Untargeted IMS Tentative Identification Lipidomics

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We use this protocol and it's working

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ABSTRACT

The purpose of this protocol is to generate tentative annotations for lipids detected using IMS.

1 Following pre-processing, tentative identification is performed using an in-house developed annotation software - annotine.

2 Generate an average mass spectrum of the dataset (in profile mode).

3 Scale the mass spectrum between 0 and 1, and peak-pick its profile to retrieve a list of m/z features (commonly 100s to 1000s).

4 Filter the peak list to retain only peaks that have a relative intensity above 0.001 (sensitive mode) or 0.01 (standard mode). Peaks whose intensity value falls below this threshold are removed.

5 (*optional*) De-isotope the peak list to remove M+1, M+2, … and other potential isotopes from further consideration.

6 Generate an internal database on the basis of a user-supplied list of molecular species databases and a set of user-supplied expected adduct types:

Databases:
a. coreMetabolome, LMSD, SHexCer, HMDB5
b. (optional) a local LC-MS database
Adducts:
a. Positive mode: [M+H]+, [M+Na]+, [M+K]+
b. Negative mode: [M-H]-, [M-CH3]-

Note

- coreMetabolome5 is retrieved from metaspace (https://metaspace2020.eu/help);
- LMSD database is retrieved from LipidMaps (https://www.lipidmaps.org/databases);
- HMDB5 database is retrieved from HMDB (https://hmdb.ca/downloads);
- SHexCer is a manually curated list, and
- an LC-MS database can be (optionally) included if prior LC-MS experiments have been conducted.

7 Perform tentative identification by comparing the peak list with the built database of species and adduct combinations. If a peak is within a ±5 ppm window of an annotation in the database, that annotation is assigned to that peak. This process is repeated until each peak has been compared to the database.

8 Evaluate each tentative annotation using metrics.

9 (*optional*) To reduce the number of unlikely annotations, calculate a false discovery rate (FDR) for every tentative identification. Annotations can be filtered based on the FDR (or any other) score.

10 (*optional*) If LC-MS results are available (see LC-MS/MS lipidomics protocol below), associate these directly with the annotine results. This allows immediate highlighting of which tentative identifications have also been observed by LC-MS/MS, increasing the confidence of the identification.

Protocol

NAME
Bulk Untargeted LC-MS/MS Lipidomics

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PREVIEW