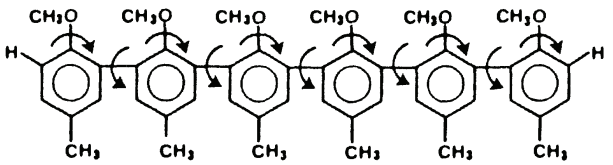
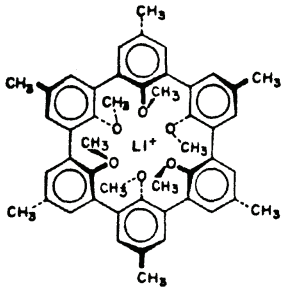
Host-guest chemistry

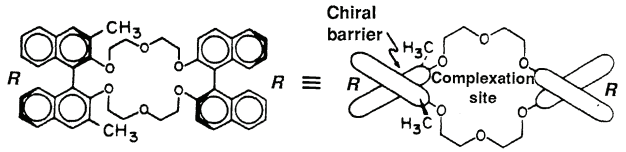
F. Edward Boas
2001-10-17

Preorganization of binding sites

Molecule	Binding energy for Li^+
	6 kcal/mol
	23 kcal/mol

Cram DJ (1988) "The design of molecular hosts, guests, and their complexes." *Science* 240: 760-7.

Chiral recognition



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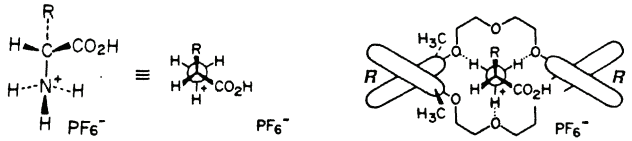
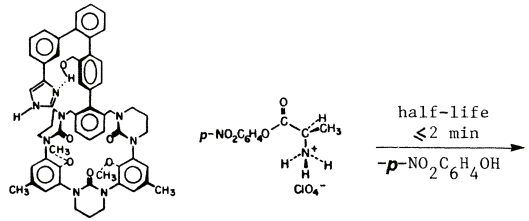


