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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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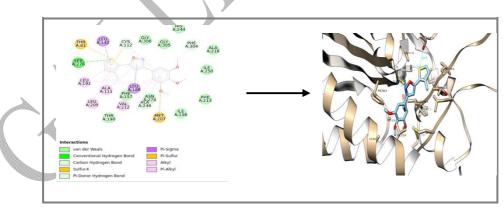
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ABSTRACT

19 The 5-(3-Methylthiophen-2yl)- 3-(3,4,5-trimethoxyphenyl) Isoxazole compound comprises three 20 distinct units, 3-methylthiophene ring, a five-membered isoxazole ring and a trimethoxyphenyl ring. 21 The compounds bearing heterocyclic ring systems such as thiophene and an isoxazole moieties are 22 reported to posses numerous useful biological activities. In the view of this authors are aimed to 23 perform molecular docking for anti-bacterial, anticancer and antidepressant activities for the protein 24 targets (1HNJ), (1JNX) and (1XRW) respectively to evaluate their binding energies to the above 25 mentioned target proteins using a tool Auto Dock 4.2. The docking results showed that the compound 26 displayed relatively better binding energy for anti-bacterial and anti-depressant activities than anti-27 cancer activity. 28

29 Graphical Abstract





31 32

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