

## Editorial

583 Nasce a PubliSBQ  
Conselho de Editores

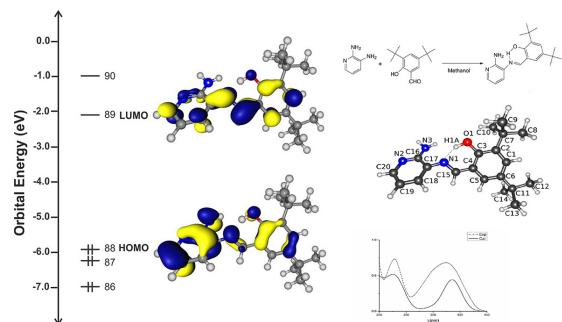
## Artigo

584 Synthesis, characterization and computational studies of (E)-2-{{(2-aminopyridin-3-yl)imino]-methyl}-4,6-di-tert-butylphenol

Alexander Carreño, Andrés Vega, Ximena Zarate, Eduardo Schott, Manuel Gacitúa, Ninnette Valenzuela, Marcelo Preite, Juan M. Manríquez and Ivonne Chávez

### Graphical Abstract

We synthesized the (E)-2-{{(2-AMINOPYRIDIN-3-YL)IMINO]-METHYL}- 4,6-DI-tert-BUTYLPHENOL ligand and characterized by FTIR, UV-vis,  $^1\text{H}$ - $^{13}\text{C}$  NMR , 1D TOCSY spectra and cyclic voltammetric. This study included theoretical calculation using DFT Theory.

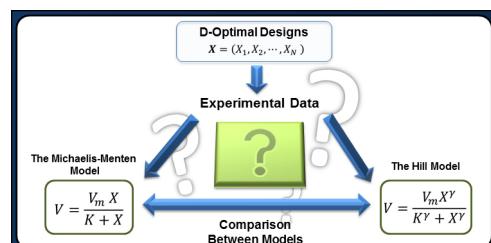


589 Delineamentos experimentais eficientes para estudos de cinética química

Iuri E. P. Ferreira, Luzia A. Trinca e Cláudia P. Ferreira

### Graphical Abstract

The D-optimal Designs allow the fitting and comparison of the Michaelis-Menten and Hill models. Furthermore, they ensure precise estimations of the kinetic parameters for both models.

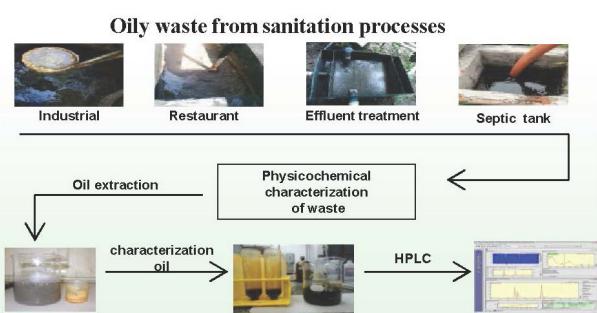


597 Caracterização físico-química de resíduos oleosos do saneamento e dos óleos e graxas extraídos visando a conversão em biocombustíveis

Jairo P. de Oliveira, Paulo W. P. Antunes, Laura M. Pinotti e Sérvio T. A. Cassini

### Graphical Abstract

Process used for the extraction and characterization of oily waste sanitation, targeting the use of biofuels.

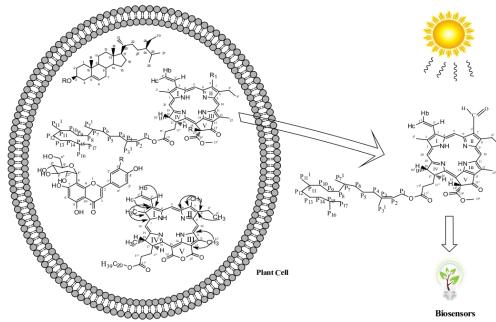


- 603 Chemical constituents isolated from *Turnera subulata* Sm. and electrochemical characterization of phaeophytin b

