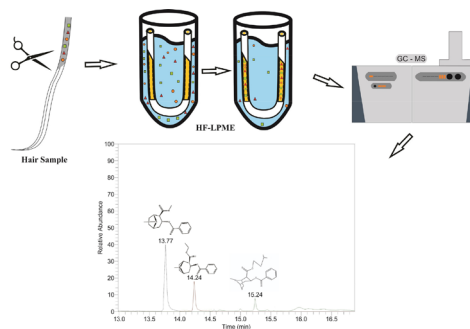


- 921 Highly selective HF-LPME-GC-MS for cocaine and biotransformation products in human hair to monitor drug addicts

Deborah T. P. Scanferla, Jessica Y. Sakurada, Luís O. de Oliveira, Renata S. Lini, Raul G. Agüera, Mariana A. O. Madia, Paula P. Moreira, Jessica C. Z. Romoli, Érika Bando, Miguel Machinski Junior, Camila Marchioni and Simone A. G. Mossini

<http://dx.doi.org/10.21577/0100-4042.20170737>

A hair segment was incubated with methanol and the analytes were extracted from the solution through a porous hollow fiber, by Liquid Phase Microextraction (HF-LPME). The extract was analysis in Gas Chromatography - Mass Spectrometry (GC-MS).

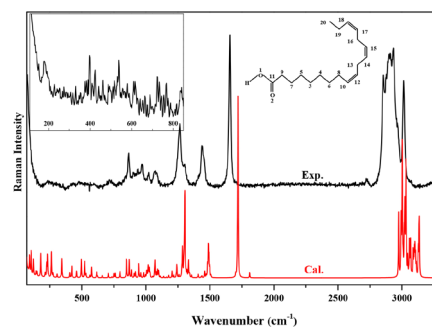


- 929 DFT calculation and Raman spectroscopy studies of α -linolenic acid

Heng Peng, Hua-Yi Hou and Xiang-Bai Chen

<http://dx.doi.org/10.21577/0100-4042.20170749>

The experimental and calculated Raman spectra of α -linolenic acid are in excellent agreement in the whole spectral range of 100-3500 cm^{-1} , and a complete vibrational modes assignment of the experimentally observed Raman peaks can be obtained basing on the DFT calculation.

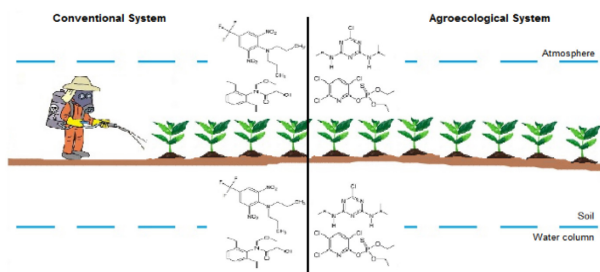


- 936 Avaliação de agrotóxicos em solo de sistemas de produção agrícola convencional e agroecológico

Fernanda G. Morro e Danielle C. Schnitzler

<http://dx.doi.org/10.21577/0100-4042.20170763>

The Graphical Abstract represents two cultivation systems, the conventional and the agroecological, which are located close to each other. Due to the application of agrochemicals in the conventional system, it is possible that they will move between environmental interfaces.

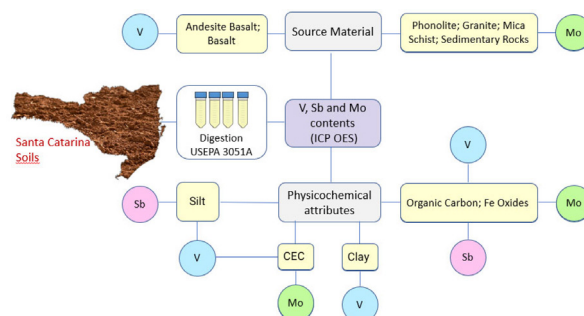


- 947 Teores de vanádio, molibdênio e antimônio em solos de diferentes litologias em Santa Catarina

Ilana M. Suppi, Mari L. Campos, David J. Miquelluti e Matheus R. Machado

<http://dx.doi.org/10.21577/0100-4042.20170768>

The analysis of vanadium, molybdenum, and antimony contents in soils without anthropic contamination of Santa Catarina state has demonstrated of these levels can be related with source material, as well with physicochemical attributes of soils.

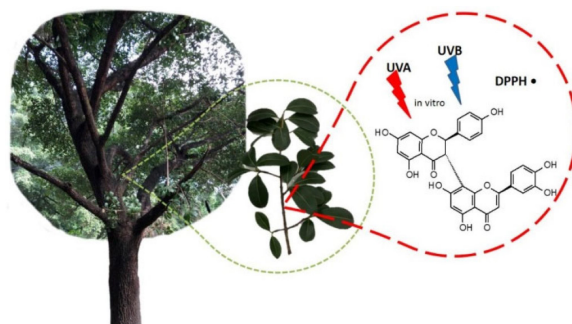


- 954 Composição química e atividades fotoprotetora e antiradicalar *in vitro* dos galhos de *Platonia insignis* (Clusiaceae)

Andréia G. A. Silva, Rodrigo de A. Moreira, Renato P. de Sousa, Evaldo dos S. M. Filho, Marcia D. A. Veras, Mariana H. Chaves e Sâmia D. L. Freitas

<http://dx.doi.org/10.21577/0100-4042.20170761>

The chemical study of the branches of *Platonia insignis* enabled the isolation of the biflavonoid morelloflavone and the identification of over 9 polyphenols. *In vitro* biological tests of solar photoprotection and antiradical activities against the crude extract and Hex and AcOEt fractions showed relevant results, which confirm the high pharmaceutical potential of the species.



