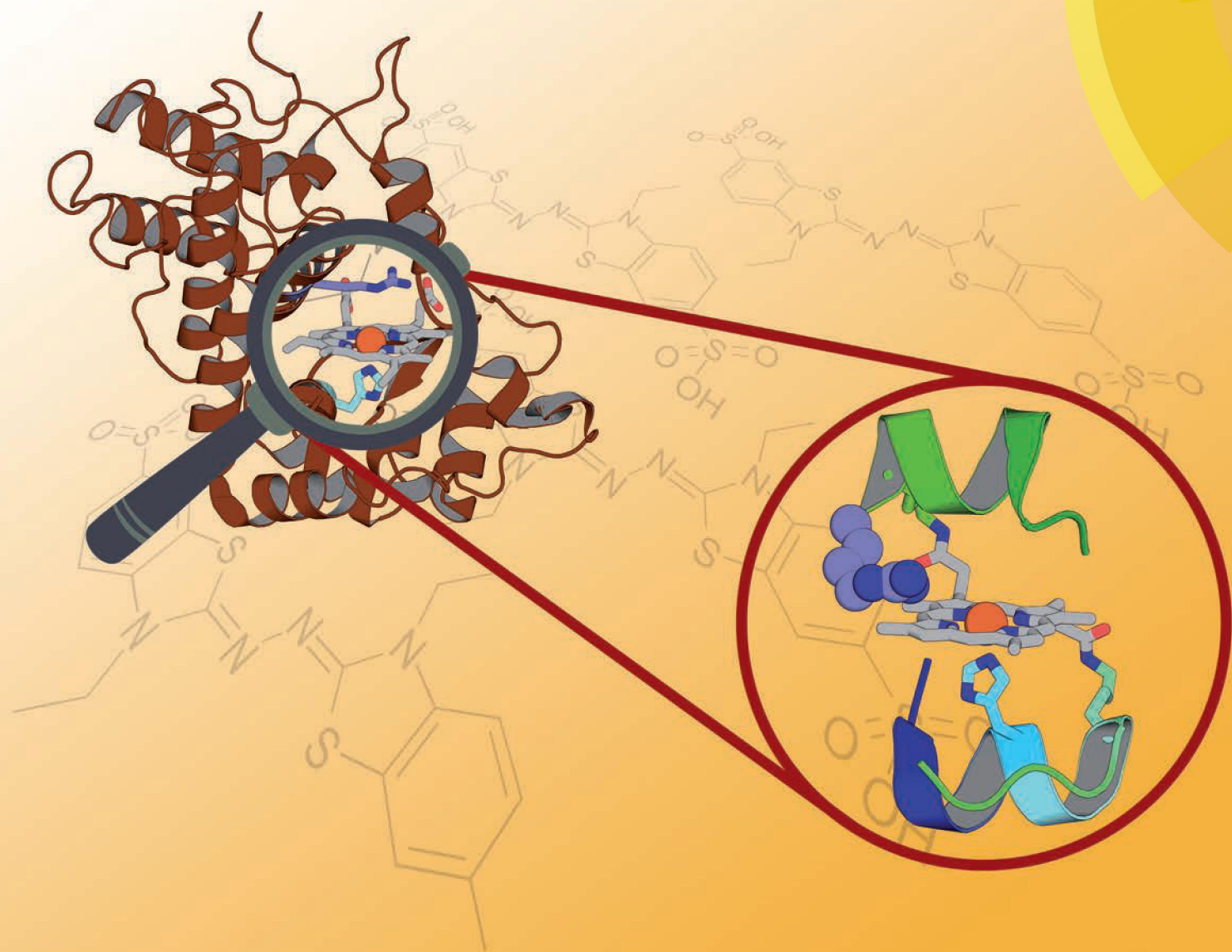


# Organic & Biomolecular Chemistry

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ISSN 1477-0520



**PAPER**

Vincenzo Pavone, Angela Lombardi *et al.*  
An artificial heme-enzyme with enhanced catalytic activity: evolution, functional screening and structural characterization

# Organic & Biomolecular Chemistry

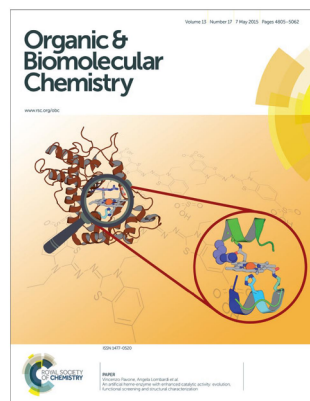
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## IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 13(17) 4805–5062 (2015)

