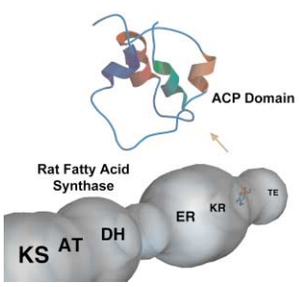
ISSN 1477–0520 OBCRAK(3) 441–608(2003)

Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica



Cover
See M. A. C. Reed, M. Schweizer, A. E. Szafranska, C. Arthur, T. P. Nicholson, R. J. Cox, J. Crosby, M. P. Crump and T. J. Simpson, page 463.
A representation of the rat fatty acid synthase (grey) and the structure of the isolated ACP domain (image by M. P. Crump).

contents

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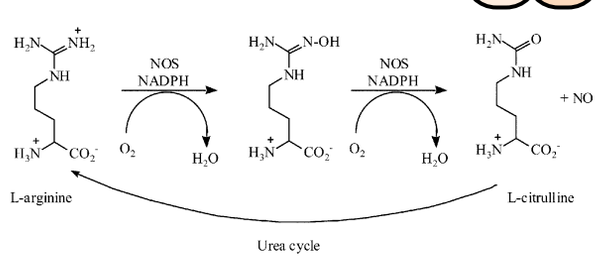
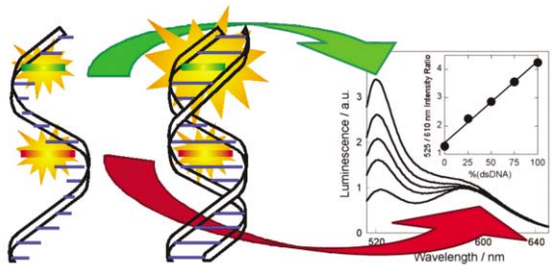
PERSPECTIVE

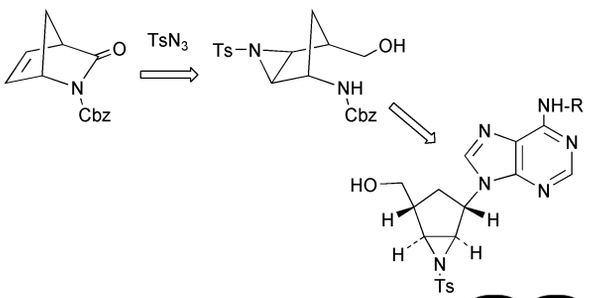




Direct determination of single-to-double stranded DNA ratio in solution using steady-state fluorescence measurements

Lori Beach, Claude Schweitzer and J. C. Scaiano

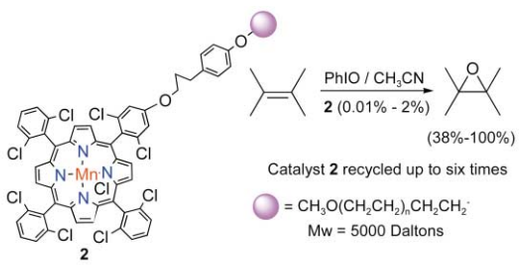
The ratio of fluorescence intensities from two simultaneously excited intercalated dyes is directly proportional to the ss : ds DNA ratio. The method constitutes a promising new approach for detection of radiation-induced DNA damage.



First synthesis of 2′,3′-epimino-carbocyclic nucleosides

Minoru Ishikura, Atsushi Murakami and Nobuya Katagiri

The first 2′,3′-epimino-carbocyclic nucleosides are prepared.



Synthesis of poly(ethylene glycol)-supported manganese porphyrins: efficient, recoverable and recyclable catalysts for epoxidation of alkenes

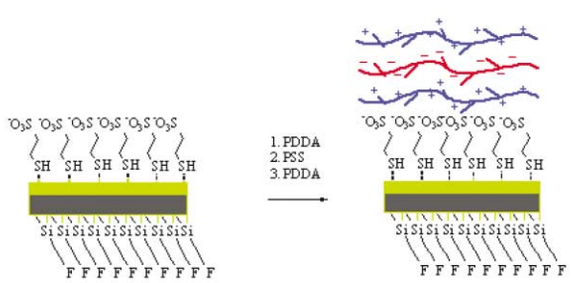
Maurizio Benaglia, Tamara Danelli and Gianluca Pozzi

We have demonstrated that soluble, PEG-supported manganese porphyrins can be easily prepared and conveniently used as recoverable and recyclable catalysts in the epoxidation of alkene with readily available oxidants.

