Viewing Multiple Interactive Plots with `plotly` And `trelliscopejs`

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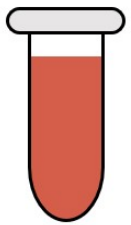
Introduction to Lipids

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

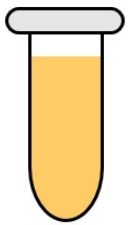
The most common ones are cholesterol and triglycerides in blood lipid panel test.

How Lipids are measured (Targeted Lipidomics)



Sample

Lipid extraction

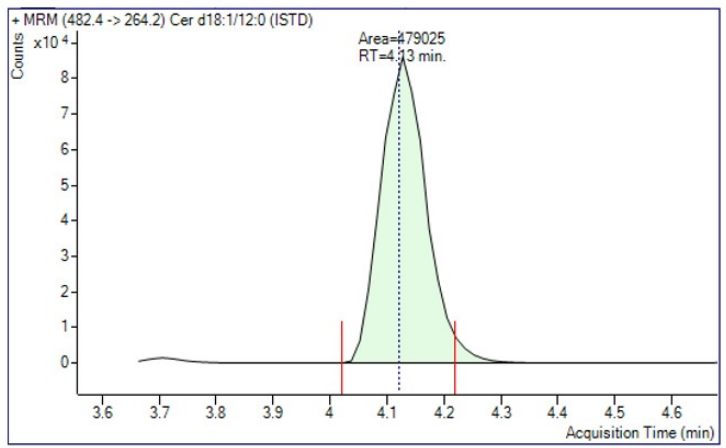


Lipid Extract

Lipid measurement

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

Liquid Chromatography/Mass Spectrometry



