

Organic & Biomolecular Chemistry

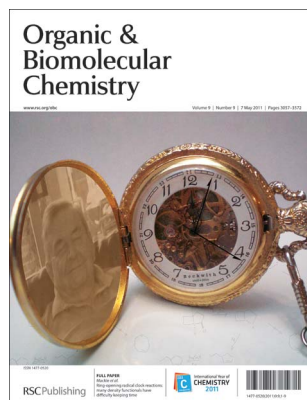
An international journal of synthetic, physical and biomolecular organic chemistry

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 9(9) 3057–3572 (2011)



Cover

See Mackie *et al.*, pp. 3158–3164.

Image reproduced by permission of Gino A. DiLabio from *Org. Biomol. Chem.*, 2011, **9**, 3158.

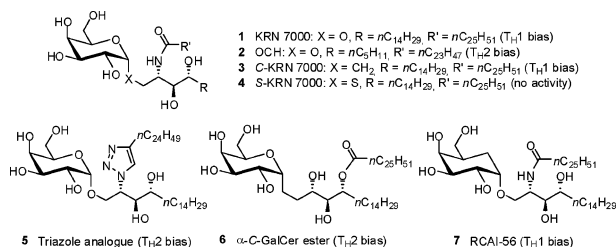
PERSPECTIVES

3080

The stimulating adventure of KRN 7000

Aline Banchet-Cadeddu,* Eric Hénon, Manuel Dauchez, Jean-Hugues Renault, Fanny Monneaux and Arnaud Haudrechy

This review presents an up-to-date library of analogues of KRN 7000, a potent synthetic α -galactosylceramide known to activate the invariant NKT immune cells.

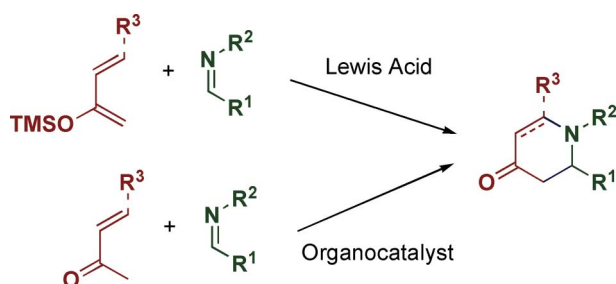


3105

Mannich–Michael *versus* formal aza–Diels–Alder approaches to piperidine derivatives

P. Ricardo Girling, Takao Kiyoi and Andrew Whiting*

A mechanistic examination is taken of the reactions we think of as aza–Diels–Alder reactions in approaching piperidines.



EDITORIAL STAFF

Editor

Richard Kelly

Deputy editor

Lorena Tomás Laudo

Senior publishing editor

Helen Saxton

Publishing editors

Nicola Burton, Sarah Dixon, Scott Gallifent-Holmes, Frances Galvin, Ben Merison, Stephen Montgomery, Roxane Owen

Publishing assistants

Jackie Cockrill, Juliet Palmer

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 24 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

2011 Annual (print+electronic) subscription price: £3726; US\$6955. 2011 Annual (electronic) subscription price: £3353; US\$6260. 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, Zürich, Switzerland

Margaret Brimble,

Auckland, New Zealand
Pauline Chiu, Hong Kong, China
Ben Davis, Oxford, UK
Veronique Gouverneur, Oxford, UK
Kenichiro Itami, Nagoya University, Japan

Stephen Kent, Chicago, USA

Stefan Matile, Geneva, Switzerland
Paolo Scrimin, Padova, Italy
Brian Stoltz, Pasadena, USA
Keisuke Suzuki, Tokyo, Japan
Qi-Lin Zhou, Nankai University, China

ADVISORY BOARD

Roger Alder, Bristol, UK
Helen Blackwell, Madison, USA
John S Carey, Tonbridge, UK
Barry Carpenter, Cardiff, UK
Michael Crimmins, Chapel Hill, USA
Antonio Echavarren, Tarragona, Spain
Jonathan Ellman, New Haven, USA
Kurt Faber, Graz, Austria
Ben Feringa, Groningen, The Netherlands
Nobutaki Fujii, Kyoto, Japan
Jan Kihlberg, Umeå, Sweden

Philip Kocienski, Leeds, UK
Steven V Ley, Cambridge, UK
Stephen Loeb, Ontario, Canada
Ilan Marek, Haifa, Israel
Manuel Martín Lomas, San Sebastián, Spain
Keiji Maruoka, Kyoto, Japan
Heather Maynard, Los Angeles, USA
E W 'Bert' Meijer, Eindhoven, The Netherlands
Eiichi Nakamura, Tokyo, Japan
Ryoji Noyori, Nagoya, Japan

Mark Rizzacasa, Melbourne, Australia
Richmond Sarpong, Berkeley, USA
Oliver Seitz, Berlin, Germany
Bruce Turnbull, Leeds, UK
Chris Welch, Rahway, USA
Helma Wennemers, Basel, Switzerland
Peter Wipf, Pittsburg, USA
Henry N C Wong, Hong Kong, China
Shuli You, Shanghai, China
Sam Zard, Palaiseau, France
Zhang Li-He, Beijing, 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 2011. 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).

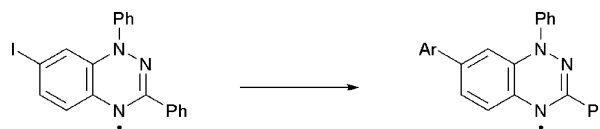
Royal Society of Chemistry: Registered Charity No. 207890.

3122

Synthesis of 7-aryl/heteraryl-1,3-diphenyl-1,2,4-benzotriazinyls *via* palladium catalyzed Stille and Suzuki-Miyaura reactions

Christos P. Constantinides, Panayiotis A. Koutentis* and Georgia Loizou

Stille and Suzuki-Miyaura reactions of 7-iodo-1,3-diphenyl-1,4-dihydro-1,2,4-benzotriazin-4-yl are presented as rare examples of cross-coupling reactions with stable organic radicals.



Suzuki-Miyaura Conditions: ArB(OH)₂ (3 equiv.), Pd(OAc)₂ (5 mol%), K₂CO₃ (3 equiv.), 1 h, 47-93% 6 examples

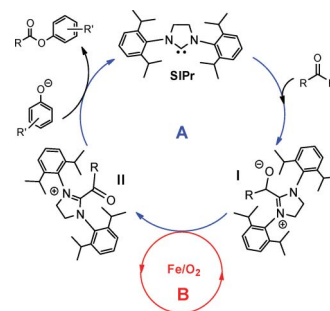
Stille Conditions: ArSnBu₃ (2 equiv.), Pd(OAc)₂ (5 mol%), 20-30 min, 82-93% 3 examples

3126

NHC/Iron cooperative catalysis: aerobic oxidative esterification of aldehydes with phenols

R. Sudarshan Reddy, João N. Rosa, Luís F. Veiros, Stephen Caddick and Pedro M. P. Gois*

An NHC/iron cooperative catalytic system mediates the aerobic oxidative esterification of aldehydes with phenols. The use of equimolar amounts of reactants led to good to excellent isolated yields of esters.

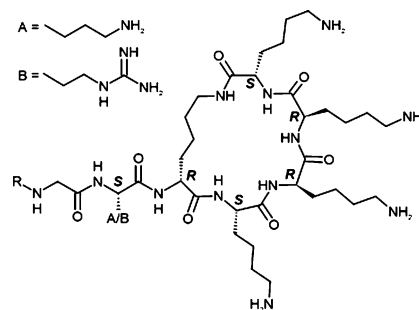


3130

Structure elucidation and biosynthesis of lysine-rich cyclic peptides in *Xenorhabdus nematophila*

Sebastian W. Fuchs, Anna Proschak, Thorsten W. Jaskolla, Michael Karas and Helge B. Bode*

The structures of thirteen novel cyclic lipoheptapeptides were elucidated from *Xenorhabdus nematophila* using a combination of different methods.

