Applied Supramolecular Chemistry: Two Stories

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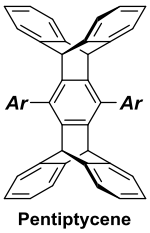
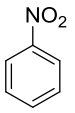
My presentation will provide a brief description of two projects we have recently undertaken in my laboratory: Supramolecular nanochemistry and Multi-analyte sensing by cross-reactive arrays.

Sensing of explosives.

Small-molecule fluorescent sensors based on pentiptycene were used for the recognition of nitroaromatic compounds such as nitrobenzene, 2,4-dinitrotoluene (DNT) and the explosive, TNT. The pentiptycene derivatives are obtained using a three-step dehydrohalogenation cycloaddition protocol. The interaction of the receptors and nitroaromatics was studied both in solution and in the solid state using fluorescence spectroscopy and X-ray crystallography, respectively. It will be shown that the pentiptycene receptors provide a cavity suitable for binding nitroaromatic compounds in an edge-to-face mode. Pentiptycene-based sensors are fluorescent and can be used as fluorescence-based sensor for organic volatile compounds, including vapors of TNT. The obtained results inspired us to develop inexpensive, reliable, and robust sensor materials suitable for CHEM-FET applications.



Pentiptycene



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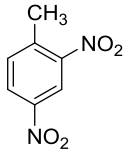
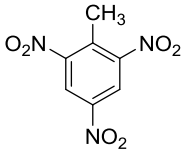
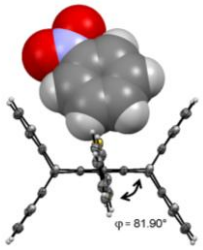


2,4-DNT



TNT



Toward assays for a carbonic anhydrase inhibitor assay.

Carbonic anhydrases (CAs) are a family of enzymes that catalyze the rapid interconversion of carbon dioxide and water to bicarbonate and protons. CA enzymes are ubiquitous in living organisms. CAs found in mammals are divided into four broad subgroups, which, in turn consist of several isoforms. Interestingly, defects and mutations in these enzymes are associated with a broad range of diseases. Thus, carbonic anhydrase inhibitors have been established as antiglaucoma agents, diuretics, antiepileptics, drugs for the management of mountain sickness, gastric and duodenal ulcers, neurological disorders, or osteoporosis. Our current research is focused on a microarray-based method aimed at identification of drugs binding into the active site of Zn-based carbonic anhydrases. Here, a series of fluorescence sensors comprising the sulfonamide moiety were synthesized and used to set up a competitive assay with a potential CA inhibitor. The sensor changes fluorescence depending on the equilibria between the CA enzyme, sensor, and inhibitor. These changes in fluorescence are recorded and evaluated to identify, which ligands display the highest affinity and can best fulfill the role of the inhibitors of the enzyme. Potential for the development of high-throughput assays will also be discussed.