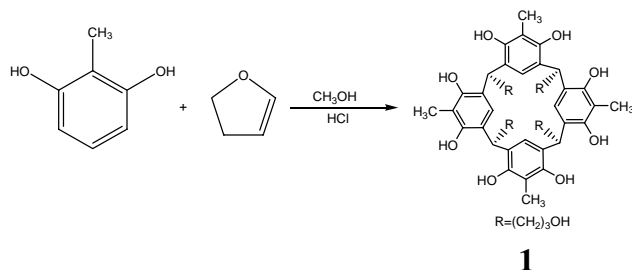
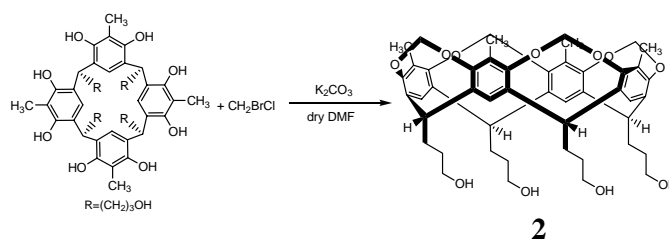


The goal of my project is to use metal ions to create a dynamic vessel whose assembly/disassembly is regulated. To create the vessel I will synthesize a molecule which has two different ligands on each of the two ends. The way I plan to do this is by varying the “foot” of a resorcinol-based cavitand, and using 2-methyl resorcinol. The methyl group will provide a handle for upper rim functionalization. Although several methods have been developed to link cavitand molecules by their tops,<sup>1</sup> to our knowledge only one way to link cavitand molecules by their lower rims has been reported.<sup>2</sup> This is most likely due to the increased flexibility of the lower rim. To create a

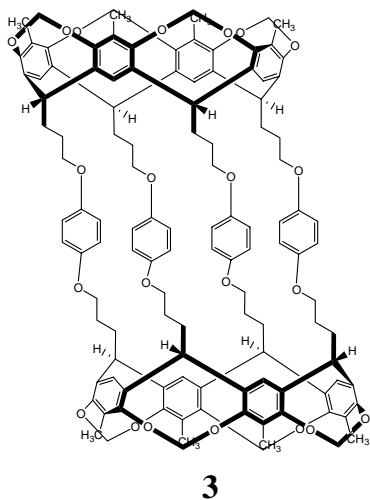


vessel which is linked by its lower rims, I will work with a propanol-footed cavitand. I have already synthesized the propanol-footed cavitand following a literature procedure.<sup>2</sup> The reaction entails the acid catalyzed condensation of 2-methyl resorcinol with 2,3-dihydrofuran to yield propanol-footed cavitand **1**.

Next, I added a methylene bridge, synthesizing cavitand **2** and providing the cavitand with the stability necessary for cage self-assembly.<sup>3</sup> A previously reported method for this reaction using a similar cavitand occurs in a sealed tube and allows for higher reaction temperatures and a significant decrease in reaction time compared to other procedures.<sup>4</sup>



In order to link the cavitands through their lower rims, I have tosylated the alcohol groups. My next step is to add hydroquinone, which will attack the carbon  $\alpha$  to the tosyl group, and the tosyl group will leave. By adding hydroquinone to the tosylated bowl in a 1:2 hydroquinone:bowl ratio, I will link four feet of one bowl to four feet of another to form the linked cavitand **3**. With the cavitands linked on the lower rims, I will add ligating groups to the other end. The methyl group of the resorcinol will be brominated, an imino diacetic acid group attached, and another metal such as  $\text{Co}^{+2}$  used to link all the tops. We will be able to control the complete assembly/disassembly of this final cage by adding competitive ligands. We expect to publish our findings and further analyze the guests which this host may encapsulate for delivery applications.



<sup>1</sup> Yamanaka, M.; Yamada, Y.; Seir, Y.; Yamaguchi, K.; Kobayashi, K. Selective Formation of a Self-Assembling Homo or Hetero Cavitand Cage via Metal Coordination Based on Thermodynamic or Kinetic Control. *J. Am. Chem. Soc.* **2006**, *128*, 1531–1539.

<sup>2</sup> Pirondini, L.; Bonifazi, D.; Menozzi, E.; Wegelius, E.; Rissanen, K.; Massera, C.; Dalcanale, E. Synthesis and Coordination Chemistry of Lower Rim Cavitand Ligands. *Eur. J. Org. Chem.* **2001**, *12*, 2311–2320.

<sup>3</sup> Pinalli, R.; Cristini, V.; Sottili, V.; Geremia, S.; Campagnolo, M.; Caneschi, A.; Dalcanale, E. Cavitand-Based Nanoscale Coordination Cages. *J. Am. Chem. Soc.* **2004**, *126*, 6516–6517.

<sup>4</sup> Román, E.; Peinador, C.; Mendoza, S.; Kaifer, A.E. Improved Synthesis of Cavitands. *J. Org. Chem.* **1999**, *64*, 2577–2578.

