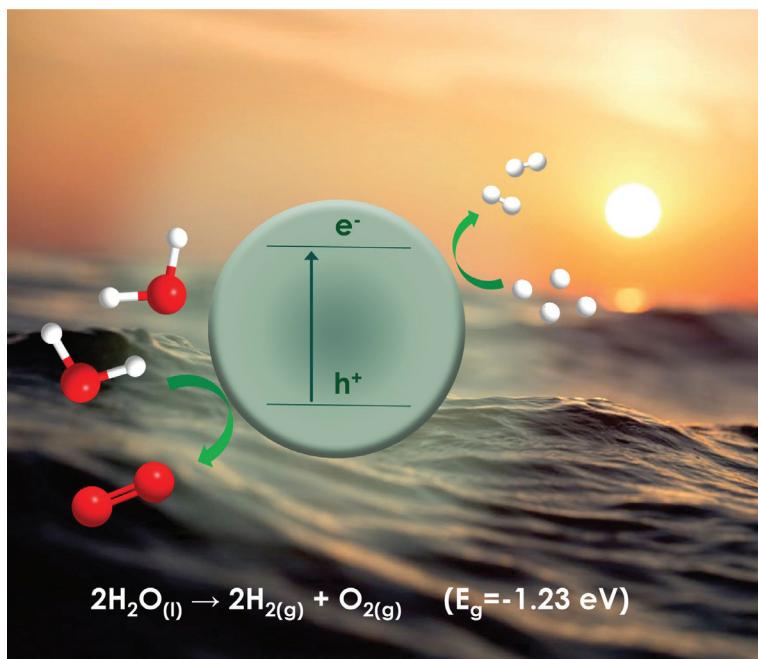


## Cover Picture



This figure illustrates the generation of charge carriers in semiconductor photocatalyst nanoparticles as a result of band gap excitation by sunlight. These charge carriers can then be employed to promote the water splitting reaction for the generation of  $H_2$ . This transformation is of paramount importance to the solar-to-chemical energy conversion. We review herein the fundamentals of  $H_2$  generation from water splitting and representative classes of photocatalytic materials. Details are presented in the Review **An Overview of the Photocatalytic  $H_2$  Evolution by Semiconductor-Based Materials for Nonspecialists** by Ivo F. Teixeira, Jhon Quiroz, Mauricio S. Homsi and Pedro H. C. Camargo on page 211.

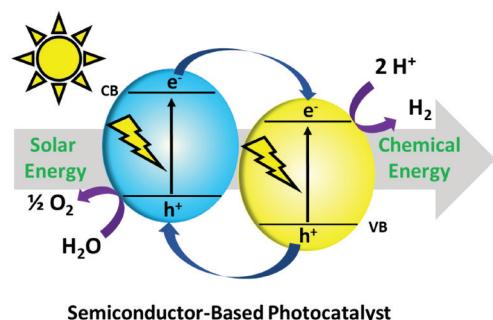
## Contents

### Reviews

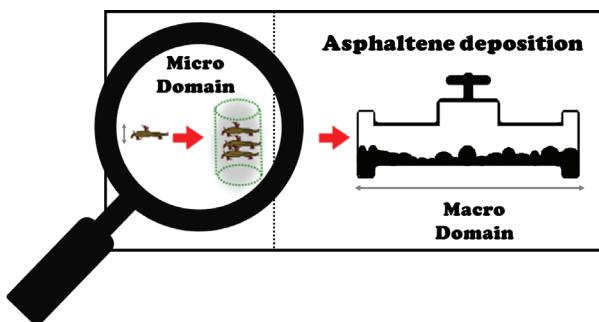
- 211 An Overview of the Photocatalytic  $H_2$  Evolution by Semiconductor-Based Materials for Nonspecialists

Ivo F. Teixeira, Jhon Quiroz, Mauricio S. Homsi and Pedro H. C. Camargo

**Graphical Abstract**  
We review semiconductor photocatalysts for the  $H_2$  evolution reaction that have displayed the best reported activities and quantum efficiencies.