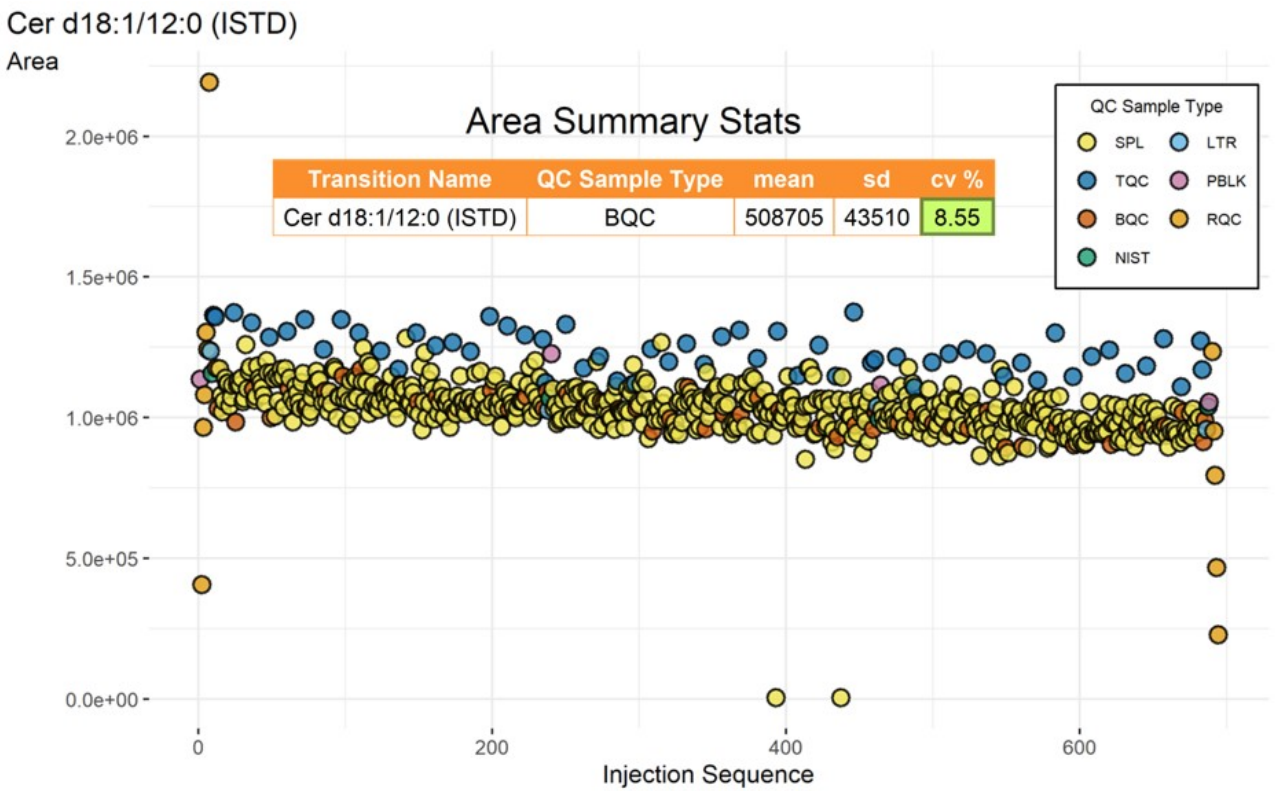
Peak integration

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

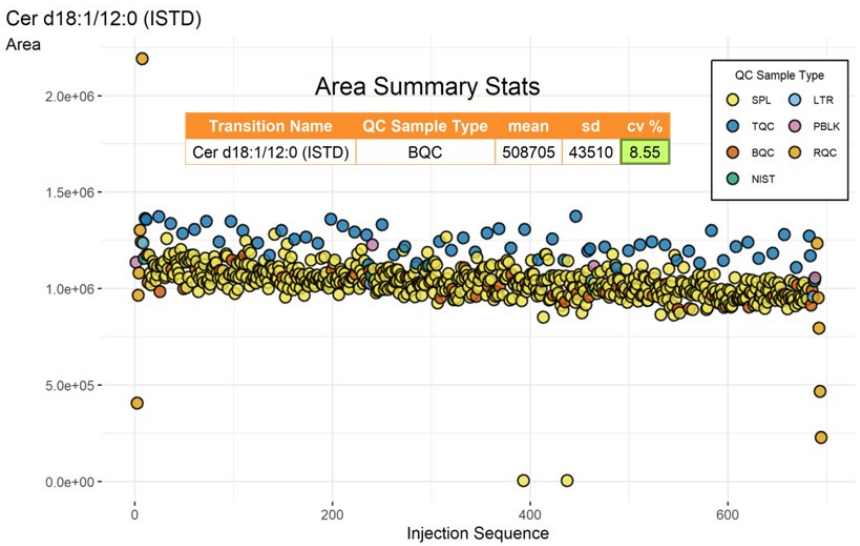
Quality Control (QC) Samples

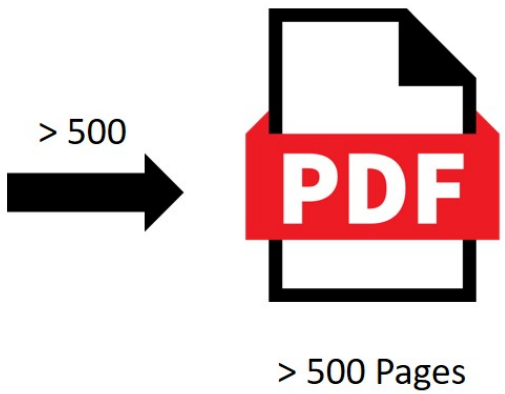
Quality control samples helps to check the severity of variation from external sources such as contaminant ions. We want to keep molecules that gives a low variation on the quality control samples. Plots are exported as pages in a pdf file.

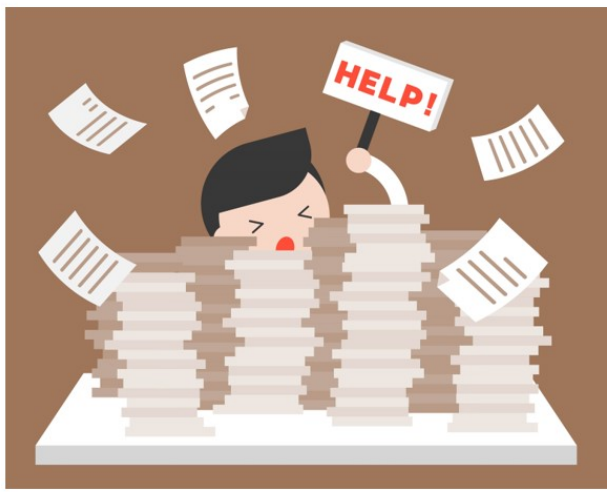


Motivation for using `plotly` and `trelliscopejs`

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.



