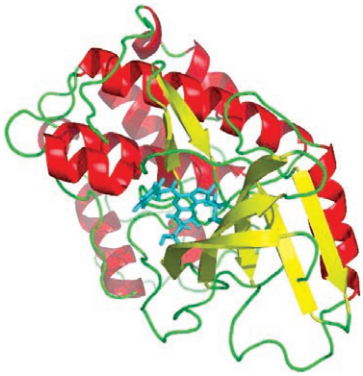
Molecular Mechanics

*P. Dobeš, M. Otyepka, M. Strnad, P. Hobza**

Interaction Energies for the Purine Inhibitor Roscovitine with Cyclin-Dependent Kinase 2: Correlated Ab Initio Quantum-Chemical, DFT and Empirical Calculations

Chem. Eur. J.
DOI: **10.1002/chem.200501269**



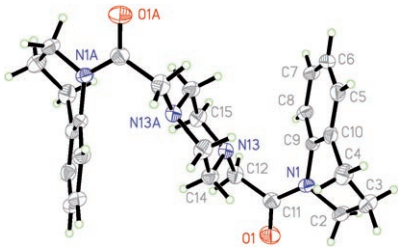
The total stabilisation energy between roscovitine and cyclin-dependent kinase 2 (shown here) is very large (66 kcal mol^{-1}) and originates predominantly from dispersion energy. A few amino acid residues contribute significantly to the binding of roscovitine and cdk2, whereas many amino acids make a negligible contribution.

Total Synthesis

L. Shen, Y.-H. Ye, X.-T. Wang, H.-L. Zhu, C. Xu, Y.-C. Song, H. Li, R.-X. Tan**

Structure and Total Synthesis of Aspernigerin: A Novel Cytotoxic Endophyte Metabolite

Chem. Eur. J.
DOI: **10.1002/chem.200501423**



Antitumor agents: Aspernigerin, a novel cytotoxic alkaloid consisting of an unprecedented structural framework (see figure) has been isolated and shown to exhibit cytotoxic activity greater than that of 5-fluorouracil. A feasible total synthetic route for aspernigerin has been established for further pharmacological research.

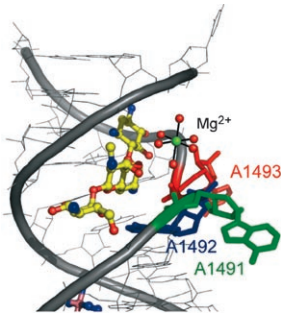
Molecular Recognition

*J. Kondo, B. François, A. Urzhumtsev, E. Westhof**

Crystal Structure of the *Homo sapiens* Cytoplasmic Ribosomal Decoding Site Complexed with Apramycin

Angew. Chem. Int. Ed.
DOI: **10.1002/anie.200600354**

On target: The crystal structure of the complex formed between apramycin and the cytoplasmic ribosomal decoding sites of human cells (see picture; complex in yellow, adenine residues numbered) was studied and compared with that of the analogous bacterial complex. The studies provide insight into apramycin toxicity in humans.



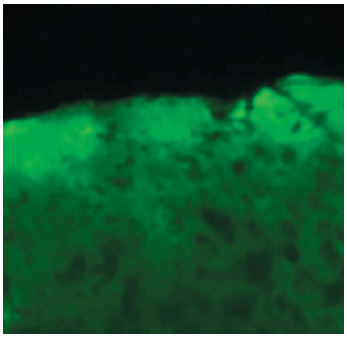
Cell-Penetrating Molecules

*K. K. Maiti, O.-Y. Jeon, W. S. Lee, D.-C. Kim, K.-T. Kim, T. Takeuchi, S. Futaki, S.-K. Chung**

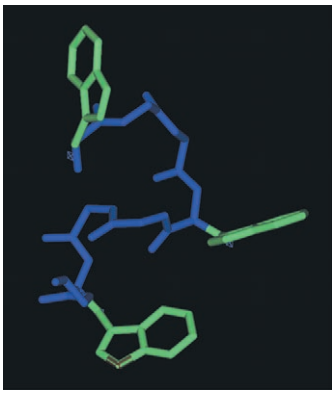
Design, Synthesis, and Membrane-Translocation Studies of Inositol-Based Transporters

Angew. Chem. Int. Ed.
DOI: **10.1002/anie.200600312**

Delivery vehicles: Novel guanidine-containing "transporters" constructed on a dimeric inositol scaffold show significant translocation across the cell membrane and the blood–brain barrier, as well as unique in vitro and in vivo distributions. Doxorubicin was efficiently delivered to mouse brain tissue by conjugating the compound with such a transporter (see fluorescence microscopy image).



Peptide Biochemistry



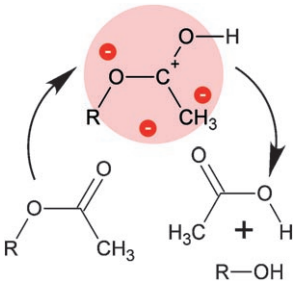
A simple hexapeptide (Ac-Nal2-Ape-Nal2-Ape-Nal2-Ile-NH_2; Nal2 = 3-naphthalen-2-yl-L-alanine, Ape = 5-aminopentanoic acid), almost entirely made up of unnatural amino acid residues, shows strong antiviral potency in vitro and markedly increased enzymatic stability relative to a normal peptide.

*A. M. D'Ursi, S. Giannecchini, C. Esposito, M. C. Alcaro, O. Sichi, M. R. Armenante, A. Carotenuto, A. M. Papini, M. Bendinelli, P. Rovero**

Development of Antiviral Fusion Inhibitors: Short Modified Peptides Derived from the Transmembrane Glycoprotein of Feline Immunodeficiency Virus

ChemBioChem
DOI: **10.1002/cbic.200500390**

Catalytic RNA



Born to cut. We have converted an RNA aptamer into a primitive ribozyme by taking advantage of transition-state stabilization during an ester hydrolysis reaction of a modified ligand/substrate inside the RNA binding pocket (see scheme).

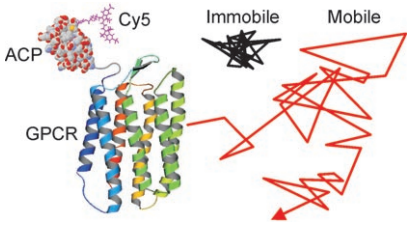
*D. M. Brackett, T. Dieckmann**

Aptamer to Ribozyme: The Intrinsic Catalytic Potential of a Small RNA

ChemBioChem
DOI: **10.1002/cbic.200500538**

Transmembrane Proteins

Tracking system. Diffusion of individual proteins in the plasma membrane of living cells plays a central role in cellular signal transduction. By using a novel labeling technique that allowed for the site-specific attachment of fluorophores to cell-surface-expressed proteins, the heterogeneous mobility distribution of neurokinin-1 receptors was revealed with single-molecule microscopy (see figure).



*M. Prummer, B. H. Meyer, R. Francini, J.-M. Segura, N. George, K. Johnsson, H. Vogel**

Post-translational Covalent Labeling Reveals Heterogeneous Mobility of Individual G Protein-Coupled Receptors in Living Cells

ChemBioChem
DOI: **10.1002/cbic.200500477**

On these pages, we feature the excellent work in chemistry that has been recently reported in our sister journals *ChemBioChem*, *Angewandte Chemie*, or *Chemistry—A European Journal*.

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