www.publish.csiro.au/journals/ajc



Metabolomics is a comprehensive analysis strategy that aims to identify and quantify the suite of metabolites in an organism. Learn more about a tool to achieve that end in the Focus by Shellie (p. 619).

Full Papers

Stereoselective Isomerizations of 4-(2'-Chloro-3'-methoxyphenyl)-2,5-dimethyl-1,3-dioxolanes: Stereochemistry and Conformation of the Product 2-Benzopyrans

Robin G. F. Giles, Ivan R. Green, Shuk-Hui Li

Aust. J. Chem. 2005, 58, 565–571.

A *uudd* Cyclic Water Tetramer and an Opened Octameric Water Cluster in the Charge-Transfer Salts of the Bipyridinium Cation

Yan-qiong Sun, Jie Zhang, Zhan-feng Ju, Guo-Yu Yang

Aust. J. Chem. 2005, 58, 572-577.

Syntheses, Structures, Properties, and Theoretical Studies of d¹⁰ Metal Complexes of Ethylenediamine

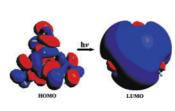
Wen-Tong Chen, Ming-Sheng Wang, Li-Zhen Cai, Guo-Cong Guo, Jin-Shun Huang

Aust. J. Chem. 2005, 58, 578-584.

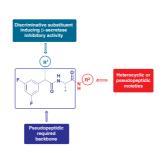
Design of β -Secretase Inhibitors by Introduction of a Mandelyl Moiety in DAPT Analogues

Nicolas Pietrancosta, Gilles Quéléver, Younes Laras, Cédrik Garino, Stéphane Burlet, Jean Louis Kraus

Aust. J. Chem. 2005, 58, 585-594.



Four tris(ethylenediamine)-chelated metal complexes have been synthesized. All of the complexes display fluorescent properties in the blue range, which are attributed to the ligand-to-metal charge-transfer mechanism, as probed by molecular orbital calculations. Spectroscopic and thermogravimetric analyses are also presented for the title compounds.



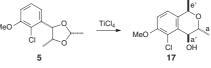
 β -secretase (BACE-1) is an important enzyme in the pathology of Alzheimer's disease. A series of new BACE-1 inhibitors bearing 3,5-difluoromandelyl-alanyl or 3,5-difluorophenylacetyl-alanyl backbones linked to various functionalized heterocyclic or aliphatic moieties (shown) have been prepared and characterized. The former proved potent BACE-1 inhibitors, while the latter appeared to have no activity.

the 1,8- and 4,5-*peri* interactions present. In the examples considered, the stereochemistry of the C-1 methyl group changes dramatically over a small temperature range when 1,8-*peri* interactions are significant.

The half-chair conformation of the dihydropyran ring in aryl-substituted

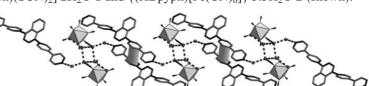
4-hydroxy-1,3-dimethyl-2-benzopyrans is determined by the magnitude of

AUSTRALIAN JOURNAL OF



AN INTERNATIONAL JOURNAL FOR CHEMICAL SCIENCE

In a continuing effort to elucidate the structure of water clusters to facilitate understanding of its vital role in nature, new observations of a *uudd* cyclic water tetramer and an opened octameric water cluster with a chair-like conformation are reported in two kinds of bipyridium charge-transfer salts: $[(Bpyph)(SCN)_2]\cdot 2H_2O$ **1** and $\{(HBpyph)[Fe(CN)_6]\}\cdot 5.5H_2O$ **2** (shown).



A Simple Approach to Micro-Patterned Surfaces by Breath Figures with Internal Structure Using Thermoresponsive Amphiphilic Block Copolymers

Alexandra Nygard, Thomas P. Davis, Christopher Barner-Kowollik, Martina H. Stenzel

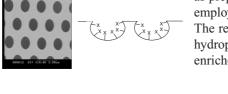
Aust. J. Chem. 2005, 58, 595-599.

