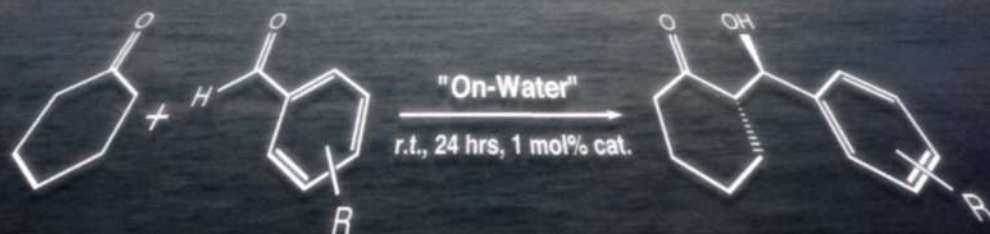


# Organic & Biomolecular Chemistry

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**PAPER**

Luke C. Henderson *et al.*  
Synergistic effects within a C<sub>2</sub>-symmetric organocatalyst: the potential formation of a chiral catalytic pocket



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# Organic & Biomolecular Chemistry

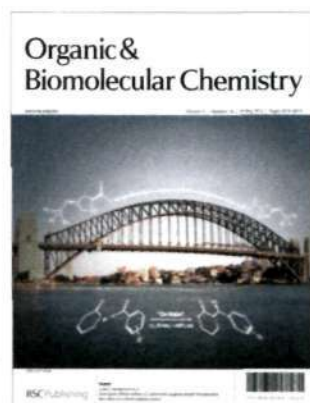
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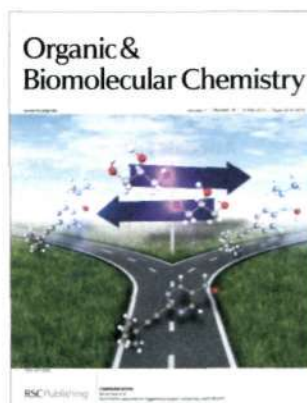
ISSN 1477-0520 CODEN OBCRAK 11(18) 2919–3074 (2013)



### Cover

See Luke C. Henderson *et al.*, pp. 2951–2960.

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### Inside cover

See Kenso Soai *et al.*, pp. 2928–2931.

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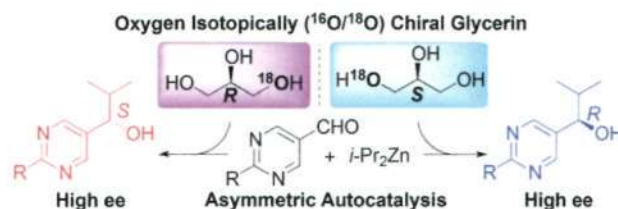
## COMMUNICATIONS

2928

### Asymmetric autocatalysis triggered by oxygen isotopically chiral glycerin

Arimasa Matsumoto, Shotaro Oji, Shizuka Takano, Kyohei Tada, Tsuneomi Kawasaki and Kenso Soai\*

Oxygen isotopic ( $^{18}\text{O}/^{16}\text{O}$ ) chirality of glycerin induces enantioselective addition of diisopropylzinc to pyrimidine-5-carbaldehyde with high enantiomeric excess in conjunction with asymmetric autocatalysis.



2932

### The development of a one pot, regiocontrolled, three-component reaction for the synthesis of thieno[2,3-c]pyrroles

Cynthia M. Hong and Alexander V. Statsyuk\*

A three-component reaction has been developed that allows the regioselective synthesis of thieno[2,3-c]pyrroles.



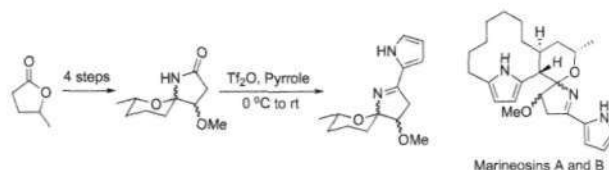


2936

### A concise approach to the spiroiminal fragment of marineosins

Guang Li, Xun Zhang, Qi Li, Pengju Feng and Yian Shi\*

A concise approach to the spiroiminal fragment of marineosins A and B is described. The key steps involve an acid-catalyzed *N*-acyliminium ion cyclization and a Vilsmeier–Haack reaction with  $\text{Tf}_2\text{O}$ .

