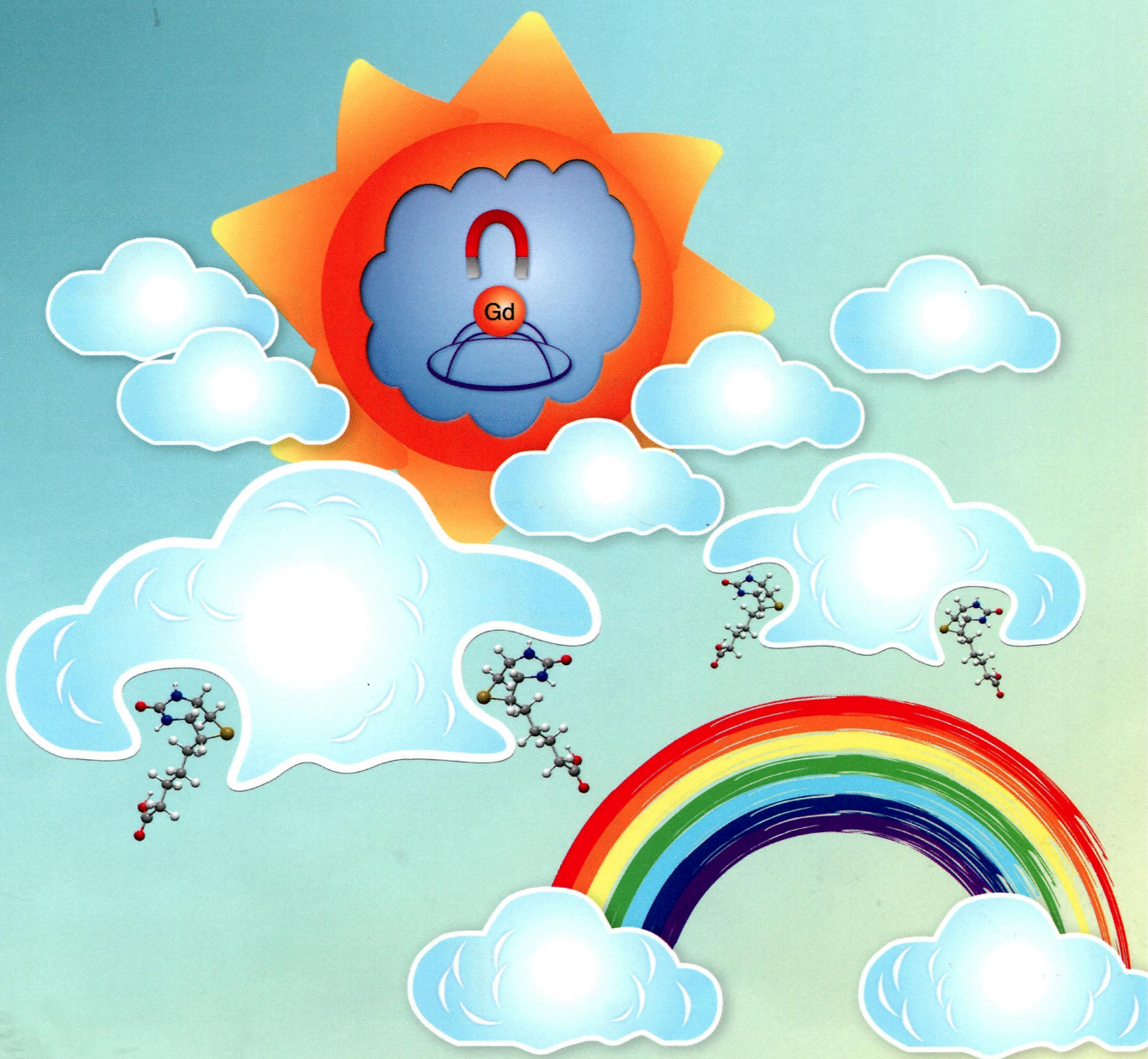


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PAPER

Goran Angelovski *et al.*

Synthesis and characterization of pH-sensitive, biotinylated MRI contrast



Organic & Biomolecular Chemistry

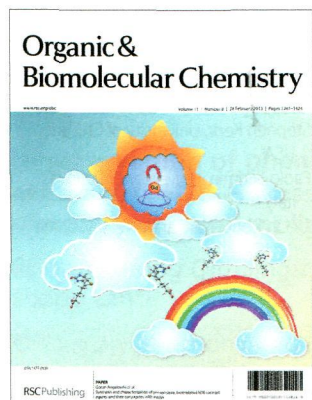
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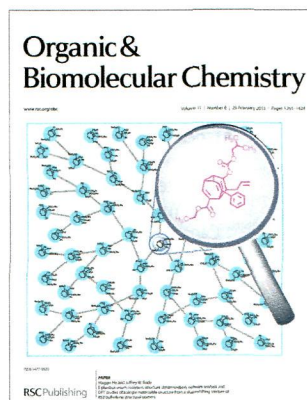
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Cover

See Goran Angelovski *et al.*, pp. 1294–1305.

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Inside cover

See Maggie He and Jeffrey W. Bode, pp. 1306–1317.

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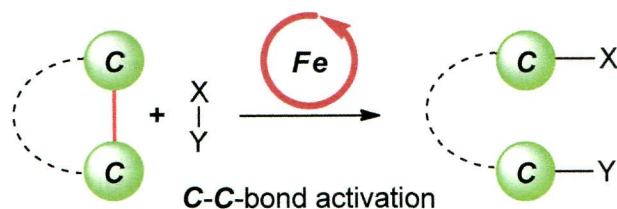
EMERGING AREA

1271

Iron-catalysed carbon–carbon single bond activation

Johannes E. M. N. Klein and Bernd Plietker*

The activation of C–C-bonds by means of Fe-catalysis is an emerging field within organometallic catalysis and offers interesting perspectives for streamlining synthetic strategies.



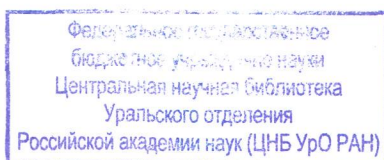
