Spotlights ...

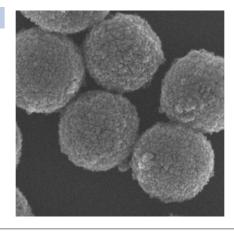
Hollow Spheres

H. Xu, W. Wei, C. Zhang, S. Ding, X. Qu, J. Liu, Y. Lu, Z. Yang*

Low-Temperature Facile Template Synthesis of Crystalline Inorganic Composite Hollow Spheres

Chem. Asian J.

DOI: 10.1002/asia.200700017



Nothing in it! Composite hollow spheres of TiO₂ (shown), BaTiO₃, and SrTiO₃ with varied crystalline phases and compositions can be synthesized under mild conditions. The sulfonated polystyrene gel templates used ensure that the crystalline hollow spheres grow without damage to their shells.

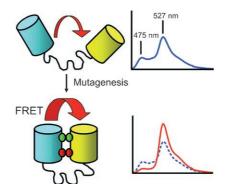
FRET Sensors

J. L. Vinkenborg, T. H. Evers, S. W. A. Reulen, E. W. Meijer, M. Merkx*

Enhanced Sensitivity of FRET-Based Protease Sensors by Redesign of the GFP Dimerization Interface

ChemBioChem

DOI: 10.1002/cbic.200700109



Close encounters. Sensor proteins based on fluorescence resonance energy transfer (FRET) often display a modest change in emission ratio upon activation. Here, we show that promoting intramolecular interactions between donor and acceptor fluorescent domains is an attractive new strategy for increasing the ratiometric change in FRET-based protease sensors.

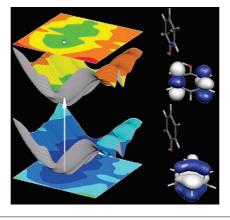
Franck-Condon Analysis

R. Brause, M. Santa, M. Schmitt,*
K. Kleinermanns*

Determination of the Geometry Change of the Phenol Dimer upon Electronic Excitation

Chem Phys Chem

DOI: 10.1002/cphc.200700127



Analysing phenol: The structural changes of phenol upon electronic excitation are quantified experimentally and theoretically. A Franck–Condon analysis of the fluorescence emission spectra confirms the local nature of the excitation.

Cheminformatics

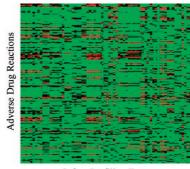
A. Bender,* J. Scheiber, M. Glick, J. W. Davies, K. Azzaoui, J. Hamon, L. Urban, S. Whitebread, J. L. Jenkins

Analysis of Pharmacology Data and the Prediction of Adverse Drug Reactions and Off-Target Effects from Chemical Structure

ChemMedChem

DOI: 10.1002/cmdc.200700026

Preclinical Safety Pharmacology attempts to anticipate adverse drug reactions (ADRs) during early phases of drug discovery by testing compounds in simple, in vitro binding assays. In this paper we describe the successful application of cheminformatics methods to predict adverse side effects of drugs to accelerate drug discovery and decrease late stage attrition in drug discovery projects.



Safety Profiling Targets



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An empty low-lying $3\sigma^*$ orbital is responsible for the catalytic activity of oxidoiron(IV) compounds in alkane hydroxylation. We study the influence of the ligand environment on the spin state and catalytic activity of simple systems, correlating these properties to the strength of the electron donation from the ligands, and in particular, we prove that systems with *weak* equatorial and axial donor ligands show superior catalytic activity.

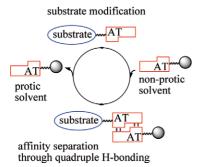
High-Valent Oxidoiron(IV) Systems

L. Bernasconi,* M. J. Louwerse, E. J. Baerends*

The Role of Equatorial and Axial Ligands in Promoting the Activity of Non-Heme Oxidoiron(IV) Catalysts in Alkane Hydroxylation

Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.200601238



A new workup and purification method based on quadruple hydrogen-bonding interactions is reported. Substrates with a hydrogen-bonding affinity tag were conveniently separated from a reaction mixture and purified using a resin with self-complementary affinity tags. Ugi reaction products and substitution products were successfully purified by this affinity separation protocol.

Affinity Separation

B. W. T. Gruijters, J. M. M. Verkade, F. L. van Delft, R. P. Sijbesma, P. H. H. Hermkens, F. P. J. T. Rutjes*

A Novel Purification Method in Organic Synthesis Using Hydrogen Bonding

Eur. J. Org. Chem.

DOI: 10.1002/ejoc.200700242

Unusual cleavage: A series of mononuclear or dinuclear Fe^{II}—phenylpyruvate enolate complexes that contain tetradentate tris (6-methyl-2-pyridylmethyl) amine (6-Me₃-TPA) or tridentate benzyl bis (2-quinolinylmethyl) amine (Bn-BQA) ligands are reported. The phenylpyruvate complexes react with dioxygen to undergo oxidative C2—C3 bond cleavage of phenylpyruvate (see scheme).

Iron Complexes

T. K. Paine, J. England, L. Que, Jr.*

Iron-Catalyzed C2—C3 Bond Cleavage of Phenylpyruvate with O₂: Insight into Aliphatic C—C Bond Cleaving Dioxygenases

Chem. Eur. J.

DOI: 10.1002/chem.200601844



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5265