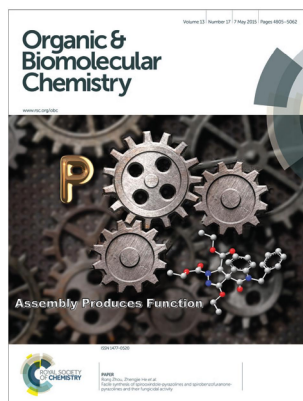


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See Vincenzo Pavone, Angela Lombardi *et al.*, pp. 4859–4868.

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### Inside cover

See Rong Zhou, Zhengjie He *et al.*, pp. 4869–4878.

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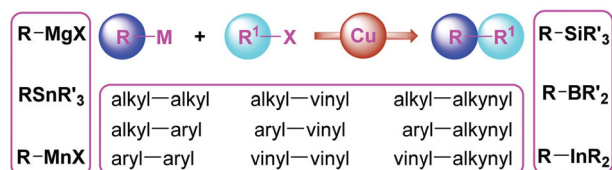
## REVIEW

4816

### Copper-catalysed cross-coupling: an untapped potential

Surendra Thapa, Bijay Shrestha, Santosh K. Gurung and Ramesh Giri\*

Copper is emerging as a viable catalytic metal for cross-coupling reactions to construct carbon–carbon (C–C) bonds.



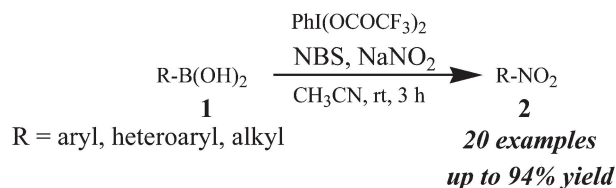
## COMMUNICATIONS

4828

### A novel transition metal free [bis-(trifluoroacetoxy)iodo]benzene (PIFA) mediated oxidative *ipso* nitration of organoboronic acids

Nachiketa Chatterjee, Divya Bhatt and Avijit Goswami\*

A mild, convenient and transition metal free methodology for oxidative *ipso* nitration of organoboronic acids, including heteroaryl- and alkylboronic acids, has been developed using a combination of [bis-(trifluoroacetoxy)]-iodobenzene (PIFA) – *N*-bromosuccinimide (NBS) and sodium nitrite as the nitro source.



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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.

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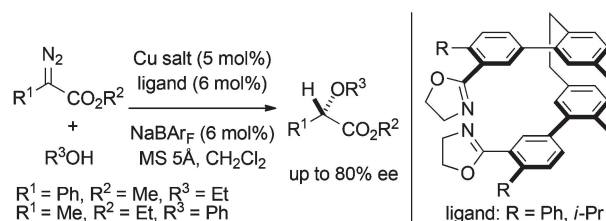
## COMMUNICATIONS

4833

### Synthesis of planar chiral [2.2]paracyclophane-based bisoxazoline ligands bearing no central chirality and application to Cu-catalyzed asymmetric O–H insertion reaction

Shinji Kitagaki,\* Kenta Sugisaka and Chisato Mukai

C<sub>2</sub>-symmetric planar chiral [2.2]paracyclophane-based bisoxazoline ligands effectively control the asymmetric induction during the Cu-catalyzed O–H insertion reaction of  $\alpha$ -diazo esters.

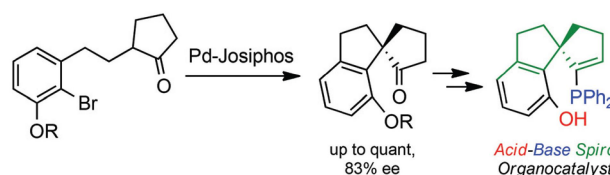


4837

### Pd-catalyzed enantioselective intramolecular $\alpha$ -arylation of $\alpha$ -substituted cyclic ketones: facile synthesis of functionalized chiral spirobicycles

Lulu Fan, Shinobu Takizawa,\* Yoshiki Takeuchi, Kazuhiro Takenaka and Hiroaki Sasai\*

Synthesis of chiral spirocyclic ketones was accomplished via the Pd-catalyzed intramolecular  $\alpha$ -arylation of  $\alpha$ -substituted cyclic ketones. The obtained spirocyclic ketone could be converted into an acid–base organocatalyst.

