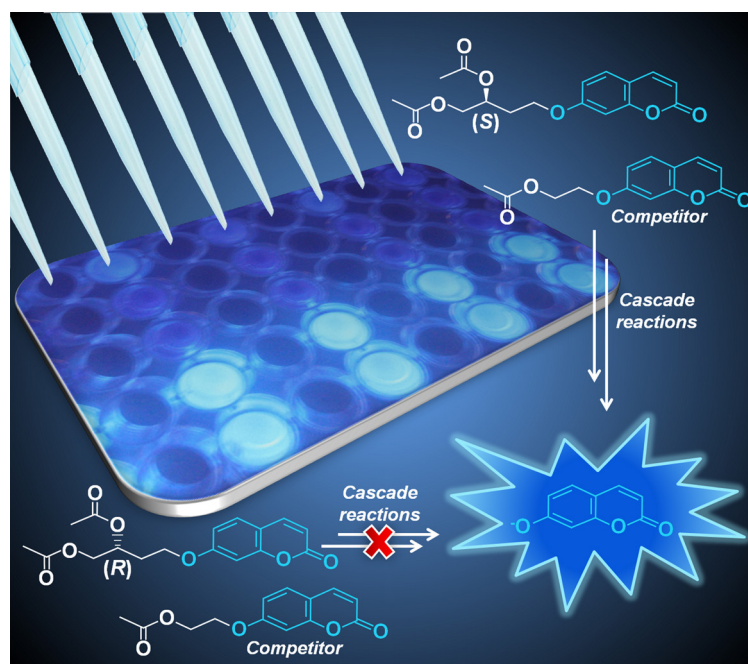


## Cover Picture



High throughput screening techniques (HTS) are fast and efficient alternatives to evaluate enzymatic activities. Here, this technique is applied to obtain enantiomeric excess and conversions values with chiral fluorogenic probes and a non fluorogenic competitor, which was named Quick-*ee*. The fluorescent signal reveals of the enantioselectivity of the enzyme. Details are presented in the Article **High Throughput Enzymatic Enantiomeric Excess: Quick-*ee*** by Maria L. S. de O. Lima, Caroline C. da S. Gonçalves, Juliana C. Barreiro, Quezia Bezerra Cass and Anita Jocelyne Marsaioli on page 319.

## Contents

### Letter

- 209 Metrological Traceability of Measurement Results in Pharmaceutical and Chemical Sciences: Selection and Use of Certified Reference Materials  
Raquel Nogueira

## Communication

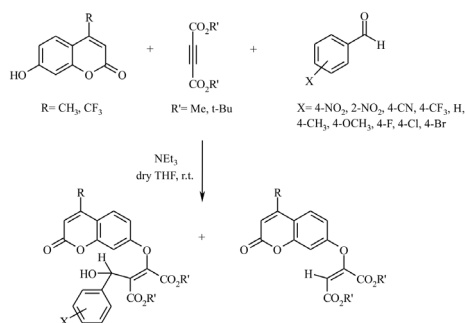
### 218 Three-Component Reactions of 7-Hydroxy Coumarin Derivatives, Acetylenic Esters and Aromatic Aldehydes in the Presence of $\text{NEt}_3$

SI online

Sakineh Asghari, Robabeh Baharfar, Samaneh Ahangar Darabi and Reza Mohammadian

#### Graphical Abstract

Novel coumarin derivatives have been synthesized in good yields by three-component reactions of 7-hydroxy coumarins, dialkyl acetylenedicarboxylates and aromatic aldehydes in the presence of  $\text{NEt}_3$  under mild reaction conditions



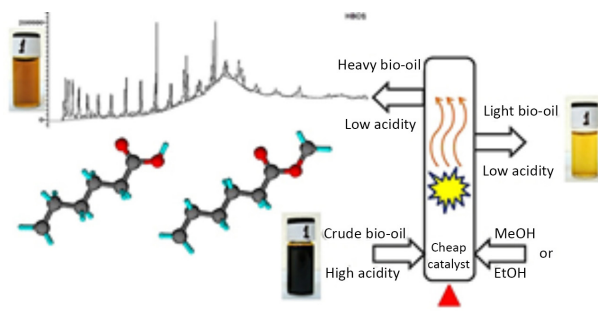
## Articles

### 224 Upgrade of Biofuels Obtained from Waste Fish Oil Pyrolysis by Reactive Distillation

Alberto Wisniewski Jr., Lorena Wosniak, Dilamara R. Scharf, Vinicyus R. Wiggers, Henry F. Meier and Edesio L. Simionatto

