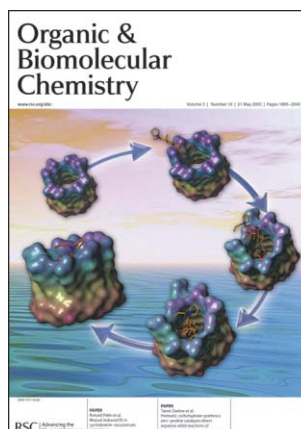
**Cover**

See Kai C. Hultzsch, pp. 1819–1824
The energy profile and transition states of the asymmetric hydroamination/cyclisation of aminopentene are promoted by a chiral catalyst. Promising new catalyst designs have appeared in recent years, which might help to lift the young field of asymmetric hydroamination out of its infancy.

Image reproduced by permission of Kai Carsten Hultzsch from *Org. Biomol. Chem.*, 2005, **3**, 1819.

**Inside Cover**

See Alan Cooper, Margaret Nutley, Elizabeth J. MacLean, Ken Cameron, Lee Fielding, Jordi Mestres and Ronald Palin, pp. 1863–1871
Rocuronium bromide (steroid, orange) enters the cavity of a cyclodextrin; changes in the conformation of both the cyclodextrin and steroid ensure efficient binding. This presents a new horizon in the field of anaesthesia.

Image reproduced by permission of Ronald Palin, Mike Toker and Grant Wishart from *Org. Biomol. Chem.*, 2005, **3**, 1863.

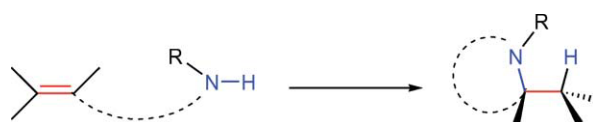
EMERGING AREA

1819

Catalytic asymmetric hydroamination of non-activated olefins

Kai C. Hultzsch*

Asymmetric hydroamination is a highly atom-economical process for the synthesis of chiral amines. In particular, early transition metal catalysts have been successful in reactions involving non-activated olefins.



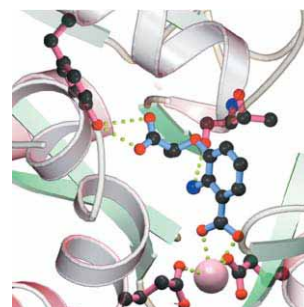
COMMUNICATIONS

1825

**Inhibition studies on salicylate synthase**

Richard J. Payne, Olivier Kerbarh, Ricardo Nunez Miguel, Andrew D. Abell and Chris Abell*

Chorismate and isochorismate analogues were designed and tested as inhibitors of *Yersinia enterocolitica* salicylate synthase.



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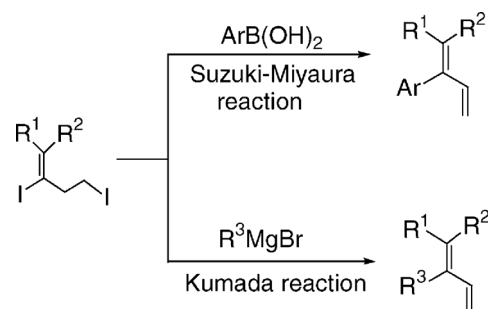
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1828

Facile synthesis of multisubstituted buta-1,3-dienes via Suzuki–Miyaura and Kumada cross-coupling strategy of 2,4-diiodobuta-1-enes with arylboronic acids and Grignard reagents

Li-Xiong Shao and Min Shi*

One-pot Suzuki–Miyaura-type and Kumada-type cross-coupling reactions of 2,4-diiodobuta-1-enes with arylboronic acids and alkyl/aryl magnesium bromides were carried out in the presence of accessibly simple catalysts under mild conditions.

