Organic & Biomolecular Chemistry

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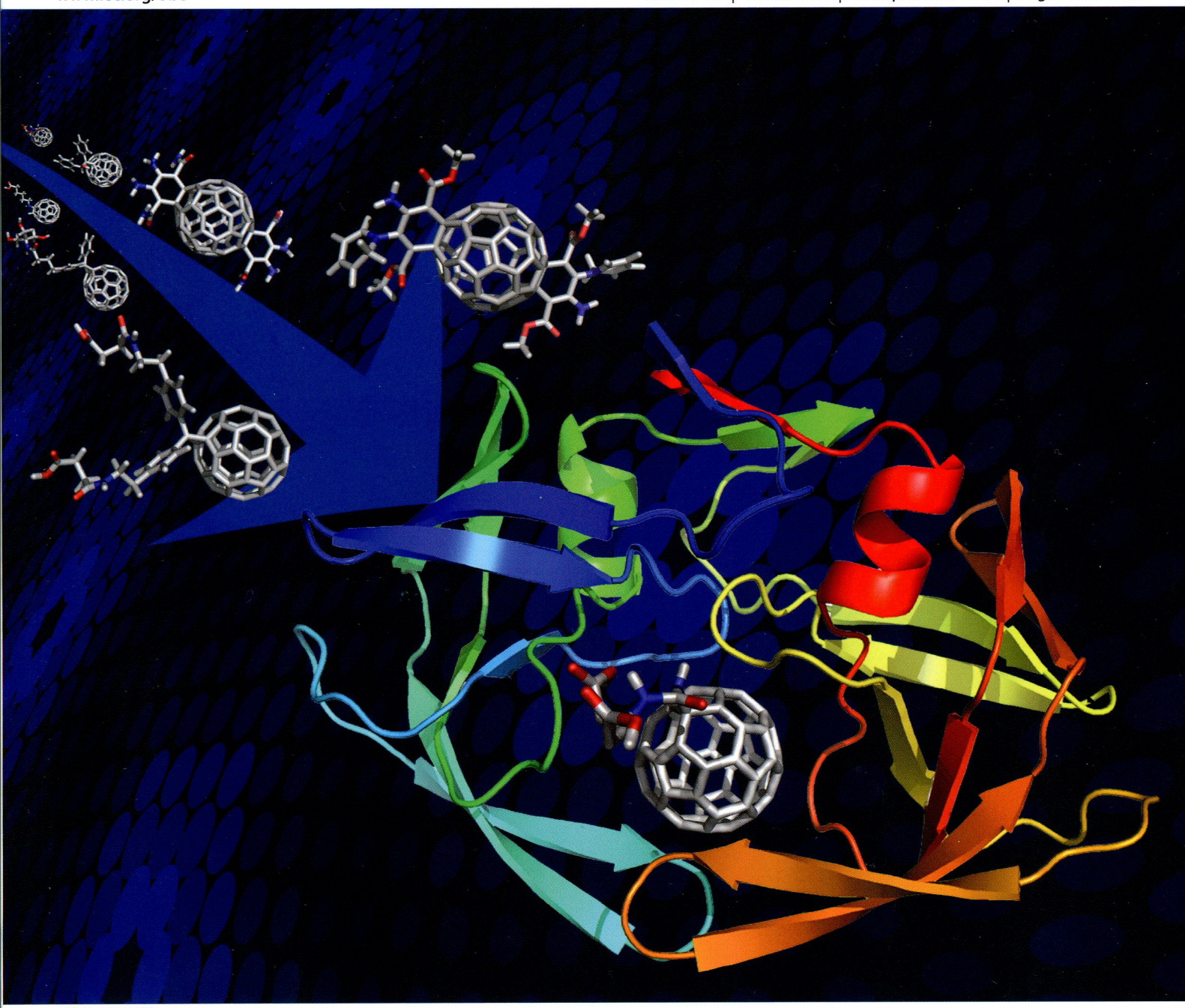
Volume 11 | Number 35 | 21 September 2013 | Pages 5737–5964



ISSN 1477-0520

PAPER

Bakhtiyor Rasulev *et al.*

Receptor- and ligand-based study of fullerene analogues: comprehensive computational approach including quantum-chemical, QSAR and molecular docking simulations

