Oral Contributions

[MS38-02] Solid State Molecular Recognition for Supramolecular Sensing. Chiara Massera, Tahnee Barboza, Elisa Biavardi, Franco Ugozzoli, Enrico Dalcanale,

Dipartimento di Chimica, Università degli Studi di Parma, Viale delle Scienze 17/A, 43124 Italy.
E-mail: chiara.massera@unipr.it

A chemical sensor is a device that transforms chemical information into an analytical useful signal. Optimal sensors for environmental, security and biomedical applications must be sufficiently responsive to allow detection of the target analyte at low concentrations, and selective enough to respond primarily to a single chemical species in presence of interferents. In this respect, cavitands, synthetic organic compounds with enforced cavities of molecular dimensions, [1] represent a very important class of molecular receptors for chemical and biochemical sensing. When designing a cavitand, the mastering of weak interactions at the molecular level is an essential feature, as well as the choice of the bridging groups which determine shape, dimensions and complexation properties of the resulting cavity. The study of host-guest complexes at the solid state through X-ray diffractions on single crystals is therefore fundamental for understanding and tailoring the weak interactions operating on the functional surfaces, which are responsible for the desired functions. Phosphonate cavitands are well-known for their ability to complex positively charged species and neutral molecules by a synergistic combination of weak interactions. [2] We have recently demonstrated [3] that a silicon surface decorated with phosphonate cavitands can selectively recognize sarcosine (whose presence in urine is linked with an aggressive form of prostate cancer) from other non-methylated amino acids in biological fluids.

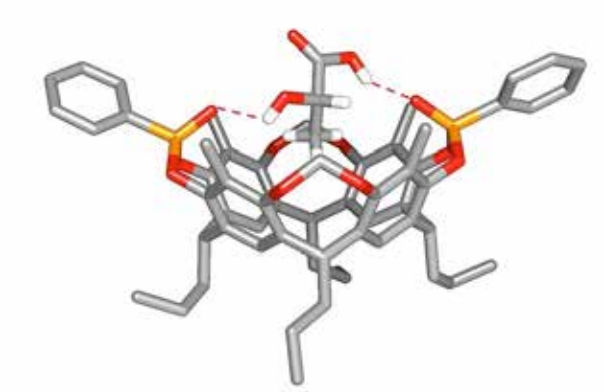

Figure 1. Molecular structure of the complex between a diphosphponate cavitand and lactic acid. C, grey; O, red; P, orange; H, white. For clarity, only the hydrogen atoms of the guest are shown. H-bonds are represented as red dotted lines.

The same ability is currently being exploited for the molecular recognition of carboxylic acids of social interest (see Fig. 1 for an example of a cavitand-acid complex in the solid state), as well as for the detection of illicit drugs and illicit drug precursors (amphetamine, metamphetamine, ecstasy, ephedrine, norephedrine, pseudoephedrine, heroin, cocaine etc.) usually transported as hydrochloride ammonium salts.

[1] Cram, D. J. (1983) Science 219, 1177-1183.
[2] (a) Dalcanale, E. et al. (2003) J. Am. Chem. Soc. 125, 12068-12069; (b) Dalcanale E et al. (2008) Chem.-Eur. J. 14, 5772-5579.
[3] Biavardi, E. et al. (2012) PNAS, 109, 2263-2268.

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