SRI VENKATESWARA COLLEGE OF ENGINEERING

COURSE DELIVERY PLAN - THEORY

Department of Biotechnology	LP: BT22035 Rev. No: 00 Date: 21.01.25
B.E/B.Tech/M.E/M.Tech : B.Tech (Biotechnology) Regulation: 2022 PG Specialisation : - Sub. Code / Sub. Name : BT22035 –Cheminformatics and Medicinal Chemistry (H & M) Unit : I	

Unit Syllabus: BASICS OF DRUG ACTION 9 hrs

Introduction to Medicinal Chemistry, Energy, Thermodynamics, Interactions, Receptorology, Enzyme Kinetics, Enzyme Inhibition, Nucleic acids, Drug Likeness, Drug action after metabolism

Objective: This unit aims to acquire the basics of drug action.

Session No *	Topics to be covered	Ref	Teaching Aids
1	Introduction to Medicinal Chemistry	TB3- Ch.5; pg.145-176 TB3- Ch.6; pg.177-206	LCD/BB
2	Energy, Thermodynamics	TB3 – Ch.4; pg. 117-122	Blended Learning-Video Lecture
3	Interactions, Receptorology	TB2- Ch.3; pg. 60-120 TB3 – Ch.8; pg. 251-264	Blended Learning-Video Lecture
4	Enzyme kinetics	TB2- Ch.8; pg. 316-402 TB3- Ch.9; pg. 303-305	Blended Learning-Video Lecture
5	Enzyme Inhibition	TB2- Ch.8; pg. 316-402 TB3- Ch.9; pg. 306-319	LCD/BB
6	Nucleic acids	TB3 – Ch.10; pg. 335-344	Blended Learning-Video Lecture
7	Drugs that act on Nucleic acids	TB3- Ch.10; pg. 362-379	Blended Learning-Video Lecture
8	Drug Likeness, Pharmacokinetics basics	TB3- Ch.11; pg. 403-408	Blended Learning-Video Lecture
9	Drug action after metabolism	TB3 – Ch.12; pg. 439-476	LCD/BB
Content beyond syllabus covered (if any): Pharmacokinetics basics			

* Session duration: 50 minutes

Sub. Code / Sub. Name: BT22035 –Cheminformatics and Medicinal Chemistry (H & M)

Unit : II

Unit Syllabus : COMPUTER-AIDED DRUG DESIGN 9 hrs

Electronic structure methods, Molecular Modeling, Structure activity relationships, QSAR, Molecular docking, Molecular dynamics, Pharmacophore, De Novo drug design.

Objective: This unit aims to illustrate the different methods of Computer-aided drug design.

Session No *	Topics to be covered	Ref	Teaching Aids
10	Electronic structure methods	AR1- Ch2; pg.9-64	LCD/BB
11	Molecular Modeling – small molecules	AR1- Ch3; pg.65-76 TB3-Ch.4; pg.114	Blended Learning-Video Lecture
12	Molecular Modeling – macromolecules	AR1- Ch3; pg.77-132 TB3-Ch.4; pg.115	Blended Learning-Video Lecture
13	Structure activity relationships	AR2 – Ch.5; pg.181-212	Blended Learning-Video Lecture
14	QSAR	AR2 – Ch.5; pg. 181-207 TB2- Ch. 5; pg. 202-252 TB3-Ch.4; pg.136-140	LCD/BB
15	Molecular docking	AR2 – Ch.3; pg.92-121 TB3- Ch.4; pg.127-129	Blended Learning-Video Lecture
16	Molecular dynamics	AR2 – Ch.5; pg. 45-77 TB3 – Ch.4; pg. 123-126	Blended Learning-Video Lecture
17	Pharmacophore	AR2 – Ch.3; pg.121-123 TB3- Ch.4; pg. 133-134	Blended Learning-Video Lecture
18	De Novo drug design	AR2 – Ch.3; pg.124-129 TB3-Ch.4; pg.128-129	LCD/BB

Content beyond syllabus covered (if any): - NIL-

* Session duration: 50 mins

Sub. Code / Sub. Name: BT22035 –Cheminformatics and Medicinal Chemistry (H & M)

Unit : III

Unit Syllabus : ORGANIC SYNTHESIS 9 hrs

Organic reaction mechanism, alkylation, metal/ammonia reduction, reaction of electron-deficient intermediates, organometallics, asymmetric synthesis, photochemistry, synthesis of complex molecules.

Objective: This unit provides an insight on different reactions in Organic synthesis.

Session No *	Topics to be covered	Ref	Teaching Aids
19	Organic reaction mechanism	TB1 -Ch.4; pg.389-404 TB1- Ch.5; pg. 548-553 TB1-Ch.7; pg.682-684	LCD/BB
20	Alkylation	TB1-Ch.9; pg.805-808	Blended Learning-Video Lecture
21	Metal/ammonia reduction	TB1-Ch.6; pg.591-600	Blended Learning-Video Lecture
22	Reaction of electron-deficient intermediates	TB1-Ch.5; pg-531-535	Blended Learning-Video Lecture
23	Organometallics	TB1-Ch.7; pg. 676-681	LCD/BB
24	Asymmetric synthesis	TB1-Ch.2; pg. 189-207	Blended Learning-Video Lecture
25	Photochemistry	TB1- Ch.8; Pg. 1073-1153	Blended Learning-Video Lecture
26	Synthesis of complex molecules -Aromatic Substitution	TB1 – Ch.9; Pg. 771-824	Blended Learning-Video Lecture
27	Synthesis of complex molecules -Concerted Pericyclic Reactions	TB1 – Ch.10; Pg. 833-951	LCD/BB

Content beyond syllabus covered (if any): -NIL-

* Session duration: 50 mins

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Sub. Code / Sub. Name: BT22035 –Cheminformatics and Medicinal Chemistry (H & M)
Unit : IV

Unit Syllabus : STRUCTURE AND FUNCTION OF BIOMOLECULES 9 hrs

Methods for the determination of structure of biomolecules, properties of amino acids and peptide bond, structure of nucleic acids and protein-nucleic acid interactions, structure and function of biomolecules pertaining to different therapeutic areas, biological crystallography, spectrofluorimetric and optical methods, Thermodynamics methods.

