

Biocatalysts in synthetic organic chemistry

Guest editor: S. M. Roberts

*Department of Chemistry, University of Liverpool, The Robert Robinson Laboratories,
Liverpool L69 7ZD, UK*

Contents

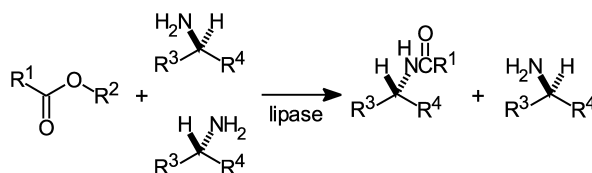
Announcement: Tetrahedron Symposia-in-Print
Preface

p 495
p 499

REPORT

Enantioselective acylation of chiral amines catalysed by serine hydrolases
Fred van Rantwijk* and Roger A. Sheldon

pp 501–519

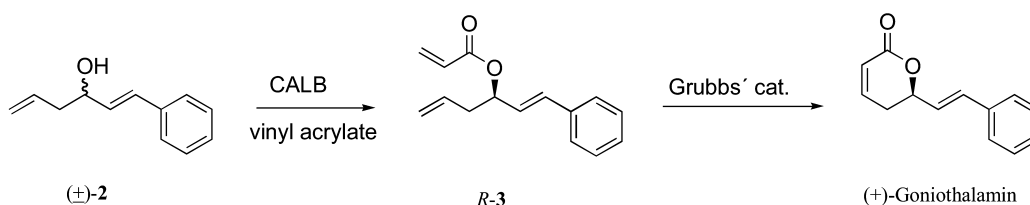


ARTICLES

Synthesis of (+)-goniothalamine and its enantiomer by combination of lipase catalyzed resolution and alkene metathesis

pp 521–524

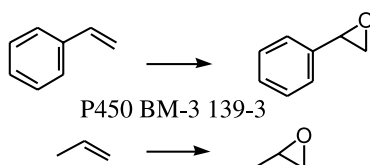
Eirik Sundby, Lars Perk, Thorleif Anthonsen,* Arne Jørgen Aasen and Trond Vidar Hansen*



Alkene epoxidation catalyzed by cytochrome P450 BM-3 139-3

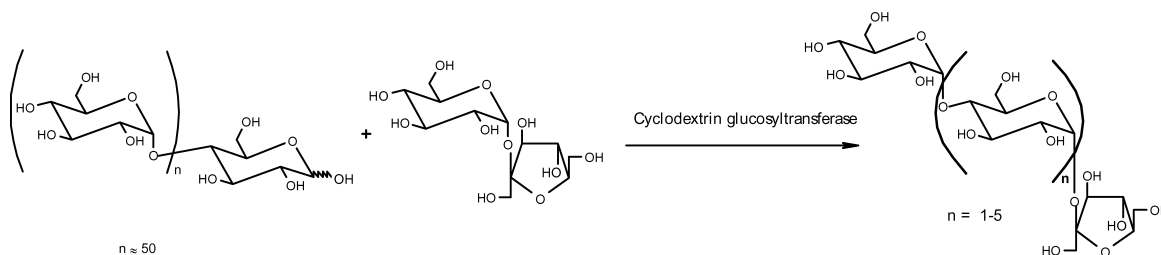
pp 525–528

Edgardo T. Farinas, Miguel Alcalde and Frances Arnold*

**Synthesis of maltooligosyl fructofuranosides catalyzed by immobilized cyclodextrin glucosyltransferase using starch as donor**

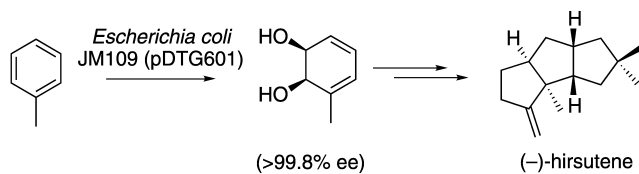
pp 529–534

M. Teresa Martín, M. Angeles Cruces, Miguel Alcalde, Francisco J. Plou, Manuel Bernabé and Antonio Ballesteros*

**A chemoenzymatic synthesis of the linear triquinane (–)-hirsutene and identification of possible precursors to the naturally occurring (+)-enantiomer**

