The Anatomy of Complex Recognition Interfaces

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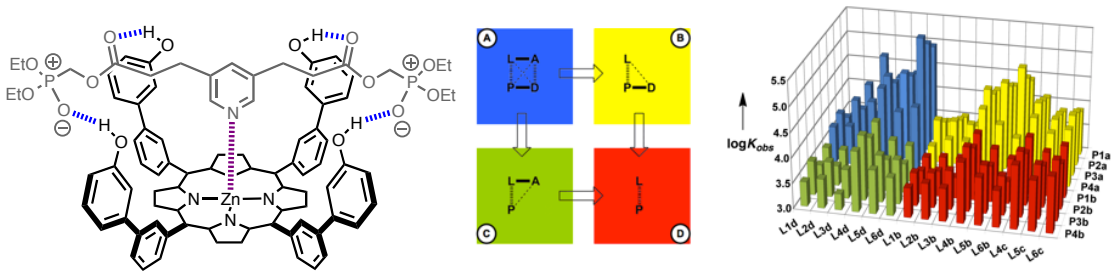
Cooperativity is the basis for a range of important phenomena in supramolecular science: chelating ligands, supramolecular catalysis, self-assembly and multivalency. It is a property that we understand very well at a qualitative level, but rather poorly at a quantitative level. Almost all functional molecular systems in biology, materials and nanotechnology involve multiple cooperative intermolecular interactions between macromolecular surfaces. Many factors contribute to the thermodynamic properties of these interfaces: electrostatic interactions between charges, H-bonds, aromatic interactions, desolvation, changes in conformation etc. This complexity makes it difficult to disentangle the relative contributions of individual interactions, so new experiments are required if we are to develop a quantitative understanding of cooperativity that can be used in molecular design. We have been using synthetic porphyrin-ligands complexes, high throughput titration systems and chemical double mutant cycles to begin to map the relationship between supramolecular architecture and cooperativity.



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