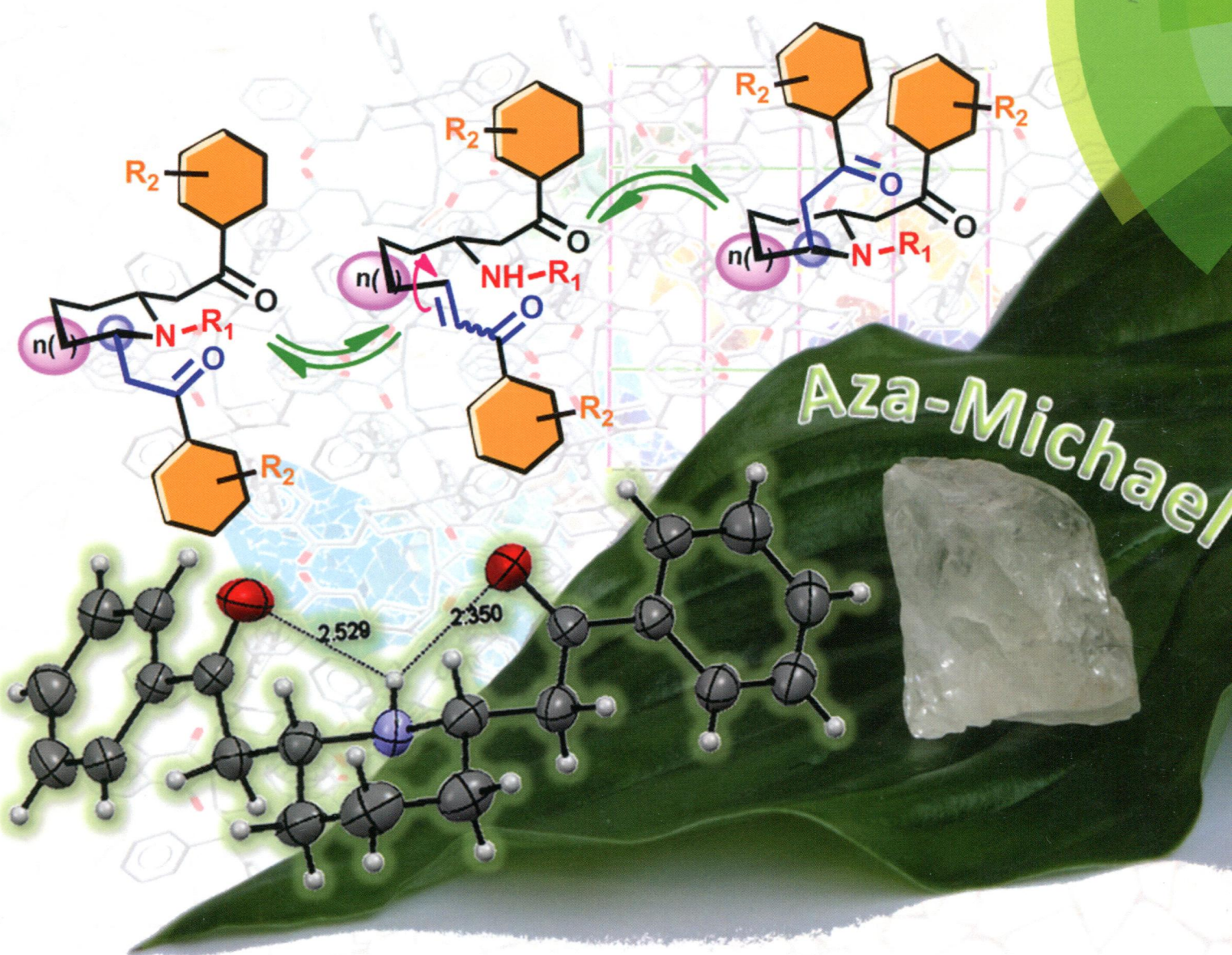


# Organic & Biomolecular Chemistry

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PAPER

F. Le Bideau, D. Joseph *et al.*

Thermodynamic epimeric equilibration and crystallisation-induced dynamic resolution of lobelanine, norlobelanine and related analogues