Enhanced π · · · π interactions in α,β-unsaturated carbonyl

Lisa D. Harris, James A. Platts and Nicholas C. O. Tomkinson

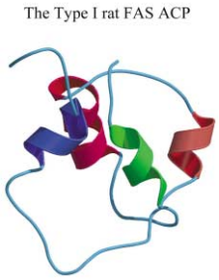
High level *ab initio* calculations on complexes of benzene with acrolein and ethene reveal that π · · · π interactions for the electron deficient acrolein are as strong as those found in the benzene dimer.



A general microcantilever surface modification method using a multilayer for biospecific recognition

Xiaodong Yan, Yuri Lvov, Hai-Feng Ji, Alok Singh and Thomas Thundat

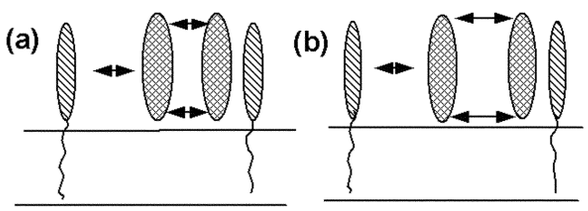
The formation of a multilayer film occurs on only one surface of a microcantilever due to the unique property of perfluorocarbons.



The type I rat fatty acid synthase ACP shows structural homology and analogous biochemical properties to type II ACPs

Michelle A. C. Reed, Michael Schweizer, Anna E. Szafranska, Chris Arthur, Thomas P. Nicholson, Russell J. Cox, John Crosby, Matthew P. Crump and Thomas J. Simpson

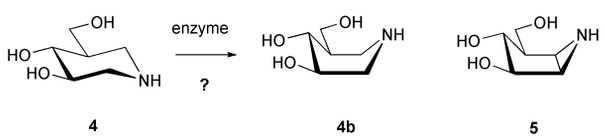
An isolated type I acyl carrier protein (ACP) domain shows considerable structural homology and analogous biochemical properties to type II ACPs.



Kinetic barriers and ordering of non-covalently bound states

Simon W. O'Brien, Hideyuki Shiozawa, Rosa Zerella, Dominic P. O'Brien and Dudley H. Williams

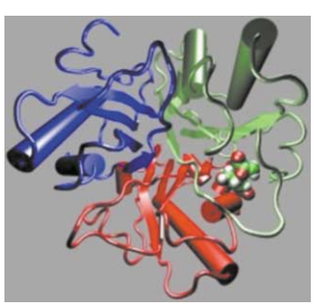
Surface cooperativity greater with tight (a) *vs.* loose (b) dimer.



Aziridines as a structural motif to conformational restriction of azasugars

Oscar Lopez Lopez, José G. Fernández-Bolaños, Vinni H. Lillelund and Mikael Bols

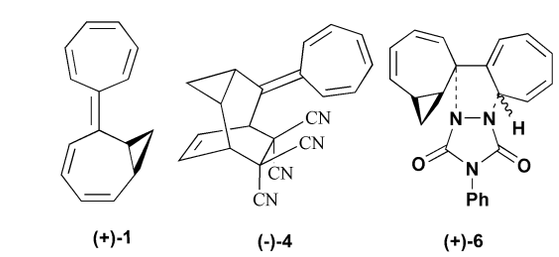
In contrast to isofagomine, its conformationally restricted analogues were found to be very poor or non glycosidase inhibitors, showing that isofagomine does not bind the investigated glycosidases in the $^{1,4}B$ conformation.



QM/MM calculations of kinetic isotope effects in the chorismate mutase active site

Sergio Martí, Vicent Moliner, Iñaki Tuñón and Ian H. Williams

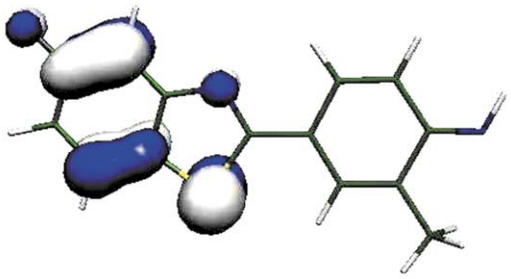
Computed KIEs probe transition states for rearrangement of chorismate to prephenate in water and catalysed by *B. subtilis* enzyme.