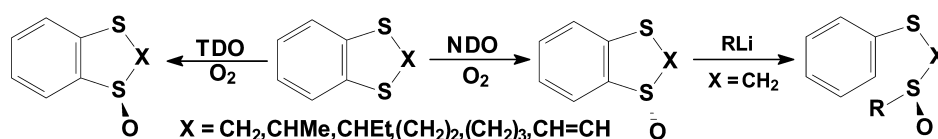
pp 535–547

Martin G. Banwell,* Alison J. Edwards, Gwion J. Harfoot and Katrina A. Jolliffe

**Dioxygenase-catalysed sulfoxidation of bicyclic alkylaryl sulfides and chemoenzymatic synthesis of acyclic disulfoxides**

pp 549–559

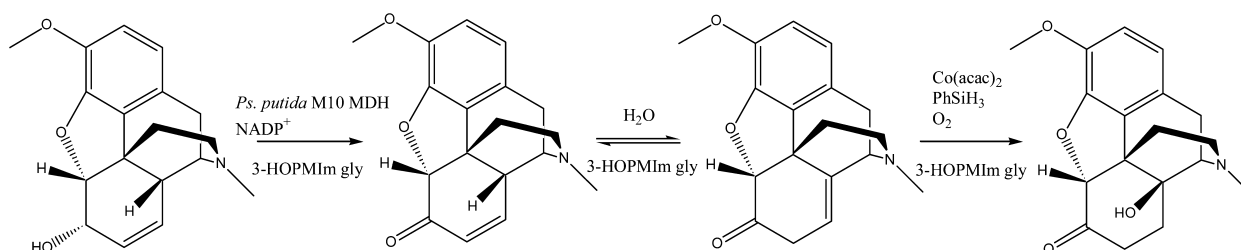
Derek R. Boyd,* Narain D. Sharma, Simon A. Haughey, Martina A. Kennedy, John F. Malone, Steven D. Shepherd, Christopher C. R. Allen and Howard Dalton



Combined biological and chemical catalysis in the preparation of oxycodone

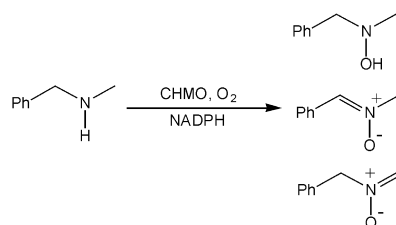
pp 561–568

Adam J. Walker and Neil C. Bruce*

**Oxidation of secondary amines by molecular oxygen and cyclohexanone monooxygenase**

pp 569–575

Stefano Colonna,* Vincenza Pironti, Giacomo Carrea, Piero Pasta and Francesca Zambianchi

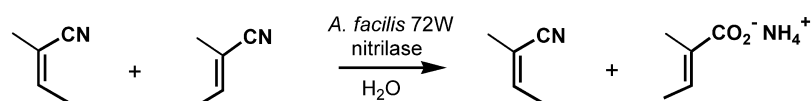


The formation of *N*-oxides, hydroxylamines and nitrones via enzymatic oxidation with cyclohexanone monooxygenase is described.

Regioselective biocatalytic hydrolysis of (*E,Z*)-2-methyl-2-butenitrile for production of (*E*)-2-methyl-2-butenoic acid

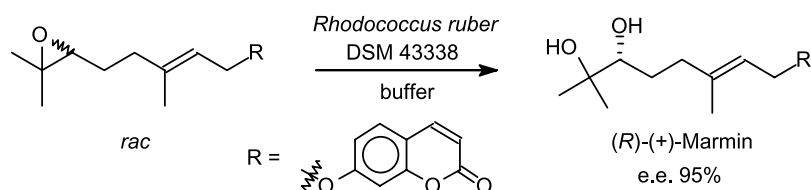
pp 577–581

Eugenia C. Hann, Amy E. Sigmund, Susan K. Fager, Frederick B. Cooling, John E. Gavagan, Michael G. Bramucci, Sarita Chauhan, Mark S. Payne and Robert DiCosimo*

**Chemo-enzymatic enantio-convergent asymmetric synthesis of (*R*)-(+)-Marmin**

pp 583–588

Klaus Edegger, Sandra F. Mayer, Andreas Steinreiber and Kurt Faber*

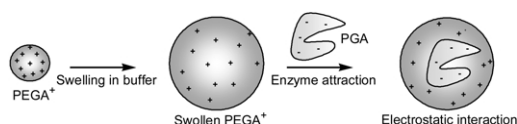


(*R*)-(+)-Marmin was obtained by asymmetric enantioconvergent biohydrolysis of the corresponding oxirane in 95% ee.

