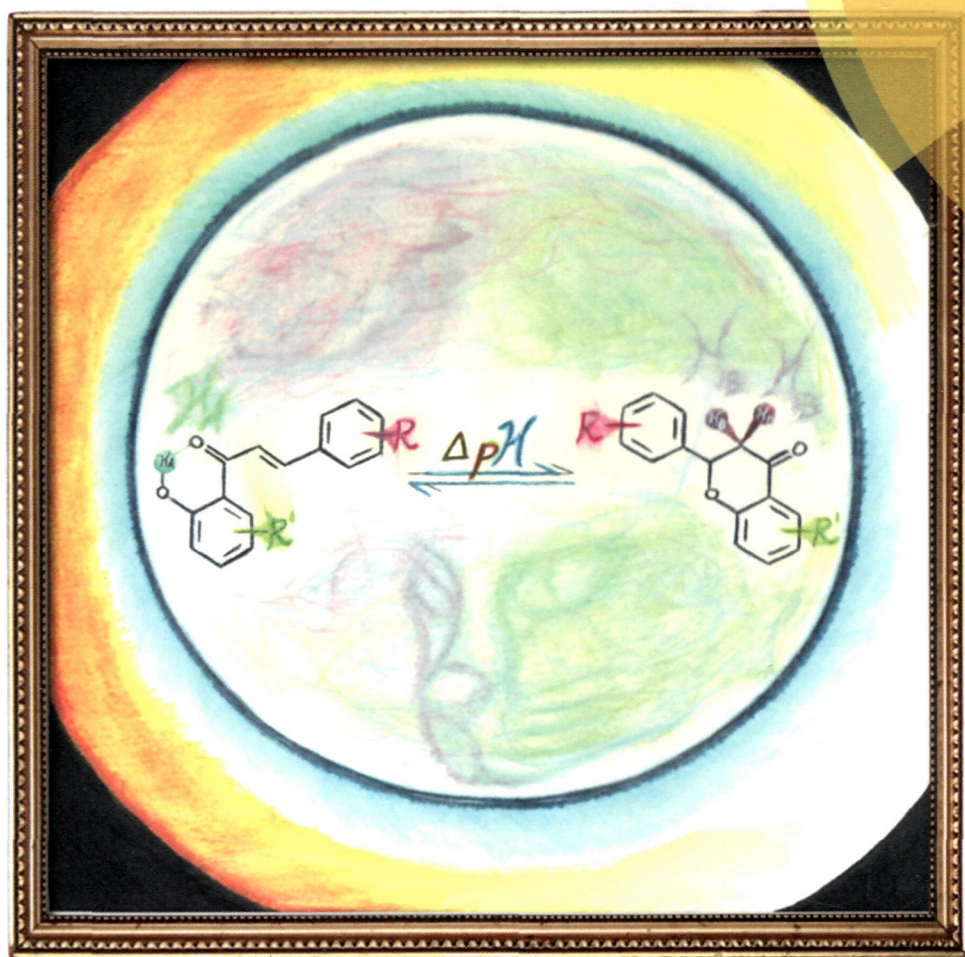


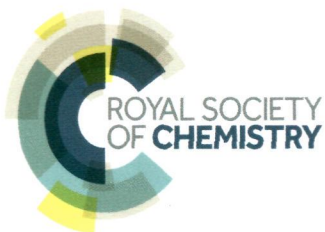
114  
0-72/6

# Organic & Biomolecular Chemistry

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ISSN 1477-0520



PAPER

Marc J. Adler *et al.*

Impact of mono- and disubstitution on the colorimetric dynamic covalent switching chalcone/flavanone scaffold

# Organic & Biomolecular Chemistry

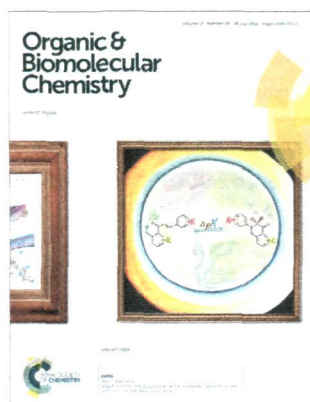
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## IN THIS ISSUE