RSC Publishing

1477-0520(2013)11:35;1-5

Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry

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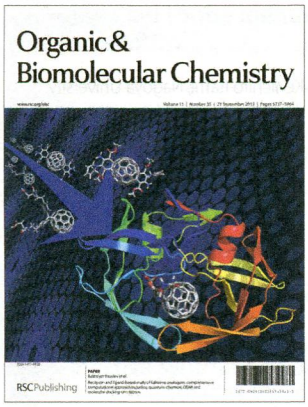
ISSN 1477-0520 CODEN OBCRAK 11(35) 5737–5964 (2013)



Cover
See Bakhtiyor Rasulev *et al.*, pp. 5798–5808.

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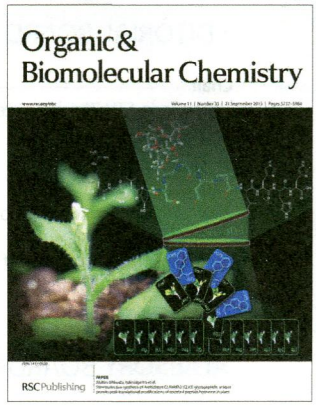

Inside cover
See Akihiro Ishiwata, Yukishige Ito *et al.*, pp. 5892–5907.

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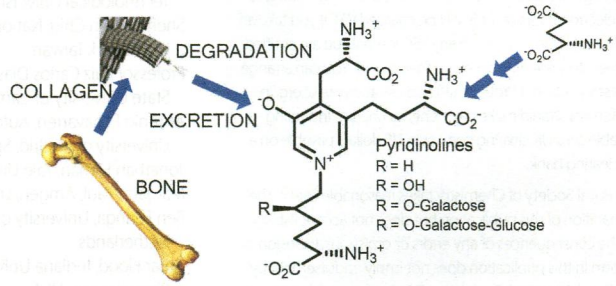
PERSPECTIVES

5747

Chemical structure, biosynthesis and synthesis of free and glycosylated pyridinolines formed by cross-link of bone and synovium collagen

Luigi Anastasia, Paola Rota, Mario Anastasia and Pietro Allevi*

Syntheses of free and glycosylated pyridinolines have been reviewed drawing support for a better rationalization of their biological origin.

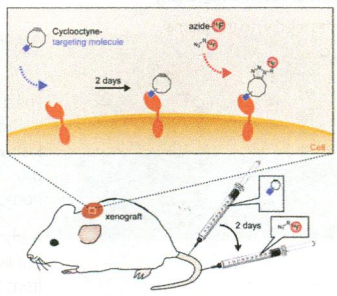


5772

Bioorthogonal chemistry for pre-targeted molecular imaging – progress and prospects

Laurence Carroll,* Helen L. Evans, Eric O. Aboagye and Alan C. Spivey

The aim of this perspective is to critically review the three most prominent bioorthogonal reactions that are used presently, on both a purely chemical level and in the context of biological systems.

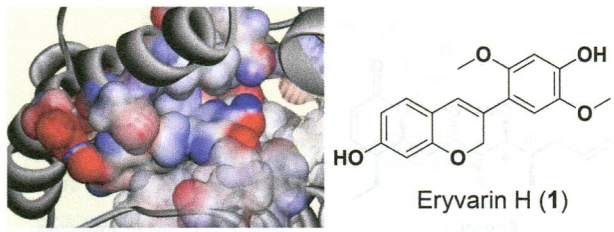


5782

Total synthesis of eryvarin H and its derivatives and their biological activity as ERRγ inverse agonist

Ja Young Koo, Sangmi Oh, Seung-Rye Cho, Minseob Koh, Won-Keun Oh, Hueng-Sik Choi* and Seung Bum Park*

A docking study and total synthesis of eryvarin H and its derivatives led to the identification of a potential inverse agonist of ERRγ.

