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Molecular Docking Study of an Isoxazole Derivative: 5-(3-Methylthiophen-2yl)- 3-(3,4,5-trimethoxyphenyl) Isoxazole

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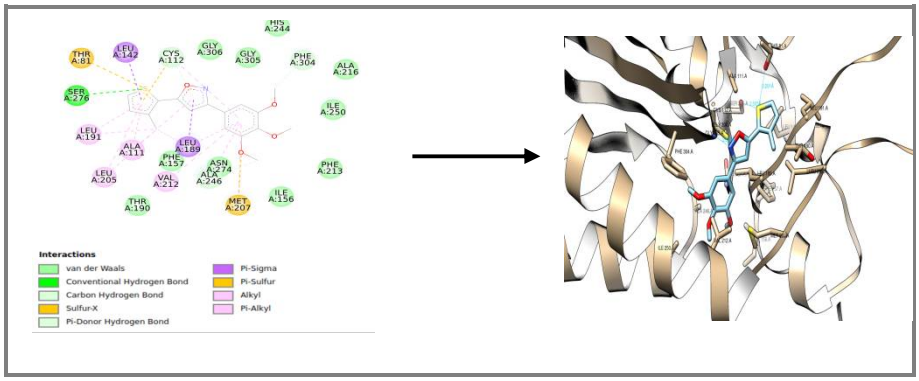
ABSTRACT

The 5-(3-Methylthiophen-2yl)- 3-(3,4,5-trimethoxyphenyl) Isoxazole compound comprises three distinct units, 3-methylthiophene ring, a five-membered isoxazole ring and a trimethoxyphenyl ring. The compounds bearing heterocyclic ring systems such as thiophene and an isoxazole moieties are reported to posses numerous useful biological activities. In the view of this authors are aimed to perform molecular docking for anti-bacterial, anticancer and antidepressant activities for the protein targets (1HNJ), (1JNX) and (1XRW) respectively to evaluate their binding energies to the above mentioned target proteins using a tool Auto Dock 4.2. The docking results showed that the compound displayed relatively better binding energy for anti-bacterial and anti-depressant activities than anti-cancer activity.

Graphical Abstract



Keywords: Molecular docking, Anti-cancer, Anti-depressant, Anti-bacterial, Binding affinities.