عنوان مقاله:

Investigation of Sup90-Dota and interaction with Carbon nanotubes; A Semi empirical study

محل انتشار:

دومین کنفرانس ملی نانو ساختارها،علوم و مهندسی نانو (سال: 1396)

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خلاصه مقاله:

The investigation of the anticancer drugs will be important because of the proliferation of cancer. We want to take steps to improve public health.The combination of two carbon nanotubes (single wall nanotube and multi wall nanotube) and Sup90-Dota (an anticancer drug) was investigated based on Molecular Mechanic and Semi Empirical methods.Our goal is to investigate the transfer of carbon nanotubes by drug Sup90- Dota and the study of structural changes caused by the interaction of this anticancer drug combination with the nanotubes.We study of different parameters such as total energy, potential energy and kinetic energy and time of simulations are 20 ns. Calculation and geometrical optimization in different temperature (295,298,310 and 315 kelvin) were conducted via Monte Carlo method (Amber, Bio+, MM+ and OPLS).The semi-empirical calculations such as total energy, binding energy, isolated atomic energy, electronic energy, core–core interaction and heat of formation in AM1 , RM1 , PM3 , MNDO , INDO and CNDO for Sup90- Dota and CNT- Sup90- Dota complex.Analysis of Sup90- Dota and it’s interaction with CNTs show that, this carrier can be applied to improve the activities of this anti cancer drug

کلمات کلیدی:

Sup90 - Dota , Nanotube , anticancer, Molecular Mechanic , Semi Empiric