# Organic & Biomolecular Chemistry

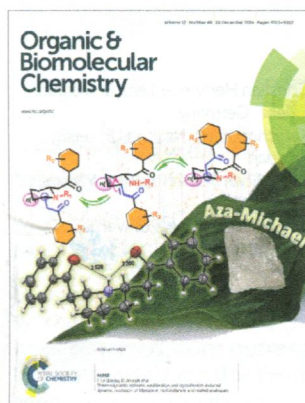
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## IN THIS ISSUE

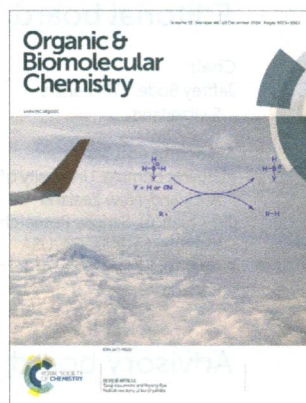
ISSN 1477-0520 CODEN OBCRAK 12(48) 9723-9922 (2014)



### Cover

See F. Le Bideau, D. Joseph *et al.*, pp. 9797–9810.

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### Inside cover

See Takuji Kawamoto and Ilhyong Ryu, pp. 9733–9742.

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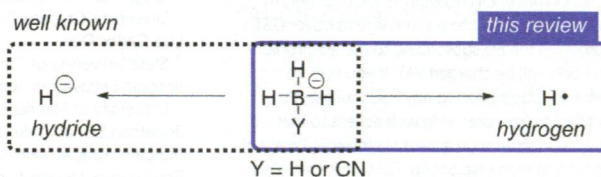
## REVIEWS

9733

### Radical reactions of borohydrides

Takuji Kawamoto and Ilhyong Ryu\*

This review article focuses on state-of-the-art borohydride based radical reactions, also covering earlier work, kinetics and some DFT calculations with respect to the hydrogen transfer mechanism.

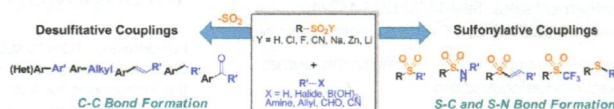


9743

### Sulfinate derivatives: dual and versatile partners in organic synthesis

Jessy Aziz, Samir Messaoudi,\* Mouad Alami\* and Abdallah Hamze\*

Recent advances in the preparation and synthetic uses of sulfinic acids and their derivatives are highlighted in this review. They are used as versatile partners in sulfonylative and desulfinitive reactions.

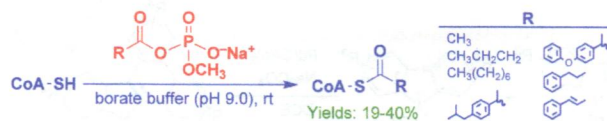


9760

### Synthesis of coenzyme A thioesters using methyl acyl phosphates in an aqueous medium

Mohan Pal and Stephen L. Bearne\*

Regioselective *S*-acylation of coenzyme A is achieved under aqueous conditions using various aliphatic and aromatic carboxylic acids activated as their methyl acyl phosphate monoesters.

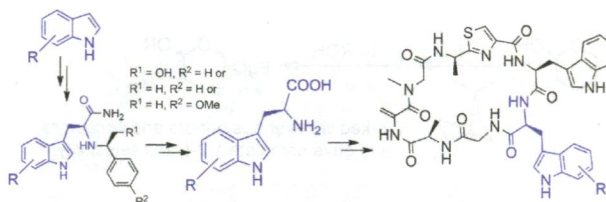


9764

### A facile approach to tryptophan derivatives for the total synthesis of argyrin analogues

Chou-Hsiung Chen, Sivanewary Genapathy, Peter M. Fischer and Weng C. Chan\*

Utilising a chiral auxiliary-facilitated Strecker amino acid synthesis strategy, indole-substituted (*S*)-tryptophans have been obtained from corresponding indoles; the former in turn were used for the synthesis of a potent antibacterial agent, argyrin and its analogues.

