

# **Theoretical Study on the Geometrical and physico chemical Properties of Paclitaxel Conjugated to Nanoparticle Chitosan Biopolymer Along with ethylene glycol chains**

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## **Abstract**

The recent years of computational chemistry has been very applied about drug delivery and release. 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 nanoparticles (LMWC) is one of the best carriers. These carriers bind to the drug succinate linker connected and form a stable complex. So it is possible to use these nanoparticles to reduce toxicity and increase its solubility. The loop connecting poly ethylene glycol (PEG) can prolong its time in the blood circulation of the drug. 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 was used, HF/6-31g\*\*.

**Keywords:** HF calculations, Paclitaxel, LMWC-PTX, geometrical parameter, PEG