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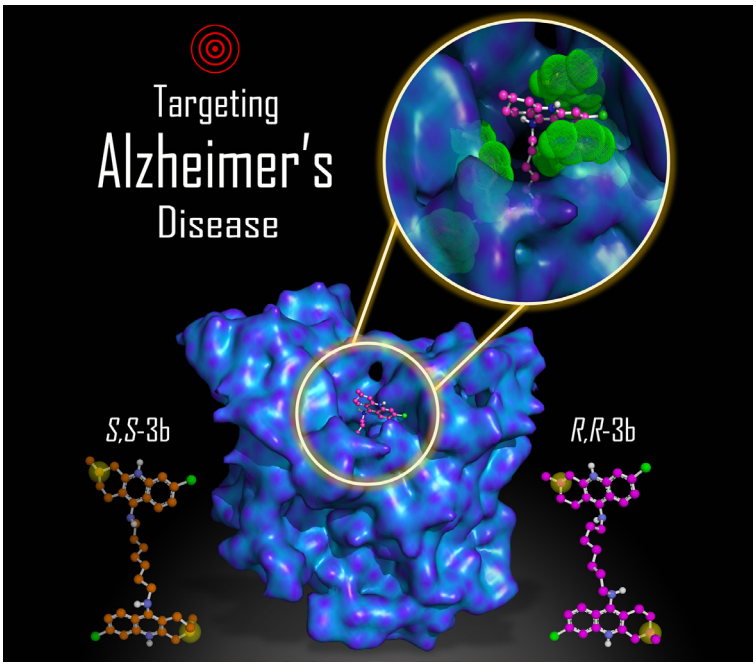
Cover Picture



Enantiomeric series of methylated and/or chorinated bis(7)-tacrine analogues were found to be potent inhibitors of AChE and BuChE with IC_{50} in the nanomolar concentration scale. The *R*,*R*-**3b** (with Cl) inhibitor is the most active homodimer against AChE and is also selective, showing no activity against BuChE. Binding mode and affinity predictions showed the importance of pi-stacking and halogen bond interactions in peripheral anionic site (PAS). Details are presented in the Article **Chiral Bistacrine Analogs: Synthesis, Cholinesterase Inhibitory Activity and a Molecular Modeling Approach** by *João P. B. Lopes, Jessie S. da Costa, Marco A. Ceschi, Carlos A. S. Gonçalves, Eduardo L. Konrath, Ana L. M. Karl, Isabella A. Guedes and Laurent E. Dardenne* on page 2218.

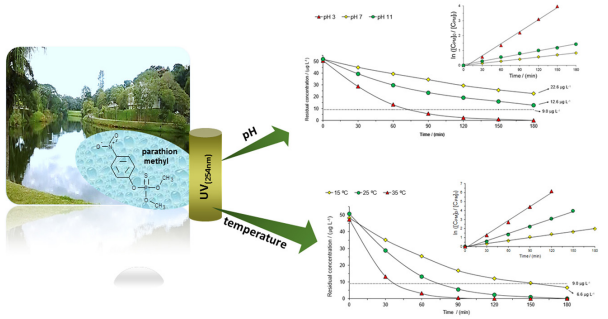
Contents

Articles

2045 **DLLME-GC/ECD Method for the Residual Analysis of Parathion-Methyl and its Application in the Study of the UV-Photodegradation Process**

SI online

Gustavo G. Pimenta, Maria E. L. R. de Queiroz, Raquel P. D. Victor, Luiz M. Noronha, Antônio A. Neves, André F. de Oliveira and Fernanda F. Heleno



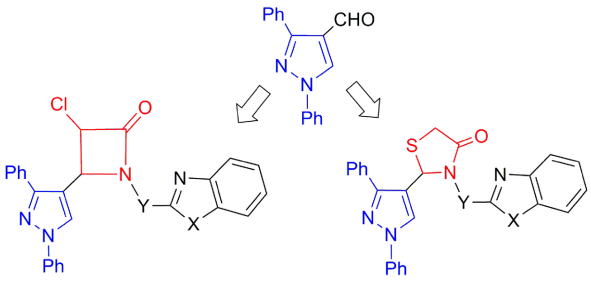
Graphical Abstract

A DLLME-GC/ECD was optimized and validated to analyze the parathion-methyl in water and evaluate its UV-photodegradation.

