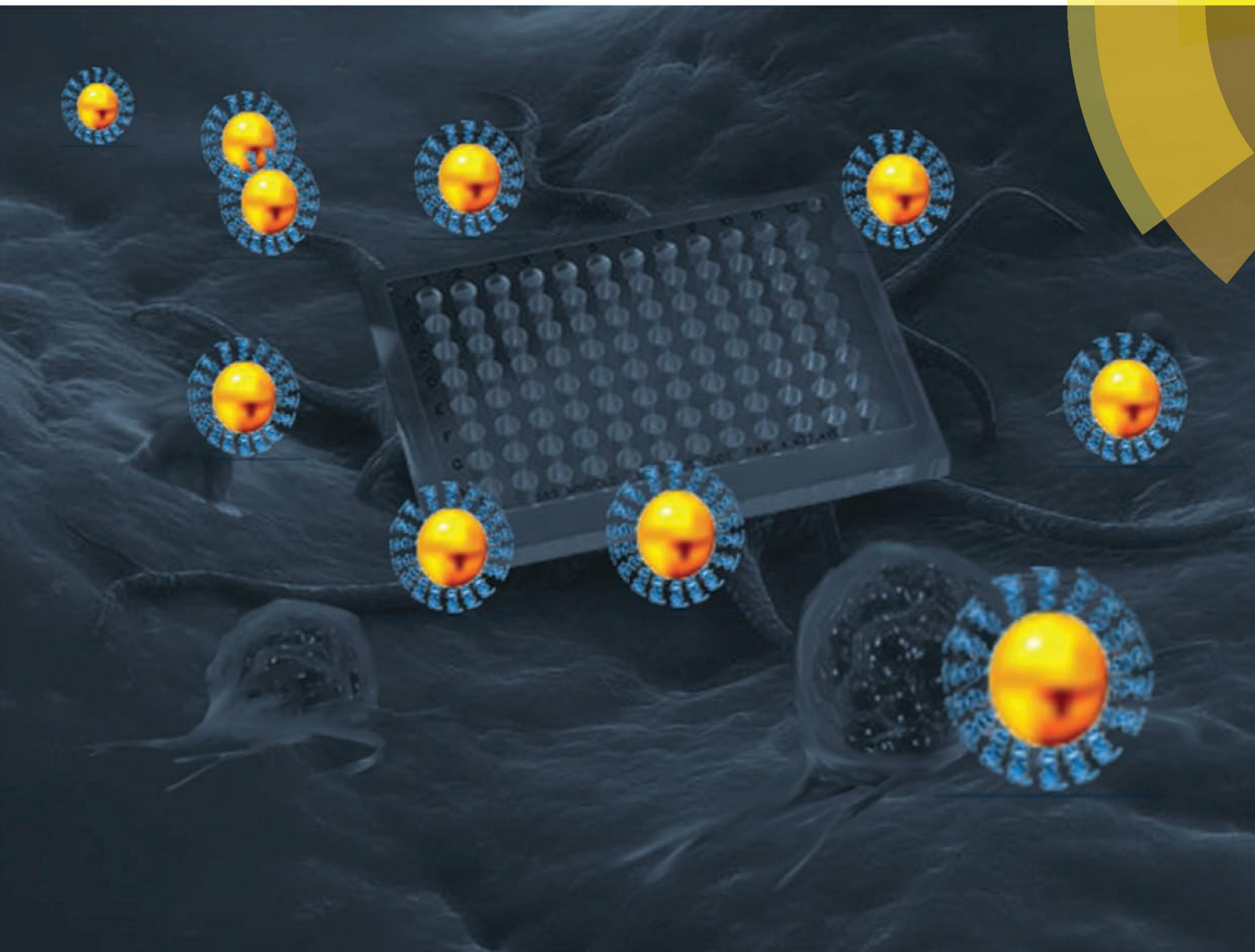


# Organic & Biomolecular Chemistry

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ISSN 1477-0520



## PAPER

Sabine Schlecht *et al.*  
Synthesis of tumor-associated MUC1-glycopeptides and their multivalent presentation by functionalized gold colloids