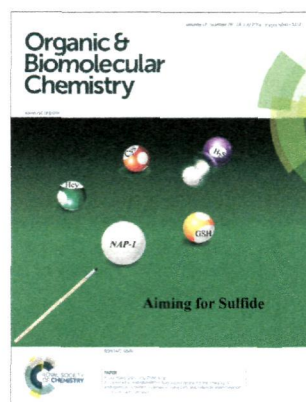
ISSN 1477-0520 CODEN OBCRAK 12(28) 5041–5312 (2014)



### Cover

See Marc J. Adler *et al.*, pp. 5108–5114.

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### Inside cover

See Yi Liu, Yong Qian, Jing Zhao *et al.*, pp. 5115–5125.

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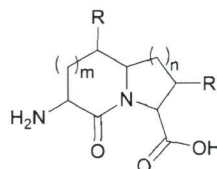
## REVIEW

5052

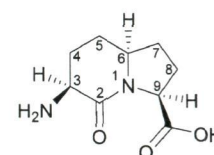
### Design, synthesis, conformational analysis and application of indolizidin-2-one dipeptide mimics

Arkady Khashper and William D. Lubell\*

Growth in the field of peptide mimicry over the past few decades has resulted in the synthesis of many new compounds and the investigation of novel pharmacological agents.



Azabicyclo[X.Y.0]alkan-2-one amino acid



(3S,6S,9S)-1

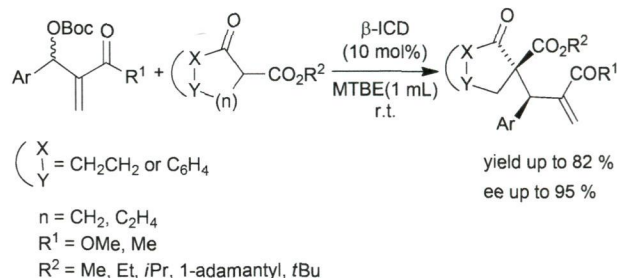
## COMMUNICATIONS

5071

### Organocatalytic enantioselective allylic alkylation of MBH carbonates with $\beta$ -keto esters

M. Kamlar, S. Hybelbauerová, I. Císařová and J. Veselý\*

The highly stereoselective allylic alkylation of Morita–Baylis–Hillman carbonates with  $\beta$ -ketoesters catalysed by  $\beta$ -ICD is described.

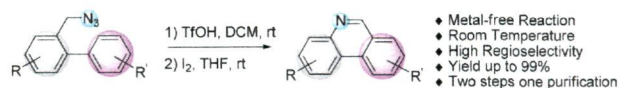


5077

### A new synthetic approach to 6-unsubstituted phenanthridine and phenanthridine-like compounds under mild and metal-free conditions

Jumreang Tummatorn,\* Suppachai Krajangsri, Krissada Norseeda, Charnsak Thongsornkleeb and Somsak Ruchirawat

A tandem azide rearrangement/intramolecular annulation and oxidation reactions of biarylmethyl azides provides a new and mild approach for the synthesis of 6-unsubstituted phenanthridine and phenanthridine-like compounds.

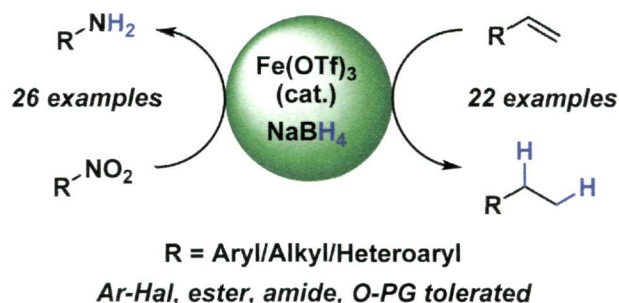


5082

### Iron-catalysed, general and operationally simple formal hydrogenation using $\text{Fe}(\text{OTf})_3$ and $\text{NaBH}_4$

Alistair J. MacNair, Ming-Ming Tran, Jennifer E. Nelson, G. Usherwood Sloan, Alan Ironmonger and Stephen P. Thomas\*

An operationally simple and environmentally benign formal hydrogenation protocol has been developed using a highly abundant iron(III) salt and an inexpensive, bench stable, stoichiometric reductant,  $\text{NaBH}_4$ , in ethanol, under ambient conditions.

