

# Organic & Biomolecular Chemistry

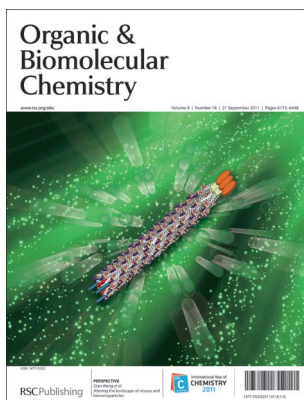
An international journal of synthetic, physical and biomolecular organic chemistry

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## IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 9(18) 6173–6448 (2011)



### Cover

See L. A. Lee *et al.*, pp. 6189–6195.

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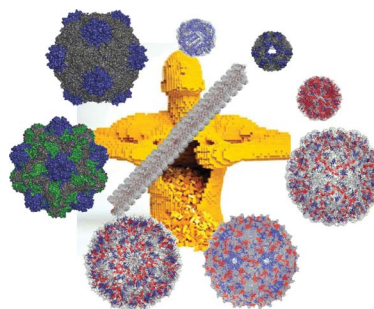
## PERSPECTIVE

6189

### Altering the landscape of viruses and bionanoparticles

L. Andrew Lee, Huong Giang Nguyen and Qian Wang\*

This review highlights some of the recent progress in the chemical modifications of bionanoparticles.



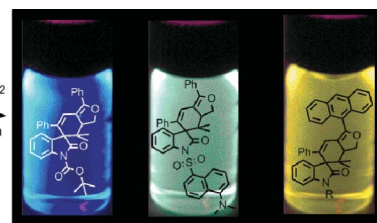
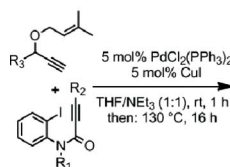
## COMMUNICATIONS

6196

### Luminescent bichromophoric spiroindolones – synthesis and electronic properties

Jan Schönhaber and Thomas J. J. Müller\*

Novel bichromophoric spirocyclic indolones with tunable emission color have been synthesized by an insertion–coupling–isomerization–Diels–Alder domino reaction.



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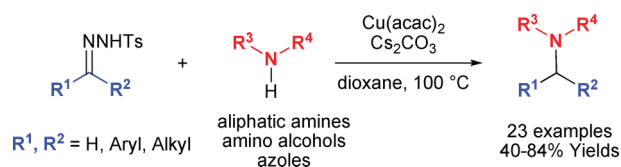
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6200

### Copper-catalyzed reductive coupling of tosylhydrazones with amines: A convenient route to $\alpha$ -branched amines

Abdallah Hamze,\* Bret Tréguier, Jean-Daniel Brion and Mouâd Alami\*

The use of primary and secondary aliphatic amines, amino alcohols as well as azole derivatives as partners in the copper-catalyzed coupling with tosylhydrazones allows the selective preparation of aryl- and diarylmethylamines in good yields.

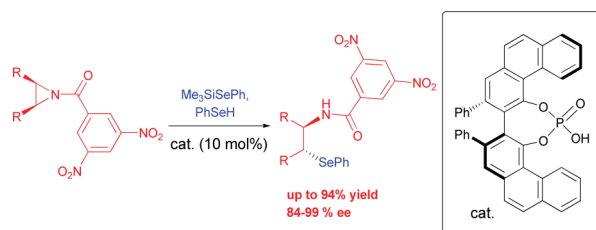


6205

### A general phosphoric acid-catalyzed desymmetrization of *meso*-aziridines with silylated selenium nucleophiles

Matilde Senatore, Alessandra Lattanzi, Stefano Santoro, Claudio Santi and Giorgio Della Sala\*

The first example of *meso*-aziridines desymmetrization with selenium nucleophiles has been reported. This general and highly enantioselective reaction is promoted by a chiral phosphoric acid using (phenylseleno)trimethylsilane as the nucleophile.

