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Cover Picture



Glutathione S-transferase (GST) catalyzes the conjugation of the reduced form of glutathione (GSH) to xenobiotic substrates, leading to their excretion. This is an important mechanism in insect-resistance to dichloro-diphenyl-trichloroethane (DDT). Molecular docking calculations positions the DDT beta-carbon for the nucleophilic addition by the thiolate group in GSH. This reaction converts DDT to dichloro-diphenyl-dichloroethylene (DDE). Punctual mutation on position 120 in GST Epsilon class isoforms from *Anopheles gambiae* influences the conformational dynamics of protein strengthening the reaction capabilities to consume DDT. Details are presented in the Article **The Role of the Conformational Dynamics of Gluthatione S-Transferase Epsilon Class on Insecticide Resistance in** *Anopheles gambiae* **by** *Frederico J. S. Pontes, Rafael T. Maia, Maria Carolina P. Lima, Constância F. J. Ayres and Thereza A. Soares* **on page 1602.**

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Articles

1521 Application of a Novel Micro-Cloud Point Extraction for Preconcentration and Spectrophotometric Determination of Azo Dyes



Sl online Elham Ghasemi and Massoud Kaykhaii

Graphical Abstract For the extraction of analytes, salt solution is added to the aqueous sample to form micelles. After centrifugation, enriched micellar phase is dissolved in a diluting solvent and was transferred to a microcell for spectrophotometric determination. 1527 Soil Organic Carbon Determination Using NIRS: Evaluation of Dichromate Oxidation and Dry Combustion Analysis as **Reference Methods in Multivariate Calibration** Karla K. Beltrame, André M. Souza, Maurício R. Coelho. Thayane C. B. Winkler, Wyrllen E. Souza and Patrícia Valderrama

Graphical Abstract A comparison between dichromate oxidation and dry combustion analysis as reference methods in multivariate calibration from near infrared spectroscopy was evaluated.

1533 **Evaluation of QuEChERS Sample Preparation and Gas** Chromatography Coupled to Mass Spectrometry for the **Determination of Pesticide Residues in Grapes** Fernanda Volpatto, Arci D. Wastowski, Gabrieli Bernardi,

Osmar D. Prestes, Renato Zanella and Martha B. Adaime

Graphical Abstract

The concern about the presence of pesticide residues in fruits has prompted the search for alternative methods able to detect low levels of these compounds in a simple and efficient way. Thus, in this work a quick, easy, cheap, effective, robust and safe (QuEChERS) method was successfully modified, validated and applied for pesticide residues determination in grape samples by gas chromatography coupled with mass spectrometry.





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Combining the Pharmacophore Features of Coumarins and 1,4-Substituted 1,2,3-Triazoles to Design New Acetylcholinesterase Inhibitors: Fast and Easy Generation SI online of 4-Methylcoumarins/1,2,3-triazoles Conjugates via Click Chemistry

> Fernando C. Torres, Guilherme A. Gonçalves, Kenia L. Vanzolini, Aloir A. Merlo, Bruna Gauer, Maribete Holzschuh, Saulo Andrade, Maristela Piedade, Solange C. Garcia, Ivone Carvalho, Gilsane L. von Poser, Daniel F. Kawano, Vera L. Eifler-Lima and Quezia B. Cass

Graphical Abstract We describe the synthesis of 4-methylcoumarins/1,4-substituted 1,2,3-triazole conjugates that are moderate inhibitors of acetylcholinesterase in vitro.



1551 Gas-Phase Polycyclic Aromatic Hydrocarbons in the Parking Lot Impacted by Light-Duty Vehicles Burning Gasoline and Ethanol Blends

Fabio C. Sabino, Jurandir P. Pinto, Ismael R. Amador, Leila D. Martins and Maria Cristina Solci



Graphical Abstract

Gaseous polycyclic aromatic hydrocarbons (PAHs) in a parking lot impacted by gasoline and ethanol blend used in flex-fuel vehicles.



