

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

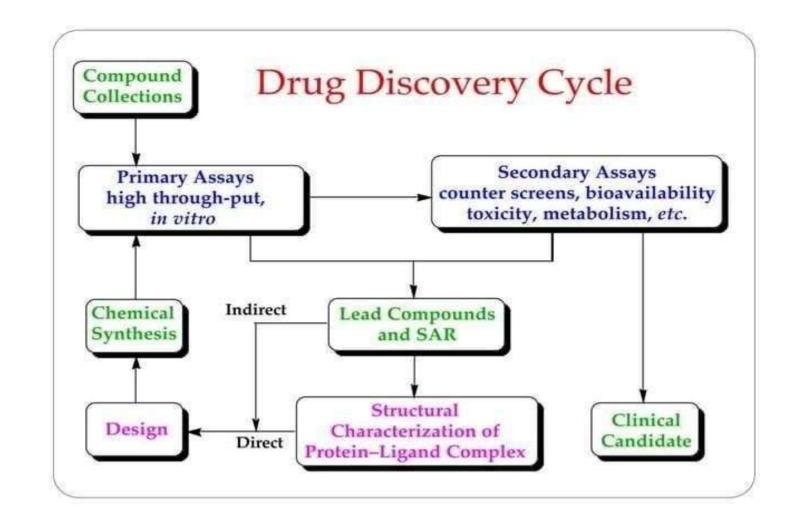
COURSE NAME: COMPUTER AIDED DRUG DESIGN(BP 807 ET)

VIII SEM / IV YEAR

TOPIC 5: ANALOG BASED DRUG DESIGN

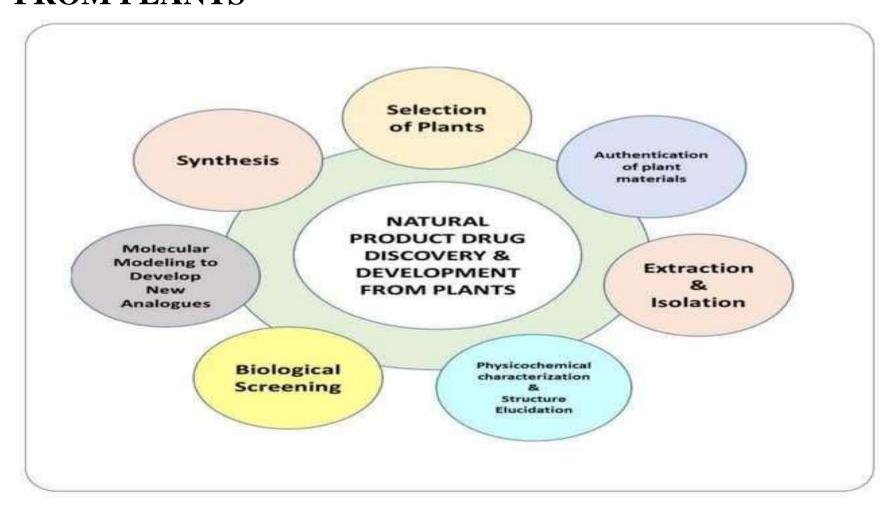
DRUG DISCOVERY CYCLE





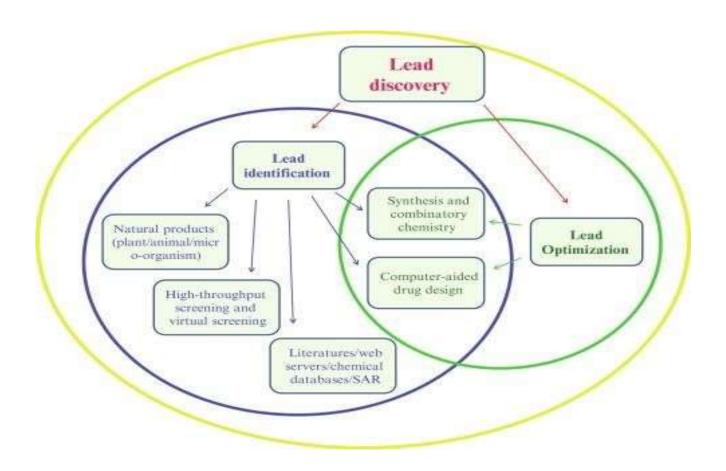
NATURAL PRODUCT DRUG DISCOVERY & DEVELOPMENT FROM PLANTS





