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Role of Organic Molecules in Drug Design & Development

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Abstract: *In the past 25 years, there have been significant changes to the function of the medicinal chemist in drug discovery, mostly as a result of the development of technologies like combinatorial chemistry and structure-based drug design. With more than 50 years of experience in medicinal chemistry, Small molecules continue to be the foundation of contemporary drug discovery. They are created and created by medicinal chemists, many of whom were trained as organic chemists in the beginning. We address this evolving function using examples from our collective experience across the last four decades. By assisting the medicinal chemist in reclaiming the creative role that contributed to previous achievements, this historical viewpoint may offer suggestions on how to enhance the current model for drug development.*

Keywords: Drug Discovery, AZT drug, discovery, drug design, toxicology, analgesics

I. INTRODUCTION

Organic molecules play important roles in biology, medicine, and technology. It functions as the primary tool for comprehending structure and responsiveness. This research has been used to synthesis complicated natural chemicals, produce molecules of commercial interest, create newer, more effective pharmacological therapeutic agents based on rational drug design, and identify creative ways to improve the effectiveness of chemical science. The bulk of novel chemical entities (NCEs) in use or being researched globally are small molecule medicines and therapeutic prospects. 1−3 These chemicals are made possible in part because to the talent and creativity of the medicinal and process chemists who create the substances. With the help of medications like atorvastatin (1), ledipasvir (2), imantinib (3), AZT (4), and linezolid (5), countless lives have been and continue to be extended and saved, providing enormous benefits to society, the families, and friends of those being treated [Figure 2]. Stereochemistry, functional groups, and structural complexity all vary depending on the target that each molecule is intended to reach. However, as chemists deal with the increasingly quick turnaround of test results that affect their daily decisions, the precise nature of the role is clearly changing. This is due to the new resources available to synthetic and medicinal chemists as well as in several important areas, particularly in drug metabolism and chemical toxicology. Designing and producing substances that can be utilized in medicine for illness prevention, treatment, and cure in humans and animals is the goal of medicinal chemistry. When seen in a retrospective light, medicinal chemistry encompasses the study of already approved medications, as well as their pharmacological characteristics and structure-activity relationships (SAR). The synthesis of Each molecule was first created on a modest scale (likely milligrams) in the lab, and it took a long time to build safe, effective, and scalable processes to produce kilograms of active pharmaceutical ingredient (API), which was then put into dosage forms for patient administration. The synthesis of a molecule that tested a project team's hypothesis was a key early stage in the difficult process of drug discovery, it is crucial to note.

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II. OVERVIEW OF SYSTEM

Organic molecules perform key functions in nature, drug, and technology. It plays as the engine for understanding structure and reactivity. This science has found application in the production of molecules of commercial interest; in the construction of newer pharmacological active therapeutic agents derived from rational drug design, into synthesize complex natural molecules, in the finding innovative approaches to render this chemical science more efficient.1 The role played by organic chemist in pharmaceutical industry continues to be one of the main drivers in the drug discovery process However, the precise nature of the role is undergoing a visible change, not only because of the new available to the synthetic and medicinal chemists, but also in several key areas, particularly in drug metabolism and chemical toxicology, as chemists deal with the ever more rapid turnaround of testing data that influences their day-to-day decision. Objective of medicinal chemistry is to design and production of compounds that can be used in medicine for prevention, treatment and cure of human or animal disease. Taken in retrospective sense medicinal chemistry includes study of already existing drugs, of their pharmacological properties and their structure activity relationship (SAR) along with above prospective sense.

Pharmacology" is derived from pharmakone = drug and logos = discourse or treatise, and hence includes allied fields such as pharmacy, pharmacognosy, toxicology, posology, chemotherapy, therapeutic and materia medica. "Pharmacy" is the study of the formulation of an active chemical entity, in the form of tablets, capsules, powders, aerosols, injections etc. The physiological activity of drugs has been found to depend upon the presence of particular functionality or structural unit.2 Part of drug which causes actual curing effect is known as "pharmacophores". There are two major considerations that have to be discussed in any drug design project. Firsts, drugs interact with molecular targets in the body and so it is important to choose the correct target for the desired pharmaceutical effect.3 In other words a drug that will interact is powerfully and selectively as possible for that target is known as "pharmacodynamics". Second, a drug after administration has an ability to travel through the body in order to reach its

