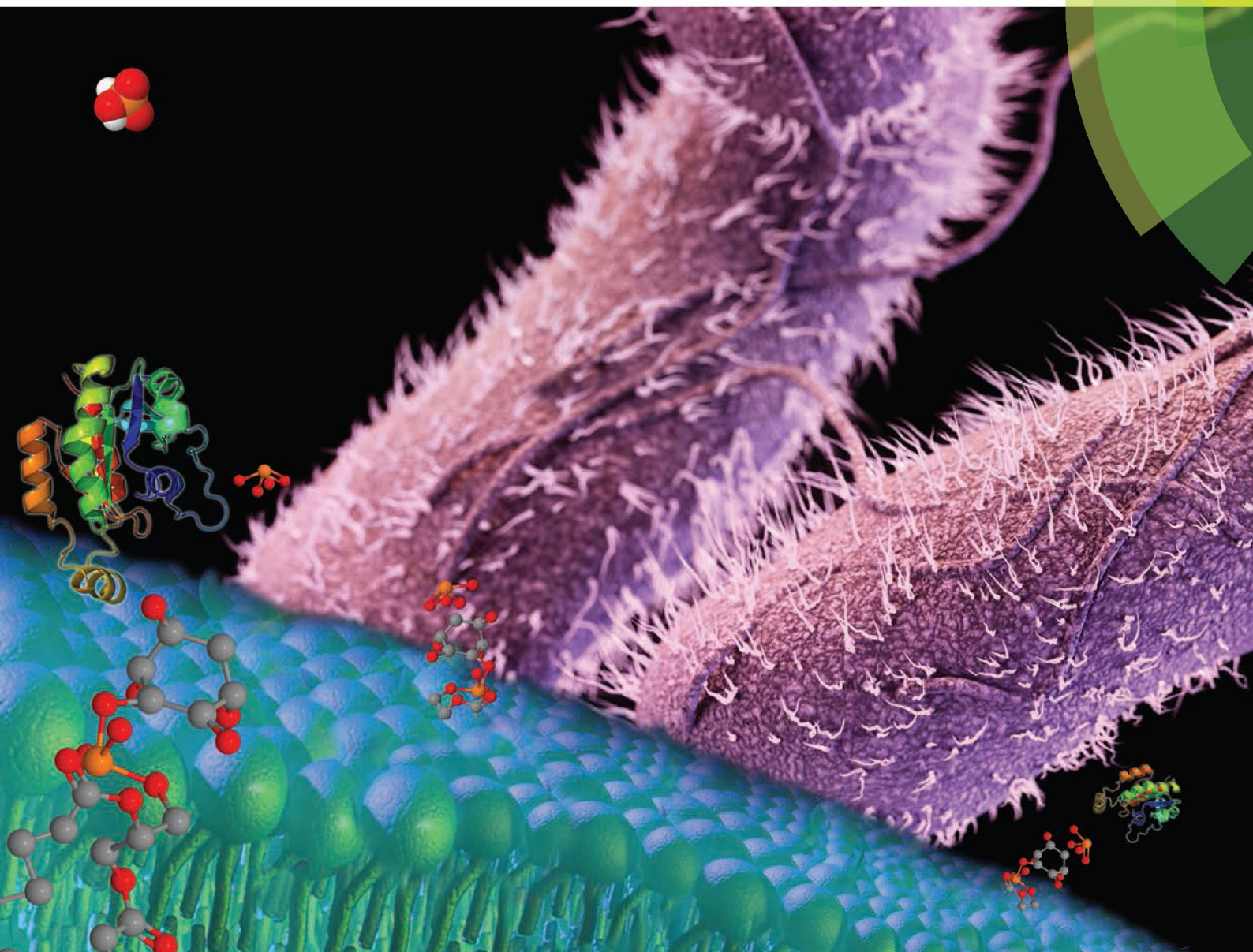


# Organic & Biomolecular Chemistry

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ISSN 1477-0520



**PAPER**

Rüdiger Woscholski, Piers R. J. Gaffney *et al.*  
Synthesis of unsaturated phosphatidylinositol 4-phosphates and the effects of substrate unsaturation on *SopB* phosphatase activity

# Organic & Biomolecular Chemistry

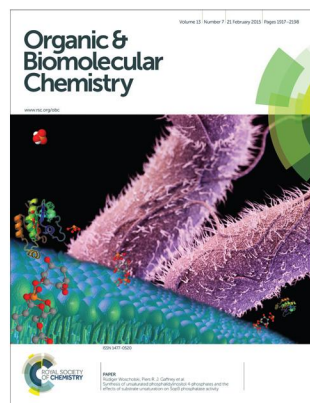
An international journal of synthetic, physical and biomolecular organic chemistry

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## IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 13(7) 1917–2198 (2015)



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Piers R. J. Gaffney *et al.*,  
pp. 2001–2011.

