

Organic & Biomolecular Chemistry

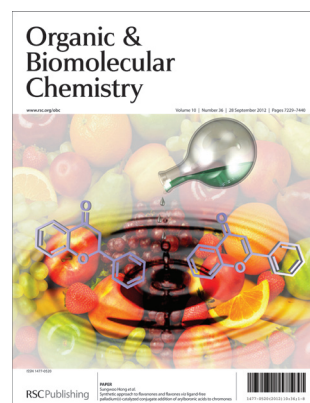
An international journal of synthetic, physical and biomolecular organic chemistry

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

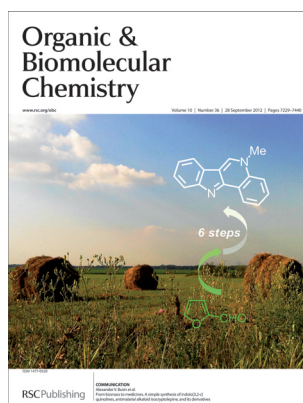
ISSN 1477-0520 CODEN OBCRAK 10(36) 7229–7440 (2012)



Cover

See Sungwoo Hong *et al.*, pp. 7305–7312.

Image reproduced by permission of Sungwoo Hong from *Org. Biomol. Chem.*, 2012, **10**, 7305.



Inside cover

See Alexander V. Butin *et al.*, pp. 7262–7265.

Image reproduced by permission of Alexander V. Butin from *Org. Biomol. Chem.*, 2012, **10**, 7262.

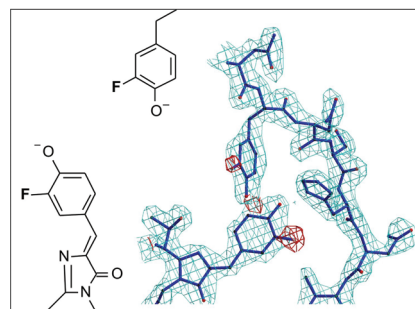
EMERGING AREA

7241

Organic fluorine as a polypeptide building element: *in vivo* expression of fluorinated peptides, proteins and proteomes

L. Merkel and N. Budisa*

The design and engineering of complex protein scaffolds with hydrocarbons partially or fully augmented with fluorocarbons is one of the most promising routes to create living systems with novel chemistries. Here we elaborate the first experimental steps in this direction.



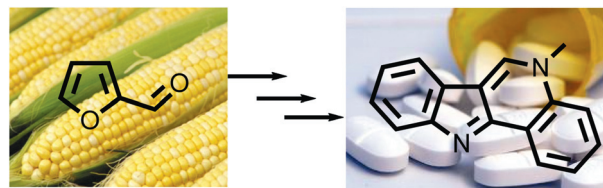
COMMUNICATIONS

7262

From biomass to medicines. A simple synthesis of indolo[3,2-*c*]quinolines, antimalarial alkaloid isocryptolepine, and its derivatives

Maxim G. Uchuskin, Arkady S. Pilipenko, Olga V. Serdyuk, Igor V. Trushkov and Alexander V. Butin*

An approach to indolo[3,2-*c*]quinolines, alkaloid isocryptolepine and its derivatives from furfural is described.



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

Nathalie Horner, Sarah Salter

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

Barry Carpenter, Cardiff University, UK

Antonio Echavarren, Autonomous

University of Madrid, Spain

Jonathan Ellman, Yale University, USA

Ben Feringa, University of Groningen,

Netherlands

Nobutaka Fujii, Kyoto University, Japan

Steven V Ley, University of Cambridge,

UK

Stephen Loeb, University of Windsor,

Canada

Ilan Marek, Israel Institute of

Technology, Israel

Keiji Maruoka, Kyoto 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

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

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.

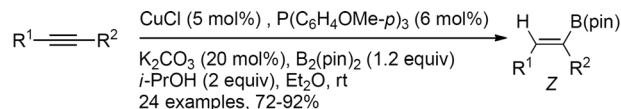
COMMUNICATIONS

7266

CuCl–K₂CO₃-catalyzed highly selective borylcupration of internal alkynes – ligand effect

Weiming Yuan and Shengming Ma*

An efficient and practical copper-catalyzed highly regio- and stereoselective borylcupration of internal alkynes with bis(pinacolato)diboron using a catalytic amount of K₂CO₃ as base producing *Z*-alkenylboron compounds has been demonstrated by applying the ligand effect of commercially available electron-rich tris(*p*-methoxyphenyl) phosphine.

