química nova

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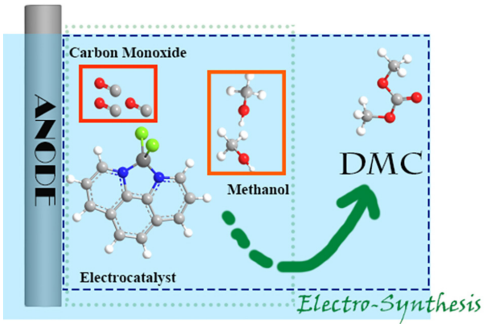
Editorial

297 Integridade científica: compromisso da SBQ
Angelo C. Pinto

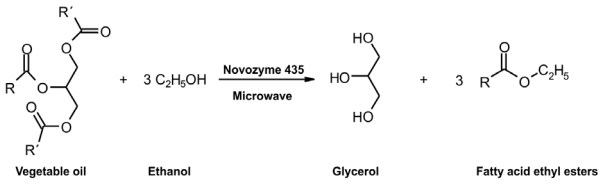
Artigo

298 A new homogeneous electrocatalyst for electrochemical carbonylation of methanol to dimethyl carbonate
Xiaoyan Wang, Gan Jia, Yuting Yu, Yanfang Gao, Wen Zhang, Hong Wang, Zhenzhu Cao and Jinrong Liu



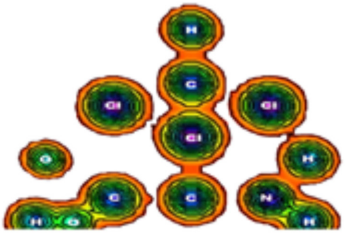
Dimethyl carbonate (DMC) is viewed as an environmentally benign intermediate because of its negligible eco-toxicity and its versatile chemical applications. In this paper, a novel homogeneous electrocatalyst based on Cu(Phen)Cl_2 was used for electrocatalytic oxidative carbonylation of methanol to DMC.

303 Microwave activation of immobilized lipase for transesterification of vegetable oils
Monna L. B. Queiroz, Rachel F. Boaventura, Micael N. Melo, Heiddy M. Alvarez, Cleide M. F. Soares, Álvaro S. Lima, Montserrat F. Heredia, Cláudio Dariva and Alini T. Fricks



Complete transesterification of soybean oil catalyzed by Novozyme 435 under microwave.

309 Trihalometanos em água potável e riscos de câncer: simulação usando potencial de interação e transformações de Bäcklund
Benjamim H. de L. Silva e Marcos A. B. de Melo

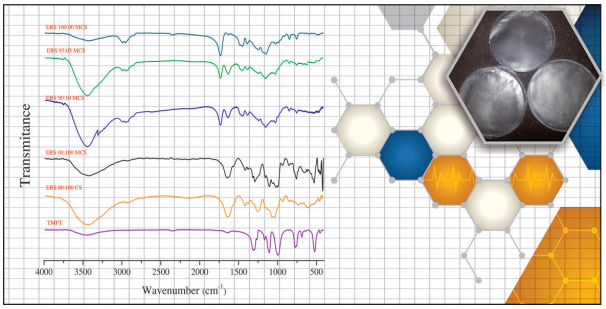


$$k\left(-\frac{\hbar^2}{2m}\left(\frac{\partial V}{\partial x}\right)^2+\left(\frac{\partial V}{\partial y}\right)^2+\left(\frac{\partial V}{\partial z}\right)^2\right)+\frac{\hbar^2}{2m}\left(\frac{\partial^2 V}{\partial x^2}+\frac{\partial^2 V}{\partial y^2}+\frac{\partial^2 V}{\partial z^2}\right)+i\hbar\frac{\partial V}{\partial t}=0$$

A simulation between trichloromethane and alanine was performed investigating amino acid changes that may arise in protein and possibly induce the formation of cancer.

