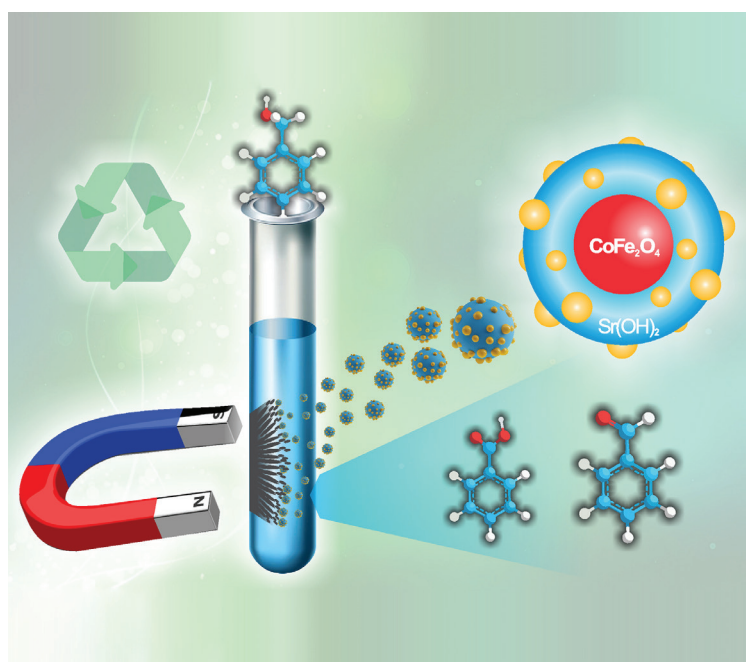


## Cover Picture



Gold-based catalysts are appealing candidates to substitute stoichiometric reagents in oxidation reactions. The major hurdle in their wide application is related to separation issues, which can be solved via the magnetic recovery potential of the cobalt ferrite ( $\text{CoFe}_2\text{O}_4$ ). Aldehydes or esters are starting materials necessary for the fine chemistry industry, which are obtained by alcohol oxidation. The performance of the proposed material is increased by metal-support interactions that use the properties of the  $\text{Sr}(\text{OH})_2$  material and Au nanoparticles. Focusing on sustainable approaches, the studies herein presented were able to oxidize the benzyl alcohol with a good balance between activity and selectivity, with a catalyst that was used five times without performance loss. Details are presented in the Article **Gold Supported on Strontium Surface-Enriched  $\text{CoFe}_2\text{O}_4$  Nanoparticles: a Strategy for the Selective Oxidation of Benzyl Alcohol** by Laise N. S. Pereira, Carlos E. S. Ribeiro, Aryane Tofanello, Jean C. S. Costa, Carla V. R. de Moura, Marco A. S. Garcia and Edmilson M. de Moura on page 1317.

## Contents

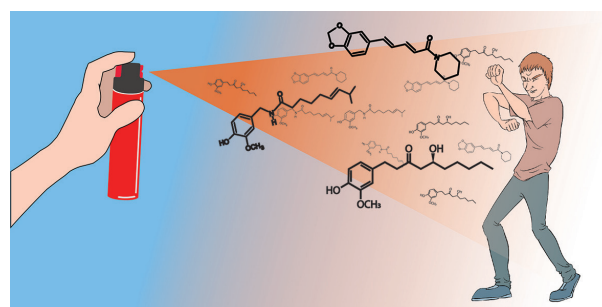
### Review

#### 1115 Perspectives and Applications of Natural Products as Civilian Defense Devices

Ananda S. Antonio, Gabriel D. Fonseca, Álvaro J. B. Mendes, Larissa S. M. Wiedemann and Valdir F. Veiga-Junior

#### Graphical Abstract

Capsaicin, piperine, gingerol and other pungent natural compounds are technologically developed bioproducts for civilian's self-defense proposes.



