Spectroscopic Analysis to Distinguish Two Cucurbit[n]urils In a Mixture

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Introduction

- A macrocycle is a cyclic molecule that consists of 12 or more atoms and is shaped to encapsulate molecules called guests.
- Cucurbit[6]uril (CB[6]) and Cucurbit[7]uril (CB[7]) are types of macrocycles that exhibit hydrogen bonds, ionic bonds, Van der Waal’s forces or hydrophobic interactions with guest molecules.
- Cucurbit[n]urils are size-complimentary to hold guests, such as 4-(1H-imidazol-1-yl)alanine (IMA) and 1,6-hexanediamine dihydrochloride (DAH). Portal, cavity and outer diameter increase from CB[6] to CB[7]. However, height stays the same throughout.

Objectives

The objectives of my research is to distinguish between CB[6] and CB[7] using fluorescence spectroscopy and detect a minimum amount of CB[6] when mixed with CB[7]. As well, find out if changing the total concentration of CB affects fluorescence.

Methods

- Steady-state fluorescence
- Experiments were done at 20 °C with a 10 mm x 10 mm fluorescence cuvette and using a gastight syringe for insertion of DAH.

Results

- CB[7] is non-selective and exhibits no fluorescence because when figure 5 is compared with figures 3 and 4 a different trend is shown and there appears to be not a lot of fluorescence detected. A complex with CB[7], if it is being formed, is not emissive.
- CB[6] is selective and its guest (IMA) exhibits fluorescence upon encapsulation. When figure 1 is compared with figures 3 and 4 the same trend of decreasing fluorescence occurs due to the displacement of the guest from its cavity.
- As the total concentration of CB changes, so does fluorescence trends. In figures 3 and 4, 20 µM of CB requires 4 additions to reach a saturation point.

Conclusions

- Overall, we answered our objectives and future work can be built on my research. Host-inclusion complexes can be used in real-life applications and more steps can be taken to fully understand Cucurbit[n]urils complexes.
- We found that CB[6] interferes with the detection of CB[7] using its specific titration procedure. However, CB[7] cannot interfere with the CB[6] titration because it either forms a non-emissive complex or, more likely, forms an unstable complex with low equilibrium constant.
- Detection as low as 0.1% CB[6] to a 99.9% CB[7] ratio was analyzed through titration.

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References