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DESIGN AND NOVEL SYNTHESIS OF SCHIFF BASE DERIVATIVE FOR ANTI INFLAMMATORY ACTIVITY

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Abstract:

This research focuses on the design, synthesis, and evaluation of coumarin Schiff basederivatives as potential anti-inflammatory agents with fewer side effects than traditional non-steroidal anti-inflammatory drugs (NSAIDs). NSAIDs are widely used but are associatedwith gastrointestinal and cardiovascular toxicity, creating a need for safer alternatives. In this study, four Coumarin-based compounds were designed and synthesized. Drug-likeness of the compounds was assessed using Lipinski's Rule of Five, confirming their suitability for oral use. Molecular docking studies were performed against the cyclooxygenase-2 (COX-2) enzyme to predict binding affinity and interaction patterns. All compounds showed better binding energy compared to the standard drug ibuprofen, indicating strong potential for anti-inflammatory activity. The synthesized compounds were further evaluated through an in vitro protein denaturation assay to measure anti-inflammatory effects. revealed that compounds 6 and 7 exhibited higher inhibition of protein denaturation than ibuprofen. Among them, compound 7 demonstrated the best overall performance, with the highest inhibition percentage and strong statistical correlation between concentration and activity. Although compound 8 showed excellent docking , its potential gastrointestinal side effects reduce its suitability as a lead compound. Overall, the study concludes that compound 7 is the most promising candidate for further development. Future research should focus on toxicity studies and clinical evaluation to confirm its safety and effectiveness.

Keywords: Coumarin, Schiff base derivatives, Anti-inflammatory activity, NSAIDs, Cyclooxygenase-2 (COX-2), Molecular docking, Drug design, Lipinski's Rule of Five, Protein denaturation assay, Binding affinity, Lead compound