## Articles

### 1130 Determination of L-Ascorbic Acid in Milk by Ultra-High-Performance Liquid Chromatography Coupled to Tandem Mass Spectrometry Analysis

Caroline D. Zappiello, Antonio E. Nicácio, Luciana P. Manin, Liane Maldaner and Jesuí V. Visentainer

#### Graphical Abstract

This study presented the development of a fast and accurate method for determination of L-ascorbic acid (L-AA) in different milk samples (raw and processed). In the sample preparation, a low toxicity organic solvent was used in the degreasing and deproteinization step, avoiding L-AA oxidation.



### 1138 A Complete and Unambiguous $^1\text{H}$ and $^{13}\text{C}$ NMR Signals Assignment of *para*-Naphthoquinones, *ortho*- and *para*-Furanonaphthoquinones

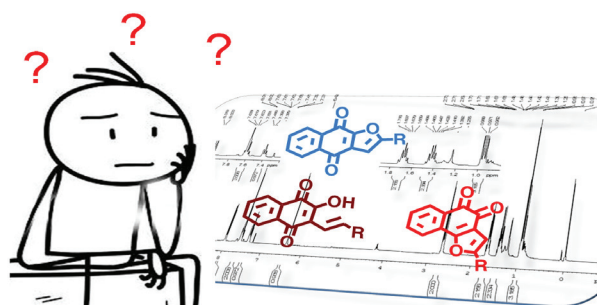


SI online

Tatiane F. Borgati, José D. de Souza Filho and Alaíde B. de Oliveira

#### Graphical Abstract

This is the first report distinguishing *para*-naphthoquinones, *ortho*- and *para*-furanonaphthoquinones by one and two-dimensional techniques of nuclear magnetic resonance (NMR).



### 1150 Human Metabolism of the Anabolic Steroid Methasterone: Detection and Kinetic Excretion of New Phase I Urinary Metabolites and Investigation of Phase II Metabolism by GC-MS and UPLC-MS/MS

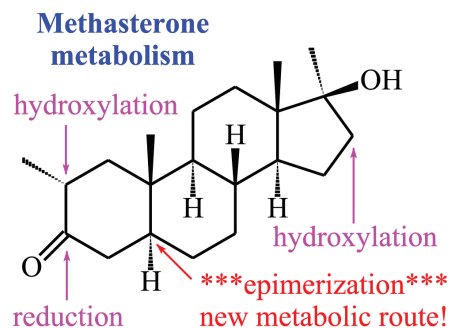


SI online

Wendell S. Magalhães, Bruno C. Garrido, Gustavo A. Cavalcanti, Monica C. Padilha, Alessandro Casilli, Henrique M. G. Pereira and Francisco R. de Aquino Neto

#### Graphical Abstract

The phase I and II metabolism of methasterone, a designer anabolic steroid prohibited for athletes and monitored by anti-doping laboratories, were studied by chromatographic techniques using human urine samples. One new metabolite is shown: 17 $\beta$ -hydroxy-2 $\alpha$ ,17 $\alpha$ -dimethyl-5 $\beta$ -androstan-3-one, obtained from the epimerization at C5.



### 1161 DFT Study of the Interaction between the $\text{Ni}^{2+}$ and $\text{Zn}^{2+}$ Metal Cations and the 1,2-Dithiolene Ligands: Electronic, Geometric and Energetic Analysis

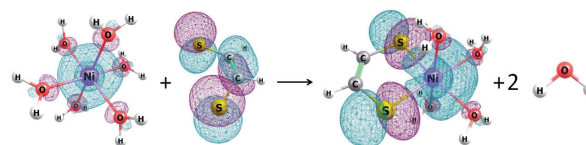


SI online

Glauber S. Melengate, Daniel G. S. Quattrociocchi, José M. Siqueira Júnior, Stanislav R. Stoyanov, Leonardo M. Costa and Glaucio B. Ferreira

#### Graphical Abstract

The affinity between the  $\text{Zn}^{2+}$  and  $\text{Ni}^{2+}$  metal cations and 1,2-dithiolene ligands was quantified from the substitution energies and rationalized through energetic, electronic and geometric parameters.



