Basecamp 2020 - Day 6 - Assignment #2

Assignment#2:

1. Why is identification necessary when conducting a targeted lipidomics experiment? **1 mark**
2. Are SRM peaks picked from a total or extracted ion chromatogram? **1 mark**
3. How does a chromatogram differ from/relate to a mass spectrum? (Hint: a picture is very helpful) **2 marks**
4. When would it be important to annotate artifactual or isotopic peaks? Why should these peaks be identified? **2 marks**
5. If BATL returns an UNASSIGNED label in the Barcode column, how should you interpret this label? (Hint: think of the reasons for a peak to not be assigned a lipid identity.) **1 mark**

R Exercises:

1. The "openxlsx" package allows you to open and export xlsx spreadsheets. Using the help() function, can you figure out which openxlsx package function writes a table in R to an xlsx spreadsheet? **1 mark**
2. I have stated that the BATL functions to annotate artifacts/isotopes and assign lipid identities can be applied to a vector of SRM peak files. Can you modify the R script to deartifact and label multiple SRM peak files? (Hint: make a vector of the same SRM peak file.) **2 marks**
3. Provide your BATL output with each peak barcoded **3 marks**
4. Compare these barcodes to the lipid identities in the Lipid Lexicon and annotate your BATL output with a column that provides the molecular identity of each barcode. **2 marks**