Introduction of permanently charged groups into PEGA resins leads to improved biotransformations on solid support

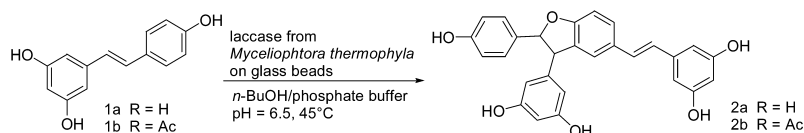
pp 589–594

Alessandra Basso, Rein V. Ulijn, Sabine L. Flitsch,* Graham Margetts, Ian Brazendale, Cynthia Ebert, Luigi De Martin, Paolo Linda, Silvia Verdelli and Lucia Gardossi


Biotransformation of resveratrol: synthesis of *trans*-dehydrodimers catalyzed by laccases from *Myceliophthora thermophyla* and from *Trametes pubescens*

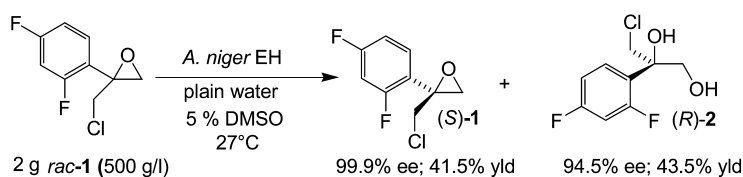
pp 595–600

Silvia Nicotra, Maria Rita Cramarossa, Adele Mucci, Ugo Maria Pagnoni, Sergio Riva and Luca Forti*

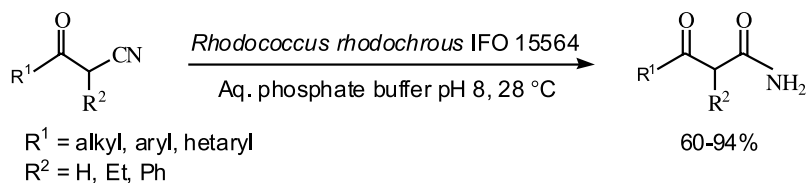

Enzymatic transformations. Part 55: Highly productive epoxide hydrolase catalysed resolution of an azole antifungal key synthon

pp 601–605

Nicolas Monfort, Alain Archelas and Roland Furstoss*


Preparation of N-unsubstituted β -ketoamides by *Rhodococcus rhodochrous*-catalysed hydration of β -ketonitriles

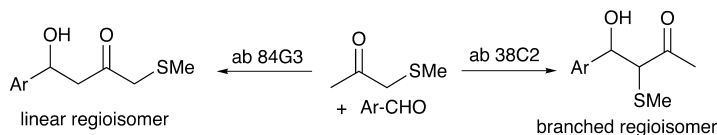
pp 607–618

 Vicente Gotor,* Ramón Liz and Ana M^e Testera


Unusual reversal of regioselectivity in antibody-mediated aldol additions with unsymmetrical methyl ketones

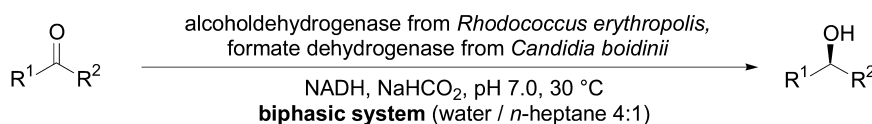
pp 619–632

V. Maggiotti, S. Bahmanyar, M. Reiter, M. Resmini, K. N. Houk and V. Gouverneur*

**Preparative asymmetric reduction of ketones in a biphasic medium with an (*S*)-alcohol dehydrogenase under in situ-cofactor-recycling with a formate dehydrogenase**

pp 633–640

Harald Gröger,* Werner Hummel,* Claudia Rollmann, Françoise Chamouleau, Hendrik Hüsken, Helge Werner, Christine Wunderlich, Kofi Abokitse, Karlheinz Drauz and Stefan Buchholz

