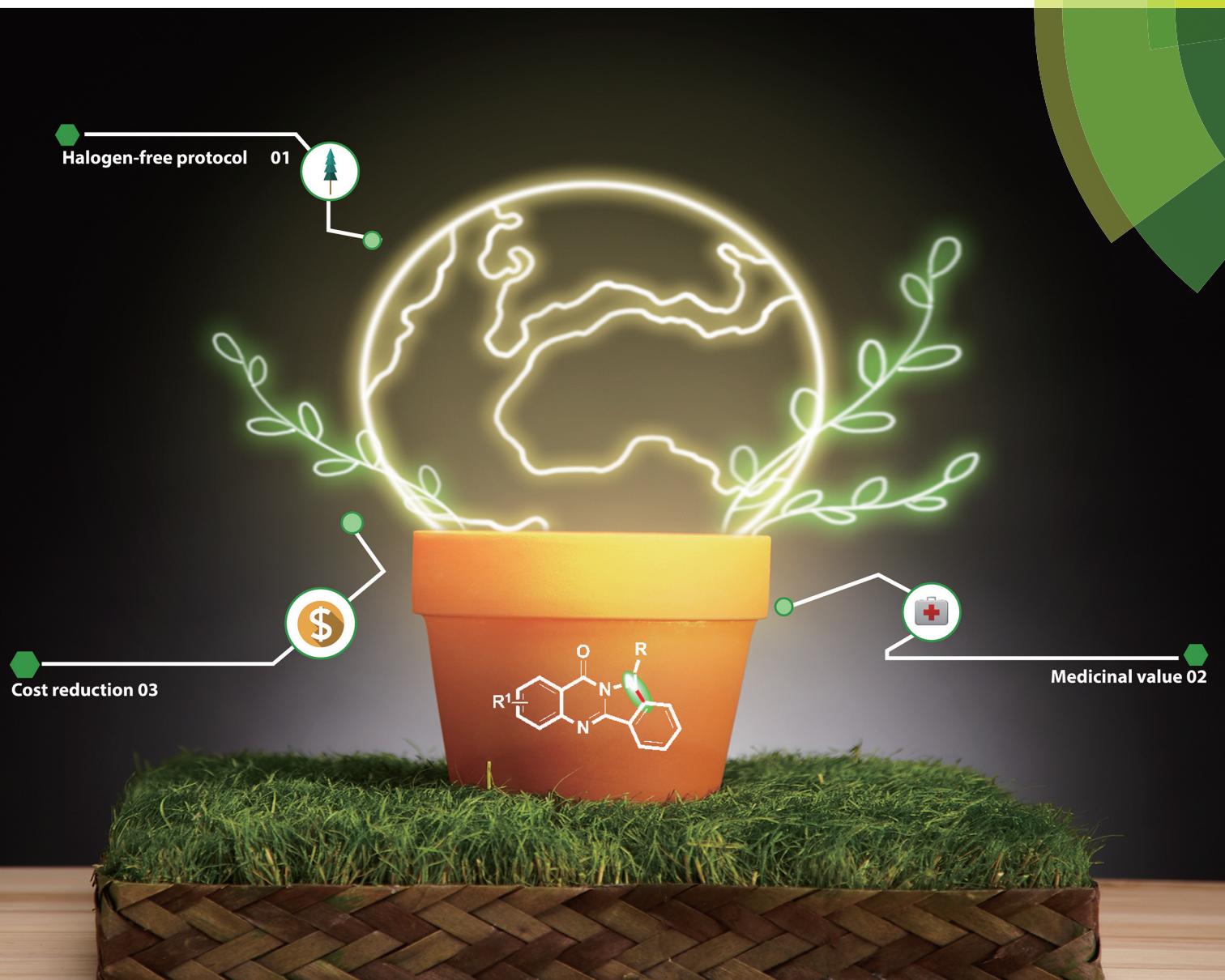


# Organic & Biomolecular Chemistry

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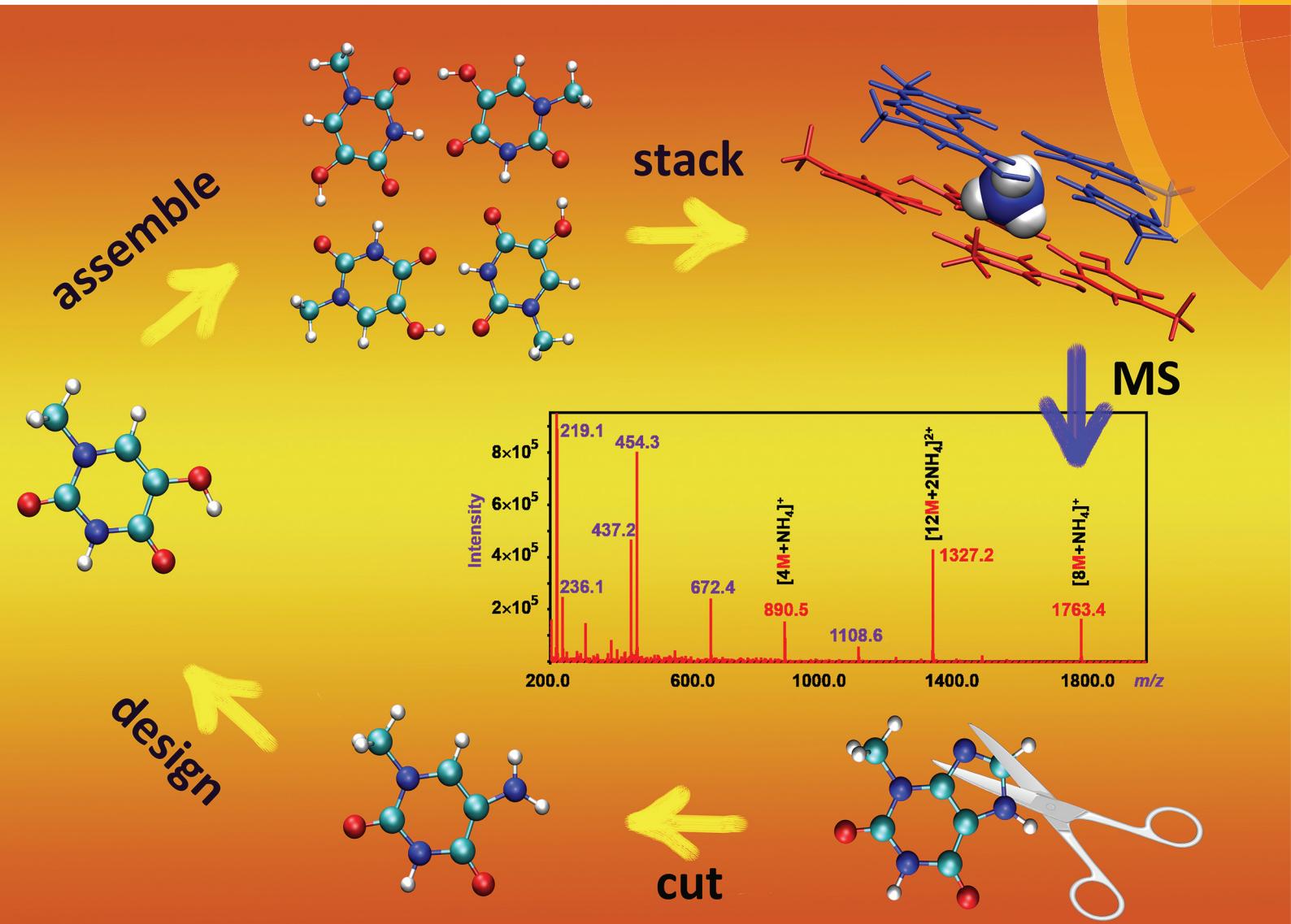
## PAPER

Jiuxi Chen, Huayue Wu *et al.*

Copper-catalyzed C–O bond cleavage and cyclization: synthesis of indazolo[3,2-*b*]quinazolinones

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## PAPER

Célia Fonseca Guerra, Lajos Kovács *et al.*

The evaluation of 5-amino- and 5-hydroxyuracil derivatives as potential quadruplex-forming agents

