Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry

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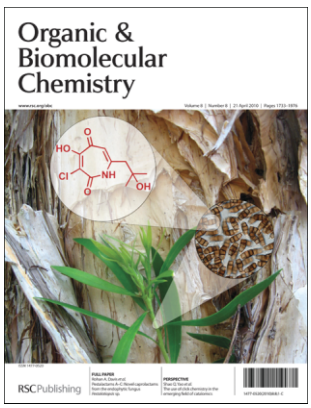
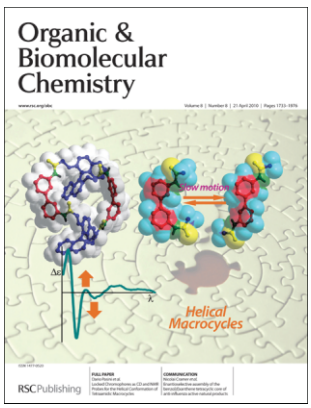
ISSN 1477-0520 CODEN OBCRAK 8(8) 1733–1976 (2010)



Cover

See Rohan A. Davis *et al.*, pp. 1790–1796.
Chemical investigations of a fermentation culture from the endophytic fungus *Pestalotiopsis* sp. yielded three novel natural products, pestalactams A–C. This fungus was isolated from the Australian plant *Melaleuca quinquenervia*.

Image reproduced by permission of Rohan A. Davis from *Org. Biomol. Chem.*, 2010, **8**, 1785.



Inside cover

See Dario Pasini, pp. 1815–1819.
Chiral macrocycles adopt an unusual helical shape when the internal rigidification induced by hydrogen bonding is counterbalanced by flexible spacers.

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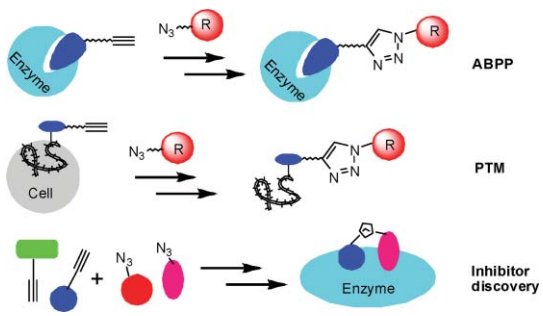
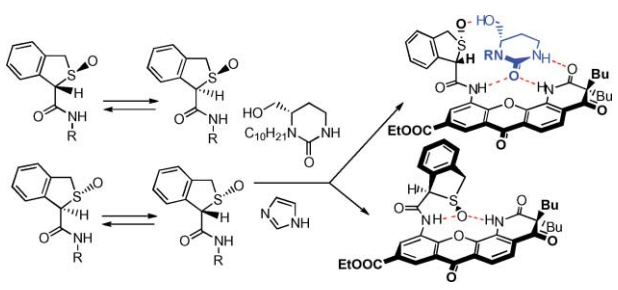
PERSPECTIVE