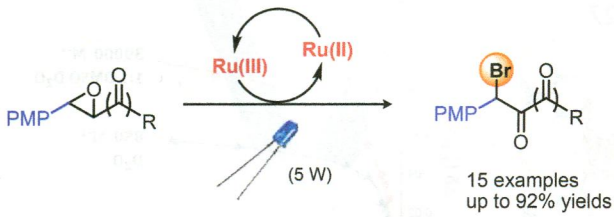


5787

Visible light-mediated oxidative quenching reaction to electron-rich epoxides: highly regioselective synthesis of α-bromo (di)ketones and mechanism study

Lin Guo, Chao Yang, Lewei Zheng and Wujiong Xia*

A novel and simple procedure was developed for the regioselective synthesis of α-bromo (di)ketones from electron-rich epoxides *via* visible light photoredox catalysis.

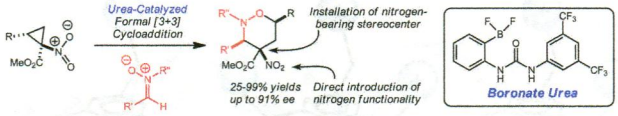


5793

Urea-catalyzed construction of oxazinanes

Andrea M. Hardman, Sonia S. So and Anita E. Mattson*

Highly functionalized oxazinanes are efficiently prepared through urea-catalyzed formal [3 + 3] cycloaddition reactions of nitrones and nitrocyclopropane carboxylates.

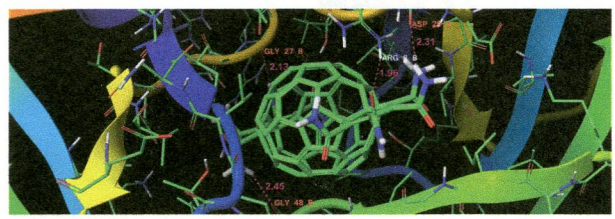


5798

Receptor- and ligand-based study of fullerene analogues: comprehensive computational approach including quantum-chemical, QSAR and molecular docking simulations

Lucky Ahmed, Bakhtiyor Rasulev,* Malakhat Turabekova, Danuta Leszczynska and Jerzy Leszczynski

A combination of comprehensive computational approaches revealed structural features responsible for fullerene derivatives anti-HIV activity.



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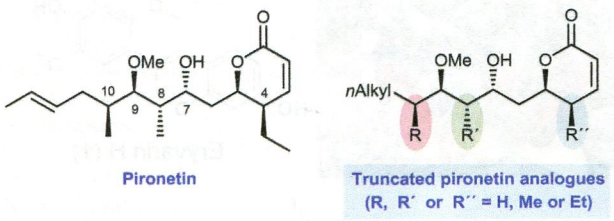
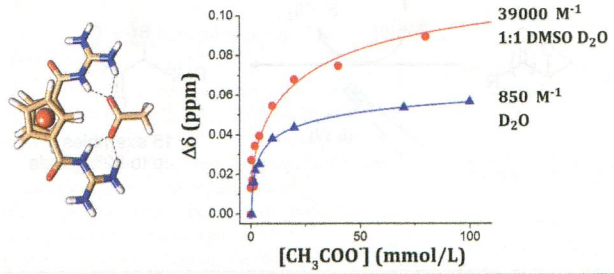


Synthesis and biological evaluation of truncated α-tubulin-binding pironetin analogues lacking alkyl pendants in the side chain or the dihydropyrone ring

J. Paños, S. Díaz-Oltra, M. Sánchez-Peris, J. García-Pla, J. Murga,* E. Falomir, M. Carda, M. Redondo-Horcajo, J. F. Díaz,* I. Barasoain* and J. A. Marco*

The stereoselective syntheses and the biological evaluation of several truncated pironetin analogues (some of the alkyl residues at C4, C-8 and C-10 are absent) are discussed. As the parent compound, these analogues are also cytotoxic and share the same mechanism of action.

5827

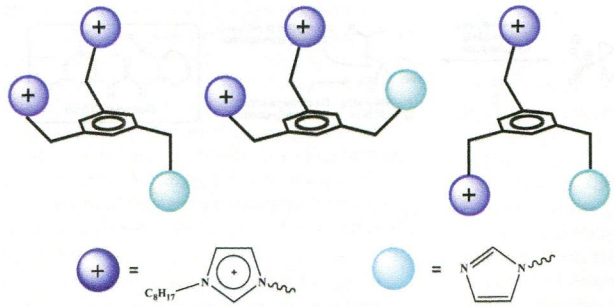


Pincher ferrocene-derived cation carboxylate ion pairs in aqueous DMSO

Christie L. Beck, Stephen A. Berg and Arthur H. Winter*

Pincher ferrocene-derived (bis)guanidinium (di)cations form complexes with monocarboxylates in competitive solvents (H_2O–DMSO).

