

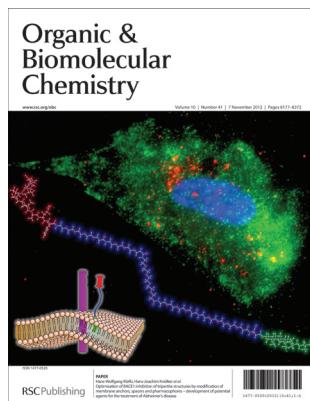
# Organic & Biomolecular Chemistry

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

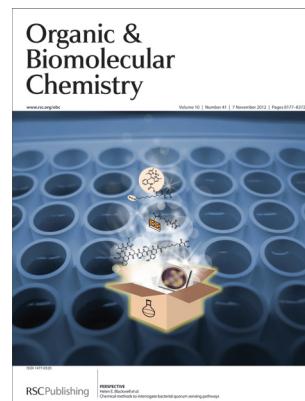
ISSN 1477-0520 CODEN OBCRAK 10(41) 8177–8372 (2012)



### Cover

See Hans-Wolfgang Klafki,  
Hans-Joachim Knölker *et al.*,  
pp. 8216–8235.

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*Org. Biomol. Chem.*, 2012, **10**,  
8216.



### Inside cover

See Helen E. Blackwell *et al.*,  
pp. 8189–8199.

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Biomol. Chem.*, 2012, **10**, 8189.

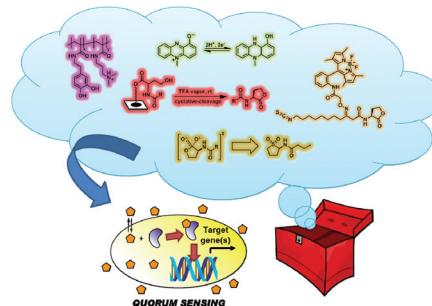
## PERSPECTIVE

8189

### Chemical methods to interrogate bacterial quorum sensing pathways

Thanit Praneenararat, Andrew G. Palmer and  
Helen E. Blackwell\*

There is considerable interest in methods to probe and modulate quorum-sensing pathways with temporal and spatial control. Such methods would be tremendously valuable for both basic and applied research. In this Perspective, we provide an overview of the use of chemical probes and techniques in quorum sensing research.



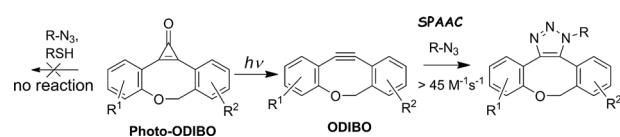
## COMMUNICATIONS

8200

### Photochemical generation of oxa-dibenzocyclooctyne (ODIBO) for metal-free click ligations

Christopher D. McNitt and Vladimir V. Popik\*

Oxa-dibenzocyclooctynes (ODIBOs) combine excellent stability and very high reactivity in strain-promoted acetylene azide cycloaddition (SPAAC). ODIBOs are prepared by photochemical decarbonylation of corresponding cyclopropenones (photo-ODIBO), which are azide-inert.



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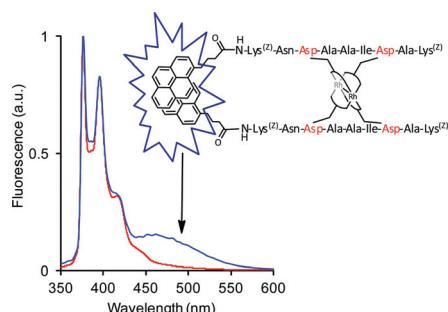
## COMMUNICATIONS

8203

**Determination of orientational isomerism in rhodium(II) metallopeptides by pyrene fluorescence**

Ramya Sambasivan and Zachary T. Ball\*

Pyrene excimer fluorescence is a useful tool to ascertain the structure of rhodium(II) metallopeptides, differentiating between parallel and antiparallel orientational isomers.



8207

**Fluorinated  $\beta$ -nitro amines by a selective  $ZrCl_4$ -catalyzed aza-Henry reaction of (*E*)-trifluoromethyl aldimines**

Stefania Fioravanti,\* Lucio Pellacani\* and Maria Cecilia Vergari

New fluorinated  $\beta$ -nitro amines are synthesized by a  $ZrCl_4$ -catalyzed aza-Henry reaction. The reactivity of the starting imines is deeply influenced by the presence of the  $CF_3$  group, while the stereochemical outcome seems to be unaffected, the *anti* isomer being always the major one.



