

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.

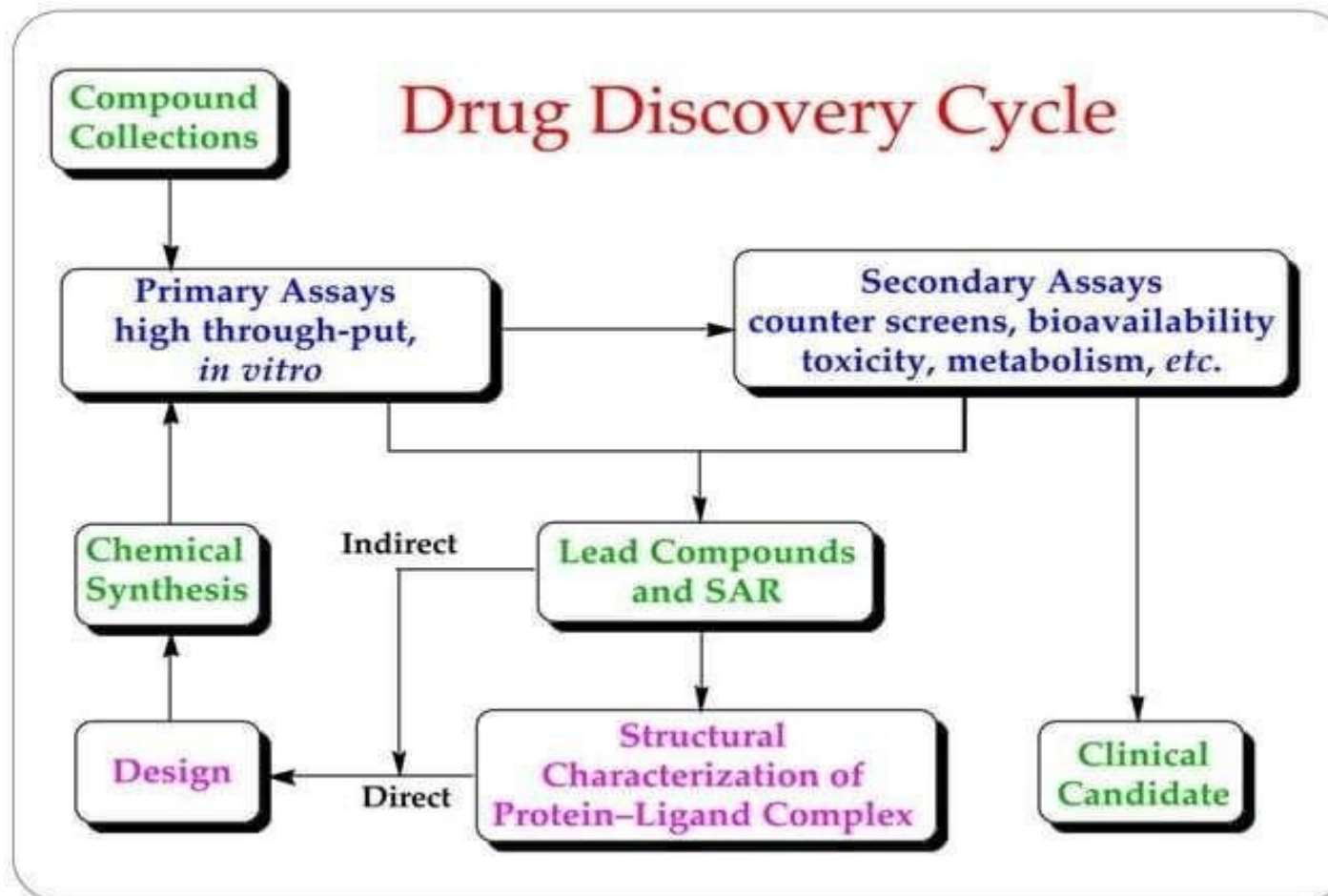
Coimbatore -641035

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

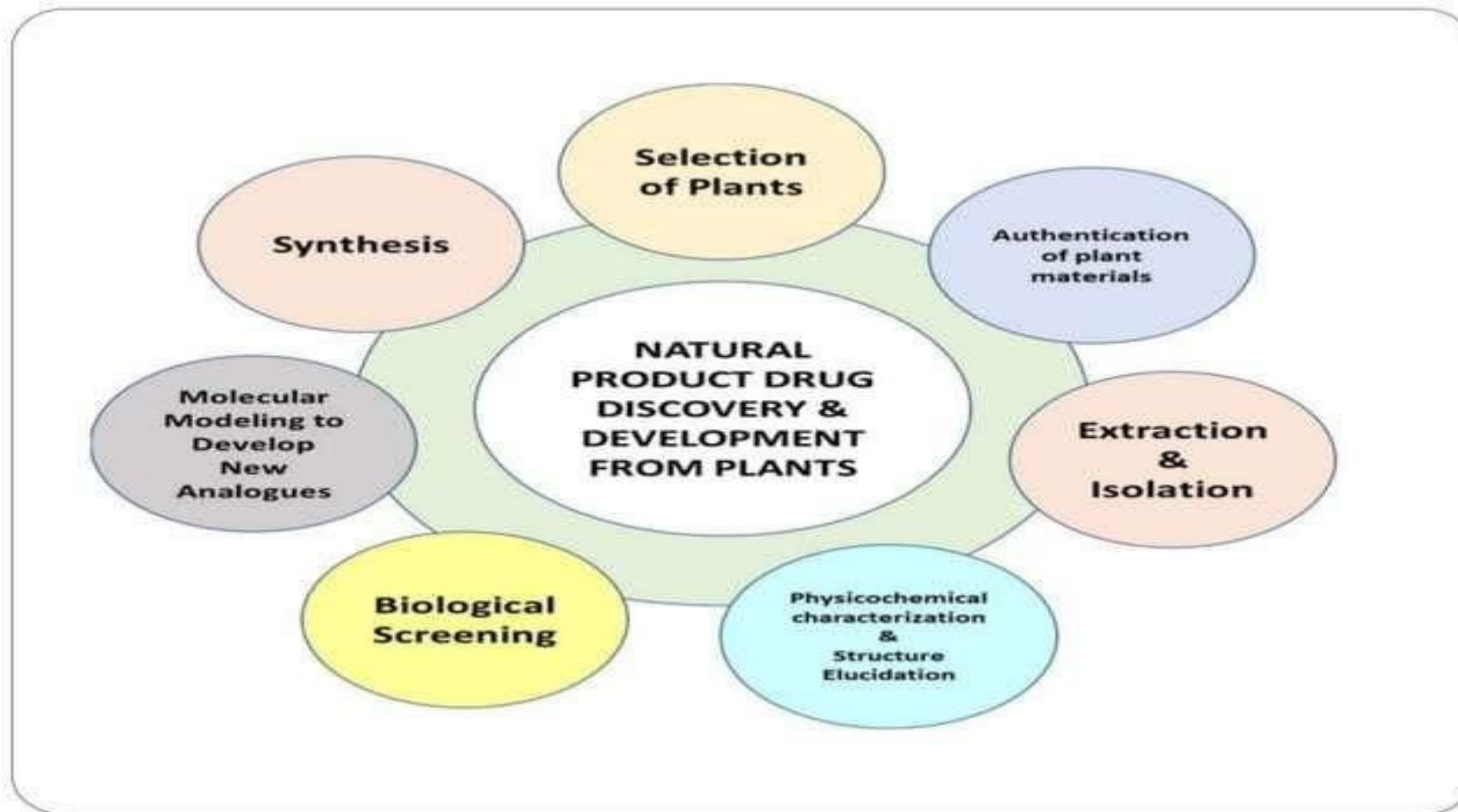
