1A3b

Allostery in Guest Binding of Homoditopic Octaphosphonate Biscavitands

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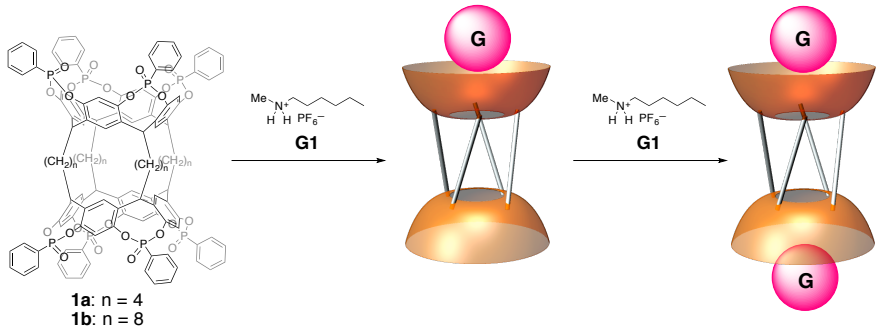
Allosteric regulations—a first guest binding influences the binding strength of subsequent guests to a multitopic receptor—are key features of many biological processes. Chemists have been developing multitopic receptors to establish artificial allosteric regulation that could be readily applicable to the efficient regulations of drug release, catalytic reactions, information transduction, etc. There are two types of mechanisms in allosteric regulation: one is homotropic, and the other is heteropic. Mimicry of a heterotropic regulation in synthetic allosteric receptors has been widely studied, whereas the development of a homotropic allosteric receptor is more difficult.

We have developed rim-to-rim connected bisresorcinarenes[1] in which each cavity is connected with four alkyl chains; therefore, it can intramolecularly communicate with the remaining cavity to give rise to cooperative guest binding events. Here, we set out to construct homotropic allosteric receptors **1a**,**b** based on bisresorcinarenes (Scheme 1)[2]



Scheme 1. Schematic representation of homotropic allostery in guest binding and the structures of biscavitands **1a, b** and guests **G1**.

The structure of **1a**, **b** was confirmed by X-ray crystals structure analysis (Figure 1). The conformational feature of **1a** can be recognized to be more rigid than that **1b**. Guest binding of **1a**, **b** demonstrated the positive and negative cooperative binding, respectively. The cooperative binding can be associated with the structural flexibilities of the four linkers.

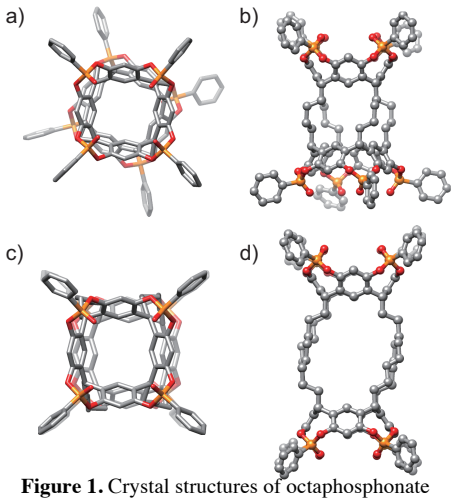


Figure 1. Crystal structures of octaphosphonate biscavitands **1a, b**: (a, c) top views; (b, d) side views. The solvent molecules are omitted for clarity.

Reference

[1] H. Yamada, T. Ikeda, T. Mizuta, T. Haino, *Org. Lett.* **2012**, *14*, 4510-4513

[2] D. Shimoyama, H. Yamada, T. Ikeda, R. Sekiya, T. Haino, *Eur. J. Org. Chem.* **2016**, *20*, 3300-3300.