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Organic & Biomolecular Chemistry

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Incorporating Acta Chemica Scandinavica

Cover

See Ernesto Quesada, Martin Stockley, Jacques P. Ragot, Michael E. Prime, Adrian C. Whitwood and Richard J. K. Taylor, pp. 2483–2495.

The cover picture depicts the coprophilous fungi *Psilocybe sp.* growing over a dung substrate (picture courtesy of the Australian National Botanic Garden Website http://www.anbg.gov.au/fungi). The lithiated key intermediate for the syntheses of the bioactive fungal metabolites preussomerins F, K and L are superimposed.

Image reproduced by permission of Heino Lepp.
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contents

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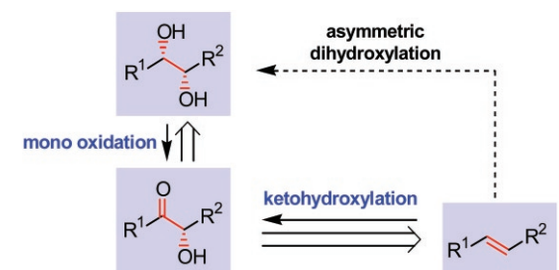
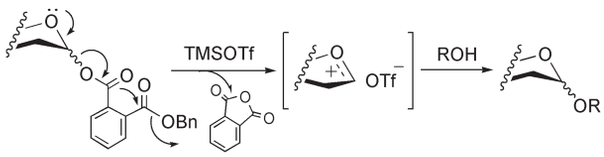


The RuO_4-catalysed dihydroxylation, ketohydroxylation and mono oxidation—novel oxidation reactions for the synthesis of diols and α-hydroxy ketones

Bernd Plietker and Meike Niggemann

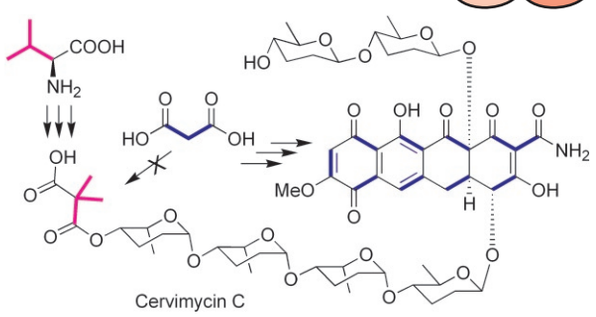
RuO_4 acts a versatile catalyst in novel oxidations of alkenes leading to unsymmetrical α-hydroxy ketones in high regio- and stereoselectivity.



Glycosylation with glycosyl benzyl phthalates as a new type of glycosyl donor

Kwan Soo Kim, Yong Joo Lee, Hye Young Kim, Sung Soo Kang and Soon Young Kwon

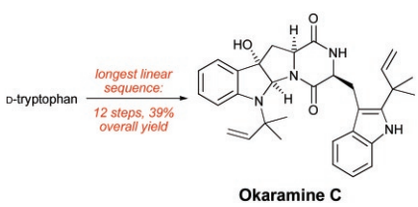
Glycosyl benzyl phthalates, which were readily prepared from 1-hydroxy sugars, have been found to be efficient glycosyl donors in their glycosylations with various glycosyl acceptors using TMSOTf as a promoter.



Biosynthesis of cervimycin C, an aromatic polyketide antibiotic bearing an unusual dimethylmalonyl moiety

Kerstin Herold, Zhongli Xu, Friedrich A. Gollmick, Udo Gräfe and Christian Hertweck

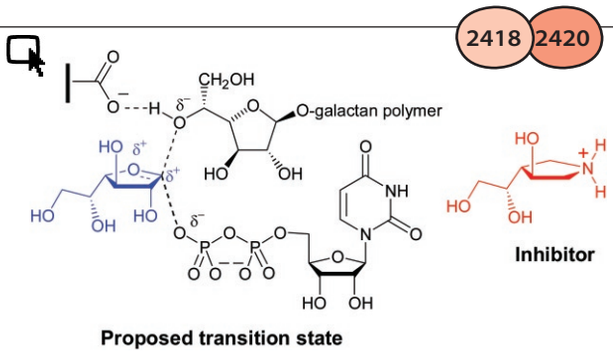
The rare dimethylmalonyl moiety of the antibiotic cervimycin is not derived from malonate, as the polyketide aglycon, but from valine.



