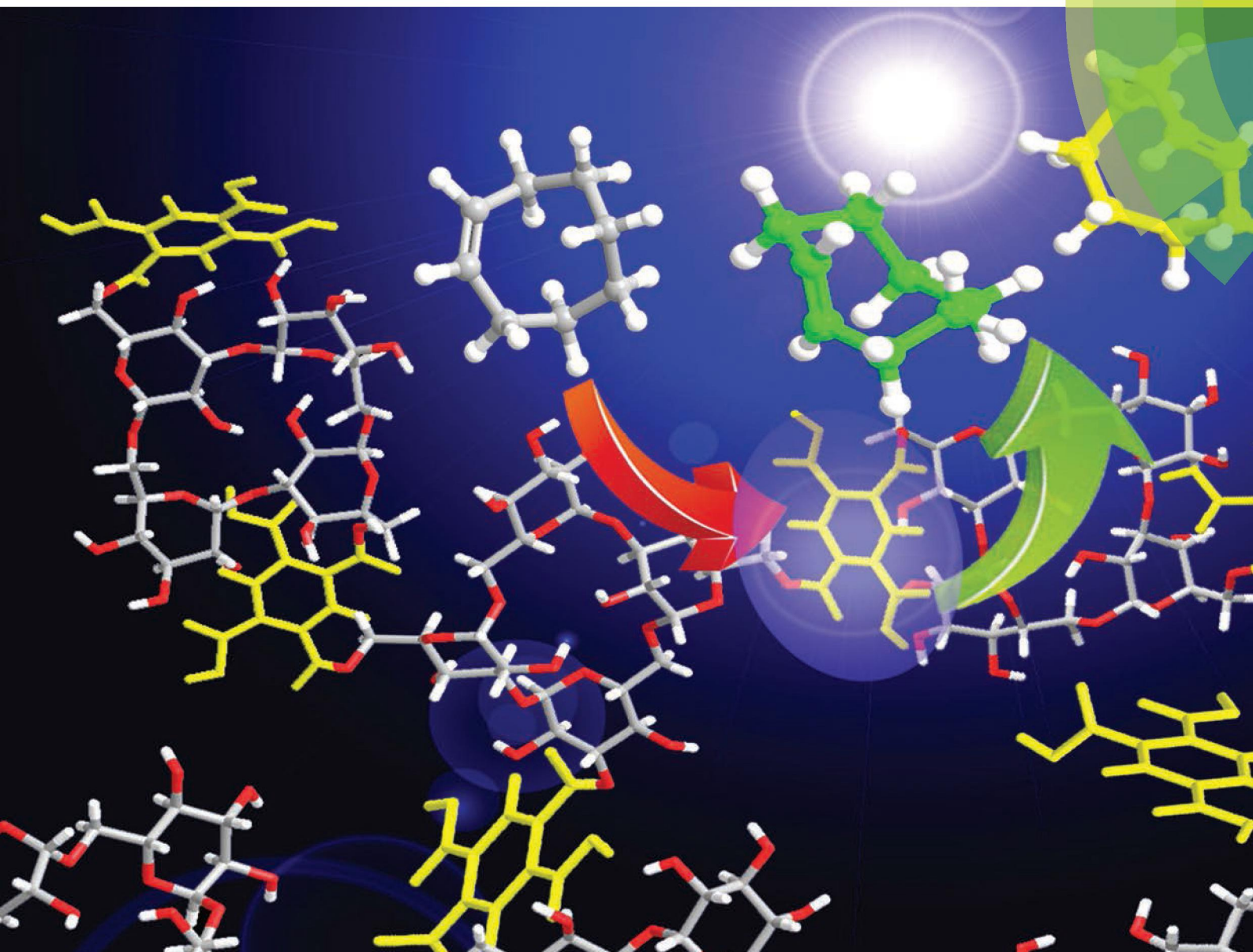


Organic & Biomolecular Chemistry

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PAPER

Cheng Yang, Francesco Trotta, Yoshihisa Inoue *et al.*
Solvent- and phase-controlled photochirogenesis. Enantiodifferentiating photoisomerization of (*Z*)-cyclooctene sensitized by cyclic nigerosylnigerose-based nanosponges crosslinked by pyromellitate

Organic & Biomolecular Chemistry

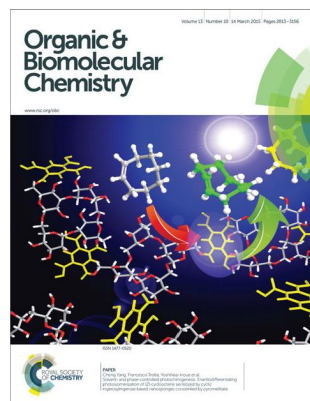
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IN THIS ISSUE

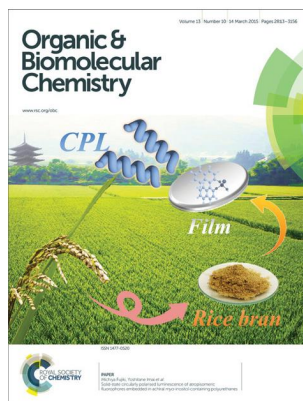
ISSN 1477-0520 CODEN OBCRAK 13(10) 2813–3156 (2015)



Cover

See Cheng Yang, Francesco Trotta, Yoshihisa Inoue *et al.*, pp. 2905–2912.

