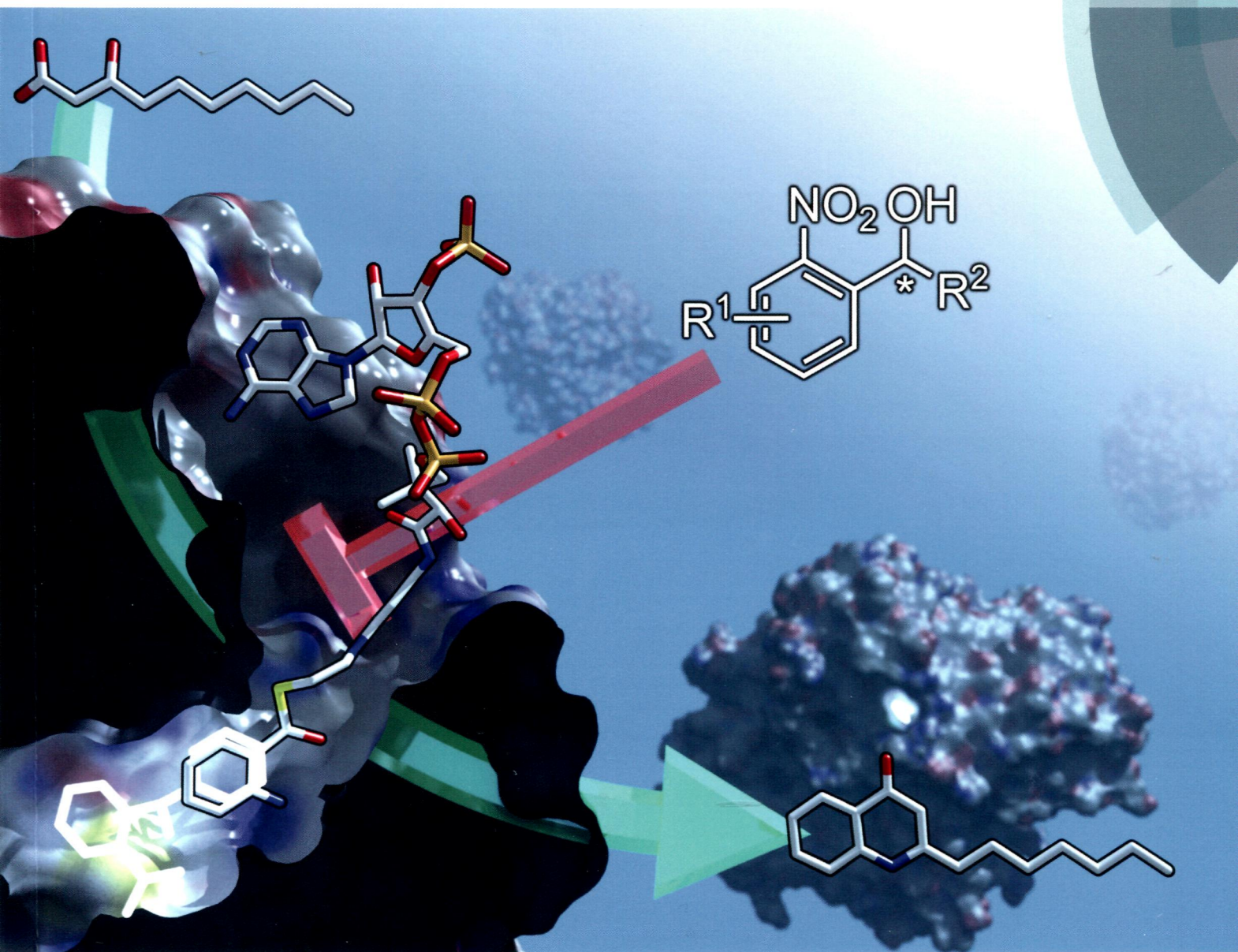


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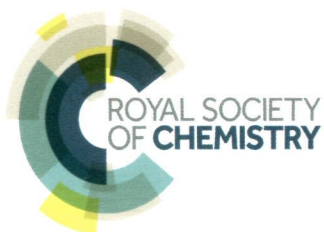
Volume 12 | Number 32 | 28 August 2014 | Pages 6017–6280

