Organic & Biomolecular Chemistry

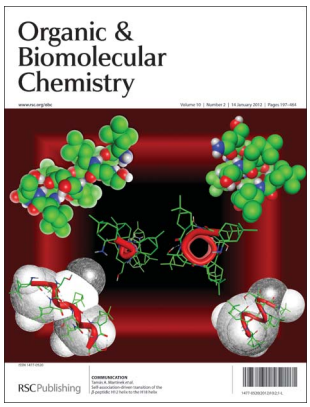
An international journal of synthetic, physical and biomolecular organic chemistry

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(2) 197–464 (2012)

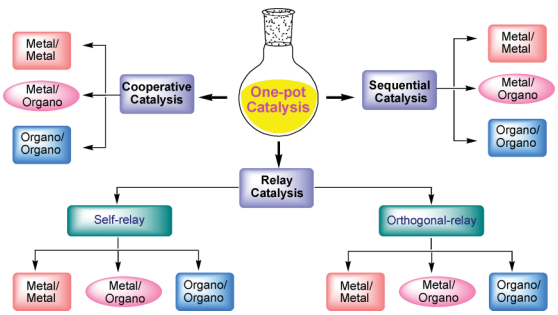


Cover

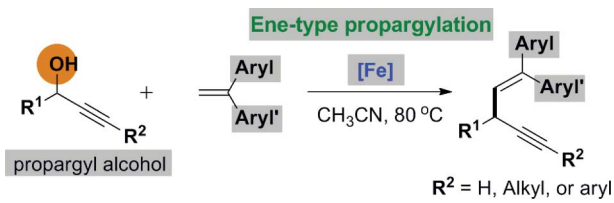
See Tamás A. Martinek *et al.*, pp. 255–259.

Image reproduced by permission of Tamás A. Martinek from *Org. Biomol. Chem.*, 2012, **10**, 255.

EMERGING AREA



COMMUNICATIONS



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.

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.

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.

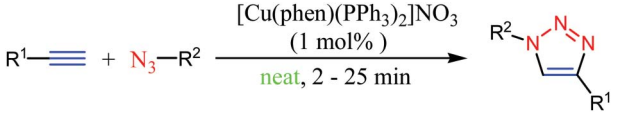
Authors may reproduce/republish portions of their published contribution without seeking permission from the RSC, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of The Royal Society of Chemistry.

229

Quick and highly efficient copper-catalyzed cycloaddition of organic azides with terminal alkynes

Dong Wang, Mingming Zhao, Xiang Liu, Yongxin Chen, Na Li and Baohua Chen*

A highly efficient catalyst $[Cu(phen)(PPh_3)_2]NO_3$ for the Huisgen cycloaddition reaction has been developed.

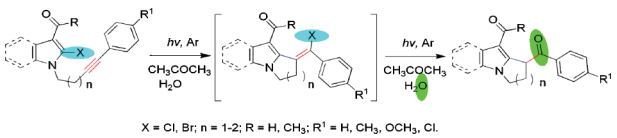


232

Photoinduced chlorine atom-transfer cyclization/ photohydrolysis of 3-acyl-2-chloro-*N*-(ω-phenylalkynyl)pyrroles: a one-pot synthesis of benzoyl-substituted fused pyrroles

Shen-Ci Lu, Wei-Xia Wang, Pan-Liang Gao, Wei Zhang* and Zhi-Feng Tu

A one-pot synthesis of benzoyl-substituted fused pyrroles and indoles has been achieved by photoinduced halogen atom-transfer cyclization and subsequent photohydrolysis.

