

Raw Data Conversion — mzML and Vendor Formats — Hands-on

Learn how to convert proprietary LC–MS/MS RAW files into open, analysis ready formats without losing critical metadata. This module focuses on the landscape of vendor formats, mzML concepts, batch conversion planning, file naming, integrity checks and archiving practices that support downstream search, quantification and public data submission.

Raw Data Conversion — mzML and Vendor Formats

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Session 1

Fee: Rs 8800 [Apply Now](#)

Vendor RAW & Open Formats Landscape

Overview of vendor RAW formats and ecosystems

[instrument specific RAW files](#) [profile vs centroid views](#) [metadata storage concepts](#)

Why open formats matter in proteomics workflows

[interoperability across tools](#) [long term accessibility](#) [compliance and FAIR data](#)

Common open formats and use cases (conceptual)

mzML for spectra **mzXML and MGF context** **raw plus derived file pairs**

Session 2

Fee: Rs 11800 Apply Now

mzML Structure & Conversion Concepts

Logical anatomy of an mzML file

spectra and chromatograms **binary data arrays**
controlled vocabulary terms

Key decisions during RAW to mzML conversion

centroiding vs profile export **precision and compression choices** **retention time and index preservation**

Capturing instrument and method metadata correctly

scan settings mapping **sample and run level annotations** **linkage to study design sheets**

Session 3

Fee: Rs 14800 Apply Now

Batch Conversion, Naming & Integrity

Planning batch conversions for full studies

folder structures and run grouping **log files and parameter templates** **parallelization considerations**

Robust file naming and mapping to metadata sheets

human readable conventions **run identifiers and barcodes** **linkage to sample and condition IDs**

Integrity checks on converted files (conceptual)

basic spectrum count comparisons **checksum and size sanity checks** **spot inspection in viewers**

Session 4

Fee: Rs 18800 Apply Now

Archiving, Reproducibility & Repositories

Organizing RAW and mzML for long term storage

theory plus folder mapping exercise

Capturing conversion parameters for reproducibility

documenting tool versions **parameter files and manifests** **linking to analysis workflows**

Preparing data packages for public repositories (conceptual)

pairing RAW, mzML and search outputs **metadata tables for submissions** **checklists for shareable datasets**