# Organic & Biomolecular Chemistry

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ISSN 1477-0520



## PAPER

Martin Empting, Rolf W. Hartmann *et al.*  
From *in vitro* to *in cellulo*: structure–activity relationship of (2-nitrophenyl)-methanol derivatives as inhibitors of PqsD in *Pseudomonas aeruginosa*



# Organic & Biomolecular Chemistry

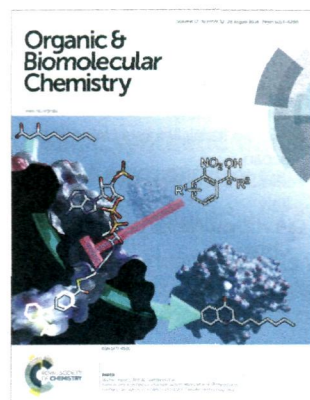
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## IN THIS ISSUE

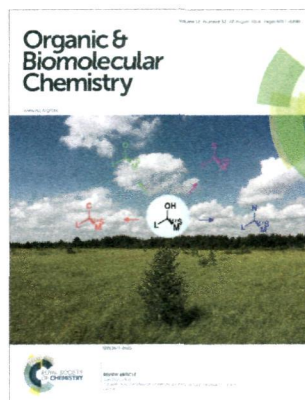
ISSN 1477-0520 CODEN OBCRAK 12(32) 6017-6280 (2014)



### Cover

See Martin Empting,  
Rolf W. Hartmann *et al.*,  
pp. 6094–6104.

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### Inside cover

See Jian Zhou *et al.*,  
pp. 6033–6048.

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**12**, 6033.

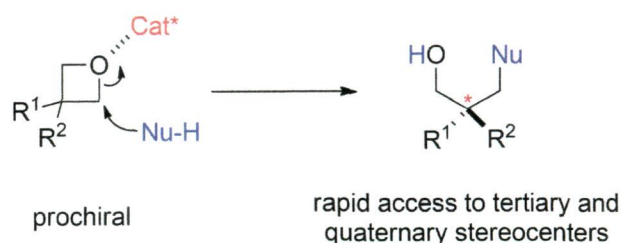
## PERSPECTIVE

6028

### Catalytic asymmetric nucleophilic openings of 3-substituted oxetanes

Zhaobin Wang, Zhilong Chen and Jianwei Sun\*

Important progress has been made in catalytic asymmetric ring-opening of 3-substituted oxetanes, but significant challenges and opportunities remain.



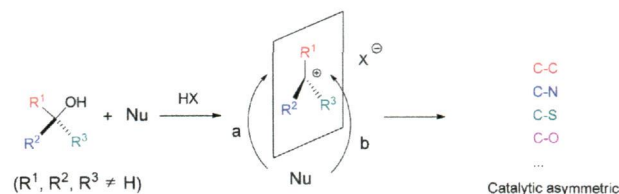
## REVIEWS

6033

### Catalytic functionalization of tertiary alcohols to fully substituted carbon centres

Long Chen, Xiao-Ping Yin, Cui-Hong Wang and Jian Zhou\*

This review summarizes the recent progresses in the catalytic nucleophilic substitution of tertiary alcohols using carbon or heteroatom based nucleophiles for the efficient, diverse and atom economical construction of fully substituted carbon centres, and discusses synthetic opportunities that are still open.



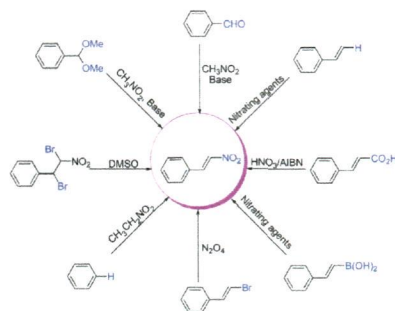
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Центральная научная библиотека  
Уральского отделения  
Российской академии наук (ЦНБ УРО РАН)

6049

### Recent advances in the synthesis of nitroolefin compounds

Guobing Yan,\* Arun Jyoti Borah and Lianggui Wang

This review focuses on recent achievements in nitroolefin synthesis and the mechanisms of the reactions are also discussed.

