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Molecular dynamics and free energy analyses of the interactions between b-cyclodextrin and some anticancer drugs

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In order to design a drug delivery system, various high-performance carrier materials are being developed to deliver the necessary amount of drug to the targeted site both efficiently and precisely. Cyclodextrins (CDs) are potential candidates for such a role, because of their ability to alter physical, chemical and biological properties of guest molecules through the formation of inclusion complexes. In this paper we analyze the possibility of forming host-guest inclusion complexes between beta-cyclodextrin (BCD) and several anticancer active principles, characterized by different mechanism of action, by molecular simulations. The trajectories of the insertion angles, rotation of the non-polar parts of the drugs inside the macrocycle and other geometrical features give detailed information on the dynamics of the complexes. The relative binding energies in all cases indicate possibilities of formation of inclusion complexes between BCD and the anticancer drugs either in a 1:1 or in a 2:2 stoichiometry.

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