VIII SEM / IV YEAR

TOPIC 5: ANALOG BASED DRUG DESIGN

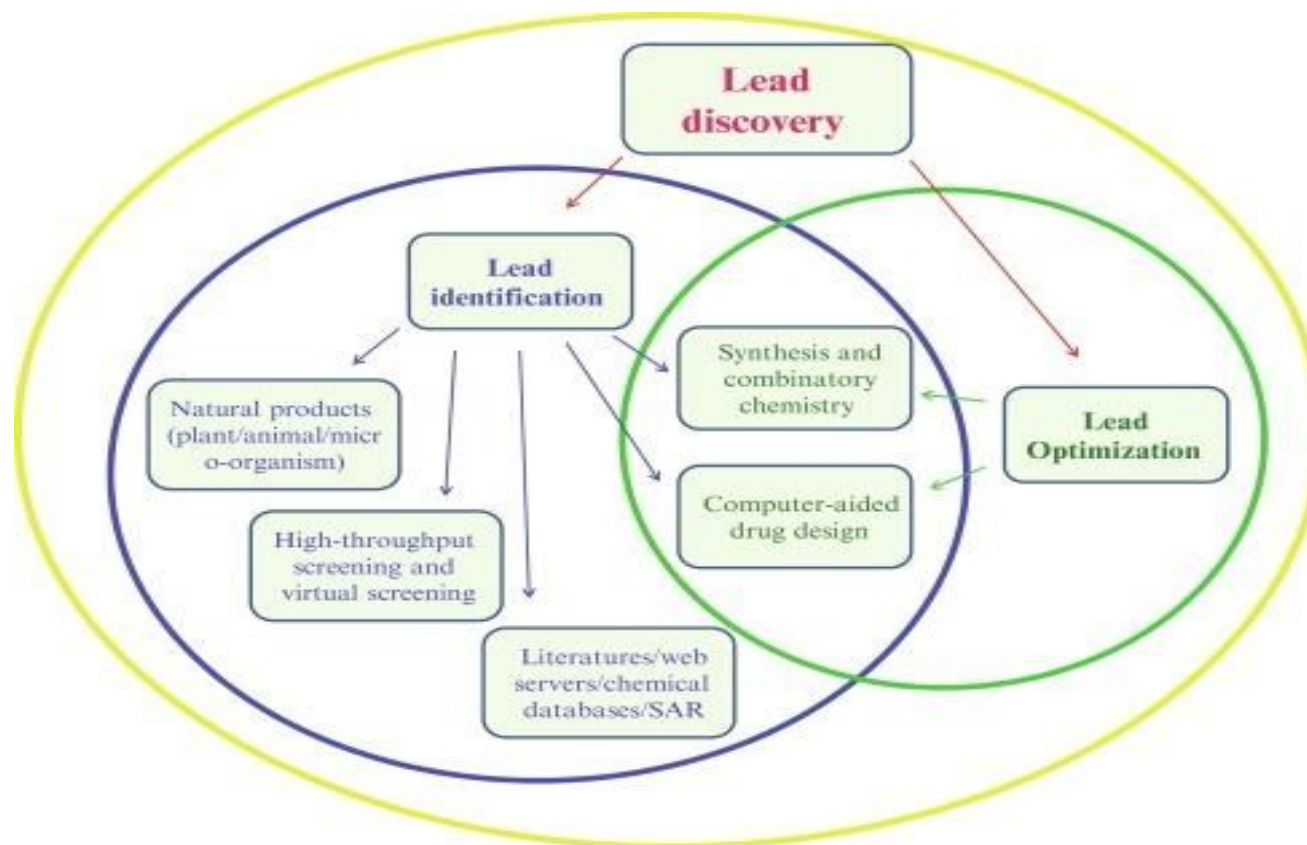
DRUG DISCOVERY CYCLE



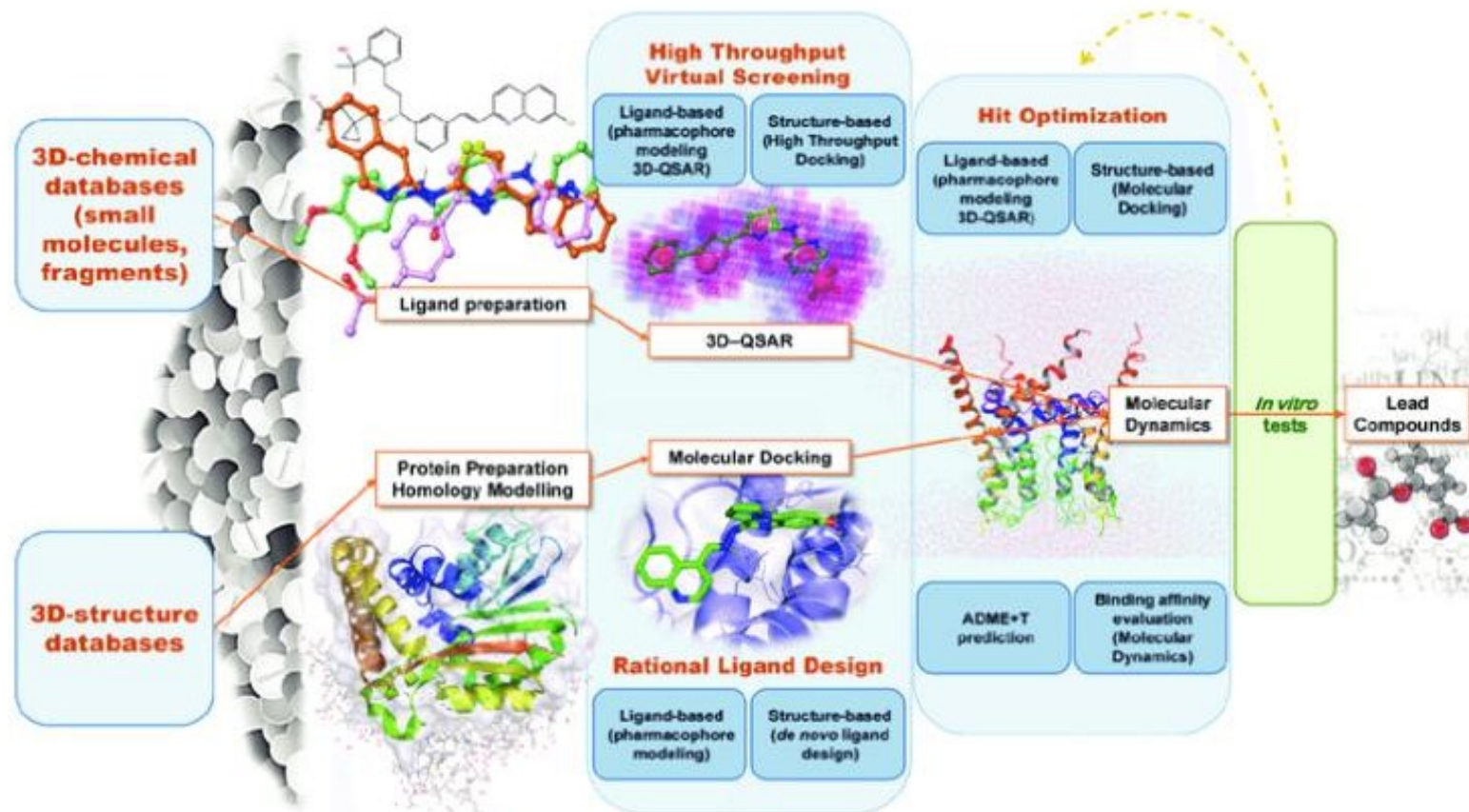
NATURAL PRODUCT DRUG DISCOVERY & DEVELOPMENT FROM PLANTS