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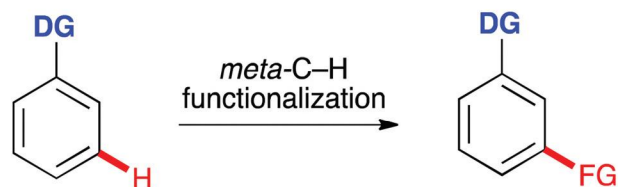
## REVIEWS

1930

### Transition metal catalyzed *meta*-C–H functionalization of aromatic compounds

Jiong Yang\*

This review summarizes synthetic methods for directing group guided, transition metal catalyzed *meta*-C–H functionalization of aromatic compounds.

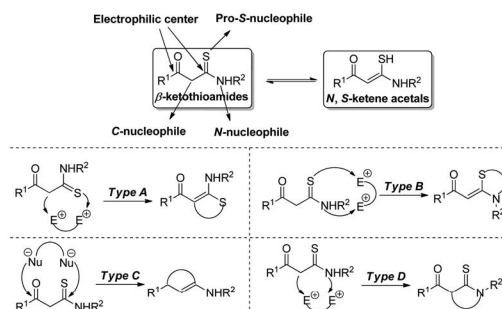


1942

### $\beta$ -Ketothioamides: efficient reagents in the synthesis of heterocycles

Wei-Si Guo, Li-Rong Wen\* and Ming Li\*

$\beta$ -Ketothioamides (KTAs) are versatile building blocks for the rapid construction of various heterocyclic compounds.



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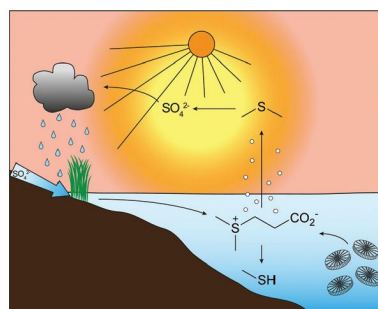
## REVIEWS

1954

### The chemical biology of dimethylsuloniopropionate

Jeroen S. Dickschat,\* Patrick Rabe and Christian A. Citron

This review addresses synthesis, biosynthesis, transport and degradation of dimethylsuloniopropionate and its derivatives.



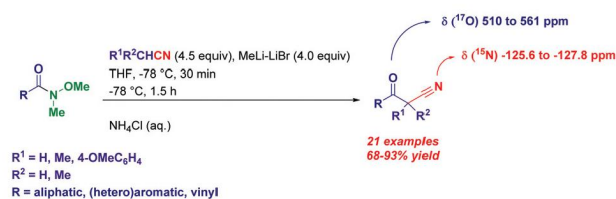
## COMMUNICATIONS

1969

### Chemoselective efficient synthesis of functionalized $\beta$ -oxonitriles through cyanomethylation of Weinreb amides

Ashenafi Damtew Mamuye, Laura Castoldi, Ugo Azzena, Wolfgang Holzer and Vittorio Pace\*

Homologation of Weinreb amides with cyanomethyl lithium: a new route to  $\beta$ -oxonitriles.

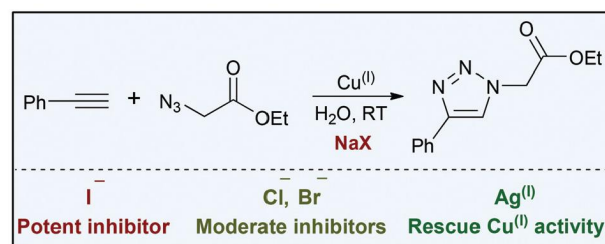


1974

### Halide inhibition of the copper-catalysed azide-alkyne cycloaddition

Rebekah M. Moorman, Matthew B. Collier, Bram H. Frohock, Michael D. Womble and Justin M. Chalker\*

Halides are inhibitors of the copper-catalysed azide-alkyne cycloaddition. Case studies in this inhibition are presented, along with experimental measures useful in accommodating halides in this widely used reaction.

