عنوان مقاله:

Molecular Modeling of 3-(1,3-Dioxoisoindolin-2-yl)benzyl Nitrate and its Molecular Docking Study with (Phosphodiesterase-5 (PDE5

محل انتشار:

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خلاصه مقاله:

In this study, the electronic properties of the novel medicinal compound 3-(1,3-dioxoisoindolin-2-yl) benzyl nitrate as a treatment of sickle cell disease are obtained using density functional theory (DFT) method. In first step, the molecular structure of the title compound is optimized at B3LYP/6-311++G(d,p) level of theory at room temperature. Then, its stability and reactivity properties are calculated by frontier molecular orbitals (FMOs) energies. The global reactivity indices show this medicinal molecule is a more stable compound and the nitrogen atom of the nitrate group has positive charge. So, the nitrate group can quit nitric oxide molecule in binding to Phosphodiesterase-5 (PDE5) enzyme. On the other hand, the docking analysis of the ligand-enzyme complex shows the steric interactions play the main role in this complex formation. Also, the data shows the PDE5 residues containing Phe [A] 820, Gln [A] 817, Ile [A] 768, Val [A] 782, Gln [A] 775, Phe [A] 786, Ile [A] 778, Leu [A] 765, Met [A] 816, Ala [A] 767 and Tyr [A] 612 play .main role in the ligand-enzyme complex formation

کلمات کلیدی:

Benzyl nitrate, Molecular docking, Molecular Simulation, Phosphodiesterase-5, Sickle cell disease