

Accepted Manuscript

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Koray Sayin, Ayhan Üngördü



PII: S1386-1425(17)30986-1
DOI: doi:[10.1016/j.saa.2017.12.013](https://doi.org/10.1016/j.saa.2017.12.013)
Reference: SAA 15658

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received date: 27 September 2017

Revised date: 22 November 2017

Accepted date: 1 December 2017

Please cite this article as: Koray Sayin, Ayhan Üngördü , Investigation of anticancer properties of caffeinated complexes via computational chemistry methods. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Saa(2017), doi:[10.1016/j.saa.2017.12.013](https://doi.org/10.1016/j.saa.2017.12.013)

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Investigation of Anticancer Properties of Caffeinated Complexes via Computational Chemistry Methods

Koray SAYIN*, Ayhan ÜNGÖRDÜ

krysayin@gmail.com or ksayin@cumhuriyet.edu.tr

Tel.: +90 346 219 10 10 / 2851, Fax: +90 346 219 11 52

Department of Chemistry, Faculty of Science, Cumhuriyet University, 58140 Sivas,
Turkey

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, ^1H -, ^{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

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