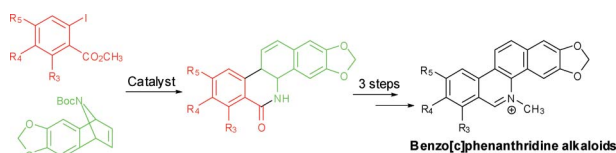


3133

Palladium-catalyzed tandem reaction to construct benzo[c]phenanthridine: application to the total synthesis of benzo[c]phenanthridine alkaloids

Pei Lv, Kanglun Huang, Longguan Xie and Xiaohua Xu*

Total synthesis of benzo[c]phenanthridine alkaloids was accomplished by palladium-catalyzed ring-opening coupling-cyclization.



Early Registration
Deadline 1st May

23rd International Congress on
Heterocyclic Chemistry

GLASGOW, SCOTLAND

ICHC2011

31st July – 4 August 2011

www.ichc2011.com



The programme will include an exciting range of cutting edge heterocyclic chemistry on offer to reflect recent advances in a truly international coverage. Five main themes of heterocyclic chemistry will be covered:

- **synthetic methodology**
- **natural product and complex molecule synthesis**
- **materials**
- **medicinal chemistry**
- **nanochemistry**
- **chemical biology**
- **chemical biology/ Biosynthesis**
- **chemical biology/ DNA nucleoside analogues**

A list of speakers participating in the programme can be found on the congress web site:

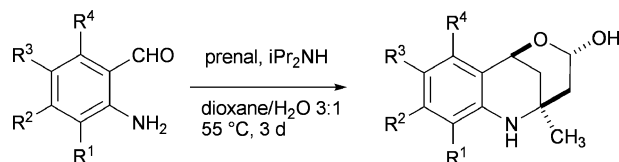
www.ichc2011.com

3136

Synthetic studies towards marmycins A and B: development of the vinylogous aldol–aza-Michael domino reaction

Emmanuel Bourcet, Manuel C. Bröhmer, Martin Nieger and Stefan Bräse*

The vinylogous aldol–aza-Michael domino reaction between 2-aminobenzaldehydes and prenal was developed to build up the core of natural products marmycin A and B without the need of protective groups.

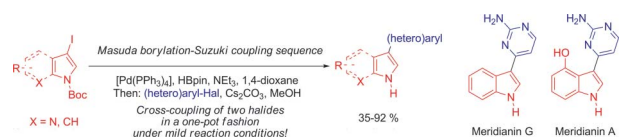


3139

Rapid synthesis of bis(hetero)aryls by one-pot Masuda borylation–Suzuki coupling sequence and its application to concise total syntheses of meridianins A and G

Eugen Merkul, Elisabeth Schäfer and Thomas J. J. Müller*

3-(Hetero)aryl substituted indoles, 7-azaindoles, and pyrroles can be obtained in a very concise fashion *via* a one-pot Masuda borylation–Suzuki coupling sequence.

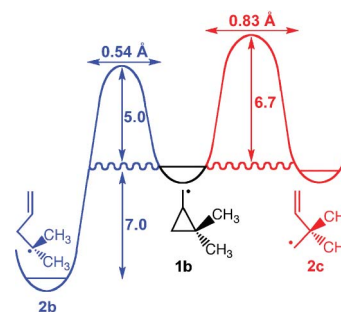


3142

Effects of geminal methyl groups on the tunnelling rates in the ring opening of cyclopropylcarbinyl radical at cryogenic temperature

Xue Zhang, David A. Hrovat, Ayan Datta and Weston Thatcher Borden*

Relative enthalpy changes for the two possible modes of ring opening of 2,2-dimethylcyclopropylcarbinyl radical. Tunnelling is indicated by wavy lines.

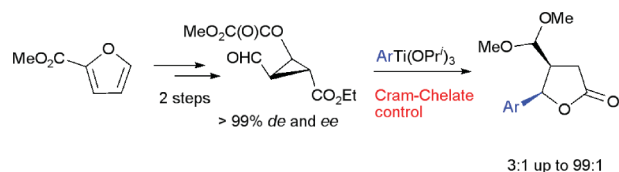


3146

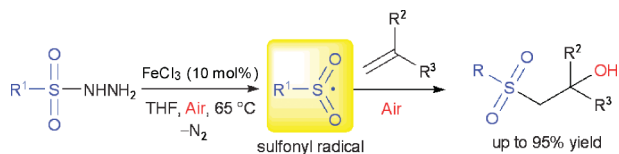
Stereoselective routes to aryl substituted γ -butyrolactones and their application towards the synthesis of highly oxidised furanocembranoids

Allan Patrick G. Macabeo, Andreas Kreuzer and Oliver Reiser*

Addition of aryltitanium compounds to cyclopropylcarbaldehyde **6** leads to *cis*-aryl disubstituted γ -butyrolactones in up to 99% *de*, contrasting with additions of allylsilanes that proceed with high Felkin–Anh-control to the corresponding *trans* disubstituted γ -butyrolactones.



3151

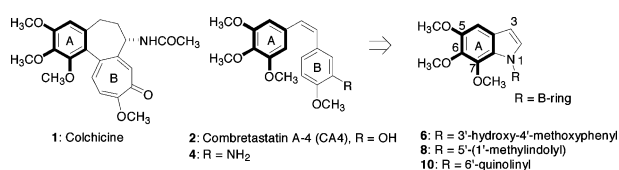


Iron-catalyzed sulfonyl radical formations from sulfonylhydrazides and oxidative addition to alkenes

Tsuyoshi Taniguchi,* Atsushi Idota and Hiroyuki Ishibashi

Sulfonyl radicals generate from sulfonylhydrazides in the presence of an iron catalyst and air. Addition of resultant radicals to alkenes affords β -hydroxy sulfones in good yield.

3154



Concise syntheses of *N*-aryl-5,6,7-trimethoxyindoles as antimitotic and vascular disrupting agents: application of the copper-mediated Ullmann-type arylation

Hsueh-Yun Lee, Jang-Yang Chang, Ling-Yin Chang, Wen-Yang Lai, Mei-Jung Lai, Kuang-Hsing Shih, Ching-Chuan Kuo, Chi-Yen Chang and Jing-Ping Liou*

A series of *N*-aryl-5,6,7-trimethoxyindoles were synthesized *via* copper-catalyzed Ullmann-type *N*-arylation through the corresponding 5,6,7-trimethoxyindole and aryl halides; the synthesized compounds demonstrated potent antiproliferative activity.

PAPERS

3158

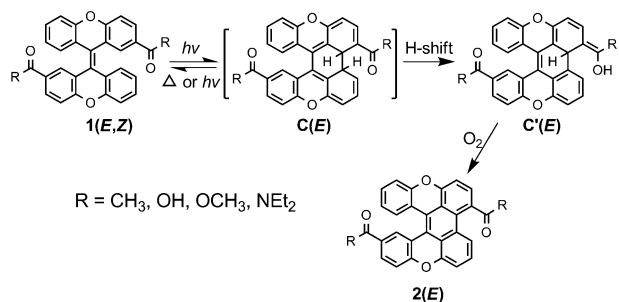


Ring-opening radical clock reactions: many density functionals have difficulty keeping time

Iain D. Mackie and Gino A. DiLabio*

Many density-functional theory methods provide poor agreement to experimental rate constants for the ring opening of radical clock species.

3165



Highly efficient and regioselective photocyclization of 2,2'-diacyl bixanthylenes

Mao Mao, Qing-Qing Wu, Ming-Guang Ren and Qin-Hua Song*

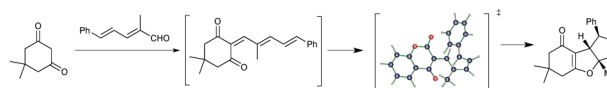
We report the conclusive mechanism for rationalizing the regioselectivity and efficiency in the photocyclization of synthesized 2,2'-substituted bixanthylenes.

