SNS COLLEGE OF PHARMACY AND HEALTH SCIENCES

Affiliated To The Tamil Nadu Dr. MGR Medical University, Chennai

Approved by Pharmacy Council of India, New Delhi.

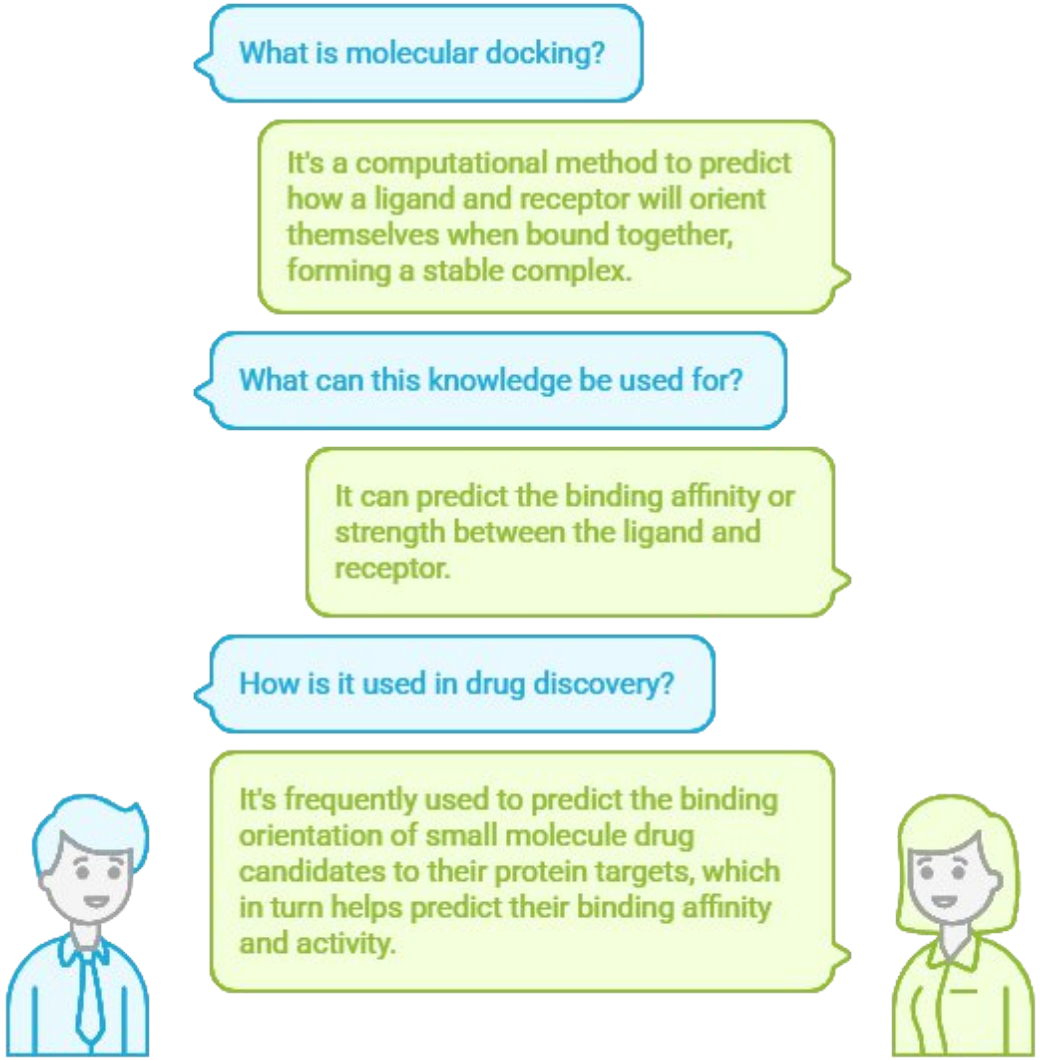
Coimbatore -641035

COURSE NAME : COMPUTER AIDED DRUG DESIGN(BP 807 ET)

VIII SEM / IV YEAR

TOPIC : DOCKING BASED SCREENING & DE NOVO DRUG DESIGN

WHAT IS MOLECULAR DOCKING ..?

