

# Organic & Biomolecular Chemistry

INDEXED IN MEDLINE

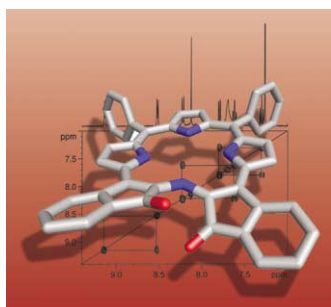
Incorporating Acta Chemica Scandinavica

**Cover**

See Jason R. McCarthy, Michael A. Hyland and Christian Brückner, pp. 1484–1491.

The cover shows a molecular model of indaphyrin, a novel class of *meso*-tetraarylsecochlorin-derived chromophores incorporating *o*-phenyl-to- $\beta$ -linkages, over its H,H-COSY spectrum. The linkage introduces some strain into the molecule, leading to a slightly ruffled conformation of the macrocycle. The ketone-linkages also force the phenyl groups nearly into co-planarity with the porphyrinoid chromophore, resulting in an extended  $\pi$ -system.

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## contents

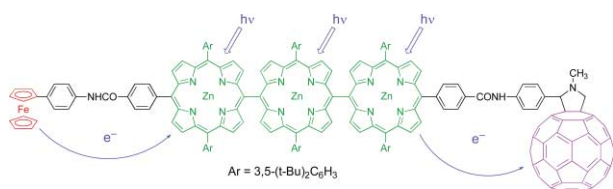
## PERSPECTIVE

1425 1433

### Porphyrin–fullerene linked systems as artificial photosynthetic mimics

Hiroshi Imahori

We have successfully prepared a variety of porphyrin–fullerene linked systems, which exhibit excellent photoinduced electron transfer properties.



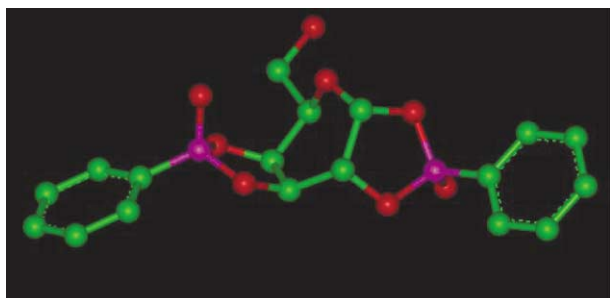
## ARTICLES

1434 1441

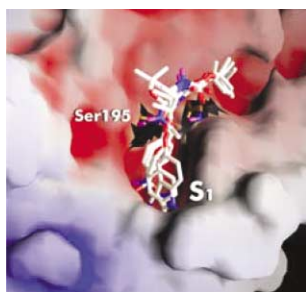
### Structures of carbohydrate–boronic acid complexes determined by NMR and molecular modelling in aqueous alkaline media

Malcolm P. Nicholls and Prem K. C. Paul

$^1\text{H}$  NMR techniques coupled with molecular modelling calculations have provided a wealth of information on the structure of boronic acid complexed carbohydrates and are useful tools in the field of molecular sensing and recognition in aqueous media.



1442 1446

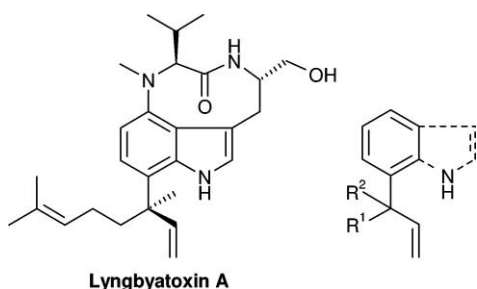


### On the rational design of substrate mimetics: the function of docking approaches for the prediction of protease specificities

Robert Günther, Christian Elsner, Stephanie Schmidt, Hans-Jörg Hofmann and Frank Bordusa

The function of an automated docking procedure in the prediction of the specificity of proteases towards substrate mimetics is reported.

