

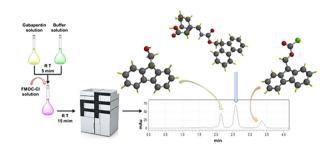
Volume 44, Número 5, 2021

Artigo/Article

543 Studies using HPLC-PDA in gabapentin N-derivatization reactions with 9-fluorenylmethyl chloroformate (FMOC-Cl) Emanoel Hottes, Carla R. G. R. Santos, Heloisa J. M. de Souza, Marco E. F. Lima e Rosane N. Castro

http://dx.doi.org/10.21577/0100-4042.20170719

FMOC-OH is a degradation product of the derivatizing agent FMOC-Cl, which is widely used as N-protecting group of amino acids and related molecules, such as gabapentin. The formation of FMOC-OH is conditioned to the pH of the reaction medium. The results obtained allowed the optimization of the gabapentin derivatization reaction with FOMOC-Cl through the analysis of the products obtained by HPLC-PDA.

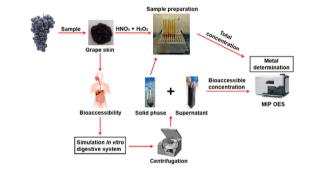


547 Avaliação da concentração total e da fração bioacessível de metais em amostras de casca de uva de cultivares Tannat e Cabernet Sauvignon por MIP OES

> Bruno Jacobs, Daisa H. Bonemann, Camila C. Pereira, Alexander O. de Souza, Ana C. B. Luckow, Meibel T. Lisboa, Anderson S. Ribeiro, Solange Cadore e Adriane M. Nunes

http://dx.doi.org/10.21577/0100-4042.20170709

This study aims a better elemental characterization of grape skin samples based on the determination of the total concentration and the bioaccessible fraction of metals by MIP OES.

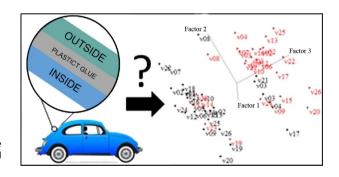


553 Vidros automobilísticos como vestígios de cena de crime: uma abordagem multivariada

Caio H. P. Rodrigues e Aline T. Bruni

http://dx.doi.org/10.21577/0100-4042.20170720

This work discusses automotive glasses as evidence in traffic forensic analysis. Chemometrics was used to evaluate Energy Dispersive X-ray Fluorescence data for different oxides concentrations according to the glasses' internal and external faces.

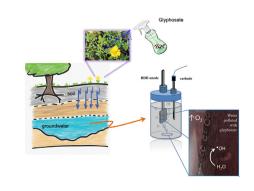


561 Oxidação anódica para descontaminação de um efluente contaminado com o herbicida glifosato utilizando anodo de diamante dopado com boro

Maycon D. de Lima, Ana S. Fajardo, Elaine C. de M. Santos, Aline M. Sales-Solano, Djalma R. da Silva e Carlos A. Martínez-Huitle

http://dx.doi.org/10.21577/0100-4042.20170715

Boron-doped diamond electrodes can be used as a potential tool for environmental applications by employing an electrochemical cell to eliminate the organic pollutants from wastewater with electrogenerated oxidants.

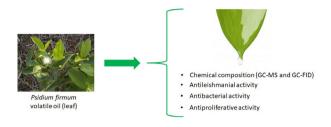


iv Quim. Nova

570 First report on chemical composition and biological properties of volatile oil from *Psidium firmum* O. Berg leaves Cassia C. Fernandes, Pietro Chrystal, Alexandra C. Pereira, Ana C. Colli, Livia Stenico, Arthur B. Ribeiro, Iara S. Squarisi, Ana C. B. B. Candido, Denise C. Tavares, Lizandra G. Magalhães, Antônio E. M. Crotti, Carlos H. G. Martins and Mayker L. D. Miranda

http://dx.doi.org/10.21577/0100-4042.20170710

Findings provided strong evidence of the promising potential of volatile oil from *Psidium firmum* fresh leaves as a nature-based antileishmanial, antibacterial and antiproliferative agent.



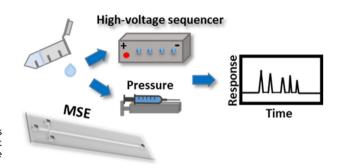
Revisão/Review

575 Métodos de injeção da amostra em microssistemas eletroforéticos

Kemilly M. P. Pinheiro, Kariolanda C. A. Rezende e Wendell K. T. Coltro

http://dx.doi.org/10.21577/0100-4042.20170700

One of the major challenges related to electrophoresis microsystems refers to the sample injection mode. In this way, this review covers the different electrokinetic and hydrodynamic approaches aiming to provide a complete overview for the readers.

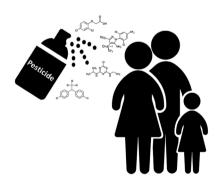


584 A química na avaliação do impacto à saúde humana diante da exposição aos pesticidas

> Jéssyca F. de Medeiros, Raphael D'Anna Acayaba e Cassiana C. Montagner

http://dx.doi.org/10.21577/0100-4042.20170699

Humans are constantly exposed to pesticides in several ways. Since most pesticides are not selective for target species, adverse effects can occur in non-target species, including humans.



