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Lipids annotation of Nano-DESI MSI datasets

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Works for me

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ABSTRACT

Scope:

Annotate lipid species detected by Nano-DESI IMS analysis.

Expected Outcome:

A list of lipid identifications with low mass errors (<5 ppm) that correlate to ion images produced by Nano-DESI IMS analysis.

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ABSTRACT

Scope:

Annotate lipid species detected by Nano-DESI IMS analysis.

Expected Outcome:

A list of lipid identifications with low mass errors (<5 ppm) that correlate to ion images produced by Nano-DESI IMS analysis.

- 1 Create mass list from the averaged spectrum.

- 2 Use LIPIDMAPS database to annotate each m/z value with the following search criteria:
https://www.lipidmaps.org/resources/tools/bulk_structure_searches.php?database=COMP_DB
 - 1a. Positive Mode Adducts: [M+H]⁺, [M+Na]⁺, [M+K]⁺
 - 1b. Negative Mode Adducts: [M-H]⁻
 2. Specify Mass Tolerance: 0.005 m/z
 3. Specify Chains: Even Chains Only
- 3 Obtain DDA MS/MS data from each sample.
- 4 Calculate ppm error associated with each assignment and remove assignments with errors larger than 5 ppm, although most have errors lower than 3 ppm.
- 5 Use the diagnostic fragments and characteristic neutral loss to narrow down the peak assignment. Remove the assignments that does not match with the CID spectrum.