Course title: Bioinformatics and computational biology			
Course code: BBP 173	**No. of credits:** 3	**L-T-P:** 29-16-0	**Learning hours:** 45
Pre-requisite course code and title (if any): Science graduate			
Department: Department of Biotechnology			
Course coordinator: Prof Mukesh Jain		**Course instructor:** Prof Mukesh Jain / Dr. Rohini Garg	
Contact details: mjain@jnu.ac.in			
Course type: Core		**Course offered in:** Semester 3	

Course description:

The area of Bioinformatics is a blend of two dynamic subject areas; biology and computing. The increasingly large volumes of biological data from genome sequencing activities cannot be stored, visualized and analysed without the power of modern information technology. In this course in the student gets an exposure to various facets of bioinformatics. It aims to provide basic understanding of how biological data is stored and retrieved from various biological databases. Further, this course deals with the methodologies of sequence analysis and phylogenetic analysis. It will also focus on in-silico prediction of protein structure, protein-ligand docking and molecular simulations. There will be emphasis on exposing the student to wide variety of tools which they can use in their day-to-day wet lab experiments.

Course objectives:

1. To learn the core areas of Bioinformatics like sequence analysis, phylogenetic trees, genomics, proteomics
2. To explore the students to applied areas of Bioinformatics like homology modeling and simulation methods.
3. To provide knowledge about predicting the structure of biomolecules, structure prediction and validation.

Course contents

Module	Topic	L	T	P
Module 1: Phylogenetics and structure prediction				
1	**Sequence analysis** Introduction to Biological sequences, Introduction to sequence editing tools (EMBOSS, BioEdit, Ensembl)	4	2	
2	**Molecular Phylogenetics** Molecular evolution, Overview and protocols, Nature of data use, Probabilistic models and associated algorithms, Probabilistic models of evolution, Maximum likelihood algorithm, Phylogenetic analysis algorithms, Distance based methods: UPGMA, Neighbour-joining method, Character based methods: Maximum likelihood, Maximum parsimony, Reliability methods: Bootstrap validation, Jack- knife validation	7	3	

3	**Protein structure prediction** Introduction to protein structure, Protein stability and folding, Protein stability and denaturation, Protein folding, Application of hydrophobicity, Protein Structure Prediction and Modeling, Critical Assessment of structure prediction (CASP) ,Secondary structure prediction (Chau-Fasman method, GOR method, Nearest neighbor method, Neural network method)	7	2	
4	**Profiles and Hidden markov models** Profiles, Hidden Markov models, Markov process, Markov models and Hidden Markov models (HMM), Components of Profile HMM, Building HMM, HMM scoring algorithms.	4	2	
Module 2: Molecular Modelling and Simulation				
1	**Homology modelling** Introduction to modelling , tools and softwares , Seven steps of homology modelling, Application in drug designing	3	3	
2	**Molecular Modelling and Simulation** Overview of molecular modelling, Molecular modelling methods (Semi-empirical methods, Empirical methods), Molecular Dynamics, Newton's equations for many particles, Types of dynamics simulation, Conformational searching using MD and other methods, Free energy calculations, Docking simulations, Rigid docking, Flexible docking, Scoring schemes.	4	4	
	Total	**29**	**16**	**0**

Evaluation criteria:

1. Test 1: 30%
2. Test 2: 30%
3. Test 3 (end semester) 40%

Learning outcomes:

1. An understanding of data analysis approaches.
2. The students will be familiar with the application of miolecular phylogenetic analysis and structural prediction approaches.
3. Ability to perform molecular modeling and simulation.

Pedagogical Approach:

Classroom/online lectures and tutorials, with a major emphasis on the detailed discussion of original research articles from scientific journals in class.

Skill Set:

1. Bioinformatics: homology searches, sequence alignment, motifs, phylogenetics, protein folding and structure prediction.
2. Molecular modeling and simulation.
3. Sequence and phylogenetic analysis

Employability:

1. Bioinformatics and software development companies.
2. Academic Institutions and Industries involving R&D.

Materials:

Suggested readings:

1. Cynthia Gibas, Per Jambeck, "Developing Bioinformatics Computer Skills", O'Reilly Media,Inc., 2001.
2. David Edwards, Jason Eric Stajich, David Hansen, "Bioinformatics: Tools and Applications", Springer, 2009.
3. David W Mount, "Bioinformatics: Sequence and genome analysis", Cold spring harbor laboratory press, 2nd edition, 2004.
4. Stan Tsai C., "Biomacromolecules: Introduction to Structure, Function and Informatics", John Wiley & Sons, 2007.
5. Attwood T K, D J Parry-Smith, "Introduction to Bioinformatics", Pearson Education, 2005.
6. Parag Rastogi, "Bioinformatics Methods And Applications: Genomics Proteomics And Drug Discovery", PHI Learning Pvt. Ltd., 3rdedition, 2008
7. David M. Webster, "Protein Structure Prediction: Methods and Protocols", Methods in molecular biology, vol.143 , 2000.
8. Arthur Lesk, "Introduction to Protein Science: Architecture, Function and Genomics", Oxford University Press, 2010.
9. Masatoshi Nei, Sudhir Kumar , "Molecular Evolution and Phylogenetics", Oxford University Press, 2000.
10. Alessandra Nurisso, Antoine Daina and Ross C. Walker, "Homology Modeling : Methods and Protocols", Springer Protocols , 2012.

Web Resources

1. ww.ncbi.nlm.nih.gov/
2. www.ddbj.nig.ac.jp/
3. www.embl.org/
4. www.ebi.ac.uk/Tools/msa/clustalo/
5. www.expasy.org/

Other readings

1. Altschul SF, Gish W, Miller W, Myers EW, Lipman DJ, "Basic local alignment search tool" , J Mol Biol., 1990.
2. Elmar Krieger, Sander B. Nabuurs, and Gert Vriend, "HOMOLOGY MODELING", Structural Bioinformatics, 2003.
3. Gregoret LM, Cohen FE ,"Novel method for the rapid evaluation ofp acking in protein structures" , J Mol Biol ,1990.
4. Hang Chen, Fei Gu,and Zhengge Huang , "Improved Chou-Fasman method for protein secondary structure prediction" , BMC Bioinformatics,2006.

Additional information (if any):

Student responsibilities:

1. Class attendance.
2. Study of course materials as specified by the instructor

Course reviewers:

1. Dr. Gitanjali Yadav, Scientist IV, NIPGR, New Delhi
2. Dr. Debasis Mohanty, NII, New Delhi