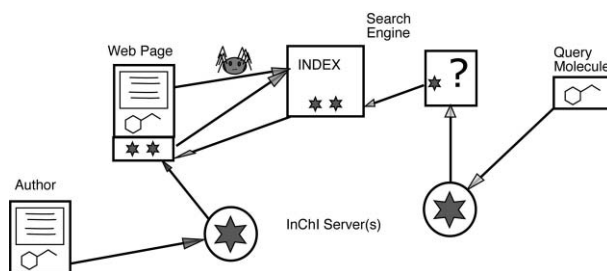


1832

Enhancement of the chemical semantic web through the use of InChI identifiers

Simon J. Coles, Nick E. Day, Peter Murray-Rust, Henry S. Rzepa and Yong Zhang

The International Chemical Identifier (InChI) precisely defines molecular structures for unique indexing by major web search engines.

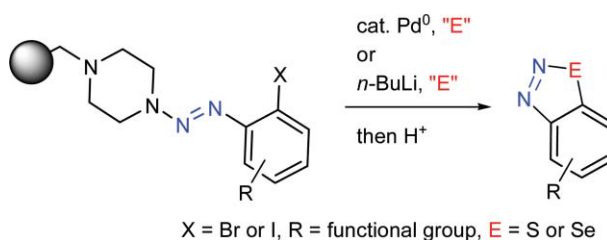


1835

Efficient solid phase synthesis of benzo[1,2,3]thiadiazoles and related structures

Michael Kreis, Carl F. Nising, Maarten Schroen, Kerstin Knepper and Stefan Bräse*

The first solid-phase synthesis of benzo[1,2,3]thiadiazoles was achieved by starting from resin bound *ortho* bromo or iodo triazenes and using a functionalisation on cleavage.



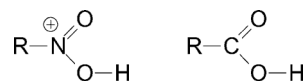
ARTICLES

1838

Protonated nitro group: structure, energy and conjugation

Otto Exner and Stanislav Böhm*

The protonated nitro group is isoelectronic with the carboxyl group but some of its properties differ significantly.

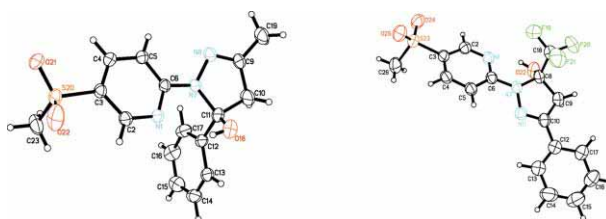


1844

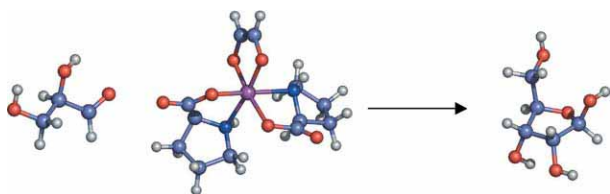
New hydroxy-pyrazoline intermediates, subtle regio-selectivity and relative reaction rate variations observed during acid catalyzed and neutral pyrazole cyclization

Timothy Norris,* Roberto Colon-Cruz and David H. B. Ripin

New hydroxypyrazolines, their formation and dehydration to pyrazoles and observed subtle regio-selectivity effects depending on conditions of formation.



1850

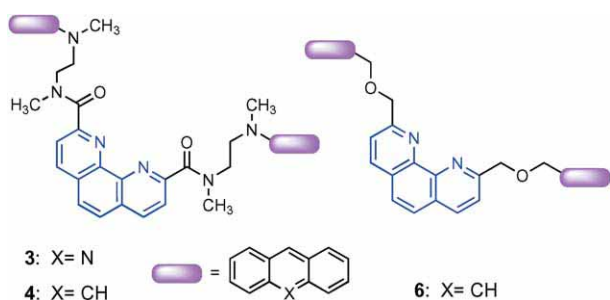


Prebiotic carbohydrate synthesis: zinc–proline catalyzes direct aqueous aldol reactions of α -hydroxy aldehydes and ketones

Jacob Kofoed, Jean-Louis Reymond and Tamis Darbre*

rac-Glyceraldehyde reacts with glycolaldehyde in the presence of zinc–proline to give pentoses. Ribose accounted for 30% of the mixture and was stable under the reaction conditions.