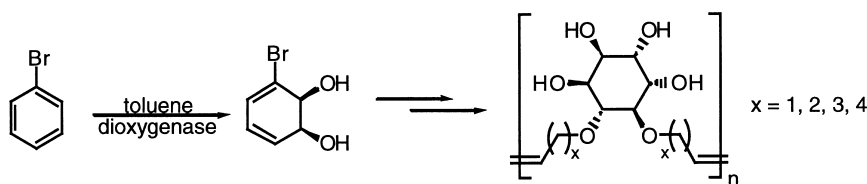


An enzyme-compatible biphasic reaction media for the asymmetric reduction of ketones with in situ-cofactor regeneration has been developed. As enzymes, a novel recombinant (*S*)-alcohol dehydrogenase from *Rhodococcus erythropolis* and a formate dehydrogenase were used.

Synthesis of chiral ADMET polymers containing repeating *D*-chiro-inositol units derived from a biocatalytically prepared diene diol

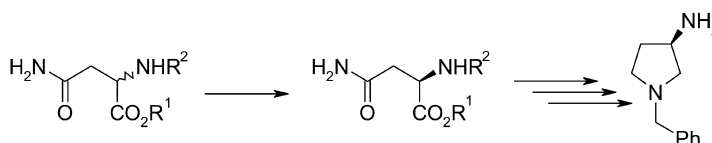
pp 641–646

Vu P. Bui and Tomas Hudlicky*

**Chemo-enzymatic preparation of chiral 3-aminopyrrolidine derivatives**

pp 647–653

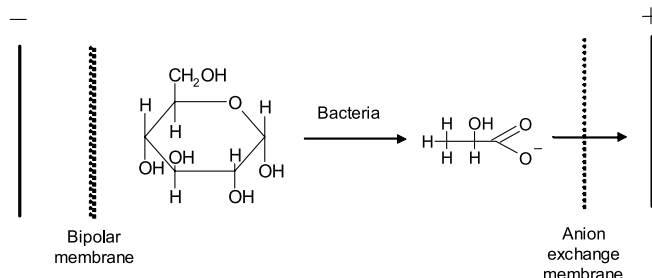
Hans Iding,* Beat Wirz and Mark Rogers-Evans



An electrokinetic bioreactor: using direct electric current for enhanced lactic acid fermentation and product recovery

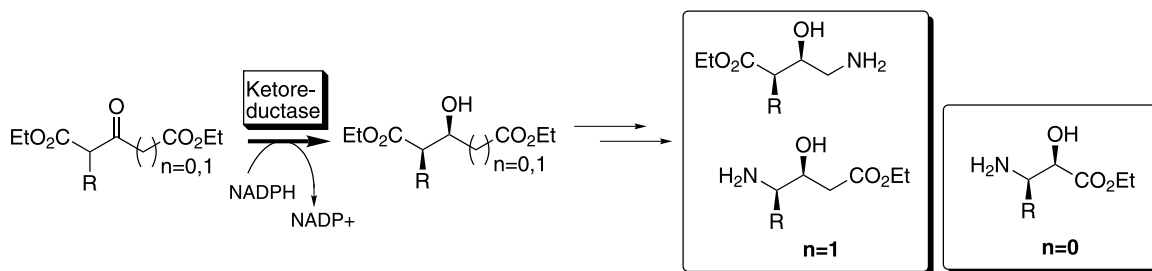
pp 655–661

Hong Li, Roberta Mustacchi, Christopher J. Knowles, Wolfgang Skibar, Garry Sunderland, Ian Dalrymple and Simon A. Jackman*


Ketoreductases in the synthesis of valuable chiral intermediates: application in the synthesis of α -hydroxy β -amino and β -hydroxy γ -amino acids

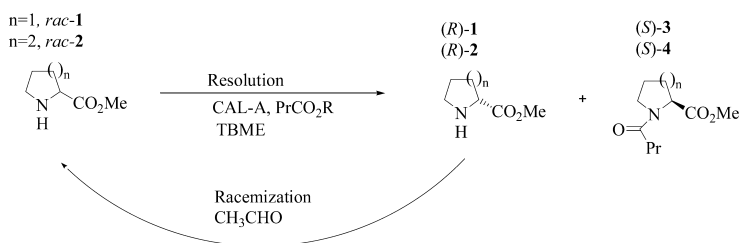
pp 663–669

Spiros Kambourakis* and J. David Rozzell


Aldehyde-based racemization in the dynamic kinetic resolution of *N*-heterocyclic α -amino esters using *Candida antarctica* lipase A

