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Understanding and rationalizing cooperativity effects between non-covalent interactions: towards more efficient anion receptor platforms

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Anions play a crucial role in various fields, including biology, medicine, catalysis and environmental sciences.^[1] Consequently, the design of new anion receptors has become an important challenge in modern organic chemistry. We have designed new anion receptors (figure 1) based on the combination of two types of fragments: a urea derivative capable of generating hydrogen bonds and a π -deficient heterocycle capable of generating anion- π interactions.^[2] The design of these anion receptors is essential because non-covalent interactions individually contribute to the structuring and properties of complex three-dimensional molecular assemblies. When combined within a single multifunctional molecular platform, they can generate cooperative, non-cooperative or anti-cooperative phenomena. The combination of molecular modelling and analytical chemistry will be presented to provide some understanding of such complex effects.

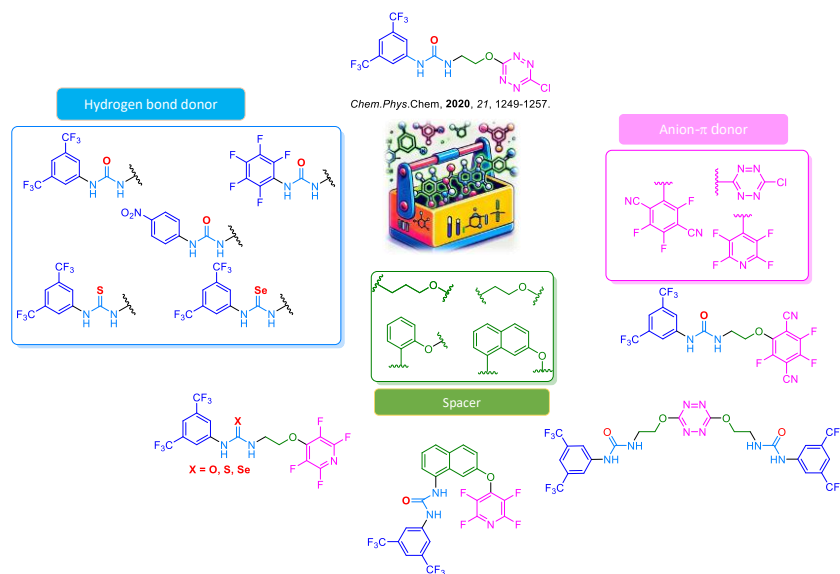


Figure 1 : supramolecular toolbox

References :

[1] Zhang, Z.; Schreiner, P. *Chem. Soc. Rev.*, 2009, 38, 1187-1198.

[2](a) Plais, R.; Gouarin, G.; Gaucher, A.; Haldys, V.; Brosseau, A.; Clavier, G.; Salpin, J.-Y.; Prim, D. *ChemPhysChem*. **2020**, 21, 1249-1257. (b) Plais, R.; Gouarin, G.; Gaucher, A.; Haldys, V.; Brosseau, A.; Clavier, G.; Salpin, J.-Y.; Prim, D. *RSC Adv.*, **2021**, 11, 9476-9487. (c) Plais, R.; Gouarin, G.; Bournier, A.; Zayene, O.; Mussard, V.; Bourdreux, F.; Marrot, J.; Brosseau, A.; Gaucher, A.; Clavier, G.; Salpin, J.-Y.; Prim, D. *ChemPhysChem* **2023**, 24, 1-8, e202200524. (c) Zayene, O.; Plais, R.; Rolhion, L.; Bourdreux, F.; Pieters, G.; Gaucher, A.; Clavier, G.; Cœuret, A.; Salpin, J.-Y.; Prim, D. *ChemistrySelect* **2024**, 9, e202302763. 10.1002/slct.202302763.