#### Graphical Abstract

The second generation biofuels produced from waste biomass material appear as a promising substitute to fossil fuels. The potential uses of the liquid biofuel have the high acidity as the main technological barrier. The bio-oil obtained from waste fish oil was submitted to reactive distillation during the refinement, in a process known as bio-oil upgrade, employing a widely available alcohols and cheap reactants as catalysts to improve their quality



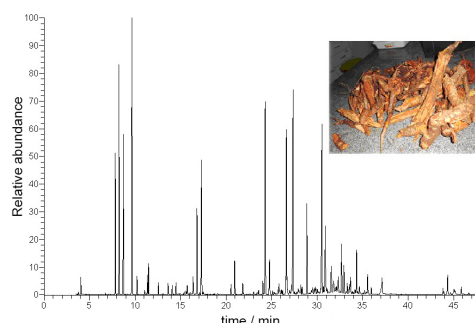
### 233 Chemical Composition and Cytotoxic Activity of the Root Essential Oil from *Jatropha ribifolia* (Pohl) Baill (Euphorbiaceae)

SI online

Celia E. L. da Silva, Sandro Minguzzi, Rogério C. L. da Silva, Maria F. C. Matos, Danilo Tofoli, João E. de Carvalho, Ana L. T. G. Ruiz, Willian F. da Costa and Euclésio Simionatto

#### Graphical Abstract

The essential oil of roots of *Jatropha ribifolia*, obtained by hydrodistillation was characterized in terms of its chemical composition by GC-FID and GC-MS. The essential oil and fractions were tested *in vitro* against nine human cancer cell lines by sulforhodamine B assay

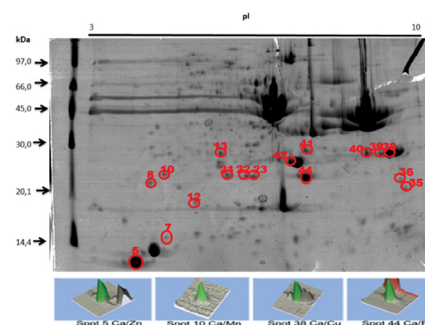


### 239 Metalloproteomic Profile Determination of Muscle Samples from Nile Tilapia (*Oreochromis niloticus*) Using AAS and ESI-MS/MS after 2D-PAGE Separation

Bruna Cavecci, Paula M. de Lima, João V. de Queiroz, Camila P. Braga, Cilene C. F. Padilha, Aline L. Leite, Marília A. R. Buzalaf, Luiz E. Pezzato and Pedro M. Padilha

#### Graphical Abstract

Metalloproteomic profile of muscle tissue samples from Nile tilapia (*Oreochromis niloticus*)



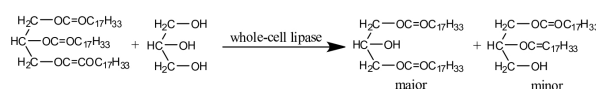
### 247 Improving Yield of 1,3-Diglyceride by Whole-Cell Lipase from *A. Niger* GZUF36 Catalyzed Glycerolysis via Medium Optimization

SI online

Cuiqin Li, Lanxiang Li, Huanjing Zhou, Chaoshuang Xia and Laping He

#### Graphical Abstract

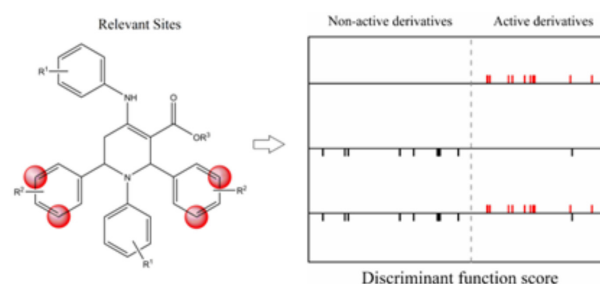
Yield of 1,3-diglyceride (1,3-DG) is improved 1.42-fold through optimization of medium via glycerolysis of triglyceride (TG) catalyzed by whole-cell lipase from a new isolated strain, *Aspergillus niger* GZUF36



## 255 The Correlation Between Electronic Structure and Antimalarial Activity of Tetrahydropyridines

Oscar A. Naranjo-Montoya, Lucas M. Martins, Luiz C. da Silva-Filho, Augusto Batagin-Neto and Francisco C. Lavarda

