química nova

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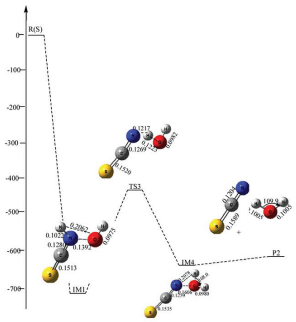
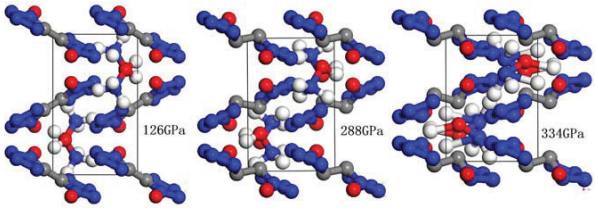
Artigo

1137 Theoretical research on the multi-channel reaction mechanism and kinetics of HNCS with OH^-
Li-Jie Hou, Bo-Wan Wu, Yan-Xia Han, Chao Kong and Li-Guo Gao



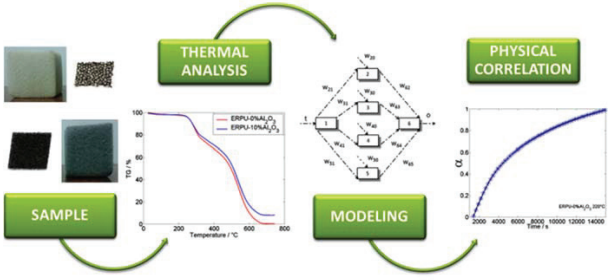
The channel of H-atom in HNCS direct extraction to OH^- (OH^-+HNCS→IM1→TS3→IM3→SCN^- +H_2O) in singlet state was the main channel.

1141 High pressure behavior of crystalline dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate: first-principles study
Guozheng Zhao and Xilin Yan



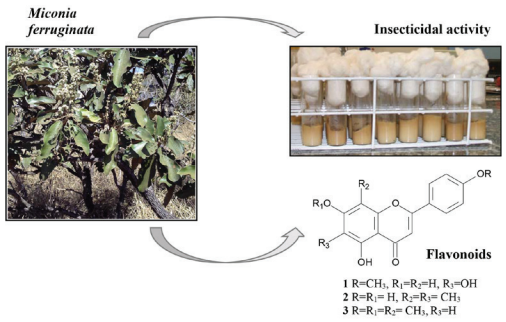
First of all, TKX-50 is rearranged in the crystal and the improvement of the molecular planarity occurs. Next, structural transformation appears with the distortion of the tetrazole rings. Finally, the rotation of molecular conformation occurs.

1149 Estudo cinético de decomposição térmica de espumas rígidas de poliuretano por rede neural artificial
Bárbara D. L. Ferreira, Virgínia R. Silva, Bruna B. Jacobsem, Mª Irene Yoshida e Rita C. O. Sebastiao



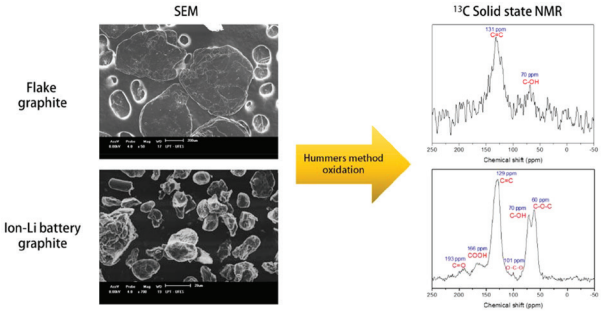
Thermal analysis data of two Rigid Polyurethane Foam samples: loaded with (Al_2O_3) and no inorganic filler are modeled by neural network supporting physical correlation.