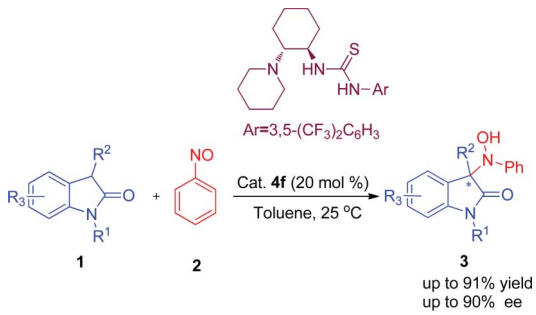


236

Asymmetric hydroxyamination of oxindoles catalyzed by chiral bifunctional tertiary amine thiourea: construction of 3-amino-2-oxindoles with quaternary stereocenters

Li-Na Jia, Jun Huang, Lin Peng, Liang-Liang Wang, Jian-Fei Bai, Fang Tian, Guang-Yun He, Xiao-Ying Xu* and Li-Xin Wang*

Chiral bifunctional tertiary amine thiourea was successfully applied to catalyze the asymmetric hydroxyamination of 3-subsituted oxindoles with nitrosobenzene to construct 3-amino-2-oxindoles in good yields (up to 91%) and enantioselectivities (up to 90% ee).

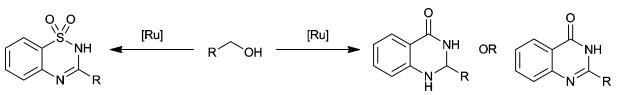


240

Ruthenium-catalysed oxidative synthesis of heterocycles from alcohols

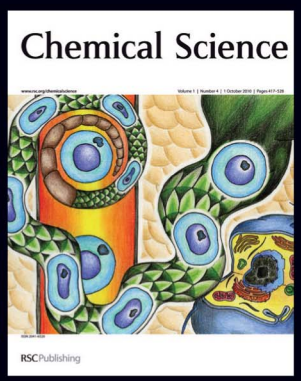
Andrew J. A. Watson,* Aoife C. Maxwell and Jonathan M. J. Williams

Ruthenium-catalysed hydrogen transfer has been successfully used for the conversion of alcohols into either 2,3-dihydroquinazolines or quinazolines.



Recognition starts here...

in the **best new journal***



011067

*Winner of ALPSP Award for Best New Journal 2011

Chemical Science

A new global impact journal for exceptional research from across the chemical sciences

What's different about *Chemical Science*, you might ask?
Firstly, we know that current approaches to selecting and publishing articles aren't always as effective as they might be. Secondly, we appreciate the challenges you face in getting your work published, noticed and recognised.

We want to change this. So *Chemical Science* will make it easier for you to get the recognition that your work deserves.

A hand-picked team of dynamic Associate Editors, led by **Editor-in-Chief David MacMillan**, will ensure that every article has a fair review. And as active researchers, they will guarantee that the journal represents the best new thinking in the chemical sciences.

Submit your next article to *Chemical Science* – and step into the spotlight.

RSC Publishing

www.rsc.org/chemicalscience

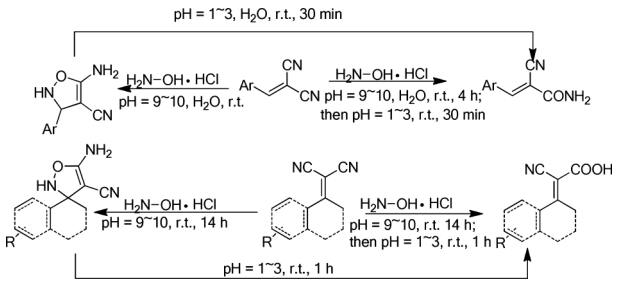
Registered Charity Number 207890

244

Synthesis of functionalized 2,3-dihydroisoxazoles by domino reactions in water and unexpected ring-opening reactions of 2,3-dihydroisoxazoles

Ping Li, Bo-Tao Teng, Fa-Gen Jin, Xin-Sheng Li, Wei-Dong Zhu and Jian-Wu Xie*

A new, mild, and environmentally benign process for the efficient synthesis of 2,3-dihydroisoxazoles, 2-cyano-3-aryl-acrylamides, and 2-cyanobut-2-enoic acid derivatives has been reported.

