# Organic & Biomolecular Chemistry

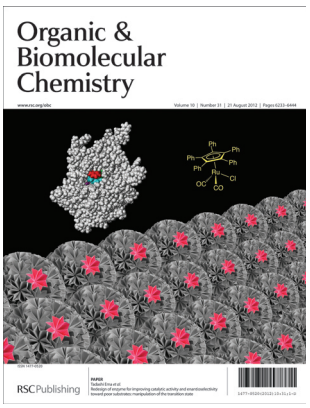
An international journal of synthetic, physical and biomolecular organic chemistry

**www.rsc.org/obc**

*RSC Publishing is a not-for-profit publisher and a division of the Royal Society of Chemistry. Any surplus made is used to support charitable activities aimed at advancing the chemical sciences. Full details are available from www.rsc.org*

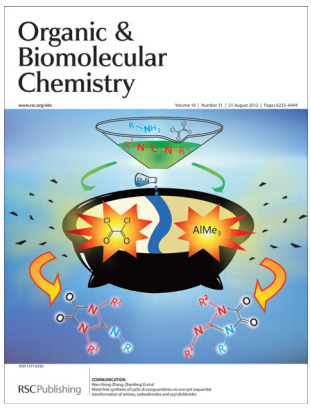

## IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 10(31) 6233–6444 (2012)




**Cover**
See Tadashi Ema *et al.*, pp. 6299–6308.

Image reproduced by permission of Tadashi Ema from *Org. Biomol. Chem.*, 2012, **10**, 6299.

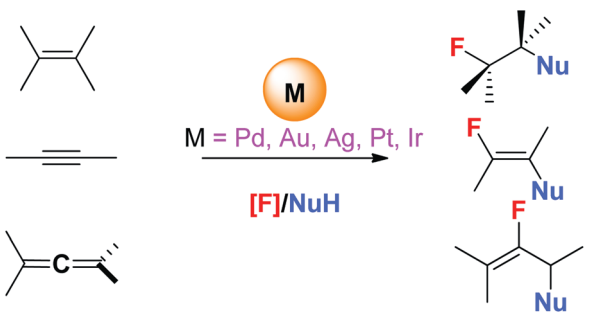



**Inside cover**
See Wen-Xiong Zhang, Zhenfeng Xi *et al.*, pp. 6266–6270.

Image reproduced by permission of Wen-Xiong Zhang from *Org. Biomol. Chem.*, 2012, **10**, 6266.

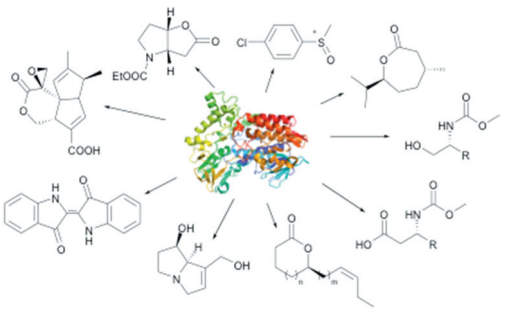
## EMERGING AREA






## PERSPECTIVE





Organic & Biomolecular Chemistry (print: ISSN 1477-0520; electronic: ISSN 1477-0539) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF. All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to RSC Distribution Services, c/o Portland Customer Services, Commerce Way, Colchester, Essex, UK CO2 8HP. Tel +44 (0)1206 226050; E-mail sales@rscdistribution.org

2012 Annual (print+electronic) subscription price: £3950; US$7373. 2012 Annual (electronic) subscription price: £3752; US$7004. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT. If you take an institutional subscription to any RSC journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip. Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank. Periodicals postage paid at Rahway, NJ, USA and at additional mailing offices. Airfreight and mailing in the USA by Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001, USA.

US Postmaster: send address changes to Organic & Biomolecular Chemistry (OBC) c/o Mercury Airfreight International Ltd., 365 Blair Road, Avenel, NJ 07001. All despatches outside the UK by Consolidated Airfreight.