A concise total synthesis of (+)-okaramine C

Peter R. Hewitt, Ed Cleator and Steven V. Ley

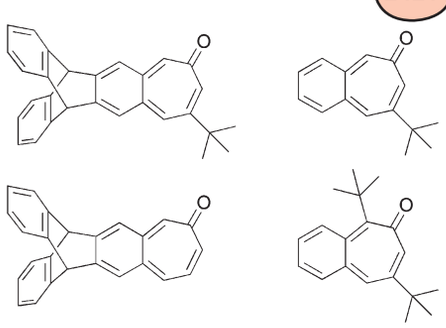
A short total synthesis of the insecticidal natural product okaramine C is described, demonstrating our selenocyclisation-oxidative deselenation sequence.



Synthesis and biological evaluation of new inhibitors of UDP-Gal*f* transferase—a key enzyme in *M. tuberculosis* cell wall biosynthesis

Sylvaine Cren, Sudagar S. Gurcha, Alexander J. Blake, Gurdyal S. Besra and Neil R. Thomas

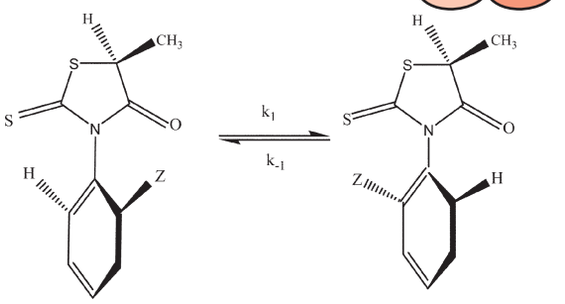
Two 1-*N*-iminosugars have been designed, synthesized and evaluated as inhibitors of UDP-D-Gal*p* mutase and UDP-α-D-Gal*f* transferase, essential enzymes involved in *Mycobacterial* cell wall biosynthesis.



Kinetic stabilization of the *o*-quinoidal 3,4-benzotropone system

Masakazu Ohkita, Kieko Sano, Katsuhiko Ono, Katsuhiro Saito, Takanori Suzuki and Takashi Tsuji

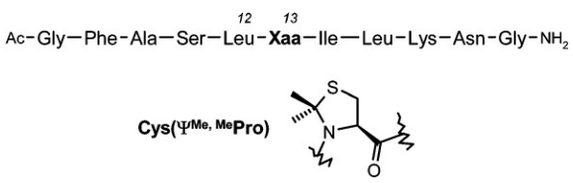
Kinetic stabilization of the *o*-quinoidal 3,4-benzotropone system was investigated by introducing a triptycene unit and/or *tert*-butyl group(s).



Barriers to internal rotation around the C–N bond in 3-(*o*-aryl)-5-methyl-rhodanines using NMR spectroscopy and computational studies. Electron density topological analysis of the transition states

Yeliz Aydeniz, Funda Oğuz, Arzu Yaman, Aylin Sungur Konuklar, Ilknur Doğan, Viktorya Aviyente and Roger A. Klein

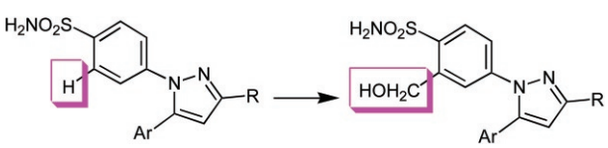
The height of the barriers to rotation for 3-(*o*-aryl)-5-methyl-rhodanines, Z = H, F, Cl, Br, OH and CH_3, using B3LYP/6-31G* are in remarkably good agreement with those obtained experimentally using NMR, supporting the use of DFT methods for problems of this type.



