# Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry

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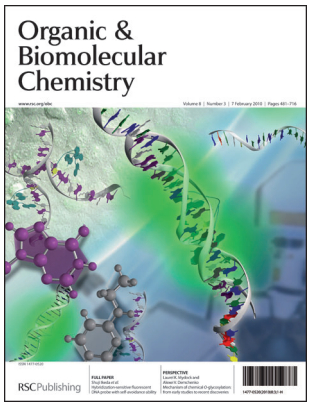
## IN THIS ISSUE

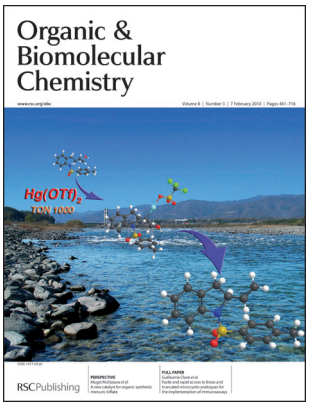
ISSN 1477-0520 CODEN OBCRAK 8(3) 481–716 (2010)




**Cover**

See Shuji Ikeda *et al.*, pp. 546–551. Inosine (purple)–ethylcytosine (gray) base pair is unstable. The probes containing inosines, ethylcytosines and thiazole orange labels can avoid their self-dimerization (left) and emit hybridization-sensitive fluorescence by hybridization with the target RNA (center).

Image reproduced by permission of Akimitsu Okamoto from *Organic & Biomolecular Chemistry*, 2010, **8**, 546.



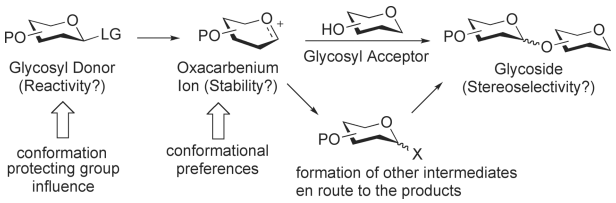

**Inside cover**

See Mugio Nishizawa *et al.*, pp. 511–521. Rich and clean stream of Yoshino-gawa river, Tokushima, Japan. $Hg(OTf)_2$-catalyzed reaction takes place smoothly in high catalytic turnover under mild conditions.

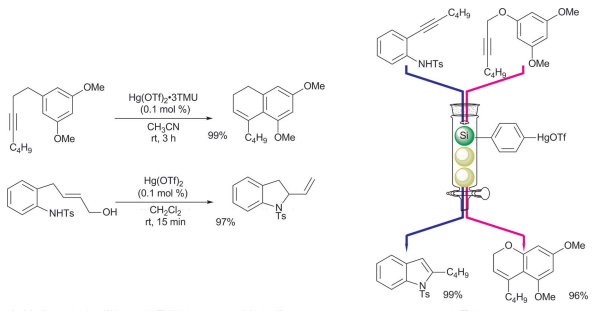
Image reproduced by permission of Mugio Nishizawa from *Organic & Biomolecular Chemistry*, 2010, **8**, 511.

## PERSPECTIVES







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# Organic & Biomolecular Chemistry

## An international journal of synthetic, physical and biomolecular organic chemistry

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*Organic & Biomolecular Chemistry* brings together molecular design, synthesis, structure, function and reactivity in one journal. It publishes fundamental work on synthetic, physical and biomolecular organic chemistry as well as all organic aspects of: chemical biology, medicinal chemistry, natural product chemistry, supramolecular chemistry, macromolecular chemistry, theoretical chemistry, and catalysis.



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Full details on how to submit material for publication in Organic & Biomolecular Chemistry are given in the Instructions for Authors (available from http://www.rsc.org/authors). Submissions should be made *via* the journal's homepage: http://www.rsc.org/obc.

