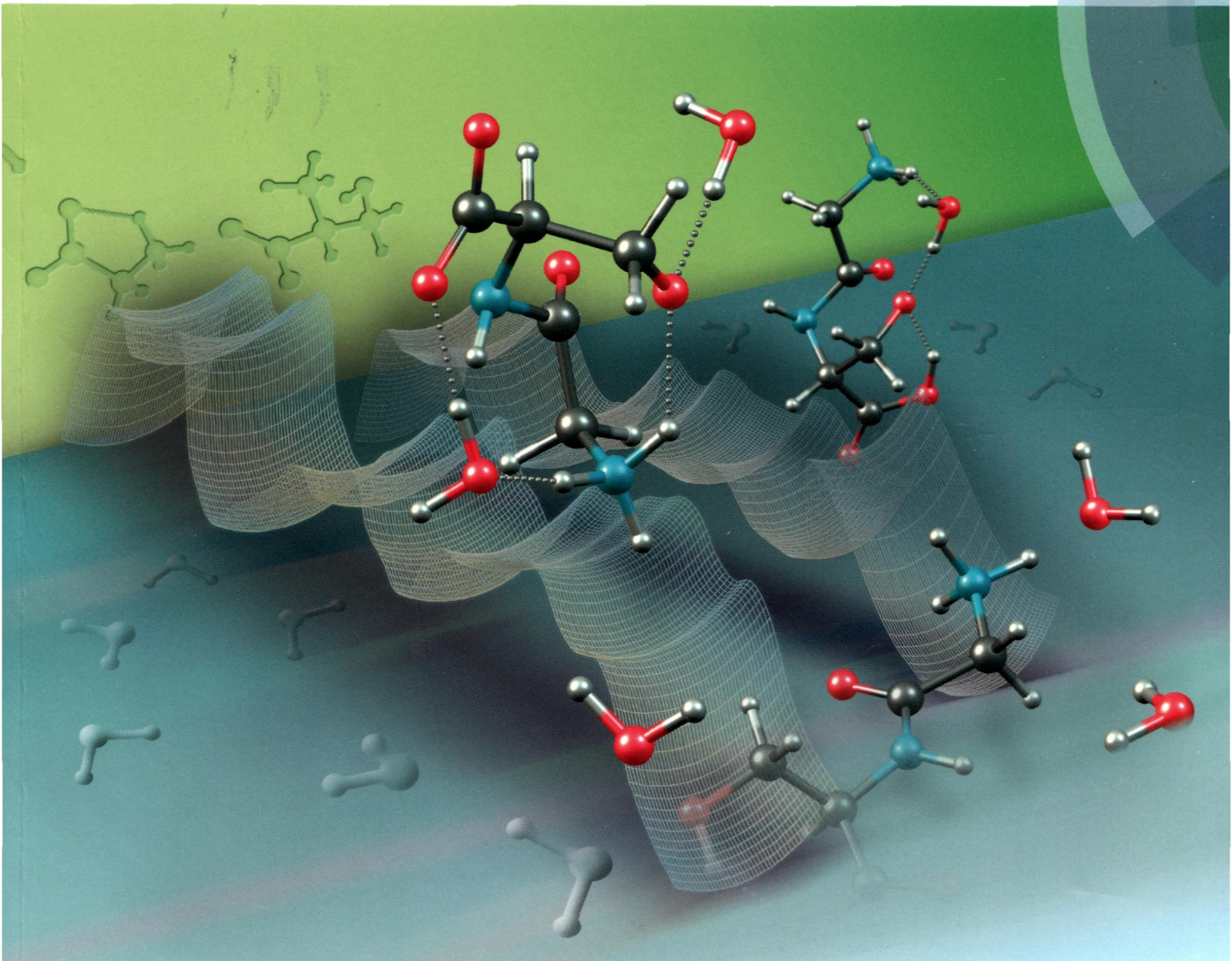
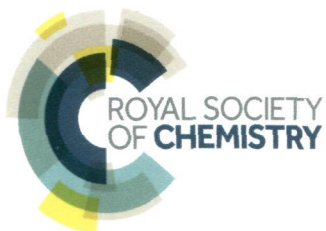