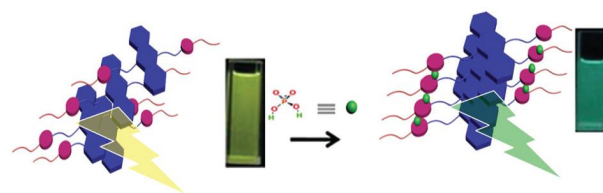


1979

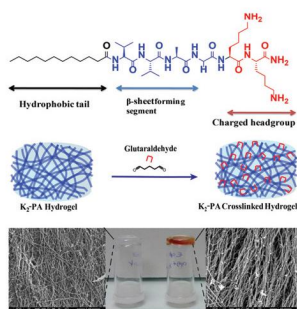
### Preassembly-driven ratiometric sensing of $\text{H}_2\text{PO}_4^-$ anions in organic and aqueous environments

Wei-tao Gong, Duo Na, Le Fang, Hassan Mehdi and Gui-ling Ning\*

The preassembly phenomenon of **R1** facilitates novel ratiometric fluorescence sensing of  $\text{H}_2\text{PO}_4^-$  in organic and aqueous environments.



1983

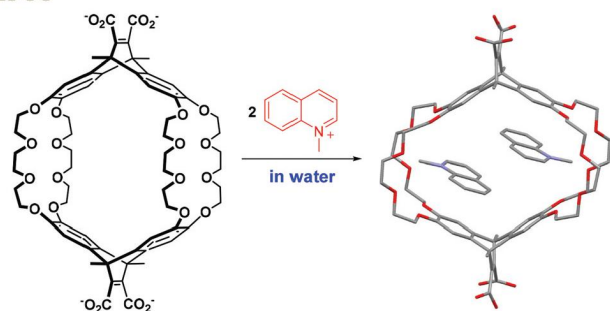


### Tuning viscoelastic properties of supramolecular peptide gels *via* dynamic covalent crosslinking

Mohammad Aref Khalily, Melis Goktas and Mustafa O. Guler\*

A dynamic covalent crosslinking approach is used to crosslink supramolecular peptide gels.

1988

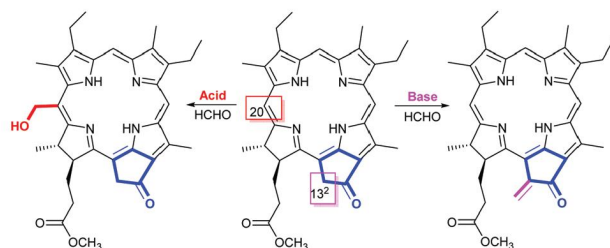


### Synthesis of a novel water-soluble cylindrical macrotricyclic host and its complexation with *N*-methylquinolinium and *N*-methylisoquinolinium salts: formation of 1 : 2 complexes in water

Fei Zeng and Chuan-Feng Chen\*

A water-soluble cylindrical macrotricyclic host could form 1 : 2 complexes with *N*-methylquinolinium or *N*-methylisoquinolinium salts in water solution and in the solid state.

1992

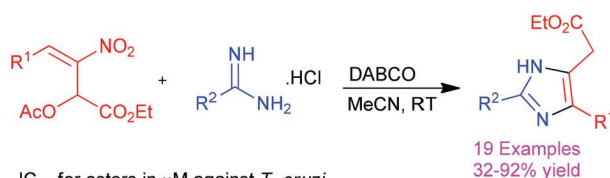


### Highly efficient synthesis of novel methyl $13^2$ -methylene mesopyropheophorbide a and its stereoselective Michael addition reaction

Jiazhu Li, Yang Liu, Xi-Sen Xu, Yan-Long Li, Shan-Guo Zhang, Il Yoon, Young Key Shim, Jin-Jun Wang\* and Jun-Gang Yin\*

pH-Dependent regioselective condensation of methyl mesopyropheophorbide a with HCHO is studied and stereoselective Michael reaction of the  $13^2$ -methylene product is also discussed.

1996



$IC_{50}$  for esters in  $\mu M$  against *T. cruzi*

$R^1 = 4-MeOC_6H_4$ ,  $R^2 = Ph$ : 111.9;  $R^1 = 2,4-(MeO)_2C_6H_3$ ,  $R^2 = Ph$ : 102.0

$R^1 = 4-Me-C_6H_4$ ,  $R^2 = Ph$ : 51.1; Standard (benzimidazole): 103.6

### Synthesis of imidazoles *via* cascade reaction of nitroallylic acetates with amidines and studies on their trypanocidal activity

Tarun Kumar, Deepti Verma, Rubem F. S. Menna-Barreto, Wagner O. Valença, Eufânio N. da Silva Júnior\* and Irishi N. N. Namboothiri\*

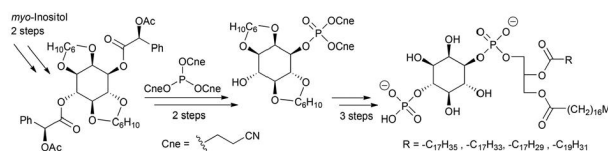
Functionalized imidazoles derived from nitroallylic acetates and amidines exhibit potent activity against *T. cruzi*, the etiological agent of Chagas disease.

