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Organic & Biomolecular Chemistry **Cover** See Yan-Song Zheng *et al.,* pp. 729–735.

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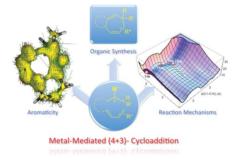
EMERGING AREA

699

Transition metal-catalysed (4 + 3) cycloaddition reactions involving allyl cations

Israel Fernández* and José Luis Mascareñas

In this emerging area article, we focus on the synthetic applications and reaction mechanisms of novel intramolecular transition metal catalysed (4 + 3)-cycloaddition reactions of allenedienes.



COMMUNICATIONS

705

Fluoride-selective optical sensor based on the dipyrrolyl-tetrathiafulvalene chromophore

Shadi Rivadehi, Ellen F. Reid, Conor F. Hogan, Sheshanath V. Bhosale and Steven J. Langford*

A chemosensor bearing dipyrrolyl motifs as recognition sites and a tetrathiafulvalene redox tag has been evaluated as an optical and redox sensor for a series of anions (F^- , $H_2PO_4^-$, CH_3COO^- , Cl^- , Br and HSO_4^-) in DCM solution.



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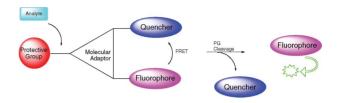
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A simple FRET-based modular design for diagnostic probes

Orit Redy, Einat Kisin-Finfer, Eran Sella and Doron Shabat*

Self-immolative dendritic adaptors were applied to the preparation of modular FRET-based molecular probes for detection of various analytes of interest.



716

Is nevirapine atropisomeric? Experimental and computational evidence for rapid conformational inversion

Edmund W. D. Burke, Gareth A. Morris, Mark A. Vincent, Ian H. Hillier and Jonathan Clayden*

We report the results of an NMR and computational study which reveal that while the non-nucleoside reverse transcriptase inhibitor nevirapine possesses two stable enantiomeric conformations, they interconvert with a barrier of about 76 kJ mol⁻¹ at room temperature. Nevirapine has a half life for enantiomerisation at room temperature of the order of seconds and is not atropisomeric.

720

Calixarene-induced aggregation of perylene bisimides

Dong-Sheng Guo, Bang-Ping Jiang, Xiang Wang and Yu Liu*

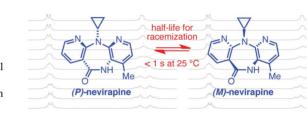
The complex-induced aggregation of perylene bisimides by *p*-sulfonatocalix[*n*]arenes was studied, where the aggregation stability, aggregation distance, as well as the degree of order of aggregation were all improved.

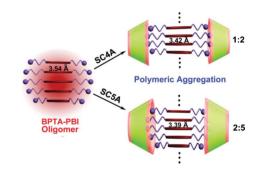
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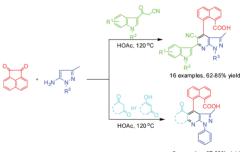
Multicomponent approaches to 8-carboxylnaphthylfunctionalized pyrazolo[3,4-b]pyridine derivatives

Yan Hao, Xiao-Ping Xu,* Tao Chen, Li-Li Zhao and Shun-Jun Ji*

A simple and novel protocol for the efficient synthesis of a series of 8-carboxylnaphthyl-functionalized pyrazolo[3,4-*b*]pyridine derivatives was developed through a one-pot, three-component reaction involving acenaphthylene-1,2-dione and 1*H*-pyrazol-5-amines in acetic acid medium. A possible reaction mechanism was proposed.







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729

Effect of carboxylic acid on micelles of a neutral amphiphilic dendro-calix[4]arene

Hong Huang, Dong-Mi Li, Weizhou Wang, Yi-Chang Chen, Khalid Khan, Song Song and Yan-Song Zheng*

Micelles formed from a neutral amphiphilic dendro-calix[4]arene could be changed from solid to hollow or to linear ones through encapsulation of carboxylic acid in the cavity of the calixarene.

736

Cyclopropane-based stereochemical diversity-oriented conformational restriction strategy: Histamine H_3 and/or H_4 receptor ligands with the 2,3-methanobutane backbone

Mizuki Watanabe, Takaaki Kobayashi, Takatsugu Hirokawa, Akira Yoshida, Yoshihiko Ito, Shizuo Yamada, Naoki Orimoto, Yasundo Yamasaki, Mitsuhiro Arisawa and Satoshi Shuto*

Conformationally restricted histamine analogs with a 2,3-methanobutane backbone were designed, synthesized and evaluated as the histamine H_3/H_4 receptor ligands.

