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The Binding Interaction of Imazapyr with Cucurbit[n]uril (n=6-8): Combined Experimental and Molecular Modeling study

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ABSTRACT

The inclusion complexes of imazapyr (IMA) with cucurbit[n]uril, CB[n] (n=6-8), have been investigated. Fluorescence spectroscopy, MALDI-TOF, and ^{1}HNMR were used to investigate and characterize the inclusion complexation of IMA and CB[n] in solutions. Whereas the solid state complexes have been characterized by Fourier transform infrared spectroscopy (FTIR), and powder X-ray diffraction (PXRD). IMA was fond to form 1:1 complexes with CB[n] with association constants ranging from 5.80×10^{2}-2.65×10^{3}. The guest molecule IMA was found to encapsulate into the larger cavities of CB[7] and CB[8], whereas with CB[6] the molecule remains outside the cavity. Molecular dynamic (MD) simulations were used to follow the inclusion process at an atomistic level to study the mechanism and stability of inclusion. The results obtained showed that inclusion complexes of IMA with both CB[7] and CB[8] are highly stable in aqueous media, but the CB[6] smaller cavity size of prohibited the formation of an inclusion complex with IMA. The results clearly show that in addition to hydrophobic effects the presence of hydrogen bonding has added greatly to the stability of these complexes.

Keywords: Imazapyr; Herbicides; Cucurbit[n]uril; Inclusion complex; Molecular dynamics.