# Organic & Biomolecular Chemistry

## An international journal of synthetic, physical and biomolecular organic chemistry

**www.rsc.org/obc**

*Organic & Biomolecular Chemistry* brings together molecular design, synthesis, structure, function and reactivity in one journal. It publishes fundamental work on synthetic, physical and biomolecular organic chemistry as well as all organic aspects of: chemical biology, medicinal chemistry, natural product chemistry, supramolecular chemistry, macromolecular chemistry, theoretical chemistry, and catalysis.



## INFORMATION FOR AUTHORS

Full details on how to submit material for publication in Organic & Biomolecular Chemistry are given in the Instructions for Authors (available from http://www.rsc.org/authors). Submissions should be made *via* the journal's homepage: http://www.rsc.org/obc.

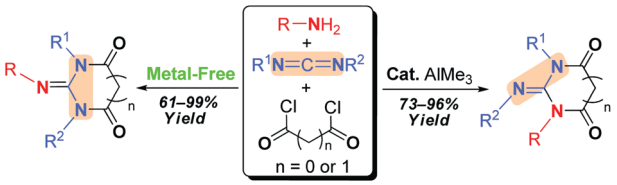
## COMMUNICATIONS

### 6266

**Metal-free synthesis of cyclic di-oxoguanidines *via* one-pot sequential transformation of amines, carbodiimides and acyl dichlorides**

Fei Zhao, Yang Wang, Wen-Xiong Zhang* and Zhenfeng Xi

Two sequential transformations from the same starting materials are achieved under metal-free or $AlMe_3$-catalyzed conditions providing structurally different cyclic di-oxoguanidines.

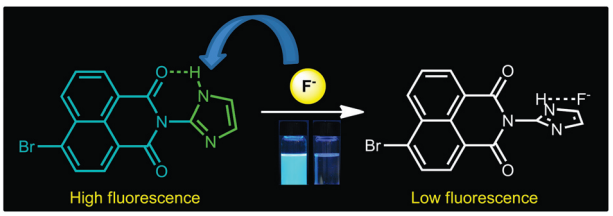



### 6271

**A new *N*-imidazolyl-1,8-naphthalimide based fluorescence sensor for fluoride detection**

Junqi Wang, Lingyun Yang, Chen Hou and Haishi Cao*

An *N*-imidazolyl-1,8-naphthalimide behaves as a fluoride sensor with high selectivity in $CH_2Cl_2$ owing to disruption of the intramolecular H-bond by fluoride.

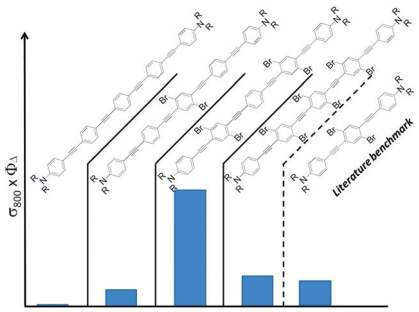



### 6275

**Influence of bromine substitution pattern on the singlet oxygen generation efficiency of two-photon absorbing chromophores**

Pierre-Henri Lanoë, Thibault Gallavardin, Aurore Dupin, Olivier Maury, Patrice L. Baldeck, Mikael Lindgren, Cyrille Monnereau* and Chantal Andraud*

Position of bromine substituents along the backbone of quadrupolar chromophores determines their two-photon induced singlet oxygen generation efficiency.



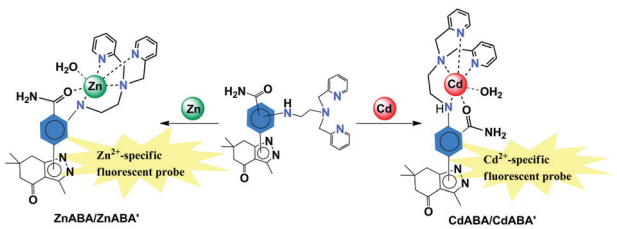

## PAPERS

### 6279

**Tetrahydroindazolone substituted 2-aminobenzamides as fluorescent probes: switching metal ion selectivity from zinc to cadmium by interchanging the amino and carbamoyl groups on the fluorophore**

Jia Jia, Qin-Chao Xu, Ri-chen Li, Xi Tang, Ying-Fang He, Meng-Yu Zhang, Yuan Zhang and Guo-Wen Xing*

Three $Cd^{2+}$ or $Zn^{2+}$-specific fluorescent probes have been developed with *N*,*N*-bis(2-pyridylmethyl)ethylenediamine as chelator and 2-aminobenzamide as fluorophore.