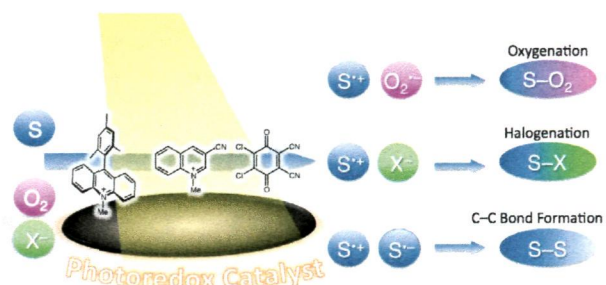


6059

### Organic synthetic transformations using organic dyes as photoredox catalysts

Shunichi Fukuzumi\* and Kei Ohkubo

This review article presents various photocatalytic transformation such as oxygenation, halogenation and C–C bond formation with organic photoredox catalysts.



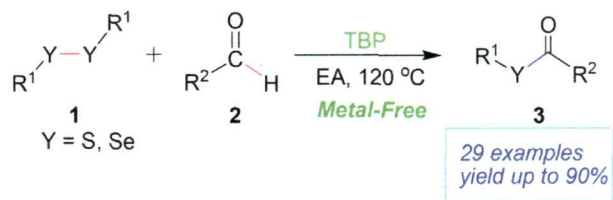
## COMMUNICATIONS

6072

### Syntheses of thiol and selenol esters by oxidative coupling reaction of aldehydes with RYYR (Y = S, Se) under metal-free conditions

Chunhuan He, Xuewei Qian and Peipei Sun\*

Thiol (selenol) esters were synthesized by a direct oxidative coupling reaction of aldehydes with disulfides (diselenides) under metal-free conditions.

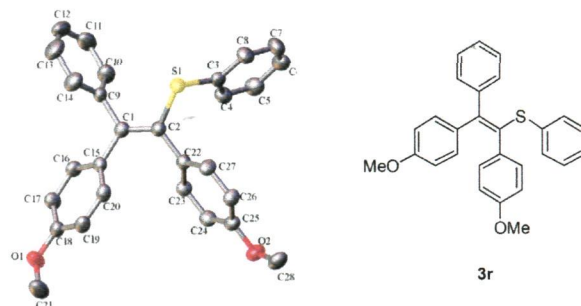


6076

### Iron-catalyzed tetrasubstituted alkene formation from alkynes and sodium sulfinates

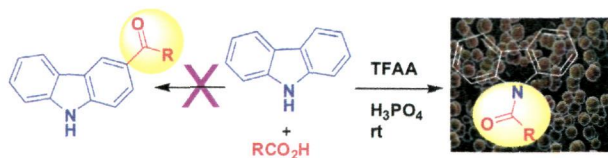
Saiwen Liu, Lichang Tang, Hui Chen, Feng Zhao and Guo-Jun Deng\*

An iron-catalyzed sulfenylation and arylation of alkynes with aryl sulfinic acid sodium salts is described.





6080

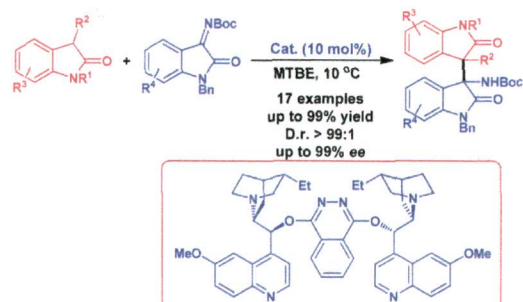


### TFAA/H<sub>3</sub>PO<sub>4</sub> mediated unprecedented N-acylation of carbazoles leading to small molecules possessing anti-proliferative activities against cancer cells

Sunder Kumar Kolli, Bagineni Prasad, P. Vijaya Babu, Mohd Ashraf Ashfaq, Nasreen Z. Ehtesham, R. Ramesh Raju\* and Manojit Pal\*

TFAA/H<sub>3</sub>PO<sub>4</sub>-mediated unusual N-acylation of carbazoles afforded potential anti-proliferative agents.

6085

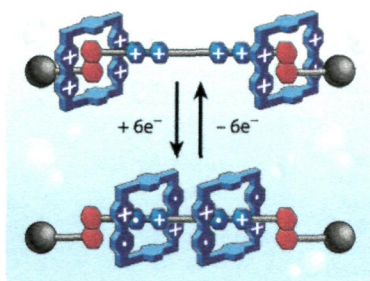


### Highly enantioselective synthesis of bisoxindoles with two vicinal quaternary stereocenters via Lewis base mediated addition of oxindoles to isatin-derived ketimines

Zhongkai Tang, Yan Shi, Haibin Mao, Xuebin Zhu, Weipeng Li, Yixiang Cheng, Wen-Hua Zheng\* and Chengjian Zhu\*

A highly efficient method provides access to the bisoxindole structure moiety with two vicinal quaternary stereogenic centers (>99 : 1 dr, >99% ee).