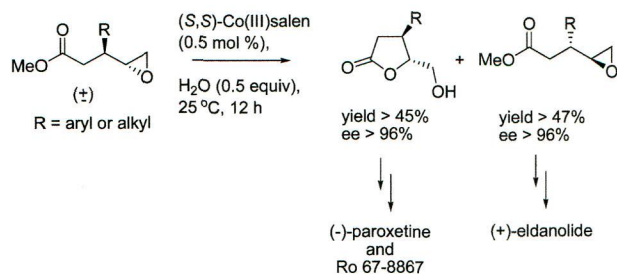
COMMUNICATIONS

1280

Optically pure γ -butyrolactones and epoxy esters via two stereocentered HKR of 3-substituted epoxy esters: a formal synthesis of (–)-paroxetine, Ro 67-8867 and (+)-eldanolide

Dattatray A. Devalankar, Pratibha U. Karabal and Arumugam Sudalai*

The HKR of racemic *anti*- or *syn*- 3-substituted epoxy esters catalyzed by Co(III)salen complex provides ready access to the corresponding enantioenriched 3,4-disubstituted γ -butyrolactones and 3-substituted epoxy esters.

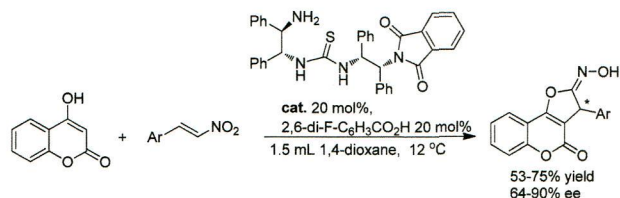


1286

Asymmetric Michael/cyclization tandem reaction of 4-hydroxycoumarin with β -nitroalkenes catalyzed by chiral bifunctional thioureas

Ren-Qiang Mei, Xiao-Ying Xu, Lin Peng, Fan Wang, Fang Tian and Li-Xin Wang*

The first asymmetric Michael/cyclization tandem reaction of 4-hydroxycoumarin with nitroolefins catalyzed by chiral bifunctional thioureas was reported and 2,3-dihydrofuro[3,2-c]-coumarin adducts were obtained in moderate yields (53–75%) and good enantioselectivities (64–90% ee).