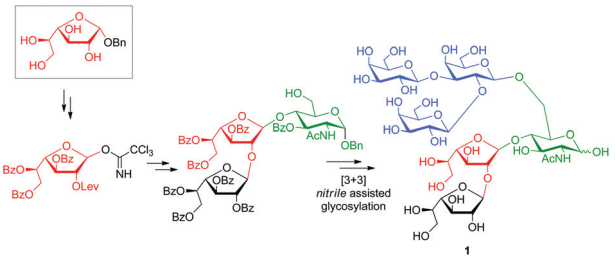
 

## 6322

### Synthesis of the *O*-linked hexasaccharide containing β-D-Gal*f*-(1→2)-β-D-Gal*f* in *Trypanosoma cruzi* mucins

Gustavo A. Kashiwagi, Verónica M. Mendoza, Rosa M. de Lederkremer and Carola Gallo-Rodriguez*

The novel hexasaccharide **1** was synthesized by a [3 + 3]-convergent strategy employing benzyl α-D-galactofuranoside, obtained in one step from galactose, as a new internal Gal*f*-precursor.

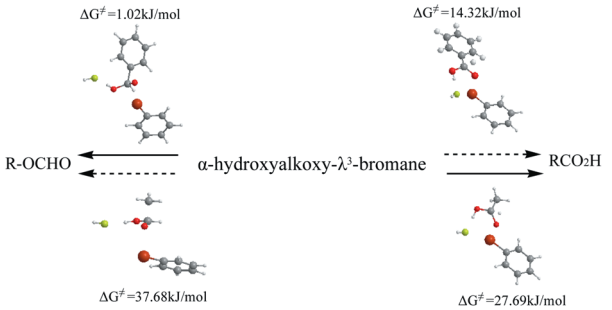



## 6333

### Theoretical study on the hypervalent $\lambda^3$-bromane strategy for Baeyer–Villiger oxidation of benzaldehyde and acetaldehyde: rearrangement mechanism

Hui Fu,* Shouwen Xie, Aiping Fu, Xufeng Lin, Hui Zhao and Tianxu Ye

DFT calculations described and explained well the key step of the novel BVO reaction of benzaldehyde and acetaldehyde.

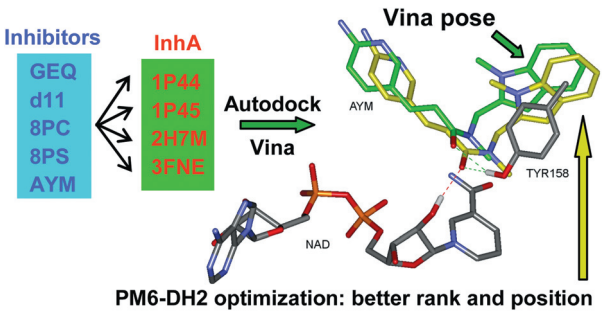



## 6341

### Cross-docking study on InhA inhibitors: a combination of Autodock Vina and PM6-DH2 simulations to retrieve bio-active conformations

Jean-Luc Stigliani,* Vania Bernardes-Génisson,* Jean Bernadou and Geneviève Pratviel

An Autodock Vina ensemble docking of InhA inhibitors followed by a PM6-DH2 post-docking allowed to select the correct ligand poses.

