عنوان مقاله:

Molecular Modeling Studies of Vinblastine as anticancer nanotechnology investigation

محل انتشار:

هشتمین همایش بیوتکنولوژی جمهوری اسلامی ایران و چهارمین همایش ملی امنیت زیستی (سال: 1392)

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خلاصه مقاله:

Vinblastine is one of the vinca alkaloids that play a major role in cancer chemotherapy by inhibiting the polymerisation of tubulin into microtubules.Antimitotic of vinblastine families binding site inhibit microtubule assembly. The ultimate action of this agent causes mitotic arrest by inhibiting normal dynamic instability at very low concentration. The investigation of vinblastine has been studied by theoretical methods. It has been established as the best structural and functional of vinblastine. In an effort to understand the conformational preferences that may be attributed to stereoelectronic effects, a number of computational chemistry studies carried out. Molecular mechanics, Monte Carlo, Molecular Dynamics and Langevin calculations have been performed on vinblastine. These results show the minimized structure of vinblastine, calculated potential energy for important dihedral angles and the effect of .temperature on geometry of optimized structure

کلمات کلیدی:

Vinblastine, Molecular Mechanic, DFT