

Delivery of Gleevec (imatinib) by carbon nanotube for cancer treatment in different solutions

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Background and Aims: single wall carbon nanotubes (SWCNTs) have potential advantages, including their ability to carry a high cargo loading, their intrinsic stability and structural flexibility, which could prolong the circulation time and hence the bioavailability of the carried drug molecules. SWCNT-based materials have already been investigated as potential delivery vehicles for intracellular transport of nucleic acids, proteins and drug molecules. Tyrosine kinase inhibitor STI571 (also called Gleevec or imatinib) is a small molecule has been used in molecularly targeted therapy for chronic myeloid leukemia (CML). Imatinib has been proved to be a cost-effective 1st-line therapy for patients with newly diagnosed chronic phase CML.

Methods: We used the methods Molecular Dynamics, Langevin Dynamics, Monte carlo, single point and Geometry optimization and The force fields are MM, AMBER, BIO and OPLS and temperatures are 290, 295, 300, 305, 310, 315. By these methods were evaluated and significant results were obtained. That the energy obtained, the study examined and compared to simulation with empirical studies. The systems were optimized at first by HF and BLYP, B3LYP methods by STO-3G, 6-31G and with the same basis sets and methods.

Results: in this research we simulated gleevec and SWCNT complex with special softwares and calculated amount of stability in different solutions by computing thermochemical functions such as kinetic energy changes (K), entropy differences (ΔS), enthalpy differences (ΔH), Gibbs energy change (ΔG). stable forms of complex can be used in laboratory for experimental studies.

Conclusions: we have employed there different theoretical methods including Hartee-Fock (RHF), density functional theory (B3LYP) methods with STO-3G, 6-31G basis sets to study the substituent effects of 1, 4-benzodiazepine derivatives as well as bioactivity caused by their structural stabilities and corresponding thermochemical parameters. The activity and stability as well as vibrational frequencies of the drug are strongly affected under thermochemical properties at the specific temperature.

Keywords: Nanotubes; Tyrosine kinase inhibitor; Gleevec