Quantifying noncovalent interactions using artificial receptors as model systems

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We are interested in supramolecular systems that form stable aggregates even under the most challenging conditions, namely in water. As the strength of most specific non-covalent interactions such as H-bonds or ion pairs significantly decreases in polar surrounding the design of such systems is still rather difficult. We use both rational design and combinatorial methods in this context. Currently, we mainly are exploring H-bond enforced ion pairing to obtain stable aggregates in water. Our focus is a better molecular understanding of the underlying recognition event and its thermodynamics and the application of such supramolecular systems.

For example, we developed a new and highly efficient binding motif for the complexation of carboxylates in water, the guanidiniocarbonyl pyrroles. Using “knock-out” analogues the energetic contributions of individual interactions within this multiple point binding sites can be assessed both experimentally and theoretically. Based on this binding motif a host of different applications such as polymers and gels, artificial gene transfection vectors or ligands for protein surface binding could be developed.

An even more challenging task besides a quantitative understanding of noncovalent interactions is to elucidate the role the solvent plays in supramolecular complexation experimentally. Some first approaches into this direction are also discussed.