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Inside cover

See Michiya Fujiki, Yoshitane Imai *et al.*, pp. 2913–2917.

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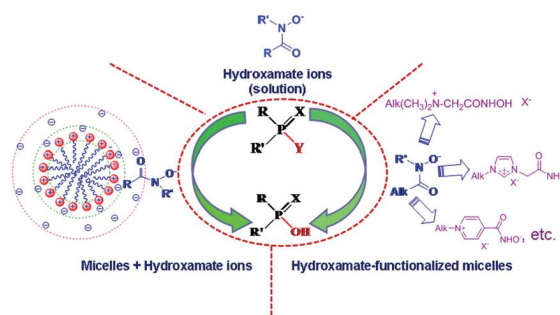
REVIEWS

2827

From α -nucleophiles to functionalized aggregates: exploring the reactivity of hydroxamate ion towards esterolytic reactions in micelles

Namrata Singh, Yevgen Karpichev, Rahul Sharma, Bhanushree Gupta, Arvind K. Sahu, Manmohan L. Satnami and Kallol K. Ghosh*

Hydroxamate ions as α -nucleophiles for esterolytic reactions in water and micelles.

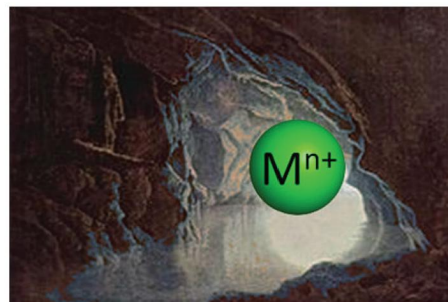


2849

Supramolecular control of transition metal complexes in water by a hydrophobic cavity: a bio-inspired strategy

Olivia Bistri and Olivia Reinaud*

Different strategies for obtaining water-soluble cavity-appended metal complexes are described, and their resulting interlocked assets are discussed in relationship with the very specific properties of water as a solvent.



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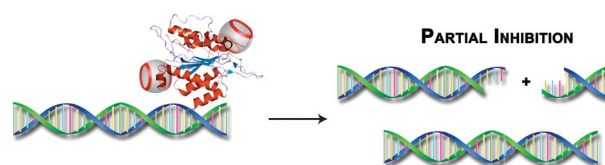
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2866

Cucurbiturils as supramolecular inhibitors of DNA restriction by type II endonucleases

Cátia Parente Carvalho, Amir Norouzy, Vera Ribeiro, Werner M. Nau and Uwe Pischel*

Cucurbiturils inactivate the restriction reaction of type II endonucleases *via* supramolecular interactions. This was monitored for different enzyme–DNA combinations in the absence and presence of organic macrocycles. The process can be re-activated by competitive displacement on addition of polyamines.

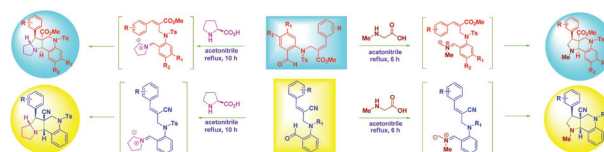


2870

Highly regio- and diastereo-selective synthesis of novel tri- and tetra-cyclic perhydroquinoline architectures *via* an intramolecular [3 + 2] cycloaddition reaction

M. Bakthadoss,* D. Kannan, J. Srinivasan and V. Vinayagam

A facile and efficient synthetic protocol was established for the construction of novel tri- and tetra-cyclic pyrrolo/ pyrrolizinoquinoline architectures *via* an intramolecular [3 + 2] cycloaddition reaction strategy.

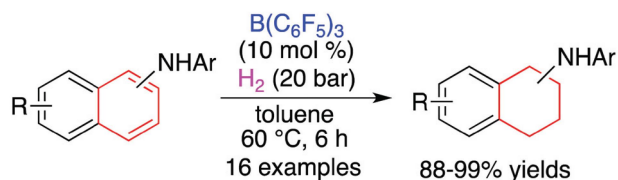


2875

B(C₆F₅)₃-catalyzed metal-free hydrogenation of naphthylamines

Gen Li, Yongbing Liu and Haifeng Du*

A catalytic metal-free hydrogenation of naphthylamines using B(C₆F₅)₃ was achieved under mild conditions for the first time to furnish tetrahydronaphthylamines in high yields.

