

IN SILICO AND EXPERIMENTAL IDENTIFICATION OF NON-ULCEROGENIC ANTIINFLAMMATORY AGENTS: SCHIFF BASES OF 4-AMINO-5-(2-CHLOROPHENYL)-4*H*-1,2,4-TRIAZOLE-3-THIOL

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ABSTRACT:

A new series of substituted (E)-4-(benzylideneamino)-5-(2-chlorophenyl)-4H-1,2,4-triazole-3-thiol have been designed, synthesized and tested for antiinflammatory activity. All the tested compounds exhibited antiinflammatory activity comparable to that of standard drug diclofenac. Compound **6e** emerged as highly potent lead compound. Ulcerogenic studies of the synthesized compounds show nil or negligible ulcerogenic effect compared to diclofenac. Compound **6e** selected for docking studies with COX-2 exhibited convincingly low energy of docked conformation with RMSD less than 2 which indicated conformation in favorable state.

KEYWORDS: 1,2,4-triazole, COX-2, Docking, MOE

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