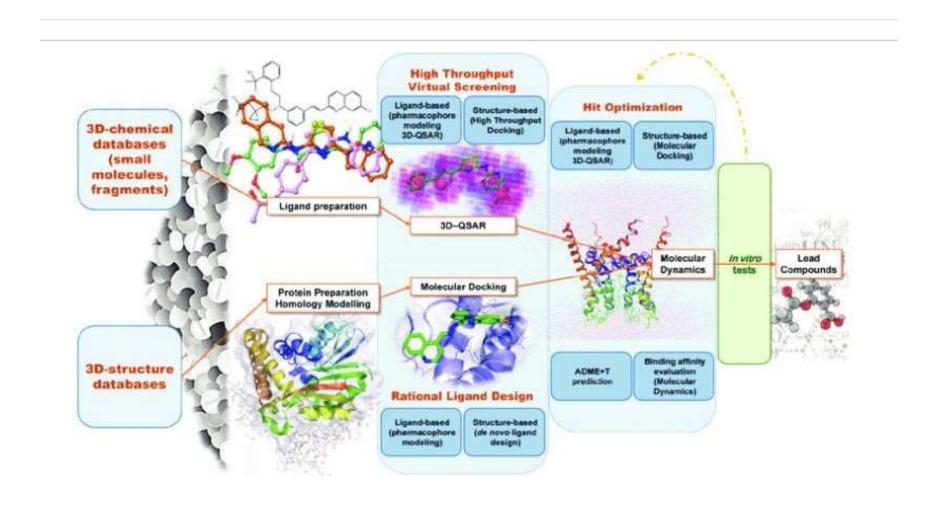
STAGES OF LEAD DISCOVERY





ANALOG BASED SCREENING MODELS

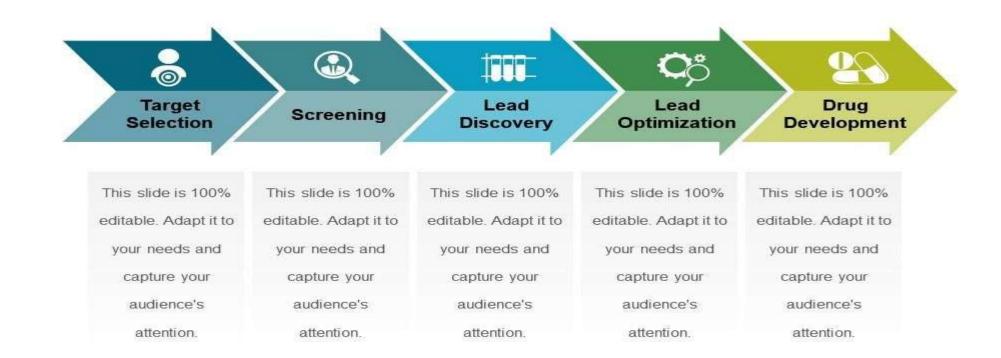




06-11-2025

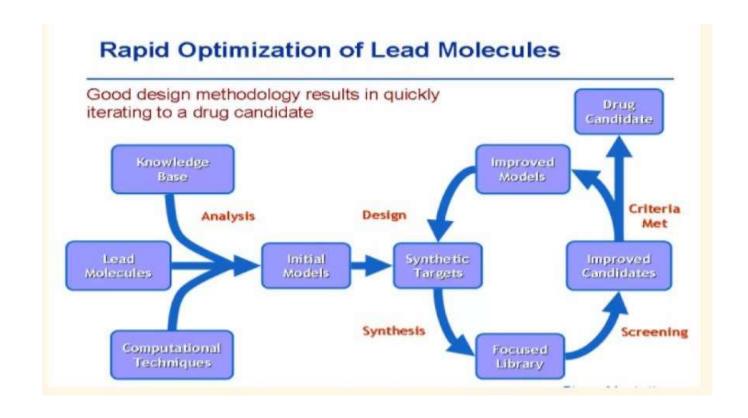


Drug Development Lead Optimization Steps With Icons



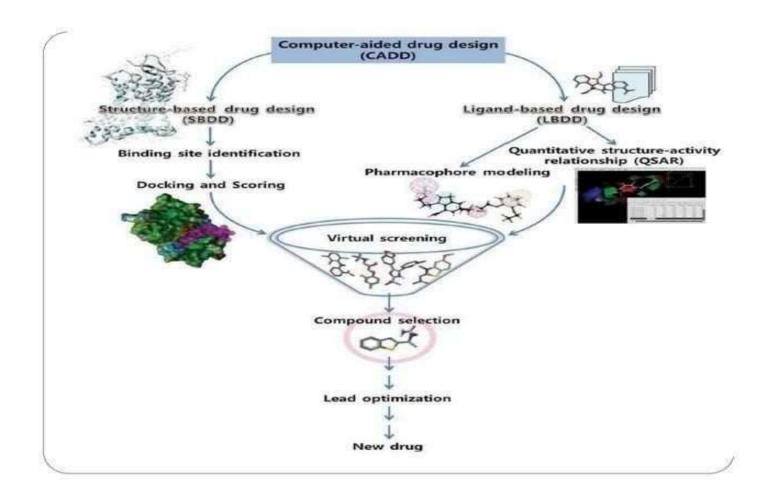


RAPID OPTIMIZATION OF LEAD MOLECULES BY ANALOG METHODS



