Volume 13 | Number 23 | 21 June 2015 | Pages 6409–6656

Organic & Biomolecular Chemistry

www.rsc.org/obc

ISSN 1477-0520

ROYAL SOCIETY OF CHEMISTRY

PAPER

Jean-François Nierengarten, Anne Imberty, Stéphane P. Vincent *et al.*

Fucofullerenes as tight ligands of RSL and LecB, two bacterial lectins

Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry

www.rsc.org/obc

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 13(23) 6409–6656 (2015)

Cover
See Jean-François Nierengarten, Anne Imberty, Stéphane P. Vincent *et al.*, pp. 6482–6492.

Image reproduced by permission of Stéphane P. Vincent from *Org. Biomol. Chem.*, 2015, **13**, 6482.

Published on 02 June 2015. Downloaded on 05/02/2016 04:23:01.

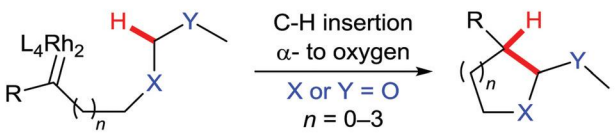
REVIEWS

6419

Rhodium(II)-catalysed intramolecular C–H insertion α- to oxygen: reactivity, selectivity and applications to natural product synthesis

Fanny J. Lombard and Mark J. Coster*

This review highlights reactivity and selectivity trends for the insertion of Rh(II) carbenes into C–H bonds that are activated by α-oxygen substituents, and the application of this reaction to the total synthesis of some natural products.



6432

"Pruning of biomolecules and natural products (PBNP)": an innovative paradigm in drug discovery

Surendar Reddy Bathula, Srirama Murthy Akondi, Prathama S. Mainkar* and Srivari Chandrasekhar*

Smart Schneider: 'Nature' is the most intelligent tailor with an ability to utilize the resources. Researchers are still at an infant stage learning this art. The present review highlights some of the man made pruning of bio-molecules and NPs (PBNP) in finding chemicals with a better therapeutic index.

View Article Online

Published on 02 June 2015. Downloaded on 05/02/2016 04:23:01.

Editorial staff

Editor
Richard Kelly

Deputy editor
Marie Cote

Editorial production manager
Helen Saxton

Development editor
James Anson

Publishing editors
Nicola Burton, Zoe Karthauser, Elisa Meschini, Roxane Owen, Simon Rankmore, Donna Smith

Publishing assistants
Emily Finney, Rosalind Searle

Publisher
Emma Wilson

For queries about submitted papers, please contact Helen Saxton, Editorial production manager 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 Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK
Tel +44 (0)1223 432398; E-mail orders@rsc.org

2015 Annual (print+electronic) subscription price: £4572; US$8534. 2015 Annual (electronic) subscription price: £4343; US$8107 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.

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**

MIX
Paper from responsible sources
FSC® C013604

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. Broad in scope, it publishes research and reviews on topics across organic synthesis, physical organic chemistry, supramolecular chemistry and chemical biology.

Editorial board

Chair
Andrei Yudin, University of Toronto, Canada

Associate editors
Margaret Brimble, University of Auckland, New Zealand
Christian Hackenberger, Free University Berlin, Germany
Lei Liu, Tsinghua University, China
Jin-Quan Yu, Scripps Research Institute, La Jolla, CA, USA

Editorial board members
Ashraf Brik, Technion-Israel Institute of Technology, Israel
Pauline Chiu, University of Hong Kong, China
Jonathan Clayden, University of Manchester, UK
Anthony Davis, University of Bristol, UK
Christian Hertweck, Leibniz-Institute Jena, Germany
Kenichiro Itami, Nagoya University, Japan
Dean Tantillo, UC Davis, USA
Qi-Lin Zhou, Nankai University, China