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PAPER

Tzvetan T. Mihaylov *et al.*

A computational study of the glycerol hydrolysis at physiological pH: a zwitterionic versus anionic mechanism

Organic & Biomolecular Chemistry

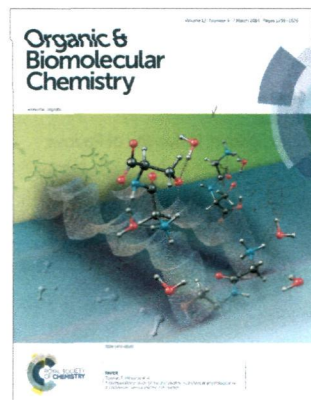
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Cover

See Tzvetan T. Mihaylov *et al.*, pp. 1395–1404.

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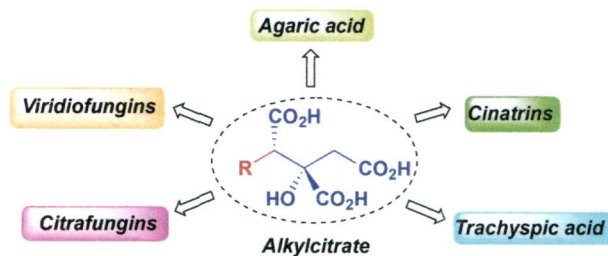
REVIEW

1367

Total synthesis of alkyl citrate natural products

Mark A. Rizzacasa* and Dayna Sturgess

This review highlights the synthesis of members of the alkyl citrate family of natural products. The focus is on the stereoselective construction of the alkyl citrate moiety common to these compounds.



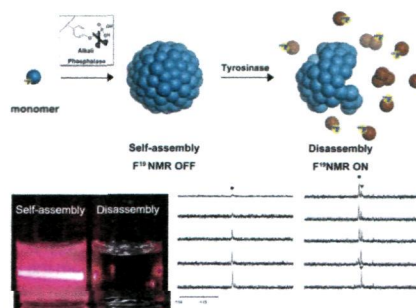
COMMUNICATIONS

1393

Enzyme-controllable F-NMR turn on through disassembly of peptide-based nanospheres for enzyme detection

Jie Gao, Yang Shi, Youzhi Wang, Yanbin Cai, Jie Shen,* Deling Kong and Zhimou Yang*

The enzyme tyrosinase could trigger the disassembly of peptide-based nanospheres, resulting in F-NMR signal turning on.

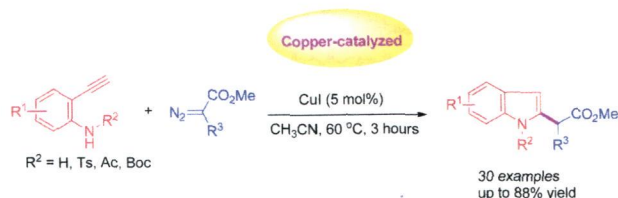


1387

Copper-catalyzed annulation of α -substituted diazoacetates with 2-ethynylanilines: the direct synthesis of C2-functionalized indoles

Gang Liu, Guangyang Xu, Jian Li, Dong Ding and Jiangtao Sun*

Copper-catalyzed direct annulation of α -substituted diazoacetates with 2-ethynylanilines leading to C2-functionalized indoles was achieved under mild reaction conditions. The C2-(carboxylate methyl) substituted indoles were obtained in moderate to high yields.

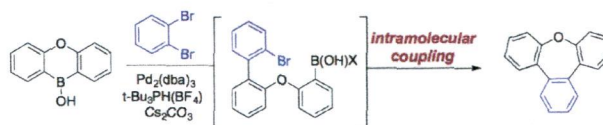


1391

Synthesis of benzannulated heterocycles by twofold Suzuki–Miyaura couplings of cyclic diarylboronic acids

Elena Dimitrijević, Madeline Cusimano and Mark S. Taylor*

Successive transmetalations of the two C–B bonds of cyclic boronic acids enable a novel synthesis of benzo-fused heterocycles from readily available precursors.