1447 1455

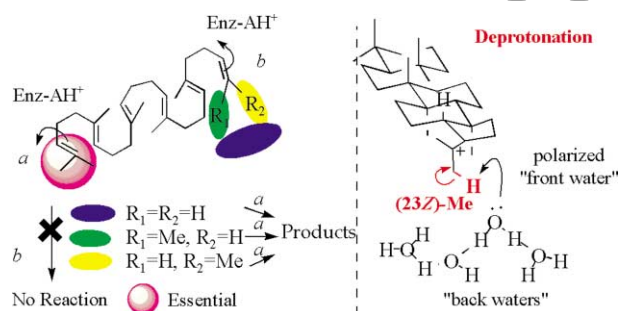


### Studies of the formation of all-carbon quaternary centres, en route to lyngbyatoxin A. A comparison of phenyl and 7-substituted indole systems

Janne E. Tønder, Masood Hosseini, Alex B. Ahrenst and David Tanner

Metal mediated allylic substitutions and conjugate additions to geranyl, cinnamyl and allylic indole compounds en route to lyngbyatoxin A.

1456 1470

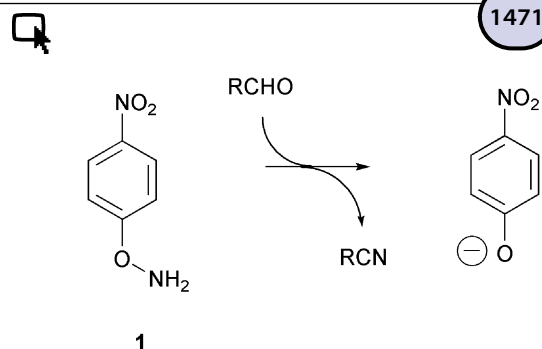


### Squalene-hopene cyclase: final deprotonation reaction, conformational analysis for the cyclization of (3*R*,*S*)-2,3-oxidosqualene and further evidence for the requirement of an isopropylidene moiety both for initiation of the polycyclization cascade and for the formation of the 5-membered E-ring

Tsutomu Hoshino, Schin-ichi Nakano, Tomohiro Kondo, Tsutomu Sato and Aya Miyoshi

Essentiality of an isopropylidene moiety and deprotonation from 23Z-Me for hopene biosynthesis by squalene cyclase.

1471 1475

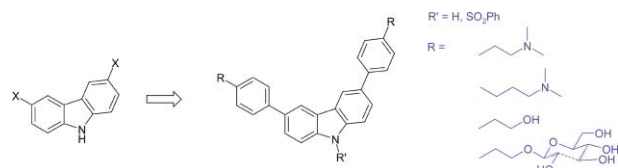


### Aldehyde detection by chromogenic/fluorogenic oxime bond fragmentation

Syed Salahuddin, Olivier Renaudet and Jean-Louis Reymond

A series of new fluorogenic and chromogenic oxyamine reagents was prepared by amination of nitrophenol and umbelliferones. The oxyamines formed oximes with carbonyl compounds in organic solvent. In water, the oximes undergo chromogenic or fluorogenic fragmentation under basic conditions. The process provides an assay for formaldehyde in water.

1476 1483



### Synthesis of diphenylcarbazoles as cytotoxic DNA binding agents

Ulrich Jacquemard, Sylvain Routier, Arnaud Tatibouët, Jérôme Kluza, William Laine, Christine Bal, Christian Bailly and Jean-Yves Mèroux

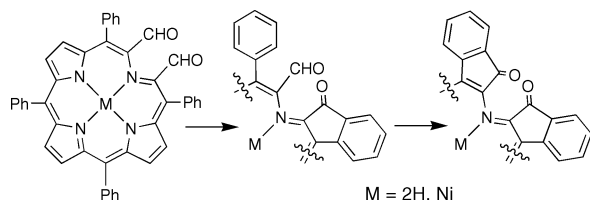
The DNA binding compounds exhibit potent cytotoxic activity toward P388 leukemia cells.

1484 1491

**Synthesis of indaphyrins: *meso*-tetraarylsecochlorin-based porphyrinoids containing direct *o*-phenyl-to- $\beta$ -linkages**

Jason R. McCarthy, Michael A. Hyland and Christian Brückner

Step-wise acid-induced cyclization of *meso*-tetraphenyl-2,3-secochlorin-2,3-dialdehyde produced *meso*-diphenylindaphyrins, novel secochlorin-based chromophores with significantly red-shifted absorption spectra as compared to porphyrins.

