Spotlights ...

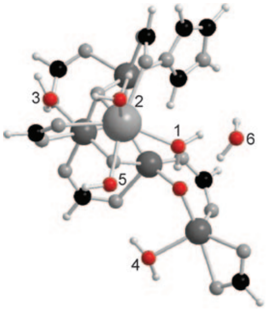
On these pages, we feature a selection of the excellent work that has recently been published in our sister journals. If you are reading these pages on a computer, click on any of the items to read the full article. Otherwise please see the DOIs for easy online access through Wiley Online Library.

Photosystem II

S. Petrie, R. Stranger,* R. J. Pace

Hydration Preferences for Mn_4Ca Cluster Models of Photosystem II: Location of Potential Substrate–Water Binding Sites

Water ways: Density functional calculations are reported on a set of three model structures of the Mn_4Ca cluster in the water-oxidizing complex of Photosystem II (see figure). The preferred hydration sites across five oxidation states and all feasible magnetic-coupling arrangements have been explored to identify the most likely substrate–water binding sites.



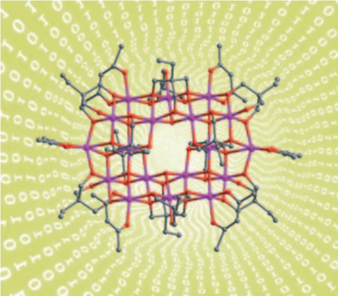
Chem. Eur. J.
DOI: **10.1002/chem.201001132**

Manganese Clusters

C.-M. Liu,* D.-Q. Zhang, D.-B. Zhu

Ring Like Octadecanuclear Mixed-valence Manganese Cluster with a Spin Ground State of 20

Big spin! In the presence of 2-aminopropane-1,2-diol, the reaction of 1,1,1-tris-(hydroxylmethyl)propane and $Mn(acac)_2$ in MeCN yielded a novel ring like octadecanuclear mixed-valence manganese cluster complex, which exhibits an overall ferromagnetic property and possesses a large spin ground state of 20.



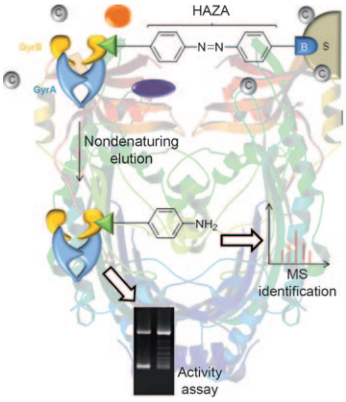
Chem. Asian J.
DOI: **10.1002/asia.201000511**

Proteomics

G. Budin, M. Moune-Dimala, G. Leriche, J.-M. Saliou, J. Papillon, S. Sanglier-Cianférani, A. Van Dorsselaer, V. Lamour,* L. Brino,* A. Wagner*

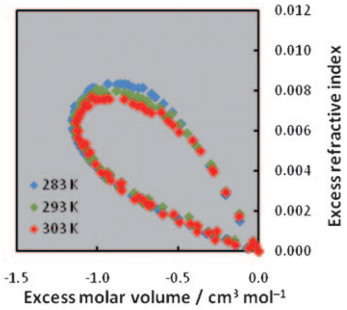
Nondenaturing Chemical Proteomics for Protein Complex Isolation and Identification

Controlled fishing: Mild cleavage conditions enabled by the use of the HAZA linker allowed smooth release of captured proteins under non-denaturing conditions. A DNA gyrase complex A2B2 was enriched then released in native form by chemical cleavage while preserving its enzymatic activity. This procedure allows the capture and release of endogenous protein complexes under native conditions.



ChemBioChem
DOI: **10.1002/cbic.201000574**

Liquid Mixtures

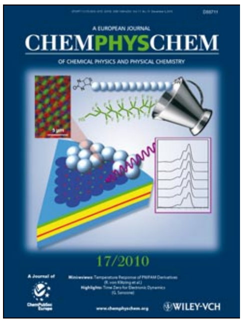


J. C. R. Reis,* I. M. S. Lampreia, Â. F. S. Santos, M. L. C. J. Moita, G. Douhéret

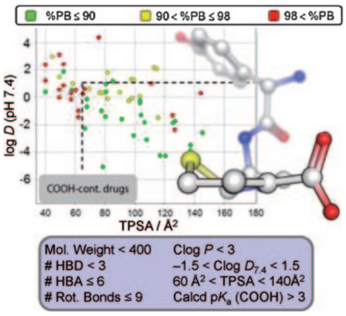
Refractive Index of Liquid Mixtures: Theory and Experiment

A thermodynamic formalism is developed to analyse refractive index data of liquid mixtures. A positive change of refractive index upon ideal mixing is predicted and interpreted in terms of London dispersion forces. The correlation between excess refractive indices and excess molar volumes is pear-shaped for an amphiphile/water system at different temperatures (see picture).