1158 Constituintes químicos e atividade inseticida de *Miconia ferruginata*
Gracielle O. S. Cunha, Andreia P. Matos, Antonio R. Bernardo, Antonio C. S. Menezes, Marcela C. de M. Burger, Paulo C. Vieira, Moacir R. Forim, João B. Fernandes e Mª Fatima das G. F. da Silva



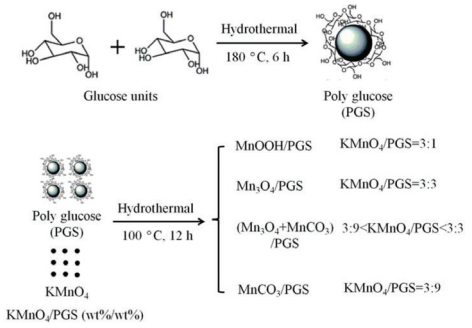
Flavonoids, triterpenes and steroids were isolated from *Miconia ferruginata*. The leaf extracts showed insecticidal effects.

1164 Estudo através de RMN de ^{13}C no estado sólido sobre a síntese de oxido de grafite utilizando diferentes precursores grafíticos
Mariana A. Vieira, Carolina Mª R. Frasson, Tainara L. G. Costa, Daniel F. Cipriano, Miguel A. Schettino Jr., Alfredo G. Cunha e Jair C. C. Freitas



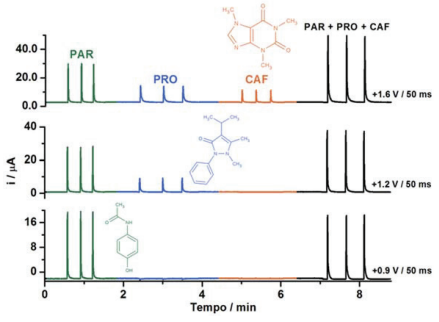
Graphite precursors with distinct particle sizes (as seen in SEM imagens) led to the production of graphite oxides with distinct degrees of oxidation (as seen in ^{13}C NMR spectra).

1172 Support effect on the structure and properties of manganese oxide electrode materials
Huatao Wu, Yongjun Han, Li Wang, Lihui Zhang and Xiang Wang



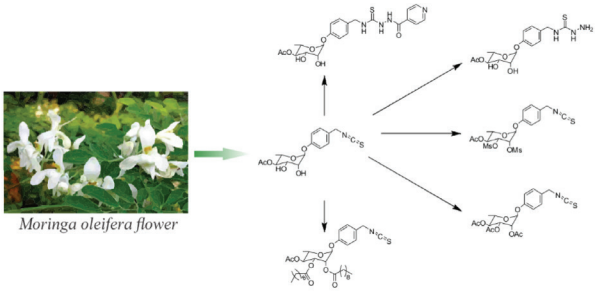
The composite electrode material of manganese oxide supported on poly glucose (PGS) was prepared by using $KMnO_4$ as manganese source. The composition of the composite electrode materials relies on the weight ratio of $KMnO_4$/PGS.

1180 Determinação rápida e simultânea de propifenazona, paracetamol e cafeína utilizando análise por injeção em batelada com detecção amperométrica
Weberson P. Silva, Luiz A. J. Silva, Rodrigo A. A. Muñoz e Eduardo M. Richter



Use of batch injection analysis with multiple pulse amperometric detection (BIA-MPA) for simultaneous determination of propyphenazone (PRO), paracetamol (PAR), and caffeine (CAF).

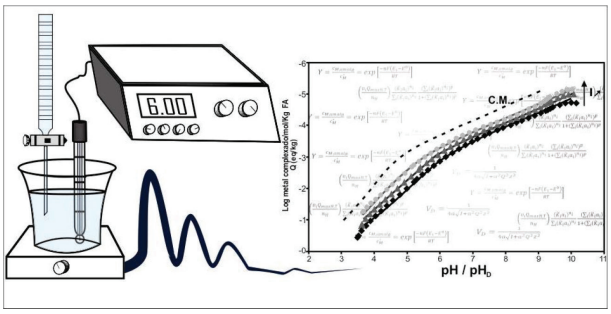
1186 New semisynthetic derivatives of a benzylisothiocyanate isolated from *Moringa oleifera* and evaluation of their cytotoxic activity
Diana K. C. de Almeida, Marcos R. da Silva, Mª Conceição F. de Oliveira, Jair Mafezoli, Marcos C. de Mattos, Andréa F. Moura, Manoel O. Moraes Filho and Francisco G. Barbosa



Semisynthetic derivatives of a benzylisothiocyanate isolated from *Moringa oleifera* were produced and evaluated for cytotoxic activity.

