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The Thesis Submitted for the Degree of Master of Science (In the field of Analytical Chemistry)

Theoretical study on the effect of weak intramolecular hydrogen bonds on the inhibitory activity of the pyrazolo[3,4-d]pyrimidine derivatives

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Abstract

Pyrazolopyrimidine derivatives are the fused heterocyclic compounds, which have been recognized as biological and pharmaceutical agents. It seems that changing electronic properties of structures affects on their inhibitory strength. In this research, geometries of some pyrazolopyrimidine derivatives are optimized using quantum mechanical computations. Then, the effect of substituents on the weak intramolecular hydrogen bond parameters including structural parameters, electron charge densities at the hydrogen bond and ring critical points and donor-acceptor energies are evaluated. The different substituents are located on the A and C rings. The electron-withdrawing substituents on the A ring lead to increase of hydrogen bond strength. While, the data do not have a regular trend when the substituents are placed on the C ring, which can be related to the spatial effects of the adjacent NH_2 group. The results of this study can be used for drug design by selecting the substitutions that can play a significant role in the tendency of these compounds to form intermolecular interactions with enzymes and thus their inhibitory activity.

Keywords: Pirazolo(3,4-d)pyrimidine, quantum mechanics, Inhibitor, Intramolecular hydrogen bond, drug design