

IN SILICO PROFILING OF THE BIOLOGICAL ACTIVITY AND ADVERSE-EFFECT SPECTRUM OF A NOVEL 2-HYDROXYNAPHTHALDEHYDE-DERIVED TOSYLHYDRAZINECARBOXAMIDE

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Hydrazone derivatives are an important class of compounds exhibiting diverse biological activities and considerable potential in medicinal chemistry. Early in silico screening enables the identification of promising pharmacological targets before experimental investigations. In this study, the biological activity and adverse-effect spectra of the newly synthesized (E)-2-((2-hydroxynaphthalen-1-yl)methylene)-N-tosylhydrazinecarboxamide were predicted using the PASS Online platform [1].

PASS analysis revealed a broad spectrum of predicted biological activities (Figure 1). The highest probability was observed for glutamyl endopeptidase II inhibition ($P_a = 0.766$, $P_i = 0.015$), followed by HMGCS2 expression enhancement ($P_a = 0.710$), polyprotein protease inhibition ($P_a = 0.708$), and anti-infective activity ($P_a = 0.707$). In addition, insulysin (insulin-degrading enzyme, IDE) inhibition was predicted with $P_a = 0.694$ and $P_i = 0.009$. Considering the role of IDE in insulin metabolism, this target appears promising for subsequent molecular docking and experimental validation [2].

The predicted adverse-effect profile (Figure 2) was mainly represented by metabolic acidosis ($P_a = 0.741$, $P_i = 0.020$) and porphyria ($P_a = 0.703$, $P_i = 0.007$), whereas the remaining predicted adverse effects demonstrated considerably lower probabilities. These findings indicate that safety-related endpoints should also be evaluated during further pharmacological investigations [1].

The obtained results demonstrate that the investigated hydrazone possesses a diverse predicted biological activity profile, while IDE inhibition represents one of the most biologically relevant targets for future studies. Overall, PASS-based prediction provides a rational basis for molecular docking, experimental validation, and further pharmacological characterization of this compound [1–3].

References:

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