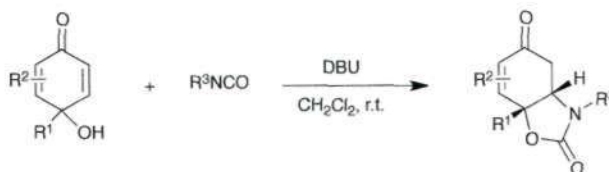


2939

### An expedient stereoselective and chemoselective synthesis of bicyclic oxazolidinones from quinols and isocyanates

Jinzhu Zhang, Jing Wu, Zhiwei Yin, Haisu Zeng, Kunal Khanna, Chunhua Hu and Shengping Zheng\*

A mild and efficient synthesis of bicyclic oxazolidinones from quinols and isocyanates, under DBU-mediated conditions at room temperature, is described. The aza-Michael addition to substituted cyclohexadienones is stereoselective and chemoselective.

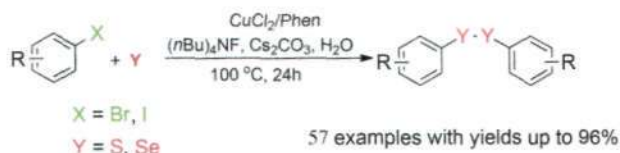


2943

### Synthesis of disulfides and diselenides by copper-catalyzed coupling reactions in water

Zhengkai Li, Fang Ke,\* Hang Deng, Hualong Xu, Haifeng Xiang and Xiangge Zhou\*

Aqueous copper-catalyzed reactions between aryl halides and elemental sulfur or selenium afford desired dichalcogenides in yields up to 96%.

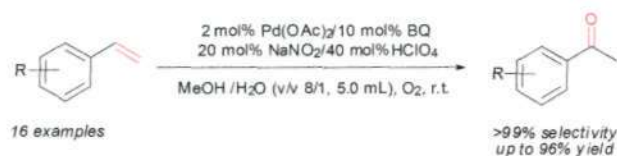


2947

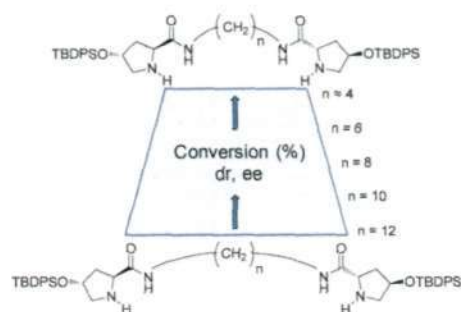
### Highly selective Wacker reaction of styrene derivatives: a green and efficient aerobic oxidative process promoted by benzoquinone/ $\text{NaNO}_2$ / $\text{HClO}_4$ under mild conditions

Guofu Zhang, Xiaoqiang Xie, Yong Wang, Xin Wen, Yun Zhao and Chengrong Ding\*

A highly efficient system for aerobic Wacker oxidation has been developed, which was selective to the oxidation of styrene derivatives.



2951

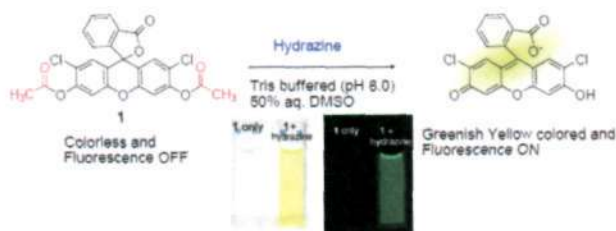


### Synergistic effects within a $C_2$ -symmetric organocatalyst: the potential formation of a chiral catalytic pocket

Joshua P. Delaney, Hannah L. Brozinski and Luke C. Henderson\*

This study describes the synthesis of five novel  $C_2$ -symmetric organocatalysts that facilitate the on-water asymmetric aldol reaction at low catalyst loading (1 mol%) without the use of additives.

2961

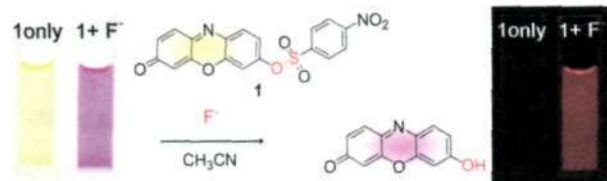


### Dual signaling of hydrazine by selective deprotection of dichlorofluorescein and resorufin acetates

Myung Gil Choi, Jung Ok Moon, Jihee Bae, Jung Woo Lee and Suk-Kyu Chang\*

Highly selective chemosignaling behaviors toward hydrazine of a reaction-based probe of dichlorofluorescein and resorufin acetates were investigated. Hydrazinolysis of latent dichlorofluorescein and resorufin acetates revealed prominent chromogenic and fluorogenic signaling.

