



Integral University, Lucknow

Effective from Session: 2020 -21							
Course Code	BE 620	Title of the Course	Computer Aided Drug Design	L	T	P	C
Year	2	Semester	3	3	1	0	4
Pre-Requisite	None	Co-requisite	None				
Course Objectives	The objective of the course is learning and understanding the entire picture of the latest developments in the field of Drug Designing. The application of the course focuses on recent insilico structure and ligand based approaches to modern day drug design.						

Course Outcomes	
CO1	Explain the stages of modern era drug designing and apply it while correlating with any drug's discovery and approval pattern.
CO2	Analyze the important drug targets and understand its significance in designing new drugs against new targets.
CO3	Understand the concept and applications of structure based drug design and apply it in corresponding case studies.
CO4	Understand the concept and applications of ligand based drug design and apply it in corresponding case studies.
CO5	Analyze the pharmacokinetic and toxicity related issues of the drug molecules.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Stages of Drug Designing	Drug Discovery Pipeline: Strategies to identify possible drug targets, Validation and Druggability of targets, Discovery of Lead compounds, Optimization of Lead compounds to Candidate drugs, Clinical Trials and its applications.	8	CO1
2	Drug Targets	Potential Drug Targets: Family of G-Protein Coupled receptors (GPCRs), Ion Channels: Molecular structure and significance; Aquaporins as Drug Targets, DNA as anti-cancer targets.	8	CO2
3	Direct Drug Design	Structure based Drug Design: Molecular Docking- principles and concepts, Representation of molecules, Searching and Scoring of potential solutions, Special aspects of docking: protein flexibility and water molecules. Common Docking programs: AUTODOCK, GOLD.	8	CO3
4	Indirect Drug Design	Ligand based Drug Design: Quantitative Structure Activity Relationship (QSAR) – principles and concepts, Statistical Methods used in QSAR analyses, Pharmacophore Modeling: Criteria for satisfactory pharmacophore model, Basics of Hip Hop and Hypogen Model, Applications of pharamacophore model.	8	CO4
5	Drug Pharmacokinetics	Pharmacokinetic analyses of Drugs: Quantitative Structure Property Relationship (QSPR) studies –important parameters and significance, ADME- TOX studies, Concept of Drug-likeness and its applicability.	8	CO5

Reference Books:

Harren Jhoti, Andrew R. Leach; Structure- based Drug Discovery, Springer, 2007, ISBN 1402044070

Andrew Leach; Molecular Modelling: Principles and Applications (2nd Edition), Prentice Hall, 2001, ISBN 13: 9780582382107

R E Hubbard; Structure-based Drug Discovery: An Overview, Royal Society of Chemistry, 2006

Barry A. Bunin, Brian Siesel, Guillermo Morales, Jurgen Bajorath; Chemoinformatics: Theory, Practice, & Products, Springer Science & Business Media, 2006.

e-Learning Source:

Zhang W, Pei J, Lai L. Computational Multitarget Drug Design, J ChemInf Model, 2017. doi: 10.1021/acs.jcim.6b00491.

National Center for Biotechnology Information, www.ncbi.nlm.nih.gov

Webinar recording: a sequel for beginners: ligand-based drug design — the basics <https://www.youtube.com/watch?v=ef5EaoBYUU>

Jenny Viklund& Fredrik Rahm (Sprint Bioscience): Marvin Live for structure-based drug design: Chem axon: https://www.youtube.com/watch?v=5gzxQC_mMX0

Course Articulation Matrix: (Mapping of COs with POs and PSOs)																		
PO-PSO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3	PSO5	PSO6	PSO7
CO1	1	2	2	3	3	2	1	2	1	2	1	2	3	2	2			
CO2	1	2	2	2	2	2	1	1	1	2	1	1	3	2	1			
CO3	3	3	3	3	2	2	1	1	1	1	1	2	3	1	2			
CO4	3	3	3	3	2	2	1	1	1	1	1	2	3	1	2			
CO5	3	2	2	1	3	2	2	1	1	1	1	2	3	2	2			

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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Integral University, Lucknow

Effective from Session: 2020-21							
Course Code	BE621	Title of the Course	Applied Genomics	L	T	P	C
Year	II	Semester	III	2	1	0	3
Pre-Requisite	BE521	Co-requisite	None				
Course Objectives	The objective of the course is to inbuilt knowledge and skills in student of the main experimental designs and tools applied in genetics and genomics and approaches for genetic and genomic data analysis, and next generation sequencing. In particular the student is able to: understand the structure of genetic variability, learn DNA sequencing methods, use software for genomic data analysis, correctly interpret results and plan genetic studies in a proper way.						