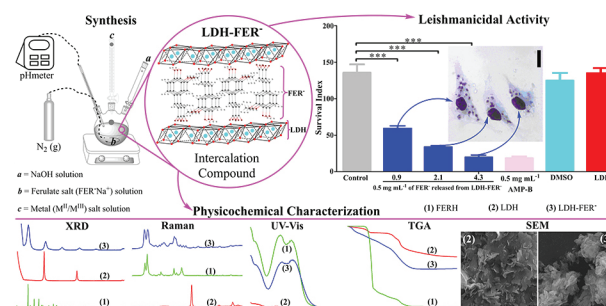
**1178 Ferulate Anion Intercalated into Zn/Al Layered Double Hydroxide: A Promising Intercalation Compound for Inhibition of *Leishmania (L.) amazonensis***

SI online

Robson Sousa, Bruno J. M. da Silva, Amarlis A. Dias, Carla C. F. Meneses, Beatriz A. Bentes, Edilene O. Silva, Cláudio M. R. Remédios, Waldecki P. Feio, Olivier Masson, Cláudio N. Alves, Mara M. S. P. Arruda and Jerônimo Lameira

**Graphical Abstract**

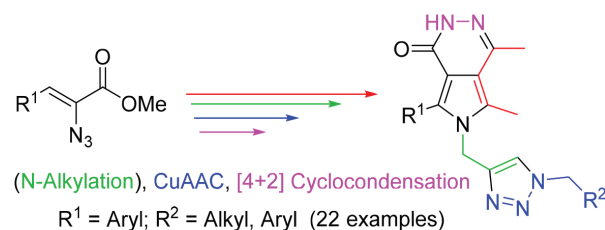
Synthesis, physicochemical characterization and leishmanicidal activity of the layered double hydroxide (LDH)-ferulate anion (FER<sup>-</sup>) intercalation compound, a potential drug delivery vehicle for potential treatment of cutaneous leishmaniasis without any side effect.



**1189 Streamlined Synthesis of 6-((1H-1,2,3-Triazol-4-yl)methyl)-1H-pyrrolo[3,4-d]pyridazin-1-one System via Sequential N-Alkylation, CuAAC, and [4 + 2] Cyclization Reactions**

SI online

Helio G. Bonacorso, Hernane T. Magalhães, Gean M. Dal Forno, Francieli M. Libero, Manfredo Hoerner, Clarissa P. Frizzo, Marcos A. P. Martins and Nilo Zanatta



**Graphical Abstract**

Useful synthesis of pyrrolo[3,4-d]pyridazin-1-ones by sequential N-alkylation, CuAAC and [4 + 2] cyclocondensation reactions.

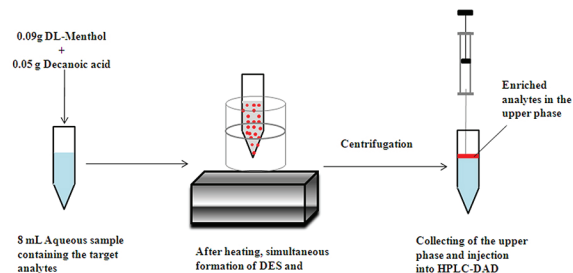
**1203 A Deep Eutectic Solvent as an Extraction Solvent to Separate and Preconcentrate Parabens in Water Samples Using *in situ* Liquid-Liquid Microextraction**

SI online

Dandan Ge, Ying Wang, Qian Jiang and Enrui Dai

**Graphical Abstract**

*In situ* deep eutectic solvent liquid-liquid microextraction method was developed as a sample preparation method for the detection of parabens. The deep eutectic solvent, formed *in situ* by the DL-menthol and decanoic acid, was used as the microextraction solvent.



