Viewing Multiple Interactive Plots with plotly And trelliscopejs
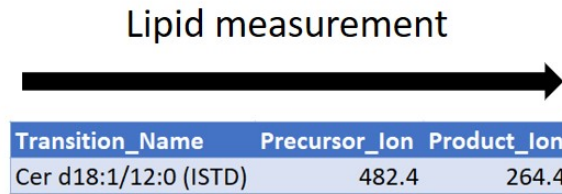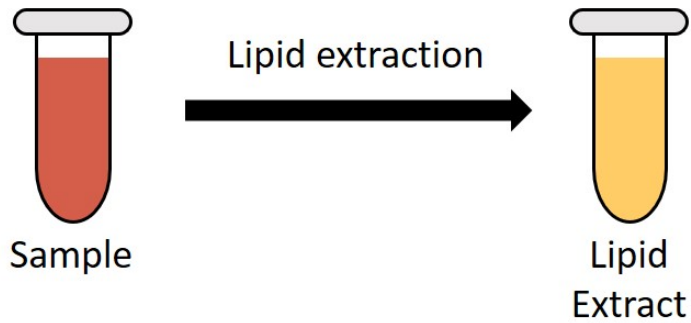
Jeremy Selva

Introduction to Lipids

Lipids are organic compounds that are mostly insoluble in polar solvents like water.

The most common ones are cholesterol and triglycerides in blood lipid panel test.


Take blood sample

How Lipids are measured (Targeted Lipidomics)

Transition_Name	Precursor_Ion	Product_Ion
Cer d18:1/12:0 (ISTD)	482.4	264.4

Sample → Lipid extraction → Lipid Extract → Lipid measurement → Liquid Chromatography/Mass Spectrometry

Sample_Name	Cer d18:1/12:0 (ISTD)
Sample 01	479025
Sample 02	570275
Sample 03	374854
Sample 04	319491
Sample 05	231691

Peak Area Data

Peak integration

+ MRM (482.4 -> 264.2) Cer d18:1/12:0 (ISTD)
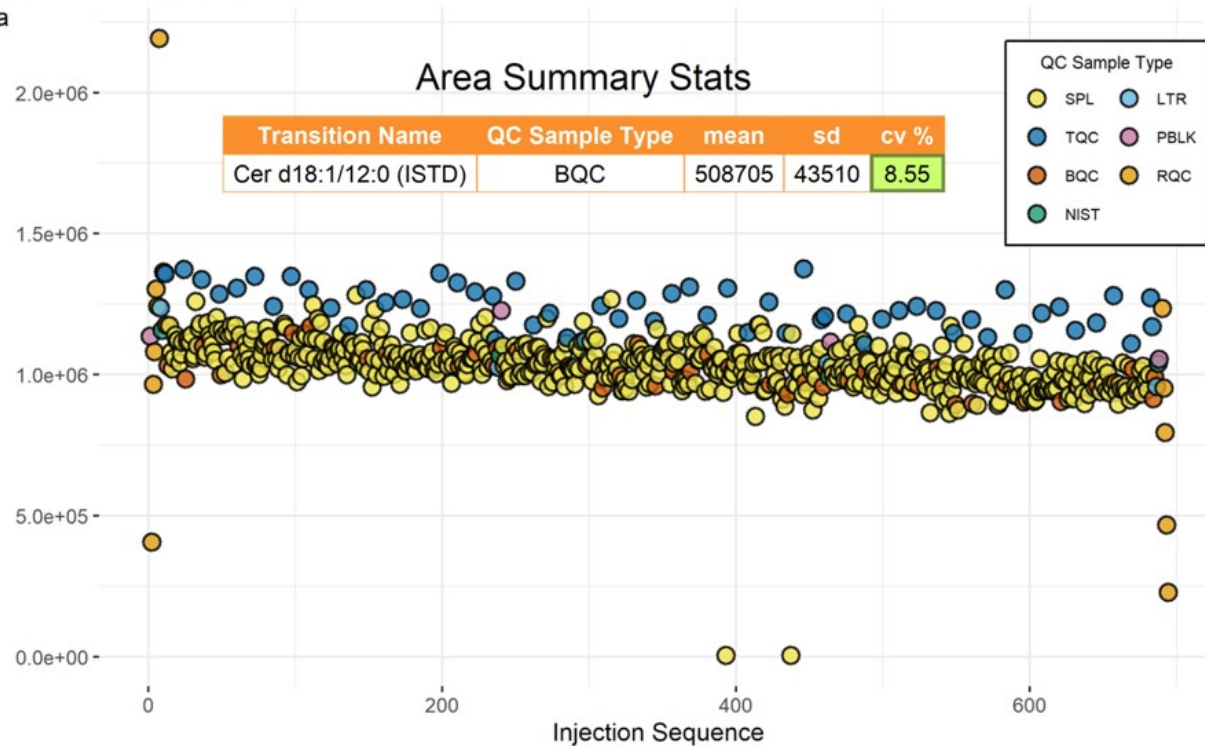Area=479025
RT=4.13 min.
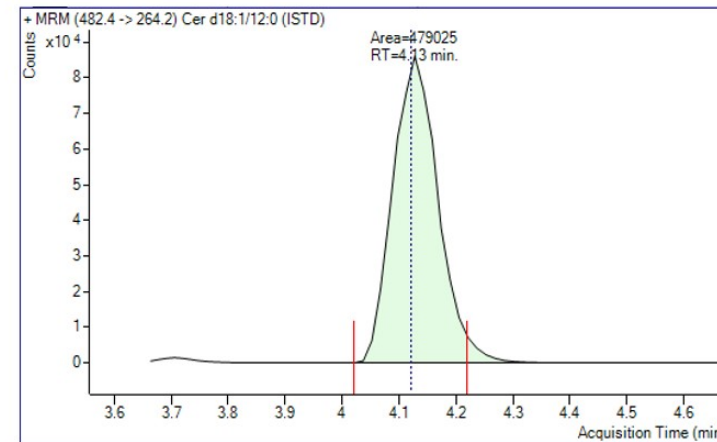
Quality Control (QC) Samples

