Guest mediated ternary complexes: a new form of supramolecular materials

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The key to supramolecular chemistry often lie within macrocycles. As macrocyclic receptors, resorcinarenes are known for their ability to bind atomic or molecular guests via non-covalent interactions within their shallow but well-defined cavities. It is very challenging to design and construct concerted ternary assemblies of purely organic components held together by weak interactions alone, and the existing assemblies take two primary forms that have other types of host-guest interactions which is different than what is included in this report. To the best of our knowledge, there are no examples where the guest molecule mediates the interaction between a host and a third component outside of the cavity. This report presents a carefully designed strategy for just such a ternary. ABC assembly is based on two set of synergistic supramolecular weak interactions: aromatic interactions between a resorcinarene host (A) and an *N*-aromatic guest (B), and the moderate to strong hydrogen bonding between the bound *N*-aromatic guest (B) and carboxylic acids (C). The ternary assemblies are analyzed in the solid state through single crystal X-ray diffraction, in solution via ^{1}H and ^{19}F NMR spectroscopy. The binding processes were quantified through ^{1}H NMR titration experiments, and the observations were further supported by DFT-based computational calculations. As computationally predicted, the cooperativity between each component of the ABC ternary complex play a key role in the formation of the energetically favored ternary systems compared to binary analogues.