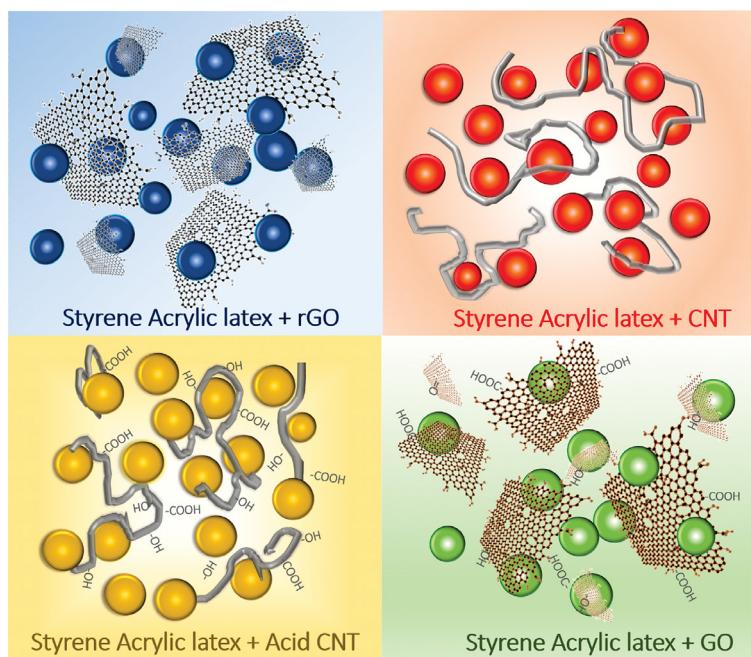


## Cover Picture



Acrylic latex-based nanocomposites have been prepared with three different carbon nanomaterials (nanotubes and graphene-like structures). Due to the unique interaction between the components, resulting materials present noticeable multifunctionality. The electrical, mechanical, magnetic and chemical properties can be modulated according the type and amount of filler, creating several different materials that can be chosen for specific applications. Details are presented in the Article **Multifunctional Nanocomposites between Different Carbon Nanostructures and Styrene Acrylic Latex** by *Carolina F. Matos, Fernando Galembeck and Aldo J. G. Zarbin* on page 1396.

## Contents

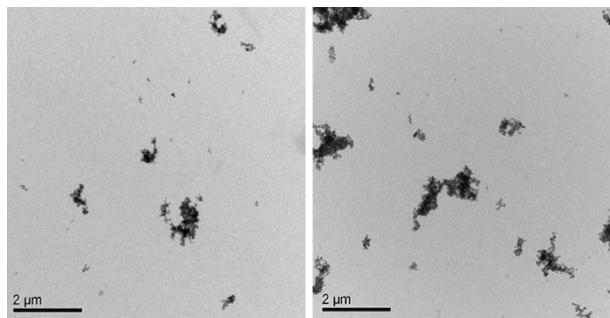
### Editorial

- 1349 Celebrating the 40<sup>th</sup> Anniversary of Brazilian Chemical Society (SBQ): Retrospective and Perspectives  
*Marília O. F. Goulart and Rossimiriam P. de Freitas*

## Articles

**1351 An Investigation on Morphology and Fractal Dimension of Diesel and Diesel-Biodiesel Soot Agglomerates**

<https://doi.org/10.1593/jbcs.2020-0001>  
Sl online

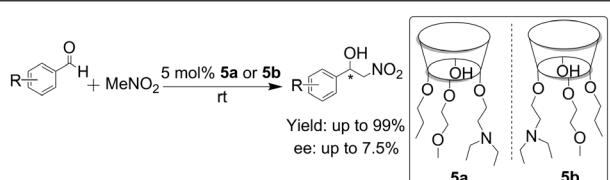


**Graphical Abstract**

Fractal-like dimension and morphology of ultrafine particles emitted by a diesel engine run with B4, B50, and B100 are evaluated.

