Peak Detection, Deconvolution & Alignment Pipelines — Hands-on

Turn raw LC–MS and GC–MS data into high quality feature tables that downstream statistics can trust. This module focuses on chromatographic peak detection, deconvolution, alignment, blank and QC filtering, and basic data curation logic so that untargeted metabolomics runs yield reproducible, analysis ready tables.

Peak Detection, Deconvolution & Alignment Pipelines

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Session Index

Session 1

Fee: Rs 8800 Apply Now

From Raw Files to Chromatographic Peaks

Raw data formats and conversion for LC–MS / GC–MS pipelines

vendor formats **open formats (mzML, mzXML)** **centroid vs profile data**

Principles of chromatographic peak detection in 2D space

m/z traces and EICs **noise vs true peaks** **smoothing and thresholds**

Key peak picking parameters and quality checks (concepts)

minimum peak width **signal to noise** **intensity and area measures**

Session 2
Fee: Rs 11800 Apply Now

Deconvolution, Isotopes & Adduct Grouping

Deconvolution of co eluting peaks and complex chromatograms

co elution patterns **mass spectral deconvolution (overview)** **peak shape based splitting**

Identifying and grouping isotope patterns

M and M plus 1 logic **natural abundance expectations** **filtering isotopic duplicates**

Adduct relationships and feature clustering

common adducts (Na, K, NH4) **adduct and neutral loss networks** **collapsing redundant features**

Session 3
Fee: Rs 14800 Apply Now

Retention Time Alignment & Feature Matrix Curation

Why alignment is needed and basic strategies

RT drift across runs **landmark peaks and warping** **alignment quality metrics**

Building the feature matrix and handling missingness

feature merging across samples **intensity vs area values** **missing value patterns**

Filtering by blanks, QCs and basic reproducibility rules

blank dominated features **CV in pooled QCs** **minimum**

presence filters

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: End to End Peak Picking Workflow

Build a peak detection and alignment pipeline on example data

Theory + Practical

Parameter tuning and evaluating impact on feature quality

peak thresholds and widths alignment and grouping options QC driven decisions

Deliverables: documented workflow & curated feature matrix

pipeline steps and parameters (PDF/HTML) final feature table (CSV/TSV) basic QC plots and summaries