Advisory board

Kyo Han Ahn, Pohang University of Science and Technology, Korea
Fredrik Almqvist, Umeå University, Sweden
Jeffrey Bode, ETH Zurich, Switzerland
Barry Carpenter, Cardiff University, UK
David Chen, Seoul National University, Korea
Shunsuke Chiba, Nanyang Technological University, Singapore
Sheng-Hsien Chiu, National Taiwan University, Chinese Taipei
Luiz Carlos Dias, State University of Campinas, Brazil
Antonio Echavarren, Autonomous University of Madrid, Spain
Jonathan Ellman, Yale University, USA
Margaret Faul, Amgen, USA
Ben Feringa, University of Groningen, The Netherlands
Amar Flood, Indiana University Bloomington, USA
Nobutaka Fujii, Kyoto University, Japan
Carmen Galan, University of Bristol, UK
Sam Gellman, University of Wisconsin, USA
Mimi Hii, Imperial College London, UK
Krishna Kaliappan, IITB, India
Steven V. Ley, University of Cambridge, UK
Shih-Yuan Liu, University of Oregon, USA
Stephen Loeb, University of Windsor, Canada
David Lupton, Monash University, Australia
Ilan Marek, Israel Institute of Technology, Israel
Keiji Maruoka, Kyoto University, Japan
Cristina Nevado, University of Zürich, Switzerland
Dhevalapally B. Ramachary, University of Hyderabad, India
Viresh Rawal, University of Chicago, USA
Mark Rizzacasa, University of Melbourne, Australia
Richmond Sarpong, University of California, Berkeley, USA
Paolo Scrimin, University of Padua, Italy
Oliver Seitz, Humboldt University of Berlin, Germany
Jay Siegel, University of Zürich, Switzerland
Tibor Soos, Hungarian Academy of Sciences, Hungary
Corey Stephenson, University of Michigan, USA
Mark Taylor, University of Toronto, Canada
Dirk Trauner, Ludwig-Maximilian University Munich, Germany
Bruce Turnbull, University of Leeds, UK
Georgios Vassilikogiannakis, University of Crete, Greece
Helma Wennemers, University of Basel, Switzerland
Peter Wipf, University of Pittsburgh, USA
Shuli You, Shanghai Institute of Organic Chemistry, China
Li He Zhang, Peking University, China
Jian Zhou, East China Normal 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 2015. 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).

Registered Charity No. 207890.

COMMUNICATIONS

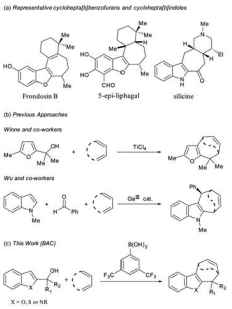
Published on 02 June 2015. Downloaded on 05/02/2016 04:23:01.

6449

Mild arylboronic acid catalyzed selective [4 + 3] cycloadditions: access to cyclohepta[*b*]-benzofurans and cyclohepta[*b*]indoles

Kou-Sen Cao, Hong-Xu Bian and Wen-Hua Zheng*

The first example of arylboronic acid catalyzed [4 + 3] cycloaddition reaction is reported.

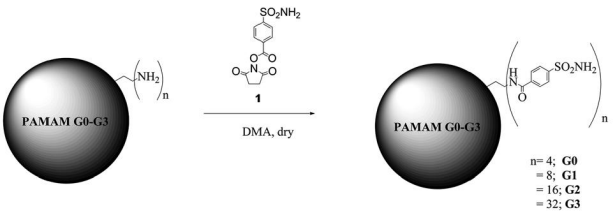


6453

Dendrimers incorporating benzenesulfonamide moieties strongly inhibit carbonic anhydrase isoforms I–XIV

Fabrizio Carta,* Sameh M. Osman, Daniela Vullo, Zeid AlOthman and Claudiu T. Supuran*

As extension of our previous study herein we report a comprehensive investigation of poly(amidoamine) (PAMAM) dendrimers as modulators of the human carbonic anhydrase (hCA, EC 4.2.1.1) isoforms I–XIV.