1856

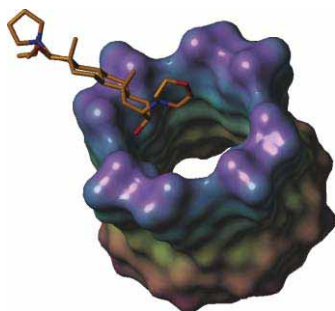


Syntheses and copper(II)-dependent DNA photocleavage by acridine and anthracene 1,10-phenanthroline conjugate systems

Lourdes Gude, María-José Fernández, Kathryn B. Grant* and Antonio Lorente*

1,10-Phenanthroline derivatives containing acridine or anthracene chromophores cleave pUC19 plasmid DNA upon irradiation with ultraviolet light. DNA cleaving activities are modulated by copper(II).

1863

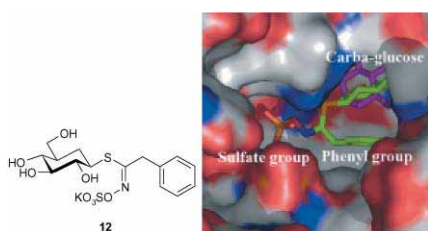


Mutual induced fit in cyclodextrin–rocuronium complexes

Alan Cooper, Margaret Nutley, Elizabeth J. MacLean, Ken Cameron, Lee Fielding, Jordi Mestres and Ronald Palin*

Thermodynamic and structural data together with theoretical calculations characterise and rationalise the nature of the sequential binding process of a modified cyclodextrin and steroid (rocuronium bromide). The recognition and mutual induced fit between cyclodextrin and steroid represents a classic example of dynamic host–guest chemistry.

1872

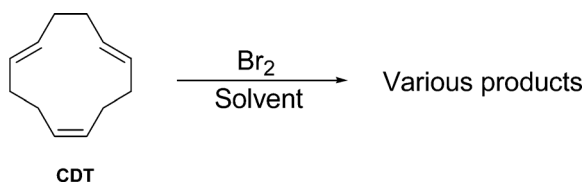


The glucosinolate–myrosinase system. New insights into enzyme–substrate interactions by use of simplified inhibitors

Aurélie Bourderioux, Myriam Lefoix, David Gueyraud, Arnaud Tatibouët,* Sylvain Cottaz, Steffi Arzt, Wim P. Burmeister and Patrick Rollin

Non-hydrolysable myrosinase inhibitors have been devised and studied. Structural tuning of the aglycon part is being used for the development of simplified and more potent inhibitors.

1880



An extensive study of bromination of *cis,trans,trans*-1,5,9-cyclododecatriene: product structures and conformations

Keith Smith,* Chia-Hui Liu, Gamal A. El-Hiti, Gurvinder S. Kang, Elfyn Jones, Simon G. Clement, Alex D. Checquer, Oliver W. Howarth, Michael B. Hursthouse and Simon J. Coles

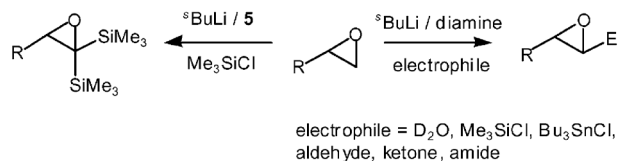
Various products of reaction of CDT with bromine have been characterised by their NMR spectra and X-ray crystallography; in some cases solution conformations were also established.

1893

Deprotonation–electrophile trapping of terminal epoxides

David M. Hodgson,* Eirene H. M. Kirton, Steven M. Miles, Stéphanie L. M. Norsikian, Nigel J. Reynolds and Steven J. Coote

Deprotonation of terminal epoxides in the presence of diamine ligands allows trapping with a range of electrophiles, yielding functionalised epoxides in good yields with control of stereochemistry at the epoxide.

