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Investigation of Anticancer Properties of Caffeinated Complexes via Computational Chemistry Methods

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Abstract

Computational investigations were performed for 1,3,7-trimethylpurine-2,6-dione, 3,7-dimethylpurine-2,6-dione, their Ru(II) and Os(III) complexes. B3LYP/6-311++G(d,p)(LANL2DZ) level was used in numerical calculations. Geometric parameters, IR spectrum, ^{1}H-, ^{13}C- and ^{15}N-NMR spectrum were examined in detail. Additionally, contour diagram of frontier molecular orbitals (FMOs), molecular electrostatic potential (MEP) maps, MEP contour and some quantum chemical descriptors were used in the determination of reactivity rankings and active sites. The electron density on the surface was similar to each other in studied complexes. Quantum chemical descriptors were investigated and the anticancer activity of complexes were more than cisplatin and their ligands. Additionally, molecular docking calculations were performed in water between related complexes and a protein (ID: 3WZE). The most interact complex was found as Os complex. The interaction energy was calculated as 342.9 kJ/mol.

Keywords: Caffeine, Transition Metal Complexes, Computational study, Anticancer Properties, Molecular Docking