

In Silico Molecular Anti-Inflammatory, Analgesic, Antipyretic and Antitubercular Study of Synthetic Ibuprofen and Naproxen Derivative 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 derivative were *in silico* evaluated for anti-inflammatory, analgesic, antipyretic (NSAIDs) and antitubercular activity and compared with reference drugs. The result showed that both compounds displayed promising NSAIDs and antitubercular activities and would be effective candidates.

RESUMEN: El ibuprofeno y el derivado de naproxeno que contienen un anillo de oxadiazol se prepararon mediante la reacción de isoniazida con ibuprofeno y naproxeno en presencia de oxicloruro de fósforo (POCl₃). El ibuprofeno y el naproxeno son fármacos antiinflamatorios no esteroideos (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 (AINE) y antituberculosa y se compararon con fármacos de referencia. El resultado mostró que ambos compuestos mostraban actividades antituberculosas y AINE prometedoras y serían candidatos eficaces.

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

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