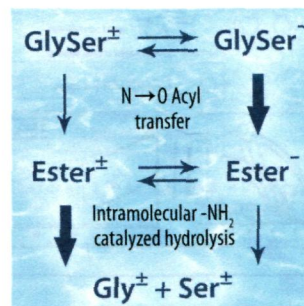
PAPERS

1395

A computational study of the glycyserine hydrolysis at physiological pH: a zwitterionic versus anionic mechanism

Tzvetan T. Mihaylov,* Tatjana N. Parac-Vogt and Kristine Pierloot

The hydrolysis of GlySer at physiological pH was investigated by modeling the most feasible reaction mechanisms in aqueous phase at the MP2/6-311+(2df,2p)//SMD-M06/6-311+(2df,2p) level of the theory.

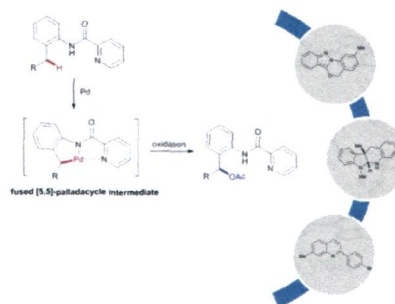


1405

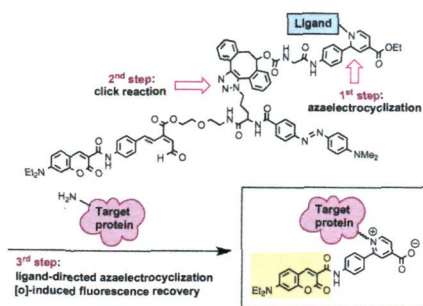
Palladium catalyzed acetoxylation of benzylic C–H bonds using a bidentate picolinamide directing group

Tao Cheng, Weiyu Yin, Yi Zhang, Yingnan Zhang and Yong Huang*

Palladium catalyzed oxygenation of inert benzylic C–H bonds offers a straightforward entry to heterocycle synthesis.



1412

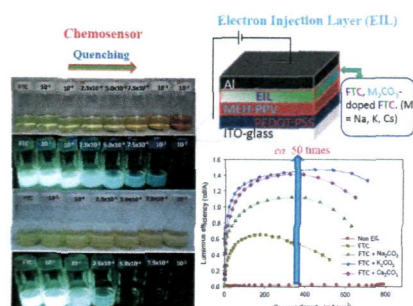


A cascading reaction sequence involving ligand-directed azaelectrocyclization and autooxidation-induced fluorescence recovery enables visualization of target proteins on the surfaces of live cells

Katsunori Tanaka,* Masataka Kitadani, Ayumi Tsutsui, Ambara R. Pradipta, Rie Imamaki, Shinobu Kitazume, Naoyuki Taniguchi and Koichi Fukase*

A general probe designed to induce a cascading sequence of reactions on a target protein was efficiently synthesized.

1419

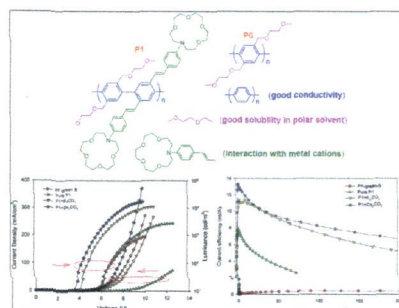


A fluorene-based material containing triple azacrown ether groups: synthesis, characterization and application in chemosensors and electroluminescent devices

Chia-Shing Wu, Ying-Ju Lin and Yun Chen*

A novel fluorene-based FTC containing triple azacrown ether groups is applied as a chemical sensor and as an electron injection layer simultaneously.

1430



Water/alcohol soluble electron injection material containing azacrown ether groups: synthesis, characterization and application to enhancement of electroluminescence

Chia-Shing Wu, Huai-An Lu, Chiao-Pei Chen, Tzung-Fang Guo and Yun Chen*

A copoly(*p*-phenylene) containing pendant azacrown ether and ethylene glycol ether groups was prepared as a highly efficient electron injection layer for PLEDs.