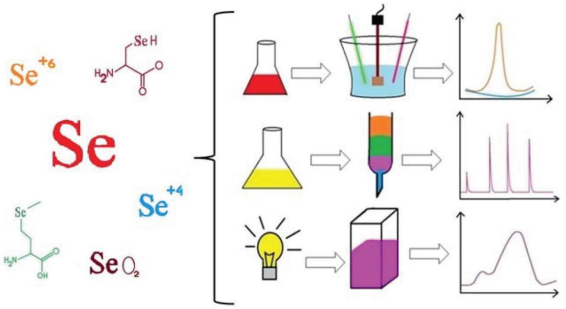
Revisão

1191 Especiação termodinâmica de metais traço com substâncias húmicas: o modelo NICA-Donnan
José P. Pinheiro, Adnívia S. C. Monteiro, Noemie Janot, Bert J. Groenenberg e André H. Rosa



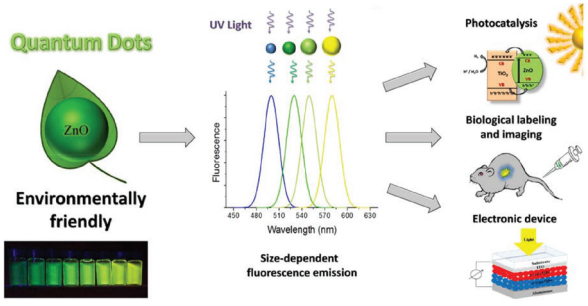
The figure shows an example of a potentiometric titratíon of humic matter at different íonic strenghts with master curve and NICA-Donnan modelling. Inset: solutions of aquatic fulvic acid, aquatic humic acid and peat humic acid after titration.

1204 Compostos orgânicos e inorgânicos contendo selênio: revisão de métodos analíticos e perspectivas para análises químicas
Fernanda C. O. L. Martins, Diego L. Franco, Rodrigo A. A. Muñoz e Djenaine De Souza



Spectrometric, chromatographic and electroanalytical methods in the quantification of organic and inorganic compounds containing Se in food, biological and natural water samples.

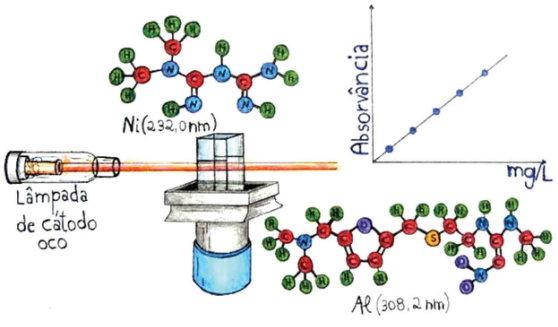
1215 Pontos quânticos ambientalmente amigáveis: destaque para o óxido de zinco
Crislaine Sandri, Mª Victória Krieger, Wallison C. Costa, Arleide R. da Silva, Ivan H. Bechtold e Lizandra Mª Zimmermann



This picture shows the fluorescence emission of the environmentally friendly zinc oxide quantum dots, being related to its size and some of its main applications.

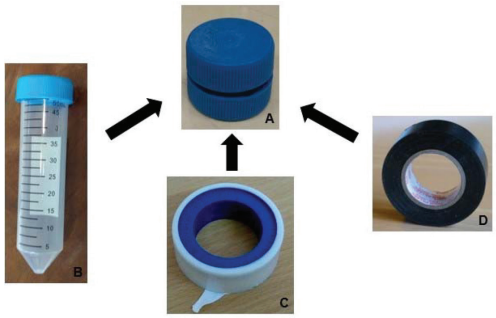
Nota Técnica

1228 Utilização do espectrômetro de absorção atômica para determinação de cloridrato de metformina e cloridrato de ranitidina em medicamentos
Mariana B. A. de Souza, Klaiani B. Fontana, Caroline Gonçalves e Eduardo S. Chaves



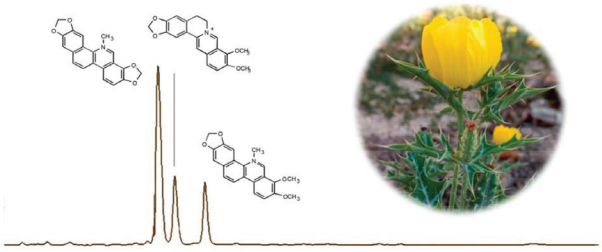
Atomic absorption spectrometer for metformin and ranitidine hydrochlorides determinations in medicines via molecular absorption.