746

Synthesis and biological activity of phosphonoacetate- and thiophosphonoacetate-modified 2'-*O*-methyl oligoribonucleotides

Richard N. Threlfall, Adrian G. Torres, Angelika Krivenko, Michael J. Gait and Marvin H. Caruthers*

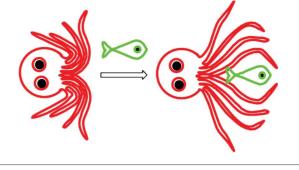
2'-O-Me oligoribonulceotides (ORNs) modified with phosphonoacetate and thiophosphonoacetate internucleotide linkages have been synthesised. Thiophosphonoacetate modifications greatly improve the efficiency of cell uptake and the potency of a 2'-O-Me-ORN miRNA122 inhibitor.

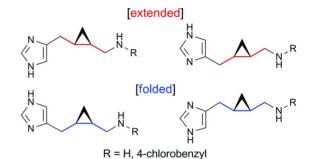
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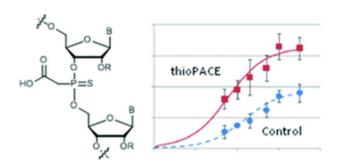
The DNA three-way junction as a mould for tripartite chromophore assembly

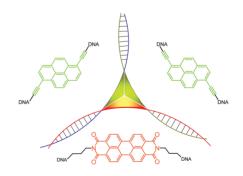
Markus Probst, Daniel Wenger, Sarah M. Biner and Robert Häner*

The arrangement of different chromophoric building blocks at the branch point of a DNA three-way junction results in characteristic spectroscopic properties.

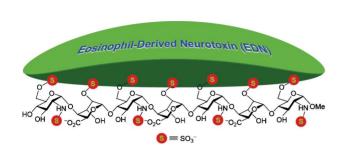


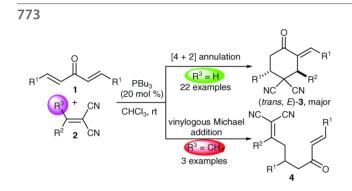






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Synthesis of heparin oligosaccharides and their interaction with eosinophil-derived neurotoxin

Shang-Cheng Hung,* Xin-An Lu, Jinq-Chyi Lee, Margaret Dah-Tsyr Chang,* Shun-lung Fang, Tan-chi Fan, Medel Manuel L. Zulueta and Yong-Qing Zhong

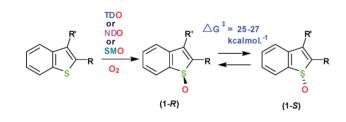
Heparin tri-, penta- and heptasaccharides were concisely synthesized and the latter strongly interfered with EDN binding to the cell surface.

Phosphine-catalyzed [4 + 2] annulation and vinylogous addition reactions between 1,4-dien-3-ones and 1,1-dicyanoalkenes

Rong Zhou, Jianfang Wang, Junjun Tian and Zhengjie He*

Two kinds of highly chemoselective phosphine-catalyzed cross-couplings between 1,4-dien-3-ones and 1,1-dicyanoalkenes are presented.

782



Bacterial dioxygenase- and monooxygenase-catalysed sulfoxidation of benzo[b]thiophenes

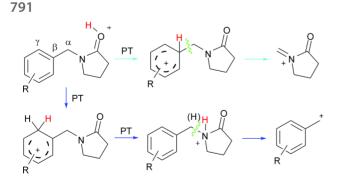
Derek R. Boyd,* Narain D. Sharma, Brian McMurray, Simon A. Haughey, Christopher C. R. Allen, John T. G. Hamilton, W. Colin McRoberts, Rory A. More O'Ferrall, Jasmina Nikodinovic-Runic, Lydie A. Coulombel and Kevin E. O'Connor*

Dioxygenase- and monooxygenase-catalysed sulfoxidation of benzo[*b*]thiophenes can yield enantioenriched chiral benzo[*b*]thiophene sulfoxides which racemize spontaneously.