STAGES OF LEAD DISCOVERY



ANALOG BASED SCREENING MODELS



Drug Development Lead Optimization Steps With Icons



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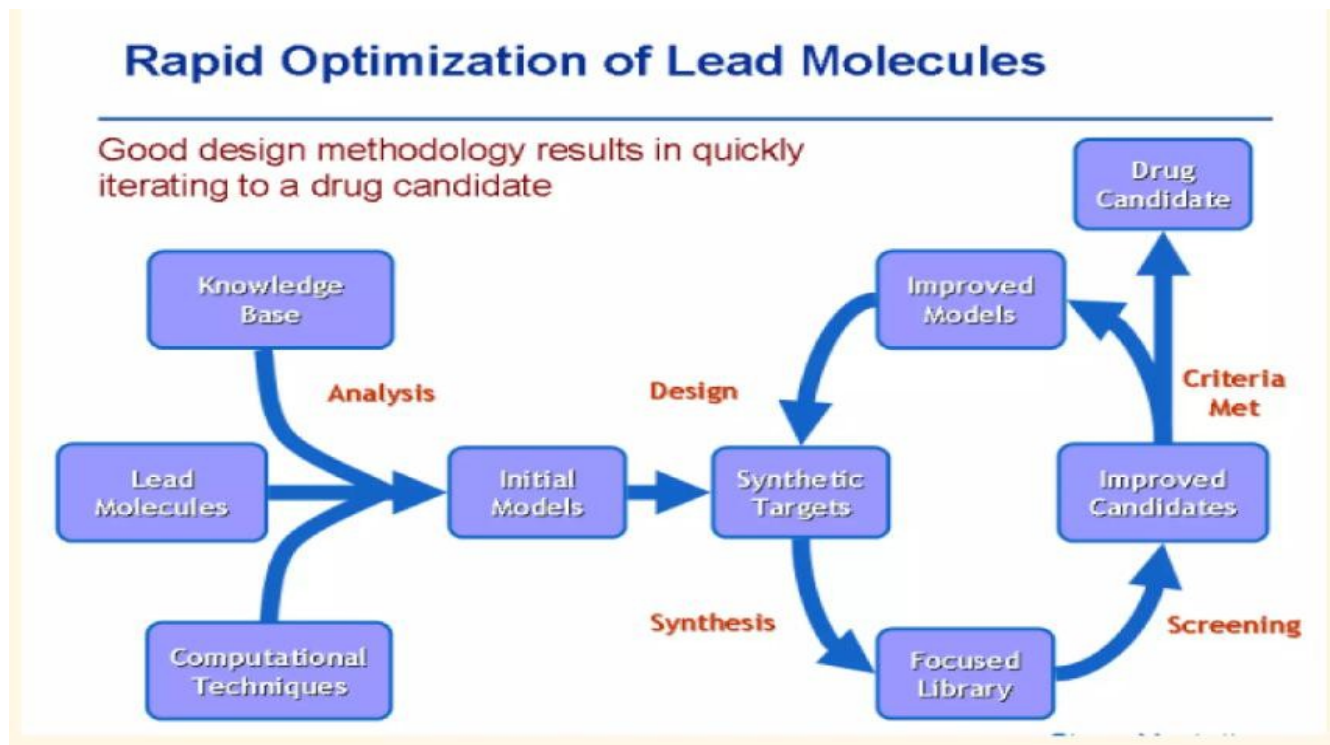
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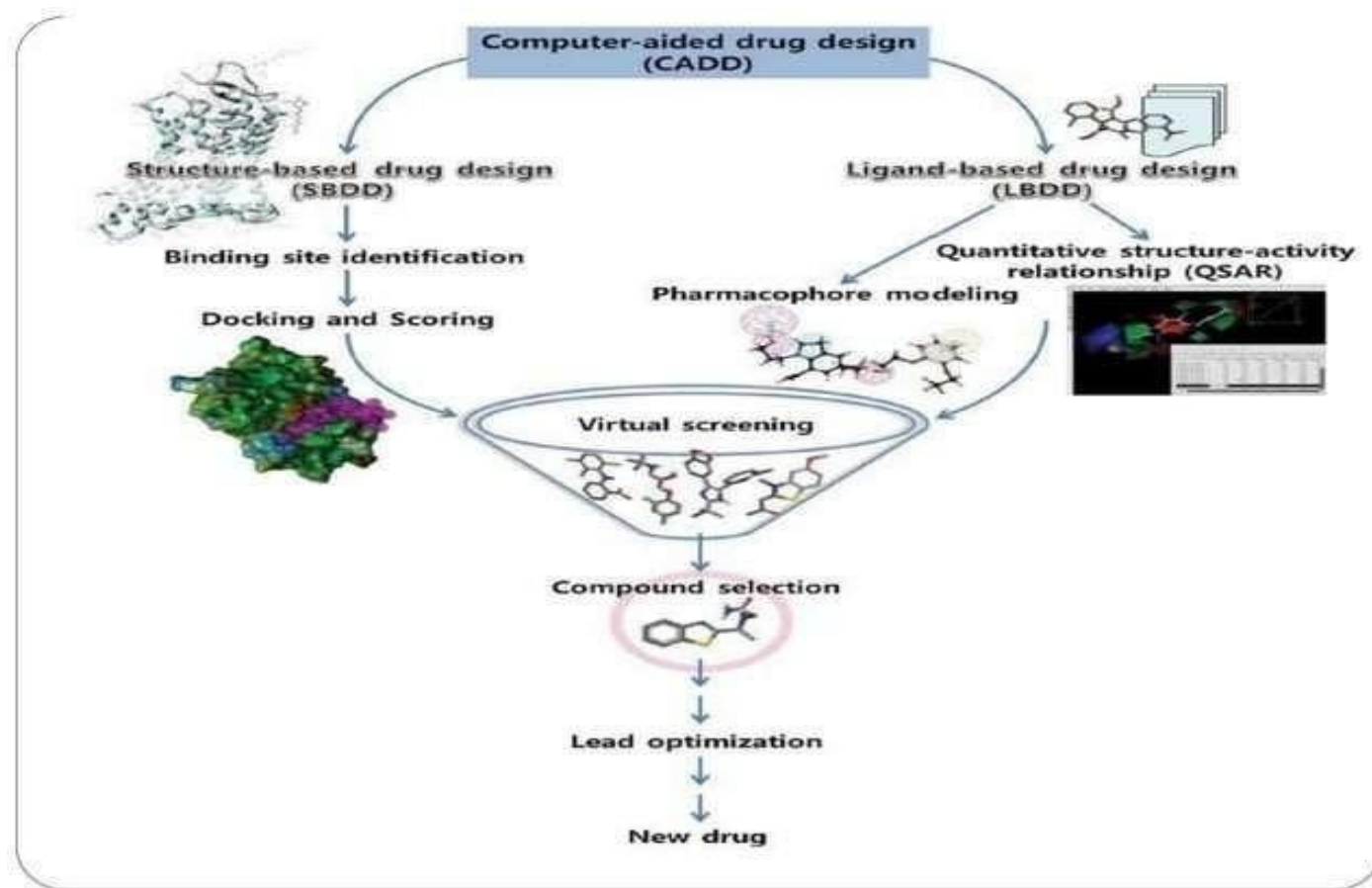
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RAPID OPTIMIZATION OF LEAD MOLECULES BY ANALOG METHODS



ANALOG BASED METHODOLOGY OF COMPUTER AIDED DRUG DESIGN (CADD)