# Organic & Biomolecular Chemistry

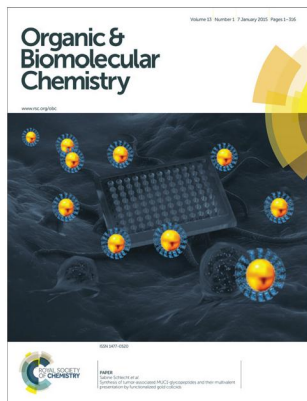
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## IN THIS ISSUE

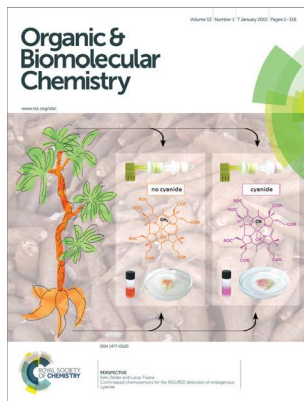
ISSN 1477-0520 CODEN OBCRAK 13(1) 1–316 (2015)



### Cover

See Sabine Schlecht *et al.*, pp. 81–97.

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### Inside cover

See Felix Zelder and Lucas Tivana, pp. 14–17.

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## PERSPECTIVES

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### Corrin-based chemosensors for the ASSURED detection of endogenous cyanide

Felix Zelder\* and Lucas Tivana\*

Cassava (*Manihot esculenta* Crantz) is a staple food for more than 500 million people, especially in Africa and South America.

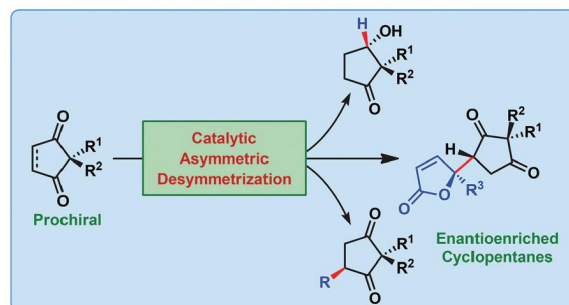


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### Catalytic asymmetric desymmetrization approaches to enantioenriched cyclopentanes

Madhu Sudan Manna and Santanu Mukherjee\*

Asymmetric desymmetrization represents an excellent strategy for obtaining highly functionalized chiral building blocks. However, the application of this strategy for the synthesis of cyclopentane derivatives remained limited, when compared to cyclohexanes. Here, we give an overview of asymmetric desymmetrization reactions leading to enantioenriched cyclopentanes.





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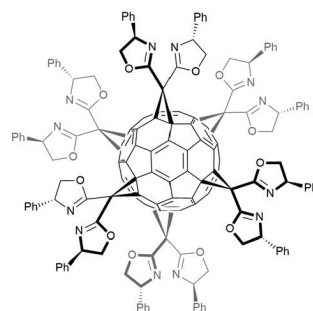
## REVIEW

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### Synthesis of highly functionalized C<sub>60</sub> fullerene derivatives and their applications in material and life sciences

Weibo Yan,\* Stefan M. Seifermann, Philippe Pierrat and Stefan Bräse\*

Highly functionalized fullerenes can be efficiently constructed by various techniques.



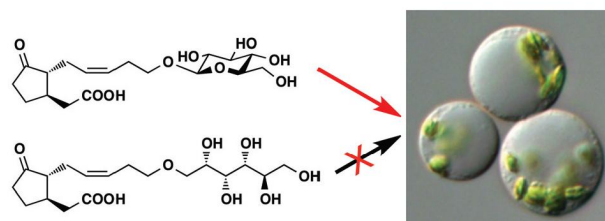
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### Functional importance of the sugar moiety of jasmonic acid glucoside for bioactivity and target affinity

Minoru Ueda,\* Gangqiang Yang, Yuuki Nukadzuka, Yasuhiro Ishimaru, Satoru Tamura and Yoshiyuki Manabe

Importance of the D-glycopyranoside structure for the bioactivity and target affinity of jasmonic acid glucoside.