3170

Unprecedented stereoselective synthesis of cyclopenta[*b*]benzofuran derivatives and their characterisation assisted by aligned media NMR and ^{13}C chemical shift *ab initio* predictions

Martín J. Riveira, Chakicherla Gayathri, Armando Navarro-Vázquez, Nicolay V. Tsarevsky, Roberto R. Gil* and Mirta P. Mischne*

A new approach to the synthesis of cyclopenta[*b*]benzofuran derivatives.

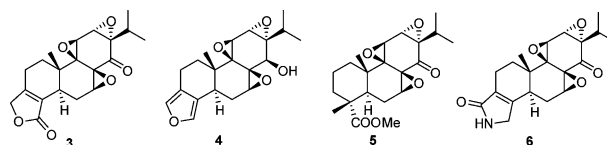


3176

Total synthesis of novel D-ring-modified triptolide analogues: structure–cytotoxic activity relationship studies on the D-ring of triptolide

Bing Zhou, Xiaomei Li, Huanyu Tang, Zehong Miao, Huijin Feng and Yuanchao Li*

The syntheses of triptolide analogues **3–6** and SAR studies on the D-ring of triptolide are reported.

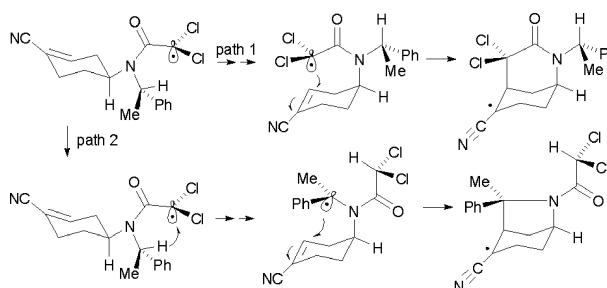


3180

Translocation *versus* cyclisation in radicals derived from *N*-3-alkenyl trichloroacetamides

M. Luisa Marin,* Ramon J. Zaragoza,* Miguel A. Miranda, Faïza Diaba and Josep Bonjoch

The dichotomy between translocation and direct radical cyclisation of *N*-3-alkenyl trichloroacetamide radicals has been experimentally and theoretically studied and the DFT calculations are in good agreement with the observed experimental results.

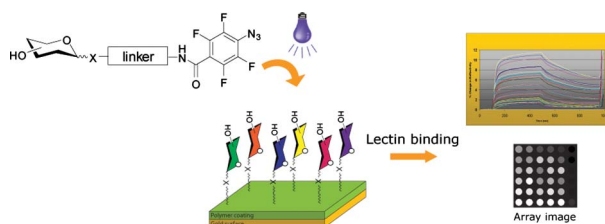


3188

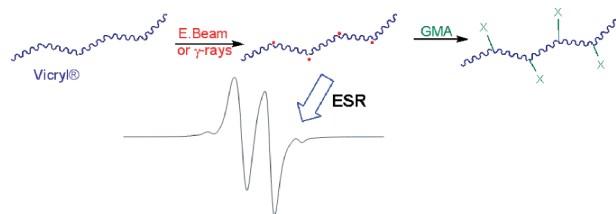
Stereoselective synthesis of light-activatable perfluorophenylazide-conjugated carbohydrates for glycoarray fabrication and evaluation of structural effects on protein binding by SPR imaging

Lingquan Deng, Oscar Norberg, Suji Uppalapati, Mingdi Yan* and Olof Ramström*

Structurally varied, photoprobe-conjugated carbohydrates were efficiently synthesized and arrayed, resulting in optimal protein binding as evaluated by SPR imaging.



3199

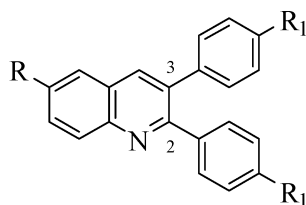


Radical-based grafting of GMA on sutures of different nature

Angelo Alberti,* Piergiorgio Fuocho, Maurizio Guerra, Dante Macciantelli, Giangiaco Torri, Antonio Valerio and Elena Vismara*

The formation of radicals upon high energy irradiation of sutures allows their easy GMA-derivatization.

3205



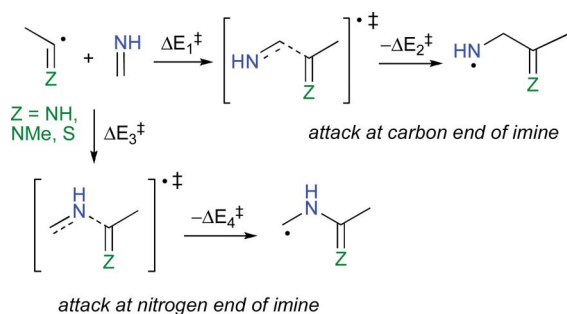
R = F, OH, OMe, or aminoalkoxy groups.
R₁ = H, OH, OMe, or aminoalkoxy groups.

Synthesis and antiproliferative evaluation of 2,3-diarylquinoline derivatives

Chih-Hua Tseng, Yeh-Long Chen, Kuin-Yu Chung, Chi-Huei Wang, Shin-I Peng, Chih-Mei Cheng and Cherng-Chyi Tzeng*

A number of 2,3-diarylquinoline derivatives were synthesized and evaluated for their antiproliferative activities against Hep G2, Hep 3B, A549, H1299, MCF-7, and MDA-MB-231 cancer cell lines.

3217

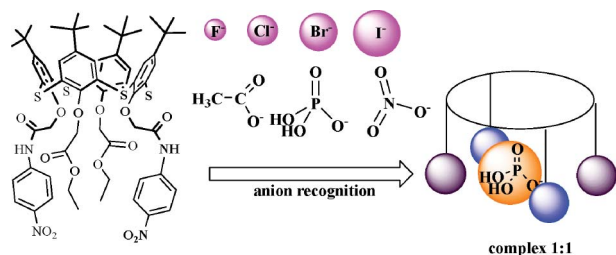


An *ab initio* and DFT study of radical addition reactions of imidoyl and thioyl radicals to methanimine

Sara H. Kyne, Carl H. Schiesser and Hiroshi Matsubara*

Imidoyl and thioyl radicals add to the nitrogen of methanimine through simultaneous multi-orbital interactions between the radicals and the imine.

3225



p-tert-Butyl thiocalix[4]arenes functionalized at the lower rim by amide, hydroxyl and ester groups as anion receptors

Ivan I. Stoikov,* Alena A. Yantemirova, Roman V. Nosov, Ildar Kh. Rizvanov, Ajdar R. Julmetov, Vladimir V. Klochkov, Igor S. Antipin, Alexander I. Konovalov and Ilya Zharov

Selective receptors for fluoride and dihydrogen phosphate salts of tetrabutylammonium were found.

RSC Advances

An international journal to further the chemical sciences



RSC Advances is a new peer-reviewed journal covering all the chemical sciences, including interdisciplinary fields. Published articles will report high quality, well-conducted research that adds to the development of the field.