2054 **Synthesis, Anti-Diabetic and Renoprotective Activity of Some New Benzazole, Thiazolidin-4-one and Azetidin-2-one Derivatives**

SI online

Ahmed Abdou O. Abeed, Mohamed Salah K. Youssef and Rehab Hegazy



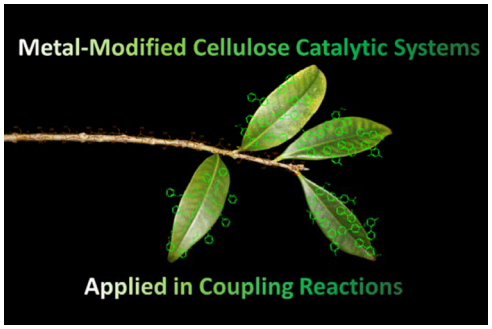
X= NH, O; Y= NH, $NHCH_2COS$, $COCH_2S$

Graphical Abstract

A new series of heterocycles were synthesized. Some of these compounds were evaluated for their anti-hyperglycemic and renoprotective activity.

2064 **Cellulose Oxidation and the Use of Carboxyl Cellulose Metal Complexes in Heterogeneous Catalytic Systems to Promote Suzuki-Miyaura Coupling and C–O Bond Formation Reaction**

Guilherme B. C. Martins, Marcelo R. dos Santos, Marcus V. R. Rodrigues, Renata R. Sucupira, Luisa Meneghetti, Adriano L. Monteiro and Paulo A. Z. Suarez



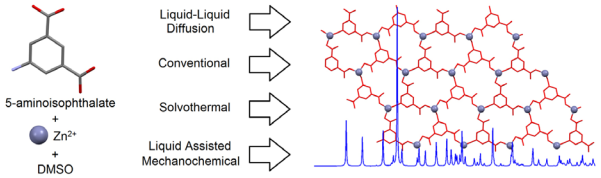
Graphical Abstract

Application of metal-modified cellulose as ligand in heterogeneous catalytic systems of coupling reactions as a new option for green and sustainable chemistry.

2073 **Structural Invariance of a Zn^{II} Coordination Polymer with 5-Aminoisophthalic Acid under Different Synthetic Conditions**

SI online

Iara M. L. Rosa, Ana C. Z. dos Santos, Luana A. R. Giusto, Carlos B. Pinheiro and Antonio C. Doriguetto

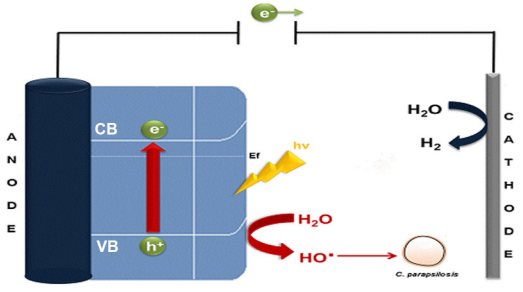


Graphical Abstract

Synthesis of coordination polymer [Zn(aip)(DMSO)] (aip: 5-aminoisophthalate and DMSO: dimethylsulfoxide) using several synthetic conditions, which show the high stability and structural invariance of the network.

2084 **Antifungal Properties of High Efficient W/WO_3 Electrodes Acting under UV-Vis and Visible Light and Chloride Medium**

Barbara C. A. Souza, Thais T. Guaraldo, Michelle F. Brugnera, Regina H. Pires, Maria J. S. M. Giannini and Maria V. B. Zanoni

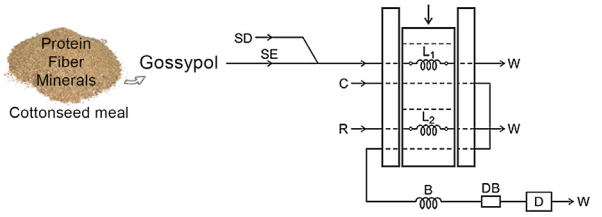


Graphical Abstract

Fast inactivation of *C. parapsilosis* by photoelectrocatalysis. The attack of HO· radicals to the cell wall of the fungus promotes rapid death and high degradation of organic compounds from the cell lyse. Photoelectrocatalysis is an efficient alternative to threat wastewater with high chloride content containing fungus.

