

# Organic & Biomolecular Chemistry

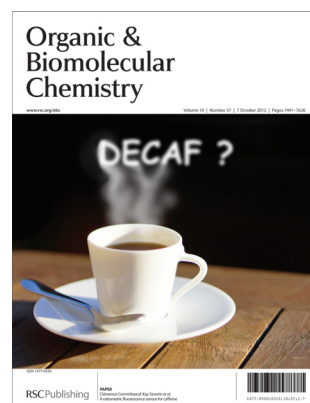
An international journal of synthetic, physical and biomolecular organic chemistry

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## IN THIS ISSUE

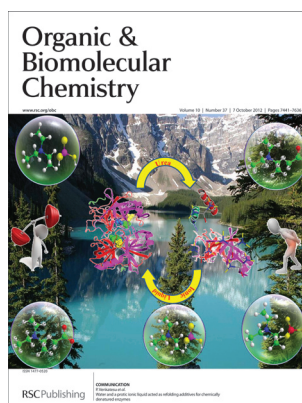
ISSN 1477-0520 CODEN OBCRAK 10(37) 7441–7636 (2012)



### Cover

See Clémence Corminboeuf,  
Kay Severin *et al.*,  
pp. 7487–7490.

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Chem.*, 2012, **10**, 7487.



### Inside cover

See P. Venkatesu *et al.*,  
pp. 7475–7478.

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Chem.*, 2012, **10**, 7475.

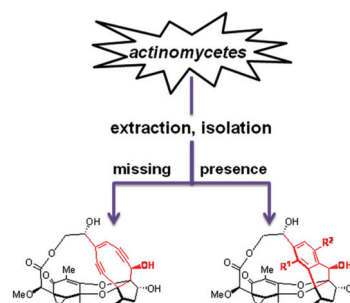
## EMERGING AREA

7453

### When the nine-membered enediynes play hide and seek

Mickaël Jean, Sophie Tomasi and Pierre van de Weghe\*

The lack of stability of the 9-membered enediynes not associated with an apoprotein may explain the low number of isolated natural compounds containing this core.



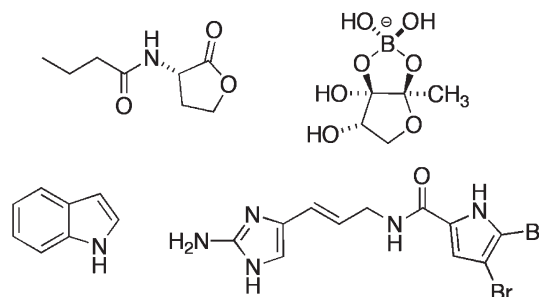
## PERSPECTIVE

7457

### Small molecule control of bacterial biofilms

Roberta J. Worthington, Justin J. Richards and  
Christian Melander\*

We report an overview of the development of small molecules that inhibit and/or disperse bacterial biofilms through non-microbicidal mechanisms.



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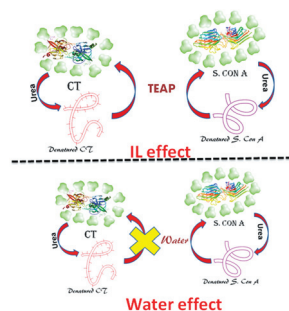
## COMMUNICATIONS

7475

**Water and a protic ionic liquid acted as refolding additives for chemically denatured enzymes**

Pankaj Attri, P. Venkatesu\* and Anil Kumar

The ability of water and a protic ionic liquid, triethyl ammonium phosphate (TEAP) to act as refolding additives for the urea-induced chemical denatured state of the two enzymes,  $\alpha$ -chymotrypsin and succinylated Con A, is reported.

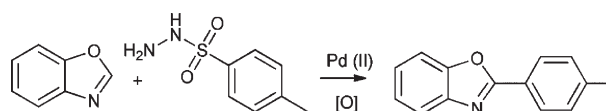


7479

**Palladium-catalyzed desulfitative arylation of azoles with arylsulfonyl hydrazides**

Xinzhang Yu, Xingwei Li\* and Boshun Wan\*

Palladium-catalyzed desulfitative and denitrogenative arylation of azoles with arylsulfonyl hydrazides has been achieved.

