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Design and Identification of Chalcone-Cyclized Derivatives as Novel PTP1B Inhibitors Using *In Silico* and *In Vitro* Approaches

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SUMMARY. In the current study, a series chalcone-cyclized derivatives (**3a-3j**) were prepared and assessed for their inhibitory activity against the protein tyrosine phosphatase 1B (PTP1B) enzyme. Four PTP1B inhibitors were obtained with IC_{50} in the micromolar range, and compound **3i** exhibited a prior activity than ursolic acid with IC_{50} of 1.54 μM. The simple structure-function relationships were discussed. The docking study was carried out, and the results suggested the extension of the H-bond group can increase the binding between ligand and protein, improving the inhibitory activity against PTP1B.

RESUMEN. En el estudio actual se prepararon una serie de derivados ciclados de chalcona (**3a-3j**) y se evaluó su actividad inhibidora contra la enzima proteína tirosina fosfatasa 1B (PTP1B). Se obtuvieron cuatro inhibidores de PTP1B con IC_{50} en el rango micromolar y el compuesto **3i** exhibió una actividad mayor que el ácido ursólico, con IC_{50} de 1,54 μM. Se discutieron las relaciones estructura-función. Se llevó a cabo el estudio de acoplamiento y los resultados sugieren que la extensión del grupo de enlaces H puede aumentar la unión entre el ligando y la proteína, mejorando la actividad inhibitoria contra PTP1B.

KEY WORDS: chalcone, docking, diabetes, PTP1B, pyrazole.

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