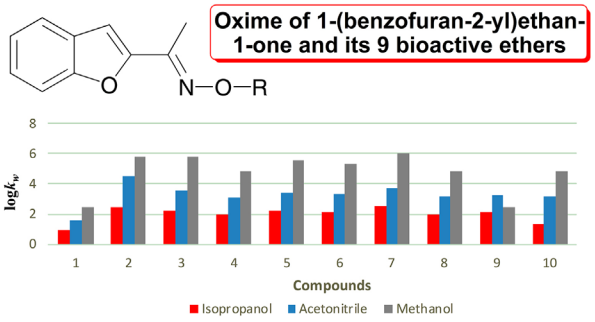
2094 **An Environmental Friendly Flow-Injection Procedure for On Line Extraction and Spectrophotometric Determination of Gossypol in Cottonseed Meal**
Bianca Daminato, Marcos Y. Kamogawa and Wanessa R. Melchert

Graphical Abstract
A fast, simple, inexpensive and green flow analysis procedure for the determination of gossypol in cottonseed meal.



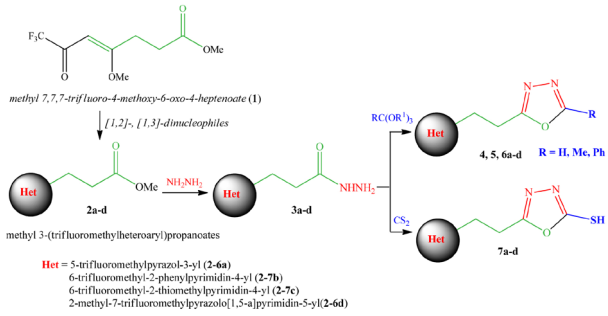
2100 **Lipophilicity Study of 1-(Benzofuran-2-yl)ethan-1-one Oxime and its Substituted *O*-Benzyl Ethers**
Tomasz Kosmalski, Renata Studzińska, Małgorzata Redka, Robert Pluskota and Bożena Modzelewska-Banachiewicz

Graphical Abstract
Lipophilicity parameters for 1-(benzofuran-2-yl)ethan-1-one oxime and its nine biological active ethers were evaluated using reversed phase high performance liquid chromatography (RP-HPLC) method. The log k_w lipophilicity parameters were compared with computed log P values using methanol, 2-propanol and acetonitrile as organic modifier of the mobile phases.



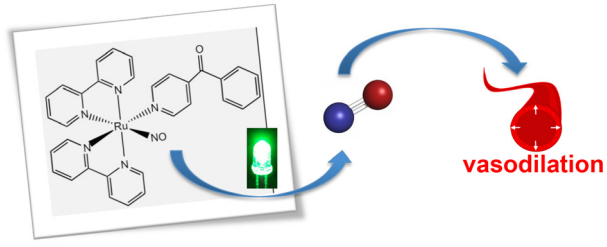
2106 **Strategies for the Efficient Synthesis of Biheterocyclic 5-[2-(Trifluoromethylheteroaryl)-ethyl]-1,3,4-oxadiazoles from Levulinic Acid**
SI online
Juliana L. Malavolta, Leandro M. Frigo, Sidnei Moura, Darlene C. Flores and Alex F. C. Flores

Graphical Abstract
New ethylene-spaced biheterocyclic 5-[2-(trifluoromethyl heteroaryl)-ethyl]-1,3,4-oxadiazoles were synthesized by two consecutive cyclocondensations from methyl 7,7,7-trifluoro-4-methoxy-6-oxo-4-heptenote derived from the renewable levulinic acid.



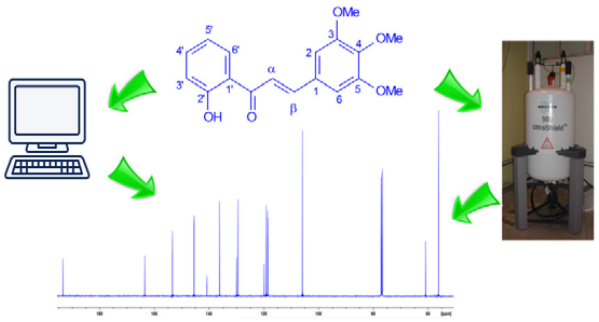
2117 **A Potential Visible-Light NO Releaser: Synthesis, Reactivity and Vasodilator Properties**
SI online
Auridéia P. de Sousa, André F. Fernandes, Iury A. Paz, Nilberto R. F. Nascimento, Javier Ellena, Eduardo H. S. Sousa, Luiz G. F. Lopes and Alda K. M. Holanda

Graphical Abstract
A new ruthenium nitrosyl complex containing benzoylpyridine ligand showed promising visible light induced release of NO and vasodilation activity.