2966

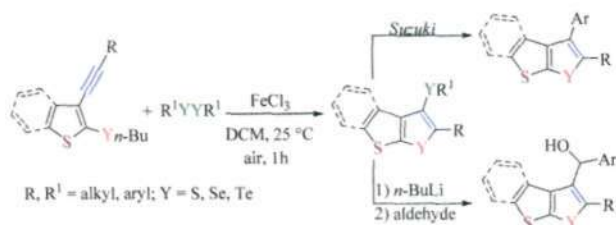


### Reaction-based dual signaling of fluoride ions by resorufin sulfonates

Hyun Gyu Im, Hong Yeong Kim, Myung Gil Choi and Suk-Kyu Chang\*

Resorufin nosylate exhibited naked-eye detectable colorimetric and fluorogenic signaling of fluoride ions in acetonitrile. The interference from sulfide ions was effectively suppressed by using the TPEN- $Cu^{2+}$  complex as a masking agent.

2972



### $FeCl_3$ -diorganyl dichalcogenides promoted cyclization of 2-organochalcogen-3-alkynylthiophenes: synthesis of chalcogenophene-[2,3-*b*]thiophenes

André L. Stein, Filipe N. Bilheri, Alisson R. Rosário and Gilson Zeni\*

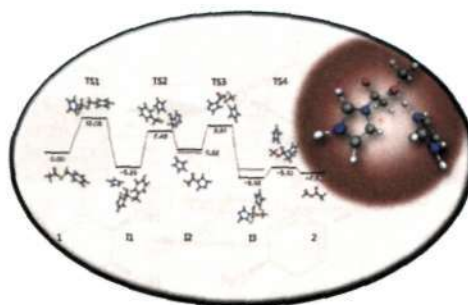
We present here our results on the  $FeCl_3$ -diorganyl dichalcogenides intramolecular cyclization of 2-organochalcogen-3-alkynylthiophenes to prepare (S)-Se-, (S)-S- and (S)-Te-heterocycles.

2979

### The role of imidazole in peptide cyclization by transesterification: parallels to the catalytic triads of serine proteases

Kendall G. Byler,\* Yangmei Li, Richard A. Houghten and Karina Martinez-Mayorga\*

This study rationalizes the need of high concentrations of imidazole in cyclization of decapeptides. The proposed concerted deprotonation step is energetically feasible, coinciding with histidine-mediated deprotonation in cleavage by serine proteases.

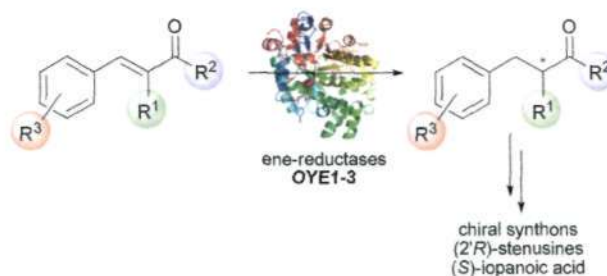


2988

### Substrate scope and synthetic applications of the enantioselective reduction of $\alpha$ -alkyl- $\beta$ -arylenones mediated by Old Yellow Enzymes

Elisabetta Brenna, Sara Lucia Cosi, Erica Elisa Ferrandi, Francesco G. Gatti, Daniela Monti, Fabio Parmeggiani\* and Alessandro Sacchetti

A systematic investigation of ene-reductases mediated bioreduction of  $\alpha$ -alkyl- $\beta$ -arylenones allowed us to assess the stereo-electronic requirements of the reaction and to obtain valuable chiral building blocks.

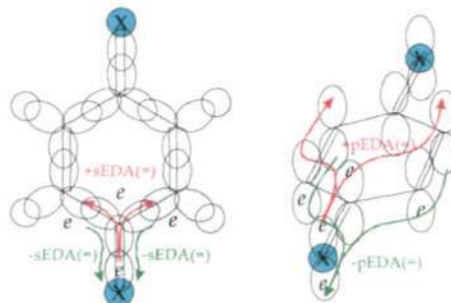


2997

### The sEDA(=) and pEDA(=) descriptors of the double bonded substituent effect

Andrzej Mazurek and Jan Cz. Dobrowolski\*

Double bonded substituent effect descriptors, sEDA(=) and pEDA(=), were constructed. They show to what extent a double bonded substituent donates electrons to or withdraws them from the substituted system.

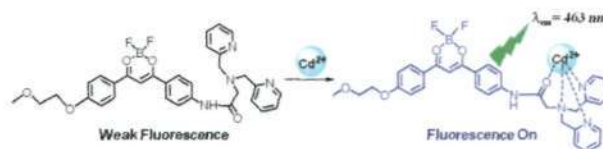


3014

### A selective turn-on fluorescent probe for $\text{Cd}^{2+}$ based on a boron difluoride $\beta$ -dibenzoyl dye and its application in living cells

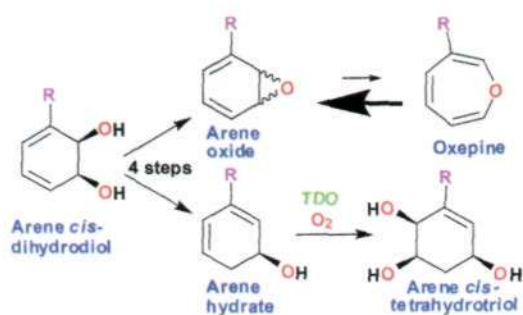
Li Xin, Yu-Zhe Chen,\* Li-Ya Niu, Li-Zhu Wu, Chen-Ho Tung, Qing-Xiao Tong\* and Qing-Zheng Yang

Herein we report the first example of difluoroboron dibenzoyl based fluorescent probes for selective  $\text{Cd}^{2+}$  detection in aqueous media.





