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Role of chemistry in drug discovery and drug design

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Abstract
The drug discovery and development process use as target of new drug. This process transform some techniques such as screening, optimization, characterization, validation, synthesis. Target based drug design is more important, long-term, successful process. Which is use as high Throughput screening (HTS). Target is synthesized by combination of chemistry. All type of chemistry use in new drug discovery such as analytical chemistry, computational chemistry, organic chemistry, inorganic chemistry, medicinal chemistry, physical chemistry, biochemistry etc. Analytical chemistry in pharmaceutical drug development providing assurance of the quality, safety and efficacy of new drug. Analytical chemistry play and important in developing a new drug. HPLC is most important Analytical process in pharmaceutical industry, other techniques are also used. It's used as investigate polymorphism in new drug. All drugs are manufacturing under GMP i.e Good manufacturing practices. 50% Analytical chemistry used in drug discovery and development. Analytical method and instrumentation is used in the preclinical testing, toxicity testing and quality control. Commonly used as purification chemistry.

Keywords: discovery, drug design, toxicology, analgesics

Introduction

Chemistry is science of the composition, structure, properties & reaction of matter, especially of atomic & molecular systems. Chemistry plays an important role in understanding disease and their remedies, i.e. Drugs. The medicines or drugs that we taken for the treatment of the various ailments are chemical, either Organic or Inorganic. However, most drugs are organic molecules. Let's take aspirin as an example. It is drug which is most popular and widely used as analgesic drug because of its structure is simple and cost is also low. Chemical name of aspirin is acetyl salicylic acid, as an organic molecule. All the drugs are chemicals, and pharmacy is mainly about the study of various aspects of the drug, including manufacture, storage, action & toxicities, manufacture & managements, chemistry still plays vital role in pharmacy education. However, the use of chemistry is become at another level. The chemistry study for pharmacy student and other are completely different but though the basics of chemistry used in both studies as a basics as well as different fundamentals study. The halogen also appear in many life-savings drugs. The recently discovered antiviral compounds, such as fialuridine (which contain both F & I, as well as N & O) are essential for the fight against HIV and AIDS. The world's selling medicine in 1998 was omeprazole, an antiulcer drug from Astra. It prevents excess acid in stomach & allows the body to heal ulcers. It contains pyridine ring and Benz imidazole ring, two aromatic heterocycles. The drug in news in 1999 was Viagra Pfizer's cure for male impotence. In the first three months after its release in 1998, 2.9 million prescription were issued for Viagra. It contain a simple benzene ring & more complex heterocyclic system, which can divided into two aromatic heterocyclic rings. The chemistry play's important role for the understanding structure and reactivity of the drugs. Nowadays, Research and Development Department (R&D) of many laboratories are working for synthesis of new medicine/drugs. They improved their quality and values, decrease the production cost. Medicinal chemistry studies & pharmaceutical chemistry studies are disciplines at the intersection of branch of chemistry, especially synthetic organic chemistry and pharmacology and various other biological specialities where they are involved with design, chemical synthesis studies and development studies for pharmaceutical agents or bio-active molecules (drugs). Compounds used as medicine are most organic compounds such divided as atorvastatin, fluticasone, clopidoqrel etc. Inorganic & organo- metallic compounds are also useful as drugs lithium & platinum - based agents such as lithium carbonate, cisplatin as well as qaullium. This chemistry has contributed In so many life processes and to the efforts regarding to advance the quality of life as well as to the development of society from synthetic, medicinal, biopharmaceutical and industrial point of view [1, 2, 4, 5, 6, 8].

Drug Discovery

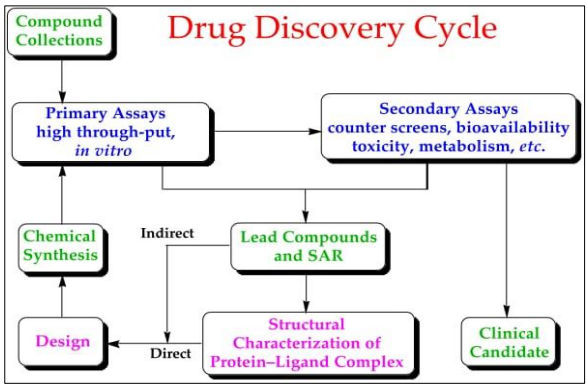

Fig 1

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

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 druggable 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.

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.

Lead Optimization

After an 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.

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.

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 interact 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.

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

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.

The Fractionation of medicines available in solid formulation [4, 6]

Fractionation of drug can be seen in clinical practice, Fractionation is mostly observed in solid dosage forms, because of intact tablets. Tablets are available of the pharmaceutical market. Factor affecting in solid drug fractionation in that patients related factor is involved in age, body weight, sex, pathological conditions, evaluation of genetics, easily to swallowing etc. It availability of a big therapeutic arsenal fractionation aspects of the tablets standard of quality, dimension, shape, hardness, presence of score, uniformity of active ingredient stability, packing material etc. This technique available for drug fractionation. Fractionation is important health and disease of people.

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Conclusion

Regarding to this Review article I am happy to conclude that this review paper is going to be one of most important topic in future related to drug discovery and development of new drug.For new scientists and researchers this paper will be very useful for further research studies.

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