- Submissions now open – first issue mid-2011
- An expert editorial team led by Professor Mike Ward, University of Sheffield, UK
- Free access to all content throughout 2011 and 2012
- Free colour, no page charges
- Published online only

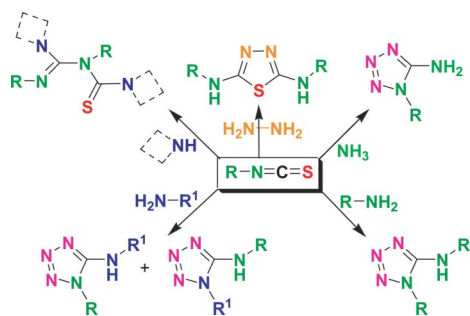
Go online today

RSC Publishing

www.rsc.org/advances

Registered Charity Number 207890

3235

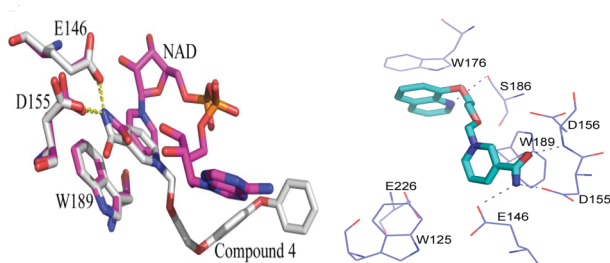


Tandem regioselective synthesis of tetrazoles and related heterocycles using iodine

Ramesh Yella, Nilufa Khatun, Saroj Kumar Rout and Bhisma K. Patel*

A one-pot, tandem process has been developed for the synthesis of a library of tetrazoles from aryl isothiocyanates.

3246

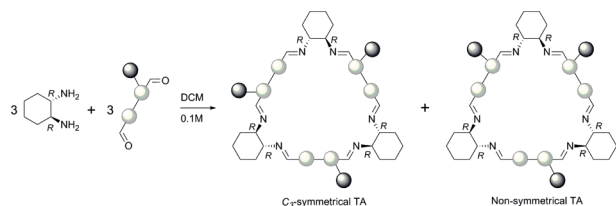


Design, synthesis and biological characterization of novel inhibitors of CD38

Min Dong, Yuan-Qi Si, Shuang-Yong Sun, Xiao-Ping Pu, Zhen-Jun Yang, Liang-Ren Zhang, Li-He Zhang,* Fung Ping Leung, Connie Mo Ching Lam, Anna Ka Yee Kwong, Jianbo Yue, Yeyun Zhou, Irina A. Kriksunov, Quan Hao and Hon Cheung Lee*

The X-ray crystal structure of CD38/**Compound 4** complex and computer simulation of **Compound 7** docking to CD38 show the significant role of nicotinamide for the substrate recognition of CD38 and the effect of aromatic group at the end of the chain.

3258

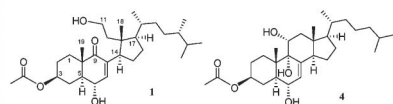


Synthesis of tri-substituted biaryl based trianglimines: formation of C_3 -symmetrical and non-symmetrical regioisomers

Hany F. Nour, Marius F. Matei, Bassem S. Bassil, Ulrich Kortz and Nikolai Kuhnert*

A new synthetic strategy for the introduction of a series of substituents into novel C_3 -symmetrical and non-symmetrical trianglimine macrocycles.

3272



Hirsutosterols A–G, polyoxygenated steroids from a Formosan soft coral *Cladiella hirsuta*

Bo-Wei Chen, Shu-Ming Chang, Chiung-Yao Huang, Jui-Hsin Su, Zhi-Hong Wen, Yang-Chang Wu and Jyh-Horng Sheu*

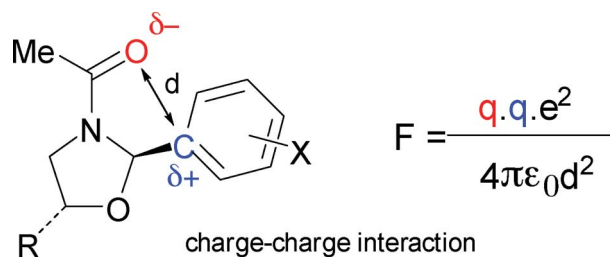
Structure elucidation and biological activities of seven new polyoxygenated steroids, isolated from a Formosan soft coral, *Cladiella hirsuta*, are described.

3279

A quantitative structure–reactivity relationship in *N*-acetyl oxazolidines: an electrostatic interaction controls rotamer population

R. Fernando Martínez,* Martín Ávalos, Reyes Babiano, Pedro Cintas, José L. Jiménez, Juan C. Palacios and Esther M. S. Pérez

A stereoelectronic effect, whose origin is a charge–charge interaction, controls the rotamer ratio in *N*-acetyl oxazolidines.

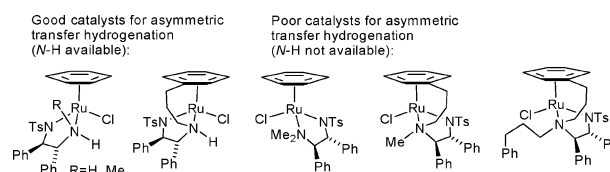


3290

The importance of the N–H bond in Ru/TsDPEN complexes for asymmetric transfer hydrogenation of ketones and imines

Rina Soni, Fung Kei Cheung, Guy C. Clarkson, Jose E. D. Martins, Mark A. Graham and Martin Wills*

N-Methylation of ruthenium/TsDPEN catalysts for asymmetric transfer hydrogenation results in a sharp decrease in their activity in ketone and imine reduction.

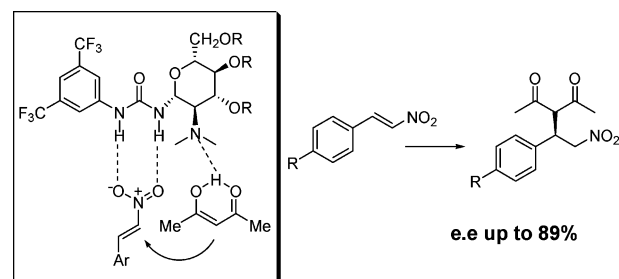


3295

Novel carbohydrate-based bifunctional organocatalysts for nucleophilic addition to nitroolefins and imines

Alessandra Puglisi, Maurizio Benaglia,* Laura Raimondi, Luigi Lay* and Laura Poletti

Novel enantiomerically pure bifunctional organocatalysts bearing a tertiary amine group in proximity to a urea group were synthesized starting from *D*-glucosamine. Enantioselectivities up to 89% were obtained in the acetylacetone addition to β -nitrostyrene. Semiempirical (AM1) computational studies allowed to find a nice theoretical rationale for the behaviour of the catalyst of choice.

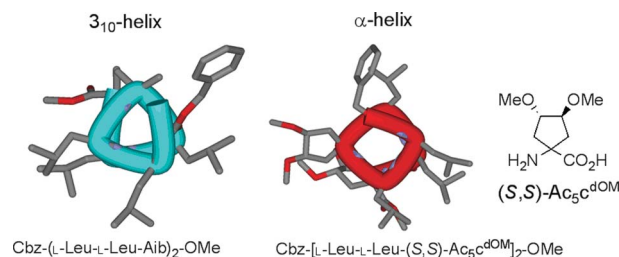


3303

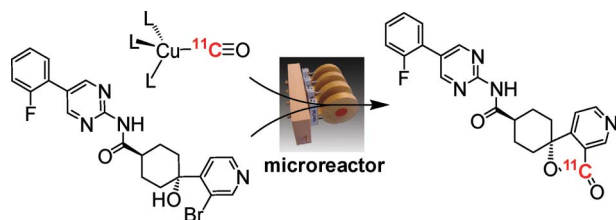
Conformational studies on peptides containing α,α -disubstituted α -amino acids: chiral cyclic α,α -disubstituted α -amino acid as an α -helical inducer

Yosuke Demizu,* Mitsunobu Doi, Masaaki Kurihara, Haruhiro Okuda, Masanobu Nagano, Hiroshi Suemune and Masakazu Tanaka*

The Aib residue has the propensity to form 3_{10} -helices in short peptides, whereas the chiral $\text{Ac}_5\text{c}^{\text{dOM}}$ residues have a penchant for forming α -helices.