# Organic & Biomolecular Chemistry

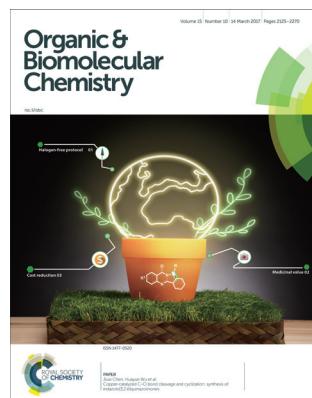
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## IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 15(10) 2125–2270 (2017)



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See Jiuxi Chen,  
Huayue Wu et al.,  
pp. 2168–2173.

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### Inside cover

See Célia Fonseca Guerra,  
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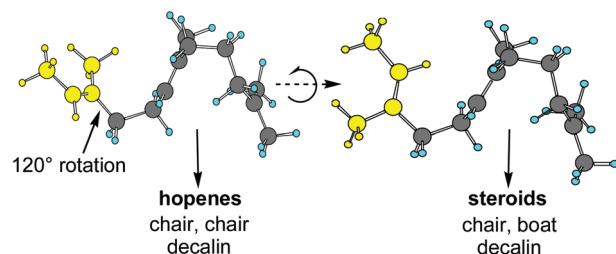
## REVIEWS

2133

### Computational studies on the cyclization of squalene to the steroids and hopenes

B. Andes Hess, Jr

A review of computational studies of the related biosyntheses of steroids and hopenes reported during the last two decades is presented.

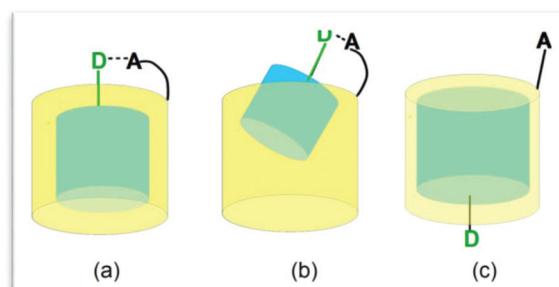


2146

### Spatial mismatch, non-additive binding energies and selectivity in supramolecular complexes

Hans-Jörg Schneider

A geometric mismatch in supramolecular complexes often leads to deviations from the additivity of binding energies with the consequence of large changes in selectivity and binding mode.



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**Organic & Biomolecular Chemistry**  
 (print: ISSN 1477-0520; electronic: ISSN 1477-0539)  
 is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK Tel +44 (0)1223 432398; E-mail [orders@rsc.org](mailto:orders@rsc.org)

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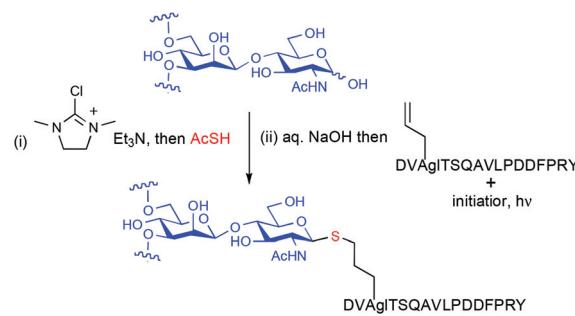
## COMMUNICATIONS

2152

**Protecting group free synthesis of glycosyl thiols from reducing sugars in water; application to the production of *N*-glycan glycoconjugates**

S. R. Alexander, D. Lim, Z. Amso, M. A. Brimble and A. J. Fairbanks\*

Un-protected 2-acetamido terminated reducing sugars may be converted into the corresponding glycosyl thiols in water, and conjugated to peptides using the thiol–ene click reaction without recourse to any protecting groups.