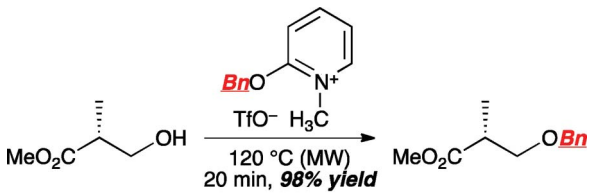


248

Microwave-assisted benzyl-transfer reactions of commercially available 2-benzyloxy-1-methylpyridinium triflate

Teng-wei Wang, Tanit Intaranukulkit, Michael R. Rosana, Rimantas Slegeris, Janet Simon and Gregory B. Dudley*

MW heating should be considered for benzylation of high-value substrates using the title reagent.



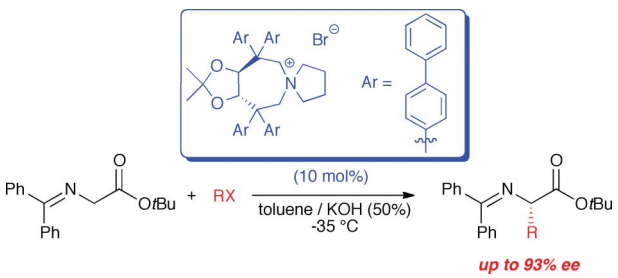
benzylation of 1°, 2°, 3° alcohol, phenol, carboxylic acid, and electron-rich arene substrates; isolated yields from 48% (3° ROH) to >90% (1° ROH and carboxylic acid)

251

Design, synthesis, and application of tartaric acid derived *N*-spiro quaternary ammonium salts as chiral phase-transfer catalysts

Mario Waser,* Katharina Gratzer, Richard Herchl and Norbert Müller

A novel class of tartaric acid-derived *N*-spiro quaternary ammonium salts was synthesised starting from known TADDOLs. These compounds were found to catalyse the asymmetric α-alkylation of glycine Schiff bases with high enantioselectivities and in good yields.



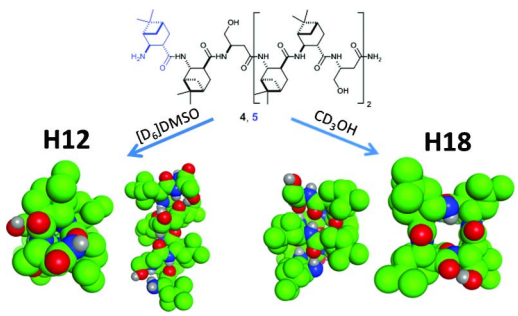
up to 93% ee

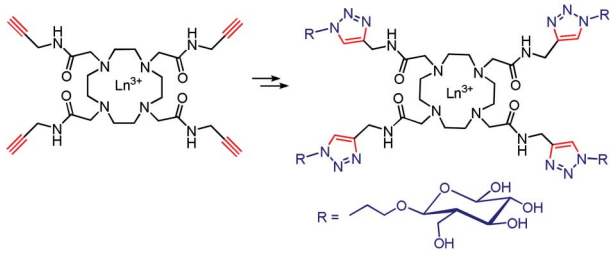
255

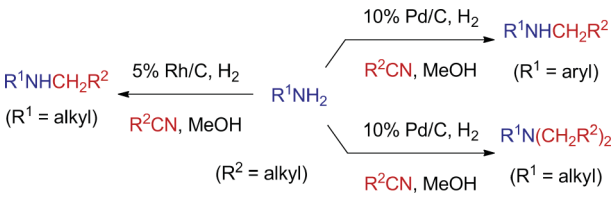
Self-association-driven transition of the β-peptidic H12 helix to the H18 helix