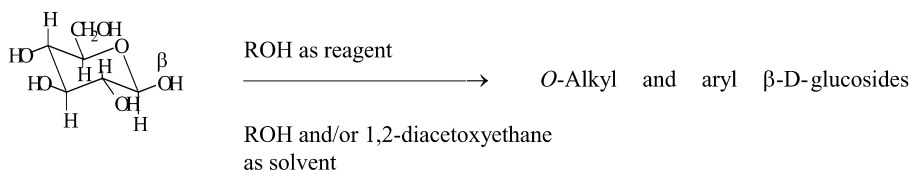
pp 671–677

Arto Liljebblad, Anu Kiviniemi and Liisa T. Kanerva*


Novel reaction systems for the synthesis of *O*-glucosides by enzymatic reverse hydrolysis

pp 679–682

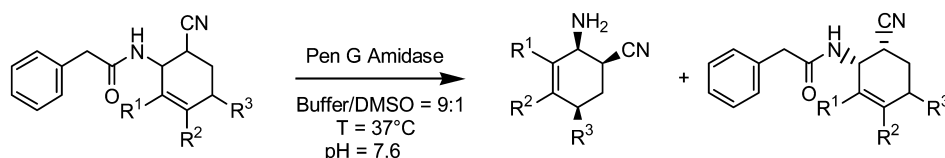
Teréz Balogh, László Boross and Judit Kosáry*



Enzymatic resolution of 4-*N*-phenylacetyl-amino-derivatives obtained from multicomponent reactions using PenG amidase and in silico studies

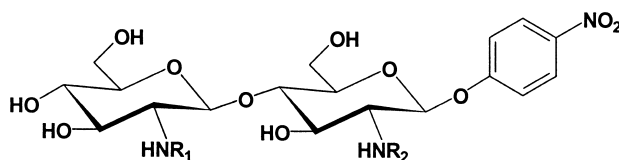
pp 683–691

Dirk Strübing, Helfried Neumann, Stefan Klaus, Axel Jacobi von Wangelin, Dirk Gördes, Matthias Beller, Paolo Braiuca, Cynthia Ebert, Lucia Gardossi and Udo Kragl*

**Hydrolytic and transglycosylation reactions of *N*-acetyl modified substrates catalysed by β -*N*-acetylhexosaminidases**

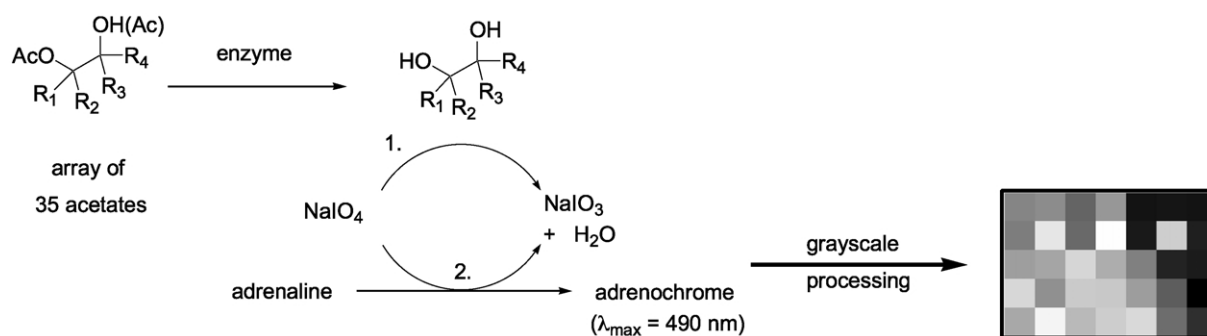
pp 693–701

Pavla Fialová, Lenka Weignerová, Jana Rauvolfová, Věra Příkrylová, Andrea Pišvejcová, Rüdiger Ettrich, Marek Kuzma, Petr Sedmera and Vladimír Křen*