*Severino G. de Brito Filho, Marianne G. Fernandes, Otemberg S. Chaves, M<sup>a</sup> Célia de O. Chaves, Felipe B. Araruna, Carla Eiras, José R. de S. de A. Leite, M<sup>a</sup> de Fátima Agra, Raimundo Braz-Filho and M<sup>a</sup> de Fátima V. de Souza*

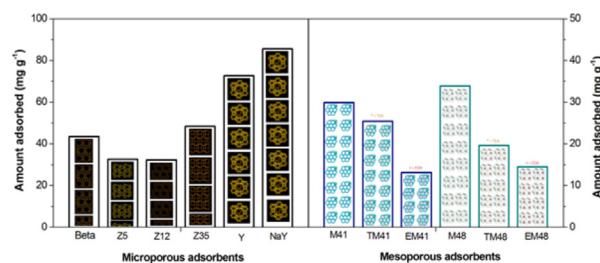
#### Graphical Abstract

Phaeophytin b, natural product of plant, arouses interest as material used in the construction of optical -electronic devices employed in photodynamic therapy and in the development of electrochemical biosensors.



- 610 Adsorção de CO<sub>2</sub> em peneiras moleculares micro e mesopórosas

*Thiago G. Oliveira, Sanny W. M. Machado, Silvia C. G. Santos, Marcelo J. B. Souza e Anne M. G. Pedrosa*

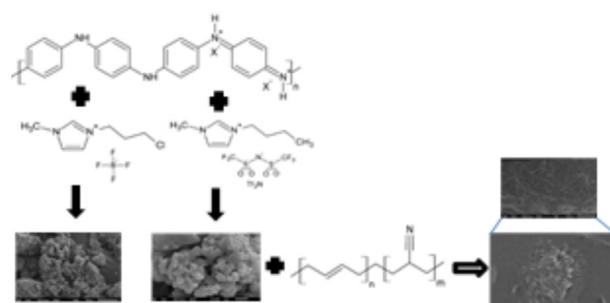


#### Graphical Abstract

The Figure shows the amounts of carbon dioxide adsorbed in micro and mesoporous molecular sieves according to different structures and also due to the presence of amines in the mesoporous molecular sieves.

- 618 Líquidos iônicos como plastificantes em blendas de borracha nitrílica/polanilina

*Leandro Prudêncio, Fernanda F. Camilo e Roselena Faez*

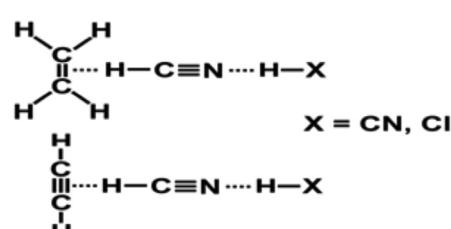


#### Graphical Abstract

The electrical conductivity of PANI having ionic liquid (IL) depends on the anion of the ionic liquid employed. Both PANI-LI as the elastomeric composite show higher conductivity and homogeneity when prepared with Tf<sub>2</sub>N ionic liquids.

- 624 A regra de Bent contextualiza a força da ligação de hidrogênio em clusters trimoleculares

*Ives T. O. Santos, Danilo G. Rego e Boaz G. Oliveira*



#### Graphical Abstract

The  $\pi \cdots H$  and  $n \cdots H$  hydrogen bond strengths of the C<sub>2</sub>H<sub>2</sub> $\cdots$ HCN $\cdots$ HX and C<sub>2</sub>H<sub>4</sub> $\cdots$ HCN $\cdots$ HX (X = CN or Cl) clusters and red-shifts on the proton donor bonds are in line with the Bent rule.

