Abstract
In this study, primary structures of some hydrazone compounds were optimized by means of quantum mechanical computations using B3LYP and M062X methods with the 6-31g (d,p) basis set set by Gaussian09 program package. Then, molecular docking studies were performed with Autodock 4. 2 software to examine the role of different substituents on inhibitory strength against the monoamine oxidase A. Results show that affinity of these compounds are in the range of -6. 80 − -8. 90 kcal mol^{-1} and compound with substituent CF_3 has the best affinity. Molecular docking studies indicate that the noncovalent π-π interactions between this compound and enzyme's aminoacids have important role on value of affinity. Thus, π-π interactions between some of these compounds and aminoacid TRP were studied at the M06-2X/6-31g (d,p) level. Results show that the best interaction energy corresponds to compound with substituent CF_3 and hydrazones with electron-withdrawing substituents can be helpful as new drugs for treatment of depression.

Keywords: hydrazone, molecular docking, monoamine oxidase, inhibitor

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Investigation of substituent effect and molecular docking study of some hydrazone derivatives as anti-depressant agents

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