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Koray Sayin, Duran Karakaş

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Investigation of Structural, Electronic Properties and Docking Calculations of Some Boron Complexes with Norfloxacin: A Computational Research

Koray SAYIN*, Duran KARAKAŞ

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

Tel.: +90 346 219 10 10 / 2851, Fax.: +90 346 219 11 86

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

ABSTRACT

Quantum chemical calculations are performed over BF_2R **(1)**, $B(NO)_2R$ **(2)**, $B(CN)_2R$ **(3)** and $B(CH_3)_2R$ **(4)** [R: 1-ethyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylate]. Mentioned boron complex with fluorine atoms which is BF_2R are optimized at HF/6-31+G(d), B3LYP/6-31+G(d) and M062X/6-31+G(d) level and the best level is determined by comparison of experimental and calculated results. The best calculation level is determined as M06-2X/6-31+G(d) level. The other complexes are optimized at this level. Structural properties, IR and NMR spectrum are examined in detail. Additionally, biological activities of mentioned complexes are investigated by some quantum chemical descriptors (E_{HOMO}, E_{LUMO}, I, A, E_{GAP}, η, σ, χ, CP, ω, N, ΔN_{max} and S) and molecular docking analyses. The interaction energies for complex **(1)**, **(2)**, **(3)** and **(4)** are calculated as -480.1, -443.6, -433.6 and -402.1 kJ mol^{-1}, respectively. As a result, it is found that boron complex with fluorine atoms (BF_2R) is the best candidate for anticancer drug.

Keywords: Norfloxacin, Boron Complexes, Modelling Studies, Spectral Analysis, Docking