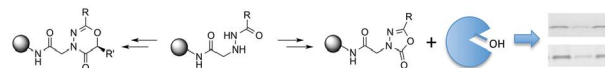


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### Solid phase synthesis of 1,3,4-oxadiazin-5 (6R)-one and 1,3,4-oxadiazol-2-one scaffolds from acyl hydrazides

Bani Kanta Sarma, Xiaodan Liu, Hao Wu, Yu Gao and Thomas Kodadek\*

Solid phase synthesis of 1,3,4-oxadiazin-5(6R)-one and 1,3,4-oxadiazol-2-one scaffolds from resin-bound acyl hydrazides is described.

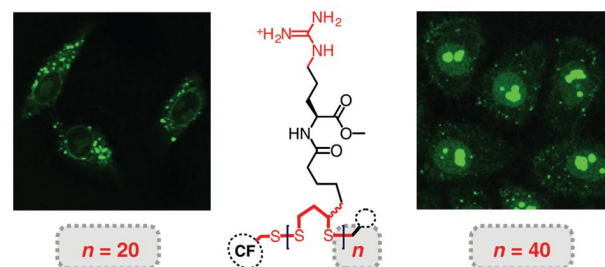


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### Cell-penetrating poly(disulfide)s: the dependence of activity, depolymerization kinetics and intracellular localization on their length

Nicolas Chuard, Giulio Gasparini, Aurélien Roux, Naomi Sakai and Stefan Matile\*

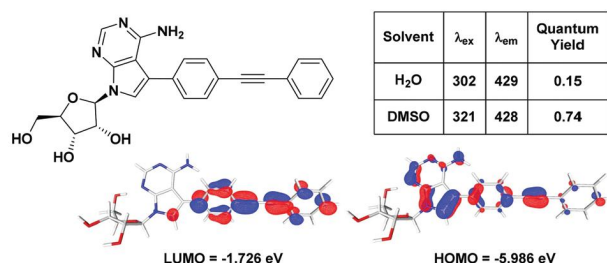
We report that, with the increasing length, cell-penetrating poly(disulfide)s preferably accumulate in the endosomes, cytosol and then the nucleoli.





## COMMUNICATIONS

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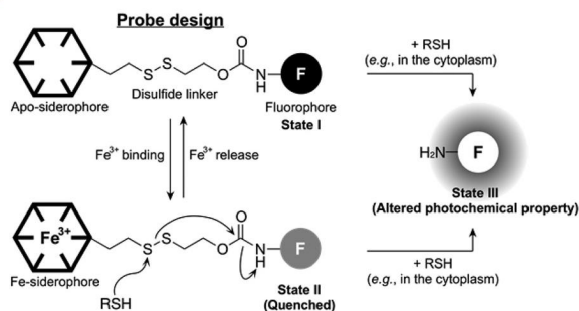


### Design and synthesis of fluorescent 7-deazaadenosine nucleosides containing $\pi$ -extended diarylacetylene motifs

Sara De Ornellas, John M. Slattery, Robert M. Edkins, Andrew Beeby, Christoph G. Baumann\* and Ian J. S. Fairlamb\*

A novel series of C-modified  $\pi$ -extended 7-deazaadenosines exhibit promising fluorescence properties.

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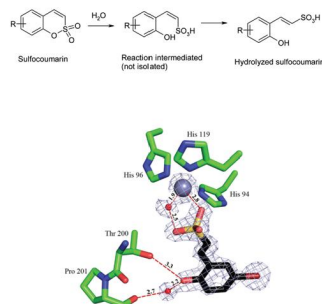


### Development of a novel fluorescence probe capable of assessing the cytoplasmic entry of siderophore-based conjugates

Hyeon Seok Kim, Woon Young Song and Hak Joong Kim\*

A novel fluorescence probe capable of assessing the cytoplasmic entry of siderophore-based conjugates was synthesized and evaluated by photochemical characterization and cell-based assays.

