

# Organic & Biomolecular Chemistry

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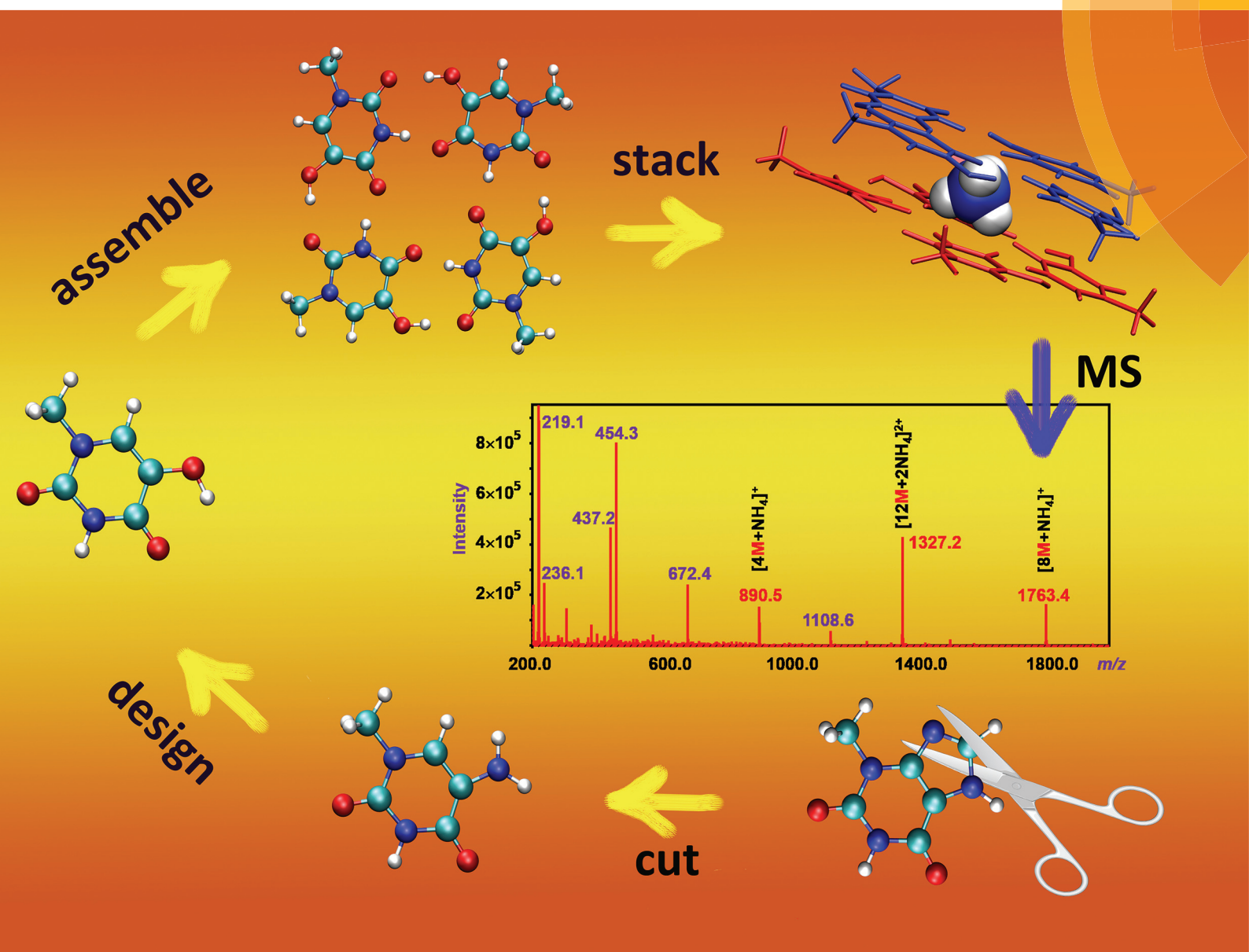