Quality control samples helps to check the severity of variation from external sources such as contaminant ions.

We want to keep molecules that gives a low variation on the quality control samples.
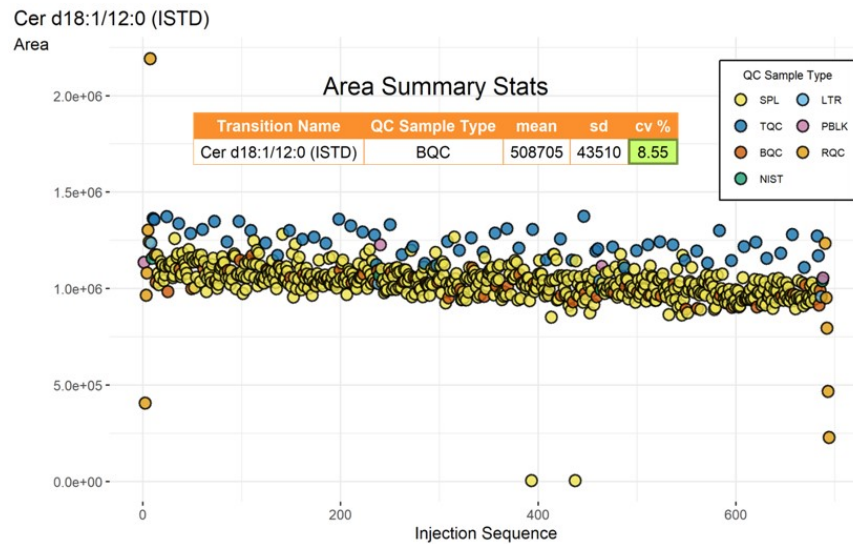
Plots are exported as pages in a pdf file.

Motivation for using `plotly` and `trelliscopejs`

Today's targeted lipidomics workflow can measure up to a few hundred molecules.
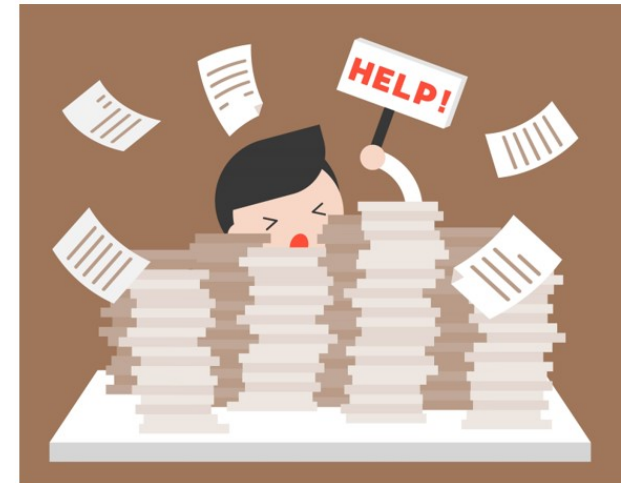
This gives a pdf file of over 500 pages.