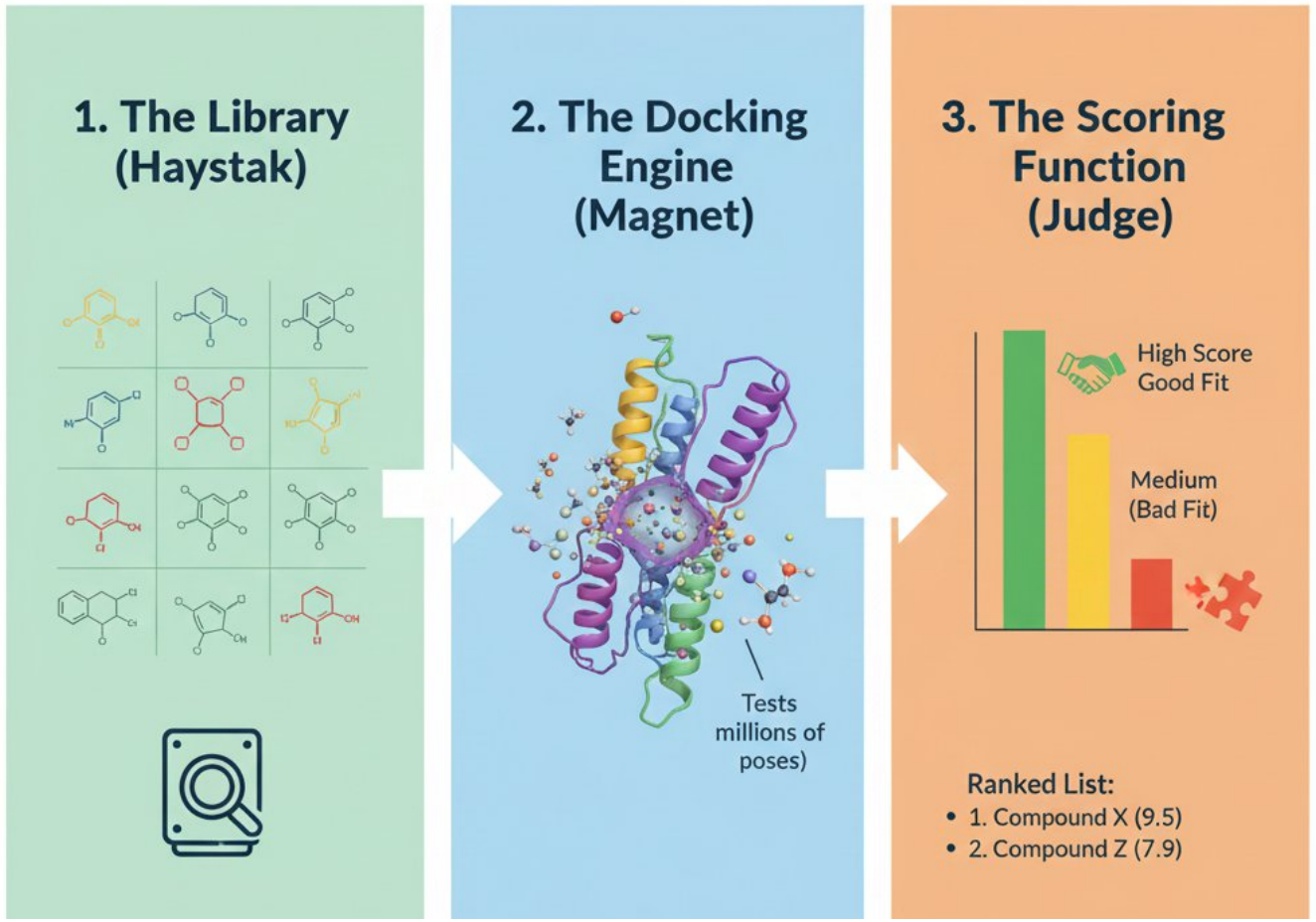


THE CORE VOCABULARY
(THE LANGUAGE OF DOCKING)

Term	Simple Definition	The Analagy
Receptor	The target protein structure that acts as "host" for travels to molecule.	The Lock Key
Ligand	The specific "pocket" or hollow area where the chemical reaction happens.	The Keyhole
