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Experimental and Theoretical Characterization of Supramolecular Complexes between 7-(Diethylamino)Quinoline-2(1H)-One and Cucurbit[7] Uril

Authors : Kevin A. Droguett, Edwin G. Pérez, Denis Fuentealba, Margarita E. Aliaga, Angélica M. Fierro

Abstract : Supramolecular chemistry is a field of growing interest. Moreover, studying the formation of host-guest complexes between macrocycles and dyes is highly attractive due to their potential applications. Examples of the above are drug delivery, catalytic process, and sensing, among others. There are different dyes of interest in the literature; one example is the quinolinone derivatives. Those molecules have good optical properties and chemical and thermal stability, making them suitable for developing fluorescent probes. Secondly, several macrocycles can be seen in the literature. One example is the cucurbiturils. This water-soluble macromolecule family has a hydrophobic cavity and two identical carbonyl portals. Additionally, the thermodynamic analysis of those supramolecular systems could help understand the affinity between the host and guest, their interaction, and the main stabilization energy of the complex. In this work, two 7-(diethylamino) quinoline-2 (1H)-one derivative (QD1-2) and their interaction with cucurbit[7]uril (CB[7]) were studied from an experimental and in-silico point of view. For the experimental section, the complexes showed a 1:1 stoichiometry by HRMS-ESI and isothermal titration calorimetry (ITC). The inclusion of the derivatives on the macrocycle lends to an upward shift in the fluorescence intensity, and the pKa value of QD1-2 exhibits almost no variation after the formation of the complex. The thermodynamics of the inclusion complexes was investigated using ITC; the results demonstrate a non-classical hydrophobic effect with a minimum contribution from the entropy term and a constant binding on the order of 106 for both ligands. Additionally, dynamic molecular studies were carried out during 300 ns in an explicit solvent at NTP conditions. Our finding shows that the complex remains stable during the simulation (RMSD ~1 Å), and hydrogen bonds contribute to the stabilization of the systems. Finally, thermodynamic parameters from MMPBSA calculations were obtained to generate new computational insights to compare with experimental results.

Keywords : host-guest complexes, molecular dynamics, quinolin-2(1H)-one derivatives dyes, thermodynamics
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