ANALOG BASED METHODOLOGY OF COMPUTER AIDED DRUG DESIGN (CADD)





ABOUT SAR (STRUCTURAL ACTIVITY RELATIONSHIP)

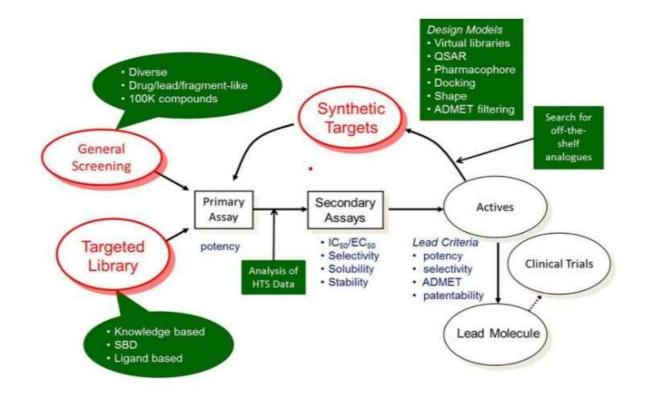


What is SAR?

- 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.

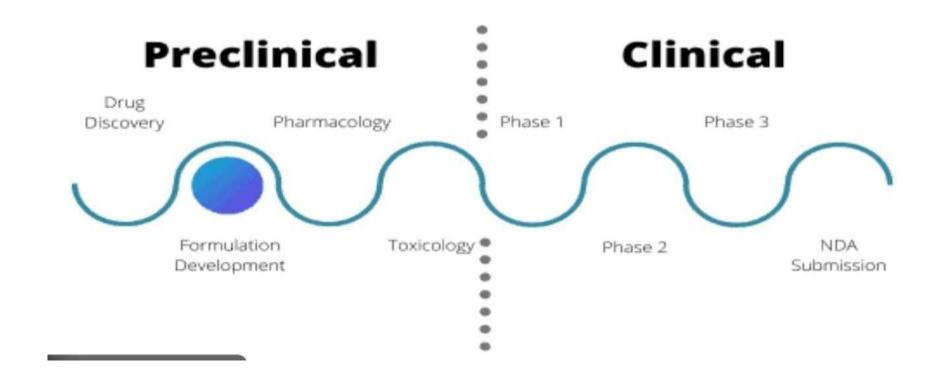
STUDY OF GENERAL SCREENING, TARGETED LIBRARY, & SYNTHETIC TARGETS BY ANALOG METHODS







