Integral University
M. TECH. BIOINFORMATICS
(w.e.f. Session 2020-21)
(Students admitted 2020 onwards)

2nd Year **3rd Semester**

S. No.	Course Category	Subject Code	Subject	Periods and Credits				Evaluation Scheme				Subject Total
								Sessional (CA)			ESE	
				L	T	P	C	CT	TA	Total		
1	DC	BE-620	Computer Aided Drug Design	3	1	0	4	40	20	60	40	100
2	DE		Departmental Elective 2	2	1	0	3	40	20	60	40	100
3	DE		Departmental Elective 3	2	1	0	3	40	20	60	40	100
4	DC	BE-604*	Advances in Molecular Techniques	2	1	0	0*	40*	20*	60*	40*	100*
5	DC	BE-603	Colloquium	0	0	4	0*	40*	20*	60*	40*	100*
6	DC	BE-699	M.Tech. Dissertation	0	0	8	4	40	20	60	40	100
7	DC	BE-625	Computer Aided Drug Design Lab	0	0	4	2	40	20	60	40	100
Total				**9**	**4**	**16**	**16**	**200**	**100**	**300**	**200**	**500**

* A zero-credit foundation course. Candidate has to pass this course by securing at least 50% marks.

L: Lecture **T**: Tutorial **P**: Practical **C**: Credit **CA**: Continuous Assessment

CT: Class Test **TA**: Teacher's Assessment **ESE**: End Semester Examination

DC: Departmental Core **DE**: Departmental Elective

Departmental Electives 2

1. Applied Genomics (BE-621)
2. Protein Informatics (BE-622)

Departmental Electives 3

1. System Biology (BE-623)
2. Chemoinformatics and Pharmacogenomics (BE-624)

COMPUTER AIDED DRUG DESIGN
BE-620

Pre-requisite	Co-requisite	L	T	P	C
None	None	3	1	0	4

Objective: 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.

UNIT I	**Stages of Drug Designing**	**8**
	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.	
UNIT II	**Drug Targets**	**8**
	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.	
UNIT III	**Direct Drug Design**	**8**
	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.	
UNIT IV	**Indirect Drug Design**	**8**
	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.	
UNIT V	**Drug Pharmacokinetics**	**8**
	Pharmacokinetic analyses of Drugs: Quantitative Structure Property Relationship (QSPR) studies –important parameters and significance, ADME- TOX studies, Concept of Drug-likeliness and its applicability.	

References Books:

1. Harren Jhoti, Andrew R. Leach; Structure- based Drug Discovery, Springer, 2007, ISBN 1402044070
2. Andrew Leach; Molecular Modelling: Principles and Applications (2nd Edition), Prentice Hall, 2001, ISBN 13: 9780582382107
3. R E Hubbard; Structure-based Drug Discovery: An Overview, Royal Society of Chemistry, 2006
4. Barry A. Bunin, Brian Siesel, Guillermo Morales, Jurgen Bajorath; Chemoinformatics: Theory, Practice, & Products, Springer Science & Business Media, 2006.

Research publications:

1. Zhang W, Pei J, Lai L. Computational Multitarget Drug Design, J ChemInf Model, 2017. doi: 10.1021/acs.jcim.6b00491.
2. Leelananda SP, Lindert S. Beilstein. Computational methods in drug discovery, J Org Chem,. 2016 Volume 12. Pg- 2694-2718.

Websites:

1. **Error! Hyperlink reference not valid.** simulation software: www.schrodinger.com
   Online document/video/audio

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

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

2. Webinar recording: a sequel for beginners: ligand-based drug design — the basics
   https://www.youtube.com/watch?v=ef5EaooBYUU

APPLIED GENOMICS
BE-621

Pre-requisite	Co-requisite	L	T	P	C
BE 521	None	**2**	**1**	**0**	**3**

Objective: 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.

UNIT I	**Genome**	**8**
	Definition of genome, GenomeMap: TypesofGenomemaps and theiruses, High and low-resolution map, Polymorphic markers: LINEs, SINEs, RFLP, SNP; Typesofmaps: Cytogeneticmap, Linkagemap, Transcript map, Physicalmap.	
UNIT II	**Gene Prediction**	**8**
	DNA sequencing: Sanger's method and Maxam Gilbert method; Large scale genome sequencing strategies: Shot gun 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.	
UNIT III	**Structural and Functional Genomics**	**8**
	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.	
UNIT IV	**Gene Expression analysis**	**8**
	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.	

References 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;
5. 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.