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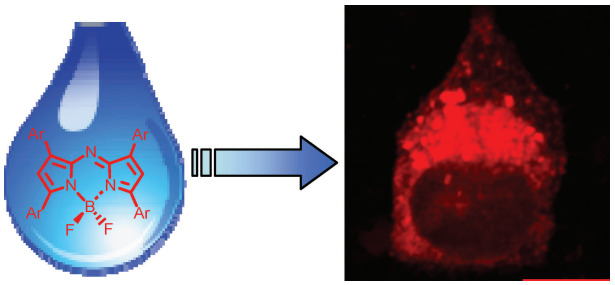



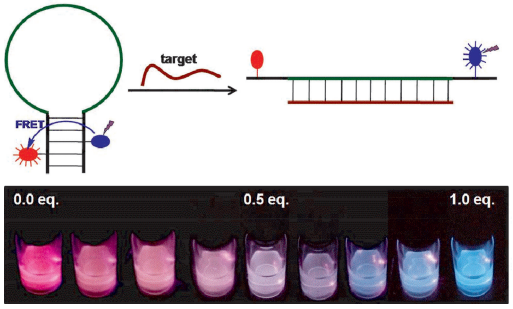




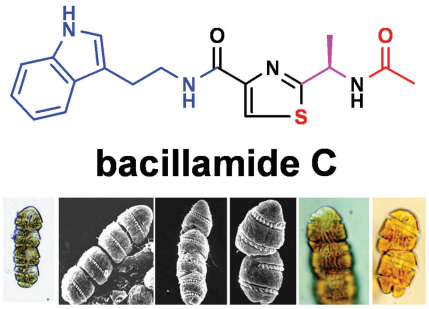




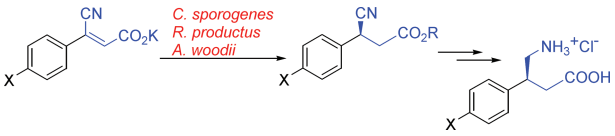

DALTON DIVISION AND ORGANIC DIVISION

# Dalton Discussion 12:
# Catalytic C-H and C-X Bond Activation

13 - 15 September 2010
Durham University, UK
www.rsc.org/DD12

## Call for posters now open

Organised jointly by the Dalton Division and Organic Division, DD12 will bring together the organic, organometallic and inorganic (coordination chemistry) communities from academia and industry to discuss the current state of the art, the development and future of late metal-catalysed cross-coupling strategies involving C-X and/or C-H bonds.

The meeting will highlight the importance of catalytic bond activation in cross-coupling chemistry. The latest research will be presented and discussed.

## Topics

- Synthetic chemistry (including applications)
- Inorganic and organometallic chemistry
- Reaction mechanism (physical organic and organometallic chemistry)
- Transition metal catalysis
- Applications of C-H and C-X bond activation in organic synthesis

## Keynote speakers

**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*

**Offers of contributed papers related to the listed themes for poster presentation are invited by 16 July 2010.**
Visit **www.rsc.org/DD12** for further information.

## Registration will open in spring 2010.

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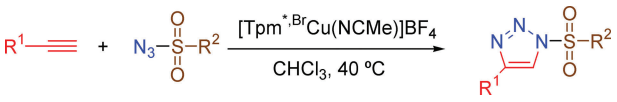




