



Knowledge that will change your world

Using MS-DIAL in SWATH-MS mode

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Access to data files at Riken

- http://prime.psc.riken.jp/?action=drop_index
- This website has a large number of downloadable data files, including those in .abf format
- Besides data-dependent data acquisition (DDA) data files, there are also SWATH-MS files where data-independent data acquisition (IDA)
- The latter may allow for quantitative data collection (poly MRM-MS).

Available files for MS-DIAL

MS-DIAL demo files

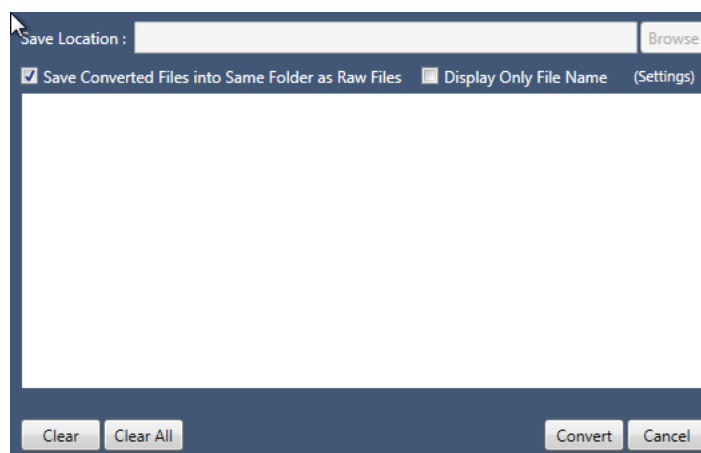
Both data independent MS/MS acquisition (SWATH) and data dependent MS/MS acquisition (IDA) data sets is downloaded as the demo files of MS-DIAL. In order to use MS-DIAL program, the user has to convert the vendor's raw data to ABF file format. The demonstration for file convert can be performed via AB Sciex raw data sets (.wiff and .wiff.scan). The file converter is available at <http://www.reifycs.com/english/AbfConverter/>. If you want to demonstrate MS-DIAL itself, please use the converted files (.abf) from the below link. Also see [MSDIAL quick start](#)

Contents:

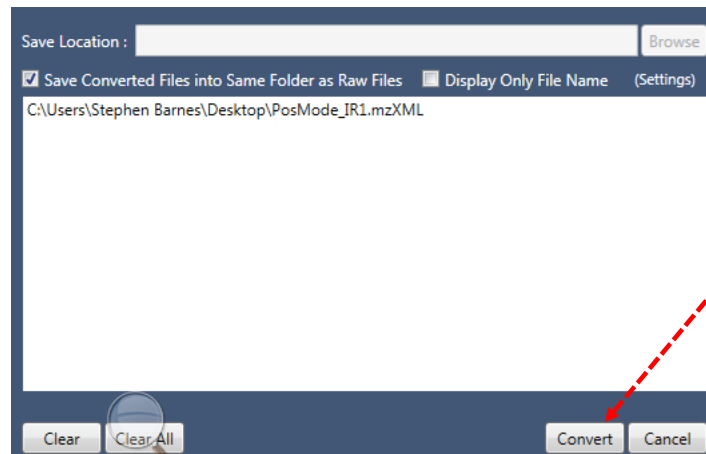
- AB Sciex raw data (.wiff & .wiff.scan), SWATH, Negative ion
mode: [20140809 MSDIAL_DemoFiles_Swath \(wiff.wiffscan\)](#) [zip archive: 691MB]
- ABF files of the raw data set, SWATH, Negative ion
mode: [20140809 MSDIAL_DemoFiles_Swath \(abf\)](#) [zip archive: 1,833MB] **These are in right format - 20 min**
- AB Sciex raw data (.wiff & .wiff.scan), IDA, Negative ion
mode: [20140809 MSDIAL_DemoFiles_Ida \(wiff.wiffscan\)](#) [zip archive: 1,394MB]
- ABF files of the raw data set, IDA, Negative ion
mode: [20140809 MSDIAL_DemoFiles_Ida \(abf\)](#) [zip archive: 4,830MB]