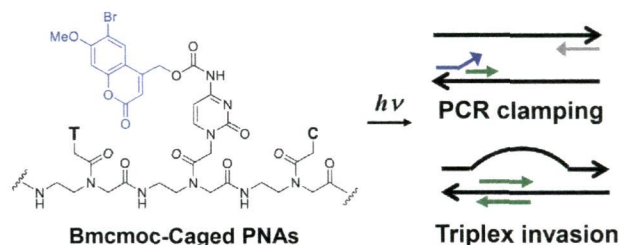


5089

### Synthesis of nucleobase-caged peptide nucleic acids having improved photochemical properties

Takayoshi Watanabe, Tomoko Hoshida, Jun Sakyo, Mariko Kishi, Satoshi Tanabe, Junichi Matsuura, Shingo Akiyama, Makiko Nakata, Yasuaki Tanabe, Akinobu Z. Suzuki, Soichiro Watanabe and Toshiaki Furuta\*

A nucleobase-caged peptide nucleic acid (PNA) having a (6-bromo-7-methoxycoumarin)-4-ylmethoxycarbonyl (Bmcmoc) caging group was newly synthesized.

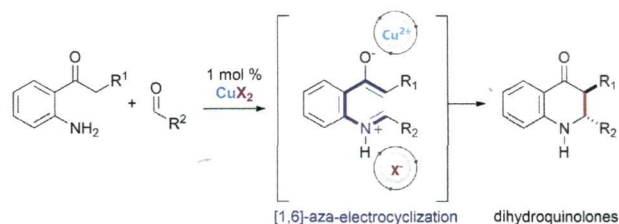


5094

### Enantioselective one-pot synthesis of dihydroquinolones via BINOL-derived Lewis acid catalysis

Peter C. Knipe and Martin D. Smith\*

A high-yielding and diastereoselective route to biologically significant 2-aryl- and 2-alkyl-3-amido dihydroquinolones has been developed in up to 90 : 10 e.r. by employing a novel Lewis acidic BINOL-derived copper(II) catalyst.



5098

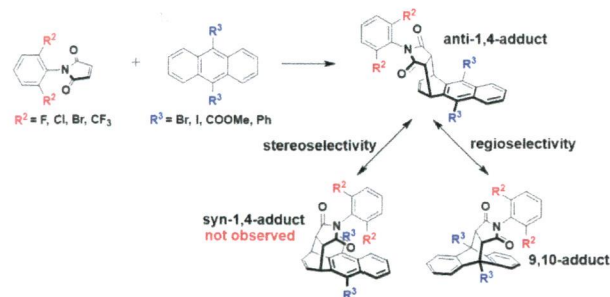


### Regioselective synthesis of 3,4,5-trisubstituted 2-aminofurans

Thi Ngoc Tram Huynh, Pascal Retailleau, Clément Denhez,\* Kim Phi Phung Nguyen and Dom Guillaume

Three series of methyl 5-substituted 2-aminofuran-4-keto-3-carboxylates have been prepared following a multicomponent reaction strategy by the addition of an isocyanide to 4-oxo-2-butynoate in the presence of an aldehyde.

5102



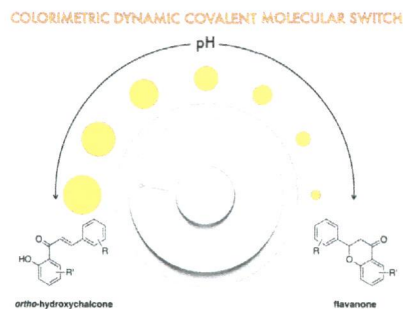
### Unusual regio- and stereo-selectivity in Diels–Alder reactions between bulky *N*-phenylmaleimides and anthracene derivatives

Hao Chen, Erdong Yao, Chi Xu, Xiao Meng and Yuguo Ma\*

Unusual regio- and stereo-selectivity in Diels–Alder (D–A) reactions were achieved between bulky *N*-phenylmaleimides and anthracene derivatives.