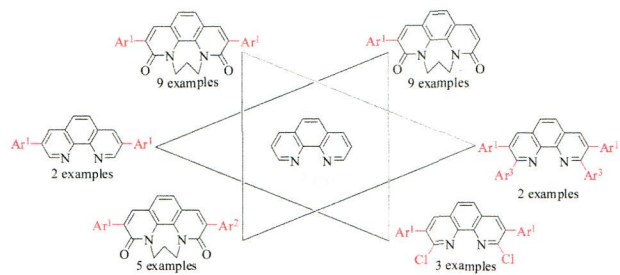


1290

Direct arylation of phenanthroline derivatives via oxidative C–H/C–H cross-coupling: synthesis and discovery of excellent ligands

Bijin Li, Xurong Qin, Jingsong You,* Xuefeng Cong and Jingbo Lan*

Various aryl functionalized phenanthrolines have been conveniently and efficiently synthesized and show excellent competence in promoting transition-metal-free direct arylation and the Pd-catalysed Heck reaction.



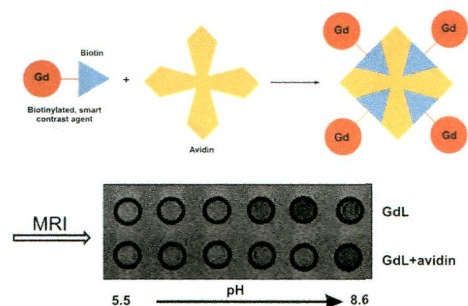
PAPERS

1294

Synthesis and characterization of pH-sensitive, biotinylated MRI contrast agents and their conjugates with avidin

Sandip M. Vibhute, Jörn Engelmann, Tatjana Verbić, Martin E. Maier, Nikos K. Logothetis and Goran Angelovski*

Two pH sensitive contrast agents which possess different types of linkers were developed and were further functionalized by biotinylation. The MRI response of their conjugates with avidin was investigated.

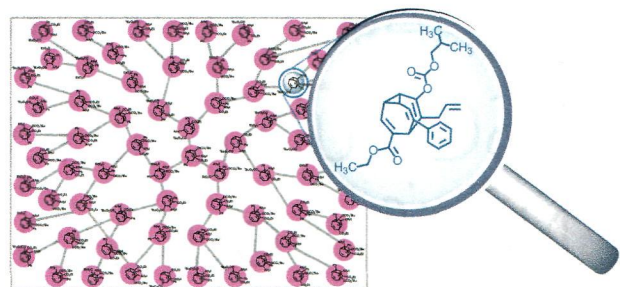


1306

E pluribus unum: isolation, structure determination, network analysis and DFT studies of a single metastable structure from a shapeshifting mixture of 852 bullvalene structural isomers

Maggie He and Jeffrey W. Bode*

A single structure is isolated from a dynamic mixture of 852 isomers in a shapeshifting organic molecule. We have determined the structure and investigated this molecule by computations and network mapping.

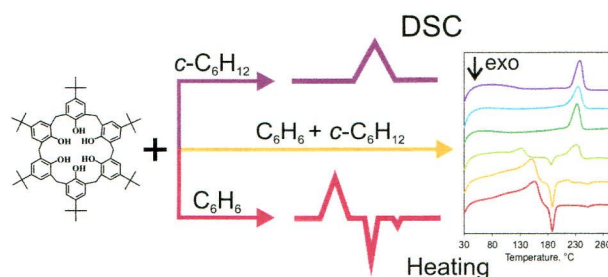


1318

Analysis of guest binary mixtures by *tert*-butylcalix[6]arene using host memory of previously bound guests

Goulnaz D. Safina, Marat A. Ziganshin, Aidar T. Gubaidullin and Valery V. Gorbatchuk*

A new principle of quantitative and qualitative analysis of binary mixtures is offered using only one receptor and its single parameter, which works even in the absence of preferential binding.

