



QSAR, Brine Shrimp Lethal Assay and antimicrobial studies on Synthesized L-Tryptophan-2,4-dihydroxy benzaldehyde Schiff Base

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Abstract : Schiff base was synthesized by the condensation reaction between L-tryptophan and 2,4-dihydroxy Benzaldehyde in double distilled water. Synthesized Schiff base was characterized by UV, fluorescence FT-IR, mass, ¹H-NMR spectral studies and FT-IR, ¹H-NMR data were compared with the theoretical Spartan 14 wave function tool values. QSAR properties of the molecule were predicted by MOLSOFT and OSIRIS online tools by submitting smiles notation. Docking affinity of the Schiff base with *E. coli* proteins was studied by online auto dock vina software through mcule server. From the outcomes of the tools, Schiff base was carried for toxicity study by brine shrimp lethal assay test with various concentrations from 25 µg/mL to 250 µg/ mL and antibacterial character against *E. coli*. From the lethal assay test L-tryptophan Schiff base lethal concentration for 50% mortality (LC₅₀) value was calculated by regression method and it was found to be 130.32 µg/ mL. Minimum inhibitory concentration (MIC) against *E. coli* was found to be 20µl of the Schiff base, which is lower than the toxicity limit.

Keywords: L-tryptophan, 2, 4-dihydroxy benzaldehyde, Schiff base, QSAR, Docking, Toxicity, Antimicrobial.

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