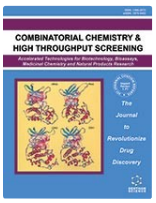

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Research Article

Synthesis of Novel Hydrazones of Levofloxacin Related Molecule and their In Vitro Evaluation as Antioxidant, and Molecular Docking Studies

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Abstract

Objective: The research work aims to synthesize novel series of hydrazones and antioxidant screening. It also aims to evaluate the binding affinities and in silico methods for identifying possible drug targets of synthesized compounds.

Methods: This report briefly explains the synthesis of a novel series of hydrazones. It was synthesized via. hydrazinolysis of esters to obtain hydrazide, treated with aldehyde and acetophenone to get hydrazones. The spectral confirmed hydrazones exhibited excellent to comparable anti-

oxidant as compared to the standard drugs Butylated hydroxytoluene (BHT) and Ascorbic acid. Molecular docking on myeloperoxidase (MPO) demonstrated the ability of this scaffold to correctly recognize the target and engage in significant bonded and non-bonded interactions with key residues therein.

Results and Discussion: In this study, we report effectively synthesized compounds BK-35, BK- 41, BK-26, BK-28, and BK-39 that showed the best DPPH radical scavenging activity. The docking results clearly showed the binding mode of hydrazones into the active site of Myeloperoxidase (MPO). In in-silico results, none of the synthesized compounds, BK-24 to BK- 41, violated Lipinski's rule of five (miLog P ≤ 5).

Conclusions: In vitro preliminary anti-oxidant screening results in support by in Silico binding affinity data of novel hydrazones of levofloxacin related molecules BK-24 to BK-41 reported here have emerged as excellent anti-oxidant agents. The inference derived from the in vitro anti-oxidant screening data and the quantitative insights derived from the per-residue interaction analysis with MPO enzyme are now being fruitfully utilized for site-specific mutation around the nucleus to identify selective and potent anti-oxidants.

Keywords: Carbohydrazide, anti-oxidant, bio-activity, computational study, organic chemistry, mutation.

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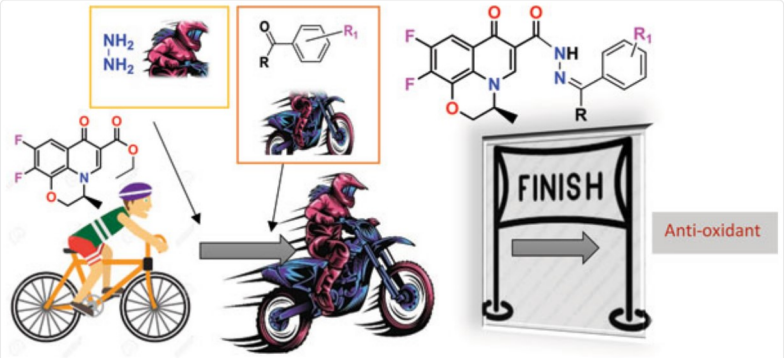
Graphical Abstract



Synthesis of novel hydrazones of levofloxacin related molecule.

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