A case study of 2,2-dimethylthiazolidine as locked *cis* proline amide bond: synthesis, NMR and molecular modeling studies of a δ-conotoxin EVIA peptide analog

Sabine Chierici, Muriel Jourdan, Mélanie Figuet and Pascal Dumy

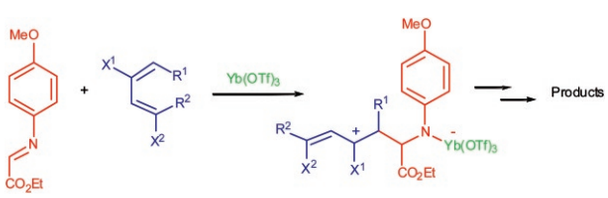
Synthesis and structural studies of a Cys($\Psi^{Me,Me}$Pro)-containing analog of the δ-conotoxin EVIA loop 2 to target the presumed bioactive *cis* conformation.



2-Hydroxymethyl-4-[5-(4-methoxyphenyl)-3-trifluoro-methyl-1*H*-1-pyrazolyl]-1-benzenesulfonamide (DRF-4367): an orally active COX-2 inhibitor identified through pharmacophoric modulation

Sunil Kumar Singh, Saibaba Vobbalareddy, Srinivasa Rao Kalleda, Shaikh Abdul Rajjak, Seshagiri Rao Casturi, Srinivasa Raju Datla, Rao N. V. S. Mamidi, Ramesh Mullangi, Ravikanth Bhamidipati, Rajagopalan Ramanujam, Venkateswarlu Akella and Koteswar Rao Yeleswarapu

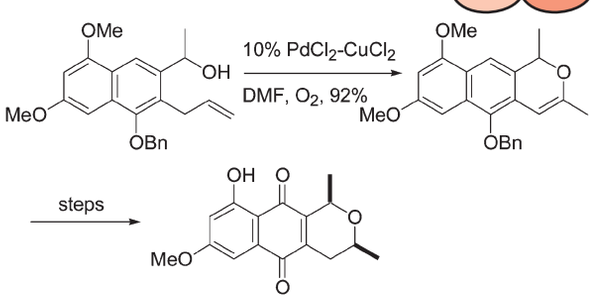
Pharmacophoric modulation of celecoxib afforded an orally effective COX-2 inhibitor for the treatment of inflammatory disorders.



Mechanistic studies on the formal aza-Diels–Alder reactions of *N*-aryl imines: evidence for the non-concertedness under Lewis-acid catalysed conditions

Stephen Hermitage, Judith A. K. Howard, David Jay, Robin G. Pritchard, Michael R. Probert and Andrew Whiting

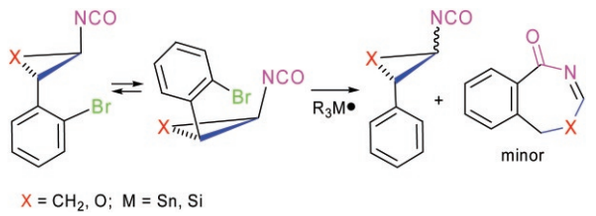
Lewis-acid catalysed reaction of various dienes with a *para*-methoxyaniline, ethyl glyoxalate-derived imine with different dienes produces products which can all be explained by a common step-wise reaction mechanism, rather than alternative concerted cycloadditions.



The synthesis of ventiloquinone L, the monomer of cardinalin 3

Edwin M. Mmutlane, Joseph P. Michael, Ivan R. Green and Charles B. de Koning

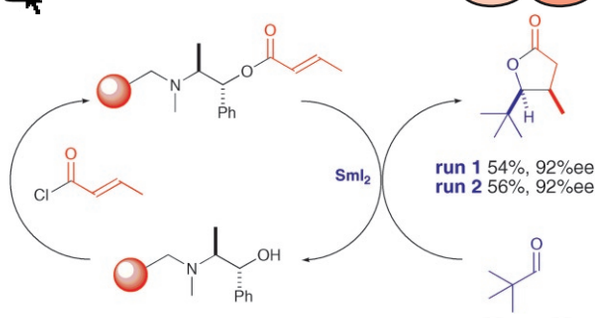
The synthesis of ventiloquinone L is described.