Binding Site	A specific 3D orientation or "posture" of ligantiod happens.	A specific "turn" of of the key
Pose	A mathemtical value (Energy) tells us how stable inside bon site.	The "Click" sound
Affinity	A mathemtical value (Energy) that atraction the attraction becepor the receptor and the ligand.	How hard of is pull pull the key out

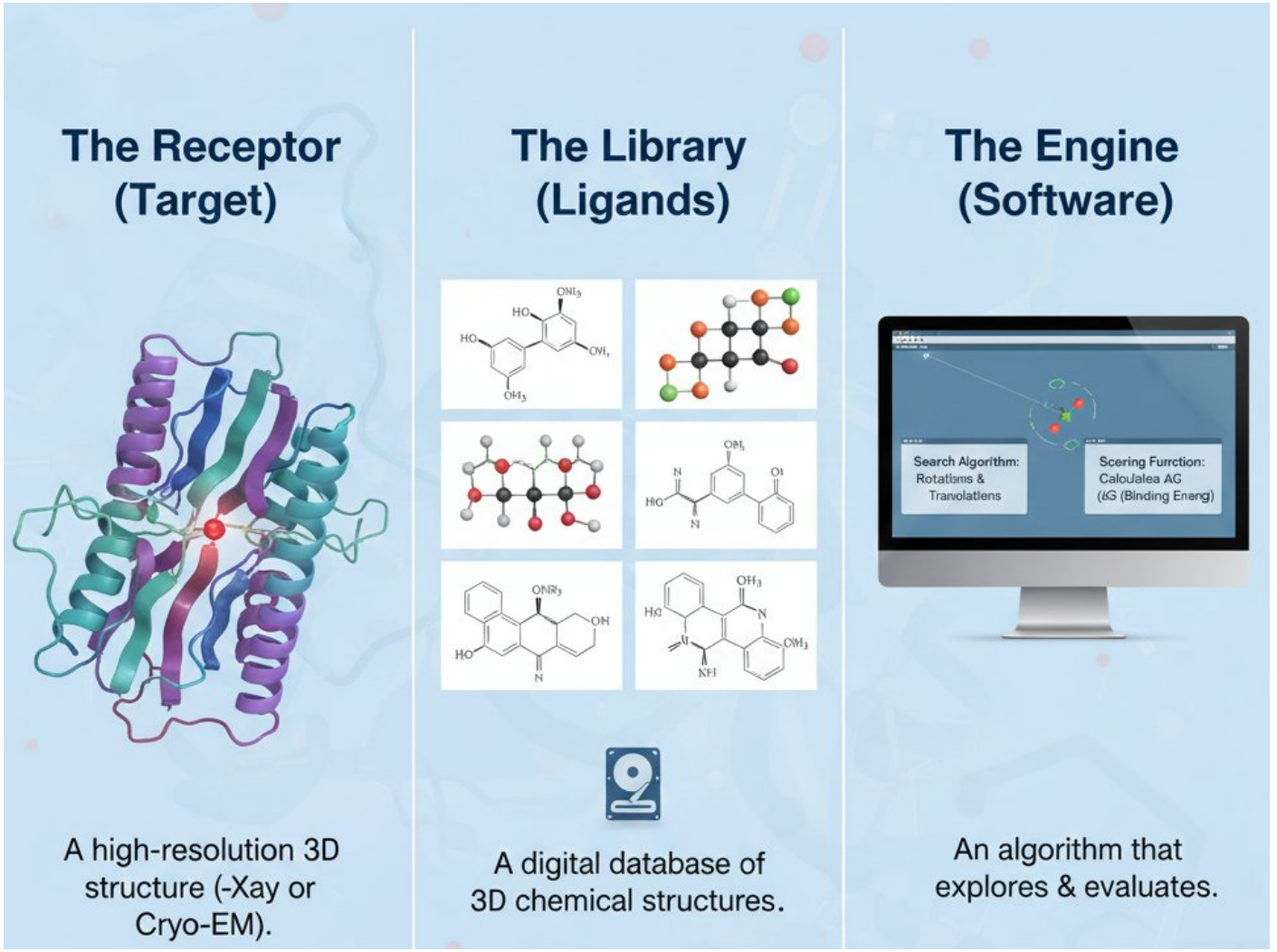
WHAT IS DOCKING BASED SCREENING..?