Course Outcomes	
CO1	Understand the term genome and the methods of genetic and physical mapping.
CO2	Learn about different methods of DNA sequencing, genome annotation, and gene prediction.
CO3	Understand the concepts of structural, functional, and computational genomics; and gain knowledge about the applications of comparative genomics.
CO4	Understand the concepts of microarray data analysis for gene expression and will gain knowledge about the bioinformatics tools used in the microarray data analysis.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Genome	Definition of genome, GenomeMap: Types of Genomemaps and their uses, High and low-resolution map, Polymorphic markers: LINEs, SINEs, RFLP, SNP; Types of maps: Cytogenetic map, Linkage map, Transcript map, Physical map.	8	CO1
2	Gene Prediction	DNA sequencing: Sanger's method and Maxam Gilbert method; Large scale genome sequencing strategies: Shotgun sequencing, Clone contig approach. Genome Annotation: Structural annotation - Various approaches for gene prediction in the case of prokaryotes and eukaryotes, ORF Finder, GenScan, Prediction of promoter sequences and splice sites.	8	CO2
3	Structural and Functional Genomics	Basic principles of structural and functional genomics: role and their applications. Comparative Genomics: Purpose and Methods of comparison, Comparison at nucleotide level, ontological comparison, phylogenetic comparison; Applications of Comparative Genomics.	8	CO3
4	Gene Expression analysis	Gene Expression and Microarray data Analysis: Exploring the microarray data set, Spatial images of microarray data, Statistics of the microarrays, Scatter plots of microarray data; Clustering gene expression profiles, Principal component analysis (PCA), Self-Organizing Maps (SOM), Bioinformatics tools for Microarray data analyses.	8	CO4

Reference Books:	
1.	Developing Bioinformatics Computer Skills: An Introduction to Software Tools for Biological Applications; Publisher: O'Reilly Media; Edition Year: 2001.
2.	Introduction to Genetic Analysis; Publisher: Freeman & Company, W. H.; Edition Year: 2017.
3.	Gene Cloning and DNA Analysis: An Introduction; Publisher: John Wiley & Sons Ltd; Edition Year: 2010.
4.	Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins. Publisher: John Wiley & Sons Ltd; Edition Year: 2005.
6.	Introduction to Bioinformatics: A Theoretical and Practical Approach; Publisher: John Wiley & Sons Ltd; Edition Year: 2005.
e-Learning Source:	
1.	Biology Animation Library
2.	https://www.dnalc.org/resources/animations/cycseq.html

Course Articulation Matrix: (Mapping of COs with POs and PSOs)																		
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	1	2	1	1	1	1	1	1	1	1		3	1	1	1			
CO2	2	3	1	1	2	2	1	1	1	1		3	2	3	1			
CO3	1	2	1	1	2	3	1	1	1	1		3	1	3	1			
CO4	2	3	3	2	3	2	1	1	1	1		3	2	3	1			

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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Integral University, Lucknow

Effective from Session: 2021-2022							
Course Code	BE622	Title of the Course	Protein Informatics	L	T	P	C
Year	II	Semester	III	2	1	0	3
Pre-Requisite	BE620	Co-requisite	None				
Course Objectives	This course will introduce students to the fundamentals of tools and techniques of computational molecular biology, and to the bioinformatics tools and databases used for the prediction of protein function and structure. It is designed to impart a substantial understanding of popular computational methods, as well as molecular tools and techniques of protein sequence and structure analysis methods applied to real data.						

Course Outcomes	
CO1	Understand the details of protein's hierarchical evolutionary classification and their associated databases.
CO2	Explain the concepts and applications of spectroscopy and their impact on display and analysis of proteomics data.
CO3	Understand the basics of chromatography and electrophoretic techniques and their implications to the analysis of biological macromolecules.
CO4	Discuss the practical aspects of protein-protein interactions using online tools of Expert Protein Analysis System (ExPASy).