Synthesis, absolute configuration and conformation of optically active 1,2-homoheptafulvalene

Shunji Ito, Mitsuhiro Kurita, Sigeru Kikuchi, Toyonobu Asao, Yoshitora Ito, Masaji Oda, Hideo Sotokawa, Akio Tajiri and Noboru Morita

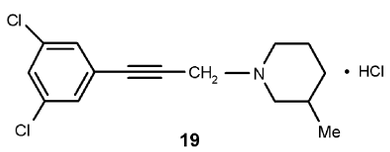
Optically active 1,2-homoheptafulvalene and heptafulvene derivatives were prepared for the first time.



Antitumor benzothiazoles. Frontier molecular orbital analysis predicts bioactivation of 2-(4-aminophenyl)-benzothiazoles to reactive intermediates by cytochrome P4501A1

Sean E. O'Brien, Helen L. Browne, Tracey D. Bradshaw, Andrew D. Westwell, Malcolm F. G. Stevens and Charles A. Laughton

HOMO plot for the nitrenium ion from 2-(4-amino-3-methyl-phenyl)-5-fluorobenzothiazole.

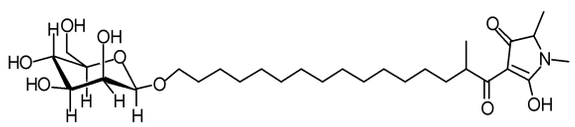


19

Novel 3-phenylprop-2-ynylamines as inhibitors of mammalian squalene epoxidase

David L. Musso, Morris J. Clarke, James L. Kelley, G. Evan Boswell and Grace Chen

The synthesis of a novel series of 3-phenylprop-2-ynylamines as selective mammalian squalene epoxidase inhibitors is described. Compound **19** is the most potent analog with an IC_{50} of 2.8 ± 0.6 μM against rat liver squalene epoxidase.

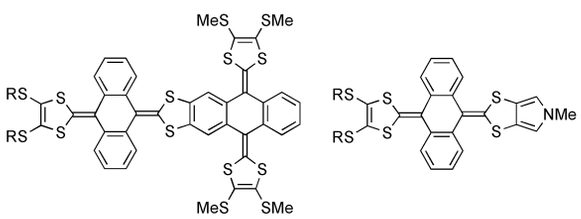


1

Epicoccamide, a novel secondary metabolite from a jellyfish-derived culture of *Epicoccum purpurascens*

Anthony D. Wright, Claudia Osterhage and Gabriele M. König

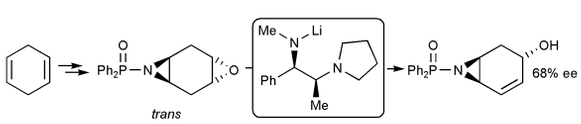
The new natural product epicoccamide (**1**) isolated from the fungus *Epicoccum purpurascens* is composed of three distinct biosynthetic subunits.



New strategies and building blocks for functionalised 9,10-bis(1,3-dithiol-2-ylidene)-9,10-dihydroanthracene derivatives, including pyrrolo-annelated derivatives and π-extended systems with intramolecular charge-transfer

Christian A. Christensen, Martin R. Bryce, Andrei S. Batsanov and Jan Becher

New derivatives of the title system have been synthesised and their electrochemical redox properties studied.



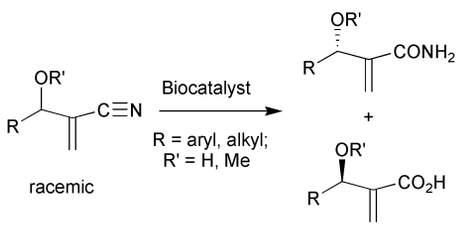
Chiral lithium amide base-mediated rearrangement of *meso*-cyclohexene oxides: asymmetric synthesis of amino- and aziridinocyclohexenols

Peter O'Brien and Christopher D. Pilgram

Two different chiral lithium amide base routes for the synthesis of amino- and aziridino-containing cyclohexenols have been explored.

Nitrile biotransformations for the synthesis of enantiomerically enriched Baylis–Hillman adducts

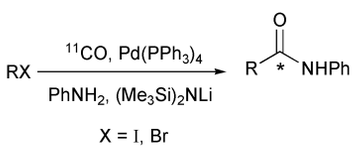
Mei-Xiang Wang and Yan Wu



Enantioselective biohydrolysis of the Baylis–Hillman nitriles produced amides and acids with ee values being dependent upon the structure of the substrates.

