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Conformational Analysis

M. Benaglia, F. Cozzi,* M. Mancinelli, A. Mazzanti*

The Intramolecular Interaction of Thiophene and Furan with Aromatic and Fluoroaromatic Systems in Some [3.3]Meta(heterocyclo)paracyclophanes: A Combined Computational and NMR Spectroscopic Study

A dive into an electron sea! Four thiophene- and furan-containing [3.3]meta(heterocyclo)paracyclophanes were designed and synthesized to study the intramolecular interaction between standard heteroaromatic rings and tetra-H- or tetra-F-substituted benzenes. The furan-derived adducts were shown by calculations and NMR spectroscopy to adopt a perpendicular edge-to-face disposition of the rings with the oxygen atom pointing toward the benzene platform (see figure).



Chem. Eur. J.
DOI: 10.1002/chem.201000783

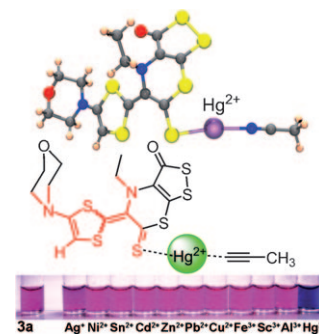


Chromogenic Probes

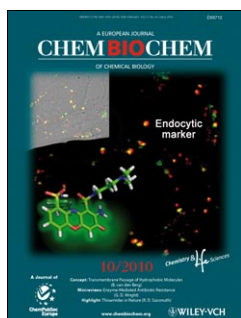
P. Fuentès, D. Moreno, J. V. Cuevas, M. García-Valverde, T. Torroba*

A Selective Chromogenic Probe for Mercury(II) and Cyanide in Aqueous Buffered Solution from a Cycloaddition Reaction of an Ynamine to Polycyclic Dithiolethiones

Mercury rising! A new polysulfur-nitrogen heterocycle is described as a new selective chromogenic probe for the naked-eye detection of mercury(II), by a dramatic change of color from purple to blue-violet in a HEPES-buffered water/acetonitrile 1:1 mixture, with sub-micromolar sensitivity. The chemical probe also changes from purple to red in the presence of cyanide.



Chem. Asian J.
DOI: 10.1002/asia.201000063

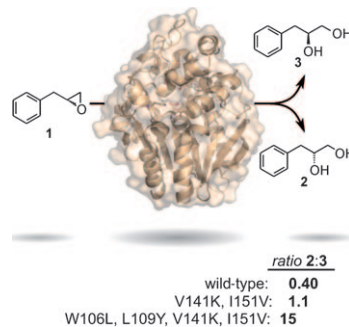


Enzyme Catalysis

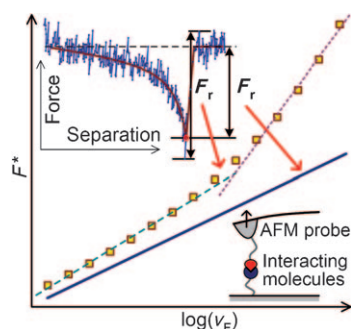
A. Gurell, M. Widersten*

Modification of Substrate Specificity Resulting in an Epoxide Hydrolase with Shifted Enantiopreference for (2,3-Epoxypropyl)benzene

Mutagenesis of the active-site residues of the epoxide hydrolase StEH1 led to enzyme variants with modified enantiopreference for (2,3-epoxypropyl)benzene. The wild-type enzyme favors the *S* enantiomer, whereas a quadruple mutant displays a 15:1 preference for the *R* enantiomer, due to crippled catalytic efficiency in the hydrolysis of the *S* enantiomer, but retained activity with the *R* enantiomer.



ChemBioChem
DOI: 10.1002/cbic.201000185



Force Spectroscopy

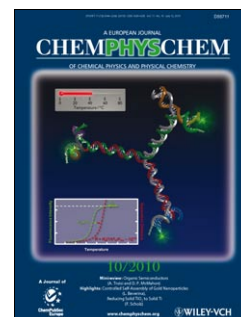
N. Li, S. Guo, B. B. Akhremitchev*

Apparent Dependence of Rupture Force on Loading Rate in Single-Molecule Force Spectroscopy

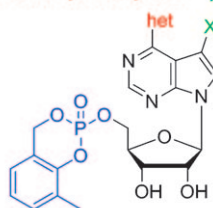
Mighty noise: Non-linear dependence of the most probable rupture force on the logarithm of the loading rate might appear if the contributions from noise are included in extracted rupture forces (see figure).

