

Synthesis and molecular modeling studies of naproxen-based acyl hydrazone derivatives

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Abstract: A series of *N*-acylhydrazone derivatives (**2a–2p**) containing 6-methoxy-naphthalene and acylhydrazone moieties were synthesized in good yield using microwave irradiation and developed as potential COX-2 inhibitors. Furthermore, the interactions between COX-2 and the compounds were examined in detail by molecular modeling studies such as structure-activity relationship and molecular docking performed using Gaussian 09 and Discovery Studio 3.5. As a result, it was found that *N*-acylhydrazone compounds displayed a different mechanism than SC-558 as COX-2 inhibitor by binding to different active sites of the protein, COX-2. Compound **2c** would be a good COX-2 inhibitor candidate for preclinical studies.

Key words: Naproxen, microwave, acyl hydrazones, molecular docking

1. Introduction

Nonsteroidal anti-inflammatory drugs (NSAIDs) are used to reduce pain, inflammation, and fever. Most NSAIDs reduce pain by preventing prostaglandin biosynthesis, by inhibiting the activity of the cyclooxygenase enzyme (COX).¹ Until 1990, only one form of the COX enzyme was known and it was thought to be responsible for both its anti-inflammatory activity and unwanted side effects. After 1990, it was found that the COX enzyme had 2 iso forms: COX-1 (constitutive form) and COX-2 (inducible form). Inhibition of the COX-1 enzyme causes some of the unwanted side effects such as gastrointestinal hemorrhage, ulceration, and decreased renal function, while inhibition of COX-2 is responsible for reducing pain, fever, etc.² An ideal NSAID would inhibit COX-2 enzyme activity without affecting COX-1 enzyme activity. To find an ideal NSAID, researchers synthesized many COX-2 selective hybrid NSAID compounds. Unfortunately, at the end of 2004, the COX-2 selective NSAID drug rofecoxib was withdrawn from the market because it was discovered that it increased the risk of cardiovascular events.³

After that many new studies were conducted to find NSAIDs that were safe in both gastrointestinal and cardiovascular terms. In these studies, naproxen showed the lowest cardiovascular risk^{4–5} but had significant gastrointestinal side effects.^{6–8} As part of the research, molecular modeling techniques⁹ were used to design and develop the optimal compound(s) with less time, labor, and cost. Such methods also became increasingly useful in many other clinically oriented studies.¹⁰

In the present study, we planned to synthesize hybrid compounds of naproxen that minimize the side

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