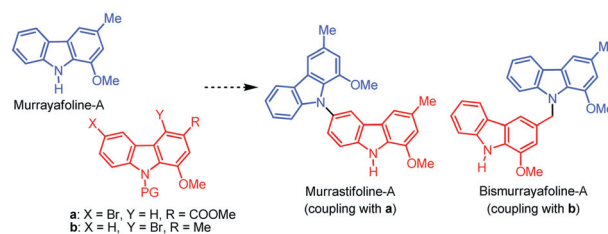
R¹ = Ar; R² = Me, *n*-Pr, *n*-Bu, *n*-C₆H₁₃R¹ = *t*-Bu; R² = ArR¹ = CH₂OH, CH₂OBn, CH₂OAc, CH₂NHTs; R² = Me

7269

Novel approach to biscarbazole alkaloids via Ullmann coupling – synthesis of murrastifoline-A and bismurrayafoline-A

Carsten Börger, Olga Kataeva and Hans-Joachim Knölker*

Unprecedented Ullmann couplings of murrayafoline-A with either 6-bromo- or 4-bromocarbazole derivatives provide highly efficient synthetic routes to the biscarbazole alkaloids murrastifoline-A (6 steps, 66% overall yield) and bismurrayafoline-A (6 steps, 28% overall yield).



7274

Palladium-catalyzed atom transfer radical cyclization of unactivated alkyl iodide

Hui Liu, Zongjun Qiao and Xuefeng Jiang*

A palladium-catalyzed atom transfer cyclization of unactivated alkyl iodide has been developed.

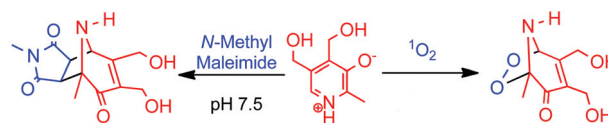


7278

Novel ring chemistry of vitamin B₆ with singlet oxygen and an activated ene: isolated products and identified intermediates suggesting an operable [3 + 2] cycloaddition

David Samuel, Kirsten Norrell and David G. Hilmey*

Reaction between pyridoxine and ¹O₂, or maleimide, demonstrates novel rearrangement, intermediate identification, and unactivated aqueous cycloaddition within the 3-hydroxypyridine ring.



RSC Prizes and Awards

Rewarding Excellence and Dedication

Organic Chemistry Awards

The Organic Chemistry awards portfolio rewards excellence in both industry and academia for original research in any aspect of organic chemistry, as well as specific areas including organometallic and physical organic chemistry.

The RSC confers a wide range of Prizes and Awards to acknowledge those undertaking excellent work. In recognition of their achievement, winners receive up to £5,000 prize money. Visit our website for further details and to make your nomination.

Reward achievement

2013 nominations open on 1 September 2012

To view our full list of Prizes and Awards, and to find out how to make a nomination, visit our website.

Closing date for nominations is 15 January 2013

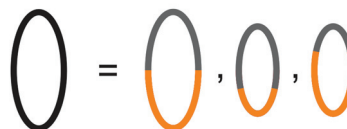
PAPERS

7282

Investigating the effect of macrocycle size in anion templated imidazolium-based interpenetrated and interlocked assemblies

Graeme T. Spence, Nicholas G. White and Paul D. Beer*

The effect of varying the size of the macrocycle component on the formation of anion templated imidazolium interpenetrated assemblies and on the recognition properties of analogous interlocked rotaxane host systems is investigated.

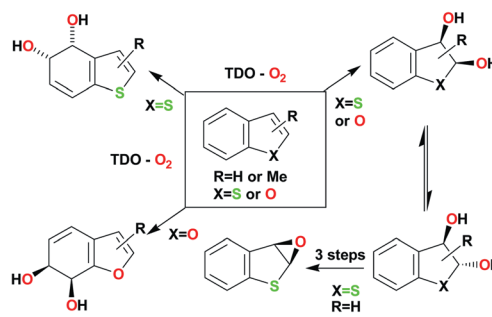


7292

Toluene dioxygenase-catalyzed *cis*-dihydroxylation of benzo[*b*]thiophenes and benzo[*b*]furans: synthesis of benzo[*b*]thiophene 2,3-oxide

Derek R. Boyd,* Narain D. Sharma, Ian N. Brannigan, Timothy A. Evans, Simon A. Haughey, Brian T. McMurray, John F. Malone, Peter B. A. McIntyre, Paul J. Stevenson and Christopher C. R. Allen

Dioxygenase-catalysed stereoselective dihydroxylation of benzo[*b*]thiophenes and benzo[*b*]furans yielded *cis* and *trans* diols having synthetic potential.