1440



Measurement of supramolecular effective molarities for intramolecular H-bonds in zinc porphyrin-imidazole complexes

Michael A. Jinks, Hongmei Sun and Christopher A. Hunter*

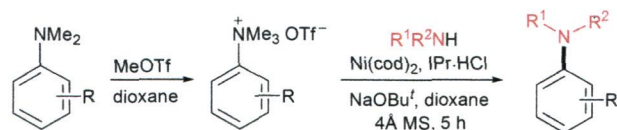
Effective molarities measured for the formation of H-bonds in a variety of zinc porphyrin-imidazole complexes are all between 3 mM and 200 mM, and the values measured for flexible and rigid ligand systems are comparable.

1448

Nickel-catalyzed cross-coupling of aryltrimethylammonium triflates and amines

Xue-Qi Zhang and Zhong-Xia Wang*

Ni(cod)₂-IPr effectively catalyzes cross-coupling of aryltrimethylammonium triflates and amines in the presence of NaOBu^t and 4 Å molecular sieves.

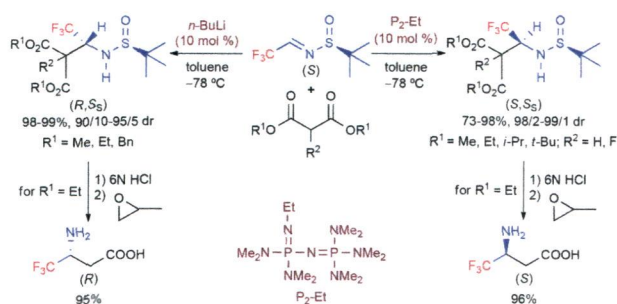


1454

Asymmetric Mannich reaction between (*S*)-*N*-(*tert*-butanesulfinyl)-3,3,3-trifluoroacetaldimine and malonic acid derivatives. Stereodivergent synthesis of (*R*)- and (*S*)-3-amino-4,4,4-trifluorobutanoic acids

Norio Shibata,* Takayuki Nishimine, Naoyuki Shibata, Etsuko Tokunaga, Kosuke Kawada, Takumi Kagawa, José Luis Aceña, Alexander E. Sorochinsky and Vadim A. Soloshonok*

Mannich additions of malonates to the title CF₃-sulfinylimine are described.

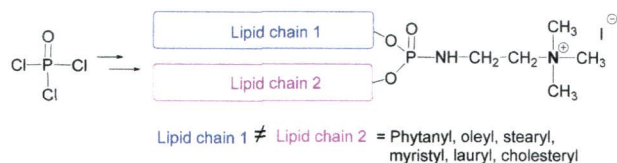


1463

Cationic lipophosphoramidates with two different lipid chains: synthesis and evaluation as gene carriers

Stéphanie S. Le Corre, Mathieu Berchel, Nawal Belmadi, Caroline Denis, Jean-Pierre Haelters, Tony Le Gall, Pierre Lehn, Tristan Montier and Paul-Alain Jaffrès*

The synthesis of a series of new cationic lipids possessing two different lipid chains is detailed. The transfection efficacies have shown the interest to associate a phytanyl chain with either, a lauryl or oleyl chain.

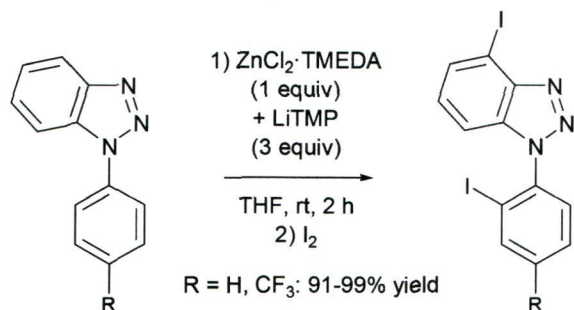


1475

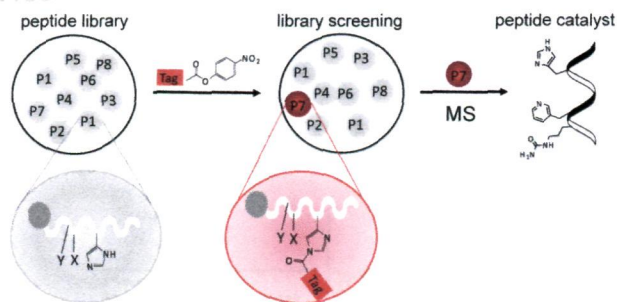
Deproto-metallation using a mixed lithium–zinc base and computed CH acidity of 1-aryl 1*H*-benzotriazoles and 1-aryl 1*H*-indazoles