**1363 Synthesis of *N,O*-Type Inherently Chiral Calix[4]arenes Substituted on the Lower Rim and their Organocatalysis Properties**

<https://doi.org/10.1593/jbcs.2020-0002>  
Sl online

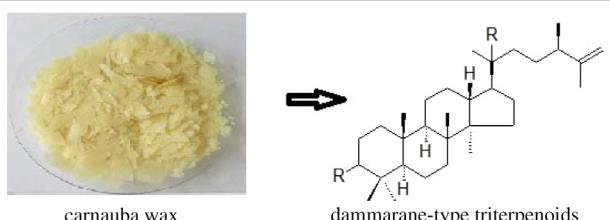


**Graphical Abstract**

Inherently chiral calix[4]arenes can catalyze Henry reaction between aromatic aldehydes and nitromethane in excellent yields but poor enantioselectivities.

**1371 Dammarane Triterpenoids from Carnauba, *Copernicia prunifera* (Miller) H. E. Moore (Arecaceae), Wax**

<https://doi.org/10.1593/jbcs.2020-0003>  
Sl online

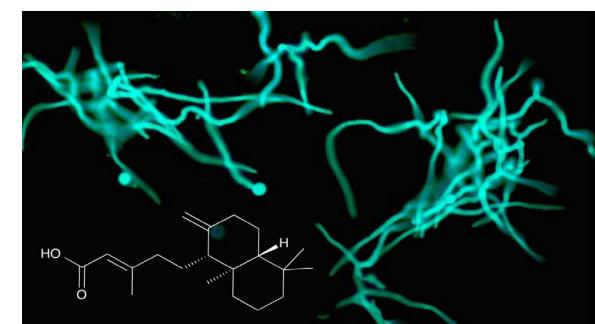


**Graphical Abstract**

Sixteen dammarane-type triterpenoids, including thirteen new, were identified from carnauba (*Copernicia prunifera*) wax (types 1 and 4).

**1377 Copaiba Oil and Its Constituent Copalic Acid as Chemotherapeutic Agents against Dermatophytes**

<https://doi.org/10.1593/jbcs.2020-0004>  
Sl online

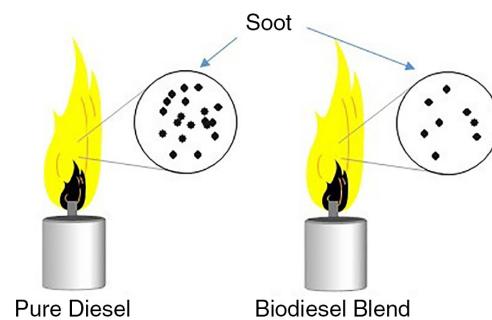


**Graphical Abstract**

Copalic acid activity against dermatophytes *Trichophyton rubrum*, *Trichophyton mentagrophytes* and *Microsporum gypseum*.

**1384 Study of the Influence of Biodiesel in Soot Emissions of Diesel Laminar Diffusion Flames**

*Lincoln Tolomelli e Tolomelli, Luiz G. Barreta, Pedro T. Lacava and Dermeval Carinhana Jr.*



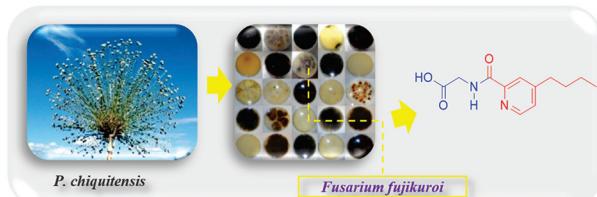
**Graphical Abstract**

Biodiesel/diesel blends flames are investigated using LII. The results showed a decrease of soot production as the amount of biodiesel was increased.