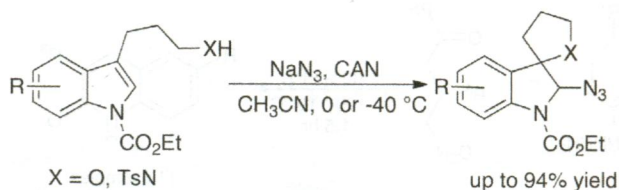


9769

### A facile approach to spirocyclic 2-azido indolines via azidation of indoles with ceric ammonium nitrate

Jing Li, Mao Liu, Qi Li, Hua Tian and Yian Shi\*

This paper describes azidation of indoles with  $\text{NaN}_3$  and ceric ammonium nitrate (CAN), giving a variety of spirocyclic 2-azido indolines in good yields and moderate diastereoselectivities.

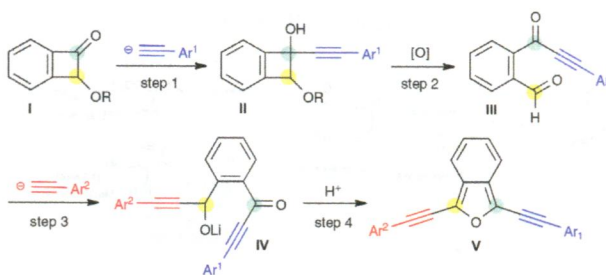


9773

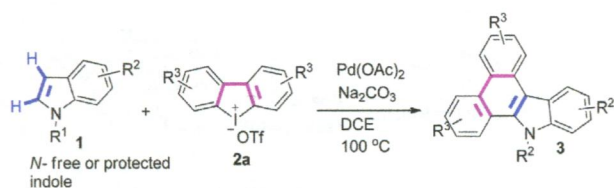
### An efficient synthetic route to 1,3-bis(arylethynyl)-isobenzofuran using alkoxybenzocyclobutenone as a reactive platform

Kenta Asahina, Suguru Matsuoka, Ryosuke Nakayama and Toshiyuki Hamura\*

An efficient synthetic method of 1,3-bis(arylethynyl)-isobenzofurans is developed.



9777

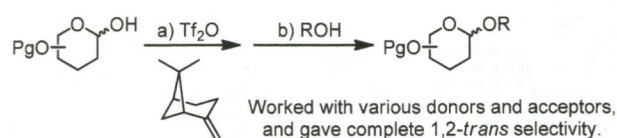


### Palladium catalyzed dual C–H functionalization of indoles with cyclic diaryliodoniums, an approach to ring fused carbazole derivatives

Yongcheng Wu, Xiaopeng Peng, Bingling Luo, Fuhai Wu,\*  
Bo Liu, Fenyun Song, Peng Huang and Shijun Wen\*

As the tile reaction shows, an array of dibenzocarbazoles were obtained *via* dual C–H functionalization of indoles with cyclic diaryliodoniums in a single operation.

9781

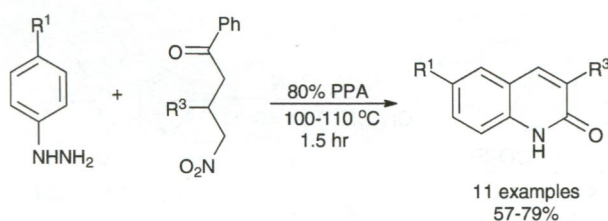


### Strained olefin enables triflic anhydride mediated direct dehydrative glycosylation

Guohua Chen,\* Qiang Yin, Jian Yin, Xiangying Gu,  
Xiao Liu, Qidong You, Yue-Lei Chen,\* Bing Xiong\* and  
Jingkang Shen\*

Tf<sub>2</sub>O mediated dehydrative glycosylation was enabled by strained olefins, including *beta*-(–)-pinene, and inhibited by other typical bases.