An exploratory study of ring closures of aryl radicals onto cyclopropyl- and oxiranyl-isocyanate acceptors

Patricia L. Minin and John C. Walton

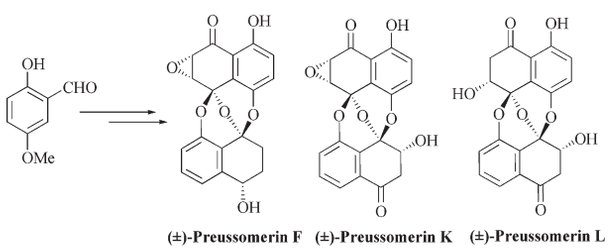
trans- and *cis*-1-bromo-(2-isocyanatocyclopropyl)benzen es interconvert, as do *trans*- and *cis*-(2-bromophenyl)-3-isocyanatooxiranes: ring closures of the corresponding radicals are minor compared to reduction.



Development of a solid-phase 'asymmetric resin-capture–release' process: application of an ephedrine chiral resin in an approach to γ-butyrolactones

Nessan J. Kerrigan, Panee C. Hutchison, Tom D. Heightman and David J. Procter

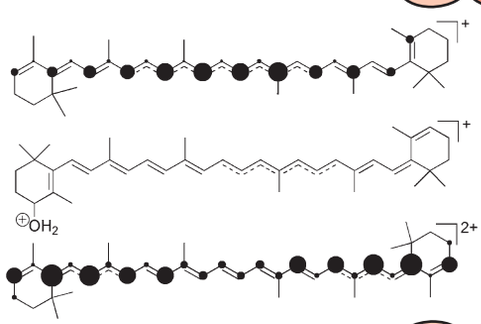
An 'asymmetric resin-capture–release' strategy has been evaluated as a tool for high throughput synthesis. An asymmetric Sm(II)-mediated approach to γ-butyrolactones employing an ephedrine chiral resin was selected to illustrate the concept. Lactones are obtained in moderate to good isolated yields with selectivities up to 96% ee.



A versatile, non-biomimetic route to the preussomerins: syntheses of (±)-preussomerins F, K and L

Ernesto Quesada, Martin Stockley, Jacques P. Ragot, Michael E. Prime, Adrian C. Whitwood and Richard J. K. Taylor

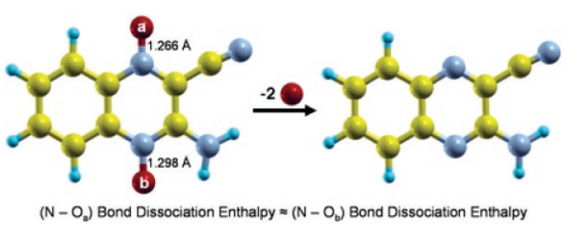
Concise total syntheses of the *title* fungal metabolites preussomerins F, K and L are described following a versatile, unified, non-biomimetic approach based on the functionalisation of 2-arylacetal anions.



Nucleophilic reactions of charge delocalised carotenoid mono- and dications

Geir Kildahl-Andersen, Liv Bruås, Bjart Frode Lutnaes and Synnøve Liaaen-Jensen

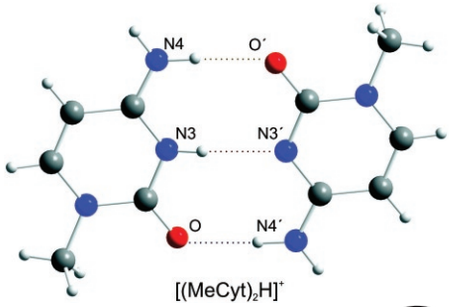
Reactions with O, N and S nucleophiles gave in total 28, including 18 new, extensively *E*/*Z* isomerised neutral carotenoid products.



Thermochemistry of 2-amino-3-quinoxalinecarbonitrile-1,4-dioxide. Evaluation of the mean dissociation enthalpy of the (N–O) bond

Maria D. M. C. Ribeiro da Silva, José R. B. Gomes, Jorge M. Gonçalves, Emanuel A. Sousa, Siddharth Pandey and William E. Acree, Jr.

