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Swiss Science Concentrates

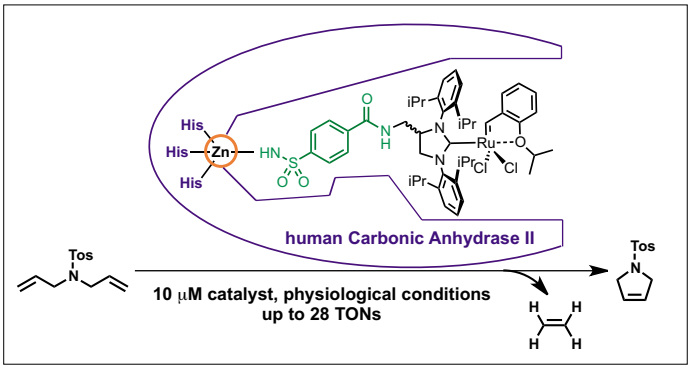
A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

Carbonic Anhydrase II as Host Protein for the Creation of a Biocompatible Artificial Metathesase

J. Zhao, A. Kajetanowicz, and T. R. Ward*, *Org. Biomol. Chem.* **2015**, *137*, 4728. University of Basel

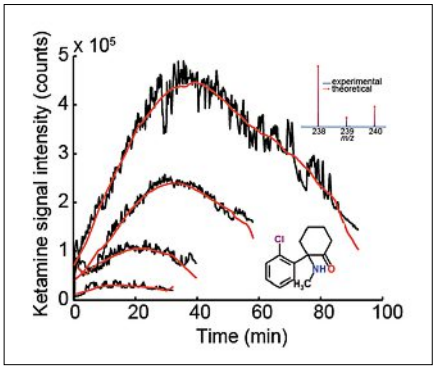
Certain forms of cancer overexpress variants of human *Carbonic Anhydrase* (*hCA*). These arylsulfonamide binding proteins represent privileged targets for cancer therapy. Ward and coauthors report on their efforts to exploit *hCA* for the creation of a biocompatible artificial metathesase by incorporation of an Hoveyda-Grubbs catalyst bearing an arylsulfonamide anchor within *hCA*. Optimization of the catalytic performance is achieved upon combining chemical and genetic means. Up to 28 turn-over-numbers were obtained within four hours under aerobic physiological conditions. Further efforts are directed at the site-specific uncaging of drugs using a cell-surface hCA variant overexpressed in various forms of cancer.



Drug Pharmacokinetics Determined by Real-Time Analysis of Mouse Breath

X. Li, P. Martinez-Lozano Sinues, R. Dallmann, L. Bregy, M. Hollmén, S. Proulx, S. A. Brown, M. Detmar, M. Kohler, and R. Zenobi*, *Angew. Chem. Int. Ed.* **2015**, *54*, 7815. ETH Zürich

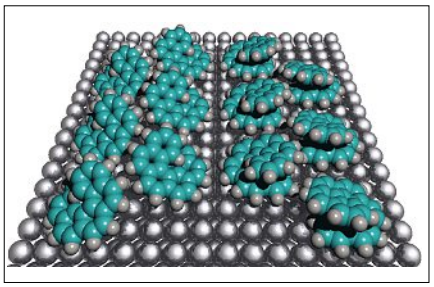
During lead optimization, pharmacokinetic (PK) parameters of each compound are determined in plasma using animal models prior to the clinical phases of development. Zenobi and coworkers developed a noninvasive, real-time PK monitoring of ketamine, propofol, and valproic acid, and their metabolites in mice, using secondary electrospray ionization and high-resolution mass spectrometry. In contrast to conventional studies that require many animals to be sacrificed even for low resolution PK curves, this novel approach yields real-time PK curves with a hitherto unmatched time resolution (10 s), and none of the animals has to be sacrificed. This thus represents a major step forward not only in animal welfare, but also major cost and time savings.



From Homochiral Clusters to Racemate Crystals: Viable Nuclei in 2D Chiral Crystallization

J. Seibel, M. Parschau, and K.-H. Ernst*, *J. Am. Chem. Soc.* **2015**, *137*, 7970. EMPA Dübendorf and University of Zürich

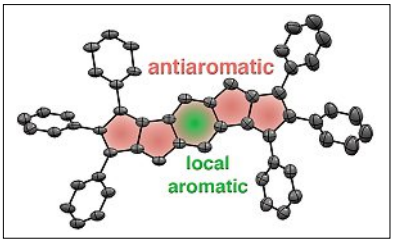
The quest for enantiopure compounds raises the question of which factors favor conglomerate crystallization over racemate crystallization. Ernst and coworkers demonstrate that studying nucleation and crystal growth at surfaces with submolecular-resolution scanning tunneling microscopy is a suitable approach to better understand intermolecular chiral recognition. Racemic heptahelicene on the Ag(100) surface shows a transition from homochiral nuclei to larger racemic motifs, although the extended homochiral phase exhibits higher density. The homochiral–heterochiral transition is explained by the higher stability of growing nuclei due to a better match of the molecular lattice to the substrate surface. These observations are direct visual proof of viable nuclei.



The Impact of Antiaromatic Subunits in [4n+2] π-Systems: Bispentalenes with [4n+2] π-Electron Perimeters and Antiaromatic Character

J. Cao, G. London, O. Dumele, M. von Wantoch Rekowski, N. Trapp, L. Ruhlmann, C. Boudon, A. Stanger*, and F. Diederich*, *J. Am. Chem. Soc.* **2015**, *137*, 7178. ETH Zürich

The concepts of aromaticity and antiaromaticity are of fundamental importance in classifying physical and chemical properties of planar, π-conjugated cyclic molecules. However, until now, no unique definition for aromaticity and antiaromaticity is generally accepted. Diederich, Stanger and coworkers prepared three series of stable, neutral, π-extended bispentalene derivatives. While these chromophores feature skeletons with [4n+2] π-electron perimeters, the two 8 π-electron pentalene subunits strongly influence bonding and spectral properties. Both experimental and computational results suggest that the molecular properties of the presented bispentalenes are dominated by the antiaromatic pentalene-subunits despite the [4n+2] π-electron perimeter of the skeletons.



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