

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 Unfortunately, at the end of 2004, the COX-2 selective NSAID drug rofecoxib was withdrawn from the market because it was discovered that it increased the risk of cardiovascular events.³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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Current Molecular Targets of Heterocyclic Compounds for Cancer Therapy discusses recently developed treatments based on molecular targets which are genetically altered in cancer cells and are essential for tumor development and survival. Considerable research effort has been devoted to the development of targeted drugs that inhibit the action of pathogenic kinases and clinical studies performed so far have validated the positive effects of kinase inhibitors for cancer treatment. Each chapter discusses a molecular target such as ALK2, ATR, CK, Src, Abl, EGFR, Fyn, Blk, Lyn, IGFs, and PAK1. The book's chapters are written by experts who actively work on the targets to help readers fully understand how they can be used. This is a valuable resource for cancer researchers, oncologists, graduate students, and members of the biomedical field who are interested in the potential of novel cancer therapies based on molecular targets. Discusses recently discovered molecular targets for cancer therapy. Brings updated literature of heterocyclic compounds, an important construction motif for the development of new anticancer drugs. Encompasses comprehensive compilation of recently introduced anticancer drugs in the market and their health outcomes and pharmacoeconomics. Nanostructured Biomaterials Bibhu Prasad

Swain, 2022-03-07. This book presents recent advances in nanostructured biomaterials. It covers the structures and applications of advanced nanostructured biomaterials. The topics covered include overview on biological activities of thiazole derivatives, imidazole derivatives, pyrazole derivatives, tetrazole derivatives, benzimidazole derivatives, oxazole, isoxazoles, etc. The book also covers the topic of nanocarriers as drug delivery vectors. Given the contents, the book will be useful for students, researchers, and professionals working in the area of biomaterials and nanomaterials. **Nitrogen Heterocycles**

in Cancer Therapy Sanjeev Kumar Sahu, Ankur Vaidya, 2025-10-17. Nitrogen Heterocycles in Cancer Therapy explores the vast array of recently discovered nitrogen-containing heterocyclic compounds utilized in combatting cancer. This comprehensive work not only highlights the fundamentals of oncology but also explains into the intricacies of designing, synthesizing, and understanding the anticancer mechanisms of these compounds. Spanning across 10 chapters, the book explores the principles underlying the design, synthesis, and anticancer mechanisms of nitrogen-containing heterocyclic compounds, drawing from the latest research findings. Its scope extends beyond molecular targeting to encompass the exploration of newly identified heterocyclic compounds with potential anticancer properties. A significant emphasis is placed on crucial evaluation techniques such as in vitro cell culture and in vivo animal models, providing insights into the performance of these compounds in combating cancer. Particularly noteworthy is the inclusion of clinical study reports detailing the efficacy of various drug candidates across different cancer conditions, coupled with an analysis of their global market impact and pharmacoeconomics. Offering profound insights, this book emerges as an indispensable resource for researchers, clinicians, and students alike, offering a comprehensive understanding of the cutting-edge approaches shaping the

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