5836

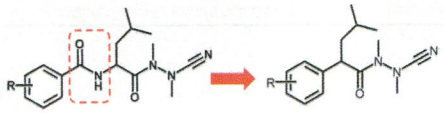


Solution and thermal behaviour of novel dicationic imidazolium ionic liquids

Francesca D'Anna,* H. Q. Nimal Gunaratne, Giuseppe Lazzara, Renato Noto,* Carla Rizzo and Kenneth R. Seddon

A new class of dicationic imidazolium ionic liquids shows the presence of different conformational isomers. Their thermal behaviour was analysed and it was observed that it is influenced by the different nature of the anion.

5847



Selectivity \ Nos.	13	13′
Cat L/K	10	320
Cat S/K	1061	1784
Cat B/K	1016	8566

Highly selective aza-nitrile inhibitors for cathepsin K, structural optimization and molecular modeling

Xiao-Yu Yuan, Ding-Yi Fu, Xing-Feng Ren, Xuexun Fang, Lincong Wang, Shuxue Zou and Yuqing Wu*

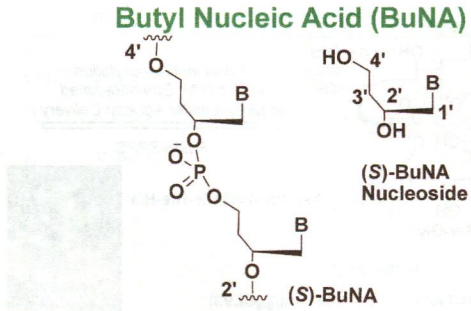
A series of selective cathepsin K inhibitors without a P2–P3 amide linker were prepared. Compound **13′** showed largely improved and best selectivity profiles against cathepsins B and S, especially toward its highly homologic cathepsin L.

5853

Design, synthesis, biophysical and primer extension studies of novel acyclic butyl nucleic acid (BuNA)

Vipin Kumar, Kiran R. Gore, P. I. Pradeepkumar and Venkitasamy Kesavan*

Synthesis and biophysical studies of novel artificial nucleic acids and the incorporation of these acyclic nucleotides in DNA strands were investigated.

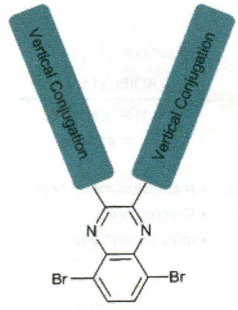


5866

Quinoxaline derivatives with broadened absorption patterns

Lidia Marin, Laurence Lutsen, Dirk Vanderzande and Wouter Maes*

A series of quinoxaline-based materials with improved light-harvesting features has been synthesized by extending the conjugation within the solubilizing side chains.

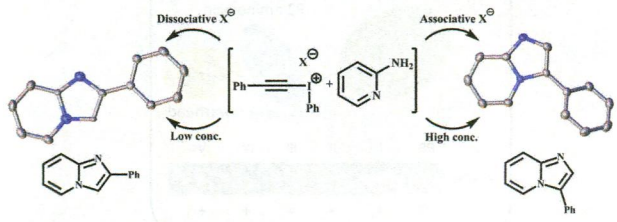


5877

Unprecedented regiochemical control in the formation of aryl[1,2-*a*]imidazopyridines from alkynyliodonium salts: mechanistic insights

Luke I. Dixon, Michael A. Carroll,* Thomas J. Gregson, George J. Ellames, Ross W. Harrington and William Clegg

Both the concentration of the alkynyliodonium salt and the choice of counter-ion have been shown to influence the regioselectivity of aryl[1,2-*a*]imidazopyridine formation.

