NMR Metabolomics — Acquisition, Processing & Annotation — Hands-on

Develop a complete, practice ready workflow for NMR based metabolomics. This module walks you from basic 1H NMR concepts and experiment setup through acquisition, spectra processing, bucketing or peak picking, and metabolite annotation using curated spectral libraries and databases for robust quantitative and qualitative readouts.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

NMR Basics, Experiments & Metabolomics Context

Principles of NMR for metabolomics applications

chemical shift & spin systems **relaxation & line width** **sensitivity & dynamic range**

1H NMR experiments commonly used in metabolomics

1D proton **CPMG / T2 filter (overview)** **NOESY presat / water suppression**

Matrices, sample tubes and basic preparation for NMR

biofluids (plasma, serum, urine) **buffers & pH control** **deuterated solvents & references**

Session 2
Fee: Rs 11800 Apply Now

Acquisition Parameters & QC for NMR Runs

Setting up NMR acquisition for metabolomics

spectral width & offset **number of scans & relaxation delay** **temperature control**

Shimming, locking, tuning and water suppression checks

lock optimization **manual vs automated shimming** **water peak management**

Run QC and system suitability for NMR metabolomics

reference compounds **reproducibility metrics** **instrument drift awareness**

Session 3
Fee: Rs 14800 Apply Now

Spectral Processing & Data Reduction

Core processing steps from FID to spectrum

zero filling & apodization **Fourier transform** **phase & baseline correction**

Alignment, reference and solvent region handling

chemical shift referencing **alignment approaches (overview)** **water and urea region treatment**

Data reduction: binning vs peak picking strategies

fixed width and adaptive binning **peak lists** **export to**

multivariate tools

Session 4

Fee: Rs 18800 Apply Now

Metabolite Annotation & Reporting

Annotation workflows with spectral libraries and databases

HMDB / BMRB (concepts) | in house libraries | confidence levels

Relative and absolute quantitation considerations in NMR

integrals vs peak heights | internal standards | dilution and linearity checks

Deliverables: processed dataset, annotation table & methods note

bucket / feature matrix (CSV) | metabolite annotation sheet | NMR metabolomics methods summary