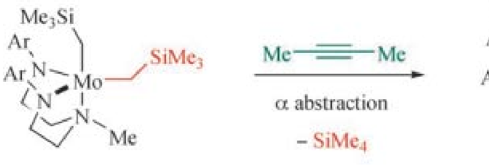
# SPOTLIGHTS …

## Dialkyl Complexes

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

### Oxidative Reactions of the $Mo^{IV}$ 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 $[(CF_3N_2NMe)Mo\text{-}(CHSiMe_3)(\eta^2\text{-}MeC{\equiv}CMe)]$, $[\{(CF_3N_2NMe)MoS\}_2]$, and $[\{(CF_3N_2NMe)Mo(CSiMe_3)Cl\}_2]$, respectively. α-H abstraction of $Mo^{VI}$ to yield (initially) $Mo{=}CHSiMe_3$ and $SiMe_4$ is the proposed route for these reactions.

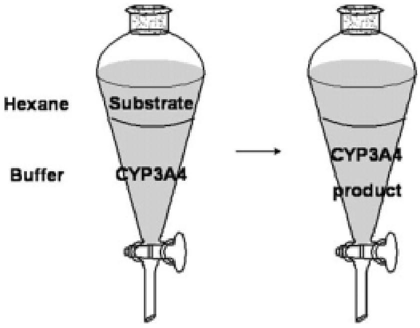
## Biocatalysis

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.



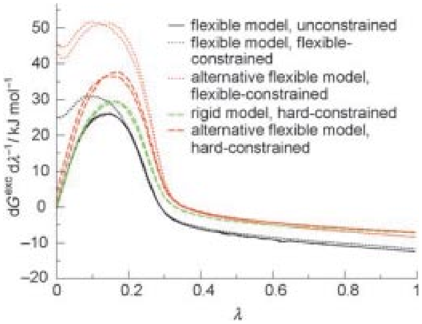
## Computational Power

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).

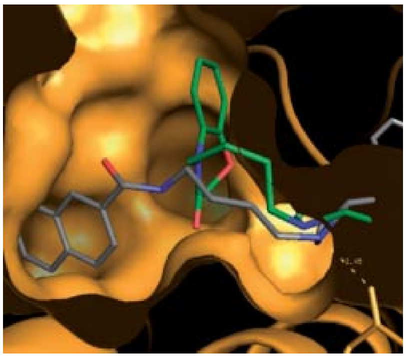


## Compound Libraries

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.

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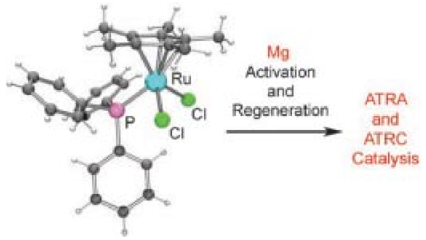
## *Ruthenium*



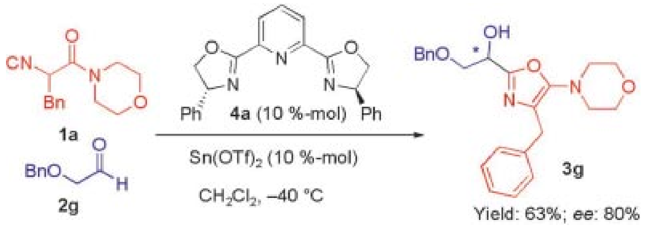
**Radical Reactions**: A combined catalyst system of the Ru complex [$RuCl_2Cp^*(PPh_3)$] (Cp*: pentamethylcyclopentadienyl) with magnesium allows atom-transfer radical addition (ATRA) and cyclization (ATRC) reactions to be performed with exceptional efficiency under mild conditions (see scheme).

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**

## *Asymmetric Synthesis*



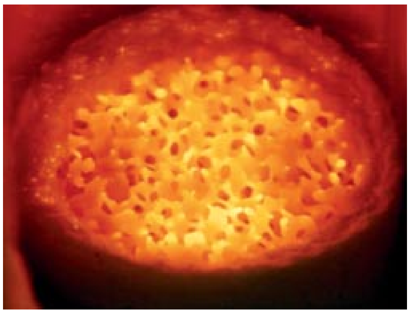
Reactions between α-isocyanoacetamides and aldehydes can be performed at low temperature in the presence of stannous chloride to furnish oxazoles in good to excellent yields. In the presence of the chiral catalyst [Sn-(*R*)-Ph-PyBox]$(OTf)_2$, the reaction between the chelating aldehyde **2g** and **1a** afforded the corresponding 5-aminooxazole **3g** in good yield and enantioselectivity.

S. Wang, M.-X. Wang,* D.-X. Wang, J. Zhu*

**Asymmetric Lewis Acid Catalyzed Addition of Isocyanides to Aldehydes – Synthesis of 5-Amino-2-(1-hydroxyalkyl)oxazoles**

*Eur. J. Org. Chem.*
DOI: **10.1002/ejoc.200700340**

## *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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