Docking-Based Screening: The Digital Filter

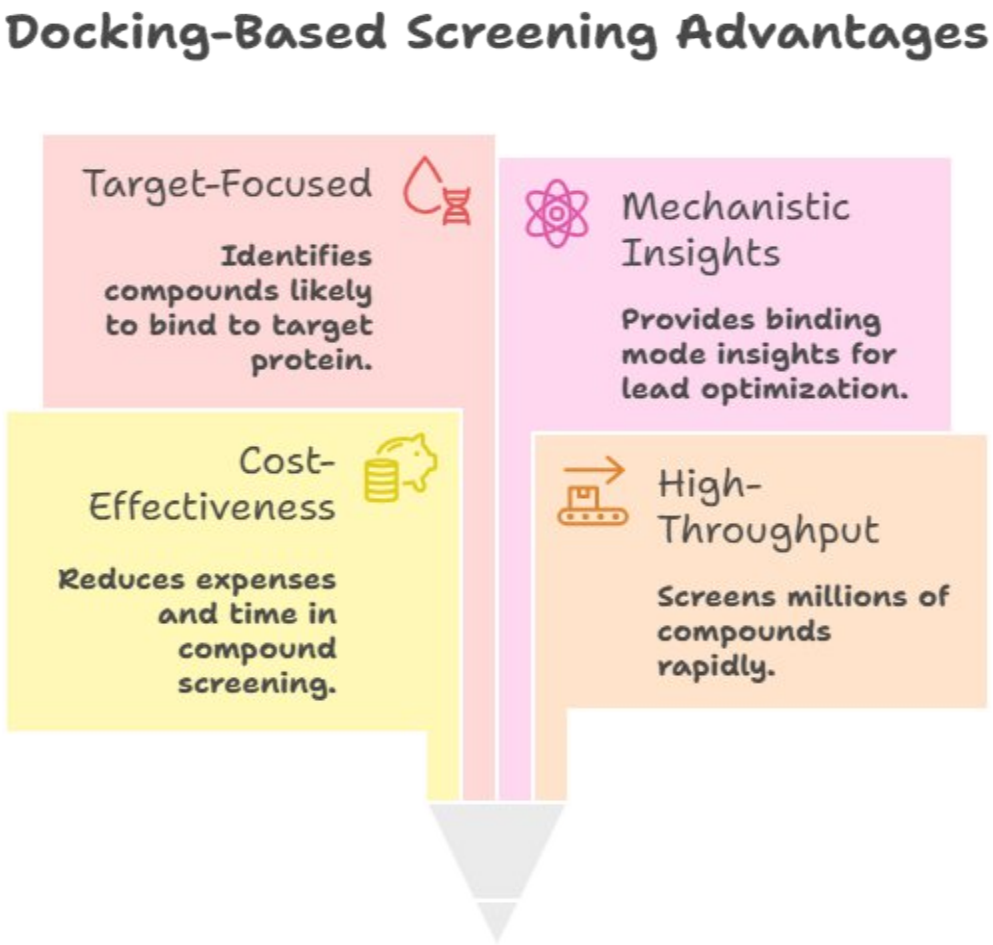


THE WORKFLOW OF DOCKINGBASED SCREENING

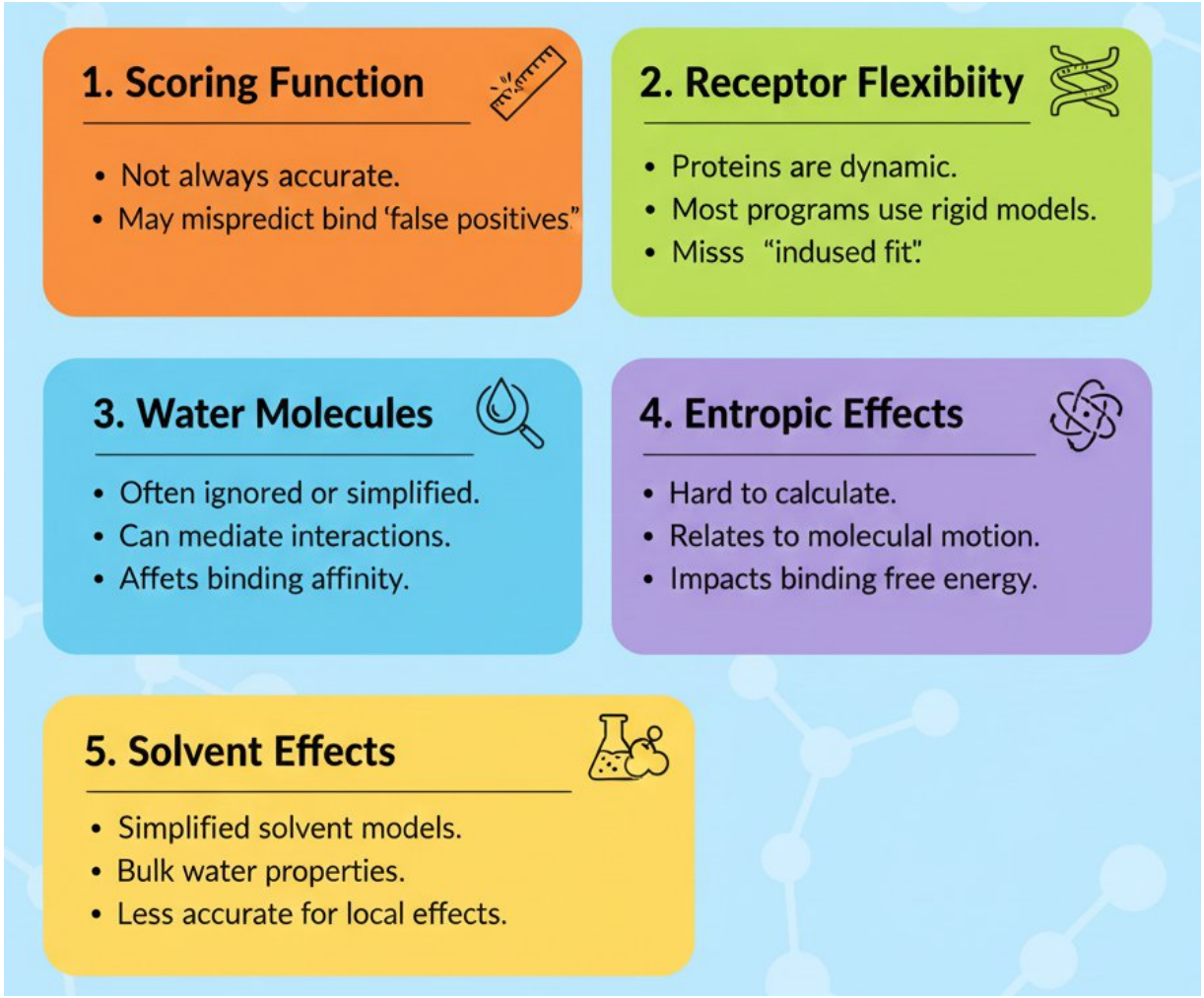
THE COMPONENTS OF DOCKING BASED SCREENING SYSTEM



