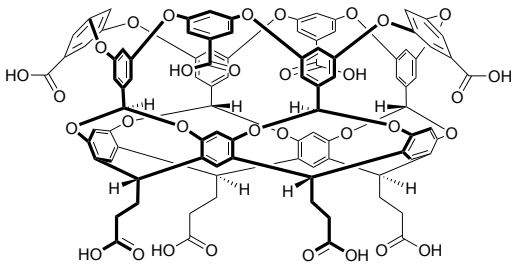
The host

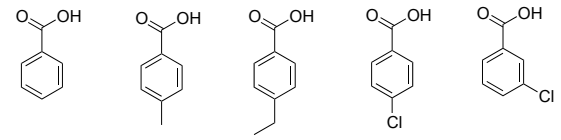
The octa-acid (**Host**) will be studied at pH 9.2 to ensure that it is fully deprotonated, i.e., that it will be the octa-sodium salt.



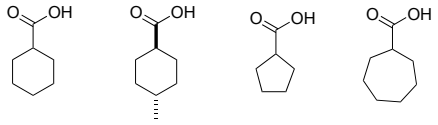
Host

List of guests

All of these guests are carboxylic acids. Their pK_a values are such that at pH 8.7 all are >99% deprotonated. The charge on the guests is needed to ensure that the host does not undergo dimerization upon guest binding.



1 **2** **3** **4** **5**



6 **7** **8** **9**

Paired Comparisons	Justification
1 and 2	Influence of *p*-substituent filling void at base of cavity, i.e., under the guest
1 and 3	Influence of *p*-substituent filling void…
2 and 3	Influence of *p*-substituent filling void…
2 and 4	Influence of C-H···Cl interactions btw. host and guest
4 and 5	Influence of orientation of molecule in pocket
1 and 6	Guest volume/saturated verses unsaturated guest
2 and 7	Guest volume/saturated verses unsaturated guest
6 and 8 and 9	Influence of volume changes
7 and 9	Influence of different shapes (at constant guest volume)

The solutions

The host will be dissolved in borate buffer (pH 9.2). All of the guests should be sufficiently water-soluble such that titrations to determine the K_a values will involve adding a concentrated solution of the guest (in aqueous DMSO with buffer) to an aqueous solution of the host. The aqueous DMSO solution of the guest will be < 40% DMSO. Consequently, the final DMSO concentration at the end of the titration will be < 5%.