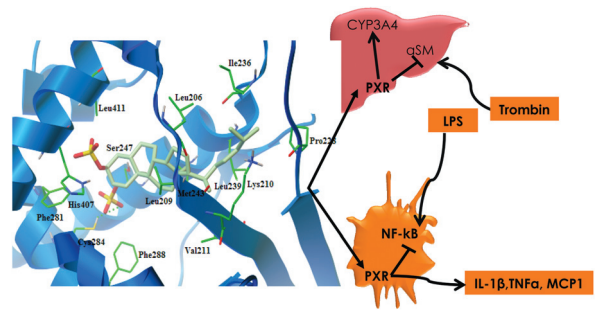


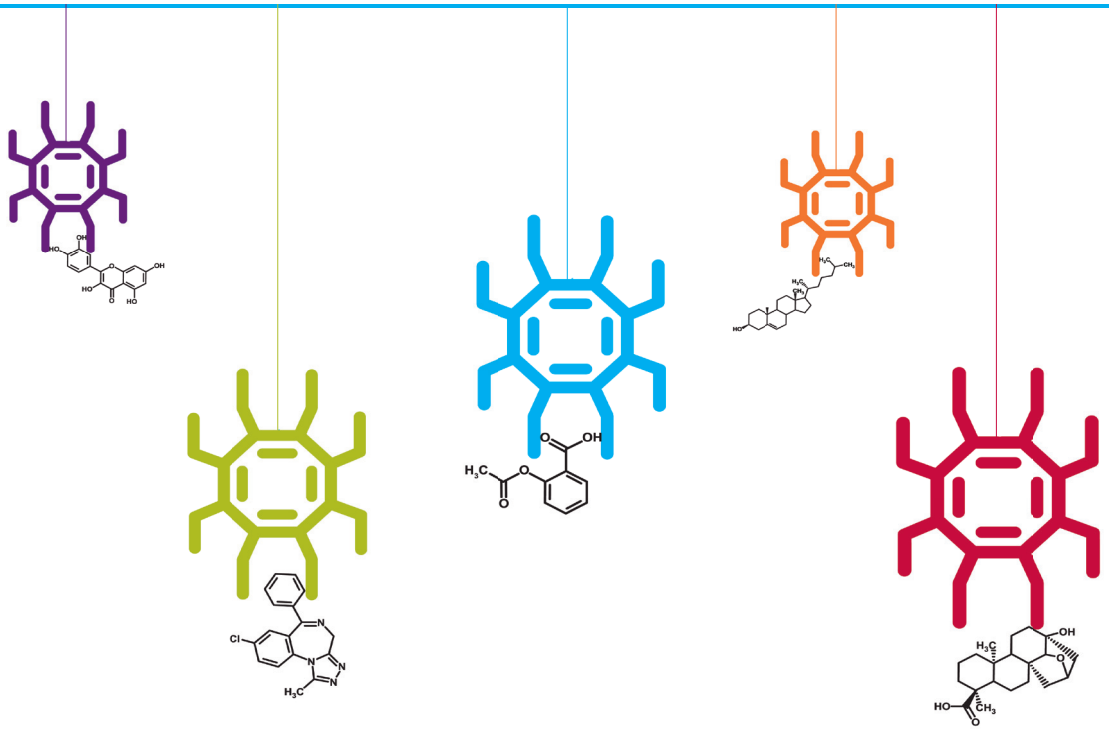

## 6350

### Modification in the side chain of solomonsterol A: discovery of cholestan disulfate as a potent pregnane-X-receptor agonist

Valentina Sepe, Raffaella Ummarino, Maria Valeria D'Auria, Gianluigi Lauro, Giuseppe Bifulco, Claudio D'Amore, Barbara Renga, Stefano Fiorucci and Angela Zampella*

Seven synthetic analogues of the PXR (pregnane-X-receptor) marine agonist solomonsterol A were prepared by total synthesis. The study discloses cholestan disulfate as a simplified new potent PXR agonist.





