

Organic & Biomolecular Chemistry

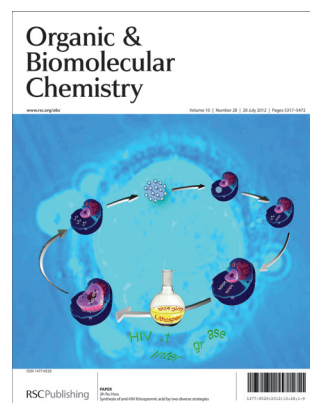
An international journal of synthetic, physical and biomolecular organic chemistry

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

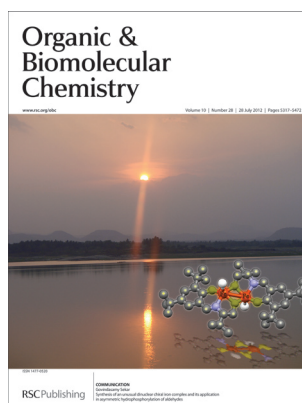
ISSN 1477-0520 CODEN OBCRAK 10(28) 5317–5472 (2012)



Cover

See Jih Ru Hwu,
pp. 5456–5465.

Image reproduced by permission of Jih Ru Hwu from *Org. Biomol. Chem.*, 2012, **10**, 5456.



Inside cover

See Govindasamy Sekar,
pp. 5347–5352.

Image reproduced by permission of Govindasamy Sekar from *Org. Biomol. Chem.*, 2012, **10**, 5347.

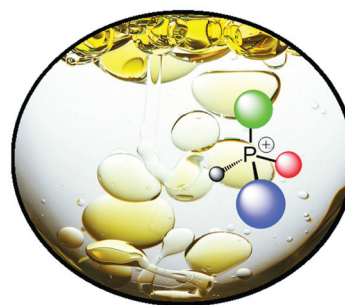
EMERGING AREA

5327

Chiral quaternary phosphonium salts: a new class of organocatalysts

Dieter Enders* and Thanh Vinh Nguyen

Chiral quaternary phosphonium salts can be used as versatile catalysts for various asymmetric chemical transformations.



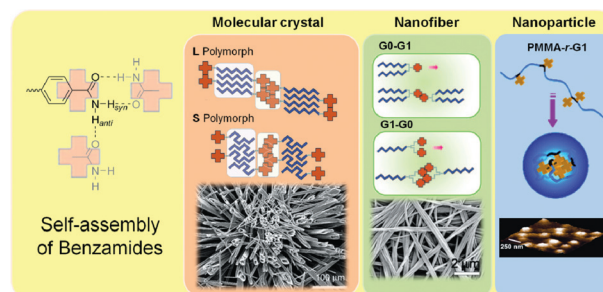
PERSPECTIVE

5332

Self-assembly driven by an aromatic primary amide motif

Myungeun Seo, Jeyoung Park and Sang Youl Kim*

This perspective highlights the key hydrogen bonding properties of primary amides determined from crystal structure studies, and a variety of supramolecular assemblies involving primary amides are discussed.



EDITORIAL STAFF

Editor

Richard Kelly

Deputy editor

Marie Cote

Development editor

James Anson

Senior publishing editor

Helen Saxton

Publishing editors

Mark Archibald, Andrea Banham, Nicola Burton, Sarah Dixon, Frances Galvin, Elisa Meschini, Roxane Owen

Publishing assistants

Aliya Anwar, Nathalie Horner

Publisher

Emma Wilson

For queries about submitted papers, please contact Helen Saxton, Senior publishing editor in the first instance. E-mail: obc@rsc.org

For pre-submission queries please contact Richard Kelly, Editor. Email: obc-rsc@rsc.org

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.

The Royal Society of Chemistry takes reasonable care in the preparation of this publication but does not accept liability for the consequences of any errors or omissions. Inclusion of an item in this publication does not imply endorsement by The Royal Society of Chemistry of the content of the original documents to which that item refers.

Advertisement sales: Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

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.

