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Abstract

Design and Bioactivity Evaluation of Chloro-Substituted Hydrazones †

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Aroylhydrazones, created by combining aromatic aldehydes and hydrazides, have numerous biological effects such as analgesic, anti-inflammatory, anticancer, antimicrobial, and antibacterial. The current study reports how the presence of a chlorine atom in hydrazone molecules affects their lipophilicity and molecular characteristics.

Methods: A series of novel chloro-substituted salicylaldehyde benzoylhydrazone derivatives was created by inserting the Cl atom in the aldehyde and hydrazide moiety and changing the substituent positions. To select the lead chloro-hydrazones with suitable pharmacological properties, the molecular and bioactivity scores of the proposed compounds were evaluated using a group contribution approach.

Results: Including a chlorine atom in the salicylaldehyde or hydrazide moiety raises the value of log P. Despite minor variances, all chloro-substituted salicylaldehyde benzoyl hydrazone derivatives show acceptable lipophilicity, with log P values up to 4.51. Cl-hydrazones have a TPSA of less than 140 $Å^2$, indicating high permeability to the cellular plasma membrane. Bioactivity scores indicate biological activity against GPCR ligands, ion channel modulators, kinase inhibitors, nuclear receptor ligands, protease inhibitors, and other enzyme targets.

Conclusions: The results revealed that all compounds are potential candidates for future drug discovery studies.

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