COMMUNICATIONS



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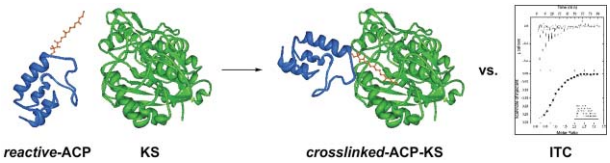
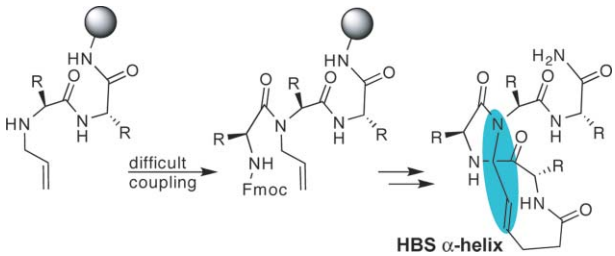
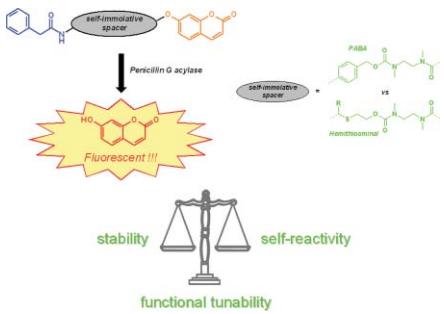
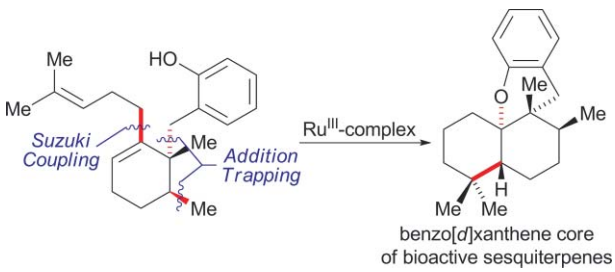
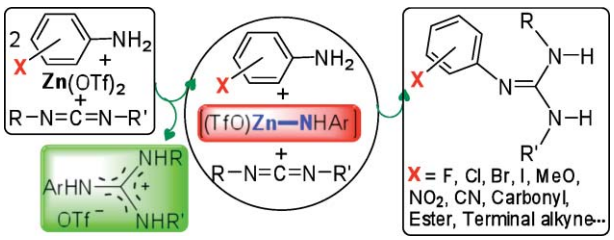








1816

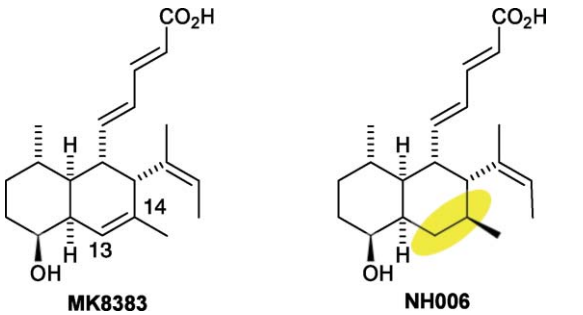


$Zn(OTf)_2$-catalyzed addition of amines to carbodiimides: efficient synthesis of guanidines and unpredicted formation of Zn–N amido species

Dongzhen Li, Jie Guang, Wen-Xiong Zhang,* Yang Wang and Zhenfeng Xi*

$Zn(OTf)_2$ acts as an excellent catalyst precursor for addition of various amines to carbodiimides under an atmosphere of air, offering a convenient synthesis of guanidines with high functional-group tolerance. A Zn–N amido species acts as the active species.

1821

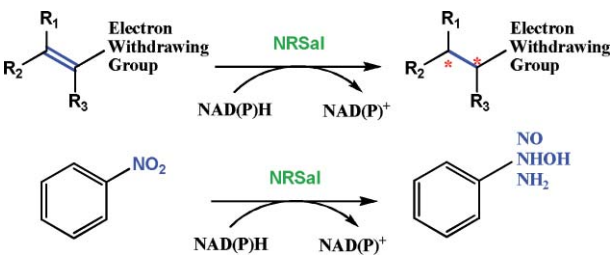


Synthesis of NH006—a photostable fungicide effective against *Botrytis cinerea*—according to the asymmetric total synthesis of MK8383

Nobuyuki Hayashi, Kentaro Yamamoto, Nobuto Minowa, Masaaki Mitomi and Masahisa Nakada*

We report the synthesis of NH006, an MK8383 derivative with a saturated C13-14 double bond and (*S*) configuration at C14, based on the asymmetric total synthesis of MK8383. NH006 exhibits good photostability and potent antifungal activity against *B. cinerea*.