26

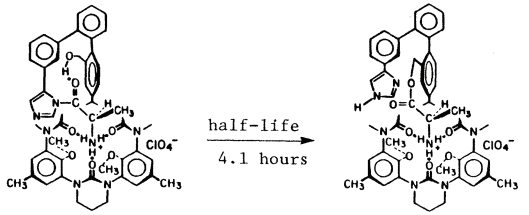
Stabler complex

Difference in binding energy of amino acid enantiomers: 0.4 – 1.9 kcal/mol

Enzyme active site analogs

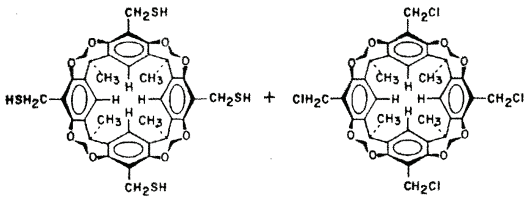


34 32

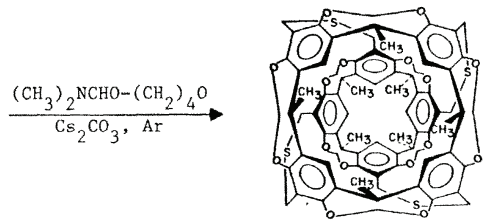


35 36

Carcerands

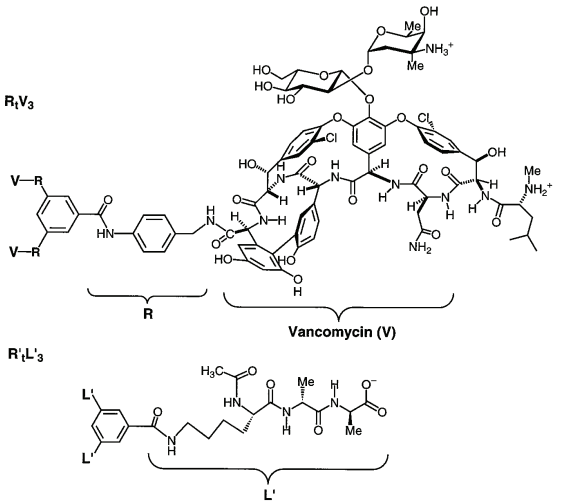


46 47



48

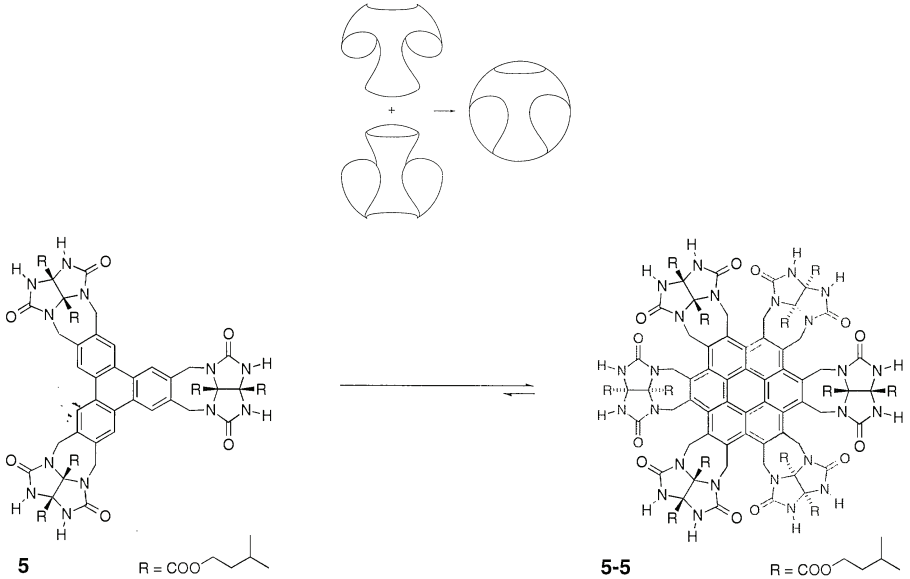
Trivalent Vancomycin • D-Ala-D-Ala



$k_d = 4\times10^{-17}$ M

Rao J and Whitesides GM et al. (1998) *Science* 280: 708-11

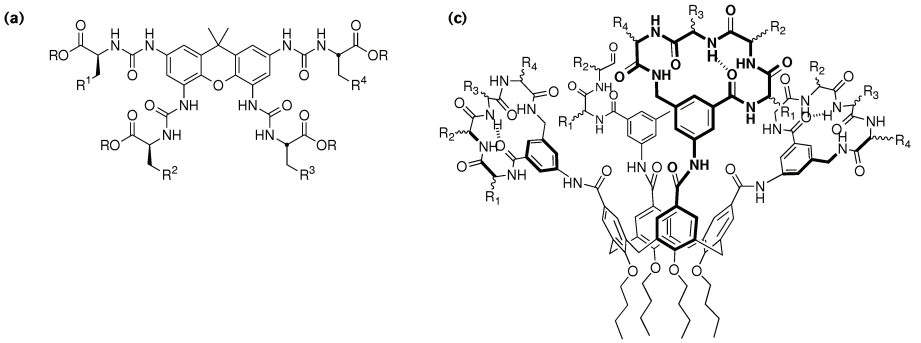
Molecular tennis ball



5 5-5

Grotzfeld RM and Rebek J et al. (1996) *Science* 271: 487-9.

Combinatorial scaffolds for molecular recognition

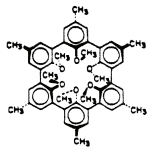


xanthene core functionalized with amino acids to bind DNA

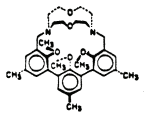
calixarene-supported cyclic tetrapeptide to bind proteins

Linton B and Hamilton AD. (1999) *Current opinion in chemical biology* 3: 307-12.

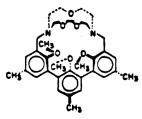
Preorganization of binding sites



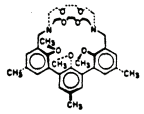
8, spherand



15, cryptaspherand



16, cryptaspherand

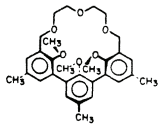


17, cryptaspherand

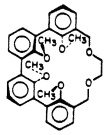
18, cryptand

19, cryptand

6, cryptand



20, hemispherand



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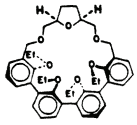
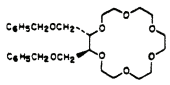
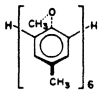


22, hemispherand

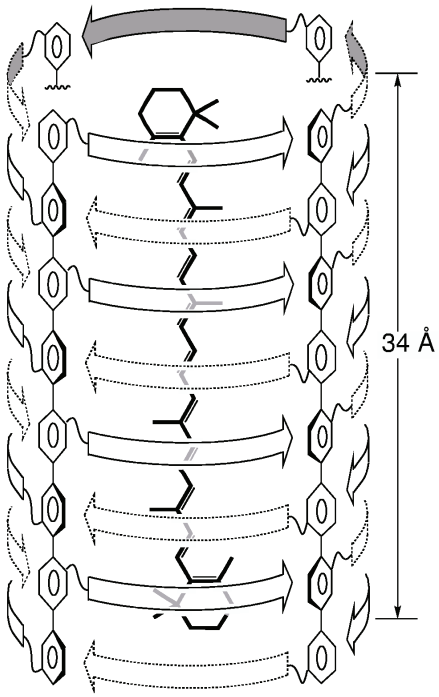


23, corand



14, podand

β-barrel encapsulating β-carotene



Arrows represent peptides: Lys-Leu-Lys and Glu-Leu-Glu

Baumeister B and Matile S. (2000) *Chem. Eur. J.* 6(10): 1739-49.