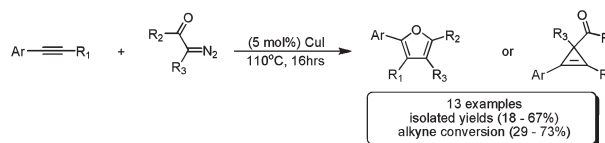


7483

**Highly selective synthesis of tetra-substituted furans and cyclopropenes: copper(I)-catalyzed formal cycloadditions of internal aryl alkynes and diazoacetates**

Andrew K. Swenson, Kate E. Higgins, Matthew G. Brewer, William W. Brennessel and Michael G. Coleman\*

Selective Cu(I)-catalyzed cycloadditions of internal alkynes and diazoacetates is a straightforward method for the synthesis of poly-substituted furans and cyclopropenes.



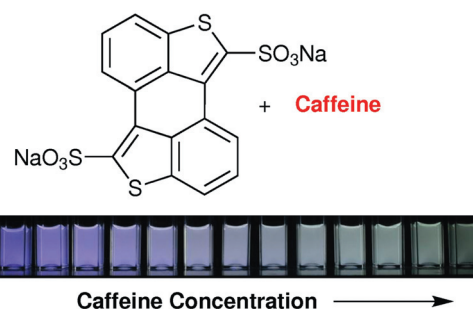
## PAPERS

7487

**A ratiometric fluorescence sensor for caffeine**

Nicolas Luisier, Albert Ruggi, Stephan N. Steinmann, Laurane Favre, Nicolas Gaeng, Clémence Corminboeuf\* and Kay Severin\*

A disulfonated bibenzo[*b*]thiophene can be used as a molecular probe for the optical detection of caffeine.



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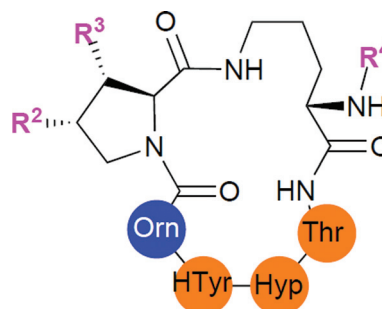
Closing date for nominations is 15 January 2013

7491

### Mutual influence of backbone proline substitution and lipophilic tail character on the biological activity of simplified analogues of caspofungin

Monique P. C. Mulder, Peter Fodran, Johan Kemmink, Eefjan J. Breukink, John A. W. Kruijtzter, Adriaan J. Minnaard\* and Rob M. J. Liskamp\*

Mutual influence of hydroxy groups ( $R^2, R^3$ ) and the lipophilic tail ( $R^4$ ) leads to selective and active simplified analogues of antifungal caspofungin.

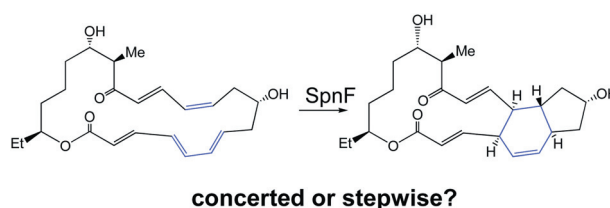


7503

### Concerted, highly asynchronous, enzyme-catalyzed [4 + 2] cycloaddition in the biosynthesis of spinosyn A; computational evidence

B. Andes Hess, Jr.\* and Lidia Smentek

Density functional calculations on the recently discovered enzymatic Diels–Alder reaction suggests the reaction is a polar, highly asynchronous, concerted reaction.

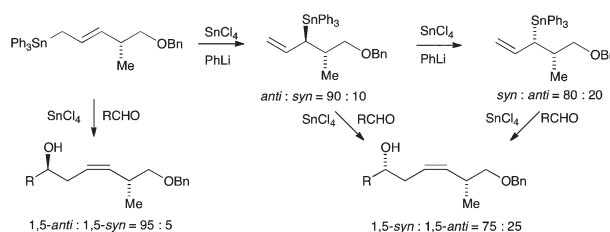


7510

### Concerning the 1,5-stereocontrol in tin(IV) chloride promoted reactions of 4- and 5-alkoxyalk-2-enylstannanes: trapping intermediate allyltin trichlorides using phenyllithium

Lindsay A. Hobson and Eric J. Thomas\*

Confirmation of the configurations of pent-1-enyltin trichlorides generated from 4- and 5-alkoxy-pent-2-enylstannanes that had been suggested on the basis of the stereoselectivities of their reactions with aldehydes has been achieved by trapping using phenyllithium.