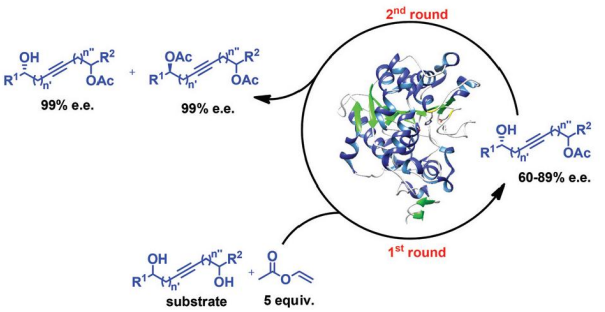


6458

Enzymatic kinetic resolution of internal propargylic diols. Part I: a new approach for the synthesis of (*S*)-pent-2-yn-1,4-diol, a natural product from *Clitocybe catinus*

Jeiely G. Ferreira, Cleverson R. Princival, Dyego M. Oliveira, Renata X. Nascimento and Jefferson L. Princival*

An efficient two round EKR of bis-substituted propargylic diols has been described and applied for synthesize (*S*)-pent-2-yn-1,4-diol, a natural product from *Clitocybe catinus*.

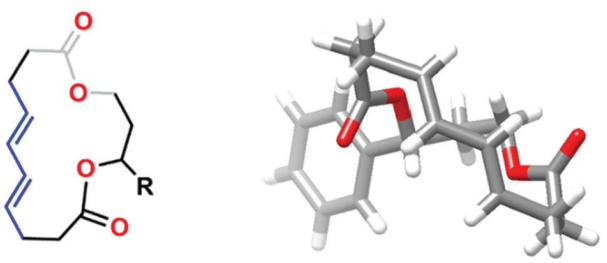


6463

Synthesis, structure and reactivity of [15]-macrodilactones

Debjani Si and Mark W. Peczuh*

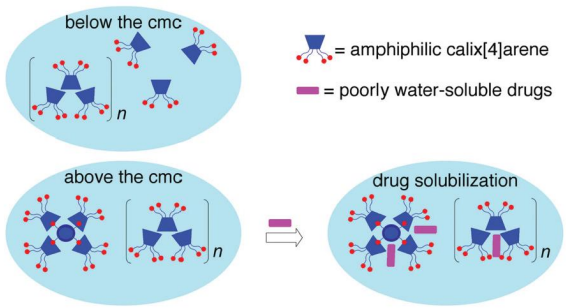
Synthesis and characterization of some new [15]-macrodilactones revealed that the interplay between three planar units, a stereogenic center and a hinge atom generated a planar chirality that governs their molecular topology.



Published on 02 June 2015. Downloaded on 05/02/2016 04:23:01.

COMMUNICATIONS

6468

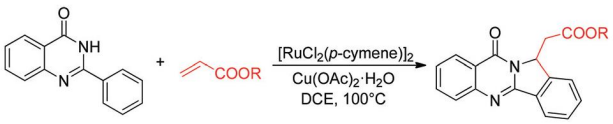


Self-assembly of amphiphilic anionic calix[4]arenes and encapsulation of poorly soluble naproxen and flurbiprofen

Lucia Barbera, Giuseppe Gattuso, Franz H. Kohnke, Anna Notti,* Sebastiano Pappalardo, Melchiorre F. Parisi, Ilenia Pisagatti,* Salvatore Patanè, Norberto Micali and Valentina Villari

The ability of an anionic calix[4]arene amphiphile to aggregate and to solubilize, as a result, the poorly water-soluble drugs naproxen and flurbiprofen is described.

6474

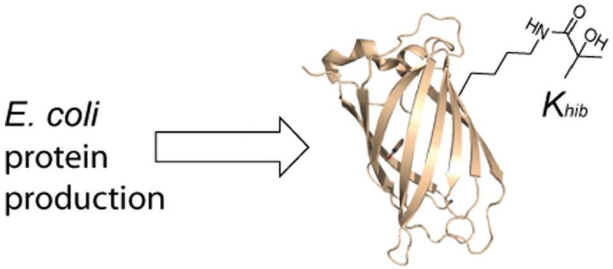


Ruthenium-catalyzed oxidative coupling of 2-aryl-4-quinazolinones with olefins: synthesis of pyrrolo[2,1-*b*]quinazolin-9(1*H*)-one motifs

Yong Zheng, Wei-Bin Song, Shu-Wei Zhang and Li-Jiang Xuan*

A ruthenium-catalyzed oxidative coupling of 2-aryl-quinazolinones with olefins *via* C–H bond activation followed by an intramolecular aza-Michael reaction is described.

