



INVESTIGATING CONCEPT RELATED TO HETROCYCLE COMPOUND AND MEDICINAL CHEMISTRY

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ABSTRACT

The current research work focusing the central theme of this dissertation entitled "Development of Green Synthetic Protocols for Biologically Relevant Heterocycles" was initiated in August, 2015 under the supervision of Prof. (Dr.) Goutam Brahmachari, Department of Chemistry, Visva-Bharati University, Santiniketan-731235, and India. The fundamental objective of the current study is to design sustainable synthesis procedures for heterocycles with potential biological applications. Concern about the potentially harmful byproducts of modern chemical processes is a modern phenomenon. One of the ultimate goals of modern chemistry is the development of organic synthesis methods that are less harmful to the environment. Traditional procedures using poisonous and/or dangerous stoichiometric reagents being phased out in favor of more atom-efficient and environmentally friendly "Green and Sustainable Chemistry" approaches. To achieve high selectivity and waste reduction, for instance, catalysis is one of the key concepts.

Keywords: - Elements, High Selectivity, Physical, Synthesis, Compounds.

I. INTRODUCTION

The study of the elements, their compounds, their physical and chemical characteristics, their uses and applications, and the laws that govern them all fall under the umbrella of chemistry.

The intricacy of the biological system makes drug discovery a difficult task. Synthesis of compounds by trial and error and random screening for biological activity is a time-consuming traditional technique. Thus, it is the hope of pharmaceutical researchers to rationally design novel compounds, i.e., to anticipate their action before synthesis. Using such methodical techniques to drug creation has both scientific and financial benefits.

Humans and the wide variety of microbes that might cause illness have been at odds for a very long time. It's safe to assume

that for about the same amount of time, people have been looking for effective treatments. Due to the serious nature of most illnesses and the near-total ignorance of their causes that prevailed until the previous century, this was an extremely challenging undertaking. No sensible treatment was possible until the discovery of bacteria three hundred years ago and the subsequent knowledge of their involvement in illness approximately 150 years ago. Whether caused by bacteria, viruses, fungus, protozoa, multicellular parasites, or prions, an infectious illness always manifests itself clinically. Diseases may be caused by these pathogens in animals and plants.

Due to their potential for transmission from one person or species to another, infectious diseases are often classified as



contagious illness (communicable disease). Physical contact between sick people is one possible route for the spread of an infectious illness. These pathogens may also be dispersed by the air, on contaminated surfaces, or through the bites of insects or other arthropods. illness infectiousness denotes the relative ease with which one illness may be spread to another host, whereas infectivity explains the capacity of organisms to enter, live, and reproduce in the host.

Following Paul Ehrlich's success in treating infections with organometallics and his ideas of vital staining, the modern anti-infective era began with the discovery of the sulfonamides in France and Germany in 1936. Although the exact procedures utilised for their discovery are much more complex now than they were 50 years ago, soil-derived microbes remain the most productive source of antibiotics. At first, fermentation extracts were tested only for their antimicrobial activity in vitro. Those who persevered were forced to undergo more intricate pathogenic and toxicological studies in pursuit of therapeutically effective medicines. These days, hundreds of such extracts from ever-more-exotic microorganisms are evaluated every week, with tests including complex assays for drugs working through a specific biochemical pathway or exhibiting desired features. The contribution of genomics to this endeavour is anticipated to be significant. This effort has resulted in a wide variety of potent, effective, and precise treatment options for some of humanity's oldest and most widespread bacterial illnesses.

II. GENERAL ASPECTS OF HETEROCYCLIC COMPOUNDS

Heterocyclic compounds are a kind of chemical compound with a carbon- and non-carbon-based cyclic skeleton. A heteroatom is any atom that is not a carbon atom. Nitrogen, oxygen, and sulfur are all examples of heteroatoms. We know that heterocyclic compounds include lactones, lactams, and cyclic ethers. Congeneric open-chain compounds with comparable characteristics will be covered in the respective chapters. Heterocyclic compounds (also known as aromatic heterocyclic compounds) with a somewhat stable ring structure are the primary focus of this chapter.

Heterocyclic compounds come in a broad variety of forms and numbers, and may be found all throughout the natural world. An essential physiological function is performed by several heterocyclic compounds found naturally in animals and plants. Some medicines, vitamins, and amino acid and nucleotide sequences, for instance, have a heterocyclic structure. Similarly, plant chlorophyll and animal hemoglobin have heterocyclic structures. Roughly 50% of currently used drugs are of the heterocyclic structural type. As a result, organic chemicals, and organic medications in particular, rely heavily on heterocyclic compounds.