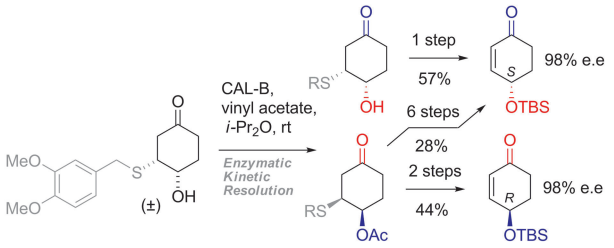




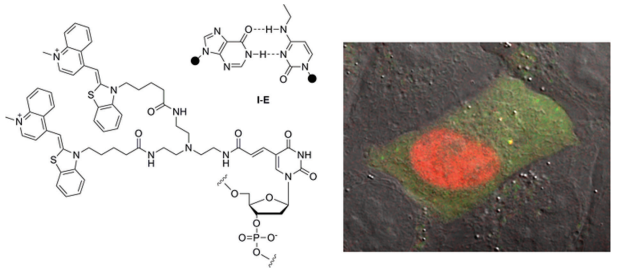




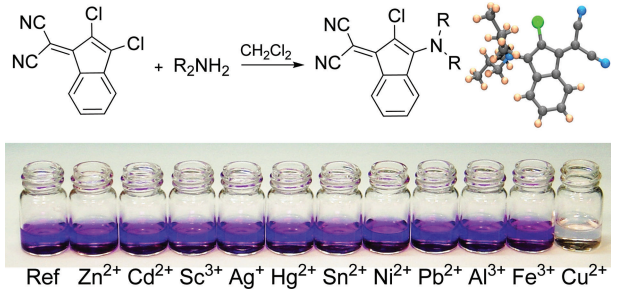

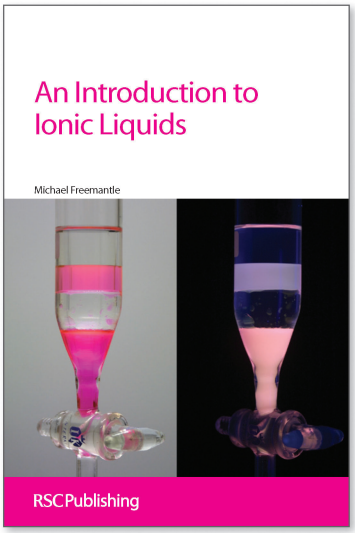


# An Introduction to Ionic Liquids

## Michael Freemantle

This is the first single-author book on ionic liquids and the first introductory book on the topic. An Introduction to Ionic Liquids is written in a clear, concise and consistent way and provides a useful introduction to ionic liquids for those readers who are not familiar with the topic. It is also wide ranging, embracing every aspect of the chemistry and applications of ionic liquids. The book draws extensively on the primary scientific literature to provide numerous examples of research on ionic liquids. These examples will enable the reader to become familiar with the key developments in ionic liquids chemistry over recent years.

Science students, researchers, teachers in academic institutions and chemists and other scientists in industry and government laboratories will find the book an invaluable introduction to one of the most rapidly advancing and exciting fields of science and technology today.

BB Hardback | 281 pages | ISBN 9781847551610 | 2009 | £39.95



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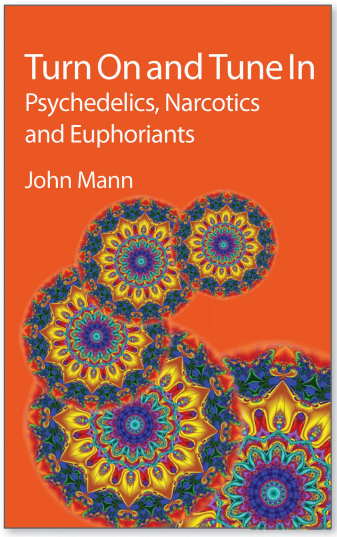


# Turn On and Tune In

## Psychedelics, Narcotics and Euphoriants

## John Mann

John Mann from Queen's University of Belfast has brought together details of the historical, anthropological and sociological importance of a range of psychoactive substances (both natural and synthetic) including LSD, opium, heroin, cocaine, cannabis, peyote, belladonna, mandrake, and absinthe. He has highlighted the colourful figures, both famous and infamous, involved in drug production, trafficking or use such as Albert Hofmann, Timothy Leary, Thomas de Quincey, Wilde, and many pop stars – John Lennon, Jerry Garcia of the Grateful Dead, Mick Jagger etc.

The basic chemistry and pharmacology are covered together with a brief account of useful drugs that have emerged from a study of the psychoactive ones. This book can be enjoyed by both the scientist and general reader and tells a fascinating story.

BB Hardback | 160 pages | ISBN 9781847559098 | 2009 | £24.95

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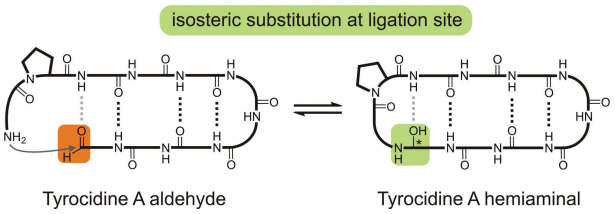
## The reversible macrocyclization of Tyrocidine A aldehyde: a hemiaminal reminiscent of the tetrahedral intermediate of macrolactamization

Sebastian Enck, Florian Kopp, Mohamed A. Marahiel* and Armin Geyer*

The carboxylate at the native ligation site of Tyrocidine A was isosterically substituted by an aldehyde, which subsequently closes reversibly and stereoselectively to a stable hemiaminal, enabling the NMR spectroscopic analysis of the macrocyclization equilibrium.

