عنوان مقاله:

Theoretical evaluation of medicinal properties for some of N-aryl-3- hydroxypyridine-4-ones derivative compounds

محل انتشار:

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خلاصه مقاله:

Nowadays, the bidentate ligands 3-hydroxypyridin-4-ones (HPOs) as orally active iron chelating agents have been demonstrated to possess potentials for the treatment of some of the human diseases such as iron-overload in thalassaemia patients and malaria. In this research, a series of HPOs with different substitutes and positions were theoretically investigated in order to extract and predict their partition coefficient values (LogP) which were experimentally determined in an aqueous/octanol system. The effective electronic parameters on logP were also investigated. The results show that the type of method, basis set, and the solvent do not basically affect on the logP values. But some parameters such as hydrophobicity, polarizability, and orbital electronic charge density (HOMO and .LUMO) are effective on logP values

کلمات کلیدی:

Hydroxypridinone, partition coefficient, chelating agent, density functional theory