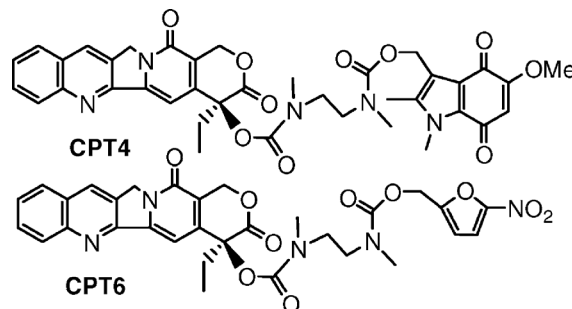


1905

Bioreduction activated prodrugs of camptothecin: molecular design, synthesis, activation mechanism and hypoxia selective cytotoxicity

Zhouen Zhang, Kazuhito Tanabe, Hiroshi Hatta and Sei-ichi Nishimoto*

Novel camptothecin prodrugs were synthesized to investigate the bioreductive activation mechanism and the hypoxia selective cytotoxicity.

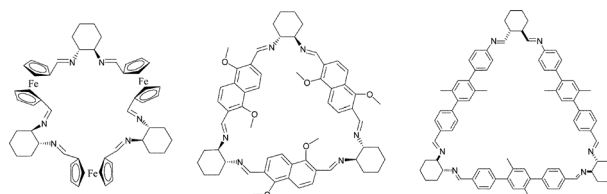


1911

Tuning the size of macrocyclic cavities in trianglimine macrocycles

Nikolai Kuhnert,* Nicolai Burzlaff, Chirag Patel and Ana Lopez-Periago

By choosing aromatic dialdehydes of different sizes it is possible to have full control over the overall size of the central hole of trianglimine macrocycles.

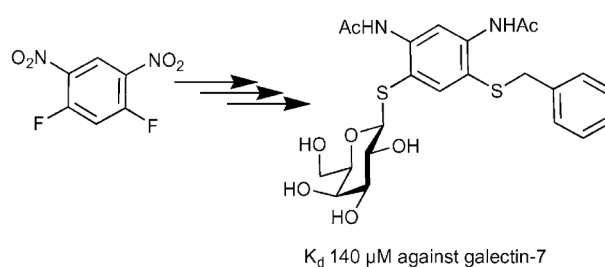


1922

Synthesis of a phenyl thio-β-D-galactopyranoside library from 1,5-difluoro-2,4-dinitrobenzene: discovery of efficient and selective monosaccharide inhibitors of galectin-7

Ian Cumpstey, Susanne Carlsson, Hakon Leffler and Ulf J. Nilsson*

Reaction of 1,5-difluoro-2,4-dinitrobenzene with 1-thio-β-D-galactose provides substituted phenyl 1-thio-β-D-galactopyranosides as potent galectin inhibitors.

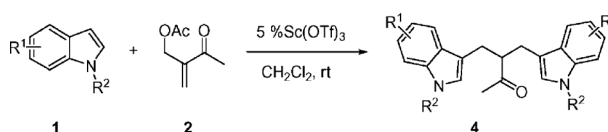


1933

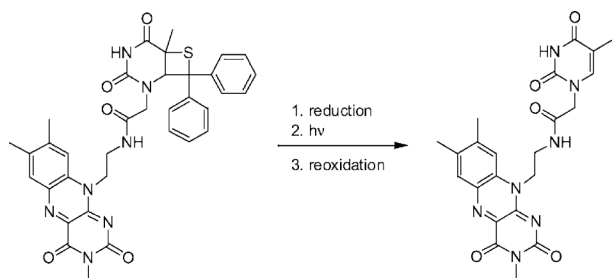
Sc(OTf)₃-catalyzed efficient synthesis of β,β-bis(indolyl) ketones by the double indoloylation of acetic acid 2-methylene-3-oxobutyl ester

Shengming Ma,* Shichao Yu and Zhihua Peng

The double indoloylation of acetic acid 2-methylene-3-oxo-butyl ester with differently substituted indoles to afford β,β-bis(indolyl) ketones is reported.