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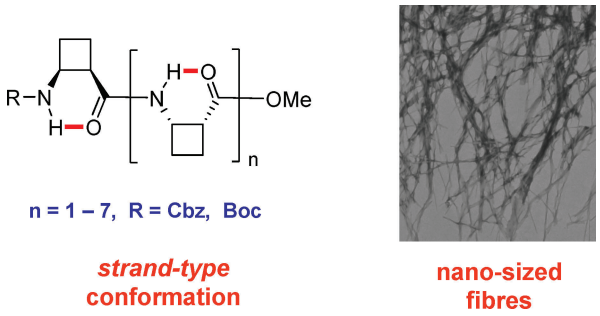
## Folding and self-assembling with β-oligomers based on (1*R*,2*S*)-2-aminocyclobutane-1-carboxylic acid

Elisabeth Torres, Esther Gorrea, Kepa K. Burusco, Eric Da Silva, Pau Nolis, Federico Rúa, Stéphanie Boussert, Ismael Díez-Pérez, Samantha Dannenberg, Sandra Izquierdo, Ernest Giralt, Carlos Jaime, Vicenç Branchadell and Rosa M. Ortuño*

All *cis*-cyclobutane β-oligomers show a strand-type preferential conformation in solution. These compounds self-assemble to give nano-sized fibres and some of them also form gels.

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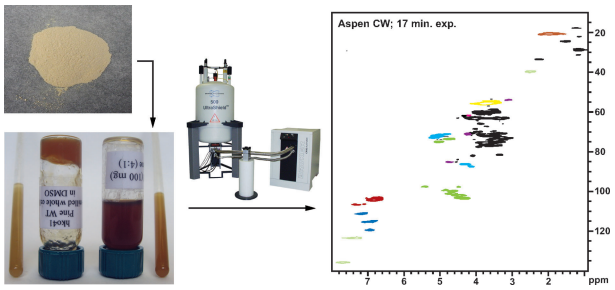
## Solution-state 2D NMR of ball-milled plant cell wall gels in DMSO-$d_6$/pyridine-$d_5$

Hoon Kim* and John Ralph

2D solution-state NMR (HSQC) fingerprinting of entire plant cell wall fractions (*i.e.* without component fractionation) has been improved by using DMSO-$d_6$/pyridine-$d_5$ (4 : 1, v/v) gels.

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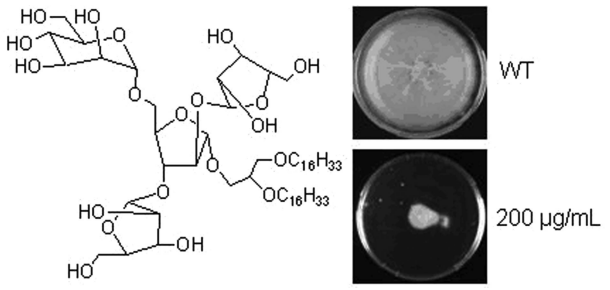
## Synthetic arabinomannan glycolipids and their effects on growth and motility of the *Mycobacterium smegmatis*

Kottari Naresh, Binod Kumar Bharati, Prakash Gouda Avaji, Narayanaswamy Jayaraman* and Dipankar Chatterji*

Synthetic arabinomannan glycolipids, relevant to mycobacterial cell-wall components, acted as inhibitors of growth through reduced biofilm formation and impaired motility of bacteria.



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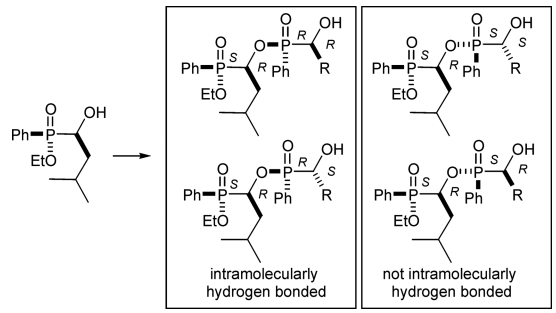
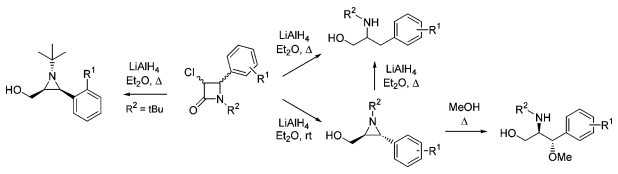



## A synthesis of oligomeric α-hydroxy phenylphosphinates and a study of the conformational preferences of the dimers

Kamyar Afarinkia,* Martin Royappa, Ian J. Scowen, Jonathan W. Steed and Hiu-wan Yu

A combination of NMR spectroscopy, X-ray crystallography and computational methods is used to show that the folding patterns of a novel class of oligomers is determined by relative configuration of the carbon and phosphorus stereocenters.