SI online



### Graphical Abstract

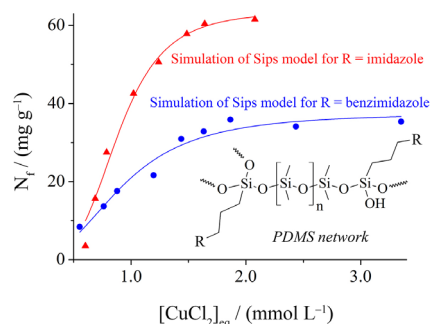
Multivariate data analysis were employed to correlate the antimalarial activity of tetrahydropyridines derivatives with electronic structure data obtained through quantum mechanical calculations. The results bring valuable insights in order to design new active compounds

## 266 Synthesis of Poly(Dimethylsiloxane) Networks Functionalized with Imidazole or Benzimidazole for Copper(II) Removal from Water

Fábio L. Pissetti, Pedro L. de Araújo, Fábio A. B. Silva and Gaél Y. Poirier

### Graphical Abstract

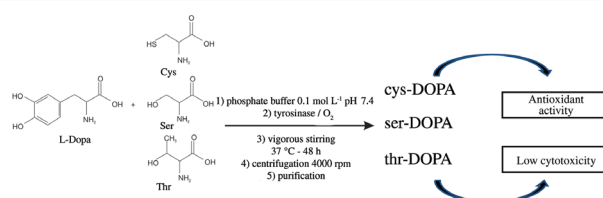
Functionalized elastomeric networks with imidazole or benzimidazole functional groups, derived from poly(dimethylsiloxane), were able to absorb copper(II) from aqueous solutions. The metal removal proceeded in accordance with the Sips adsorption model



## 273 Preparation, Characterization, Cytotoxicity and Antioxidant Activity of DOPA Melanin Modified by Amino Acids: Melanin-Like Oligomeric Aggregates

Thiago G. Costa, Mateus J. Feldhaus, Felipe S. Vilhena, Melina Heller, Gustavo A. Micke, Aldo S. Oliveira, Inês M. C. Brighente, Fabiola B. F. Monteiro, Tânia B. Creczynski-Pasa and Bruno Szpoganicz

SI online



### Graphical Abstract

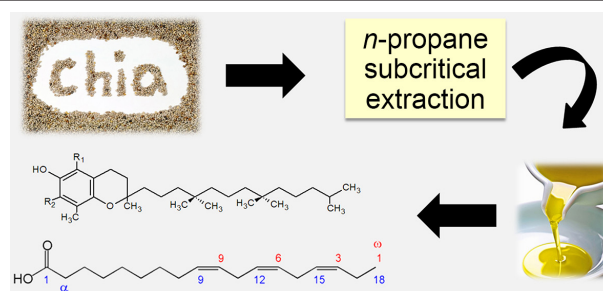
Preparation and characterization of new melanin chemically modified with serine and threonine amino acids, with low toxicity and high antioxidant capacity, potential molecules for pharmaceutical industry and food chemistry

## 282 Subcritical Extraction of *Salvia hispanica* L. Oil with *n*-Propane: Composition, Purity and Oxidation Stability as Compared to the Oils Obtained by Conventional Solvent Extraction Methods

Ana B. Zanqui, Damila R. de Moraes, Cláudia M. da Silva, Jandysen M. Santos, Lucas U. R. Chiavelli, Paulo R. S. Bittencourt, Marcos N. Eberlin, Jesui V. Visentainer, Lúcio Cardozo-Filho and Makoto Matsushita

### Graphical Abstract

This work presents an evaluation study of *Salvia hispanica* L. oil extracted by subcritical *n*-propane, compared to different conventional lipid extraction methods. Subcritical *n*-propane method is better than other methods, this is a promising alternative for oil extraction and results in a product with great composition, oxidative capacity and high purity

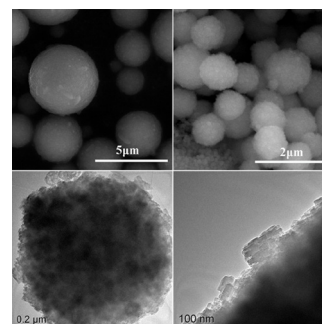


## 290 Synthesis of SAPO-34/ZSM-5 Composite and Its Catalytic Performance in the Conversion of Methanol to Hydrocarbons

Liping Li, Xiaojing Cui, Junfen Li and Jianguo Wang

### Graphical Abstract

SAPO-34/ZSM-5 composite was synthesized with nano-sized ZSM-5 zeolite as seeds. It has a sphere-like morphology and a large quantity of mesopores. Owing to its proper acidity and mesoporosity, the composite exhibits high stability in the conversion of methanol to hydrocarbons (MTH reaction)