Heterocyclic compounds with a five- or six-membered ring, or their fused heterocyclic compounds, are the most abundant and the most significant. There are two main types of heterocyclic compounds, those with five members of the ring and those with six members of the ring. Five-membered heterocyclic compounds include furan, thiophene,



pyrrole, imidazole, triazole, and their fused heterocyclic compounds; six-membered heterocyclic compounds include pyridine, pyrimidine, and their fused heterocyclic compounds; quinoline, and quinazoline.

Five- and six-membered heterocyclic compounds may be further subdivided into one-hetero-atom-containing heterocyclic compounds, two-hetero-atom-containing heterocyclic compounds, and multiple-hetero-atom-containing heterocyclic compounds. For instance, furan, thiophene, pyridine, indole, quinoline, dibenzofuran, etc. all contain exactly one hetero atom; imidazole, pyrimidine, benzimidazole, quinazoline, etc. all contain exactly two; and purine, which contains more than two, is a heterocyclic compound with multiple hetero atoms. Single heterocyclic compounds and fused heterocyclic compounds are two types of heterocyclic compounds that are distinguished by the ring structure of their molecules. For instance, indole, quinoline, dibenzofuran, purines, etc. are all examples of fused heterocyclic compounds, whereas furan, pyridine, pyrimidine, imidazole, etc. are all single heterocyclic compounds.

Heterocycles with five or six members and nitrogen, oxygen, or sulfur heteroatoms are the most prevalent kind. These four simple heterocyclic compounds—pyridine, pyrrole, furan, and thiophene—are among the most well-known in the chemical world. Five carbon and one nitrogen atoms form a ring inside a molecule of pyridine. Five-membered rings made up of four carbon atoms and one nitrogen, oxygen, or sulfur atom are found in pyrrole, furan, and thiophene compounds.

Both pyridine and pyrrole have nitrogen atoms in their molecules, making them

nitrogen heterocycles. Many biological materials include modest quantities of pyridine and pyrrole that are released during high-temperature decomposition. Both of these chemicals were first identified in the 1850s, when they were found in an oily combination created by intensely heating bones. These days, pyridine and pyrrole are both made in laboratories by chemical synthesis. The most lucrative use for these chemicals is in the production of colors and pharmaceuticals. In addition to its usage as a dyeing additive, pyridine is used as a solvent, waterproofing agent, rubber additive, and alcohol denaturant.

III. MEDICINAL CHEMISTRY

Formulation, production, and research of medicines are the focus of medical chemistry, often known as pharmaceutical chemistry. Discovering, synthesizing, and developing new chemical entities having therapeutic potential is the goal of medicinal chemistry. The physiology of presently used drugs is also a part of this field of study. Pharmaceutical chemists put a premium on quality control measures to ensure that their drugs work as intended. The goal of a medicinal chemist is to develop or discover a new chemical with therapeutic applications. This endeavor calls for the combined efforts of many experts in areas as varied as chemistry, biology, biochemistry, pharmacology, mathematics, medicine, and computers. Any chemical compound used for the diagnosis, cure, mitigation, or prophylaxis of illness in people, animals, or plants is known as a drug. When discussing the medicinal effects of a substance, such as analgesic or b-blocker, the terms "activity" and "potency" are sometimes used



interchangeably. The media and the general people, however, often incorrectly use the word "drug" to items that are not drugs. Diamorphine, a heroin derivative, is used to alleviate pain in terminal cancer patients.

Understanding such interactions can provide fundamental, basic knowledge that is both general and compound-specific, and can be used to improve the overall profile of a given molecular display or to design an NCE (New Chemical Entities), for example, by effecting small molecule-driven perturbations of discrete biological processes or of overall biological pathways to elicit a specified therapeutic endpoint. The focus of small molecule displays should be on low molecular weight compounds, frequently of xenobiotic origin, rather than polymers created from biotechnology. While the latter are being tackled by other disciplines, it is still the domain of medicinal chemistry to think about the finer points of how tiny molecule components of larger complicated biomolecular systems interact with one another. In contrast, it is more advantageous to adopt a wide perspective of the biological domain, one that takes into account not just the conventional variety of biological surfaces that may be exploited for successful interaction, but also the whole spectrum of innovative ADMET-related systems. By definition, technologies that may be utilized as instruments to research these interactions at the basic level are not included in the concept of medicinal chemistry. Biotechnological techniques like site-directed mutagenesis, combinatorial chemistry in tandem with knowledge-generating structural databases, and classic synthetic chemistry for systematic

