

Apr 11, 2023

Untargeted IMS Tentative Identification Lipidomics

DOI

<https://dx.doi.org/10.17504/protocols.io.4r3l27j7qg1y/v1>

Lukasz Migas¹, Madeline E. Colley², Katerina Djambazova², Martin Dufresne², Angela Kruse², David Anderson², Olof Isberg², Jamie Allen², ali.zahraei², Melissa Farrow², Jeff Spraggins², Raf Van De Plas², Martin Dufrense²

¹Delft University of Technology; ²Vanderbilt University

VU Biomolecular Multim...

Human BioMolecular Atl...



Angela R.S. Kruse

Ohio State University, Columbus

Create & collaborate more with a free account

Edit and publish protocols, collaborate in communities, share insights through comments, and track progress with run records.

Create free account

OPEN  ACCESS



DOI: <https://dx.doi.org/10.17504/protocols.io.4r3l27j7qg1y/v1>

Protocol Citation: Lukasz Migas, Madeline E. Colley, Katerina Djambazova, Martin Dufresne, Angela Kruse, David Anderson, Olof Isberg, Jamie Allen, ali.zahraei, Melissa Farrow, Jeff Spraggins, Raf Van De Plas, Martin Dufrense 2023. Untargeted IMS Tentative Identification Lipidomics. **protocols.io** <https://dx.doi.org/10.17504/protocols.io.4r3l27j7qg1y/v1>

License: This is an open access protocol distributed under the terms of the **Creative Commons Attribution License**, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited

Protocol status: Working

We use this protocol and it's working

Created: April 07, 2023

Last Modified: October 18, 2023

Protocol Integer ID: 80191

Keywords: untargeted ims tentative identification lipidomics the purpose, untargeted ims tentative identification lipidomic, tentative annotations for lipid, lipid, using im, tentative annotation, im

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

CREATED BY

Madeline E. Colley

Preview