599 Recentes avanços na funcionalização seletiva de quinolinas Dartagnan S. P. Ferreira, Valter E. Murie, Thiago dos Santos, Paulo C. Vieira, Giuliano C. Clososki

http://dx.doi.org/10.21577/0100-4042.20170701

In the last twenty years, quinolines have received much attention due to their wide spectrum of attractive chemical and biological properties. This review describes recent strategies for obtaining structurally diverse quinolines as well relevant synthetic applications.



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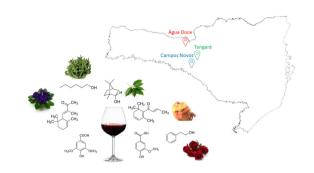
Nota Técnica/Technical Notes

616 Aroma profile and phenolic content of Merlot red wines produced in high-altitude regions in Brazil

Stefany G. Arcari, Vinícius Caliari, Edson L. de Souza and Helena T. Godoy

http://dx.doi.org/10.21577/0100-4042.20170687

Merlot red wines from Água Doce, Campos Novos and Tangará presented borneol, high concentrations of 1-hexanol, 2-phenylethanol, β -damascenone, α -ionone and, syringic and vanillic acids, the last two effective in capturing the free radicals DPPH and ABTS.

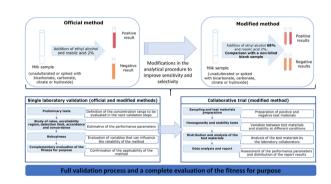


625 Detection of acid neutralizers in fraudulent milk: full validation of a classical qualitative method

Carina de S. Gondim, Marina P. e Palhares, Pedro P. B. dos Santos, Roberto C. de Sousa, Roberto G. Junqueira e Scheilla V. C. de Souza

http://dx.doi.org/10.21577/0100-4042.20170703

The classical rosolic acid method for detection of neutralizing compounds in milk was fully validated for four adulterants, in official and modified versions. Modifications in the analytical procedure improved the method performance.



Educação/Education

636 Relações sociedade-natureza em perspectiva: educação ambiental nas Licenciaturas em Química dos Institutos Federais no Brasil

Wesley F. Magela e Nyuara A. S. Mesquita

http://dx.doi.org/10.21577/0100-4042.20170694

Considering the increase in the number of training courses for Chemistry teachers offered by Federal Institutes from the first decade of the $21^{\rm st}$ century, it is important to investigate the formative elements of these courses, such as Environmental Education.



646 Basic concepts of self-organized phenomena in chemical systems

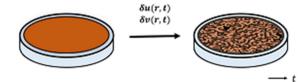
Leonardo Silva-Dias

http://dx.doi.org/10.21577/0100-4042.20170684

The BZ reaction is a typical oscillating reaction, which can spontaneously evolve to organized states under the influence of small perturbations. Such features make this reaction a suitable kinetic mechanism to theoretically study the emergence of oscillations, waves, and stationary patterns.

$$BrO_3^- + 2Br^- + 3H^+ \rightarrow 3HOBr$$

 $BrO_3^- + HBrO_2 + 3H^+ + 2\mathbf{M_{rcd}} \rightarrow 2HBrO_2 + 2\mathbf{M_{ox}} + H_2O$
 $2\mathbf{M_{ox}} + BrMA + MA \rightarrow fBr^- + 2\mathbf{M_{rcd}} + O.P.$



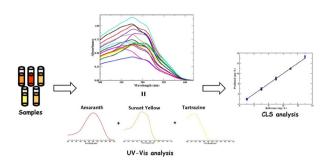
vi Quim. Nova

655 Simultaneous spectrophotometric determination and classical least squares method: a simple experiment to introduce the concept of multivariate calibration

Jhonatas R. Carvalho, Larissa R. Lopes, Luciano N. Vidal and Poliana M. Santos

http://dx.doi.org/10.21577/0100-4042.20170686

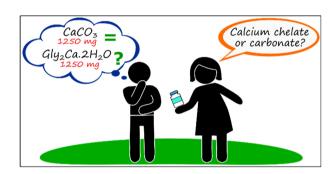
All data produced in a measurement may contain useful information that can be employed to build a more robust and reliable calibration model, through multivariate analysis.



659 Carbonato de cálcio ou cálcio quelado? Elucidando essa dúvida por meio de estudo de caso

Adriana N. de Macedo, Mariana R. Almeida e Ana L. de Quadros

http://dx.doi.org/10.21577/0100-4042.20170706



A case study involving a question about calcium supplementation using calcium carbonate or calcium chelate.

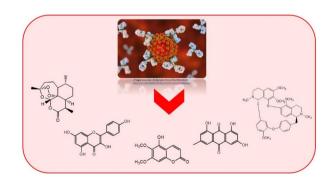
Assuntos Gerais/General Subject

667 Phytochemicals as potential antiviral agents in SARS-CoV-2 therapy: an update

Nerilson M. Lima, Teresinha de J. A. S. Andrade, Kojo S. Acquah, Marcone A. L. de Oliveira, Kellyane F. Gois and Lis C. M. Medeiros

http://dx.doi.org/10.21577/0100-4042.20170714

This work describes some medicinal plant species, and phytochemicals and their derivatives, with promising antiviral potential against coronavirus, which could be explored as potential candidates for drug prototypes in the treatment of COVID-19.



Errata/Erratum

673 The fundamental importance of basic science: examples of high-impact discoveries from an international Chemistry Network

Review, with DOI number: https://dx.doi.org/10.21577/0100-4042.20170584, published in the journal *Quim. Nova*, Vol. 43, No. 8, 1176-1189, 2020.

http://dx.doi.org/10.21577/0100-4042.20170775