EDITORIAL BOARD

Chair

Jeffrey Bode, ETH Zürich, Switzerland

Associate Editors

Jin-Quan Yu, Scripps Research

Institute, La Jolla, CA, USA

Andrei Yudin, University of Toronto,

Canada

Ashraf Brik, Ben-Gurion University of the Negev, Israel

Margaret Brimble, University of Auckland, New Zealand

Pauline Chiu, University of Hong Kong, China

Anthony Davis, University of Bristol, UK

Veronique Gouverneur, University of Oxford, UK

Christian Hertweck, Leibniz-Institute Jena, Germany

Kenichiro Itami, Nagoya University, Japan

Stephen Kent, University of Chicago, USA

Paolo Scrimin, University of Padova, Italy

Qi-Lin Zhou, Nankai University, China

ADVISORY BOARD

Helen Blackwell, University of Wisconsin-Madison, USA

Barry Carpenter, Cardiff University, UK

Michael Crimmins, University of North Carolina, USA

Antonio Echavarren, Autonomous University of Madrid, Spain

Jonathan Ellman, Yale University, USA

Kurt Faber, University of Graz, Austria

Ben Feringa, University of Groningen, Netherlands

Nobutaka Fujii, Kyoto University, Japan

Jan Kihlberg, Umeå University, Sweden

Philip Kocienski, University of Leeds, UK

Steven V Ley, University of Cambridge, UK

Stephen Loeb, University of Windsor, Canada

Ilan Marek, Israel Institute of Technology, Israel

Manuel Martín Lomas, CCRB, San Sebastián, Spain

Keiji Maruoka, Kyoto University, Japan

Heather Maynard, University of California, Los Angeles, USA

E W' Bert' Meijer, Eindhoven University of Technology, Netherlands

Eiichi Nakamura, University of Tokyo, Japan

Ryoji Noyori, Nagoya University, Japan

Mark Rizzacasa, University of Melbourne, Australia

Richmond Sarpong, University of California, Berkeley, USA

Oliver Seitz, Humboldt University of Berlin, Germany

Jay Siegel, University of Zürich, Switzerland

Bruce Turnbull, University of Leeds, UK

Chris Welch, Merck & Co., Rahway, NJ, USA

Helma Wennemers, University of Basel, Switzerland

Peter Wipf, University of Pittsburgh, USA

Henry N C Wong, Chinese University of Hong Kong, China

Shuli You, Shanghai Institute of Organic Chemistry, China

Sam Zard, Ecole Polytechnique, France

Li He Zhang, Peking University, China

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>.

Authors may reproduce/republish portions of their published contribution without seeking permission from the RSC, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of The Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2012. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

The Royal Society of Chemistry takes reasonable care in the preparation of this publication but does not accept liability for the consequences of any errors or omissions.

Ⓢ The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

Royal Society of Chemistry: Registered Charity No. 207890.

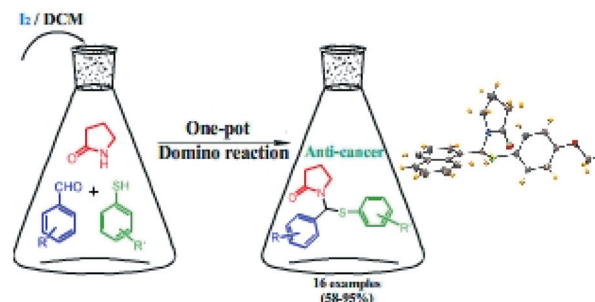
COMMUNICATIONS

5343

Efficient iodine catalyzed three components domino reaction for the synthesis of 1-((phenylthio)(phenyl)methyl)pyrrolidin-2-one derivatives possessing anticancer activities

Gunasekar Ramachandran, Natesan S. Karthikeyan, Periyasamy Giridharan and Kulathu I. Sathiyarayanan*

A three components domino reaction of γ -butyrolactam, benzaldehyde and thiophenol catalyzed by elemental iodine results in anticancer agents.

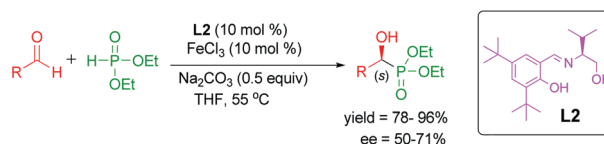


5347

Synthesis of an unusual dinuclear chiral iron complex and its application in asymmetric hydrophosphorylation of aldehydes

Pandi Muthupandi and Govindasamy Sekar*

An unusual dinuclear chiral iron complex has been synthesized and effectively utilized in the asymmetric hydrophosphorylation of aldehydes to synthesize optically active α -hydroxy phosphonates with excellent yield and good enantioselectivity.