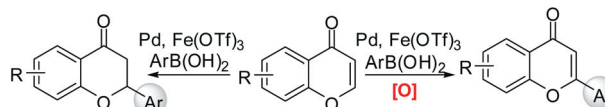


7305

Synthetic approach to flavanones and flavones *via* ligand-free palladium(II)-catalyzed conjugate addition of arylboronic acids to chromones

Donghee Kim, Kyungrok Ham and Sungwoo Hong*

The remarkable catalytic effects of $\text{Fe}(\text{OTf})_3$ in the context of the Pd(II)-catalyzed conjugate addition of arylboronic acids to chromones were observed to yield a variety of flavanones under mild conditions. The addition of catalytic amounts of DDQ and KNO_2 to the reactions exclusively yielded flavone analogs.

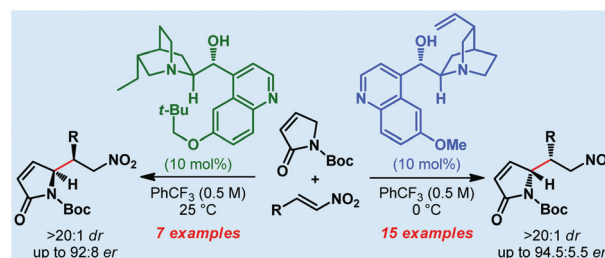


7313

Organocatalytic asymmetric direct vinylogous Michael addition of α,β -unsaturated γ -butyrolactam to nitroolefins

Abhijnan Ray Choudhury and Santanu Mukherjee*

The first organocatalytic enantioselective direct vinylogous Michael reaction of α,β -unsaturated γ -butyrolactam to nitroolefins is developed using cinchona alkaloids as the catalysts. Both product enantiomers are accessible with moderate to good enantioselectivity.