1826

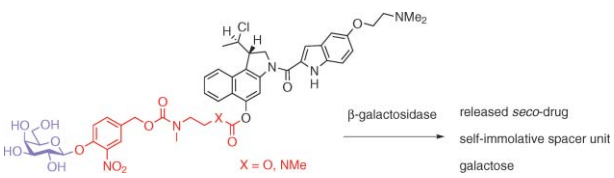


Nitroreductase from *Salmonella typhimurium*: characterization and catalytic activity

Yanto Yanto, Mélanie Hall and Andreas S. Bommarius*

Nitroreductase NRSal from *Salmonella typhimurium* displays both nitroreductase and enoate reductase activity in the asymmetric reduction of C=C bonds and aromatic nitro compounds. It also demonstrated the first single isolated enzyme-catalyzed reduction of nitrobenzene to aniline.

1833



Synthesis of the first spacer containing prodrug of a duocarmycin analogue and determination of its biological activity

Heiko J. Schuster, Birgit Krewer, J. Marian von Hof, Kianga Schmuck, Ingrid Schuberth, Frauke Alves and Lutz F. Tietze*

The synthesis of a spacer prodrug is presented, which allows selective activation at the tumour site releasing the cytostatic after sufficient self-immolation of an introduced spacer unit with an $IC_{50} = 750$ pM.

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- Applications of C-H and C-X bond activation in organic synthesis

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Jennifer Love
The University of British Columbia, Canada

William D. Jones
University of Rochester, USA

Aiwen Lei
Wuhan University, China

Zhang-jie Shi
Peking University, China

Invited speakers

Robin Bedford
University of Bristol, UK

John M. Brown
University of Oxford, UK

Stuart Macgregor
Heriot-Watt University, Edinburgh, UK

Hans de Vries
DSM Pharmaceutical Products, The Netherlands

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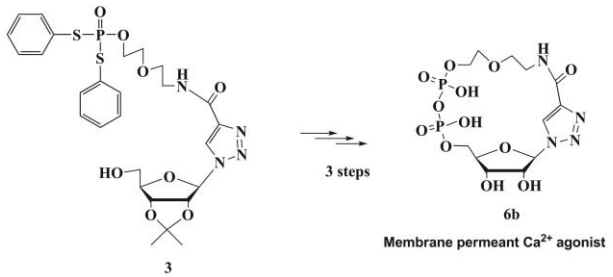
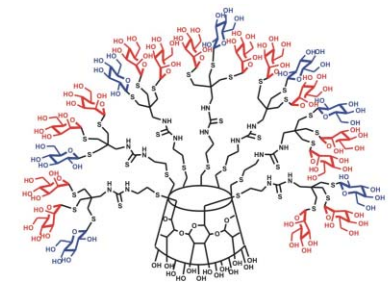


Novel nucleobase-simplified cyclic ADP-ribose analogue: A concise synthesis and Ca^{2+}-mobilizing activity in T-lymphocytes

Lingjun Li, Cornelia C. Siebrands, Zhenjun Yang, Liangren Zhang, Andreas H. Guse and Lihe Zhang*

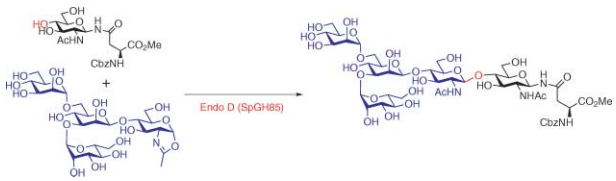
A purine nucleobase-simplified cyclic ADP ribose (cADPR) analogue was synthesized. It exhibits calcium release activity in intact T-lymphocytes, and indicates that it is a membrane-permeable cADPR mimic.



Comparative studies on lectin–carbohydrate interactions in low and high density homo- and heteroglycoclusters

Marta Gómez-García, Juan M. Benito, Ricardo Gutiérrez-Gallego, Alfredo Maestre, Carmen Ortiz Mellet, José M. García Fernández and José L. Jiménez Blanco*

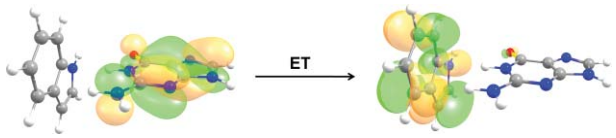
A versatile synthetic procedure to construct a series of high- and low-density homo- and heteroglycoclusters is reported. The binding properties of these multivalent glycoconjugates to Con A, a model lectin, have been assessed by using a range of competitive and non-competitive binding assays including ELLA, ITC and SPR.



