



Department of Biotechnology		LP: BY22313
		Rev. No: 00
M.Tech : Biotechnology	Regulation: 2022 (Autonomous)	Date: 03.07.2024
PG Specialisation : Biotechnology		
Sub.Code/Sub. Name : BY22313 - Molecular Modeling and Drug Design Laboratory		

Session No*	List of Experiments
1	Small molecules from Biological Databases — PUBCHEM, Drugbank, ZINC15
2	Checking Lipinski's rule five and ADME properties — SWISSADME
3	Drawing Chemical molecules - ACD ChemsSketch
4	Protein Sequence and Structure Annotation — Genpept, UniprotKB, PDB
5	Pairwise and Multiple Sequence Alignment — BLAST, CLUSTALW
6	Modeling of Proteins & Structure Assessment — SWISS Modeller
7	Phylogenetic Analysis — PHYLIP
8	QSAR Analysis — QSAR toolbox
9	Pharmacophore generation & Mapping — Pharm-mapper
10	Pathways search - KEGG, Protein-Protein Interactions — StringDB
11	Network pathways — Cytoscape
12	Bioinformatics Toolbox — MATLAB
13	Molecular Docking — Autodock
14	Protein- Protein Docking — Patchdock, Firedock
15	Docking Analysis and Validation — Discovery Studio
Content beyond syllabus (if any): Biochemical test to identify microorganism	



* Session Duration: 300 minutes



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REFERENCES:

1. Rebecca C. Wade and Outi M.H. Salo- Ahen, "Molecular Modeling in Drug Design", MDPI publishers, 2019.
2. Anand Solomon K, "Molecular Modelling and Drug Design", 1st Edition, MJP Publishers, 2015.
3. Om Silakari, Pankaj Kumar Singh, "Concepts and Experimental Protocols of Modelling and Informatics in Drug Design", Academic Press Inc., 2020.
4. Shao Li, "Network Pharmacology", 1st Edition, Springer Verlag, 2021.
5. Rastogi S.C, Rastogi Paraag and Namita Medritta, "Bioinformatics: Methods and applications — Genomics, Proteomics and Drug Discovery", 5th Edition, PHI Learning Pvt. Ltd, 2022.

	Prepared by	Approved by
Signature		
Name	J. Hariharan	Dr. E. Nakkeeran
Designation	Assistant Professor	HOD-BIO
Date	08.07.2024	08.07.2024
Remarks*: Nil		

* If the same lab plan is followed in the subsequent semester/year it should be mentioned and signed by the Faculty and the HOD