$C^{\alpha}-C^{\beta}$ and $C^{\alpha}-N$ bond cleavage in the dissociation of protonated *N*-benzyllactams: dissociative proton transfer and intramolecular proton-transport catalysis

Yunfeng Chai, Cheng Guo, Kezhi Jiang, Yuanjiang Pan* and Cuirong Sun*

Intramolecular dissociative proton transfers, from oxygen to C^{β} directly or from oxygen to nitrogen stepwise, lead to bond cleavages on the two sides of C^{α} , respectively.



798

Synthesis and antidepressant-like activity of selenophenes obtained *via* iron(III)–PhSeSePh-mediated cyclization of *Z*-selenoenynes

Bibiana M. Gai, André L. Stein, Juliano A. Roehrs, Filipe N. Bilheri, Cristina W. Nogueira and Gilson Zeni*

We present the antidepressant-like action of

2,5-disubstituted-3-(organoseleno)selenophenes prepared by a novel synthetic route, the intramolecular cyclization of (Z)-chalcogenoenynes.

808

Pd nanoparticle catalysed one-pot sequential Heck and Suzuki couplings of bromo-chloroarenes in ionic liquids and water

Pietro Cotugno, Antonio Monopoli,* Francesco Ciminale, Nicola Cioffi and Angelo Nacci*

Pd nanoparticles in green reaction media (*viz*. ionic liquids and water) catalyze the one-pot sequential Heck and Suzuki coupling of bromo-chloroarenes to afford unsymmetrically substituted arenes.

814

Hydrogen bond donating ability of *meta* and *para* hydroxy phenoxyl radicals

Riccardo Amorati* and Gian Franco Pedulli

The ability of protonated semiquinones to donate hydrogen bonds to various acceptors has been investigated by EPR spectroscopy and DFT calculations.



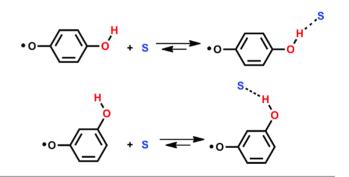
Fusaroside, a unique glycolipid from *Fusarium* sp., an endophytic fungus isolated from *Melia azedarach*

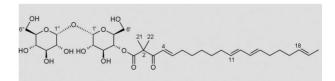
Sheng-Xiang Yang, Hong-Peng Wang, Jin-Ming Gao,* Qiang Zhang, Hartmut Laatsch* and Yi Kuang

Fusaroside (1), a unique trehalose-containing glycolipid, was produced by an endophytic fungus *Fusarium* sp. isolated from *Melia azedarach* L. The structure of fusaroside (1) was determined by spectroscopic data and chemical degradation.









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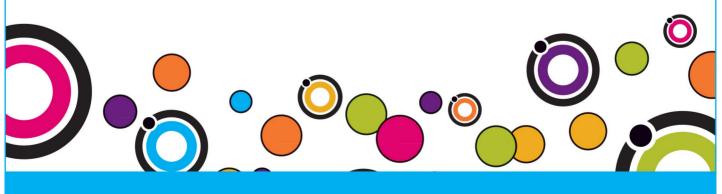
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LAUNCHED

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A formal [3+3]-annulation-based approach to pancratistatins: total synthesis of (\pm) -7-deoxy-pancratistatin and its 2-*epi* and 2,4-di*epi* analogues

Olaia Nieto-García, Hugo Lago-Santomé, Fernando Cagide-Fagín, Juan Carlos Ortiz-Lara and Ricardo Alonso*

(\pm)-7-Deoxy-pancratistatin and its 2-*epi*- and 2,4-di*epi*- analogues are prepared from a total of four commercially-available fragments.

835

C–H functionalization of tertiary amines by cross dehydrogenative coupling reactions: solvent-free synthesis of α-aminonitriles and β-nitroamines under aerobic condition

Kaliyamoorthy Alagiri and Kandikere Ramaiah Prabhu*

Environmentally benign CDC reactions to accomplish α -aminonitriles and β -nitroamines are developed using aerobic conditions under solvent-free conditions.

843

Syntheses of furo[3,4-c]coumarins and related furyl coumarin derivatives *via* intramolecular Wittig reactions

Yeong-Jiunn Jang, Siang-en Syu, Yu-Jhang Chen, Mei-Chun Yang and Wenwei Lin*

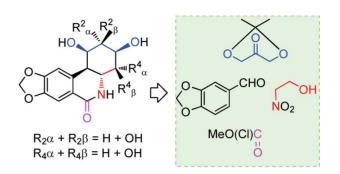
Novel preparation of polysubstituted furo[3,4-*c*]coumarins and related furocoumarin derivatives, starting from the Michael acceptors, tributylphosphine, and acyl chlorides, is realized.

