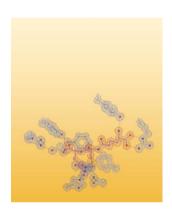
# Organic Biomolecular hemistry

## Incorporating Acta Chemica Scandinavica



**Cover**See J. M. Elkins, P. J. Rutledge, N. I. Burzlaff, I. J. Clifton, R. M. Adlington, P. L. Roach and J. E. Baldwin, page 1455 The active site of isopenicillin N synthase with an unsaturated substrate analogue.





## PROFILE

Profile: Organic & Biomolecular Chemistry profiles Professor Andrew D. Hamilton



## COMMUNICATIONS

PBG synthase + NH3  $+\dot{N}H_3$ (R)-[2- $^{2}$ H]ALA PBG

Stereochemistry and mechanism of the conversion of 5-aminolaevulinic acid into porphobilinogen catalysed by porphobilinogen synthase

Catherine E. Goodwin and Finian J. Leeper

(R)-[2-2H]ALA shows a much larger isotope effect than the (S)-isomer; a detailed mechanism is proposed based on this stereochemistry and crystal structures.

### COMMUNICATIONS

## 5-Formyl-2-furylboronic acid as a versatile bifunctional reagent for the synthesis of $\pi$ -extended heteroarylfuran systems

Paul R. Parry, Martin R. Bryce and Brian Tarbit

5-Formyl-2-furylboronic acid reacts cleanly with a range of heteroaryl bromides under Suzuki-Miyaura cross-coupling conditions to produce 2-formyl-5-heteroarylfuran derivatives. Subsequent Wittig olefination reactions afford  $\pi$ -conjugated alkene-pyridyl-furan derivatives.

## Tandem RCM-Pauson-Khand reaction for access to tricycles in one step

Marta Rosillo, Luis Casarrubios, Gema Domínguez and Javier Pérez-Castells

Only one step is used to obtain tricyclic structures by means of a tandem RCM and Pauson-Khand reaction.

Efficient radical scavenging ability of artepillin C, a major component of Brazilian propolis, and the mechanism

Ikuo Nakanishi, Yoshihiro Uto, Kei Ohkubo, Kentaro Miyazaki, Haruko Yakumaru, Shiro Urano, Haruhiro Okuda, Jun-Ichi Ueda, Toshihiko Ozawa, Kiyoshi Fukuhara, Shunichi Fukuzumi, Hideko Nagasawa, Hitoshi Hori and Nobuo Ikota

Artepillin C, a major component of Brazilian propolis, can scavenge cumylperoxyl radical via a one-step hydrogen atom transfer mechanism at a rate comparable to that of (+)-catechin.

## PhCMe<sub>2</sub>OO PhCMe<sub>2</sub>OOH COOH ĊOOH Artepillin C

## ARTICLES

## Crystallographic studies on the reaction of isopenicillin N synthase with an unsaturated substrate analogue

Jonathan M. Elkins, Peter J. Rutledge, Nicolai I. Burzlaff, Ian J. Clifton, Robert M. Adlington, Peter L. Roach and Jack E. Baldwin

A pseudo-time-resolved strategy is used to follow the reaction of isopenicillin N synthase with an unsaturated substrate analogue in the crystalline state.



1460

## Oligonucleotide based artificial nuclease (OBAN) systems. Bulge size dependence and positioning of catalytic group in cleavage of RNA-bulges

Hans Åström, Nicholas H. Williams and Roger Strömberg

OBAN cleavage of bulge-forming oligoribonucleotides display different bulge size preferences for different linker positions, turnover and Michaelis-Menten behaviour.

Cyclosporin H (CsH) Cyclosporin G (CsG)

Two new cyclosporin folds observed in the structures of the immunosuppressant cyclosporin G and the formyl peptide receptor antagonist cyclosporin H at ultra-high resolution

Brian Potter, Rex A. Palmer, Robert Withnall, Terence C. Jenkins and Babur Z. Chowdhry

The detailed structures of the immunosuppressant cyclosporin G and the formyl peptide receptor antagonist cyclosporin H are presented.