Research Publications:

1. Lilian T. C. Franca, Emanuel Carrilho and Tarso B. L. Kist; A review of DNA sequencing techniques; Quarterly Reviews of Biophysics; Volume number: 35; Page: 169-200; Year: 2002.
2. Adi L. Tarca, Roberto Romero and Sorin Draghici, Analysis of microarray experiments of gene expression profiling; Am J Obstet Gynecol.; Volume number: 195; Page: 373-388; Year: 2006.
3. Hrmova M. and Fincher GB.; Functional genomics and structural biology in the definition of gene function.; Methods Mol Biol. Volume number: 513; Page: 199-227; Year: 2009.

Websites:

1. Biology Animation Library
2. https://www.dnalc.org/resources/animations/cycseq.html

Online document/video/audio:

1. DNA sequence analysis methods-I
   Dr. Vikash Kumar Dubey
   http://nptel.ac.in/courses/102103017/pdf/lecture%2029.pdf

2. DNA Sequence Analysis Methods-II
   Dr. Vikash Kumar Dubey
   http://nptel.ac.in/courses/102103017/pdf/lecture%2030.pdf

3. Artificial Intelligence & Molecular Biology
   Lawrence Hunter
   http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.104.662&rep=rep1&type=pdf

4. Lecture Notes for Methods in Cell Biology
   http://www.tulane.edu/~wiser/methods/notes.pdf
   Mark F. Wiser

PROTEIN INFORMATICS
BE-622

Pre-requisite	Co-requisite	L	T	P	C
BE528	**BE-620**	**2**	**1**	**0**	**3**

Objective: 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 substantial understanding of popular computational methods, as well as molecular tools and techniques of protein sequence and structure analysis methods applied to the real data.

UNIT I	**Introduction to Protein Structure and Databases**	**8**
	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.	
UNIT II	**Principles and Applications of Spectroscopy**	**8**
	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.	
UNIT III	**Introduction to Chromatography and Electrophoresis**	**8**
	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.	
UNIT IV	**Applied Proteomics**	**8**
	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.	

References Books:

1. Protein Bioinformatics: From Sequence to Function; Academic Press, 2011; ISBN 0123884241, 9780123884244.
2. Principles and Techniques of Practical Biochemistry; Cambridge University Press, 16-Mar-2000Reprint 4 March 2010; ISBN 0521731674; 978-0521731676.
3. Essential Bioinformatics; Cambridge University Press, 2006; ISBN 113945062X, 9781139450621.
4. Lehninger Principles of Biochemistry; W. H. Freeman; 13 February 2013; ISBN 1464109621, 978-1464109621.

Research publications:

1. Saeys Y, Inza I, Larrañaga P; A review of feature selection techniques in bioinformatics; Bioinformatics; Volume 19; 2507-2517; 2007

Websites:

1. Predicting Protein-Protein Interactions from the Molecular to the Proteome Level; https://www.ncbi.nlm.nih.gov/pubmed/

2. Keskin O, Tuncbag N, Gursoy A.; DOI: 10.1021/acs.chemrev.5b00683

Online document/video/audio:

1. Analytical Biochemistry Dr. Ashwani K. Sharma, IIT Roorkee; http://nptel.ac.in/courses/102107028/
2. Bioanalytical Techniques and Bioinformatics; Dr. Vishal Trivedi and Dr. Nitin Chaudhary, IIT Guwahati;
    a. http://nptel.ac.in/courses/102103044/
3. Introduction to Proteomics; Dr. Sanjeeva Srivastava, IIT Bombay; https://onlinecourses.nptel.ac.in/noc16_bt07

SYSTEM BIOLOGY
BE-623

Pre-requisite	Co-requisite	L	T	P	C
BE-525	**None**	**2**	**1**	**0**	**3**

Objective: 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 *in vitro* and *in vivo* studies.

UNIT I	**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**
UNIT II	**System Biology Tools 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**
UNIT III	**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**
UNIT IV	**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**

References Books:

1. 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.
2. L. Alberghina, H.V. Westerhoff. Systems Biology: Definitions and perspectives, Springer, 2005, ISBN 978 3-540-74269-2.
3. A. Kriete, R.Eils. Computational systems biology, Academic press, 2005, ISBN 0-12-088786-X.
4. 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.

Websites:

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

Online document/video/audio:

1. Introduction to Computational and Systems Biology. Foundations of Computational and Systems Biology, Spring 2014, MIT OpenCourseWare, http://ocw.mit.edu/7-91JS14.
2. Computational Methods in Systems Biology, Douglas Lauffenburger, MIT, GEM4 Summer School 2012, https://www.youtube.com/watch?v=hGR_gJjRWsc.

