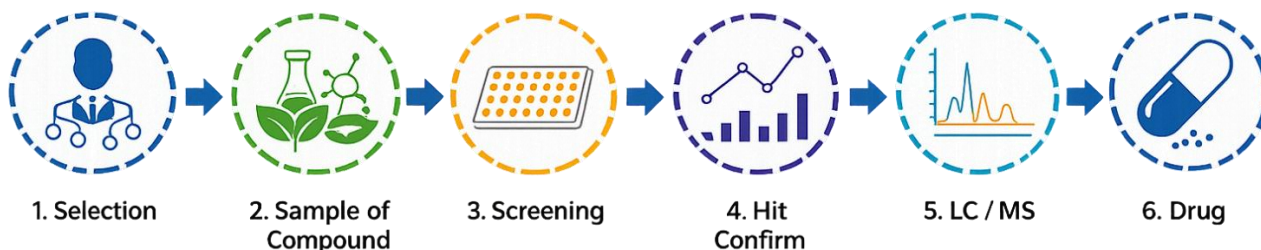


Rational Drug Design

Traditional vs Rational Drug Design

Traditional Drug Design

- **Traditional drug design** is based on trial-and-error methods where compounds are tested without complete knowledge of the biological target.



Characteristics of Traditional Drug Design

1. Empirical Approach

- Drugs are discovered by testing many compounds without detailed knowledge of the target

2. Random Screening

- Large numbers of natural or synthetic compounds are tested

3. Observation-Based Discovery

- Drug effects are observed and then studied further

4. Time-Consuming Process

- It requires long time due to repeated testing

Methods Used in Traditional Drug Design

1. Natural Product Screening

- Compounds are obtained from plants, animals, or microorganisms

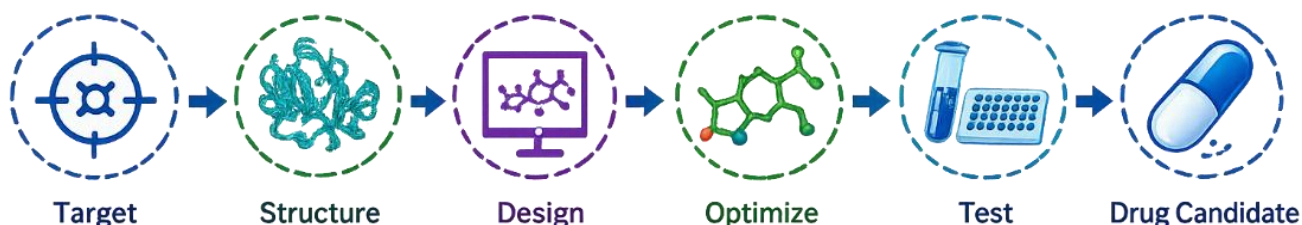
2. Chemical Modification

- Existing compounds are modified to improve activity

3. Serendipity (Accidental Discovery)

- Drugs are discovered by chance observations

Rational Drug Design



- **Rational drug design** is a scientific approach where drugs are designed based on knowledge of the biological target and its structure.

Characteristics of Rational Drug Design

1. Target-Based Approach

- Drug design is based on a specific biological target

2. Structure-Based Design

- Uses 3D structure of the target protein

3. Knowledge-Driven Process

- Uses information about disease mechanisms

4. Efficient and Focused

- Reduces unnecessary testing

Differences Between Traditional and Rational Drug Design

Basis of Difference	Traditional Drug Design	Rational Drug Design
Approach	Uses trial-and-error methods	Uses scientific knowledge and planned strategies
Target Information	Does not require detailed knowledge of the biological target	Requires detailed information about the drug target
Time and Cost	Takes more time and is usually more costly	More efficient, saving time and cost
Accuracy	Less precise	More precise and targeted