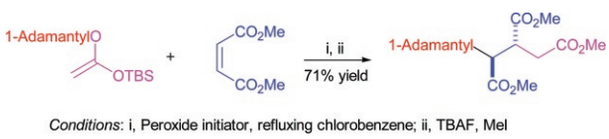
Experimental and computational studies on this Tirapazamine structurally related compound allowed determination of the 1st, 2nd and mean N–O bond dissociation enthalpies. Hydrogen bonding, N–O_b···H–NH, explains the similar enthalpy values to remove the oxygens.



Synthesis of [(MeCyt)$_2$H]I—structure and stability of a dimeric threefold hydrogen-bonded 1-methylcytosinium 1-methylcytosine cation

Thomas Krüger, Clemens Bruhn and Dirk Steinborn

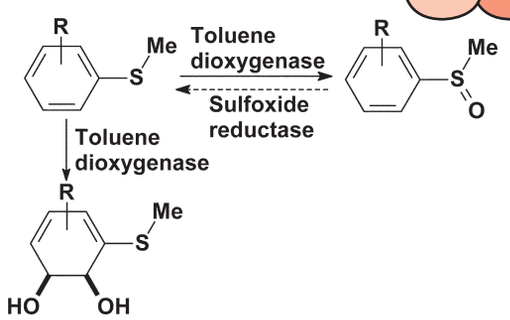
The threefold hydrogen bond in the cation [(MeCyt)$_2$H]$^+$ was shown to be much stronger than that in the triply hydrogen-bonded Watson–Crick Cyt-Gua dimer (−42.4 *vs.* −24.2 kcal mol^{-1}).



Carbon–carbon bond formation by radical addition–fragmentation reactions of *O*-alkylated enols

Yudong Cai, Brian P. Roberts, Derek A. Tocher and Sarah A. Barnett

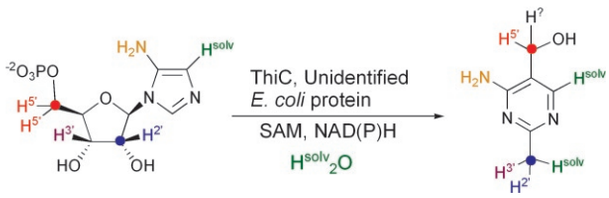
Electron-rich alkenes of the type H$_2$C=C(OR)Ph and H$_2$C=C(OR)OSiBu^{t}Me$_2$, in which R is a secondary or tertiary alkyl group, undergo C–C bond-forming radical-chain reactions with organic halides and with electron-poor alkenes.



Dioxygenase-catalysed oxidation of alkylaryl sulfides: sulfoxidation *versus cis*-dihydrodiol formation

Derek R. Boyd, Narain D. Sharma, Breige E. Byrne, Simon A. Haughey, Martina A. Kennedy and Christopher C. R. Allen

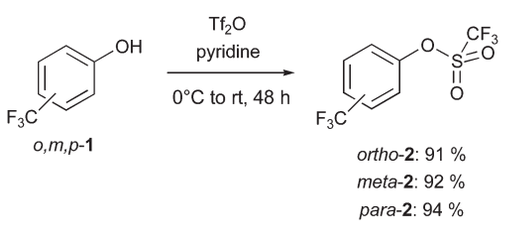
Factors that determine whether dioxygenase-catalysed sulfoxidation or *cis*-dihydroxylation of substituted phenylmethylsulfides occurs are discussed.



Biosynthesis of the thiamin pyrimidine: the reconstitution of a remarkable rearrangement reaction

Brian G. Lawhorn, Ryan A. Mehl and Tadhg P. Begley

Biosynthesis of the thiamin pyrimidine has been reconstituted in a cell-free system, and a comprehensive set of labeling studies that reveal a complex rearrangement reaction are described.



On the preparation of *ortho*-trifluoromethyl phenyl triflate

Duncan Gill, Alison J. Hester and Guy C. Lloyd-Jones

Use of a pyridine as a nucleophilic catalyst allows the ready preparation of trifluoromethyl phenyl triflates by reaction of the corresponding phenols with triflic anhydride.

ADDITIONS AND CORRECTIONS

2549

Martin Ohsten Rasmussen, Bridget Hogg, Jean-Jacques Bono, Eric Samain and Hugues Driguez

New access to lipo-chitooligosaccharide nodulation factors

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