316 Análises físico-químicas de biofilmes de sulfato de condroitoina modificado

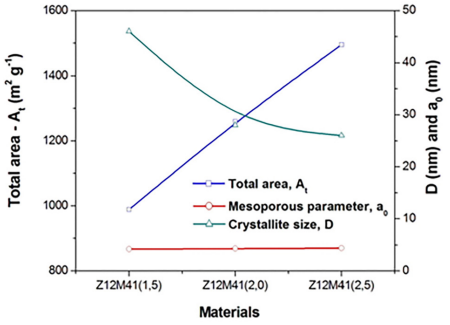
Élcio J. Bunhak, Elisabete S. Mendes, Nehemias C. Pereira, Edgardo A. G. Pineda, Ana A. W. Hechenleitner e Osvaldo A. Cavalcanti



The physicochemical and surface analyses of free films are important tools for research and the development of new materials for coating of solid dosage forms to control drug delivery.

321 Desenvolvimento de materiais híbridos micro-mesoporosos do tipo ZSM-12/MCM-41

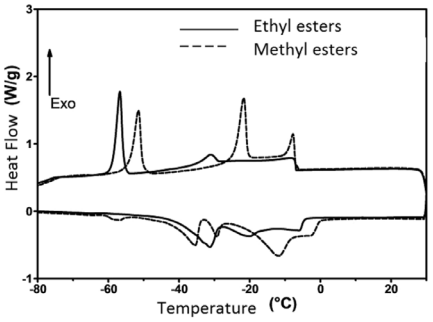
Joselaine C. Santana, Sanny W. M. Machado, Marcelo J. B. Souza e Anne M. G. Pedrosa



The figure shows that the parameters total area, crystallite size of the microporous phase and the mesoporous parameter value are dependent on the alkaline treatment carried out on different hybrid materials and indicate the different contributions of micro- and mesoporosity in these materials.

328 Composição química e temperatura de cristalização de ésteres obtidos de quatro óleos vegetais extraídos de sementes de plantas do cerrado

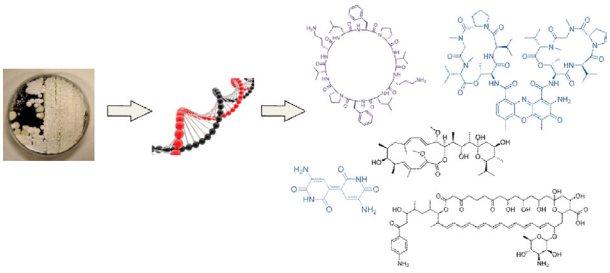
Luciane Pierezan, Márcia R. P. Cabral, Deluana Martins Neto, Jusinei M. Stropa, Lincoln C. S. de Oliveira, Dilamara R. Scharf, Edésio L. Simionatto, Rogério C. de L. da Silva e Euclésio Simionatto



Chemical composition and thermal behavior was reviewed in mixtures of four esters obtained from vegetable oils.

333 Triagem metabólica por PKS e NRPS em actinobactérias endofíticas de *Citrus reticulata*

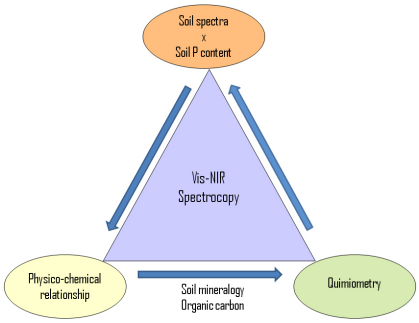
Pedro L. R. da Cruz, Leila R. Giarola, Suellen da S. Moraes, Déborah E. S. G. da Silva, Joelma Marcon, João L. Azevedo, Welington L. Araújo e Luciana G. de Oliveira



A molecular fingerprint approach was employed to evaluate the biosynthetic potential of endophytic actinobacteria from *Citrus reticulata* in the production of PKs and NRPs metabolites.

342 VIS-NIR spectrometry, soil phosphate extraction methods and interactions of soil attributes

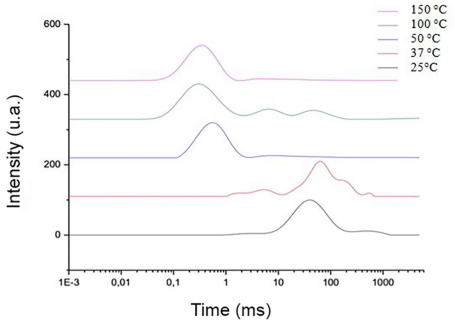
José F. de Oliveira, Michel Brossard, Edemar J. Corazza, Robélio L. Marchão, Pedro R. S. Vendrame, Osmar R. Brito and Mª de Fátima Guimarães



Understanding the interrelations between P content, extraction method and their effect on prediction by Vis-Nir spectroscopy.

