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Evaluation of inhibitory potential of phosphoramide compound OP[NH-^{2}Py(4-CH_3)]$_3$ against acetylcholinesterase and urease enzymes by using molecular docking method

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Phosphoramide compounds with the main skeleton O═P─N have received much attention in various medical fields such as their application as acetylcholinesterase and urease inhibitors [1,2]. Therefore, in the present work, a compound of the phosphoramide family with the formula OP[NH-^{2}Py(4-CH_3)]$_3$ (tris(4-methylpyridin-2-yl)phosphoric triamide) was selected and its inhibitory effect against acetylcholinesterase (1EEA) and urease (4GY7) enzymes is investigated by using the molecular docking method. The results show that this compound with the binding energy of −7.4 kcal/mol can be suggested as a suitable candidate to inhibit acetylcholinesterase enzyme. Moreover, the appropriate inhibitory effect of this compound on urease enzyme is confirmed by the binding energy of −6.2 kcal/mol.

Keywords: Phosphoramide, Acetylcholinesterase, Urease, Molecular docking

References

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