ASMS Short Course - Computational Approaches and Practical Data Analysis for Untargeted Metabolomics

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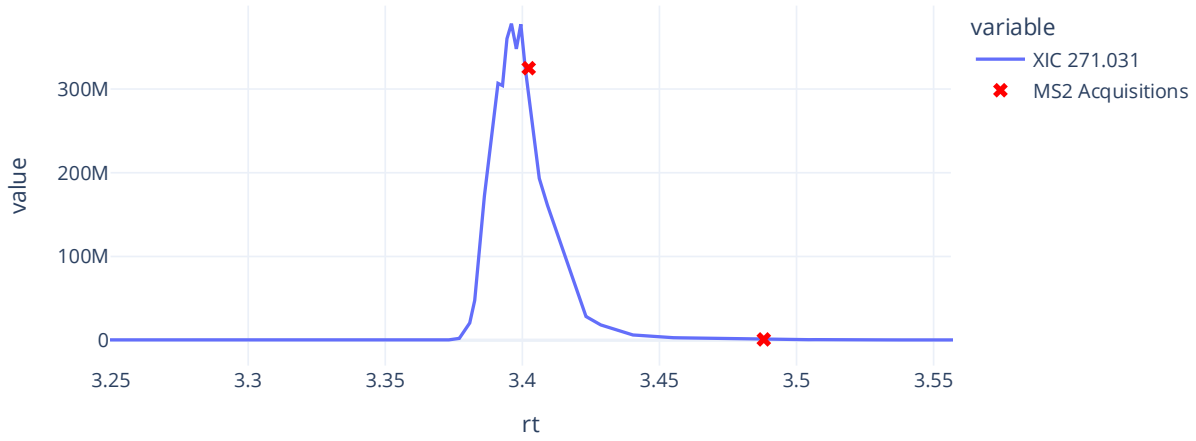
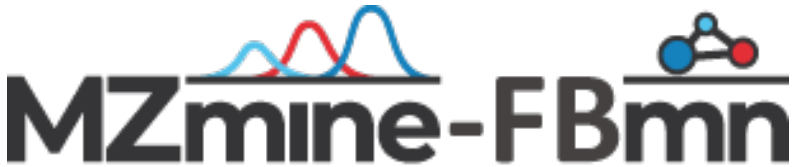
Untargeted Metabolomics Data Acquisition

- Learning Objectives
  - Concepts
    - Liquid Chromatography
    - Mass Spectrometry and Tandem Mass Spectrometry Data Acquisition
    - Opportunities and Limitations of Annotation by MS/MS
    - Opportunities and Limitations of Quantification with MS



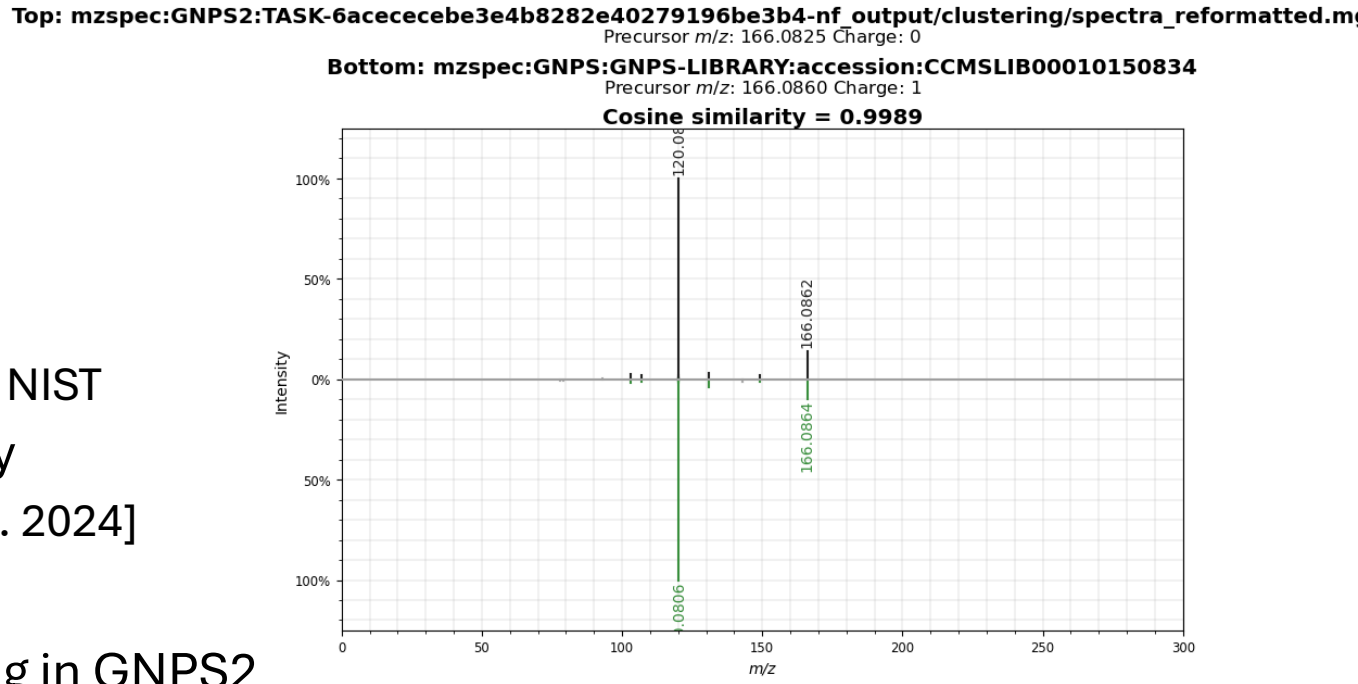
Data preprocessing and Relative Quantification