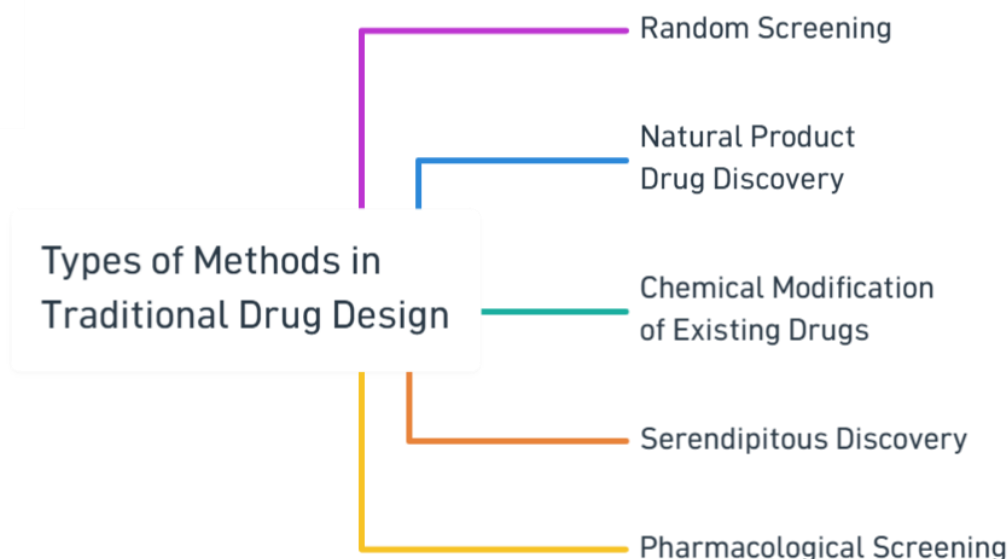
Methods Followed in Traditional Drug Design

- Traditional drug design uses various methods to discover and develop drugs mainly based on experimental testing and observation.

Why These Methods are Used

- To identify compounds with biological activity
- To improve existing drugs
- To discover new therapeutic agents

Types of Methods in Traditional Drug Design



1. Random Screening

- Large numbers of compounds are tested against biological systems

Subtypes of Random Screening

a) In vitro Screening

- Testing is done in laboratory conditions using cells or enzymes

b) In vivo Screening

- Testing is done in living organisms such as animals

2. Natural Product Drug Discovery

- Drugs are obtained from natural sources

Subtypes of Natural Sources

a) Plant Sources

- Medicinal plants are used to extract compounds

b) Microbial Sources

- Bacteria and fungi produce useful compounds

c) Marine Sources

- Compounds are obtained from marine organisms

3. Chemical Modification of Existing Drugs

- Existing drugs are modified to improve their properties

types of Chemical Modification

a) Addition of Functional Groups

- New chemical groups are added

b) Removal of Functional Groups

- Unnecessary parts are removed

c) Substitution Reactions

- One group is replaced with another

4. Serendipitous Discovery

- Drugs are discovered by chance during experiments

Examples of Observations

a) Unexpected Effects

- A compound shows a different useful effect

b) Side Effect Utilization

- Side effects of drugs are used for new purposes

5. Pharmacological Screening

- Compounds are tested for biological activity

types of Pharmacological Screening

a) Primary Screening

- Initial testing for activity

b) Secondary Screening

- Detailed testing of active compounds

High Throughput Screening (HTS)

- High throughput screening is a modern technique used in drug discovery to quickly test a very large number of chemical compounds against a biological target to identify active compounds called hits.

Why High Throughput Screening is Important

- It helps to test thousands to millions of compounds in a short time
- It increases the efficiency of drug discovery
- It helps to identify active compounds quickly

Key Features of High Throughput Screening

1. Automation

- Machines and robots are used to perform experiments

2. Miniaturization

- Very small quantities of chemicals are used

3. Parallel Processing

- Many experiments are performed at the same time

4. Data Handling Systems

- Computer systems are used to store and analyze large data

Types of High Throughput Screening

1. Biochemical Assays

- These assays test interaction with isolated proteins or enzymes

2. Cell-Based Assays

- These assays test the effect of compounds on living cells

3. Binding Assays

- These assays measure how strongly a compound binds to a target

4. Functional Assays

- These assays measure the biological response produced by a compound

Steps in High Throughput Screening

1. Preparation of Compound Library

- A large collection of chemical compounds is prepared

2. Assay Development

- A suitable test system is designed

3. Screening Process

- Compounds are tested using automated systems

4. Data Collection

- Results are recorded and stored

5. Hit Identification

- Active compounds are identified for further study

Applications of High Throughput Screening

1. Lead Identification

- Helps to find initial lead compounds

2. Target Validation

- Confirms if a target is suitable for drug development

3. Toxicity Testing

- Helps to identify harmful effects early



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