Anand Panigrahy

Center for Patient Derived Models

Data Wrangling RShiny

Note: All functions in R package "CPDMTools"

Note: For each TabPanel, please have the UI buttons be displayed above the DT table respectively

Note: Please turn off scientific notation, R Code: options(scipen = 999)

Note: Sample dataset descriptions listed below

* SideBarPanel
  + “Import Labguru Plate Map (xlsx)" - Import File Button
    - Function: labguru\_plate\_prep
      * file\_path
    - Action: Imports and prepares plate map data
    - Output: plate\_map\_long data frame
    - Reveals: TabPanel: “Labguru Plate Map”
  + "Tecan Drugging Data" - Radio Button
    - Button 1: "Yes" (Default)
      * Displays: "Drugging Type" - Radio Button
        + Button 1: "Monotherapy" (Default)
        + Button 2: "Synergy"
      * Displays: "Import Tecan Report File (.xlsx)" - Import File Button
        + Function: tecan\_report\_prep

file\_path

drugging\_type

remove\_na = TRUE (if no Labguru plate map uploaded, please set this to FALSE)

* + - * + Action: Imports and prepares tecan report based on drugging type
        + Output: tecan\_plate\_map data frame
        + Reveals: TabPanel: “Tecan Report”
    - Button 2: “No”
  + "Data File Type" - Radio Button
    - Button 1: "Imaging" (Default)
      * Displays: "Imaging File Type" - Radio Button
        + Button 1: "Incucyte" (Default)
        + Button 2: "Cytation"
      * Displays: "Import Growth File (.txt)" - Import File Button
        + Function: tecan\_report\_prep

file\_path

drugging\_type

* + - * + Action: Imports and prepares tecan report based on drugging type
        + Output: growth\_data data frame
        + Display: Reveals TabPanel: “Growth Data”
    - Button 2: "CTG"
      * Displays: "Import CTG File (.xlsx)" - Import File Button
        + Function: ctg\_data\_prep
        + Action: Imports and prepares ctg data
      * Output: ctg\_data data frame
      * Display: Reveals TabPanel “CTG”
  + “Join Datasets” – Click Button
    - NOTE - is only revealed when one of the minimum following criteria is met
      * Labguru plate map is imported AND an Imaging/CTG File is imported
      * Tecan Report is imported AND an Imaging/CTG File is imported
    - Function: plate\_data\_join (please note that the inputs for the function are based on the inputs of the user)
      * labguru\_plate\_data\_frame = NULL (input must be the filtered labguru plate map data frame if applicable)
      * tecan\_plate\_map\_data\_frame = NULL (input must be the filtered tecan data frame if applicable)
      * growth\_data\_frame = NULL
      * ctg\_data\_frame = NULL
    - E.g. if a user inputs a labguru plate map, a tecan report, and a growth file, the function would be: plate\_data\_join(labguru\_plate\_data\_frame = plate\_map\_long, tecan\_plate\_map\_data\_frame = tecan\_plate\_map, growth\_data\_frame = growth\_data, ctg\_data\_frame = NULL)
    - Output: A data frame called joined\_data
    - Display: Reveal TabPanel “Joined Data”
* TabPanel: “Labguru Plate Map”
  + Displays plate\_map\_long data frame as a DT interactive table
  + Displays: “Filter Data By” - Radio Button
    - Button 1: "Labguru Model Name" (Default)
      * Reveals a drop-down menu of unique inventory\_item\_name values, defaults to first one
      * Action: Filters the plate\_map\_long data frame to respective inventory\_item\_name
      * Display: Updates the displayed plate\_map\_long DT table
    - Button 2: "Well Range"
      * Reveals the following
        + "Enter Labguru Model Name" - Text Field

Please have the default text be the first unique inventory\_item\_name value

* + - * + "Row Letter Range" - Sliding Bar

Range A - max letter value for row variable (e.g. P), default to A and max row value

Action: Filters the plate\_map\_long data frame variable row by the range

Display: Updates the displayed plate\_map\_long DT table

* + - * + "Column Number Range" - Sliding Bar

Range 1 - max number value for column variable (e.g. 24), default to 1 and max column value

