In-silico Design, Synthesis and Characterization of Isatin based clicked scaffold as an antibacterial Agent

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Abstract

Human health is having a severe threat by bacterial infection. As it attracted researchers to work and synthesize antibacterial agents. This work develops Isatin-1,2,3-triazole as an antibacterial agent using one-pot synthesis i.e., click chemistry. In-vitro antibacterial activity of Isatin-1,2,3-triazole was evaluated against common pathogens, Gram-negative (Escherichia coli) and Gram-positive (Staphylococcus aureus) pathogens by microdilution method as well as well-diffusion method. The results showed that Triazole has enhanced antibacterial activity of Isatin against E. coli, and S. aureus. Structure-activity analysis and molecular docking studies revealed that the antibacterial activity of Triazole-tethered Isatin tosyl azide is particularly better as compared to N-propargyl Isatin. Furthermore, Isatin triazole showed best binding affinity with Staphylococcus aureus (PDB ID:4TU5) and E. coli (PDB ID:6YD9) bacteria proteins which are -10.44KJ/mol and -8.4KJ/mol. Isatin triazole showed high GI absorption and low toxicity parameters and its satisfied Lipinski's rule of five and passed Veber, and Ghose rules. It's also maintained the stability with the proteins during md simulation for 100 ns. Overall, the study found that these Isatin triazole molecules have considerable therapeutic qualities, and their in-silico analysis strongly suggests that more clinical research can be conducted to gain insight into the mechanisms of action in healing a range of bacterial diseases.

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