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Introduction to protein structure and databases	Overview of Amino acids, Secondary, Tertiary, and Quaternary structure of proteins, Motifs and Domain, Significance of Leucine zipper and Zing finger, Principles of classification of proteins based on structural features: CATH and SCOP, Structural databases: PDB and MMDB.	8	CO1
2	Principles and applications of spectroscopy	Introduction to principles and applications of UV-Visible Spectroscopy, Fluorescent Spectroscopy, CD Spectroscopy and basic concepts of NMR and Mass Spectrometry and their significance in structural biology.	8	CO2
3	Introduction to chromatography and electrophoresis	Basic principle of Chromatography and Electrophoresis techniques in isolating, separating and purifying protein molecules, Brief overview of different types of Chromatography and Electrophoresis & their applications.	8	CO3
4	Applied proteomics	Study of transcriptome and proteome; Concept of protein-protein interactions and their databases such as DIP. Tools for analysis of protein-protein interactions: PPI server. Protein arrays: basic principles; bioinformatics-based tools for analysis of proteomics data, ExPASy Proteomics server.	8	CO4

Reference Books:	
Protein Bioinformatics: From Sequence to Function; Academic Press, 2011; ISBN 0123884241, 9780123884244	
Principles and Techniques of Practical Biochemistry; Cambridge University Press, 16-Mar-2000 Reprint 4 March 2010; ISBN 0521731674; 978-0521731676	
Essential Bioinformatics; Cambridge University Press, 2006; ISBN 113945062X, 9781139450621	
Lehninger Principles of Biochemistry; W. H. Freeman; 13 February 2013; ISBN 1464109621, 978-1464109621	
e-Learning Source:	
Analytical Biochemistry; Dr. Ashwani K. Sharma, IIT Roorkee; http://nptel.ac.in/courses/102107028/	
Bioanalytical Techniques and Bioinformatics; Dr. Vishal Trivedi and Dr. Nitin Chaudhary, IIT Guwahati; http://nptel.ac.in/courses/102103044/	
Introduction to Proteomics; Dr. Sanjeeva Srivastava, IIT Bombay; https://onlinecourses.nptel.ac.in/noc16_bt07	

Course Articulation Matrix: (Mapping of COs with POs and PSOs)																			
PO-PSO- CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	PSO6
CO1	2	2	2	2	3	2	2	1	1	3	2	3	2	2	2				
CO2	2	2	1	3	3	1	1	1	1	3	2	3	2	2	2				
CO3	1	2	2	2	3	1	1	1	1	2	1	3	2	2	2				
CO4	1	2	2	2	2	1	1	1	1	2	1	3	2	2	2				

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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Integral University, Lucknow

Effective from Session: 2020-21							
Course Code	BE623	Title of the Course	System Biology	L	T	P	C
Year	II	Semester	III	2	1	0	3
Pre-Requisite	BE525	Co-requisite	None				
Course Objectives	The objective of the course is learning and developing thoughtful process in understanding and modelling the biological processes in living system. The modelling ranges from simple molecules to cell based systems as an alternate platform to <i>in vitro</i> and <i>in vivo</i> studies.						

Course Outcomes	
CO1	Understand the basic concepts and principles of computational modeling and its advantages.
CO2	Understand the concepts and utility of system biology tools such as modeling tools and databases such as Gene Ontology and Reactome.
CO3	Understand the concepts of simulation related to pathways and gene networks.
CO4	Understand the basic concepts of designing of gene circuits and database related to system biology.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Basics to Modeling	Basic Terminology & Principles – The Biology – Modeling – Properties of Models - Advantages of Computational Modeling - Typical Aspects of Biological Systems and Corresponding Models - Network Versus Elements – Modularity- Robustness and Sensitivity - Data integration – Living Science - The human genome landscape.	8	CO1
2	System Tools Biology and Databases	Computer-based Information Retrieval and Examination – Systems Biology Databases and Tools on the Internet- Gene Ontology – Reactome - TRANSFAC and EPD - Genome Matrix - Modeling Tools - Modeling and Visualization- Mathematica and Matlab – Gepasi - E-Cell – PyBioS - Systems Biology Workbench – Cell Designer.	8	CO2
3	Simulations of Pathways	Simulation and pathways: - Whole-cell: Principle and levels of simulation – Virtual Erythrocytes, Pathological analysis. Flux Balance Analysis – metabolomics- and enzymes, Gene Networks: basic concepts, computational model such transcription networks basic concepts.	8	CO3
4	Gene Circuits	Design of Circuits and Databases: Introduction-, databases KEGG and EMP; MetaCyc and AraCyc .Expression databases and various databases related to systems biology. Optional design of gene circuits I: cost and benefit: gene circuits II selection of regulation.	8	CO4

Reference Books:

- Uri Alon. An Introduction to Systems Biology-Design principles of Biological circuits, Chapman and Hall/CRC Taylor francis group, 2007, ISBN 1-58488-642-0.
- L. Alberghina, H.V. Westerhoff. Systems Biology: Definitions and perspectives, Springer, 2005, ISBN 978 3-540-74269-2.
- A. Kriete, R.Eils. Computational systems biology, Academic press, 2005, ISBN 0-12-088786-X.
- E. Klipp, R. Herwig, A. Kowlad, C. Wierling and H. Lehrach. Systems Biology in practice: Concepts, Implementation and applications, 2006, ISBN 10-3-527-31078-9.

e-Learning Source:

- Institute for Systems Biology | Seattle, WA. <https://www.systemsbiology.org>.
- Systems Biology | ISBE Project Website. project.isbe.eu/systems-biology.

PO-PSO CO	Course Articulation Matrix: (Mapping of COs with POs and PSOs)																		
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6	
CO1	2	1	1	2	2	1			2	1		3	2	3	3				
CO2	2	2	2	2	3	1			2	1		3	2	3	3				
CO3	2	2	2	2	3	1			2	1		3	2	3	3				
CO4	2	2	2	2	3	1			2	1		3	2	3	3				

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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Integral University, Lucknow

Effective from Session: 2020 -21							
Course Code	BE 624	Title of the Course	Chemoinformatics and Pharmacogenomics	L	T	P	C
Year	2	Semester	3	2	1	0	3
Pre-Requisite	None	Co-requisite	BE 620				
Course Objectives	The objective of the course is to introduce the student of the main experimental designs and tools applied in genetics and genomics and approaches for genetic and genomic data analysis, and next generation sequencing to different chemoinformatics methods, use of chemoinformatics in modern drug research, design, organisation, management, retrieval, analysis and visualisation of chemical information. In particular the student is able to: understand the role of SNP's genetic variability, pharmacogenomics and its application in drug design personalized medicine.						

Course Outcomes				
CO1	Explain the concept of design and applications of chemical databases.			
CO2	Analyze the important chemoinformatics tools required in the process of drug discovery.			
CO3	Understand the concept of pharmacogenomics and its current developments.			
CO4	Understand the concept of drug metabolism and correlate it with drug response pattern in human pharmacokinetic studies.			
Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Computers in chemical research	Introduction to Chemoinformatics, Representation and manipulation of 2D and 3D molecular structures, Chemical Databases - Design, Storage & Retrieval methods, Overview of PubChem and ChEBI databases.	8	CO1
2	HTS	Design and Analysis of High-throughput screening, Virtual Screening, Common tools for Virtual screening, Prediction of ADME-TOX properties of chemical compounds, Chemoinformatics tools for drug discovery.	8	CO2
3	Pharmacogenomics	History and overview, Concept of Genomic medicine: current status and application in various diseases. Role of SNP's in pharmacogenomics and case study, Construction and application of Genomic library.	8	CO3
4	Pharmacogenomics and drug design	Need for protein structure information, Mutation in drug targets, In silico drug design of small molecules at genetic level, Drug metabolism: Role of cytochromes P450; The genetics of drug metabolism and pharmacogenomics. Challenges of Pharmacogenomics.	8	CO4

Reference Books:

Proteome Research: New Frontiers in Functional Genomics; Publisher: Springer; Edition Year: 2007

Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins; Publisher: John Wiley & Sons Ltd; Edition Year: 2005.

Bioinformatics for Systems Biology; Publisher: Springer; Edition Year: 2009.

Chemoinformatics: A Textbook; Publisher: John Wiley & Sons Ltd; Edition Year: 2005.

e-Learning Source:

The Drug Discovery Pipeline; Chloé-Agathe Azencott

<http://cazencott.info/dotclear/public/lectures/2014-S1133-drugdiscovery.notes.pdf>

Chemoinformatics J. Polanski

<http://booksite.elsevier.com/brochures/compchemometrics/PDF/Chemoinformatics.pdf>

Pharmacogenomic step toward personalized medicine; Hong-Guang Xie

<https://www.fda.gov/downloads/Drugs/ScienceResearch/ResearchAreas/Pharmacogenetics/m119614.pdf>

