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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  $\text{BF}_2\text{R}$  (**1**),  $\text{B}(\text{NO})_2\text{R}$  (**2**),  $\text{B}(\text{CN})_2\text{R}$  (**3**) and  $\text{B}(\text{CH}_3)_2\text{R}$  (**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  $\text{BF}_2\text{R}$  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 ( $E_{\text{HOMO}}$ ,  $E_{\text{LUMO}}$ , I, A,  $E_{\text{GAP}}$ ,  $\eta$ ,  $\sigma$ ,  $\chi$ , CP,  $\omega$ , N,  $\Delta N_{\text{max}}$  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  $\text{kJ mol}^{-1}$ , respectively. As a result, it is found that boron complex with fluorine atoms ( $\text{BF}_2\text{R}$ ) is the best candidate for anticancer drug.

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

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