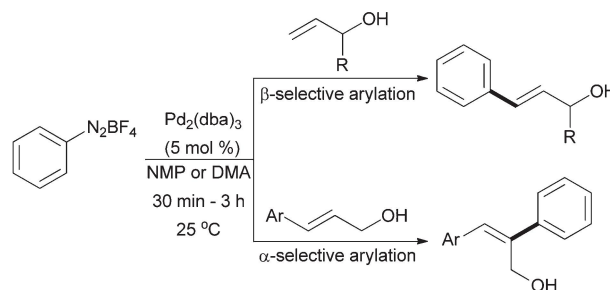


4841

### Chemo-, regio-, and stereoselective Heck–Matsuda arylation of allylic alcohols under mild conditions

Tohasib Yusub Chaudhari, Asik Hossian, Manash Kumar Manna and Ranjan Jana\*

Chemo-, regio-, and stereoselective Heck–Matsuda arylation of allylic and cinnamyl alcohols with inexpensive and readily available arenediazonium salts is reported.

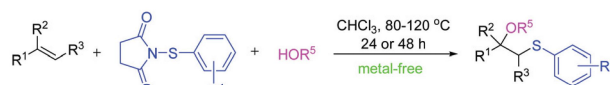


4846

### Metal-free oxysulfenylation of alkenes with 1-(aryltio)pyrrolidine-2,5-diones and alcohols

Jipan Yu, Chang Gao, Zhixuan Song, Haijun Yang and Hua Fu\*

An easy and efficient metal-free approach to  $\beta$ -alkoxy sulfides has been developed. The protocol uses readily available 1-(aryltio)pyrrolidine-2,5-diones and alcohols as the oxysulfenyating agents, chloroform as the solvent, and no ligand, additive and exclusion of air were required.



## COMMUNICATIONS

4851

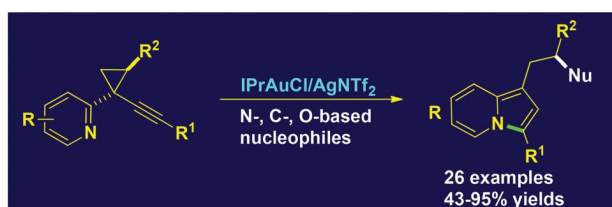


### An efficient approach to 1,2,3-trisubstituted indole *via* rhodium catalyzed carbene C<sub>sp<sup>3</sup></sub>-H bond insertion

Mei-Hua Shen,\* Ying-Peng Pan, Zhi-Hong Jia, Xin-Tao Ren, Ping Zhang and Hua-Dong Xu\*

A method for convenient synthesis of *N*-alkyl-2-aryl-indole-3-carbaldehyde *via* carbene C-H bond insertion.

4855



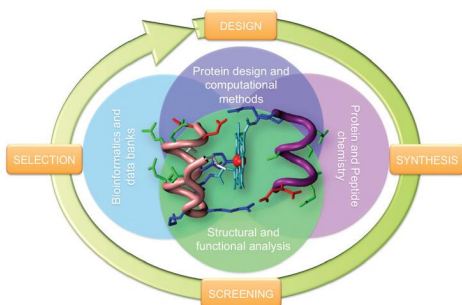
### Au-catalyzed ring-opening reactions of 2-(1-alkynyl-cyclopropyl)pyridines with nucleophiles

Ren-Rong Liu, Shi-Chun Ye, Chuan-Jun Lu, Bin Xiang, Jianrong Gao and Yi-Xia Jia\*

A novel method for the C-C bond cleavage of cyclopropanes was developed by gold-catalyzed cycloisomerization of 2-(1-alkynyl-cyclopropyl)pyridine with nucleophiles, which provides efficient access to structurally diverse indolizines under mild conditions.