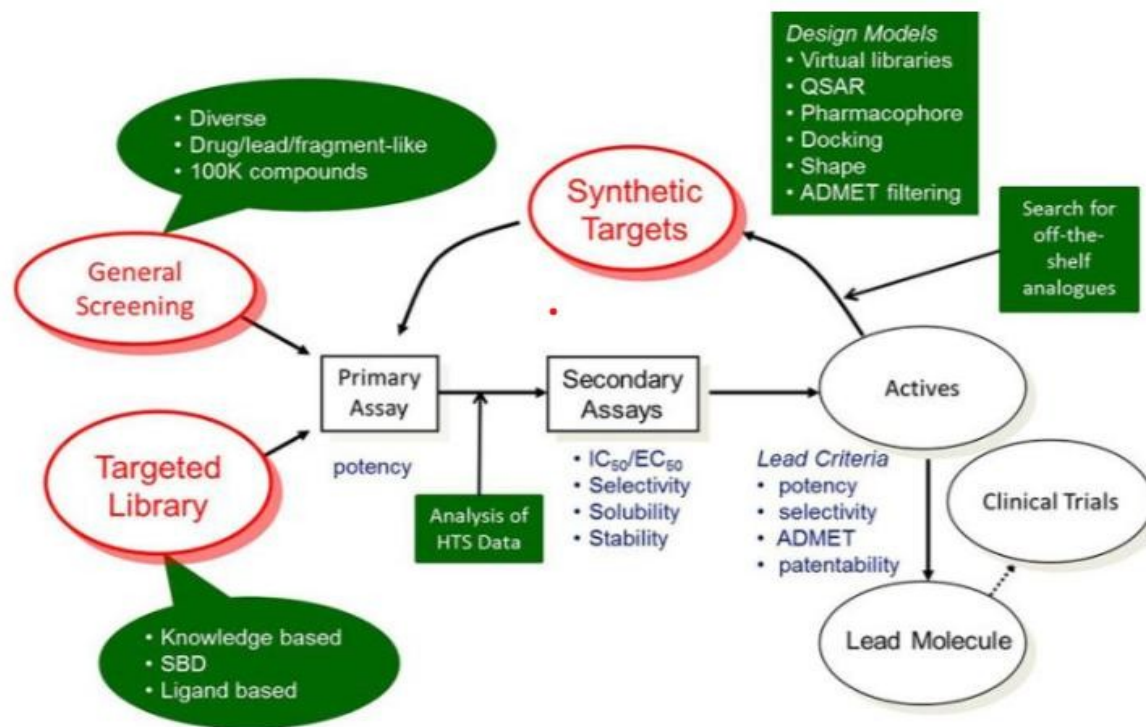


ABOUT SAR (STRUCTURAL ACTIVITY RELATIONSHIP)

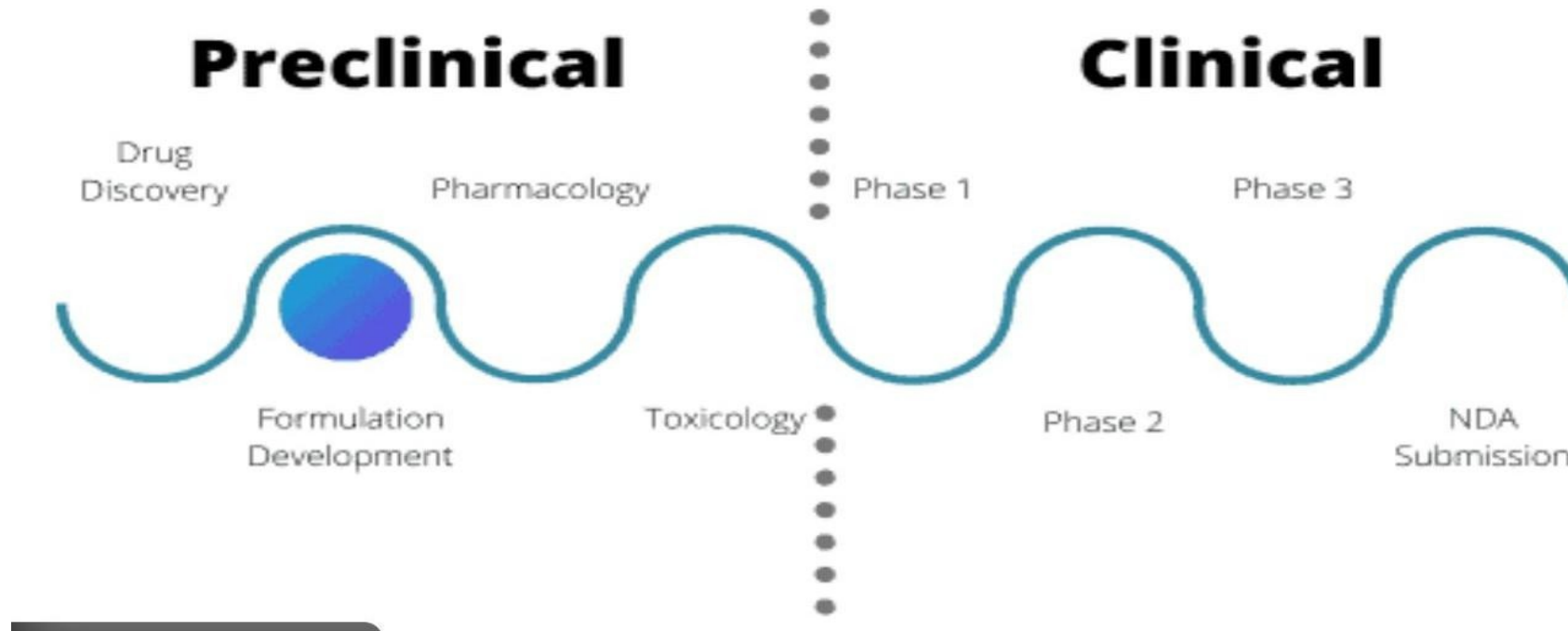
What is SAR ?

- SAR – It stands for Structure – Activity Relationship .
- It is basically defined as the relationship between the 3D structure of molecules and their biological activity.