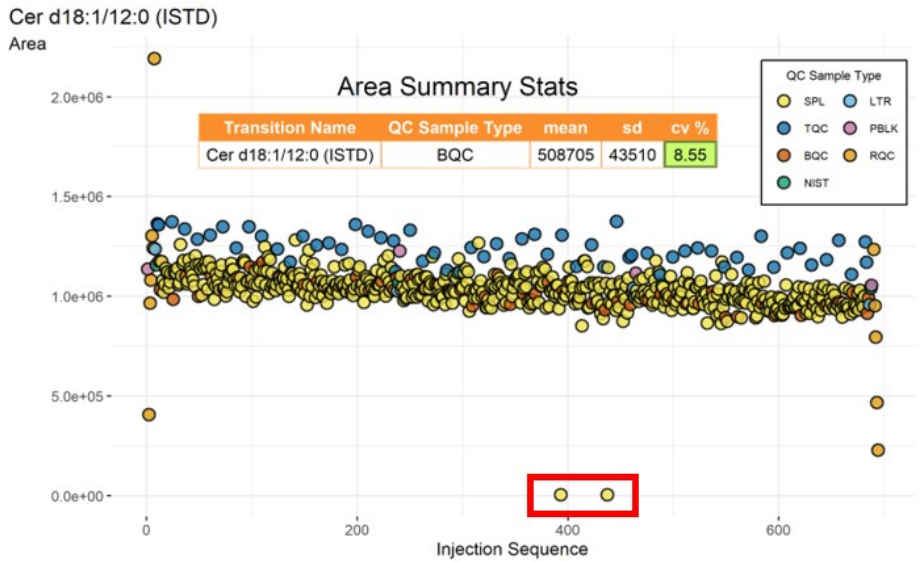


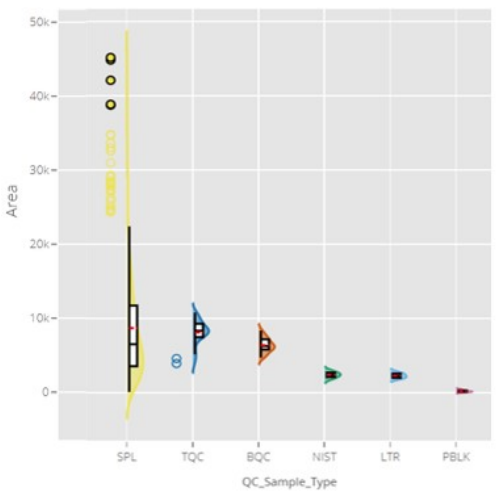


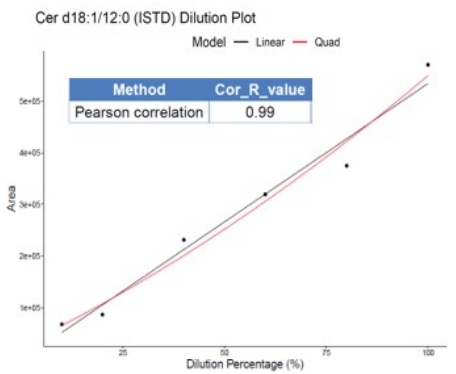
Motivation for using `plotly` and `trelliscopejs`

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`

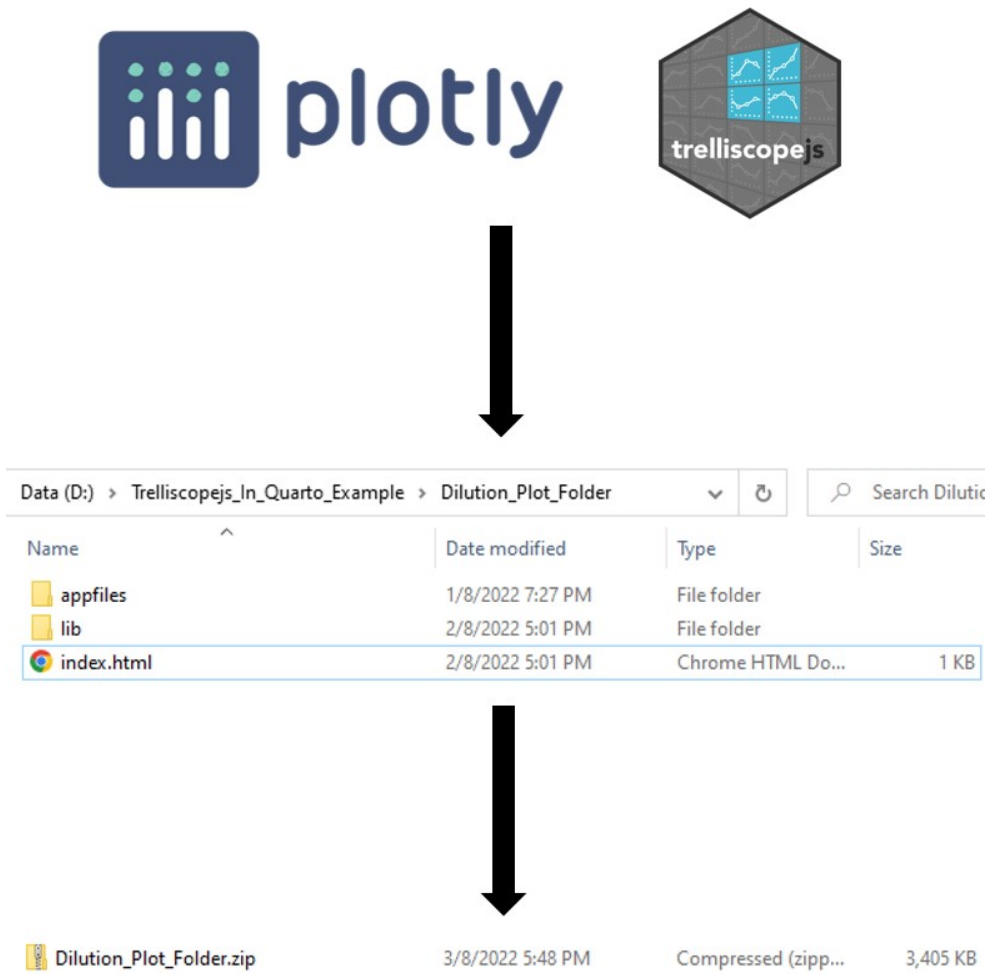
Using `plotly` to create interactive plots is moving in the right direction.