Interaction of β-Carbolines with DNA: Spectroscopic Studies, Correlation with Biological Activity and Molecular Docking Marina M. Silva, Franciele C. Savariz, Edeíldo F. Silva-Júnior, Sl online Thiago M. de Aquino, Maria Helena Sarragiotto, Josué C. C. Santos and Isis M. Figueiredo

Graphical Abstract This work reports the interaction evaluation of twelve B-carboline derivatives with deoxyribonucleic acid (DNA) using spectroscopic techniques, correlation of binding constants (K_h) with IC_{50} of seven human cancer cell lines and molecular docking.



1569 Microwave-Induced Combustion of Coal for Further Sulfur **Determination by Inductively Coupled Plasma Optical Emission Spectrometry or Ion Chromatography** Gabriela Corazza, Alessandra S. Henn, Marcia F. Mesko, Fabio A. Duarte, Erico M. M. Flores and Paola A. Mello

Graphical Abstract

A careful optimization of the microwave-induced combustion method for Brazilian coal digestion for further determination of sulfur by inductively coupled plasma optical emission spectrometry (ICP OES) and ion chromatography was developed.

Microwave-induced combustion



1577 Novel Non Enzymatic TBHO Modified Electrochemical Sensor for Hydrogen Peroxide Determination in Different Beverage Samples

Navid Nasirizadeh, Masoud Ghaani, Zahra Shekari and SI online Mohammad Shateri-Khalilabad

Graphical Abstract

Graphical Abstract

A new electrochemical sensor based on glassy carbon electrode which is modified by nation, graphene oxide, silver nanoparticles and tertbutylhydroquinone (TBHQ) for hydrogen peroxide determination in real beverage samples was developed.



1587 Lipophilicity Study of Thiazolo[3,2-a]pyrimidine Derivatives as Potential Bioactive Agents

Renata Studzińska, Renata Kołodziejska, Małgorzata Redka, Bożena Modzelewska-Banachiewicz and Beata Augustyńska



27 potentially active thiazolo[3,2-a]pyrimidine derivatives were analyzed by two methods: reversed phase high performance liquid chromatography (RP-HPLC) and reversed phase thin layer chromatography (RP-TLC) methods. Determined lipophilicity parameters are in the range from 0 to 5. It is mean that there are hydrophobic substances, soluble in the lipid phase and in case of being used as drugs, they will be active after oral application.



Leonardo S. G. Teixeira

UV-Assisted Digestion of Petrochemical Industry Effluents Prior to the Determination of Zn, Cd, Pb and Cu by Differential Pulse Anodic Stripping Voltammetry Sl online Daniela Domingos, Maria de Lourdes S. Ferreira Neta, Ana Rosa C. G. Massa, Marcio V. Reboucas and



Graphical Abstract

The feasibility of applying differential pulse anodic stripping voltammetry technique for the determination of metals species in the petrochemical industry effluent was demonstrated after UV-assisted digestion procedure.



The Role of the Conformational Dynamics of Glutathione S-Transferase Epsilon Class on Insecticide Resistance in Anopheles gambiae

Frederico J. S. Pontes, Rafael T. Maia, Maria Carolina P. Lima, SI online Constância F. J. Ayres and Thereza A. Soares



Graphical Abstract

Influence of conformational dynamics of glutathione S-transferases (GSTs) on dichloro-diphenyl-trichloroethane (DDT) metabolizing was investigated through molecular dynamics simulations.



Cholinesterases Inhibition by Novel cis- and trans-3-Arylaminocyclohexyl N,N-Dimethylcarbamates: Biological Evaluation and Molecular Modeling

Sl online Diego A. S. Yamazaki, Augusto A. Cândido, Mariane C. Bagatin, Miguel Machinski Jr., Simone A. G. Mossini, Rodrigo M. Pontes, Fernanda A. Rosa, Ernani A. Basso and Gisele F. Gauze

Graphical Abstract

Novel 3-arylaminocyclohexyl N,N-dimethyl carbamates synthesized showed selectivity for the butyrylcholinesterase (BuChE) inhibition. Kinetics studies indicated a mixed-type inhibition against BuChE which is compatible with molecular modeling studies.





