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Research Article

Synthesis, Computational Studies of New Chalcone Derivatives as Anxiolytics and Skeletal Muscle Relaxants

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Abstract

Introduction: Chalcone derivatives are known for their diverse biological activities, including anxiolytic and skeletal muscle relaxant properties. Recent studies indicate that structural modifications can enhance their therapeutic effectiveness. This study aimed to synthesize and biologically evaluate novel chalcone derivatives, investigating their structure-activity relationship through computational studies and assessing their pharmacological potential.

Methods: Five chalcone derivatives (P1–P5) were synthesized via Claisen-Schmidt condensation and characterized using infrared spectroscopy (IR) and nuclear magnetic resonance (NMR) spectroscopy. Their physicochemical and pharmacokinetic profiles were analyzed via SWISS ADME, confirming drug-likeness. Biological assessments, including the Elevated Plus Maze (EPM), Open Field Test (OFT), Hole Board Test (HBT), and Rotarod Test, were conducted to evaluate anxiolytic and muscle-relaxant activities.

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