- 631 Determinação espectrofotométrica indireta de capsaicinoides em pimentas *Capsicum* a partir da reação com o complexo de Co(II) com 4-(2-piridilazo) resorcinol  
Patrícia T. de Souza e Adriana V. Rossi

**Graphical Abstract**

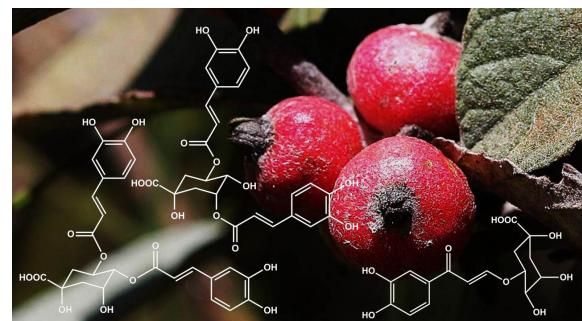
Total capsaicinoids in *Capsicum* pepper extract obtained with cachaça were quantified spectrophotometrically from the effect of capsaicinoids in absorbance of the Co(II) with 4-(2-piridilazo) resorcinol (PAR) complex.



- 638 Constituintes químicos e avaliação das atividades antioxidante e anti-inflamatória das raízes de *Sabicea brasiliensis* Wernh (Rubiaceae)  
Jucilene C. Batista, Silvana M<sup>a</sup> de O. Santin, Ivânia T. A. Schuquel, Laura L. M. de Arruda, Ciomar A. Bersani-Amado, Cecília M<sup>a</sup> A. de Oliveira, Lucilia Kato, Heleno D. Ferreira e Cleuza C. da Silva

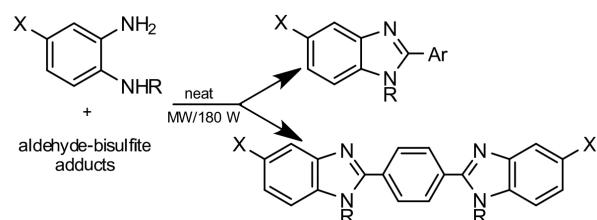
**Graphical Abstract**

In this paper we report the isolation of the main chemical constituents from the roots of *Sabicea brasiliensis* and evaluation of the antioxidant and anti-inflammatory activities.



- 643 Simple, mild, and highly efficient synthesis of 2-substituted benzimidazoles and bis-benzimidazoles

Bilge Eren and Yunus Bekdemir

**Graphical Abstract**

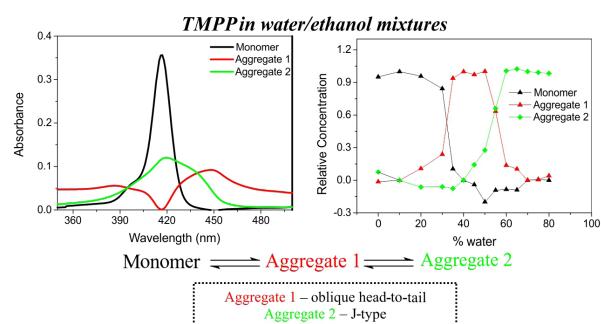
A series of benzimidazole derivatives were synthesized in very short times under microwave heating conditions with an easy purification procedure.

- 648 Autoagregação da 5,10,15,20-tetrakis(4-metoxifenil)porfirina (TMPP): estudos espectroscópicos e análises multivariadas

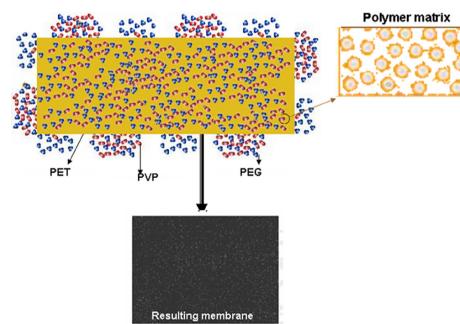
Gustavo Braga, Jader L. Aparicio, Bruno H. Vilsinski, André L. Tessaro, Adriana P. Gerola, Noboru Hioka e Wilker Caetano

**Graphical Abstract**

Self-aggregation studies of TMPP were carried out in water/ethanol mixtures. The TMPP was kept monomeric up to 25 % of water. The formation of oblique head-to-tail and J-type aggregates were observed with increasing percentage of water.