9786

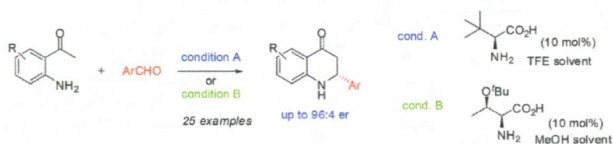


### Highly efficient modular metal-free synthesis of 3-substituted 2-quinolones

Alexander V. Aksenov,\* Alexander N. Smirnov,  
Nicolai A. Aksenov, Inna V. Aksenova, Asiyat S. Bijieva  
and Michael Rubin\*

A modular approach to 3-substituted 2-quinolones *via* a cascade annulation reaction between 4-nitroketones and hydrazines has been developed.

9789



### Primary amino acid catalyzed asymmetric intramolecular Mannich reaction for the synthesis of 2-aryl-2,3-dihydro-4-quinolones

Buddhadeb Mondal and Subhas Chandra Pan\*

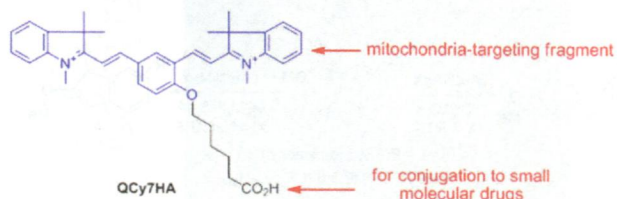
A high enantioselective synthesis of 2-aryl-2,3-dihydro-4-quinolones has been developed *via* intramolecular Mannich reaction using primary amino acids as catalysts.

9793

### Design and synthesis of a mitochondria-targeting carrier for small molecule drugs

Junyan Han,\* Tae Hoon Lee, Ching-Hsuan Tung and Daniel Y. Lee\*

A novel mitochondria-targeting carrier QCy7HA was developed, which transported the covalently attached doxorubicin (DOX) to mitochondria specifically, resulting in the limitation of the effects of P-glycoprotein efflux pumps of multidrug-resistant cells on DOX.



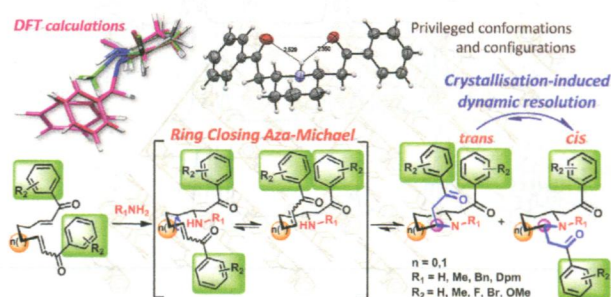
PAPERS

9797

### Thermodynamic epimeric equilibration and crystallisation-induced dynamic resolution of lobelanine, norlobelanine and related analogues

Z. Amara, G. Bernadat, P.-E. Venot, P. Retailleau, C. Troufflard, E. Drège, F. Le Bideau\* and D. Joseph\*

The step-economical synthesis of lobelanine involving a ring closing double aza-Michael (RCDAM) reaction is revisited and successfully extended to the synthesis of various configurationally more stable analogues.

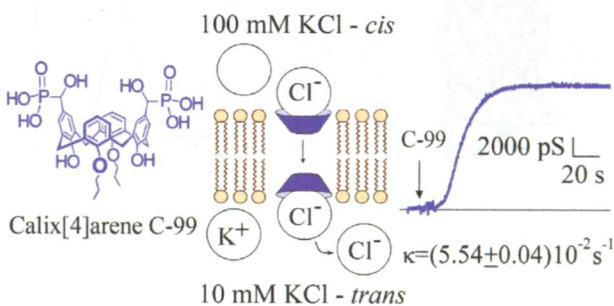


9811

### Anion carrier formation by calix[4]arene-bis-hydroxymethylphosphonic acid in bilayer membranes

Oleg Ya. Shatursky,\* Ludmila A. Kasatkina, Roman V. Rodik, Sergiy O. Cherenok, Alexander A. Shkrabak, Tatiana O. Veklich, Tatiana A. Borisova, Sergiy O. Kosterin and Vitaly I. Kalchenko