## PAPERS

4859

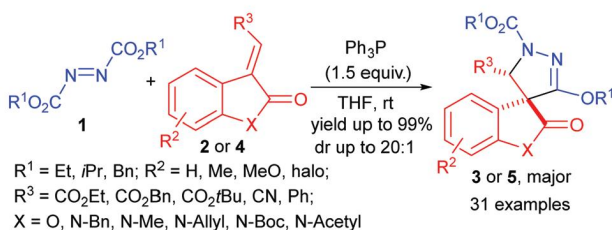


### An artificial heme-enzyme with enhanced catalytic activity: evolution, functional screening and structural characterization

Rosa Vitale, Liliana Lista, Corinne Cerrone, Giorgio Caserta, Marco Chino, Ornella Maglio, Flavia Nastri, Vincenzo Pavone\* and Angela Lombardi\*

The rational refinement of function into the heme-protein model Mimochrome VI (MC6) resulted in a new analogue, Fe<sup>III</sup>-E<sup>2</sup>L(TD)-MC6, with an improved peroxidase activity.

4869



### Facile synthesis of spirooxindole-pyrazolines and spirobenzofuranone-pyrazolines and their fungicidal activity

Changjiang Yang, Juanjuan Li, Rong Zhou,\* Xiangyu Chen, Yunpeng Gao and Zhengjie He\*

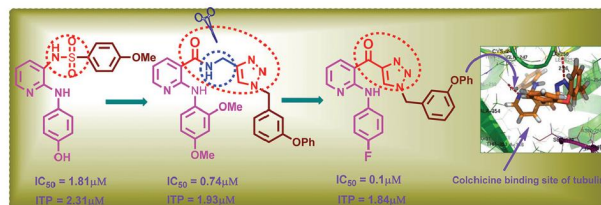
A new and facile synthetic method is developed for biologically important spirooxindole-pyrazolines and spirobenzofuranone-pyrazolines.

4879

### Synthesis of 2-anilinopyridyl–triazole conjugates as antimetabolic agents

Ahmed Kamal,\* A. V. Subba Rao, M. V. P. S. Vishnuvardhan, T. Srinivas Reddy, Konderu Swapna, Chandrakant Bagul, N. V. Subba Reddy and Vunnam Srinivasulu

The newly synthesized 2-anilinopyridyl–triazole conjugates with excellent pharmacological profile could serve as leads for further optimization.



4896

### Manganese(III)-mediated alkenyl C<sub>sp2</sub>–P bond formation from the reaction of β-nitrostyrenes with dialkyl phosphites

Jian-Fei Xue, Shao-Fang Zhou, Ye-Ye Liu, Xiangqiang Pan,\* Jian-Ping Zou\* and Olayinka Taiwo Asekun

Mn(OAc)<sub>3</sub>-mediated tandem phosphonyl radical addition to β-nitrostyrenes followed by denitration to form (*E*)-2-alkenyl phosphonates is described.

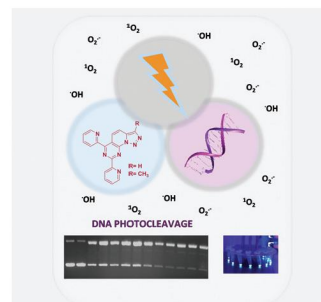


4903

### Triazolopyridopyrimidines: an emerging family of effective DNA photocleavers. DNA binding. Antileishmanial activity

Rosa Adam, Pablo Bilbao-Ramos, Belén Abarca,\* Rafael Ballesteros,\* M. Eugenia González-Rosende, M. Auxiliadora Dea-Ayuela, Francisco Estevan and Gloria Alzuet-Piña\*

Triazolopyridopyrimidine compounds behave as DNA photocleavers through both type I and type II mechanisms.

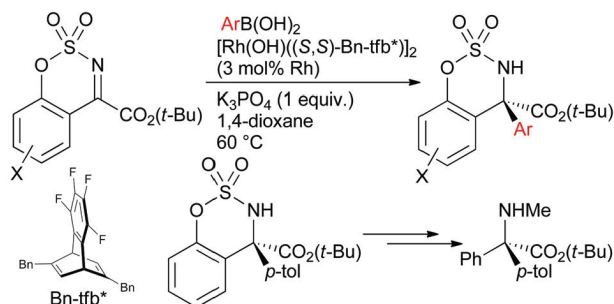


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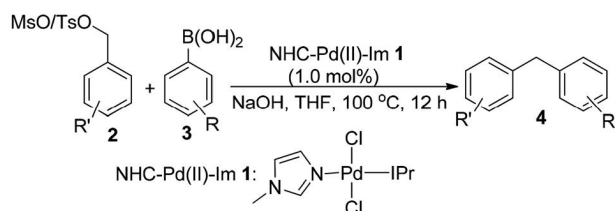
### Rhodium-catalyzed asymmetric addition of arylboronic acids to cyclic *N*-sulfonyl ketimines towards the synthesis of α,α-diaryl-α-amino acid derivatives

Ryosuke Takechi and Takahiro Nishimura\*

Rhodium/chiral diene complex-catalyzed asymmetric addition of arylboronic acids to cyclic ketimines having an ester group proceeded to give the corresponding α-amino acid derivatives in high yields with high enantioselectivity.