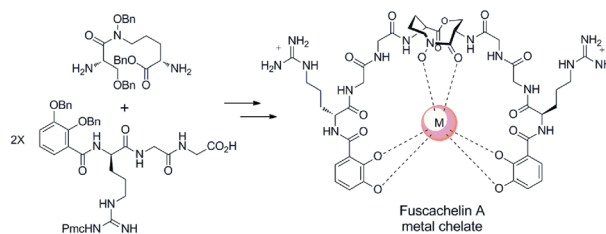


5353

Synthesis and structure confirmation of fuscachelins A and B, structurally unique natural product siderophores from *Thermobifida fusca*

Eric J. Dimise, Heather L. Conductor, Geoffrey E. Stoker and Steven D. Bruner*

The fuscachelin siderophores have been prepared synthetically as have their metal chelation complexes.

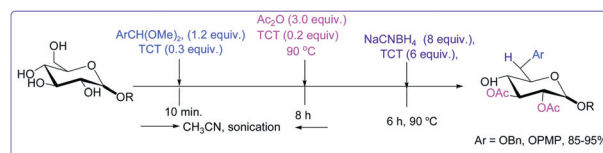


5357

2,4,6-Trichloro-1,3,5-triazine (TCT) mediated one-pot sequential functionalisation of glycosides for the generation of orthogonally protected monosaccharide building blocks

Madhubabu Tatina, Syed Khalid Yousuf and Debaraj Mukherjee*

Orthogonally protected monosaccharide building blocks have been prepared using TCT in a one-pot multicomponent transformation. The process involves successive steps of arylidene acetalation, esterification and regioselective reductive acetal cleavage.

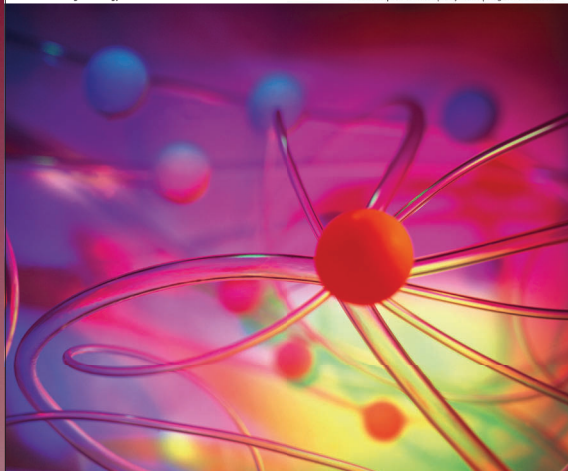


New
Journal

Toxicology Research

www.rsc.org/toxicology

Volume 1 | Number 00 | May 2012 | Pages 0000-0000



ISSN 2045-452X

RSC Publishing



THE BRITISH TOXICOLOGY SOCIETY

Toxicology Research

A new, multi-disciplinary journal covering the best research in both fundamental and applied aspects of toxicology

Published in partnership with the British Toxicology Society and Chinese Society of Toxicology

The journal is led by Editor-in-Chief, Nigel Gooderham, professor of molecular toxicology at Imperial College London and provides a home to communications, full papers and reviews.

Authors benefit from wide exposure for their work with free online access to content published during 2012 and 2013. Published work can also be made more visible through integration with *ChemSpider*, the RSC's free chemical structure database.

Authors can expect a speedy peer review and publication process, with the option of publishing research as an Accepted Manuscript, making work available quickly after acceptance.

The first issue is scheduled for publication mid-2012, and the first articles are now freely available online.

Submit your work now!



THE BRITISH TOXICOLOGY SOCIETY



Chinese Society Of Toxicology

RSC Publishing

www.rsc.org/toxicology

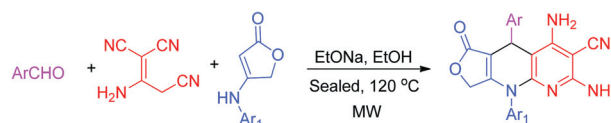
Registered Charity Number 207890

5361

New domino heteroannulation of enamines: synthesis of diverse fused naphthyridines

Jing Li, Yan Yu, Man-Su Tu, Bo Jiang,* Shu-Liang Wang and Shu-Jiang Tu*

A series of new poly-functionalized fused naphthyridine derivatives were synthesized *via* a three-component reaction of aldehyde, 2-aminoprop-1-ene-1,1,3-tricarbonitrile and enaminone in EtOH using EtONa as a base promoter. During these reaction processes, the domino construction of fused naphthyridine skeleton was readily achieved in one-pot.