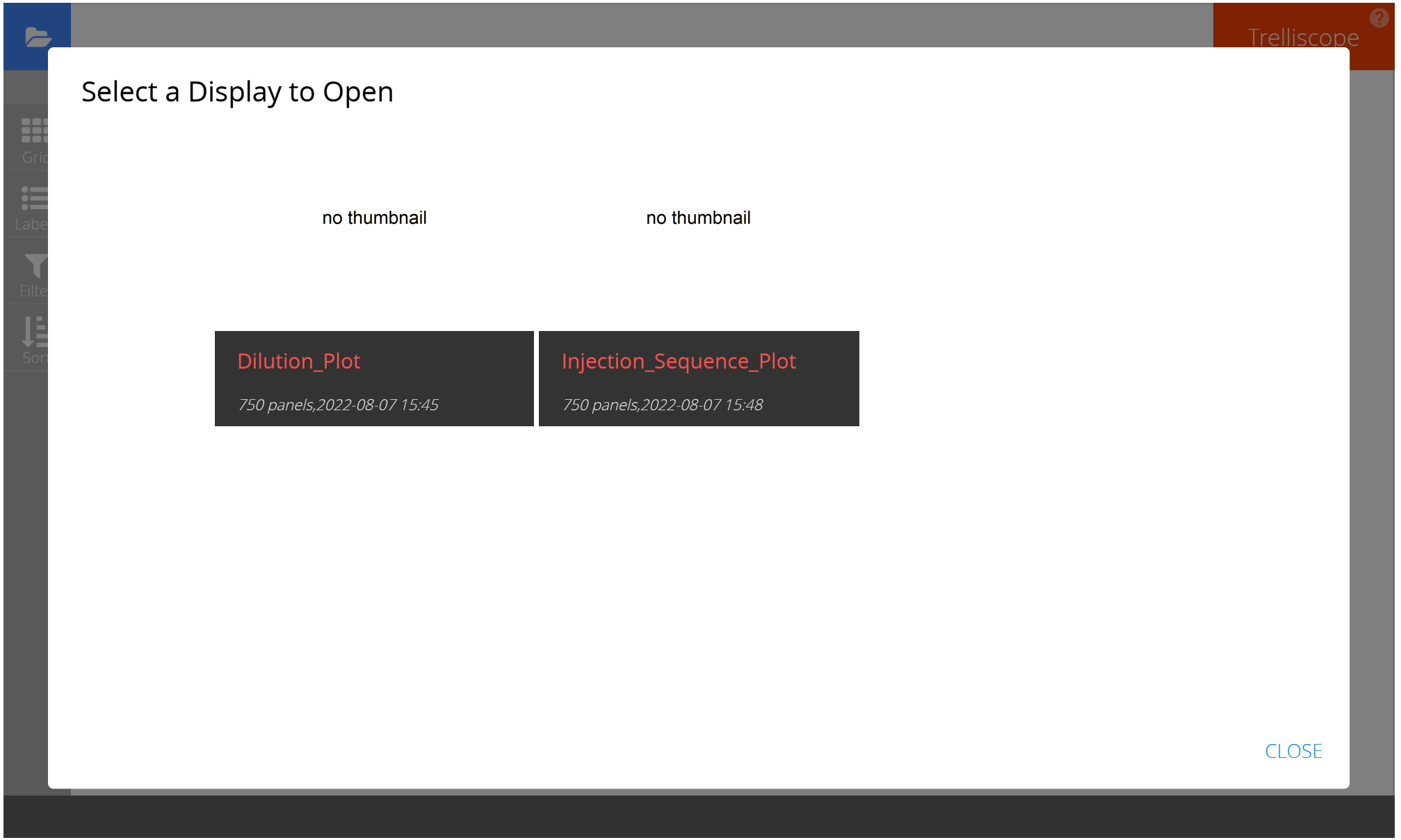
However, distribution of such results to collaborators/managers remains a challenge.

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.**




Trelliscope
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

Quarto Example

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

Article | Open Access | Published: 10 January 2022

Lipidomic profiling of human serum enables detection of pancreatic cancer

Denise Wolrab, Robert Jirásko, ... Michal Holčapek + Show authors

Nature Communications **13**, Article number: 124 (2022) | Cite this article

9421 Accesses | **5** Citations | **41** Altmetric | Metrics

Data availability

All data necessary to support the conclusions are available in the manuscript or supplementary information. Source data are provided with this paper. Raw data, instructions for software handling, and the software are deposited at figshare.com:https://figshare.com/s/cc087785ca362af7118e–(UHPSFC/MS; Phase I and Phase II). https://figshare.com/s/e336bdf3a52f04c2de1f–(Shoutgun-MS (LR and HR); Phase II). https://figshare.com/s/cb071be45cd91a7c90e2–(MALDI-MS; Phase I). https://figshare.com/s/1fd10f273b049b93fa24–(RP-UHPLC/MS; Phase II). Source data are provided with this paper.

