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Computational Investigation of Bioactive Compounds from *Zanthoxylum armatum* DC. for Their Anti-Inflammatory Potential

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Abstract

Zanthoxylum armatum DC. locally named *Mukthrubi* is a medicinally important plant widely used plant in Manipur. It is recognised for its rich phytochemical profile and traditional use in managing inflammatory disorders. This study presents a comprehensive computational investigation of various major bioactive compounds to evaluate their anti-inflammatory potential.

To assess how well these compounds bind to important inflammatory proteins such as COX-2, TNF-α and IL-1β, molecular docking simulation was performed to measure predicted affinity for binding as well as types of interactions. Density Functional Theory (DFT) was applied to establish the electronic nature of each compound by determining HOMO–LUMO distributions, energy gaps between them, and molecular reactivity indices which are indicative of their potential ability to interact with target sites.

Furthermore, ADMET profiling was evaluated for drug-likeness, pharmacokinetics, and toxicity characteristics, followed by molecular dynamics (MD) simulations analysis to observed the stability of the ligand–protein complexes.

The Docking simulations identified key compounds of *Zanthoxylum armatum* DC. as the potent inhibitor of COX-2, TNF-α and IL-1β compared to the control inhibitors and reference compounds. The DFT simulations confirmed the favorable electronic characteristics necessary for a high level of interaction between the ligands and their target. Additionally, ADMET simulation predicted a good oral absorption and safety profile for all the investigated compounds. The combined data from docking, DFT and MD simulations provide a promising anti-inflammatory activity of the Phytocompounds in *Zanthoxylum armatum* DC. and serve as a rational base for subsequent experimental validation.

Keywords: Molecular Docking, Anti-inflammatory, ADMET, DFT, MD Simulations

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