New process for crystal data files

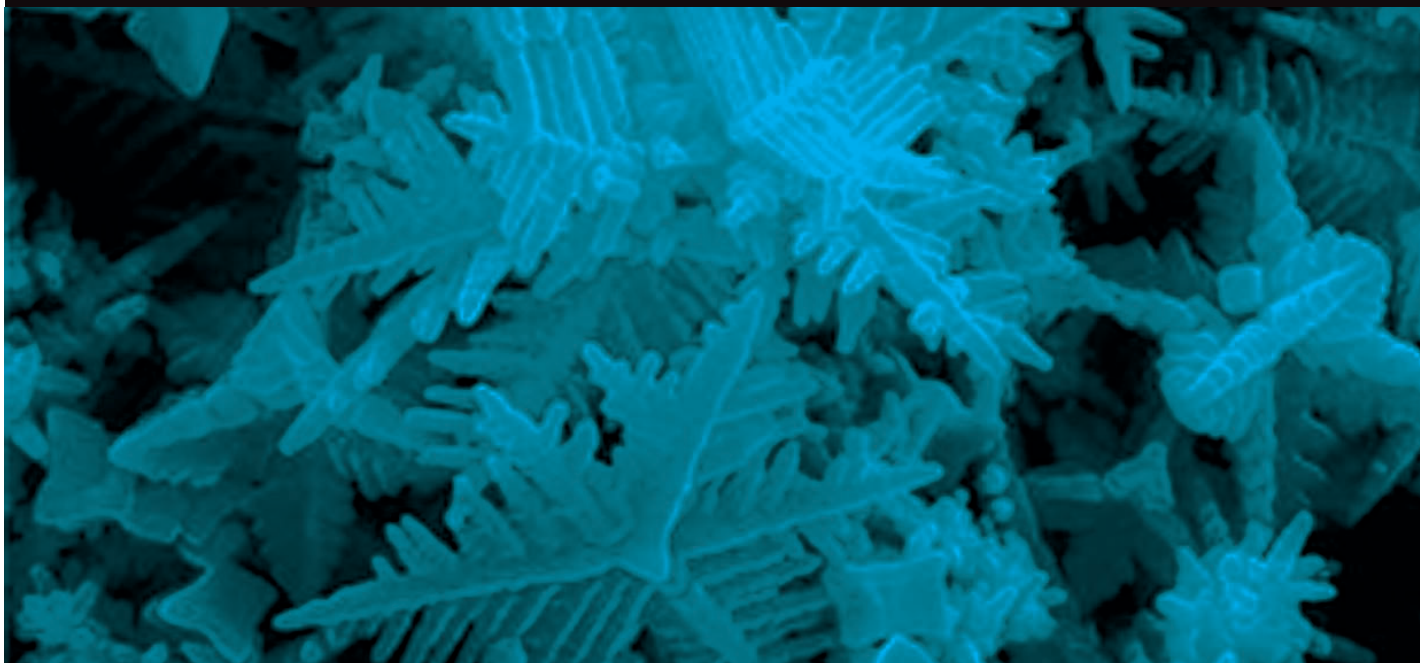


Image courtesy of Professor Gang Chen and Dr Rencheng Jin DOI: 10.1039/C2CE06417K

Do you submit crystallographic data with your articles? Confused by what you need to do?

Then you'll be glad to hear that we are making it easier for you: from September 1st, all crystal data files (CIFs) must be accompanied by the CCDC reference number(s) when you submit your article.

As this change also aligns us with preferred CCDC practices, it means a more streamlined process for everyone involved.

Full details are available on our website.

RSC Publishing

www.rsc.org/crystal_data

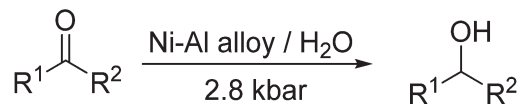
Registered Charity Number 207890

7321

Selective reduction of ketones using water as a hydrogen source under high hydrostatic pressure

Anna Tomin, Alexander Lazarev, Matthew P. Bere, Hana Redjeb and Béla Török*

High hydrostatic pressure-assisted reduction of acyclic, cyclic and aryl ketones to alcohols was achieved with high yields and excellent selectivities.

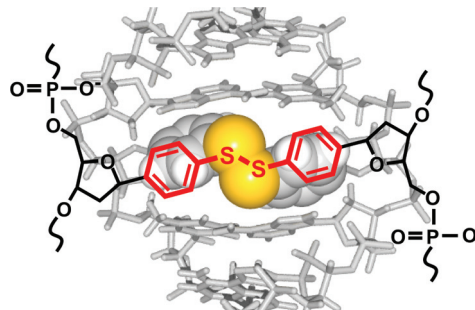


7327

Solution structure of S-DNA formed by covalent base pairing involving a disulfide bond

Akihiko Hatano,* Munehiro Okada and Gota Kawai

We determined the solution structure of the S-DNA containing a disulfide bond at the central position in the duplex by NMR. It was found that the disulfide base pair was intercalated into the sequence and DNA is bent at the point of the disulfide base pair to face the major groove.

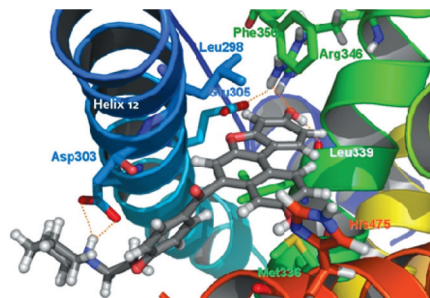


7334

Towards β -selectivity in functional estrogen receptor antagonists

Jose Juan Rodríguez, Kamila Filipiak, Maciej Maslyk, Jakub Ciepielski, Sebastian Demkowicz, Sonia de Pascual-Teresa, Sonsoles Martín-Santamaría,* Beatriz de Pascual-Teresa and Ana Ramos*

Novel estrogen receptor ligands with functional β -selectivity were synthesized and evaluated. The figure shows the docked binding mode obtained for one of the described antagonists.