2001

### Synthesis of unsaturated phosphatidylinositol 4-phosphates and the effects of substrate unsaturation on *SopB* phosphatase activity

Samuel Furse, LokHang Mak, Edward W. Tate, Richard H. Templer, Oscar Ces, Rüdiger Woscholski\* and Piers R. J. Gaffney\*

Single enantiomers of PI-4-*P*, with a range of *sn*-2-fatty acid esters, were prepared efficiently. The effects of the degree of *sn*-2-unsaturation on the kinetic parameters of *SopB* were determined.

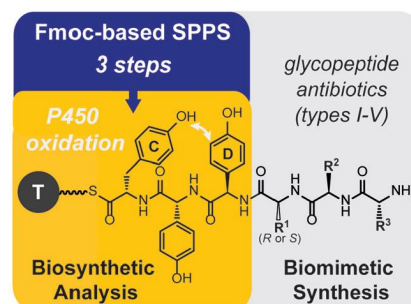


2012

### Rapid access to glycopeptide antibiotic precursor peptides coupled with cytochrome P450-mediated catalysis: towards a biomimetic synthesis of glycopeptide antibiotics

Clara Brieke, Veronika Kratzig, Kristina Haslinger, Andreas Winkler and Max J. Cryle\*

One Cytochrome P450 enzyme performs the phenolic crosslinking of a range of chemically synthesized, carrier-protein loaded glycopeptide antibiotic precursor peptides.



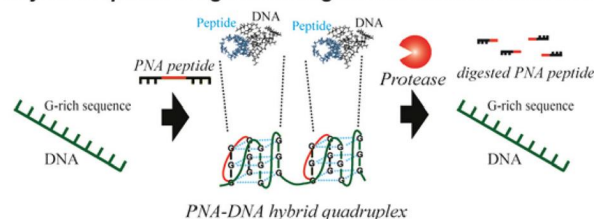
2022

### Control of guanine-rich DNA secondary structures depending on the protease activity using a designed PNA peptide

Kenji Usui,\* Arisa Okada, Keita Kobayashi and Naoki Sugimoto\*

A regulation system for DNA secondary structure formation of G-rich sequences using a designed PNA peptide exhibiting an enzyme-responsive functionality, depending on the protease activity was constructed.

#### Enzyme-responsive ligand for regulation of DNA structures

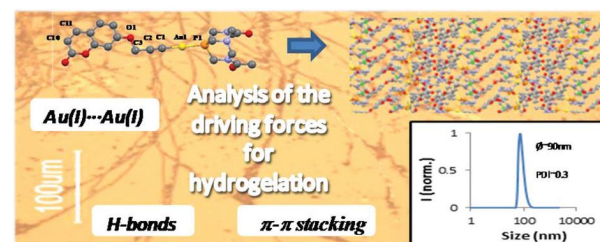


2026

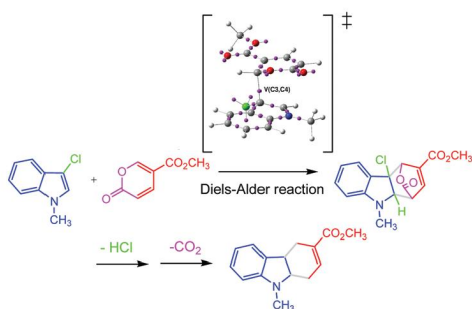
### A coumarin based gold(i)-alkynyl complex: a new class of supramolecular hydrogelators

Artur J. Moro, Bertrand Rome, Elisabet Aguiló, Julià Arcau, Rakesh Puttreddy, Kari Rissanen, João Carlos Lima\* and Laura Rodríguez\*

A phosphine-gold(i)-alkynyl-coumarin complex, [Au(7-(prop-2-ine-1-yloxy)-1-benzopyran-2-one)(DAPTA)] (**1**), was synthesized and the formation of long luminescent fibers in solution was characterized *via* fluorescence microscopy and dynamic light scattering.