**1389 Antimicrobial Screening of Endophytic Fungi Isolated from the Aerial Parts of *Paepalanthus chiquitensis* (Eriocaulaceae) Led to the Isolation of Secondary Metabolites Produced by *Fusarium fujikuroi***

*SI online*

*Felipe Hildário, Vanessa M. Chapla, Angela R. Araujo, Paulo T. Sano, Taís M. Bauab and Lourdes C. dos Santos*



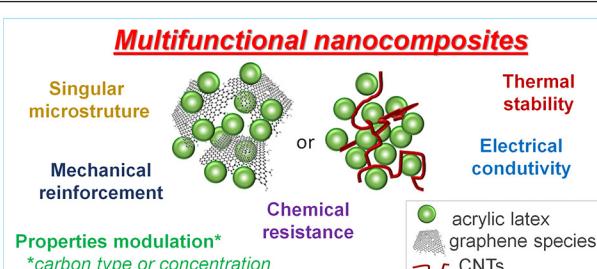
**Graphical Abstract**

Metabolite produced by *Fusarium fujikuroi* isolated from the capitulae of *Paepalanthus chiquitensis* (Eriocaulaceae). Photo of *P. chiquitensis* was taken by Marcelo T. L. de Oliveira.

**1396 Multifunctional Nanocomposites between Different Carbon Nanostructures and Styrene Acrylic Latex**

*SI online*

*Carolina F. Matos, Fernando Galembeck and Aldo J. G. Zarbin*



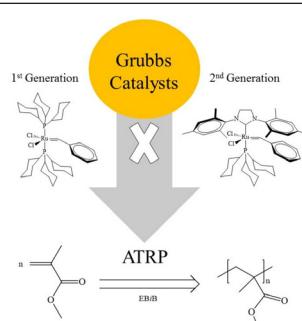
**Graphical Abstract**

Multifunctional nanocomposites between carbon nanostructures and acrylic latex were successfully prepared, with improved and tunable properties compared to the neat polymer.

**1407 Atom Transfer Radical Polymerization of Methyl Methacrylate Mediated by Grubbs 1<sup>st</sup> and 2<sup>nd</sup> Generation Catalysts: Insight into the Active Species**

*SI online*

*Maria Beatriz A. Afonso, Lucas G. Gonçalves, Patrícia Borim, José Luiz S. Sá, Beatriz E. Goi and Valdemiro P. Carvalho-Jr.*

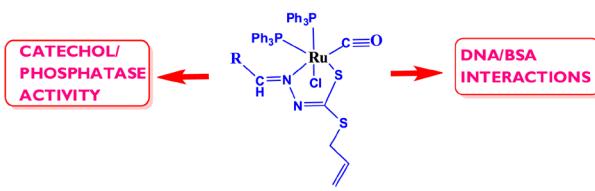


**Graphical Abstract**

Grubbs 1<sup>st</sup> and 2<sup>nd</sup> generation catalyst were evaluated as catalyst in atom-transfer radical polymerization (ATRP) of methyl methacrylate (MMA) and their yet unknown mechanism for ATRP was investigated.

**1414 Catechol Oxidase, Phosphatase-Like Activity, DNA/BSA Binding Studies of Ru<sup>II</sup> Complexes of S-Allyldithiocarbazate: Synthesis and Spectral Studies**

Si online Ponnusamy Selvakumar, Ramaswamy Narayanasamy, Nanjan Nanjundan, Krishnaswamy Velmurugan and Raju Nandhakumar

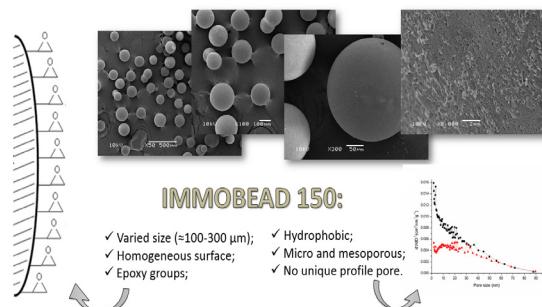


**Graphical Abstract**

Ruthenium(II) complexes containing S-allyldithiocarbazate derivatives, potentially active towards *in vitro* biomolecular interactions and bio-catalytic transformations such as catechol oxidation and phosphate hydrolysis.

