Lecture Plan for BT 305

1. Genes and Proteins
2. Analysis of protein content and organization
3. Analysis of protein structures
4. Comparative modeling structure prediction algorithms and tools, threading.
5. Empirical force field models; Bond stretching, angle bending and torsional terms, the harmonic oscillator model for molecules.
6. Non-bonded interactions; Van der Waals, electrostatic and hydrogen bonding, United atom force fields and reduced representations,
7. Force field parameterization. Potential Energy Surface; Convergence Criteria, Optimization.
8. multivariable optimization algorithms, minimization methods, steepest descent and conjugate gradient methods.
9. Quiz 1
10. Molecular Dynamics Simulations; Newtonian dynamics; Integrators - Leapfrog and Verlet algorithms,
11. Truncated and shifted-force potentials. implicit and explicit solvation models, periodic boundary conditions. temperature and pressure control in molecular dynamics simulations.
12. Conformational Analysis; Evolutionary algorithms and simulated annealing, clustering and pattern recognition techniques.
13. Monte Carlo Simulation methods; Theoretical aspects and implementation to the Metropolis method, Configurationally biased Monte Carlo simulations.
14. Computational Protein Design
15. Application lecture 1
16. Mid Semester Evaluation, Mid Sem subject and QP discussion
17. Methods in Drug design; Chemical databases, 2D and 3D database search, Similarity Search
18. Scaffold hoping, Lead identification, optimization and validation, Docking
19. De Novo Drug Design, Virtual screening.
20. Quantitative Structure Activity Relationship; Introduction to QSAR, Descriptors QSARs.
21. Regression Analysis and Partial Least Squares Analysis, Combinatorial Libraries.
22. Application lecture 2
23. Quiz 2
24. The human Interactome
25. Elements of Network Theory
26. Protein-Protein Interaction Networks
27. Disease Networks, Diseasome
28. Concluding lecture - Perspectives