NMR Spectroscopy for Biomacromolecules: Assignments & Restraints — Hands-on

Gain a practical, workflow oriented understanding of NMR spectroscopy for biomacromolecules. From experimental design and isotope labeling strategies to resonance assignments, restraint generation, structure calculation and validation, this module prepares you to read, interpret and generate NMR based structural models for proteins and nucleic acids.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

NMR Fundamentals & Experimental Design

NMR principles for biomacromolecules

spin, magnetization and relaxation | **chemical shifts and linewidths** | **solution vs solid state overview**

Sample preparation and isotope labeling strategies

15N / 13C labeling concepts | **deuteration overview** | **buffer and stability considerations**

Key 1D and 2D experiments for biomolecules

1D 1H, 2D COSY / TOCSY | 1H–15N HSQC | 1H–13C HSQC / NOESY

Session 2

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Backbone & Side Chain Assignments

Backbone assignment strategies for proteins

triple resonance experiments | HNCA / HNCO overview | CBCA(CO)NH style logic

Side chain assignments and aromatic regions

aliphatic side chain mapping | aromatic ring assignments | 13C edited NOESY concepts

Peak picking and assignment software workflows

peak lists and connectivity | assignment validation | handling ambiguous peaks

Session 3

Fee: Rs 14800 Apply Now

Restraints, Structure Calculation & Ensembles

Generating structural restraints from NMR data

NOE distance restraints | J coupling derived dihedrals | RDC and other restraints overview

Structure calculation workflows

restraint preparation | simulated annealing concepts | iterative refinement cycles

Ensemble analysis and convergence metrics

RMSD within ensembles | restraint violation checks

selection of representative models

Session 4

Fee: Rs 18800 Apply Now

Validation, Dynamics & Reporting

Validation of NMR structures and restraints

Theory + Practical

Solution dynamics and NMR observables

relaxation measurements overview chemical exchange concepts conformational ensembles

Deposition and figure ready reporting

BMRB and PDB deposition validation reports and checklists panels and methods text for manuscripts