SRM UNIVERSITY
FACULTY OF ENGINEERING & TECHNOLOGY
DEPARTMENT OF BIOINFORMATICS

BI0306-MOLECULAR SIMULATION OF BIOMOLECULES

LESSON PLAN

Semester: VI **Course: Molecular Simulation Of Biomolecules**
Sub Code: BI0306 **Staff Handling: Mrs. S.Shobana**

Lecture Hour	Contents	Learning Outcome
	Unit 1:	
	APPLICATION OF MOLECULAR MODELING IN DRUG DESIGN	Fundamentals of Computer Aided Drug Designing (CADD)
	Introduction to Molecular Modelling.	
1	What are models used for?	
	Areas of application – Single molecule calculation, assemblies of molecules. Reaction of the molecules.	
2	Drawbacks of mechanical models as compared to graphical models.	
3	Co-ordinate systems two – matrix, potential energy surface.	Further Applications On The Design Of New Molecules
4	Molecular modeling in drug discovery	
5	Three dimensional pharmacophores	
6	molecular docking	
7	De-novo ligand designing	
8	structure-based methods	To Understand The Basis Of Structure Based Drug Design
9	electrostatic and non-electrostatic contribution to free energies.	
10	3D data base searching and virtual screening, Sources of data	
11	molecular similarity and similarity searching combinatorial libraries generation and utility	
	DRUG DISCOVERY	
12	Introduction	
13	Drug discovery: targets and receptors	
14	Drug Discovery Processes Medical Needs Target Identification	
15	Target Validation Drug Interactions with Targets or Receptors Enzymes	
16	Receptors and Signal Transduction Assay Development	
17	Case Study target identification and validation drug interactions	Drug development Methods and applications
18	small molecule drugs Introduction	

19	Irrational Approach Rational Approach Antisense Approach RNA Interference Approach Chiral Drugs	
20 21 22 23	**DRUG DEVELOPMENT** Pharmacodynamics Pharmacokinetics Toxicology animal tests formulations and delivery systems future perspectives	
24&25 26&27 28&29 30&31	**APPLICATIONS OF CADD-Introduction** Application and methods in protein engineering Protein design principles and examples Applications in pharmacophores mapping	
34&35 36&37 38&39 40&41 42&43 44&45	**QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP (QSAR)** Introduction to QSAR. Analysis of QSAR- computational approaches to chemical libraries lead module linear and nonlinear modeled equations, biological activities physicochemical parameter and molecular descriptors molecular modelling in drug discovery.	

TEXTBOOKS

1. Andrew R. Leach, *Molecular Modelling- Principles and application*, Prentice hall, II edition, 1996. (Unit I, unit V)
2. Rick NG, *Drugs: from Discovery to Approval***,** John Wiley & sons, 2004. (Units II, III,).
3. Moody PCE and Wilkinson AJ, *Protein Engineering*- IRL press oxford 1990(unit IV)

REFERENCE BOOK

1. Thomas J. Perun, Catherine Lamb Propst, *Computer-Aided Drug Design: Methods and Applications,* Informa Health Care, 1989.
2. Paul S Charifson, P*ractical Application of Computer-Aided Drug Design,* Informa Health Care, 1997.

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