化学科講演会

Helical Foldamers: Highly Modular Scaffolds for Molecular Recognition

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Abstract

Our group has developed helical foldamers – oligomers that adopt stable helical folded conformations – derived from aromatic amino acids. Some of these folded objects have shown unprecedented conformational stability even in water, and constitute convenient building blocks to elaborate synthetic, very large (protein-sized) folded architectures. Cavities can be designed within such synthetic molecules that enable them to act as artificial receptors for chiral polar guests. This design offers unmatched modularity in that each and every monomer may be varied in order to tune the structure, the dynamics and host-guest properties. Iterative evolution of oligoamide sequences was used to develop receptors able to bind a given guest with high affinity and selectivity. Rounds of selection have been made possible through the extensive use of crystallography, NMR and circular dichroism.

Removing the peripheral substituents from helical capsule sequences (these residues serve as end-caps of the helix hollow) allows the incorporation of guests that are longer than the hollow itself. The terminal stoppers of the guests are too large to go through the helix hollow, implying that the complex cannot form by a threading mechanism but through helix winding around the guest. The winding process requires helix unfolding and refolding, as well as a strict match between helix length and anchor points on the rods. The time scales of folding/unfolding being relatively slow, the helices can undergo some motions without dissociation, such as shuttling or screwing, on guest molecules having several binding sites. The strong analogy between this system and rotaxanes hints at possible applications of such constructs in the vast field of artificial molecular machines.

References

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