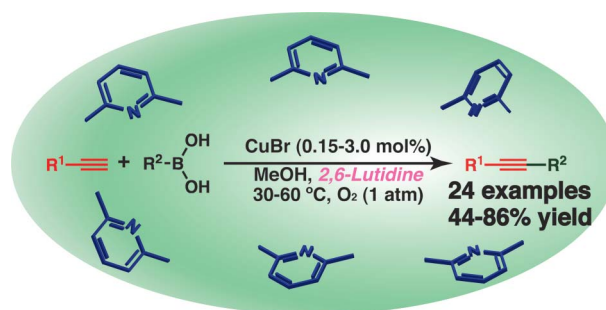


6208

### Copper-catalyzed, aerobic oxidative cross-coupling of alkynes with arylboronic acids: remarkable selectivity in 2,6-lutidine media

Tomohiro Yasukawa, Hiroyuki Miyamura and Shū Kobayashi\*

Aerobic oxidative cross-coupling reactions between alkynes and boronic acids under mild conditions catalyzed by low loadings of a copper salt are reported. 2,6-Lutidine accelerated the reactions dramatically, and the desired coupling products were obtained in high yields with high selectivity.

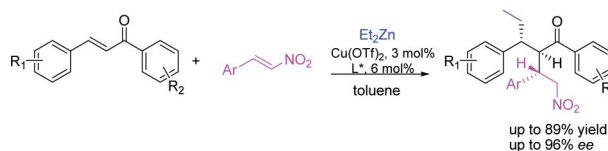


6211

### Diastereoselective and enantioselective capture of chiral zinc enolate using nitroolefins: a rapid access to chiral $\gamma$ -nitro carbonyl compounds

Cheng-Yan Ni, Sha-Sha Kan, Quan-Zhong Liu\* and Tai-Ran Kang

Highly diastereoselective and enantioselective capture of chiral zinc enolate using nitroolefins was developed. The product  $\gamma$ -nitro carbonyl compounds were readily transformed to enantiomerically enriched pyrrolidine derivatives with four contiguous chiral centers.





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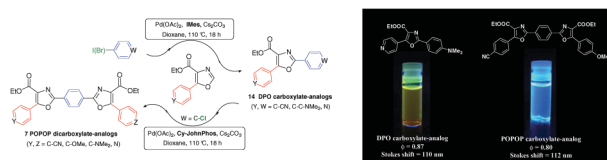
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6215

### DPO and POPOP carboxylate-analog sensors by sequential palladium-catalysed direct arylation of oxazole-4-carboxylates

Cécile Verrier, Catherine Fiol-Petit, Christophe Hoarau\* and Francis Marsais

Sequential Pd(0)-catalysed direct (het)arylation of oxazole-4-carboxylates is achieved to give rapid access to DPO and POPOP (di)carboxylate-analogs.



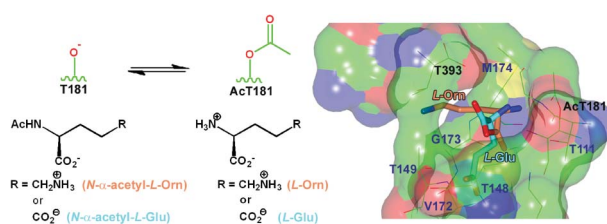
## PAPERS

6219

### Structural and biochemical analyses reveal how ornithine acetyl transferase binds acidic and basic amino acid substrates

Aman Iqbal, Ian. J. Clifton, Rasheduzzaman Chowdhury, David Ivison, Carmen Domene and Christopher J. Schofield\*

Ornithine acetyl transferases catalyze the transfer of an acetyl group via an acetyl-enzyme intermediate. Structural and biochemical studies were used to investigate how an ornithine acetyl transferase binds acidic (L-glutamate) and basic (L-ornithine) substrates.

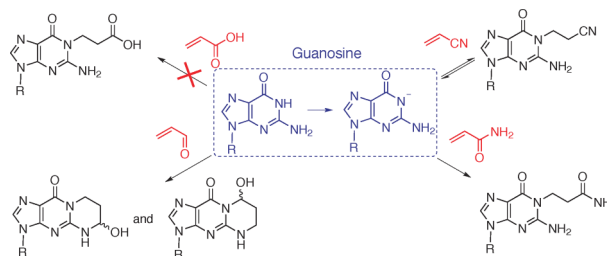


6226

### Alkylating potential of α,β-unsaturated compounds

José A. Manso, Isaac F. Céspedes Camacho, Emilio Calle and Julio Casado\*

Alkylation reactions of guanosine by some relevant α,β-unsaturated compounds occur through different mechanisms. A good correlation between chemical reactivity and mutagenicity of the alkylating agents was found.