**230 Recent Developments on the Elucidation of Colloidal Aspects of Asphaltenes and Their Relevance to Oilfield Problems**  
*Lia B. S. Balestrin and Watson Loh*

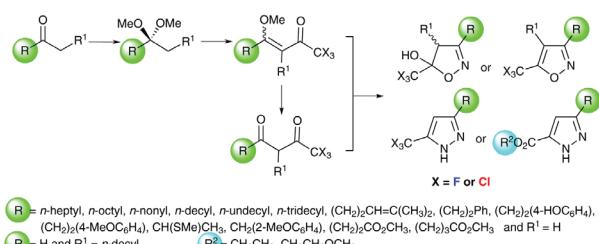
**Graphical Abstract**

This review discusses colloidal aspects of crude oil asphaltenes and their impact on oil production issues.

**Articles**

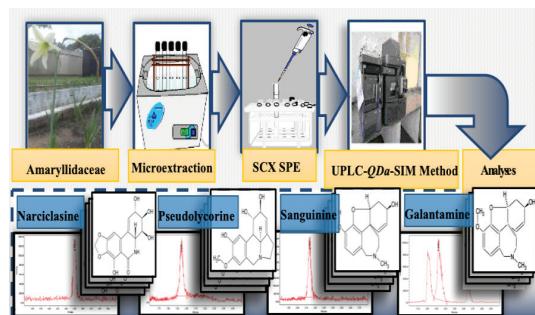
**244 An Acetal Acylation Methodology for Producing Diversity of Trihalomethyl-1,3-dielectrophiles and 1,2-Azole Derivatives**

<https://doi.org/10.1593/jbcs.2020-0011>  
*Valéria D. O. Bareño, Daiane S. Santos, Leandro M. Frigo, Debora L. de Mello, Juliana L. Malavolta, Rogerio F. Blanco, Lucas Pizzuti, Darlene C. Flores and Alex F. C. Flores*



**265 Development and Validation of a UPLC-ESI-MS Method for Quantitation of the Anti-Alzheimer Drug Galantamine and other Amaryllidaceae Alkaloids in Plants**

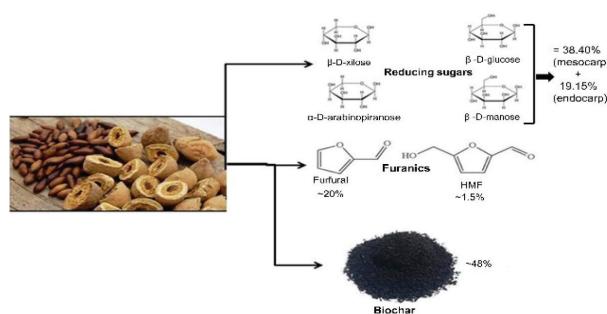
<https://doi.org/10.1593/jbcs.2020-0012>  
*José R. de Paiva, Ana S. Q. Souza, Rita C. A. Pereira, Paulo R. V. Ribeiro, Guilherme J. Zocolo, Edy S. de Brito, Otilia D. L. Pessoa and Kirley M. Canuto*

**Graphical Abstract**

Ultra-performance liquid chromatography coupled to mass spectrometry (UPLC-ESI-MS) method for quantitation of Amaryllidaceae alkaloids.

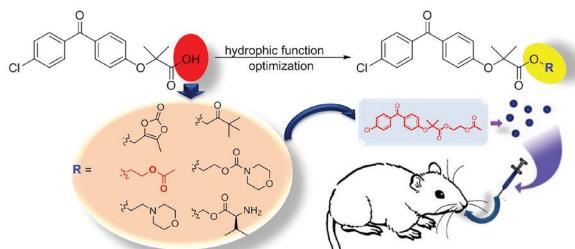
**273 Sustainability of Biorefinery Processes Based on Baru Biomass Waste**

*Magale K. D. Rambo, Michele C. D. Rambo, Polyanne M. Melo, Nayara Morgana L. de Oliveira, Yara K. S. Nemet, Elisandra Scapin, Guenther C. C. Viana and Daniel A. Bertuol*



**280 Synthesis and Evaluation of Fenofibric Acid Ester Derivatives: Studies of Different Formulation with Their Bioavailability and Absorption Conditions**

Si online Zhixiang Lv, Zhou Wang, Fuyan Xiao and Guofan Jin

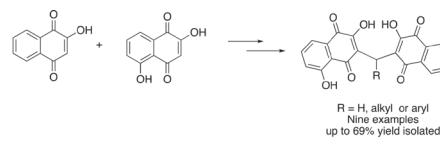


**Graphical Abstract**

A series of fenofibric acid ester pro-drugs were synthesized. The oral administration ( $20 \text{ mg kg}^{-1}$ ) of JF-2 showed a relative bioavailability of approximately 272.8% compared to fenofibrate.