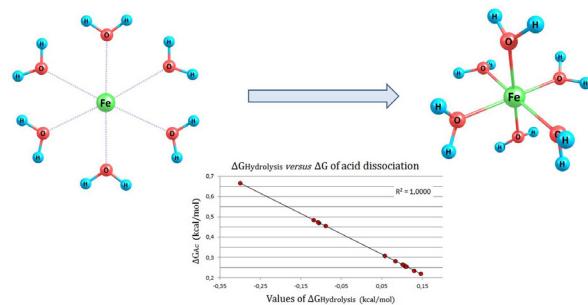
- 653 Ultrafiltration membranes from waste polyethylene terephthalate and additives: synthesis and characterization  
*Smitha Rajesh and Z. V. P. Murthy*



#### Graphical Abstract

The incorporation of additives into a membrane prepared from recycled waste polymer has been confirmed. The uniform distribution of the additive in the membrane leads to a change in the surface properties. The recycling of any polymeric material into a usable and durable product is of significant interest from an environmental viewpoint.

- 658 Propriedades relacionadas à acidez e basicidade a partir da abordagem em Química Computacional  
*Sérgio R. B. Silva, Caio L. Firme e Cássio M. G. Lima*



#### Graphical Abstract

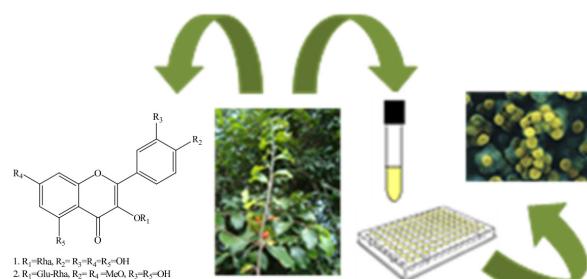
Linear relation of between  $\Delta G$  of acid dissociation and  $\Delta G$  of hydrolysis of the corresponding conjugate base.

- 663 Flavonoides glicosilados de *Erythroxylum pulchrum* A. St.-Hil. (Erythroxylaceae)

*Camila H. de Albuquerque, Josean F. Tavares, Steno L. de Oliveira, Tainá S. Silva, Gregório F. Gonçalves, Vicente C. de O. Costa, M<sup>a</sup> de Fátima Agra, Hilzeth de L. F. Pessôa e Marcelo S. da Silva*

#### Graphical Abstract

The phytochemical investigation of *Erythroxylum pulchrum* led to the isolation of quercetin-3-O-*a*-L-rhamnoside, ombuin-3-ruthinoside e ombuin-3-ruthinoside-5-glucoside. The methanol extract inhibited the growth of bacteria *S. aureus* ATCC 25925.

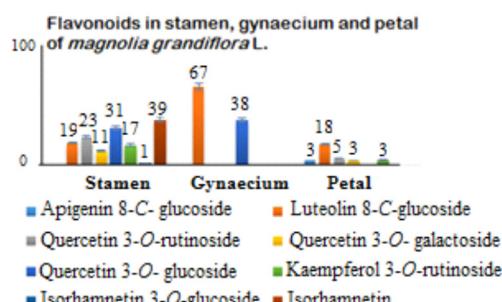


- 667 Determination of flavonoids in stamen, gynoecium, and petals of *Magnolia grandiflora* L. and their associated antioxidant and hepatoprotection activities

*Nadia M. Sokkar, Mohamed A. Rabeh, Gamal Ghazal and Amani M. Slem*

#### Graphical Abstract

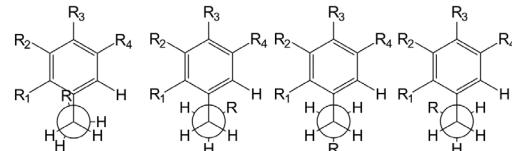
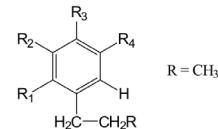
A chromatographic analysis of the flavonoids in stamen, gynoecium and petal of *Magnolia grandiflora* L. was done by HPLC-PDA-MS/MS-ESI. Antioxidant and hepatoprotective effects of their ethanolic extracts were carried out against hepatotoxicity induced by CCl<sub>4</sub> as compared by silymarin.