Looking at these static plot individually to gain insights is tedious.
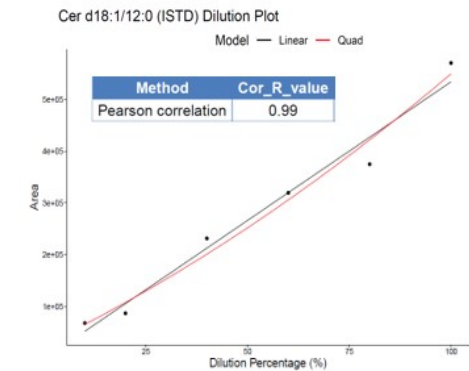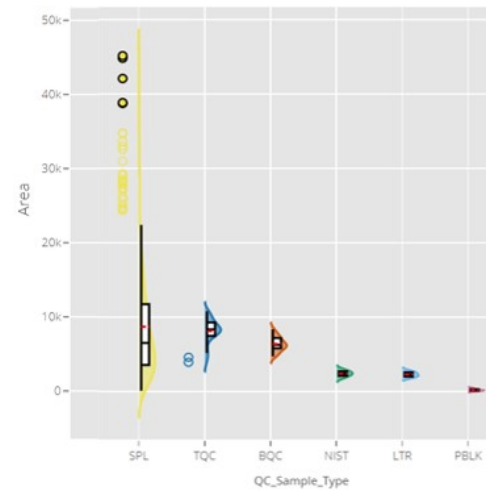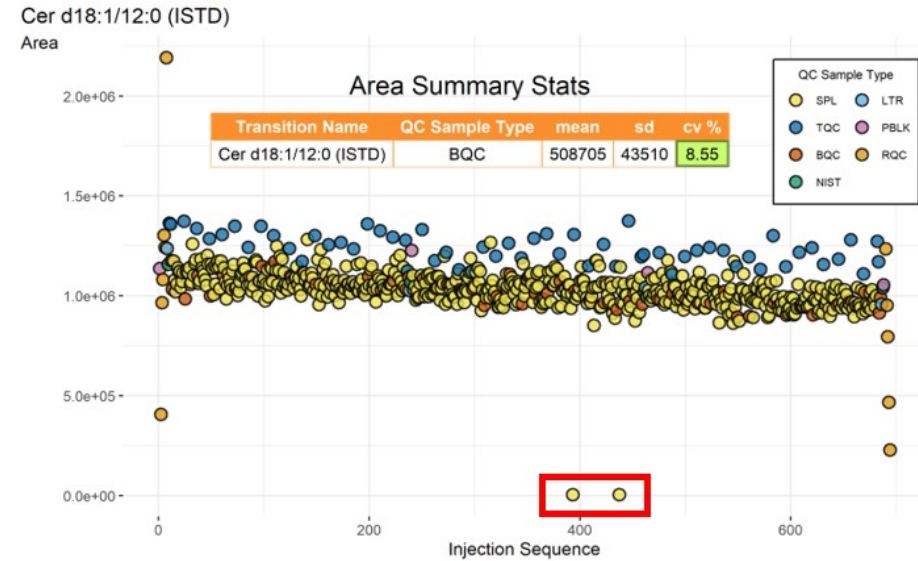

> 500

> 500 Pages

Motivation for using `plotly` and `trelliscopejs`

Out of > 500 molecules,

- Can I have more info about the outlying samples in the red box ?

- How many Ceramides have BQC CV over 20% ?

- Can you plot the same data as a Raincloud Plot ?

Motivation for using **plotly** and **trelliscopejs**

Using `plotly` to create interactive plots is moving in the right direction.

However, distribution of such results to collaborators/managers remains a challenge.

Interactive plots cannot be stored in pdf files.

