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含硫接受子的設計、合成及其反應性的研究
The Rational Design of Trithiol Ligands and Their Disulfide Linked Supramolecules as Natural Molecule Receptors

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中文摘要

研究超分子化學的目標之一是發展出一套通用的設計策略,設計出一種合成的接受子,此接受子可以有選擇性地和目標物交互作用,目標物通常包含和生物有關的分子,例如:醣類、天然物、金屬離子、氣體和帶陰電性的離子。設計的最終目的就是合成出和酵素或抗體一樣有選擇性地和目標物鍵結的接受子。這些合成而來的接受子,其選擇性和親和力通常是受到一種平台的控制與調整。目標物就是鍵結在此平台所造就出來的口袋裡面。爲了更加瞭解目標物和生物性接受子之間的交互作用,我們計畫利用一種常見的平台去構築一些超分子。我們選擇了三乙基取代的苯環當作構築平台,因爲它有著固定的、預先組織好的三芽基結構。我們將會合成出一些具有三硫基的接受子,和其雙硫鍵形成後所塑造出的籠子分子。這些超分子和目標物之間的交互作用將會是我們研究的目的之一,我們將會用各種不同的儀器去探究和測量。我們也會去研究合成的超分子和目標物鍵結後所得產物的反應性,並探討可能的立體選擇性化學反應的發生。

Abstract

One goal of supramolecular chemistry is the development of general design strategies for selective binding of a target molecule by a rationally designed synthetic receptor. The targets often include biologically important guests such as saccharides, natural products, metals, gas, and ions. Ultimately, the goal is to achieve selectivity and affinity comparable to those attained by natural receptors such as enzymes and antibodies. The selectivity and affinity of synthetic hosts is controlled and modulated by careful choice of a scaffold upon which binding moieties are appended, creating a binding pocket. To better understanding the interactions between host and guest molecules in bio-relevant systems, we plan to build up several supramolecules based on a common scaffold. Tris-substituted 1,3,5-triethylbenzene derivatives are our choices as the scaffolds for constructing the host receptors due to their rigid pre-organized facial architectures. Several tri-thiol ligands and their disulfide bond crossed-linked cage molecules will be synthesized based on this 1,3,5-triethylbenzene platform. Their covalent or noncovalent (mostly hydrogen bonding) interactions between the artificial hosts and the guest molecules, including Fe4S4 clusters, metal ions, anions, and gases, will be characterized by X-ray, NMR, Mass Spec., UV-vis, FTIR…etc. The reactivity of the host-guest complexed supramolecules, for instance 3:1 subsited Fe4S4 clusters, and the potential rate enhancement or stereo-specific chemical reactions within the binding pocket will be further studied.