2034

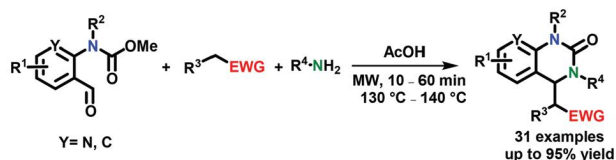


### Understanding the domino reaction between 3-chloroindoles and methyl coumalate yielding carbazoles. A DFT study

Luis R. Domingo,\* José A. Sáez and Saeed R. Emamian

The elimination of HCl and CO<sub>2</sub> in the corresponding cycloadducts makes the unfavourable polar Diels–Alder reaction of 3-chloroindole irreversible.

2044

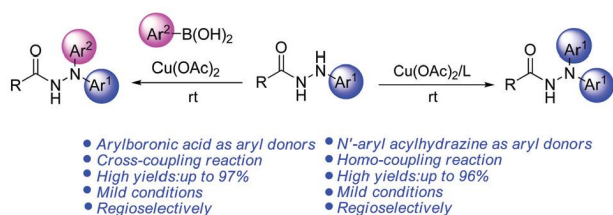


### A microwave-assisted multicomponent synthesis of substituted 3,4-dihydroquinazolinones

Marc Y. Stevens, Krzysztof Wieckowski, Peng Wu, Rajiv T. Sawant and Luke R. Odell\*

A series of structurally diverse 3,4-dihydroquinazolinones was synthesized via a novel cascade imine/cyclization/aza-Henry reaction in moderate to excellent yields.

2055

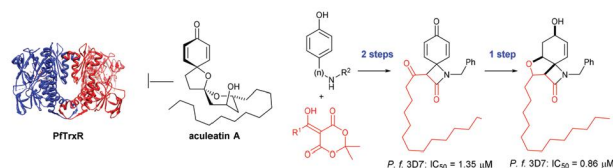


### Copper(II)-catalyzed coupling reaction: an efficient and regioselective approach to N',N'-diaryl acylhydrazines

Ji-Quan Zhang, Gong-Bin Huang, Jiang Weng, Gui Lu\* and Albert S. C. Chan

An efficient and regioselective copper(II)-catalyzed coupling reaction of N'-aryl acylhydrazines for the synthesis of N',N'-diaryl acylhydrazines has been developed.

2064



### Uncovering new structural insights for antimalarial activity from cost-effective aculeatin-like derivatives

Matthias Winkler, Marjorie Maynadier, Sharon Wein, Marie-Ange Lespinasse, Giovanna Boumis, Adriana E. Miele, Henri Vial and Yung-Sing Wong\*

An expedient synthesis of aculeatin-like analogues results in finding PfTrxR as putative cellular target and a promising new antimalarial chemotype.

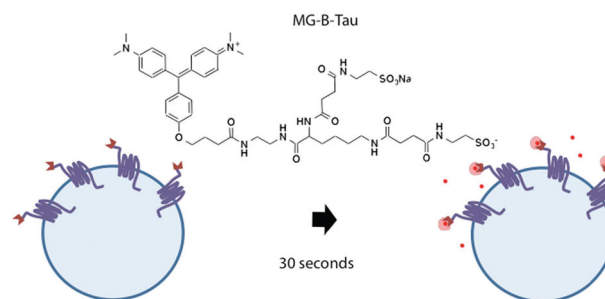
## PAPERS

2078

### Near-instant surface-selective fluorogenic protein quantification using sulfonated triarylmethane dyes and fluorogen activating proteins

Qi Yan, Brigitte F. Schmidt, Lydia A. Perkins, Matharishwan Naganbabu, Saumya Saurabh, Susan K. Andreko and Marcel P. Bruchez\*

A bis-sulfonate linker modified malachite green fluorogen improves its specificity and allows rapid, no-wash labeling of receptors on living cells.

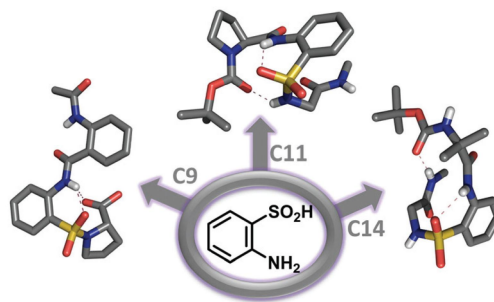


2087

### Conformational modulation of peptides using $\beta$ -amino benzenesulfonic acid ( $^S$ Ant)

Gowri Priya, Amol S. Kotmale, Debamitra Chakravarty, Vedavati G. Puranik, Pattuparambil R. Rajamohanam and Gangadhar J. Sanjayan\*

This communication describes the utility of the conformationally restricted aromatic  $\beta$ -amino acid (2-aminobenzenesulfonic acid,  $^S$ Ant) for inducing various folding interactions in short peptides.