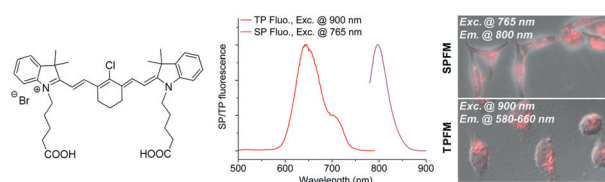


5366

A cyanine based fluorophore emitting both single photon near-infrared fluorescence and two-photon deep red fluorescence in aqueous solution

Lu Wang, Jiefu Jin, Xishan Chen, Hai-Hua Fan, Billy King Fai Li, Kok-Wai Cheah, Ning Ding, Shenghong Ju,* Wing-Tak Wong* and Cong Li*

A novel cyanine based fluorophore that emits both single-photon (SP) near-infrared fluorescence and two-photon (TP) deep red fluorescence under physiological conditions was developed.

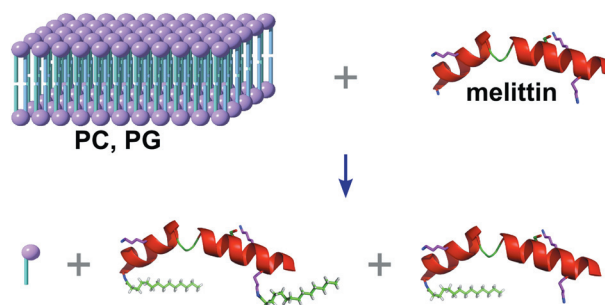


5371

The innate reactivity of a membrane associated peptide towards lipids: acyl transfer to melittin without enzyme catalysis

Robert H. Dods, Jackie A. Mosely* and John M. Sanderson*

The innate reactivity of the peptide melittin (H-GIGAVLKVLTTGLPALISWIKRKRQQ-NH₂) towards membrane lipids has been explored using LC-MS methods.

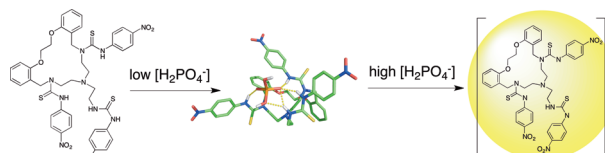


5379

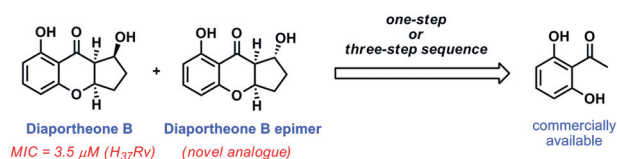
A chemosensor for dihydrogenphosphate based on an oxoazamacrocycle possessing three thiourea arms

Anxela Aldrey, Alejandro Macías, Rufina Bastida,* Guillermo Zaragoza, Gustavo Rama and Miguel Vázquez López*

A new H-bond macrocyclic chemosensor in organic media is reported. This system displayed marked changes in its UV-vis spectra and showed selectivity for dihydrogenphosphate over other inorganic anions, such as acetate or fluoride.



5385

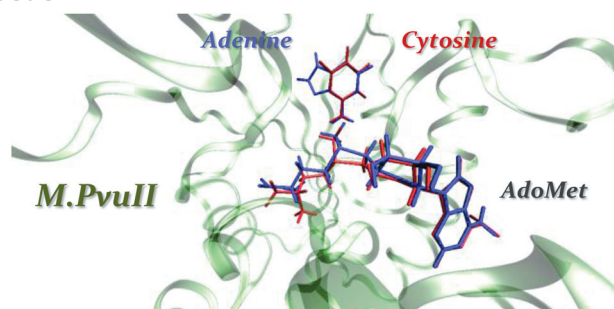


Antituberculosis agent diaportheone B: synthesis, absolute configuration assignment, and anti-TB activity of its analogues

Pandrangi Siva Swaroop, Gajanan N. Raut, Rajesh G. Gonnade, Priyanka Verma, Rajesh S. Gokhale and D. Srinivasa Reddy*

First total synthesis of diaportheone B, an antituberculosis agent isolated from endophytic fungus is reported. The absolute configuration of diaportheone B was determined using the X-ray crystal structure of its dibromo derivative.