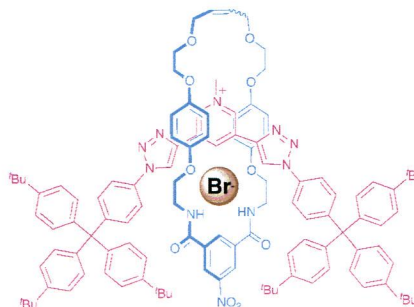


1326

A rotaxane host system containing integrated triazole C–H hydrogen bond donors for anion recognition

Nicholas G. White and Paul D. Beer*

A novel bis-triazole pyridinium axle containing rotaxane, prepared by a chloride anion templated ring closing metathesis clipping strategy, exhibits selectivity for halide anions over oxoanions with a notable preference for bromide being shown amongst the halides.

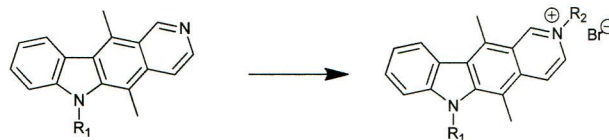


1334

Synthesis and evaluation of novel ellipticines as potential anti-cancer agents

Fiona M. Deane, Elaine C. O'Sullivan, Anita R. Maguire, Jayne Gilbert, Jennette A. Sakoff, Adam McCluskey* and Florence O. McCarthy*

Cytotoxicity Vs 12 cancer cell lines Av. GI₅₀ < 1 μM.

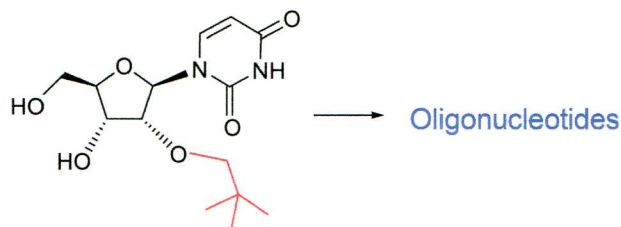


1345

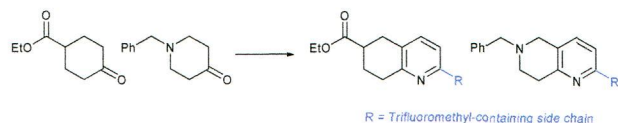
Synthesis and properties of 2'-O-neopentyl modified oligonucleotides

Gérald Mathis, Stéphane Bourg, Samia Aci-Sèche, Jean-Christophe Truffert and Ulysse Asseline*

Synthesis of 2'-O-neopentyldeoxyuridine modified oligodeoxyribonucleotides. Base-pairing with DNA and RNA was studied by absorption spectroscopy, circular dichroism and molecular dynamic simulations.



1358

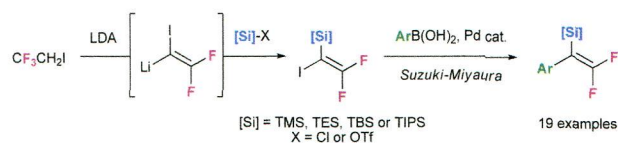


A concise one-pot synthesis of trifluoromethyl-containing 2,6-disubstituted 5,6,7,8-tetrahydroquinolines and 5,6,7,8-tetrahydronaphthyridines

Russell J. Johnson, Donogh J. R. O'Mahony,*
William T. Edwards and Matthew A. J. Duncton*

A three-step/one-pot procedure for the synthesis of the title compounds is presented. The methodology is particularly useful for installing a trifluoromethyl-group as part of a tertiary-substituent.

1367

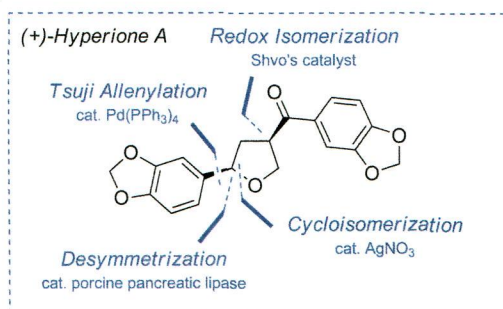


Efficient synthesis of silylated 2,2-difluorostyrene derivatives through Suzuki-Miyaura cross-coupling of 2,2-difluoro-1-iodo-1-silylethenes

Marc-Olivier Turcotte-Savard and Jean-François Paquin*

We report a new synthetic sequence for the preparation of silylated 2,2-difluorostyrene derivatives.

