

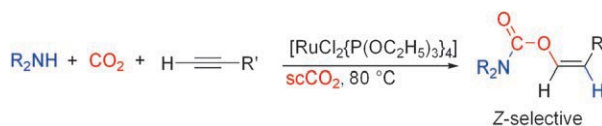
## Stereoselective Synthesis

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  $\text{CO}_2$ -Soluble Ruthenium- $\text{P}(\text{OC}_2\text{H}_5)_3$  Catalyst**

Chem. Asian J.

DOI: 10.1002/asia.200800204



**An extremely critical condition:** The addition of carbamic acids generated from secondary amines and supercritical  $\text{CO}_2$  ( $\text{scCO}_2$ ) to terminal alkynes proceeds efficiently in the presence of *trans*- $[\text{RuCl}_2\{\text{P}(\text{OC}_2\text{H}_5)_3\}_4]$ . The  $\text{CO}_2$ -

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

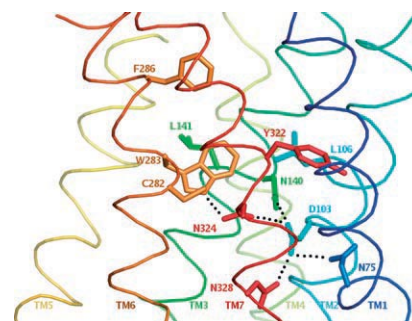
A. Gieldon, J. J. Lopez, C. Glaubitz, H. Schwalbe\*

**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

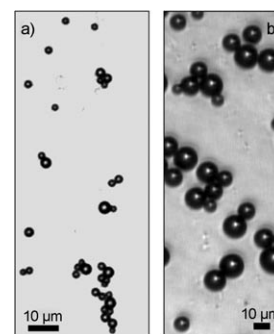
S. Rossi, G. Waton, M. P. Krafft\*

**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.



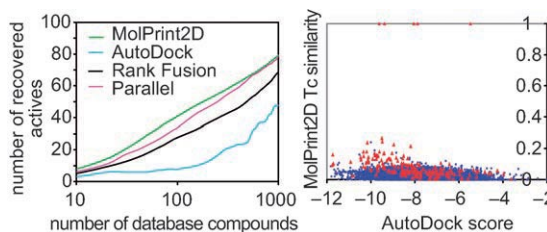
## Virtual Screening

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

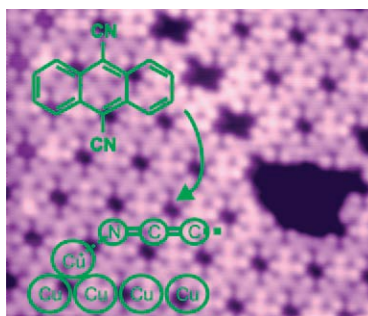


**Docking and similarity search** calculations using 2D fingerprints were carried out in parallel to identify inhibitors of nine target enzymes. By combining the results of docking and similarity searching, compound recall achieved by the individual methodologies

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.

## ... ON OUR SISTER JOURNALS

**Surface safari:** 9,10-Anthracenedicarbonitrile (DCA) molecules adsorbed on a Cu(111) surface can be titrated by gradual annealing of the substrate to form trigonal planar Cu(DCA)<sub>3</sub> complexes and, ultimately, a hexagonal network (see picture) with a Cu<sub>2</sub>-(DCA)<sub>3</sub> stoichiometry. As a result of charge donation from the substrate, the coordinated Cu adatom remains electrically neutral despite donating approximately 1/3 charge to each Cu–N bond.



### Coordination Networks

G. Pawin, K. L. Wong, D. Kim, D. Sun, L. Bartels,\* S. Hong, T. S. Rahman, R. Carp, M. Marsella

#### A Surface Coordination Network Based on Substrate-Derived Metal Adatoms with Local Charge Excess

*Angew. Chem. Int. Ed.*  
DOI: 10.1002/anie.200802543



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

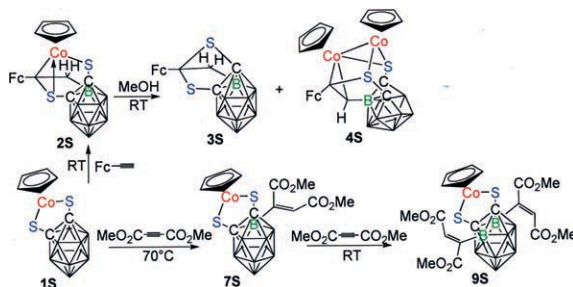
of enantioselection (*ee* values up to 89 %) by prototypical Pd<sup>II</sup>-catalyzed allylic alkylation. Further functionalization of 2-cyclobutyl-Quinazolinap has been achieved.

### 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

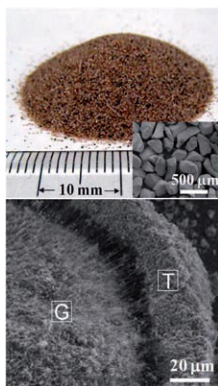
MeO<sub>2</sub>CC≡CCO<sub>2</sub>Me, the stepwise substitution of the *o*-carborane cage at the B(3)/B(6)-positions leads to **7S** and **9S**, respectively.

### 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