B. Tech Biosciences and Bioengineering

BT 305 Computational Biology

2-0-2-6

Syllabus: Analysis of protein content and organization; Analysis of protein structures, comparative modeling, structure prediction algorithms and tools, threading empirical force field models; Bond stretching, angle bending and torsional terms, the harmonic oscillator model for molecules. Non-bonded interactions; Van der Waals, electrostatic and hydrogen bonding, united atom force fields and reduced representations, Force field parameterization. Potential energy surface; Convergence criteria, Optimization; multivariable optimization algorithms, minimization methods, steepest descent and conjugate gradient methods. Molecular dynamics Simulations; Newtonian dynamics; Integrators - Leapfrog and Verlet algorithms, truncated and shifted-force potentials. Implicit and explicit solvation models, periodic boundary conditions. Temperature and pressure control in molecular dynamics simulations. Conformational analysis; Evolutionary algorithms and simulated annealing, clustering and pattern recognition techniques. Monte Carlo Simulation methods; Theoretical aspects and implementation to the Metropolis method, configurationally biased Monte Carlo simulations. Methods in Drug design; Chemical databases, 2D and 3D database search, Similarity Search, Scaffold hoping, Lead identification, optimization and validation, Docking, De Novo Drug Design, Virtual screening. Quantitative structure activity relationship; Introduction to QSAR, descriptors QSARs, regression analysis and partial least squares analysis, combinatorial libraries.

Texts:

1. A. R. Leach, *Molecular Modeling Principles and Applications*, 2nd Edition, Prentice Hall USA, 2001.
2. T. Schlick *Molecular Modeling and Simulation - An Interdisciplinary Guide*, Springer verlag, 2000.
3. B. R. Donald, *Algorithms in Structural Molecular Biology*, Massachusetts Institute of Technology Press, 2011.

References:

1. A. Hinchliffe, *Molecular Modeling for Beginners*, 2nd Edition, John Wiley & Sons Ltd, 2008.
2. P. E. Bourne, *Structural Bioinformtics*, 2nd Edition, Wiley, 2009.
3. D. W. Mount, *Bioinformatics: Sequence and Genome Analysis*, 2nd Edition, CSH Press, 2005.
4. S. G. Kochan and P. Wood, *UNIX Shell Programming*, 3rd Edition, SAMS, 2003.
5. P. Bultinck, *Computational Medicinal Chemistry for Drug Discovery*, Marcel Dekker Inc., 2004.