2130 **Conformational Analysis, Experimental and GIAO-DFT ^{13}C NMR Chemical Shift Calculation on 2'-Hydroxy-3,4,5-trimethoxy-chalcone**

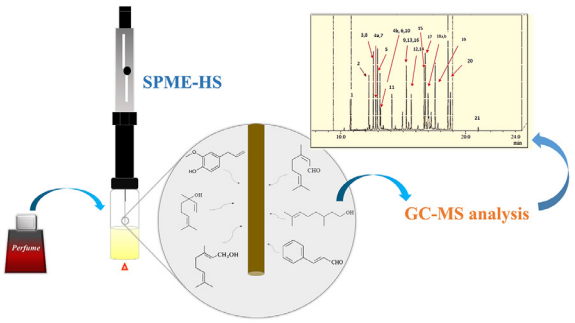
SI online *Fabio Luiz P. Costa, Paulo F. Gomes, Andressa K. Silva and Luciano M. Lião*



Graphical Abstract
Experimental and computational data: a robust protocol to complete ^{13}C NMR chemical shifts assignment of substituted chalcones.

2136 **Allergenic Fragrances Analysis in Brazilian Perfumes by Headspace Solid Phase Microextraction and Gas Chromatography-Mass Detector (HS-SPME-GC-MS)**

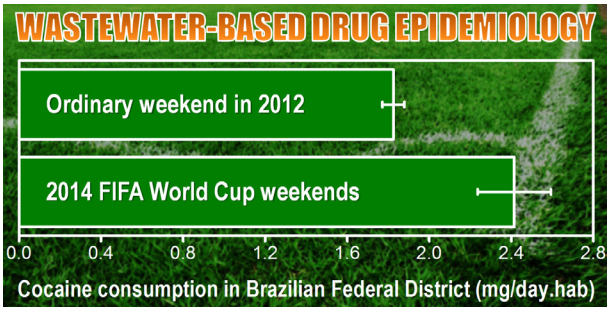
SI online *Clérton L. Gomes, Ari C. A. de Lima, Pablo G. A. Barbosa, Rouse S. Costa, Diego Q. Melo and Ronaldo F. Nascimento*



Graphical Abstract
The image depicts the first step of sample preparation process starting from the extraction of volatile perfume by solid phase microextraction (SPME) in headspace mode with subsequent identification and quantification by gas chromatography mass spectrometry (GC-MS).

2146 **Illicit Drugs, Metabolites and Adulterants in Wastewater: Monitoring Community Drug Abuse in the Brazilian Federal District during the 2014 Soccer World Cup**

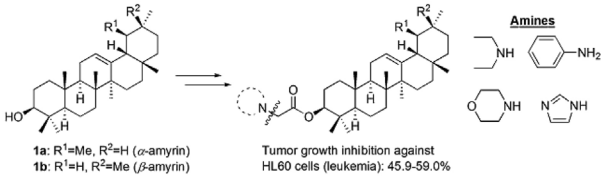
SI online *Fernando F. Sodré, Gustavo B. Souza, Rafael S. Feitosa, Carlos Eduardo B. Pereira and Adriano O. Maldaner*



Graphical Abstract
Wastewater analyses indicate high cocaine consumption during Soccer World Cup as well as different forms of used cocaine.

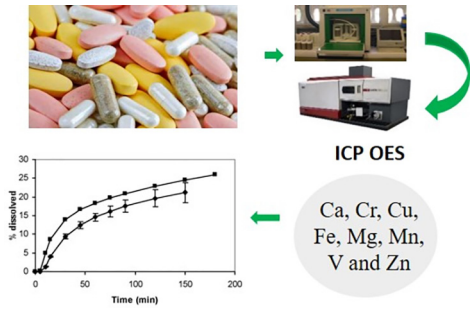
2155 **Synthesis and Evaluation of Cytotoxic Effects of Amino-ester Derivatives of Natural α,β-Amyrin Mixture**