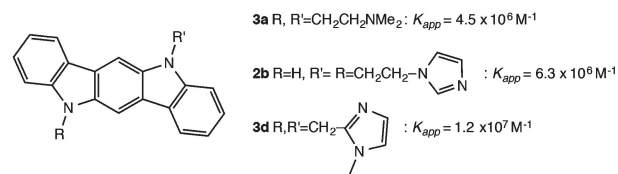


2879

Synthesis and DNA binding profile of *N*-mono- and *N,N'*-disubstituted indolo[3,2-*b*]carbazoles

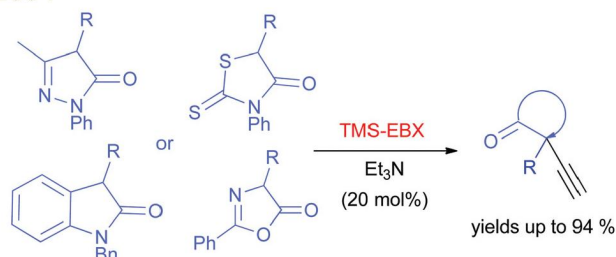
Harmanpreet Kaur Panesar, Jennifer Solano and Thomas G. Minehan*

N-Monosubstituted and *N,N'*-disubstituted indolo[3,2-*b*]carbazole derivatives bind DNA with micromolar to submicromolar affinities and a preference for intercalation at purine-pyrimidine steps.



COMMUNICATIONS

2884

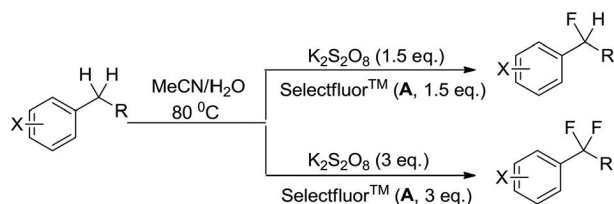


Alkylation of heterocyclic compounds using hypervalent iodine reagent

M. Kamlar, I. Císařová and J. Veselý*

The alkylation of various nitrogen- and/or sulphur-containing heterocyclic compounds using hypervalent iodine TMS-EBX by utilization of tertiary amines under mild conditions is described.

2890

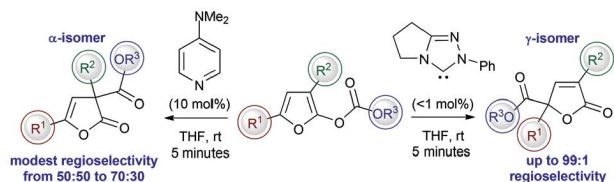


Transition-metal-free C–H oxidative activation: persulfate-promoted selective benzylic mono- and difluorination

Jing-jing Ma, Wen-bin Yi,* Guo-ping Lu and Chun Cai

An operationally simple and selective method for the direct conversion of benzylic C–H to C–F to obtain mono- and difluoromethylated arenes using Selectfluor™ as a fluorine source is developed.

2895

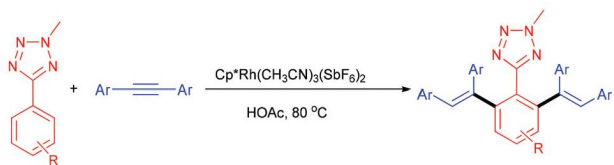


Regiodivergent Lewis base-promoted O- to C-carboxyl transfer of furanyl carbonates

Craig D. Campbell, Caroline Joannesse, Louis C. Morrill, Douglas Philp and Andrew D. Smith*

Triazolinylienes promote γ-selective C-carboxylation (up to 99 : 1 regioselectivity) in the O- to C-carboxyl transfer of furanyl carbonates in contrast to DMAP that promotes preferential α-C-carboxylation with moderate regiocontrol (typically 60 : 40 regioselectivity).

2901



Rhodium-catalyzed hydroarylation of alkynes via tetrazole-directed C–H activation

Bin Chen, Yan Jiang, Jiang Cheng and Jin-Tao Yu*

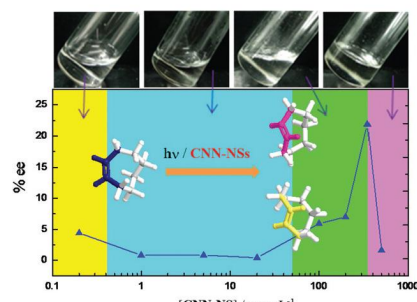
A rhodium-catalyzed hydroarylation of alkynes with aryl tetrazoles through tetrazole-directed C–H activation was developed.

2905

Solvent- and phase-controlled photochirogenesis. Enantiodifferentiating photoisomerization of (*Z*)-cyclooctene sensitized by cyclic nigerosylnigerose-based nanosponges crosslinked by pyromellitate

X. Wei, W. Liang, W. Wu, C. Yang,* F. Trotta,* F. Caldera, A. Mele, T. Nishimoto and Y. Inoue*

The enantioselectivity of the (*E*)-cyclooctene produced critically depended on the solvent and also on the phase evolved, maximizing at the flowing/rigid gel border.