4925

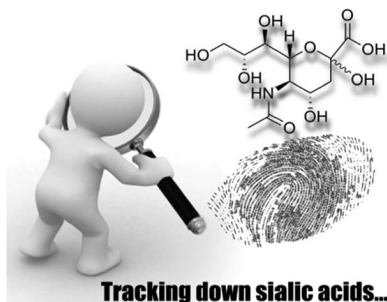


### N-heterocyclic carbene–palladium(II)–1-methylimidazole complex-catalyzed Suzuki–Miyaura coupling of benzyl sulfonates with arylboronic acids

Xiao-Xia Wang, Bin-Bin Xu, Wen-Ting Song, Kai-Xin Sun and Jian-Mei Lu\*

The first example of palladium-catalyzed coupling between benzyl sulfonates and arylboronic acids was reported.

4931



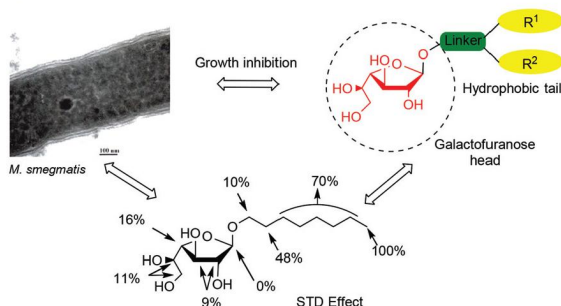
Tracking down sialic acids...

### Elucidation of several neglected reactions in the GC–MS identification of sialic acids as heptafluorobutyrate calls for an urgent reassessment of previous claims

Paola Rota,\* Luigi Anastasia and Pietro Allevi

A revision of the analytical protocol for the GC–MS determination of free or 1,7-lactonized sialic acids as heptafluorobutyrate is reported.

4940

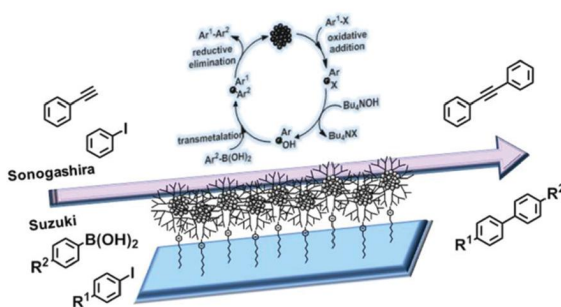


### Synthesis and evaluation of 1,2-*trans* alkyl galactofuranoside mimetics as mycobacteriostatic agents

Rémy Dureau, Maxime Gicquel, Isabelle Artur, Jean-Paul Guégan, Bertrand Carboni, Vincent Ferrières, Fabienne Berrée\* and Laurent Legentil\*

The strong interaction of an octyl chain with *M. smegmatis* cells was paired with high specificity of the galactofuranose ring against mycobacteria growth.

4953



### Dendrimer-encapsulated Pd nanoparticles as catalysts for C–C cross-couplings in flow microreactors

Roberto Ricciardi, Jurriaan Huskens and Willem Verboom\*

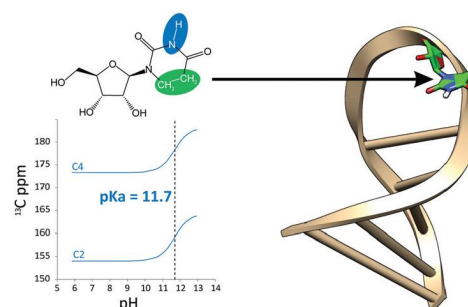
Dendrimer-encapsulated Pd nanoparticles anchored within continuous flow microreactors are efficient for C–C cross-coupling reactions. This is witnessed by the good catalytic performance for the Heck–Cassar and Suzuki–Miyaura couplings.

4960

### Contribution of dihydrouridine in folding of the D-arm in tRNA

N. Dyubankova, E. Sochacka, K. Kraszewska, B. Nawrot, P. Herdewijn and E. Lescrinier\*

NMR studies of the D-arm of tRNA<sup>Met</sup> revealed the crucial role of dihydrouridine nucleoside in folding of the oligo.

