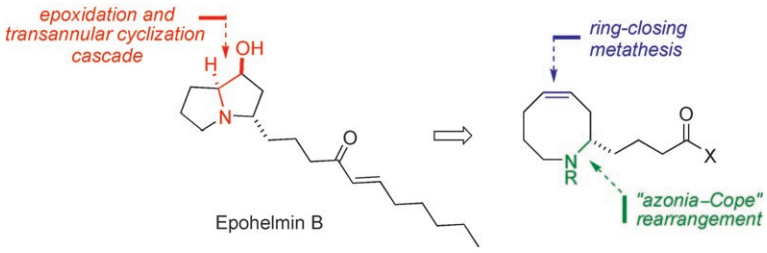
Total Synthesis

A. Fürstner,* A. Korte

Total Synthesis of Epohelmin B and Its Analogues



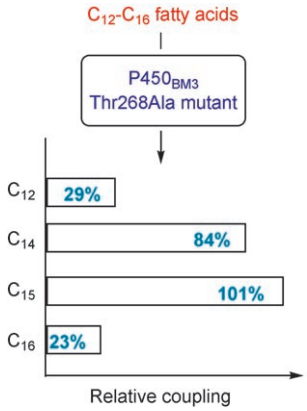
Lower your cholesterol: Epohelmin B is an interesting new lead in the quest for selective inhibitors of lanosterol synthase, the key enzyme in the cholesterol biosynthesis pathway in humans. A highly efficient and largely reagent-controlled total synthesis of this pyrrolizidine alkaloid is presented, which also opens access to a first collection of epohelmin-like compounds.

Chem. Asian J.
DOI: **10.1002/asia.200700288**

Enzyme Catalysis

M. J. Cryle, J. J. De Voss*

The Role of the Conserved Threonine in $P450_{BM3}$ Oxygen Activation: Substrate-Determined Hydroxylation Activity of the Thr268Ala Mutant



Handle with care: The ability of a mutant $P450_{BM3}$ that lacks a catalytically important threonine residue (Thr268Ala) to hydroxylate fatty acids has been found to be dependant upon the chain length of the substrate (see graph). This indicates that caution is required in assuming a loss of activity with such threonine to alanine mutants of P450 enzymes, as activity with certain substrates might be maintained.

ChemBioChem
DOI: **10.1002/cbic.200700537**

Ionic Liquids

B. L. Bhargava, M. L. Klein, S. Balasubramanian*

Structural Correlations and Charge Ordering in a Room-Temperature Ionic Liquid

Molecular dynamics simulations of a room-temperature ionic liquid show evidence of charge ordering (see figure). The intermolecular structure is investigated by calculating the neutron- and X-ray-weighted structure factors.

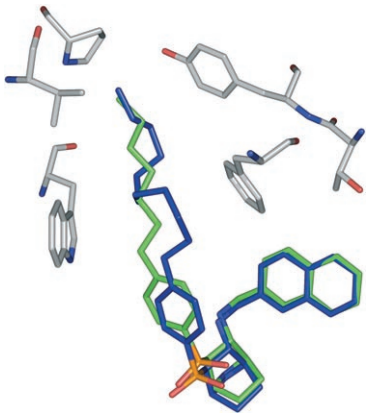
ChemPhysChem
DOI: **10.1002/cphc.200700666**

Active Site Modeling

M. Zürcher, T. Gottschalk, S. Meyer, D. Bur, F. Diederich*

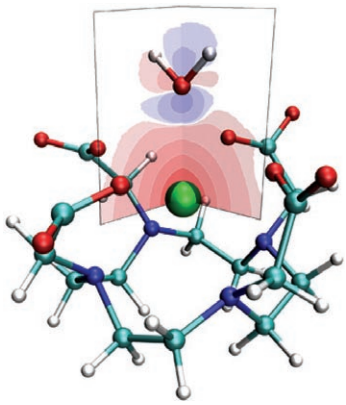
Exploring the Flap Pocket of the Antimalarial Target Plasmepsin II: The "55% Rule" Applied to Enzymes

The flap pocket of plasmepsin II was examined in terms of molecular recognition properties. It was found that *n*-alkyl chains of different length bind best to this cavity when the packing coefficient is around 0.55, and it is suggested that the chains adopt their conformation in order to fill the available space properly. The concept of ideal volume occupancy previously demonstrated for synthetic guest–host systems has been applied to an enzyme environment.