Supplementary information

Supplementary Information

Peer Review File

Description of Additional Supplementary Files

Supplementary Data 1-20

Reporting Summary

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- Package References
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Quarto Report Example With Plotly and Trelliscopejs

Code

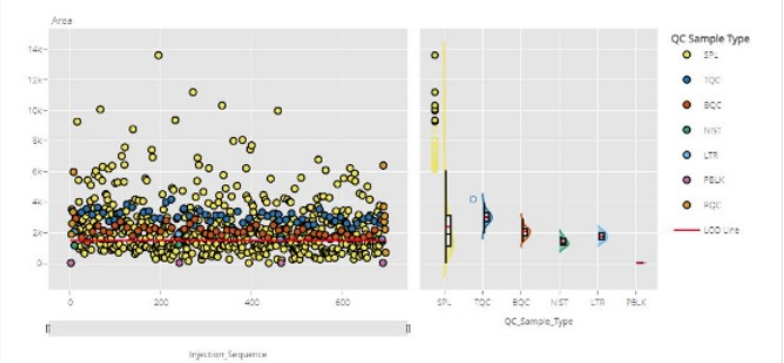
Show All Code
Hide All Code
View Source

Written by Jeremy Selva

Introduction

Here is a report showing how to create injection sequence plot and dilution plot using `plotly` for each Multiple Reaction Monitoring (MRM) transition in Mass Spectrometry.

Injection Sequence Plot | Dilution Plot



Column Of Plots

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

```
dilution_plot_table <- summary_data |>
  dplyr::mutate(
    dilution_panel = trelliscopejs::pmap_plot(
      list(dilution_data = .data[["dilution_data"]]),
      plot_dil_curve_plotly,
      dilution_title = "",
      dilution_pal = dilution_pal,
      sample_name_var = "Sample_Name",
      dil_batch_var = "Dilution_Batch_Name",
      conc_var = "Relative_Sample_Amount_[%]",
      conc_var_units = "%",
      conc_var_interval = 25,
      signal_var = "Area",
      x_axis_title = "Relative Sample Amount",
      y_axis_title = "Area",
      y_axis_rangemode = "normal",
      lin_reg_name = "lin reg",
      quad_reg_name = "quad reg",
      show_legend = TRUE,
      show_y_axis_title = TRUE,
      annotation_var = c("Dilution_Batch_Name",
                         "Injection_Sequence",
                         "Acqusition_Time_Stamp",
                         "Vial_Position")
    )
  ) |>
  dplyr::select(-c("dilution_data", "sample_data"))
```

Map over multiple inputs simultaneously and return a vector of plots

Source: R/tidy.R

Map over multiple inputs simultaneously and return a vector of plots

```
map2_plot(.x, .y, .f, ...)
pmap_plot(.l, .f, ...)
```

Trelliscopejs_In_Quarto_Example - main - RStudio

File Edit Code View Plots Session Build Debug Profile Tools Help

dilution_plot_table

Filter

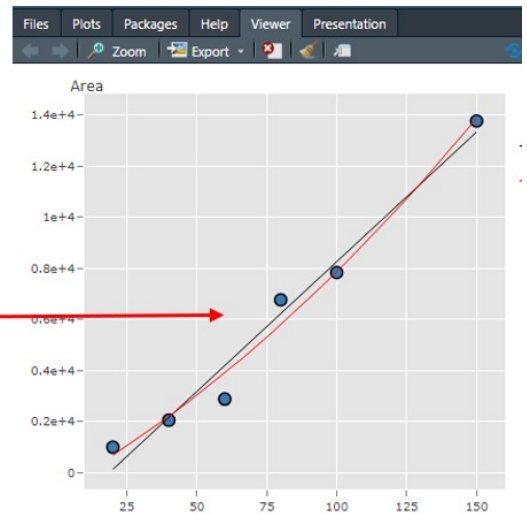
	Transition_Name	dilution_panel	Lipid_Name
1	AcylCarnitine 10:0	list(x = list(visdat = list(`77644c483021` = funct [...]	CAR 10:0
2	AcylCarnitine 10:1	list(x = list(visdat = list(`776423dd5818` = funct [...]	CAR 10:1
3	AcylCarnitine 12:0	list(x = list(visdat = list(`776449445435` = funct [...]	CAR 12:0
4	AcylCarnitine 12:1	list(x = list(visdat = list(`77647ac9148a` = funct [...]	CAR 12:1
5	AcylCarnitine 13:0	list(x = list(visdat = list(`77642fcb50cb` = funct [...]	CAR 13:0
6	AcylCarnitine 14:0	list(x = list(visdat = list(`7764393e52d3` = funct [...]	CAR 14:0