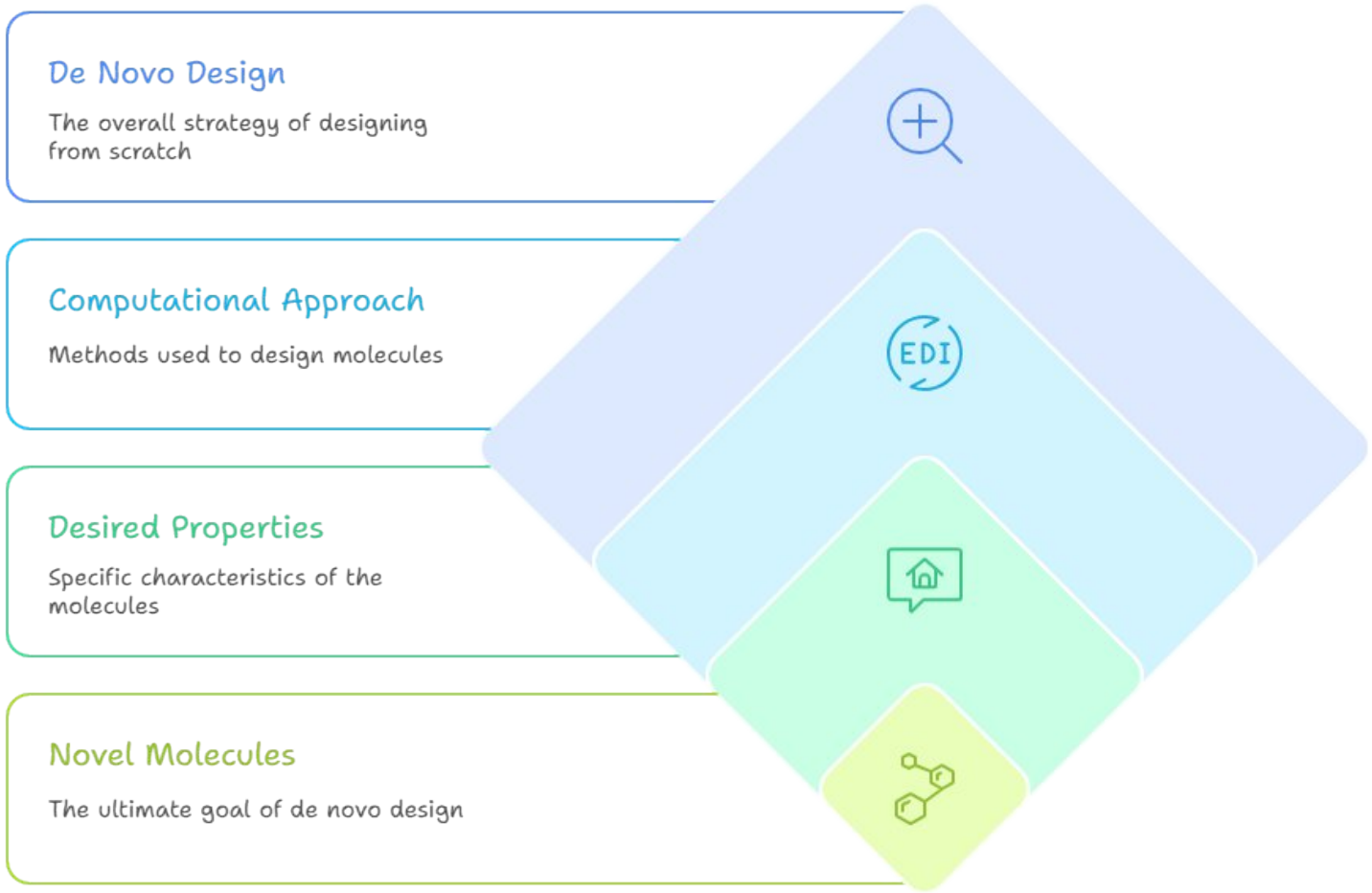
ADVANTAGES OF DOCKING BASED SCREENING



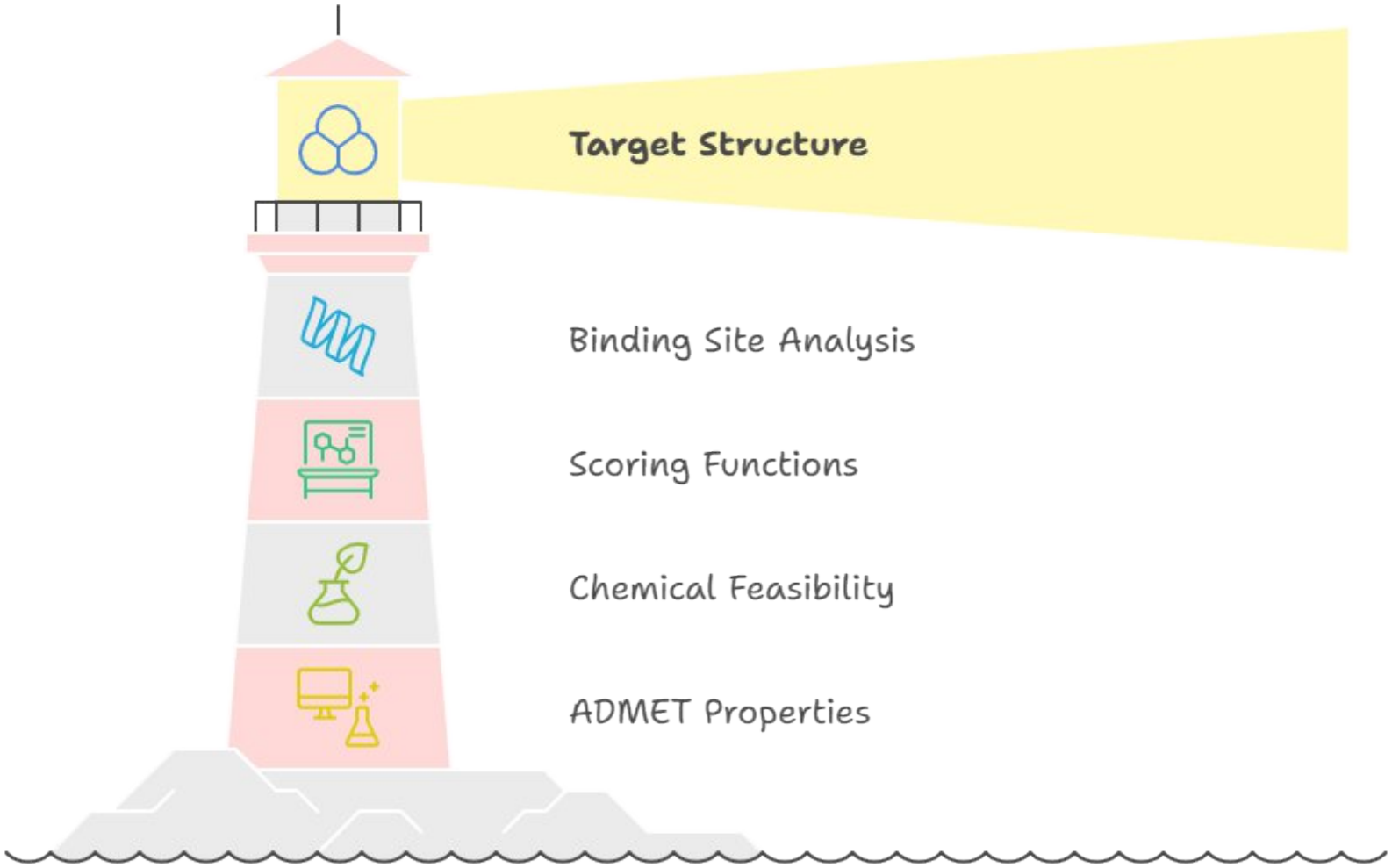
DISADAVANTAGES OF DOCKING BASED SCREENING



