VIVEKANANDHA COLLEGE OF ENGINEERING FOR WOMEN
(Autonomous Institution, Affiliated to Anna University, Chennai)
Elayampalayam, Tiruchengode – 637 205

DEPARTMENT OF BIOTECHNOLOGY

Course Code / Name : U15BT738& MOLECULAR MODELING AND DRUG DESIGNING

Class (Year / Programme / Department / Section): IV/ B.TECH/ BT

UNIT-1 CONCEPTS IN MOLECULAR MODELING				
S.No	**Topics To Be Covered**	**Duration in Minutes**	**Teaching Aid**	**Books Referred**
1.	Introduction	45	BB	T1
2.	Molecular modeling	45	BB	T1,R1
3.	Coordinate systems	45	BB	T1
4.	Energy surfaces	45	BB	T1
5.	Introduction to Quantum mechanics	45	PPT	T1,R1
6.	Schrodinger wave equation	45	BB	R1,R2
7.	Born	45	PPT	T1,R1
8.	Oppenheimer Approximation.	45	BB	T1
9.	Problems in molecular modelling	45	PPT	T2
UNIT-II DRUGS				
	Topics To Be Covered	**Duration in Minutes**	**Teaching Aid**	**Books Referred**
10.	Prodrugs- classification	45	PPT	T1
11.	Soft drugs. Drug targets	45	BB	T1,R1
12.	Enzymes, Receptors, Proteins	45	PPT	T1

13.	Nucleic acids, Lipids	45	BB	T1
14.	Drug solubility	45	PPT	T2,R1
15.	Effect of Ph	45	BB	R1
16.	Effect of polarity and pKa	45	PPT	T1,R1
17.	Drug Metabolism- Absorption, Distribution	45	PPT	R1
18.	Metabolism, Elimination.	45	PPT	R1

UNIT-III MOLECULAR MECHANICS

	Topics To Be Covered	**Duration in Minutes**	**Teaching Aid**	**Books Referred**
19.	Force field	45	BB	T1
20.	Bond Stretching	45	PPT	T1,R1
21.	Angle bending	45	BB	T1
22.	Torsion angle	45	PPT	T1
23.	Non-bonding interactions	45	BB	T1,R1
24.	Introduction to Energy	45	PPT	R1
25.	Energy minimization	45	BB	T1,R1
26.	Computer simulations	45	PPT	T1
27.	Conformational analysis	45	BB	T1
28.	Problems discussing	45	BB	T2

UNIT-IV DRUG DESIGN

	Topics To Be Covered	**Durationin Minutes**	**Teaching Aid**	**Books Referred**
29.	Steps in drug Development	45	BB	T1
30.	Lead discovery	45	BB	T1,R1

31.	Molecular modeling in drug design	45	PPT	T1
32.	Pharmacophore	45	BB	T1
33.	Concepts of comparative modelling	45	BB	T1,R1
34.	Molecular docking, AUTODOCK & HEX	45	PPT	R1
35.	Structure based methods to identify lead compound	45	BB	T1,R1
36.	De novo ligand design , Drug Discovery	45	BB	T1
37.	QSAR	45	BB	T1
38.	Drug approval process	45	PPT	R2

UNIT-V COMPUTATIONAL REPRESENTATION OF MOLECULES

	Topics To Be Covered	**Duration in Minutes**	**Teaching Aid**	**Books Referred**
39.	Introduction	45	BB	T1
40.	Chemical Databases	45	PPT	T1,R1
41.	Software Resources: Molecular Mechanics (MM3 and MM4)	45	PPT	T2
42.	Huckel-MO-Calculator, Semiempirical (MOPAC)	45	BB	T1
43.	Ab Initio (GAUSSIAN), Alchemy	45	BB	T1,R1
44.	SciQSAR , Chem3D, PDB	45	BB	R1
45.	SYBYL, CHARMM force field, HyperChem	45	PPT	T1,R1
46.	MM+, AMBER, MOE	45	BB	R1
47.	Discovery Studio, FlexX, GOLD, Schroedinger	45	PPT	T1

TEXT BOOK:

1)Andrew Leach - Molecular Modelling: Principles and Applications, 2nd Edition. Pearson Education EMA, 2001.

REFERENCES:

1)R.K. Prasad - Quantum Chemistry, 3rd Edition, 2006