672 Flavonoides de *Lonchocarpus araripensis* (Leguminosae)

- isolamento, atribuição inequívoca dos sinais de RMN  $^1\text{H}$  e  $^{13}\text{C}$  e análise conformatacional

*Almi F. Lima, Daniele A. Ferreira, Francisco J. Q. Monte  
e Raimundo Braz-Filho*

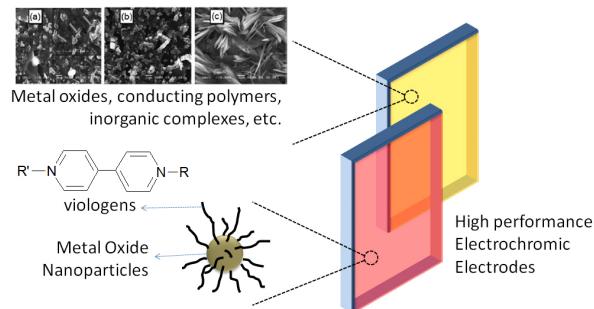
**Graphical Abstract**

Stable conformations of aromatics substituted compounds.

**Revisão**

## 677 Eletrocromismo: fundamentos e a aplicação de nanomateriais no desenvolvimento de eletrodos de alto desempenho

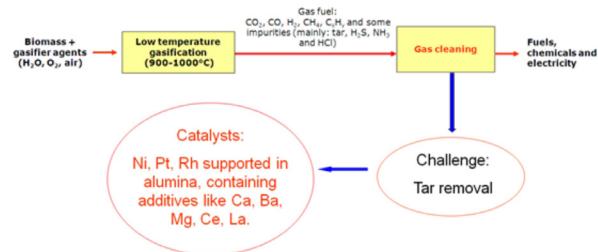
*Ronaldo C. Quintanilha, Igor Rocha, Raquel B. Vichessi,  
Emili Lucht, Karine Naidek, Herbert Winnischofer e  
Marcio Vidotti*

**Graphical Abstract**

In this review we discuss the most recent trends in electrochromism, describing the basic aspects and the new methodologies employed for the construction of high performance electrodes based on nanostructures of different materials.

## 689 Remoção do alcatrão de correntes de gaseificação de biomassa: processos e catalisadores

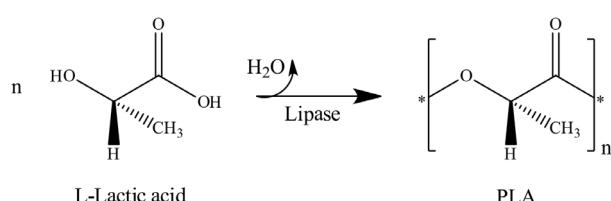
*Cristina P. B. Quitete e Mariana M. V. M. Souza*

**Graphical Abstract**

Catalysts for tar removal must have resistance to deactivation by coke and sulfur.

## 699 Aplicações de enzimas na síntese e na modificação de polímeros

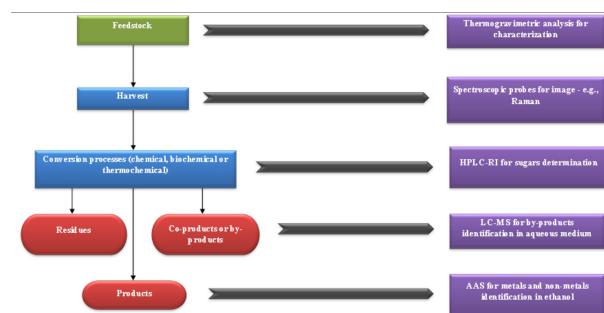
*Marcos de C. C. de Albuquerque, Claudia M<sup>a</sup> S. Ribeiro,  
Carlos R. K. Rabelo, Bernardo G. Siqueira, Ana B. A. Santa  
Marinha e Aline M. de Castro*

**Graphical Abstract**

Polyester synthesis is one of the main applications of enzymes in polymer technology. In the reaction below, a lipase acts as biocatalyst for the synthesis of poly(lactic acid) (PLA).

