LARGE-SCALE EXPLORATION OF CARBOXYLATE BINDING AFFINITY

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Carboxylates are attractive target analytes in supramolecular analytical chemistry. We report a large-scale study on binding of 11 carboxylate anions of widely differing basicity, hydrophobicity and steric demand with synthetic receptors having a different number and geometric arrangement of hydrogen bond donor (HBD) fragments, resulting in 242 accurately determined binding constants. Results reveal main structural factors of anions and receptors governing the binding and demonstrate the ability of selected receptors to discriminate between anions according to structural features (hydrophilicity, substitution at α-carbon, etc.).

Carboxylates binding to 22 urea-, carbazole- and indolocarbazole-based receptors was measured. Binding affinities were determined using ^{1}HNMR-based relative binding affinity measurement method [1]. Principal component analysis (PCA) was performed to elucidate the trends of binding selectivity of carboxylates to different receptors. The results show that most of the investigated carboxylates can be discriminated by the used receptors to a statistically significant extent. For example, receptor **10** forms additional hydrogen bonds with lactate's 2-OH group (Fig.1). Such additional HBs are probably the reason that lactate binds stronger with **10** than could be expected from its low basicity. The results obtained are an important step closer to the practical output where the use of a series of receptors that are known to have different affinities to various carboxylates could be used in sensor arrays for fingerprinting mixtures of carboxylates.

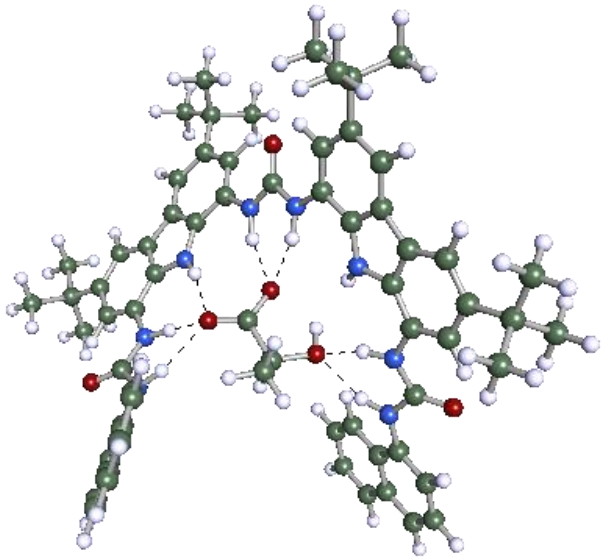

Fig.1 Complex of receptor 10 and lactate.

References

1. Kadam, S. A.; Haav, K.; Toom, L.; Haljasorg, T.; Leito, I. *J. Org. Chem.* **2014**, *79* (6), 2501–2513.

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