Jenny Viklund & Fredrik Rahm (Sprint Bioscience): Marvin Live for structure-based drug design: Chem axon:

https://www.youtube.com/watch?v=5gzxQC_mMX0

Course Articulation Matrix: (Mapping of COs with POs and PSOs)																		
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3	PSO5	PSO6	PSO7
CO1	2	1	1	2	2	1	1	1	2	1	1	2	3	2	3			
CO2	2	2	2	2	3	1	1	1	2	1	1	3	2	3	3			
CO3	2	2	2	2	3	1	1	1	2	1	2	3	1	2	2			
CO4	2	2	2	2	3	2	1	2	1	2	2	3	1	2	2			

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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Integral University, Lucknow

Effective from Session:							
Course Code	BE-625	Title of the Course	COMPUTER-AIDED DRUG DESIGN LAB	L	T	P	C
Year	II	Semester	III	0	0	4	4
Pre-Requisite	None	Co-requisite	None				
Course Objectives	To obtain hands-on-training on the different tools for computer-aided drug design						

Course Outcomes	
CO1	Retrieve the protein structures from PDB and perform energy minimization studies. The students will become efficient in visualizing and commenting on the active sites of the retrieved protein structures using Accelrys Discovery studio visualizer.
CO2	Identify the ligand binding sites in the protein molecules using Q-site Finder.
CO3	Retrieve the chemical compounds from the PubChem database and convert them into suitable pdb, asn and mol formats using Open Babel.
CO4	Perform the protein-ligand docking experiments using AutoDock Tools and the protein-protein docking experiments using the Z-DOCK server; and draw out important inferences.
CO5	Check the Drug-Likeliness properties of the given chemical compound using Lipinski's Rule of Five, and the <i>in silico</i> toxicity studies of the given chemical compound and draw out the important inferences.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Experiment No. 1 and 2	To retrieve the protein structures from PDB and perform its energy minimization studies by applying suitable force fields. To visualize and comment on the active sites of the retrieved protein structures using the Accelrys Discovery studio visualizer.	8	1
2	Experiment No. 3	To identify the ligand binding sites in the protein molecules using Q-site Finder.	8	2
3	Experiment No. 4	To retrieve the chemical compounds from the PubChem database in the sdf format and convert it into suitable pdb, asn and mol format using Open Babel.	8	3
4	Experiment No. 5 and 6	To perform the protein-ligand docking experiments using AutoDock Tools and draw out important inferences. To perform the protein-protein docking experiments using Z-DOCK the server and draw out important inferences.	8	4
5	Experiment No. 7 and 8	To check the Drug-Likeliness properties of the given chemical compound using Lipinski's Rule of Five. To carry out the <i>in silico</i> toxicity studies of the given chemical compound and draw out the important inferences.	8	5

Reference Books:

- Andrew Leach; Molecular Modelling: Principles and Applications (2nd Edition), Prentice Hall, 2001, ISBN 13: 9780582382107.
- Barry A Bunin, Brian Siesel, Guillermo Morales, Jurgen Bajorath; Chemoinformatics: Theory, Practice, & Products, Springer Science & Business Media, 2006.
- Wolff, M E Ed.; Burger's Medicinal Chemistry and Drug Discovery, John Wiley and Sons, 2010, New York.
- H. Fenniri; Combinatorial Chemistry—A practical Approach, Oxford University Press, 2000, UK.

e-Learning Source:

- Computational chemistry in drug discovery. European Bioinformatics Institute EMBL <https://www.youtube.com/watch?v=9DESu1CWbRQ>.
- Andrew McCammon: Molecular Dynamics and Drug discovery, **Error! Hyperlink reference not valid.** <https://www.youtube.com/watch?v=uilZysMFcKk>.

PO-PSO CO	Course Articulation Matrix: (Mapping of COs with POs and PSOs)														
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	3	2	1		3	2		1				2	3	2	2
CO2	3	1	2	1	3		1	1				1	3	3	1
CO3	2	1	1	2	3				2			1	3	2	1
CO4	2	2	2	1	3				1			1	3	2	2
CO5	3	2	3	2	2			1	1			2	2	2	2

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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Integral University, Lucknow

Effective from Session: 2020-21							
Course Code	BE 699	Title of the Course	M Tech Dissertation	L	T	P	C
Year	2	Semester	3	0	0	8	4
Pre-Requisite	None	Co-requisite	None				
Course Objectives	To make students familiar with essential biomedical and life sciences R&D components that will facilitate the successful completion of their dissertation work in the following semester.						

