MS34-P17 Selective Encapsulation of Neutral Molecules by *endo*-Functionalized Molecular Tubes

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Biological functions heavily rely on selective recognition of neutral molecules. As in an enzyme binding pocket and a membrane channel, catalysis and transportation are initiated by selective recognition. These natural receptors select guest molecules with complementary size and shape which can fill the cavity appropriately. In the meantime, the converging functional groups in the cavity pose another level of selectivity: the substrate must be electrostatically complementary to the functional groups in the cavity as well. Thus, high binding selectivity and/or affinity to neutral molecules are achieved by combining the cavity and the converging functional groups. For example, *endo*-functionalized receptors reject the guests with appropriate shape but inappropriate electrostatic surface, and show a high binding affinity to the guests with both shape and electrostatic complementarity.[1,2]

The title compounds of this presentation, *endo*-functionalized molecular tubes, have rarely been reported in the literature.[2] Recently, it has been demonstrated that naphthalene and the bisnaphthalene cleft are very good scaffolds for constructing molecular receptors. [3-5] On this basis, we reported molecular tubes with *endo*-functionalized urea and thiourea groups and carefully studied their molecular recognition behaviour to neutral molecules.[2,6] In this presentation our continued efforts to encapsulate neutral guests inside these *endo*-functionalized molecular tubes and the obtained crystallographic results are demonstrated.

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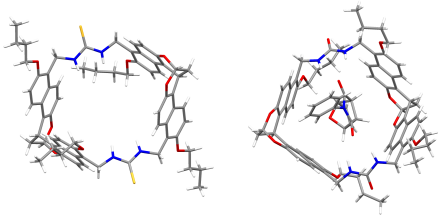

Figure 1. A structure of *endo*-funtionalized thiourea derivative (left) and urea derivative with neutral guest molecule inside (right).

Keywords: Molecular tubes, neutral guest molecules, endo-functionalization