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A tight 1:1 complex between an allosteric receptor and an organic effector with hydrogen and coordination bonds

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ABSTRACT

An allosteric system **1** was constructed by introducing a linear conjugated chain at position 1 and two side chains at positions 2 and 6 on the benzene ring. The conjugated chain consists of a zinc diethynyldiphenylporphyrin center (ZnDEDPP) extended to a diamidopyridine terminal. The side arm has a zinc tetraphenylporphyrin terminal (ZnTPP) linked by flexible ethylenedioxy groups. The organic effector **2**, possessing a uracil and two pyridine units, formed a tight 1:1 supramolecular complex with **1**. The binding constant of ZnDEDPP in **1** with 4-phenylpyridine was 4.2 times larger than that of ZnDEDPP in **1•2**, indicating that compound **2** function as an allosteric effector for the complexation of **1** and 4-phenylpyridine.

Introduction

The design and study of artificial allosteric systems are important for a better understanding of molecular recognition, which can be applied to the development of stimuli-responsive functional materials.[1] Metal ions are a typical effector (an external chemical stimulus) because the formation of a metal complex provides enough energy for a conformational alternation for activity switching.[2,3] Only a few studies have been conducted on allosteric system that recognizes neutral organic molecules as effectors because of the difficulty of generating enough driving force for the conformational alternation.[4] This is an essential process for the modulation of the degree of preorganization or the shielding or deshielding of the active sites in allosteric systems. Compared with these artificial allosteric systems, biological systems utilize combination of several kinds of supramolecular interactions such as hydrogen bonding, coordination, and hydrophobic and hydrophilic interactions. Thus, tight-binding complexes are produced in a highly selective manner, making sufficient energy for the conformational alternation. As far as we know, limited number of an allosteric system, where the conformational alternation is achieved by the recognition of a neutral organic effector with different kinds of supramolecular interactions, has reported.[5] In this study, an artificial allosteric system is applied using multiple supramolecular interactions through hydrogen bonding and metal coordination. An allosteric receptor **1** and an organic effector **2** were prepared (Fig. 1).

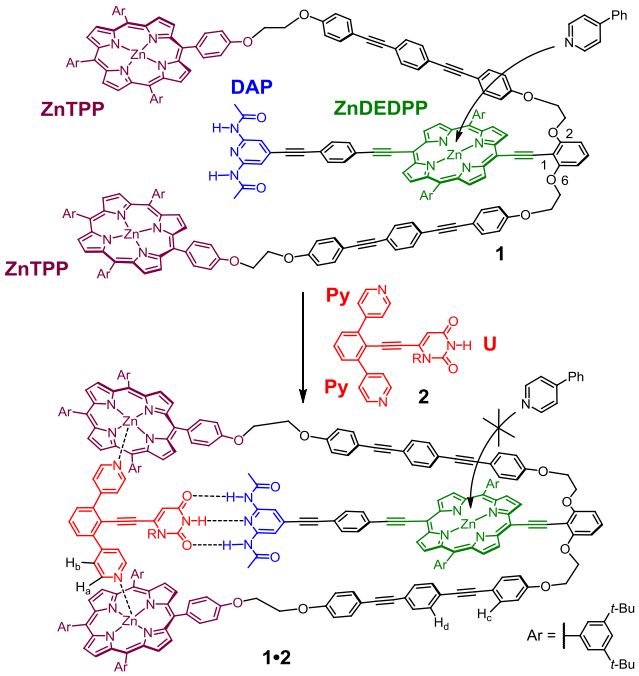

Figure 1. Mechanism of the allosteric regulation of the complexation of **1** and 4-phenylpyridine using **2** (red) as an effector.

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