SRI VENKATESWARA COLLEGE OF ENGINEERING

COURSE DELIVERY PLAN - THEORY

Department of Biotechnology	LP: BT22034 Rev. No: 00 Date: 11.06.2024
B.E/B.Tech/M.E/M.Tech : Biotechnology Regulation:2022 PG Specialisation : NA Sub. Code / Sub. Name : BT22034 / MOLECULAR MODELING IN DRUG DISCOVERY Unit : I	

Unit Syllabus: Introduction to molecular modeling in drug discovery

Objective: Understand the principles and theoretical foundations of molecular modeling in drug discovery

Session No *	Topics to be covered	Ref	Teaching Aids
1	Overview of molecular modeling	TB1(21-23) ,TB2 (57-62) , VL	Blended Learning
2	Molecular modeling techniques	TB1 (35-43), TB3 (10-14), VL	Blended Learning
3	Molecular geometry and coordinate systems	TB3 (9-15), VL	Blended Learning
4	Potential energy surfaces	TB3 (148 -153), VL	Blended Learning
5	Introduction to quantum mechanics	TB3 (118, 148), VL	Blended Learning
6	Schrodinger wave equation - hydrogen molecule	RB1(3.1-3.8), IS2 VL	Blended Learning
7	Born-Oppenheimer approximation	RB1(10.1.1 -10.1.8), VL	Blended Learning
8	Role of computational methods in drug discovery	TB 1(118-126),TB 2 76-89), VL	Blended Learning
9	Introduction to molecular visualization software	IS 1, TB3 (179-185)	Blended Learning
Content beyond syllabus covered (if any):			

* Session duration: 50 minutes

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Unit : II

Unit Syllabus : Molecular mechanics and energy minimization

Objective: Learn about molecular mechanics, fore fields and energy minimization.

Session No *	Topics to be covered	Ref	Teaching Aids
10	Empirical force field models	TB3 (196-200), RB1 (1.1.2-1.1.4) VL	Blended Learning
11	Bond stretching, angle bending, torsional term	TB3 (39-41), RB1(6.2), VL	Blended Learning
12	Nonbonding interactions	TB3 (39-41), VL	Blended Learning
13	Thermodynamics properties using a forcefield, derived energy minimization method	TB3 (47-50), VL	Blended Learning
14	Thermodynamics properties using a forcefield, non-derived energy minimization method	TB3 (49-53), VL	Blended Learning
15	Simplex and sequential univariate method	TB4 (129-134), VL	Blended Learning
16	Steepest descent method	TB3 (27-29), VL	Blended Learning
17	Conjugate gradient method	TB3 (136-139), VL	Blended Learning
18	Newton-Rapson method	IS4, TB3(138-140), VL	Blended Learning

Content beyond syllabus covered (if any):

* Session duration: 50 mins

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Unit : III

Unit Syllabus : Molecular dynamics and monte carlo simulation

Objective: Gain knowledge of molecular dynamics simulations and their applications in drug design.

Session No *	Topics to be covered	Ref	Teaching Aids
19	Introduction to Molecular Dynamics	TB4 (264-266), TB3 (47- 68), VL	Blended Learning
20	Molecular dynamics by single model and time steps	TB4 (264-266), TB3 (47- 68), VL	Blended Learning
21	Multiple steps MD	TB3 (50- 56), VL	Blended Learning
22	Setting up MD	TB3 (41- 44), VL	Blended Learning
23	Energy conservation in MD Simulation	TB5 (4-9), VL	Blended Learning
24	MD Simulation platforms and examples	TB3 (46- 53), IS 1, VL	Blended Learning
25	Monte Carl simulations	TB3 (203- 206), TB4 (398-402), VL	Blended Learning
26	Random number generation in MD	IS3, VL	Blended Learning
27	Difference in Classical Monte Carlo (MC) and Classical Molecular Dynamics (MD)	TB3 (203- 212), VL	Blended Learning
Content beyond syllabus covered (if any):			

* Session duration: 50 mins

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Unit : IV

Unit Syllabus : Insilico molecular modeling, structure activity relationship

Objective: Learn computational methods for predicting molecular structures, properties of drug candidates and quantitative structure-activity relationship (QSAR) analysis for predicting drug activity and toxicity

Session No *	Topics to be covered	Ref	Teaching Aids
28	Basics of In-silico molecular modeling	TB4 (321-322), IS1, VL	Blended Learning
29	Homology Modeling, Threading and Abinitio modeling	TB4(111-127), VL	Blended Learning
30	Types of physicochemical parameters	TB4(231-240), VL	Blended Learning
31	Experimental and theoretical approaches for the determination of physicochemical parameters	TB4(240-251), VL	Blended Learning
32	3D QSAR applications and limitations	TB4 (112-126), VL	Blended Learning
33	Virtual Screening and Molecular Descriptors	TB4 (29-81), VL	Blended Learning
34	Free Wilson analysis, MFA, CoMFA and PLS Method	TB4(103-110), VL	Blended Learning
35	Non-Linear QSAR Methods	TB4(111-127), VL	Blended Learning
36	Descriptor Selection and Virtual Screening with QSAR.	TB4 (150-168), VL	Blended Learning

Content beyond syllabus covered (if any):

* Session duration: 50 mins

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Unit : V

Unit Syllabus: Informatics & methods in drug design

Objective: Learn various tools used for molecular modelling in drug development.

