

## Untargeted Metabolomics Discovery Pipelines — Hands-on

Design and run complete untargeted metabolomics discovery pipelines. You will connect LC MS feature extraction, QC and normalization with multivariate statistics, hit selection and annotation ready outputs that support biological discovery and follow up validation.

# Untargeted Metabolomics Discovery Pipelines

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### Session 1

**Fee: Rs 8800** [Apply Now](#)

## Untargeted Workflow Overview & Data Flow

Goals of untargeted metabolomics discovery

[pattern discovery](#) [biomarker hypothesis generation](#)  
[mechanistic clues](#)

End to end pipeline building blocks

[raw to mzML to feature table](#) [QC and normalization](#)  
[statistics and annotation loop](#)

Data model and file organization for projects

raw data and processed data folders metadata sheets  
analysis notebooks and reports

### Session 2

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## Feature Matrices, QC & Normalization

From feature tables to analysis ready matrices

samples by features layout linking to sample  
metadata basic completeness checks

Quality checks using QC and blanks

RSD filters on pooled QC blank subtraction rules  
intensity drift patterns

Normalization and transformation options

total area and probabilistic quotient internal  
standard based log and scaling choices

### Session 3

Fee: Rs 14800 Apply Now

## Multivariate Statistics & Hit Finding

Exploratory analysis and batch assessment

PCA score plots QC clustering outlier detection

Supervised models for group separation

PLS DA style thinking cross validation awareness  
overfitting pitfalls

Feature ranking and candidate hit lists

univariate tests and FDR effect sizes and fold  
changes multi metric ranking tables

**Session 4**

**Fee: Rs 18800** [Apply Now](#)

## Annotation, Reporting & Review

Preparing feature lists for annotation tools

**export formats and required columns**

Visual summaries for stakeholders

**volcano plots** **heatmaps** **pathway level summaries**

Documenting pipeline and decisions

**parameter manifests** **notebooks and reports** **checklist  
for internal review**