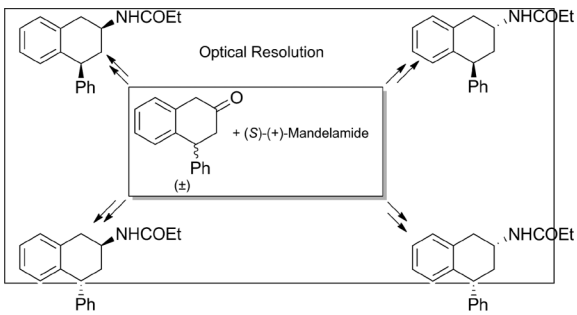
Éva Szolnoki, Anasztázia Hetényi, Tamás A. Martinek,* Zsolt Szakonyi and Ferenc Fülöp

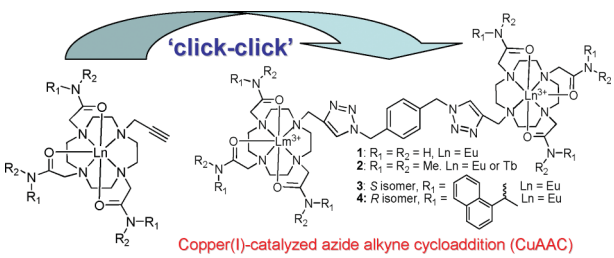
Foldamer sequences constructed by using *trans*-ABHC and β³-hSer residues produce β-H18 helix in a solvent- and concentration-dependent way.











New Journal

Toxicology Research

A new, multi-disciplinary journal covering the best research in both fundamental and applied aspects of toxicology
Published in partnership with the British Toxicology Society and Chinese Society of Toxicology

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

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

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

The first issue is scheduled for publication around May 2012.

Submit your work now!

bts THE BRITISH TOXICOLOGY SOCIETY

Chinese Society Of Toxicology

RSC Publishing

www.rsc.org/toxicology

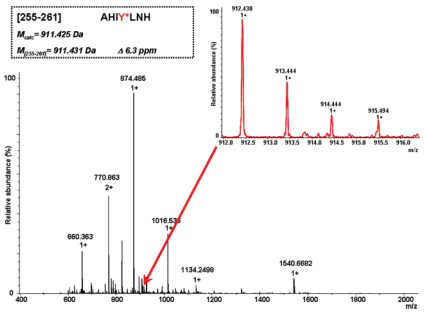
Registered Charity Number 207890

323

Tyrosine nitration affects thymidylate synthase properties

E. Dąbrowska-Maś, T. Frączyk, T. Ruman, K. Radziszewska, P. Wilk, J. Cieśla, Z. Zieliński, A. Jurkiewicz, B. Gołos, P. Wińska, E. Wałajtys-Rode, A. Leś, J. Nizioł, A. Jarmuła, P. Stefanowicz, Z. Szewczuk and W. Rode*

Purified endogenous calf thymus and L1210 thymidylate synthase proteins were found nitrated on tyrosine residues. Chemical nitration of human, mouse and *C. elegans* recombinant enzyme proteins distinctly affected catalytic potency.

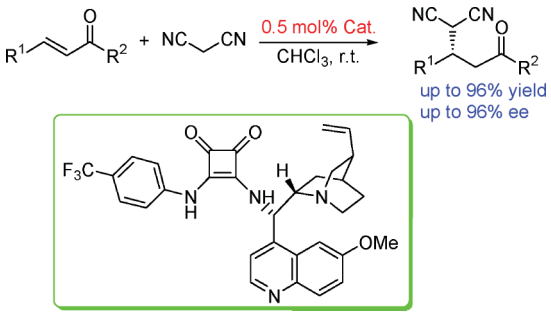


332

Squaramide-catalyzed enantioselective Michael addition of malononitrile to chalcones

Wen Yang, Yang Jia and Da-Ming Du*

A highly enantioselective Michael addition of malononitrile to chalcones catalyzed by a chiral squaramide catalyst at a very low catalyst loading (0.5 mol%) led to chiral γ-cyano carbonyl compounds in good yields with high enantioselectivities (up to 96% ee) under mild reaction conditions.

