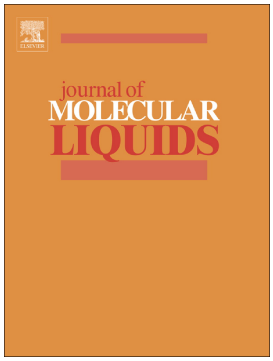

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Evaluation of solvent and ion effects upon leflunomide adsorption characteristics on (6,0) zigzag single-walled carbon nanotube and immobilized dihydroorotate dehydrogenase activity: A computational DFT and experimental study

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Abstract

In this paper, we have investigated the influence of non-aqueous and aqueous solvents (DMF, methanol, n-propanol, DMSO, water-based buffer solution) on the dihydroorotate dehydrogenase activity and leflunomide inhibitory effect. Due to the negative effect of organic solvents on the activity and inhibitory, the water solution selected as a suitable medium. The effect of ions (Si^{+2}, Ge^{+2}, Li^{+}, Na^{+} and K^{+}) was also studied, experimentally. Results confirmed that the Li^{+} has a positive effect on activity and did not opposite the effect of leflunomide. Fluorescence intensity showed a more compact conformation of the enzyme after incubation with Li^{+} ion. In the theoretical part, based on DFT results, when a Si, Ge, and mono metal cations are substituted with a single C in the SWCNT, the dopant atom extends outward from the surface of the nanotube. Our results reveal that the interaction between leflunomide molecule and pristine, Si- and Ge- doped SWCNTs are weak so that the adsorption of leflunomide onto above-mentioned nanotubes is physisorption process. Moreover, our calculated results showed that mono metal cations doped-SWCNTs had much higher adsorption energy and shorter binding distances than pure SWCNTs owning to chemisorption of the leflunomide molecule. Based on polarizable continuum model results, the relative stabilities of the investigated systems variation considerably when the solvent influence was applied. It is noteworthy to mention that the adsorption energy decreases when the dipole moment of the solvent increases. The obtained results within the AIM theory also confirm outcomes based on the geometrical data.

Keyword: Doped SWCNTs; Drug adsorption; DFT method; Solvent effect; Experimental Methods.

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