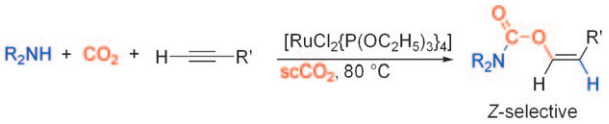
Stereoselective Synthesis

Y. Kayaki, T. Suzuki, T. Ikariya*

Utilization of *N*,*N*-Dialkylcarbamic Acid Derived from Secondary Amines and Supercritical Carbon Dioxide: Stereoselective Synthesis of *Z* Alkenyl Carbamates with a CO_2-Soluble Ruthenium–$P(OC_2H_5)_3$ Catalyst

Chem. Asian J.
DOI: **10.1002/asia.200800204**



An extremely critical condition: The addition of carbamic acids generated from secondary amines and supercritical CO_2 ($scCO_2$) to terminal alkynes proceeds efficiently in the presence of *trans*-$[RuCl_2\{P(OC_2H_5)_3\}_4]$. The CO_2-soluble Ru catalyst affords alkenyl carbamates with high regio- and stereoselectivity and decreases the formation of enynes from the catalytic dimerization of alkynes.

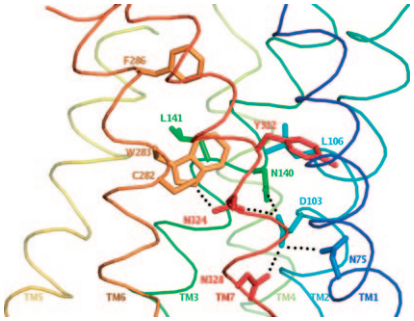
Ligand–Receptor Interactions

A. Gieldon, J. J. Lopez, C. Glaubitz, H. Schwalbe*

Theoretical Study of the Human Bradykinin–Bradykinin B2 Receptor Complex

ChemBioChem
DOI: **10.1002/cbic.200800324**

The forces of stabilization: The interaction of bradykinin (BK) with the bradykinin B2 receptor (B2R) was analyzed by using molecular modeling (MM) and molecular dynamics (MD) simulations. The specific geometries and hydrogen-bonding interactions of the inactive and active (shown) states of the BK receptor were explored in detail, and comparisons to the known partially activated rhodopsin molecule, were made.



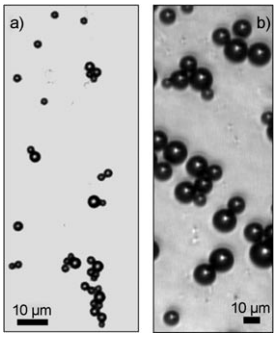
Microbubbles

S. Rossi, G. Waton, M. P. Krafft*

Small Phospholipid-Coated Gas Bubbles Can Last Longer than Larger Ones

ChemPhysChem
DOI: **10.1002/cphc.200800386**

Breaking a creed: Ultrasound attenuation measurements reveal that small microbubbles (see picture, left) with a fluid phospholipid shell and stabilized by a fluorocarbon gas can last longer in aqueous media than larger ones of the same composition (see picture, right). Such small and stable microbubbles may be useful for intravascular oxygen and drug delivery, where the use of microbubbles is promising.

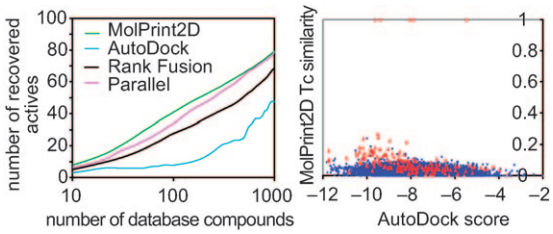


Virtual Screening

L. Tan, H. Geppert, M. T. Sisay, M. Gütschow, J. Bajorath*

Integrating Structure- and Ligand-Based Virtual Screening: Comparison of Individual, Parallel, and Fused Molecular Docking and Similarity Search Calculations on Multiple Targets

ChemMedChem
DOI: **10.1002/cmdc.200800129**



Docking and similarity search calculations using 2D fingerprints were carried out in parallel to identify inhibitors of nine target enzymes. By combining the results of docking and similarity searching, compound recall achieved by the individual methodologies was further increased in several cases. As a compound selection scheme, parallel selection of candidate compounds from docking and similarity search rankings overall produced higher recall than rank fusion.