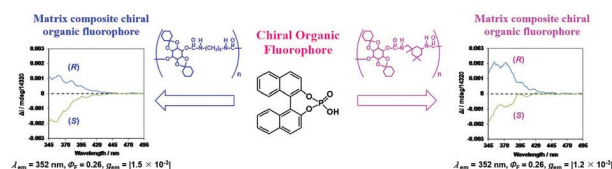


2913

Solid-state circularly polarised luminescence of atropisomeric fluorophores embedded in achiral *myo*-inositol-containing polyurethanes

Tomoyuki Amako, Kazuki Nakabayashi, Atsushi Sudo, Michiya Fujiki* and Yoshitane Imai*

Two chiral binaphthyl fluorophores in two *myo*-inositol based polyurethane matrices with high glass transition temperatures emitted circularly polarised luminescence with a high circular anisotropy factor.

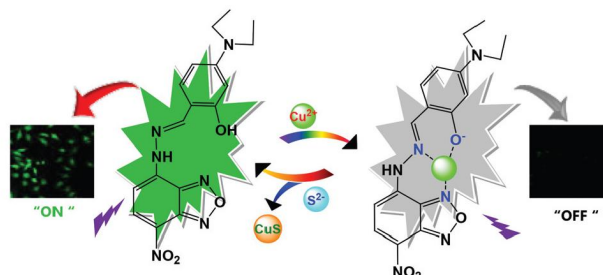


2918

NBD-based fluorescent chemosensor for the selective quantification of copper and sulfide in an aqueous solution and living cells

Qingtao Meng, Yu Shi, Cuiping Wang, Hongmin Jia, Xue Gao, Run Zhang,* Yongfei Wang and Zhiqiang Zhang*

A fluorescent chemosensor (NL) has been developed for the selective quantification of copper and sulfide in aqueous solutions and living cells.

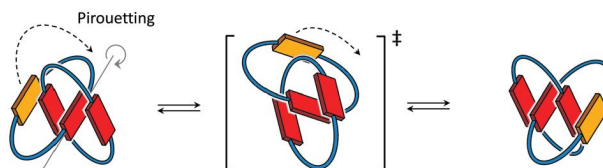


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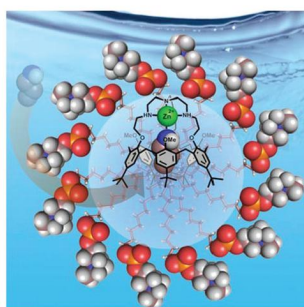
Molecular motion of donor–acceptor catenanes in water

Fabien B. L. Cougnon,* Nandhini Ponnuswamy,* G. Dan Pantoş and Jeremy K. M. Sanders

In this article, we use ¹H NMR spectroscopy to study the spontaneous molecular motion of donor–acceptor [2]catenanes in water.



2931

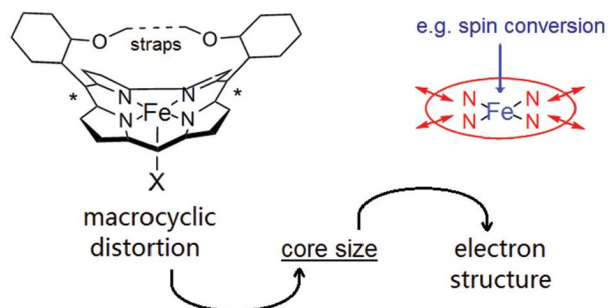


Primary amine recognition in water by a calix[6]aza-cryptand incorporated in dodecylphosphocholine micelles

Emilio Brunetti, Alex Inthasot, Flore Keymeulen, Olivia Reinaud, Ivan Jabin* and Kristin Bartik*

A zinc calix[6]azacryptand complex was incorporated into dodecylphosphocholine micelles. This complex can strongly and selectively bind linear primary amines in an aqueous medium.

2939

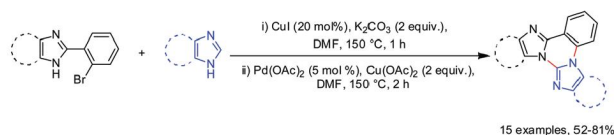


Fractional transfer of a free unpaired electron to overcome energy barriers in the formation of Fe⁴⁺ from Fe³⁺ during the core contraction of macrocycles: implication for heme distortion

Qihua Liu, Xiaochun Zhou, Haomin Liu, Xi Zhang and Zaichun Zhou*

The free unpaired electron in Fe³⁺ ions cannot be directly removed, and needs a transfer pathway with at least four steps to overcome the high energy barriers to form Fe⁴⁺ ions.

2947

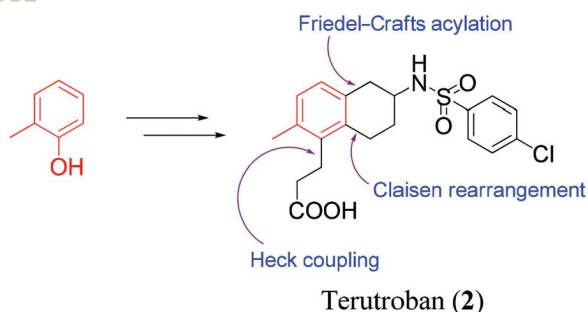


Synthesis of novel azole-fused quinazolines via one-pot, sequential Ullmann-type coupling and intramolecular dehydrogenative C–N bonding

Nitesh Kumar Nandwana, Kasiviswanadharaju Pericherla, Pinku Kaswan and Anil Kumar*

An efficient one-pot sequential procedure is described for the synthesis of novel azole-fused quinazolines through Ullmann-type coupling followed by cross dehydrogenative coupling of various azoles with 2-(2-bromophenyl)-1H-imidazole/benzimidazoles.