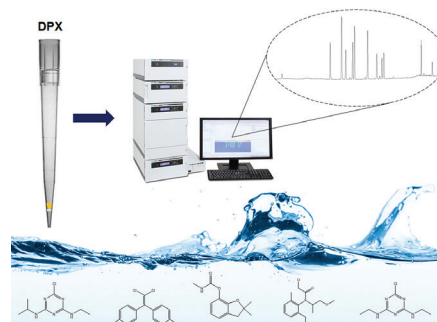
**1211 Assessment of a Fully Optimized DPX-Based Procedure for the Multiclass Determination of Pesticides in Drinking Water Using High-Performance Liquid Chromatography with Diode Array Detection**

SI online

Gabriela Corazza, Josias Merib, Sângela N. do Carmo, Leila D. Mendes and Eduardo Carasek

**Graphical Abstract**

Disposable pipette extraction (DPX)-based procedure was fully optimized for determination of multiclass of pesticides in 20 drinking water samples by high-performance liquid chromatography coupled with diode array detection (HPLC-DAD).

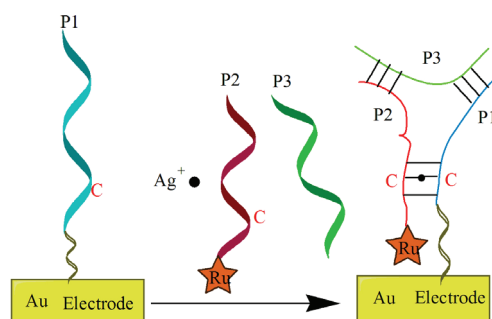


**1222 Electrochemiluminescence Detection of Silver Ion Based on Trigeminal Structure of DNA**

Zhejiang Li, Xuemei Fan, Baoyue Cao, Fei Yuan, Fengying Chen and Shumin Wang

**Graphical Abstract**

A novel electrochemiluminescence sensor for highly sensitive detection of  $\text{Ag}^+$  is developed based on the sensitive "turn-on" three-way junction of deoxyribonucleic acid (DNA).

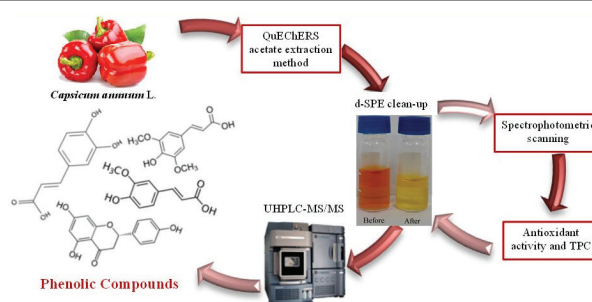


**1229 Determination of Phenolic Compounds in Red Sweet Pepper (*Capsicum annuum* L.) using a Modified QuEChERS Method and UHPLC-MS/MS Analysis and Its Relation to Antioxidant Activity**

Carina A. Rodrigues, Antonio E. Nicácio, Isabel C. S. F. Jardim, Jesuí V. Visentainer and Liane Maldaner

**Graphical Abstract**

A fast, easy and efficient analytical method based on a modified quick, easy, cheap, effective, rugged and safe (QuEChERS) method and ultra-high performance liquid chromatography tandem mass spectrometry (UHPLC-MS/MS) analysis was developed and validated for the determination of phenolic compounds in red sweet pepper.

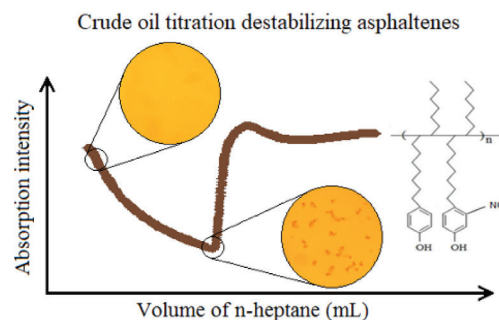


**1241 Model Molecules for Evaluating Asphaltene Precipitation Onset of Crude Oils**

Rita C. P. Nunes, Michel R. T. Valle, William R. D. Reis, Thiago M. Aversa, Sofia D. Filipakis and Elizabete F. Lucas

**Graphical Abstract**

The asphaltenes precipitation onset point of crude oil samples that do not have well-defined curves can be ascertained by adding a solution of toluene containing an additive.