5395

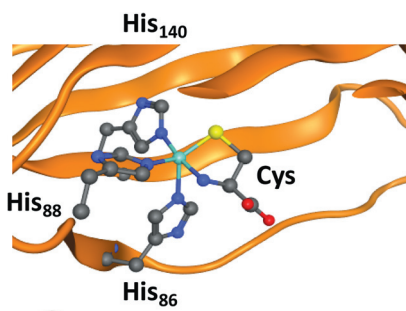


Substrate promiscuity in DNA methyltransferase *M.PvuII*. A mechanistic insight

Juan Aranda, Maite Roca* and Iñaki Tuñón*

M.PvuII is a DNA methyltransferase that catalyzes methylation of N4-cytosine but also displays promiscuous activity catalyzing methylation of N6-adenine. The nature of the residues of the active site determines the reaction mechanism.

5401

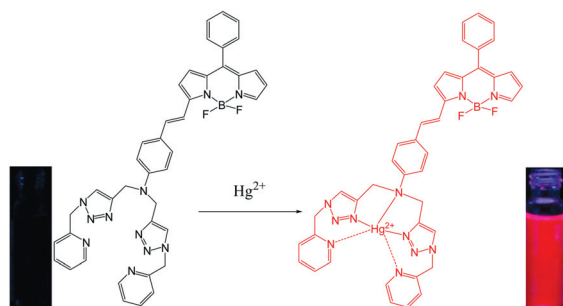


Axial and equatorial ligand effects on biomimetic cysteine dioxygenase model complexes

Luis E. Gonzalez-Ovalle, Matthew G. Quesne, Devesh Kumar,* David P. Goldberg* and Sam P. de Visser*

Density functional theory (DFT) calculations are presented on biomimetic model complexes of cysteine dioxygenase and focus on the effect of axial and equatorial ligand placement.

5410



A BODIPY-based colorimetric and fluorometric chemosensor for Hg(II) ions and its application to living cell imaging

Mani Vedamalai and Shu-Pao Wu*

A BODIPY-based chemosensor MS1 detects only the presence of Hg²⁺ ions among other transition metal ions by red emission.

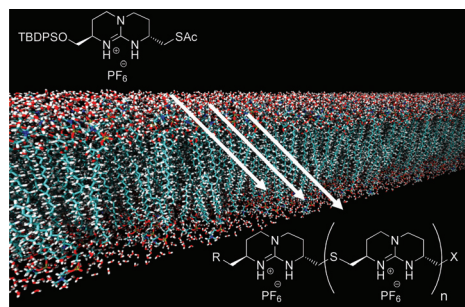
PAPERS

5417

Non-peptidic cell-penetrating agents: synthesis of oligomeric chiral bicyclic guanidinium vectors

Julián Valero, Michiel Van Gool, Ruth Pérez-Fernández, Pilar Castreño, Jorge Sánchez-Quesada, Pilar Prados and Javier de Mendoza*

We report improved and selective procedures for the preparation of oligoguanidinium scaffolds, with identical or different groups and functions at both ends of the chain.

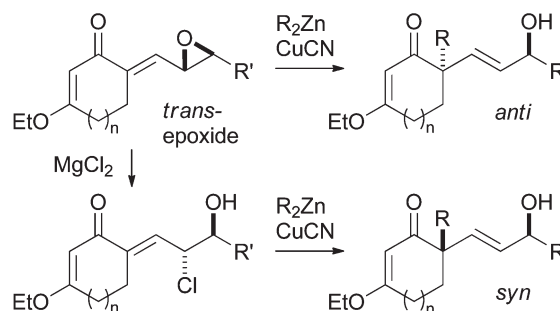


5431

Stereocontrolled synthesis of carbocyclic compounds with a quaternary carbon atom based on S_N2' alkylation of γ,δ -epoxy- α,β -unsaturated ketones

Fumihiko Yoshimura,* Ayano Kowata and Keiji Tanino*

An efficient method for stereodivergent construction of an all-carbon quaternary stereogenic center on a carbocyclic ring is reported *via* stereoselective S_N2' alkylation reactions of γ,δ -epoxy- α,β -unsaturated cyclic ketones.



