## Computational Biology I (MTH950)

Fundamentals of biological sciences. (1) Mechanical foundation: Quantum mechanics of biomolecules. The Schrodinger equation; Interaction potentials; Chemical bondings; Intermolecular forces; Classical mechanics and its role in biology; Interconnection between classical mechanics and quantum mechanics. (2) Structure and catalysis: Protein structure and function; single cell DNA and RNA sequences and structures; carbohydrates; Lipids; Enzyme and chemical dynamics; Membranes and transport; Biosignaling; (3) Bioenergetics and metabolism: Principles of bioenergetics; Glycolysis; Fatty acid catabolism; Carbohydrate biosynthesis in plants and bacteria; Metabolic regulations. (4) Information pathways: Genes and chromosomes, Metabolism of DNA, RNA, and protein; Regulation of gene expression. (5) Cellular structure and function; Cellular dynamics and transport. (6) Omics.

## Computational Biology II (MTH950)

Principles of thermodynamics; Statistical ensembles; Maxwell-Boltzmann statistics; Fermi-Dirac and Bose-Einstein statistics; Random work; Stochastic process; Markov process; Master equation; Fokker-Planck equation; Brownian motion and Langevin equation; Autocorrelation; Density matrix; Liouvelle equation; Zwanzig's equation; Linear response theory; Boltzmann equation; Master equation; Theory of liquids; Brownian ratchets; Molecular motor; Biomechanics; Protein membrane interaction; Evolutionary genomics; mathematical approaches to the discovery of gene motifs; Gene regulation; Explanatory and predictive models of cellular growth and interaction; Metabolic circuitry and dynamics; Signal transduction and enzyme dynamics; Phylogenetic analysis; Biosensors; Neuroscience; Electrostatics in metabolic process; Fluid-macromolecule interaction and impact to metabolism; Molecular dynamics and force fields; Monte Carlo; Implicit solvent modeling; Poisson-Boltzmann equation; Poisson-Nernst-Planck (PNP) equations.