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## 3-(1-phenyl-4-((2-(4-arylthiazol-2-yl) hydrazono) methyl)-1H-pyrazol-3-yl)-2H-chromen-2-ones: One-pot three component condensation, *in vitro* antimicrobial, antioxidant and molecular docking studies

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In an attempt to find a new class of heterocyclic bio-active agents, a series of novel 3-(1-phenyl-4-((2-(4-arylthiazol-2-yl) hydrazono) methyl)-1H-pyrazol-3-yl)-2H-chromen-2-one derivatives (5a-l) have been synthesized efficiently in both quantitatively and qualitatively via three-component one-pot manner by Hantzsch condensation. Structures of all the newly synthesized compounds were established by their spectral data and elemental analyses, and evaluated for their *in vitro* antimicrobial and antioxidant activities. Among the tested compounds (5a-l), the derivatives 5k, 5h and 5a have displayed broad spectrum antibacterial activity, whereas the compounds 5b and 5f were found to be potent antifungal agents. Antioxidant activity results revealed that, the compounds 5a, 5b and 5i have exhibited high radical scavenging ability than the positive control drug Trolox. Further, molecular docking of synthesized compounds (5a-l) in to binding site of crystal structure of *E. coli* MurB enzyme (PDB Id: 1MBT), a key enzyme in the peptidoglycan biosynthesis was performed to gain a comprehensive understanding into plausible binding modes and also to compare the theoretical and experimental results of these compounds. Docking results revealed that the docking scores and H-bonding interactions of the ligands are in good agreement with the *in vitro* results and also indicated that the compounds 5k, 5h and 5a have considerable binding energies and greater affinity towards the active site of MurB enzyme. Thus, they can be further optimized and developed as lead compounds.

### Biography

Ramesh Gondru has completed his MSc in Organic Chemistry in 2011 from Vivekavardhani PG College (affiliated to Kakatiya University) and he is currently pursuing PhD from National Institute of Technology, Warangal. He has published 6 papers in reputed journals.

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