CHEMOINFORMATICS AND PHARMACOGENOMICS
BE-624

Pre-requisite	Co-requisite	L	T	P	C
None	**BE 620**	**2**	**1**	**0**	**3**

Objective: 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'sgenetic variability, pharmacogenomics and its application in drug design personalized medicine.

UNIT I	**Computers in chemical research**	**8**
	Introductionto Chemoinformatics, Representation and manipulation of 2D and 3D molecularstructures, Chemical Databases - Design, Storage & Retrievalmethods, Overviewof PubChem and ChEBIdatabases.	
UNIT II	**HTS**	**8**
	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.	
UNIT III	**Pharmacogenomics**	**8**
	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.	
UNIT IV	**Pharmacogenomics and drug design**	**8**
	Need for protein structure information, Mutation in drug targets, Insilico drug design of small molecules at genetic level, Drug metabolism: Role of cytochromes P450; The genetics of drug metabolism and pharmacogenomics. Challenges of Pharmacogenomics.	

References Books:

1. Proteome Research: New Frontiers in Functional Genomics; Publisher: Springer; Edition Year: 2007.
2. Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins; Publisher: John Wiley & Sons Ltd; Edition Year: 2005.
3. Bioinformatics for Systems Biology; Publisher: Springer; Edition Year: 2009.
4. An Introduction to Chemoinformatics;
5. Publisher: springer; Edition Year: 2007.
6. Chemoinformatics: A Textbook; Publisher: John Wiley & Sons Ltd; Edition Year: 2005.
7. Concepts in Pharmacogenomics; Publisher: American Society of Health-System Pharmacists; Edition Year: 2010.

Research Publications:

1. Thomas Engel; Basic Overview of Chemoinformatics; Journal of Chemical Information and Modeling; Volume number: 46; Page: 2267-77; Year: 2006.
2. Chen WL; Chemoinformatics: past, present, and future. J ChemInf Model. Volume number: 46; Page: 2230-55; Year: 2006.
3. Margret R. Hoehe; Genetic variation and pharmacogenomics: concepts, facts, and challenges; Dialogues ClinNeurosci; Volume number: 6; Page: 05-26; Year: 2004.
   A. Surendiran, S.C. Pradhan, and C. Adithan; Role of pharmacogenomics in drug discovery and development.
4. Indian J Pharmacol.; Volume number: 40; Page: 137-143; Year: 2008.

Online document/video/audio:

1. ChemoinformaticsJ. Polanski
   http://booksite.elsevier.com/brochures/compchemometrics/PDF/Chemoinformatics.pdf
2. Pharmacogenomic step toward personalized medicine; Hong-GuangXie
   https://www.fda.gov/downloads/Drugs/ScienceResearch/ResearchAreas/Pharmacogenetics/m119614.pdf
3. The Drug Discovery Pipeline; Chloé-AgatheAzencott
   http://cazencott.info/dotclear/public/lectures/2014-S1133-drugdiscovery.notes.pdf

COMPUTER AIDED DRUG DESIGN LAB
BE-625

Pre-requisite	Co-requisite	L	T	P	C
None	**None**	**0**	**0**	**4**	**2**

Objective: To obtain hands-on-training on the different tools for computer-aided drug design

List of Experiments	1. To retrieve the protein structures form PDB and perform its energy minimization studies by applying suitable force fields. 2. To visualize and comment on the active sites of the retrieved protein structures using Accelrys Discovery studio visualizer. 3. To identify the ligand binding sites in the protein molecules using Q-site Finder. 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. 5. To perform the protein-ligand docking experiments using AutoDock Tools and draw out important inferences. 6. To perform the protein-protein docking experiments using Z-DOCK server and draw out important inferences. 7. To check the Drug-Likeliness properties of the given chemical compound using Lipinski's Rule of Five. 8. To carry out the *in silico* toxicity studies of the given chemical compound and draw out the important inferences.

References Books:

1. Andrew Leach; Molecular Modelling: Principles and Applications (2nd Edition), Prentice Hall, 2001, ISBN 13: 9780582382107.
2. Barry A Bunin, Brian Siesel, Guillermo Morales, Jurgen Bajorath; Chemoinformatics: Theory, Practice, & Products, Springer Science & Business Media, 2006.
3. Wolff, M E Ed.; Burger's Medicinal Chemistry and Drug Discovery, John Wiley and Sons, 2010, New York.
4. H. Fenniri; Combinatorial Chemistry–A practical Approach, Oxford University Press, 2000, UK.
5. D. Frenkel, B. Smit; Understanding Molecular Simulation: From Algorithms to Applications, Elsevier 2012.
6. Stephen Misener, Stephen A. Krawetz . Bioinformatics Methods and Protocols, Humana Press, 1999, ISBN 978-0-89603-732-8.

