Lipid Annotation of MALDI IMS Datasets

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1 Works for me

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ABSTRACT

Scope:

Annotate lipid species detected by MALDI IMS analysis.

Expected Outcome:

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

1 Perform a quadratic recalibration of the IMS dataset using common well-characterized lipids: *m/z* 734.5694, 760.5851, 782.5670, 788.6164, 798.5410, 810.6007, 832.5827, and 848.5566
Software used are DataAnalysis or Mmass, and ppm error calculated in excel.

2 Create mass list from the averaged, re-calibrated IMS data set.

3 Calculate ppm error associated with common lipids, such as $[PC(32:0)+H]^+$ and $[PC(34:1)+H]^+$, for mass errors. If mass error is above 3 ppm, re-calibrate.

4 If LC-MS/MS has been performed, annotate each *m/z* value against the LC-MS/MS list, otherwise move to 4.1

4.1 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: $[M+H]^+$, $[M+H-H_2O]^+$, $[M+Na]^+$, $[M+K]^+$

1b. Negative Mode Adducts: $[M+H]^-$, $[M+Cl]^-$, $[M+HCOO]^-$, $[M+OAc]^-$

2. Specify Mass Tolerance: 0.005 *m/z*
3. Specify Chains: Even Chains Only
4. Sort: Delta

5 Calculate ppm error associated with each assignment and remove assignments with errors larger than 5 ppm, although most have errors lower than 3 ppm.