

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

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Received: 03.02.2014 • Accepted: 15.07.2014 • Published Online: 23.01.2015 • Printed: 20.02.2015

**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).<sup>1</sup> 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.<sup>2</sup> 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 Unfortunately, at the end of 2004, the COX-2 selective NSAID drug rofecoxib was withdrawn from the market because it was discovered that it increased the risk of cardiovascular events.<sup>3</sup>

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<sup>4,5</sup> but had significant gastrointestinal side effects.<sup>6-8</sup> As part of the research, molecular modeling techniques<sup>9</sup> 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.<sup>10</sup>

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

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## **Synthesis And Molecular Modeling Studies Of Naproxen Based:**

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.

**Current Molecular Targets of Heterocyclic Compounds for Cancer Therapy** Vivek Asati, Ankur Vaidya, 2024-04-10 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.

**Metalloenzymes** Claudiu T. Supuran, William Alexander Donald, 2023-08-30 Metalloenzymes: From Bench to Bedside offers a thorough overview of metalloenzymes spanning biochemical and structural features, pharmacology, and biotechnological applications. After a brief overview, international experts in the field discuss a wide range of magnesium, calcium, zinc, manganese, nickel, iron, copper, cadmium, molybdenum, and tungsten enzymes along with catalytic roles within their active sites. With a uniform approach throughout, each chapter includes the structure and function of the enzyme, physiologic and pathologic roles, inhibitors, and activators of the enzyme, and their design and clinical agents or compounds applied in medicine and drug discovery. This book enables scientists across academia and industry to adopt ongoing metalloenzyme research and continuous discovery of novel metalloenzymes in new life science studies and clinical applications. Examines a range of metalloenzymes from biochemistry to pharmacology and drug design. Each chapter examines enzyme structure and function, physiologic and pathologic roles, inhibitors, and activators, and clinical application. Features chapter contributions from international experts in the field.

**Host-Guest Polymer Complexes** Alan Edward Tonelli, Ganesh Narayanan, Alper Gurarslan, 2018-10-02 This book is a printed edition of the Special Issue Host Guest Polymer Complexes that was published in Polymers. **Dissertation**

**Abstracts International** ,2006      **Cumulated Index Medicus** ,1996      **Handbook of Engineering and Specialty Thermoplastics, Volume 2** Johannes Karl Fink,2011-04-12 This book focuses on common types of polymers belonging to the class of water soluble polymers It covers a wide range of applications food cosmetic medical lithography and ink jet printing agricultural wastewater cleaning and oilfield The text is arranged according to the chemical constitution of polymers and reviews the developments that have taken place in the last decade Each chapter follows the same template A brief introduction to the polymer type is given and previous monographs and reviews dealing with the topic are listed for quick reference The text continues with monomers polymerization fabrication techniques properties applications as well as safety issues Providing a rather encyclopedic approach to water soluble polymers the Handbook of Engineering and Specialty Thermoplastics Presents a listing of suppliers and commercial grades Reviews current patent literature essential for the engineer developing new products Contains an extensive tradenames index with information that is fairly unique Concludes with an index of acronyms and a general index The Handbook of Engineering and Specialty Thermoplastics Water Soluble Polymers provides a comprehensive reference for chemical engineers and offers advanced students a textbook for use in courses on chemically biased plastics technology and polymer science      *Index Medicus* ,2004 Vols for 1963 include as pt 2 of the Jan issue Medical subject headings      *Pharmaceuticals in Aquatic Environments* Vinod Kumar Garg,Ashok Pandey,Navish Kataria,Caterina Faggio,2023-11-13 1 Explores the management of the environment through green chemistry 2 Describes phytoremediation technology for decontamination of pharmaceuticals laden water and wastewater 3 Covers the detection methods and quantification of pharmaceutical residues in various contaminated sources 4 Discusses ecotoxicological aspects and risk assessment of pharmaceuticals in the aquatic environment 5 Reviews degradation and treatment technologies including nanotechnology biomaterials biochar      **Comprehensive Organic Synthesis** ,2014-02-14 The second edition of Comprehensive Organic Synthesis winner of the 2015 PROSE Award for Multivolume Reference Science from the Association of American Publishers builds upon the highly respected first edition in drawing together the new common themes that underlie the many disparate areas of organic chemistry These themes support effective and efficient synthetic strategies thus providing a comprehensive overview of this important discipline Fully revised and updated this new set forms an essential reference work for all those seeking information on the solution of synthetic problems whether they are experienced practitioners or chemists whose major interests lie outside organic synthesis In addition synthetic chemists requiring the essential facts in new areas as well as students completely new to the field will find Comprehensive Organic Synthesis Second Edition Nine Volume Set an invaluable source providing an authoritative overview of core concepts Winner of the 2015 PROSE Award for Multivolume Reference Science from the Association of American Publishers Contains more than170 articles across nine volumes including detailed analysis of core topics such as bonds oxidation and reduction Includes more than10 000 schemes and images Fully revised and updated important growth areas

including combinatorial chemistry new technological industrial and green chemistry developments are covered extensively