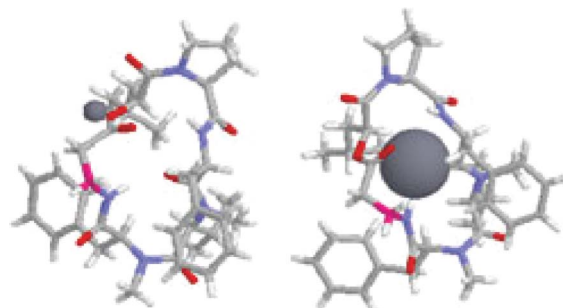


6234

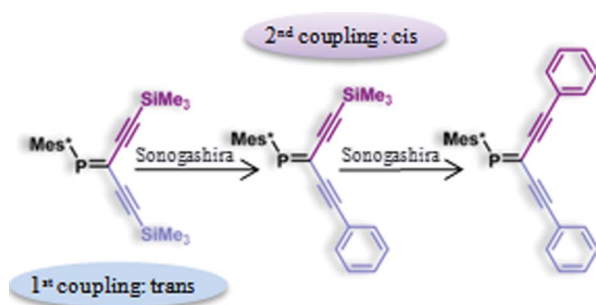
### Effect of ester chemical structure and peptide bond conformation in fragmentation pathways of differently metal cationized cyclodepsipeptides

Raja Banerjee,\* S. Sudarslal, R. S. Ranganayaki and S. Raghothama

Interacting site of metal ions differ for isaridin due to its chemical structure and peptide bond conformation, leading to different fragmentation pathway.



6246

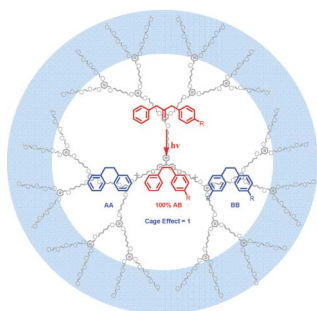


### *C,C*-Diacetylenic phosphalkenes in palladium-catalyzed cross-coupling reactions

Elisabet Öberg, Xue-Li Geng, Marie-Pierre Santoni and Sascha Ott\*

Sequential TMS removal on *C,C*-diacetylenic phosphalkenes ( $A_2PA$ ) allows for selective aryl substitutions and the preparation of an arene-bridged bis- $A_2PA$ .

6256

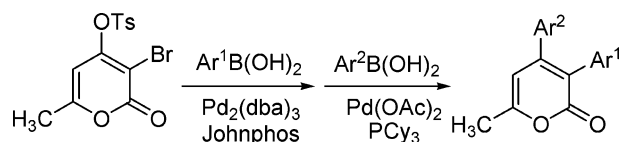


### Unsurpassed cage effect for the photolysis of dibenzyl ketones in water-soluble dendrimers

Zhao Yuan, Jinping Chen,\* Yi Zeng, Ying-Ying Li, Yongbin Han and Yi Li\*

Amphiphilic water-soluble dendrimers, terminated with charge-neutral tetraethylene glycol monomethyl ethers, were used as microreactors to conduct the photolysis of dibenzyl ketone derivatives, affording an unsurpassed cage effect of 1.00.

6265

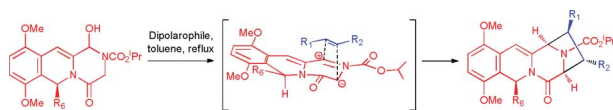


### Generation of diverse 2-pyrones *via* palladium-catalyzed site-selective Suzuki-Miyaura couplings of 3-bromo-4-tosyloxy-2-pyrone

Xiaoli Lei, Liang Gao, Qiuping Ding, Yiyuan Peng\* and Jie Wu\*

Based on different reactivity of the (pseudo)halide substituents in the 2-pyrone (3-Br and 4-OTs), palladium-catalyzed sequential site-selective Suzuki–Miyaura cross-coupling reactions of 3-bromo-6-methyl-4-tosyloxy-2-pyrone are described, which afford the diverse 2-pyrones in good yields.