## PAPER

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

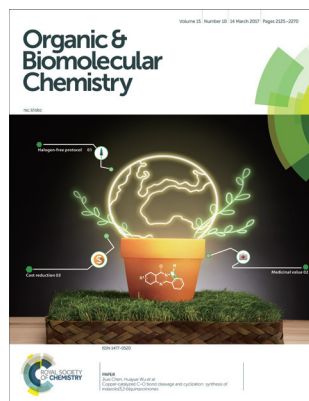
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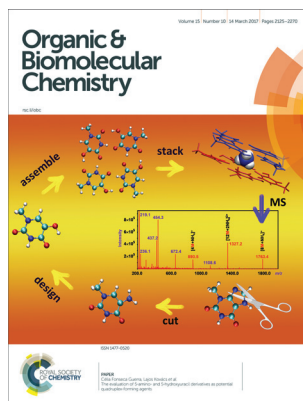
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See Jiuxi Chen,  
Huayue Wu *et al.*,  
pp. 2168–2173.

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2017, **15**, 2168.



### Inside cover

See Célia Fonseca Guerra,  
Lajos Kovács *et al.*,  
pp. 2174–2184.

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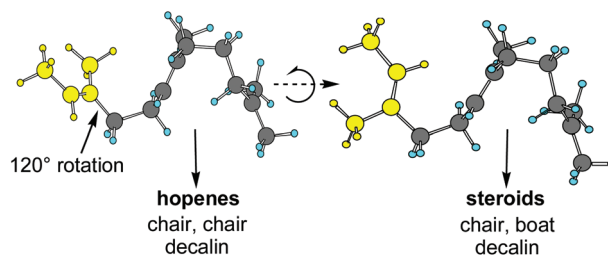
## REVIEWS

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.

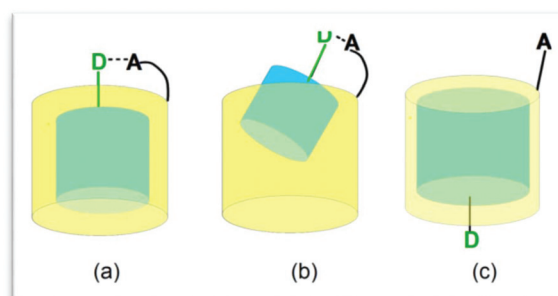


2146

### 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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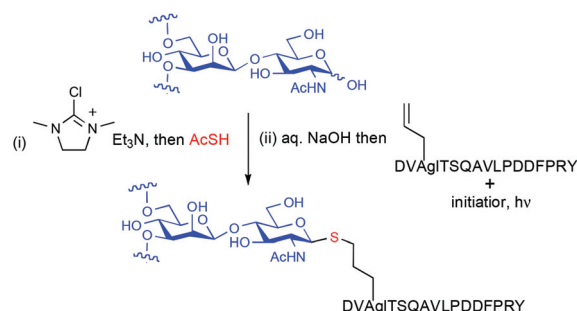
## COMMUNICATIONS

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.

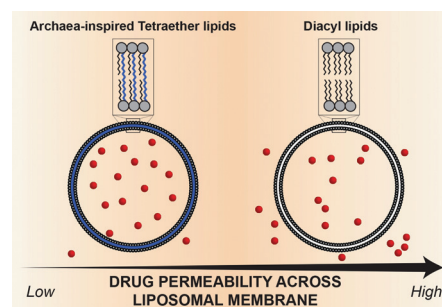


2157

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

Geoffray Leriche, Jessica L. Cifelli, Kevin C. Sibucio, 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.