6479



Genetic encoding of the post-translational modification 2-hydroxyisobutyryl-lysine

William A. Knight and T. Ashton Cropp*

Adding 2-hydroxyisobutyryl lysine to the genetic code of *E. coli* is reported.

PAPERS

6482

Fucofullerenes as tight ligands of RSL and LecB, two bacterial lectins

Kevin Buffet, Emilie Gillon, Michel Holler, Jean-François Nierengarten,* Anne Imberty* and Stéphane P. Vincent*

A series of water-soluble glycofullerenes containing up to 24 fucose residues were tested against the two bacterial lectins LecB and RSL, and $\mathbf{C_{60}(E)_{12}}$ bearing 24 fucose residues appeared to be the best known inhibitor of both lectins to date.

This journal is © The Royal Society of Chemistry 2015

Published on 02 June 2015. Downloaded on 05/02/2016 04:23:01.

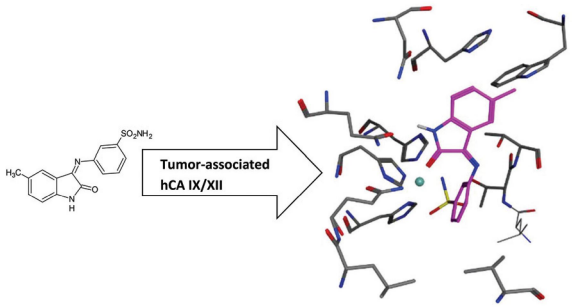
PAPERS

6493

Discovery of novel isatin-based sulfonamides with potent and selective inhibition of the tumor-associated carbonic anhydrase isoforms IX and XII

Özlen Güzel-Akdemir, Atilla Akdemir,* Nilgün Karalı and Claudiu T. Supuran*

A series of 2/3/4-[(2-oxo-1,2-dihydro-3*H*-indol-3-ylidene)amino]benzenesulfonamides, obtained from substituted isatins and 2-, 3- or 4-aminobenzene-sulfonamide, showed low nanomolar inhibitory activity against the tumor associated carbonic anhydrases IX and XII.

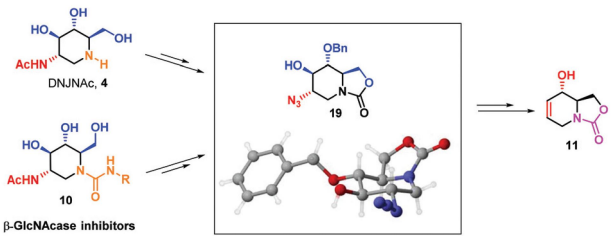


6500

Stereoselective synthesis of 2-acetamido-1,2-dideoxynojirimycin (DNJNAc) and ureido-DNJNAc derivatives as new hexosaminidase inhibitors

Alex de la Fuente, Teresa Mena-Barragán, Ronald A. Farrar-Tobar, Xavier Verdaguer, José M. García Fernández, Carmen Ortiz Mellet* and Antoni Riera*

A novel approach to the synthesis of 2-acetamido-1,2-dideoxynojirimycin (DNJNAc) and ureido-DNJNAc derivatives as potent hexosaminidase inhibitors is reported.

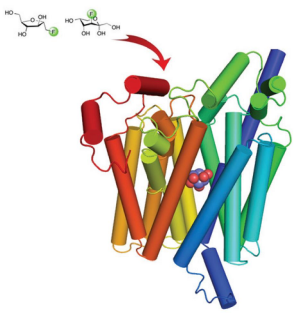


6511

New fluorinated fructose analogs as selective probes of the hexose transporter protein GLUT5

Olivier-Mohamad Soueidan, Brendan J. Trayner, Tina N. Grant, Jeff R. Henderson, Frank Wuest, F. G. West* and Chris I. Cheeseman*

Two fluorinated fructose analogs are taken up by tumor cells in culture. Their high affinity for the transporter protein GLUT5 provides information on the structural demands of its binding site, and suggests approaches towards new molecular imaging probes.