1937

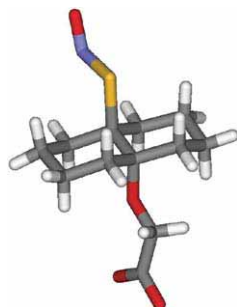


Model compounds for (6–4) photolyases: a comparative flavin induced cleavage study of oxetanes and thietanes

Marcus G. Friedel, Michaela K. Cichon and Thomas Carell*

A flavin–thietane model compound was prepared in order to analyze a reductive cycloreversion process employed by the DNA repair enzyme (6–4) photolyase.

1942

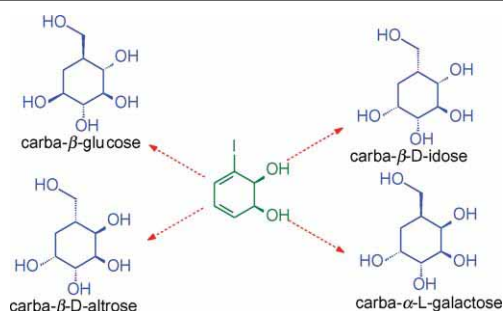


The synthesis of water soluble decalin-based thiols and S-nitrosothiols—model systems for studying the reactions of nitric oxide with protein thiols

Alan C. Spivey,* Jacqueline Colley, Lindsey Sprigens, Susan M. Hancock, D. Stuart Cameron, Kordi I. Chigboh, Gemma Veitch, Christopher S. Frampton and Harry Adams

The synthesis of novel aqueous soluble decalin-based thiols for the study of nitric oxide–thiol interactions and X-ray structures of S-nitroso thiol derivatives are described.

1953

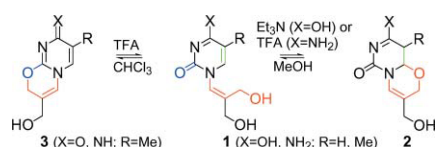


Chemoenzymatic synthesis of carbasugars from iodobenzene

Derek R. Boyd,* Narain D. Sharma, Nuria M. Llamas, John F. Malone, Colin R. O'Dowd and Christopher. C. R. Allen

The four pyranose carbasugars, carba-β-D-altrose, carba-α-L-galactose, carba-β-D-idose, and carba-β-L-glucose were obtained from the *cis*-dihydrodiol metabolite of iodobenzene *via* chemoenzymatic synthesis.

1964

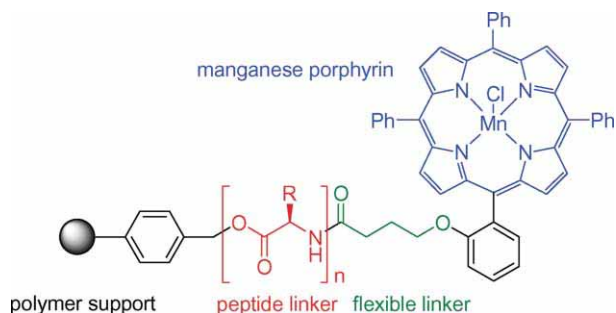


Cyclization reactions of 1-[3'-hydroxy-2'-(hydroxymethyl)-prop-1'-enyl]pyrimidine nucleobases: intramolecular Michael additions to the C(5)=C(6) bonds and intramolecular dehydrations

Otto Dahl, Jacob Jensen, Michael Åxman Petersen and Ulla Henriksen*

The nucleoside analogues **1** undergo Michael addition when treated with TFA or/and Et₃N in MeOH, but form anhydro compounds (**3**) with TFA under anhydrous conditions.

1971



Polymer-supported manganese porphyrin catalysts—peptide-linker promoted chemoselectivity

Emilie Brulé, King Kuok (Mimi) Hii and Yolanda R. de Miguel*

A novel polymer-supported manganese porphyrin catalyst with a histidine-containing peptide linker displays good chemoselectivity in the epoxidation of limonene.