Streptococcus pneumoniae endohexosaminidase D; feasibility of using *N*-glycan oxazoline donors for synthetic glycosylation of a GlcNAc-asparagine acceptor

Thomas B. Parsons, Mitul K. Patel, Alisdair B. Boraston, David J. Vocadlo and Antony J. Fairbanks*

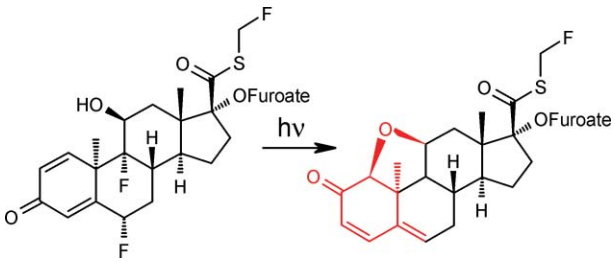
Endohexosaminidase D, a family 85 glycoside hydrolase from *S. pneumoniae*, catalyses the glycosylation of a GlcNAc-bearing glycosyl amino acceptor using *N*-glycan oxazoline oligosaccharides as donors, demonstrating the synthetic potential of this enzyme as a biocatalyst for the synthesis of defined glycoconjugates.

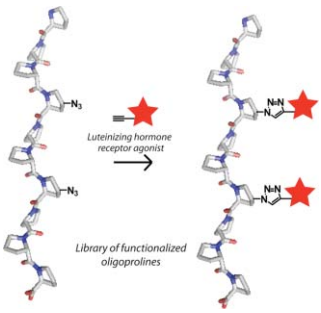


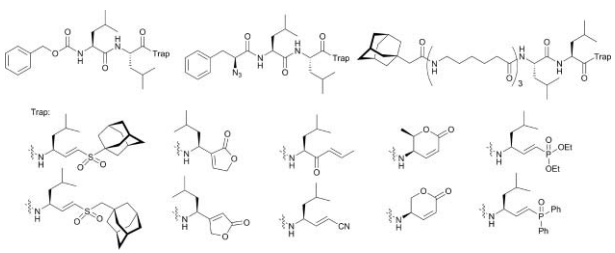
Electron transfer from aromatic amino acids to guanine and adenine radical cations in π stacked and T-shaped complexes

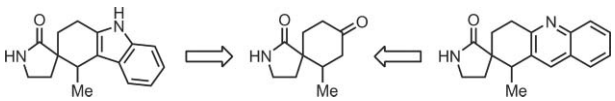
Cristina Butchosa, Sílvia Simon* and Alexander A. Voityuk*

Efficient electron transfer (ET) from aromatic amino acid residues to guanine and adenine radical cations has been found in T-shaped complexes. Thus, π stacking of the donor and acceptor sites is not required for the repair of oxidized nucleobases.









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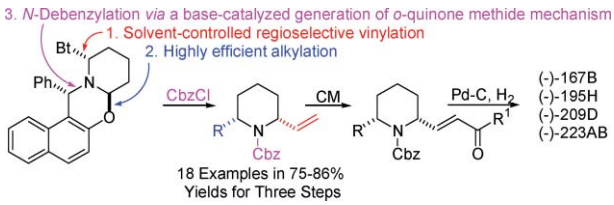
1899

Enantiopure 2,6-disubstituted piperidines bearing one alkene- or alkyne-containing substituent: preparation and application to total syntheses of indolizidine-alkaloids

Hui Liu, Deyong Su, Guolin Cheng, Jimin Xu, Xinyan Wang* and Yuefei Hu*

A general and efficient preparation of enantiopure 2,6-disubstituted piperidines bearing one alkene- or alkyne-containing substituent was developed. By using this method, total syntheses of (–)-167B, (–)-195H, (–)-209D and (–)-223AB were accomplished efficiently.