**Adrenaline profiling of lipases and esterases with 1,2-diol and carbohydrate acetates**

pp 703–710

Denis Wahler, Olivier Boujard, Fabrice Lefèvre* and Jean-Louis Reymond*

**The use of a thermostable signature amidase in the resolution of the bicyclic synthon (*rac*)- γ -lactam**

pp 711–716

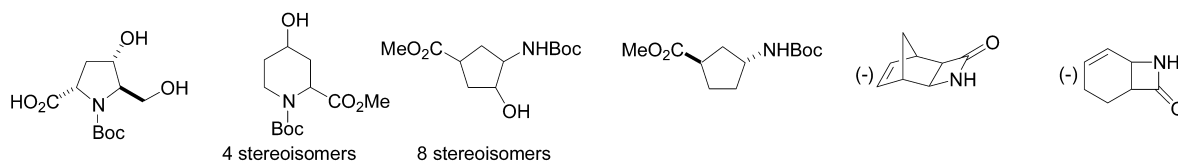
Helen S. Toogood, Rob C. Brown, Kirsty Line, Phil A. Keene, Stephen J. C. Taylor, Ray McCague and Jennifer A. Littlechild*

An enzyme that selectively cleaves the (+)-enantiomer from a racemic mix of γ -lactam has been isolated from the thermophilic archaeon *Sulfolobus solfataricus* MT4. The temperature optimum for the cleavage reaction of the γ -lactam substrate was 85 °C in phosphate buffer at pH 7.0. The enzyme also exhibits general amidase activity by cleaving linear and branched aliphatic and aromatic amides. It can catalyse the synthesis of benzoic hydrazide from benzamide preferentially to benzamide cleavage in the presence of excess hydrazine. It has potential for use in industrial biotransformations for the production of both carbocyclic nucleosides and hydrazides.

Use of hydrolases for the synthesis of cyclic amino acids

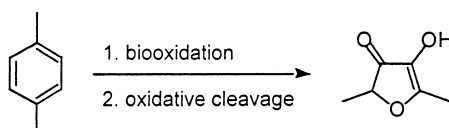
pp 717–728

Richard C. Lloyd,* Michael C. Lloyd, Mark E. B. Smith, Karen E. Holt, Jonathan P. Swift, Philip A. Keene, Stephen J. C. Taylor and Raymond McCague

**Directed evolution of the dioxygenase complex for the synthesis of furanone flavor compounds**

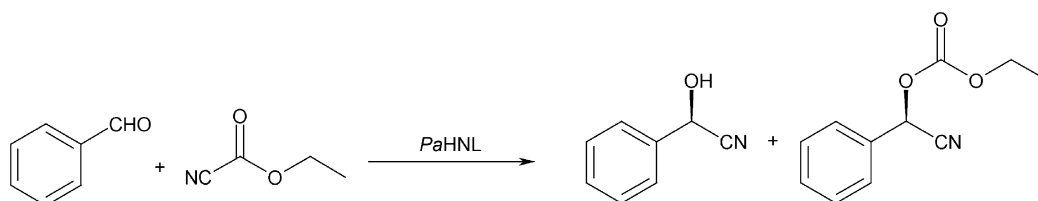
pp 729–734

Lisa M. Newman,* Henry Garcia, Tomas Hudlicky and Sergey A. Selifonov

**One-pot chemoenzymatic synthesis of protected cyanohydrins**

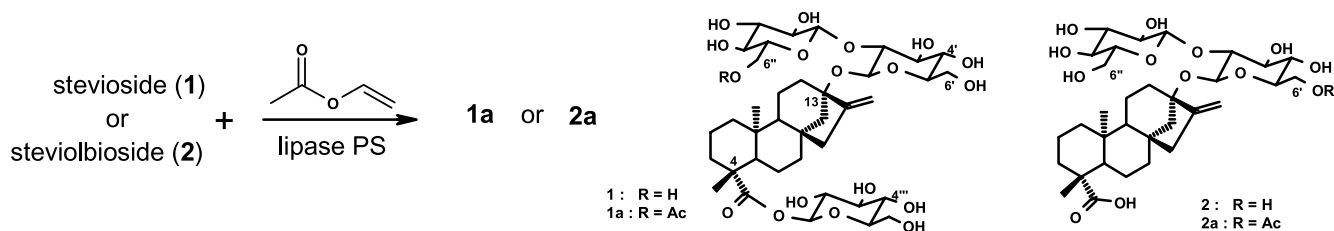
pp 735–739

Thomas Purkarthofer, Wolfgang Skranc, Hansjörg Weber, Herfried Griengl, Marcel Wubbolts, Gerald Scholz and Peter Pöchlauer*