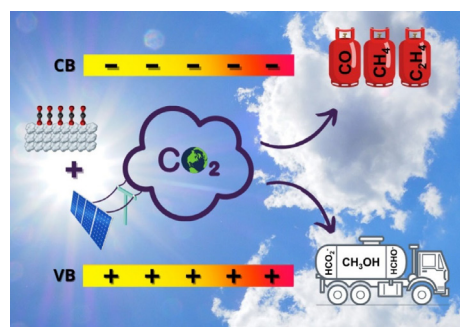
Revisão/Review

- 963 Redução de CO₂ em hidrocarbonetos e oxigenados: fundamentos, estratégias e desafios

Gelson T. S. T. da Silva, Osmando F. Lopes, Eduardo H. Dias, Juliana A. Torres, André E. Nogueira, Leandro A. Faustino, Fernando S. Prado, Antônio O. T. Patrocínio e Caue Ribeiro

<http://dx.doi.org/10.21577/0100-4042.20170745>

The image shows the use of electrical and light-activated catalysts, as well as the combine energy in the process for CO₂ reduction into some liquid and gas products.

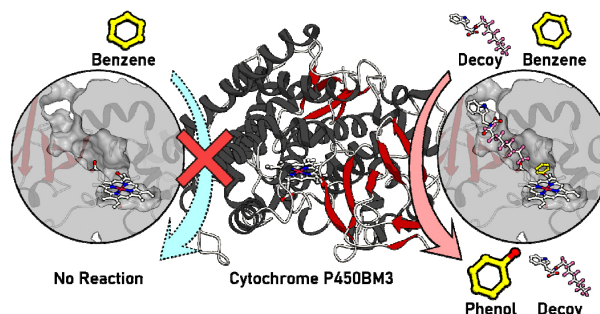


- 982 Enganando o citocromo P450BM3: catálise de várias transformações de substratos não nativos usando moléculas-traíçoeriras

Joshua K. Stanfield, Kazuto Suzuki, Kai Yonemura, Talita Malewschik e Osami Shoji

<http://dx.doi.org/10.21577/0100-4042.20170747>

Cytochrome P450BM3 is a highly selective enzyme that, barring extensive engineering, will not hydroxylate non-native substrates, such as benzene. However, upon the simple addition of a native substrate mimic (decoy molecule), P450BM3 can be “tricked” into hydroxylating non-native substrates.

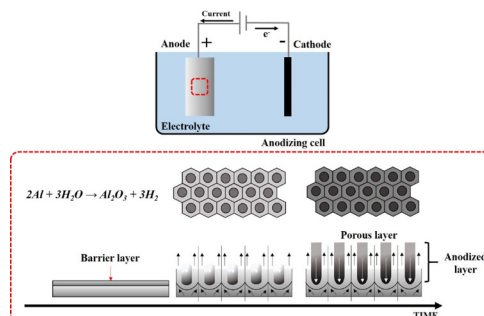


- 999 O processo de anodização do alumínio e suas ligas: uma abordagem histórica e eletroquímica

João V. de S. Araujo, Rejane M. P. da Silva, Rafael E. Klumpp e Isolda Costa

<http://dx.doi.org/10.21577/0100-4042.20170748>

Aluminum anodizing process and the formation of the anodized layer as a function of time.

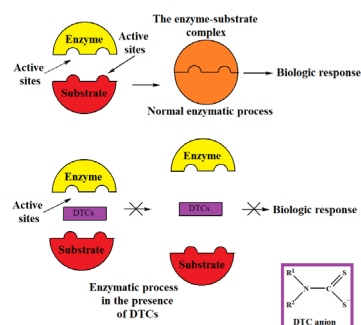


- 1012 Aspectos gerais da química dos ditiocarbamatos e de seus complexos metálicos e interações dessas espécies químicas com importantes enzimas – uma breve revisão

Daniele C. Menezes e Geraldo M. de Lima

<http://dx.doi.org/10.21577/0100-4042.20170755>

Dithiocarbamates (DTC) are ligands well explored in coordination chemistry. A number of works also report how some biologic processes behave in the presence of DTC-bearing complexes. These studies show that DTCs deactivate important enzymes.