ANALOG BASED DRUG DESIGN IN PRECLINICAL & CLINICAL PROCESS

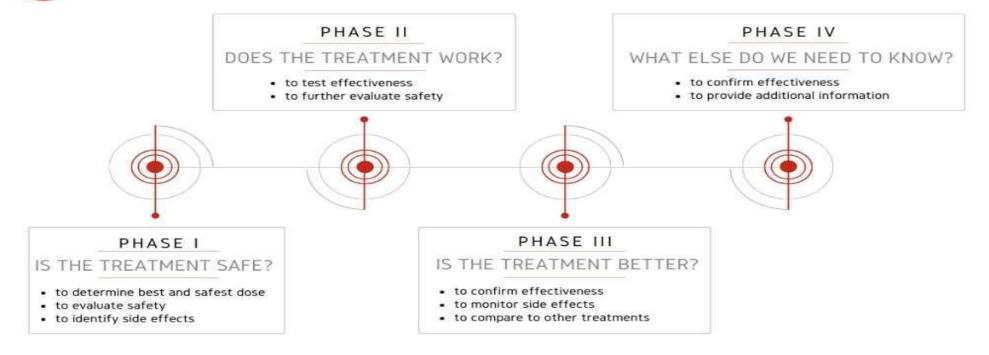


PHASES INVOLVED IN CLINICAL TRAILS



THE 4 PHASES IN CLINICAL TRIALS

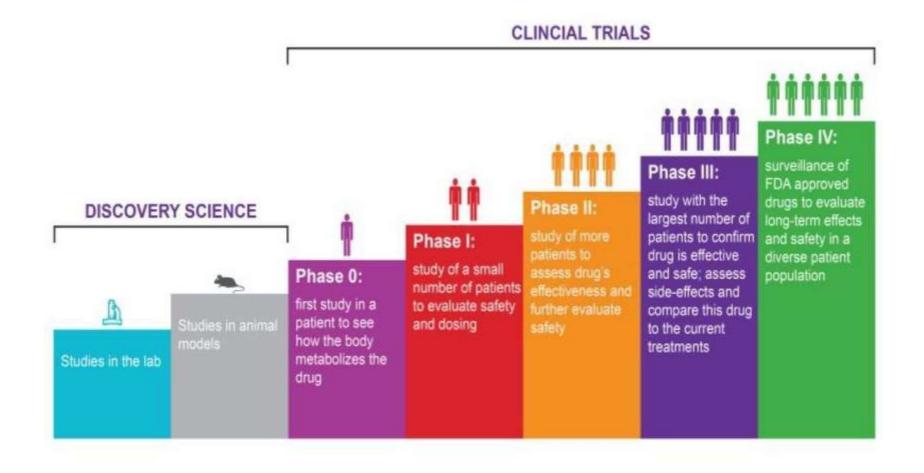




I.S

www.snsgroups.com

STUDY OF DRUG DISCOVERY SCIENCE & CLINICAL TRAILS



PHASES OF DRUG DISCOVERY & DRUG DEVELOPMENTS

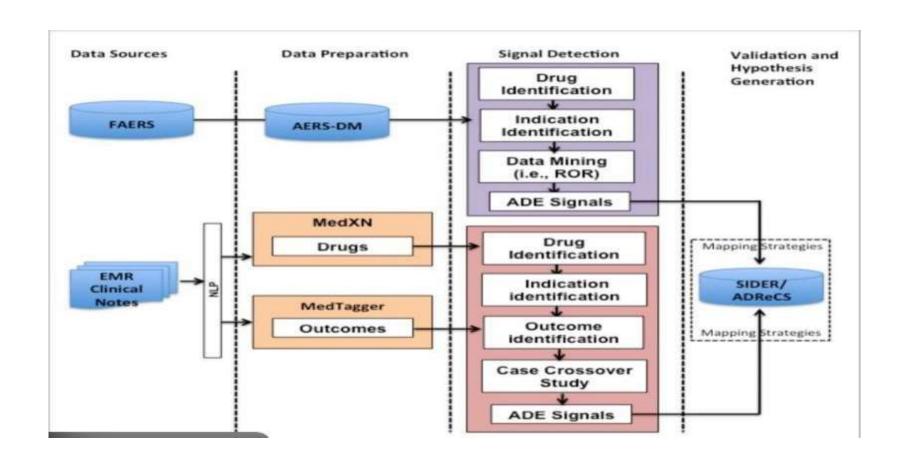


Phases of drug development

Laboratory		Early clinical			Late clinical			Market
Discovery	Preclinico	Phase 0	la	1b	2a	2b	3	4
		***	5		PoPo	16 ^{(P}	26666666666666666666666666666666666666	
Target finding & drug design	1 (1-10-0-1-10)	Preliminary trial D, ADME, pound selection	Safei MT SAD		Safety & Dose finding in-patient	assessment	Efficacy & Side effects, comparison to existing treatment	Post-market surveillance
Laboratory	Animal	Patients 10-15	Healthy vo (sometimes 20-1	patients)		Patients 50-300	Patients 300-3.000	