351 Uso da RMN de baixa resolução na avaliação da dinâmica molecular do *Origanum vulgare*

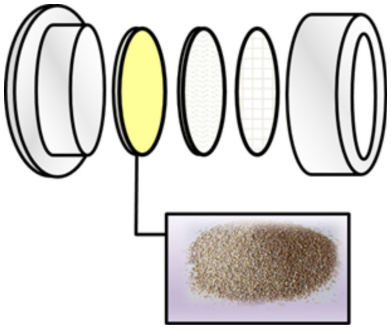
Vanessa C. dos S. P. de Oliveira, Mª Inês B. Tavares, Eduardo M. B. da Silva, Bianca N. B. de Lima e Roberto P. Cucinelli Neto



The evaluation of thermal treatment of *Origanum vulgare* using the domain curves of proton spin-lattice relaxation time, which discloses the structural changes or degradation process occurring in the sample when it is submitted to thermal treatment.

356 Dispositivos DGT modificados com materiais alternativos para uso na especiação de elementos traço

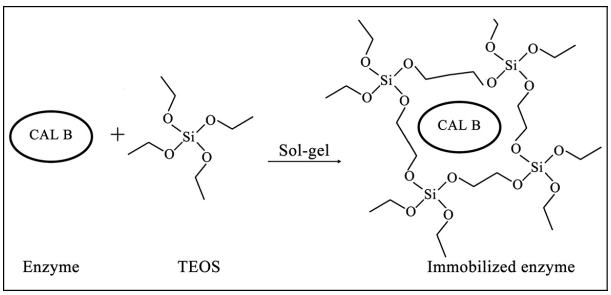
Cristiano L. Chostak, Mônica S. de Campos, Simone B. da Silva, Gilberto Abate e Marco T. Grassi



Alternative DGT devices prepared using montmorillonite MT-K10 as the ligand phase and agarose as the diffusive phase, for the speciation of trace metals in natural waters.

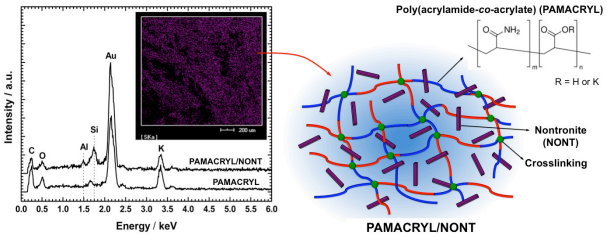
364 Estudo da imobilização de lipase em sílica obtida pela técnica sol-gel

Aline M. M. Ficanha, Nádia L. D. Nyari, Katarine Levandoski, Marcelo L. Mignoni e Rogério M. Dallago



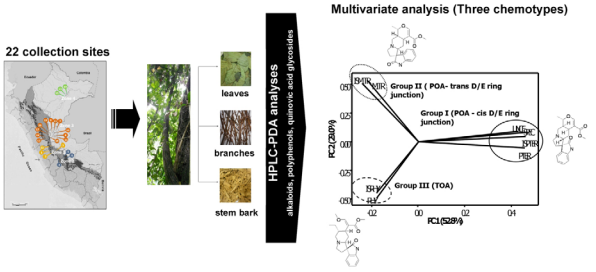
Matrix sol-gel production created by partial hydrolysis of the precursor (TEOS) results in an oligomer. This is completely hydrolyzed and forms a colloidal dispersion (sol) which upon addition of the enzyme starts the process of polycondensation. The end of the process results in an immobilized enzyme.

370 Novel superabsorbent hydrogel composite based on poly(acrylamide-*co*-acrylate)/nontronite: characterization and swelling performance
Renan C. F. Leitão, Cícero P. de Moura, Lindomar R. D. da Silva, Nágila M. P. S. Ricardo, Judith P. A. Feitosa, Edvani C. Muniz, André R. Fajardo and Francisco H. A. Rodrigues



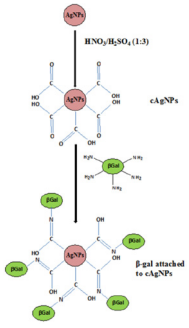
A novel superabsorbent hydrogel composite based on a poly(acrylamide-*co*-acrylate) matrix filled with nontronite with highly attractive swelling properties and potential uses in agriculture was designed and characterized in this manuscript.

