عنوان مقاله:

Computational study of Folat-conjugated Gold nanopartical and 6Mercapto-1-Hexanol linker for cancer treatment with nanotechnology applications

محل انتشار:

سومین همایش ملی کاربردهای شیمی در فناوریهای نوین (سال: 1392)

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خلاصه مقاله:

Cancer is a disease that humans have been involved with, and scientists have done great efforts to treat it. But they have not had much success, On the other hand Nano science as a new scientific in various branches of science have been made many changes.Gold nanoparticles (AuNPs) provide non-toxic carriers for drug and gene delivery applications. An additional attractive feature of AuNPs is their interaction with thiols, providing an effective and selective means of controlled intracellular release. We also know that folate receptor (FR) is a confirmed tumor-associated antigen that binds folate and folate–drug conjugates with very high affinity and shuttles these bound molecules inside cells via an endocytic mechanism. Now we have a folate connecting by the linker 6-mercapto-1-hexzanol to gold nanoparticles (AuNP). In this report, the Molecular Structure, and some Geometrical properties (Bond lengths and Bond angles) folate-6mercapto-1-hexzanol-AuNP were investigated using the Density Functional .Theory (DFT) and Hartree Fock (HF) calculations

کلمات کلیدی:

DFT and HF calculations, cancer, 6-mercapto-1-hexanol, folate, folate receptor, folic acid, gold nanoparticle nanoconjugate