ChemMedChem
DOI: **10.1002/cmdc.200700236**

Fundamental parameters for nuclear spin relaxation such as quadrupole coupling constants and hyperfine interaction tensors can be obtained from quantum chemical calculations combined with molecular dynamics simulations. Recent results are reviewed on the Gd^{3+} ion in aqueous solution and on the MRI contrast agent $[Gd(DOTA)(H_2O)]^-$.

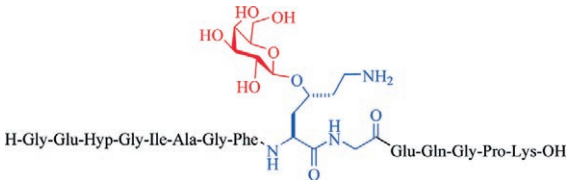


MRI Contrast Agents

O. V. Yazyev, L. Helm*

Nuclear Spin Relaxation Parameters of MRI Contrast Agents – Insight from Quantum Mechanical Calculations

Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.200701013**



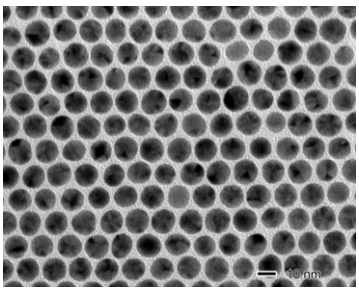
The preparation of a *N*-Fmoc-protected galactosylated (2*S*,4*R*)-4-hydroxylysine derivative and its incorporation into the sequence of an immunodominant glycopeptide from type II collagen is described. The synthesis of the 4-hydroxylysine aglycon started from (2*S*,4*S*)-4-hydroxy-6-oxo-1,2-piperidinedicarboxylate and involved the formation of a γ-lactone and its *N*-acylation with glycyl esters.

Glycopeptide Synthesis

J. Marin, J.-P. Briand, G. Guichard*

Synthesis of a Galactosylated 4-Hydroxylysine Building Block and Its Incorporation into a Collagen Immunodominant Glycopeptide

Eur. J. Org. Chem.
DOI: **10.1002/ejoc.200700806**



Control your size! Gold(I) halides, including AuCl and AuBr, were employed for the first time as precursors in the preparation of Au nanoparticles (see figure) with a narrow size distribution through a facile synthetic approach.

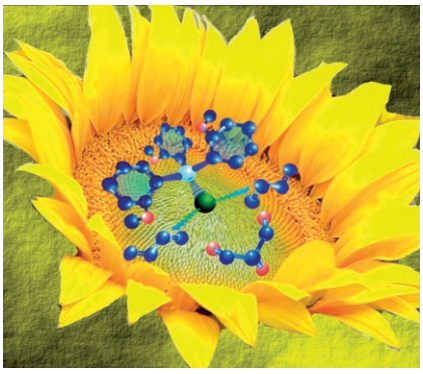
Gold

X. Lu, H.-Y. Tuan, B. A. Korgel, Y. Xia*

Facile Synthesis of Gold Nanoparticles with Narrow Size Distribution by Using AuCl or AuBr as the Precursor

Chem. Eur. J.
DOI: **10.1002/chem.200701570**

The chain gang: Crude glycerol, a by-product in the production of biodiesel, can be telomerized with 1,3-butadiene to form C_8-chain ethers. The development of suitable catalyst systems for the direct telomerization of crude glycerol at the biodiesel plant provides a route to useful building blocks from cheap starting materials for commercially valuable products such as detergents and surfactants.



Glycerol Conversion

R. Palkovits, I. Nieddu, R. J. M. Klein Gebbink, B. M. Weckhuysen*

Highly Active Catalysts for the Telomerization of Crude Glycerol with 1,3-Butadiene

ChemSusChem
DOI: **10.1002/cssc.200700147**

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