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Rehm, Gerald Reed, 1991 **Application of Ionic Liquids in Biotechnology** Toshiyuki Itoh, Yoon-Mo Koo, 2019-07-24 This volume explores how ionic liquids are used in different areas of biotechnology It also provides insights on the interaction of ionic liquids with biomolecules and biomaterials Ionic liquids have become essential players in the fields of synthesis catalysis extraction and electrochemistry and their unique properties have opened a wide range of applications in biotechnology Readers will discover diverse examples of the application of ionic liquids as solvents for biomaterials extraction and pretreatment in enzymatic and whole cell catalysed reaction and as activation agents for biocatalysis Particular attention is given to the biologically functionalized ionic liquids employed in medical and pharmaceutical applications Although ionic liquids are considered green solvents the contributing authors will also explore their environmental impact when applied to biotechnology Chemical biological and medical scientists interested in ionic liquids and biotechnology will find this work instructive and informative *CRC Handbook of Organic Photochemistry and Photobiology, Volumes 1 & 2* William M. Horspool, Francesco Lenci, 2003-09-29 The second edition of this best selling handbook is bigger more comprehensive and now completely current In addition to thorough updates to the discussions featured in the first edition this edition includes 66 new chapters that reflect recent developments new applications and emerging areas of interest Within the handbook's 145 critically reviewed articles **Journal of the National Cancer Institute**, 2008

Ionic Liquids and Deep Eutectic Solvents for Application in Pharmaceutics Miguel M. Santos, Luís C. Branco, 2021-09-01 Dear Colleagues In recent years functional coating technology has attracted increased attention due to its effective potential for improved engineered materials Growing demand for new materials with synergistic properties pushed research toward a new field to obtain innovative and smart coatings with functional capabilities that greatly differ from the conventional ones In such a context the expression of functional coatings has acquired specific relevance This Special Issue will assess cutting edge developments in this research area for the improvement and growth of actual performance industrial scale up and marketability of functional coatings This Special Issue is useful for researchers who are approaching this application context to improve their knowledge with the aim of providing valuable scientific support for new research paths concerning functional surface engineering design and tailoring Prof Luigi Calabrese Prof Edoardo Proverbio Guest Editors Business Modeling for Life Science and Biotech Companies Alberto Onetti, Antonella Zucchella, 2014-03-21 Most books on the

biotechnology industry focus on scientific and technological challenges ignoring the entrepreneurial and managerial complexities faced bio entrepreneurs The Business Models for Life Science Firms aims to fill this gap by offering managers in this rapid growth industry the tools needed to design and implement an effective business model customized for the unique needs of research intensive organizations Onetti and Zucchella begin by unpacking the often used business model term examining key elements of business model conceptualization and offering a three tier approach with a clear separation between the business model and strategy focus exploring the different activities carried out by the organization locus evaluating where organizational activities are centered and modus testing the execution of the organization s activities The business model thus defines the unique way in which a company delivers on its promise to its customers The theory and applications adopt a global approach offering business cases from a variety of biotech companies around the world *Index to Theses with Abstracts Accepted for Higher Degrees by the Universities of Great Britain and Ireland and the Council for National Academic Awards* ,2006 *Wastewater Treatment with the Fenton Process* Dominika Bury, Michał Jakubczak, Jan Bogacki, Piotr Marcinowski, Agnieszka Jastrzębska, 2023-12-11 The presence of refractory organic compounds in wastewater is a global problem Advanced oxidation processes in general and the Fenton oxidation process are alternative technologies for wastewater and water treatment This book gives an overview of Fenton process principles explains the main factors influencing this technology includes applications kinetic and thermodynamic calculations and presents a strong overview on the heterogeneous catalytic approach It demonstrates that the iron based heterogeneous Fenton process including nanoparticles a new complex solution is highly efficient environmentally friendly and can be suitable for wastewater treatment and industrial wastewater FEATURES Describes in detail the heterogeneous Fenton process and process applications Analyzes the advantages and disadvantages of different catalysts available and their suitability to specific processes Provides economic analysis of the Fenton process in a ready to use package for industrial practitioners for adaptation into already existing industrially viable technologies Promotes a modern solution to the problem of degradation of hazardous compounds through ecological and environmentally friendly processes and the use of a catalyst that can be recycled Explains highly complex data in an understandable and reader friendly way Intended for professionals researchers upper level undergraduate and graduate students in environmental engineering materials science chemistry and those who work in wastewater management Chapters 3 4 and 9 of this book are freely available as a downloadable Open Access PDF at <http://www.taylorfrancis.com> under a Creative Commons Attribution Non Commercial No Derivatives CC BY NC ND 4.0 license **Chemistry of Biologically Potent Natural Products and Synthetic Compounds** Shahid Ul Islam, Javid Ahmad Banday, 2021-06-29 In view of their promising biological and pharmaceutical activities natural product inspired and heterocyclic compounds have recently gained a reputation in the field of medicinal chemistry Over the past decades intensive research efforts have been ongoing to understand the synthesis biochemistry and engineering involved in their preparation

and action mechanisms Several novel natural product derivatives heterocyclic and other synthetic compounds have been reported to have shown interesting biological activities including anticancer antimicrobial anti inflammatory anti glyceimic anti allergy and antiviral etc Chemistry of Biologically Potent Natural Products and Synthetic Compounds provides up to date information on new developments and most recent medicinal applications of the natural products and derivatives as well as the chemistry and synthesis of heterocyclic and other related compounds

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