3020



### Chemoenzymatic synthesis of monocyclic arene oxides and arene hydrates from substituted benzene substrates

Derek R. Boyd,\* Narain D. Sharma, Vera Ljubez, Peter K. M. McGeehin, Paul J. Stevenson,\* Marine Blain and Christopher C. R. Allen

Monocyclic arene *cis*-dihydrodiols were converted to the corresponding arene oxides, which racemize *via* oxepine tautomers, and arene hydrates, which can yield *cis*-tetrahydrotriols by dioxygenase-catalysed dihydroxylation.

3030

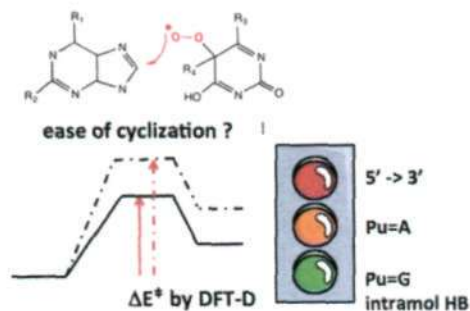


### FRET-based imaging of transbilayer movement of pepducin in living cells by novel intracellular bioelectrochemically activatable fluorescent probes

Mieko Tsuji, Satoshi Ueda, Tasuku Hirayama, Kensuke Okuda, Yoshiaki Sakaguchi, Aoi Isono and Hideko Nagasawa\*

We developed two types of intracellular bioelectrochemically activatable FRET probes based on pepducins targeting the intracellular juxtamembrane region and the cytosol, respectively.

3038

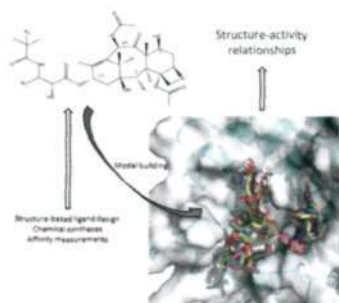


### Addressing the competitive formation of tandem DNA lesions by a nucleobase peroxy radical: a DFT-D screening

C. Dupont, C. Patel, J. L. Ravanat and E. Dumont\*

DFT-D calculations are performed on dinucleoside monophosphates to infer a reactivity ordering for the intrastrand attack of a peroxy nucleobase on guanine and adenine.

3046



### A structure-based design of new C2- and C13-substituted taxanes: tubulin binding affinities and extended quantitative structure-activity relationships using comparative binding energy (COMBINE) analysis

C. Coderch, Y. Tang, J. Klett, S.-E. Zhang, Y.-T. Ma, W. Shaorong, R. Matesanz, B. Pera, A. Canales, J. Jiménez-Barbero, A. Morreale, J. F. Díaz, W.-S. Fang\* and F. Gago\*

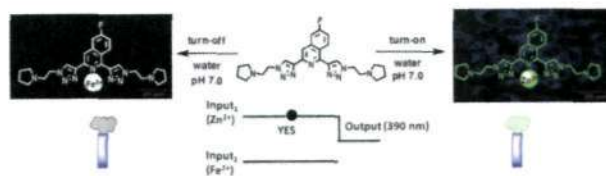
Ten novel taxanes have been synthesized and their binding affinities for mammalian tubulin have been measured.

3057

### Design and synthesis of an on-off "click" fluorophore that executes a logic operation and detects heavy and transition metal ions in water and living cells

Ganesh Chandra Midya, Sushovan Paladhi, Sudipta Bhowmik, Subhadeep Saha and Jyotirmayee Dash\*

A fluorescent molecule that shows selective "on-off" switch like behaviour with heavy and transition metal ions in water and living cells and mimics the function of a YES logic gate.



3064

### Synthesis of 2-amino-imidazo[4,5-*b*]pyridines

Adam J. Rosenberg, Theresa M. Williams, Abraham J. Jordan and Daniel A. Clark\*

The C2 amination of imidazo[4,5-*b*]pyridines was accomplished through C2 halogenation followed by substitution ( $S_NAr$ ) with functionalized primary and secondary amines.

