# A Study of Drug-Like Properties of Regioisomers of Chloroaspirin Using QSAR and Molecular Docking

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## Abstract:

Chloroaspirin, a chlorinated derivative of aspirin, has drawn interest due to its potential pharmacological applications. There are four regioisomers of chloroaspirin i.e., 3-chloroaspirin, 4-chloroaspirin, 5-chloroaspirin and 6-chloroaspirin. In this study, we evaluate the drug-like properties of all the regioisomers of chloroaspirin using Quantitative Structure-Activity Relationship (QSAR) modeling and molecular docking with cyclooxygenase enzyme-1(COX-1). Various computational approaches are employed to predict physicochemical properties, bioavailability, and interaction with target enzymes. The order of binding affinity of the regioisomers with the enzyme is as '4-chloroaspirin > 3-chloroaspirin > 5-chloroaspirin > 6-chloroaspirin'. Our findings provide insights into the suitability of these regioisomers as potential therapeutic agents.

## Keywords:

Chloroaspirin, Regioisomers, QSAR, Molecular Docking, ADMET, COX-1, Drug-likeness.