عنوان مقاله:

A DFT Study of Selenium-Cyclic Peptide Anticancer Nanocarrier

محل انتشار:

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نویسندگان:

Sara Moghimi - *Department of Chemistry, Mashhad Branch, Islamic Azad University, Mashhad, Iran*

Ali Morsali - *Department of Chemistry, Mashhad Branch, Islamic Azad University, Mashhad, Iran*

Mohammad Heravi - *Department of Chemistry, Mashhad Branch, Islamic Azad University, Mashhad, Iran*

S. Ali Beyramabadi - *Department of Chemistry, Mashhad Branch, Islamic Azad University, Mashhad, Iran*

خلاصه مقاله:

Using Se۸ selenium and cyclic peptides and nanoparticles (SeCPNP), six configurations for the adsorption of the ۵-fluorouracil (FU) anticancer drug on SeCPNP have been examined (SeCPNP/FU۱-۶). Binding energies, solvation energies and quantum molecular descriptors such as electrophilicity (ω) and global hardness (η) in the aqueous solution and gas phase were studied at the density functional level of M۰۶-۲X. The most stable structure by binding energy calculations was determined. The values obtained from solvation energies indicate that SeCPNPs can increase the solubility of FU, which is a key factor in drug delivery. According to quantum molecular descriptors, the reactivity of cyclic peptide (CP) and FU drug in all structures (SeCPNP / FU ۱-۶) increases. AIM calculations for all structures show that Se-A interactions (A = O, H, N, F, C) and intermolecular hydrogen bonding play an important role for this drug delivery system. In structures where FU is parallel to SeCPNP and undergoes interactions concurrently with Se۸ and CP, it is more stable than structures in which the drug undergoes interactions only with Se۸ and CP.

کلمات کلیدی:

fluorouracil, Anticancer, AIM analysis, DFT, Selenium cyclic peptide nanoparticles-۵