicardo A.S. Gonçalves, Rafael S. Dutra, Leandro O. Pereira, Ronaldo V. Pereira e Renato P. Freitas

<http://dx.doi.org/10.21577/0100-4042.20170826>



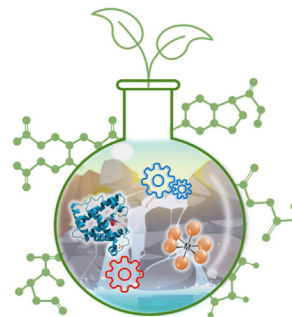
The macro multi-element mapping b XRF technique allows performing images about the distribution of elements present in a sample. In artworks, these elemental mappings are related to the pigments present on the canvases. Therefore, images enable the investigation of the creative process of the artworks and also are useful in the forensic study of canvases.

Revisão/Review

- 304 Reações em cascata enzimática, quimioenzimática e fotoenzimática: perspectivas para uma síntese orgânica mais sustentável

Shirley A. Castilho, Humberto M. S. Milagre e Cintia D. F. Milagre

<http://dx.doi.org/10.21577/0100-4042.20170829>

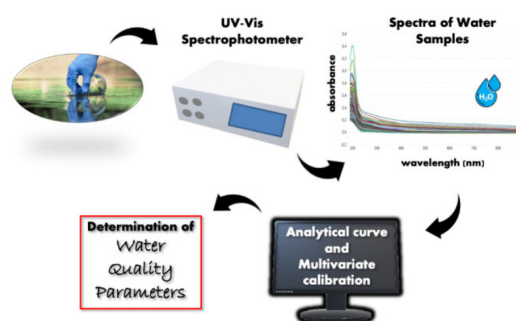


Pot-economy, step-economy and atom-economy are key issues that can be addressed by enzymatic cascade reactions, an efficient and sustainable approach in synthetic organic chemistry.

- 314 Avanços analíticos baseados em modelos de calibração de primeira ordem e espectroscopia UV-VIS para avaliação da qualidade da água: uma revisão - parte 1

Grazielle R. Santos, Gabriela S. P. Paulino, Grazielle P. I. Borges, Aníbal F. Santiago e Gilmare A. da Silva

<http://dx.doi.org/10.21577/0100-4042.20170830>



Use of ultraviolet-visible (UV-Vis) spectrophotometry and calibration methods for determination of water quality parameters.

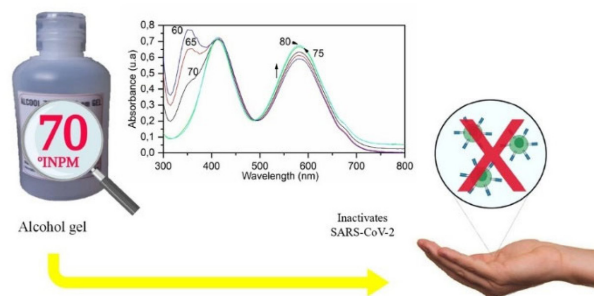
Nota Técnica/Technical Notes

- 324 Álcool em gel para assepsia das mãos – formulação adequada e eficiência garantida em meio à pandemia da COVID-19

Kleber Q. Ferreira, Isabel C. Rigoli, Marcus V. S. da Silva, Alexandre de F. Espeleta e Zênis N. da Rocha

<http://dx.doi.org/10.21577/0100-4042.20170831>

“A good looking” alcohol gel containing ethanol less than 68.25 %INPM may trick the customer. However, it does not trick the coronavirus, with remains active. This is worrying fact amidst COVID-19 crisis.



Educação/Education

- 335 O químico e o meio ambiente: aspectos históricos e as contribuições do ensino de gestão ambiental

Suellen A. Alves

<http://dx.doi.org/10.21577/0100-4042.20170837>

Environmental management is essential nowadays for any productive sector. In this sense, teaching environmental management and disciplines that encourage sustainable thinking and clean practices in undergraduate courses in Bachelor of Chemistry is necessary.

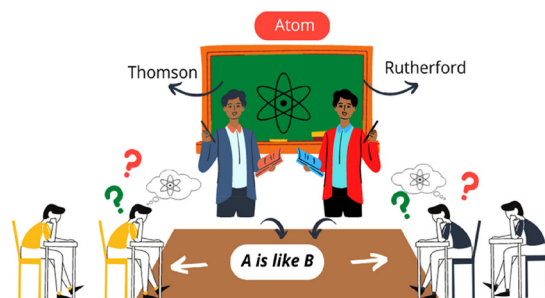


- 345 Usando analogias para lecionar sobre o átomo nas aulas de química geral no ensino superior

José Arão, Laurinda Leite e Emília Nhalevilo

<http://dx.doi.org/10.21577/0100-4042.20170845>

Analogies are comparisons between two knowledge domains: a familiar domain and an unknown or inaccessible one. They are twofold educational tools as they may help you to think and to visualize scientific entities, like the atom, and may cause unintended understandings.



Assuntos Gerais/General Subject

- 355 Análises de amostras ambientais para fins de salvaguardas nucleares no Brasil

Carina C. Lisbôa, Olívio P. de Oliveira Júnior e Delvonei A. de Andrade

<http://dx.doi.org/10.21577/0100-4042.20170839>

Through a simple kit containing clean swipe cloths, plastic bags, gloves, forms, a pen, labels and a roll of aluminum foil (used to establish a clean working surface) is possible to collect environmental samples in nuclear facilities and obtain essential data for nuclear safeguards.



