Abstract

This work deals with the butterfly conformation control of the anti-HIV TIBO molecule confined into carbon nanotubes (CNT). This theoretical study concerns the variation of some pertinent conformation descriptors such as butterfly angle, wingspan, volume, dipole moment, solvation energy and confinement energy versus carbon nanotube diameters. Obtained results show that it is possible to describe the configurations of actual drugs as 8-Cl or 9-Cl TIBO as the parent molecule TIBO encapsulated in an adequate CNT. Our approach indicates that drug confinement inside CNTs may be a promising way to use a same drug in order to fellow HIV virus mutations