2951



Total synthesis of a thromboxane receptor antagonist, terutroban

Wasim Ahmed, Prathama S. Mainkar, Srihari Pabbaraja and Srivari Chandrasekhar*

Synthesis of terutroban (2) is achieved following a non-Diels–Alder approach using cost-effective chemicals.

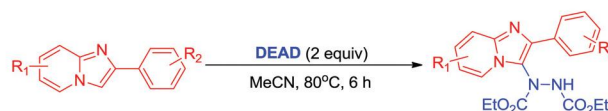
PAPERS

2958

Metal-free, efficient hydrazination of imidazo[1,2-*a*]pyridine with diethyl azodicarboxylate in neutral media

Yuanxiang Wang, Brendan Frett, Nick McConnell and Hong-yu Li*

The first example of metal-free regioselective hydrazination of imidazo[1,2-*a*]pyridine with diethyl azodicarboxylate is accomplished.

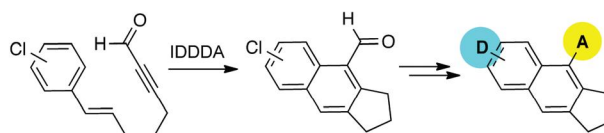


2965

Cyclopenta[*b*]naphthalene cyanoacrylate dyes: synthesis and evaluation as fluorescent molecular rotors

Laura S. Kocsis, Kristyna M. Elbel, Billie A. Hardigree, Kay M. Brummond,* Mark A. Haidekker* and Emmanuel A. Theodorakis*

The application of an intramolecular dehydrogenative dehydro-Diels–Alder (IDDDA) reaction to the construction of fluorescent molecular rotors (D- π -A motif) containing a cyclopenta[*b*]naphthalene ring system is described.

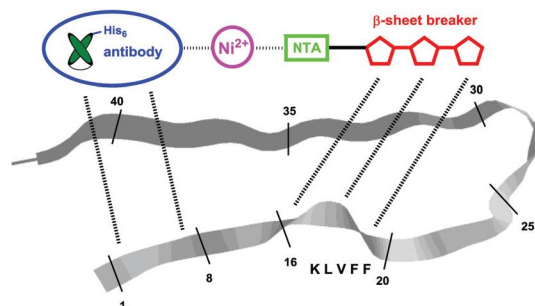


2974

Hybridization of an A β -specific antibody fragment with aminopyrazole-based β -sheet ligands displays striking enhancement of target affinity

Marco Hellmert, Andreas Müller-Schiffmann, Max Sena Peters, Carsten Korth* and Thomas Schrader*

A His-tagged antibody is combined with an NTA- β -sheet breaker and displays a striking increase in A β affinity.

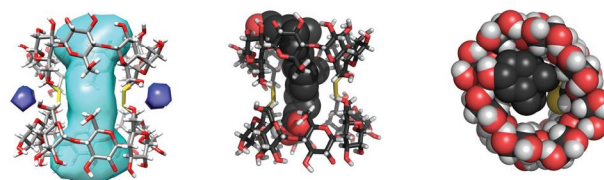


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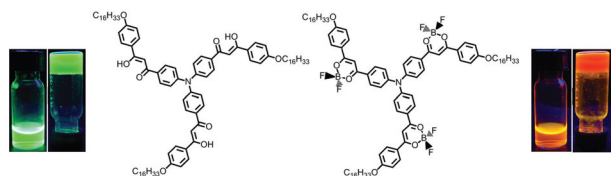
A γ -cyclodextrin duplex connected with two disulfide bonds: synthesis, structure and inclusion complexes

Sergey Volkov, Lukáš Kumprecht, Miloš Buděšínský, Martin Lepšík, Michal Dušek and Tomáš Kraus*

Oxidative dimerization of 6^I,6^V-disulfanyl- γ -cyclodextrin yields a duplex tubular structure with internal volume of $\sim 740 \text{ \AA}^3$ allowing formation of very stable inclusion complexes with medium to large organic molecules in water ($K_a \sim 10^8 \text{ M}^{-1}$).



2986

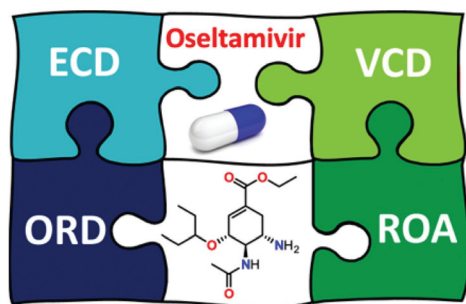


Luminescent organogels based on triphenylamine functionalized β -diketones and their difluoroboron complexes

Chong Qian, Mingyang Liu, Guanghui Hong, Pengchong Xue, Peng Gong and Ran Lu*

New organogelators based on triphenylamine functionalized β -diketones and their difluoroboron complexes were synthesized.

