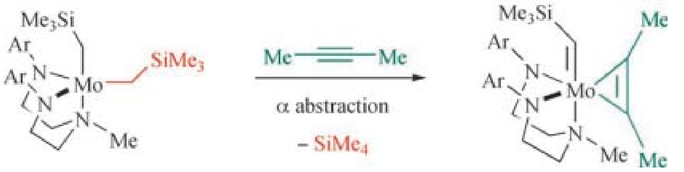
SPOTLIGHTS …

Dialkyl Complexes

A. S. Hock, R. R. Schrock*

Oxidative Reactions of the $\mathrm{Mo^{IV}}$ Dialkyl Complex $[\{(3\text{-}CF_3C_6H_4NCH_2CH_2)_2\text{-}NMe\}Mo(CH_2SiMe_3)_2]$

Chem. Asian J.
DOI: **10.1002/asia.200700093**



Silicon replacement therapy: $[(CF_3N_2NMe)Mo(CH_2SiMe_3)_2]$ ($(CF_3N_2NMe)^{2-} = [(3\text{-}CF_3C_6H_4\text{-}NCH_2CH_2)_2NMe]^{2-}$) reacts with 2-butyne, cyclohexene sulfide, and C_2Cl_6 to give $[(CF_3N_2NMe)Mo(CHSiMe_3)(\eta^2\text{-}MeC{\equiv}CMe)]$, $[\{(CF_3N_2NMe)MoS\}_2]$, and $[\{(CF_3N_2NMe)Mo(CSiMe_3)Cl\}_2]$, respectively. α-H abstraction of $\mathrm{Mo^{VI}}$ to yield (initially) $Mo{=}CHSiMe_3$ and $SiMe_4$ is the proposed route for these reactions.

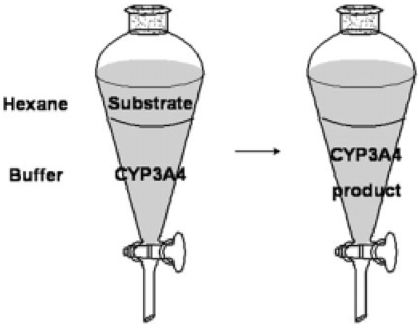
Biocatalysis

A. Chefson, K. Auclair*

CYP3A4 Activity in the Presence of Organic Cosolvents, Ionic Liquids, or Water-Immiscible Organic Solvents

ChemBioChem
DOI: **10.1002/cbic.200700128**

Selective hydroxylation of inactivated C–H bonds. While tolerating only low amounts of water-miscible cosolvents or water-miscible ionic liquids, human CYP3A4 functions acceptably in organic solvents, with optimum activity in buffer/hexane biphasic solvent systems; this offers considerable potential for future applications of P450s in synthesis.



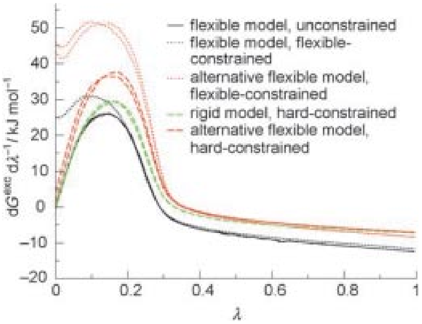
Computational Power

M. Christen, C. D. Christ,
W. F. van Gunsteren*

Free Energy Calculations Using Flexible-Constrained, Hard-Constrained and Non-Constrained Molecular Dynamics Simulations

ChemPhysChem
DOI: **10.1002/cphc.200700176**

Turning the water into methanol: One of the most important quantities that can be obtained from simulations are relative free energies. The difference in the free energy of liquid water and liquid methanol is calculated by molecular dynamics simulations using three different models for water and methanol: a flexible model, an alternative flexible model and a rigid model (see picture).