The downloads need to be done in the Windows platform

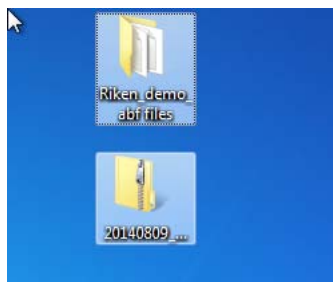
ABF converter



Add .mzxml file



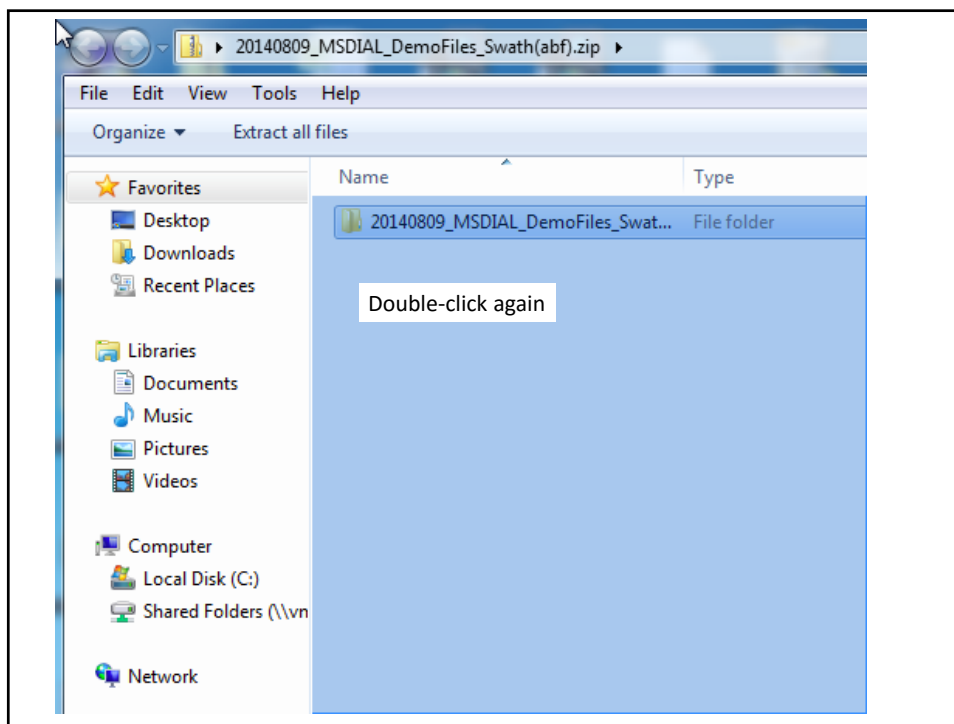
Extracting the data



New folder for the .abf files

Downloaded .zip file

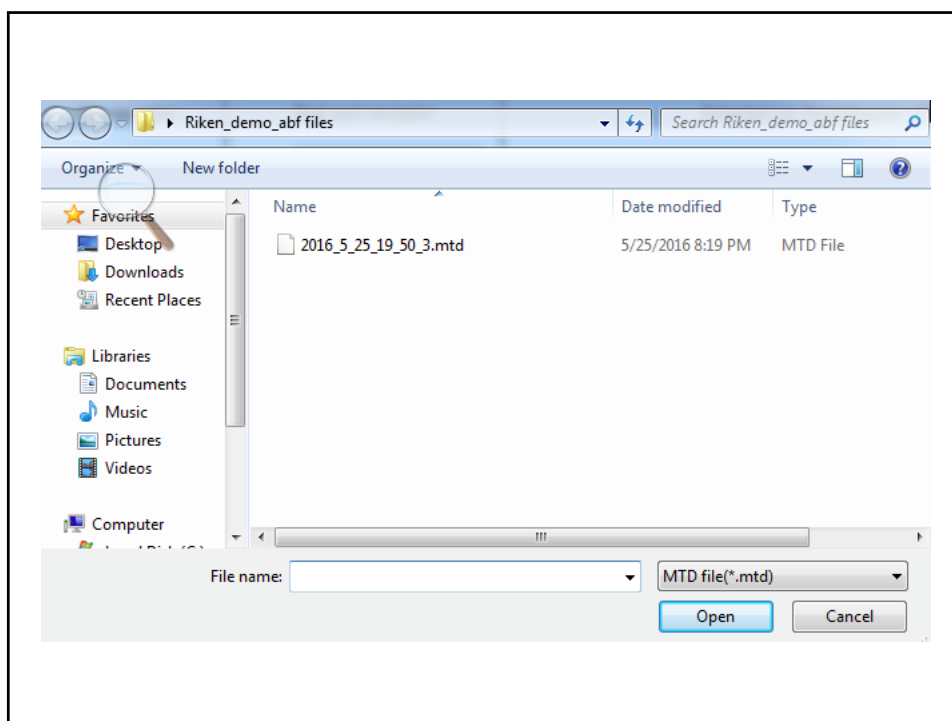
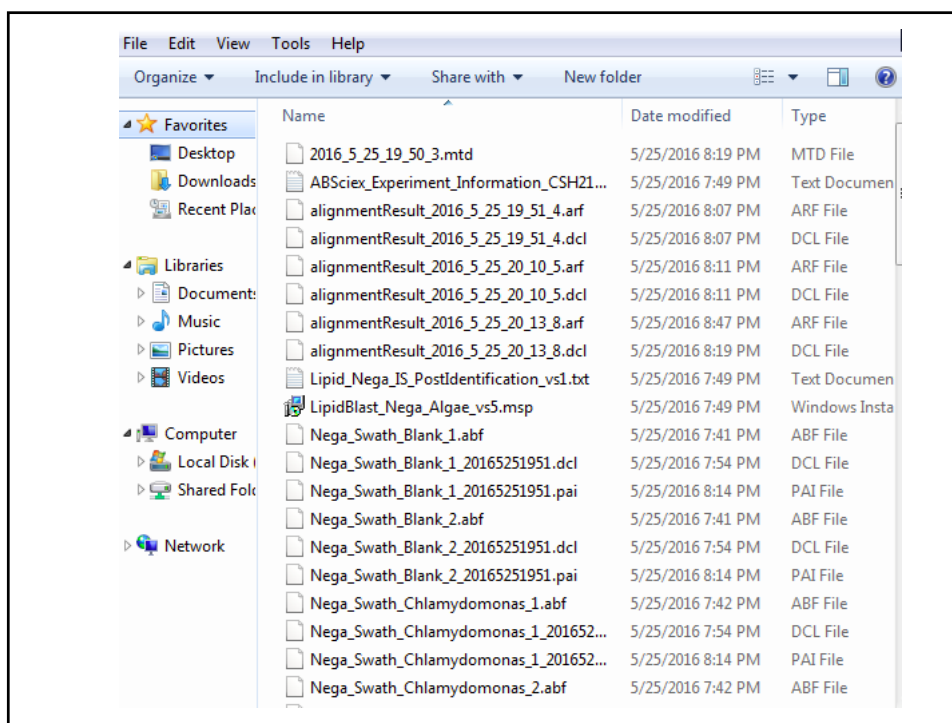
Double-click on it



