# Spotlights ...

#### **Molecular Rotations**

S. Nishihara, T. Akutagawa,\* D. Sato, S. Takeda, S.-i. Noro, T. Nakamura\*

Multirotations of (Anilinium) ([18]Crown-6) Supramolecular Cation Structure in Magnetic Salt of [Ni(dmit)<sub>2</sub>]<sup>-</sup>

Chem. Asian J.

DOI: 10.1002/asia.200700010

Round and round we go: (Anilinium)-([18]crown-6) dynamic supramolecular cations undergo different modes of rotation in the solid state. The 180° flip-flop motion of anilinium and the rotation of [18]crown-6 were confirmed from solid-state NMR spectra. Multimolecular rotations of different motional freedoms were also observed simultaneously.



### Enzyme Catalysis

Y. Liu, C. Mihai, R. J. Kubiak, M. Rebecchi, K. S. Bruzik\*

Phosphorothiolate Analogues of Phosphatidylinositols as Assay Substrates for Phospholipase C

**ChemBioChem** 

DOI: 10.1002/cbic.200700061

RO : SH N SS N RO : 
$$A_{324nm} = 19\,800 \text{ cm}^{-1} \text{ m}^{-1}$$

Unnaturally superior. Analogues of all naturally occurring phosphatidylinositols in which the scissile P—O bond is replaced by a P—S bond have been synthesized and shown to be useful assay substrates for the determination of phosphatidylinositol-specific phospholipase C activity.

#### **Proton Transfer**

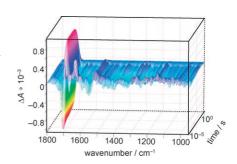
T. Majerus, T. Kottke, W. Laan, K. Hellingwerf, J. Heberle\*

Time-Resolved FT-IR Spectroscopy Traces Signal Relay within the Blue-Light Receptor AppA

**ChemPhysChem** 

DOI: 10.1002/cphc.200700248

Revealing intermediates: Time-resolved step-scan FT-IR difference experiments (see figure) on flavin-containing photoreceptors reveal photocycle intermediates which have been spectrally silent in previous UV/Vis experiments on Appa—BLUF. The data indicate blue-light induced proton transfer or a change in H-bonding in the vicinity of a carboxylic side chain which represent an important step in signal transfer from the chromophore to the protein surface.



#### Virtual Screening

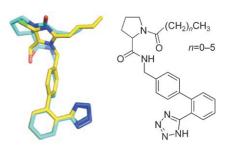
C. Lamanna, A. Catalano, A. Carocci, A. Di Mola, C. Franchini,\* V. Tortorella, P. M. L. Vanderheyden, M. S. Sinicropi, K. A. Watson, S. Sciabola

AT<sub>1</sub> Receptor Ligands: Virtual-Screening-Based Design with TOPP Descriptors, Synthesis, and Biological Evaluation of Pyrrolidine Derivatives

ChemMedChem

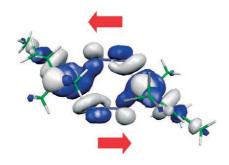
DOI: 10.1002/cmdc.200700082

A virtual approach that uses TOPP 3D descriptors to explore the AT<sub>1</sub> receptor is presented. It features a new series of sartan analogues (shown), which were synthesized and biologically evaluated on CHO-hAT<sub>1</sub> cells stably expressing the human AT<sub>1</sub> receptor.



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Prediction of the magnetic properties of binuclear Cu<sup>II</sup> compounds containing asymmetric azide bridges remains a challenge. A combination of correlated ab initio calculations and the analysis of the experimental data shows that the asymmetry of the coordination of the azido bridge is a determining factor in the tuning of the coupling constant value.

## Molecular Magnetism

M. Angels Carvajal, C. Aronica, D. Luneau,\* V. Robert\*

Shearing-Like Distortion in Binuclear End-to-End Cu<sup>II</sup> Azido Compounds: An Ab Initio Study of the Magnetic Interactions

Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.200700456

The Pd-catalyzed stereoselective cyclization of dicarbamates proceeded with 1,3asymmetric induction under either thermodynamic or kinetic control to afford

enantioselectively six-membered-ring cyclic carbamates. Calculations enabled us to rationalize the observed stereoselectivity.

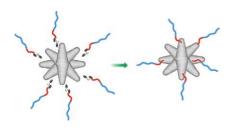
#### **Pd-Catalyzed Cyclizations**

G. Broustal, X. Ariza, J.-M. Campagne,\* J. Garcia,\* Y. Georges, A. Marinetti, R. Robiette\*

A Stereoselective Approach to 1,3-Amino Alcohols Protected as Cyclic Carbamates: Kinetic vs. Thermodynamic Control

Eur. J. Org. Chem.

DOI: 10.1002/ejoc.200700503



Taking the nanotube by the horn! The covalent functionalization of the newly discovered carbon nanohorns with welldefined homopolymers and block copolymers is described (see scheme). The synthesis and the properties of the above hybrid materials are elucidated using complementary techniques.

#### **Carbon Nanohorns**

G. Mountrichas, S. Pispas,\* N. Tagmatarchis\*

Grafting Living Polymers onto Carbon Nanohorns

Chem. Eur. J.

DOI: 10.1002/chem.200700770



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