6271



### 1,3-Dipolar cycloadditions from tricyclic hemiaminals. Synthesis of the quinocarcin core through catalyst-free generation of azomethine ylides

Lena Huck, J. Francisco González, Elena de la Cuesta, J. Carlos Menéndez and Carmen Avendaño\*

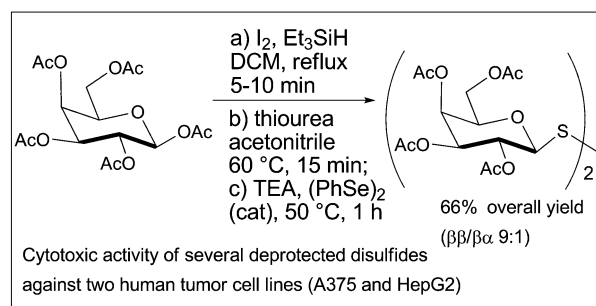
A 1,3-dipolar cycloaddition approach to the quinocarcin core has been developed that affords highly functionalized cycloadducts from readily accessible hemiaminals *via* a catalyst-free dehydration process.

6278

### A straightforward synthetic access to symmetrical glycosyl disulfides and biological evaluation thereof

Matteo Adinolfi, Domenica Capasso,\* Sonia Di Gaetano, Alfonso Iadonisi,\* Loredana Leone and Antonello Pastore

Cytotoxic activity of several deprotected disulfides against two human tumor cell lines (A375 and HepG2).

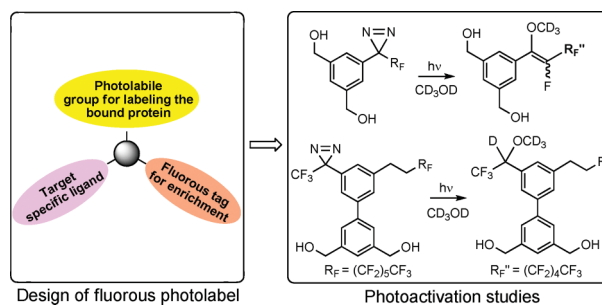


6284

### Design, synthesis and photoactivation studies of fluorous photolabels

Arun Babu Kumar, Jordan Micheal Anderson and Roman Manetsch\*

Two perfluorinated photoprobes have been synthesized and their photoactivation reactions have been studied in detail. The photoprobe, in which the photoreactive diazine ring is incorporated on the fluorous tag, is prone to self-deactivation and thus less suitable for photoaffinity studies.

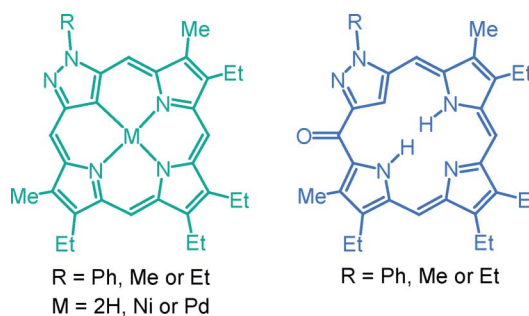


6293

### Pyrazole analogues of porphyrins and oxophlorins

Alexandra M. Young, Amber L. Von Ruden and Timothy D. Lash\*

Pyrazoloporphyrins, a new class of carbaporphyrinoid macrocycles, are reported and syntheses of related oxophlorins and organometallic derivatives are described.