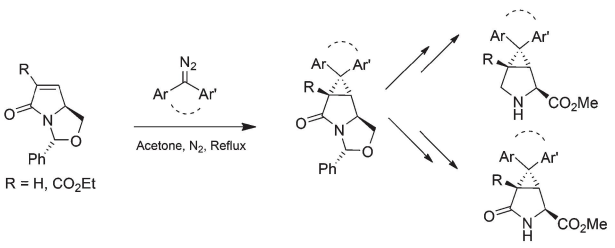


6522

Uncatalysed diaryldiazo cyclopropanations on bicyclic lactams: access to annulated prolines

Lawrence Harris, Martin Gilpin, Amber L. Thompson, Andrew R. Cowley and Mark G. Moloney*

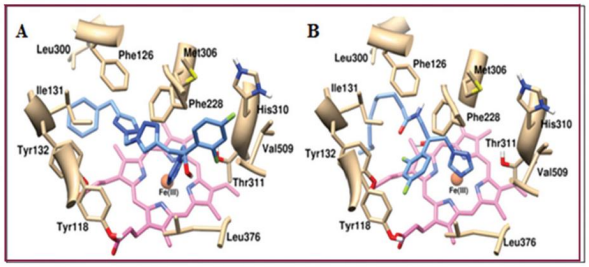
The uncatalysed cycloaddition of substituted diaryldiazo compounds onto bicyclic unsaturated lactams derived from pyroglutamic acid efficiently leads to highly functionalised azatricyclononanes.



Published on 02 June 2015. Downloaded on 05/02/2016 04:23:01.

PAPERS

6551

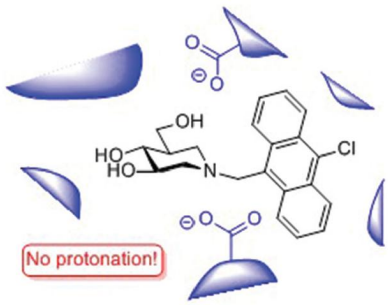


Design and synthesis of new fluconazole analogues

Vandana S. Pore,* Sandip G. Agalave, Pratiksha Singh, Praveen K. Shukla, Vikash Kumar and Mohammad I. Siddiqi

The synthesis of new fluconazole analogues containing two different 1,2,3-triazole units and an amide group is described. All the compounds showed very high antifungal activity and no toxicity.

6562

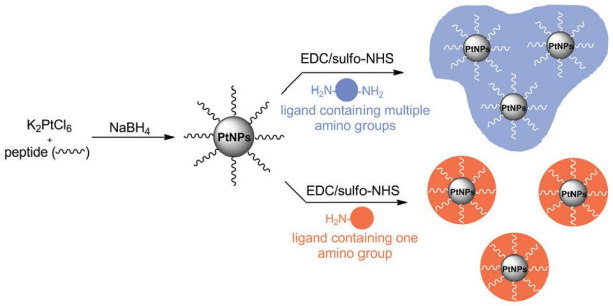


A fluorescence study of isofagomine protonation in β-glucosidase

Emil Lindbäck, Bo Wegge Laursen, Jens Christian Navarro Poulsen, Kristine Kilså, Christian Marcus Pedersen and Mikael Bols*

N-(10-Chloro-9-anthracenemethyl)isofagomine **5** inhibits β-glucosidase strongly yet the nitrogen atom plays little role in binding.

