

Annotation & Identification — Libraries & In-Silico — Hands-on

Learn how to turn LC–MS/GC–MS feature tables into biologically meaningful metabolite and lipid identities. This module focuses on spectral library searching, in-silico fragmentation and formula prediction, adduct/isotope handling and reporting of identification levels so that your untargeted and targeted studies produce traceable, defensible annotations.

Annotation & Identification — Libraries & In-Silico

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Session 1

Fee: Rs 8800 [Apply Now](#)

Concepts, Evidence Levels & Data Readiness

From features to identities: terminology & workflows

[feature, peak group, compound](#) [annotation vs identification](#) [small-molecule ID challenges](#)

Reporting standards & identification levels

[MSI levels 1–4](#) [library vs in-silico evidence](#) [when to claim putative IDs](#)

Preparing data for annotation workflows

clean feature tables & MS/MS links | adduct & isotope information | export formats (mzML, MGF, CSV)

Session 2

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Spectral Libraries, Matching & Curation

Reference databases & spectral libraries

HMDB, MassBank, METLIN, GNPS | mzCloud, NIST and vendor libs | coverage & limitations

MS/MS library matching fundamentals

precursor tolerance & fragment tolerance | dot product & entropy scores | match filters & FDR concepts

Curation of library hits and conflicts

reviewing spectra and structures | isomer/anologue discrimination | documenting rationale & notes

Session 3

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In-Silico Tools, Networks & Structural Hints

Formula prediction & in-silico fragmentation

accurate mass & isotope patterns | tools like SIRIUS/MS-FINDER | ranking & pruning candidates

Molecular networking & chemotype grouping

GNPS molecular networks | spectral similarity & clusters | propagating annotations in networks

Combining library & in-silico evidence

adduct, RT and MS/MS consistency **pathway context**
and biochemistry **assigning confidence levels**

Session 4

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Mini Capstone: Annotation Strategy & Report

Designing an annotation workflow for a study

untargeted dataset from LC-MS/GC-MS

Prioritizing features & documenting decisions

rank by effect size & QC **traceable annotation tables**
linking to pathways and figures

Deliverables: annotation table, confidence tags & methods text

feature-to-metabolite mapping file **MSI level &**
evidence columns **ready-to-use methods paragraph**