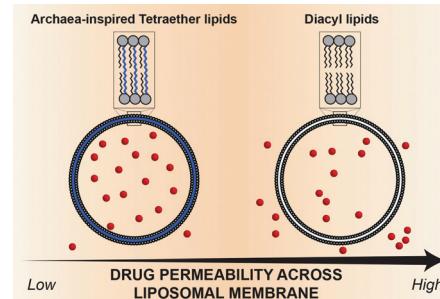


2157

**Characterization of drug encapsulation and retention in archaea-inspired tetraether liposomes**

Geoffrey Leriche, Jessica L. Cifelli, Kevin C. Sibucao, Joseph P. Patterson, Takaoki Koyanagi, Nathan C. Gianneschi and Jerry Yang\*

Archaea-inspired lipids exhibit reduced membrane permeability and increased retention of hydrophilic drugs in liposomes.

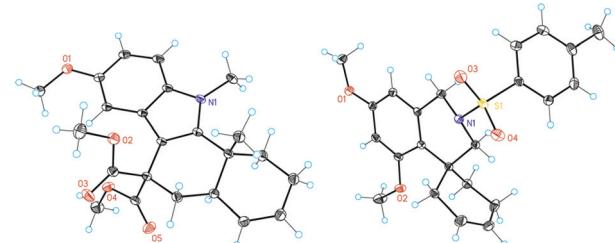


2163

**Broad scope gold(II)-catalysed polyenyne cyclisations for the formation of up to four carbon–carbon bonds**

Zhouting Rong and Antonio M. Echavarren\*

The polycyclisation of polyenyynes catalyzed by gold(II) has been extended for the first time to the simultaneous formation of up to four carbon–carbon bonds, leading to steroid-like molecules with high stereoselectivity in a single step with low catalyst loadings.



## PAPERS

2168

**Copper-catalyzed C–O bond cleavage and cyclization: synthesis of indazolo[3,2-*b*]-quinazolinones**

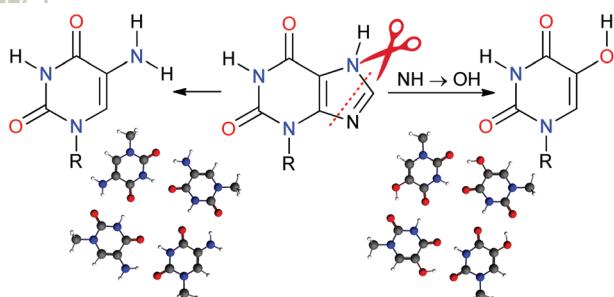
Rui Qiao, Leping Ye, Kun Hu, Shuling Yu, Weiguang Yang, Miaochang Liu, Jiuxi Chen,\* Jinchang Ding and Huayue Wu\*

Cu-catalyzed sequential inert C–O bond cleavage followed by intramolecular C–N bond formation for the synthesis of indazolo[3,2-*b*]quinazolinones.



## PAPERS

2174

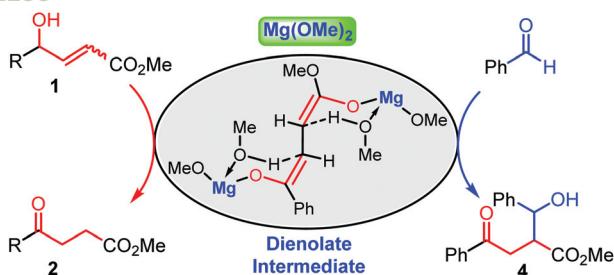


**The evaluation of 5-amino- and 5-hydroxyuracil derivatives as potential quadruplex-forming agents**

Gábor Paragi, Zoltán Kupihár, Gábor Endre, Célia Fonseca Guerra\* and Lajos Kovács\*

5-Hydroxyuracil has been identified as a building block for supramolecular quadruplex assemblies.

2185

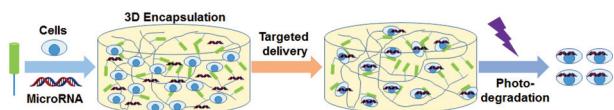


**Mg(OMe)<sub>2</sub> promoted allylic isomerization of  $\gamma$ -hydroxy- $\alpha,\beta$ -alkenoic esters to synthesize  $\gamma$ -ketone esters**

Luhao Lai, A-Ni Li, Jiawei Zhou, Yarong Guo, Li Lin,\* Wei Chen and Rui Wang\*

Herein we report a facile Mg(OMe)<sub>2</sub> promoted allylic isomerization to afford  $\gamma$ -keto esters involving an *in situ* dienolate intermediate.

