Indian Journal of Chemistry
Vol. 63, October 2024, pp. 945-958
DOI: 10.56042/ijc.v63i10.10916

Computational studies and *in silico* evaluation of Cd (II) and Zn (II) complexes revealing their anti-cancer trait

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Received 6 May 2024; accepted (revised) 23 September 2024

Computational studies offer to explore mechanistic aspects of molecular interactions with the potential to deliver practical strategies and enable rational *in silico* drug design. New powerful cancer drugs are crucial, as evidenced by the prevalence of extensively and multi-drug-resistant tuberculosis. This research work describes the use of DFT for the optimization of zinc and cadmium metal complexes. FMO distribution and its based electronic properties, and electrostatic potential have been studied. According to ADMET analysis, every substance is safe for biological use and non-carcinogenic. Both complexes have been docked to human-GTPase-K-Ras protein to determine binding ability and modes. The stability of protein-drug complexes has been probed through MD simulations, focusing on the most tightly bound complex. The Zn-complex is more thermodynamically stable compared to Cd-complex. Good ligand binding interaction with the receptor protein has been identified through molecular docking analysis mainly because of non-bonding interactions. Finally, these results might help develop a novel anti-cancer agent.

Keywords: Cd(II) and Zn(II) complexes, Computational studies, DFT, Molecular docking studies, Anti-cancer mannerism