Session No *	Topics to be covered	Ref	Teaching Aids
37	Cheminformatics and their role in molecular designing and analysis	RB2 (2-9), VL	Blended Learning
38	ADME databases	TB4 (243 -260), TB3 (198-199), VL	Blended Learning
39	Chemical, Biochemical and Pharmaceutical databases	TB4 (243 -260), VL	Blended Learning
40	General approach to discovery of new drugs	TB4 (262 -268), VL	Blended Learning
41	Lead discovery and lead modification	IS5, VL	Blended Learning
42	Physiochemical principles of drug action	TB4 (243 -260), VL	Blended Learning
43	Drug stereo chemistry	RB (10.1.1 - 10.1.7), VL	Blended Learning
44	Drug action	TB4 (243 -260), VL	Blended Learning
45	Drug Discovery and Medicinal Chemistry	TB5 (26-48), TB4(260-271), VL	Blended Learning

Content beyond syllabus covered (if any):

* Session duration: 50 mins

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REFERENCES:

TEXT BOOK(S)

1. Leach AR., "Introduction to Molecular Modeling", 1st Edition, Oxford University Press, 2001.
2. Voth G.A., "Principles of Molecular Modeling and Simulation: A Guide for Biomolecular Scientists", 1st Edition, Springer, 2018.
3. Rebecca C. Wade and Outi M. H. Salo-Ahen, "Molecular Modeling in Drug Design", 1st Edition, MDPI, 2019.
4. Tomasz P, Jerzy L, and Mark TC., "Recent Advances in QSAR Studies", 1st Edition, Springer, 2010.
5. Leach AR., "Molecular Modeling: Principles and Applications", 1st Edition, Pearson, 2001.

REFERENCE BOOK(S)

1. Zielinksi et al., "QUANTUM STATES OF ATOMS AND MOLECULES", 1st Edition ,Chemical Education Digital Library, Libretexts.org , 2024.
2. David S. Wishart, "Introduction to Cheminformatics", 1st , Edition Curr Protoc Bioinformatics, 2007.

INTERNET SOURCE(S)

1. https://www.bioinformatics.org/gary/Lecture_3.4_Stucture_Tools_and_Visualization.pdf
2. https://batch.libretexts.org/print/url=https://chem.libretexts.org/Courses/University_of_California_Davis/Chem_107B%3A_Physical_Chemistry_for_Life_Scientists/Chapters/4%3A_Quantum_Theory/4.10%3A_The_Schr%C3%B6dinger_Wave_Equation_for_the_Hydrogen_Atom.pdf
3. https://reference.wolfram.com/language/tutorial/RandomNumberGeneration.html
4. https://www.geeksforgeeks.org/newton-raphson-method/
5. https://lifesciences.danaher.com/us/en/library/lead-optimization-drug-discovery-guide.html

COURSE YOUTUBE LINK:

https://www.youtube.com/playlist?list=PLvDocy_6Jwl80E0dCIRiXGcjeQRDFcocO

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1. Leach AR., "Introduction to Molecular Modeling", 1st Edition, Oxford University Press, 2001.
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1. Zielinksi et al., "QUANTUM STATES OF ATOMS AND MOLECULES", 1st Edition ,Chemical Education Digital Library, Libretexts.org , 2024.
2. David S. Wishart, "Introduction to Cheminformatics", 1st , Edition Curr Protoc Bioinformatics, 2007.

INTERNET SOURCE(S)

1. https://www.bioinformatics.org/gary/Lecture_3.4_Stucture_Tools_and_Visualization.pdf
2. https://batch.libretexts.org/print/url=https://chem.libretexts.org/Courses/University_of_California_Davis/Chem_107B%3A_Physical_Chemistry_for_Life_Scientists/Chapters/4%3A_Quantum_Theory/4.10%3A_The_Schr%C3%B6dinger_Wave_Equation_for_the_Hydrogen_Atom.pdf
3. https://reference.wolfram.com/language/tutorial/RandomNumberGeneration.html
4. https://www.geeksforgeeks.org/newton-raphson-method/
5. https://lifesciences.danaher.com/us/en/library/lead-optimization-drug-discovery-guide.html

COURSE YOUTUBE LINK:

https://www.youtube.com/playlist?list=PLvDocy_6Jwl80E0dCIRiXGcjeQRDFcocO

	Prepared by	Approved by
Signature		
Name	Dr M Nareshkumar	Dr E Nakkeeran
Designation	Assistant Professor	Professor & HOD
Date	08/07/2024	08/07/2024
Remarks *:		
Remarks *:		

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