378 Chemical composition variability in the *Uncaria tomentosa* (cat's claw) wild population
Evelyn M. C. Peñaloza, Samuel Kaiser, Pedro E. de Resende, Vanessa Pittol, Ânderson R. Carvalho and George González Ortega



No clear correlation between chemical composition and geographic origin, altitude or season of collection was found. Nevertheless, three chemotypes were distinguished based on the oxindole alkaloid profile of the cat's claw samples.

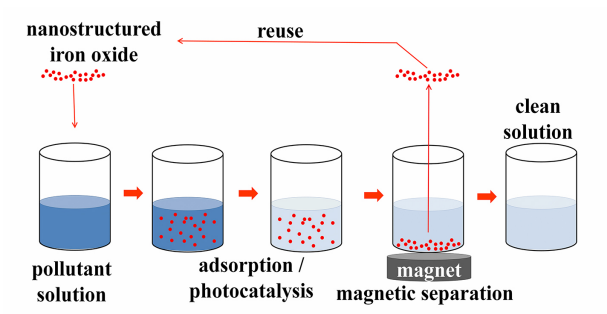
387 Carboxylation of silver nanoparticles for the immobilization of β-galactosidase and its efficacy in galacto-oligosaccharides production
Shakeel A. Ansari, Rukhsana Satar and Syed K. Zaidi



Attachment of ß-galactosidase on carboxylated AgNPs.

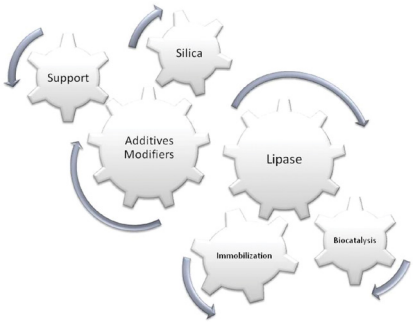
Revisão

393 Aplicação de óxidos de ferro nanoestruturados como adsorventes e fotocatalisadores na remoção de poluentes de águas residuais
Marcela F. Silva, Edgardo A. Gómez Pineda e Rosangela Bergamasco



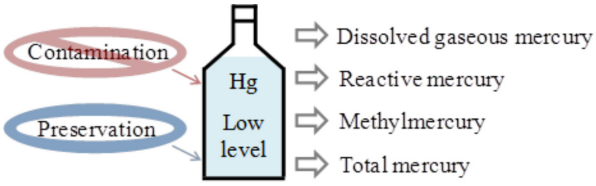
The use of iron oxides as adsorbent and photocatalyst for the removal or degradation of pollutants has proved a promising approach. The separation and reuse of iron oxides is very simple, effective and economical while also being more environmentally friendly.

399 Uso de sílicas modificadas para imobilização de lipases
Nayara B. Carvalho, Álvaro S. Lima e Cleide M. F. Soares



Strategies for surface modification of supports using different additives for lipase immobilization in order to replace conventional immobilization methods and improve biocatalyst efficiency.

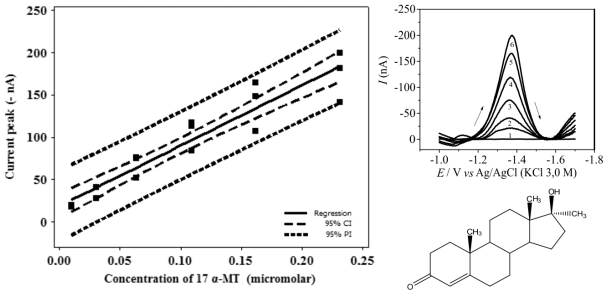
410 Metodologias de coleta, preservação e armazenamento de amostras de água para análise de mercúrio - uma revisão
Daniele Kasper, Bruce R. Forsberg, Ronaldo de Almeida, Wanderley R. Bastos e Olaf Malm



Analysis of mercury in water is a challenge because of its low levels. Sample preservation methods and protocols that avoid contamination are discussed for the most commonly evaluated mercury species.

