عنوان مقاله:

Theoretical study on the geometrical properties of paclitaxel usingdensity functional theory and Hartree–Fock method

محل انتشار:

همایش ملی نانو فناوری و شیمی سبز (سال: 1391)

تعداد صفحات اصل مقاله: 3

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خلاصه مقاله:

Paclitaxel is a natural occurring diterpene alkaloid originally isolated from the bark of Taxusbrevifolia. It is now one of the most important chemotherapeutic agents for clinical treatment ofovarian and breast cancers. Recent clinical trials have also shown paclitaxel's potential for thetreatment of non-small-cell lung cancer, head and neck cancer, and other types of cancers. Whiletremendous chemical research efforts have been made in the past years, which established theundamental structure-activity relationships of the paclitaxel molecule, and provided analogs forbiochemical studies to elucidate the precise mechanism of action and for the development of secondgenerationagents, many areas .remain to be explored

کلمات کلیدی:

Anti-cancer drug; DFT and HF calculations; Paclitaxel