Calix[4]arene **C-99**-mediated ionic transport follows mobile carrier mode of facilitated diffusion (relative permeability  $P_{Cl^-}/P_{K^+} \sim 3$ ) with the passage of 20 ions per second.

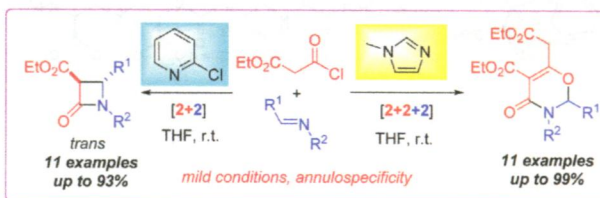


9822

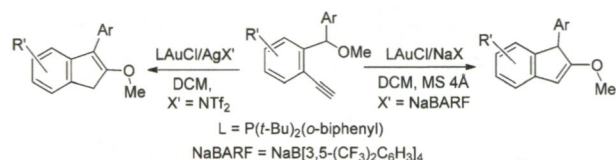
### Base-switched annuloselectivity in the reactions of ethyl malonyl chloride and imines

Zhanhui Yang, Siqi Li, Zhong Zhang and Jiayi Xu\*

The [2 + 2] and [2 + 2 + 2] annuloselectivity in the reactions of ethyl malonyl chloride with imines was controlled by different bases, providing a simple synthesis of  $\beta$ -lactam-3-carboxylates and 2,3-dihydro-1,3-oxazin-4-ones.



9831

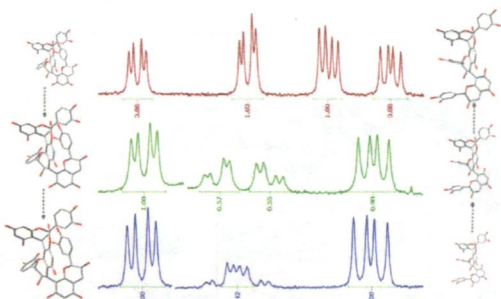


### Gold-catalyzed carboalkoxylation of 2-ethynylbenzyl ethers to form 1- and 3-substituted 2-methoxy-1-*H*-indenes: Brønsted acids versus gold catalysis

Chun-Hao Chen, Chiou-Dong Wang, Yi-Feng Hsieh and Rai-Shung Liu\*

Selective synthesis of 1- and 3-substituted 2-methoxyindenes from the carboalkoxylation of 2-ethynylbenzyl ethers is described.

9837

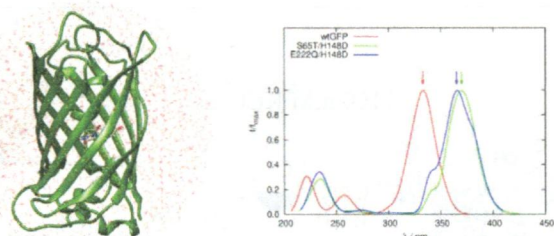


### Conformational equilibria in selected A-type trimeric procyanidins

Marta K. Dudek (Jamróz),\* Sławomir Kaźmierski, Kamil Stefaniak, Witold B. Gliński and Jan. A. Gliński

There are two favored conformations of A-type procyanidin trimers: the (+ $\varphi$ )-rotamer and the (− $\varphi$ ) one. Their ratio depends on the procyanidin structure and solvent – different solvents favor different conformers.