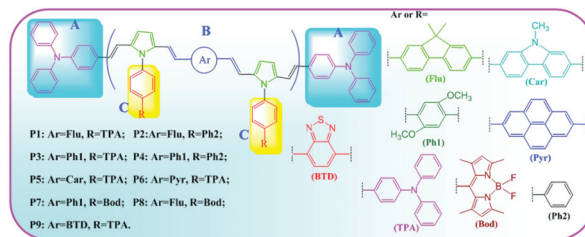


7527

### Theoretical insight into linear optical and two-photon absorption properties for a series of N-arylpyrrole-based dyes

Xiao-Ting Liu, Jing-Fu Guo, Ai-Min Ren,\* Zhong Xu, Shuang Huang and Ji-Kang Feng

Structural modifications are made to improve two-photon spectra of N-arylpyrrole-based chromophores and enlarge the repertoire of biomolecular fluorescent probes.





# New process for crystal data files

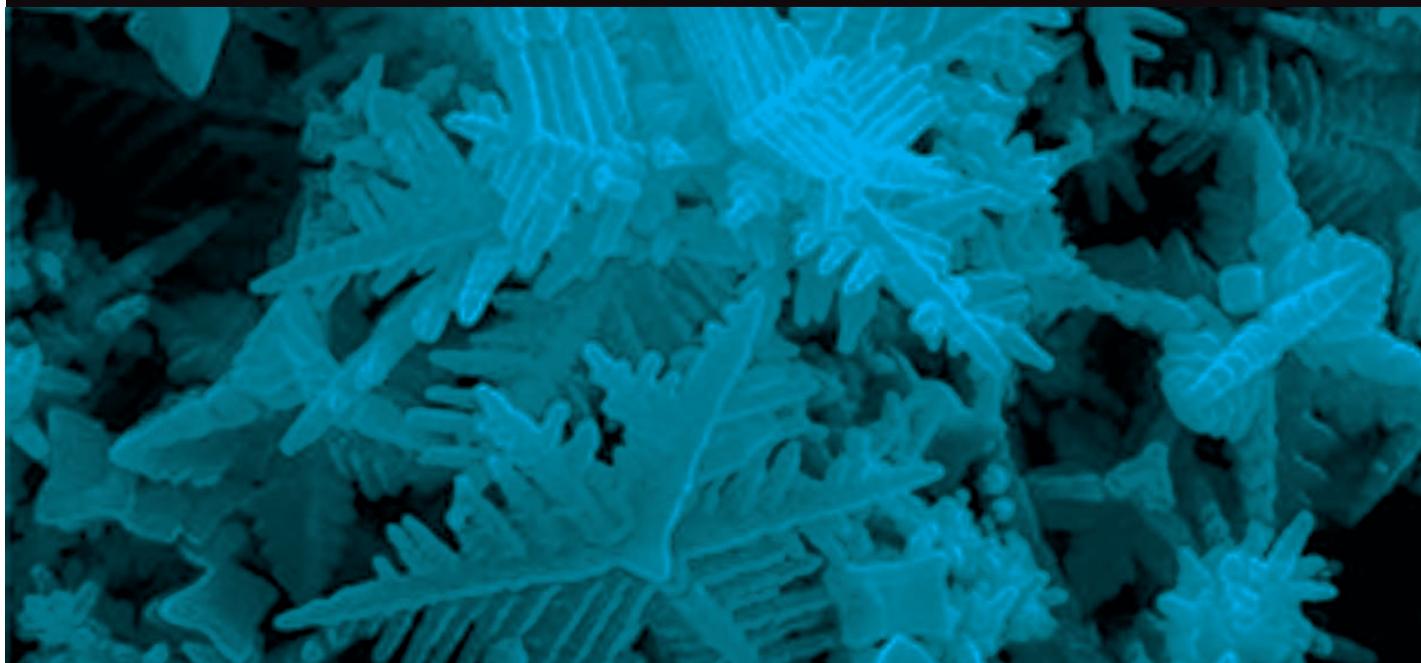


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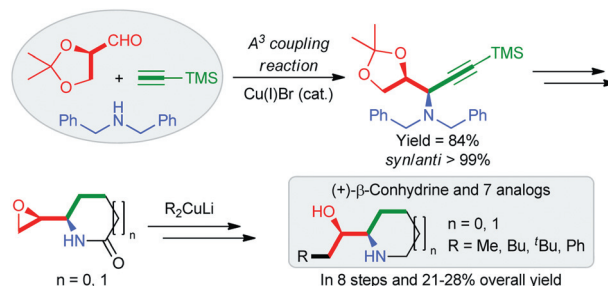
## PAPERS

7536

### Diastereoselective construction of *syn*- $\alpha$ -oxyamines via three-component $\alpha$ -oxyaldehyde–dibenzylamine–alkyne coupling reaction: application in the synthesis of (+)- $\beta$ -conhydrine and its analogues

Sharad Chandrakant Deshmukh, Arundhati Roy and Pinaki Talukdar\*

A Cu(I) catalyzed  $\alpha$ -oxyaldehyde–dibenzylamine–alkyne coupling reaction with excellent diastereoselective construction of *syn*- $\alpha$ -oxyamine is reported which is applied in the synthesis of (+)- $\beta$ -conhydrine, and related piperidine and pyrrolidine analogues.

