

Title: Bowls not Balls: Using Cyclotrimeratrylene Derivatives as Xenon Hosts in the Development of Biosensors.

Abstract: Xenon-129 (^{129}Xe) is a magnetic resonance imaging (MRI) active noble gas that binds to a tri-amino functionalized cyclotrimeratrylene (CTV) making it a unique candidate for development as a biosensor. ^{129}Xe has a large chemical shift that is responsive to its environment, is safe to be administered orally, and passes through the blood brain barrier making it a good candidate for a biosensor reporter using current MRI technology. Up until now research has focused on cryptophane structures, which are ball-shaped molecular hosts that can encapsulate ^{129}Xe , as the avenue for making selective contrasting agents. The two main drawbacks of cryptophanes are the low yield of the current synthetic strategies and the difficulty in functionalizing them to make them selective and water-soluble. In contrast, the tri-amino CTV has a shorter synthetic route with an overall yield of 47.5%, and it is obtained from readily available inexpensive starting materials. The tri-amino functionalized CTV binds ^{129}Xe and has a rapid exchange rate, making it the lead compound in a hereto undiscovered class of ^{129}Xe molecular hosts that are easily functionalized.