Abstract

In this research, the electronic structure of pyrimidine-based derivatives were optimized at both M062X level of theory with 6-31G(d, p) basis set using the Gaussian 09 package. The Docking study of these derivatives was then performed using the Auto dock 4.2 software to investigate the role of various substitutions on the inhibitory strength against the 3V8S enzyme. The results show that the binding energy of these compounds is in the range of - 5.8 to -7.0 kcal / mol, and the composition bearing the CF_3 substituent has the lowest binding energy. Moreover, Molecular docking calculations have revealed that non-covalent π-π interactions between these compounds and the enzyme amino acids play an important role in the amount of the binding energy. More precise *ab intio* studies of the π-π interactions between some of these compounds with phenylalanine amino acids at the M062X / 6-31G (d, p) level were accomplished. The results confirmed that probably the best binding energy of ligand-enzyme complex related to those ligands with the more electron-withdrawing groups in particular the adduct bearing CN substituent. Therefore, it is likely that this derivative has a more effective role in the treatment of cardiovascular disease, and might be a suitable candidate for synthesis.

Keywords: Kinase protein, Molecular docking, Cardiovascular disease, Inhibitor.

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Molecular docking study of some kinase protein inhibitors for treatment of cardiovascular disease

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