Title : Design and Molecular Simulation of 5-Hydroxy-7-Methoxyflavanone Derivatives Derived from Extraction for Potential Anti-Inflammatory Agents

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ABSTRACT

This study aimed to isolate pinostrobin, a major bioactive compound from *Boesenbergia rotunda* with reported anti-inflammatory activity, and to develop pinostrobin derivatives for inhibiting cyclooxygenase enzymes (COX-1 and COX-2), which play crucial roles in the inflammatory process. Pinostrobin was extracted from *B. rotunda* with a yield of 19%. Subsequently, molecular docking studies were performed to investigate the interactions between the compounds and the target proteins COX-1 (PDB ID: 1EQG) and COX-2 (PDB ID: 3LN1). The results revealed that the cinnamic acid–pinostrobin derivative exhibited the most favorable binding energy toward COX-2, with a value of −9.1 kcal/mol. This interaction involved **π**–**π** T-shaped interactions with amino acid residues Tyr341, Tyr371 and Trp373, as well as **π**-Alkyl and **π**-Sigma interactions with several residues within the active site. In contrast, the 4-nitrocinnamic acid–pinostrobin derivative showed the strongest binding affinity toward COX-1, with a binding energy of −9.0 kcal/mol. This compound formed a conventional hydrogen bond with Tyr355 and electrostatic interactions with Arg120 and Met522, in addition to **π**–**π** T-shaped, **π**-Alkyl and **π**-Sigma interactions with multiple amino acid residues in the active site. Based on these findings, the precursor compound 5-hydroxy-7-methoxyflavanone was structurally modified through esterification reactions with cinnamic acid and 4-nitrocinnamic acid to enhance its binding affinity toward the target enzymes. The esterification with cinnamic acid yielded 5-*O*-cinnamoylpinostrobin with a yield of 82%, while the reaction with 4-nitrocinnamic acid produced 5-*O*-(4-nitrocinnamoyl)pinostrobin with a yield of 57%. The chemical structures of the synthesized compounds were confirmed using Nuclear Magnetic Resonance (NMR) spectroscopy. These results suggest that pinostrobin derivatives possess potential as lead compounds for the future development of anti-inflammatory agents.

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