Effect of substituents on mutual induced-fit controlled hydrogen-bonded capsule formation

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ABSTRACT

The mutual induced-fit process, well known in biological systems, involves the cooperative interaction of multiple components. However, mimicking this process in artificial systems, particularly using purely organic components, presents a significant challenge. In this study, we explore the role of substituents in enhancing the mutual induced-fit effect, leading to signal amplification in hydrogen-bonded capsule formation. Two distinct, highly flexible ligands an N-bridged tripodal ligand and a triazine-bridged ligand were employed. The N-bridged ligand acts as a molecular clip, inducing a cone-shaped conformation in the triazine-bridged adduct. This conformation undergoes solvent polarity-dependent hydrogen-bonded capsule formation, yielding a single product. In the absence of the N-bridged ligand, only 50% capsule formation was observed through ^{1}H NMR at 100 mM concentration. However, in its presence, mutual interactions drive the system into a stable cone-shaped conformation, achieving 100% capsule formation, independent of concentration. The entire process is characterized by IR spectroscopy, ^{1}H and ^{13}C NMR spectra, concentration-dependent ^{1}H NMR titration, ^{1}H-^{1}H COSY, ^{1}H-^{1}H NOESY, DOSY NMR, high-resolution ESI mass spectrometry, and energy-minimized structural analysis.

Keywords: Hydrogen-bond, N-bridged ligand, Substitution effect, Supramolecular-assembly, Dynamic self-assembly