Course Outcomes	
CO1	Students will learn the searching of useful and authentic scientific literature.
CO2	Students will learn to analyze the structural biology data
CO3	Students will get the knowledge of proper information mining
CO4	Students will learn the metabolic pathway modeling
CO5	Students will learn the combinatorial chemistry concepts.

Unit No.	Title of the Experiment	Content of Unit	Contact Hrs.	Mapped CO
1	Literature survey	Retrieval of articles from PubMed and PubMed Central.	10	1
2	Structural biology	Retrieval of structural data of biological macromolecules using 3D repository databases.	10	2
3	Data mining	Information mining of drug molecules and their trends towards data-powered health.	10	3
4	Pathway modeling	Creation of publishable pathway models using online tools.	10	4
5	Combinatorial modeling	Combinatorial design of small molecules and their optimization.	8	5

Reference Books:
Bioinformatics for Systems Biology; Publisher: Springer; Edition Year: 2009.
Gupta, S.P., Statistical Methods; S. Chand & Sons, NewDelhi.
Andrew Leach; Molecular Modelling: Principles and Applications (2nd Edition), Prentice Hall, 2001, ISBN 13: 9780582382107
e-Learning Source:
Mendeley: https://www.mendeley.com

Course Articulation Matrix: (Mapping of COs with POs and PSOs)																		
PO-PSO CO	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	1	2	1	3	1	2	1	1	1	1	1	3	3	2	3			
CO2	1	2	3	1	1	2	1	1	1	1	1	3	3	1	3			
CO3	1	2	1	1	1	2	3	1	1	1	1	3	3	3	3			
CO4	1	2	1	3	1	2	1	1	1	1	1	3	3	3	3			
CO5	1	2	1	3	1	2	1	1	1	1	1	3	3	2	3			

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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Integral University, Lucknow

Effective from Session: 2020-2021							
Course Code	BE699	Title of the Course	M. Tech Dissertation	L	T	P	C
Year	II	Semester	IV	0	0	4	2
Pre-Requisite	None	Co-requisite	None				
Course Objectives	To make students familiar with essential biomedical and life sciences R&D components that will facilitate the successful completion of their dissertation work in the following semester.						

Course Outcomes	
CO1	Skill to perform a review of available literature effectively to present the research gap.
CO2	Capability to build, retrieve, and optimize the 3D structures of biological macromolecules using in-silico tools.
CO3	Empower users with relevant drug information and advanced insights using clinical drug data API
CO4	Competency in applying various engineering and technological tools to create biological pathways.
CO5	Capability to design and optimize small molecules using different tools of combinatorial chemistry.

Unit No.	Title of the Unit	Content of Unit	Contact Hrs.	Mapped CO
1	Retrieval of research articles	Retrieval of articles from PubMed and PubMed Central.	5	CO 1
2	3D structure retrieval of biological macromolecules	Retrieval of structural data of biological macromolecules using 3D repository databases.	5	CO 2
3	Drug data mining	Information mining of drug molecules and their trends towards data-powered health.	5	CO 3
4	Construction of biological pathways	Creation of publishable pathway models using online tools.	5	CO 4
5	Combinatorial Design	Combinatorial design of small molecules and their optimization.	5	CO 5

Reference Books:

1. Fundamental Concepts of Bioinformatics - Dan E. Krane, Michael L. Raymer, Pearson education.
2. Sequence structure and Database – Des Higgins, Willice Taylor, oxford press
3. Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, by Andreas D. Baxeavanis, B. F. Francis Ouellette, Wiley-Interscience,
4. Sequence and Genome Analysis by David W. Mount - Cold Spring Harbor Laboratory
5. Bioinformatics and Functional Genomics; by Jonathan Pevsner; Wiley-Liss
6. Introduction to Bioinformatics; Arthur M. Lesk; Oxford University Press

e-Learning Source:

<https://www.vlab.co.in/broad-area-biotechnology-and-biomedical-engineering>

PO-PSO CO	Course Articulation Matrix: (Mapping of COs with POs and PSOs)														
	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12	PSO1	PSO2	PSO3
CO1	0	0	0	3	3	0	0	3	3	3	0	3	3	2	2
CO2	0	0	0	3	3	0	0	3	3	3	0	3	3	3	1
CO3	0	0	0	0	3	0	0	0	3	3	0	3	3	2	1
CO4	0	0	0	3	3	0	0	0	3	0	0	3	3	2	2
CO5	0	0	0	3	3	0	0	3	3	3	0	3	2	2	2

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Name & Sign of Program Coordinator	Sign & Seal of HoD
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