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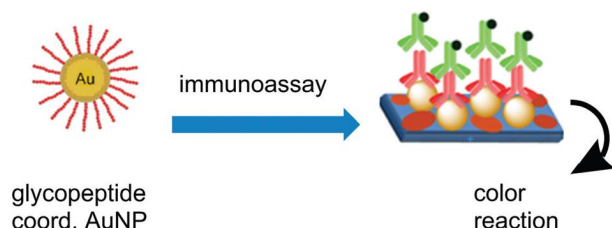
### 6-Substituted 1,2-benzoxathiine-2,2-dioxides are isoform-selective inhibitors of human carbonic anhydrases IX, XII and VA

Muhammet Tanc, Fabrizio Carta,\* Andrea Scozzafava and Claudiu T. Supuran\*

A series of 6-substituted 2-benzoxathiine-2,2-dioxides were synthesized starting from 2,5-dihydroxybenzaldehyde, and then screened *in vitro* for their inhibition properties against five human carbonic anhydrase (hCA, EC 4.2.1.1) isoforms.

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### Synthesis of tumor-associated MUC1-glycopeptides and their multivalent presentation by functionalized gold colloids

Isabella Tavernaro, Sebastian Hartmann, Laura Sommer, Heike Hausmann, Christian Rohner, Martin Ruehl, Anja Hoffmann-Roeder and Sabine Schlecht\*

The authors present the synthesis of novel MUC1-glycopeptide antigens and their multivalent presentation by gold colloids. Their biological activity was tested in a dot-blot immunoassay experiment.

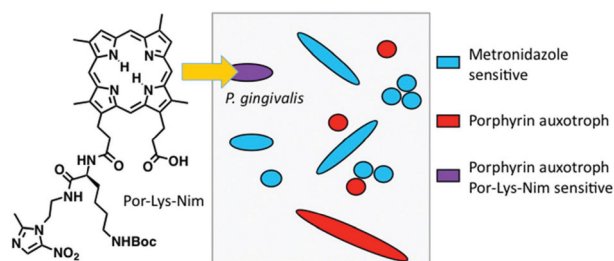
## PAPERS

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**Amino acid-linked porphyrin-nitroimidazole antibiotics targeting *Porphyromonas gingivalis***

Simon A. Dingsdag, Benjamin C-M. Yap, Neil Hunter and Maxwell J. Crossley\*

Amino acid-linked porphyrin-nitroimidazole adducts, as potent as metronidazole, are highly selective for *Porphyromonas gingivalis*.



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**Pd-catalyzed oxidative C–H alkenylation for synthesizing arylvinyltriazole nucleosides**

Jingjie Tang, Mei Cong, Yi Xia, Gilles Quéléver, Yuting Fan, Fanqi Qu and Ling Peng\*

Pd-catalyzed oxidative C–H alkenylation: an effective method for synthesizing arylvinyltriazole nucleosides in good yields and with large functional group tolerance.

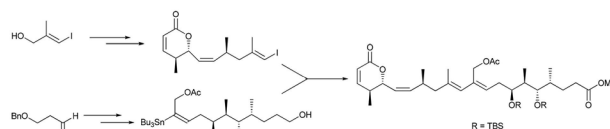


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**Synthesis of fully functionalized aglycone of lycoperdinoside A and B**

Balla Chandrasekhar, Sudhakar Athe, P. Purushotham Reddy and Subhash Ghosh\*

Synthesis of fully functionalized aglycone of lycoperdinoside A and B is achieved via Pd-catalyzed Stille–Migita cross coupling and Evans *syn*- and *anti* aldol reactions as key steps.

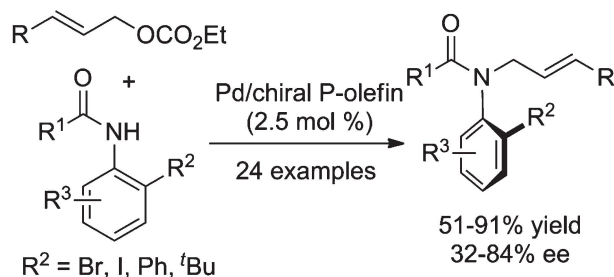


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**Asymmetric synthesis of axially chiral anilides by Pd-catalyzed allylic substitutions with P/olefin ligands**

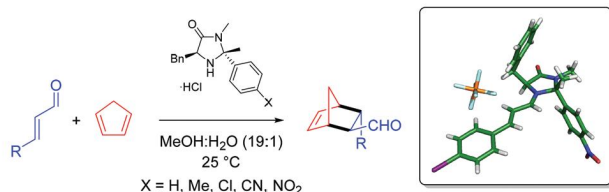
Yilin Liu, Xiangqing Feng\* and Haifeng Du\*

Palladium-catalyzed allylic substitutions of *ortho*-substituted anilides using P/olefin ligands were achieved to afford chiral anilides with up to 84% ee.





