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Investigations of Inclusion Complexes of Imazapyr with 2-Hydroxypropyl(β/γ) Cyclodextrin Experimental and Molecular Modeling Approach

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Abstract : The inclusion complexes of imazapyr (IMA) with 2-hydroxypropyl(β/γ) cyclodextrins (HP β/γ-CD), have been studied in aqueous media and in the solid state. In this work, fluorescence spectroscopy, electrospray-ionization mass spectrometry (ESI-MS), and HNMR were used to investigate and characterize the inclusion complexes of IMA with the cyclodextrins in solutions. The solid-state complexes were obtained by freeze-drying and were characterized by Fourier transform infrared spectroscopy (FTIR), and powder X-ray diffraction (PXRD). The most predominant complexes of IMA with both hosts are the 1:1 guest: host complexes. The association constants of IMA-HP β-CD and IMA-HP γ -CD were 115 and 215 L mol^{-1}, respectively. Molecular dynamic (MD) simulations were used to monitor the mode of inclusion and also to investigate the stability of these complexes in aqueous media at atomistic levels. The results obtained have indicated that these inclusion complexes are highly stable in aqueous media, thereby corroborating the experimental results. Additionally, it has been demonstrated that in addition to hydrophobic interactions and van der Waals interactions the presence of hydrogen bonding interactions of the type H---O and CH---O between the guest and the host have enhanced the stability of these complexes remarkably.

Keywords : imazapyr, inclusion complex, herbicides, 2-hydroxypropyl-β/γ-cyclodextrin
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