6089



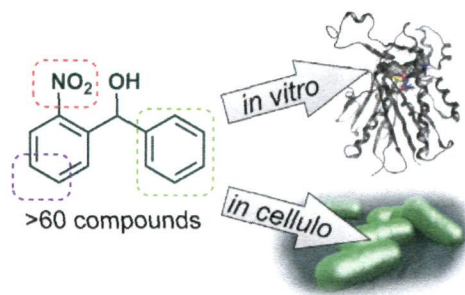
### Relative contractile motion of the rings in a switchable palindromic [3]rotaxane in aqueous solution driven by radical-pairing interactions

Leah S. Witus, Karel J. Hartlieb, Yuping Wang, Aleksandrs Prokofjevs, Marco Frasconi, Jonathan C. Barnes, Edward J. Dale, Albert C. Fahrenbach and J. Fraser Stoddart\*

This communication describes a mechanically interlocked molecule (MIM), capable of switchable and reversible linear molecular motion.

## PAPERS

6094



### From *in vitro* to *in cellulo*: structure–activity relationship of (2-nitrophenyl)methanol derivatives as inhibitors of PqsD in *Pseudomonas aeruginosa*

Michael P. Storz, Giuseppe Allegretta, Benjamin Kirsch, Martin Empting\* and Rolf W. Hartmann\*

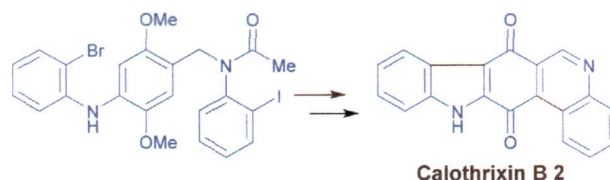
More than 60 derivatives of (2-nitrophenyl)methanol were synthesized and evaluated regarding their potency to inhibit PqsD. *In vitro* and *in cellulo* structure–activity relationships were derived.

6105

### Palladium mediated intramolecular multiple C–X/C–H cross coupling and C–H activation: synthesis of carbazole alkaloids calothrixin B and murrayaquinone A

Srinivasan A. Kaliyaperumal, Shyamapada Banerjee and Syam Kumar U. K.\*

Straightforward palladium mediated syntheses of calothrixin B and murrayaquinone A are described.

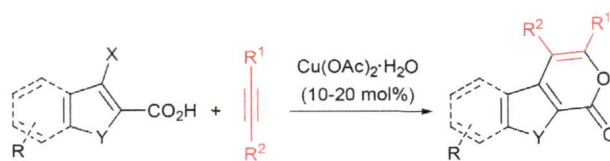


6114

### Copper-catalyzed annulation of heteroaromatic $\beta$ -halo- $\alpha,\beta$ -unsaturated carboxylic acids with alkynes for the synthesis of indolo[2,3-c]pyrane-1-ones and thieno[2,3-c]pyrane-7-ones

Da-Wei Gu and Xun-Xiang Guo\*

Efficient synthesis of indolo[2,3-c]pyrane-1-ones and thieno[2,3-c]pyrane-7-ones was achieved *via* annulation of heteroaromatic  $\beta$ -halo- $\alpha,\beta$ -unsaturated carboxylic acids with alkynes.

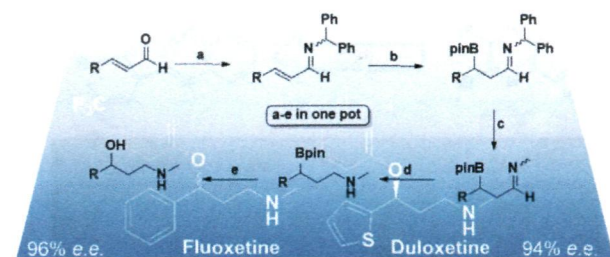


6121

### Total synthesis of fluoxetine and duloxetine through an *in situ* imine formation/borylation/transimination and reduction approach

Adam D. J. Calow, Elena Fernández\* and Andrew Whiting\*

Efficient, catalytic, asymmetric total syntheses of both (*R*)-fluoxetine and (*S*)-duloxetine from  $\alpha,\beta$ -unsaturated aldehydes are reported.

