UB/HWI Department of Structural Biology
Topical Content of the Courses in Structural Biology

The "functional literacy" background "primer" courses

STB 530. Mathematics and Physics Topics for Biology, Biochemistry and Chemistry

- Selected mathematics topics
  - Matrix and linear algebra
  - Vector and tensor analysis
  - Symmetry group theory
  - Coordinate transformations
  - Fourier analysis
  - Convolutions
  - Probability and statistics
  - Data fitting
  - Error analysis
  - Elementary computer programming (Fortran and/or C)
- Selected physics topics
  - Wave motion
  - Standing waves
  - Traveling waves
  - Electromagnetic radiation
  - Physical optics
  - Scattering theory
  - Electronic and photonic information transmission

STB ###. Molecular Biology and Biochemistry Topics for Mathematics, Physics, Chemistry, Computer Science, and Engineering Students

- Biomolecular Structure and Function
  - Proteins — amino acids, peptides
  - Nucleic acids — bases, sugars, nucleosides, sugar phosphates, nucleotides
  - Carbohydrates — mono-, di-, and poly-saccharides
  - Lipids — triglycerides, phospholipids
- Metabolic chemistry
  - Enzymes
  - Cofactors — Ions, NAD, NADP, Co-A,…
- Biological phosphorylations
  - Bioenergetics — ATP, ADP, AMP
  - Signaling — cAMP, protein phosphorylation
- Prokaryotic and Eukaryotic Cells
  - Biomembranes
  - Organelles
- Molecular Genetics
  - DNA, cDNA
  - RNA, t-, m-, and r-RNAs

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The core structural methods courses

STB 531. Protein Expression, Purification, and Crystallization

- Target selection
- Molecular biology of gene isolation and amplification
- Biotechnology of gene expression and protein tagging
  - Bacterial cells
  - Baculovirus/insect cells
  - Mammalian tissue cells
- Chromatographic protein purification
- Screening for crystallization and crystal growth conditions
  - Acids, bases, and buffers; pH, pK, pI.; salts and ionic strength
  - Solubility phenomena
    - Undersaturation, saturation, supersaturation
    - Aggregation
      - Monodisperse
      - Polydisperse
    - Precipitation
    - Inclusion bodies
    - Solvation; salting-in and salting-out
  - Nucleation, crystallization, and crystal growth

STB 533-534. Crystallographic Methods of Structural Biology I and II

- Diffraction Physics
  - X-Rays
  - Neutrons
  - Electrons (electron crystallography and cryo-electron microscopy)
- Structure determination
  - refinement
  - validation
  - interpretation
  - Crystal specimen mounting and cryopreservation
  - X-ray sources, monochromators, and detectors
  - Crystal symmetry and diffraction symmetry
  - Optical Fourier transforms and X-ray diffraction patterns
  - Diffraction measurements, data reduction, and error analysis
  - Crystal structure analysis
    - The crystallographic phase problem
      - Harker-Patterson-Fourier methods
      - SIR, MIR, SAS, SIRAS, MAD heavy-atom methods
      - Molecular replacement, rotation-translation methods
      - Direct methods
      - Solvent flattening
      - Noncrystallographic symmetry averaging
    - Structure modeling, refinement, and interpretation
      - Independent-atom models at atomic resolution
      - Stereochemically restrained models at polyatomic functional-group resolution

STB. Spectroscopic Methods of Structural Biology
(Cross-listed CHE 512. NMR and Biomolecular Structure)

- Nuclear magnetic resonance spectroscopy
  - Magnetic moments
  - Bloch equations
    - Signal Strength
    - Relaxation times – Line widths
  - Chemical shifts
    - Spin-spin coupling – Line splitting
  - Biomolecular systems
    - ^{1}H, ^{13}C, ^{15}N, ^{31}P, ^{19}F NMR
    - One-dimensional ^{1}H NMR spectra of proteins
    - Two-dimensional ^{1}H–^{15}N and ^{1}H–^{13}C correlation spectra
    - Multidimensional spectra and the Product Operator Formalism
- Other spectroscopies
  - Electron paramagnetic resonance
  - Electronic absorption (XFAS, UV, Vis)
  - Vibration/rotation (IR, Raman)
  - Mass spectrometry
- Optical methods (ORD, CD, Fluorescence)
- Ultracentrifugation methods

STB. Computational Modeling of Biomolecular Structure
(Cross-listed BIO 608. Topics in Macromolecular Structure)

- Quantum mechanics
  - Molecular orbitals theory
  - Density functional theory
- Molecular mechanics
  - Force fields
  - Simulated annealing
  - Molecular dynamics
- Bioinformatic databases – Searches and analyses
  - Genomics data
    - Gene prediction
    - Gene expression
  - Proteomics data
  - Sequence alignment
  - Sequence similarity searching
  - Protein domain families
  - 3-D protein structures
- Structure-based rational drug design
  - Structure-activity relationships
  - Intermolecular interactions
  - Interaction pharmacophores