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Significance: Cucurbiturils and hemicucurbiturils have been studied as molecular receptors. Pittelkow and co-workers report the synthesis of a new hemicucurbit[6]uril from acid-catalyzed, halide-templated, regioselective condensation of biotin and formaldehyde. Halide binding constants for this cavitand, spanning about two orders of magnitude, are determined by titration experiments using NMR spectroscopy and isothermal titration calorimetry. A procedure to isolate halide-free cavitand is also presented, opening up the potential for future binding studies on chiral guests.

Comment: It is remarkable that of the nine possible regioisomers, only the alternating hexamer is observed. The thioether and carboxylic acid moieties of the biotin-formaldehyde hexamer hold potential for binding metal clusters/surfaces. Curiously, although the cavitand is found to bind iodide more strongly than chloride or bromide, the optimized conditions for 6+6 cyclocondensation use sodium bromide.