Objective: This unit helps to demonstrate on methods for determination of structure and function of biomolecules.

Session No *	Topics to be covered	Ref	Teaching Aids
28	Methods for the determination of structure of biomolecules	AR4- Ch.8; pg. 241-245	LCD/BB
29	Properties of amino acids	AR4-Ch.4; pg.67-70	Blended Learning-Video Lecture
30	Properties of peptide bond	AR4-Ch.4; pg.70	Blended Learning-Video Lecture
31	Structure of nucleic acids	TB3- Ch.10; pg. 341-344	Blended Learning-Video Lecture
32	Structure of protein-nucleic acid interactions	TB3- Ch.10; pg. 350-361	LCD/BB
33	Biological crystallography	TB4- Ch.4; pg. 59-90	Blended Learning-Video Lecture
34	Spectrofluorimetric methods	TB4- Ch.10; pg. 175-196	Blended Learning-Video Lecture
35	Other Optical Methods	TB4- Ch.3; pg. 37-58 AR4- Ch.4; pg. 73-77	Blended Learning-Video Lecture
36	Thermodynamics methods	AR4-Ch.3; pg. 52-64	LCD/BB

Content beyond syllabus covered (if any): -NIL-

* Session duration: 50 mins

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Sub. Code / Sub. Name: BT22035 –Cheminformatics and Medicinal Chemistry (H & M)

Unit : V

Unit Syllabus : DRUG METABOLISM 9 hrs

Biotransformation of drugs, factors influencing enzyme induction and inhibition, factors affecting drug metabolism, dose-effect relationships, metabolism pathways, excretion of drugs, adverse drug reactions and drug interactions; toxic reactions, allergic reactions, idiosyncracy.

Objective: This unit provides broad knowledge on drug metabolism

Session No *	Topics to be covered	Ref	Teaching Aids
37	Biotransformation of drugs	AR3 – Ch. 5; pg. 111-146 RB1 – Ch. 9; pg. 116-124	LCD/BB
38	Factors influencing enzyme induction and inhibition	AR3 – Ch. 5; pg. 147-150	Blended Learning-Video Lecture
39	Factors affecting drug metabolism	TB3- Ch.12; pg. 439-443	Blended Learning-Video Lecture, Quiz
40	Dose-effect relationships	AR3 – Ch. 14; pg. 325-334 RB2 – Ch.12; pg. 530-534	Blended Learning-Video Lecture
41	Metabolism pathways	TB3- Ch.9; pg. 329-331	LCD/BB
42	Excretion of drugs, Adverse drug reactions	AR3 – Ch. 7; pg. 178-203 RB1 – Ch.57; pg. 692 RB1 – Ch.9; pg. 122-124	Blended Learning-Video Lecture, Animations
43	Drug interactions	TB3- Ch.12; pg. 460-474 RB1 – Ch.9; pg. 120-121	Blended Learning-Video Lecture
44	Toxic reactions, Allergic reactions	TB3- Ch.12; pg. 444 RB1 – Ch.57; pg. 693-695	Blended Learning-Video Lecture
45	Idiosyncracy	Lecture Notes	LCD/BB

Content beyond syllabus covered (if any):

* Session duration: 50 mins

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REFERENCES:

TEXT BOOK (TB):

1. Francis A. Carey, Richard J. Sundberg, Advanced organic chemistry: part A structure and mechanisms, Springer, 5th Ed, 2008.
2. John Smith H, Hywel Williams, Introduction to the principles of drug design and action, CRC press, 4th Ed, 2005.
3. Gareth Thomas, Medicinal chemistry, John Wiley, 2nd Ed, 2007.
4. Notling B, Methods in modern biophysics, Springer, 2nd Ed, 2012.

REFERENCE BOOK (RB):

1. Rang H.P, Dale M.M, Ritter J.M, Flower R.J, Rang and Dale‟s Pharmacology, Churchil Livingstone, Elsevier, 8th Ed, 2015.
2. Adeboye Adejare, Remington‟s the science and practice of pharmacy, Elsevier, 23rd Ed, 2021.

ADDITIONAL REFERENCES (AR):

1. Mannhold R, Kubinyi H, Timmerman H., Methods and Principles of Medicinal Chemistry, Wiley-VCH, 3rd Ed, 1996
2. Anand Solomon K, Molecular Modeling and Drug Design, MJP Publishers, 1st Ed, 2008.
3. Brahmankar DM, Sunil B. Jaiswal, Biopharmaceutics and Pharmacokinetics A Treatise, Vallabh Prakashan, 1st Ed, 2004.
4. Donald Voet, Judith G. Voet, Biochemistry, John Wiley & Sons, 4th Ed, 2011.

YOUTUBE CHANNEL VIDEOS LINK

https://www.youtube.com/playlist?list=PLvDocy_6Jwl-jY6PnuHRnrxXXzoVicLu7

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Designation	PROFESSOR	PROFESSOR & HOD
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Remarks *:		