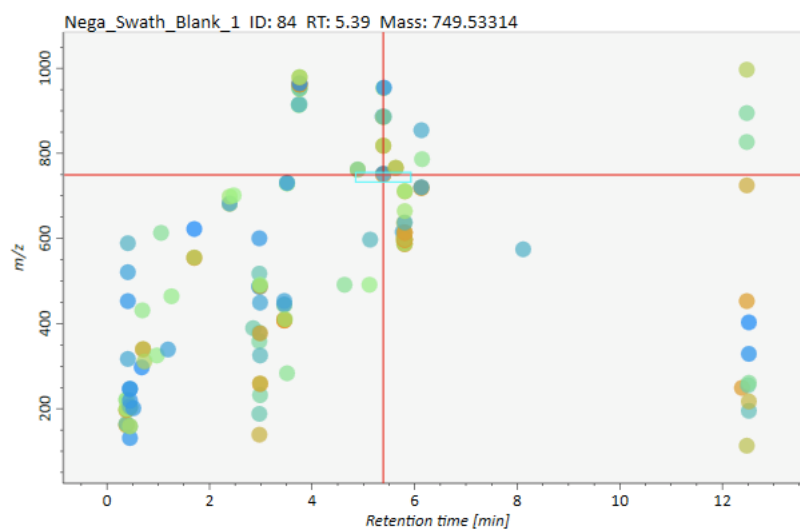
.Zip Folder with .abf files

A screenshot of a Windows Explorer window showing the contents of a zip folder. The window displays a list of files with columns for Name, Type, Compressed size, Password, Size, Ratio, and Date modified. The files listed include text documents, a Windows Installer Patch, and numerous ABF files.

