PGDBD-Elective course I

IT 604 Molecular modeling and simulation

Simulation of biological processes. Equilibrium and steadt state calculations. Hill plot. Van't Hoff equation. Steady state enzyme kinetis. Lineweaver Burk fitting. Eadie-Hifstee fitting. Competitive ingibition.

Simulation of diffusion and transport. Fick's law. Electrophoresis. Countercurrent diffusion. Compartment models in physiology and pharmacokinetics. Periodic dose administration. Oscillations in calcium metabolism.

Regulation and control in metabolism. One-substrate, one-product reactions. Steady state flux calculation. Flux control coefficients.
Models of regulation. Feed-forward loops. Regulation of signaling. Bacterial chemotaxis. Morphogenesis.

Protein and nucleic acid structures and their interactions. Protein structural hierarchy. Turns and loops. Homology modeling.

Basics of molecular dynamics. Software tools for MD simulation in public domain. Gromacs, Amber, NAMD, VMD, Pymol.
Symplectic transformation. Harmonic oscillator example. Linear stability. Resonance condition and artifacts. Multiple-timestep methods. Langevin dynamics. Brownian dynamics. Sampling methods. Coarse graining methods. Biasing approaches.
Similarity and diversity in chemical drugs. Molecular modeling in rational drug design. Problems in chemical libraries. Similarity and diversity sampling.

Advanced topics and current trends.