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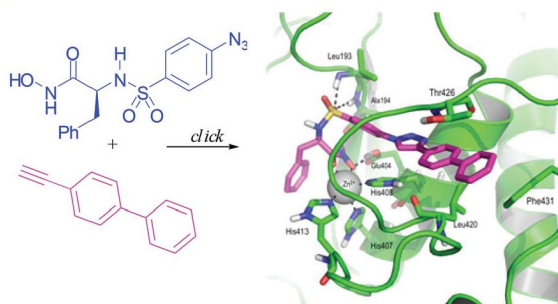


### Improving catalyst activity in secondary amine catalysed transformations

John B. Brazier, Timothy J. K. Gibbs, Julian H. Rowley, Leopold Samulis, Sze Chak Yau, Alan R. Kennedy, James A. Platts and Nicholas C. O. Tomkinson\*

Improved catalytic efficiency has been observed in the Diels-Alder cycloaddition by modification of the imidazolidinone architecture.

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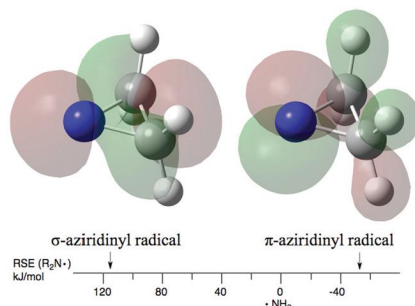


### Design and synthesis of potent hydroxamate inhibitors with increased selectivity within the gelatinase family

José María Zapico, Anna Puckowska, Kamila Filipiak, Claire Coderch, Beatriz de Pascual-Teresa\* and Ana Ramos\*

Triazole-based inhibitors with high potency and selectivity for MMP-2 were obtained through a click chemistry approach.

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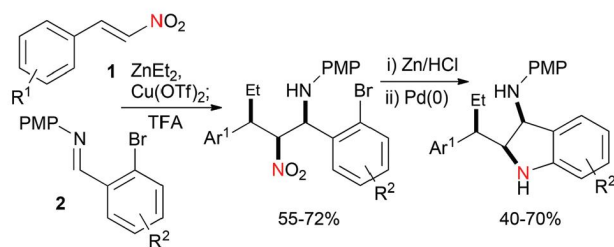


### The stability of nitrogen-centered radicals

Johnny Hioe, Davor Šakić, Valerije Vrček\* and Hendrik Zipse\*

Radical stabilization energies (RSEs) for a large variety of aminyl and protonated amine radical cations have been calculated using high-level composite procedures.

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### Stereoselective synthesis of 1,2-diamine containing indolines by a conjugate addition nitro-mannich reaction

James C. Anderson,\* Ian B. Campbell, Sebastien Campos, Jonathan Shannon and Derek A. Tocher

The sequential use of the conjugate addition nitro-Mannich reaction, nitro reduction and then Pd-catalyzed intramolecular cyclisation allows the concise, stereodivergent synthesis of complex indolines.

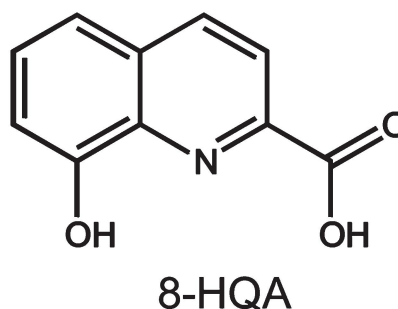
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### Biosynthesis of 8-hydroxyquinoline-2-carboxylic acid, an iron chelator from the gut of the lepidopteran *Spodoptera littoralis*

Jelena Pesek, Jiří Svoboda, Martina Sattler, Stefan Bartram and Wilhelm Boland\*

8-HQA is generated in the gut of Noctuid larvae from tryptophan as an iron chelator to control the gut microbiome.