Online document/video/audio:

1. Computational chemistry in drug discovery. European Bioinformatics Institute - EMBL-EBIhttps://www.youtube.com/watch?v=9DESulCWbRQ.
2. Andrew McCammon: Molecular Dynamics and Drug discovery, https://www.youtube.com/watch?v=ui1ZysMFcKk.

COLLOQUIUM

BE-603

Pre-requisite	Co-requisite	L	T	P	C
None	None	0	0	4	0

Objective: To acquaint the student with the various techniques used in contemporary research in food technology that will be useful in successful completion of their project work in the fourth semester**.**

1. Searching for scientific literature (Sciencedirect, SCOPUS, Google Scholar etc.)
2. Exposure to different manuscript forms (Review, Short note, Research article, Communication).
3. Design of experiments in research.
4. Basic statistical analysis (ANOVA, RSM, ANN).
5. Different manuscript formats and referencing styles (Use of Mendeley, Endnotes.).
6. Publishing manuscripts (plagiarism check, cover letters, suggesting reviewers etc).
7. Thesis writing and presentation.
8. Exposure of students to research in laboratory.
9. Ethics in conducting research.

References:

1. Sciencedirect:https://www.sciencedirect.com/
2. Mendeley:https://www.mendeley.com

Books:

1. Gupta, S.P., Statistical Methods; S. Chand & Sons, NewDelhi.
2. Jerold H.Zar (2009): Bio-statistical Analysis, 4th Edition, Pearson EducationInc.

ADVANCES IN MOLECULAR TECHNIQUES
BE-604

Pre-requisite	Co-requisite	L	T	P	C
None	None	2	1	0	0

Objective: To acquaint the students with the principles and application of the latest techniques in molecular biology.

UNIT I	**PCR-based Techniques** Principle and applications of PCR; RACE; DD-RTPCR; Degenerate PCR, TA cloning, Realtime PCR, Scorpion probes, Site directed mutagenesis, PCR-based mutagenesis, Error-prone PCR.	**8**
UNIT II	**Gene Silencing** Antisense RNA technique, Sense co-supression in plants and animals, RNAi, Gene silencing, Ribozymes.	**8**
UNIT III	**Sequencing Techniques** Rapid DNA and RNA sequencing techniques, Sanger method, Maxam and Gilbert procedure, Automated DNA sequencing, Pyrosequencing, Genomics: High throughput, Shot gun, Clone contig, Microarray, Protein microarray	**8**
UNIT IV	**Molecular Markers and other Molecular Techniques** Molecular markers, RFLP, RAPD, AFLP, SCAR, STS, Microsatellites, SSCP, Yeast two-hybrid system, DNase foot printing.	**8**

References Books:

1. Molecular Cloning; Sambrook and Russel, Cold Spring Harbor Laboratory.
2. Gene Cloning and DNA Analysis: An Introduction, T.A. Brown; Blackwell Publications.
3. Principles of Gene manipulation and genomics; Primrose and Twyman; Wiley Publishing.

Integral University
M. TECH. BIOINFORMATICS
(w.e.f. Session 2020-21)
(Students admitted 2020 onwards)

2nd Year **4th Semester**

S. No	Course Category	Subject code	Name of the Subject	Periods				Evaluation Scheme				Subject Total
				L	T	P	C	Sessional (CA)			ESE	
								CT	TA	Total		
1.	DC	BE-699	M.Tech. Dissertation	0	0	0	4	40	20	60	40	100
2.	DC	BE-699	M.Tech. Dissertation	0	0	0	4	40	20	60	40	100
3.	DC	BE-699	M.Tech. Dissertation	0	0	0	4	40	20	60	40	100
4.	DC	BE-699	M.Tech. Dissertation	0	0	0	4	40	20	60	40	100
Total				**0**	**0**	**0**	**16**	**160**	**80**	**240**	**160**	**400**

L: Lecture **T**: Tutorial **P**: Practical **C**: Credit **CA**: Continuous Assessment

CT: Class Test **TA**: Teacher's Assessment **ESE**: End Semester Examination

DC: Departmental Core