Specialised searching



requires specialised tools

Registered charity Number 207890

The graphical abstracting services at the RSC are an indispensable tool to help you search the literature.

Methods in Organic Synthesis focuses on key primary journals covering: functional group changes, the introduction of chiral centres, and enzyme and biological transformations.

The online database has excellent functionality. Search by: authors, products, reaction, reactants and reagents.

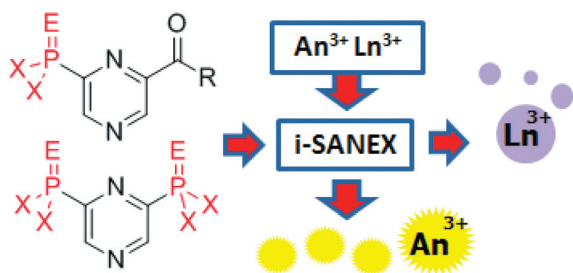
With Methods in Organic Synthesis you can find exactly what you need. Also available as a print bulletin.

For more information visit

RSC Publishing

www.rsc.org/databases

5443

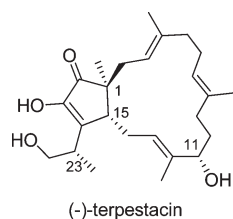


Palladium-catalyzed cross-coupling of various phosphorus pronucleophiles with chloropyrazines: synthesis of novel Am(III)-selective extractants

Nicolai I. Nikishkin, Jurriaan Huskens, Jana Assenmacher, Andreas Wilden, Giuseppe Modolo and Willem Verboom*

Pd-catalyzed cross-coupling of (di)chloropyrazines with phosphorus pronucleophiles in the presence of a base gives phosphorylated pyrazines in 81–95% yields. Hydrophilic derivatives exhibit a very good selectivity for Am³⁺ over Eu³⁺.

5452

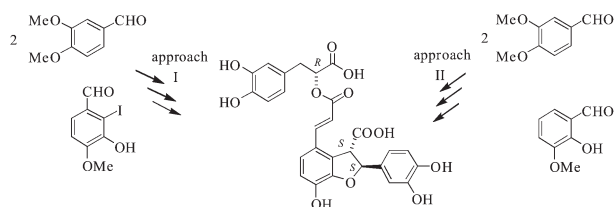


A convergent stereocontrolled total synthesis of (–)-terpestacin

Yehua Jin and Fayang G. Qiu*

A stereocontrolled total synthesis of (–)-terpestacin has been achieved starting from (*R*)-(–)-carvone as a chiral pool and (*E,E*)-farnesol *via* a highly convergent approach.

5456

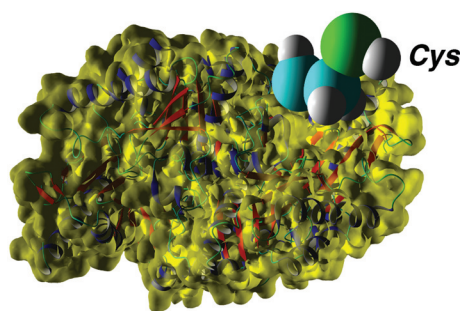


Synthesis of anti-HIV lithospermic acid by two diverse strategies

Tirumala G. Varadaraju and Jih Ru Hwu*

An efficient and convergent route for the synthesis of the natural product (+)-lithospermic acid, which possesses anti-HIV activity, was accomplished.

5466



Chromobacterium violaceum ω -transaminase variant Trp60Cys shows increased specificity for (*S*)-1-phenylethylamine and 4'-substituted acetophenones, and follows Swain–Lupton parameterisation

Karim Engelmark Cassimjee, Maria Svedendahl Humble, Henrik Land, Vahak Abedi and Per Berglund*

An improved ω -transaminase variant (Trp60Cys) from *Chromobacterium violaceum* shows increased specificity, altered cofactor dependence, different pH-optimum and higher resonance dependence; indicators of an altered reaction mechanism.