

What is a PhD thesis? Psychological and social factors during PhD, student's role in thesis work, supervisor's role in thesis work, overview of research planning, time management, fair scientific practices.

Ethics in natural sciences, avoiding research that cause unjustified risk to people, jeopardizing the environment or convert public resources into private profits, striving for objectivity (in the research process and in presentation of results), handling uncertainties.

Literature survey, critical use of existing knowledge, finding out a research problem, scientific publishing, classification of conferences and journals, judging whether a material is publishable, refereeing process, criticizing own and others work.

How to give seminars, how to use various softwares, how to use various instruments, how to interact with people, how to apply for jobs, plagiarism in science – what to do and not to do.

As a concrete example, each student will be asked to produce a “prototype thesis” in a given area under a “prototype supervisor”. The student will apply the knowledge, ethics and best scientific practices to produce the thesis. Students will be evaluated based on the thesis and its defence.

## 2. Advanced Level Optional Courses (to choose any 2 from each Group - A, B and C)

### A. Advanced Biophysical techniques (OPT1)

#### (i) Macromolecular crystallography (Udayaditya Sen & Sampa Biswas)

Structure factors, Atomic scattering factor, temperature factor, structure factor calculation, Phase problem and electron density calculation. Advanced phasing techniques (like MAD/SAD). Phasing by MR, Model building and refinement. Fiber Diffraction.

High throughput crystallography; Cryo-crystallography and its application in trapping reaction intermediates; X-ray crystallography to elucidate structure-function relationship for some important biological pathways; crystallography of large macromolecular assembly.

Crystallization techniques, handling protein crystals using cryo techniques, diffraction data collection, electron density map interpretation, crystallographic data analysis.

#### (ii) Chromatography and Mass Spectrometry (Soumen Kanti Manna)

**Chromatography:** General principles of chromatography, common types of chromatography<sup>1</sup>, factors affecting chromatographic separation and considerations for choosing mode of chromatography, applications.

**Mass Spectrometry:** General principles, ion source<sup>2</sup>, types of mass analyzers<sup>3</sup>, ion fragmentation and rearrangements, mass spectrometry of protein and peptides, mass spectrometry of small molecules, imaging mass spectrometry, applications.

<sup>1</sup>normal phase, reverse phase, HILIC, ion exchange, size exclusion, affinity, GC and chiral.

<sup>2</sup>ESI, APCI, MALDI, EI, DESI, LAESI, FAB, SIMS, NIIMS.

<sup>3</sup>quadrupole, TOF, ion trap, orbitrap, ICR.