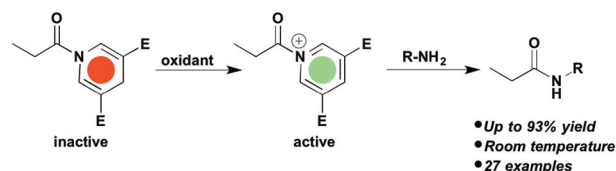


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### Oxidative activation of dihydropyridine amides to reactive acyl donors

Erik Daa Funder, Julie B. Trads and Kurt V. Gothelf\*

Amides of 1,4-dihydropyridine (DHP) are activated by oxidation for acyl transfer to amines, alcohols and thiols.

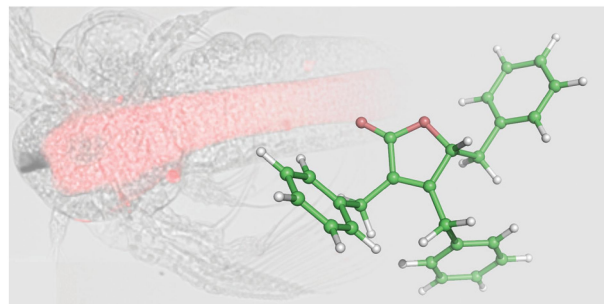


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### Synthesis of maculactone A and derivatives for environmental fate tracking studies

Samuel L. Bader, Michael U. Luescher and Karl Gademann\*

Labelled probes of the antifouling natural product, maculactone A, allow for distribution studies in *Artemia salina*.



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### The rapid synthesis of oxazolines and their heterogeneous oxidation to oxazoles under flow conditions

Steffen Glöckner, Duc N. Tran, Richard J. Ingham, Sabine Fenner, Zoe E. Wilson, Claudio Battilocchio and Steven V. Ley\*

A flow process to access oxazolines and oxazoles via a rapid and practical protocol is described.





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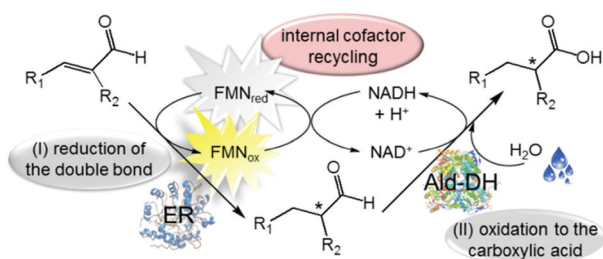


### Cationic azacryptands as selective three-way DNA junction binding agents

Jana Novotna, Aurelien Laguerre, Anton Granzhan, Marc Pirrotta, Marie-Paule Teulade-Fichou and David Monchaud\*

Azacryptands are promising candidates for assessing the therapeutic potential of three-way DNA junctions.

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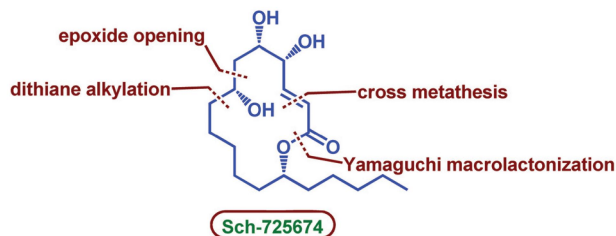


### Systematic methodology for the development of biocatalytic hydrogen-borrowing cascades: application to the synthesis of chiral $\alpha$ -substituted carboxylic acids from $\alpha,\beta$ -unsaturated aldehydes

Tanja Knaus, Francesco G. Mutti, Luke D. Humphreys, Nicholas J. Turner and Nigel S. Scrutton\*

The development of hydrogen-borrowing biocatalytic cascades is presented and applied to the synthesis of diverse  $\alpha$ -chiral substituted carboxylic acids.

