Proforma for course plan

Course Name: Statistical Mechanics of Biomolecules: Theory and simulation
Course Code: IT 452
Credit: 3 +1 Credits
Course offered to: M.Sc (Sem-III)

Course description: This course aims to provide an elementary introduction to statistical mechanics with special emphasis to molecular systems. Topics include: Boltzmann distribution, ensembles, application of theory to various problems involving discrete and continuous cases. Usage of software like AMBER will be illustrated.

Pre-requisites:

Course Outcome(s) (CO): At the end of the course, the students should be able to

1. Explain the basics of statistical mechanics.
2. Can apply to simple discrete systems.
3. Should have a basic understanding of the usage of statistical mechanics for biomolecular phenomena.

Tentative plan:

Week number	**Lecture topic**	CO met
1-2	A test will be conducted to check students' knowledge of basic physics and maths (to decide the level of teaching). Introduction to statistical mechanics with simple examples. Concept of probability distribution of energies for a system of particles; Boltzmann distribution	CO-1
3-6	Concept of temperature, entropy. Review of the three laws of thermodynamics. Thermodynamics of protein folding. Introduction to literature in protein folding. HP model of protein folding.	CO-1 and CO-2.
7-11	Different ensembles. Exact statistical mechanics of helix-coil transition. Introduction to Molecular dynamics and Monte Carlo simulation. Concept of free energy. Importance of free energy in biology.	CO-1 and CO-2
12-14	Using molecular dynamics package like AMBER real calculations of biomolecules will be introduced.	CO-3

Text Books and References

(1) Statistical Physics (Berkeley lecture series – volume 5) by F. Reif. McGraw-Hill

(2) Statistical Physics of Biomolecules: An Introduction, Dan Zuckerman. CRC Press.

Related articles from journals

Related topics from authentic sources