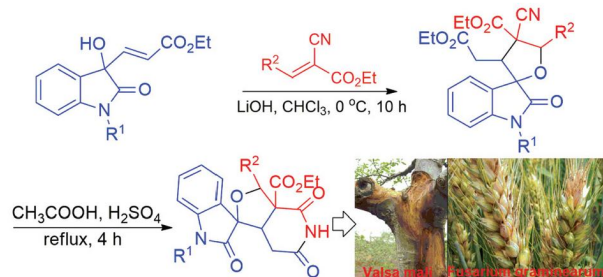


4967

### Synthesis and antifungal activities of novel polyheterocyclic spirooxindole derivatives

Jia-Shou Wu,\* Xue Zhang, Ying-Lao Zhang and Jian-Wu Xie\*

A series of spirooxindole tetrahydrofuran derivatives were obtained in moderate to good yields *via* base-mediated cascade [3 + 2] double Michael reactions under mild conditions. Their antifungal effects on selected five target phytopathogenic fungi were investigated, and their structure antifungal activity relationships were also discussed.



4976

### Efficient approach to 2-hydroxy-2,3-dihydrofuran derivatives and its application for the synthesis of novel 4-(1H-pyrazol-4-yl)pyridazines

Jun-Rui Ma, Wen-Ming Shu, Kai-Lu Zheng, Fan Ni, Guo-Dong Yin\* and An-Xin Wu\*

A highly efficient method for the synthesis of 2-hydroxy-2,3-dihydrofuran derivatives from 1,4-enediones and phenacyl pyridinium halides *via* a domino reaction has been developed. At the same time, we also synthesize the novel 4-(1H-pyrazol-4-yl)pyridazine skeleton.

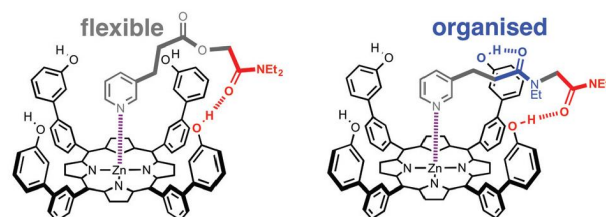


4981

### Influence of non-covalent preorganization on supramolecular effective molarities

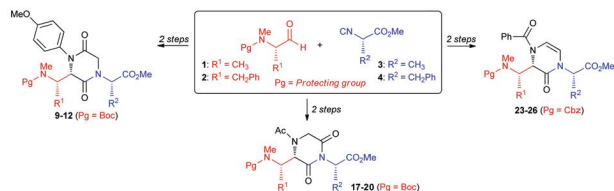
Hongmei Sun, Cristina Navarro and Christopher A. Hunter\*

Formation of H-bonding interactions, which restrict the conformational mobility of a flexible linker, have no effect on chelate cooperativity in a family of porphyrin-pyridine complexes.





4993

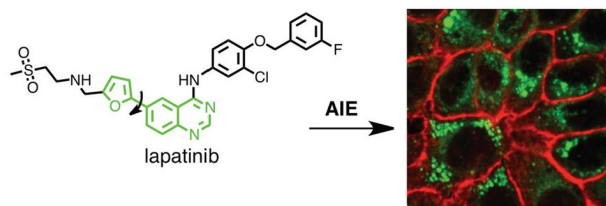


### Application of the Ugi reaction with multiple amino acid-derived components: synthesis and conformational evaluation of piperazine-based minimalist peptidomimetics

Mattia Stucchi, Silvia Cairati, Rengul Cetin-Atalay, Michael S. Christodoulou, Giovanni Grazioso, Gennaro Pescitelli, Alessandra Silvani,\* Deniz Cansen Yildirim and Giordano Lesma

Three different chiral piperazine-based scaffolds have been synthesized using a Ugi/cyclization strategy.

5006



### Binding-induced, turn-on fluorescence of the EGFR/ERBB kinase inhibitor, lapatinib

James N. Wilson,\* Wenjun Liu, Adrienne S. Brown and Ralf Landgraf

The photophysical properties, fluorescence imaging, cellular uptake and distribution of lapatinib, an EGFR/ERBB inhibitor are reported.