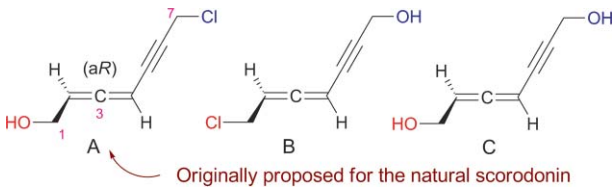


1905

Synthesis of the structure proposed for the natural allenic antibiotic scorodonin

Ya-Jun Jian and Yikang Wu*

The structure originally proposed for the natural scorodonin (A) is supported by enantioselective synthesis despite the *ca.* 2 ppm differences in ^{13}C NMR, while B and C are excluded.

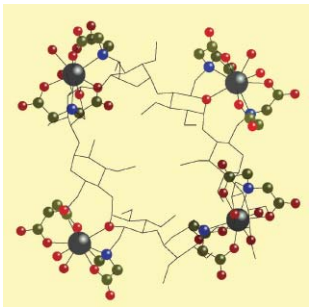


1910

Novel polycarboxylated EDTA-type cyclodextrins as ligands for lanthanide binding: study of their luminescence, relaxivity properties of Gd(III) complexes, and PM3 theoretical calculations

D. Maffeo, M. Lampropoulou, M. Fardis, Y. G. Lazarou, I. M. Mavridis, D. A. I. Mavridou, E. Urso, H. Pratsinis, D. Kletsas and K. Yannakopoulou*

Polycarboxylated **EDTA**-type CDs coordinate with lanthanide cations. The complexes with Gd(III) display exceptionally high relaxivity values and low toxicity, and thus are promising MRI contrast agents.

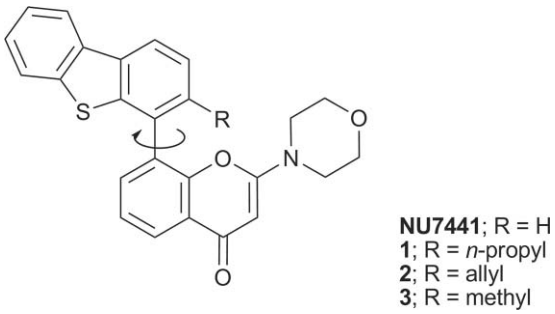


1922

Atropisomeric 8-arylchromen-4-ones exhibit enantioselective inhibition of the DNA-dependent protein kinase (DNA-PK)

Céline Cano,* Bernard T. Golding, Karen Haggerty, Ian R. Hardcastle, Marcus Peacock and Roger J. Griffin

We describe the development and resolution of the first atropisomeric DNA-PK inhibitors. Interestingly and as predicted, the biological evaluation of the pairs of atropisomers showed a marked difference in potency, with only one enantiomer being biologically active.

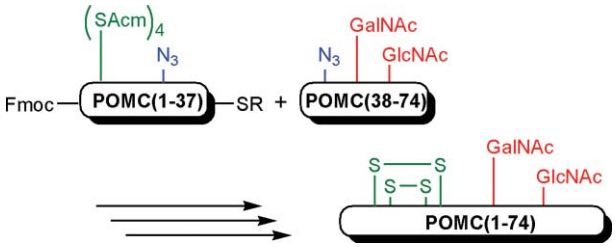


1966

Chemical synthesis of mouse pro-opiomelanocortin(1–74) by azido-protected glycopeptide ligation *via* the thioester method

Hidekazu Katayama,* Hironobu Hojo,* Ichiko Shimizu, Yuko Nakahara and Yoshiaki Nakahara

The use of azidopeptide as a building block facilitated the chemoselective peptide ligation by the thioester method. A glycoprotein was successfully synthesized by this method.



* Indicates the author for correspondence: see article for details.

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