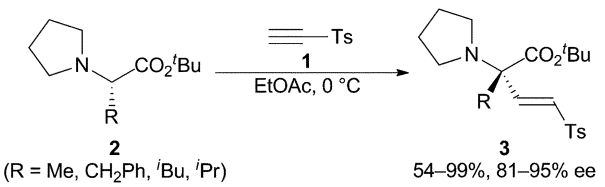


339

Asymmetric α-2-tosylethenylation of *N*,*N*-dialkyl-L-amino acid esters *via* the formation of non-racemic ammonium enolates

Eiji Tayama,* Tomohito Igarashi, Hajime Iwamoto and Eietsu Hasegawa

Asymmetric α-2-tosylethenylation of **2** with **1** was shown to produce good yields with high enantioselectivities. The reaction proceeds *via* the formation of a non-racemic ammonium enolate without an external source of chirality.



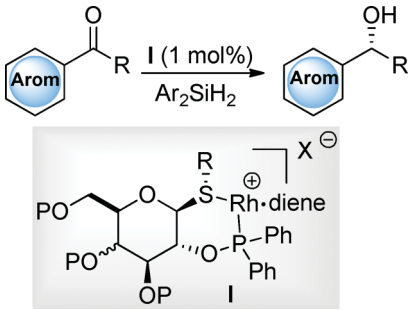
346

Acidic-functionalized ionic liquid as an efficient, green and reusable catalyst for hetero-Michael addition of nitrogen, sulfur and oxygen nucleophiles to *α*,*β*-unsaturated ketones

Feng Han, Lei Yang,* Zhen Li and Chungu Xia*

An efficient, green and reusable acidic-functionalized ionic liquid catalyst was used for hetero-Michael addition to construct C–X bonds.

355

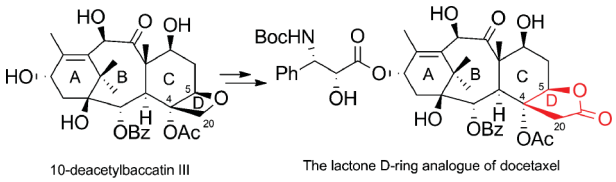


P/S ligands derived from carbohydrates in Rh-catalyzed hydrosilylation of ketones

Noureddine Khiar,* Manuel Pernía Leal, Raquel Navas, Juan Francisco Moya, María Victoria García Pérez and Inmaculada Fernández*

Diastereomerically pure cationic Rh(I)-complexes derived from phosphinite thioglycosides are highly efficient catalysts in the asymmetric hydrosilylation of aromatic prochiral ketones.

361

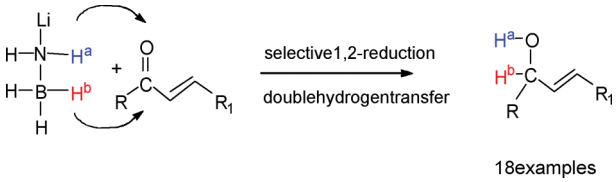


A novel D-ring modified taxoid: synthesis and biological evaluation of a γ-lactone analogue of docetaxel

Feng Gao, Zhan-Kun Yang, Qiao-Hong Chen, Xiao-Guang Chen and Feng-Peng Wang*

The synthesis of a novel D-ring modified docetaxel analogue, in which the oxetane ring is replaced with a γ-lactone, was achieved from 10-deacetylbaccatin III. Key steps of the synthesis include direct acetylation of the secondary hydroxyl group at C-5 and D-ring opening and intramolecular aldol reaction to form the γ-lactone.

