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Synthesis, biological activity evaluation, and molecular docking studies of amino acid and amine-derived Schiff basesA. K. T. D. Sandaruwan¹, H. M. I. Herath¹, H. G. N Rajapaksha², M. G. A. N. Perera^{1*}¹Department of Physical Science and Technology, Faculty of Applied Sciences,
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This study aimed to synthesize and evaluate a series of amino acid and aromatic amine-derived Schiff bases specifically as targeted antioxidant agents and antifungal inhibitors of ergosterol biosynthesis. Eight compounds five amino acid-based and three amine-based were successfully synthesized. Structural formation of the azomethine linkage was confirmed by UV-Visible and FTIR spectroscopy, supplemented by melting and boiling point literature comparisons. Biological screening assessed DPPH radical scavenging, cell hemolysis, *Saccharomyces cerevisiae*-based antifungal activity, and brine shrimp lethality. Additionally, molecular docking was performed against Lanosterol 14- α -demethylase to evaluate specific binding interactions relevant to fungal cell membrane formation. Experimental data revealed that the imine derived from para-aminophenol and benzaldehyde exhibited the most potent antioxidant activity ($IC_{50} = 15.12 \mu\text{g/mL}$) while maintaining excellent hemocompatibility. Antifungal spot assays demonstrated a dose-dependent inhibitory effect against *S. cerevisiae*, with the imine

derived from alanine and salicylaldehyde displaying the highest efficacy. Docking studies supported this by confirming a strong binding affinity of -8.3 kcal/mol with Lanosterol 14- α -demethylase. Systemic toxicity screening identified the imine derived from glycine and nitrobenzaldehyde as the most toxic compound ($LC_{50} = 49.98 \mu\text{g/mL}$), while overall *in silico* profiling (SwissADME, ProTox-3.0) confirmed high gastrointestinal absorption, optimal bioavailability, and broad Class 5 safety across the series. Ultimately, these findings highlight the alanine-salicylaldehyde imine as a promising targeted candidate for antifungal development, and the para-aminophenol-benzaldehyde imine as a viable biocompatible antioxidant.

Keywords:Schiff bases; Molecular docking; Antioxidant activity; Biocompatibility; Lanosterol 14- α -demethylase.