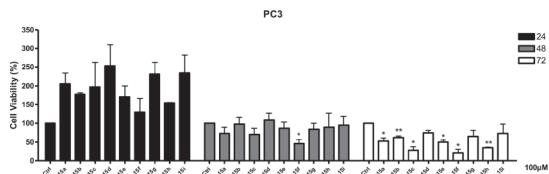
**288 A New Strategy for the Synthesis of Nonsymmetrical 3,3'-(Aryl/alkyl-methylene)bis-2-hydroxy-1,4-naphthoquinones and Their Cytotoxic Effects in PC3 Prostate Cancer Cells**

Si online Ruan Carlos B. Ribeiro, Paula Priscilla de Freitas, Caroline S. Moreira, Leonardo G. C. de Moraes, Matheus G. de Moraes, Fernando C. da Silva, David R. Rocha, Etel R. Pereira Gimba and Vitor F. Ferreira



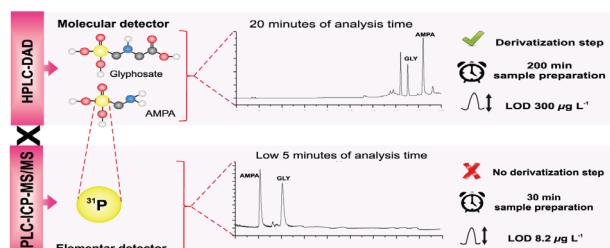
**Graphical Abstract**

A novel method for the synthesis of nonsymmetrical 3,3'-(aryl/alkyl-methylene)bis-2-hydroxy-1,4-naphthoquinones was developed by using the Mannich adduct of naphthoquinone and the reaction with another moiety of 2-hydroxy-1,4-naphthoquinone.



**298 Quantification of Glyphosate and AMPA by HPLC-ICP-MS/MS and HPLC-DAD: A Comparative Study**

Si online Emanuella M. Pimenta, Fabio F. da Silva, Érica S. Barbosa, Ane P. Cacique, Douglas L. Cassimiro, Gevany P. de Pinho and Flaviano O. Silvério

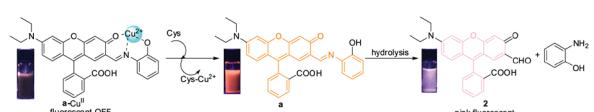


**Graphical Abstract**

The image represents the parameters in which high performance liquid chromatography using inductively coupled plasma with triple quadrupole mass spectrometer (HPLC-ICP-MS/MS) was superior to high performance liquid chromatography with diode array detector (HPLC-DAD) in determining glyphosate and aminomethylphosphonic acid (AMPA).

**305 A Highly Selective Colorimetric Sensor for Cysteine Detection**

Si online Mengjiao Peng, Hui Wang, Gregory L. Gibson, Hua Shang, Jianmin Yang, Yan Chen and Yin Lu



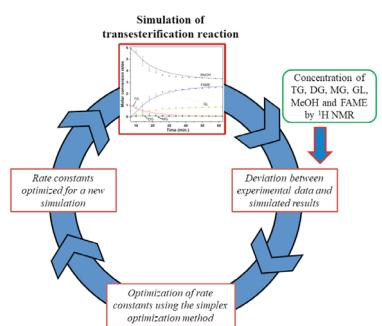
**Graphical Abstract**

Cysteine (Cys) can release Cu<sup>II</sup> ion from the non-fluorescent a-Cu<sup>II</sup> complex. Then hydrolytic cleavage of Schiff base (*E*)-2-(6-(diethylamino)-2-((2-hydroxyphenylimino)methyl)-3-oxo-3*H*-xanthen-9-yl)benzoic acid (**a**) produces a pink fluorescent compound 2-(6-(diethylamino)-2-formyl-3-oxo-3*H*-xanthen-9-yl)benzoic acid (**2**). Thus, Cys residues act as a "switch" in an off-on fluorescence system.

