عنوان مقاله:

A computational investigation on the connection between physico chemical and geochemical properties of paclitaxel and paclitaxel conjugated to nanoparticles

محل انتشار:

همایش ملی کاربرد سیستم های هوشمند (محاسبات نرم) در علوم و صنایع (سال: 1392)

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خلاصه مقاله:

Computational chemistry is a branch of chemistry that uses principles of computer science to assist in solving chemical problems. The recent years of computational chemistry have been very application about delivery and release drugs.paclitaxel (PTX) is a well known anti-cancer agent. The cytotoxicity of paclitaxel can be minimized by linking it to an affinity succinate linkage is used to improve the interaction between an anti-cancer agent, paclitaxel and a chitosan biopolymer.This chitosan sheet could be used as drug carrier for controlled release. [1,2] Low molecular weight chitosan conjugated with paclitaxel (LMWC-PTX) was also synthesized by chemical conjugation of LMWC and PTX through a succinate linker, which can be cleaved at physiological conditions. [1,3] In this report, the Molecular Structure, Dipole Moment (DM)and some physicochemical properties,some geometrical parameter ,such as bond length, bond angle and energy structures of paclitaxel , chitosan and paclitaxel conjugated to nanoparticle chitosan were investigated using the Hartree Fock (HF) calculations.The computational method which were used, HF/6-31g**.

کلمات کلیدی:

computational, Paclitaxel, chitosan , geometrical parameter, nanoparticle

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