Showing 1 to 6 of 750 entries, 44 total columns

Console Background Jobs

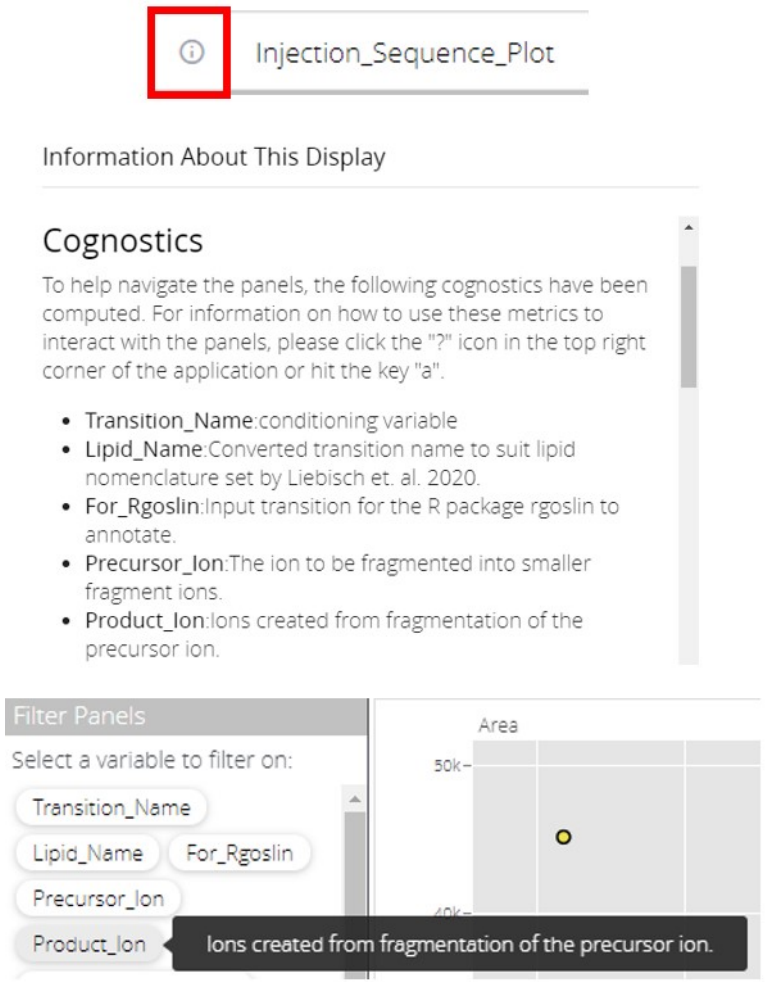
R 4.2.1 · D:/Trelliscopejs_In_Quarto_Example/

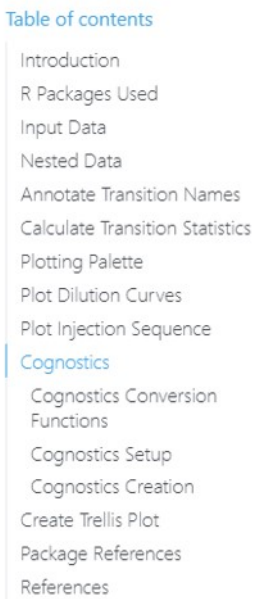
```
> dilution_plot_table$dilution_panel[[1]]
```

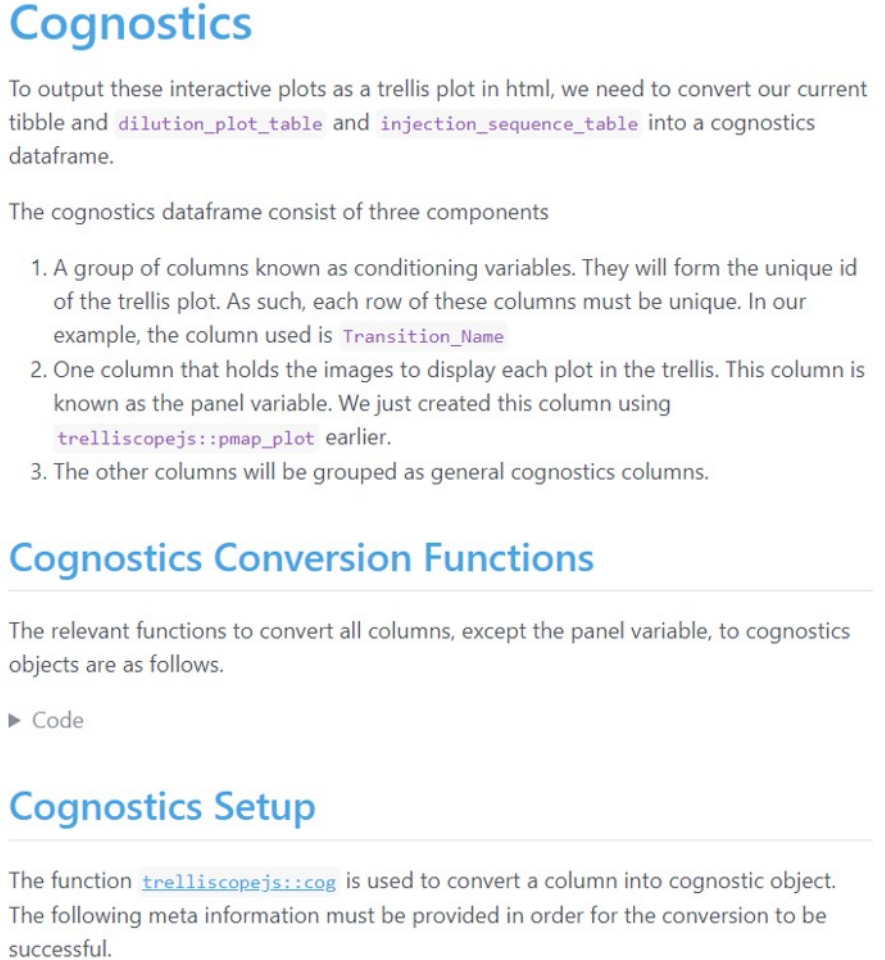


`trelliscopejs` cognostics

Providing metadata information as `trelliscopejs` cognostics can help to improve the user experience. Refer to the Quarto example on how to do it.