## 1475 1479

## An improved approach for the synthesis of $\alpha,\alpha$ -dialkyl glycine derivatives by the Ugi–Passerini reaction

Susana P. G. Costa, Hernâni L. S. Maia and Sílvia M. M. A. Pereira-Lima

General strategy for routine synthesis of bulky  $\alpha$ , $\alpha$ -dialkyl glycines by the Ugi–Passerini reaction.

$$\begin{array}{c} \text{CH}_3\text{CO}_2\text{H} + \\ \text{Pmb} \cdot \text{NCR}_2 + \\ \text{CNR'} \end{array} + \begin{array}{c} \text{O} \\ \text{R} \\ \text{H}_3\text{C} \end{array} + \begin{array}{c} \text{R} \\ \text{N} \\ \text{Pmb} \cdot \text{O} \end{array} + \begin{array}{c} \text{O} \\ \text{R} \\ \text{N} \\ \text{Pmb} \cdot \text{O} \end{array} + \begin{array}{c} \text{O} \\ \text{R} \\ \text{N} \\ \text{Pmb} \cdot \text{O} \end{array} + \begin{array}{c} \text{O} \\ \text{R} \\ \text{N} \\ \text{O} \end{array} + \begin{array}{c} \text{O} \\ \text{N} \\ \text{O} \end{array} + \begin{array}{c} \text{R} \\ \text{O} \\ \text{N} \\ \text{O} \end{array} + \begin{array}{c} \text{O} \\ \text{O} \end{array} + \begin{array}{c} \text{O} \\ \text{O} \end{array} + \begin{array}{c} \text{O} \\ \text{O} \\ \text{O} \end{array} + \begin{array}{c$$

## Q



1480 1483

$$Dpa = Me_2N \longrightarrow N=N$$

$$CO-$$

$$Dpa^*OH + NH_2CHR-CO_2R^1$$

$$1. DCC / HOBt$$

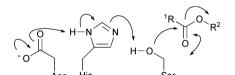
$$Dpa-N(Boc)-CHR-CO_2R^1$$

$$1. DCC / HOBt$$

Dpa<sup>-</sup>OH + Z-Lys-OMe

1486

Z-Lys(N-Boc,w-Boc,w-Dpa)-OMe



## Development of a temporary marker for peptides

M. Sameiro T. Goncalves and Hernâni L. S. Maia

Labelling of amino acid esters followed by investigation of the conditions of cleavage of the chromophore by nucleophiles or electrolysis.

Synthesis and hydrolysis studies of a peptide containing the reactive triad of serine proteases with an associated linker to a dye on a solid phase support

John M. Clough, Ray V. H. Jones, Hannah McCann, David J. Morris and Martin Wills

The synthesis of a model system to probe the capacity for a simple linear peptide incorporating the reactive triad to cleave ester bonds *via* intramolecular hydrolysis.

## 1498 1502

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## Stability against enzymatic hydrolysis of endomorphin-1 analogues containing $\beta$ -proline

Giuliana Cardillo, Luca Gentilucci, Alessandra Tolomelli, Maria Calienni, Ahmed R. Qasem and Santi Spampinato

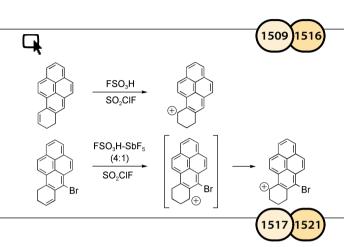
Endomorphin-1 analogues containing  $\beta\text{-proline}$  display good affinity towards  $\mu\text{-opioid}$  receptors and enhanced stability against enzymatic hydrolysis.



# Biosynthesis of anthecotuloide, an irregular sesquiterpene lactone from *Anthemis cotula* L. (Asteraceae) *via* a nonfarnesyl diphosphate route

John van Klink, Hans Becker, Susannah Andersson and Wilhelm Boland

Stable isotope labelling studies have shown that anthecotuloide is biosynthesized from the head-to-head coupling of geranyl-PP with dimethylallyl-PP.



Stable ion study of benzo[a]pyrene (BaP) derivatives: 7,8-dihydro-BaP, 9,10-dihydro-BaP and its 6-halo derivatives, 1- and 3-methoxy-9,10-dihydro- BaP-7(8H)-one, as well as the proximate carcinogen BaP 7,8-dihydrodiol and its dibenzoate, combined with a comparative DNA binding study of regioisomeric (1-, 4-, 2-) pyrenylcarbinols

T. Okazaki, K. K. Laali, B. Zajc, M. K. Lakshman, S. Kumar, W. M. Baird and W.-M. Dashwood

A comparative stable ion and DNA binding study was conducted on a series of BaP derivatives.