**1430 Physical-Chemical Properties of the Support Immobead 150 Before and After the Immobilization Process of Lipase**

Si online Carla R. Matte, Carolina Bordinhão, Jakeline K. Poppe, Edilson V. Benvenutti, Tania M. H. Costa, Rafael C. Rodrigues, Plinio F. Hertz and Marco A. Z. Ayub



**Graphical Abstract**

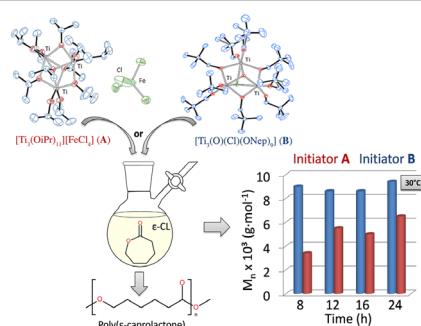
Immobead 150 possess interesting features to be used as a support for immobilization of lipases.

**1440 Improved Reactivity in the Ring-Opening Polymerization of  $\epsilon$ -Caprolactone with a Trinuclear Titanium(IV) Oxochloroneopentoxide as Initiator**

Si online Siddhartha O. K. Giese, Thiago A. da Silva, David L. Hughes, André Luis Rüdiger, Eduardo L. de Sá, Sônia F. Zawadzki, Jaisa F. Soares and Giovana G. Nunes

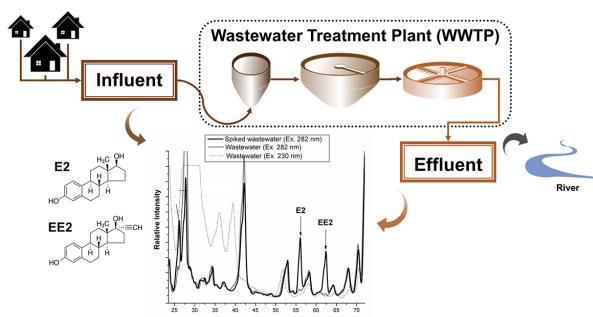
**Graphical Abstract**

Complexes  $[\text{Ti}_3(\text{O}^{\prime}\text{Pr})_{11}][\text{FeCl}_4]$  and  $[\text{Ti}_3(\text{O})(\text{Cl})(\text{ONep})_9]$  were employed as initiators for the polymerization of  $\epsilon$ -caprolactone ( $\epsilon$ -CL). The better polymerization reactivity of  $[\text{Ti}_3(\text{O})(\text{Cl})(\text{ONep})_9]$  seems to be associated with the maintenance of its polynuclear structure in the reaction mixture.



**1453 Sensitive Estrogens Determination in Wastewater Samples by HPLC and Fluorescence Detection**

Marcus Vinicius de Liz, Bianca do Amaral, Sandra Stets, Noemi Nagata and Patricio Peralta-Zamora

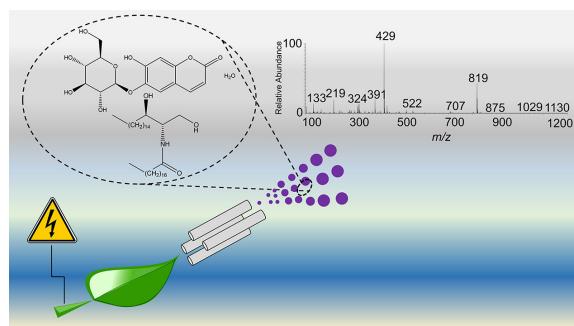


**Graphical Abstract**

Fluorescence-based HPLC method for quantification of estrogens ( $17\beta$ -estradiol and  $17\alpha$ -ethynodiol) in both influent and effluent wastewater samples.

**1461 Differentiation of Toxic and Non-Toxic Leaves of *Jatropha curcas* L. Genotypes by Leaf Spray Mass Spectrometry**

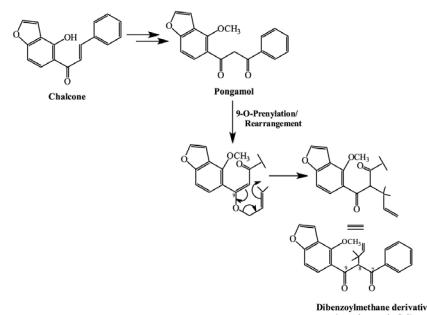
Igor Pereira, Thays C. de Carvalho, Wanderson Romão,  
SI online Paulo R. Filgueiras, Bruno G. Laviola, Clenilson M.  
Rodrigues, Patrícia V. Abdenur and Boniek G. Vaz

**Graphical Abstract**

A recent ambient ionization mass spectrometry technique known as leaf spray (LS-MS) is a simple and fast method for screening of plant samples. In this work, toxic and non-toxic *Jatropha curcas* leaves were differentiated by LS-MS.