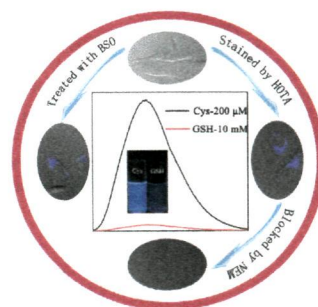


6128

### A fluorescent probe for intracellular cysteine overcoming the interference by glutathione

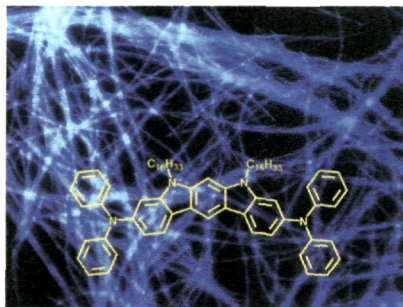
Minggang Tian, Fuqiang Guo, Yuming Sun, Weijia Zhang, Fang Miao, Yong Liu, Guofen Song, Cheuk-Lam Ho, Xiaoqiang Yu,\* Jing Zhi Sun\* and Wai-yeung Wong\*

A fluorescent probe was reported to discriminate 30–200  $\mu$ M cysteine, overcoming the interference by 1–10 mM glutathione. The selectivity was also proved by cellular experiments.





6134

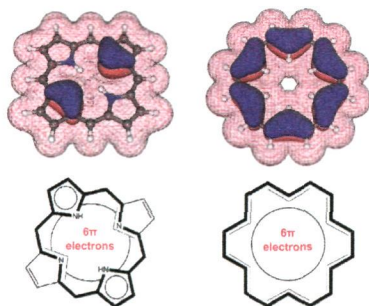


### Balanced $\pi$ - $\pi$ interactions directing the self-assembly of indolocarbazole-based low molecular mass organogelators

Peng Gong, Pengchong Xue, Chong Qian, Zhenqi Zhang and Ran Lu\*

New indolocarbazole-based organogelators emitting strong blue light have been synthesized.

6145

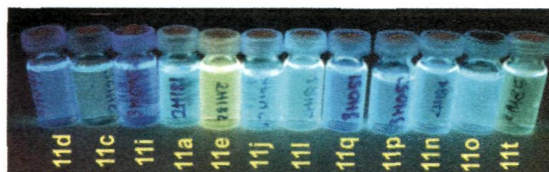
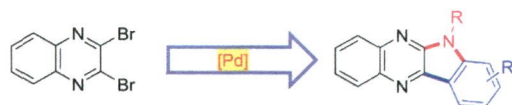


### Deciphering aromaticity in porphyrinoids via adaptive natural density partitioning

Alexander S. Ivanov and Alexander I. Boldyrev\*

Aromaticity in porphyrins is described by the adaptive natural density partitioning analysis.

6151

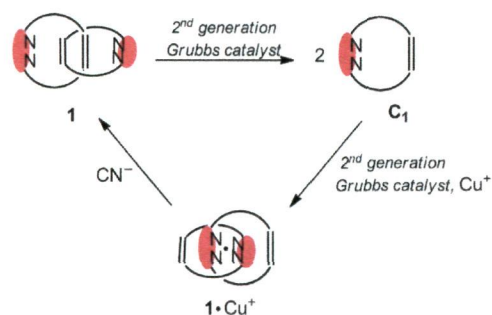


### Palladium catalyzed synthesis and physical properties of indolo[2,3-*b*]quinoxalines

Tran Quang Hung, Do Huy Hoang, Ngo Ngoc Thang, Tuan Thanh Dang,\* Khurshid Ayub, Alexander Villingner, Aleksej Friedrich, Stefan Lochbrunner, Gerd-Uwe Flechsig and Peter Langer\*

A series of indolo[2,3-*b*]quinoxaline derivatives were efficiently synthesized from 2,3-dibromoquinoxaline by two pathways.

6167



### Copper(I)-induced amplification of a [2]catenane in a virtual dynamic library of macrocyclic alkenes

José Augusto Berrocal, Marko M. L. Nieuwenhuizen, Luigi Mandolini, E. W. Meijer and Stefano Di Stefano\*

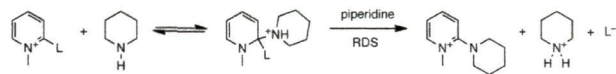
The interlocked virtual component **1** of a well-behaved dynamic library of cyclic olefins is resuscitated by means of the template effect.