- The analysis of SAR enables the determination of the chemical group responsible for evoking a target biological effect in any living organism.

STUDY OF GENERAL SCREENING, TARGETED LIBRARY, & SYNTHETIC TARGETS BY ANALOG METHODS



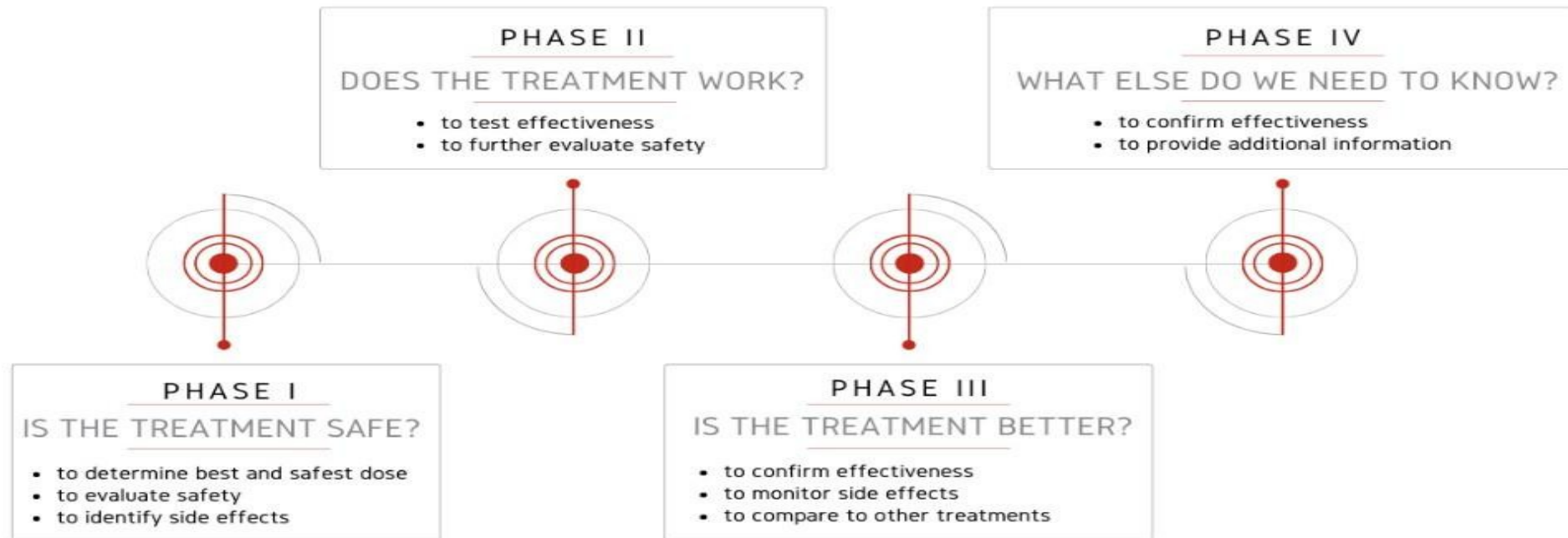
ANALOG BASED DRUG DESIGN IN PRECLINICAL & CLINICAL PROCESS