## PAPERS

5108

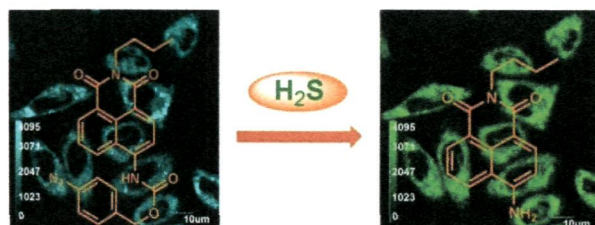


### Impact of mono- and disubstitution on the colorimetric dynamic covalent switching chalcone/flavanone scaffold

Brian M. Muller, Jesse Mai, Reid A. Yocum and Marc J. Adler\*

The impact of substitution on a novel colorimetric dynamic covalent switching scaffold was investigated using UV/Vis and NMR spectroscopy.

5115



### A colorimetric and ratiometric fluorescent probe for the imaging of endogenous hydrogen sulphide in living cells and sulphide determination in mouse hippocampus

Ling Zhang, Sai Li, Mei Hong, Yuqing Xu, Shuashuai Wang, Yi Liu,\* Yong Qian\* and Jing Zhao\*

A naphthalimide-azide based colorimetric and ratiometric fluorescent probe has been developed for the selective and sensitive detection of hydrogen sulphide.

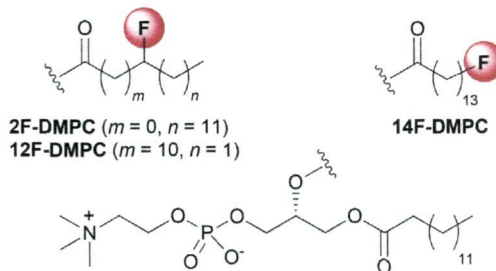
5126

### Evaluation of the effect of fluorination on the property of monofluorinated dimyristoylphosphatidylcholines

Marie-Claude Gagnon, Bianka Turgeon, Jean-Daniel Savoie, Jean-François Parent, Michèle Auger\* and Jean-François Paquin\*

The synthesis and characterization of three monofluorinated dimyristoylphosphatidylcholines, with the fluorine atom located at the extremities of the acyl chain in position 2 of the glycerol (*sn*-2), is described.

New monofluorinated dimyristoylphosphatidylcholines (F-DMPC's)

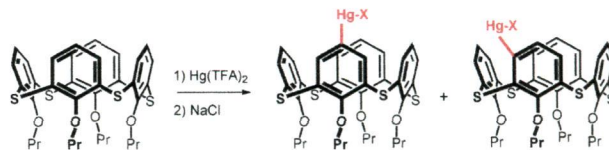


5136

### Mercuration of thiacalix[4]arenes in the *cone* and 1,3-*alternate* conformations

F. Botha, S. Böhm, H. Dvořáková, V. Eigner and P. Lhoták\*

A monomercuration reaction of thiacalix[4]arenes immobilized in the *cone* or 1,3-*alternate* conformations gave a mixture of two regioisomers (*meta* and *para*) in approx. 4 : 1 and 2 : 1 ratios, respectively.

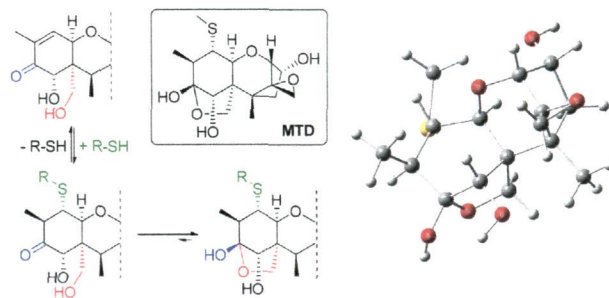


5144

### Methylthioethoxynivalenol (MTD): insight into the chemistry, structure and toxicity of *thia*-Michael adducts of trichothecenes

Philipp Fruhmann, Theresa Weigl-Pollack, Hannes Mikula,\* Gerlinde Wiesenberger, Gerhard Adam, Elisabeth Varga, Franz Berthiller, Rudolf Krska, Christian Hametner and Johannes Fröhlich

Synthesis and investigation of MTD revealed characteristic hemiketalisation and partial detoxification as effects of *thia*-Michael addition to type B trichothecenes.

