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An experimental and theoretical investigation of inclusion complexes of Indole Chalcones in β -cyclodextrin

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Indole Chalcone (IC) derivatives form an important group of chalcones with biological activities such as anti-inflammatory, neuro-protective, anti-amoebic, anti-cancer, etc. In addition, various chalcones are also recognized for their wide antimicrobial activity and they can be employed as efficient drugs for the treatment of several diseases like malaria or tuberculosis. Despite a variety of potential applications of chalcones in medicinal chemistry, these compounds generally have limited pharmacological uses because of low dissolution rate and bioavailability. There are multiple techniques designed to increase the solubility of a drug, including the use of micelles, liposomes, nanoparticles and nanodispersions. Among the existing techniques, the formation of inclusion complexes with encapsulating agents such as β -Cyclodextrin (β -CD) is frequently employed. The present study focuses on the formation of inclusion complexes of IC derivatives with β -CD, which involves absorption and steady state fluorescence spectroscopies. The stoichiometries and binding constants (K_{in}) of these complexes have been investigated by monitoring their absorbance and fluorescence spectral profiles. The data are analyzed by Benesi-Hildebrand plots as well as Job's method, which indicate 1:1 stoichiometry of IC: β -CD complexes. Fluorescence measurements are also used to investigate the effect of temperature on the stability of inclusion complexes. Stability of IC: β -CD complexes are significantly affected with variation in substituents on the phenyl ring and temperature. The stability of the inclusion complex observed to decrease with increase in temperature. All the experimental results and the geometrical data obtained using PM3 semi-empirical method illustrate the partial inclusion of IC derivatives from the phenyl ring side in β -CD cavity. The binding process of IC derivatives with β -CD is found to be exothermic in nature and seems to be controlled by electrostatic and hydrophobic forces.

Biography

Manju K Saroj has her expertise in working experimentally and theoretically on photo-physical properties of the biologically active molecules like Isatin Chalcone, Indole Chalcones and thymol based Schiff's bases. She has done extensive study related to specific and non-specific interaction of various probe in heterogeneous and homogenous media by considering their absorption and fluorescence spectral profile.

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