Shiny was considered but

- Lack expertises to maintain a secure web server to run Shiny applications.
- Cannot expect collaborators/managers to install/run R packages and code to rebuild the Shiny application just to view the results.
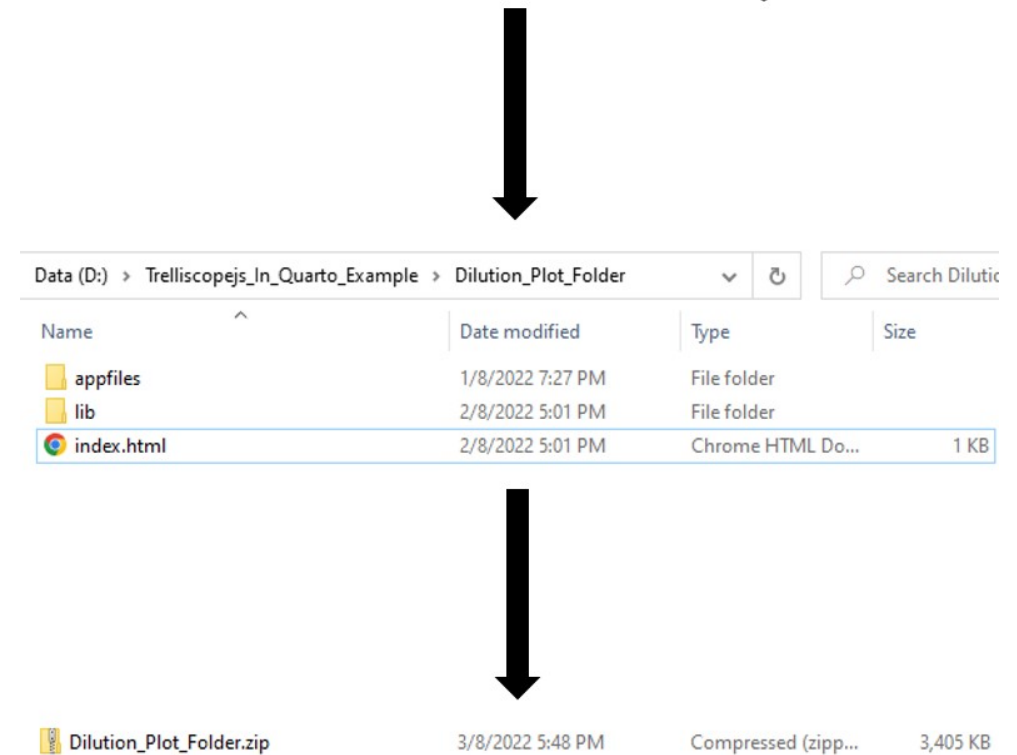
Select a Display to Open

no thumbnail   no thumbnail

Dilution_Plot

750 panels,2022-08-07 15:45

Injection_Sequence_Plot

750 panels,2022-08-07 15:48

CLOSE

8

Quarto Example

Thanks to open science, I am able to create a walk through example using Quarto 🔗 .

Column Of Plots

Use `dplyr::mutate` and `trelliscopejs::pmap_plot` to save `plotly` plots as a new column.

`trelliscopejs` cognostics

Providing metadata information as `trelliscopejs` cognostics can help to improve the user experience.

Refer to the Quarto 🔗 🐙 example on how to do it.

Cognostics

To output these interactive plots as a trellis plot in html, we need to convert our current tibble and `dilution_plot_table` and `injection_sequence_table` into a cognostics dataframe.

The cognostics dataframe consist of three components

1. A group of columns known as conditioning variables. They will form the unique id of the trellis plot. As such, each row of these columns must be unique. In our example, the column used is `Transition_Name`
2. One column that holds the images to display each plot in the trellis. This column is known as the panel variable. We just created this column using `trelliscopejs::pmap_plot` earlier.
3. The other columns will be grouped as general cognostics columns.

Cognostics Conversion Functions

The relevant functions to convert all columns, except the panel variable, to cognostics objects are as follows.

▶ Code

Cognostics Setup

The function `trelliscopejs::cog` is used to convert a column into cognostic object. The following meta information must be provided in order for the conversion to be successful.

Information About This Display (from screenshot)
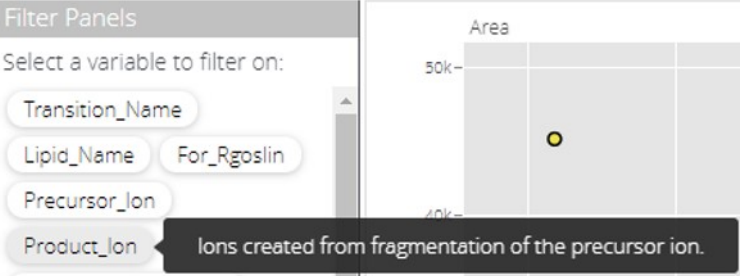
Injection_Sequence_Plot

Information About This Display

Cognostics

To help navigate the panels, the following cognostics have been computed. For information on how to use these metrics to interact with the panels, please click the "?" icon in the top right corner of the application or hit the key "a".

- Transition_Name:conditioning variable
- Lipid_Name:Converted transition name to suit lipid nomenclature set by Liebisch et. al. 2020.
- For_Rgoslin:Input transition for the R package rgoslin to annotate.
- Precursor_Ion:The ion to be fragmented into smaller fragment ions.
- Product_Ion:Ions created from fragmentation of the precursor ion.