Short Communications

Crystal Structure of 1-Methyl-5,8dihydroxynaphtho[2,3-c]furan-4,9-dione

Brian W. Skelton, Matthew J. Piggott

Aust. J. Chem. 2005, 58, 600-602.



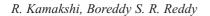
Surface tension measurements were utilized to study the internal structure of honeycomb-structured porous films, as prepared using breath figures when employing amphiphilic block copolymers. The resulting structure was found to have hydrophobic surfaces while the pores are enriched with hydrophilic polymer.

a similar preference for the 5,8-dihydroxynaphtho[2,3-c]furan-4,9-dione tautomer, necessitating revision of the published structures of ventilone F and G. $O^{H} O = O^{H} O$

The determined and modelled structures of the title natural product (right

structure) revealed none of the isobenzofuranoid tautomer (left). This prompted modelling of the structure of ventilone G. The results confirmed

Solventless Rapid Synthesis of Oxime, Semicarbazone, and Phenylhydrazone Derivatives from Carbonyl Compounds under Microwave Conditions

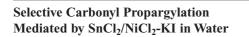


Aust. J. Chem. 2005, 58, 603-606.

Iron(III) Fluoride: A Highly Efficient and Versatile Catalyst for the Protection of Carbonyl Compounds under Solvent-Free Conditions

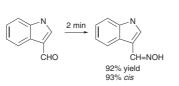
Babasaheb P. Bandgar, Vinod T. Kamble, Ashwini Kulkarni

Aust. J. Chem. 2005, 58, 607-610.

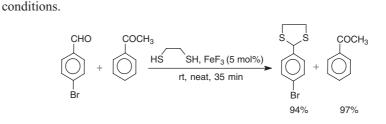


Jun Wang, Xiao-Peng Miao, Gu Yuan





A rapid and efficient solventless method for the synthesis of oximes, semicarbazones, and phenylhydrazones using microwave irradiation is described. The method is simple and it is stereo-selective.



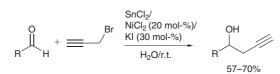
Iron(III) fluoride is a superior catalyst for the conversion of aldehydes into

oxathioacetals and dithioacetals under solvent-free conditions. Catalysis by

iron(III) fluoride provides chemoselective protection of aldehydes in the

presence of ketones, high yields, operational simplicity, and mild reaction

Catalyzed by NiCl₂-KI, SnCl₂ can efficiently mediate the reaction of propargyl bromide and aldehydes to produce homopropargylic alcohols as the major products at room temperature.



Lupane-Triterpene Esters from the Leaves of *Ceriops decandra* (Griff.) Ding Hou

Chanita Ponglimanont, Pakakrong Thongdeeying

Aust. J. Chem. 2005, 58, 615-618.

Focus

Comprehensive Two-Dimensional Gas Chromatography–Mass Spectrometry and its Use in High-Resolution Metabolomics

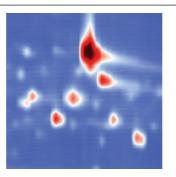
Robert A. Shellie

Aust. J. Chem. 2005, 58, 619.

CH₃ 1: R = H, β-O-*E*-feruloyl

2: R = H, β -O-Z-feruloyl

The extraction and isolation of two novel triterpene esters (shown) from the leaves of *C. decandra* is reported in addition to their structural assignment based on rigorous NMR techniques. The fastidious extraction process employed also yielded an additional 16 known triterpenes, which were also identified.



The coupling of two-dimensional gas chromatography to time-of-flight mass spectrometry gives rise to a powerful tool for comprehensively analyzing large numbers of metabolites. The attractive features of this technique (such as high resolution) and examples of its use are presented here.

Book Reviews			
Chris Whiteley	620		
Simon W. Lewis	621		
A. David Ward, Prudence Cowled	621		
Forest E. Michael	622		