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targets is known as "pharmacokinetics". Nowadays, nanomedicine research played significant role in drug discovery. Generally, nanomedicine is a field of medicine to facilitate the information tools of nanotechnology to the prevention and cure against several lethal diseases viz.4 microbial, malaria, HIV, TB, cancer etc. The development of newer pharmaceuticals is currently a critical and challenging task to the pharmaceutical industry. The vital interest of the medicinal and agrochemical industries in organic synthesis is often related with their natural occurrence. Similarly, medicinal and pharmaceutical field, there has always been and continue to be a need for newer chemical entities with diverse biological properties.5 Many works are still needed to minimize the time, expenditure, and attrition rate in the drug discovery process simultaneously addressing the huge unmet medical need across the world. Referencing the study report, poor pharmacokinetic and preclinical toxicity were the main reasons for the failure in the drug development, in addition to the lack of efficiency and adverse effects.6 New drugs are necessitated to cure new diseases, to find less hazardous drug and to cure diseases whose drugs have become ineffective due to resistant strains of microorganisms. Besides these causes, new drug discovery and researches are required to recognize pharmacophore present in the effective drugs.7,8 We must always continue to search for drugs which exhibit clear advantages over the already existing respective drugs. Such advantages may be: improvement in bioactivity, partial or total absence of adverse effects, minor toxicity, more nutritive value, improved stability and decrease in production cost.9–12 Nowadays, research development department (R&D) of many organic and pharmaceutical laboratories are working for synthesis of newer biophores/pharmacophores having improved their potential in drug activity and increasing yields of existing drugs. Finally, this chemistry has contributed to life processes and to the efforts to advance the quality of life as well as to the development of society from synthetic, medicinal, biopharmaceutical and industrial point of view (Figures 1–3).

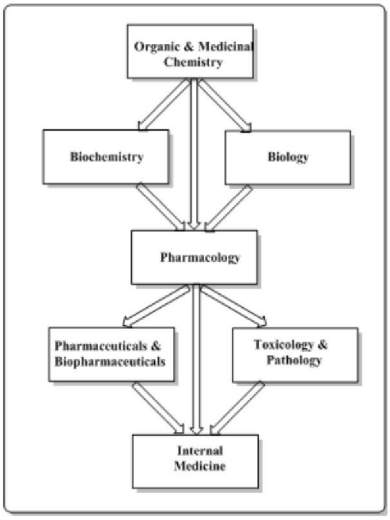

Fig 1: Ramifications of Organic, Medicinal & Pharmaceutical Chemistry

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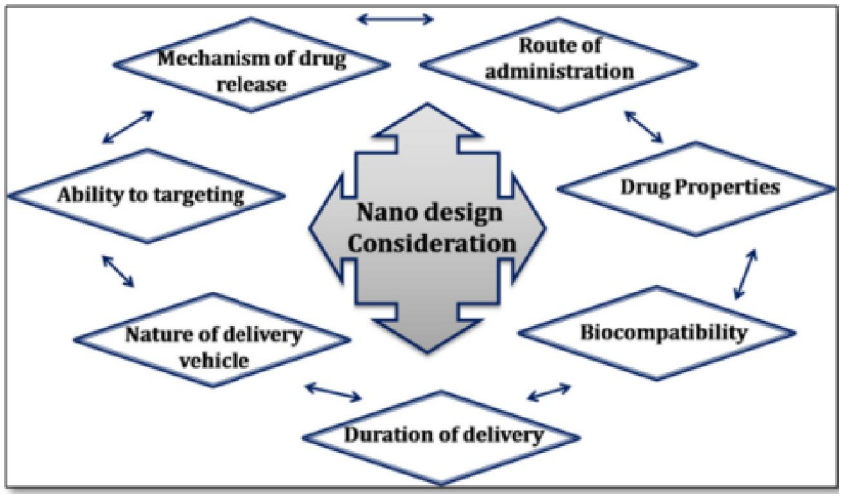