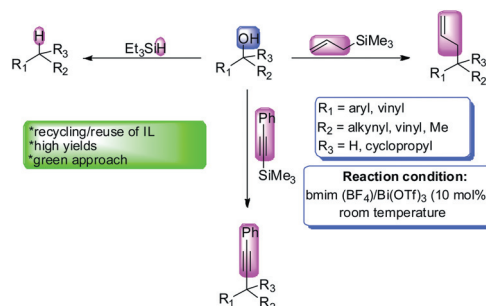


7347

Facile coupling of propargylic, allylic and benzylic alcohols with allylsilane and alkynylsilane, and their deoxygenation with Et_3SiH , catalyzed by $\text{Bi}(\text{OTf})_3$ in $[\text{BMIM}][\text{BF}_4]$ ionic liquid (IL), with recycling and reuse of the IL

G. G. K. S. Narayana Kumar and Kenneth K. Laali*

Facile coupling of pi-activated alcohols (propargylic, allylic, benzylic) with allyl-TMS and alkynyl-TMS and their deoxygenation with Et_3SiH using $\text{Bi}(\text{OTf})_3/\text{bmim}(\text{BF}_4)$.



RSC Books

Let us provide you with the best and most diverse choice of chemical science titles

Cutting-edge high-quality content, outstanding excellence across the chemical sciences and beyond, the RSC continues to lead as one of the fastest chemical science print and online book publishers in the world



New Series



Food and Nutritional Components in Focus



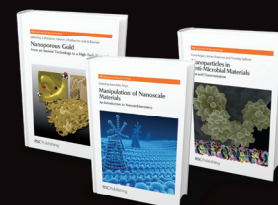
RSC Drug Discovery Series



RSC Green Chemistry Series



RSC Energy & Environment Series



RSC Nanoscience & Nanotechnology Series



RSC Biomolecular Sciences Series



General Science



Seminal Texts

Register

with our alerting service to receive all the latest RSC book news - tailored to your subject specialist area

Visit www.rsc.org/alerts

RSC Publishing

www.rsc.org/books

Registered Charity Number 207890

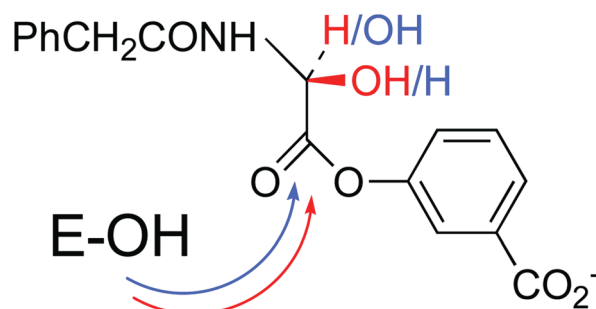
PAPERS

7356

Kinetics and stereochemistry of hydrolysis of an *N*-(phenylacetyl)- α -hydroxyglycine ester catalyzed by serine β -lactamases and α -peptidases

Ryan B. Pelto and R. F. Pratt*

β -Lactam-recognizing enzymes make a choice between an *R* and an *S* α -hydroxyl group.

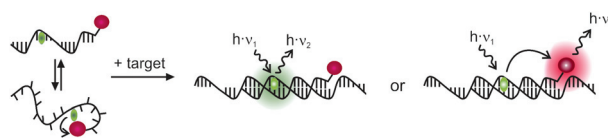


7363

Dual fluorophore PNA FIT-probes – extremely responsive and bright hybridization probes for the sensitive detection of DNA and RNA

Elke Socher, Andrea Knoll and Oliver Seitz*

The energy transfer between a “smart” thiazole orange nucleotide and carefully selected terminally appended acceptor dye provides dual labeled peptide nucleic acid probes with up to 450-fold enhancements of fluorescence upon hybridization with complementary nucleic acids.

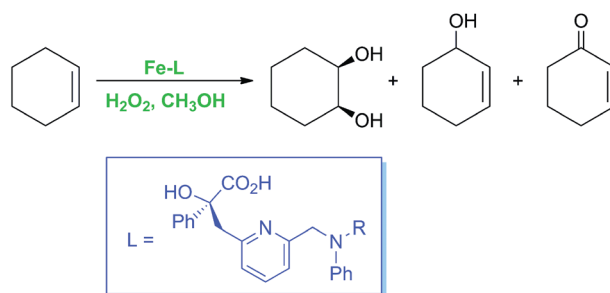


7372

Investigating the oxidation of alkenes by non-heme iron enzyme mimics

Sarah M. Barry, Helge Mueller-Bunz and Peter J. Rutledge*

Ligands inspired by non-heme iron enzyme architectures combine with ferrous acetate and hydrogen peroxide to promote hydrocarbon oxidation, and self-destruction.