R = H, Me,  ${}^{n}C_{8}H_{17}$ ,  ${}^{i}Pr$ ,  ${}^{t}Bu$ , Me<sub>3</sub>Si, Ph X = S, Se, Te

# Synthesis of 1-alkynyl(diphenyl)onium salts of group 16 elements *via* heteroatom transfer reaction of 1-alkynyl(phenyl)-λ<sup>3</sup>-iodanes

Masahito Ochiai, Takema Nagaoka, Takuya Sueda, Jie Yan, Da-Wei Chen and Kazunori Miyamoto

1-Alkynyl(phenyl)- $\lambda^3$ -iodanes undergo selective transfer of the alkynyl groups onto diphenyl chalcogens to give 1-alkynyl-(diphenyl)sulfonium, -selenonium, and -telluronium salts.

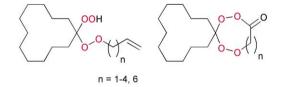
## Q

## 1522 1527

## New approaches to the synthesis of spiro-peroxylactones

Kevin J. McCullough, Hidekazu Tokuhara, Araki Masuyama and Masatomo Nojima

(Alkenyldioxy)cyclododecyl hydroperoxides are transformed into peroxylactones *via* a two-step ozonolysis–dehydration (or oxidation) sequence.





 $d[F-TEDA] / dt = k_2x[F-TEDA]x[fluorene]$ 

The role of geometry on regioselectivity and rate of fluorination of fluorene and diphenylmethane with Selectfluor<sup>TM</sup> F-TEDA-BF $_4$ 

Jernej Iskra, Marko Zupan and Stojan Stavber

To study the direct introduction of fluorine into aromatic molecules, the reactions of diphenylmethane and fluorene with F-TEDA-BF<sub>4</sub> have been investigated.



## Preparation of diamines by lithiationsubstitution of imidazolidines and pyrimidines

Neil J. Ashweek, Iain Coldham, Thomas F. N. Haxell and Steven Howard

Chiral 1,2-diamines have been prepared by cyclization to an imidazolidine, asymmetric lithiation then substitution, followed by hydrolysis.

## DOTTADs - readily made novel metal ligands with multivariant functionality

Andrea Arany, Otto Meth-Cohn and Miklós Nyerges

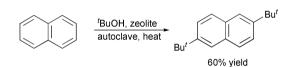
A general multi-purpose synthesis of a new class of heterocyclic ligands has been established.



## Study of regioselective dialkylation of naphthalene in the presence of reusable zeolite catalysts

Keith Smith, Simon D. Roberts and Gamal A. El-Hiti

Highly regioselective dialkylation of naphthalene has been achieved using an easily regenerated catalyst.

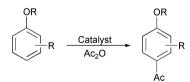




Acetylation of aromatic ethers using acetic anhydride over solid acid catalysts in a solvent-free system. Scope of the reaction for substituted ethers

Keith Smith, Gamal A. El-Hiti, Anthony J. Jayne and Michael Butters

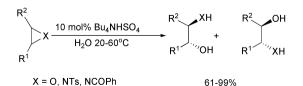
Regioselective acetylation of aryl ethers under modest conditions is achieved with the help of zeolite catalysis.



## Tetrabutylammonium bisulfate: a new effective catalyst for the hydrolysis of aziridines or epoxides

Ren-Hua Fan and Xue-Long Hou

High yields of β-amino alcohols and 1,2-diols are afforded by Bu<sub>4</sub>NHSO<sub>4</sub>-catalyzed ring-opening reaction of aziridines and epoxides with water.





# H<sub>2</sub>O<sub>2</sub>/Catalyst: Colourless products

# 1578 1583



planar 2,6-disubstitution (non-photochromic) twisted (photochromic)

## ARTICLES

Azo dye oxidation with hydrogen peroxide catalysed by manganese 1,4,7-triazacyclononane complexes in aqueous solution

Bruce C. Gilbert, John R. Lindsay Smith, Maurice S. Newton, John Oakes and Roger Pons i Prats

A mechanism is presented for the bleaching of azonaphthol dyes with  $H_2O_2$  catalysed by manganese 1,4,7-triazacyclononane complexes in aqueous solution.