9845

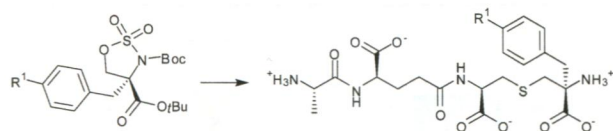


### New insights into the structure–spectrum relationship in S65T/H148D and E222Q/H148D green fluorescent protein mutants: a theoretical assessment

Pau Armengol, Ricard Gelabert,\* Miquel Moreno and José M. Lluch

Dynamic simulations and excited state calculations track the origin of the absorption spectrum red-shift in two green fluorescent protein mutants.

9853



### Enantioselective synthesis of $\alpha$ -benzylated lanthionines and related tripeptides for biological incorporation into *E. coli* peptidoglycan

Thibaut Denoël, Astrid Zervosen,\* Christian Lemaire, Bernard Joris, Mireille Hervé, Didier Blanot, Guillermo Zaragoza and André Luxen

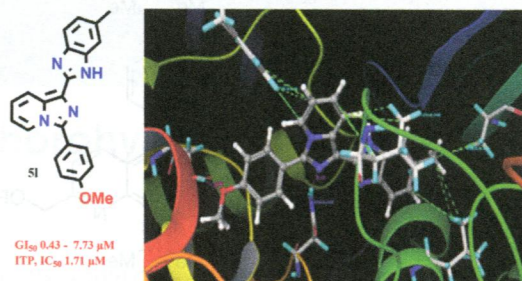
The synthesis of modified tripeptides (*S*)-Ala- $\gamma$ -(*R*)-Glu-X, where X = (*R,S*) or (*R,R*) diastereomers of  $\alpha$ -benzyl or  $\alpha$ -(4-azidobenzyl)lanthionine, was carried out.

9864

### Synthesis and biological evaluation of imidazo-[1,5-a]pyridine-benzimidazole hybrids as inhibitors of both tubulin polymerization and PI3K/Akt pathway

Ahmed Kamal,\* A. V. Subba Rao, V. Lakshma Nayak, N. V. Subba Reddy, Konderu Swapna, G. Ramakrishna and Mallika Alvala

Imidazo[1,5-a]pyridine-benzimidazole hybrids are firstly reported herein to induce cytotoxicity by targeting microtubules.



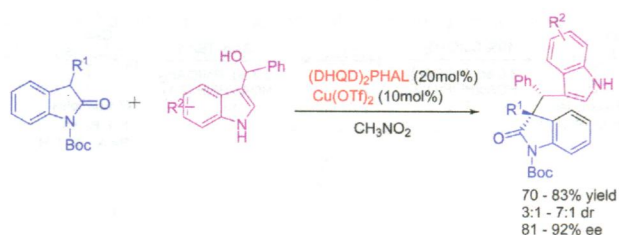
Docked pose of 5l in colchicine binding site of tubulin

9881

### Highly enantioselective reaction of 2-oxindoles with (3-indolyl)methanols by cooperative Catalysis of a Lewis acid and organocatalyst

Chuan-Li Ren, Tao Zhang, Xing-Yong Wang, Tao Wu, Jing Ma,\* Qing-Qing Xuan, Feng Wei, Hong-Yan Huang, Dong Wang and Li Liu\*

An efficient cooperative bispinchnona alkaloid and Lewis acid catalytic system was developed in the enantioselective  $\alpha$ -alkylation of 2-oxindoles with (3-indolyl)(phenyl)methanols.

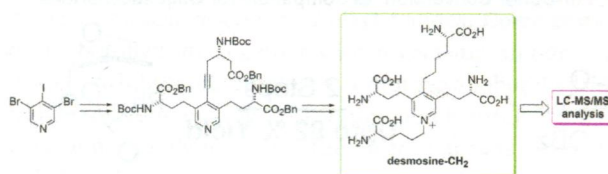


9887

### Synthesis and LC-MS/MS analysis of desmosine-CH<sub>2</sub>, a potential internal standard for the degraded elastin biomarker desmosine

Yuko Murakami, Rina Suzuki, Hiroto Yanuma, Jiangtao He, Shuren Ma, Gerard M. Turino, Yong Y. Lin and Toyonobu Usuki\*

Chemical synthesis and LC-MS/MS analysis of desmosine-CH<sub>2</sub>, a potential internal standard for the degraded elastin biomarker desmosine, are achieved.