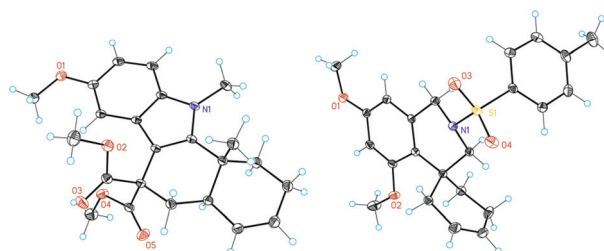


2163

### Broad scope gold(i)-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(i) 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

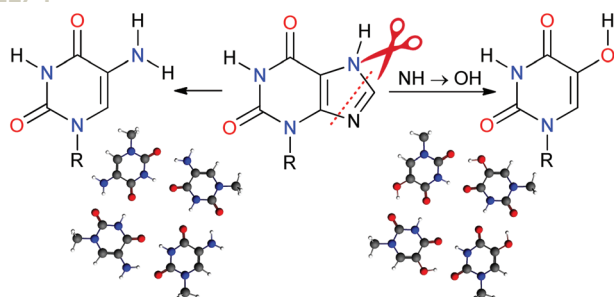
Rui Qiao, Leping Ye, Kun Hu, Shuling Yu, Weiguang Yang, Miaochar Liu, Jiuxi Chen,\* Jinchang Ding and Huayue Wu\*

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

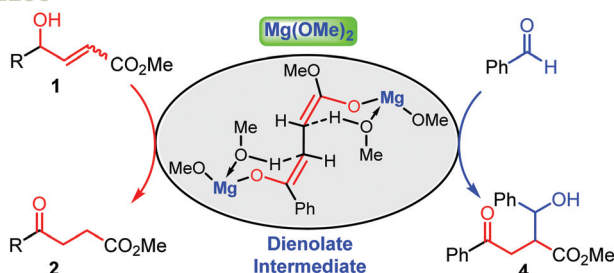


### The evaluation of 5-amino- and 5-hydroxyuracil derivatives as potential quadruplex-forming agents

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

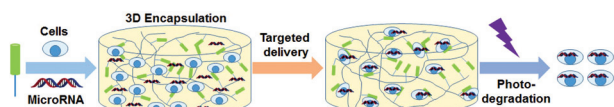


### Mg(OMe)<sub>2</sub> promoted allylic isomerization of $\gamma$ -hydroxy- $\alpha,\beta$ -alkenoic esters to synthesize $\gamma$ -ketone esters

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

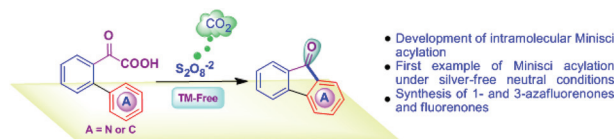


### A photo-degradable supramolecular hydrogel for selective delivery of microRNA into 3D-cultured cells

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.

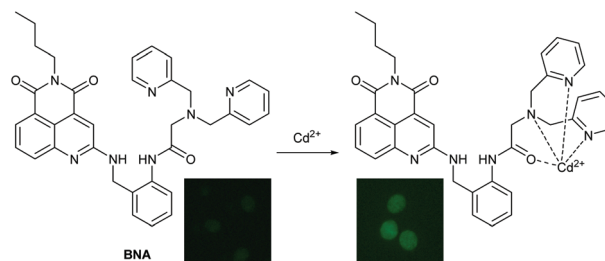
## PAPERS

2211

A 4,5-quinolimine-based fluorescent sensor for the turn-on detection of  $\text{Cd}^{2+}$  with live-cell imaging

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

The first 4,5-quinolimine sensor, **BNA**, bearing the amide-DPA receptor, was reported for sensing  $\text{Cd}^{2+}$  with live-cell imaging.

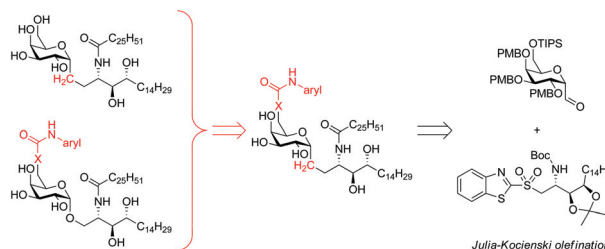


2217

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.