## PAPERS

8211

**Concise construction of the tetracyclic core of lycorine-type alkaloids and the formal synthesis of  $\alpha$ -lycorane based on asymmetric bifunctional thiourea-catalyzed cascade reaction**

Yao Wang, Yong-Chun Luo, Hong-Bo Zhang and Peng-Fei Xu\*

A concise and stereoselective construction of the tetracyclic core of lycorine-type alkaloids and the formal synthesis of  $\alpha$ -lycorane has been achieved based on an asymmetric bifunctional thiourea-catalyzed cascade reaction.



8216

**Optimisation of BACE1 inhibition of tripartite structures by modification of membrane anchors, spacers and pharmacophores – development of potential agents for the treatment of Alzheimer's disease**

Philipp Linning, Ute Haussmann, Isaak Beyer, Sebastian Weidlich, Heike Schieb, Jens Wiltfang, Hans-Wolfgang Klafki\* and Hans-Joachim Knölker\*

Systematic structural variation leads to an optimisation of the inhibitory effect of tripartite structures towards BACE1-induced cleavage of the amyloid precursor protein (APP).



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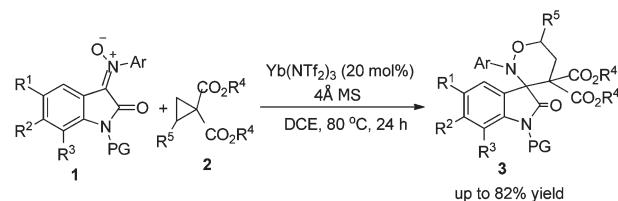
## PAPERS

8236

**Yb(NTf<sub>2</sub>)<sub>3</sub>-catalyzed [3 + 3] cycloaddition between isatin ketonitrones and cyclopropanes to construct novel spiro[tetrahydro-1,2-oxazine]oxindoles**

Hai-Bin Yang and Min Shi\*

A highly regioselective Yb(NTf<sub>2</sub>)<sub>3</sub>-catalyzed [3 + 3] cycloaddition between isatin ketonitrones and cyclopropanes to construct spiro[tetrahydro-1,2-oxazine]oxindoles in moderate to good yields is described.

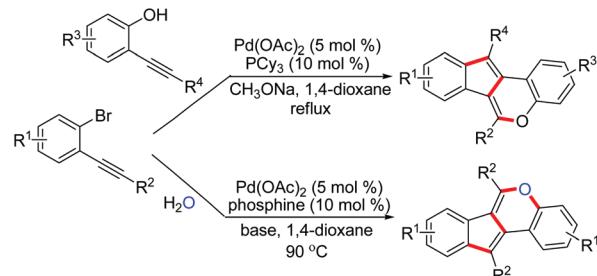


8244

**Facile assembly of indeno[1,2-*c*]chromenes via a palladium-catalyzed reaction of 2-alkynylhalobenzene**

Xiaolin Pan, Hongming Nie, Yong Luo, Yueqiu Gao\* and Jie Wu\*

The scaffold of indeno[1,2-*c*]chromene could be constructed *via* a palladium-catalyzed reaction of 2-alkynylbromobenzene with water, in which four bonds are formed with high efficiency.

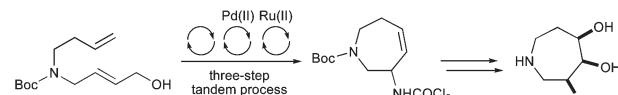


8251

**Stereoselective synthesis of hydroxylated 3-aminoazepanes using a multi-bond forming, three-step tandem process**

Sajjad Ahmad and Andrew Sutherland\*

A multi-bond forming, three-step tandem process has been utilised for the diastereoselective synthesis of hydroxylated aminoazepanes.

