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Muath Suliman <sup>a</sup>, , , Mazin Hadi Kzar <sup>b</sup>, Ameena S.M. Juma <sup>c</sup>, Israa Abbas Ali <sup>d</sup>, Yaser Yasin <sup>e</sup>, Nidhal Hassan Sayyid <sup>f</sup>, Adnan Taan Alkhafaji <sup>g</sup>, Abed J. Kadhim <sup>h</sup>, Majeed M. Abid <sup>i</sup>, Ahmed Hussien Alawadi <sup>j</sup>, <sup>n</sup>, <sup>o</sup>, Ali Alsalamy <sup>p</sup>, Jupinder Kaur <sup>l</sup>, , , Elham Tazikeh-Lemeski <sup>k</sup>, , , Sahar Moazen Rad <sup>l</sup>, Alireza Soltani <sup>m</sup>, , 

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## Abstract

In this paper, density functional theory calculations have been employed to study the interaction of curcumin through  $\beta$ -diketone- and enol- forms with the borospherene molecule ( $B_{40}$ ) and its silicon-doped variant ( $SiB_{39}$ ) for application as a nanocarrier for designing a drug delivery system. The obtained results from binding energies analysis indicated that the enol form (state II:  $-1.32\text{ eV}$ ) and  $\beta$ -diketone form (state III:  $-2.51\text{ eV}$ ) of curcumin prefers a strong polar covalent B-O and Si-O bonds through carbonyl groups after the interaction with  $B_{40}$  and  $SiB_{39}$  fullerenes. The boron fullerene doped with silicon atom improves the adsorption of  $\beta$ -diketone form and has higher binding energy values and increased dipole moment. So,  $SiB_{39}$  fullerene is more sensitive to the presence of  $\beta$ -diketone (state III: 76.84%) and enol form is (state IV: 93.68%) compared to the  $B_{40}$  fullerene due to the alteration in energy gap. According to molecular docking analysis the  $\beta$ -diketone curcumin conjugated with  $SiB_{39}$  (state III) and  $B_{40}$  fullerenes (state I) revealed the best binding affinity with the tumor necrosis factor alpha (TNF- $\alpha$ ) receptor ( $-8.9\text{ kcal/mol}$ ) and the cyclooxygenase-1 (COX-1) receptor ( $-8.8\text{ kcal/mol}$ ). The anticancer activities of  $\beta$ -diketone curcumin conjugated  $B_{40}$  and  $SiB_{39}$  fullerenes improved in comparison with curcumin towards Epidermal growth factor and Human Epidermal Growth Factor Receptor 2 receptors. Molecular docking simulation analysis illustrated that the interaction of curcumin conjugated  $B_{40}$  and  $SiB_{39}$  fullerenes have great potential for the anticancer and anti-inflammatory activities in contrast to Curcumin. Thus, the molecular docking and density functional theory analysis confirm that curcumin decorated  $B_{40}$  and  $SiB_{39}$  fullerenes have significant potential to be explored further in cancer and inflammation treatments.