**Remote control of enzyme selectivity: the case of stevioside and steviolbioside**

pp 741–746

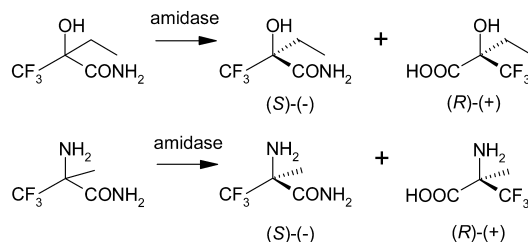
Giorgio Colombo, Sergio Riva* and Bruno Danieli



The substrate specificity of the heat-stable stereospecific amidase from *Klebsiella oxytoca*

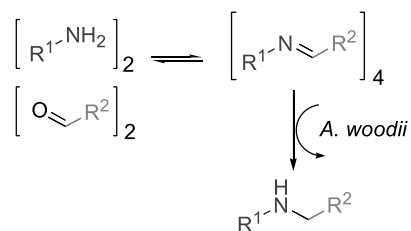
pp 747–752

Nicholas M. Shaw* and Andrew B. Naughton

**A dynamic combinatorial screen for novel imine reductase activity**

pp 753–758

Hong Li, Paul Williams, Jason Micklefield, John M. Gardiner and Gill Stephens*

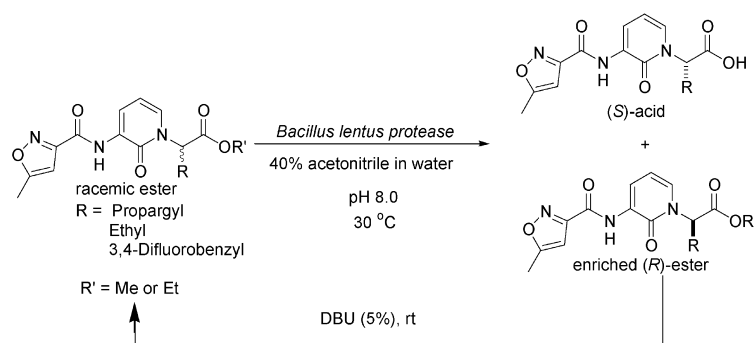


A new screen has been developed for novel biocatalytic imine reduction using virtual dynamic combinatorial libraries. Imine reductase activity has been detected in the strict anaerobe, *Acetobacterium woodii*.

An efficient enzymatic preparation of rhinovirus protease inhibitor intermediates

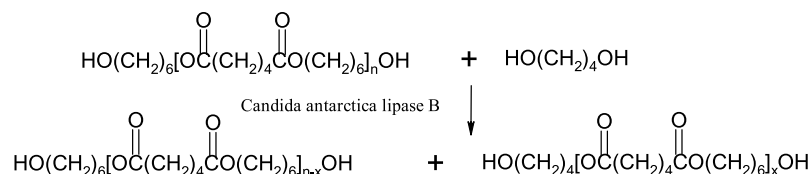
pp 759–764

Carlos A. Martinez, Daniel R. Yazbeck and Junhua Tao*

**Mechanistic studies on the enzymatic transesterification of polyesters**

pp 765–770

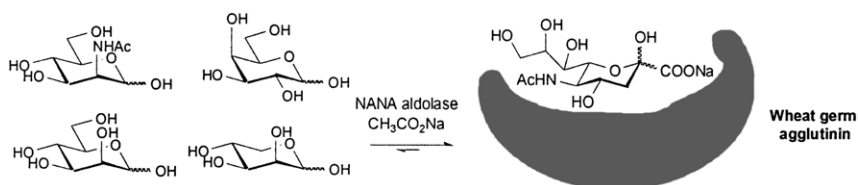
R. W. McCabe and A. Taylor*



Generation of a dynamic combinatorial library using sialic acid aldolase and in situ screening against wheat germ agglutinin

pp 771–780

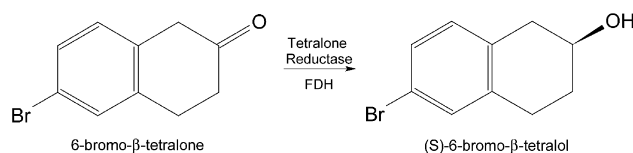
Roger J. Lins, Sabine L. Flitsch, Nicholas J. Turner,* Ed Irving and Stuart A. Brown