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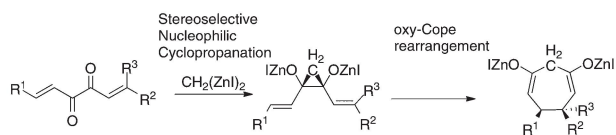


### An enantioselective total synthesis of Sch-725674

Kota Ramakrishna and Krishna P. Kaliappan\*

An enantioselective total synthesis of Sch-725674 using dithiane alkylation, cross metathesis reaction, Yamaguchi macrolactonization and a substrate controlled stereoselective reduction as key steps is described.

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### Preparation of cycloheptane ring by nucleophilic cyclopropanation of 1,2-diketones with bis(iodozincio)methane

Ryosuke Haraguchi, Yoshiaki Takada and Seiji Matsubara\*

The nucleophilic cyclopropanation of hexa-1,5-diene-3,4-diones with bis(iodozincio)methane afforded the Zn alkoxides of cyclohepta-2,7-diene-1,2-diols stereospecifically *via* Zn alkoxides of *cis*-dialkenylcyclopropane-1,2-diols.

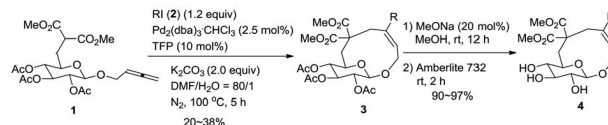
## PAPERS

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**Palladium(0)-catalyzed synthesis of cyclic glucosides**

Xin Huang, Chunling Fu and Shengming Ma\*

A highly regio- and stereo-selective synthesis of cyclic  $\beta$ -D-glucosides **3** via Pd(0)-catalyzed coupling cyclization of allenyl  $\beta$ -D-glucoside **1** and organic iodides in 20–38% yields is reported.

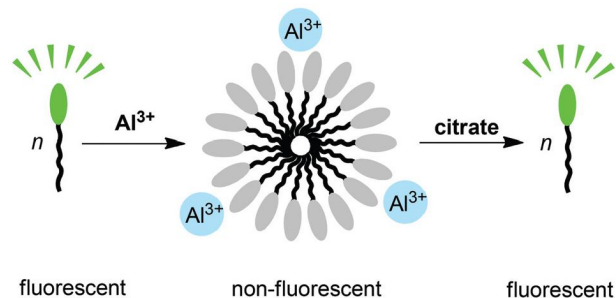


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**Selective detection of  $\text{Al}^{3+}$  and citric acid with a fluorescent amphiphile**

Ziya Köstereli and Kay Severin\*

The assembly and disassembly of a fluorescent amphiphile by  $\text{Al}^{3+}$  and citrate, respectively, can be used to sense these analytes by fluorescence spectroscopy.

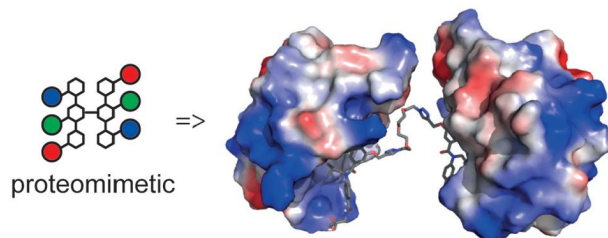


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**Multivalent helix mimetics for PPI-inhibition**

Anna Barnard, Jennifer A. Miles, George M. Burslem, Amy M. Barker and Andrew J. Wilson\*

A multivalent helix mimetic is developed that inhibits the p53/*h*DM2 and induces dimerization/aggregation of its target – *h*DM2.

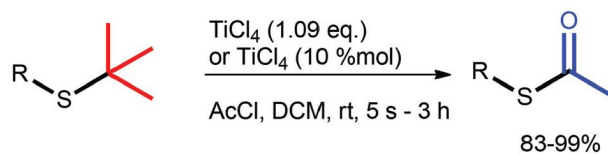


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**Mild Ti-mediated transformation of *t*-butyl thio-ethers into thio-acetates**

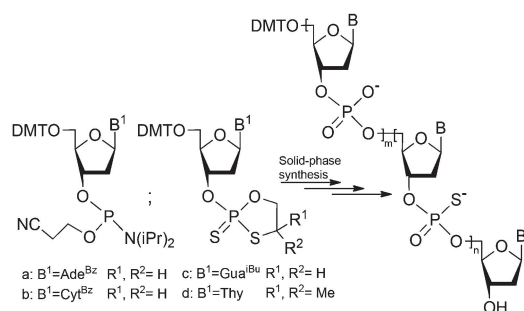
Thomas C. Pijper, Jort Robertus, Wesley R. Browne and Ben L. Feringa\*

Rapid conversion of thio-ethers to thio-acetates using  $\text{TiCl}_4$  that tolerates a wide variety of functionalities, in good to excellent yields.