3313

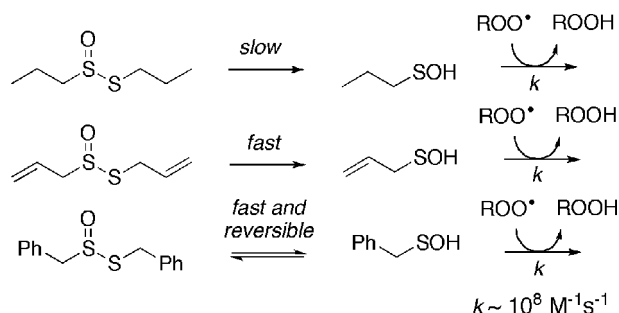


Microfluidic reactions using [¹¹C]carbon monoxide solutions for the synthesis of a positron emission tomography radiotracer

Steven Kealey, Christophe Plisson, T. Lee Collier, Nicholas J. Long, Stephen M. Husbands, Laurent Martarello and Antony D. Gee

A copper(I)-[¹¹C]CO solution has been used to perform carbonylation reactions for the synthesis of [¹¹C]MK-0233, a radioligand for the neuropeptide Y Y5 receptor, using both microfluidics and conventional techniques.

3320

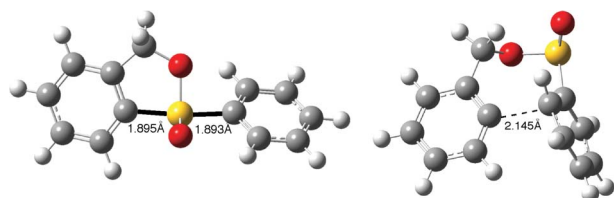


The mechanism of radical-trapping antioxidant activity of plant-derived thiosulfonates

Philip T. Lynett, Krista Butts, Vipraja Vaidya, Graham E. Garrett and Derek A. Pratt*

The ease with which plant-derived thiosulfonates undergo Cope elimination to form the corresponding sulfenic acids accounts for their differences in antioxidant activity.

3331

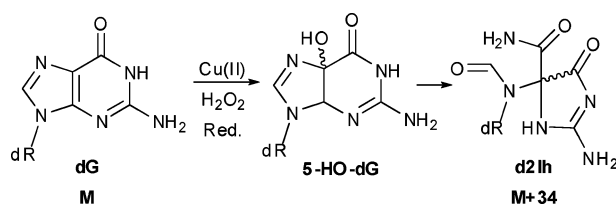


Intramolecular homolytic substitution of sulfinates and sulfenamides – a computational study

Sara H. Kyne,* Heather M. Aitken, Carl H. Schiesser, Emmanuel Lacôte, Max Malacria, Cyril Ollivier and Louis Fensterbank*

BHandHLYP/6-311++G(d,p) calculations predict that intramolecular homolytic substitution by aryl radicals at the sulfur atom in phenylsulfonates and sulfenamides competes with intramolecular addition to the phenyl ring.

3338



Characterization of 2'-deoxyguanosine oxidation products observed in the Fenton-like system Cu(II)/H₂O₂/reductant in nucleoside and oligodeoxynucleotide contexts

Aaron M. Fleming, James G. Muller, Insun Ji and Cynthia J. Burrows*

Copper-mediated Fenton oxidation of 2'-deoxyguanosine leads to predominant formation of 5-carboxamido-5-formamido-2-iminohydantoin (d2Ih) via C5 hydroxylation.



Who's who in *Chemical Science*



David MacMillan
Editor-in-Chief
Princeton University, USA



Christopher Bielawski
Polymer Science University
of Texas at Austin, USA



Stephen Buchwald
Organic Chemistry
MIT, USA



Thomas Carell
Chemical Biology and
Bioorganic Chemistry
LMU, München, Germany



Benjamin F Cravatt
Chemical Biology
Scripps, USA



Christopher C Cummins
Inorganic and
Organometallic Chemistry
MIT, USA



Kazunari Domen
Physical Chemistry
Energy and Surface
Science, University
of Tokyo, Japan



Matthew Gaunt
Organic Chemistry
University of
Cambridge UK



Hubert Girault
Analytical Science
EPFL, Switzerland



David A Leigh
Supramolecular
Chemistry University of
Edinburgh, UK



Kopin Liu
Physical Chemistry
Academia Sinica, Taiwan



Jeffrey R Long
Inorganic Chemistry
UC Berkeley, USA



Wonwoo Nam
Bioinorganic Chemistry
Ewha Womans
University, Korea



Colin Nuckolls
Organic Materials
Columbia University, USA



Teri Odom
Nanoscience
Northwestern
University USA



Matthew J Rosseinsky
Inorganic Materials
University of
Liverpool, UK



F Dean Toste
Organic Chemistry
UC Berkeley, USA

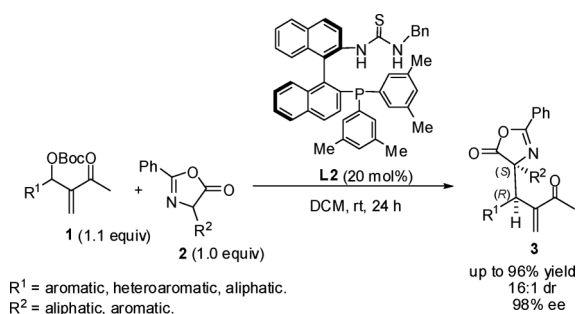


Haw Yang
Physical Chemistry
Princeton University, USA

All our Associate Editors ensure that every article submitted to *Chemical Science* has a fair review. And, as active researchers, they guarantee that the journal represents the best new thinking in the chemical sciences.

The proof is in the content – go online today

3349

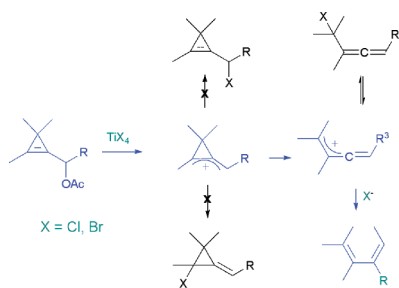


Multifunctional chiral phosphines-catalyzed highly diastereoselective and enantioselective substitution of Morita–Baylis–Hillman adducts with oxazolones

Yuan-Liang Yang, Cheng-Kui Pei and Min Shi*

Multifunctional chiral phosphine (phosphine–thiourea type) **L2**-catalyzed allylic substitutions of MBH adducts **1** with oxazolones **2** produce the corresponding optically active adducts **3** in good to excellent yields and ee's as well as moderate to good de's under mild conditions.

3359



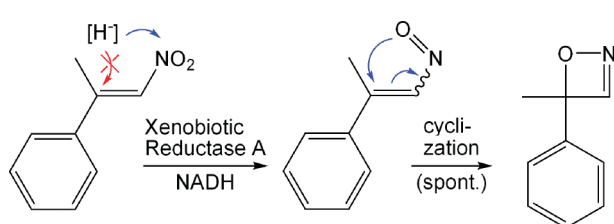
12 examples - complete regioselectivity and Z-stereoselectivity!

Titanium-mediated rearrangement of cyclopropenylmethyl acetates to (*E*)-halodienes

Gary Gallego, Alireza Ariafard,* Kiet Tran, David Sandoval, Leera Choi, Yi-Hsun Chen, Brian F. Yates, Fu-Ming Tao and Christopher J. T. Hyland*

TiCl₄ and TiBr₄ rapidly transform cyclopropenylmethyl acetates to (*E*)-halodienes with complete regio- and stereoselectivity.

3364

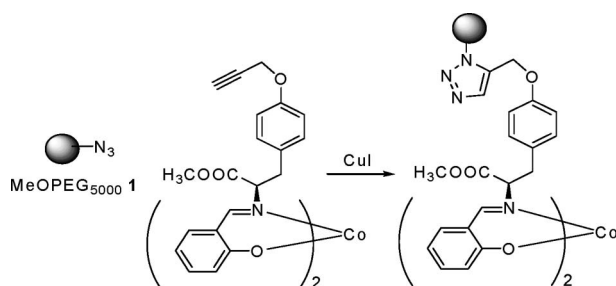


Reductive biotransformation of nitroalkenes via nitroso-intermediates to oxazetes catalyzed by xenobiotic reductase A (XenA)

Katharina Durchschein, Walter M. F. Fabian, Peter Macheroux, Klaus Zangger, Gregor Trimmel and Kurt Faber*

Bioreduction of a nitroalkene by xenobiotic reductase A (XenA) furnished the corresponding nitrosoalkene, which underwent electrocyclic cyclization to yield a highly strained 1,2-oxazete derivative.

