Specific Electrostatic Molecular Recognition in Water - DTU Orbit (09/11/2017)

Specific Electrostatic Molecular Recognition in Water

The identification of pairs of small peptides that recognize each other in water exclusively through electrostatic interactions is reported. The target peptide and a structure-biased combinatorial ligand library consisting of ≈78 125 compounds were synthesized on different sized beads. Peptide–peptide interactions could conveniently be observed by clustering of the small, fluorescently labeled target beads on the surface of larger ligand-containing beads. Sequences of isolated hits were determined by MS/MS. The interactions of the complex showing the highest affinity were investigated by a novel single-bead binding assay and by 2D NMR spectroscopy. Molecular dynamics (MD) studies revealed a putative mode of interaction for this unusual electrostatic binding event. High binding specificity occurred through a combination of topological matching and electrostatic and hydrogen-bond complementarities. From MD simulations binding also seemed to involve three tightly bound water molecules in the interface between the binding partners. Binding constants in the submicromolar range, useful for biomolecular adhesion and in nanostructure design, were measured.

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