SI online *Mauricio M. Victor, Jorge M. David, Marcelo A. S. dos Santos, André L. B. S. Barreiros, Marizeth L. Barreiros, Fernanda S. Andrade, Adriana A. Carvalho, Maria Claudia S. Luciano, Manoel O. de Moraes, Francisco W. A. Barros-Nepomuceno and Claudia Pessoa*



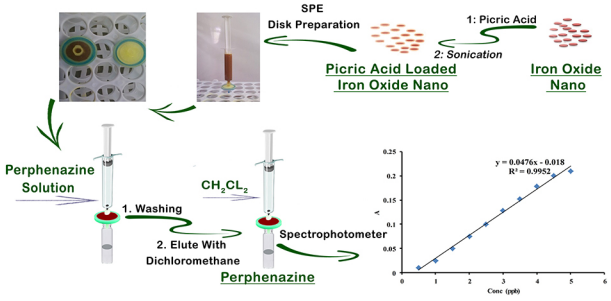
Graphical Abstract
Natural α,β-amyrin mixtures isolated from *Esenbeckia grandiflora* were transformed into aminoesters and their cytotoxic activities were evaluated against PC-3, HCT-116 and HL-60 tumor cells. Diethyl, aniline, morpholine and imidazole derivatives showed moderate activity against HL60.

2163 ***In vitro* Monitoring of Macro and Microelements in Multimineral Preparations across Dissolution Profiles by Inductively Coupled Plasma Optical Emission Spectrometry (ICP OES)**
Aníbal de F. Santos Júnior, Ramon R. Sá, Laiana O. B. Silva, Hemerson I. F. Magalhães, Taiana B. Tarantino and Maria Graças A. Korn



Graphical Abstract
The metal content across dissolution profiles of five multivitamin supplements was evaluated by inductively coupled plasma optical emission spectrometry (ICP OES).

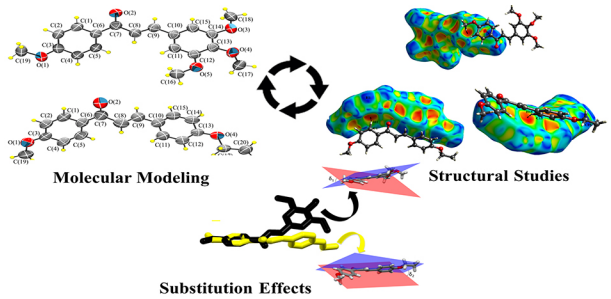
2172 **Pre-Concentration and Separation of Perphenazine Using Picric Acid Loaded α-Fe_2O_3 Nanoparticles: HPLC Syringe Filter as the Particles Support**
Zahra Ramezani, Marzieh Shekarriz, Abdol Azim Behfar and Somayeh Kiamarzi



Graphical Abstract
Picric acid loaded iron oxide nanoparticles were retained on HPLC (high-performance liquid chromatography) syringe disk and used as SPE (solid phase extraction) sorbent for perphenazine pre-concentration and clean up.

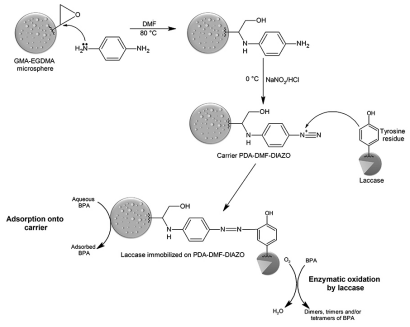
2180 **The Influence of Methoxy and Ethoxy Groups on Supramolecular Arrangement of Two Methoxy-chalcones**
Jean M. F. Custodio, Eduardo C. M. Faria, Lóide O. Sallum, Vitor S. Duarte, Wesley F. Vaz, Gilberto L. B. de Aquino, Paulo S. Carvalho Jr. and Hamilton B. Napolitano

SI online



Graphical Abstract
What is the influence of substituents on methoxy-chalcones? A combined structural and theoretical investigation.