607

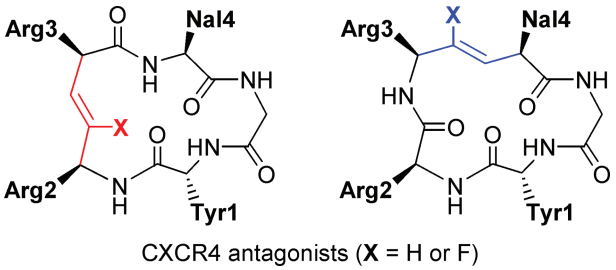


## Stereoselective synthesis of *trans*- and *cis*-2-aryl-3-(hydroxymethyl)aziridines through transformation of 4-aryl-3-chloro-β-lactams and study of their ring opening

Matthias D'hooghe, Karen Mollet, Stijn Dekeukeleire and Norbert De Kimpe*

*trans*- and *cis*-1-Alkyl-4-aryl-3-chloroazetidin-2-ones were transformed into *trans*- and *cis*-2-aryl-3-(hydroxymethyl)aziridines *via* reductive ring contraction.

616




## Synthesis and biological evaluation of selective CXCR4 antagonists containing alkene dipeptide isosteres

Tetsuo Narumi, Ryoko Hayashi, Kenji Tomita, Kazuya Kobayashi, Noriko Tanahara, Hiroaki Ohno, Takeshi Naito, Eiichi Kodama, Masao Matsuoka, Shinya Oishi* and Nobutaka Fujii*

A set of cyclic peptide analogues of a selective CXCR4 antagonist FC131 were synthesized and bioevaluated. The CXCR4 antagonism and anti-HIV activity was demonstrated. FC131 and the analogues were shown to selectively inhibit SDF-1 binding to CXCR4.

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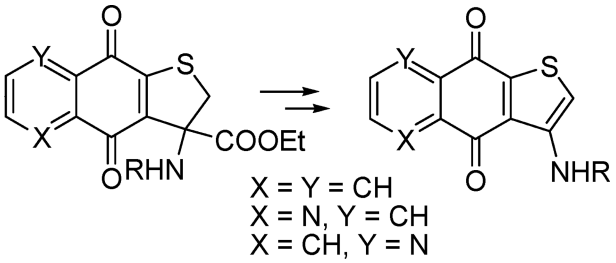


## Unprecedented synthesis of a novel amino quinone ring system *via* oxidative decarboxylation of quinone-based α,α-amino esters

Pietro Campiglia, Claudio Aquino, Alessia Bertamino, Nicoletta De Simone, Marina Sala, Sabrina Castellano, Marisabella Santoriello, Paolo Grieco, Ettore Novellino and Isabel M. Gomez-Monterrey*

An efficient synthesis of new quinone derivatives through an α,α-amino ester oxidative decarboxylation provides access to new building blocks for the development of potential antitumoral agents.

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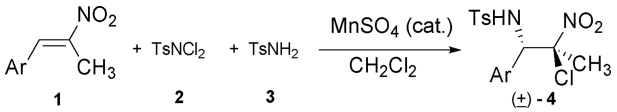
## New catalytic system for aminohalogenation of β-methyl-β-nitrostyrenes to give opposite regiochemistry

San-Jun Zhi, Hao Sun, Guangqian Zhang, Guigen Li* and Yi Pan*

A new combination of catalyst and co-additive was found for the aminohalogenation of β-methyl-β-nitrostyrenes with 4-$TsNCl_2$ by using $MnSO_4$ as the catalyst. A mechanism involving the formation of chloronium intermediate was proposed.

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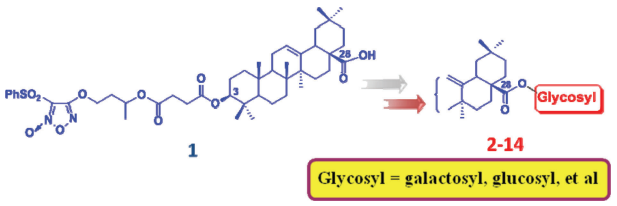
## Synthesis and *anti*-human hepatocellular carcinoma activity of new nitric oxide-releasing glycosyl derivatives of oleanolic acid

Zhangjian Huang, Yihua Zhang,* Li Zhao, Yongwang Jing, Yisheng Lai, Luyong Zhang,* Qinglong Guo, Shengtao Yuan, Jianjun Zhang, Li Chen, Sixun Peng and Jide Tian

A series of NO-releasing glycosyl derivatives (**2–14**) of oleanolic acid were synthesized, and **3** exhibited better solubility and strong cytotoxicity against human HCC than the active compound **1**.

