Integrating 4D peak picking of LC-TIMS-MS/MS data into GNPS feature based molecular networking for 4D Metabolomics and 4D Lipidomics analysis.

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Introduction

As throughput of metabolomic and lipidomic analyses continuously expands, effective workflows for analyzing the resulting datasets are of increasing importance. Molecular networking in recent years has become a vital tool in the metabolomics community as it quickly allows the identification of compounds with similar fragmentation patterns which are often structurally related.

While this approach mainly focusses on the fragment spectra, important information can be deduced from the precursor spectra, i.e. intensity, accurate mass and isotopic pattern of the analytes. Herein, we present a workflow to integrate analyte information for untargeted profiling from the software MetaboScape into GNPS feature based molecular networking.

Results

The presented workflow (Fig. 1) allows the enrichment of molecular networks with additional information from MetaboScape (Fig. 2) and also allows the processing of 4D LC-TIMS-QTOF and PASEF data using GNPS molecular networking (Fig. 3).

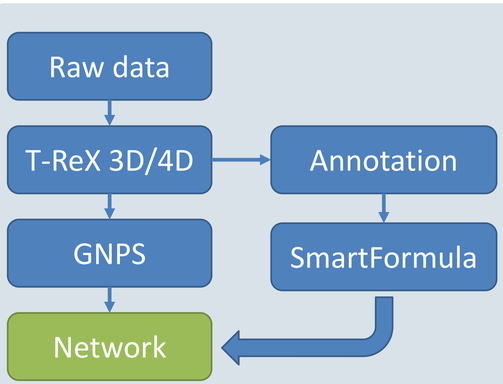

Fig. 1: Workflow of MetaboScape and GNPS integration. First, Peak picking is performed by T-ReX algorithms. Dedicated mgf export allows processing in GNPS while further annotations can be used to enrich the resulting network.

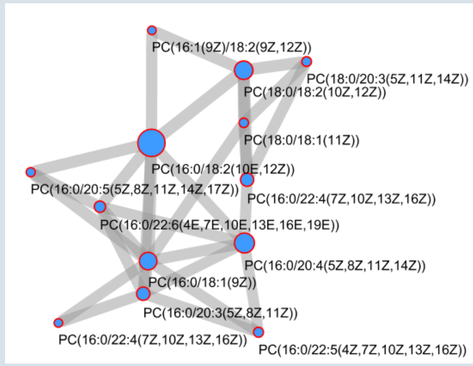

Fig. 3: Subset of a PC cluster from a 4D Lipidomics experiment. Peak picking by T-ReX 4D enables processing of 4D data in GNPS feature based networking.

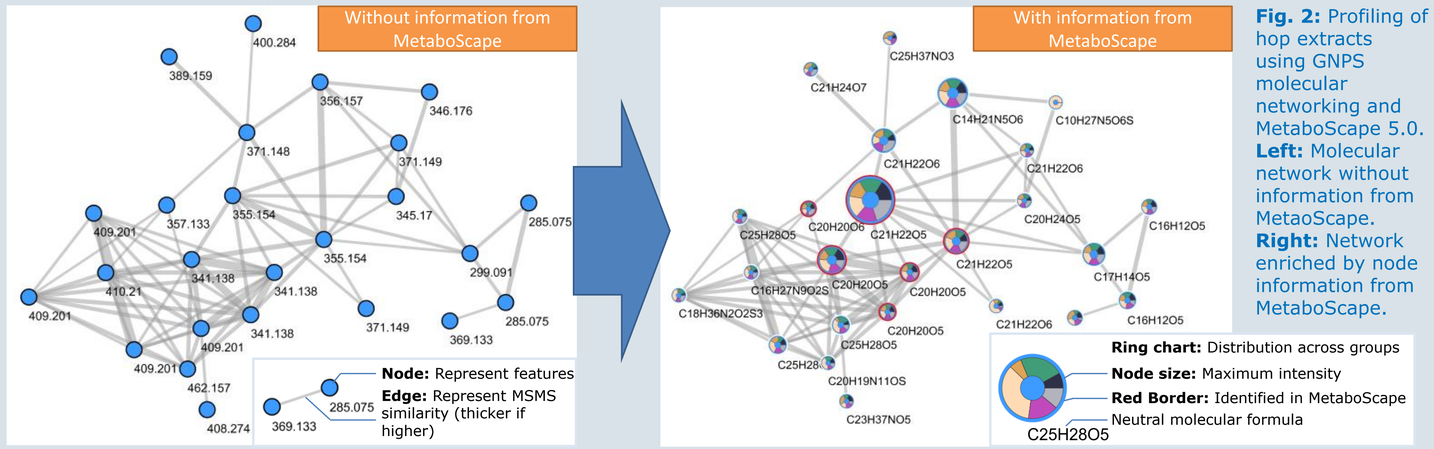

Fig. 2: Profiling of hop extracts using GNPS molecular networking and MetaboScape 5.0. **Left:** Molecular network without information from MetaoScape. **Right:** Network enriched by node information from MetaboScape.

Summary

To the best of our knowledge, this workflow enables the integration of 4D Metabolomics/Lipidomics data into GNPS molecular networking for the first time. Furthermore, the additional metadata greatly eases the interpretation of resulting networks.

This allows to easily assess distribution of analytes from distinct compound classes between sample groups and asses if purification of a compound is feasible (by maximum intensity).

References

(1) Wang, Mingxun, et al.; Nature Biotechnology, 34, 828 (2016)

Conclusions

- The presented workflows leverages the peak picking performance of T-ReX algorithms for use in GNPS feature based molecular networking.
- Allows integration of 4D data into GNPS for 4D Metabolomics and Lipidomics.
- Integrates reliable sum formula generation based on HRAM and isotopic pattern.
- Easily assess CCS values, intensity distribution, maximum intensity and molecular formulas of nodes in the network.

4D Metabolomics