ORIGINAL RESEARCH ARTICLES

GREEN SYNTHESIS OF 5-ARYL-1,2,4-TRIAZOLIDINE-3-THIONES USING GLYCEROL–WATER MEDIUM, AND THEIR MOLECULAR DOCKING STUDIES AS POTENTIAL ANTIMALARIAL AGENTS

Shivangi P. Sawant[a], Sai Srinivas Ponugoti[a], Priya C. Saroj[a], Abhishek S. Kardile[a] and Shreerang V. Joshi[a]*

(Received 01 November 2025) (Accepted 20 December 2025)

ABSTRACT

The emergence of drug-resistant malaria strains continues to challenge global malaria control efforts. Misuse and overuse of existing antimalarial therapies have contributed to the development of resistant variants of *Plasmodium falciparum*. In this work, we report the synthesis, characterization and *in silico* analysis of 5-aryl-1,2,4-triazolidine-3-thione derivatives as potential agents against drug-resistant *P. falciparum*. Their interactions with two essential parasitic targets: PfDHFR-TS and Falcipain-2, were investigated through molecular docking to assess their potential antimalarial activity. The compounds 3a-3o were synthesized using an eco-friendly method that uses glycerol and water as solvents. The reaction conditions were gentle, making the process more sustainable and efficient, with good results in a shorter time. NMR and FT-IR tests confirmed that the compounds were formed correctly. The docking results suggest that these compounds bind well to PfDHFR-TS and FP-2.