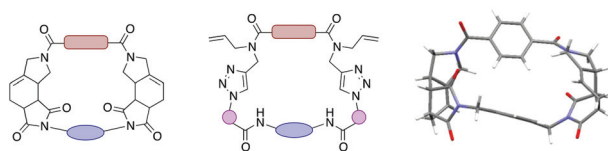


7545

### A two-directional strategy for the diversity-oriented synthesis of macrocyclic scaffolds

Kieron M. G. O'Connell, Henning S. G. Beckmann, Luca Lariaia, Helen T. Horsley, Andreas Bender, Ashok R. Venkitaraman and David R. Spring\*

The efficient synthesis of a range of complex macrocyclic compounds is achieved using two-directional synthesis.

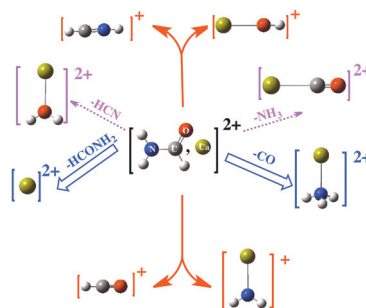


7552

### Modelling peptide–metal dication interactions: formamide–Ca<sup>2+</sup> reactions in the gas phase

Ane Eizaguirre, Otilia M3, Manuel Y3ñez,\* Jean-Yves Salpin\* and Jeanine Tortajada

The collision induced dissociation of formamide–Ca<sup>2+</sup> complexes produced in the gas phase through nanoelectrospray ionization yields as main products ions [CaOH]<sup>+</sup>, [HCNH]<sup>+</sup>, [Ca(NH<sub>2</sub>)]<sup>+</sup>, HCO<sup>+</sup> and [Ca(NH<sub>3</sub>)]<sup>2+</sup> and possibly [Ca(H<sub>2</sub>O)]<sup>2+</sup> and [C,O,Ca]<sup>2+</sup>, the latter being rather minor.

