Lipids annotation of Nano-DESI MSI datasets

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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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PROTOCOL

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

   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 do not match with the CID spectrum.