1977

Absolute configuration and predominant conformations of 1,1-dimethyl-2-phenylethyl phenyl sulfoxide

Ana G. Petrovic, Jiangtao He, Prasad L. Polavarapu,*
Ling S. Xiao and Daniel W. Armstrong

The absolute configuration of 1,1-dimethyl-2-phenylethyl phenyl sulfoxide was determined from a comparison of predicted and observed VCD, OR, and ECD.

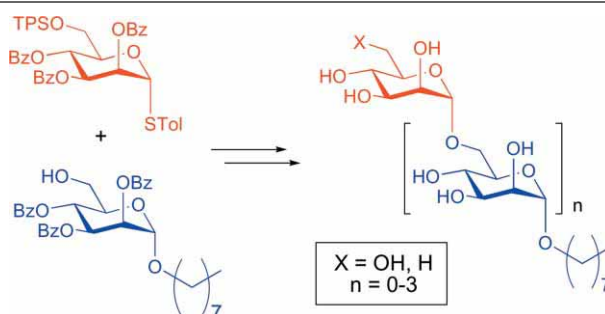


1982

Rapid, iterative assembly of octyl α -1,6-oligomannosides and their 6-deoxy equivalents

Jacinta A. Watt and Spencer J. Williams*

A simple iterative route to hydrophobic α -1,6-linked oligomannosides and their 6-deoxy congeners from a single glycosyl donor and acceptor alcohol is described.

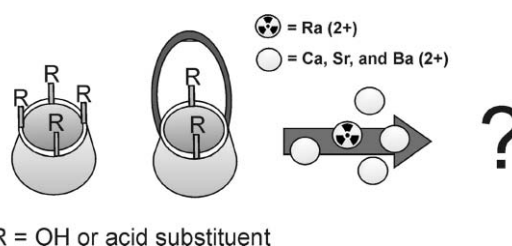


1993

Thiacalix[4]arene derivatives as radium ionophores: a study on the requirements for Ra^{2+} extraction

Fijs W. B. van Leeuwen, Hans Beijleveld, Aldrik H. Velders,
Jurriaan Huskens, Willem Verboom* and
David N. Reinhoudt*

A systematic study on selective Ra^{2+} extractants, based on synergistic, anionic, and ionizable crown ether derivatives as extractants, is reported.

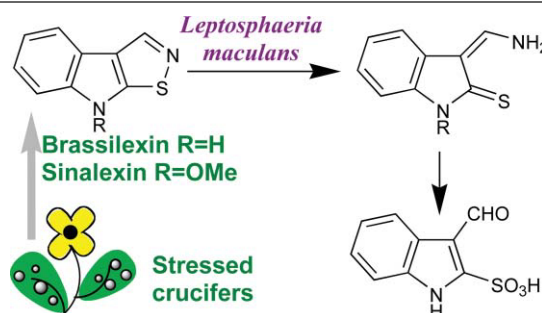


2002

Detoxification pathways of the phytoalexins brassilexin and sinalexin in *Leptosphaeria maculans*: isolation and synthesis of the elusive intermediate 3-formylindolyl-2-sulfonic acid

M. Soledade C. Pedras* and Mojmir Suchy

Detoxification of the potent antifungal phytoalexins brassilexin and sinalexin involves reductive bioconversion to the corresponding 3-aminomethyleneindole-2-thiones. Brassilexin is ultimately transformed to the new metabolite 3-formylindolyl-2-sulfonic acid.