Synthesis of ^{11}C-amides using [^{11}C]carbon monoxide and *in situ* activated amines by palladium-mediated carboxaminations

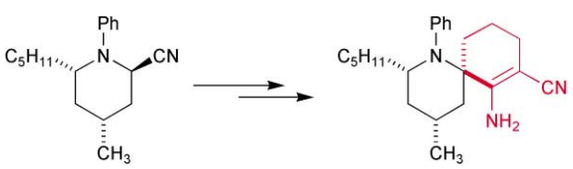
Farhad Karimi and Bengt Långström



[^{11}C]Carbon monoxide, aryl halides and amines have been used in the palladium-mediated synthesis of twenty ^{11}C-amides; this method gave improved yields compared with previous methods.

Diastereoselective preparation of 2,4,6-trisubstituted-2′-cyanopiperidines: application to the construction of the carbon framework of perhydrohistrionicotoxin

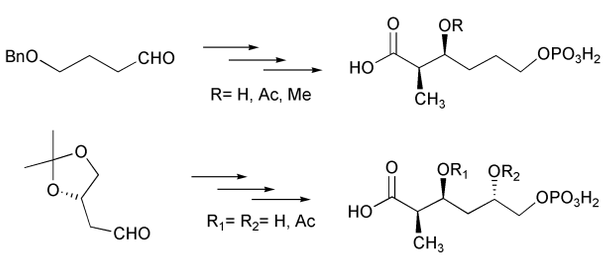
Richard Malassene, Enguerran Vanquelef, Loic Toupet, Jean-Pierre Hurvois and Claude Moinet



A diastereoselective preparation of the basic carbon framework of the perhydrohistrionicotoxin employing anodic cyanation and Thorpe–Ziegler cyclization is described.

Synthesis of (*R*)-2-methyl-4-deoxy and (*R*)-2-methyl-4,5-dideoxy analogues of 6-phosphogluconate as potential inhibitors of 6-phosphogluconate dehydrogenase

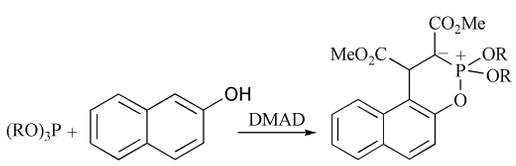
Christophe Dardonville and Ian H. Gilbert



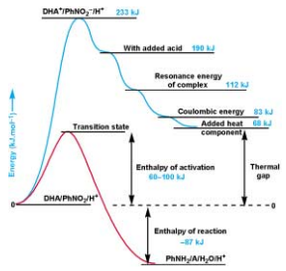
4-Benzyloxybutanol and L-malic acid were used as starting materials and boron aldol methodology was used for the incorporation of the 2*S*,3*R* chiral centres.

Reaction between naphthols and dimethyl acetylene-dicarboxylate in the presence of phosphites. Synthesis of stable oxa-2λ^5-phosphaphenanthrenes, and benzochromene derivatives

Issa Yavari, Mohammad Anary-Abbasinejad and Zinatossadat Hossaini



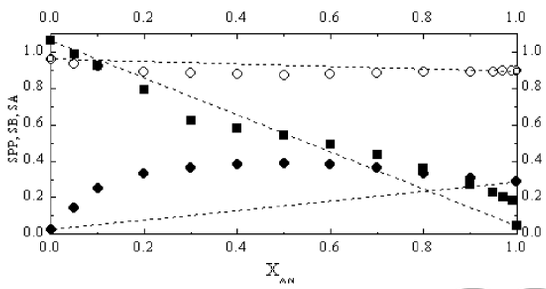
The addition reaction of DMAD, 2-naphthol and trimethyl or triphenyl phosphite gave oxaphosphaphenanthrene derivatives.



Investigations into the mechanism of action of nitrobenzene as a mild dehydrogenating agent under acid-catalysed conditions

M. Lurdes S. Cristiano, David J. P. Gago, Antonio M. d'A. Rocha Gonsalves, Robert A. W. Johnstone, Moya McCarron and Jorge M. T. B. Varejão

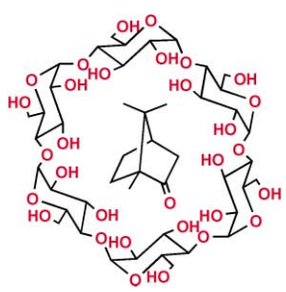
The kinetics of dehydrogenation of hydrocarbons with protonated nitrobenzenes are interpreted as resulting from an initial electron transfer process.



