Organo-N-heterocyclic Carbene Catalyzed Regioselective Synthesis of Some New Phenothiazine- Isoxazole Hybrids and their Anti-bacterial Screening, Molecular Docking Studies

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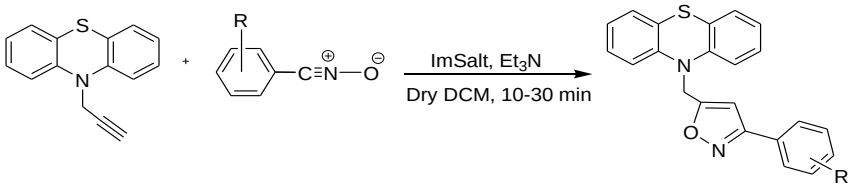
Some new phenothiazine-isoxazole hybrids were regioselectively synthesized in high yields by organo-NHC catalyzed 1, 3-dipolar cycloaddition (DC) reaction of 10-(pro-2-yn-1-yl)-10H-phenothiazine with nitrile oxides. These new phenothiazine--isoxazole compounds were evaluated for *in vitro* antibacterial activity against a panel of gram-positive *Bacillus sphericus, Staphylococcus epidermidis* and gram-negative *Klebsiella pneumonia, Escherichia coli* species. Most of these newly synthesized compounds were found to possess excellent growth inhibition activity compared to commercial standards like Penicillin-G and Streptomycin. Molecular docking studies are also performed for the compounds showed positive results.

Scheme



R= H, 4-Me. 4-OMe, 4-Cl, 4-Br, 4-F, 4-NO_2, 2-NO_2, 4-OH, 4-CN, 2-OH,2, 4-di-Cl, 2-Cl and 2-Br

Keywords: 10-(pro-2-yn-1-yl)-10H-phenothiazine, 1, 3-Dipolar cycloaddition, organo-NHC catalyst Phenothiazine-isoxazole hybrids, Antibacterial activity, Molecular docking studies.