Design, Synthesis of novel 4-aryl quinoline-2-carboxylates as antimycobacterial agents.

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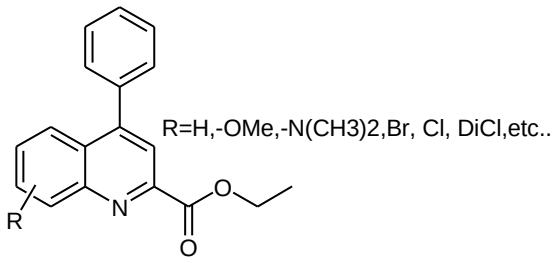
Abstratct:

A new series of 4-aryl quinoline-2-carboxylates **4a-4k** were synthesized by using standard protocol. Synthesized compounds were characterized byIR, ^{1}H NMR and Mass spectra. Molecular docking simulation studies were carried out in order to better understand the hypothetical interaction of the compounds with target site. Docking studies of the compounds were performed on the DNA Gyrase and ATP ase site of mycobacterium tuberculosis (H37Rv strain) with PDB Codes of 3UC1 and 3zkb respectively. The results showed that the compound **4b** &**4k** exhibited good binding affinity with the DNA Gyrase and compound **4h** showed good binding affinity with ATP ase with the docking scores of **-4.702,-4.642&-8.313** respectively. Further synthesized compounds were screened for anti-bacterial activity against different Gram positive & Gram negative strains and also in vitro anti-tubercular activity against H37Rv strains. SAR of the compounds is discussed.



General structure-IV

Key words: Mycobacterium, Quinoline, H37Rv strain, ATP ase, DNA Gyrase.