

In Silico Molecular Anti-inflammatory, Analgesic, Antipyretic and Antitubercular Study of Synthetic Ibuprofen and Naproxen Derivatives Containing Isoniazid Moiety

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SUMMARY. Ibuprofen and naproxen derivative containing oxadiazole ring were prepared by the reaction of isoniazid with ibuprofen and naproxen in presence of phosphorous oxy chloride (POCl₃). Ibuprofen and naproxen are well known non selective non steroidal anti-inflammatory drugs (NSAIDs). These synthesized compounds were identified by their melting points, FT-IR, ¹H-NMR, and mass spectroscopy. These ibuprofen and naproxen derivatives were *in silico* evaluated for anti-inflammatory, analgesic, antipyretic (NSAIDs), and antitubercular activity and compared with reference drug. The result showed that these compounds (1, 2) displayed promising NSAIDs and antitubercular activities and would be effective candidates for pharmacology.

RESUMEN. Los derivados de ibuprofeno y naproxeno que contienen un anillo de oxadiazol se prepararon mediante la reacción de isoniazida con ibuprofeno y naproxeno en presencia de oxiclورو de fósforo (POCl₃). El ibuprofeno y el naproxeno son fármacos antiinflamatorios no esteroides (AINEs) no selectivos bien conocidos. Estos compuestos sintetizados se identificaron por sus puntos de fusión, FT-IR, ¹H-NMR y espectroscopía de masas. Estos derivados de ibuprofeno y naproxeno se evaluaron *in silico* para determinar su actividad antiinflamatoria, analgésica, antipirética (AINEs) y antituberculosa y se compararon con el fármaco de referencia. El resultado mostró que estos compuestos (1, 2) mostraban actividades antituberculosas y AINE prometedoras y serían eficaces candidatos farmacológicos.

KEYWORDS: analgesic, antiinflammatory, antitubercular, ibuprofen, isoniazid, naproxen, NSAIDs, oxadiazole derivatives, pyridine.

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