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Article

Quantum Mechanical Study on the Mechanistic, Energetic, and Structural Properties of Adsorption of 6Ãƒ Â¢Ã‚€Ã‚•Thioguanine onto Ãƒ ÂŽÃ‚³Ãƒ Â¢Ã‚€Ã‚•Fe_2O_3 Nanoparticles

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Abstract

Using density functional theory, noncovalent interactions and four mechanisms of covalent functionalization of 6Ãƒ Â¢Ã‚Â€Ã‚Â•thioguanine anticancer drug onto Ãƒ ÂŽÃ‚Â³Ãƒ Â¢Ã‚Â€Ã‚Â•Fe_2O_3 nanoparticles have been investigated. Quantum molecular descriptors of noncovalent configurations were studied. It was specified that binding of 6Ãƒ Â¢Ã‚Â€Ã‚Â•thioguanine onto Ãƒ ÂŽÃ‚Â³Ãƒ Â¢Ã‚Â€Ã‚Â•Fe_2O_3 nanoparticles is thermodynamically suitable. Hardness and the gap of energy between LUMO and HOMO of 6Ãƒ Â¢Ã‚Â€Ã‚Â•thioguanine are higher than the noncovalent configurations, showing the reactivity of 6Ãƒ Â¢Ã‚Â€Ã‚Â•thioguanine increases in the presence of Ãƒ ÂŽÃ‚Â³Ãƒ Â¢Ã‚Â€Ã‚Â•Fe_2O_3 nanoparticles. 6Ãƒ Â¢Ã‚Â€Ã‚Â•thioguanine can bond to Ãƒ ÂŽÃ‚Â³Ãƒ Â¢Ã‚Â€Ã‚Â•Fe_2O_3 nanoparticles through NH_2 (k_1 mechanism), NH in sixÃƒ Â¢Ã‚Â€Ã‚Â•membered ring (k_2 mechanism), NH in fiveÃƒ Â¢Ã‚Â€Ã‚Â•membered ring (k_3 mechanism), and S (k_4 mechanism) groups. The activation energies, the activation enthalpies and the activation Gibbs free energies of these reactions were calculated. Thermodynamic data indicate that k_3 mechanism is exothermic and spontaneous and can take place at room temperature. These results could be generalized to other similar drugs.

Citing Literature

Number of times cited: 1

- Hadi Lari, Ali Morsali and Mohammad Momen Heravi, Quantum Mechanical Study of Ãƒ ÂŽÃ‚Â³-Fe2O3 Nanoparticle as a Nanocarrier for Anticancer Drug Delivery, *Zeitschrift fÃƒ ÂƒÃ‚Â¼r Physikalische Chemie*, **0**, 0, (2018).
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