Understanding and Rationalizing Cooperativity Effects Between Non-Covalent Interactions : Towards More Efficient Anion Receptor Platforms

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Anions are widely spread in several areas such as biology, medicine, catalysis, or environment.[1] Therefore, the molecular recognition of anions is a promising branch of supramolecular chemistry. However, unlike the extensive use of cation receptors, anion recognition is still in its infancy.

The development of receptors is based on the use of one or multiple weak interactions. Many of these interactions such as anion-π interaction, halogen or hydrogen bonding have been extensively studied independently. A combination of several weak interactions within a single polyfunctional molecular platform is likely to generate (anti)-cooperative effects on anion binding, but they remain difficult to highlight, predict and/or understand.[2,3]

Based on these considerations, we recently focused on the emerging area of anion receptors combining hydrogen-bond donor groups and π-deficient heterocycles able to generate anion-π interactions.[2,4,5,6] Only a few theoretical publications reported the study of cooperativity effects in such combination to date.[3] Moreover, the accuracy between predicted properties and experimental results has to be improved.

In this communication, the combination of molecular modelling and analytical chemistry will be discussed to deliver some understanding of such complex effects. DFT calculations will provide some structural information on complexes formed.[4,5] Correlation between calculated interaction energies and experiments will be assessed, enabling the establishment of a predictive model.[4] Then, (anti)-cooperative effects between the different interactions will be evidenced and explained.[5] As perspectives, the influence of small structural modulations on chloride binding will be highlighted.[6]

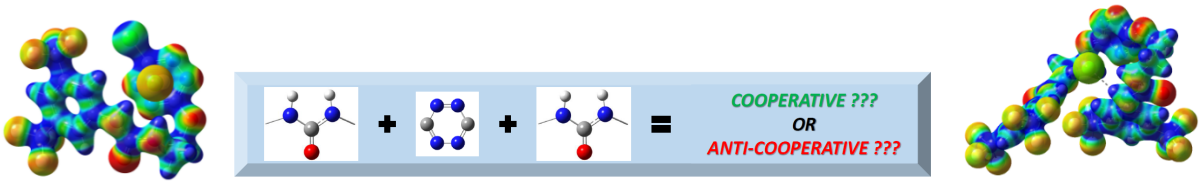

Fig. 1 Molecular designs and cooperativity effects

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