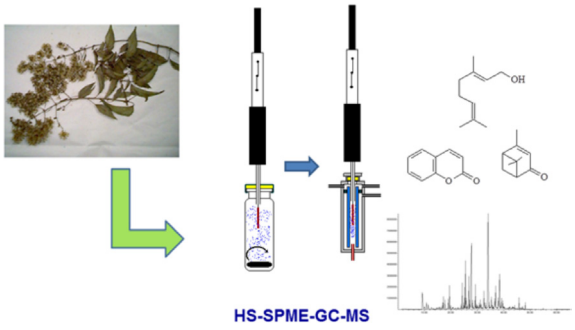
Nota Técnica

419 Validação intralaboratorial da determinação de metiltestosterona em águas naturais por voltametria usando eletrodo de gota pendente de mercúrio
Luciane Miranda, Maria L. Felsner, Yohandra R. Torres, Ivonete Hoss, Andressa Galli e Sueli P. Quináia



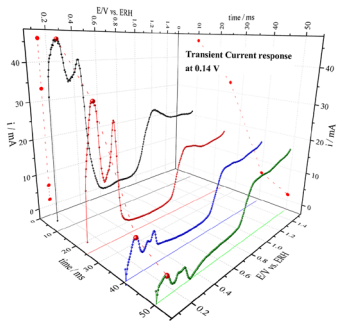
This study presents the in-house validation of a new voltammetric methodology for 17α-MT analysis in natural water. The methodology exhibited selectivity, linearity, accuracy and precision.

427 HS-SPME-GC-MS analysis of volatile and semi-volatile compounds from dried leaves of *Mikania glomerata* Sprengel
Esmeraldo A. Cappelaro and Janete H. Yariwake



This paper describes the identification of volatile and semi-volatile compounds and a comparison of the HS-SPME-GC-MS chromatographic profiles of dried leaves of *Mikania glomerata* Sprengel (Asteraceae), also known in Brazil as “guaco”.

431 Considerações técnicas quanto ao uso da voltametria de varredura escalonada em processos adsortivos
Khallil H. A. A. Fernandes, João P. T. da S. Santos, Vinicius Del Colle, Janaina Souza-Garcia e Camilo A. Angelucci



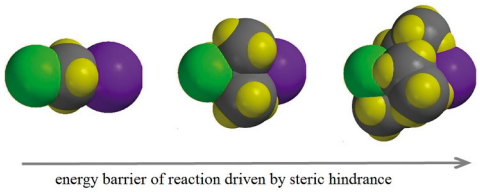
Cyclic voltammogram profile of platinum in acid media obtained by *Staircase Sweep Voltammetry (SCV)*. The data displays the current recorded at different periods during each step comprising the SCV signal.

Educação

436 Química verdadeiramente verde – propriedades químicas do cloro e sua ilustração por experimentos em escala miniaturizada
Martin Wallau, Daniela Bianchini, Camila P. Ebersol, José A. dos Santos Júnior e Thiago M. Barboza

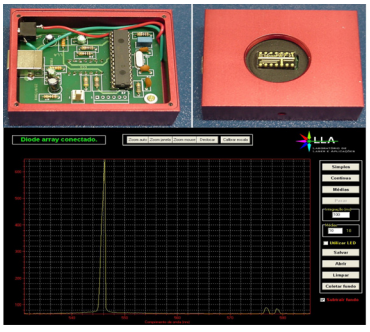
Chlorine, the only element which appears greenish, is presented as one of the fundamental but also most criticised industrially used chemicals. By miniaturised experiments, chlorine´s applications and properties can be easily demonstrated.

446 Una propuesta para enseñar el efecto de la forma de las moléculas en la reactividad química
José G. Cermeños-Estrada, John J. Pérez-Moncada y Daniel Barragán



Steric effects or steric hindrance can be explained to freshman students clearly by using correlations between properties of molecules and the energy barrier height of series of S_N2 reactions.

451 O uso de um sensor de luz linear como recurso didático para demonstrar princípios de difração e espectroscopia
Fernando A. M. de Oliveira, Eduardo R. de Azevedo e Luiz A. de O. Nunes



Picture of the light intensity acquisition apparatus developed including: the electronic control circuit, linear diode array and software graphics interface with a Hg lamp spectrum displayed.