Statistics & Chemometrics — PCA PLS-DA & MVA — Hands-on

Learn how to convert metabolomics feature tables into trustworthy statistical and chemometric insights. This module covers normalization, transformation, unsupervised and supervised multivariate methods, model validation and interpretation so that you can defend your results in manuscripts, theses and regulatory facing reports.

Statistics & Chemometrics — PCA PLS-DA & MVA

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Data Structures, QC & Normalization

Feature matrices and metadata for metabolomics

- samples x features layout
- phenotype and batch factors
- long vs wide representations

QC based diagnostics before analysis

- missingness patterns & filters
- RSD of pooled QC samples
- drift, outliers and batch trends

Normalization, transformation and scaling choices

total area, Probabilistic Quotient, IS based | log and power transforms | auto, pareto and range scaling

Session 2

Fee: Rs 11800 Apply Now

Unsupervised Analysis: PCA & Clustering

PCA for global structure and QC

variance explained and scree plots | scores and loadings interpretation | detecting batch effects and outliers

Distance metrics and clustering basics

Euclidean vs correlation distances | hierarchical clustering and heatmaps | k means and cluster selection

Practical visualization for metabolomics data

score plots with groups and QCs | feature clustering heatmaps | R (ggplot) and Python plotting

Session 3

Fee: Rs 14800 Apply Now

Supervised MVA: PLS-DA & Validation

When and how to use supervised models

classification vs regression questions | overfitting risks in omics | train test splits and cross validation

PLS and PLS-DA for metabolomics

model components and variance (R2X, R2Y) | Q2, permutation tests and CV | VIP scores and feature ranking

Model validation and honest performance estimates

nested CV and repeated CV ROC and PR curves, confusion matrix avoiding information leakage

Session 4
Fee: Rs 18800 Apply Now

Mini Capstone: Model Building & Reporting

End to end analysis of a metabolomics dataset

from raw feature table to models

Linking multivariate results to biology

top features and volcano plots pathway enrichment inputs integrating with prior knowledge

Deliverables: analysis notebook, figures & methods text

R / Python notebook with code PCA and PLS-DA publication plots ready to edit methods and results text