

عنوان مقاله:

Computational study of Folate-conjugated with two platinum nanoparticle and 6-Mercapto-1-Hexanol linker for cancer treatment with nanotechnology applications

محل انتشار:

دومین کنفرانس ملی توسعه کاربردهای صنعتی اطلاعات، ارتباطات و محاسبات (سال: 1392)

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خلاصه مقاله:

There are over 220 different known cancers that afflict humans. The causes of cancer are diverse, complex, and only partially understood. Many things are known to increase the risk of cancer, including tobacco use, dietary factors, certain infections, exposure to radiation, lack of physical activity, obesity, and environmental pollutants. Platinum nanoparticles (PtNPs) provide non-toxic carriers for drug and gene delivery applications. An additional attractive feature of PtNPs is their interaction with thiols, providing an effective and selective means of controlled intracellular release. selective targeting of folate-receptor positive cancerous cells. The linker chosen was 6-mercapto-1-hexanol (MH) with nanoconjugate products named Folate-MH-PtNP. We report the folate-receptor tissue. This demonstrates that folate targeting is effective in selecting for specific cell populations. 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-hexanol to two Platinum nanoparticles (PtNP). In this report, the Molecular Structure, and some Geometrical properties (Bond lengths and Bond angles) of folate-6mercapto-1-hexanol- PtNP were investigated using [the Density Functional Theory (DFT) calculations].

کلمات کلیدی:

DFT calculations, cancer, 6-mercapto-1-hexanol, folate, folate receptor, folic acid, Platinum nanoparticle

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