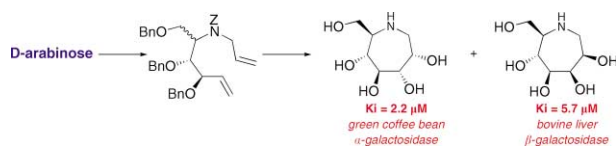


1492 1499

**The first synthesis of substituted azepanes mimicking monosaccharides: a new class of potent glycosidase inhibitors**

Hongqing Li, Yves Blériot, Caroline Chantreau, Jean-Maurice Mallet, Matthieu Sollogoub, Yongmin Zhang, Eliazar Rodríguez-García, Pierre Vogel, Jesús Jiménez-Barbero and Pierre Sinaÿ

The first synthesis of 1,6-dideoxy-1,6-iminoheptitols, displaying selective and potent glycosidase inhibition in the low micromolar range, is described.

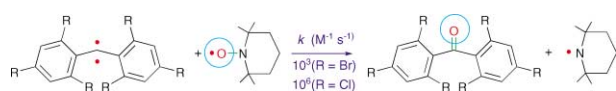


1500 1503

**Reaction of tetramethylpiperidine *N*-oxides with persistent triplet diphenylcarbenes**

Jun-ichi Nakajima, Katsuyuki Hirai and Hideo Tomioka

Triplet carbene reacts with amine *N*-oxide radical to form ketone faster than abstracting H from H donors but much slower than reacting with triplet oxygen.

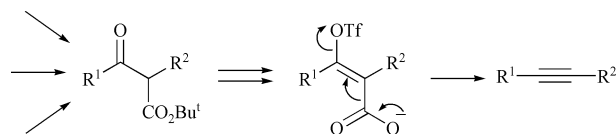


1504 1510

**Decarboxylative elimination of enol triflates as a general synthesis of acetylenes**

Ian Fleming and Chandrashekar Ramarao

The decarboxylative elimination of enol triflates is a general method for the regiocontrolled synthesis of acetylenes with  $R^1$  = alkyl or ethynyl, and  $R^2$  = alkyl,  $CO_2H$  or H, extending the method using the decarboxylative elimination of enol arenesulfonates, which only worked when the group  $R^1$  was aryl, ethenyl or cyclopropyl.

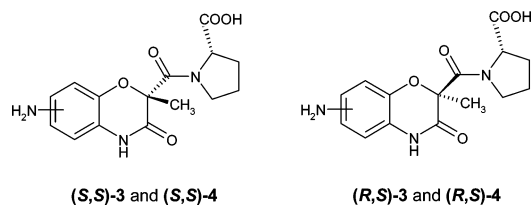


1511 1517

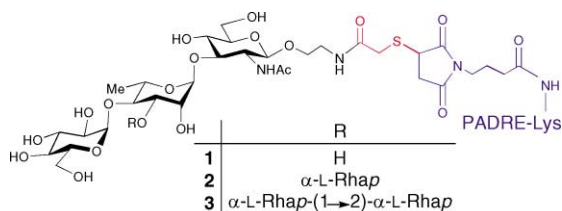
**Conformationally tailored *N*-[(2-methyl-3-oxo-3,4-dihydro-2*H*-1,4-benzoxazin-2-yl)carbonyl]proline templates as molecular tools for the design of peptidomimetics.****Design and synthesis of fibrinogen receptor antagonists**

Petra Štefanič, Zvone Simončič, Matej Breznik, Janez Plavec, Marko Anderluh, Elisabeth Addicks, Athanassios Giannis and Danijel Kikelj

(*S,S*)-3, (*S,S*)-4, (*R,S*)-3 and (*R,S*)-4 were used as conformationally tailored peptidomimetic templates for the design of fibrinogen receptor antagonists.



1518 1527

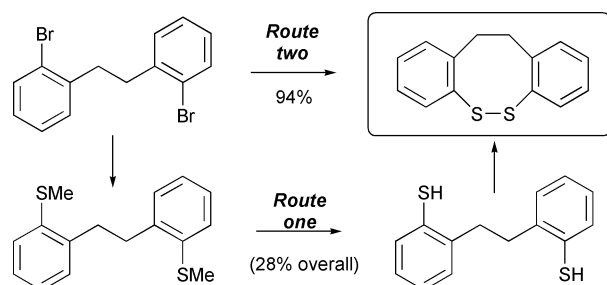


### Preparation of synthetic glycoconjugates as potential vaccines against *Shigella flexneri* serotype 2a disease

Karen Wright, Catherine Guerreiro, Isabelle Laurent, Françoise Baleux and Laurence A. Mulard

Synthesis of neoglycopeptides **1**, **2** and **3** using a modular approach.