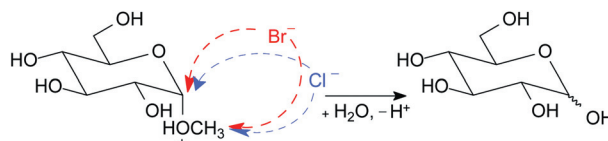


7382

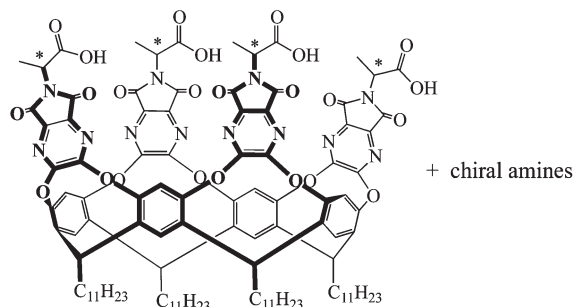
Direct participation of counter anion in acid hydrolysis of glycoside

Hung Duy Phan, Tomoya Yokoyama* and Yuji Matsumoto

The direct participation of Br^- and Cl^- in acid hydrolysis of glycoside was suggested.



7392

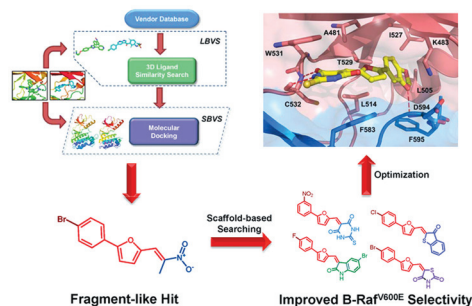


Resorcinarene-based cavitands with chiral amino acid substituents for chiral amine recognition

Na Li, Fan Yang, Hillary A. Stock, David V. Dearden, John D. Lamb and Roger G. Harrison*

Cavitands with amino acid substituents along their upper rim have been synthesized, characterized by MS, and used for chiral recognition of benzyl amines.

7402

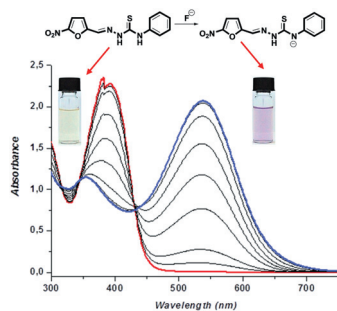


Development of a novel class of B-Raf^{V600E}-selective inhibitors through virtual screening and hierarchical hit optimization

X. Kong, J. Qin, Z. Li, A. Vultur, L. Tong, E. Feng, G. Rajan, S. Liu, J. Lu, Z. Liang, M. Zheng, W. Zhu, H. Jiang, M. Herlyn, H. Liu,* R. Marmorstein* and C. Luo*

Identification of B-Raf^{V600E} selective inhibitors.

7418

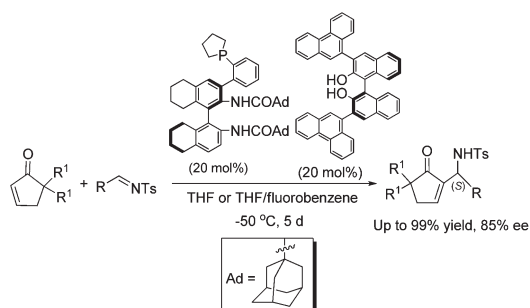


Synthesis and evaluation of thiosemicarbazones functionalized with furyl moieties as new chemosensors for anion recognition

Luis E. Santos-Figueroa, María E. Moragues, M. Manuela M. Raposo,* Rosa M. F. Batista, Susana P. G. Costa, R. Cristina M. Ferreira, Félix Sancenón, Ramón Martínez-Mañez,* José Vicente Ros-Lis and Juan Soto

A family of heterocyclic thiosemicarbazone dyes containing furyl groups was synthesized and their response in the presence of selected anions studied.

7429



New multifunctional chiral phosphines and BINOL derivatives co-catalyzed enantioselective aza-Morita-Baylis-Hillman reaction of 5,5-disubstituted cyclopent-2-enone and *N*-sulfonated imines

Yuan-Liang Yang, Yin Wei and Min Shi*

New multifunctional chiral phosphine and BINOL derivative co-catalyzed aza-MBH reaction of 5,5-disubstituted cyclopent-2-enone **1** with *N*-sulfonated imines **2** afforded the corresponding optically active adducts **3** in good to outstanding yields with moderate to good ee's under mild conditions.