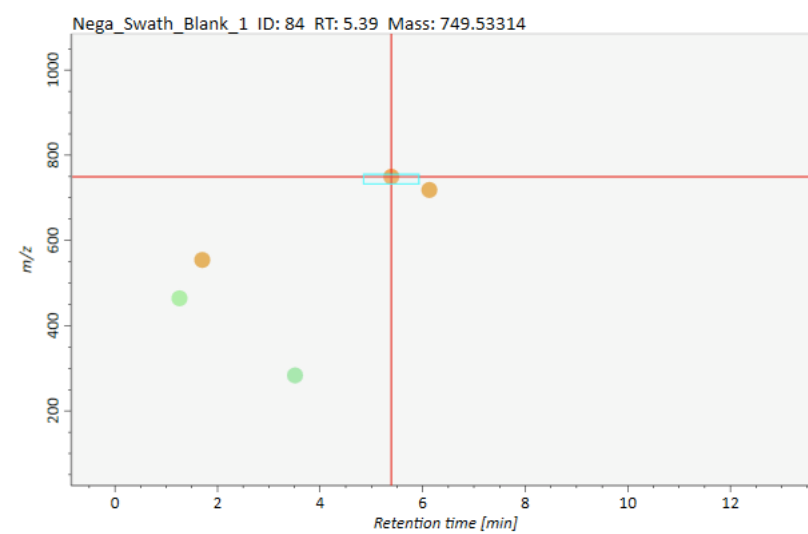
Name	Type	Compressed size	Password ...	Size	Ratio	Date modified
ABSciex_Experiment_Information_...	Text Document	1 KB	No	2 KB	59%	3/4/2014 6:14 AM
Lipid_Nega_IS_Postidentification_v...	Text Document	1 KB	No	1 KB	43%	8/31/2014 11:28 PM
LipidBlast_Nega_Algae_vs5.msp	Windows Installer Patch	1,258 KB	No	19,646 KB	94%	7/30/2014 8:18 PM
Nega_Swath_Blank_1.abf	ABF File	84,242 KB	No	229,279 KB	64%	8/9/2014 5:39 PM
Nega_Swath_Blank_2.abf	ABF File	84,325 KB	No	229,248 KB	64%	8/9/2014 5:40 PM
Nega_Swath_Chlamydomonas_1.abf	ABF File	80,618 KB	No	215,367 KB	63%	8/9/2014 5:40 PM
Nega_Swath_Chlamydomonas_2.abf	ABF File	80,111 KB	No	214,010 KB	63%	8/9/2014 5:41 PM
Nega_Swath_Chlamydomonas_3.abf	ABF File	80,526 KB	No	215,331 KB	63%	8/9/2014 5:41 PM
Nega_Swath_Chlamydomonas_4.abf	ABF File	80,061 KB	No	213,331 KB	63%	8/9/2014 5:42 PM
Nega_Swath_Chrollera_Utez2341_1...	ABF File	82,156 KB	No	221,266 KB	63%	8/9/2014 5:42 PM
Nega_Swath_Chrollera_Utez2341_2...	ABF File	81,602 KB	No	219,308 KB	63%	8/9/2014 5:43 PM
Nega_Swath_Chrollera_Utez2341_3...	ABF File	81,338 KB	No	218,253 KB	63%	8/9/2014 5:43 PM
Nega_Swath_Chrollera_Utez2341_4...	ABF File	82,446 KB	No	222,420 KB	63%	8/9/2014 5:44 PM
Nega_Swath_Chrollera_Utez2805_1...	ABF File	81,248 KB	No	217,841 KB	63%	8/9/2014 5:44 PM
Nega_Swath_Chrollera_Utez2805_2...	ABF File	81,660 KB	No	218,883 KB	63%	8/9/2014 5:45 PM
Nega_Swath_Chrollera_Utez2805_3...	ABF File	81,089 KB	No	217,171 KB	63%	8/9/2014 5:45 PM
Nega_Swath_Chrollera_Utez2805_4...	ABF File	80,687 KB	No	215,992 KB	63%	8/9/2014 5:46 PM
Nega_Swath_QC_1_1.abf	ABF File	80,346 KB	No	215,176 KB	63%	8/9/2014 5:46 PM
Nega_Swath_QC_1_3.abf	ABF File	82,124 KB	No	219,564 KB	63%	8/9/2014 5:47 PM
Nega_Swath_QC_1_5.abf	ABF File	82,041 KB	No	219,418 KB	63%	8/9/2014 5:47 PM



