Unraveling the Role of Non–Covalent Interactions in Recognition and Catalysis.

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Abstract

Non-covalent intermolecular forces, including hydrogen bonding, ion-pairing and π-interactions, are being increasingly recognised as crucial factors determining selectivity in numerous catalytic processes.\[^1\] Excellent examples include asymmetric hydrogen-bonding and counteranion-directed catalysis. In parallel, new possibilities of supramolecular catalysis have also been demonstrated using multicomponent assemblies.\[^2\] Despite these promising results, a molecular understanding of these interactions and their influence in recognition and reaction outcome remains difficult.

In this talk I will present two examples in the area of protein recognition and catalysis which have provided us with deeper understanding on the critical influence of non-covalent interactions for selectivity. In the former one, I discuss the nature of cation–π interactions and their importance on protein-ligand binding via \textit{ab initio} and data-mining methods.\[^3\] In the second example, I will discuss the enantioselective ring-opening reaction of \textit{meso}-aziridinium and episulfonium cations promoted by asymmetric counteranion-directed catalysis (ACDC) in the condensed phase. The influence of electrostatic interactions and CH···O interactions on the stability and stereoselectivity is studied employing both classical and quantum methods.\[^4\]

Reference and notes


