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Synthesis, antibacterial activity and molecular docking studies of some new imine derivatives

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The aim of this research work was to synthesize some new imine derivatives (Schiff bases) by using the reaction between different heterocyclic amines and aromatic aldehydes. We have synthesized nine compounds (imine derivatives), five of them are not known yet. These products are synthetized under reflection condition. The structure of the synthesized products was determined based on IR and 1H NMR spectra. Compounds were screened for their antibacterial activity against gram positive bacteria *Staphylococcus aureus* (clinical isolate), *Staphylococcus aureus* (food isolate), *Listeria monocytogenes*, and against gram negative bacteria *Escherichia coli*. Compounds were found to be potent antimicrobial agent against gram positive bacteria. All the compounds were subjected to molecular docking studies for the inhibition of the enzyme L-glutamine D-fructose-6-phosphate amidotransferase [GlcN-6- P] (EC 2.6.1.16). The *in silico* molecular docking study results showed that from nine synthesized compounds, seven of them shows minimum binding energy and have good affinity toward the active pocket, thus, they may be considered as good inhibitor of GlcN-6-P synthase. From this research work we can conclude that this synthesized compounds show antibacterial activities. The synthesized compounds can be used further by modifying their structure with the aim to increase their biological activity.

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