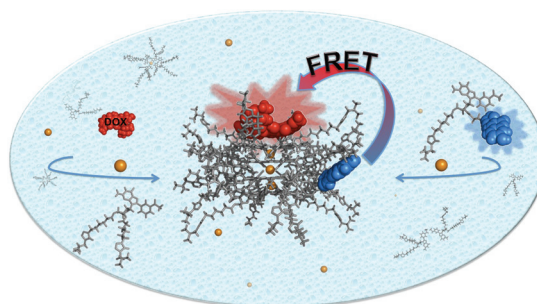


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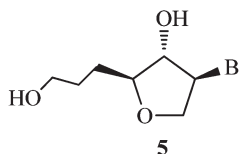
### An aquatic host–guest complex between a supramolecular G-quadruplex and the anticancer drug doxorubicin

Jos3 M. Rivera,\* Mariana Mart3n-Hidalgo and Jean C. Rivera-R3os

This article describes the synthesis of a fluorescent deoxyguanosine derivative and studies of its self-assembly, in water, into a supramolecular G-quadruplex capable of binding to the drug doxorubicin.



7566



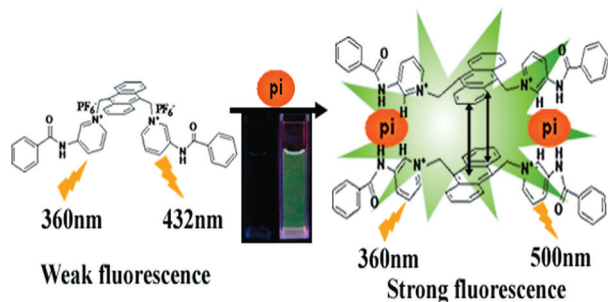
B = adenine or thymine

### Synthesis and properties of novel L-isonucleoside modified oligonucleotides and siRNAs

Jun Zhang, Yue Chen, Ye Huang, Hong-Wei Jin, Ren-Ping Qiao, Lei Xing, Liang-Ren Zhang, Zhen-Jun Yang\* and Li-He Zhang\*

A novel isonucleoside **5** containing a 5'-CH<sub>2</sub> extended chain at the sugar moiety was synthesized. In siRNA, passenger strand modified with isonucleoside (**5a/b**) at 3' or 5' terminal can retain the silencing activity and minimize the passenger strand specific off-target effect.

7578

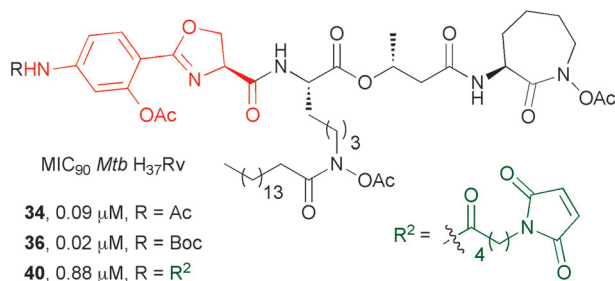


### Selective sensing of H<sub>2</sub>PO<sub>4</sub><sup>-</sup> (Pi) driven by the assembly of anthryl pyridinium ligands

Weitao Gong,\* Qinglan Zhang, Furui Wang, Bei Gao, Yuan Lin and Guiling Ning\*

A new strategy for selective sensing of Pi by the assembly of pyridinium moieties exhibiting a strong excimer emission is presented.

7584

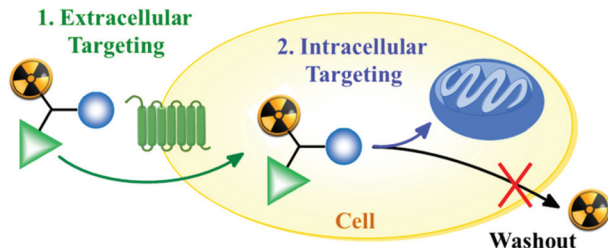


### Syntheses of mycobactin analogs as potent and selective inhibitors of *Mycobacterium tuberculosis*

Raúl E. Juárez-Hernández, Scott G. Franzblau and Marvin J. Miller\*

Three analogs of mycobactin T, the siderophore secreted by *Mycobacterium tuberculosis* (*Mtb*) were synthesized and screened for their antibiotic activity against *Mtb* H<sub>37</sub>Rv and a broad panel of Gram-positive and Gram-negative bacteria.

7594



### Dual-targeting conjugates designed to improve the efficacy of radiolabeled peptides

Christiane A. Kluba, Andreas Bauman, Ibai E. Valverde, Sandra Vomstein and Thomas L. Mindt\*

The synthesis and *in vitro* evaluation of dual-targeting conjugates designed to improve the efficacy of peptide based radiopharmaceuticals is described.