2999

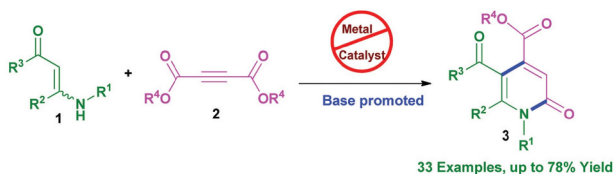


A configurational and conformational study of (–)-Oseltamivir using a multi-chiroptical approach

Marcin Górecki*

Four chiroptical methods, *i.e.* electronic circular dichroism (ECD), optical rotatory dispersion (ORD), vibrational circular dichroism (VCD), and Raman optical activity (ROA) were employed to discover a set of the most probable conformations of (–)-Oseltamivir in solution.

3011

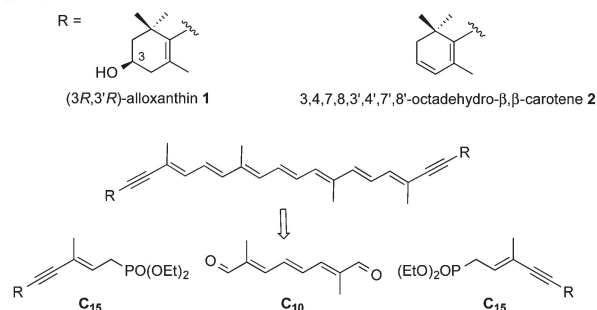


Reaction of β -enaminones and acetylene dicarboxylates: synthesis of substituted 1,2-dihydropyridinones

Vemu Nagaraju, Dalovai Purnachander, N. S. V. M. Rao Mangina, Suriseti Suresh, Balasubramanian Sridhar and Galla V. Karunakar*

Synthesis of dihydropyridinones was achieved by reaction of β -enaminones with acetylene dicarboxylates without using transition metal/catalyst.

3024



Synthesis of labile all-*trans*-7,8,7',8'-bis-acetylenic carotenoids by bi-directional Horner–Wadsworth–Emmons condensation

Belén Vaz,* Noelia Fontán, Marta Castiñeira, Rosana Álvarez* and Ángel R. de Lera*

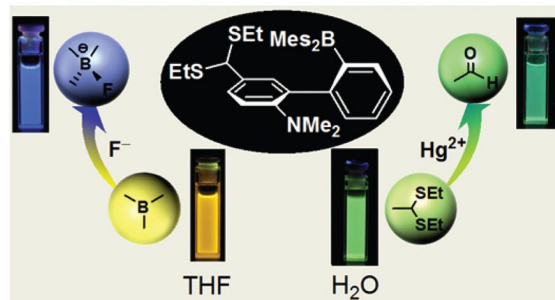
Two symmetrical C_7,C_8 -acetylenic carotenoids have been stereoselectively prepared using a bi-directional Horner–Wadsworth–Emmons condensation of the C_{10} -dialdehyde and C_{15} -phosphonates.

3032

A highly selective ratiometric bifunctional fluorescence probe for Hg²⁺ and F⁻ ions

Qing-Wen Xu, Chen Wang, Zuo-Bang Sun and Cui-Hua Zhao*

A dithioacetal-containing triarylborane behaves as a promising ratiometric bifunctional fluorescence probe to detect Hg²⁺ and F⁻ simultaneously.

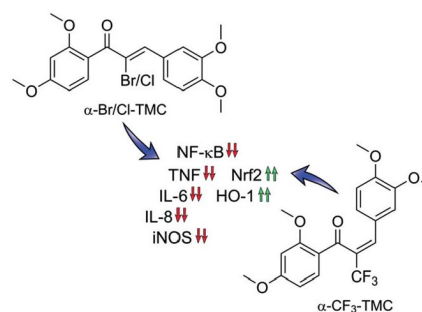


3040

Enhancing the anti-inflammatory activity of chalcones by tuning the Michael acceptor site

Hannelore Rucker, Nafisah Al-Rifai, Anne Rasclé, Eva Gottfried, Lidia Brodziak-Jarosz, Clarissa Gerhäuser, Tobias P. Dick and Sabine Amslinger*

Boosting the alkylation power of chalcones creates new anti-inflammatory agents. Thus NF-κB-dependent proteins are inhibited and Nrf2-dependent ones activated. The activity enhancement relies solely and very effectively on the α-substituent of the α,β-unsaturated carbonyl unit.

