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Ibuprofen: A Review of its Use in Pain Management, Inflammation, and Fever Reduction

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Abstract: *Ibuprofen is a non-steroidal anti-inflammatory drug (NSAID) commonly used to reduce pain, inflammation, and fever. However, it is known to cause side effects such as stomach ulcers, bleeding in the digestive tract, and harmful effects on the liver, kidneys, and heart.*

The aim of this study is to design new ibuprofen (IBU) analogues that are safer and more effective than the original drug. To achieve this, new chemical groups like CH_3, F, CF_3, OCF_3, Cl, and OH were added to the basic structure of ibuprofen. These changes were expected to improve both the chemical properties and biological activity of the drug.

The new compounds were studied using computational methods such as Density Functional Theory (DFT) and time-dependent DFT for geometry optimization. Molecular docking studies were carried out with the human prostaglandin synthase protein (PDB ID: 5F19) to test how well these compounds bind, their interaction patterns, and the stability of the drug-protein complex.

In addition, ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) and PASS (Prediction of Activity Spectra for Substances) tools were used to check the pharmacokinetic behavior and safety of the new molecules. Results showed that most of the analogues had lower risks of liver, kidney, and cancer-related toxicity compared to ibuprofen. Molecular docking also suggested that these analogues may provide better therapeutic effects, which was supported by pharmacokinetic predictions.

Overall, the findings suggest that the modified ibuprofen analogues may be safer and more effective than the parent drug..

Keywords*:* Cyclooxygenase (COX) inhibitor, COX-1 and COX-2 inhibition, Prostaglandin synthesis inhibition, Anti-inflammatory, Analgesic, Antipyretic, Pain relief, Fever reduction, Anti-inflammatory mechanism

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