SYNTHESIS, CHARACTERIZATION, BIOLOGICAL EVALUATION AND MOLECULAR DOCKING STUDIES OF NOVEL 6-(2-(4-PHENYLTHIAZOL-2-YL)HYDRAZONO)INDOLO[2,1-B]QUINAZOLIN-12(6H)-ONE ANALOGS AS ANTI-OXIDANT, ANTI-BACTERIAL AGENTS.

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ABSTRACT

In the present study, we report herewith anovel series of newly synthesized compounds 6-(2-(4-phenylthiazol-2-yl) hydrazono)indolo[2,1-b]quinazolin-12(6H)-one and their derivatives(T1-T16). These synthesized compounds were characterized by elemental analyses, FT-IR, ^{1}H &^{13}C NMR and mass spectroscopic techniques. The compounds were screened for their anti-oxidant activity by DPPH radical scavenging assay. Out of all the tested compounds, T3, T10, T9 and T10 showed portent anti-oxidant activity. These synthesized compounds were also screened for their anti-bacterial activity. The compounds of T2, T1, T7, and T4are found to be the most potent and remaining compounds exhibited moderate to poor activity against all the tested strains. Molecular docking studies were done against the MurB protein receptor to illustrate the binding abilities of the synthesized compounds to the active site of protein, The compounds T2,T1,T7 and T4 with -11.71 Kcal/mol, -11.32 Kcal/mol, -10.87 Kcal/mol, and -10.84 Kcal/mol exhibited lowest binding energies which correlates with in vitro anti-bacterial activity results.

Key word: *MurB protein, anti-oxidant activity, anti-bacterial activity, DPPH scavenging method, molecular docking studies.*

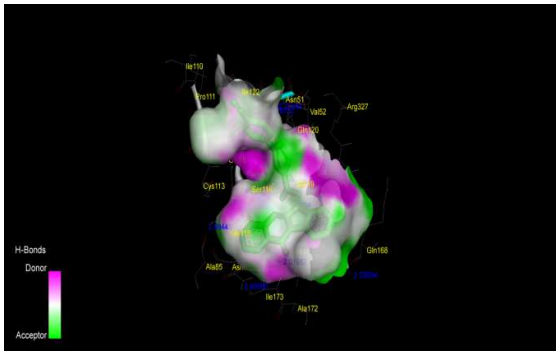

Fig: This shows the binding poses and interaction of 6-(2-(4-phenylthiazol-2-yl)hydrazono)indolo[2,1-b]quinazolin-12(6H)-one analoge T2 to binding site of MurB receptor (PDB id: 1MBT)