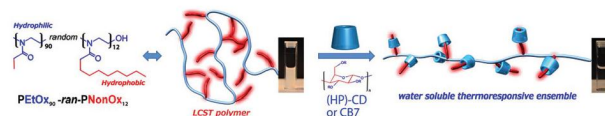


3048

Tuning temperature responsive poly(2-alkyl-2-oxazoline)s by supramolecular host-guest interactions

Victor R. de la Rosa, Werner M. Nau and Richard Hoogenboom*

A poly[(2-ethyl-2-oxazoline)-*ran*-(2-nonyl-2-oxazoline)] random copolymer was synthesized and its thermoresponsive behavior in aqueous solution modulated by the addition of different supramolecular host molecules.

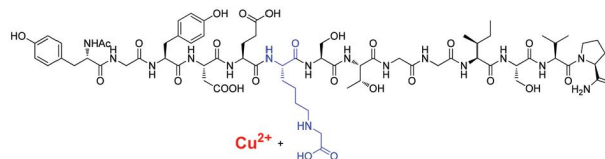


3058

Physicochemical studies on the copper(II) binding by glycated collagen telopeptides

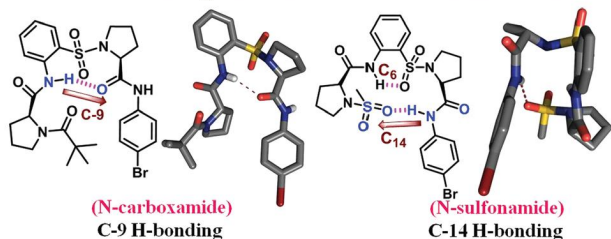
Meder Kamalov, Paul W. R. Harris, Christian G. Hartinger, Gordon M. Miskelly, Garth J. S. Cooper and Margaret A. Brimble*

The strong interaction between advanced glycation end-products and Cu(II) ions has been revealed using site-specifically glycated collagenous peptides.



3064

Reversal of H-bonding direction: Effect of N-terminal sulfonation

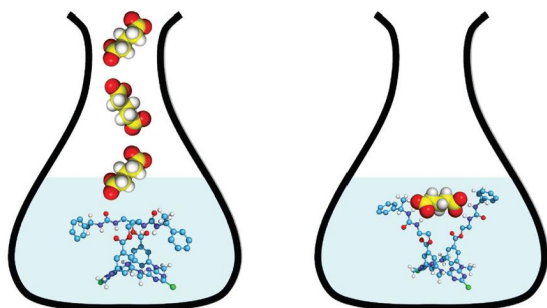


Reversal of H-bonding direction by N-sulfonation in a synthetic reverse-turn peptide motif

Kuruppanthara N. Vijayadas, Amol S. Kotmale, Shridhar H. Thorat, Rajesh G. Gonnade, Roshna V. Nair, Pattuparambil R. Rajamohanam and Gangadhar J. Sanjayan*

This manuscript depicts an intriguing example of H-bonding reversal upon introduction of a sulfonamide linkage at the N-terminus of a synthetic reverse-turn peptide.

3070

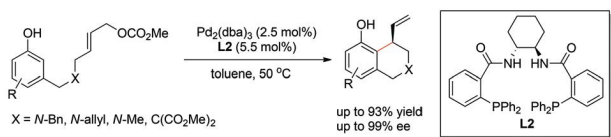


Recognition of bio-relevant dicarboxylate anions by an azacalix[2]arene[2]triazine decorated with urea moieties

Miguel M. Santos, Igor Marques, Silvia Carvalho, Cristina Moiteiro* and Vítor Félix*

The binding affinity of a dichlorocalix[2]arene[2]triazine based bis-urea azamacrocycle was investigated towards a wide range of bio-relevant dicarboxylate anions by a combination of ^1H NMR titrations in CDCl_3 and molecular dynamics simulations.

3086

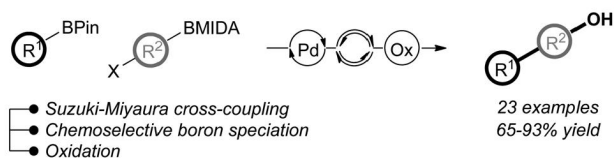


Enantioselective synthesis of 4-substituted tetrahydroisoquinolines via palladium-catalyzed intramolecular Friedel-Crafts type allylic alkylation of phenols

Zheng-Le Zhao, Qing-Long Xu, Qing Gu, Xin-Yan Wu* and Shu-Li You*

Pd-catalyzed asymmetric intramolecular allylic alkylation reaction of phenols was developed, affording C4 substituted tetrahydroisoquinolines in moderate to excellent yields, enantioselectivity and regioselectivity.

3093



A modular synthesis of functionalised phenols enabled by controlled boron speciation

John J. Molloy, Robert P. Law, James W. B. Fyfe, Ciaran P. Seath, David J. Hirst and Allan J. B. Watson*

Functionalised biaryl phenols can be rapidly accessed via one-pot Suzuki-Miyaura cross-coupling, chemoselective control of boron solution speciation, and oxidation.