2191



**A photo-degradable supramolecular hydrogel for selective delivery of microRNA into 3D-cultured cells**

Zhengquan Zhou, Qikun Yi, Tingting Xia, Wencui Yin, Adnan A. Kadi, Jinbo Li\* and Yan Zhang\*

A multi-functional supramolecular hydrogel was developed for long-term 3D cell culture, targeted miRNA delivery and easy collection of encapsulated cells.

2199



**Intramolecular Minisci acylation under silver-free neutral conditions for the synthesis of azafluorenones and fluorenones**

Joydev K. Laha,\* Ketul V. Patel, Gurudutt Dubey and Krupal P. Jethava

An intramolecular Minisci acylation under silver-free neutral conditions providing access to azafluorenones and fluorenones has been developed.

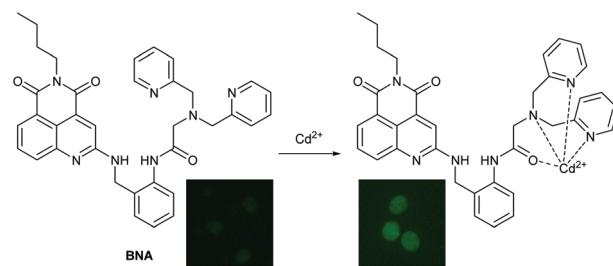
## PAPERS

## 2211

**A 4,5-quinolimide-based fluorescent sensor for the turn-on detection of Cd<sup>2+</sup> with live-cell imaging**

Yu Zhang, Xiangfeng Guo,\* Mengmeng Zheng, Rui Yang, Hongming Yang, Lihua Jia\* and Mengmeng Yang

The first 4,5-quinolimide sensor, **BNA**, bearing the amide-DPA receptor, was reported for sensing Cd<sup>2+</sup> with live-cell imaging.

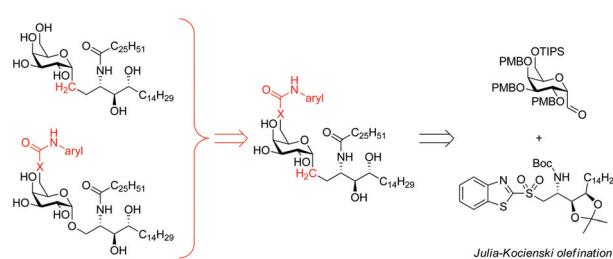


## 2217

**Synthesis of C6''-modified  $\alpha$ -C-GalCer analogues as mouse and human iNKT cell agonists**

Joren Guillaume, Toshiyuki Seki, Tine Decruy, Koen Venken, Dirk Elewaut, Moriya Tsuji and Serge Van Calenbergh\*

$\alpha$ -GalCer analogues that combine known Th1 polarizing C6''-modifications with a C-glycosidic linkage were synthesized and evaluated as iNKT cell antigens.

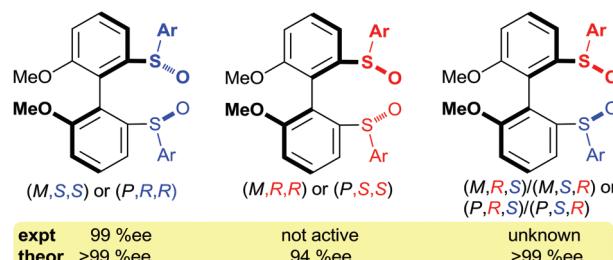


## 2226

**Cooperativity of axial and centre chirality in the biaryl disulfoxide/Rh(I)-catalysed asymmetric 1,4-addition of arylboronic acids to 2-cyclohexenone: a DFT study**

Gao-Feng Zha, Hua-Li Qin\* and Eric Assen B. Kantchev\*

Atropisomeric biaryl disulfoxides contain two synergistic chiral elements.