- 709 Análise química da biomassa – uma revisão das técnicas e aplicações

*Silvio Vaz Júnior e Itânia P. Soares*



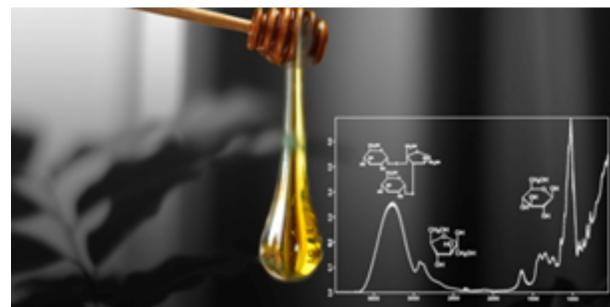
#### Graphical Abstract

Flowchart for a biomass chain (left). Chemical analyses could be used in all steps, from raw material to residues (right).

## Nota Técnica

- 716 Preliminary data on Brazilian monofloral honey from the northeast region using FT-IR ATR spectroscopic, palynological, and color analysis

*Ligia B. de Almeida-Muradian, Renato J. Sousa, Ortud M. Barth and Peter Gallmann*

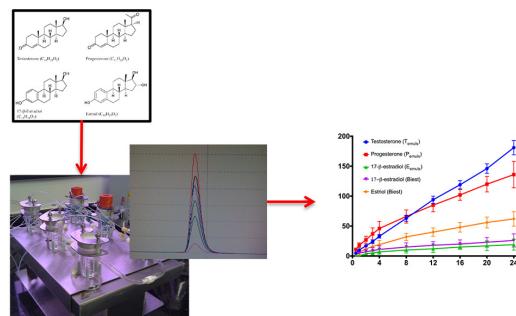


#### Graphical Abstract

FT-IR/ATR was used to predict 14 different measurands in northeast Brazilian honey samples. The results showed that mid-infrared spectrometry can be used as a screening method for the routine analysis of Brazilian honey with the advantages to be rapid, non-destructive and accurate.

- 720 Transdermal formulations containing human sexual steroids: development and validation of methods and *in vitro* drug release

*Hudson C. Polonini, Pedro P. Soldati, Marcone A. L. de Oliveira, Marcos A. F. Brandão, M<sup>a</sup> das Graças M. Chaves and Nádia R. B. Raposo*

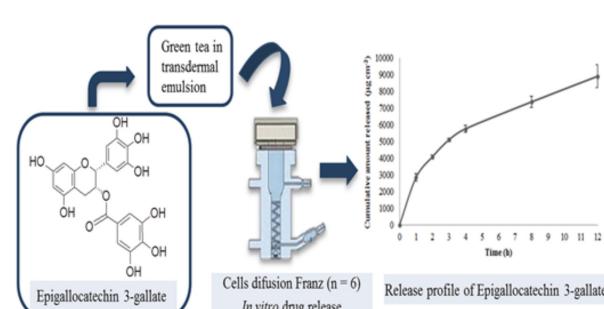


#### Graphical Abstract

In this work, we assessed the *in vitro* release of bioidentical human sexual hormones in four different liposomal transdermal emulsions (containing testosterone or progesterone or estradiol or estradiol + estriol).

- 728 Green tea in transdermal formulation: HPLC method for quality control and *in vitro* drug release assays

*Michele C. Alves, Priscila A. de Almeida, Hudson C. Polonini, Nádia R. B. Raposo, Anderson de O. Ferreira and Marcos A. F. Brandão*

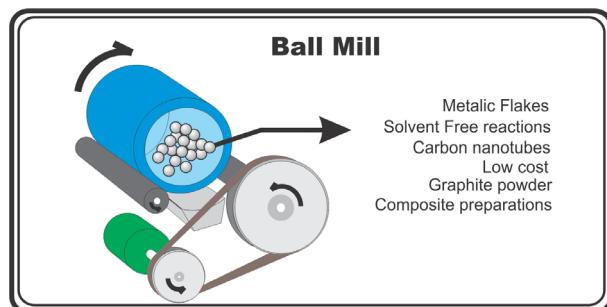


#### Graphical Abstract

An analytical method by RP-HPLC was developed and validated to be used both for quality control of green tea in a semisolid formulation and for *in vitro* drug release assays. Epigallocatechin 3-gallate showed a good flux rates in synthetic membrane when used from tested formulation.