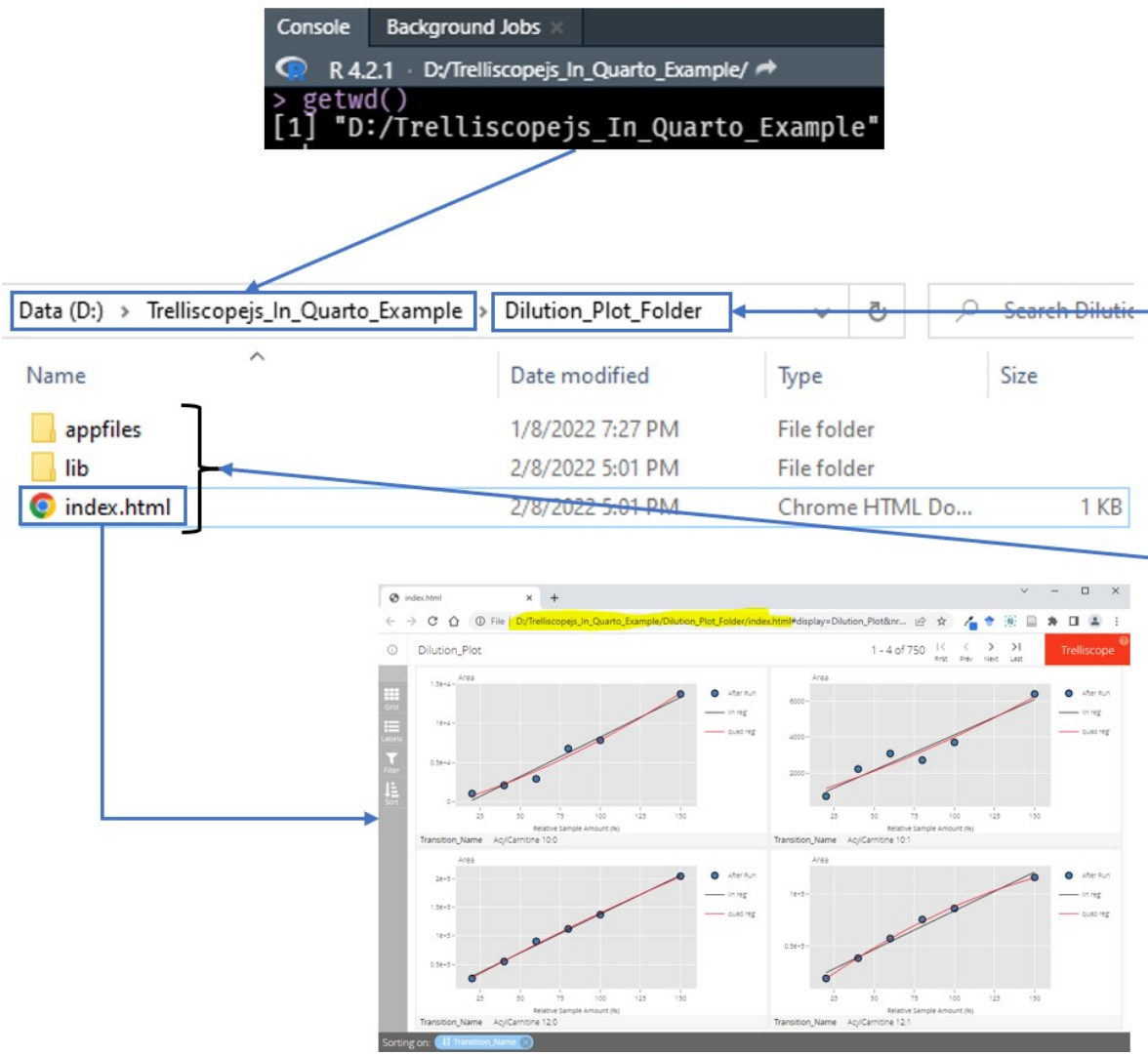




Results Distribution

To export a `trelliscopejs` object.