- Learning Goals
  - Concepts
    - Data Sharing and Public Data Visualization
    - Feature Finding for Relative Quantification
  - Practical Skills
    - Downloading Data from Public Repositories [Abeied et al. 2025]
    - Public Data Visualization with the GNPS Dashboard – [Petras et al. 2020]
    - High-Throughput Feature Finding with MZmine for Feature Based Molecular Networking - [Schmid et al. 2023]



Compound Annotation – MS/MS Libraries

- Learning Goals
  - Concepts
    - Public MS/MS Library
      - Massbank [Horai et al. 2010],
        GNPS [Wang et al. 2016], MoNA, NIST
    - MS/MS Library Matching Similarity
      - Cosine, Spectral Entropy [Li et al. 2024]
  - Practical Skills
    - High-Throughput MS/MS searching in GNPS2
    - MS/MS matching visualization and sharing
      in metabolomics resolver [Bittrimieux et al. 2020]



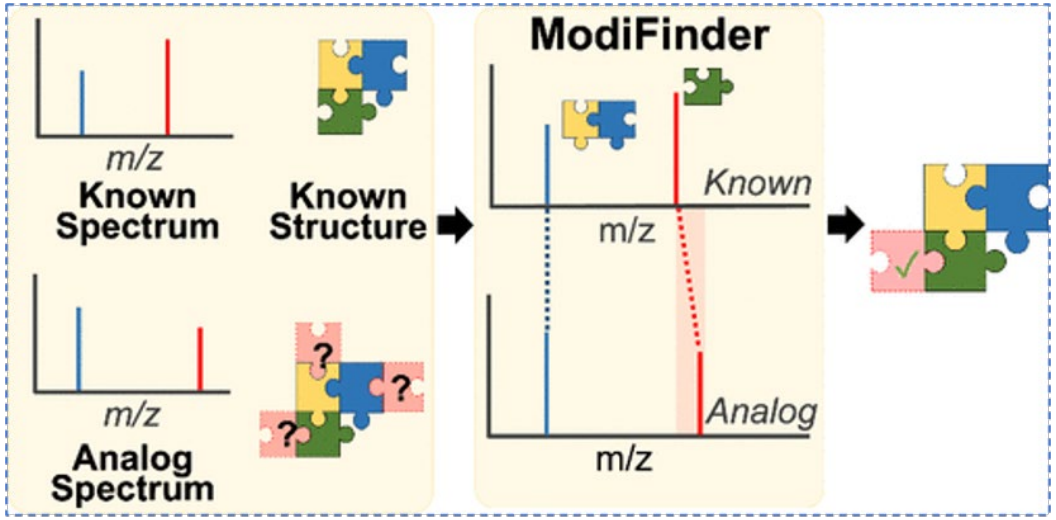
MassBank
High Quality Mass Spectral Database

GNPS

Compound Annotation – Molecular Networking/Annotation Propagation

- Learning Goals
  - Concepts
    - MS/MS Modified Cosine Similarity Theory
    - Molecular Networking Construction
      - Transitive Alignments [Wang et al. 2024] and Multiple Spectrum Alignments [Lau et al. 2025]
    - Annotation Propagation with ModiFinder [Shahneh et al. 2024]
  - Practical Skills
    - Creating Molecular Networks in GNPS2
    - Interactive Network Exploration in GNPS2
    - Using ModiFinder to localize structural modification

GNPS2



Compound Annotation – In Silico Annotation

- Learning Goals
  - Concepts
    - Fingerprint Prediction with machine learning [Duhrkop et al. 2015]
    - In Silico Database Searching
    - MS/MS spectrum prediction
    - Computational Structure Prediction
  - Practical Skills
    - Interactive structure prediction with ModiStruct in GNPS2

Statistical Analysis and Downstream Data Priorization

- Statistical Analysis of Molecular Networking Results
  - Metabolomics Data Normalization
  - Metabolomics Data Imputation
  - Statistical Analysis with Interactive Web Hitchhiker's Metabolomics Stats Guide [Shah et al. 2025]

- Network Visualization and Enrichment Analysis
  - Network Vizualization with Cytoscape
  - Integration of Statistical Results into Molecular Networks
  - GNPS2 Metaboapps for Network Enrichment Analysis