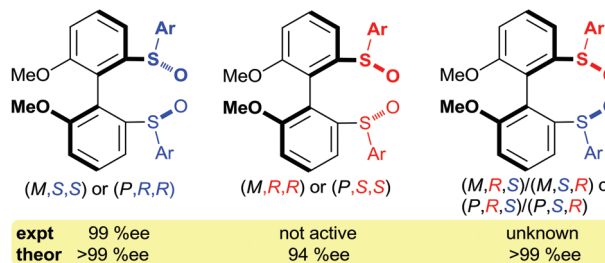


2226

## 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.

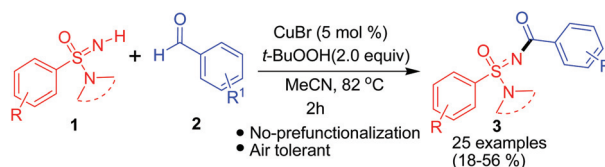


2234

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

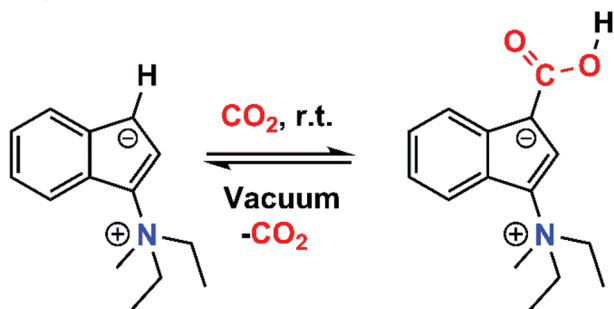
Ganesh Chandra Nandi\* and Cijil Raju

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



## PAPERS

2240

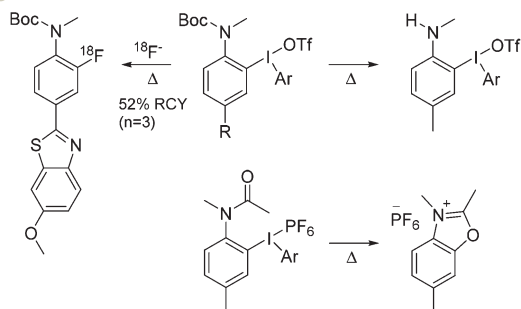


### Zwitterionic indenylammonium with carbon-centred reactivity towards reversible CO<sub>2</sub> binding and catalytic reduction

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

Zwitterionic indenylammonium can reversibly insert CO<sub>2</sub> into its C–H bond at ambient temperature and catalyze CO<sub>2</sub> hydroboration.

2246

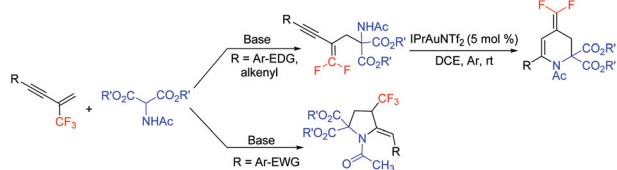


### Thermolysis and radiofluorination of diaryliodonium salts derived from anilines

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

Mechanistic and theoretical studies reveal new reactions of Ar<sub>2</sub>I salts that can interfere with radiolabeling of these substrates.

2253

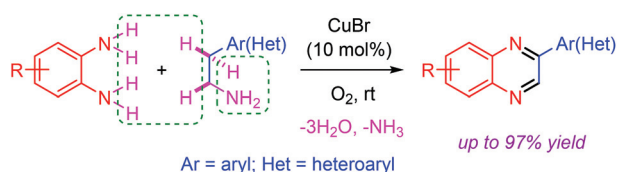


### Divergent synthesis from reactions of 2-trifluoromethyl-1,3-conjugated enynes with *N*-acetylated 2-aminomalonates

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.