Spotlights ...

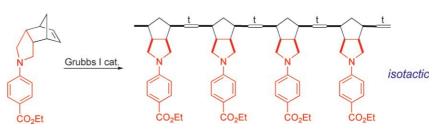
Polymers

W.-Y. Lin, H.-W. Wang, Z.-C. Liu, J. Xu, C.-W. Chen, Y.-C. Yang, S.-L. Huang, H.-C. Yang, T.-Y. Luh*

On the Tacticity of Polynorbornenes with 5,6-endo Pendant Groups That Contain Substituted Aryl Chromophores

Chem. Asian J.

DOI: 10.1002/asia.200700011



The fashion in necklaces: Polynorbornenes with electron-withdrawing substituents on the 5,6-endo aryl pendant groups may adopt isotactic stereochemistry with all pendant groups aligned in one direction. The nature of the interactions between neighboring chromophores may be a very important factor in directing the stereoregularity and conformation of these polymers. t=trans double bond.

Signal Transduction

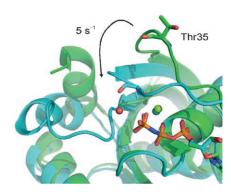
C. Kötting,* A. Kallenbach, Y. Suveyzdis, C. Eichholz, K. Gerwert*

Surface Change of Ras Enabling Effector Binding Monitored in Real Time at Atomic Resolution

ChemBioChem

DOI: 10.1002/cbic.200600552

RasoffGTP. When GTP is bound to Ras the molecular switch is usually "on"; however, in the Ras_{off}GTP state characterized here, it is "off" and signal transduction is blocked. This state and the time course of the switching process were investigated by FTIR spectroscopy at the atomic level by using para-hydroxyphenacyl-caged GTP and Ras labelled with a threonine isotope.



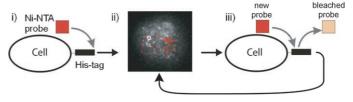
Membrane Proteins

E. G. Guignet, J.-M. Segura, R. Hovius,* H. Vogel*

Repetitive Reversible Labeling of Proteins at Polyhistidine Sequences for Single-Molecule Imaging in Live Cells

Chem Phys Chem

DOI: 10.1002/cphc.200700065



Single-molecule trajectories of cell surface proteins on live cells are recorded during repeated cycles of i) binding of fluorescent Ni-NTA probes to oligohistidine sequences of the proteins; ii) acquisition of image series and iii) replacement of bleached probes for subsequent imaging. The reversibility and repetitivity of this process overcomes photobleaching, which often hampers single-molecule experiments.

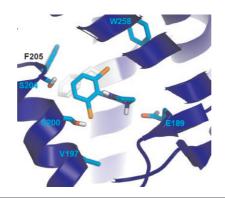
Homology Modeling

B. Balogh, C. Hetényi,* M. G. Keserű, P. Mátyus*

Structure-Based Calculation of Binding Affinities of α_{2A} -Adrenoceptor Agonists

ChemMedChem

DOI: 10.1002/cmdc.200600251



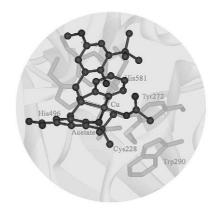
An atomic resolution structure of α_{2a} adrenoceptor was constructed and 15 known agonists were docked into the optimized model and experimental binding free energies were estimated. The figure shows the binding of the agonist clonidine (sticks) to the core binding pocket of the adrenoceptor (blue cartoon, key residues are marked with sticks).



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Galactose oxidase is an enzyme whose active site exhibits several unusual features, such as a coordinated tyrosyl radical, post-translationally modified amino acids, and π -stacked residues. The structural attributes, reactivity, electronic properties, self-processing, and many more of its properties have been addressed successfully during the last decade using model complexes.



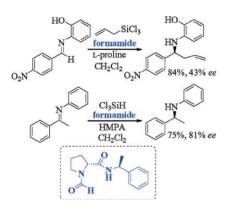
Copper-Based Enzymes

F. Thomas*

Ten Years of a Biomimetic Approach to the Copper(II) Radical Site of Galactose Oxidase

Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.200601091



Asymmetric allylation and reduction of imines in the presence of chiral *N*-formylproline derivatives as well as different additives is reported. The role of the second formamide moiety in the activator is shown to be crucial to bring about the enhancement of the reaction rate and enantioselectivity in the allylation reaction.

Allylation and Reduction of Imines

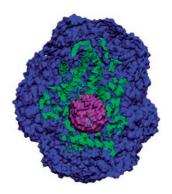
C. Baudequin, D. Chaturvedi, S. B. Tsogoeva*

Organocatalysis with Chiral Formamides: Asymmetric Allylation and Reduction of Imines

Eur. J. Org. Chem.

DOI: **10.1002/ejoc.200700058**

A QM/MM-arranged marriage between protein X-ray crystallography and solid-state ⁵¹V NMR spectroscopy is brought about by computations of the ⁵¹V NMR parameters of an entire enzyme, vanadium-dependent chloroperoxidase. A small number out of many possible candidates with different protonation states and hydrogen-bond networks can be reconciled with the experimental solid-state MAS ⁵¹V NMR data.



Bioinorganic Chemistry

M. P. Waller, M. Bühl,* K. R. Geethalakshmi, D. Wang, W. Thiel

⁵¹V NMR Chemical Shifts Calculated from QM/MM Models of Vanadium Chloroperoxidase

Chem. Eur. J.

DOI: 10.1002/chem.200700295



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