Questions on 4th Unit

1. Explain the process of Drug discovery in detail.
2. Explain the Early drug Discovery step of Drug discovery.
3. State the difference between ligand based drug discovery and Structure Based Drug discovery.
4. Explain Pharmacophore model mapping in detail.
5. What is meant by Computer Aided Drug Design.

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Question

① Drug discovery in detail?

→ Drug discovery is a long and complex process that they can take anywhere from 10 to 15 years and cost billion of dollars. It involves a series of steps, each with its own challanges and risk.

① Early Drug discovery:

- Target Identification → find disease-causing molecules that could be drug targets
- Hit Identification → Test millions of compounds to see if they bind to the target
- lead optimization → Improve promising compounds to become "leads"

② pre-clinical phase:

In the pre-clinical phase, the substances identified during early drug discovery are refined, optimized, and extensively tested in a laboratory and in animal or alternative models.

③ clinical phases:

clinical trials are composed of four phases.

Is drug safe

what does can be given without side effect

How does the substrance behave in the body

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④ Regulatory approval:

When all the trials are done the data is collected and analyzed. Then it can be submitted to the appropriate authorities for review. Before a drug or vaccine can be sold. approval from a national regulatory authority or centrained process is required.

Question

② Early drug discovery steps.

→ The early drug discovery stage lays to the foundation for developing new treatments.

- a) Target Identification - identify disease-causing molecules (proteins, genes)
- b) High Throughout screening - testing millions of compounds to find target molecule.
- c) Hit identification and discovery - find and validate a hit molecule.
- d) Assay development and screening - create test systems
- e) lead generation and optimization - improve the most promising compound product.
- f) In vivo and vitro assays - Test The safety and potential toxic effect of a compound

Question

③ Difference between ligand based drug discovery and structured based drug discovery

LBDD	SBDD
a) Existing knowledge of known ligand	a) Focus on 3D structure of target molecule.
b) doesnot require 3D structure	b) required (high resolution) 3D structure.
c) more suitable for target difficult to study direcny	c) limited by the availability of 3D str.
d) generally fast and cheaper	d) more expensive and time consuming
e) data-driven, empirical ~~knowledge~~ approach	e) hypothesis-driven, rational approach
f) Template base design method is used	f) Docking and virtual screening method is used.
g) used to identify initial leads in early stages of drug discovery.	g) used to identify promising leads in letter stages of drug discovery.

Question

④ Pharmacophore model mapping

→

Pharmacore model mapping is a crucial step in drug discovery and development. it involves identifying and aligning the key features of a molecule (known as a pharmaphore) with the corresponding features of a target protein or receptor. This allows researchers to understand how the molecule interact with the target and design new drug with improved potency and selectivity.

- pharmacophore mapping step involves mapping the feature of a potential drug molecule with the corresponding feature of re pre defined pharamacophore model.

- After mapping re molecule is evaluated based on its fit within re pharmacophore model. if re fit is not optimal re molecule can be further optimized to improve its alignment within re pharmacophore model.

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⑤ computer-aided drug design.

→ CADD is an interdisciplinary field that ~~combines~~ uses computational tools and technique to facilitate the discovery and development of new drugs. it's a powerful tool that has revolutionized drug discovery by:

① speeding up the process
② reducing costs
③ Improving accuracy and efficiency

CADD is used to

- to identify and validate new drug targets.
- predict the properties and toxicity of potential drugs.
- understand the mechanism of action of drugs