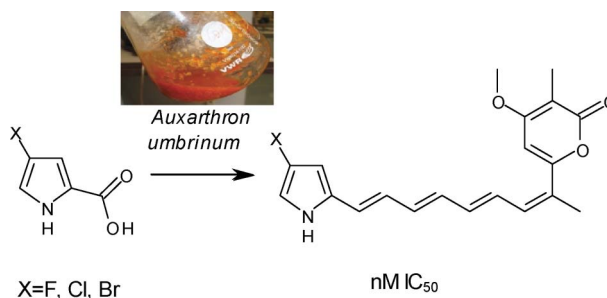


6306

### Production of anticancer polyenes through precursor-directed biosynthesis

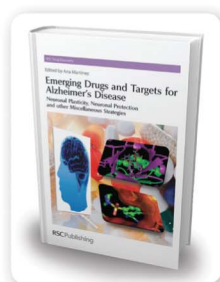
Benjamin R. Clark, Stephen O'Connor, Deirdre Fox, Jacques Leroy and Cormac D. Murphy\*

Incubation of *A. umbrinum* with substituted pyrrole-2-carboxylic acids yields novel polyenyl-pyrroles with altered cytotoxic properties.





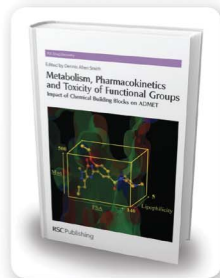
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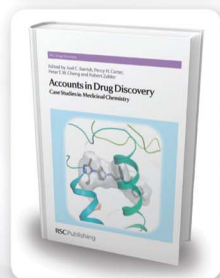
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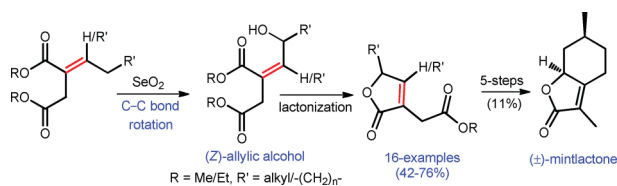


6312

### Regio- and stereoselective selenium dioxide allylic oxidation of (*E*)-dialkyl alkylidenesuccinates to (*Z*)-allylic alcohols: Synthesis of natural and unnatural butenolides

Ramesh M. Patel, Vedavati G. Puranik and Narshinha P. Argade\*

SeO<sub>2</sub> induced (*Z*)-selective allylic alcohol formation of dialkyl alkylidenesuccinates has been demonstrated to accomplish syntheses of essential butenolides/fused butenolides.

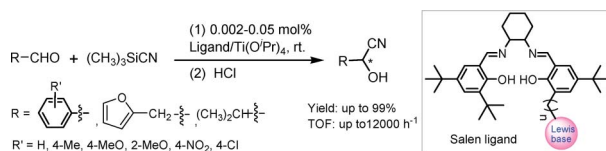


6323

### Unsymmetric salen ligands bearing a Lewis base: intramolecularly cooperative catalysis for cyanosilylation of aldehydes

Ye-Qian Wen, Wei-Min Ren and Xiao-Bing Lu\*

Unsymmetric ligands bearing an appended Lewis base in conjunction with Ti(O<sup>i</sup>Pr)<sub>4</sub> exhibited excellent activity in cyanosilylation *via* intramolecularly cooperative catalysis.



6331

### Efficient and simple zinc-mediated synthesis of 3-amidoindoles

Anahit Pews-Davtyan and Matthias Beller\*

A general synthesis of 3-amidoindoles from easily available arylhydrazines and acylated propargylamines is described. In the presence of inexpensive Zn salts, alkyne amination and subsequent Fischer indole-cyclization took place in good yields with excellent regioselectivity providing an interesting scaffold for potentially bio-active compounds.

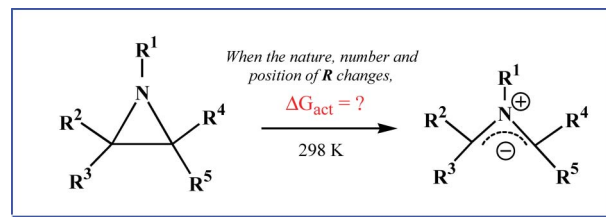


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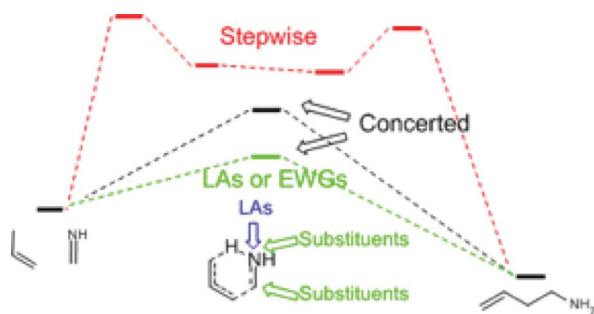
### Substituent effects on the rate of formation of azomethine ylides. A computational investigation

Harold D. Banks\*

Substituent effect on the rate of formation of azomethine ylides from aziridines was studied computationally to identify compounds that would react at room temperature in reasonable periods of time.



