Technichal:

1. Use Midar for import.
2. Use r package “rhandsontable”, only show the sample names and some annotation, adding columns “sample amounts”, “dilution series ID” ( “replicates ID” if needed).
3. Two tabs “unfiltered” and “filtered” data.

User:

1. Use Radio buttons to choose the type of data.
2. Upload either Masshunter, plain csv files or MRMkit.
3. Select the samples with curtain names by text input, separated by “,”.
4. Use the checkbox to choose the needed samples.
5. User fill columns “sample amounts”, “dilution series ID”.
6. Can choose one of the tabs “unfiltered” and “filtered” data.
7. Choose how many rows and columns of plots per page (default 4\*5).
8. Download pdf files of plots and the excel files with the information of lancer.

Chatgpt

use shiny in R to build. Left part: choose data type (csv or excel) upload the data. Right part: use r package “rhandsontable” to filter the data and show the filtered data. Choose the number of rows and columns of plots per page for the pdf file. download the pdf and excel file.

Tab view

**20240813**

1. Get the path of the data, use Midar to read and transform to long table. Select file
2. Create a new table, only show unique “raw\_data\_filename”, create empty column “is\_rqc”, “rqc\_series\_id”, “relative\_sample\_amount”.
3. Suppose is\_rqc is FALSE, the “rqc\_series\_id”, “relative\_sample\_amount” will be freezed.

**20240815**

1. Filter the rhandsontable
2. Scroll the rhandsontable

**20240820**

1. Modal popup window shiny: Please wait, spinning wheel or progress bar when plotting the data
2. Above the table:

Text box to select. Use “,” to separate. (don’t automatically select ‘rqc’)

Button: Unselect all

1. Add the table
2. Sort by TRUE/FALSE
3. For the relative\_sample\_amount, internally 100% is assigned to 1.

relative\_sample\_amount = .data$relative\_sample\_amount / 100

can allow user to enter percent (maybe inddicate in thow shown column name) then divide by 100 internally

**Problem:**

1. rqc\_series\_id and relative\_sample\_amount in filtered data won’t follow the change of rhansontable

reactive valuable

**20240909**

1. Instead of “filtered table”, add a button “filter” showing the filtered table
2. Add back the pdf plot

**20240911**

1. Rhandsone table filter function: no filter function in R, only in JavaScript
2. Download table: RwithSling for R2

**20240916**

1. Check before downloading pdf and excel, check NA. Make a function. Modal dialog. “Invalid data”
2. ~~Check whether need to add isolate()~~.
3. ~~Add the plots directly in the shiny~~
4. ~~File imput MH must be .csv; while MRMkit data must be .tsv. Update function (https://shiny.posit.co/r/reference/shiny/1.7.0/fileinput)~~
5. Turn on Wireguard A black dragon in a red circle

   Description automatically generated ->

if Macbook, then install “Microsoft Edge” A blue and green swirly logo

Description automatically generated ->

login posit (<https://posit.lsi.nus.edu.sg:3443/>) A black and white logo

Description automatically generated

**To be fixed:**

1. Popup when downloading or preparing table and plots
2. Download plots
3. ~~Column (3, selectInput("select\_page", NULL,~~ **~~choices = 1:15~~**~~)). Should 15 be flexable?~~

**Future plan for RQCee:**

1. Check before downloading pdf and excel, check NA. Make a function. Modal dialog. “Invalid data”
2. Excel output includes the original data
3. Excel output has the R and R2. Highlight r2<0.8 or y0rel>0.6 as red, opposite as green. In the codes, add a flag whether to add more information.
4. Numbers in Excel output is in 3 digits
5. ~~Color the “Poor Linearity” in the excel~~
6. Filtered table
7. X axis is not in %
8. ~~In the excel output, add one sheet explaining the classification of “Good Linearity” like~~ [~~https://github.com/SLINGhub/lancer~~](https://github.com/SLINGhub/lancer)

Prism:

1. Scatter plots
2. Bar plots
3. Boxplot
4. ­­­­­