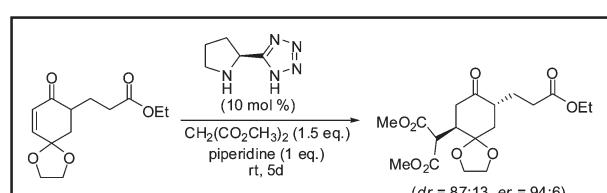


8260

**Organocatalytic dynamic kinetic resolution *via* conjugate addition: synthesis of chiral *trans*-2,5-dialkylcyclohexanones**

Ganesh Pandey,\* Priyanka A. Adate and Vedavati G. Puranik

A novel strategy of initiating an organocatalysed dynamic kinetic resolution (dr up to 99 : 1 and er up to 94 : 6) for the synthesis of chiral *trans*-2,5-dialkylcyclohexanones by an asymmetric conjugate addition of dimethyl malonate on to 6-substituted cyclohexenones is reported.



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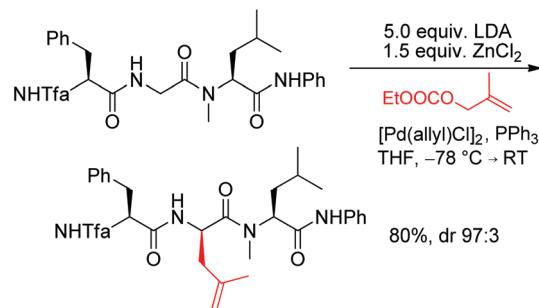
## PAPERS

8268

**Highly stereoselective modifications of peptides via Pd-catalyzed allylic alkylation of internal peptide amide enolates**

Swarup Datta, Anton Bayer and Uli Kazmaier\*

Reactions of peptide amide enolates with Pd–allyl complexes proceed not only with high yields, but also excellent regio- and diastereoselectivities.

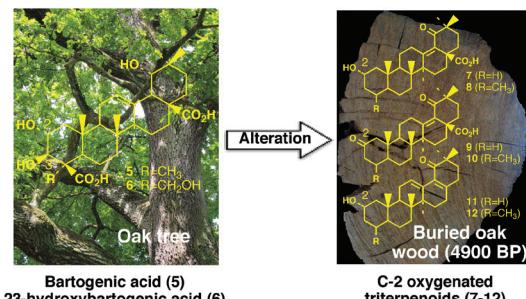


8276

**Triterpenoids functionalized at C-2 as diagenetic transformation products of 2,3-dioxygenated triterpenoids from higher plants in buried wood**

Gilles Schnell, Philippe Schaeffer, Estelle Motsch and Pierre Adam\*

C-2 functionalized triterpenoids have been identified in ancient wood as transformation products of 2,3-dioxygenated triterpenoids precursors from oak wood. They are potential specific molecular tools for palaeoenvironmental and archaeological investigations.

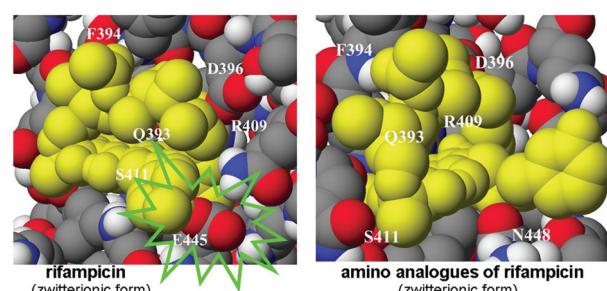


8283

**A new model of binding of rifampicin and its amino analogues as zwitterions to bacterial RNA polymerase**

Krystian Pyta, Piotr Przybylski,\* Katarzyna Klich and Joanna Stefańska

Spectroscopic, biological and molecular recognition studies of **1** and its new amino analogues led to the proposition of a new model of bacterial RNA polymerase inhibition in which a very important role is assigned to salt type interactions between a protonated substituent at the C-3 atom and E<sub>445</sub>.

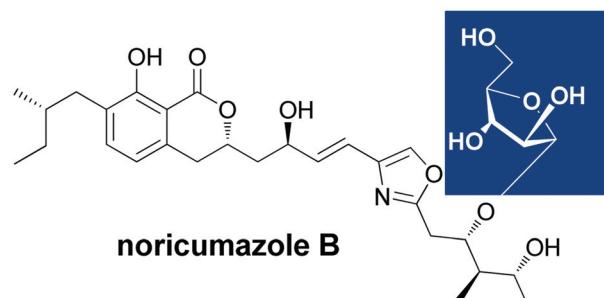


8298

**Total synthesis of noricumazole B establishes D-arabinose as glycan unit**

Jenny Barbier, Klaus Gerth, Rolf Jansen and Andreas Kirschning\*

The total synthesis of noricumazole B establishes the glycan moiety to be D- $\alpha$ -arabinoside.