Fig 2: Nano design consideration of drug discovery

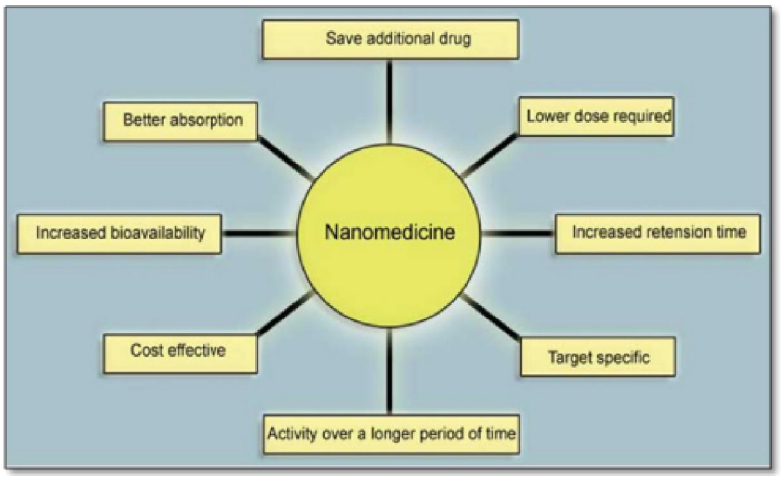

Fig 2: Importance of Nanomedicine

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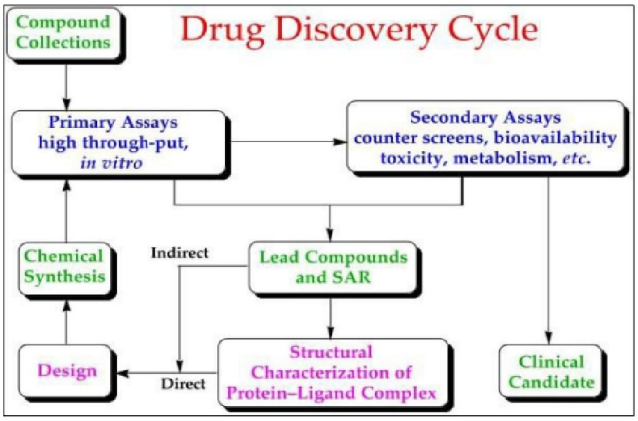
III. DRUG DISCOVERY



Drug discovery is the process which aims at identifying the compound useful is the curing & treating disease. In this process involves the identification of candidates, synthesis, validation, optimization, characterization, screening and assays for therapeutic efficacy [5,9,10] . Stages of drug discovery [1, 2, 3, 7, 9]

1. Target Identification
2. Target Validation
3. Lead compound Identification
4. Lead Optimization
5. Product Characterization
6. Formulation & Development
7. Preclinical Research
8. Investigation of New Drug
9. Clinical Trial
10. New Drug Application
11. Approval

A. Target Identification

It is first step in drug discovery. Identification of target is followed by characterization of the molecular mechanism addressed by the target. Identifying target must be efficacious safe, meet clinical and commercial requirement & be drug gable also. It also based on Molecular Biology & Biochemistry.

Tools for Target Identification & Validation

- Disease association (genetic & expression change)
- Bio-active molecules.
- Cell based models.
- Protein interaction (Pull-down assay, yeast 2 hybrid)
- Analysis of signalling pathways.
- Functional analysis (Overexpression, gene variants, transgenic) Target Validation It shows that a molecular target is directly involved in a disease process & that modulation of target is likely to have a Therapeutic effect. Approaches
- Genetic manipulation of target genes
- Antibodies
- Chemical genomic.

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Lead compound Identification

The identification of lead is the process of identifying & creating a compound that interact with the target. The drugs are tested how it metabolized and how it affects various complete functions.

B. Lead Optimization

After identification they need to be optimized for the safety & efficiency. It is process in which drug designed after initial lead compound is identified. NMR & Mass spectrometry is helpful in discovery & optimization of lead molecules. Product Characterization Any new drug molecules show the promising therapeutic action. Therefore molecule is characterized by its shape, size, strength, weakness, toxicity, use & biological activity.

C. Formulation & Development

The physicochemical property of an active pharmaceutical ingredient (API) are characterized to produce the stable, bioavailable and optimal dosage from for a specific administration route. Preclinical Research This stage involves the evaluation of the drugs safety and efficacy in animal species. The preclinical trial also have to acquire approval by corresponding regulatory authorities. Specially, side effects of the drugs need to be monitored and addressed in this stage. Investigation of New Drug (IND) At beginning to the clinical trial. IND application submitted to a FDA and it includes following steps –

- Animal study data & toxicity
- Manufacturing information
- Clinical protocol for the proposed human trials
- Data from any prior human research
- Information about the preclinical investigators Clinical trials Laboratory Source: Cell or animal studies test to see if the new treatment will be safe and can it work on people.
- PHASE 1: Safety of medication & treatment on people
- PHASE 2: Safety & effectiveness on people
- PHASE 3: Safety, effectiveness & dosing on people
- PHASE 4: Studies the long term effectiveness & compares new treatment to standard treatment on people. New drug application The new drug application express full story of drug & purpose to verify the drug is safe and effective for it's proposed use in the people studied.

D. Drug design

1. Identify structure activity relationship
2. Identify the pharmacophore
3. Improve target interaction (Pharmacodynamics)
4. Improve pharmacokinetic property.

Identify structure activity relationship

The physiological action of molecule and it's function and chemical constituents. This observation in the basis of SAR studies. SAR includes interpretation of Drug and structure features of Drug molecule. Identify the pharmacophore Pharmacophore is a group of vital properties of Drug. Pharmacophore is a geometrical description of the chemical functionalities necessary of ligand; it’s directly interacting with receptor. The goal of computer aided molecule design methods in modern medicinal chemistry. It's to reduce costs of associated with the discovery and development of new Drug.

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E. Improve target interaction

(pharmacodynamics) Pharmacodynamics is defined as the branch of pharmacology concerned with the effect of medicine in body. Pharmacodynamics is study of biochemical and physiological 18 effect of Drug and it's bind with receptor. Interact with cellular protein. Improve Pharmacokinetic properties Pharmacokinetic is a study of ADME process Absorption Distribution Metabolism Excretion All process cross the biological membranes.

Advantages

- Its ability to reduce the time and cost.
- The goal of drug design is the chemical entities with desirable pharmacological properties.
- Structure based drug design played a large role in the discovery.

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