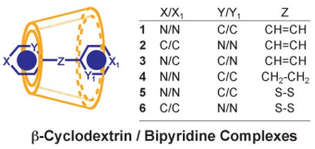
Host–Guest Systems

Y.-L. Zhao, D. Benítez, I. Yoon, J. F. Stoddart*

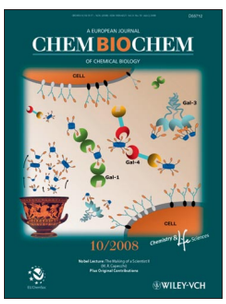
Inclusion Behavior of β-Cyclodextrin with Bipyridine Molecules: Factors Governing Host-Guest Inclusion Geometries

Guest Effect: The differences of nitrogen atom positions and the bridge bonds linked to two pyridine rings of some bipyridine guests can significantly affect the binding abilities and inclusion geometries of β-cyclodextrin with the guests in both the solution and solid states.



β-Cyclodextrin / Bipyridine Complexes

Chem. Asian J.
DOI: **10.1002/asia.200800373**

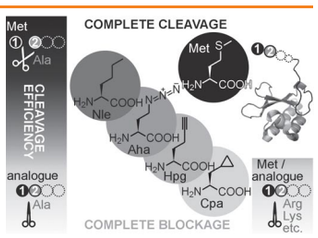


Post-translational Modification

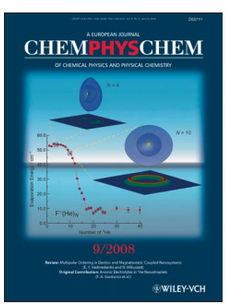
B. Wiltschi, L. Merkel, N. Budisa*

Fine Tuning the N-Terminal Residue Excision with Methionine Analogues

The amino acid composition of the N terminus of a protein determines whether the first methionine residue is excised or not. Its replacement by a chemically distinct noncanonical analogue by an expanded genetic code affects the overall efficiency of this process. Recent advances have provided novel insight into the N-terminal residue excision rules; this certainly will enrich the repertoire of chemical protein engineering.



ChemBioChem
DOI: **10.1002/cbic.200800605**

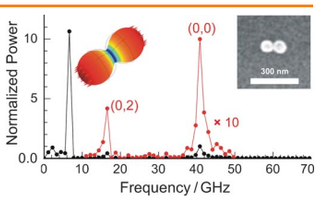


Gold Nanoparticles

A. L. Tchebotareva, M. A. v. Dijk, P. V. Ruijgrok, V. Fokkema, M. H. S. Hesselberth, M. Lippitz, M. Orrit*

Acoustic and Optical Modes of Single Dumbbells of Gold Nanoparticles

Gold vibrations: A new elastic (stretching) mode, appearing in individual dumbbells of gold nanospheres at 5–7 GHz (see figure), is a function of the contact area. This can be used to estimate the contact area between the particles, which plays an important role in the local enhancement of electromagnetic fields in such nanoantenna structures.



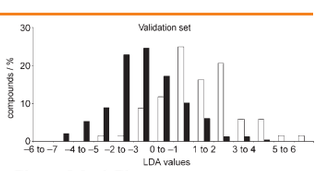
ChemPhysChem
DOI: **10.1002/cphc.200800289**

QSAR Modeling

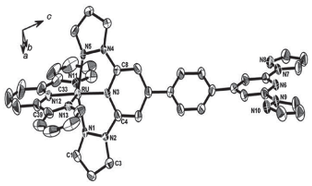
R. Gozalbes,* F. Barbosa, E. Nicolaï, D. Horvath, N. Froloff

Development and Validation of a Pharmacophore-Based QSAR Model for the Prediction of CNS Activity

A QSAR model for the prediction of CNS activity was developed and validated based on data from an in-house database of "drug-like" compounds. The model has demonstrated its applicability for novel chemical structures and its usefulness for the design of CNS-focused compound libraries.



ChemMedChem
DOI: **10.1002/cmdc.200800282**



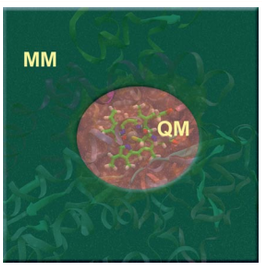
Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.200800628**

Polypyridylruthenium Complexes

F. Schramm, R. Chandrasekar, T. A. Zevaco, M. Rudolph, H. Görls, W. Poppitz, M. Ruben*

(Polypyridyl)ruthenium(II) Complexes Based on a *Back-to-Back* Bis(pyrazolylpyridine) Bridging Ligand

Two ruthenium(II) complexes were synthesised by using a linear *back-to-back* bridging ligand based on a dipyrazolylpyridine coordination unit. The structural, electrochemical and spectroscopic properties show that this new bridging ligand can be considered as structural and electronic alternative to the widely used terpyridine-based bridging ligand systems.



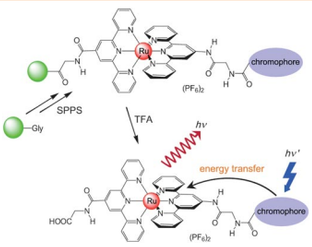
Angew. Chem. Int. Ed.
DOI: **10.1002/anie.200802019**

Theoretical Chemistry

H. M. Senn,* W. Thiel*

QM/MM Methods for Biomolecular Systems

Two are better than one: Quantum mechanics/molecular mechanics (QM/MM) methods are the state-of-the-art computational technique for treating reactive and other "electronic" processes in biomolecular systems. This Review presents the general methodological aspects of the QM/MM approach, its use within optimization and simulation techniques, and its areas of application, always with a biomolecular focus.



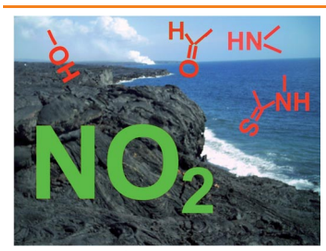
Chem. Eur. J.
DOI: **10.1002/chem.200801864**

Solid-Phase Synthesis

K. Heinze,* K. Hempel

Solid-Phase Synthesis of Peptide Libraries Combining α-Amino Acids with Inorganic and Organic Chromophores

It works for metals too! Solid-phase peptide synthesis procedures were employed for the selective stepwise assembly of bis(terpyridine)ruthenium(II) chromophores and organic antennas to yield peptidic dyads. Electrochemistry, absorption spectroscopy and DFT calculations suggest electronically isolated chromophores in the ground state, while energy transfer processes from the organic dye to the ruthenium complex occur in the excited dyads (see scheme).



ChemSusChem
DOI: **10.1002/cssc.200800193**

Sustainable Chemistry

M. R. Naimi-Jamal,* H. Hamzeali, J. Mokhtari, J. Boy, G. Kaupp*

Sustainable Synthesis of Aldehydes, Ketones or Acids from Neat Alcohols Using Nitrogen Dioxide Gas, and Related Reactions

Simply sustainable: Ubiquitous NO_2 is a poisonous gas, yet a highly reactive and chemospecific oxidation reagent for various functional groups under solvent-free conditions. The yield is quantitative in most cases, while further reactions are impeded by salt formation or hydrogen bonding with the reaction gas. The products are isolated pure enough for further use after simple evaporation of the reaction gases.