



Development Of New Synthetic Route For Small Target Molecules & Retro- Synthesis.

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Abstract :

The main goal of the study is to get knowledge about How the process of drug design and development of new drug are carried out?. To get Information about Computer Aided Drug Design & Molecular Docking Software's. Also to study of retrosynthesis with its example.

Introduction :

New methods of synthesizing new compounds and new molecules are rapidly evolving and more new technologies are developing in the field of drug discovery.

A suitable route is the key to ensuring the rapid development drug discovery project. A viable synthetic route is also required to meet all requirements, such as cost reduction.

Chemical and pharmaceutical companies carry out research into the development of new chemical compounds, work on its efficiency, safety, potency etc.

Target Identification:

Target:

Target is a molecule on which the new developed drug acts & produce its effect. They may be :-

- Receptor
- Enzymes
- Nucleic acid
- Hormones
- Ion Channel

Characteristics of Drug Target:

- The drug target is a biomolecule, normally a protein that could exist in isolated.
- The biomolecules have binding sites on which drug molecules binds. These molecules could be endogenous (produced naturally by body) or extraneous substances such as chemical molecules (drugs).
- The binding of molecules are reversible (it means after the effects of drug molecules, it must detached from target).
- The response changes in biomolecule structure play a major role in complex regulation and have a therapeutic effect on pathological conditions.

Criteria for selection of the synthetic route:

- A role of pharmaceutical chemist and a material chemist are more important to developing fast synthetic routes for a chosen molecule.
- The main aim of the pharmaceutical industry is to synthesis of a large number of molecules within a short time.
- It carries different Studies & focus on developing new drug molecules with special properties.
- The company tries the development of economical synthetic procedures, which includes not only the cost of the chemicals but also the cost of waste treatment, recycling and environmental cleaning.
- The pharmaceutical industry also focus about eco-friendly reactions and procedures.
- In an pharmaceutical company R&D laboratory looks at very large-scale reactions, their reproducibility, safety and cost parameters.

Computer added drug design:

- It is a part of modern drug discovery.
- It includes developing & analysing medicines by use of different computer methods.
- Their are many challenges for a pharmaceutical company is to develop drugs with better efficacy & no side effects.
- Traditional approach of drug discovery were very complex, time taking & costly but the CADD software are very useful, precise & efficient.
- The main goal in drug design is to find whether a drug molecule will bind to a target and if so how strongly.
- Molecular mechanics is most often used to check the strength of the intermolecular interaction between the molecule and its biological target Drug design with the help of computers used in drug discovery:

Molecular Docking:

- Molecular Docking is a tool in structural molecular biology.
- It is used to find best matching between two molecules.
- The main aim of molecular docking is to give a prediction of the ligand-receptor complex structure using computer methods.
- By using molecular docking we can Calculate the differential binding of a ligand to two different macromolecular receptors.

Retrosynthesis :

It is a important for discovering different synthetic routes.

Retrosynthesis means planning a synthesis backwards. i.e conversion of final product into starting materials.

Retrosynthesis is the process of deconstructing a target molecule into starting materials by means of imaginary breaking of bonds i. e disconnections and by the conversion of one functional group into another i.e. functional group interconversions.

The evaluation of synthesis depends on the aim of the synthesis

1. Shortest synthesis,
2. Cheapest synthesis
3. A new synthesis
4. Environmental benign synthesis
5. Synthesis without toxic risk
6. Reliable synthesis.

Properties Of ideal chemical compound :

The ideal chemical compound is

- Safe and non-toxic
- Cheap
- Shows high performance during its life cycle
- Then completely degrades to minerals
- Can be recycled to safe energy and material resources
 - Non reactive
 - Not react with container.

Disconnection :

The disconnection is a process in that the bond get breaks & convert molecule into starting material.

Synthon :

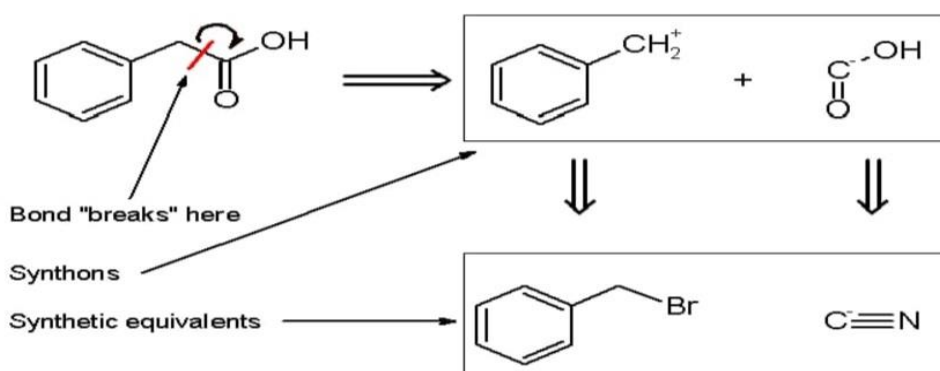
It is a structural unit in molecule which related to possible synthetic operation. The fragments are obtained from disconnection.

Retron:

It is a simplest chemical compound that allows transformation.

Example:

- An example will allow the concept of retrosynthetic analysis to be easily understood.



Conclusion:

The development of new drug molecules are challenging to the pharmaceutical companies. There are many challenges for pharmaceutical company to develop a new drug molecules with better efficacy, potency with minimum side effects. The traditional approach for developing new drug are requires a lot of time & cost, Instead of traditional approach the use of computer software are very useful methods for developing new drug molecules. Also the computer methods are more accurate, precise & carried out in short period.

References :

1. R.Balaji Rao, A Book of Logic Of Organic Synthesis, Bananas Hindu University, Published On 2022, Page No : 3.1
2. Tetsuhiko Takabatake, Senior Research Associate, A paper Of Synthetic route design system Sumitomo Chemical Co. Ltd. Organic Synthesis Research Laboratory, Vol-II, 2009,Page No : 1
3. Janet Thornton, David Vallenet, A book of Computer Aided Design Tools, Published On Dec 2017, Page No : 6
4. Rani T. Bhagat, Santosh R. Butle, Deepak S.Khobragade Sagar B. Wankhede ,A Journal of Pharmaceutical Research International, Molecular Docking in Drug Discovery, Published in 2021, Page No: 46.
5. Dr. Sumanta Mondal, A publication of Synthon approach and retrosynthesis applications, Published in 2021, Page No : 01