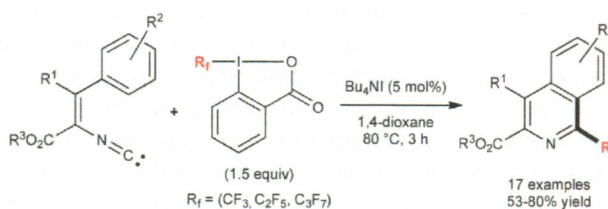


9895

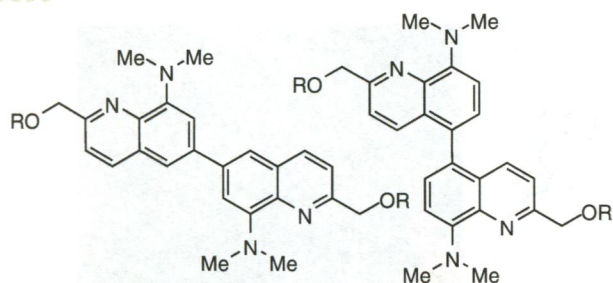
### 1-Trifluoromethylated isoquinolines via radical trifluoromethylation of isonitriles

Bo Zhang and Armido Studer\*

A simple and efficient approach to biologically important 1-trifluoroalkylated isoquinolines starting with readily prepared  $\beta$ -aryl- $\alpha$ -isocyano-acrylates and R<sub>f</sub>-I(III)-reagents (R<sub>f</sub> = CF<sub>3</sub>, C<sub>2</sub>F<sub>5</sub>, C<sub>3</sub>F<sub>7</sub>) is described.



9899

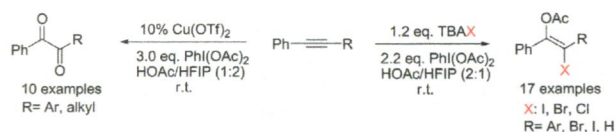


### Quinoline-derived two-photon sensitive quadrupolar probes

Petra Dunkel, Christine Tran, Thibault Gallavardin, Hamid Dhimane, David Ogden and Peter I. Dalko\*

Quadrupolar 8-dimethylaminoquinoline-derived photosensitive probes underwent photolysis under UV (365 nm) and NIR (730 nm two-photon (TP)) irradiation conditions.

9909



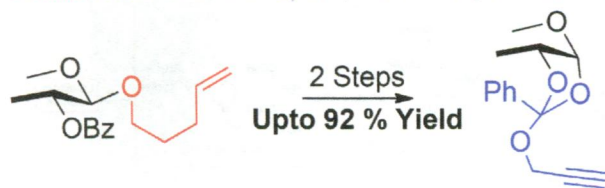
### Selective oxygenation of alkynes: a direct approach to diketones and vinyl acetate

Xiao-Feng Xia,\* Zhen Gu, Wentao Liu, Ningning Wang, Haijun Wang, Yongmei Xia, Haiyan Gao and Xiang Liu

Convenient and expedient methods for the synthesis of  $\alpha$ -diketones and  $\beta$ -haloenol acetates from arylalkynes using  $\text{PhI}(\text{OAc})_2$  as an oxidant are developed at room temperature.

9914

● Donor-Donor Conversion ● Compatible for Oligosaccharides



### Efficient synthesis of oligosaccharyl 1,2-O-orthoesters from *n*-pentenyl glycosides and application to the pentaarabinofuranoside of the mycobacterial cell surface

Shivaji A. Thadke and Srinivas Hotha\*

Conversion of *n*-pentenyl glycosides to glycosyl 1,2-orthoesters that is mild, high yielding, and importantly suitable for oligosaccharide synthesis is identified.