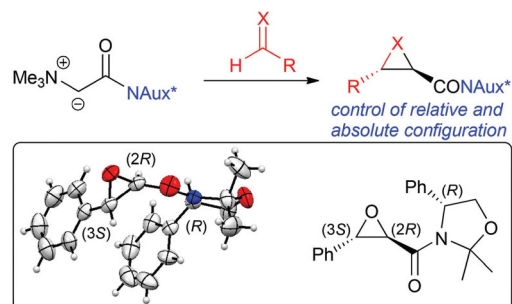


2092

### Asymmetric syntheses of three-membered heterocycles using chiral amide-based ammonium ylides

Mathias Pichler, Johanna Novacek, Raphaël Robiette, Vanessa Poscher, Markus Himmelsbach, Uwe Monkowius, Norbert Müller and Mario Waser\*

Phenylglycinol serves as a powerful chiral auxiliary in ammonium ylide-mediated reactions to obtain chiral epoxides/aziridines with excellent stereoselectivities.

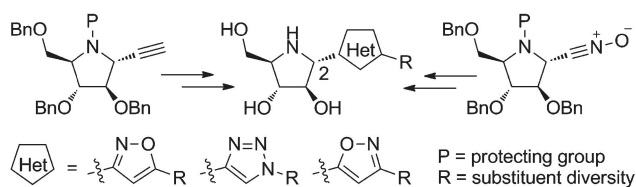


2100

### Synthesis of novel polyhydroxylated pyrrolidine-triazole/-isoxazole hybrid molecules

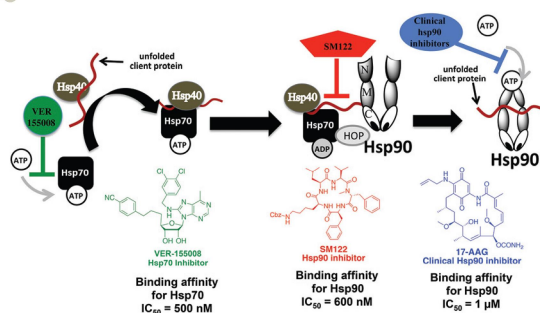
Cheng-Kun Lin, Li-Wei Cheng, Huang-Yi Li, Wen-Yi Yun and Wei-Chieh Cheng\*

A straightforward synthesis of novel, 2-heterocycl polyhydroxylated pyrrolidines is described.





2108

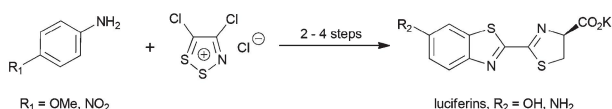


## Regulating the cytoprotective response in cancer cells using simultaneous inhibition of Hsp90 and Hsp70

Y. Wang and S. R. McAlpine\*

Both heat shock protein 90 and 70 (Hsp90, Hsp70) are cytoprotective proteins that regulate cell function and facilitate cell growth by stabilizing and folding proteins.

2117

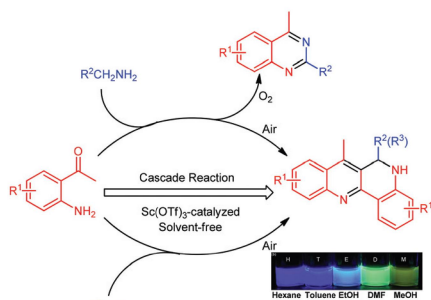


## Rapid and scalable assembly of firefly luciferase substrates

David C. McCutcheon, William B. Porterfield and Jennifer A. Prescher\*

Improved access to luciferins will bolster bioluminescence imaging applications.

2122

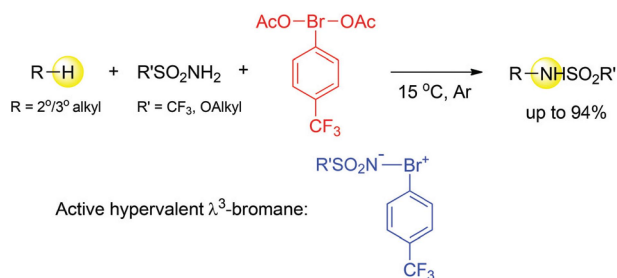


## A $\text{Sc}(\text{OTf})_3$ -catalyzed cascade reaction of *o*-aminoacetophenone with methanamine: construction of dibenzo[*b,h*][1,6]naphthyridine derivatives

Dan Mao, Jun Tang, Wenbo Wang, Xin Liu, Shengying Wu, Jianjun Yu and Limin Wang\*

A  $\text{Sc}(\text{OTf})_3$ -catalyzed and air-mediated cascade reaction was discovered as an efficient approach to the novel fluorescent fused-four-ring dibenzo[*b,h*][1,6]naphthyridine derivatives.