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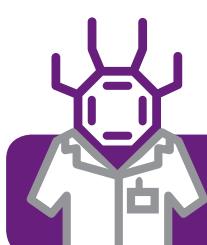
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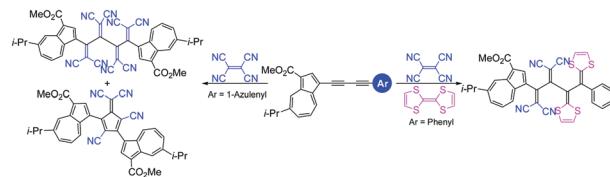
## PAPERS

## 8308

**Synthesis of push–pull chromophores by the sequential [2 + 2] cycloaddition of 1-azulenylbutadiynes with tetracyanoethylene and tetrathiafulvalene**

Taku Shoji,\* Shunji Ito, Tetsuo Okujima and Noboru Morita

Azulene-substituted butadiynes have been prepared by Cu-mediated cross- and homo-coupling reactions. The butadiynes reacted with tetracyanoethylene in a formal [2 + 2] cycloaddition reaction to afford the corresponding 1,1,4,4-tetracyanobutadienes, in excellent yields. Further [2 + 2] cycloaddition with TTF and TCNE gave novel donor–acceptor chromophores and novel 6,6-dicyanofulvene.

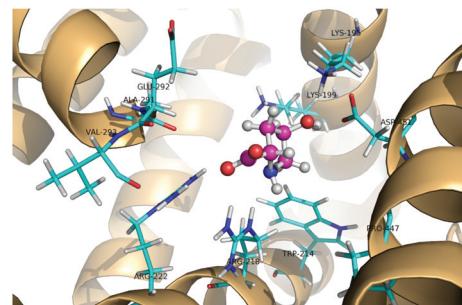


## 8314

**The binding affinity of amino acid–protein: hydroxyproline binding site I on human serum albumin**

Ximin Zhou, Wenjuan Lü, Li Su, Yafei Dong, Qianfeng Li and Xingguo Chen\*

The binding of hydroxyproline (Hyp) to HSA was studied by multispectroscopic and molecular modeling under simulated physiological conditions.

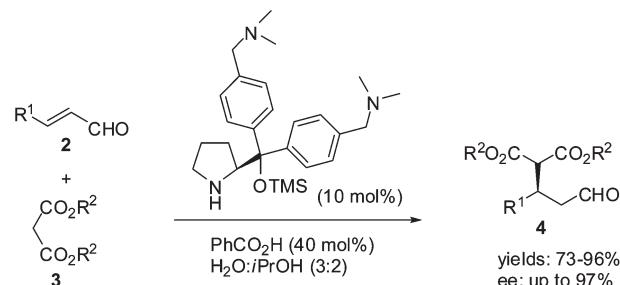


## 8322

**Highly enantioselective and recyclable organocatalytic Michael addition of malonates to  $\alpha,\beta$ -unsaturated aldehydes in aqueous media**

Subrata K. Ghosh, Kritanjali Dhungana, Allan D. Headley\* and Yukuo Ni\*

A new type of pyrrolidine-based organocatalyst, which was developed earlier in our lab, has been found to be very effective for the Michael addition reaction in aqueous solvents involving a wide range of  $\alpha,\beta$ -unsaturated aldehydes and malonate derivatives.

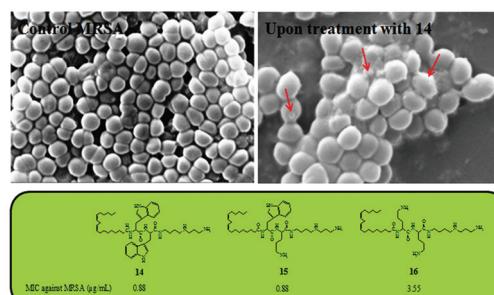


## 8326

**Synthesis, antibacterial activity and mode of action of novel linoleic acid–dipeptide–spermidine conjugates**

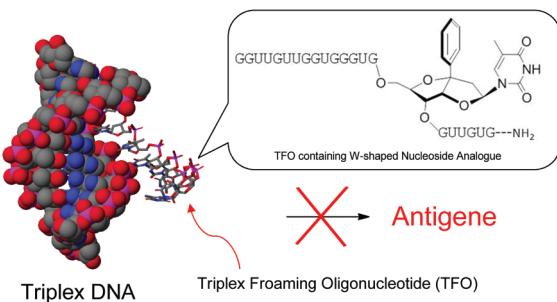
Seema Joshi, Rakeshwar P. Dewangan, Shruti Yadav, Diwan S. Rawat and Santosh Pasha\*