2192 **Synergistic Effect of Adsorption and Enzymatic Conversion in the Bisphenol-A Removal by Laccase Immobilized on Poly(glycidyl methacrylate-*co*-ethyleneglycol dimethacrylate)**
Claudinei F. Melo, Leandro A. Silva, Luciana C. Costa and Monica R. C. Marques

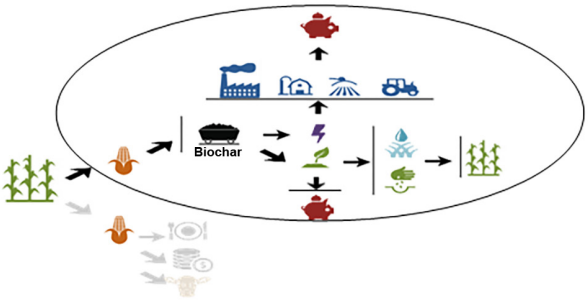


Graphical Abstract
Synthesis of the resin after diazotization and the mechanisms of removal of bisphenol-A by adsorption and enzymatic oxidation.

2202 **Investigation on Prospective Energy Power from Corncob Husk Biomass and its Biochars by Kinetic Parameters and Isoconversional Models**
Carolina C. Bueno, Amanda A. D. Maia, Leandro C. de Morais and André H. Rosa

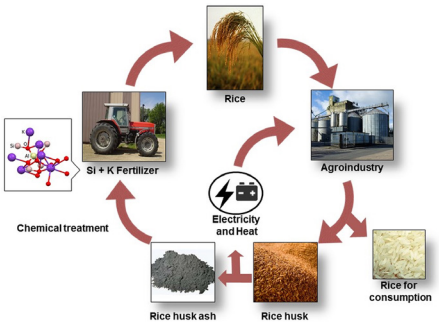
SI online

Graphical Abstract
Corncob husk biomass requires low input of energy on pyrolysis to be produced and it is an indicator for worthy carbon based biofuels. Some biochars are prone to oxidation reactions.



2211 **Rice Husk Ash as Raw Material for the Synthesis of Silicon and Potassium Slow-Release Fertilizer**
Amanda A. França, Juliana Schultz, Roger Borges, Fernando Wypych and Antonio S. Mangrich

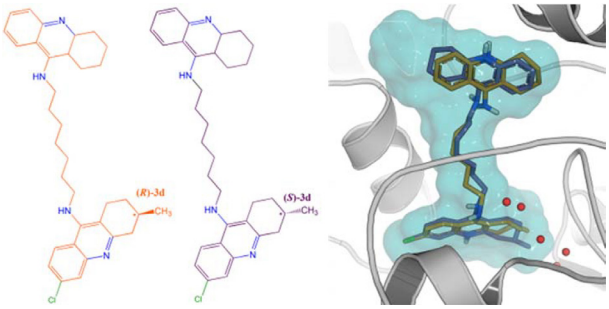
Graphical Abstract
Rice husk ash was used to synthesize a silicon and potassium slow-release fertilizer. The method is an attractive way of enabling the reuse of a waste.



2218 **Chiral Bistacrine Analogues: Synthesis, Cholinesterase Inhibitory Activity and a Molecular Modeling Approach**
João P. B. Lopes, Jessie S. da Costa, Marco A. Ceschi, Carlos A. S. Gonçalves, Eduardo L. Konrath, Ana L. M. Karl, Isabella A. Guedes and Laurent E. Dardenne

SI online

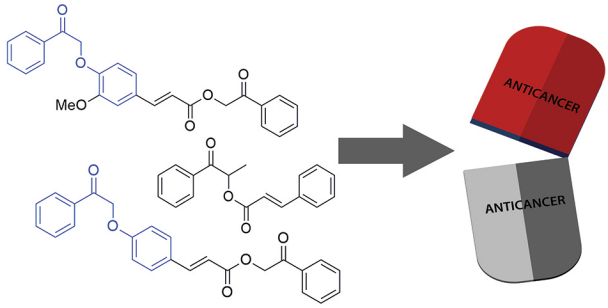
Graphical Abstract
Chiral bis(7)-tacrine compounds were synthesized in yields ranging from 40 to 80%. Both enantiomeric series were found to be potent AChE and BuChE inhibitors *in vitro*, with IC_{50} values ranging from 2 to 16 nM and from 30 to 140 nM, respectively.