**313 Mathematical Modeling of the Transesterification Reaction by Finite Elements: Optimization of Kinetic Parameters Using the Simplex Sequential Method**

Diego Galvan, Letícia Thaís Chendynski,  
Ana Carolina G. Mantovani, Marintho B. Quadri,  
Mário Killner, Hágata Cremasco and Dionisio Borsato

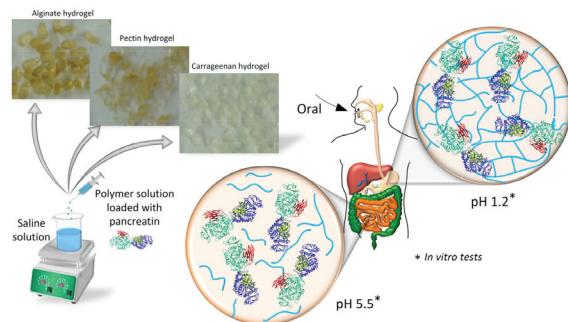
**Graphical Abstract**  
The transesterification reaction of soybean oil was modeled considering the 3 steps of the direct and reverse reactions following a second order general kinetics by the finite element method.



**320 Preparation and Delayed Release Study on Pancreatin Encapsulated into Alginate, Carrageenan and Pectin Hydrogels**

Si online <http://dx.doi.org/10.1593/jbcs.170011>  
Fernanda M. P. Olímpio, Adriano A. Mendes,  
Marcello G. Trevisan and Jerusa S. Garcia

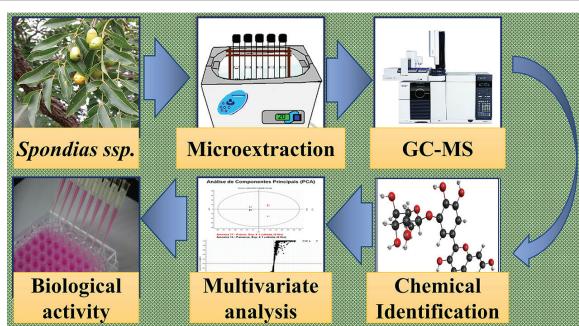
**Graphical Abstract**  
Three hydrogels were prepared and applied in pancreatin encapsulation. Alginate hydrogel presented better encapsulation efficiency and enzyme release representing as an alternative to replace the commercial formulation.



**331 GC-MS-Based Metabolomic Profiles Combined with Chemometric Tools and Cytotoxic Activities of Non-Polar Leaf Extracts of *Spondias mombin* L. and *Spondias tuberosa* Arr. Cam.**

Jhonyson A. C. Guedes, Elenilson G. Alves Filho, Maria F. S. Silva, Tigressa H. S. Rodrigues, Christiane M. C. Ramires, Maria A. C. Lima, Gisele S. Silva, Cláudia Ó. Pessoa, Kirley M. Canuto, Edy S. Brito, Ricardo E. Alves, Ronaldo F. Nascimento and Guilherme J. Zocolo

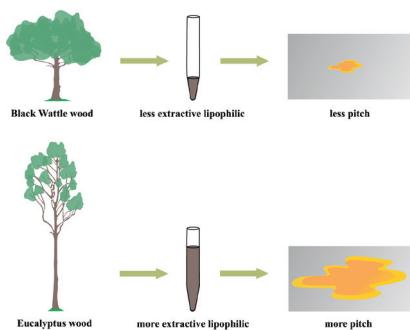
**Graphical Abstract**  
Analytical procedures, from the collection of samples to the correlation of chemical identification with biological activity.



**341 Characterizing the Chemical Composition of Lipophilic Extracts from *Acacia mearnsii* Wood**

Si online <http://dx.doi.org/10.1593/jbcs.170012>  
Gliciane R. A. Oliveira, Fábio S. Grasel, Gevany P. de Pinho and Flaviano O. Silvério

**Graphical Abstract**  
The constituents that can generate the pitch are in smaller quantities in the extracts of *Acacia mearnsii* wood in relation to the eucalyptus wood.

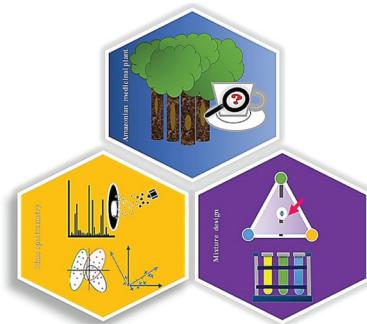


**351 Integrative Approach Based on Simplex-Centroid Design, ESI-MS and Chemometric Analysis for Comprehensive Characterization of Phenolic Compounds from *Endoplectura uchi* Bark**

*SI online*

Lilian M. Bastos, Felipe M. A. da Silva, Leonard R. S. de Souza, Ingrity S. C. Sá, Rochelly M. da Silva, Afonso D. L. de Souza and Rita de Cássia S. Nunomura

**Graphical Abstract**  
The integrative approach based on simplex-centroid design, electrospray ionization mass spectrometry (ESI-MS), and multivariate analysis provided an effective way to assess the phenolic composition of *Endoplectura uchi* bark.



