SEMESTER S7

COMPUTATIONAL BIOLOGY

Course Code	**PEBBT743**	**CIE Marks**	40
Teaching Hours/Week (L: T:P: R)	2:0:1:0	**ESE Marks**	60
Credits	3	**Exam Hours**	2 Hrs. 30 Min.
Prerequisites (if any)	Basic Knowledge of Bioinformatics	**Course Type**	Theory

Course Objectives:

This course will enable students to

1. Utilize network-based methods to model biological systems and analyze biological networks.
2. Critically assess and apply recent research papers and developments in the field of AI-driven computational biolog

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SYLLABUS

Module No.	Syllabus Description	Contact Hours
1	**Electronic Structure Methods** Quantum chemical methods are semi-empirical and ab initio methods. Conformational analysis, energy minimization, and predicting the mechanism of organic reactions using electronic structure methods.	**8**
2	**Molecular Modeling** Bioactive vs. global minimum conformations. Automated methods of conformational search. Advantages and limitations of available software. Molecular graphics. Computer methodologies behind molecular modeling including artificial intelligence methods.	**8**
3	**Structure-Activity Relationships In Drug Design** Qualitative versus quantitative approaches advantages and disadvantages. Random screening, Non-random screening, rational approaches to lead discovery. Homologation, chain branching, ring-chain transformations. Insights into molecular recognition phenomenon. Structure-based drug design, ligand-based drug design.	**8**

4	**QSAR: Electronic Effects** Hammett equation, lipophilicity effects. Hansch equation, steric effects. Taft equation. Experimental and theoretical approaches for the determination of physicochemical parameters, parameter interdependence: Regression analysis, Descriptor calculation. The importance of biological data in the correct form; 2D QSAR; and 3D-QSAR examples of CoMFA and CoMSIA. **Molecular Docking** Rigid docking, flexible docking, manual docking. Advantages and disadvantages of Flex-X, FlexS, Autodock, and Dock software, with successful examples. Dynamics of drugs, biomolecules, drug-receptor complexes, Monte Carlo simulations, and Molecular dynamics in performing conformational search and docking.	**12**

Course Assessment Method
(CIE: 40 marks, ESE: 60 marks)

Continuous Internal Evaluation Marks (CIE):

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Attendance	Assignment/ Microproject	Internal Examination-1 (Written)	Internal Examination- 2 (Written)	Total
5	15	10	10	40

End Semester Examination Marks (ESE)

In Part A, all questions need to be answered and in Part B, each student can choose any one full question out of two questions

Part A	Part B	Total
• 2 Questions from each module. • A total of 8 Questions, each carrying 3 marks (8x3 =24marks)	• Each question carries 9 marks. • Two questions will be given from each module, out of which 1 question should be answered. • Each question can have a maximum of 3 sub-divisions. (4x9 = 36 marks)	60

Course Outcomes (COs)

At the end of the course, students should be able to:

Course Outcome		Bloom's Knowledge Level (KL)
CO1	Develop and apply algorithms for structural bioinformatics and healthcare.	**K6, K3**
CO2	Interpret and practice the fundamental concepts of Molecular Modeling and Computer-aided Drug Design	**K3**
CO3	Develop practical skills in computational approaches to analyze, predict, and engineer biomolecules and biomolecular systems	**K6, K5, K4, K3**
CO4	Find a chemical compound that can fit into a specific cavity on a protein target both geometrically and chemically.	**K3, K5**
CO5	Apply appropriate tools for such modeling, ranging from electronic Structure methods, Molecular modeling, Structure-Activity Relationships in drug design, QSAR, Molecular docking and Molecular dynamics and docking, modeling, and electronic structure methods which leads to new drug target design	**K3**

Note*: K1- Remember, K2- Understand, K3- Apply, K4- Analyse, K5- Evaluate, K6- Create*

CO-PO Mapping Table:

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	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
CO1	3	3			2							2
CO2	3	3	2	2	2				2			2
CO3	3	3	2	2	2	2			2			2
CO4	3	3	2	2	3	2			2			2
CO5	3	3	2		2				2			2

Text Books				
Sl. No	**Title of the Book**	**Name of the Author/s**	**Name of the Publisher**	**Edition and Year**
1	Understanding bioinformatics	Zvelebil, Marketa J., and Jeremy O. Baum	Garland Science	2007
2	Essential bioinformatics.	Xiong, Jin	Cambridge University Press	2006
3	Introduction to Bioinformatics	Teresa K. Attwood, David J Parry-Smith	Pearson Education	1999
4	Bioinformatics – A Practical Guide to the Analysis of Genes and Proteins	Baxevanis AD,Francis Ouellellette BF	Wiley Interscience	2009

Reference Books				
Sl. No	**Title of the Book**	**Name of the Author/s**	**Name of the Publisher**	**Edition and Year**
1	Applied bioinformatics. An introduction	Selzer, Paul M., Richard J. Marhöfer, and Andreas Rohwer	Springer, Verlag	2008
2	Bioinformatics: Methods and Applications	S C Rastogi, N Mendiratta and PRastogi	PHI Learning Private Limited, New Delhi	2015
3	D E Krane and M L Raymer	Fundamental Concepts of Bioinformatics	Pearson Education	2006

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