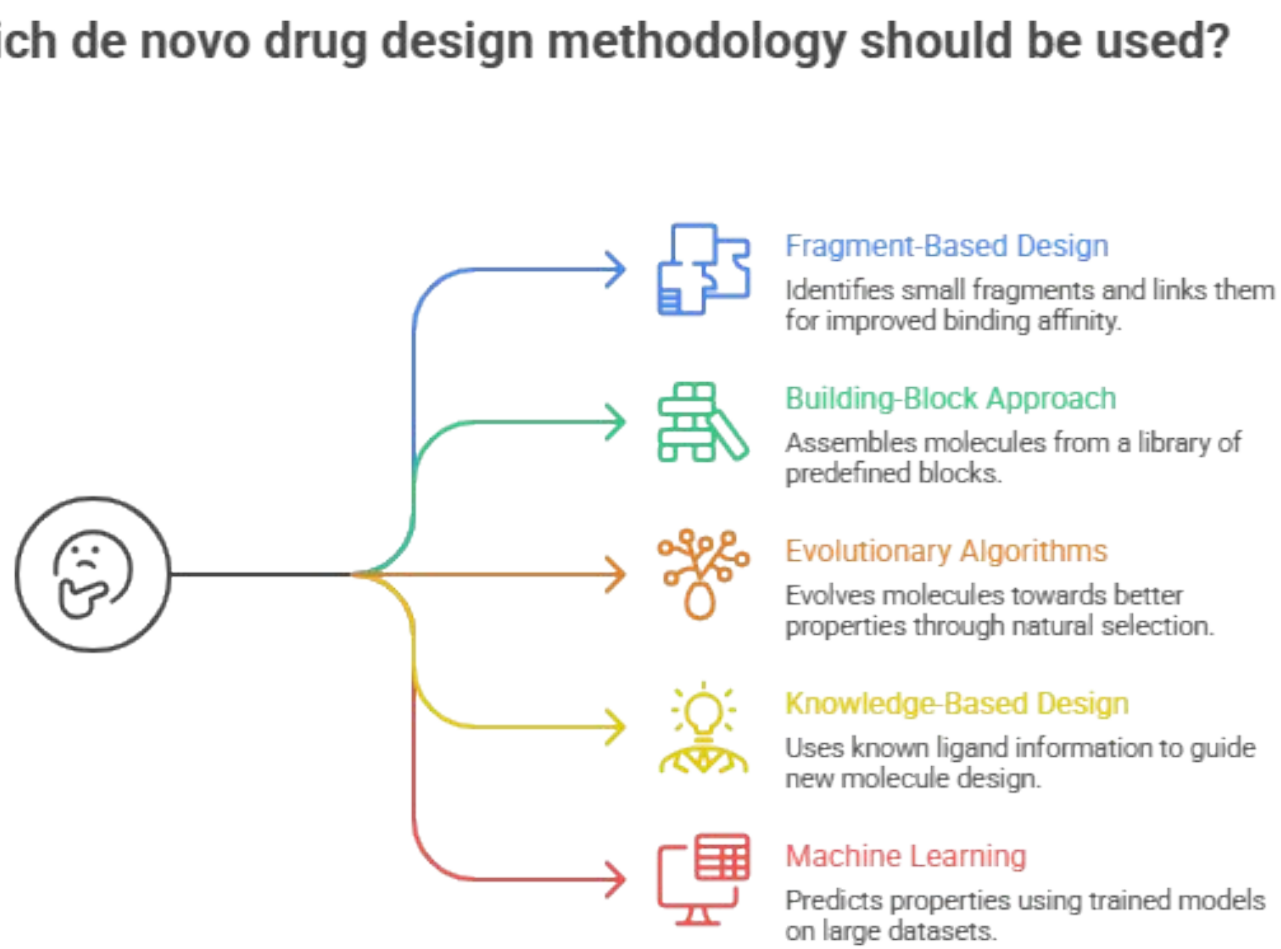
DE NOVO DRUG DESIGN PROCESS



PRINCIPLES OF DE NOVO DRUG DESIGN APPROACHES

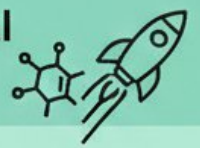


METHODOLOGIES IN DE NOVO DRUG DESIGN



ADVANTAGES OF DE NOVO DRUG DESIGN

1. Novel Chemical Space



- Explore beyond existing molecules.
- Create unique structures.
- Avoid "me-too drugs.

2. Tailored to Target

- Designed for specific pocket.
- Optimize interactions.
- Maximize potency.

