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Evaluation of inhibitory potential of phosphoramide compound [2,6-F_2-$C_6H_3C(O)NH]P(O)[N(CH_2CH_3)_2]_2$ against coronavirous and monkeypox by using molecular docking method

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In recent years, two infectious viral diseases, coronavirus and monkeypox, and the preparation of compounds with suitable biological properties as drug to inhibit these diseases have attracted attention of the world health organization and medical association[1]. Phosphoramide compounds with the main skeleton O═P─N are among the chemical compounds that show appropriate biological and medicinal activities against various illnesses such as cancer[2], hepatitis[3] and coronavirous[4]. Therefore, in the present work, a compound of the phosphoramide family with the name *N*-(2,6-difluorobenzoyl)-*N*',*N*',*N*'',*N*''-(tetraethyl) phosphoric triamide has been selected and its inhibitory effect against coronavirous and monkeypox are investigated by using the molecular docking method. Survay of the protein-ligand interactions by docking simulation on the studied compound shows that this compound with the binding energy of –5.4 kcal/mol can be proposed as a suitable candidate to inhibit the coronavirus (7ACS). Moreover, suitable inhibitory effect of this compound against monkeypox virus (4QWO) is confirmed by the binding energy of –6.4 kcal/mol.

Keywords: Phosphoramide, Molecular docking, Coronavirous, Monkeypox

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