**297 Interlaboratory Comparison of Quantifying Hydrocarbons and Trace Elements in Sediment Samples from a Tropical Estuary**

Adriana H. Nudi, Angela Wagener, Irene T. Gabardo,  
Rafael A. Lourenço and Arthur Scofield

**Graphical Abstract**

A homogeneous and stable sediment material (SED 001) was produced for quality assurance when quantifying hydrocarbons and trace elements in sediment samples

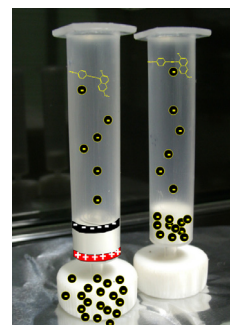


**310 Electric Field-Assisted Solid Phase Extraction: Study of Electrochromatographic Parameters with an Anionic Model Compound**

Ricardo M. Orlando, Jarbas J. R. Rohwedder and  
Susanne Rath

**Graphical Abstract**

Comparison of elution efficiency of the anionic model compound (sunset yellow) using conventional solid phase extraction (right cartridge) and electric field-assisted solid phase extraction (left cartridge)

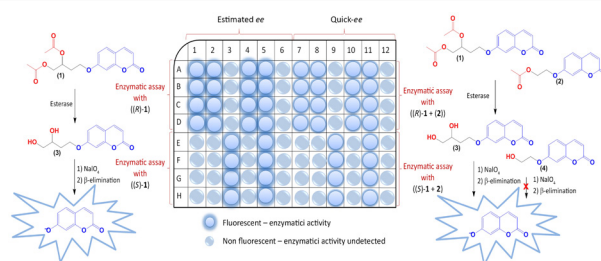


**319 High Throughput Enzymatic Enantiomeric Excess: Quick-ee**

Maria L. S. O. Lima, Caroline C. S. Gonçalves,  
Juliana C. Barreiro, Quezia B. Cass and Anita J. Marsaioli



SI online



**Graphical Abstract**

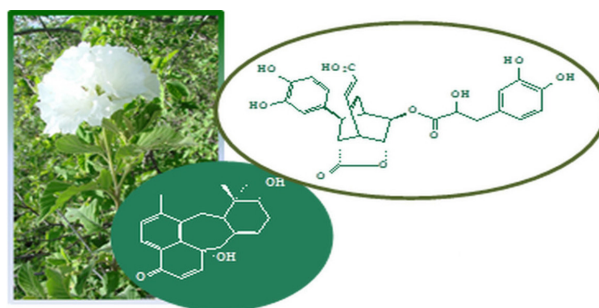
A schematic representation of the fluorogenic assays with (Quick-ee) and without competitor

**325 An Uncommon Naphthaquinoid and a New Lignan Derivative from the Roots of *Cordia leucocephala* Moric**

Jaécio C. Diniz, Francisco A. Viana, Maria da Conceição M.  
Torres, Raimundo Braz-Filho, Edilberto R. Silveira and  
Otilia D. L. Pessoa



SI online



**Graphical Abstract**

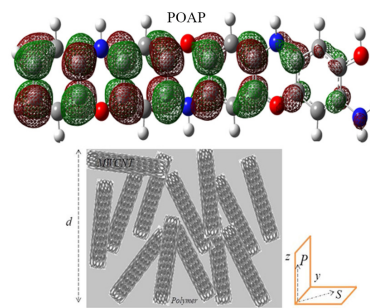
Two uncommon compounds, a meroterpen naphthaquinoid (cordiaquinone P) and a new lignan derivative were isolated from the roots of *Cordia leucocephala*. Their structures, including the relative stereochemistry, were determined by spectrometric methods

**331 Electrochemical and Optical Investigation of Conductive Polymer and MWCNT Nanocomposite Film**

Ali Ehsani, Ferydon Babaei and Hossein Mostaanzadeh

**Graphical Abstract**

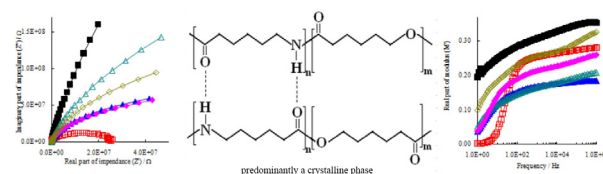
Composites of multi-walled carbon nanotubes and poly *ortho* aminophenol (POAP) were prepared by electropolymerization. Density functional theory calculation, optical properties and electrocatalytic activity of the composite have been investigated





