ABSTRACT

In the first section of this work, the effect of different substitution of (6-R-3-yl)-2-oxo-propionic acid on the acidity have been investigated. Also, the strength of intramolecular hydrogen bond have been studied. For this purpose, the effects of electron donating (ED) and electron withdrawing (EW) substituents located at the R position on the hydrogen bond have been investigated. Meaningful correlations were found between structural parameters for the hydrogen bond, the changes of charge distributions on the ring with substituent and AIM data. The EW substituents increase the acidity as well as the strength of intramolecular hydrogen bond. On the other hands, more stability of the intramolecular hydrogen bond increases the acidity of the compounds. In the second section, intercalation between these compounds and the amino acids of Integrase enzyme which is a factor of proliferation of the AIDS virus, has been studied using the molecular docking calculations. The CHO-C_6H_5 compounds is the best inhibitor for Integrase enzyme. Therefore, the effects of π-π stacking interactions on the intercalation of these compounds have also been investigated using the geometrical parameters data, AIM and NCI index analyses.

Keywords: Chromone derivatives, Hydrogen bond interaction, Acidity, Cation-π interaction, Integrase enzyme, Molecular Docking.

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