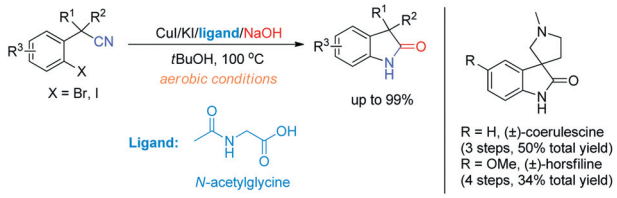
# ChemSpider

The free chemical database

ChemSpider is a free chemical structure database providing fast access to over 25 million structures, properties and associated information. By integrating and linking compounds from more than 400 data sources, ChemSpider enables researchers to discover the most comprehensive view of freely available chemical data from a single online search.

Access ChemSpider anyplace, anytime, anywhere with the ChemSpider mobile website **http://cs.m.chemspider.com** or use the ChemSpider **mobile app** – just search for it on the apple app store and download it for free.

## www.chemspider.com

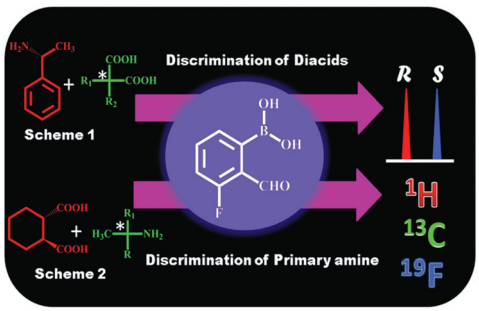



## Copper-catalyzed domino coupling reaction: an efficient method to synthesize oxindoles

Jen-Chieh Hsieh,* An-Yi Cheng, Jun-Hao Fu and Ting-Wei Kang

An efficient and novel procedure for a copper catalyzed domino coupling reaction has been developed, which afforded various oxindoles in good to excellent yields with tolerance of various substituents. In addition, this method could be applied to synthesize horsfiline and coerulescine in few steps with high total yields.



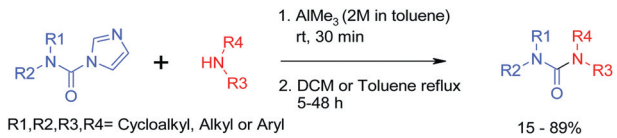



## Simple and efficient methods for discrimination of chiral diacids and chiral alpha-methyl amines

Sachin R. Chaudhari and N. Suryaprakash*

The three-component chiral derivatization protocols have been developed for testing the enantiopurity of chiral diacids and primary amines by $^{1}H$, $^{13}C$ and $^{19}F$ NMR spectroscopy.



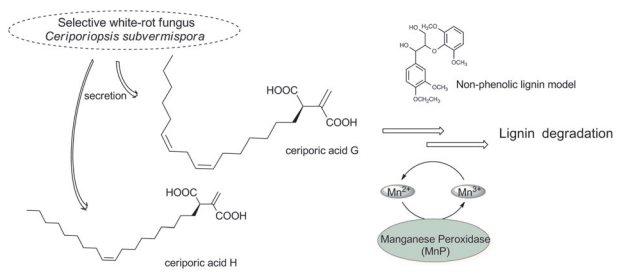



## Unsymmetrical tetrasubstituted ureas from tertiary carbamoylimidazole: activation by $AlMe_3$

A. Velavan, S. Sumathi* and K. K. Balasubramanian*

An efficient method for the synthesis of unsymmetrical tetrasubstituted ureas from carbamoylimidazole is described. The conversion is achieved by the concurrent quarternization of the imidazole nitrogen and activation of amines with $AlMe_3$.






## Alkadienyl and alkenyl itaconic acids (ceriporic acids G and H) from the selective white-rot fungus *Ceriporiopsis subvermispora*: a new class of metabolites initiating ligninolytic lipid peroxidation

Hiroshi Nishimura, Midori Sasaki, Hirofumi Seike, Masaharu Nakamura and Takashi Watanabe*

New alkadienyl and alkenyl itaconic acids (ceriporic G and H) were isolated from wood cultures of the selective white-rot fungus *Ceriporiopsis subvermispora*. The metabolites were chemically synthesized and characterized. Ceriporic acid G degraded a recalcitrant non-phenolic lignin substructure model compound in the presence of MnP.