

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

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Intermolecular forces, including hydrogen bonding, ion-pairing and π -interactions, are being increasingly recognised as crucial factors determining selectivity in numerous recognition and catalytic processes. Excellent examples include protein-binding processes, asymmetric hydrogen-bonding and counteranion-directed catalysis. In parallel, new possibilities for biomimetic catalysis have also been demonstrated using multicomponent assemblies. Despite these promising results, a molecular understanding of these interactions in condensed-phase and their influence in the reaction outcome remains challenging.

In this talk, I discuss some of the inherent challenges involved in the quantitative characterization of these interactions in solution and our ongoing work to overcome them. I will present examples in the area of protein recognition and supramolecular chemistry, which have provided us with a deeper understanding of the critical influence of non-covalent interactions for reactivity and selectivity.