### 338 Anionic Aliphatic Polyesteramide Copolymers: Evaluation of Dielectric Properties

Gheorghe Rusu and Elena Rusu

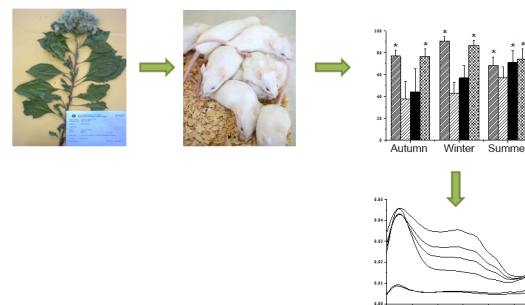


#### Graphical Abstract

The dielectric properties of anionic aliphatic polyesteramides were investigated by analyzing the complex dielectric permittivity, complex electric modulus, and complex impedance in the frequency range  $10^0$  Hz to  $10^6$  Hz, at room temperature

### 350 Seasonal Effects on HPLC-DAD-UV and UPLC-ESI-MS Fingerprints and Analgesic Activities of *Vernonia Condensata* Baker Extracts

Sabrina Afonso, Aldair C. de Matos, Vitor A. Marengo, Estefânia G. Moreira, Daniely X. Soares, Héctor Henrique F. Koolen and Ieda S. Scarminio

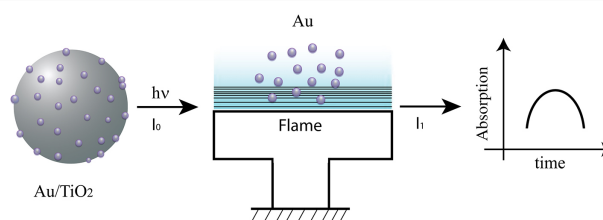


#### Graphical Abstract

HPLC-DAD-UV spectra were used to compare the chemical compositions in the different seasons. The results confirm a peripherally-mediated anti-inflammatory activity of *V. condensata*. The seasons had significant effects on the relative abundances of the metabolites

### 359 Determination of Metal Loading in Heterogeneous Catalyst by Slurry Sampling Flame Atomic Absorption Spectrometry

Marco A. S. Garcia, Daniel M. Silvestre, Cassiana S. Nomura and Liane M. Rossi

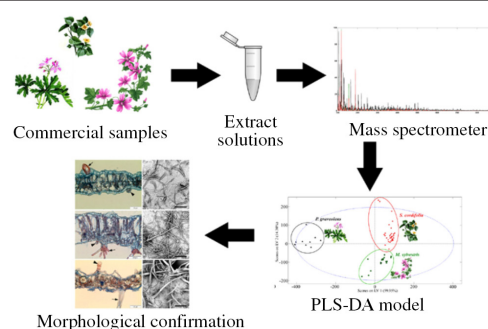


#### Graphical Abstract

This paper describes a new method for quantification of metal in supported catalysts using slurry sampling flame atomic absorption spectrometry. The slurry method allowed satisfactory results with no need for laborious extraction procedures

### 365 Non-Targeted Electrospray Mass Spectrometry-Based Metabolic Fingerprinting and PLS-DA-Based Classification of Brazilian “Malvas”

Cleverson A. F. Martins, Mário S. Piantavini, Rômulo P. Ribeiro, Erika Amano, Bruna V. Dal Prá and Roberto Pontarolo

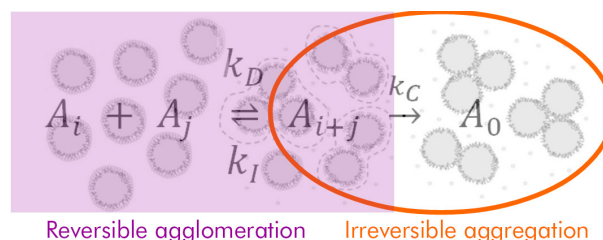


#### Graphical Abstract

Besides *Malva sylvestris*, other plants are also known as “malvas” in Brazil. Direct infusion was used to differentiate three distinct species via electrospray ionization mass spectrometry fingerprintings and a partial least squares discriminant analysis method