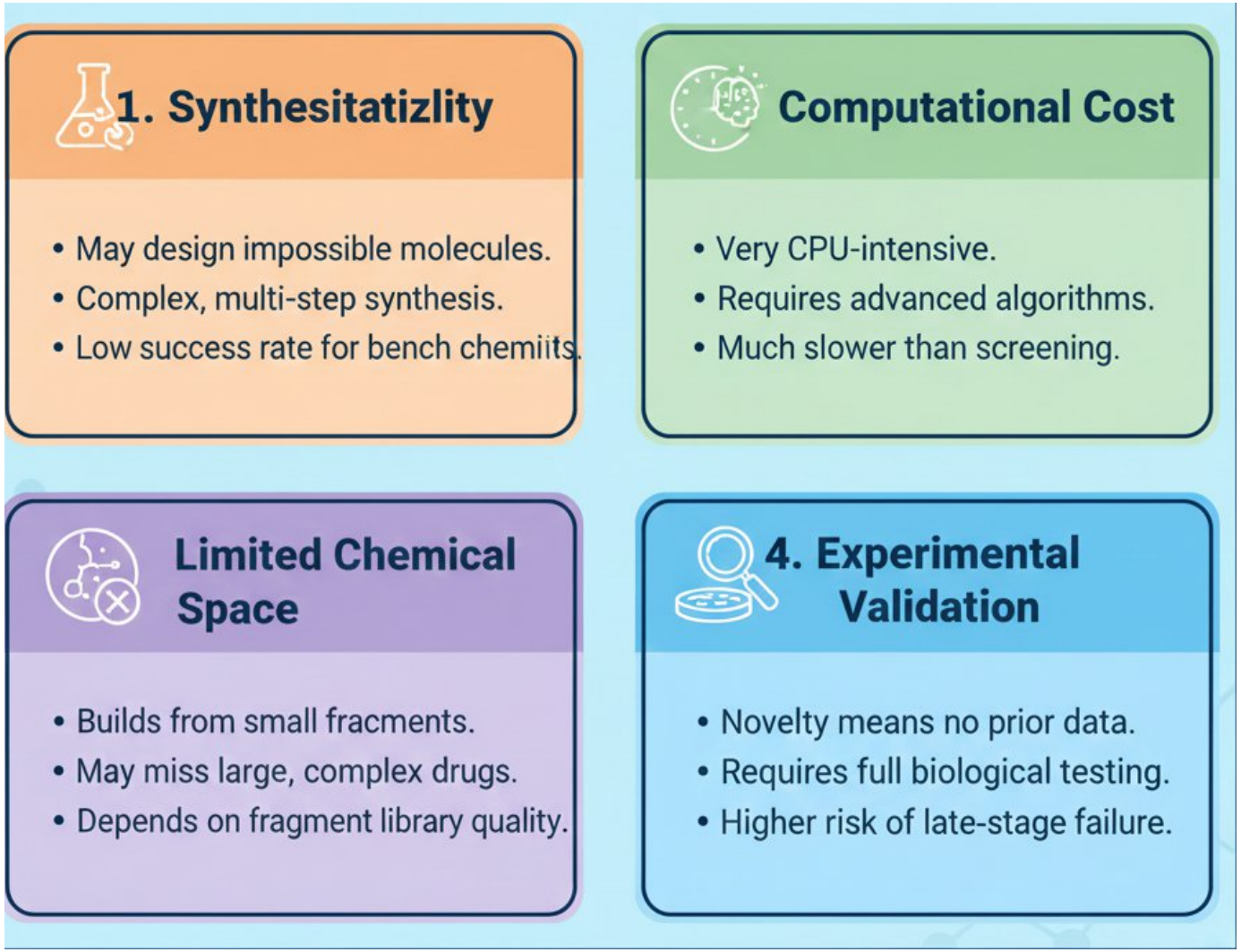
3. Intelectual Property

- Generates patentable molecules.
- Stronger market position.
- Avoidance of prior art.

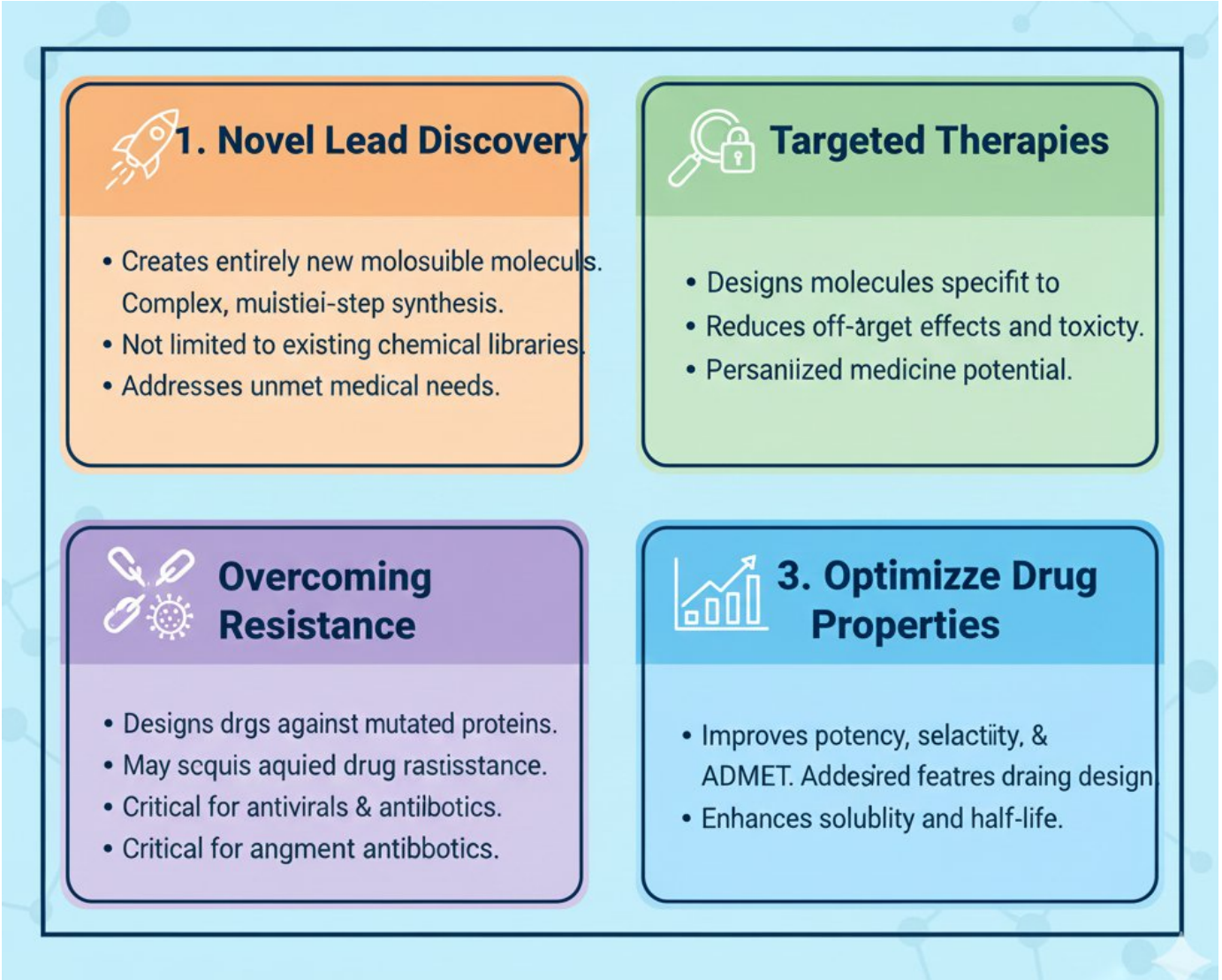
4. Overcome Resistance

- New mechanisms of action.
- Effective against mutated targets.
- Addresses drug resistance.