Filter Panels

Select a variable to filter on:

Transition_Name
Lipid_Name   For_Rgoslin
Precursor_Ion
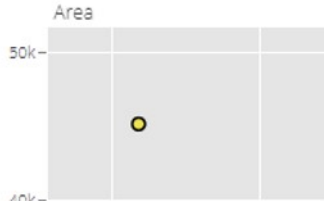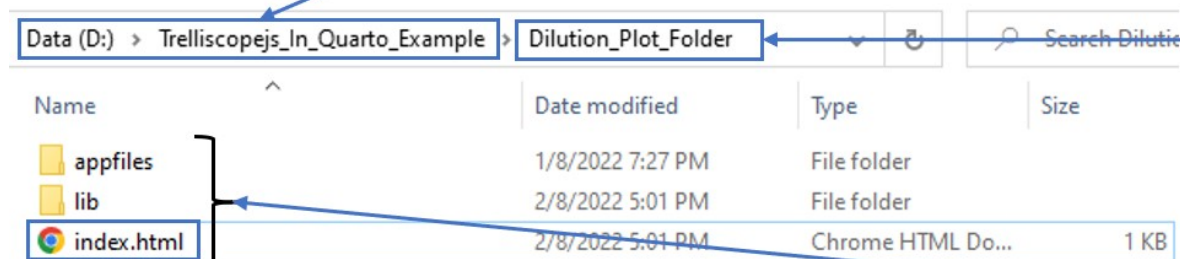Product_Ion   Ions created from fragmentation of the precursor ion.

Area
50k
40k

Results Distribution

To export a `trelliscopejs` **object.**

Step 1. Set working directory

Step 2. Call script in console

```r
trelliscope_name <- "Dilution Plot"

dilution_trellis |>
  trelliscopejs::trelliscope(
    name = trelliscope_name,
    panel_col = "dilution_panel",
    path = "Dilution_Plot_Folder",
    state = list(sort = list(trelliscope
    nrow = 2,
    ncol = 2,
    height = 520,
    width = 1100,
    self_contained = FALSE,
    thumb = FALSE,
    auto_cog = FALSE
  )
```
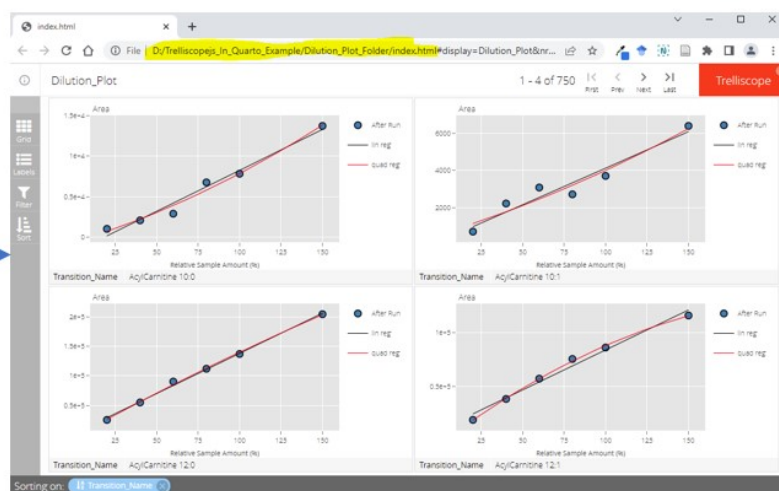
Step 3. Compress Folder

Dilution_Plot_Folder.zip   3/8/2022 5:48 PM

Results Distribution

To export a Quarto document with `trelliscopejs` **object.**

Results Distribution

Exported examples are found under the Releases section in the below GitHub page.

Other Resources

`trelliscopejs` **Examples**

- **https://ryanhafen.com/blog/pokemon/**
- **https://hafen.github.io/trelliscopejs-demo/mri/**
- **https://hafen.github.io/trelliscopejs-demo/network/**
- **https://www.rostrum.blog/2019/06/20/goat-scope/**

Presentation

- **https://www.rstudio.com/resources/rstudioconf-2017/trelliscopejs/**
- **https://www.youtube.com/watch?v=TgFJrfSEKuQ**
    - **See talk at around 54.55**
    - **Slides**

Hope to see more examples...

Conclusion

Summary

- **Quality control samples are useful to check for unwanted variation in a targeted lipidomics workflow.**

- `plotly` **and** `trelliscopejs` **can help to explore many interactive plots in an effective way.**

- **Hope that the Quarto 🔗 🐱 example and advice provided are useful.**