Novel linoleic acid–dipeptide–spermidine conjugates were synthesized with excellent anti-MRSA activity and a predominant membrane perturbing mode of action.



## PAPERS

8336

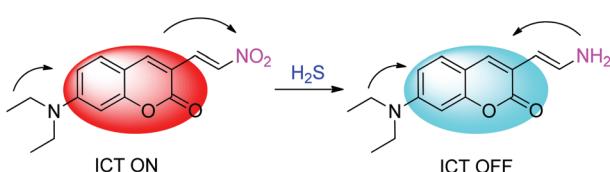


**An efficient antigenic activity and antiproliferative effect by targeting the Bcl-2 or survivin gene with triplex forming oligonucleotides containing a W-shaped nucleoside analogue (WNA- $\beta$ T)**

Yosuke Taniguchi\* and Shigeki Sasaki\*

Triplex forming oligonucleotides (TFOs) are some of the most promising tools in the antigenic strategy for the development of gene targeting therapeutics.

8342

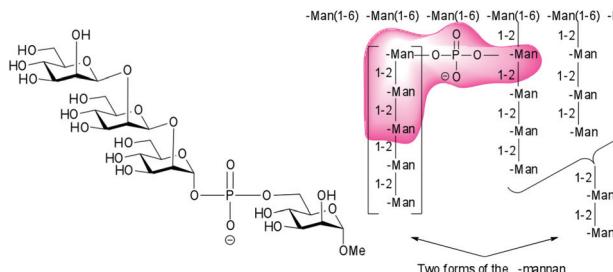


**A selective colorimetric and ratiometric fluorescent probe for hydrogen sulfide**

Ming-Yu Wu, Kun Li,\* Ji-Ting Hou, Zheng Huang and Xiao-Qi Yu\*

A ratiometric probe for selective detection of H<sub>2</sub>S with 120 nm blue shift and 4750 fold emission intensity ratio change was presented.

8348

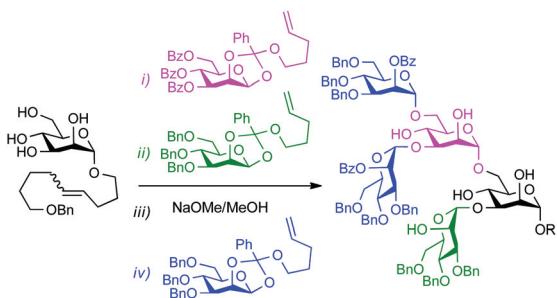


**Synthesis of a *Candida albicans* tetrasaccharide spanning the  $\beta$ 1,2-mannan phosphodiester  $\alpha$ -mannan junction**

Anh-Thu Dang, Margaret A. Johnson and David R. Bundle\*

Recognition of the synthetic tetrasaccharide, Man( $\beta$ 1-2)Man( $\beta$ 1-2)-Man( $\alpha$ 1-6)Man6P( $\alpha$ OMe) by a protective monoclonal antibody suggests an optimal  $\beta$ 1,2-mannan vaccine epitope for *Candida albicans*.

8361



**Ready access to a branched Man<sub>5</sub> oligosaccharide based on regioselective glycosylations of a mannose-tetraol with *n*-pentenyl orthoesters**

Clara Uriel, Ana M. Gómez,\* J. Cristóbal López\* and Bert Fraser-Reid

A branched Man<sub>5</sub> oligosaccharide has been synthesized by sequential regioselective glycosylations on a mannose-tetraol with *n*-pentenyl orthoester glycosyl-donors promoted by NIS/BF<sub>3</sub>·Et<sub>2</sub>O, in CH<sub>2</sub>Cl<sub>2</sub>.