DISADVANTAGES OF DE NOVO DRUGDESIGN

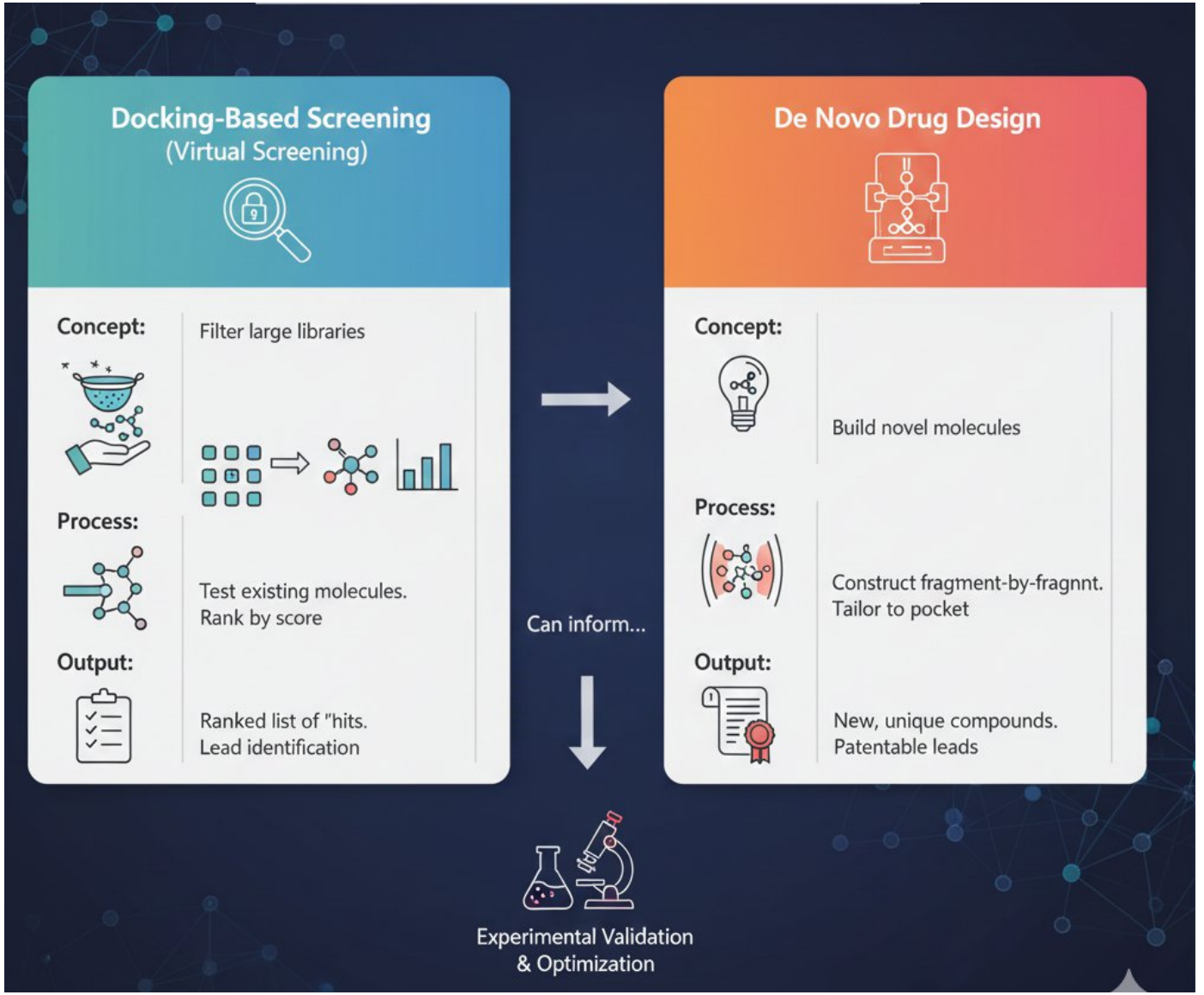


KEY APPLICATIONS OF DE NOVO DRUG DESIGN



RECENT ADVANCEMENTS IN DE NOVO DRUG DESIGN

SUMMARY


Docking-Based Screening
(Virtual Screening)
Concept:
Filter large libraries
Process:
Test existing molecules.
Rank by score
Output:
Ranked list of "hits.
Lead identification
Can inform...
De Novo Drug Design
Concept:
Build novel molecules
Process:
Construct fragment-by-fragnnt.
Tailor to pocket
Output:
New, unique compounds.
Patentable leads
Experimental Validation
& Optimization

ASSESMENTS

Question 1 : In Virtual Screening, what is the primary purpose of the "Scoring Function"?

A) To synthesize the drug molecule in the lab.

B) To rank molecules based on their predicted binding affinity.

C) To determine the 3D structure of the protein.

D) To name the chemical compound.

Question 2: Which of the following best describes "De Novo" drug design?

A) Searching the ZINC database for existing drugs.

B) Testing drugs on animal models.

C) Building a new molecule fragment-by-fragment inside a target site.

D) Using X-ray crystallography to see a protein.

REFERENCES

1. Molecular Docking for Computer-Aided Drug Design by Mohane Selvaraj Coumar, 1st Edition, pg. no: 120 – 145 (chapter 6).

2. Molecular Modeling: Principles and Applications by Andrew R. Leach, 2nd edition , pg.no :618–625.

3. Computer-Aided Drug Design by Aman Thakur, Vineet Mehta, Priyanka Nagu , 1st edition pg.no: 92/105.


Thank You!