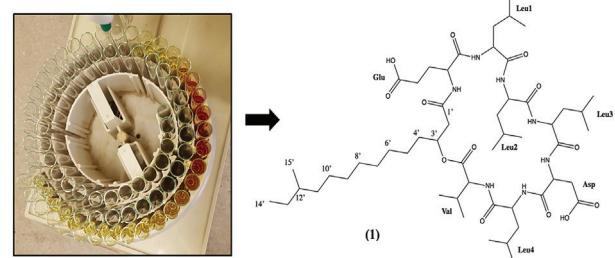
**357 Pumilacidins A-E from Sediment-Derived Bacterium *Bacillus* sp. 4040 and Their Antimicrobial Activity Evaluation**

*SI online*

Josiane A. M. de Oliveira, David E. Williams, Raymond J. Andersen, Maria H. Sarragiotto and Debora C. Baldoqui

**Graphical Abstract**

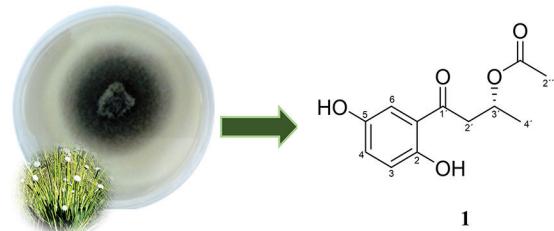
A series of pumilacidins were isolated from the solid culture of the marine-derived bacterium *Bacillus* sp. 4040. The structures were determined using a combination of mass spectrometry, nuclear magnetic resonance (NMR) spectroscopy and comparison with reported data.



**364 Aromatic Polyketides and Macrolides from *Microsphaeropsis arundinis***

*SI online*

Weslei Bruno Botero, Marcelo R. de Amorim, Iracilda Z. Carlos, Marisa C. Polesi and Lourdes C. dos Santos



**Graphical Abstract**

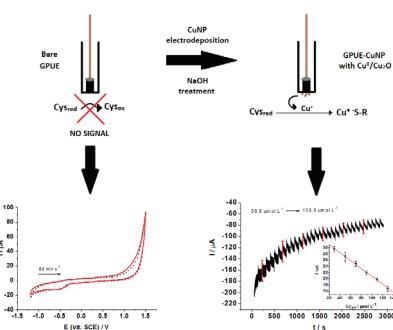
A novel aromatic polyketide isolated from *Microsphaeropsis arundinis*.

**370 Evaluation of a Graphite-Polyurethane Composite Electrode Modified with Copper Nanoparticles as an Amperometric Flow Detector in a Wall-Jet System for the Determination of Cysteine**

Isabela A. Mattioli, Letícia F. L. Schildt, Priscila Cervini, Thalita R. Sacilotto and Éder T. G. Cavalheiro

**Graphical Abstract**

Cysteine (Cys) does not present voltammetric response at bare graphite-polyurethane composite electrode (GPUE) or even at non-treated GPUE containing electrodeposited copper nanoparticles (CuNP). When GPUE-CuNP is electrochemically pretreated in basic medium the Cys response can be observed based on its interaction with Cu oxides at electrode surface allowing analytical applications in an amperometric wall-jet procedure.

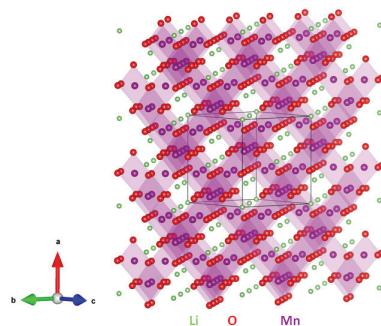


**381 Experimental and Theoretical Study of LiMn<sub>2</sub>O<sub>4</sub> Synthesized by the Solution Combustion Method Using Corn Starch as Fuel**

SI online José M. Siqueira Jr., Carolina T. Machado,  
Daniel S. G. Quattrociochi, Francisco M. S. Garrido,  
Leonardo M. da Costa, Eduardo A. Ponzio,  
Glaucio B. Ferreira and Jackson A. L. C. Resende