## 2234

**CuBr/TBHP-mediated synthesis of *N*-acyl sulfonimidamides via the oxidative cross-coupling of sulfonimidamides and aldehydes**

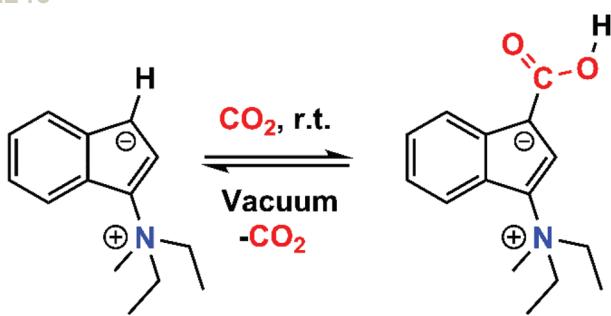
Ganesh Chandra Nandi\* and Cijil Raju

*N*-Acyl sulfonimidamides were synthesized via a Cu-catalyzed double C–H/N–H activation protocol.



## PAPERS

2240

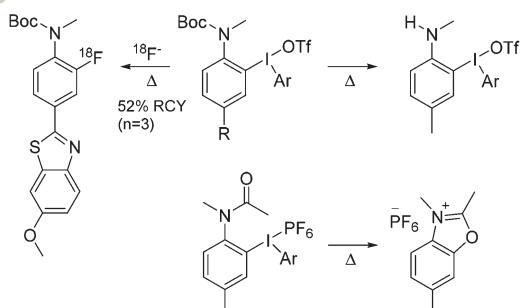


**Zwitterionic indenylammonium with carbon-centred reactivity towards reversible  $\text{CO}_2$  binding and catalytic reduction**

Yanxin Yang, Linfan Yan, Qinyu Xie, Qiuming Liang and Datong Song\*

Zwitterionic indenylammonium can reversibly insert  $\text{CO}_2$  into its C-H bond at ambient temperature and catalyze  $\text{CO}_2$  hydroboration.

2246

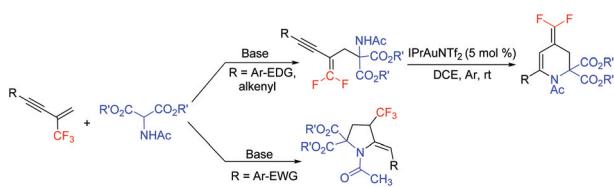


**Thermolysis and radiofluorination of diaryliodonium salts derived from anilines**

Ethan J. Linstad, Amy L. Vävere, Bao Hu, Jayson J. Kempinger, Scott E. Snyder and Stephen G. DiMagno\*

Mechanistic and theoretical studies reveal new reactions of  $\text{Ar}_2\text{I}$  salts that can interfere with radiolabeling of these substrates.

2253

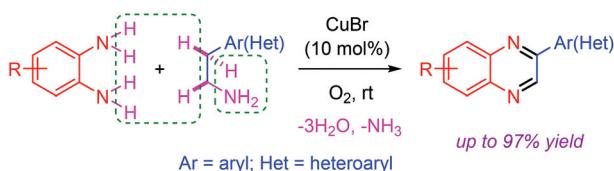


**Divergent synthesis from reactions of 2-trifluoromethyl-1,3-conjugated enynes with *N*-acetylated 2-aminomalonates**

Jieru Yang, Xiaofan Zhou, Yu Zeng, Chaoqian Huang, Yuanjing Xiao\* and Junliang Zhang\*

Divergent synthesis of fluorinated heterocycles from the reactions of 2-trifluoromethyl-1,3-conjugated enynes with *N*-acetylated 2-aminomalonates and subsequent gold-catalysed cyclization were developed.

2259



**Copper-catalyzed aerobic oxidative coupling of *o*-phenylenediamines with 2-aryl/heteroarylethylamines: direct access to construct quinoxalines**

Kovuru Gopalaiah,\* Anupama Saini, Sankala Naga Chandrudu, Devarapalli Chenna Rao, Harsh Yadav and Binay Kumar

A versatile method for synthesis of quinoxalines by Cu-catalyzed oxidative coupling of *o*-phenylenediamines with 2-arylethylamines is presented.