1376

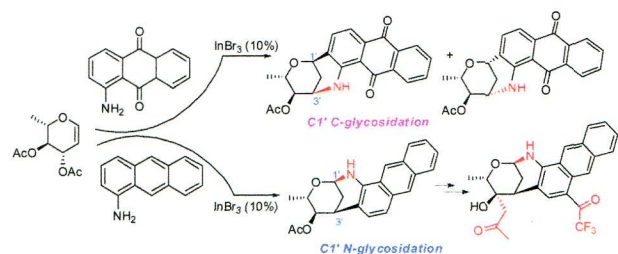


Chemoenzymatic total synthesis of hyperiones A and B

Chicco Manzuna Sapu and Jan Deska*

The first asymmetric total synthesis of hyperiones A and B based on a chemoenzymatic approach is described.

1383



Unexpected N-glycosidation reaction of glycols with 1-amino-anthracene: structure revision and application to the synthesis of new analogues of marmycin A

Xuefeng Zhang, Xiaolong Jiang, Chunyong Ding,
Qizheng Yao* and Ao Zhang*

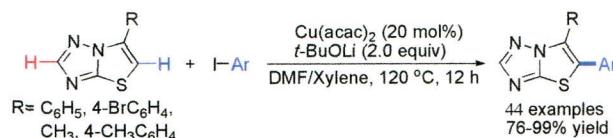
An unexpected N-glycosidation reaction of anthracen-1-amine with glycols was identified, and novel compounds bearing a quaternary carbon center were obtained as analogs of natural product marmycin A.

1390

Cu-catalyzed direct C–H bond functionalization: a regioselective protocol to 5-aryl thiazolo[3,2-*b*]-1,2,4-triazoles

Zengyang Xie, Xiaojun Zhu, Yangfan Guan, Dunru Zhu, Hongwen Hu, Chen Lin, Yi Pan, Juli Jiang* and Leyong Wang

An efficient, regioselective C-5 arylation of thiazolo[3,2-*b*]-1,2,4-triazoles catalyzed by a simple copper catalyst was developed. This arylation proceeded smoothly and tolerated a variety of functional groups (44 examples).

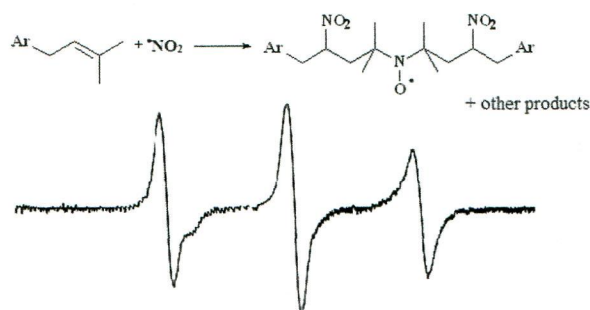


1399

Reactions of nitric oxide and nitrogen dioxide with coenzyme Q: involvement of the isoprenic chain

Paola Astolfi,* Laurence Charles, Didier Gimes, Lucedio Greci, Corrado Rizzoli, Federico Sorana and Pierluigi Stipa

A di-*tert*-alkyl nitroxide is formed when coenzymes CoQ react with nitrogen dioxide ($\cdot\text{NO}_2$) after $\cdot\text{NO}_2$ addition to the isoprenic chain of the coenzymes.

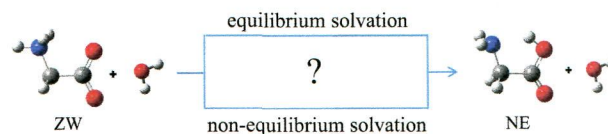


1407

Comprehensive studies on the tautomerization of glycine: a theoretical study

Chang Kon Kim, Byung-Ho Park, Hai Whang Lee and Chan Kyung Kim*

The tautomerization process of glycine between the zwitterionic (ZW) and neutral (NE) forms in aqueous solution was explained using the non-equilibrium solvation models in the CPCM calculations.



1414

Theoretical study of the proton transfer wires influence on the one- and two-photon absorption properties of green fluorescent protein chromophore

Min-Yi Zhang, Can Xu, Chen-Sheng Lin, Xiangfeng Guan and Wen-Dan Cheng*

The H-bonding complex of intermediate state of GFP is crucial for the TPA properties of GFP.