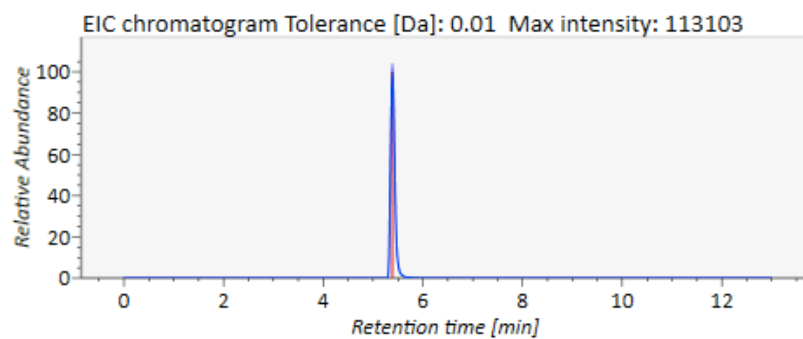
All ions in Blank 1



Identified ions in Blank 1

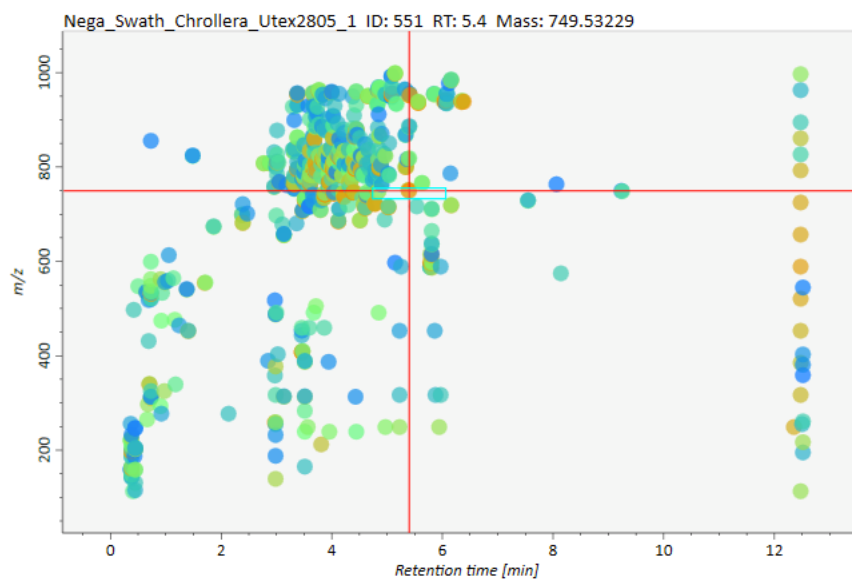


Blank sample PG 34:0

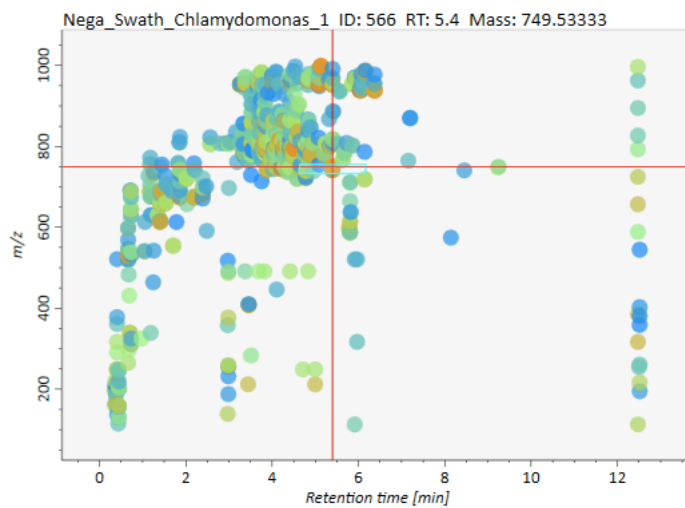


This may be an added internal standard

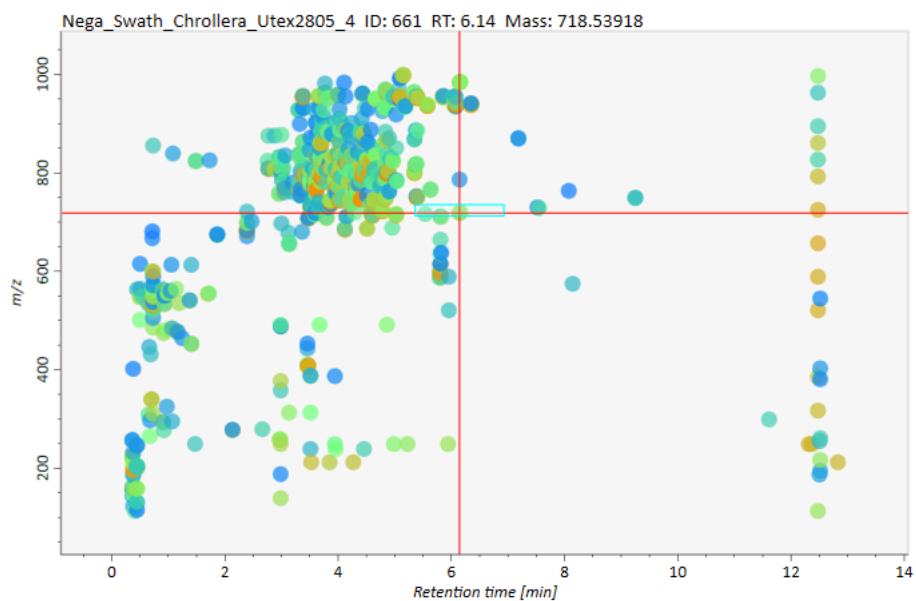
Data from *Chrorella Utex* 1