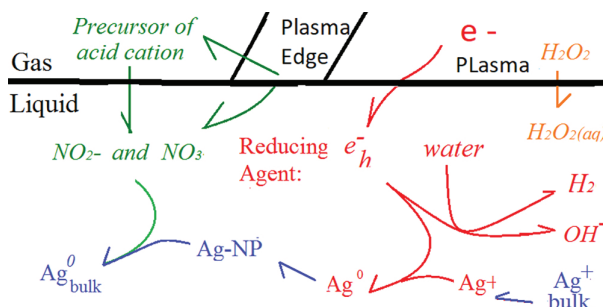


**1252 Reduction of Aqueous  $\text{Ag}^+$  Steered by Electrochemical Plasma: Connecting the Bulk pH Variation with the Reaction Pathways for Hydrated Electrons**

SI online Ingrid A. Gonçalves, Jairo Barauna, Fernando J. Cunha-Filho, Osvaldo Chiavone-Filho, Jussier O. Vitoriano, Clodomiro Alves Júnior and Andressa Mota-Lima

**Graphical Abstract**

The fast acidification promoted by a discharge in nitrogen-based gas phase interferes in the nanoparticles (NP) formation; hydrated electrons induced by an electrochemical discharge are competitively consumed through scavenger reaction (silver reduction) and through the second-order recombination reaction; fact that could only be perceived for discharge in the helium because NP formation and basification are simultaneously observed.

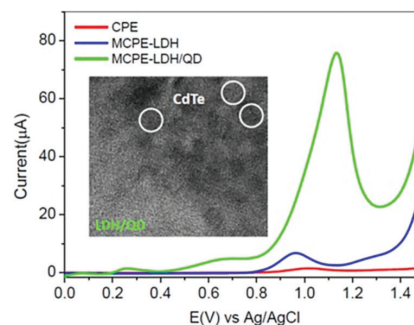


**1266 Synthesis of Hydrotalcite-Supported CdTe Semiconductor Nanocrystals for Electrochemical Detection of Ciprofloxacin**

Sanny W. M. M. Carvalho, Tiago B. S. Santana,  
SI online Charlene R. S. Matos, Luiz P. Costa, Eliana M. Sussuchi and  
Iara F. Gimenez

**Graphical Abstract**

Stable CdTe nanocrystals were prepared in a single step route onto the surface of layered double hydroxide as modifier to carbon paste electrodes.

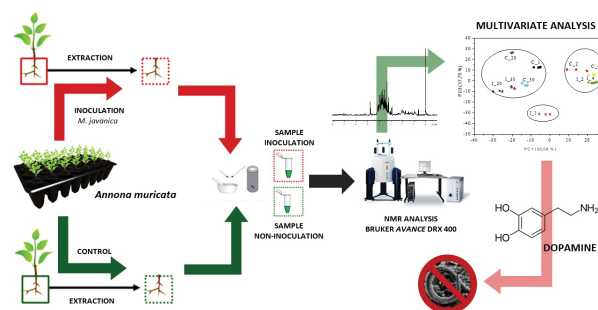


**1276 NMR-Based Metabolomic Screening for Metabolites Associated with Resistance to *Meloidogyne javanica* in *Annona muricata* Roots**

SI online Alan R. T. Machado, Felipe S. Medeiros, José D. de Souza Filho,  
Marcelo M. Sena, Willian C. Terra and Lúcia P. S. Pimenta

**Graphical Abstract**

Induced and pre-formed mechanism defense of *Annona muricata* against *Meloidogyne javanica* were detected by nuclear magnetic resonance (NMR)-based metabolomic analysis.