Determination of Pesticides in Grape Juices by QuEChERS and Liquid Chromatography-Tandem Mass Spectrometry Deise F. Souza, Edson L. Souza and Endler M. Borges

SI online

Graphical Abstract

Development of a liquid chromatography-tandem mass spectrometry (LC-MS/MS) method for the determination of 25 pesticides, which are widely used in grape culture in Brazil, in grape juice. The method was validated according with INMETRO (Instituto Nacional de Metrologia Qualidade e Tecnologia).



Sl online César F. Santos, Cleydson B. R. Santos and Carlos H. T. P. Silva



Graphical Abstract

This molecule is a promising drug lead for the development of derivatives and treatment of metabolic syndrome with the benefits of a peroxisome proliferator-activated receptor pan activation.



Marcone A. L. de Oliveira, Nádia R. B. Raposo, Anderson O. Ferreira and Marcos A. F. Brandão

Graphical Abstract

Taxifolin is the major individual polyphenol in the aqueous extract of the bark of Pinus pinaster and may be a chemical marker for quality control of this extract. It was analyzed by reversed phase liquid chromatography with photodiode array detector.



Rapid injection of mixtu us analyte solution Cloudy state Orga Aque diment IMS analysis

1657 Rapid and Highly Sensitive Determination of Melamine in Different Food Samples by Corona Discharge Ion Mobility Spectrometry after Dispersive Liquid-Liquid Microextraction Sl online Roya Mirzajani and Nahid Tavaf

Graphical Abstract

A novel and sensitive method based on dispersive liquid-liquid microextraction coupled with positive corona discharge ion mobility spectrometry has been evaluated as a fast and inexpensive technique for the direct determination of melamine in milk, dairy products and egg volk.



Graphical Abstract

Modified carbon paste electrode -1.0 -0.8 -0.6 -0.4 -0.2 E / V vs. Ag/AgCl 3 mol L⁻¹ -1.2 Ion solution Eletrochemical response

In this work carbon paste electrodes modified with Eichhornia crassipes roots were employed to study the adsorption of thallium (Tl⁺) and cadmium (Cd^{2+}) ions. Ions interact with different functional groups that are present in the roots. Eichhornia crassipes is an effective alternative for the removal of $Tl^{\scriptscriptstyle +}$ and $Cd^{2\ast}$ ions from an aqueous medium.

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Characterization of Polylactide-Stabilized Gold Nanoparticles and Its Application in the Fabrication of Electrochemical DNA Biosensors

SI online Noordiana Nordin, Nor Azah Yusof, Jaafar Abdullah, Son Radu and Reza Hajian



Graphical Abstract

Two different gold nanoparticles (AuNPs and polylactic acid-AuNPs) were prepared for construction of biosensors on screen-printed electrode. The performance of fabricated biosensor based on polylactic-stabilized AuNPs shows better sensitivity and stability.



Caroline S. Oliveira, Glaucia B. Alcantara, Luciano M. Lião, Glenda M. Mesquita, Silvia S. Freitas and Fernando Petacci

Graphical Abstract

The degradation of *Typha angustifolia* L. is accompanied by the remaining mass and ash percentage showing the liberation of polyphenols and phosphorous compounds from lignocellulosic tissue, which consequently generates humic substances. Different phosphorous compounds were identified in the remaining mass by ³¹P NMR (nuclear magnetic resonance).



1694 Phytochemical Profile of Seed Extracts of Plants Typical of the Brazilian Semiarid and their Potential Application in Brackish Water Desalination Tadeu A. C. Costa, Vânia P. Campos, Joilma S. Menezes,

Sergio T. Oliva and Chirlene B. West

Graphical Abstract

Umbu can be even more useful in the semiarid areas, where it is a native plant and where there is a lack of good quality drinking water. Coal prepared with its seed contains no toxic substances and can used for domestic desalination of brackish water.