InterScience
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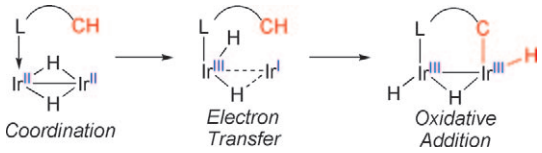


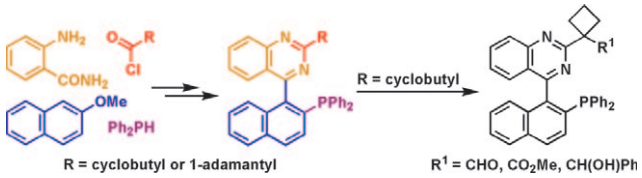
Mild oxidative addition of C–H bonds took place by the reaction of a hydrido-bridged dinuclear iridium(II) complex, $[Cp^*Ir(\mu\text{-}H)]_2$, with donor ligands such as phosphorus compounds and sulfoxides. The proximity of the two iridium centers combined with the characteristic electron configuration (Ir^{II}–Ir^{II}) of $[Cp^*Ir(\mu\text{-}H)]_2$ provides unique reactivities for these systems based on cooperative effects.

C–H Bond Activation

Y. Takahashi, K.-i. Fujita,* R. Yamaguchi*

Mild Oxidative Addition of C–H Bonds to a Hydrido-Bridged Dinuclear Complex of Iridium(II) Induced by the Coordination of Heteroatomic Ligands

Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.200800469**



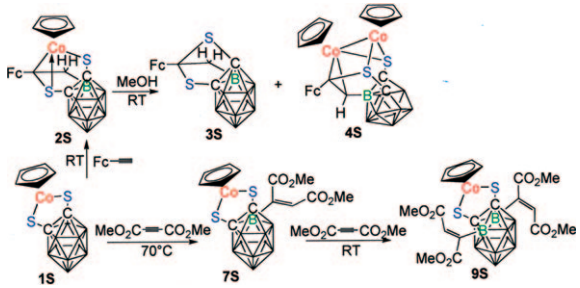
An expedient synthesis and resolution of atropisomeric P,N ligands, 2-cyclobutyl- and 2-(1-adamantyl)-Quinazolinaps, has been developed. The enantioenriched ligands provide good levels of enantioselection (*ee* values up to 89%) by prototypical Pd^{II}-catalyzed allylic alkylation. Further functionalization of 2-cyclobutyl-Quinazolinap has been achieved.

Asymmetric Catalysis

T. Fekner, H. Müller--Bunz, P. J. Guiry*

Synthesis, Resolution, and Application of Cyclobutyl- and Adamantyl-Quinazolinap Ligands

Eur. J. Org. Chem.
DOI: **10.1002/ejoc.200800650**



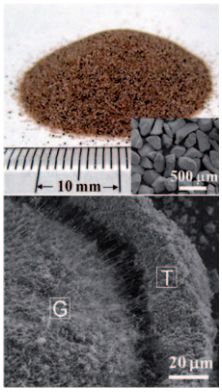
Sandwich course: Reaction of **1S** with HC≡C–Fc (Fc: ferrocenyl) leads to **2S**, which converts to **3S** and **4S** in MeOH (see scheme). However, in the case of $MeO_2CC{\equiv}CCO_2Me$, the stepwise substitution of the *o*-carborane cage at the B(3)/B(6)-positions leads to **7S** and **9S**, respectively.

Half-Sandwich Complexes

B.-H. Xu, X.-Q. Peng, Y.-Z. Li, H. Yan*

Reactions of 16e CpCo Half-Sandwich Complexes Containing a Chelating 1,2-Dicarba-*closo*-dodecaborane-1,2-dichalcogenolate Ligand with Ethynylferrocene and Dimethyl Acetylenedicarboxylate

Chem. Eur. J.
DOI: **10.1002/chem.200801136**



Bucket-and-spade chemistry: An environmentally friendly and highly efficient method for growing multiwalled carbon nanotubes (T) on a large scale has been developed which uses naturally abundant resources, namely garnet sand (G) as a catalyst precursor and support, and city gas as the carbon source. The as-produced carbon nanotubes have a well-crystallized wall structure and are easily separated from the garnet sand by sonication.

Renewable Resources

M. Endo,* K. Takeuchi, Y. A. Kim, K. C. Park, T. Ichiki, T. Hayashi, T. Fukuyo, S. Iinou, D. S. Su, M. Terrones, Mildred S. Dresselhaus

Simple Synthesis of Multiwalled Carbon Nanotubes from Natural Resources

ChemSusChem
DOI: **10.1002/cssc.200800150**

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