**1467 Antiproliferative Activity of Dibenzoylmethanes from Root Bark of *Muellera filipes* (Benth) M.J. Silva & A.M.G. Azevedo**

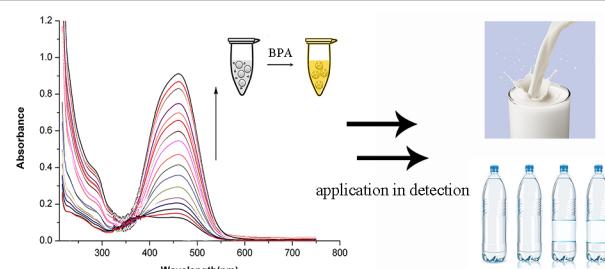
Érica L. Santos, Juliana Jo, Francisco A. Marques,  
Ana Maria G. A. Tozzi, Ana Lícia T. G. Ruiz and  
Beatriz Helena L. N. S. Maia

**Graphical Abstract**

Dibenzoylmethane derivatives with a substituent on C-8 are extremely rare in nature. These compounds can potentially be used as biomarkers of closely related genera. Two compounds showed strong activity against human cancer cell lines.

**1475 Development of a Novel Spectrophotometric Method Based on Diazotization-Coupling Reaction for Determination of Bisphenol A**

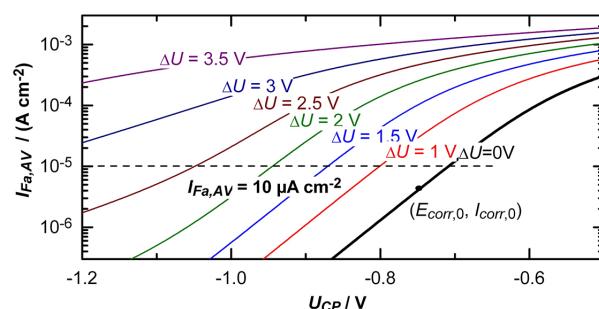
Zhiqun Xu, Qiao Wu, Yunjian Duan, Meixia Yang,  
Minrui Ou and Xiaoping Xu

**Graphical Abstract**

A novel, rapid, and easy method for quantification of BPA via diazo coupling reaction and its applications in the actual food samples.

**1483 AC Induced Corrosion of Underground Steel Pipelines under Cathodic Protection: III. Theoretical Approach with Electrolyte Resistance and Double Layer Capacitance for Mixed Corrosion Kinetics**

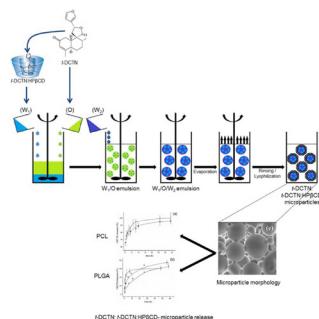
Ibrahim Ibrahim, Michel Meyer, Hisasi Takenouti and  
Bernard Tribollet

**Graphical Abstract**

Cathodic protection potential in presence of a stray AC voltage for steel pipe buried in a mildly corrosive soil provided that AC corrosion does not induce any change of soil chemistry.

**1494 Coencapsulation of *trans*-Dehydrocrotonin and *trans*-Dehydrocrotonin:hydroxypropyl- $\beta$ -cyclodextrin into Microparticles**

Waldenice A. Morais, Benício de Barros Neto, Isabella M. F. Cavalcanti, Francisco H. Xavier Junior, Nereide S. Santos-Magalhães and Maria Aparecida M. Maciel

