

Swiss Science Concentrates

A CHIMIA Column

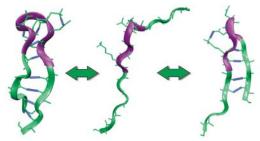
Short Abstracts of Interesting Recent Publications of Swiss Origin

The Unfolded Ensemble and Folding Mechanism of the C-terminal GB1 β -Hairpin

M. Bonomi, D. Branduardi*, F. L. Gervasio*, and M. Parrinello, *J. Am. Chem. Soc.* **2008**, *130*, 13938

ETH Zürich (USI Campus, Lugano)

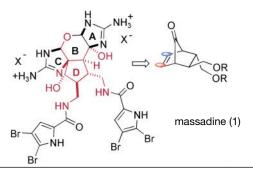
The water-soluble β -hairpin, namely the C-terminal domain of immunoglobulin binding protein GB1, is intensely studied to help understand the factors that govern β -sheet folding. In this article, new light is shed by means of advanced molecular dynamics simulations. The authors show that the folding mechanism is a multiscale process where the turn region conformation leads to two different energy pathways that are connected by elongated structures; structures are fully characterized in the article. This perspective is fully consistent with experimental evidence while it redefines the nature of the unfolded state.



Enantioselective Synthesis of the Carbocyclic D-Ring Subunit of Massadine

A. Breder, G. M. Chinigo, A. W. Waltman, and E. M. Carreira*, *Angew. Chem.*, *Int. Ed.* **2008**, *47*, 8514 ETH Zürich

Pyrrole-imidazole marine alkaloids have attracted considerable attention as a consequence of their complex architecture and potent biological activity. In this article, an efficient asymmetric synthesis of the D-ring subunit embedded in massadine (1) is presented. It includes: application of a cationic norbornyl rearrangement, ozonolytic cleavage displaying remarkable end-group differentiation, and a carboxy-inversion reaction for the installation of the key hindered secondary alcohol. The construction of the target intermediate was realized with an overall yield of 8% in a sequence of 24 linear steps (average: ~90% per step).

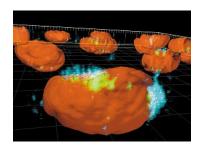


Superparamagnetic Nanoparticles as a Powerful Systems Biology Characterization Tool in the Physiological Context

J. Salaklang, B. Steitz, A. Finka, C. P. O'Neil, M. Moniatte, A. J. van der Vlies, T. D. Giorgio, H. Hofmann, J. A. Hubbell, and A. Petri-Fink*, *Angew. Chem., Int. Ed.* **2008**, *47*, 7857

EPF Lausanne; Vanderbilt University, USA

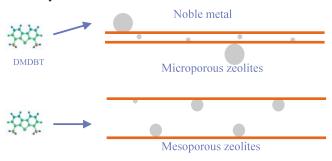
Recently, functionalized superparamagnetic iron oxide nanoparticles (SPIONs) have been utilized for protein separation and therapeutic delivery of DNA and drugs. In this article, SPIONs bearing a mitochondrial targeting peptide (MTP), a cyclic RGD peptide for internalization (cRGD), and a fluorophore for tracking were prepared to target mitochondria. After magnetic isolation from the cells, 48 proteins were identified by mass spectrometry to be interacting with the MTP-cRGD-SPIONs in a network that consists of 308 interactions.



Hydrodesulfurization of 4, 6-Dimethyldibenzothiophene over Noble Metals Supported on Mesoporous Zeolites

Y. Sun and R. Prins*, Angew. Chem., Int. Ed. 2008, 47, 8478 ETH Zürich

The reduction of the sulfur content in gasoline and diesel fuel is a subject of intense investigation for environmental reasons. In this article, it is shown that noble-metal (Pt, Pd) catalysts supported on mesoporous zeolites are much more efficient than on microporous zeolites and $\gamma\text{-Al}_2\text{O}_3$ for the hydrodesulfurization of 4,6-dimethyl-dibenzothiophene (DMBT), a classical contaminant. This increased efficiency arises because the relatively large DMBT molecules can fit into the relatively large pores of the mesoporous zeolites and so reach many active centers.



Prepared by M. Austeri, R. Bach, N. Mehanna, A. Sharma, F. Torricelli, W. Zeghida, J. Lacour **Do you want your article to appear in this SWISS SCIENCE CONCENTRATES highlight?** Please contact concentrates@chimia.ch