2129



## Metal-free C–H amination of unactivated hydrocarbons with sulfonylimino- $\lambda^3$ -bromanes generated *in situ* from (diacetoxybromo)benzene

Kazunori Miyamoto,\* Taiga Ota, Md. Mahbulul Hoque and Masahito Ochiai

A simple method for direct metal-free C–H amination of unactivated hydrocarbons using easy-handling diacetoxy- $\lambda^3$ -bromane and triflylamide or sulfamate esters was developed.

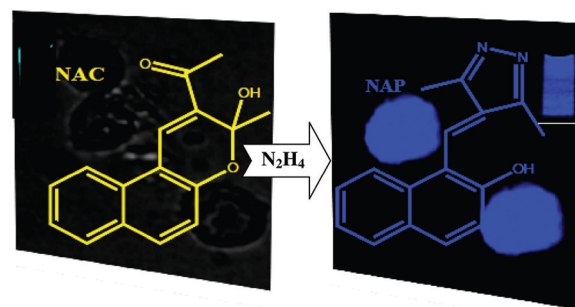
## PAPERS

2134

### Rapid detection of hydrazine in a naphthol-fused chromenyl loop and its effectiveness in human lung cancer cells: tuning remarkable selectivity via the reaction altered pathway supported by theoretical studies

Shyamaprosad Goswami,\* Avijit Kumar Das, Urmila Saha, Sibaprasad Maity, Kalyani Khanra and Nandan Bhattacharyya

A new chemosensor (NAC) is reported for fast and selective detection of  $N_2H_4$  in a novel way.

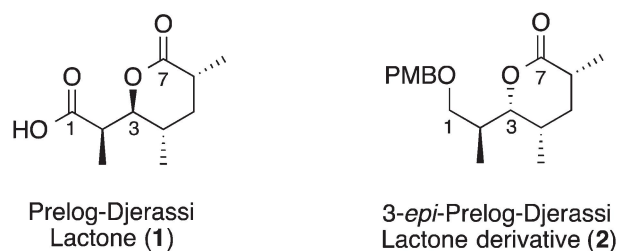


2140

### $^1H$ chemical shift differences of Prelog–Djerassi lactone derivatives: DFT and NMR conformational studies

Túlio J. Aímola, Dimas J. P. Lima, Luiz C. Dias, Cláudio F. Tormena and Marco A. B. Ferreira\*

This work reports an experimental and theoretical study of the conformational preferences of several Prelog–Djerassi lactone derivatives, to elucidate the  $^1H$  NMR chemical shift differences in the lactonic core that are associated with the relative stereochemistry of these derivatives.

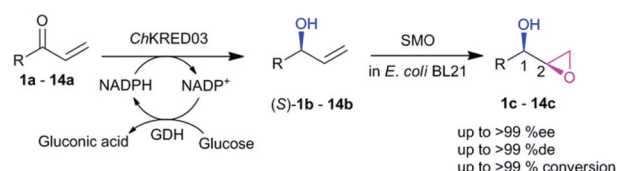


2146

### Synthesis of enantiopure glycidol derivatives via a one-pot two-step enzymatic cascade

Yu-Chang Liu, Yan Liu and Zhong-Liu Wu\*

An enzymatic cascade reaction employing an *S*-specific ketoreductase and a styrene monooxygenase to synthesize enantiopure glycidol derivatives is described.

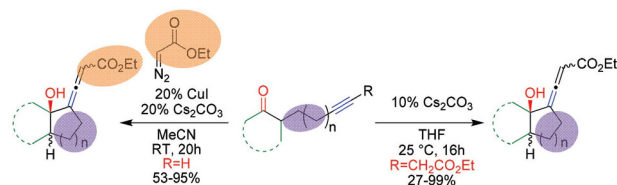


2153

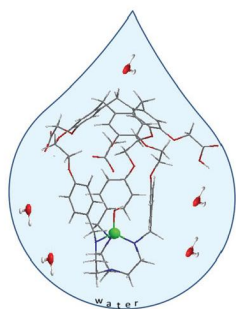
### *In situ* intramolecular catalytic 1,2-addition of allenates to cyclic ketones towards polycyclic allenates

Clément F. Heinrich, Michel Miesch and Laurence Miesch\*

Sequential deprotonation, isomerization of 3-alkynoates and subsequent 1,2-addition led to bicyclic allenate in the presence of a catalytic amount of  $Cs_2CO_3$ .