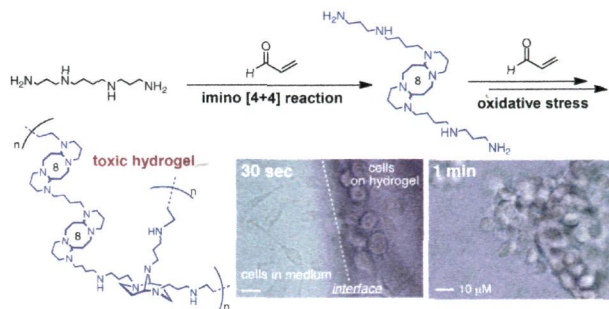


5151

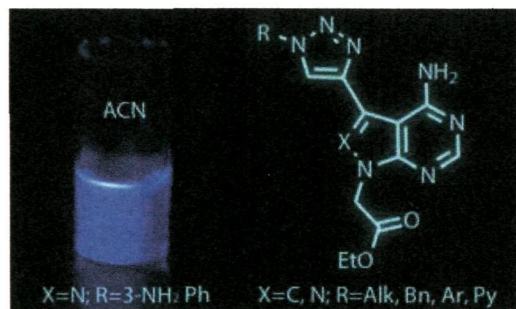
### Polyamine modification by acrolein exclusively produces 1,5-diazacyclooctanes: a previously unrecognized mechanism for acrolein-mediated oxidative stress

Ayumi Tsutsui, Rie Imamaki, Shinobu Kitazume, Shinya Hanashima, Yoshiki Yamaguchi, Masato Kaneda, Shinya Oishi, Nobutaka Fujii, Almira Kurbangalieva, Naoyuki Taniguchi and Katsunori Tanaka\*

Polyamines were found to react with acrolein to produce 1,5-diazacyclooctane.



5158

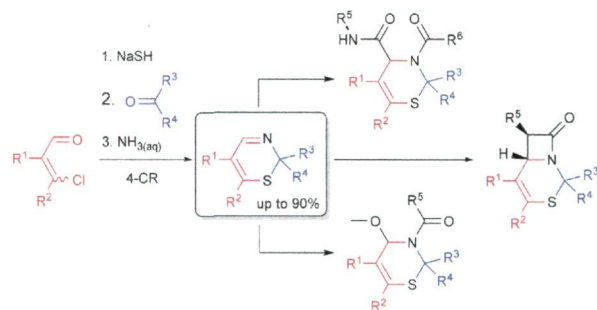


### Synthesis and photophysical characterisation of new fluorescent triazole adenine analogues

Christopher P. Lawson, Anke Dierckx, Francois-Alexandre Miannay, Eric Wellner, L. Marcus Wilhelmsson\* and Morten Grøtli\*

Novel fluorescent triazole adenine derivatives have been synthesised and their photo-physical properties characterised.

5168

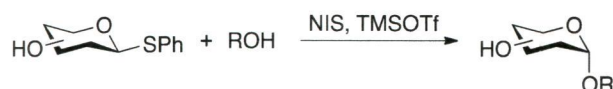


### Multicomponent reaction for the first synthesis of 2,2-dialkyl- and 2-alkyl-2-aryl-5,6-diaryl-2H-1,3-thiazines as scaffolds for various 3,4-dihydro-2H-1,3-thiazine derivatives

Fabian Brockmeyer, Robin Schoemaker, Marc Schmidtman and Jürgen Martens\*

2H-1,3-thiazines, prepared via a novel and efficient multicomponent reaction, can be used as scaffolds for the synthesis of diverse 3,4-dihydro-2H-1,3-thiazines.