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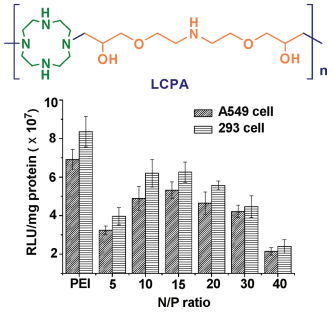
## Linear cyclen-based polyamine as a novel and efficient reagent in gene delivery

Yong-Zhe Xiang, Zhi-Hua Feng, Ji Zhang,* Yi-Le Liao, Chuan-Jiang Yu, Wen-Jing Yi, Wen Zhu* and Xiao-Qi Yu*

Novel linear cyclen-based polyamine (LCPA) could act as an effective non-viral gene vector towards both A549 and 293 cell lines.

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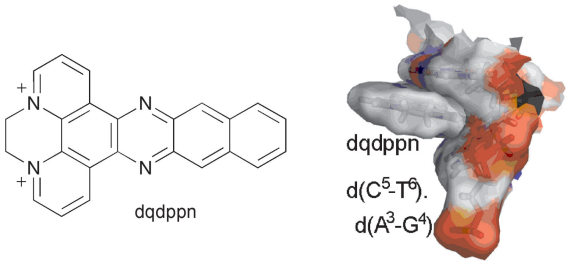
## Structural analysis of the binding of the diquaternary pyridophenazine derivative dqdppn to B-DNA oligonucleotides

Philip Waywell, James A. Thomas* and Mike P. Williamson*

The interaction of dqdppn with several hexa- and octanucleotide duplexes has been studied. The NMR-derived structural model of two of the binding complexes demonstrates that dqdppn intercalates from the major groove in an unusual 'side-on' geometry, rather than threading through the helix.



# Advances in Synthetic Biology

## 4 - 5 March 2010, London, England

Synthetic biology is the design and construction of new biological parts, devices and systems (and the re-design of existing, natural biological systems) for useful purposes. Its interdisciplinary nature between science and engineering, as well as the many potential applications in the health, material and energy sectors, make this a particularly interesting conference.

**Confirmed Speakers include:**

**Alfonson Jaramillo**, Professor, Ecole Polytechnique
**Yannis Kaznessis**, Associate Professor, University of Minnesota
**Neil Cameron**, Professor, University of Durham
**Wilfried Weber,** Professor, Swiss Federal Institute of Technology
**Peer Staehler,** Chief Scientific Officer, Febit
**Milan Stojanovic,** Head of Group, Columbia University
**Ralph Wagner,** Chief Executive Officer, GeneArt
**Gerard Markx,** Research Group Leader, Heriot Watt University
**Alistair Elfick,** Professor, Edinburgh University
**Howard Salis,** Assistant Professor, Pennsylvania State University
**Douglas Densmore,** PostDoc, Synthetic Biology Engineering Research Centre
**John Ward,** Professor, University College London
**Andreas Herrmann,** Professor, University of Groningen
**Raphael Gubeli,** Professor, University of Freiburg
**Sitta Sittampalam,** Professor, Unviersity of Kansas Cancer Centre
**James Brown,** University of Cambridge

Be part of the event

We are currently accepting poster submissions.
Details can be found online.

For sponsorship and exhibition opportunities contact Aaron Woodley
tel: +44 (0) 1787 315117 email: a.woodley@selectbiosciences.com

Agenda Topics to include:

- The Chemistry of Synthetic Biology
- Protein, Metabolic & Therapeutic Engineering
- Bioinformatics and Software Modelling in Synthetic Biology
- Cell & Tissue Engineering
- The Road Towards the Rational and Systemic Design of Novel Biological Systems

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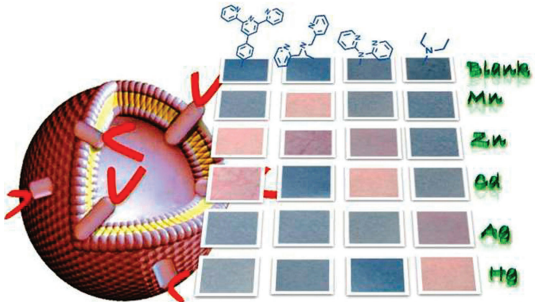