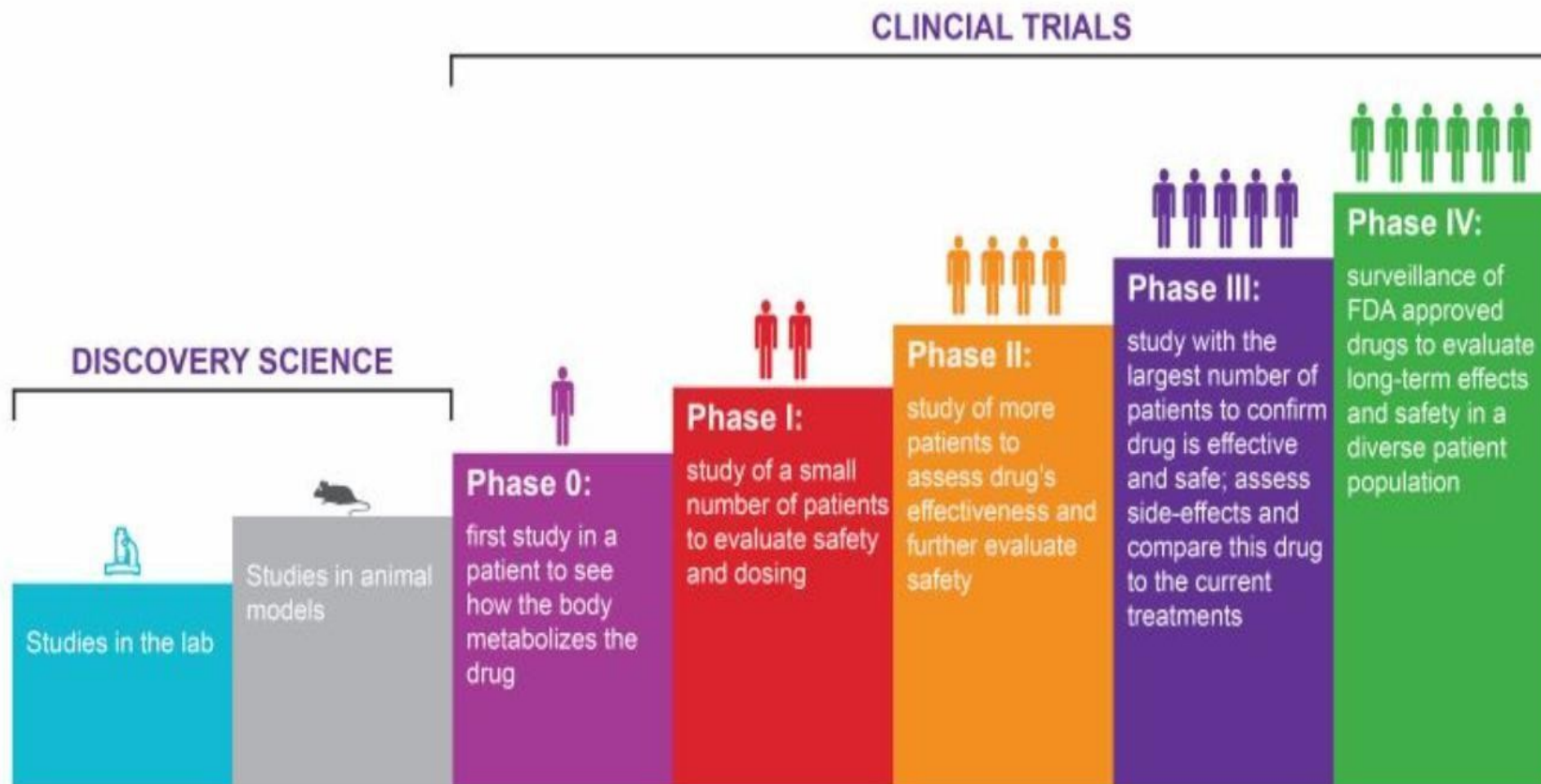
PHASES INVOLVED IN CLINICAL TRIALS

THE 4 PHASES IN CLINICAL TRIALS

DIAGRAM RESEARCH

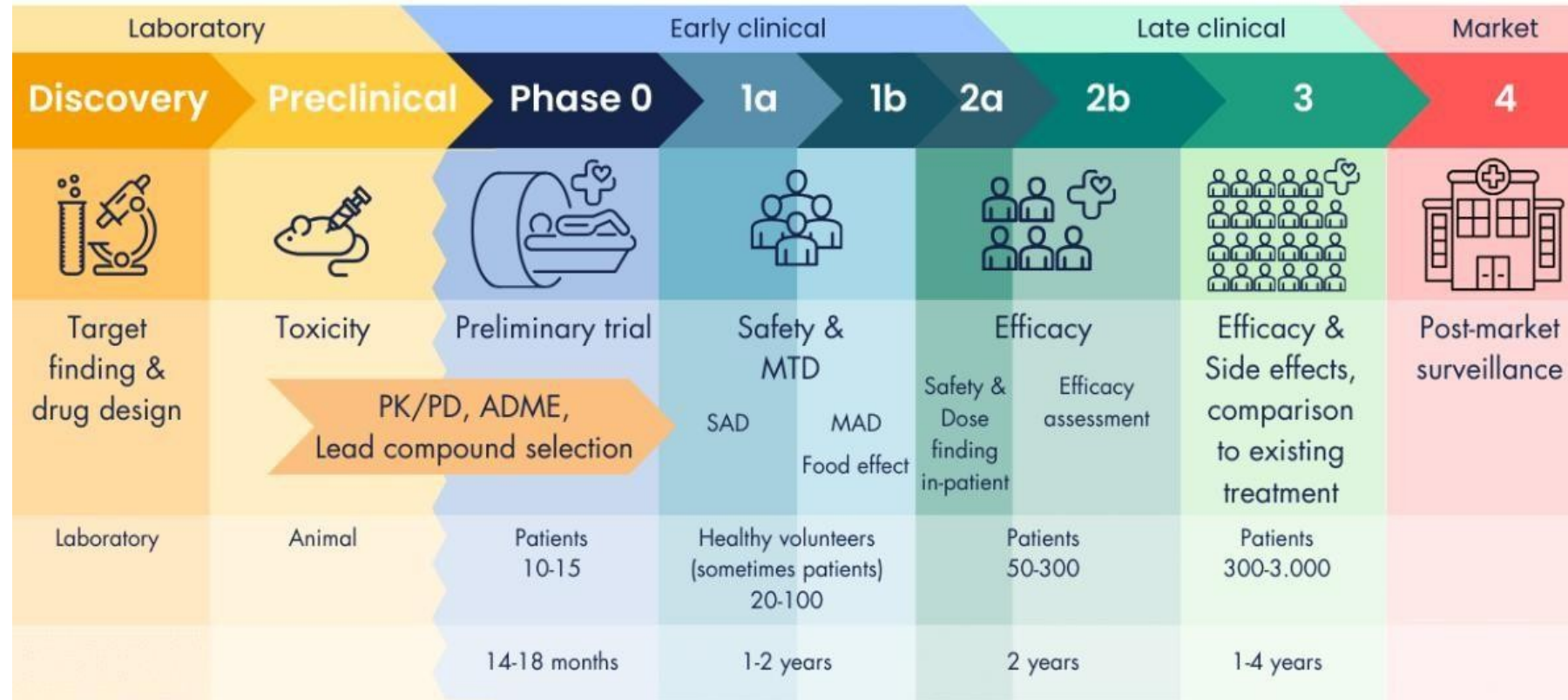


STUDY OF DRUG DISCOVERY SCIENCE & CLINICAL TRIALS



PHASES OF DRUG DISCOVERY & DRUG DEVELOPMENTS

Phases of drug development



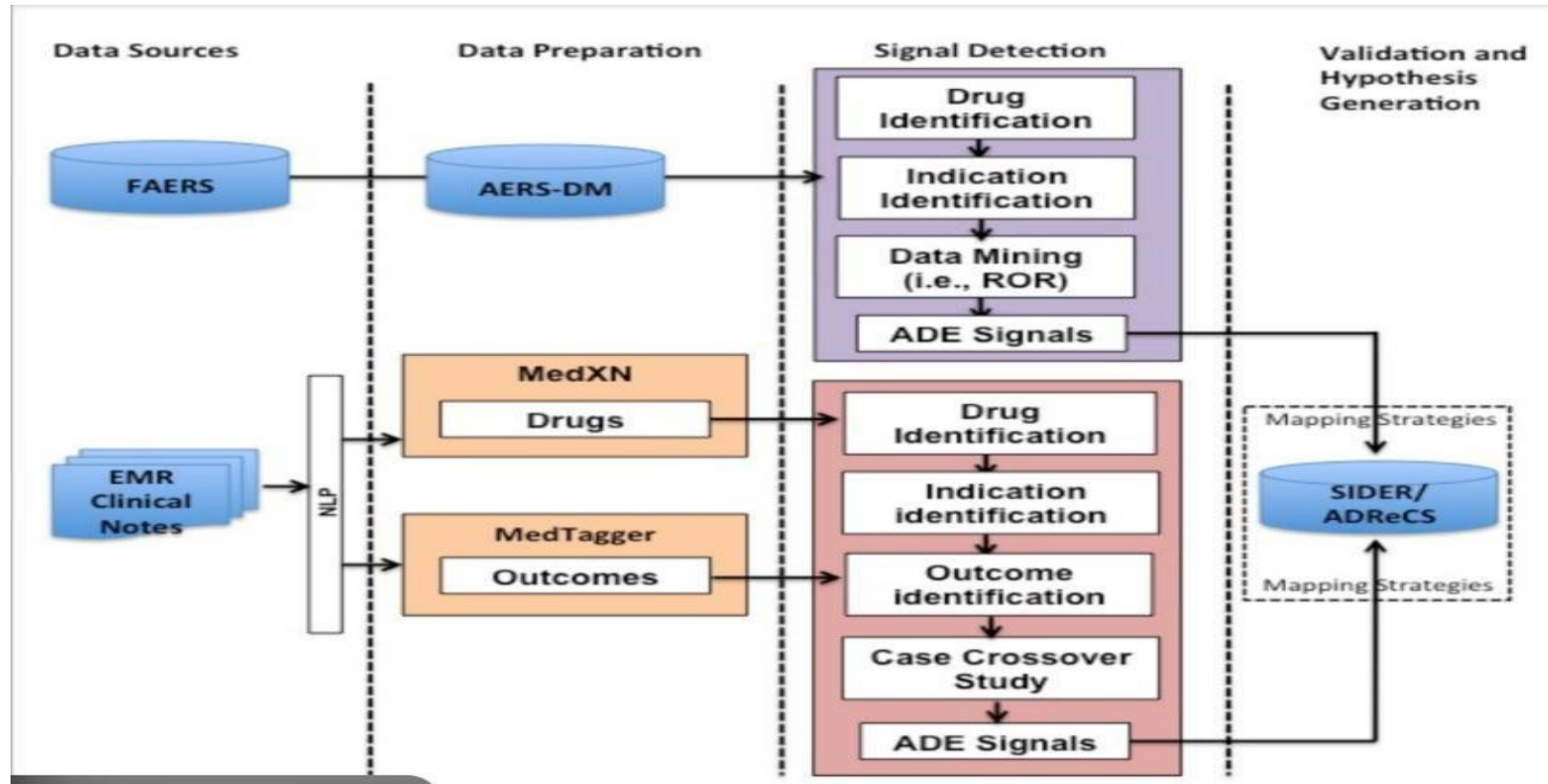
PK Pharmacokinetics
PD Pharmacodynamics

ADME Absorption, Distribution, Metabolism and Excretion
MTD Maximum Tolerated Dose

TRACFR

Simplified representation of phases in drug development. Study content and dates and numbers given may vary between studies. No rights can be derived from this figure.

