PHYSICOCHEMICAL CHARACTERISTICS OF NATURAL ANTICANCER COMPOUNDS

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In the present work the adsorption properties of the molecule Curcumin ((1E,6E)-1,7-bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione) on CNT(8,0-6) nanotube were investigated by Density Functional Theory (DFT) in the water solvent for the first time.

Keywords: quantum-chemical modeling, antioxidant activity, Curcumin, nanotube, electronic spectrum.

In this work the electronic properties, UV/Vis, FT-IR and NMR spectra of the complex between the molecule of curcumin and carbon nanotube (CNT) (8,0-6) have been calculated [1]. The electronic spectrum of the given complex between the molecule of curcumin and CNT (8,0-6) in the solvent (water) have been calculated by the time dependent method (TD-DFT) [2]. The absorption spectrum of curcumin and CNT (8,0-6) were compared with the absorption spectrum of the resulting complex to determine the effect of CNTs (8,0-6) on the shift of the absorption spectrum of the complex into the visible region of the spectrum. It is found a new method to deliver curcumin in diseased cells by the complex formed between the molecule of curcumin and CNT (8,0-6) [3].

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