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Inclusion Complexes of Some Imidazoline Drugs with Cucurbit[N]Uril (N=7,8): Preparation, Characterization and Theoretical Calculations

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Abstract : This work explored the interaction of three different imidazoline drugs, naphazoline nitrate (NPH), oxymetazoline hydrochloride (OXY) and xylometazoline hydrochloride (XYL) with two different synthesized cucurbit[n]urils CB[n], cucurbit[7]uril (CB[7]) and cucuribit[8]uril (CB[8]). Three binary inclusion complexes have been investigated in solution and in the solid state. The solid complexes were obtained by lyophilization, whereas the physical mixtures of guests and hosts at a stoichiometric ratio of 1:1 were obtained for each drug. 1HNMR, electrospray ionization mass spectrometry (ESI-MS), and matrix-assisted laser desorption-ionization time-of-flight (MALDI-TOF) mass spectrometry was used to study the complexes prepared in aqueous media. The lyophilized solid complexes were characterized by Fourier transform-infrared spectroscopy (FT-IR), powder X-ray diffractometry (PXRD), thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC). MS, FT-IR and PXRD experimental results established in this work reveal that NPH, OXY and XYL molecules form stable inclusion complexes with the two hosts. The TGA and DSC confirmed the enhancement of the thermal stability of each drug and the production of a thermally stable solid complex. The 1HNMR has shown that the protons of the guests faced shifting in ppm and broadening of their peaks upon the formation of inclusion complexes with the selected CB[n]. The aromatic protons of the guest exhibited the highest changes in the chemical shifts and shape of the NMR peaks, suggesting their inclusion into the cavity of the CB[n]. The diffusion coefficients (D), developed from the diffusion-controlled NMR Spectroscopy (DOSY) measurements, for the complexation of the selected imidazoline drugs with CB[7] and CB[8], were decreased in the presence of hosts compared to the free guests indicating the formation of the guest-host adduct. Furthermore, we conducted molecular dynamic simulations and quantum mechanics calculations on these complexes. The results of the theoretical study corroborate the experimental findings and have also shed light on the mechanism of inclusion of the guests into the two hosts. This study generates initial data for potential drug delivery or drug formulation systems for these three selected imidazoline drug compounds based on their inclusion into the CB[n] cavities.

Keywords : cucurbit[n]urils, imidazoline, inclusion complexes, molecular dynamics, DFT calculations, mass spectrometry
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