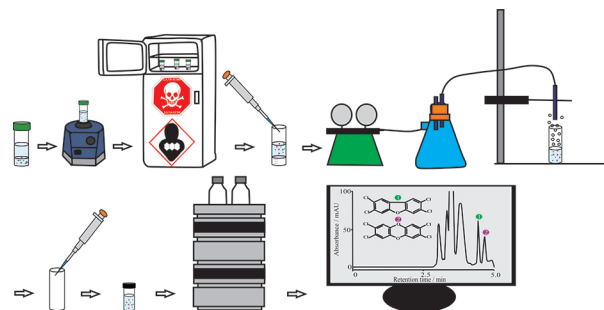


**1284 Simultaneous Determination of 2,3,7,8-TCDD and 2,3,7,8-TCDF in Water Samples by LLE-LTP and HPLC-DAD**

Lázaro C. Sicupira, João P. F. Tiago, Gevany P. de Pinho and  
SI online Flaviano O. Silvério

**Graphical Abstract**

The image represents liquid-liquid extraction with low-temperature partition (LLE-LTP) methodology combined with high-performance liquid chromatography coupled a diode array detector (HPLC-DAD) used in the present study.

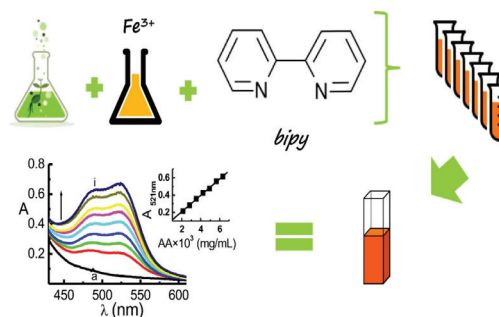


**1293 A Procedure for Assessment of the Reducing Capacity of Plants-Derived Beverages Based on the Formation of the  $\text{Fe}^{II}/2,2'$ -Bipyridine Complex**

Rafaela L. Sacchi, Waila E. L. Santana, Cecilia V. Nunez and  
Horacio D. Moya

**Graphical Abstract**

In the present study the reduction reaction of  $\text{Fe}^{III}$  to  $\text{Fe}^{II}$  in aqueous solution containing 2,2'-bipyridine (pH 4.6; acetate buffer) was used as an alternative spectrophotometric method to measure the total reducing capacity of teas and herbs. The method suggested here is fast, simple, reliable and easy to perform.





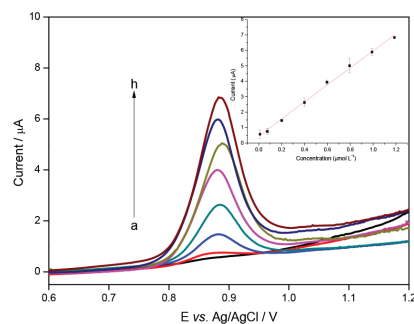
**1302 Semiconductor Nanocrystals-Reduced Graphene Composites for the Electrochemical Detection of Carbendazim**

*Paula C. A. Santana, Jéssica B. S. Lima, Tiago B. S. Santana, Luís F. S. Santos, Charlene R. S. Matos, Luiz P. da Costa, Iara F. Gimenez and Eliana M. Sussuchi*

SI online

**Graphical Abstract**

A new nanocomposite based on ZnCdTe semiconductor nanocrystals synthesized *in situ* on reduced graphene oxide (rGO) was obtained. The modified electrodes were prepared and successfully applied for the determination of carbendazim in orange juice samples.