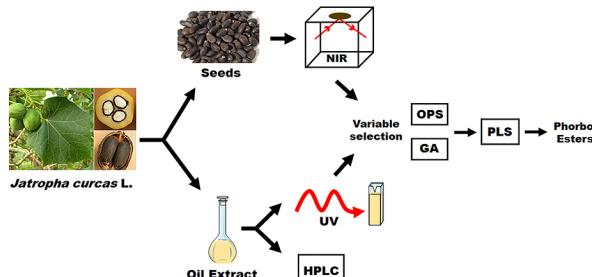


**Graphical Abstract**

Coencapsulation of *t*-DCTN and *t*-DCTN:HP- $\beta$ -CD into PCL and PLGA microspheres were developed using factorial design. Oral formulations of PLGA microparticles containing *t*-DCTN and/or *t*-DCTN:HP- $\beta$ -CD were obtained to be applied in *in vivo* studies.

**1506 Multivariate Calibration to Determine Phorbol Esters in Seeds of *Jatropha curcas* L. Using Near Infrared and Ultraviolet Spectroscopies**

Jussara V. Roque, Luiz A. S. Dias and Reinaldo F. Teófilo



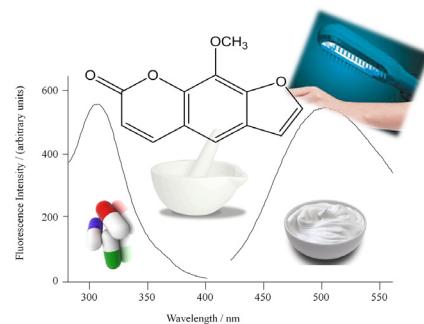
**Graphical Abstract**

Determination of phorbol esters of *Jatropha curcas* L. using NIR and UV spectroscopies employing PLS regression and variable selection.

**1517 Implementation of a Spectrofluorimetric Method to the Determination of 8-Methoxysoralen in Capsules and Creams Used in Treatment of Psoriasis and Vitiligo: an Evaluation of the Quality of Compounding Pharmacies in Rio de Janeiro**

Catarina A. Oliveira, Marcos M. Gouvêa, Flávio H. S. A.

Ribeiro, Eduardo Ricci-Júnior and Flávia F. C. Marques

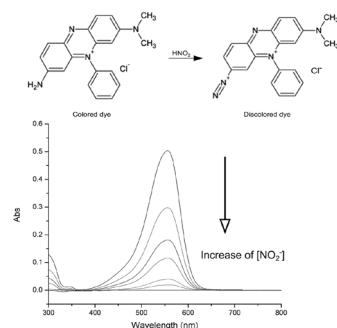


**Graphical Abstract**

The spectrofluorimetric determination of 8-methoxysoralen was applied to assessing the quality of medicines produced by compounding pharmacies.

**1528 Methylene Violet 3 RAX Dye as a New Reagent for the Determination of Nitrite in Cured Meats and Vegetables**

Caroline O. da Rocha, João Flávio S. Petrucci and Arnaldo A. Cardoso

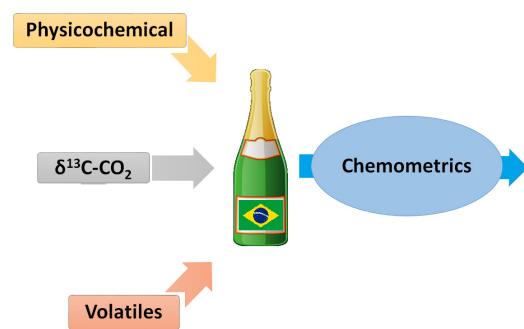


**Graphical Abstract**

Methylene Violet 3 RAX dye as a new reagent for the determination of nitrite in cured meats and vegetables.