1528 1530

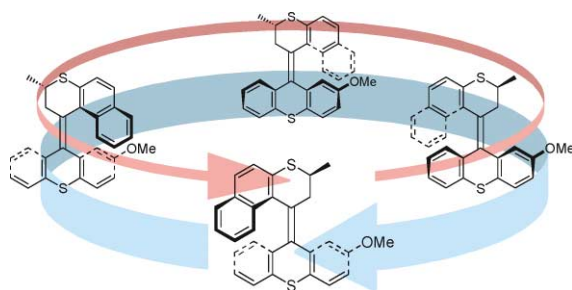


### Two routes to (11,12)-dihydrodibenzo[*c,g*][1,2]dithiocine

Paul Wyatt and Andrew Hudson

Route One features the separate introduction of two sulfur atoms and a double Pummerer reaction while Route Two uses an alternative strategy with direct introduction of both sulfur atoms using disulfur diimidazole.

1531 1541

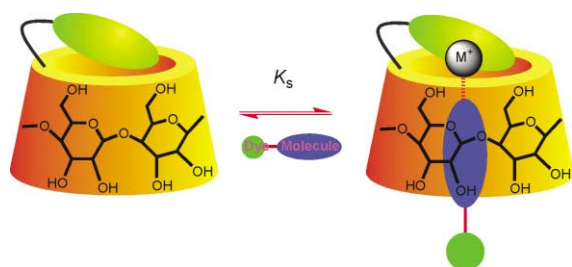


### Exploring the boundaries of a light-driven molecular motor design: new sterically overcrowded alkenes with preferred direction of rotation

Richard A. van Delden, Matthijs K. J. ter Wiel, Harmen de Jong, Auke Meetsma and Ben L. Feringa

A newly designed molecular motor based on a sterically overcrowded alkene allows preferential clockwise intramolecular rotation driven by light.

1542 1548

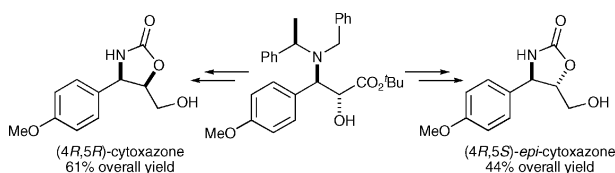


### Cooperative molecular recognition of dyes by dyad and triad cyclodextrin-crown ether conjugates

Yu Liu, Ying-Wei Yang, Lei Li and Yong Chen

Cooperative attracting or anti-cooperative repulsive interactions by an  $\text{Na}^+$ -crown ether cap actively contribute to the molecular recognition of cyclodextrin-crown ether-guest ternary systems.

1549 1553



### Asymmetric synthesis of (4*R*,5*R*)-cytoxazone and (4*R*,5*S*)-epi-cytoxazone

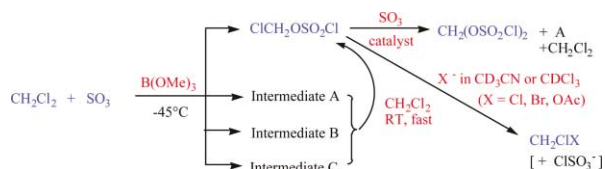
Stephen G. Davies, Deri G. Hughes, Rebecca L. Nicholson, Andrew D. Smith and Angela J. Wright

(4*R*,5*R*)-Cyttoxazone has been prepared in four steps and in 61% overall yield, while (4*R*,5*S*)-epi-cytoxazone has been prepared in six steps and in 44% overall yield.

1554 1562

**Chloromethyl chlorosulfate: a new, catalytic method of preparation and reactions with some nucleophiles**

Nicholas P. Power, Donald Bethell, Lee Proctor, Elliot Latham and Paul Dawson

Possible structures for the intermediates A, B and C are discussed and mechanistic pathways consistent with the observed kinetic form of the reaction of  $\text{CH}_2\text{Cl}_2$  with  $\text{SO}_3$  are suggested.

## CONFERENCE DIARY

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Dates, venues and contact details of forthcoming events.

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