

SPOTLIGHTS ...

Molecular Rotations

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Multirotations of (Anilinium)([18]Crown-6) Supramolecular Cation Structure in Magnetic Salt of $[\text{Ni}(\text{dmit})_2]^-$

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.

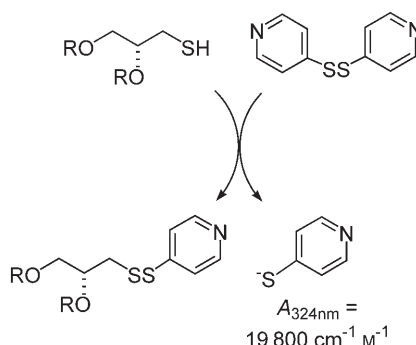


Enzyme Catalysis

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



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.

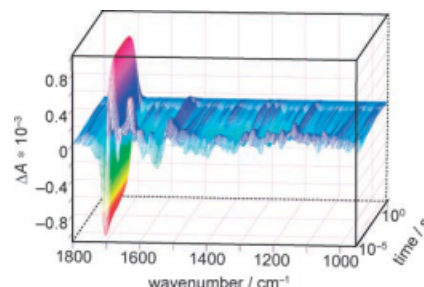
Proton Transfer

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.



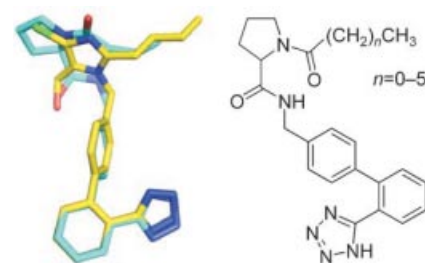
Virtual Screening

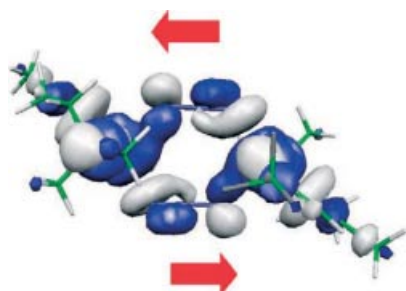
C. Lamanna, A. Catalano,
A. Carocci, A. Di Mola,
C. Franchini,* V. Tortorella,
P. M. L. Vanderheyden,
M. S. Sinicropi, K. A. Watson,
S. Sciabola

AT₁ 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 AT₁ receptor is presented. It features a new series of sartan analogues (shown), which were synthesized and biologically evaluated on CHO-hAT₁ cells stably expressing the human AT₁ receptor.





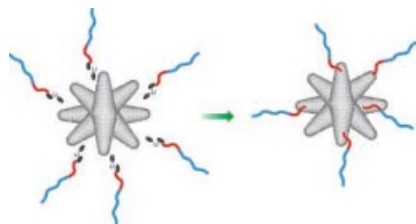
Prediction of the magnetic properties of binuclear Cu^{II} compounds containing asymmetric azide bridges remains a challenge. A combination of correlated ab initio calculations and the analysis of the experimental data shows that the asymmetry of the coordination of the azido bridge is a determining 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^{II} Azido Compounds: An Ab Initio Study of the Magnetic Interactions

Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.200700456



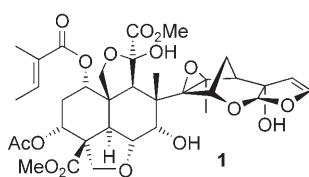
Taking the nanotube by the horn! The covalent functionalization of the newly discovered carbon nanohorns with well-defined homopolymers and block copolymers is described (see scheme). The synthesis and the properties of the above hybrid materials are elucidated using complementary techniques.

Carbon Nanohorns

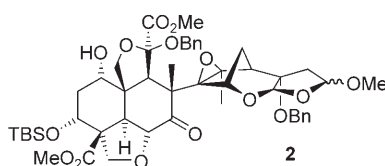
G. Mountrichas, S. Pispas,*
N. Tagmatarchis*

Grafting Living Polymers onto Carbon Nanohorns

Chem. Eur. J.
DOI: 10.1002/chem.200700770



22 Years in the making: Azadirachtin (**1**) was synthesized for the first time by a highly convergent approach, utilizing a Claisen rearrangement and a radical cyclization as key steps. End-



game strategies relied on intermediate **2**, which could be obtained by synthetic methods as well as by degradation of **1**. Bn = benzyl, TBS = *tert*-butyldimethylsilyl.

Total Synthesis

G. E. Veitch, E. Beckmann,
B. J. Burke, A. Boyer, S. L. Maslen,
S. V. Ley*

Synthesis of Azadirachtin: A Long but Successful Journey

Angew. Chem. Int. Ed.
DOI: 10.1002/anie.200703027



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