2157

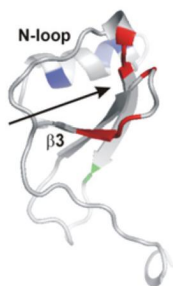
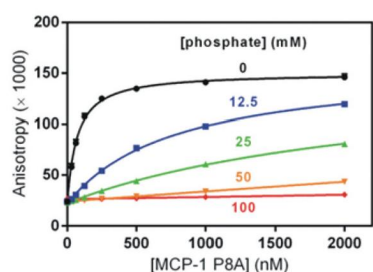


### Synthesis and physico-chemical properties of the first water soluble Cu(II)@hemicryptophane complex

Aline Schmitt, Solène Collin, Christophe Bucher, Vincent Maurel, Jean-Pierre Dutasta\* and Alexandre Martinez\*

A water-soluble metallo-enzyme model featuring a copper(II) site encaged in a closed-shell cavity of a hemicryptophane has been synthesized and studied.

2162

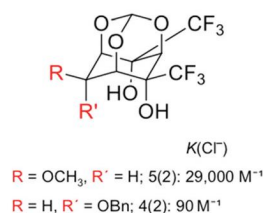
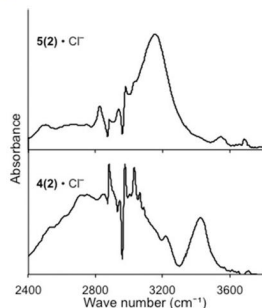


### Phosphate modulates receptor sulfotyrosine recognition by the chemokine monocyte chemoattractant protein-1 (MCP-1/CLL2)

Justin P. Ludeman, Mahdiah Nazari-Robati, Brendan L. Wilkinson, Cheng Huang, Richard J. Payne and Martin J. Stone\*

Fluorescence anisotropy shows that the physiological buffer phosphate competes with a chemokine receptor sulfopeptide for binding to a cognate chemokine.

2170

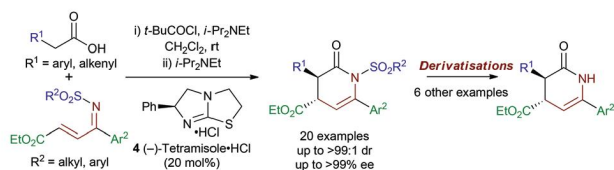


### Stereoelectronic effects: a simple yet powerful tool to manipulate anion affinity

Masoud Samet, Alireza Fattahi and Steven R. Kass\*

Stereoelectronic effects on anion binding were examined, IR spectroscopy was used to probe structures, and a well aligned non-interacting group can be more significant than a hydrogen bond donor.

2177



### Exploring the scope of the isothiurea-mediated synthesis of dihydropyridinones

Pei-Pei Yeh, David S. B. Daniels, Charlene Fallan, Eoin Gould, Carmen Simal, James E. Taylor, Alexandra M. Z. Slawin and Andrew D. Smith\*

The exploration and expansion of the scope of the isothiurea-mediated synthesis of dihydropyridinones is presented.

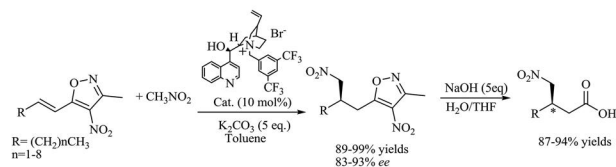
## PAPERS

2192

### An improved procedure to prepare 3-methyl-4-nitroalkylenethylisoxazoles and their reaction under catalytic enantioselective Michael addition with nitromethane

Maria Moccia,\* Robert J. Wells and Mauro F. A. Adamo\*

A two-step preparation of 3-methyl-4-nitro-5-alkylethenyl isoxazoles is herein reported. These were reacted with nitromethane under phase-transfer catalysis to provide highly enantioenriched adducts (up to 93% ee).



## CORRECTION

2196

### Correction: Studies towards asymmetric synthesis of 4(S)-11-dihydroxydocosaheptaenoic acid (diHDHA) featuring cross-coupling of chiral stannane under mild conditions

Rui Wang,\* Anyu He, Errabelli Ramu and John R. Falck