5182

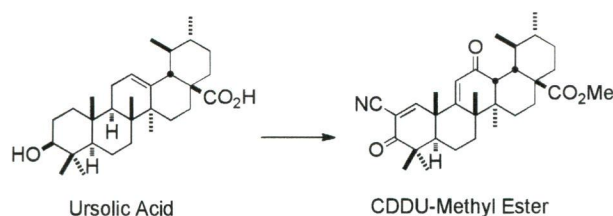


### 1,2-*cis* Alkyl glycosides: straightforward glycosylation from unprotected 1-thioglycosyl donors

Bo Meng, Zhenqian Zhu and David C. Baker\*

A simple, straightforward 1,2-*cis*-selective glycosidation method from an unprotected 1-thioglycoside is presented.

5192



### An efficient synthesis of methyl 2-cyano-3,12-dioxoursol-1,9-dien-28-oate (CDDU-methyl ester): analogues, biological activities, and comparison with oleanolic acid derivatives

Liangfeng Fu, Qi-Xian Lin, Karen T. Liby, Michael B. Sporn\* and Gordon W. Gribble\*

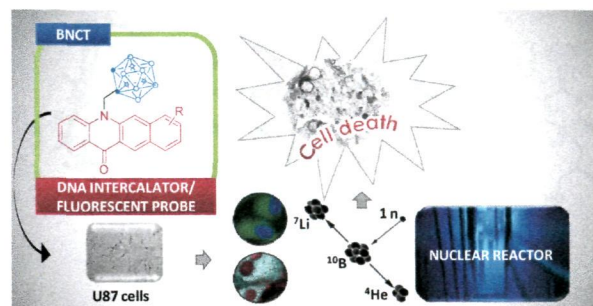
An efficient synthesis of methyl 2-cyano-3,12-dioxoursol-1,9-dien-28-oate (CDDU-methyl ester).

5201

### Synthesis, characterization and biological evaluation of carboranyl methylbenzo[*b*]acridones as novel agents for boron neutron capture therapy

A. Filipa F. da Silva, Raquel S. G. R. Seixas, Artur M. S. Silva, Joana Coimbra, Ana C. Fernandes, Joana P. Santos, António Matos, José Rino, Isabel Santos and Fernanda Marques\*

Acridone derivatives bearing carboranyl moieties as fluorescent probes for boron neutron capture therapy (BNCT) of the glioblastoma.

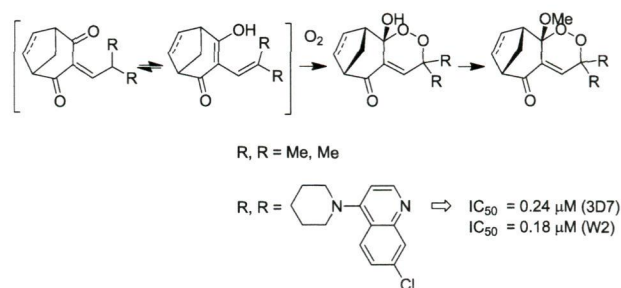


5212

### Design, synthesis and evaluation of new tricyclic endoperoxides as potential antiplasmodial agents

Jérémy Ruiz, Sonia Mallet-Ladeira, Marjorie Maynadier, Henri Vial and Christiane André-Barrès\*

New tricyclic endoperoxides were obtained by a diastereoselective autoxidation; combined with 7-chloro-4-aminoquinoline, they display good antiplasmodial activities.

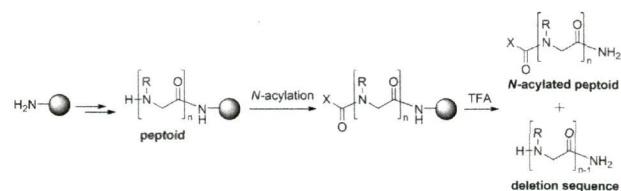


5222

### Unusual truncation of *N*-acylated peptoids under acidic conditions

Soomin Kim, Goutam Biswas, Shinae Park, Arim Kim, Hyunjung Park, Eunsook Park, Jeongmi Kim and Yong-Uk Kwon\*

Systematic studies on the unusual truncation of *N*-acylated peptoids were carried out to examine the electronic effects of acyl groups, and thus to control the formation of deletion sequences based on a plausible mechanism.

