NMR Metabolomics — 1D 2D & Chemometrics — Hands-on

Gain practical skills in NMR based metabolomics, from pulse sequences and sample preparation to spectral processing, peak picking and multivariate analysis. This module focuses on 1D and 2D NMR workflows, quality checks and chemometrics so that you can turn spectra into robust metabolite profiles and biologically meaningful patterns.

NMR Metabolomics — 1D 2D & Chemometrics

Help Desk · WhatsApp

Session Index

Session 1

Fee: Rs 8800 Apply Now

NMR Principles & Hardware for Metabolomics

NMR basics in the context of metabolomics

nuclear spin and resonance | **chemical shift and J coupling** | **sensitivity vs concentration range**

Magnets, probes and spectrometer configuration

field strength and resolution | **probe types and temperature control** | **autosamplers and throughput**

Sample preparation and reference standards for NMR

deuterated solvents and buffers **TSP, DSS and internal references** **pH control and ionic strength**

Session 2
Fee: Rs 11800 Apply Now

1D NMR Acquisition, Processing & QC

1D pulse sequences for metabolomics

standard 1H experiments **NOESY presat and CPMG water suppression strategies**

Data acquisition parameters and optimization

number of scans and relaxation delays **spectral width and resolution** **shim and line shape quality**

Processing, QC metrics and export formats

Fourier transform, phase and baseline correction **referencing and binning options** **FID and spectrum QC checklists**

Session 3
Fee: Rs 14800 Apply Now

2D NMR, Assignment & Feature Extraction

Key 2D experiments for metabolite assignment

COSY and TOCSY **HSQC and HMBC** **trade offs in time and sensitivity**

Metabolite identification and libraries

chemical shift databases and tools **peak picking and manual curation** **levels of identification in NMR**

Feature extraction approaches

bucketing and spectral bins | targeted integration of peaks | export to matrix for statistics

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Chemometrics and Interpretation

Preparing NMR data for multivariate analysis

normalization and scaling choices | handling missing features | batch and drift checks

Chemometrics on NMR metabolomics data

PCA for overview and outliers | PLS DA and validation concepts | loading plots and spectral back mapping

Deliverables: NMR workflow and analysis summary

acquisition and processing SOP | feature matrix and QC report | chemometrics figures and narratives