ChemPhysChem

DOI: 10.1002/cphc.201000251



het = furyl, thienyl etc. X = H or F



cytostatic activity (GI₅₀ = 9 nm - 5 μM)
inhibition of human adenosine kinase
(IC₅₀ = 0.08 - 5 μM)

ChemMedChem

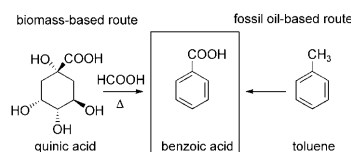
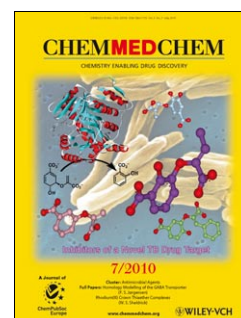
DOI: 10.1002/cmdc.201000192

Prodrugs

P. Spáčilová, P. Nauš, R. Pohl, I. Votruba, J. Snášel, H. Zábranská, I. Pichová, R. Ameral, G. Birkuš, T. Cihlár, M. Hocek*

CycloSal-phosphate Pronucleotides of Cytostatic 6-(Het)aryl-7-deazapurine Ribonucleosides: Synthesis, Cytostatic Activity, and Inhibition of Adenosine Kinases

Inhibiting ADK: CycloSal-phosphate prodrugs of nucleoside cytostatics (6-hetaryl-7-deazapurine ribonucleosides) were prepared. The pronucleotides display nanomolar cytostatic activities similar to those of the parent nucleosides. In addition, they exhibit pronounced inhibitory effects toward human adenosine kinase.



ChemSusChem

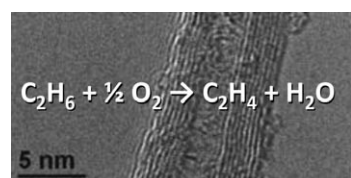
DOI: 10.1002/cssc.201000111

Renewable Resources

E. Arceo, J. A. Ellman,* R. G. Bergman*

A Direct, Biomass-Based Synthesis of Benzoic Acid: Formic Acid-Mediated Deoxygenation of the Glucose-Derived Materials Quinic Acid and Shikimic Acid

Shikimic Gimmick: An alternative biomass-based route to benzoic acid from the renewable starting materials quinic acid and shikimic acid is described. Benzoic acid is obtained selectively using a highly efficient, one-step formic acid-mediated deoxygenation method.



Carbon Nanotubes

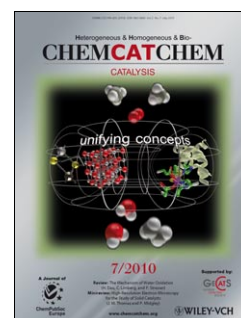
B. Frank, M. Morassutto, R. Schomäcker, R. Schlögl, D. S. Su*

Oxidative Dehydrogenation of Ethane over Multiwalled Carbon Nanotubes

At eye level: The high C–H bond strength of ethane challenges the stability of metal-free carbon nanotubes (CNTs) as a catalyst for oxidative dehydrogenation (ODH). However, surface modification of the CNTs with B₂O₃ or P₂O₅ leads to drastically enhanced oxidation resistance of the catalysts during ODH and increases alkene selectivity due to the suppression of electrophilic oxygen intermediates on the carbon surface.

ChemCatChem

DOI: 10.1002/cctc.201000035



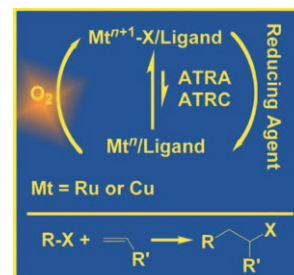


Catalyst Regeneration

T. Pintauer*

Catalyst Regeneration in Transition-Metal-Mediated Atom-Transfer Radical Addition (ATRA) and Cyclization (ATRC) Reactions

Recent advances in the area of catalyst regeneration in copper- and ruthenium-mediated atom transfer radical addition (ATRA) and cyclization (ATRC) reactions in the presence of free-radical diazo initiators or magnesium as reducing agents were reviewed. Reducing agents regenerate the activator in both processes, enabling selective ATRA and ATRC reactions using very small amounts of metal catalysts.



Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.201000234

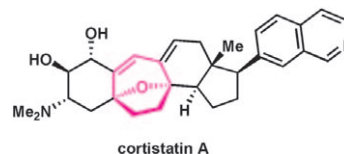


Natural Products

A. R. Hardin Narayan, E. M. Simmons, R. Sarpong*

Synthetic Strategies Directed Towards the Cortistatin Family of Natural Products

The cortistatin family of natural products have captured the attention both of synthetic chemists and of workers interested in understanding and exploiting their potent anti-angiogenic activity. Many synthetic strategies have been devised to build the rearranged steroidal cortistatin core, which has in turn enabled studies probing the origins and mechanism of these compounds' biological activity.



Eur. J. Org. Chem.
DOI: 10.1002/ejoc.201000247

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