6567

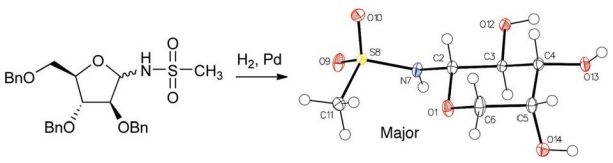


Cell-targeted platinum nanoparticles and nanoparticle clusters

Stefanie Papst, Margaret A. Brimble,* Clive W. Evans, Daniel J. Verdon, Vaughan Feisst, P. Rod Dunbar, Richard D. Tilley and David E. Williams*

The facile preparation of cell-targeted platinum nanoparticles (PtNPs) is described, using designed peptides that as a single molecule control PtNP cluster growth, stabilise clusters in aqueous suspension and enable attachment of a versatile range of cell-targeting ligands.

6573



Unexpected furanose/pyranose equilibration of *N*-glycosyl sulfonamides, sulfamides and sulfamates

Kajitha Suthagar, Matthew I. J. Polson and Antony J. Fairbanks*

Arabino N-glycosyl sulfamides, sulfonamides and sulfamates convert from the furanose to the thermodynamically preferred pyranose form in aqueous solution.

This journal is © The Royal Society of Chemistry 2015

Published on 02 June 2015. Downloaded on 05/02/2016 04:23:01.

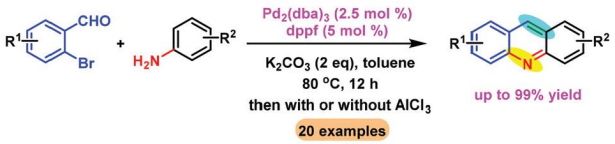
PAPERS

6580

Facile synthesis of acridines *via* Pd(0)-diphosphine complex-catalyzed tandem coupling/cyclization protocol

Ting-Jun Wang, Wen-Wen Chen, Yi Li and Ming-Hua Xu*

A facile and efficient approach for the synthesis of a variety of acridines *via* the tandem coupling/cyclization of substituted 2-bromobenzaldehydes and anilines is described.

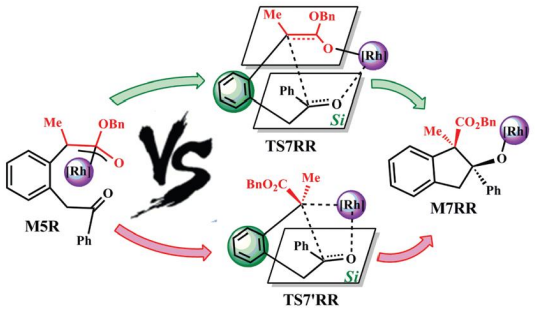


6587

Mechanisms and stereoselectivities of the Rh(I)-catalyzed carbenoid carbon insertion reaction of benzocyclobutenol with diazoester

Yanyan Wang, Yang Wang, Wenjing Zhang, Yanyan Zhu, Donghui Wei* and Mingsheng Tang*

Mechanisms and stereoselectivities of a Rh(I)-catalyzed carbenoid carbon insertion reaction of benzocyclobutenol with diazoester have been investigated using the DFT method.

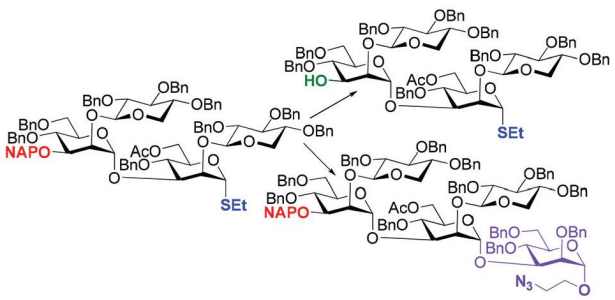


6598

A synthetic strategy to xylose-containing thioglycoside tri- and tetrasaccharide building blocks corresponding to *Cryptococcus neoformans* capsular polysaccharide structures

Lorenzo Guazzelli, Rebecca Ulc, Lina Rydner and Stefan Oscarson*

C. neoformans thiosaccharide building blocks were prepared and their conversion to glycosyl acceptors as well as use as glycosyl donors investigated.