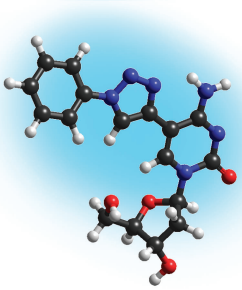



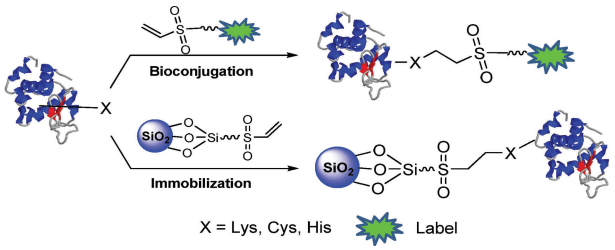




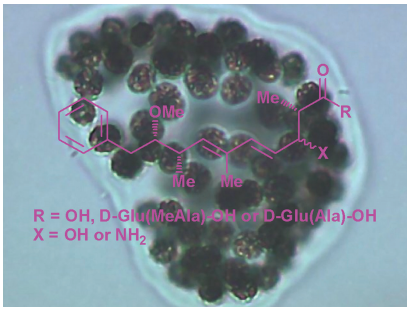

## 2010 Meetings (in chronological order)

NF-κB in Inflammation & Disease
Advances in Biopharmaceuticals
Structural Biology
Structural Genomics: Expanding the Horizons of Structural Biology
Triglycerides & Triglyceride-Rich Particles in Health & Disease (new!)
Alzheimer's Disease Beyond Aβ
Molecular Basis for Biological Membrane Organization & Dynamics
HIV Biology & Pathogenesis
RNA Silencing: Mechanism, Biology & Application
Molecular Basis for Chromatin Structure & Regulation
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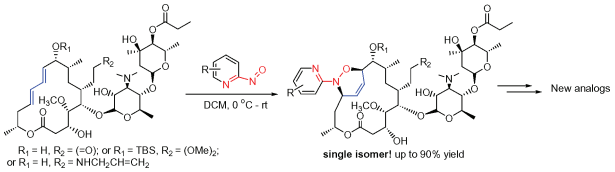
## Preparation and biological evaluation of novel leucomycin analogs derived from nitroso Diels–Alder reactions

Baiyuan Yang, Tina Zöllner, Peter Gebhardt, Ute Möllmann and Marvin J. Miller*

Novel macrolide analogs were synthesized using nitroso Diels–Alder reactions of leucomycin A7 and subsequent chemical modifications. Hetero cycloaddition reactions proceeded in a highly regio- and stereoselective fashion. Most analogs retained antibiotic profiles similar to leucomycin A7, and, in contrast to leucomycin itself, several exhibited moderate antiproliferative and cytotoxic activity.

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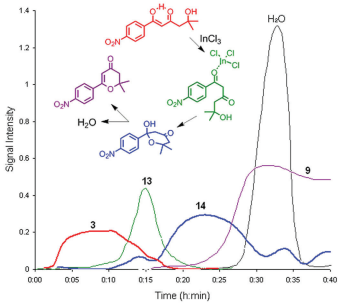
## Highly efficient indium(III)-mediated cyclisation of 5-hydroxy-1,3-diketones to 2,3-dihydro-4*H*-pyran-4-ones; mechanistic insights from *in situ* Fourier transform infrared spectroscopy

P. C. Andrews,* W. J. Gee, P. C. Junk and H. Krautscheid

Cyclisation of δ-hydroxy-β-diketones to 2,3-dihydro-4*H*-pyran-4-ones occurs efficiently in the presence of a catalytic amount of anhydrous $InCl_3$ and a dehydrating agent, with *in situ* FTIR studies indicating a reaction mechanism sensitive to both temperature and reagent concentration.

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## Reaction of carbon nucleophiles with alkylideneindazolium and alkylideneindolium ions generated from their 3-(1-arylsulfonylalkyl) indazole and indole precursors

Laura Marsili, Alessandro Palmieri and Marino Petrini*

Nucleophilic substitution of *p*-toluenesulfinate anion on sulfonyl indazoles and sulfonyl indoles is carried out *via* the corresponding iminium ion generated by reaction with $AlEtCl_2$.