- 736 Diretrizes para a construção de um moinho de bolas para a moagem de sólidos em laboratórios

*Lucas F. de Paula, Alberth C. Alves, Heden C. S. Alves, Edimar A. Ribeiro, Ana G. B. Maduro e João M. Maduro*



**Graphical Abstract**

Schematic representation of a ball mill which has its main components and describes some of their laboratory applications.

## Educação

- 740 Propuesta de un test para determinar el conocimiento conceptual de estudiantes universitarios sobre la constante de equilibrio químico y su aplicación en estudiantes españoles

*Manel Martínez-Grau, Joan J. Solaz-Portolés y Vicent Sanjosé*

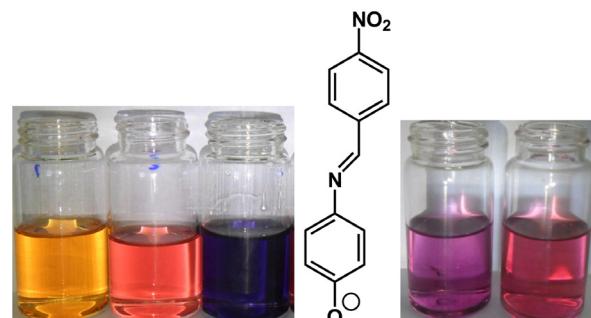
$$K_c = \frac{[C]^c [D]^d}{[A]^a [B]^b}$$

**Graphical Abstract**

The chemical equilibrium constant can generate didactic problems. In this study, we propose a way to determine students' conceptual knowledge of this constant.

- 745 Preparation and properties of perichromic dye: an undergraduate laboratory

*Priscilla Abarca, Patricia Silva, Iriux Almodovar and Marcos C. Rezende*

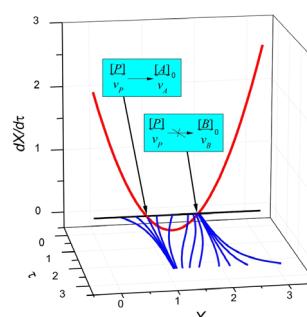


**Graphical Abstract**

In a colorful undergraduate lab, perichromism is illustrated with an easily prepared dye whose solutions are sensitive to the solvent ("solvatochromism"), to the addition of salts ("halochromism"), and to the temperature ("thermochromism").

- 748 Dinâmica não-linear e reagente limitante: um exemplo de bifurcação transcritica

*Diego J. R. da Silva*



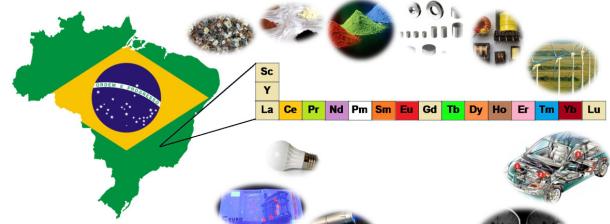
**Graphical Abstract**

The limiting reagent influence on the nonlinear dynamics of a bimolecular reaction is investigated by phase plane plots (in red) and integral curves (in blue).

## Assuntos Gerais

753 Terras raras no Brasil: histórico, produção e perspectivas

*Paulo C. de Sousa Filho e Osvaldo A. Serra*



### Graphical Abstract

This contribution discusses the properties, the applications and the current scenario of the rare earth elements in Brazil, and some perspectives regarding the prospection, the market and the government policy about these valuable resources are pointed.