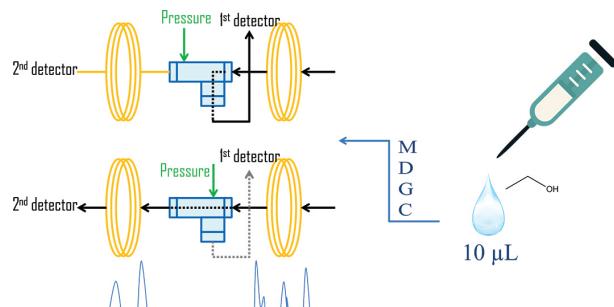
**Graphical Abstract**

LiMn<sub>2</sub>O<sub>4</sub> was synthesized by the solution combustion method using corn starch as fuel with temperature below 700 °C. This synthesis is ecofriendly and has a lower cost than the standard methods. The influence of the Li<sup>+</sup> cations amount on the MnO<sub>2</sub> oxide structural and electronic properties was also evaluated by the density functional theory (DFT) method.



**394 Ethanol Content Determination in Medicine Syrups Using Headspace and Multidimensional Heart-Cut Gas Chromatography Coupled to Mass Spectrometry**

SI online Lilian R. Batista and Nelson R. Antoniosi Filho



**Graphical Abstract**

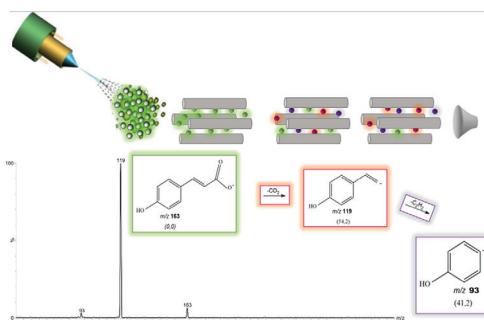
Multidimensional gas chromatography method for ethanol monitoring in medicated syrups in order to question quality certificates from regulatory agencies.

**402 Structural Study of Phenolic Acids by Triple Quadrupole Mass Spectrometry with Electrospray Ionization in Negative Mode and H/D Isotopic Exchange**

SI online Nayane B. M. Sinosaki, Angélica P. P. Tonin, Marcos A. S. Ribeiro, Camila B. Poliseli, Sharise B. Roberto, Roberta da Silveira, Jesuí V. Visentainer, Oscar O. Santos and Eduardo C. Meurer

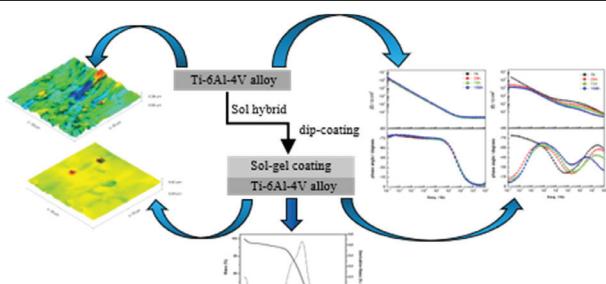
**Graphical Abstract**

Five phenolic acids were evaluated according to the fragmentation profile by collision-induced dissociation (CID) using triple quadrupole mass spectrometry by electrospray ionization in negative ionic mode (ESI(-)-MS/MS), combined with thermochemical data obtained by computational chemistry and hydrogen by deuterium (H/D) exchange.



**409 PMMA-SiO<sub>2</sub> Organic-Inorganic Hybrid Coating Application to Ti-6Al-4V Alloy Prepared through the Sol-Gel Method**

Joseane A. Santana, Sandra R. Kunst, Cláudia T. Oliveira, Antonio A. Bastos, Mario G. S. Ferreira and Victor H. V. Sarmento



**Graphical Abstract**

Hybrid coating application to Ti-6Al-4V alloy prepared through the sol-gel method.

**421 Thermal Infrared Enthalpimetry in Paper Microzone Plates for Green and High Throughput Determination of Wine Acidities**

SI online  *Daniele F. Ferreira, Bruna Tischer, Alexandre J. Cichoski, Cristiano R. Menezes, Roger Wagner, Adilson B. Costa and Juliano S. Barin*

**Graphical Abstract**

Wine samples were added in the hydrophilic microzones of a paper device followed by addition of NaOH solution in stoichiometric excess.

An infrared camera was used to record the analytical operations. The neutralization reaction releases heat, and the temperature of solutions rises, and it could be directly related to the wine acidity.