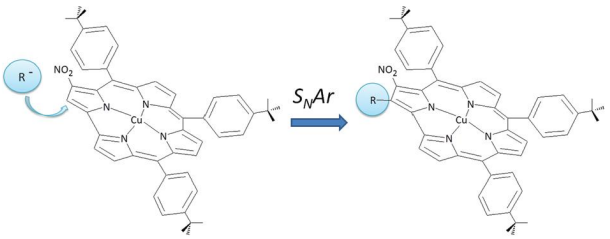


6611

Corrole and nucleophilic aromatic substitution are not incompatible: a novel route to 2,3-difunctionalized copper corrolates

M. Stefanelli,* F. Mandoj, S. Nardis, M. Raggio, F. R. Fronczek, G. T. McCandless, K. M. Smith and R. Paolesse

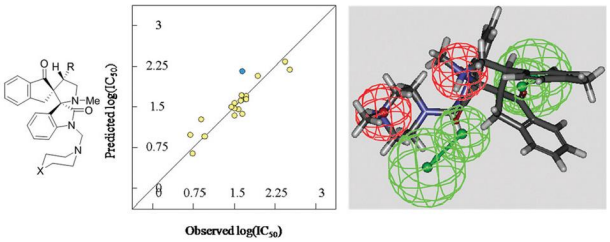
Although corrole is an electron rich macrocycle, nucleophilic aromatic substitution reactions can be used to peripherally elaborate this contracted porphyrinoid.



Published on 02 June 2015. Downloaded on 05/02/2016 04:23:01.

PAPERS

6619

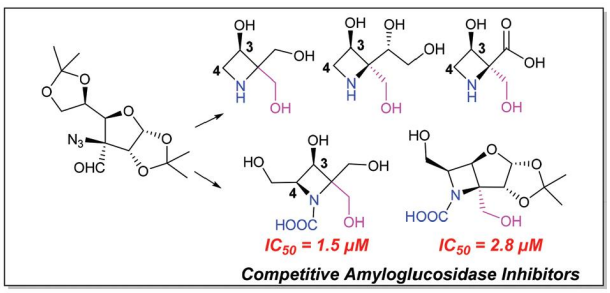


Rational design, synthesis and molecular modeling studies of novel anti-oncological alkaloids against melanoma

Adel S. Girgis,* Siva S. Panda, Aladdin M. Srour, Hanaa Farag, Nasser S. M. Ismail, Mohamed Elgendy, Amal K. Abdel-Aziz and Alan R. Katritzky

Anti-oncological active spiro-alkaloids were synthesized exhibiting promising antitumor properties against melanoma cell lines. Molecular modeling studies describe the observed properties.

6634

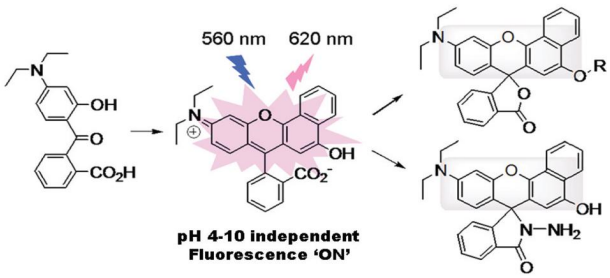


Azetidine- and *N*-carboxylic azetidine-iminosugars as amyloglucosidase inhibitors: synthesis, glycosidase inhibitory activity and molecular docking studies

Kishor S. Gavale, Shrawan R. Chavan, Ayesha Khan, Rakesh Joshi and Dilip D. Dhavale*

Azetidine and an unprecedented *N*-carboxylic azetidine iminosugars were synthesized from D-glucose, which showed prominent amyloglucosidase inhibitory activity.

6647



Molecular design and synthesis of a pH independent and cell permeant fluorescent dye and its applications

Xiaojie Jiao, Chang Liu, Kun Huang, Siwen Zhang, Song He, Liancheng Zhao and Xianshun Zeng*

A novel xanthene fluorescent dye with a combination of the desirable characters for fluorescent chemosensors and biomarkers including low molecular weight, water solubility, cell permeability, good biocompatibility, and strong tolerance to pH has been designed and synthesized.

This journal is © The Royal Society of Chemistry 2015