Characterization of binary solvent mixtures: the water–acetonitrile mixture

Javier Catalán, Cristina Díaz and Francisco García-Blanco

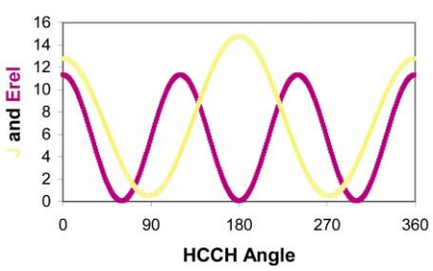
Several properties of binary water–acetonitrile mixtures are described in terms of their polarity, acidity and basicity.



On the impossibility of determination of stepwise binding constants for the 1 : 2 complex of (+)-camphor with α-cyclodextrin

Helena Dodziuk, Krzysztof S. Nowinski, Wiktor Kozminski and Grigory Dolgonos

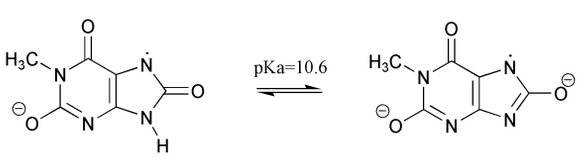
A detailed analysis of partitioning of the overall binding constant (from NMR titrations) for the 1 : 2 complex of (+)-camphor with α-cyclodextrin into the stepwise ones K_1 and K_2 revealed that the accepted procedures are equivocal for $K_1 << K_2$.



The influence of chain elongation on Karplus-type relationships: a DFT study of scalar coupling constants in polyacetylene derivatives

Ibon Alkorta and José Elguero

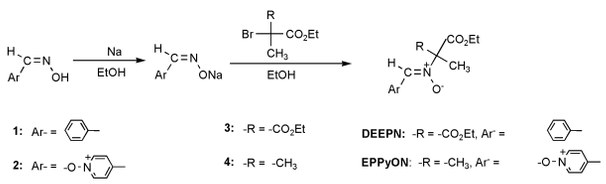
Karplus-type relationships have been obtained for coupling constants of hydrogen atoms separated by up to 15 bonds in dimethylated polyacetylenic derivatives.



Radicals derived from uric acid and its methyl derivatives in aqueous solution: an EPR spectroscopy and theoretical study

João P. Telo

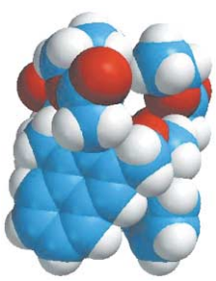
The oxidation of uric acid and of *N*-methyluric acids in aqueous solution was studied by using EPR spectroscopy and DFT calculations.



Preparation and use as spin trapping agents of new ester-nitrones

Ahmad Allouch, Valérie Roubaud, Robert Lauricella, Jean-Claude Bouteiller and Béatrice Tuccio

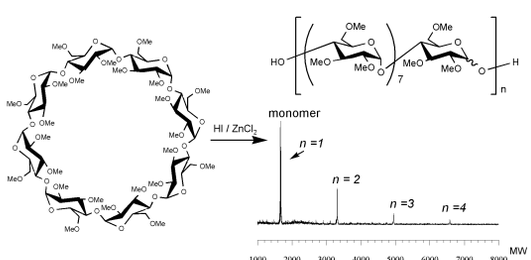
DEEPN and EPPyON efficiently trap various carbon- and oxygen-centred radicals, including superoxide, in aqueous media.



Ester derivatives of hexahomotrioxacalix[3]naphthalenes: conformational and binding properties with alkali metal cations

Muhammad Ashram, Shehadeh Mizyed and Paris E. Georghiou

Synthesis conditions dictate the conformation of the triesters formed between ethyl bromoacetate and hexahomotrioxacalix[3]-naphthalene, and its *tert*-butyl analogue.



Preparation of a unique glucan with large intervals in molecular weight distribution. Controlled ring-opening polymerization of *O*-permethylcyclodextrin

Masato Suzuki and Tomofumi Shimazaki

A combination of HI and $ZnCl_2$ was found to effectively conduct the well-controlled polymerization of γ-MeCD, confirmed by TOF-MS.

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Dates, venues and contact details of forthcoming events.

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