**1534 Exploratory Analysis of Sparkling Wines Based in the Combined Data of Stable Isotope Analysis with Physicochemical Variables and Volatile Profile**

*SI online* Victor H. J. M. dos Santos, Paulo G. Celso, Artur L. G. Rocha, Samuel Giovanaz, Carolina Z. Guerra, Jessica P. Pires, Pamela M. Engelmann and Luiz F. Rodrigues

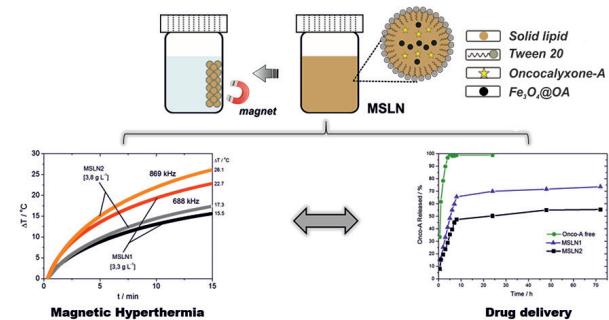


**Graphical Abstract**

The chemometric tool was applied to the physicochemical, volatiles and stable isotope data to perform the exploratory analysis and classification of sparkling wines samples.

**1547 Preliminary Evaluation of Novel Triglyceride-Based Nanocomposites for Biomedical Applications**

Raimundo R. de Almeida, Juan Gallo, Aiêrtá C. C. da Silva, Ana K. O. da Silva, Otilia D. L. Pessoa, Tamara G. Araújo, Luzia K. A. M. Leal, Pierre B. A. Fehinne, Manuel Bañobre-López and Nágila M. P. S. Ricardo

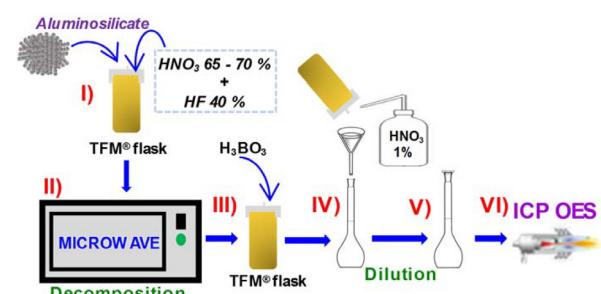


**Graphical Abstract**

Magnetic solid lipid nanoparticles (MSLN) for application in magnetic hyperthermia and controlled delivery of oncocalyxone-A.

**1557 A Straightforward Method for Determination of Al and Na in Aluminosilicates Using ICP OES**

*SI online* Francisca S. O. Ramos, Ramon K. S. Almeida, Cícero A. Lopes Júnior, Marco Aurélio Z. Arruda and Heloise O. Pastore

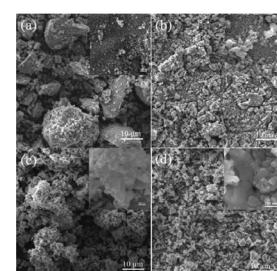


**Graphical Abstract**

Microwave-assisted acid decomposition using closed vessels was applied to aluminosilicates in order to quantify Na and Al, reducing the time consumed for samples preparation step. This procedure avoided analytes losses and contamination.

**1564 Effect of PVA Concentration on Structure and Performance of Precipitated Iron-Based Catalyst for Fischer-Tropsch Synthesis**

Cailian Ma, Guanghua Dong, Xia Liu and Jiangang Chen



**Graphical Abstract**

Polyvinyl alcohol (PVA) concentration has a significant effect on the structure of catalysts and dispersion of their active phase. Therefore, the catalyst prepared with 15 wt.% PVA, exhibits high performance and good thermal stability for Fischer-Tropsch synthesis.

## Short Reports

**1573 Suzuki-Miyaura Coupling between 3-Iadolawsone and Arylboronic Acids. Synthesis of Lapachol Analogues with Antineoplastic and Antileishmanial Activities**

 <https://doi.org/10.1593/jbcs.2020-001573>  
*S. L. S. Gomes, Gardenia C. G. Militão, Arinice M. Costa,  
 Cláudia Ó. Pessoa, Letícia V. Costa-Lotufo, Edézio F.  
 Cunha-Junior, Eduardo C. Torres-Santos,  
 Paulo R. R. Costa and Alcides J. M. da Silva*

### Graphical Abstract

Suzuki-Miyaura cross coupling reaction between 2-hydroxy-3-iodonaphthalene-1,4-dione and a series of arylboronic acids/esters followed by OH-protection as the corresponding *N,N*-diethyl carbamates is reported. The synthesized compounds were evaluated regarding their antineoplastic and antileishmanial activities furnishing promising results.

