Course Type	Course Code	Name of Course	L	T	P	Credit
DC	NCYC506	Computer Aided Drug Design	3	1	0	4

Course Objective
• Introduction to different computational methods for drug discovery and development.
Learning Outcomes
• Introductory knowledge of Computer aided drug design and drug discovery stages consisting target identification and validation • To be well equipped with of modern cheminformatics and bioinformatics approaches including QSAR, pharmacophore modelling, molecular docking, Protein structure prediction etc.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Steps in drug discovery, target identification and lead identification, drugs and drug database, issues in drug discovery, drug likeness-properties of drugs, pharmacokinetics and pharmacodynamics, importance of drug solubility and permeability, Drug ADME, toxicity of drugs, brief introduction to bioinformatics, cheminformatics, and their relation to drug design.	10L+3T	Overview of various stages of drug discovery and the important properties to be investigated during drug design in computational studies
2	Molecular modelling, molecular dynamics simulations, ensembles, potential energy surface, force field methods , energy minimization, geometry optimization , conformational analysis , global conformational minima determination , approaches and problems , Bioactive Vs global minimum conformations , Automated methods of conformational search , Dynamics of drugs , biomolecules drug-receptor complexes, Estimation of free energy and other properties from simulations	11L+4T	Learn different steps involved in protein structure prediction and molecular dynamics simulations with hands-on experience.
3	Protein-ligand docking, types of docking: rigid docking and flexible docking , manual docking ; algorithms involved in docking and docking score calculations, Advantages and disadvantages of various docking softwares	11L+4T	Discussion on various docking methods and in-hand experience of docking methods with model systems.
4	Qualitative versus quantitative approaches-advantages and disadvantages ; Random screening , Non-random screening, Insights into molecular recognition phenomenon, Structure based drug design, ligand-based drug design, pharmacophore mapping. QSAR: Electronic effects Hammett equation , Lipophilicity effects; Hansch equation , Steric	10L+3T	Learn about different screening techniques and various ligand based drug design methods

	Effects; 2D-QSAR; 3D-QSAR		
	Total	**42L+14T**	

Text Books:

1) Computational Drug Design: A Guide for Computational and Medicinal Chemists, D. C. Young, Wiley-Blackwell, ISBN: 978-0470126851, 2009.

Reference Books:

1) Understanding Molecular Simulations: From Algorithms to Applications, D. Frenkel and B. Smit, Academic Press, 2002.
2) Molecular modeling Principles and Applications. A. R. Leach. Pearson, ISBN-13: 978-0582382107, 2001.
3) An Introduction to Cheminformatics, A. R. Leach., Springer, ISBN: 978-1-4020-6291-9, 2007.
4) In Silico Drug Discovery and Design: Theory, Methods, Challenges, and Applications. C. N. Cavasotto, CRC Press, ISBN: 978-1138747586, 2017.