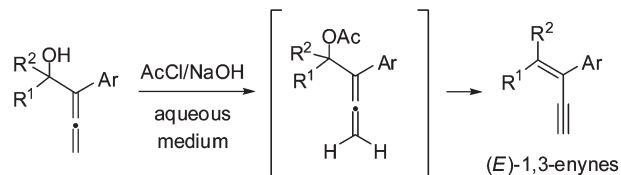
## PAPERS

7603

**Direct allenol-based stereocontrolled access to substituted (*E*)-1,3-enynes**

Benito Alcaide,\* Pedro Almendros\* and Teresa Martínez del Campo

A stereoselective synthesis of 1-substituted (*E*)-2-aryl-but-1-en-3-ynes, including tetrasubstituted alkenes, has been developed from aryl-substituted  $\alpha$ -allenols by treatment with the AcCl–NaOH (aqueous) system.

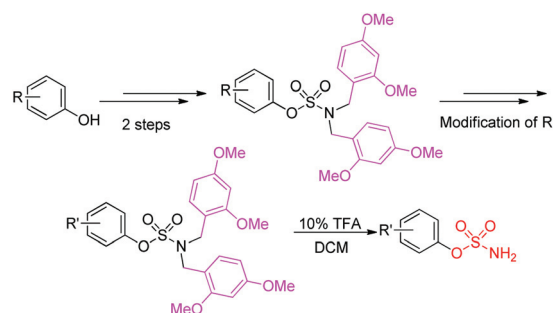


7610

**Efficacious *N*-protection of *O*-aryl sulfamates with 2,4-dimethoxybenzyl groups**

Tristan Reuillon, Annalisa Bertoli, Roger J. Griffin, Duncan C. Miller and Bernard T. Golding\*

To facilitate synthesis of phenolic *O*-sulfamates, hydrogens ( $\text{OSO}_2\text{NH}_2$  or  $\text{OSO}_2\text{NHR}$ ) have each been replaced by a 2,4-dimethoxybenzyl protecting group, which block E1cB elimination, but can be readily removed with 10% TFA in dichloromethane (17 examples, excellent yields).

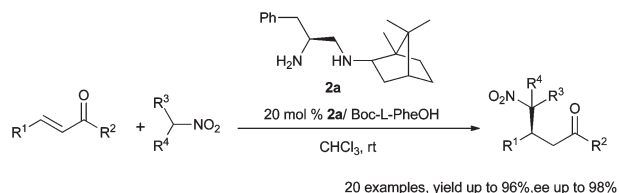


7618

**Camphor-derived  $C_1$ -symmetric chiral diamine organocatalysts for asymmetric Michael addition of nitroalkanes to enones**

Yirong Zhou, Qiang Liu and Yuefa Gong\*

A novel  $C_1$ -symmetric chiral primary–secondary diamine **2a** proved to be an efficient organocatalyst to promote the Michael addition of nitroalkanes to a broad scope of enones with high yields (up to 96%) and excellent enantioselectivities (up to 98%) under mild conditions.

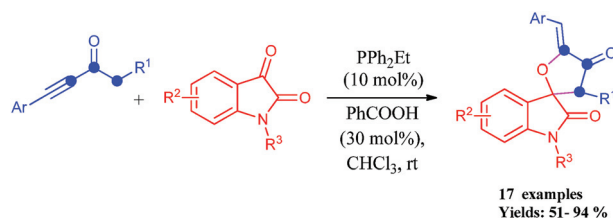


7628

**Phosphine-catalyzed domino reaction: an efficient method for the synthesis of highly functionalized spirooxazolines**

Lihua Yang, Peizhong Xie, Erqing Li, Xin Li, You Huang\* and Ruyu Chen

A novel phosphine-catalyzed intermolecular [3 + 2] cycloaddition of ynones and *N*-substituted isatins was developed.



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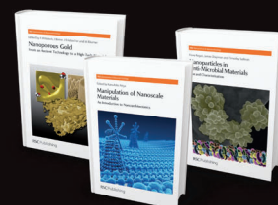
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