doi:10.2533/chimia.2013.921

Swiss Science Concentrates

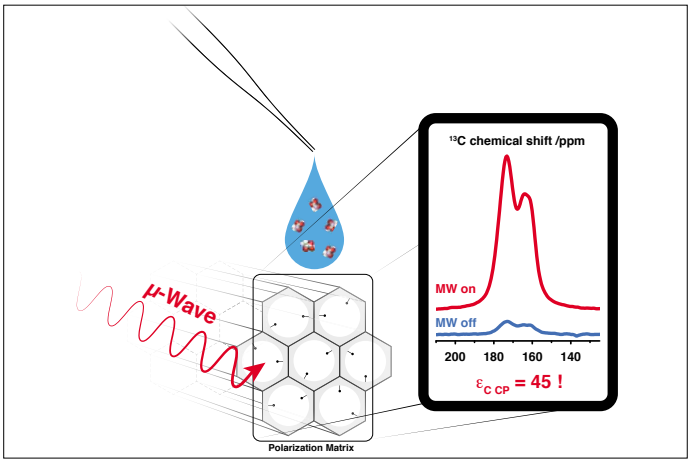
A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

Solid-phase DNP Polarizing Matrices from Homogeneously Distributed Radicals in Mesostructured Hybrid Silica Materials

D. Gajan, M. Schwarzwälder, M. P. Conley, W. R. Gruening, A. J. Rossini, A. Zagdoun, M. Lelli, M. Yulikov, G. Jeschke, C. Sauvee, O. Ouari, P. Tordo, L. Veyre, A. Lesage, C. Thieuleux,* L. Emsley,* and C. Copéret*, *J. Am. Chem. Soc.* **2013**, *135*, 15459. ETH Zürich

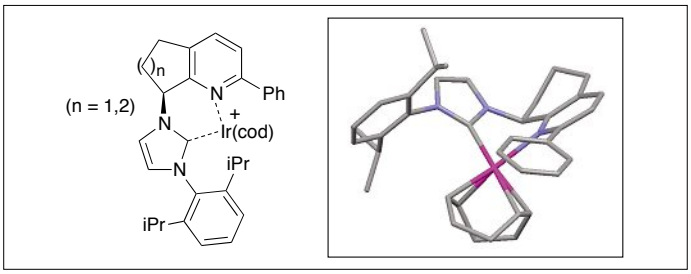
Polarization of a solution by a radical contained in a solid matrix is an attractive technology to significantly increase NMR sensitivity. Here, Dynamic Nuclear Polarization is efficiently induced by the homogeneous distribution of nitroxide radicals in the mesopores of a silica material and the fine-tuning of the total concentration and the distance between radicals. Balancing all competing effects leads to materials that can polarize solvents or small molecules, thus opening fascinating perspectives towards molecular imaging *in vivo*.



Chiral *N*-Heterocyclic Carbene/Pyridine Ligands for the Iridium-Catalyzed Asymmetric Hydrogenation of Olefins

A. Schumacher, M. Bernasconi, and A. Pfaltz*, *Angew. Chem. Int. Ed.* **2013**, *52*, 7422. University of Basel

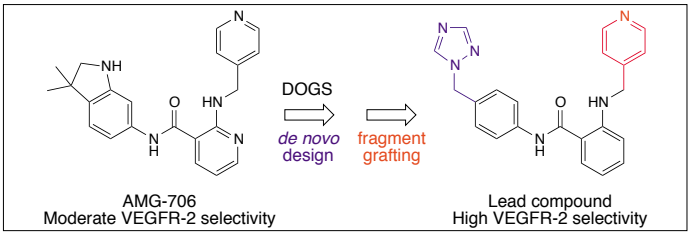
Chiral iridium complexes offer an attractive alternative to rhodium- and ruthenium-based catalysts for the enantioselective hydrogenation of olefins because they do not require a coordinating functional group in the substrate. Pfaltz *et al.* present iridium catalysts containing *N*-heterocyclic carbene (NHC)/pyridine ligands. These catalysts display high catalytic activity and excellent enantioselectivity in the hydrogenation of various olefins. Importantly, the strong donating properties of the NHC significantly decrease the acidity of the Ir–H moiety, thus allowing the hydrogenation of thus far challenging acid-sensitive substrates.



Steering Target Selectivity and Potency by Fragment-Based *De Novo* Drug Design

T. Rodrigues, T. Kudoh, F. Roudnicky, Y. F. Lim, Y.-C. Lin, C. P. Koch, M. Seno, M. Detmar, and G. Schneider*, *Angew. Chem. Int. Ed.* **2013**, *52*, 10006. ETH Zürich

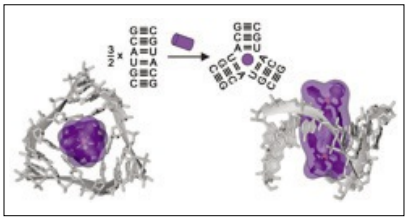
The computer-aided design and *in silico* screening of drug candidates enables faster lead development for specific drug targets. The vascular endothelial growth factor receptor-2 (VEGFR-2) has been identified as a drug target for antiangiogenic therapy. By utilizing the DOGS software (*D*esign *O*f *G*enuine *S*tructures) and starting from the patented VEGFR-1/2 inhibitor AMG-706, the authors created a library of remarkable structural diversity. By selecting two compounds with related structures to AMG-706 and elaborating one further, they identified a lead compound (IC_{50} = 64 nM) with the highest kinase selectivity profile known to date among VEGFR-2 inhibitors.



Binding of a Designed Anti-cancer Drug to the Central Cavity of an RNA Three-Way Junction

S. Phongtongpasuk, S. Paulus, J. Schnabl, R. K. O. Sigel*, B. Spingler*, M. J. Hannon*, and E. Freisinger*, *Angew. Chem. Int. Ed.* **2013**, *52*, 11513. University of Zurich, University of Birmingham

In the past fifty years, DNA has been a privileged target for transition metal complexes. In stark contrast, much less is known about their binding to RNA. The two teams from Zurich and Birmingham describe a supramolecular architecture resulting from the inclusion of a chiral cylindrical di-iron(II) complex within an RNA three-way junction (3WJ). The binding is investigated by X-ray crystallography as well as in solution. Despite their very different morphology, the cylinder is found to bind both DNA and RNA 3WJs with similar affinities.



Prepared by Christoph Daeppen, Adrian von der Höh, Valentin Köhler, Raphael Reuter, Mariana Spulber and Thomas R. Ward*

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