ANALOG BASED DRUG DESIGN DATA SOURCES



ASSESSMENTS

Question 1 : Discuss the stages of lead discovery in the drug development process. Include: Target identification, hit discovery, lead identification, lead optimization. Mention techniques such as High-Throughput Screening (HTS), computational approaches, and natural product leads.

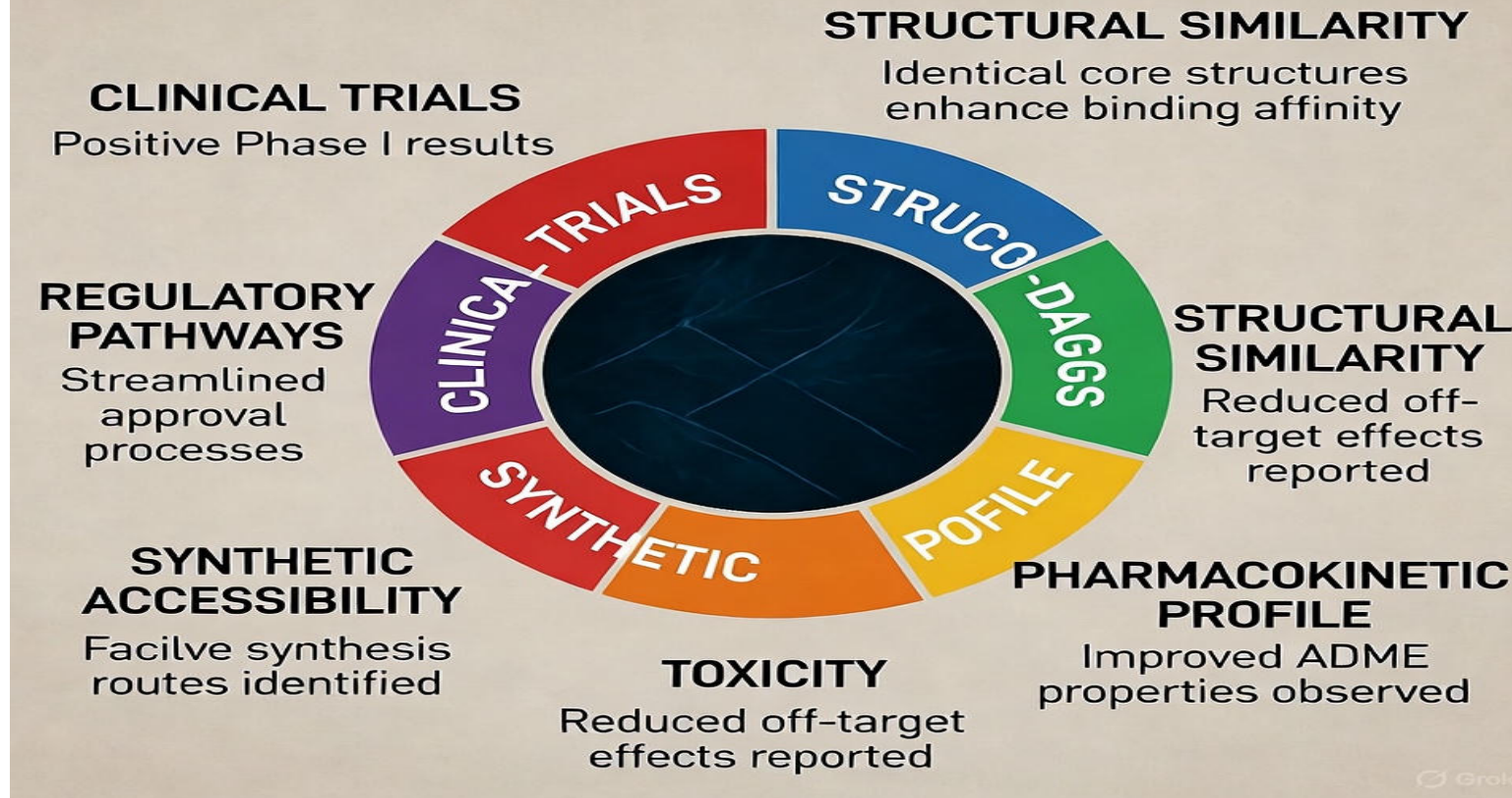


Question 2: Explain the concept and process of Analog-Based Drug Design. Define the approach. Discuss methods: structural modification, homologation, ring transformation, bioisosteric replacement. Provide a suitable example (e.g., modification of salbutamol from adrenaline).



SUMMARY

Conclusions for Key:



REFERENCES

1. Patrick, G. L. (2017). An Introduction to Medicinal Chemistry (6th ed.). Oxford University Press.
2. Silverman, R. B., & Holladay, M. W. (2014). The Organic Chemistry of Drug Design and Drug Action (3rd ed.). Academic Press.
3. Lemke, T. L., Williams, D. A., Roche, V. F., & Zito, S. W. (2013). Foye's Principles of Medicinal Chemistry (7th ed.). Wolters Kluwer/Lippincott Williams & Wilkins.
4. Nogrady, T., & Weaver, D. F. (2005). Medicinal Chemistry: A Molecular and Biochemical Approach (3rd ed.). Oxford University Press.
5. Hughes, J. P., Rees, S., Kalindjian, S. B., & Philpott, K. L. (2011). Principles of early drug discovery. British Journal of Pharmacology, 162(6), 1239–1249.