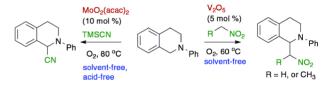
848

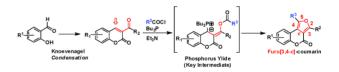
N-Heterocyclic carbene catalysed aerobic oxidation of aromatic aldehydes to aryl esters using boronic acids

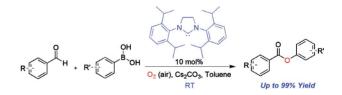
Panjab Arde, B. T. Ramanjaneyulu, Virsinha Reddy, Apurv Saxena and R. Vijaya Anand*

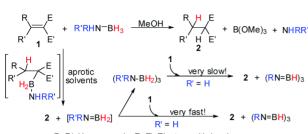
A mild protocol for the aerobic oxidation of aromatic aldehydes to the corresponding aryl esters with boronic acids using *N*-heterocyclic carbene as a catalyst is described.













861 NHCb NHCb

ribbon β-sheet-like



Xianghua Yang, Thomas Fox and Heinz Berke*

Synthetic and mechanistic studies of metal-free transfer hydrogenations applying polarized olefins as hydrogen

acceptors and amine borane adducts as hydrogen donors

Metal-free transfer hydrogenation of polarized olefins were studied

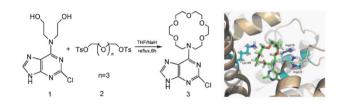
using amine borane adducts (RR'NH-BH₃) as hydrogen donors.

Designing hybrid foldamers: the effect on the peptide conformational bias of β - versus α - and γ -linear residues in alternation with (1R,2S)-2-aminocyclo-butane-1-carboxylic acid

Sergio Celis, Esther Gorrea, Pau Nolis, Ona Illa and Rosa M. Ortuño*

Conformational bias can be tuned from ribbon-type structures to β-sheet-like and helical motifs by intercalating suitable linear segments between cis-cyclobutane residues.

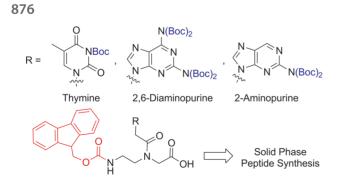
869



Synthesis of N-(2-chloro purin-6-yl) aza-18-crown-6 and its interaction with human serum albumin

Cui Li, Fengling Cui,* Runze Mao, Ruina Huo and Guirong Qu

The novel purine nucleosides-linked azacrown ether in the C6 position was synthesized. This new nucleoside analogue can be prepared from a series of N9-modified nucleosides. The N-(2-chloro purin-6-vl) aza-18-crown-6 can bind to human serum albumin through hydrophobic forces.



Synthesis and oligomerization of Fmoc/Boc-protected PNA monomers of 2,6-diaminopurine, 2-aminopurine and thymine

André H. St. Amant and Robert H. E. Hudson*

The synthesis and oligomerization of Fmoc/Boc protected PNA monomers is described for 2,6-diaminopurine, 2-aminopurine, and thymine. The mismatch discrimination and fluorescence properties of the PNA were examined.

882

Atropisomerism of a monosubstituted perfluoro[2.2]paracyclophane. A combined synthetic, kinetic, spectroscopic and computational study

Ion Ghiviriga, Henry Martinez, Christian Kuhn, Lianhao Zhang and William R. Dolbier, Jr.*

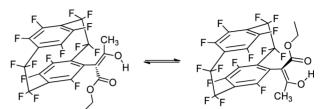
The product of S_NAr addition of ethyl acetoacetate to perfluoro[2.2]paracyclophane produces an enol tautomer which exhibits two NMR signals for its enolic proton, shown to derive from the presence of two atropisomers.

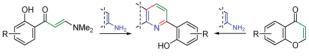
890

2,3-Unsubstituted chromones and their enaminone precursors as versatile reagents for the synthesis of fused pyridines

Viktor O. Iaroshenko,* Satenik Mkrtchyan, Ashot Gevorgyan, Mariia Miliutina, Alexander Villinger, Dmytro Volochnyuk, Vyacheslav Ya. Sosnovskikh and Peter Langer*

A divergent and regioselective approach to fused pyridines was developed through formal [3 + 3] cyclocondensations from simple 2,3-unsubstituted chromones or their enaminone precursors.





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