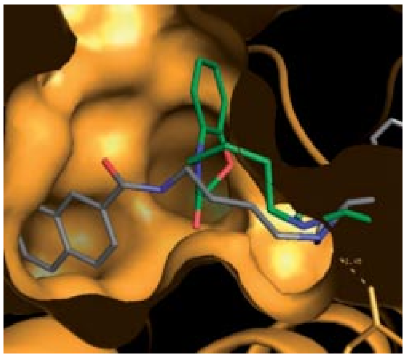


Compound Libraries

A. Böcker, B. C. Sasse , M. Nietert,
H. Stark, G. Schneider*

GPCR Targeted Library Design: Novel Dopamine D_3 Receptor Ligands

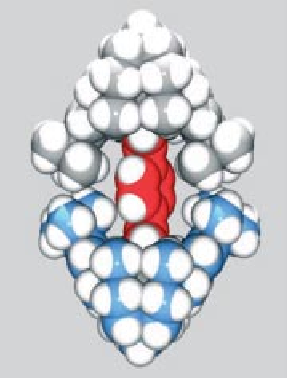
ChemMedChem
DOI: **10.1002/cmdc.200700067**



GPCR-focused compound libraries were designed by strategic iterative virtual screening. The most potent ligands yielded K_i values of 65 nM at the dopamine D_3 receptor subtype. Two potential binding modes were observed for receptor antagonists in a homology-based model of the dopamine D_3 receptor. Results demonstrate opportunities for a combination of different virtual screening methods in early stages of GPCR drug discovery for new lead finding.

Ligand Encapsulation

The ability of 4,4′-bipyrazolate type ligands to link dinuclear LNi_2 units has been examined. The formation of the Ni_4 complexes depends critically on the steric bulkiness of the supporting ligand L and the length of the organic spacer between the connecting heterocycles. The ability of the bipyrazolate moiety to transmit magnetic exchange interactions has also been examined.

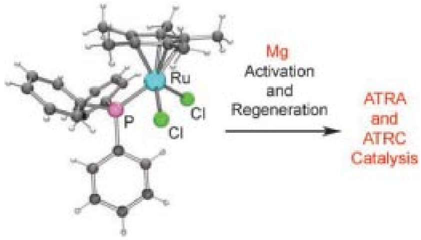


V. Lozan, P. Y. Solntsev, G. Leibeling, K. V. Domasevitch,* B. Kersting*

Tetranuclear Nickel Complexes Composed of Pairs of Dinuclear LNi_2 Fragments Linked by 4,4′-Bipyrazolyl, 1,4-Bis(4′-pyrazolyl)benzene, and 4,4′-Bipyridazine: Synthesis, Structures, and Magnetic Properties

Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.200700317**

Ruthenium



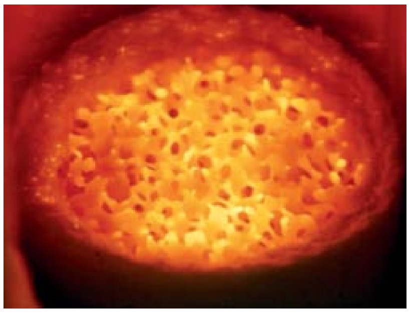
Radical Reactions: A combined catalyst system of the Ru complex [$RuCl_2Cp^*(PPh_3)$] (Cp*: pentamethylcyclopentadienyl) with magnesium allows atom-transfer radical addition (ATRA) and cyclization (ATRC) reactions to be performed with exceptional efficiency under mild conditions (see scheme).

K. Thommes, B. Içli, R. Scopelliti, K. Severin*

Atom-Transfer Radical Addition (ATRA) and Cyclization (ATRC) Reactions Catalyzed by a Mixture of [$RuCl_2Cp^*(PPh_3)$] and Magnesium

Chem. Eur. J.
DOI: **10.1002/chem.200700442**

Heterogeneous Catalysis



Breaking the coke habit: By coupling thermal decomposition with catalytic partial oxidation, an effective method has been developed to convert solid biomass such as cellulose into synthesis gas (see photo of a hot Rh catalyst surface). Not only is the process fast (<70 ms), it also avoids the formation of coke, which is known to deactivate catalyst surface sites and block surface reactions.

P. J. Dauenhauer, B. J. Dreyer, N. J. Degenstein, L. D. Schmidt*

Millisecond Reforming of Solid Biomass for Sustainable Fuels

Angew. Chem. Int. Ed.
DOI: **10.1002/anie.200701238**

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