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Molecular structure, molecular docking, molecular dynamics simulation, and drug likeness evaluation of 3,7-dihydroxy-1,2-dimethoxyxanthone for its anticancer activity

A naturally occurring xanthone, named 3,7-dihydroxy-1,2-dimethoxyxanthone was experimentally and computationally investigated for its anticancer activity. Single crystal X-ray diffraction (XRD) analysis revealed that the compound crystallizes in the triclinic space group P1. Vibrational frequencies, electronic properties, chemical reactivity descriptors, the molecular structure, and stability of the compound were investigated by DFT calculations using the Gaussian 09 W program at the B3LYP/6−311+G(2d,p) level of theory. All calculations showed correlations to experimental data. Its thermodynamic parameters at various temperatures are presented. The title molecule was docked on the proteins of prostate, cervical, breast, and melanoma cancer cells, and the results showed comparable binding energies to the standard chemotherapeutic agent, doxorubicin with small differences in the range 0.2−0.7 kcal mol−1. Given that the compound showed significant potential on the proteins of prostate and cervical cancer cells, the dynamic properties of the bound state of the title ligand with the two selected proteins were further examined through a 200 ns molecular dynamics simulation. The results showed relatively overall higher stability through the simulation time than the free target. All these findings were afterward confirmed by the good in vitro inhibition activity of the compound against human prostate and cervical cancer cell lines with IC50 values of 9.55 and 9.19 μM, respectively in comparison to the standard drug, and additionally demonstrated innocuousness towards normal human kidney cancer cell lines. Moreover, the drug-likeness properties indicated that the title compound has a high bioavailability, good water solubility, good gastrointestinal absorption, and can be easily synthesized.

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