6175

### Reactivity in the nucleophilic aromatic substitution reactions of pyridinium ions

Jeannette T. Bowler, Freeman M. Wong, Scott Gronert,\* James R. Keeffe\* and Weiming Wu\*

The nucleophilic aromatic substitution reactions of piperidine with *N*-methylpyridinium ions in methanol occur via rate determining preassociation of a second piperidine molecule with the addition intermediate followed by barrier-free deprotonation. Loss of leaving group is concurrent with deprotonation for Cl, Br, and I (E2), but subsequent to deprotonation, although rapid, for CN and F (E1cB<sub>RR</sub>).

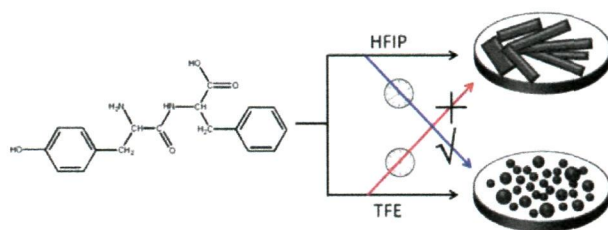


6181

### 1,1,1,3,3,3-Hexafluoro-2-propanol and 2,2,2-trifluoroethanol solvents induce self-assembly with different surface morphology in an aromatic dipeptide

Samala Murali Mohan Reddy, Ganesh Shanmugam\* and Asit Baran Mandal\*

1,1,1,3,3,3-Hexafluoro-2-propanol and 2,2,2-trifluoroethanol solvents, which are known to disaggregate self-assembled peptides, induce the self-assembly of aromatic dipeptides to give structures with different surface morphologies.



6193

### Synthetic and mechanistic aspects of the regioselective base-mediated reaction of perfluoroalkyl- and perfluoroarylsilanes with heterocyclic *N*-oxides

David E. Stephens, Gabriel Chavez, Martin Valdes, Monica Dovalina, Hadi D. Arman and Oleg V. Larionov\*

Novel and efficient method of direct perfluoroalkylation of azine *N*-oxides has been developed and interesting mechanistic details have been provided.

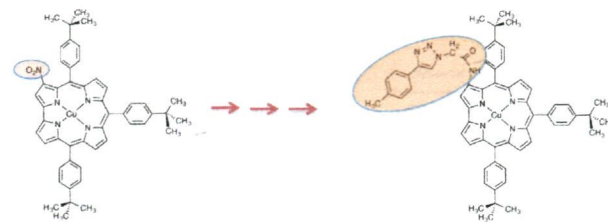


6200

### 3-NO<sub>2</sub>-5,10,15-triarylcorrolato-Cu as a versatile platform for synthesis of novel 3-functionalized corrole derivatives

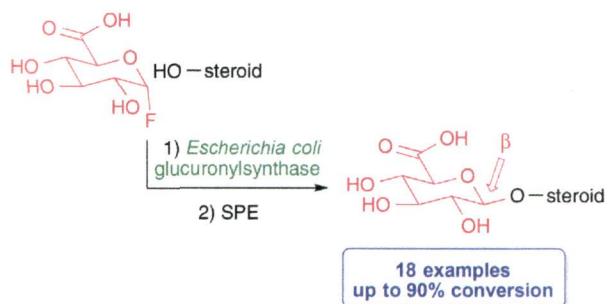
M. Stefanelli, M. Mancini, M. Raggio, S. Nardis,\* F. R. Fronczek, G. T. McCandless, K. M. Smith and R. Paolesse

By way of a  $\beta$ -acylated copper corrolate, a novel corrole derivative bearing an alkyl azide group on the peripheral positions was obtained and successfully exploited in click chemistry reactions.





6208

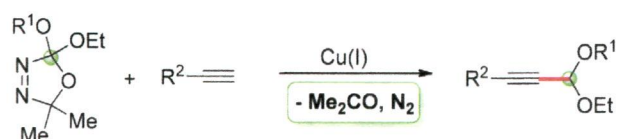


### The *Escherichia coli* glucuronyltransferase promoted synthesis of steroid glucuronides: improved practicality and broader scope

Paul Ma, Nicholas Kanizaj, Shu-Ann Chan, David L. Ollis and Malcolm D. McLeod\*

Steroid glucuronides can be quickly and conveniently prepared on the milligram scale using the *E. coli* glucuronyltransferase enzyme followed by purification with solid-phase extraction.

