

Feature Annotation & Library Matching (MZmine/MS-DIAL/GNPS) — Hands-on

Move beyond anonymous m/z features and start naming chemistry with confidence. This module focuses on practical feature annotation strategies, spectral library matching in MZmine/MS-DIAL, and GNPS molecular networking so that your untargeted metabolomics datasets yield interpretable metabolite IDs with documented confidence levels.

Feature Annotation & Library Matching (MZmine/MS-DIAL/GNPS)

[Help Desk](#) · [WhatsApp](#)

Session Index

[Session 1 — Annotation Concepts & Confidence Levels \(MSI\)](#) [Session 2 — Library Matching in MZmine / MS-DIAL](#) [Session 3 — GNPS, Molecular Networking & Library Workflows](#) [Session 4 — Mini Capstone: Annotation Workflow & ID Table](#)

Session 1

Fee: Rs 8800 [Apply Now](#)

Annotation Concepts & Confidence Levels (MSI)

From feature tables to putative IDs — the annotation problem

[m/z & RT to candidate lists](#) [MS/MS evidence](#) [in-silico vs experimental spectra](#)

Metabolomics Standards Initiative (MSI) levels of identification

[Level 1: confirmed ID](#) [Levels 2–3: putative ID / class](#)
[Level 4: unknown features](#)

Evidence types: accurate mass, RT, MS/MS, isotopes & adducts

mass error and ppm windows **RT matching to standards** **fragmentation pattern similarity**

Session 2

Fee: Rs 11800 Apply Now

Library Matching in MZmine / MS-DIAL

Preparing feature lists and MS/MS spectra for matching

export from peak picking pipelines **linking MS1 features to MS/MS scans** **data formats for MZmine/MS-DIAL**

Spectral library search settings and score interpretation

mass tolerances (MS1/MS2) **similarity scores (dot product, cosine)** **minimum matched peaks / intensity**

Working with public and in-house libraries (concepts)

MassBank / HMDB / MoNA (overview) **importing custom libraries** **curating and updating reference sets**

Session 3

Fee: Rs 14800 Apply Now

GNPS, Molecular Networking & Library Workflows

Preparing and submitting data to GNPS (concepts & workflow)

MS/MS spectra export **metadata tables** **choosing GNPS workflows**

Classical and feature-based molecular networking interpretation

cosine score & network edges **cluster and subnetwork exploration** **propagating annotations to neighbors**

GNPS library matches and chemical class-level insights

viewing library hits on networks **chemical**
class/ontology layers **unknown clusters and follow-**
ups

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Annotation Workflow & ID Table

Running an end-to-end annotation workflow on example data

Theory + Practical

Consolidating MZmine/MS-DIAL/GNPS hits into a single ID table

merging feature IDs **choosing best candidate per**
feature **flagging conflicts and unknowns**

Deliverables: annotation table with MSI levels & evidence
columns

feature-to-metabolite table (CSV/TSV) **MSI level &**
evidence documentation **short methods and**
limitations note