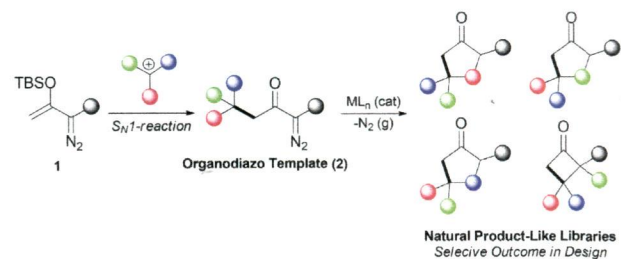


5227

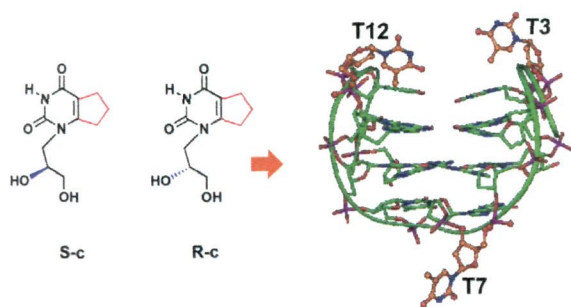
### A survey of enoldiazo nucleophilicity in selective C–C bond forming reactions for the synthesis of natural product-like frameworks

Yuxiao Liu, Yu Liu, Charles S. Shanahan, Xichen Xu and Michael P. Doyle\*

Sc(OTf)<sub>3</sub>-catalyzed S<sub>N</sub>1-like couplings of enoldiazo compounds with carbocations for construction of carbocyclic and heterocyclic scaffolds has been realised.



5243

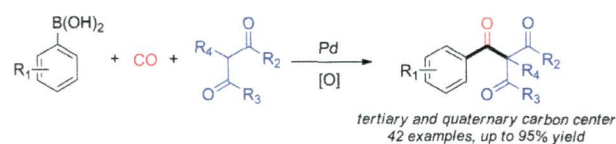


### Outstanding effects on antithrombin activity of modified TBA diastereomers containing an optically pure acyclic nucleotide analogue

M. Scutto, M. Persico, M. Bucci, V. Vellecco, N. Borbone, E. Morelli, G. Oliviero, E. Novellino, G. Piccialli, G. Cirino, M. Varra,\* C. Fattorusso\* and L. Mayol

Optically pure modified acyclic nucleosides offer unique advantages in exploring the effect on thrombin inhibition of single residue modifications at key positions of TBA.

5243

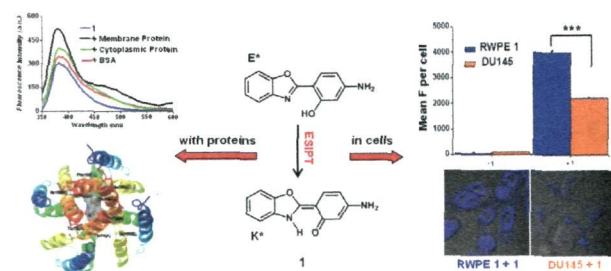


### Pd-catalyzed carbonylation for the construction of tertiary and quaternary carbon centers with $sp^3$ carbon partners

Wei Lu, Yang Li, Chao Wang, Dong Xue,\* Jian-Gang Chen and Jianliang Xiao\*

The first examples of a Pd-catalyzed carbonylation of aryl boronic acids with  $sp^3$  carbon partners are presented.

5250

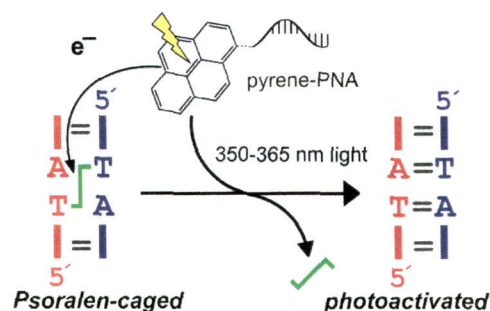


### An ESIPT fluorescent probe sensitive to protein $\alpha$ -helix structures

Nan Jiang, Chanli Yang, Xiongwei Dong, Xianglang Sun, Dan Zhang\* and Changlin Liu\*

A benzazole derivative, **1**, was observed to undergo the excited-state intramolecular proton transfer (ESIPT) process with  $\alpha$ -helical proteins. The cell images showed a difference in the staining of normal and cancerous prostate cells by **1**, which might be due to the different membrane protein levels.