3370



Polyethylene glycol clicked Co(II) Schiff base and its catalytic activity for the oxidative dehydrogenation of secondary amines

Praveen K. Khatri, Suman L. Jain,* L. N. Sivakumar K. and Bir Sain*

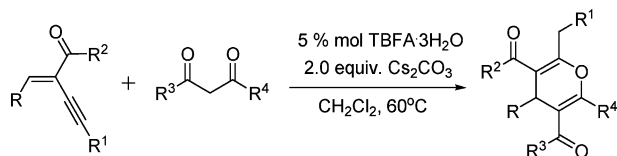
Click reaction provided an efficient synthesis of PEGylated Co(II) Schiff base for the oxidative dehydrogenation of secondary amines in high yield.

3375

Phase-transfer-catalyzed cyclization reaction of nucleophilic addition to electron-deficient 1,3-conjugated enynes for the synthesis of functionalized 4*H*-pyrans

Jie Hu, Lei Liu, Shangdong Yang* and Yong-Min Liang*

A variety of substituted 4*H*-pyrans are readily prepared in moderate to good yields under the mild reaction conditions by nucleophilic addition to electron-deficient 1,3-conjugated enynes with phase-transfer catalysis (PTC).

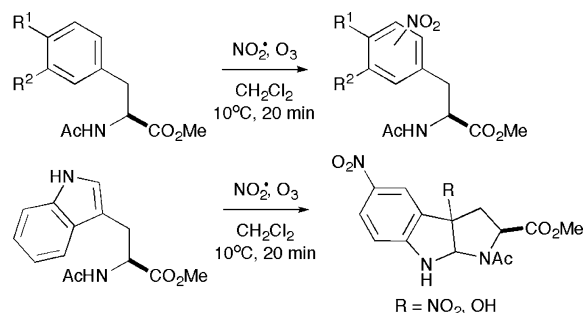


3380

Damage of aromatic amino acids by the atmospheric free radical oxidant NO₃[·] in the presence of NO₂[·], N₂O₄, O₃ and O₂

Catrin Goeschen, Natalia Wibowo, Jonathan M. White and Uta Wille*

Damage of aromatic amino acids by the most important atmospheric free-radical oxidant, NO₃[·], was studied under simulated environmental conditions.

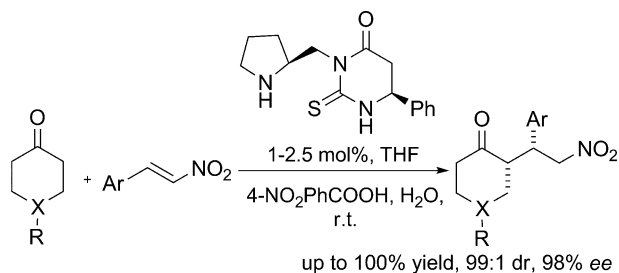


3386

Novel pyrrolidine-thiohydantoin/thioxotetrahydropyrimidinones as highly effective catalysts for the asymmetric Michael addition

Christoforos G. Kokotos, Dimitris Limnios, Despoina Triggidou, Maria Trifonidou and George Kokotos*

The synthesis of novel organocatalysts consisting of a pyrrolidine and a thiohydantoin or a thioxotetrahydropyrimidinone ring and their efficient application in the Michael reaction is described.

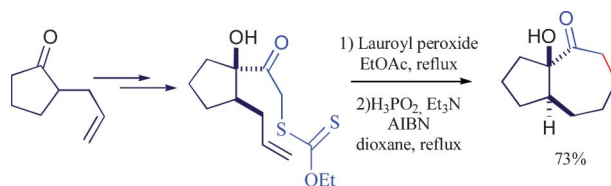


3396

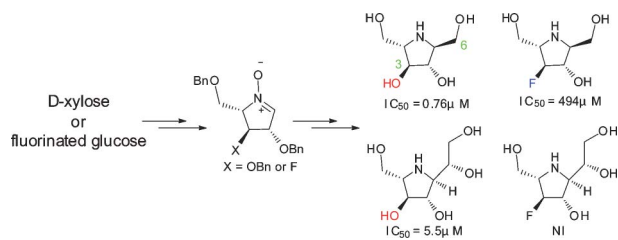
A flexible, unified radical-based approach to polycyclic structures

Rama Heng and Samir Z. Zard*

Cis- and *trans*-decalins, *trans*-perhydroazulenes, and [5.3.1]bicyclo-undecanone scaffolds can be readily constructed starting from unsaturated ketones and using the degenerative xanthate transfer technology to accomplish unusual and otherwise difficult radical cyclisations



3405



L-DMDP, L-homoDMDP and their C-3 fluorinated derivatives: synthesis and glycosidase-inhibition

Yi-Xian Li, Mu-Hua Huang, Yukiko Yamashita, Atsushi Kato, Yue-Mei Jia, Wu-Bao Wang, George W. J. Fleet, Robert J. Nash and Chu-Yi Yu*

L-DMDP, L-homoDMDP and their 3-deoxy-3-fluorinated analogues were synthesized from D-xylose or fluorinated glucose derived nitrones. Bioactivities of these iminosugars against various glycosidases were evaluated, and the C-3 hydroxyl group of these compounds was found to play an important role in their interaction with enzymes.

3415

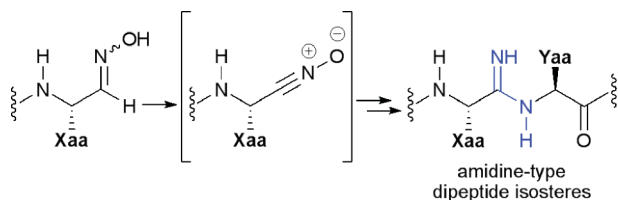


Radical reductions of alkyl halides bearing electron withdrawing groups with *N*-heterocyclic carbene boranes

Shau-Hua Ueng, Louis Fensterbank,* Emmanuel Lacôte,* Max Malacria* and Dennis P. Curran*

Stable, readily available, low molecular weight *N*-heterocyclic carbene boranes reduce halides bearing electron withdrawing substituents. Product isolation is convenient.

3421

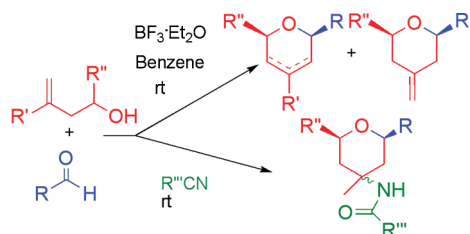


Design and synthesis of amidine-type peptide bond isosteres: application of nitrile oxide derivatives as active ester equivalents in peptide and peptidomimetics synthesis

Eriko Inokuchi, Ai Yamada, Kentaro Hozumi, Kenji Tomita, Shinya Oishi, Hiroaki Ohno, Motoyoshi Nomizu and Nobutaka Fujii*

Amidine-type peptidomimetics were designed and synthesized *via* nitrile oxide-mediated C–N bond formation.