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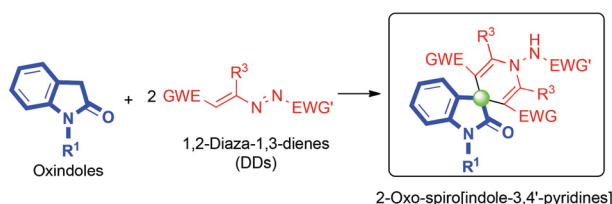


### Synthesis of PS/PO-chimeric oligonucleotides using mixed oxathiaphospholane and phosphoramidite chemistry

Ewa Radzikowska and Janina Baraniak\*

Chimeric oligonucleotides containing stereoregular phosphorothioate and natural phosphodiester linkages have been obtained on the solid phase support using nucleoside oxathiaphospholanes and commercially available nucleoside phosphoramidites.

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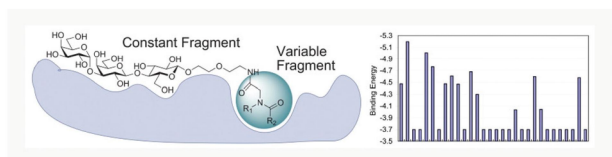


### Synthesis of novel symmetrical 2-oxo-spiro[indole-3,4'-pyridines] by a reaction of oxindoles with 1,2-diaza-1,3-dienes

Orazio A. Attanasi, Linda A. Campisi, Lucia De Crescentini, Gianfranco Favi and Fabio Mantellini\*

Synthesis of symmetrical 2-oxo-spiro[indole-3,4'-pyridines]: a novel example of spirocyclic oxindoles bearing a quaternary centre at the 3-position.

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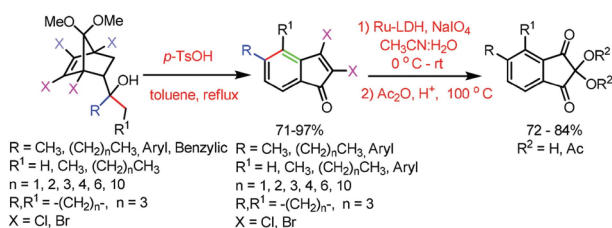


### Evaluation of a focused virtual library of heterobifunctional ligands for *Clostridium difficile* toxins

Carlos A. Sanhueza, Jonathan Cartmell, Amr El-Hawiet, Adam Szpacenko, Elena N. Kitova, Rambod Daneshfar, John S. Klassen, Dean E. Lang, Luiz Eugenio, Kenneth K.-S. Ng, Pavel I. Kitov and David R. Bundle\*

Higher activity glycopeptoid ligands for two large *Clostridium difficile* toxins TcdA and TcdB were discovered via modular fragment-based design and virtual screening.

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### A domino reaction of tetrahalo-7,7-dimethoxybicyclo[2.2.1]heptenyl alcohols leading to indenones and a *de novo* synthesis of ninhydrin derivatives

Kaki Raveendra Babu and Faiz Ahmed Khan\*

An acid mediated synthesis of indenones and a *de novo* synthesis of ninhydrin derivatives.

## Copper-catalyzed regioselective synthesis of furan *via* tandem cycloaddition of ketone with an unsaturated carboxylic acid under air

Monoranjan Ghosh, Subhajit Mishra, Kamarul Monir and Alakananda Hajra\*

A catalytic decarboxylative annulation has been developed for the regioselective synthesis of furans by the cycloaddition of ketones with  $\alpha,\beta$ -unsaturated carboxylic acids in ambient air.

