

Synthesis, Characterization, and Exploring the *In Silico* Insights of Oxadiazole Derivatives Derived from Ibuprofen and Naproxen

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SUMMARY. The synthesis, characterization, and *in-silico* analyses of oxadiazole derivatives are presented in this paper. The compounds were created by reacting Ibuprofen and naproxen with hydrazides of various aromatic acids in the presence of phosphorous oxychloride. The hydrazides were made by reacting aromatic acid with thionyl chloride to create aroyl chloride, which was then combined with 100 percent ethanol to create ethyl benzoate derivatives. These substances were created to enhance the biological effects of these nonsteroidal anti-inflammatory drugs (NSAIDs) and explore potential therapeutic uses. The synthesized compounds were characterized using FT-IR, ¹H-NMR, mass spectroscopy, and elemental analysis. *In silico* analyses indicated their favorable binding affinities towards protein targets involved in pain and inflammation such as COX-I (PDB: 1EQG) and COX-II (PDB: 1CX2). The findings suggest that oxadiazole derivatives could be used to make new NSAIDs with improved therapeutic efficacy.

RESUMEN. En este artículo se presentan la síntesis, caracterización y análisis *in silico* de derivados de oxadiazol. Los compuestos se crearon haciendo reaccionar ibuprofeno y naproxeno con hidrazidas de varios ácidos aromáticos en presencia de oxicluro de fósforo. Las hidrazidas se obtuvieron haciendo reaccionar ácido aromático con cloruro de tionilo para crear cloruro de aroilo, que luego se combinó con etanol al 100 por ciento para crear derivados de benzoato de etilo. Estas sustancias se crearon para mejorar los efectos biológicos de estos fármacos antiinflamatorios no esteroides (AINE) y explorar posibles usos terapéuticos. Los compuestos sintetizados se caracterizaron mediante FT-IR, ¹H-NMR, espectroscopia de masas y análisis elemental. Los análisis *in silico* indicaron sus afinidades de unión favorables hacia dianas proteicas implicadas en el dolor y la inflamación, como la COX-I (PDB: 1EQG) y la COX-II (PDB: 1CX2). Los hallazgos sugieren que los derivados de oxadiazol podrían usarse para fabricar nuevos AINE con mayor eficacia terapéutica.

KEYWORDS: ADMET, anti-inflammatory, heterocyclic, ibuprofen, molecular docking, naproxen, oxadiazole derivatives.

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