367

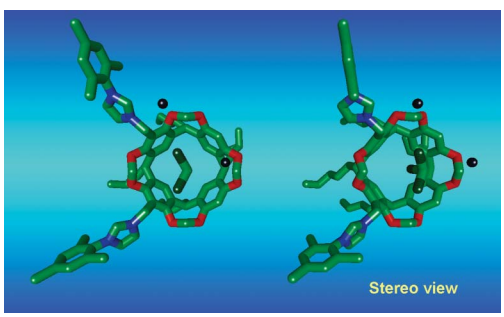


Lithium amidoborane, a highly chemoselective reagent for the reduction of α,β-unsaturated ketones to allylic alcohols

Weiliang Xu, Yonggui Zhou, Ruimin Wang, Guotao Wu and Ping Chen*

LiAB selectively reduces α,β-unsaturated ketones to allylic alcohols *via* a double hydrogen transfer process.

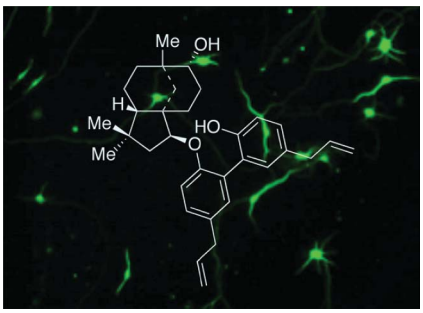
372

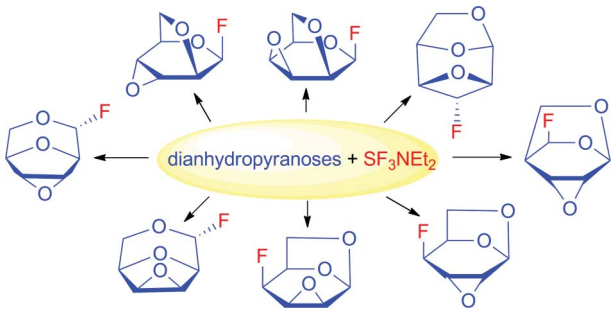


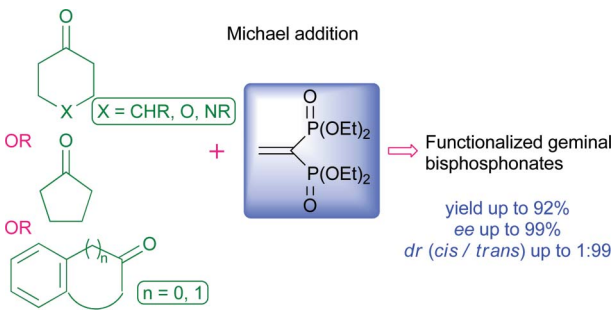
Resorcin[4]arene-derived mono-, bis- and tetra-imidazolium salts as ligand precursors for Suzuki–Miyaura cross-coupling

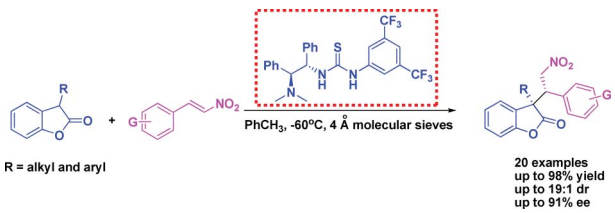
Hani El Moll, David Sémeril,* Dominique Matt,* Loïc Toupet and Jean-Jacques Harrowfield

Resorcinarene-cavitands substituted by imidazolium units were synthesised and used for the first time in Suzuki–Miyaura cross coupling. The highest activities were observed with a resorcinarene having two (1-imidazolylium)-methyl groups grafted on two proximal positions.