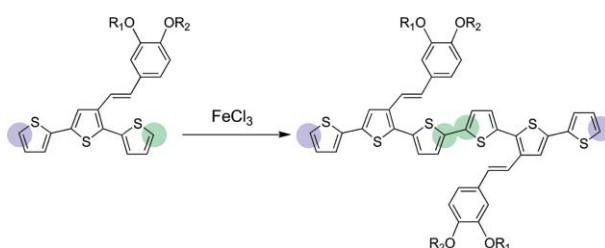


2008

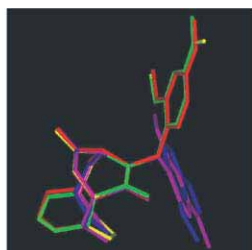
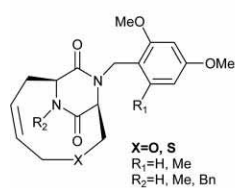
Towards functionalized poly(terthiophenes): regioselective synthesis of oligoether-substituted bis(styryl)sexithiophenes

Daina K. Grant,* Kenneth W. Jolley, David L. Officer,
Keith C. Gordon and Tracey M. Clarke

Chemical oxidation of ether-substituted styrylterthiophenes affords a single step preparation of a variety of new regioisomerically pure bis(oligo(oxyethylene)styryl)sexithiophenes.



2016

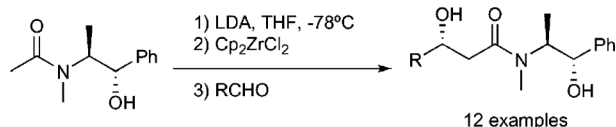
X=O
R₁, R₂=H

Design and synthesis of new bicyclic diketopiperazines as scaffolds for receptor probes of structurally diverse functionality

Pedro Besada, Liaman Mamedova, Craig J. Thomas, Stefano Costanzi and Kenneth A. Jacobson*

A new bicyclic scaffold that combines a diketopiperazine (DKP) bridged with a 10-membered ring has been synthesized and found to provide inhibitors of P2Y receptor signalling.

2026

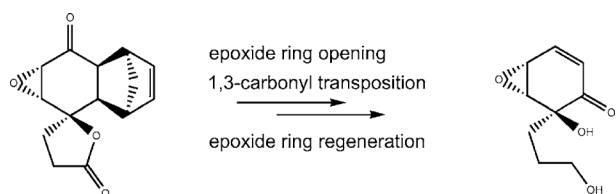


(*S,S*)-(+)-Pseudoephedrine as chiral auxiliary in asymmetric acetate aldol reactions

Mónica Rodríguez, Jose L. Vicario, Dolores Badía* and Luisa Carrillo

The ability of the aminoalcohol (*S,S*)-(+)-pseudoephedrine as chiral auxiliary in asymmetric acetate aldol reactions has been evaluated.

2031



Synthesis of a 4,5-epoxy-2-cyclohexen-1-one derivative via epoxide ring opening, 1,3-carbonyl transposition and epoxide ring regeneration: a synthetic study on a scyphostatin analogue

Ryukichi Takagi, Kengo Tojo, Masato Iwata and Katsuo Ohkata*

A 6-alkyl-4,5-epoxy-6-hydroxy-2-cyclohexen-1-one derivative was synthesized from the Diels–Alder adduct via epoxide ring opening, 1,3-carbonyl transposition and epoxide ring regeneration.

ADDITIONS AND CORRECTIONS

2037

Peter Murray-Rust, Henry S. Rzepa, Simon M. Tyrrell and Yong Zhang

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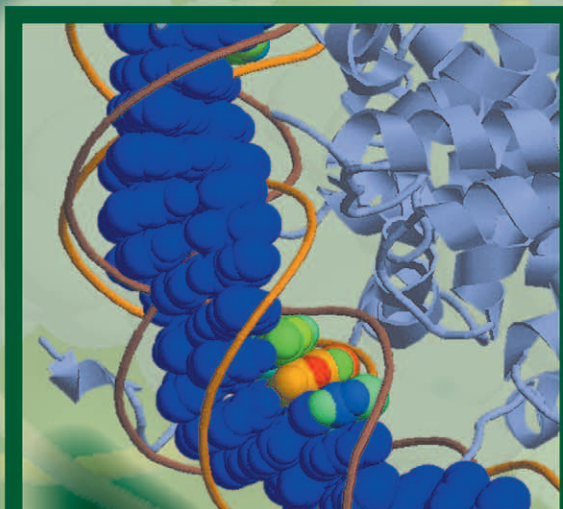
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