6343

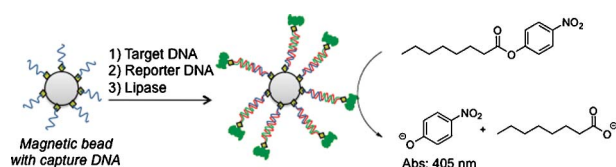


### A theoretical study of imine-ene reaction influencing factors

Qiwu Yang, Yan Liu and Wenqin Zhang\*

The mechanism and influence factors of imine-ene reaction have been studied by DFT at the B3LYP level. A concerted mechanism with an *exo* configuration transition structure was confirmed. Lewis acids (LAs) and electron-withdrawing groups (EWGs) on methanimine facilitate the reaction, and a good correlation was found between the reaction barrier and the imine electrophilicity.

6352

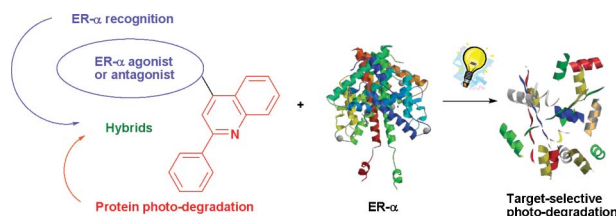


### Development of a lipase-based optical assay for detection of DNA

Suttiporn Pinijsuwan, Stepan Shipovskov, Werasak Surareungchai, Elena E. Ferapontova and Kurt V. Gothelf\*

The enzymatic cleavage of *p*-nitrophenyl octanoate by lipase from *Candida antarctica* was used to amplify the binding of a specific DNA strand in a magnetic bead-linked sandwich assay.

6357

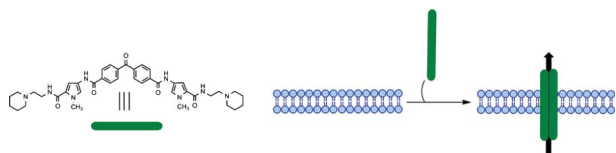


### Molecular design, chemical synthesis, and biological evaluation of agents that selectively photo-degrade the transcription factor estrogen receptor- $\alpha$

K. Tsumura, A. Suzuki, T. Tsuzuki, S. Tanimoto, H. Kaneko, S. Matsumura, M. Imoto, K. Umezawa, D. Takahashi and K. Toshima\*

The designed and synthesized 2-phenylquinoline-estradiol and 2-phenylquinoline-4-hydroxytamoxifen hybrids effectively and selectively photo-degraded the target transcription factor, estrogen receptor- $\alpha$  (ER- $\alpha$ ), in both glass vessels and MCF-7 breast cancer cells, which are dependent upon ER- $\alpha$  for growth.

6367



### Examination of a synthetic benzophenone membrane-targeted antibiotic

Sunil K. Vooturi, Mahender B. Dewal and Steven M. Firestine\*

The membrane disruption activity of benzophenone-containing antibiotics was explored. These agents depolarize membranes, release potassium from bacteria, promote dye efflux from LUVs and rescue mice from lethal MRSA infection.

A decorative graphic at the top of the page featuring a network of glowing blue nodes connected by thin lines, set against a dark blue background with vertical light streaks.

