



Comparison of nanotubes and Calixarenes in delivery of Fluorouracil as an anticancer drug

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Fluorouracil (brand names: Adrucil, Carac, Efudex and Fluoroplex) is an analog of pyrimidine which has been used as an anticancer drug for 40 years [1]. These days use of Calixarenes and Nanotubes are widely spread in the world of drug delivery [2-5]. This subject that which of these containers are better in this field has not been investigated yet. In this paper the differences between these two groups of agents are studied. For this aim Calix[6]arene and Nanotube (6,6) with the same number of atoms as containers and an anticancer drug named fluorouracil were selected. Two complexes: one, between Nanotube and the drug, another between Calixarene and the drug were formed. The structures were optimized by DFT method and B3LYP/6-31G(d) level. Results show the complex between Nanotube and fluorouracil is more stable. Mulliken charges, bond lengths and hybrids of atoms are calculated. The Nanotube-Fluorouracil complex is more stable than Calixarene-Fluorouracil complex. So Nanotubes are better containers for drugs than Calixarenes. Maybe because of more instability of single Calixarene, the released formation energy in Calixarene-Fluorouracil complex is a little more than another complex. Mulliken charges in Calixarene-Fluorouracil complex are both negative in two neighbor atoms (O and N) and this subject confirms instability of this complex.

Keywords: Calixarene, Nanotube, Fluorouracil, Anticancer, DFT.

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