Elisabeth Nagaradja, Floris Chevallier,* Thierry Roisnel, Vincent Dorcet, Yury S. Halauko,* Oleg A. Ivashkevich, Vadim E. Matulis and Florence Mongin*

1-Aryl-1*H*-benzotriazoles have been deproto-metallated using a 2,2,6,6-tetramethylpiperidino-based Li–Zn combination. The regioselectivity has been discussed in the light of DFT-calculated CH acidities (THF solution).



1488

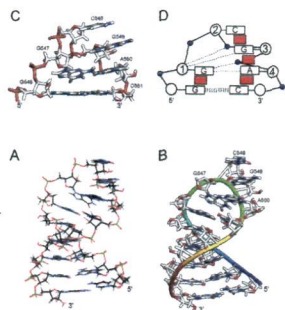


Identification and optimization of short helical peptides with novel reactive functionality as catalysts for acyl transfer by reactive tagging

Silvia Bezer, Masaomi Matsumoto, Michael W. Lodewyk, Stephen J. Lee, Dean J. Tantillo, Michel R. Gagné* and Marcey L. Waters*

A high-throughput screening method is used for identification of new catalytic functionalities for transesterification reaction in organic solvent.

1495

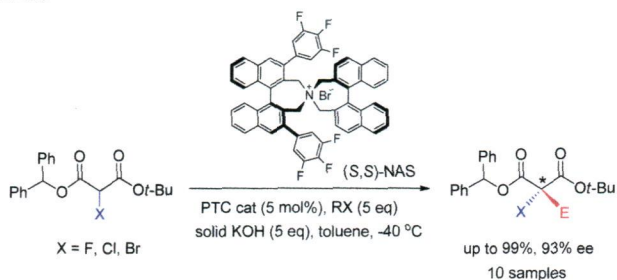


NMR elucidation of the role of Mg²⁺ in the structure and stability of the conserved RNA motifs of the EMCV IRES element

Sadia Mohammed, Marie M. Phelan, Usman Rasul and Vasudevan Ramesh*

NMR structure of the highly conserved and functionally significant 16mer RNA motif endowed with a classic "GNRA" tetraloop of the novel EMCV IRES element.

1510

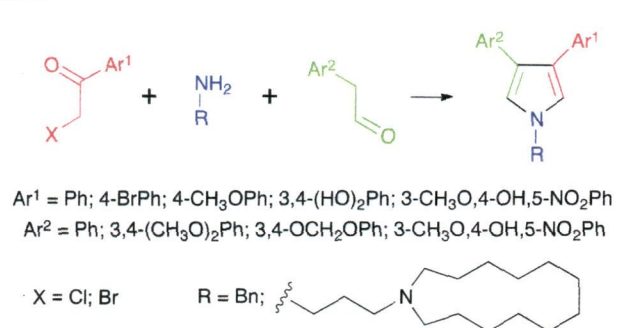


Enantioselective synthesis of α -halo- α -alkylmalonates via phase-transfer catalytic α -alkylation

Suckchang Hong, Minsik Kim, Myunggi Jung, Min Woo Ha, Myungmo Lee, Yohan Park, Mi-hyun Kim, Taek-Soo Kim, Jihoon Lee and Hyeung-geun Park*

A new enantioselective synthetic method for α -halo- α -alkylmalonates is reported.

1518



A concise formation of *N*-substituted 3,4-diarylpyrroles – synthesis and cytotoxic activity

Maxim Egorov, Bernard Delpech,* Geneviève Aubert, Thierry Cresteil, Maria Concepcion Garcia-Alvarez, Pascal Collin and Christian Marazano

Sequential condensation of a phenacyl halide with a primary amine and a phenylacetaldehyde led to *N*-substituted 3,4-diarylpyrroles. Synthesis of analogs of the marine alkaloid halitulin and cytotoxic studies are reported.