3428



where R = R' = R'' = H / alkyl / aryl; R''' = alkyl, aryl

An efficient synthesis of dihydro- and tetrahydropyrans *via* oxonium-ene cyclization reaction

Somasekhar Bondalapati, Udagandla C. Reddy, Pipas Saha and Anil K. Saikia*

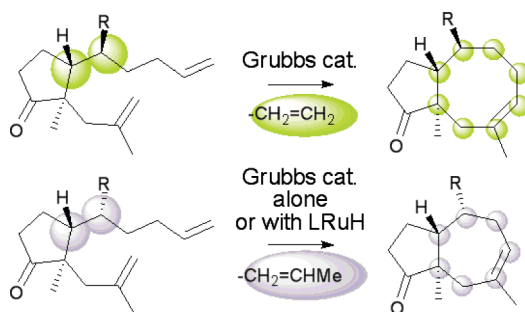
Dihydro- and tetrahydropyrans can be efficiently synthesised from aldehydes and homoallylic alcohols *via* oxonium-ene reaction with good diastereoselectivity and yields.

3439

Application of a metathesis reaction in the synthesis of sterically congested medium-sized rings. A direct ring closing *versus* a double bond migration–ring closing process

Michał Michalak and Jerzy Wicha*

1,9-Dienes related to *trans*-1-allyl-2-(pent-4-enyl)cyclopentane undergo either ring closing metathesis to form cyclooctene derivatives or tandem double bond migration–metathesis to afford cycloheptene derivatives, depending on the relative configuration and substitution pattern.

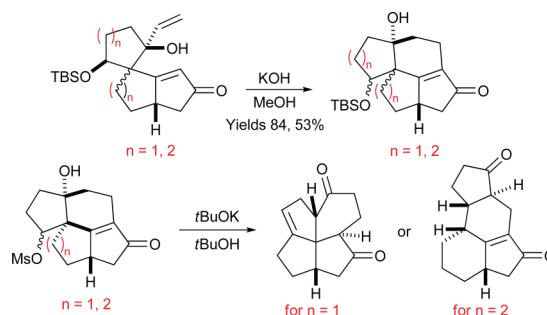


3447

Vinylogous anionic processes in the formation and interconversion of tetracyclic ring systems

Paul D. Thornton, T. Stanley Cameron and D. Jean Burnell*

Anionic ring-opening and ring-closing reactions gave the final annulated products. Rearrangement then involved ring-opening and alternative ring-closing pathways.

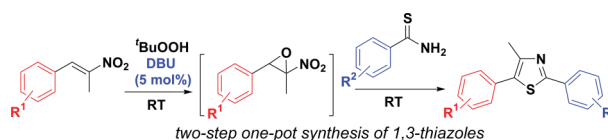


3457

Novel one-pot process for the synthesis of 1,3-thiazoles *via* organocatalysed epoxidation of nitro-olefins

Katharina M. Weiß, Shengwei Wei and Svetlana B. Tsogoeva*

The reaction of nitro-olefins with the *t*-BuOOH/DBU system gives rise to the corresponding α -nitro-epoxides, which are suitable for a subsequent reaction with thioamides under mild conditions to yield thiazole heterocycles.

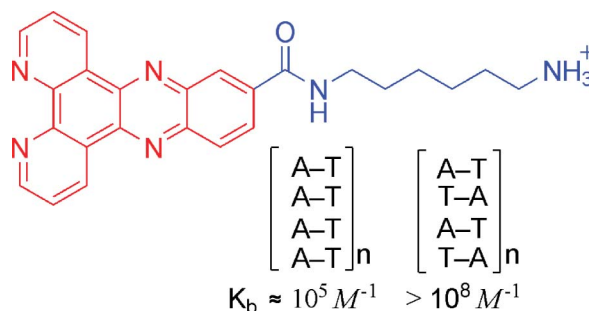


3462

Water-soluble amino derivatives of free-base dppz – syntheses and DNA binding studies

Tim Phillips, Itshamul Haq and Jim A. Thomas*

The synthesis of, and DNA binding studies on prototype water-soluble amino derivatives of dppz are described.

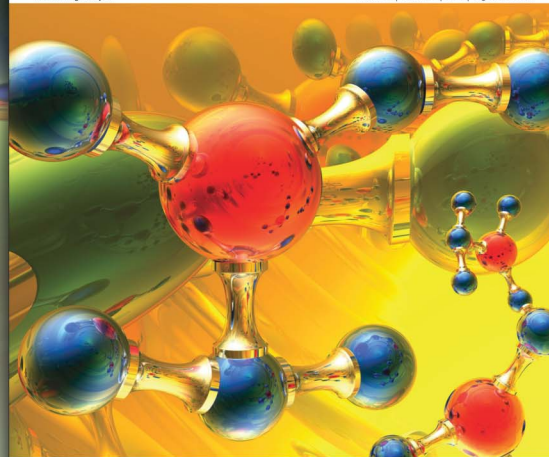


New
Journal

Catalysis Science & Technology

www.rsc.org/catalysis

Volume 1 | Number 1 | 2011 | Pages 0001-0100



ISSN 2044-4753

RSC Publishing



Catalysis Science & Technology

A multidisciplinary journal focusing on all fundamental science and technological aspects of catalysis.

Containing a mix of fundamental applied, experimental and computational work, *Catalysis Science & Technology* brings together homogeneous, heterogeneous and bio-catalysis research. The journal will provide a home to communications, full papers, perspectives and mini-reviews and is relevant to academic and industrial scientists.

Catalysis Science & Technology is led by a dynamic editorial team of active researchers in the field, including co-Editors-in-Chief Piet van Leeuwen (Institute of Chemical Research of Catalonia, Spain) and Cynthia Friend (Harvard University, USA) and Associate Editors Paul Chirik (Cornell University, USA), Noritaka Mizuno (University of Tokyo, Japan) and Paul Kamer (University of St Andrews, UK). With an international presence, the journal is well placed to publish the best research from authors spanning the catalysis community.

Work published in *Catalysis Science & Technology* will benefit from wide exposure, with free online access to all content published during 2011 and 2012 giving maximum visibility to your research.

Visit the website to register for free access

RSC Publishing

www.rsc.org/catalysis

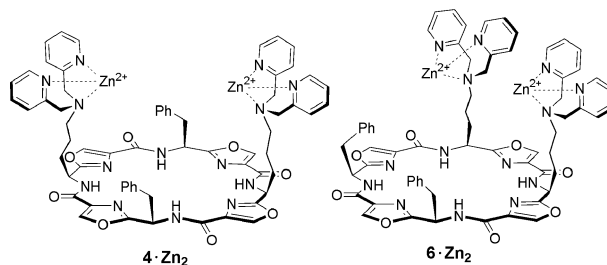
Registered Charity Number 207890

3471

Synthesis of a family of cyclic peptide-based anion receptors

Stephen J. Butler and Katrina A. Jolliffe*

A family ofazole-modified cyclic peptides bearing dipicolylamine side chains (e.g. **4** and **6**) has been prepared and the ability of their bis-Zn(II) complexes to bind polyphosphate anions investigated.

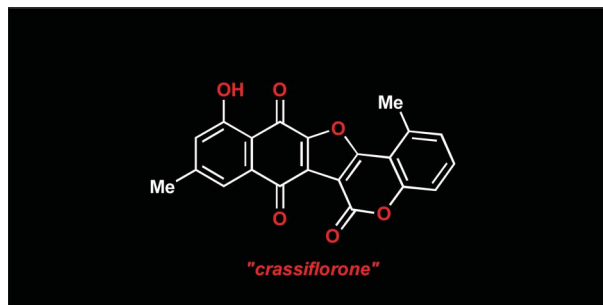


3484

Synthesis of the reported structure of crassiflorone, a naturally occurring quinone isolated from the African ebony *Diospyros crassiflora*, and regioisomeric pentacyclic furocoumarin naphthoquinones

Jalindar Padwal, William Lewis and Christopher J. Moody*

The synthesis of the reported structure of crassiflorone from the African Ebony is described, together with three isomeric furocoumarin naphthoquinones, none of which match the natural product.