1233 Desenvolvimento de amostrador passivo sensível para monitoramento de poluição atmosférica por dióxido de nitrogênio
Pedro A. F. Souza, Karen C. A. Francisco e Arnaldo A. Cardoso



A new passive sampler for measurement of ambient NO_2 was developed (A) using parts of 50 mL conical centrifuge tubes (B), Teflon tape (C) and black insulant tape (D).

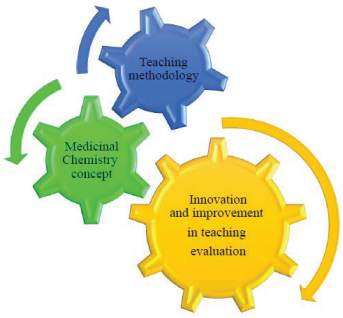
1238 HPLC-DAD determination of berberine, chelerythrine and sanguinarine in the mexican prickly poppy (*Argemone mexicana* L. Papaveraceae), a medicinal plant
Jorge F. Xool-Tamayo, Manlio Graniel-Sabido, Gumersindo Mirón-López, Gonzalo J. Mena-Rejón, Miriam Monforte-González and Felipe Vázquez Flota



The three main alkaloids of *Argemone mexicana* plants were separated in a single chromatographic run using an incremental gradient of acetonitrile in 1% acetic acid in water.

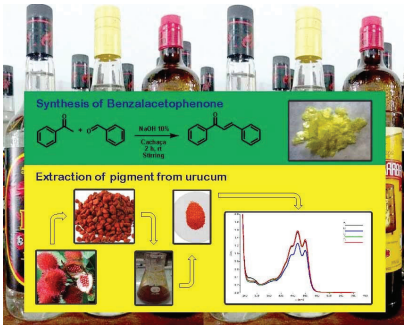
Educação

1244 Avaliação de competências desenvolvidas na disciplina de Química Medicinal da pós-gradução strictu sensu: uma experiência de sala de aula
Davidson P. Mendes, Carla J. Santos, César A. Ribeiro, Fabiana C. Guedes, Wanderlin F. Duarte e Daniel C. F. Soares



The competencies developed in Medicinal Chemistry can be considered as an engine, where the gears are related to professional, scientific and docent development.

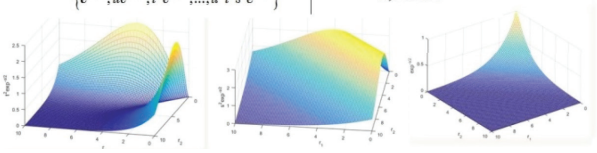
1253 Além da caipirinha: cachaça como solvente para síntese orgânica e extração de pigmento
Silvio Cunha e Jamille S. Matos



Cachaça was applied for the first time as solvent in undergraduate experiments of benzalacetophenone and dibenzalacetone syntheses, and natural pigment of urucum (*Bixa orellana L.*) was obtained using as extractor solvent a 5% NaOH solution in *cachaça*.

1259 O método de Hylleraas para átomos de dois elétrons
Felipe S. Carvalho e João P. Braga

Basis	Calculated energies
$\{e^{-s/2}, e^{-t/2}\}$	−2,847656
$\{e^{-s/2}, ue^{-t/2}\}$	−2,891120
$\{e^{-s/2}, ue^{-t/2}, t^2e^{-s/2}\}$	−2,902432
$\{e^{-s/2}, ue^{-s/2}, t^2e^{-s/2}, se^{-s/2}, s^2e^{-s/2}, u^2e^{-s/2}\}$	−2,903329
$\{e^{-s/2}, ue^{-s/2}, t^2e^{-s/2}, ..., u^6t^8s^3e^{-s/2}\}$	−2,903724



A table with the calculated electronic energies and the surfaces for some Hylleraas basis functions.