		14-18 months	1-2 ye	ears		2 years	1-4 years	
PK PharmacoKinetics ADME Absorption, Distribution, Metabolism and Excretion PD PharmacoDynamics MTD Maximum Tolerated Dose			TR	CFR		Z/C (1/4)	phases in drug development. St ween studies. No rights can be	

ANALOG BASED DRUG DESIGN DATA SOURCES







ASSESMENTS

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.

•





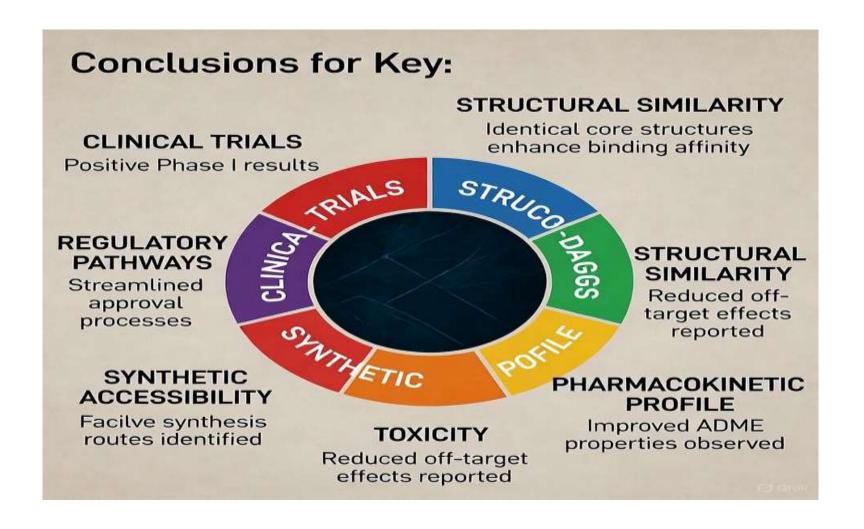
Question 2: Explain the concept and process of Analog-Based Drug Design. Define the approach. Discuss methods: structural modification, homologation, ring transformation, bioisosteric replacement. Provide a suitable example (e.g., modification of salbutamol from adrenaline).



06-11-2025 CADD|Mr. S.SRI VIKRAM |AP|SNSCPHS . 17/20

SUMMARY





CADD | Mr. S.SRI VIKRAM | AP | SNSCPHS



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.