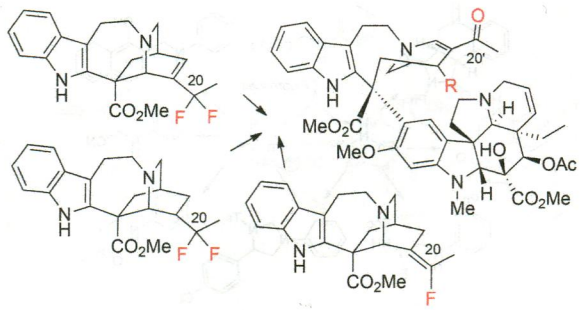


5885

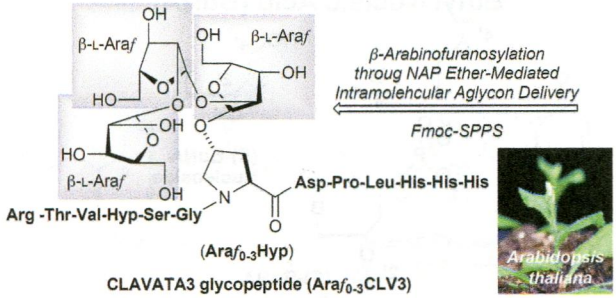
Synthesis of fluorinated catharanthine analogues and investigation of their biomimetic coupling with vindoline

Emerson Giovanelli, Lionel Moisan, Sébastien Comesse, Sébastien Leroux, Bernard Rousseau, Paul Hellier, Marc Nicolas and Eric Doris*

20,20-Difluorocatharanthine and congeners were investigated as potential precursors to dimeric *Vinca* alkaloids of the vinflunine family.



5892

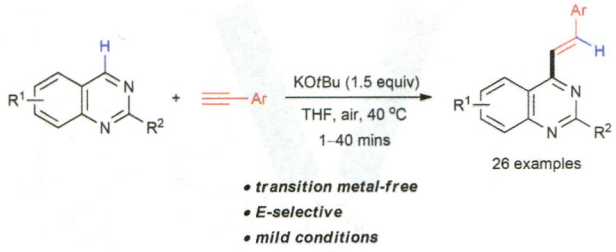


Stereoselective synthesis of *Arabidopsis* CLAVATA3 (CLV3) glycopeptide, unique protein post-translational modifications of secreted peptide hormone in plant

Sophon Kaeothip, Akihiro Ishiwata* and Yukishige Ito*

The synthesis of CLAVATA3 glycopeptide with all glycoforms (Araf$_{0-3}$CLV3) of *A. thaliana* plants has been achieved through highly stereoselective β-arabinofuranosylation of Hyp derivatives by NAP ether-mediated IAD, and Fmoc-solid phase peptide synthesis.

5908

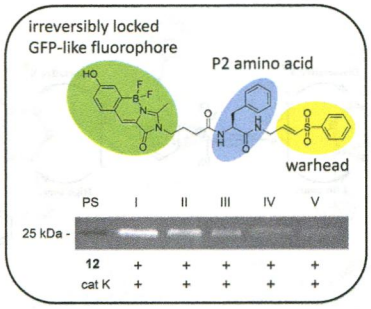


KO*t*Bu-mediated stereoselective addition of quinazolines to alkynes under mild conditions

Dan Zhao, Qi Shen, Yu-Ren Zhou and Jian-Xin Li*

A facile alkenylation of quinazolines with terminal alkynes mediated by KO*t*Bu has been achieved. The reaction is carried out under very mild conditions and shows a high stereoselectivity.

5913

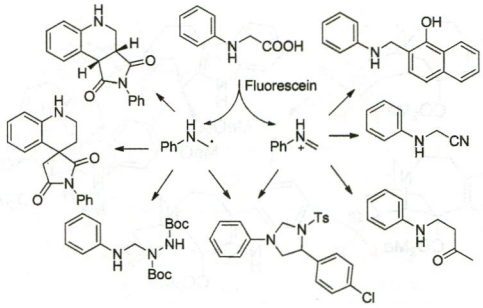


Chemical introduction of the green fluorescence: imaging of cysteine cathepsins by an irreversibly locked GFP fluorophore

Maxim Frizler, Ilia V. Yampolsky, Mikhail S. Baranov, Marit Stirnberg and Michael Gütschow*

An activity-based probe to chemically introduce green fluorescence was developed for *ex vivo* imaging of human cysteine cathepsins.

