

*Binding of Cucurbit[n]uril, n = 5, 6, or 7, with Alkali Metal Ions Via ESI-MS*

Presenters Oreoluwa Adebajo, Chemistry major; Olivia Basant, Chemistry and Psychology major; Cameron Cummings, Chemistry major; Jeffery Davison, Chemistry major; Fatima Ghiathi, Psychology major; Kimora Hudson, undeclared major; Betelhem Lonse, Chemistry major; Kaitlin Watkins, Chemistry major; Anjelina Webb, Biology major; Phillip Wooten, Chemistry major; and Mailei Zhang-Smith, Chemistry major  
Mentored by Dr. Farooq Khan

Cucurbit[n]urils, or CBn, where n = 5, 6, 7, 8 or 10 are “molecular containers” well-suited for binding of a wide array of molecules, and are of immense interest in drug delivery, photochemical reactions and catalysis. Of considerable interest in understanding the fundamental properties of these molecules are their binding properties with metal ions. In our study, we have explored the binding selectivities of CB5 with alkali metal ions via electrospray ionization (ESI) mass spectrometry in aqueous solutions. We find that CB5 binds with one or two alkali metal ions. The relative binding energies for CBn, n = 5, 6 or 7 were determined via collision-induced dissociation (CID) experiments, and found to be  $\text{Li}^+ > \text{Na}^+ > \text{K}^+ > \text{Rb}^+ > \text{Cs}^+$ . Species containing CBn, two metal ions and chloride ions were also observed, which upon CID, result in the loss of a neutral MCl species.