An alternative bioreactor concept for application of an isolated oxidoreductase for asymmetric ketone reduction

pp 781–788

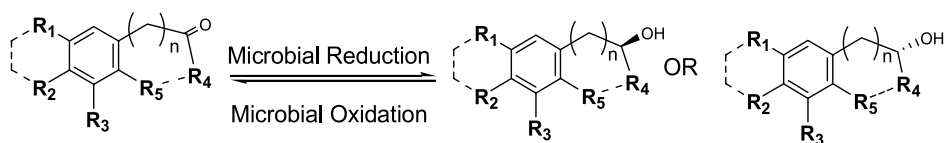
Vicky J. Shorrock, Michel Chartrain and John M. Woodley*



Rapid identification of enantioselective ketone reductions using targeted microbial libraries

pp 789–797

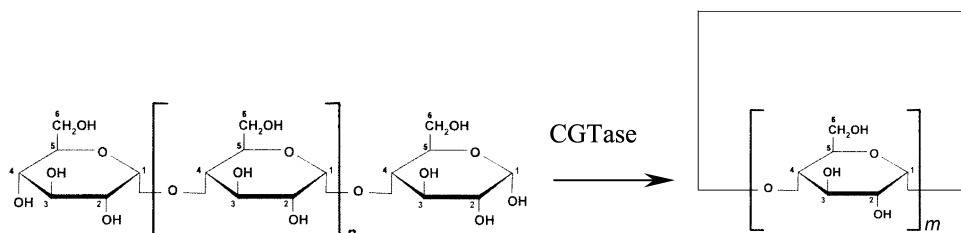
Michael J. Homann,* Robert B. Vail, Edward Previte, Maria Tamarez, Brian Morgan, David R. Dodds and Aleksey Zaks*



Effect of the reaction temperature on the transglycosylation reactions catalyzed by the cyclodextrin glucanotransferase from *Bacillus macerans* for the synthesis of large-ring cyclodextrins

pp 799–806

Qingsheng Qi, Xiaoyan She, Tomohiro Endo and Wolfgang Zimmermann*



OTHER CONTENTS**Contributors to this issue**
Instructions to contributors**I**
III–VI

*Corresponding author

①⁺ Supplementary data available via ScienceDirect**COVER**

This picture shows the active site of the *Aureobacterium* (-) γ -lactamase enzyme (PDB code 1HK7). The catalytic triad made up of Ser98, His259 and Asp230, is shown as ball and stick and the secondary structure elements are shown as ribbons. A tetrahedral intermediate of the cyclic carbonate, (3aR,7aS)-3a,4,7,7a-tetrahydro-benzo [1,3] dioxol-2-one, is shown in pale blue covalently bound to the catalytic serine residue. (*J. Mol. Biol.* **2004**, submitted)

Authors: Kirsty Line, Michail N. Isupov and Jennifer A. Littlechild

© 2004 J. A. Littlechild. Published by Elsevier Ltd.



Full text of this journal is available, on-line from **ScienceDirect**. Visit www.sciencedirect.com for more information.

CONTENTS
direct

This journal is part of **ContentsDirect**, the *free* alerting service which sends tables of contents by e-mail for Elsevier books and journals. You can register for **ContentsDirect** online at: <http://contentsdirect.elsevier.com>

Indexed/Abstracted in: AGRICOLA, Beilstein, BIOSIS Previews, CAB Abstracts, Chemical Abstracts. Current Contents: Life Sciences, Current Contents: Physical, Chemical and Earth Sciences, Current Contents Search, Derwent Drug File, Ei Compendex, EMBASE/Excerpta Medica, Medline, PASCAL, Research Alert, Science Citation Index, SciSearch

**ELSEVIER**

ISSN 0040-4020