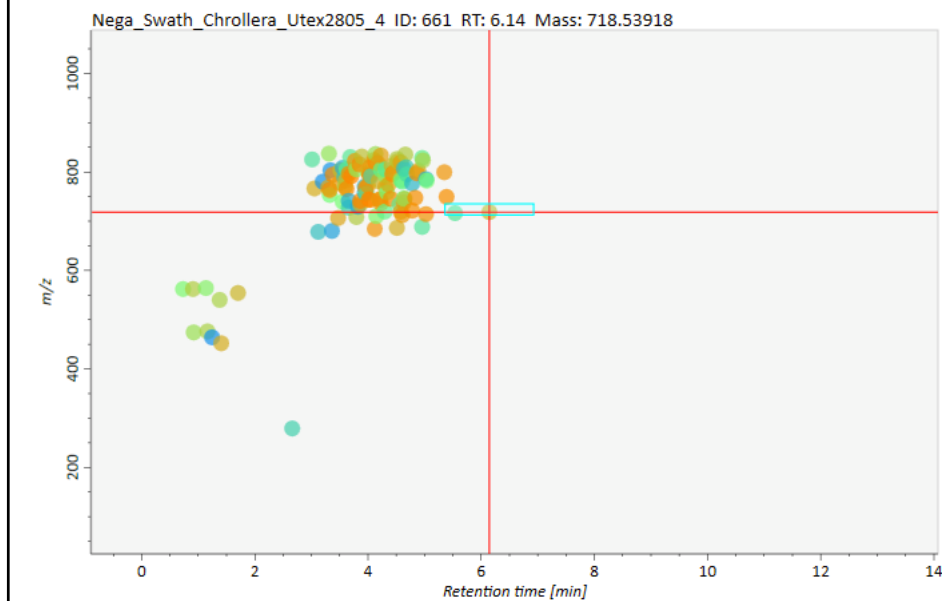
All lipid ions from *Chlamydomonas* 1



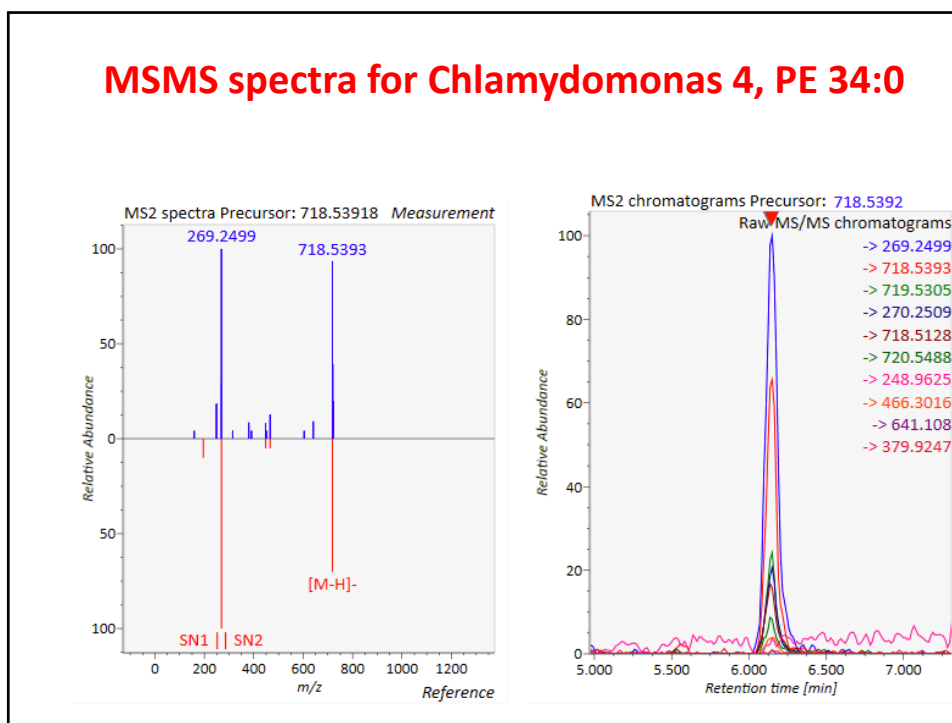
All lipid ions from *Chlamydomonas* 4



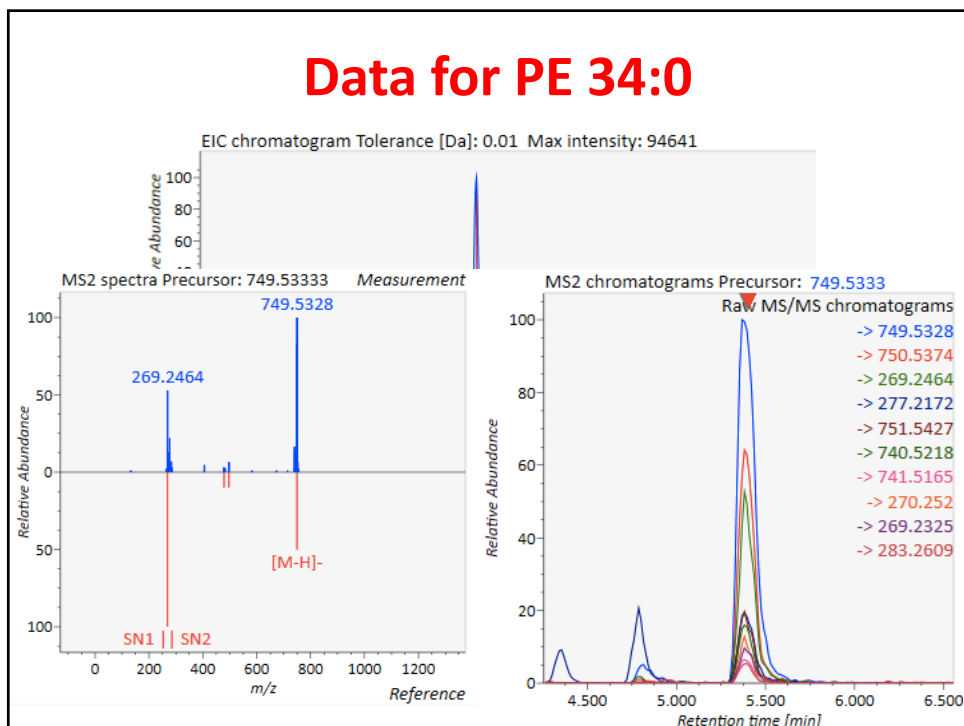
Identified ions in Chlamydomonas 4



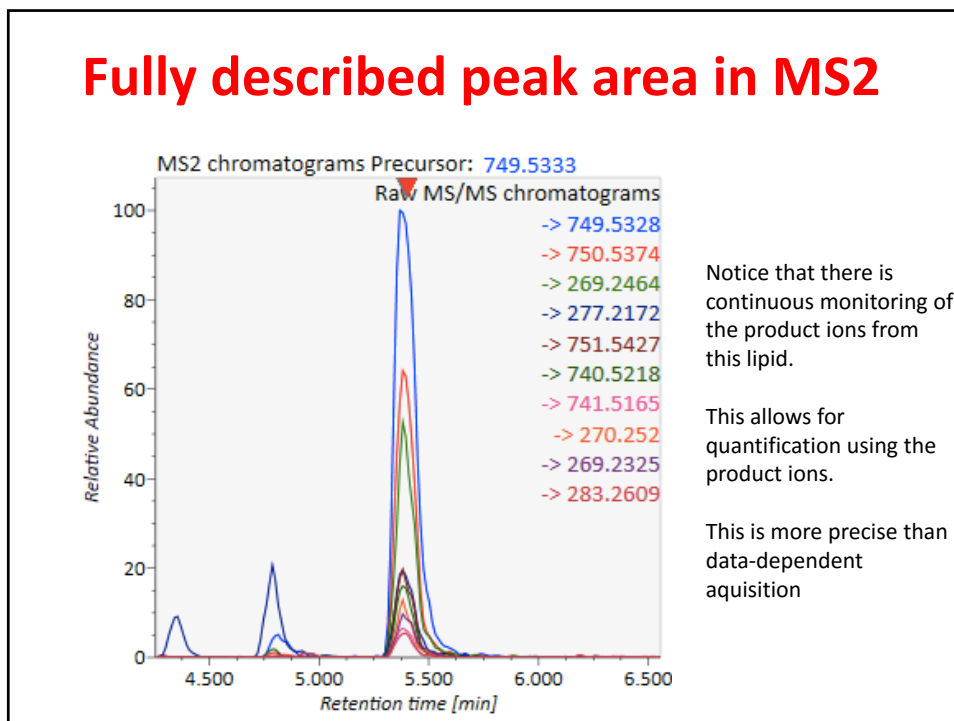
MSMS spectra for Chlamydomonas 4, PE 34:0