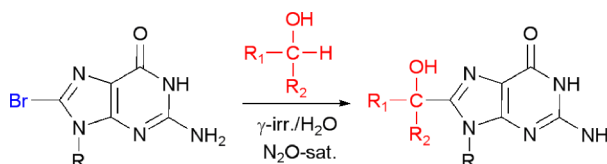


3494

Radical-based alkylation of guanine derivatives in aqueous medium

Chryssostomos Chatgililoglu,* Clara Caminal and Quinto G. Mulazzani

The addition of α -hydroxyalkyl radicals to 8-bromoguanine derivatives results in the efficient formation of intermolecular C–C bonds in aqueous media.

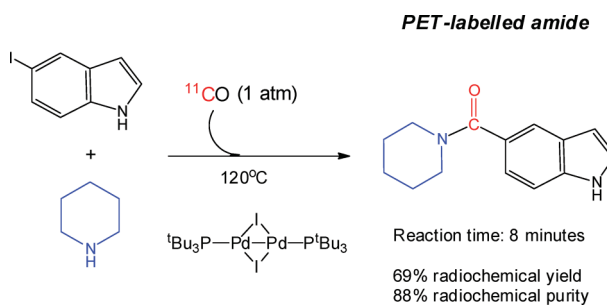


3499

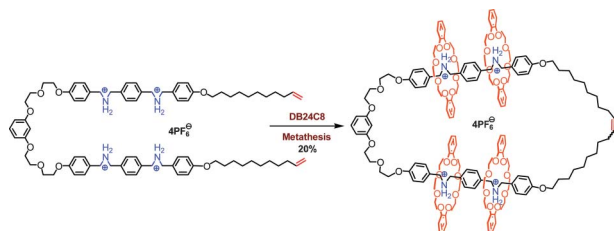
Rapid carbonylative coupling reactions using palladium(I) dimers: applications to ^{11}C -radiolabelling for the synthesis of PET tracers

Gabiella Buscemi, Philip W. Miller, Steven Kealey, Antony D. Gee, Nicholas J. Long, Jan Passchier and Ramon Vilar*

Palladium dimers with sterically hindered phosphines have been shown to be excellent pre-catalysts for the aminocarbonylation of aryl halides to yield amides and one of them has been successfully employed as a pre-catalyst for the synthesis of ^{11}C -radiolabelled amides for PET imaging.



3504

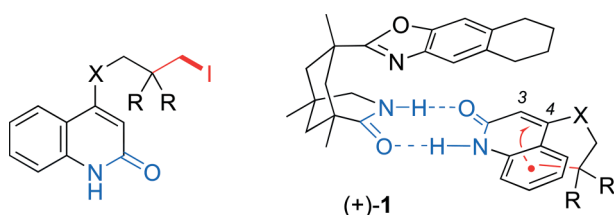


Template-directed synthesis of kinetically and thermodynamically stable molecular necklace using ring closing metathesis

Suvankar Dasgupta and Jishan Wu*

A kinetically and thermodynamically stable [5] molecular necklace is synthesized for the first time using a “threading-followed-by-ring-closing-metathesis” approach.

3516

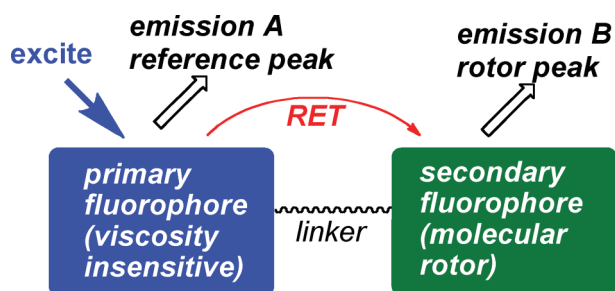


Enantioselective radical cyclisation reactions of 4-substituted quinolones mediated by a chiral template

Aline Bakowski, Martina Dressel, Andreas Bauer* and Thorsten Bach*

Upon association of quinolones to template (+)-1 the chirality information is provided for the enantioselectivity determining cyclisation step.

3530

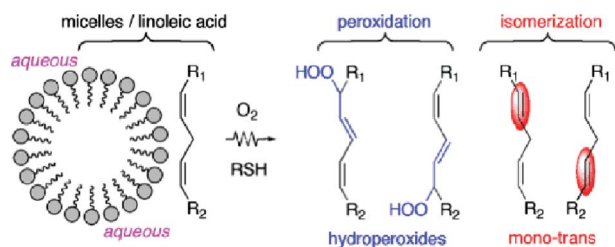


Synthesis and evaluation of self-calibrating ratiometric viscosity sensors

Hyung-Jo Yoon, Marianna Dakanali, Darcy Lichlyter, Willy M. Chang, Karen A. Nguyen, Matthew E. Nipper, Mark A. Haidekker* and Emmanuel A. Theodorakis*

Linking a viscosity-independent fluorophore with a viscosity-dependent secondary fluorophore creates a new class of viscosity sensors with self-calibrating ratiometric properties.

3541



Linoleic acid peroxidation vs. isomerization: a biomimetic model of free radical reactivity in the presence of thiols

Branka Mihaljević*, Ivana Tartaro, Carla Ferreri* and Chrystostomos Chatgililoglu*

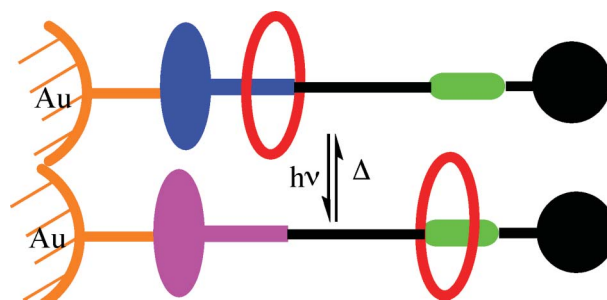
A biomimetic model offers for the first time the parallel estimation of peroxidation and isomerization as results of oxidative free radical conditions in the presence of thiols.

3549

Photoswitchable rotaxanes on gold nanoparticles

Yingxin Duo, Sabine Jacob and Werner Abraham*

Photons switch the position of the teracationic ring of a rotaxane relative to the surface of gold nanoparticles.

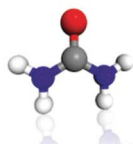
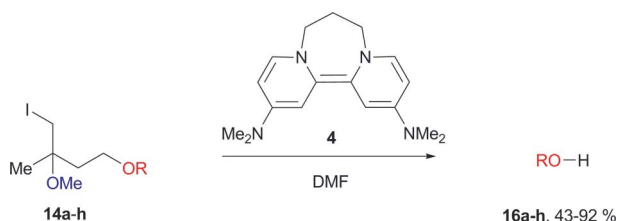


3560

Fragmentations observed in the reactions of α -methoxy- γ -alkoxyalkyl iodide substrates with super-electron-donors derived from 4-DMAP and *N*-methylbenzimidazole

Ryan Sword, Luke A. Baldwin and John A. Murphy*

Interception of alkyl radicals leads to fragmentation, detected by release of alcohols.

**ESOC 2011**10th - 15th July 2011, Crete, Greece17th European Symposium on Organic Chemistrywww.esoc2011.com**Conference Chair**

Michael Orfanopoulos, Department of Chemistry, University of Crete, Greece

You are cordially invited to participate in the 17th European Symposium of Organic Chemistry (ESOC-17) the largest European Symposium, which will be held in Crete, Greece, from 10th to 15th July 2011.

This well established conference will provide a forum for broad scientific and technological exchange among researchers from Europe and elsewhere. The conference will emphasize on new achievements in the following fields:

- Total Synthesis of Natural Products
- Catalysis in Organic Synthesis
- New Methods in Organic Synthesis
- Medicinal Chemistry
- Bioorganic Chemistry & Chemical Biology
- Supramolecular Chemistry
- Synthesis of Functional Materials
- Physical Organic Chemistry

The program will include an outstanding line up of invited speakers.

Keep up to date with the latest program information, deadlines and news. We look forward to welcoming you in Crete in July 2011.

Michael Orfanopoulos, Congress Chair