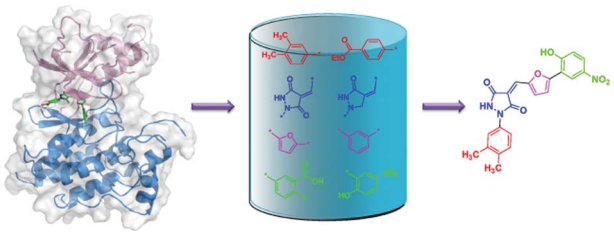








421

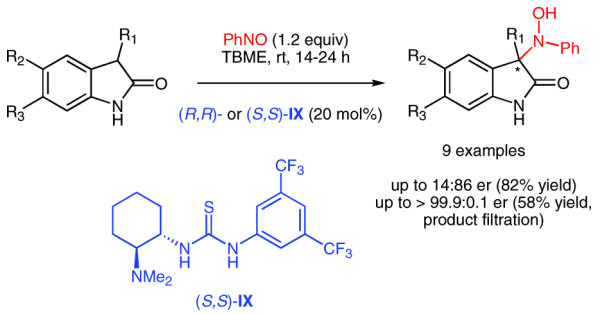


Discovering potent inhibitors against c-Met kinase: molecular design, organic synthesis and bioassay

Zhongjie Liang, Xiao Ding, Jing Ai, Xiangqian Kong, Limin Chen, Liang Chen, Cheng Luo,* Meiyu Geng,* Hong Liu,* Kaixian Chen and Hualiang Jiang

The receptor tyrosine kinase c-Met is an attractive target for therapeutic treatment of cancers.

431

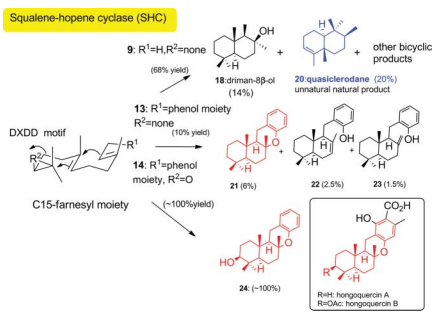


Enantioselective organocatalytic oxyamination of unprotected 3-substituted oxindoles

Xavier Companyó, Guillem Valero, Oriol Pineda, Teresa Calvet, Mercè Font-Bardía, Albert Moyano* and Ramon Rios*

The enantioselective α-oxyamination of 3-substituted oxindoles with nitrosobenzene catalyzed by amine–thiourea bifunctional organocatalysts affords 3-amino-2-oxindole derivatives in good yields and enantioselectivities.

440

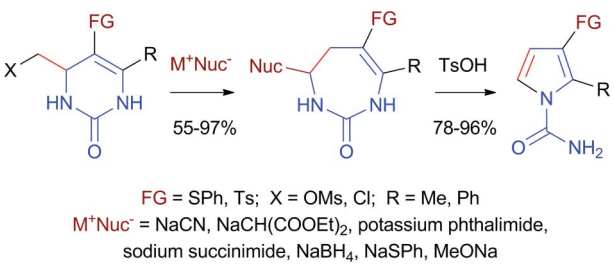


Chemo-enzymatic syntheses of drimane-type sesquiterpenes and the fundamental core of hongoquercin meroterpenoid by recombinant squalene–hopene cyclase

Yukie Yonemura, Takuro Ohyama and Tsutomu Hoshino*

A linear sesquiterpene, (6*E*,10*E*)-2,6,10-trimethyldodeca-2,6,10-triene, underwent cyclization catalyzed by squalene–hopene cyclase, affording six bicyclic sesquiterpenes (drimane skeleton) in relatively high yield (68%).

447



Synthesis of functionalized tetrahydro-1,3-diazepin-2-ones and 1-carbamoyl-1*H*-pyrroles *via* ring expansion and ring expansion/ring contraction of tetrahydropyrimidines

Anastasia A. Fesenko, Ludmila A. Trafimova and Anatoly D. Shutalev*

Nucleophile-promoted ring expansion of 4-mesyloxymethyl- and 4-chloromethyl-1,2,3,4-tetrahydropyrimidin-2-ones gave functionalized 2,3,4,5-tetrahydro-1*H*-1,3-diazepin-2-ones which were converted into 3-substituted 1-carbamoyl-1*H*-pyrroles under acidic conditions.