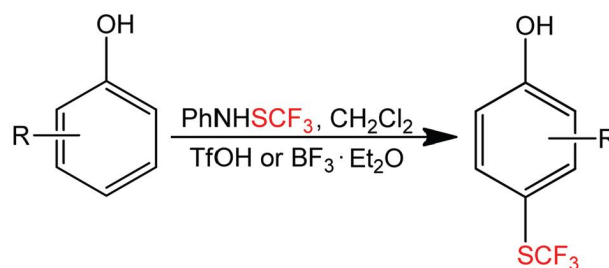
PAPERS

3103

Acid-promoted direct electrophilic trifluoromethylthiolation of phenols

Marjan Jereb* and Kaja Gosak

A highly selective and effective, acid-promoted, electrophilic trifluoromethylthiolation of phenols is described.

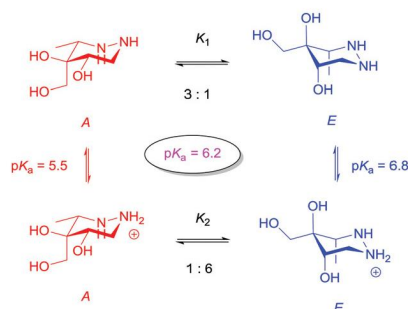


3116

Exploring the relationship between the conformation and pK_a: can a pK_a value be used to determine the conformational equilibrium?

Jacob Ingemar Olsen, Stephan P. A. Sauer, Christian Marcus Pedersen and Mikael Bols*

For the first time it is shown that the pK_a directly reflects the conformational equilibrium of conformers.

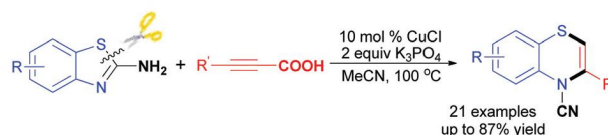


3122

Copper-catalyzed ring expansion of 2-amino-benzothiazoles with alkynyl carboxylic acids to 1,4-benzothiazines

Jing-Wen Qiu, Bo-Lun Hu, Xing-Guo Zhang,* Ri-Yuan Tang, Ping Zhong and Jin-Heng Li*

A novel copper-catalyzed ring expansion of 2-aminobenzothiazoles to 1,4-benzothiazines is described.

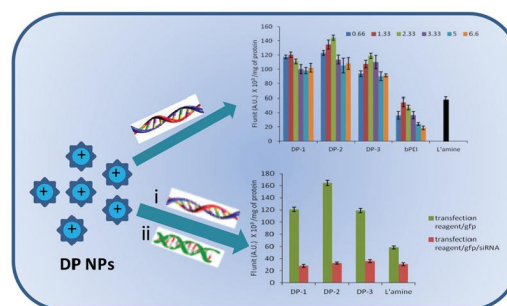


3128

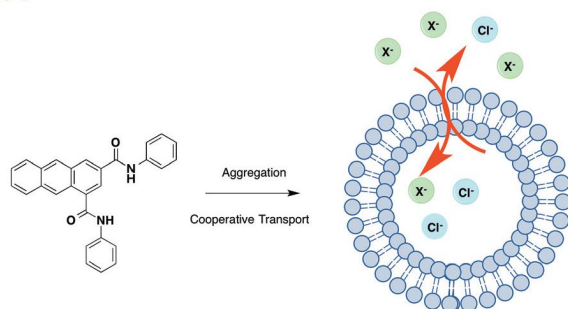
Bioreducible polyethylenimine nanoparticles for the efficient delivery of nucleic acids

Ruby Bansal, Shweta Tayal, K. C. Gupta and Pradeep Kumar*

Electrostatically crosslinked bioreducible nanoparticles of polyethylenimine (DP NPs) have been prepared and evaluated for their cytotoxicity and capability to transport nucleic acids inside the cells.



3136

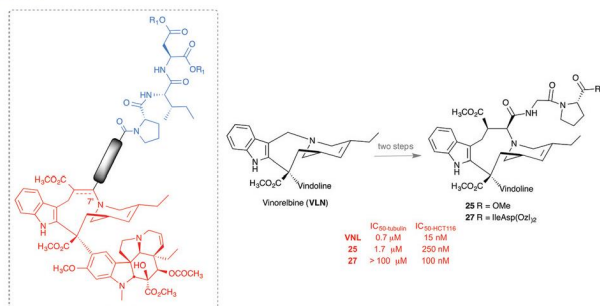


Aromatic isophthalamides aggregate in lipid bilayers: evidence for a cooperative transport mechanism

Stuart N. Berry, Nathalie Busschaert, Charlotte L. Frankling, Dale Salter and Philip A. Gale*

The synthesis and anion transport properties of a series of aromatic transmembrane anion transporters based on an isophthalamide scaffold are reported.

3144



Synthesis and evaluation of hybrid molecules targeting the vinca domain of tubulin

O. Gherbovet, Pedro A. Sánchez-Murcia, M. C. García Alvarez, J. Bignon, S. Thoret, F. Gago and F. Roussi*

Hybrids of vinca alkaloids and phomopsin A, linked by a glycine pattern, have been synthesized in one or two steps, by an insertion reaction.