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The formation, structure, and electronic properties of anticancer doxorubicin drug and cucurbit[n]urils complexes, n= 7, 8 (Theoretical Study)

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Abstract : The present theoretical study deals with host-guest complex formation between cucurbit [n] urils,n= 7,8 as a host and doxorubicin as a guest using semi-empirical calculation (PM3 level). In these complexes, the formation of Hydrogen bonding it could be occurred through portal oxygen atoms of cucurbit [n] urils and hydroxyl groups of the drug. The energies of HOMO orbital and LUMO orbital have been calculated for the host- guest complexes and their components. The result of stabilization energy is explained the complex formation.
Key words : PM3, Cucurbit [n]urils, molecular capsules.

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