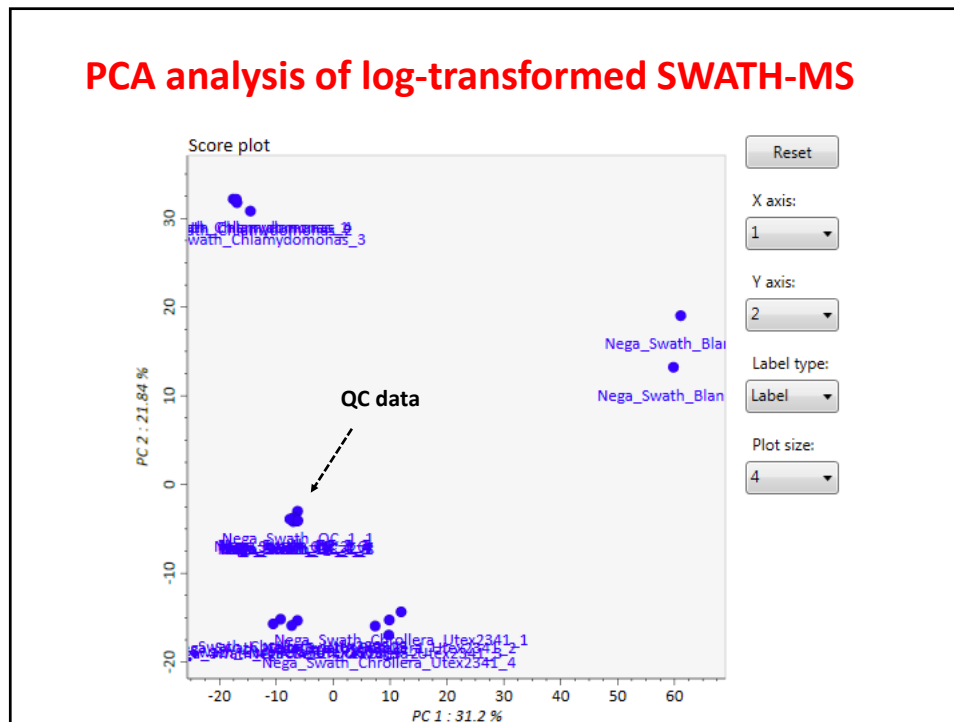
Data for PE 34:0



Fully described peak area in MS2



PCA analysis of log-transformed SWATH-MS



Conclusions about the differences

- It's well known that organisms each have a discrete profile of fatty acids
 - GC and GC-MS of fatty acid methyl esters have been used to identify microorganisms
 - Did this in our lab during the development stage of the International Space Station (1990-1993) to determine which organisms grew in the water reprocessing unit (sub-contract with Boeing)
- Since now we can also include the variation coming from the phospholipid head group, the discrimination of the organisms may be even better