Untargeted Metabolomics — Peak Picking & Alignment — Hands-on

Develop a robust untargeted metabolomics preprocessing pipeline, from vendor raw files to a high quality feature matrix. This module focuses on peak detection, deconvolution, adduct and isotope handling, and retention time alignment so that you can generate reproducible data sets for downstream statistics, biomarker discovery and pathway level interpretation.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Raw Data & Preprocessing Concepts

Vendor formats, open formats and converters

- vendor RAW files
- mzML, mzXML, netCDF
- conversion tools overview

Profile vs centroid data and spectra structure

- profile mode vs centroid mode
- m/z, intensity and retention time
- MS1 vs MS/MS levels

Overview of untargeted preprocessing workflow

peak detection and building peak lists alignment and feature grouping export to feature matrix

Session 2

Fee: Rs 11800 Apply Now

Peak Detection, Deconvolution & Filtering

Algorithms and parameters for peak picking

centroiding and noise thresholds minimum peak height and width chromatographic peak shape checks

Deconvolution, isotopes and adducts

co eluting features and deconvolution isotope pattern grouping adduct annotation strategies

Filtering low quality and redundant peaks

signal to noise and detection frequency blank subtraction concepts removing duplicated or unstable features

Session 3

Fee: Rs 14800 Apply Now

Alignment, Grouping & Feature Matrix

Retention time correction and alignment

reference based alignment warping and non linear correction monitoring alignment quality

Feature grouping across samples

clustering peaks by m/z and RT handling missing peaks intensity summarization choices

Exporting and curating the feature matrix

sample by feature table | feature metadata and identifiers | pre checks before statistics

Session 4

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Mini Capstone: End to End Untargeted Pipeline

Building a practical untargeted preprocessing workflow

from RAW files to feature matrix

Tool based implementation walkthrough

example with MZmine or MS DIAL | parameter template creation | export formats for statistics packages

Deliverables: preprocessing SOP, parameter file & QC report

stepwise SOP document | saved parameter configuration | summary plots and checks