5922



Amphiphilic methyleneamino synthon through organic dye catalyzed-decarboxylative aminoalkylation

Li Chen, Chin Sheng Chao, Yuanhang Pan, Sheng Dong, Yew Chin Teo, Jian Wang* and Choon-Hong Tan*

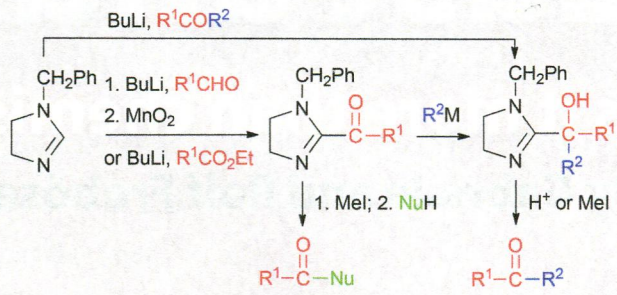
A photo-induced synthon which could be coupled with either a radical or a nucleophile in a simple operation.

5926

Coenzyme-inspired chemistry 2: 4,5-dihydroimidazolium ylides (NHCs) and the reactions of 2-(1-hydroxyalkyl)-4,5-dihydroimidazoles

Raymond C. F. Jones* and John R. Nichols

Adducts of 2-lithio-4,5-dihydroimidazoles with carbonyl compounds fragment by loss of an NHC in C–C bond formation/cleavage processes inspired by thiamine.

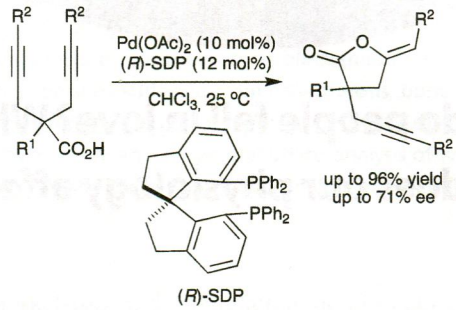


5936

Pd(II)–SDP-catalyzed enantioselective 5-*exo-dig* cyclization of γ-alkynoic acids: application to the synthesis of functionalized dihydofuran-2(3*H*)-ones containing a chiral quaternary carbon center

Vellaisamy Sridharan,* Lulu Fan, Shinobu Takizawa, Takeyuki Suzuki and Hiroaki Sasai*

The Pd(II)–SDP-catalyzed enantioselective intramolecular 5-*exo-dig* cyclization of α,α-disubstituted γ-alkynoic acids afforded dihydrofuran-2(3*H*)-ones in excellent yields with enantioselectivities up to 71%.

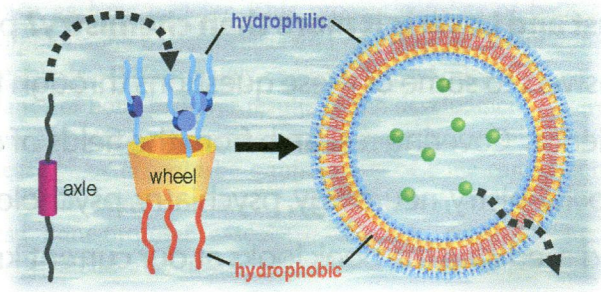


5944

Hierarchical self-assembly of amphiphilic calix[6]-arene wheels and viologen axles in water

Rocco Bussolati, Pasquale Carrieri, Andrea Secchi, Arturo Arduini,* Alberto Credi, Monica Semeraro, Margherita Venturi, Serena Silvi,* Diana Velluto, Romina Zappacosta and Antonella Fontana*

Amphiphilic calix[6]arenes self-assemble in water to generate micelles or vesicles; the formation of pseudorotaxanes with viologens increases the vesicles permeability, triggering the release of their content.



5954

Pd-catalyzed reaction of aryl halides and propargyl furylmethyl ethers: a novel pathway to functionalized dihydroisobenzofurans

Lingzhu Chen, Ruwei Shen, Luling Wu* and Xian Huang

An interesting sequential reaction has been realized, providing a facile method for the synthesis of functionalized dihydroisobenzofurans with a decent diastereoselectivity.