6215

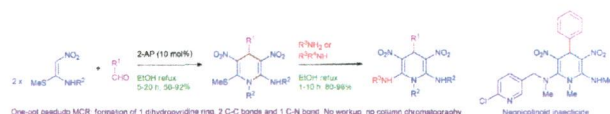


### CuI-catalyzed cross-coupling of terminal alkynes with dialkoxy-carbenes: a general method for the synthesis of unsymmetrical propargylic acetals

Tiebo Xiao, Ping Zhang, Yang Xie, Jun Wang and Lei Zhou\*

A general source of dialkoxy-carbenes, 2,2-dialkoxy-5,5-dimethyl- $\Delta^3$ -1,3,4-oxadiazolines, have been successfully employed as coupling partners in CuI-catalyzed cross-coupling reactions with terminal alkynes, which afforded various unsymmetrical propargylic acetals in good yields.

6223

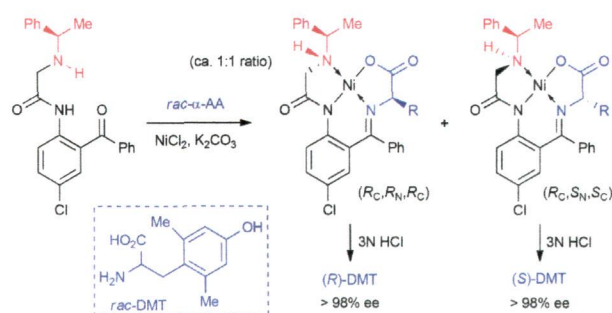


### One-pot pseudo three-component reaction of nitroketene-*N,S*-acetals and aldehydes for synthesis of highly functionalized hexa-substituted 1,4-dihydropyridines

H. Surya Prakash Rao\* and A. Parthiban

Pseudo three-component condensation of aliphatic/aromatic/ $\alpha,\beta$ -unsaturated aldehydes and nitroketene-*N,S*-acetals to afford diversely functionalized hexa-substituted 1,4-dihydropyridines under 2-aminopyridine catalysis was achieved.

6239



### Design and synthesis of (*S*)- and (*R*)- $\alpha$ -(phenyl) ethylamine-derived NH-type ligands and their application for the chemical resolution of $\alpha$ -amino acids

Ryosuke Takeda, Akie Kawamura, Aki Kawashima, Hiroki Moriwaki, Tatsunori Sato, José Luis Aceña\* and Vadim A. Soloshonok\*

A chiral ligand reacts with racemic amino acids to produce easily separable Ni(II) complexes which can be disassembled to afford both enantiomers of target amino acids.

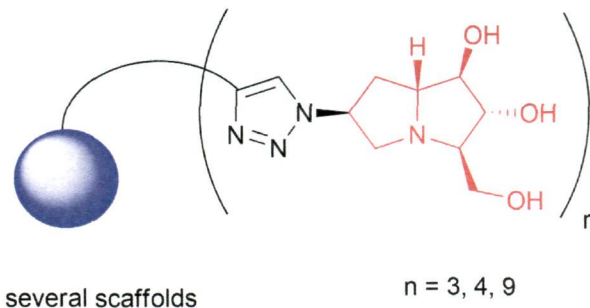


6253

### 6-Azido hyacinthacine A<sub>2</sub> gives a straightforward access to the first multivalent pyrrolizidine architectures

Giampiero D'Adamio, Camilla Parmeggiani, Andrea Goti,\* Antonio J. Moreno-Vargas, Elena Moreno-Clavijo, Inmaculada Robina and Francesca Cardona\*

The synthesis of the first multivalent pyrrolizidine iminosugars is reported, with up to 9 bioactive molecules on the same scaffold.



6267

### Synthesis, and the antioxidant, neuroprotective and P-glycoprotein induction activity of 4-arylquinoline-2-carboxylates

Jaideep B. Bharate, Abubakar Wani, Sadhana Sharma, Shahi Imam Reja, Manoj Kumar, Ram A. Vishwakarma,\* Ajay Kumar\* and Sandip B. Bharate\*

An efficient synthesis of 4-arylquinoline-2-carboxylates and their antioxidant, neuroprotective and P-glycoprotein induction activity have been described.