### 373 Colloidal Dispersion Stability: Kinetic Modeling of Agglomeration and Aggregation

Guilherme K. Gonzatti, Paulo A. Netz, Luana A. Fiel and Adriana R. Pohlmann



#### Graphical Abstract

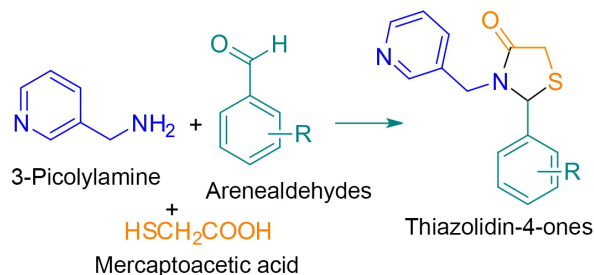
Mechanism for coalescence of colloidal particles occurs in a two-step mechanism: a rapid reversible agglomeration and a slow irreversible aggregation

**381** **Thiazolidin-4-ones from 3-(Aminomethyl)pyridine, Arenealdehydes and Mercaptoacetic Acid: Synthesis and Radical Scavenger Activity**



SI online

Adriana M. Neves, Auri R. Duval, Gabriele A. Berwaldt, Daniela P. Gouvêa, Natália P. Flores, Pâmela G. da Silva, Francieli M. Stefanello and Wilson Cunico



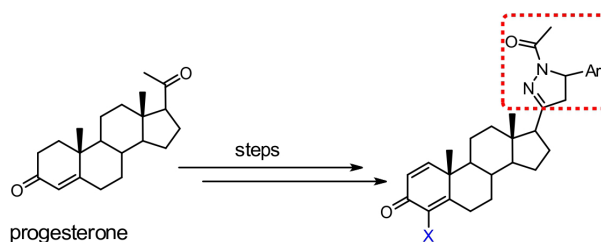
**Graphical Abstract**

The synthesis and radical scavenger activity of 2-aryl-3-(pyridin-3-ylmethyl)thiazolidin-4-ones were reported

## Short Reports

**389** **Potential Insecticidal Activity of Steroidal C-17 Pyrazolinyl Derivatives**

Ning-Juan Fan, Shao-Peng Wei, Jin-Ming Gao and Jiang-Jiang Tang

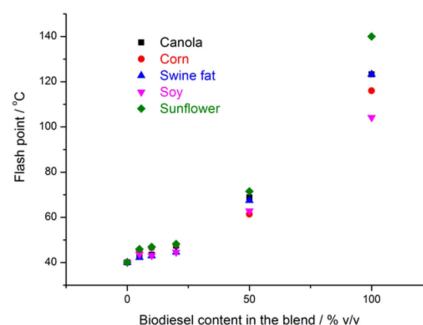


**Graphical Abstract**

Eight steroids-based pyrazolinyl derivatives were synthesized by several steps and the compound where Ar = ph exerted marked insecticidal activity, comparable to that of the natural product insecticide celangulatin V

**393** **Correlation Between the Composition and Flash Point of Diesel-Biodiesel Blends**

Rodrigo A. de Mattos, Flávio A. Bastos and Matthieu Tubino



**Graphical Abstract**

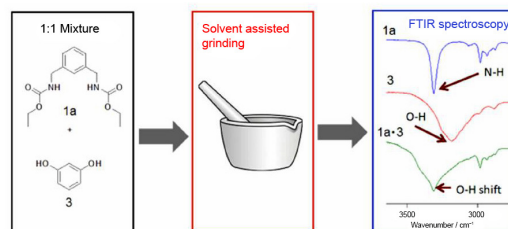
There is a clear correlation between the biodiesel quantity in a diesel-biodiesel blend and its flash point. This means that the experimental determination of a flash point temperature also provides information regarding the biodiesel content of diesel-biodiesel blends

**396** **Synthesis, Molecular Structure of Diethyl Phenylenebis(Methylene)Dicarbamates and FTIR Spectroscopy Molecular Recognition Study with Benzenediols**



SI online

Marlene M. Saucedo-Balderas, Rogelio A. Delgado-Alfaro, Francisco J. Martínez-Martínez, David Ortigón-Reyna, Margarita Bernabé-Pineda, Oscar Zúñiga-Lemus and Juan S. González-González



**Graphical Abstract**

Mechanochemical complexation of phenylenebis(methylene)dicarbamates and benzenediols confirmed by Fourier transform infrared spectroscopy