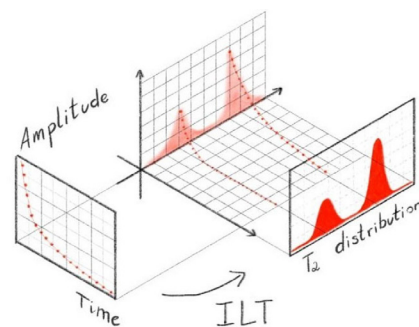
Nota Técnica/Technical Notes

- 1020 Transformada Inversa de Laplace para análise de sinais de ressonância magnética nuclear de baixo campo

Tiago B. Moraes

<http://dx.doi.org/10.21577/0100-4042.20170751>

Applying Inverse Laplace Transform (ILT) to process a Time-Domain NMR signal for the obtention of the distribution of relaxation times.

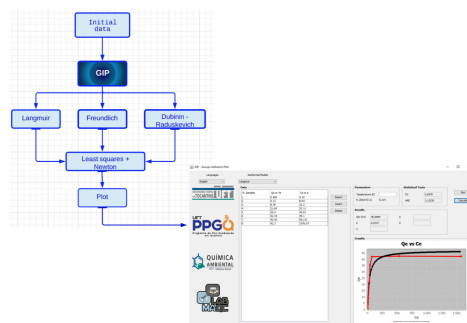


- 1028 Gurupi isotherms plot (GIP): uma ferramenta com interface gráfica intuitiva e gratuita como alternativa para o cálculo de parâmetros de isoterma de adsorção

Douglas A. Castro, Mateus P. S. Milhomem, Douglas H. Pereira e Paulo V. B. Leal

<http://dx.doi.org/10.21577/0100-4042.20170752>

Gurupi Isotherms Plot (GIP) is a new free software, has a friendly graphical interface and that uses the minimum squares and Newton method to calculate adsorption isotherm parameters with precision and fast performance.



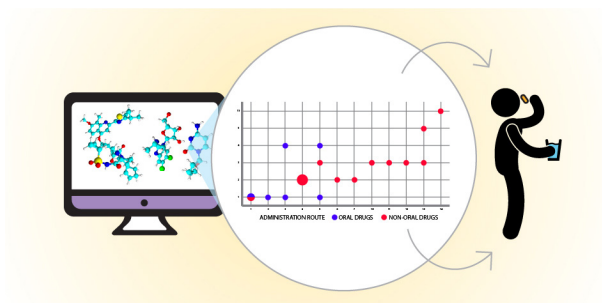
Educação/Education

- 1036 O uso de softwares livres em aula prática sobre filtros moleculares de biodisponibilidade oral de fármacos

Gabriela dos S. Rodrigues, Júnior A. Avelino, Ariane L. N. Siqueira, Luciana F. P. Ramos e Gabriela B. dos Santos

<http://dx.doi.org/10.21577/0100-4042.20170739>

A novel teaching methodology to show the importance of the physical chemical properties for the oral bioavailability of drugs.



1045 Simetria molecular e reações de dessimetrização em síntese orgânica

Bruno M. Paz, Emilio C. de Lucca Júnior e Ronaldo A. Pilli

<http://dx.doi.org/10.21577/0100-4042.20170760>

Ubiquitous in Nature, symmetry is a pervasive concept as it encompasses creativity in Arts and Science. The GA illustrates a C₂-symmetric musical piece, known as Der Spiegel, designed to be played simultaneously by two violinists, one facing each other, and both reading from the same score but from opposite sides with one starting from the beginning and the other from the end resulting in a coherent play. Taking the planning of a synthesis as a parallel to the process of composing a symphony, the recognition of symmetry in a target can be seen as the synthetic equivalent to writing a mirrored music score.



1078 Coverage of intermolecular forces in organic chemistry textbooks

José N. da Silva Júnior, José M. de S. Oliveira, Francisco S. O. Alexandre and Antonio J. M. Leite Junior

<http://dx.doi.org/10.21577/0100-4042.20170766>

The paper analyzes fifteen organic chemistry textbooks commonly used in Brazilian universities to examine intermolecular forces' coverage in them.



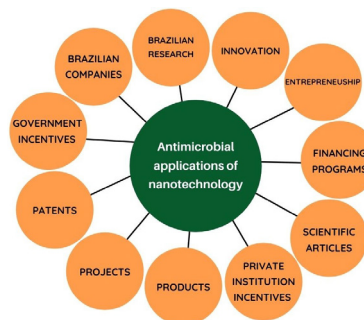
Assuntos Gerais/General Subject

1084 A nanotecnologia no Brasil e o desenvolvimento de produtos com atividade antimicrobiana

Bruna de P. Dias, Erica M. de C. Ribeiro, Ricardo L. Gonçalves, Diego S. Oliveira, Tiago H. Ferreira e Breno de M. Silva

<http://dx.doi.org/10.21577/0100-4042.20170743>

The use of nanotechnology rushes the development of new products and applications for microbial control and lever the country's entrepreneurship, innovation, research, and economy.



1093 O jardim venenoso: a química por trás das intoxicações domésticas por plantas ornamentais

Ana T. C. Aguiar e Valdir F. da Veiga Júnior

<http://dx.doi.org/10.21577/0100-4042.20170746>

Several ornamental plants are potentially dangerous to humans and animals due to the presence of various toxins. Children from 0 to 14 years old are the main victims of the intoxication cases (two thirds), mainly related to calcium oxalate, terpenes, alkaloids and glycosides.