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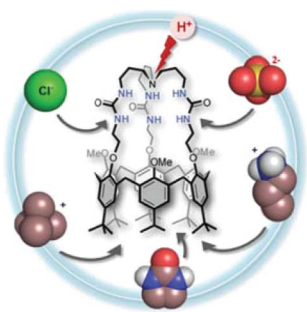
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6373

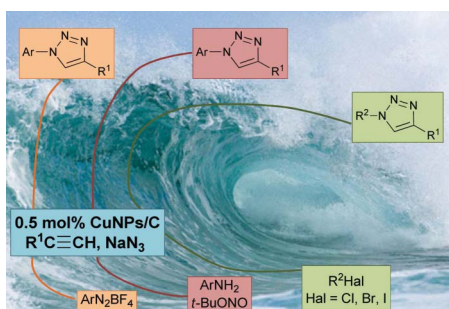


### Acid–base modulation of a versatile heteroditopic calix[6]arene based receptor

Damien Cornut, Jérôme Marrot, Johan Wouters and Ivan Jabin\*

A new calix[6]crypturea that displays acid–base controllable and versatile binding properties toward either neutral or charged species is described.

6385

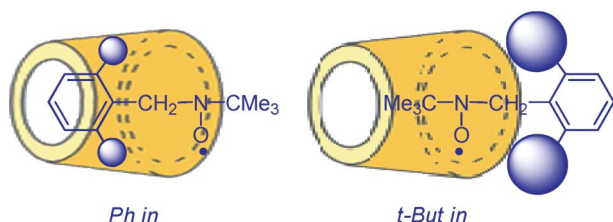


### Click chemistry from organic halides, diazonium salts and anilines in water catalysed by copper nanoparticles on activated carbon

Francisco Alonso,\* Yanina Moglie, Gabriel Radivoy and Miguel Yus\*

Copper nanoparticles on activated carbon catalyse the multicomponent synthesis of 1,2,3-triazoles from organic halides, diazonium salts, and anilines in water.

6396

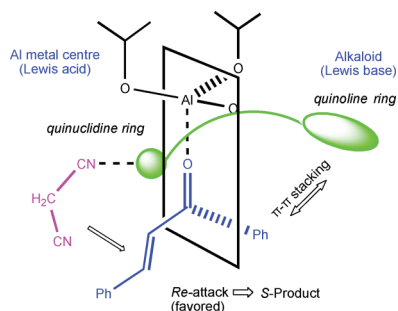


### Kinetic control of the direction of inclusion of nitroxide radicals into cyclodextrins

Paola Franchi, Costanza Casati, Elisabetta Mezzina and Marco Lucarini\*

Control of the direction of incorporation of nitroxide radicals into cyclodextrins has been demonstrated by the combined use of EPR and NMR.

6402



### Theoretical investigation on mechanism of asymmetric Michael addition of malononitrile to chalcones catalyzed by Cinchona alkaloid aluminium(III) complex

Zhishan Su, Hai Whang Lee and Chan Kyung Kim\*

A dual activation mechanism involves Al<sup>III</sup> and Cinchona alkaloid acting as Lewis acid and base, respectively.

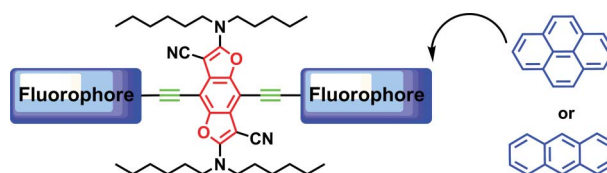


6410

### Synthesis, structures, redox and photophysical properties of benzodifuran-functionalised pyrene and anthracene fluorophores

Stephan Keller, Chenyi Yi, Chen Li, Shi-Xia Liu,\*  
Carmen Blum, Gabriela Frei, Olha Sereda, Antonia Neels,  
Thomas Wandlowski and Silvio Decurtins

Benzodifuran-functionalised pyrene and anthracene fluorophores act as highly luminescent materials that undergo two one-electron oxidations.

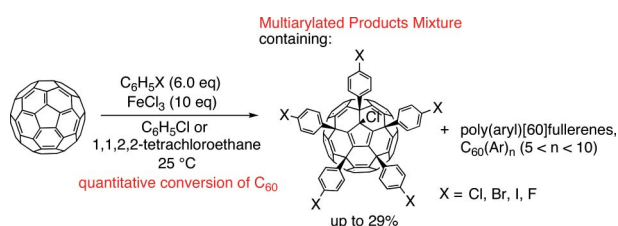


6417

### Facile fullerene modification: FeCl<sub>3</sub>-mediated quantitative conversion of C<sub>60</sub> to polyarylated fullerenes containing pentaaryl(chloro)[60]fullerenes

Masahiko Hashiguchi,\* Kazuhiro Watanabe and  
Yutaka Matsuo\*

A facile, one-step reaction using inexpensive reagents has been developed for functionalization of [60]fullerene.