Step 1. Set working directory



Step 2. Call script in console

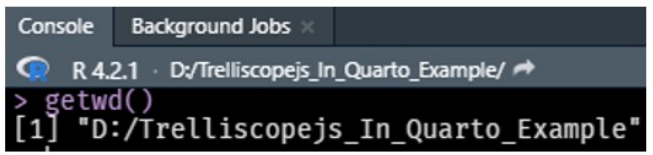
```
trelliscope_name <- "Dilution Plot"

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
  )
```

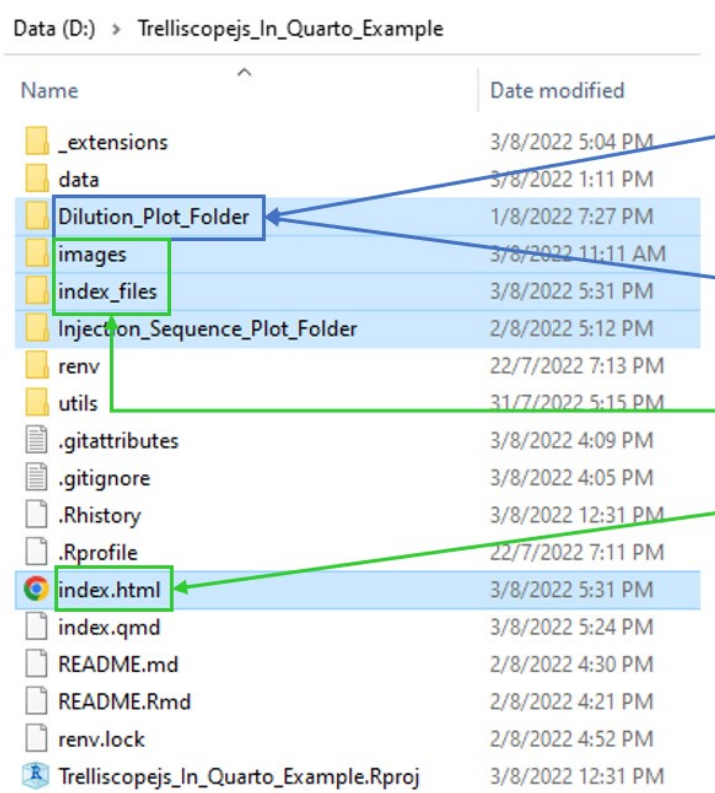
Step 3. Compress Folder

Results Distribution

To export a Quarto document with `trelliscopejs` object.

Step 1. Set working directory





Step 2. Render Quarto script


```
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
  )
```

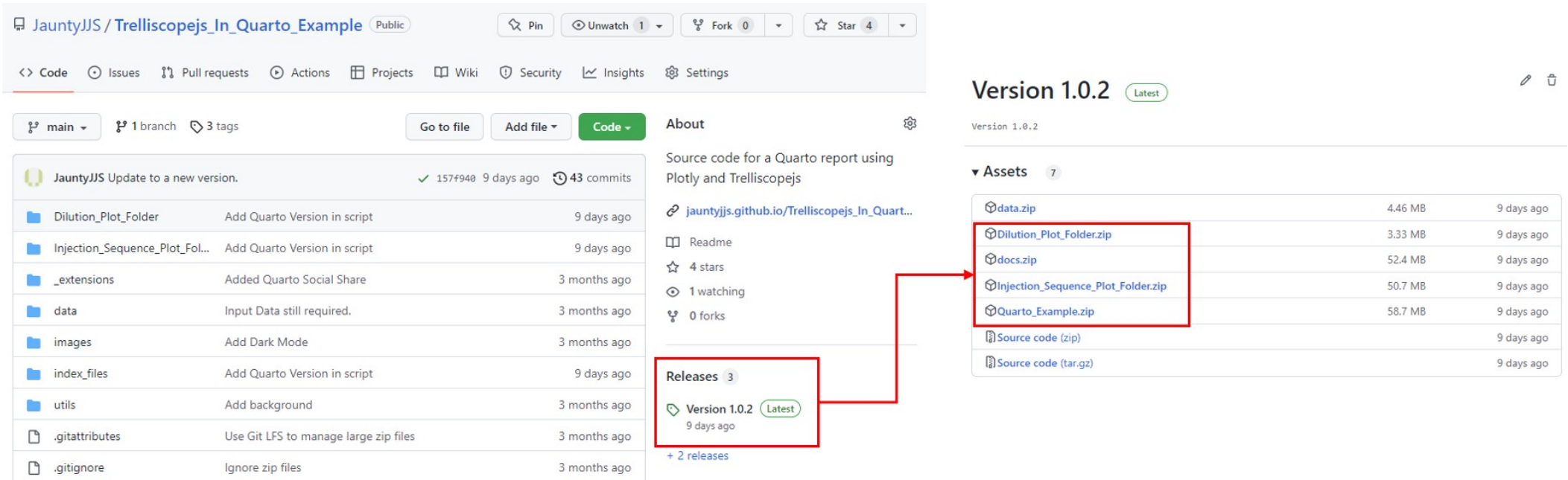
Source Code

```
    tidyverse-quiet: TRUE
format:
  html:
    theme:
      light: cerulean
      dark: cyborg
    toc: true
    toc-depth: 3
    toc-location: left
    number-sections: false
    code-fold: show
    code-overflow: scroll
    code-line-numbers: true
    code-copy: hover
    code-tools: true
    self-contained: false
    smooth-scroll: true
```

Step 3. Compress Highlighted Files/Folders

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.