## Crystalline photochromism of *N*-salicylidene-2,6-dialkylanilines: advantage of 2,6-dialkyl substituents of aniline for preparation of photochromic Schiff base crystals

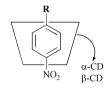
Hisatane Fukuda, Kiichi Amimoto, Hiroyuki Koyama and Toshio Kawato

Alkyl substituents in N-(3,5-dihalosalicylidene)-2,6-dialkylanilines act as space openers in the crystals that exhibit photochromism.

# Spectrophotometric study on the thermodynamics of binding of $\alpha$ - and $\beta$ -cyclodextrin towards some p-nitrobenzene derivatives

Paolo Lo Meo, Francesca D'Anna, Serena Riela, Michelangelo Gruttadauria and Renato Noto

The analysed hosts show different binding behaviour towards examined guests. For example,  $\alpha CD$  also forms 1 : 2 complexes.



## 1591 1597

1590

# $(EtO)_{2}(O)P \\ \downarrow \\ O - 1, (DEPMPO) \\ (EtO)_{2}(O)P \\ \downarrow \\ 1 - d_{2} O - 1 \\ 1 - d_{5} O - 1 \\ (EtO)_{2}(O)P \\ \downarrow \\ D_{3}C \\ \downarrow \\ D_{3}C \\ \downarrow \\ 1 - d_{7} O - 1 \\ (EtO)_{2}(O)P \\ \downarrow \\ D_{3}C \\ \downarrow \\ D_{4}C \\ \downarrow \\ D_{5}C \\ \downarrow \\ D_{5}C$

## Deuterated analogues of the free radical trap DEPMPO: synthesis and EPR studies

Jean-Louis Clément, Jean-Pierre Finet, Claudine Fréjaville and Paul Tordo

Three analogues of DEPMPO (1) labelled with two  $(1-d_2)$ , five  $(1-d_5)$  or seven  $(1-d_7)^2H$  were synthesized and used to trap the *tert*-butylperoxyl radical.

# H<sub>2</sub>N NH<sub>2</sub> NH<sub>2</sub>

Specificity in template syntheses of hexaaza-macrobicyclic cages:  $[Pt(Me_s-tricosatrieneN_6)]^{4+}$  and  $[Pt(Me_s-tricosaneN_6)]^{4+}$ 

Kylie N. Brown, Rodney J. Geue, Trevor W. Hambley, David C. R. Hockless, A. David Rae and Alan M. Sargeson

 $[Pt(tame)_2]^{4+} \ with formaldehyde and propanal stereospecifically yields a $C_3$ tri-imine cage complex <math>[Pt(Me_5\text{-tricosatrieneN}_6)]^{4+}$  which reduces with NaBH4 to a  $C_3$  saturated  $[Pt(Me_5\text{-tricosaneN}_6)]^{4+}$  ion.







Combinatorial organic materials research (COMR): design, synthesis and screening of a 225-membered materials library of liquid crystalline fluorinated p-quaterphenyls

Oliver Deeg and Peter Bäuerle

The rapid solution phase synthesis of novel liquid crystalline materials is demonstrated by utilising combinatorial and parallel methods for the preparation of a library of 225 differently fluorinated 4,4"'-dipropyl-p-quaterphenyls.

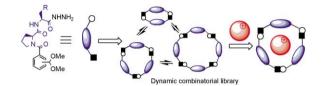




Metal-ion induced amplification of three receptors from dynamic combinatorial libraries of peptide-hydrazones

Sarah L. Roberts, Ricardo L. E. Furlan, Sijbren Otto and Jeremy K. M. Sanders

Dynamic combinatorial chemistry is used to identify three receptors which undergo substantial conformational rearrangement upon metal-ion guest binding.



## ADDITIONS AND CORRECTIONS



Yoshio Kosugi, Yoshio Imaoka, Fumisato Gotoh, Mohammad A. Rahim, Yoshihisa Matsui and Kinya Sakanishi

Carboxylations of alkali metal phenoxides with carbon dioxide

Yuji Kazuta, Satoshi Shuto, Hiroshi Abe and Akira Matsuda

The bisected s-trans conformation-controlled highly stereoselective addition of Grignard reagents to C-cyclopropylaldo-nitrone. An efficient synthesis of 1-phenyl-2-[(S)-1-aminoalkyl]-N,N-diethylcyclopropanecarboxamides, a new class of potent NMDA receptor antagonists



Dates, venues and contact details of forthcoming events.

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