ChemPhysChem
DOI: **10.1002/cphc.201000566**



Computational Medicinal Chemistry



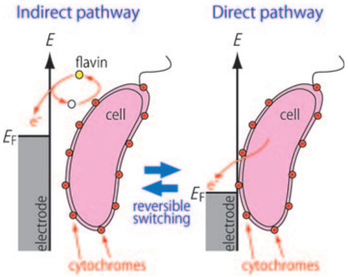
A. Böcker, P. R. Bonneau,* O. Hucke, A. Jakalian, P. J. Edwards

Development of Specific "Drug-Like Property" Rules for Carboxylate-Containing Oral Drug Candidates

Acid rules! The carboxylate moiety is an important pharmacophore in medicinal chemistry and is often irreplaceable in drug–target interactions. Based on an analysis of key physicochemical and ADMET-PK properties of oral drugs, we propose "drug-like" property rules for carboxylic acids that can help in the design of better drug candidates and decrease liabilities generally associated with acids.

ChemMedChem
DOI: **10.1002/cmdc.201000355**

Electron Transfer

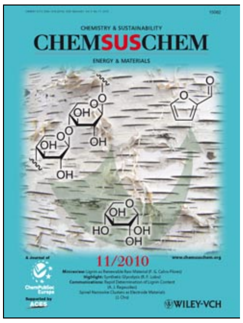


H. Liu, S. Matsuda, S. Kato, K. Hashimoto,* S. Nakanishi*

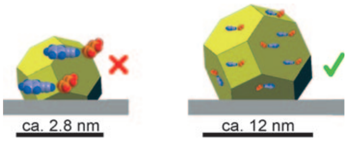
Redox-Responsive Switching in Bacterial Respiratory Pathways Involving Extracellular Electron Transfer

Go with the flow: *Shewanella* is capable of transferring respiratory electrons to solid-state metal-oxides through physical contact (direct pathway) or by using electron shuttles (indirect pathway). We reveal, by using an electrochemical approach, that these pathways are switched depending on the redox state of the cytochromes.

ChemSusChem
DOI: **10.1002/cssc.201000213**



Cross-Coupling Reactions

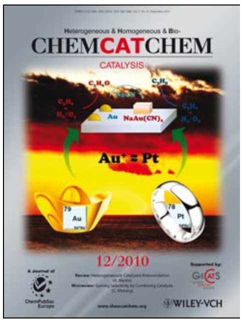


G. Kyriakou, S. K. Beaumont, S. M. Humphrey, C. Antonetti, R. M. Lambert*

Sonogashira Coupling Catalyzed by Gold Nanoparticles: Does Homogeneous or Heterogeneous Catalysis Dominate?

Some kind of 'geneous: Gold nanoparticles catalyze the Sonogashira cross coupling of iodobenzene with phenylacetylene. Large particles are much more selective than small ones and gold species leached into solution are catalytically inert, consistent with the view that the dominant reaction pathway is heterogeneous.

ChemCatChem
DOI: **10.1002/cctc.201000154**

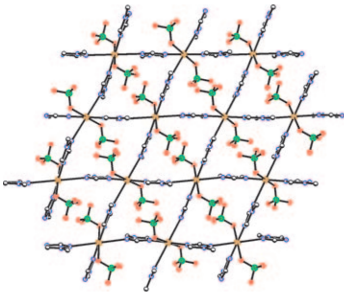


Models for Metal-Mediated Base Pairs

D. A. Megger, J. Kösters, A. Hepp, J. Müller*

Silver(I) and Mercury(II) Complexes with 1-Methyl-1,2,4-triazole as Models for Metal-Mediated Base Pairs – Formation of Discrete Complexes in Solution vs. One- and Two-Dimensional Coordination Polymers in the Solid State

The metal ion coordination behaviour of 1-methyl-1*H*-1,2,4-triazole, serving as a model for the artificial 1,2,4-triazole nucleoside, has been determined. In solution, the 2:1 stoichiometry necessary for the formation of metal-mediated base pairs is adopted. In accordance with stability constants, one- and two-dimensional cationic coordination polymers are observed in the solid state.



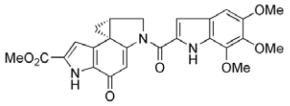
Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.201000509**

Novel Fluorescence-Labelled Prodrugs

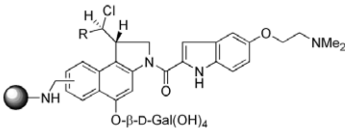
L. F. Tietze,* F. Behrendt, F. Major, B. Krewer, J. M. von Hof

Synthesis of Fluorescence-Labelled Glycosidic Prodrugs Based on the Cytotoxic Antibiotic Duocarmycin

Fluorescence-labelled compounds can be used for verification of interaction with cellular targets on the molecular level by use of confocal laser scanning microscopy for cell cultures and the Explore-Optics instrument (GE) for mice. The described fluorescence-labelled glycosidic prodrugs based on the cytotoxic antibiotic duocarmycine SA have high potential for selective treatment of cancer.



(+)-Duocarmycine SA



Eur. J. Org. Chem.
DOI: **10.1002/ejoc.201000966**