manipulation of one of the interacting species are all examples of current tools used to probe SARs. Because of its broad meaning, medicinal chemistry will need to be adaptable to new tools and techniques as they become available. Last but not least, it is crucial to acknowledge that this definition combines the basic and applied aspects of medicinal chemistry into a key mixture of endeavors for which a new research paradigm has also recently been proposed as a significant trend, albeit potentially "dangerous" in that it could compromise the longer-term pursuit of fundamental knowledge by bringing applied science decision criteria into the funding programs that have traditionally supported the former.

IV. DRUGS

Throughout the whole process of developing a new medicine, biologists and medicinal chemists are in regular contact with one another. Experts in pharmaceutical research and development must work closely with clinical research teams consisting of physicians, nurses, and other healthcare professionals in order to successfully create a new treatment. The hunt for novel molecular or chemical structures is central to the pharmaceutical industry's massive scientific issue of new medication development. For the latter, the development of medicines with new modes of action against disease-specific biological targets is the ultimate goal.

Classification of drugs

There are many methods to classify drugs:

1. One common method for organizing medications is according to their intended use, such as analgesics for pain.



2. Histamine is a molecule that contributes to inflammation, and antihistamines work by preventing its manufacture and release.
3. Penicillin, like other antibiotics, contains a β -lactum ring and kills bacteria in a manner that is similar to other antibiotics, hence these drugs are often grouped together into classes because they have a common structural characteristic and related pharmacological action.
4. A medicinal chemist's preferred classification is based on the compounds they want to block. Anticholinesterases are one family of such drugs that inhibit acetyl cholinesterase.

Medications often come in the form of salts of organic acids or organic bases. Changes in (a) solubility, stability, photosensitivity, and organoleptic characteristics are the outcome of these processes. This research was conducted with the intentions of improving (b) bioavailability by changing absorption, (c) efficacy, and (d) safety.

Applications of drugs

- A. Exogenous substances, such as vitamins, mineral salts, protein hydrolysates, and hormones, may be given to make up for shortages.
- B. To protect against disease or infection, as with vaccines and serums.
- C. To treat a disease with chemotherapeutic drugs like antibiotics.
- D. Inhibiting the normal operation of a system for a short time, as with general and local anesthetics and oral contraceptives.
- E. Modification of an aberrant function, including (i) disfunction, such as in the therapy of congestive heart failure with cardiotonics; (ii) hypofunction, such as in the treatment of suprarenal insufficiency with hydrocortisone; and (iii) hyperfunction, such as in the treatment of arterial hypertension with methyldopa.
- F. Body detoxification, using means such as antidotes, is method F.

V. CONCLUSION

To sum up, we've created a green alternative that's straightforward, catalyst-free and water-mediated, energy-efficient, and practically handy for gaining access to a wide variety of unique and functionalized biologically-interesting compounds. A 5-alkyl-, aryl-, or heteroaryl-2,8-dioxo or dithio-9,10-dihydropyrido[2,3-d:6,5-d']pyrimidine derivatives of the dipyrimidine-4,6-(1H,3H,5H,7H)-dione Four (4-1-42) and five (5,5'-(1,4-phenylene)bis(10-alkyl/aryl-2,8-dioxo/dithio-9,10-dihydropyrido[2,3-d:6,5']quinolines)This pseudo-six component reaction involving barbituric/2-thiobarbituric acids (1), substituted amines (2), and aldehydes (3) in aqueous medium at normal temperature yields dipyrimidine-4,6(1H,3H,5H,7H)-dione 4' (4'-1 - 4'-8). The key benefits of the present protocol include good to excellent yields, high atom-economy, and a low E-factor; energy-efficiency; the use of commercially available low-cost starting materials; and the ease of product isolation/purification without the aid of tedious column chromatography; all of which satisfy the triple bottom line. Additionally, this procedure has the additional benefits of



gram-scale synthesis being possible and the reaction medium being reusable.

The current approach is, at most, environmentally acceptable. The present catalyst-free methodology, featuring mild reaction conditions and operational simplicity, offers the possibility of its use with cost-effective and environmentally friendly ways for large-scale syntheses, which is especially important in light of the synthetic importance of such multi-heterocentric organic scaffolds in biologically relevant applications.

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