5260



### Pyrene chromophores for the photoreversal of psoralen interstrand crosslinks

Jens M. Stadler and Thorsten Stafforst\*

Peptide nucleic acids carrying various pyrene chromophores have been investigated to reverse psoralen DNA interstrand crosslinks in a photolyase-like manner.

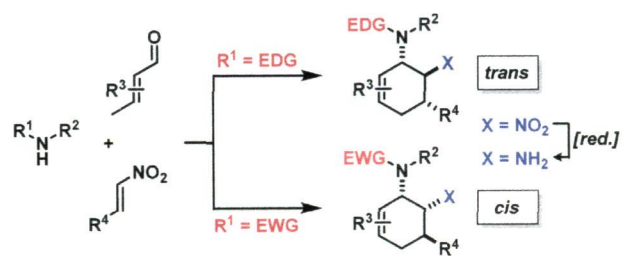


5267

### Modular synthesis of cyclic *cis*- and *trans*-1,2-diamine derivatives

Anna K. Weber, Josef Schachtner, Robert Fichtler, Timo M. Leermann, Jörg M. Neudörfel and Axel Jacobi von Wangelin\*

Structurally diverse carbocycles with two vicinal nitrogen-substituents were prepared in expedient three-component reactions from simple amines, aldehydes, and nitroalkenes.

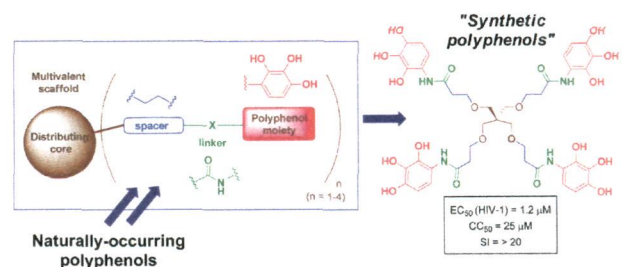


5278

### Multivalent agents containing 1-substituted 2,3,4-trihydroxyphenyl moieties as novel synthetic polyphenols directed against HIV-1

Aida Flores, María José Camarasa, María Jesús Pérez-Pérez, Ana San-Félix, Jan Balzarini and Ernesto Quesada\*

A series of synthetic polyphenols inspired by the multivalent architecture of naturally-occurring hydrolysable tannins exhibited selective inhibitory activity against HIV-1.

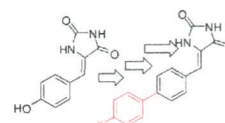


5295

### Marine natural products-inspired phenylmethyle hydantoin with potent *in vitro* and *in vivo* antitumor activities *via* suppression of Brk and FAK signaling

Asmaa A. Sallam, Mohamed M. Mohyeldin, Ahmed I. Foudah, Mohamed R. Akl, Sami Nazzal, Sharon A. Meyer, Yong-Yu Liu and Khalid A. El Sayed\*

The synthetic marine-inspired PMH analog **7** showed promising *in vitro* and *in vivo* antitumor effects against breast cancer *via* targeting Brk and FAK signaling pathways.



Antiproliferative activity (IC <sub>50</sub> , μM)		Antimigratory activity (IC <sub>50</sub> , μM)	
TC-3	MDA-MB-231	TC-3	MDA-MB-231
6.8	3.8	1.5	15.9

5304

### Exploring mutasynthesis to increase structural diversity in the synthesis of highly oxygenated polyketide lactones

J. M. Botubol-Ares, M. J. Durán-Peña, A. J. Macías-Sánchez, J. R. Hanson, I. G. Collado and R. Hernández-Galán\*

Four new highly oxygenated 11-membered lactones (**11–14**) were synthesized by a combination of metabolic engineering techniques with complex chemical substrate synthesis.