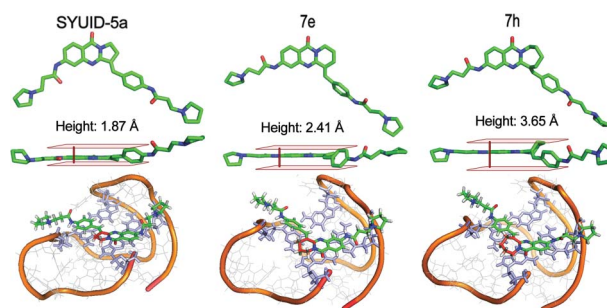


6422

### Impact of planarity of unfused aromatic molecules on G-quadruplex binding: Learning from isaindigotone derivatives

Jin-Qiang Hou, Jia-Heng Tan, Xiao-Xiao Wang, Shuo-Bin  
Chen, Si-Yuan Huang, Jin-Wu Yan, Shu-Han Chen,  
Tian-Miao Ou, Hai-Bin Luo, Ding Li, Lian-Quan Gu\* and  
Zhi-Shu Huang\*

A series of new isaindigotone derivatives were synthesized to investigate effects of planarity of unfused aromatic molecules on G-quadruplex DNA binding.

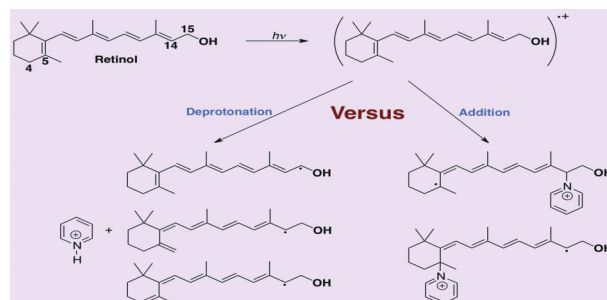


6437

### Laser flash photolysis study on the retinol radical cation in polar solvents

Ali El-Agamey\* and Shunichi Fukuzumi\*

Laser flash photolysis of retinol in polar solvents leads to the formation of retinol radical cation.





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Registration deadline 2 March 2012  
[www.rsc.org/FD156](http://www.rsc.org/FD156)

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25–27 June 2012, Assisi, Italy  
Poster abstracts by 27 April 2012  
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[www.rsc.org/FD157](http://www.rsc.org/FD157)

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Poster abstracts by 11 May 2012  
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## Analytical Research Forum 2012

2–4 July 2012, Durham, UK  
Poster abstracts by 4 May 2012  
Registration deadline 1 June 2012  
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Registration deadline 22 June 2012  
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## Ion Specific Hofmeister Effects (Faraday Discussion 160)

3–5 September 2012, Oxford, UK  
Poster abstracts by 6 July 2012  
Registration deadline 3 August 2012  
[www.rsc.org/FD160](http://www.rsc.org/FD160)

## 21st IUPAC International Conference on Physical Organic Chemistry (ICPOC 21)

9–13 September 2012, Durham, UK  
Poster abstracts by 6 July 2012  
Registration deadline 3 August 2012  
[www.rsc.org/ICPOC21](http://www.rsc.org/ICPOC21)

## Inorganic Photophysics and Photochemistry – Fundamentals and Applications (Dalton Discussion 13)

10–12 September 2012, Sheffield, UK  
Poster abstracts by 6 July 2012  
Registration deadline 3 August 2012  
[www.rsc.org/DD13](http://www.rsc.org/DD13)

## Lipids and Membrane Biophysics (Faraday Discussion 161)

11–13 September 2012, London, UK  
Poster abstracts by 13 July 2012  
Registration deadline 10 August 2012  
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