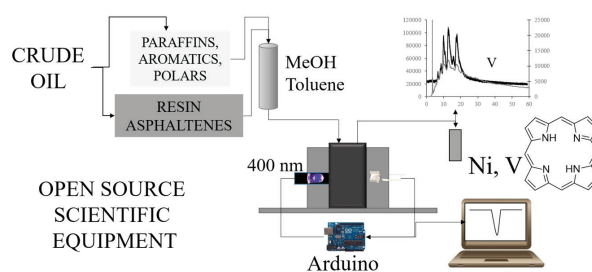
**1309 Automatized Separation of Fractions from Petroleum Based on Spectrophotometric Signal Derivative Using Open-Source Hardware for the Determination of Ni and V Linked to Porphyrins**

*Daniel M. Silva, Álvaro J. Pereira, Tatiana D. Saint'Pierre, Pierre M. Esteves, Anderson A. Rocha, Rainério Escalfoni Jr. and Christiane Duyck*

SI online

**Graphical Abstract**

Open-source device based on Arduino for separation of porphyrins fractions from crude oil is presented and successfully tested.



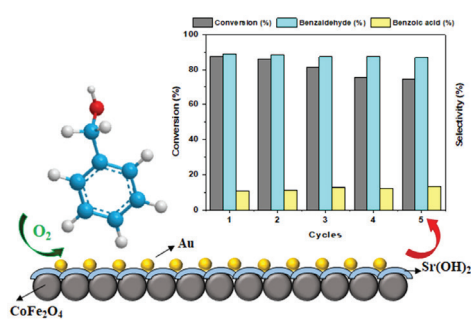
**1317 Gold Supported on Strontium Surface-Enriched CoFe<sub>2</sub>O<sub>4</sub> Nanoparticles: a Strategy for the Selective Oxidation of Benzyl Alcohol**

*Laise N. S. Pereira, Carlos E. S. Ribeiro, Aryane Tofanello, Jean C. S. Costa, Carla V. R. de Moura, Marco A. S. Garcia and Edmilson M. de Moura*

SI online

**Graphical Abstract**

This paper deals with the interaction between Sr(OH)<sub>2</sub> and CoFe<sub>2</sub>O<sub>4</sub> and their role in the oxidation reaction of benzyl alcohol with gold nanoparticles.



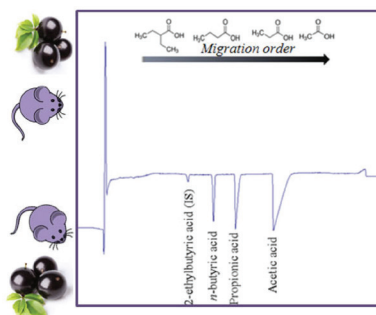
**1326 Determination of Short Chain Fatty Acids in Mice Feces by Capillary Electrophoresis**

*Leticia A. Marques, Cinthia B. B. Cazarin, Juliano Bicas, Mário R. Maróstica Junior, Emanuel Carrilho and Stanislaw Bogusz Junior*

SI online

**Graphical Abstract**

Short-chain fatty acids (SCFA) are enteric end-products essential to health. Quantification of SCFA in a small amount of mice feces sample is a big challenge. We developed, validated and applied a method based on capillary electrophoretic with indirect ultraviolet detection for determination of SCFA in mouse feces to evaluate the effect of the consumption of aqueous extract of jabuticaba on mice with induced colitis.



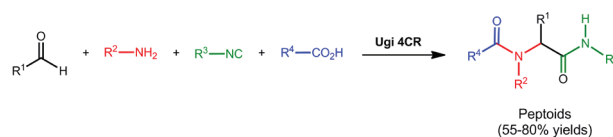
## Short Report

### 1334 Synthesis and Antileishmanial Activity of Some Functionalized Peptoids



SI online

Daniel Previdi, Stephanie Rodrigues, Mike G. Coelho,  
Ana Carolina B. B. Candido, Lizandra G. Magalhães and  
Paulo M. Donate



#### Graphical Abstract

This paper describes the microwave-assisted synthesis of thirteen functionalized peptoids and evaluates their *in vitro* antileishmanial activity against *Leishmania (Leishmania) amazonensis* promastigotes.