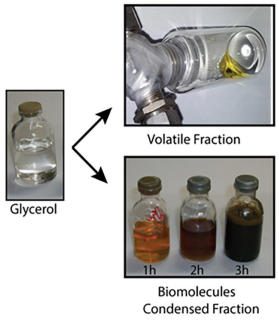
2229 **Synthesis, Characterization and *in vitro* Anticancer Activity of Novel 8,4'-Oxyneolignan Analogues**
Gisele C. Souza, Gilberto C. Franchi Jr., Alexandre E. Nowill, Lourivaldo S. Santos, Cláudio N. Alves, Lauro E. S. Barata and Carlos K. Z. Andrade

SI online

Graphical Abstract
A new subclass of 8,4'-oxyneolignans presented a promising antiproliferative activity against human cancer cells.

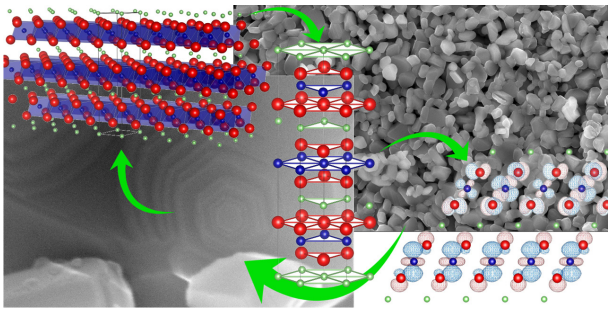


2244 **Synthetic Niobium Oxyhydroxide as a Bifunctional Catalyst for Production of Ethers and Allyl Alcohol from Waste Glycerol**
SI online *Henrique S. Oliveira, Jarbas M. Resende, Patterson P. Souza, Patricia S. O. Patrício and Luiz C. A. Oliveira*



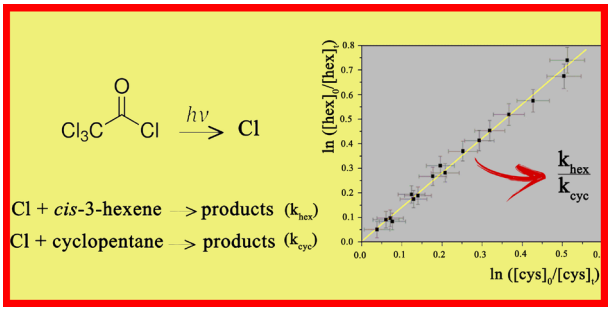
Graphical Abstract
Glycerol products in volatile fraction and condensed fraction using niobium oxyhydroxide as catalyst.

2254 **Synthesis and Characterization of $LiCoO_2$ from Different Precursors by Sol-Gel Method**
SI online *Bruno G. A. Freitas, José M. Siqueira Jr., Leonardo M. da Costa, Glaucio B. Ferreira and Jackson A. L. C. Resende*



Graphical Abstract
HT-$LiCoO_2$ synthesized by sol-gel method with the citric acid, starch, glycine and gelatin complexing agents to obtain the rhombohedral crystalline system of the $R\bar{3}m$ space group.

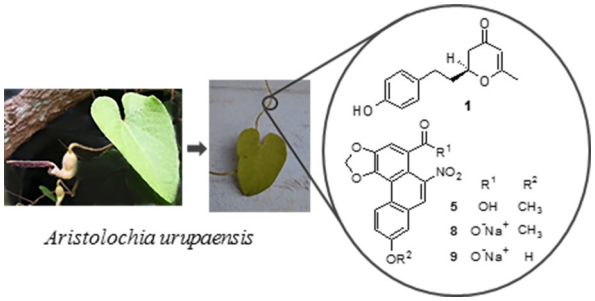
2267 **Rate Coefficient for the Reaction of Cl Atoms with *cis*-3-Hexene at 296 ± 2 K**
Thaís S. Barbosa, Javier A. Barrera, Rafael Jara Toro, Glauco F. Bauerfeldt, Graciela Arbilla and Silvia I. Lane



Graphical Abstract
The rate coefficient of the *cis*-3-hexene + Cl atoms reaction was determined by the relative rate technique using trichloroacetyl chloride to produce chlorine atoms.

Short Reports

2275 **Phenylethylpyranone and Aristolochic Acid Derivatives from *Aristolochia urupaensis***
SI online *Juliana C. Holzbach, Isabele R. Nascimento and Lucia M. X. Lopes*



Graphical Abstract
A new pyranone and three new aristolochic acid derivatives were isolated from *Aristolochia urupaensis* stems together with 31 known compounds.