Spectral Libraries, In Silico Fragmentation & GNPS — Hands-on

Master MS MS spectral library search, in silico fragmentation and GNPS style molecular networking for small molecule annotation. You will configure library matching, understand scoring and FDR like thinking, run GNPS workflows and integrate annotated networks into untargeted metabolomics and natural products studies.

Spectral Libraries, In Silico Fragmentation & GNPS

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Spectral Libraries & Reference Data

Public and commercial MS MS spectral libraries

- GNPS style community libraries
- MassBank and related resources
- vendor specific collections

Spectrum quality and metadata requirements

- collision energy and polarity fields
- instrument and acquisition details
- compound identifiers and

structures

Organising local project specific libraries

curated in house reference spectra | versioning and documentation | sharing libraries within teams

Session 2

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In Silico Fragmentation Concepts & Tools

Basics of small molecule fragmentation logic

common bond cleavages | neutral losses and diagnostic ions | energy dependence of patterns

In silico fragmentation tools and workflows

the idea of rule based engines | structure input and output spectra | matching experimental and predicted spectra

Scoring, candidate ranking and limitations

cosine like scores intuition | decoy and target thinking | ambiguity in isomers and analogs

Session 3

Fee: Rs 14800 Apply Now

GNPS Molecular Networking Workflows

From MS MS data to GNPS compatible formats

exporting mzML and mgf style files | metadata tables for GNPS | basic pre processing expectations

Setting up classical and feature based networks

similarity thresholds and minimum peaks | library search options | analog search concepts

Visualising and filtering networks for biology

cluster level inspection mapping sample groups and intensities identifying molecular families of interest

Session 4

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Integrating Library Hits into Studies

Annotation levels and confidence reporting

library hit versus in silico support analog style annotations linking scores to levels of certainty

Combining networks, statistics and pathways

mapping significant features on networks connecting to pathway maps prioritising molecular families for follow up

Exporting results and documenting workflows

tables of hits with scores and metadata network figures for presentations checklists for reproducible annotation pipelines