5012

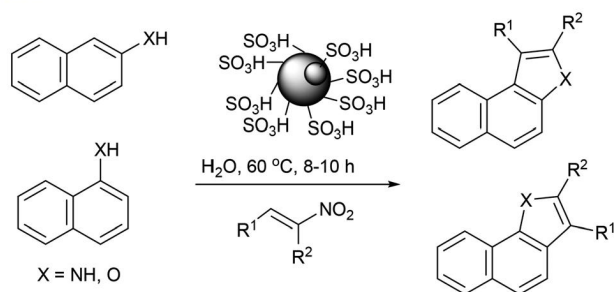


### Hot water-promoted cyclopropylcarbinyl rearrangement facilitates construction of homoallylic alcohols

Pei-Fang Li, Cheng-Bo Yi and Jin Qu\*

Hot water can promote the rearrangements of various types of cyclopropyl carbinols to afford acyclic or cyclic homoallylic alcohols in high yields.

5022



### Facile synthesis of benzoindoles and naphthofurans through carbonaceous material-catalyzed cyclization of naphthylamines/naphthols with nitroolefins in water

Furen Zhang, Chunmei Li, Chen Wang and Chenze Qi\*

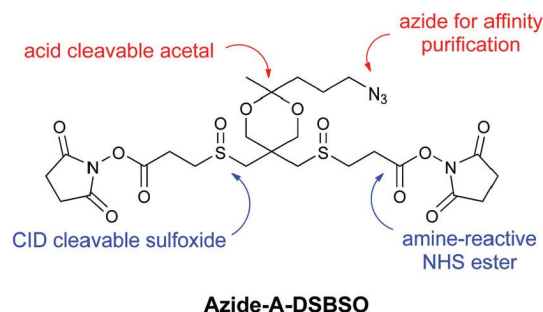
A facile and efficient approach has been established for the synthesis of benzoindole and naphthofuran derivatives via the metal-free cyclization reaction of nitroolefins with naphthylamines/naphthols.

5030

### Synthesis of two new enrichable and MS-cleavable cross-linkers to define protein–protein interactions by mass spectrometry

Anthony M. Burke, Wynne Kandur, Eric J. Novitsky, Robyn M. Kaake, Clinton Yu, Athit Kao, Danielle Vellucci, Lan Huang and Scott D. Rychnovsky\*

The cross-linking Mass Spectrometry (XL-MS) technique extracts structural information from protein complexes without requiring highly purified samples, crystallinity, or large amounts of material.

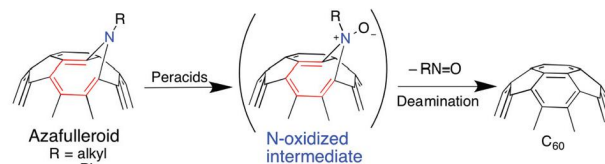


5038

### Oxidative deamination of azafulleroids into C<sub>60</sub> by peracids

Naohiko Ikuma,\* Koichi Fujioka, Yusuke Misawa, Ken Kokubo and Takumi Oshima

Oxidation of azafulleroids with peracids regenerate C<sub>60</sub> via oxidation of the bridged nitrogen, depending on the basicity of N-substituents.

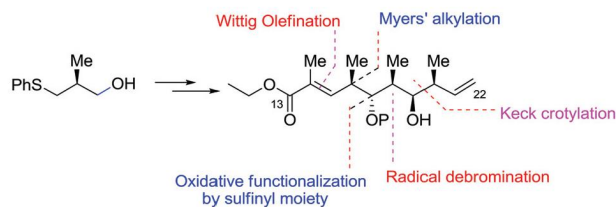


5044

### Stereoselective synthesis of the C13–C22 fragment of callistatin A by a non-aldol approach

Sadagopan Raghavan\* and Sheelamanthula Rajendar

A stereoselective route to the C13–C22 subunit of callistatin A is disclosed.



5054

### Novel ferrocene-based bifunctional amine–thioureas for asymmetric Michael addition of acetylacetone to nitroolefins

Xiaochen Ren, Chunyan He, Yingle Feng, Yonghai Chai,\* Wei Yao, Weiping Chen and Shengyong Zhang\*

An efficient method was developed to synthesize the ferrocene-based bifunctional amine–thioureas bearing multiple hydrogen-bonding donors. Asymmetric Michael addition of acetylacetone to nitroolefins catalyzed by these novel bifunctional catalysts affords the Michael adducts in high yield and moderate to excellent enantioselectivities.