Action: Filters the plate\_map\_long data frame variable column by the range

Display: Updates the displayed plate\_map\_long DT table

* + Display: “Export Prepared Labguru Plate Map” – Click Button
    - Action: Exports a .xlsx version of the Labguru plate map with respect to the filtering criteria
      * Extract the "Plate\_##" from the Labguru Plate File Name and make lower case:
        + e.g. "plate\_01"
      * If the button “Labguru Model Name" is selected, use that selected value as all lower case to name the output file (append “labgugu\_prep” at end):
        + e.g. "plate\_01\_cpdm\_2951\_labguru\_prep.xlsx"
      * If the button "Well Range" use that selected value as all lower case to name the output file (append “labgugu\_prep” at end):
        + e.g. "plate\_01\_custom \_name\_labguru\_prep.xlsx"
* TabPanel: “Tecan Report”
  + Displays tecan\_plate\_map data frame as a DT interactive
  + Display: Plate Number Range - Sliding Bar
    - Range 1 - max(plate) from tecan\_plate\_map data frame, defaults to 1 - max(plate)
    - Action: Filters the tecan\_plate\_map data frame by the plate range
    - Display: Updates the displayed tecan\_plate\_map DT table
  + Display ONLY IF Labguru Plate Map is NOT Present (used for older datasets/Ligon lab):
    - Display a message that remains present: "Warning: When Labguru plate map is not present, any well within the filtered row and column range of the Tecan plate map that did NOT contain dispensing data will be converted to Media Controls when joined with Imaging or CTG data (assumes your cells are platted in a complete rectangular matrix)".
    - "Row Letter Range" - Sliding Bar
      * Range A - max letter value for row variable (e.g. P), default to A and max row value
      * Action: Filters the tecan\_plate\_map data frame variable row by the range
      * Display: Updates the displayed tecan\_plate\_map DT table
    - "Column Number Range" - Sliding Bar
      * Range 1 - max number value for column variable (e.g. 24), default to 1 and max column value
      * Action: Filters the tecan\_plate\_map data frame variable column by the range
      * Display: Updates the displayed tecan\_plate\_map DT table
  + Display: "Concentration Units of Tecan Report" - Drop Down Menu
    - "Molar (M)"
    - "Millimolar (mM)"
    - "Micromolar (µM)" (Default)
    - "Nanomolar (nM)"
    - "Picomolar (pM)"
  + Display: “Export Prepared Tecan Report” – Click Button
    - Action: Exports a .xlsx version of the prepared Tecan report with respect to the filtering criteria
    - Take the name of the imported Tecan Report file and append “prep” to it:
      * e.g. “DT-24.0001\_Tecan\_Report\_20230804\_prep.xlsx”
* TabPanel: “Growth Data”
  + Display: growth\_data data frame as a DT interactive table
  + Display: "Please Select First Time Point Recorded After Treatment Was Given" - Drop-Down Menu
    - Reveals a drop-down menu of unique time variable values as well as a value for "No Treatment". Defaults to "No Treatment" if Tecan File is not present. Defaults to the minimum time value present if Tecan File is present.
    - Action: If a time is selected (i.e. does not equal "No Treatment"), the variable treatment\_period\_yn is updated such that all times greater than and equal to the time point selected are "Yes", otherwise "No". If "No Treatment" is selected, please update all the values of treatment\_period\_yn to be "No".
  + Display: "Select Growth Metric Type of Growth File" - Drop Down Menu
    - "Confluency (%)" (Default)
    - "Object Sum Area (µM2)"
    - "Largest Object Area (µM2)"
    - "Relative Fluorescence Intensity (AU)"
  + Displays: "Select Time Unit of Growth File" - Drop Down Menu
    - "Minutes"
    - "Hours" (Default)
    - "Days"
  + Displays: “Export Prepared Growth Metric File” – Click Button
    - Action: Exports a .xlsx version of the prepared Tecan report
    - Take the name of the imported Tecan Report file and append “prep” to it:
      * e.g. “CPDM\_1279X\_Incucyte\_Confluency\_prep.xlsx”
* TabPanel: “CTG Data”
  + Display: ctg\_data data frame as a DT interactive table
  + Display: “Export Prepared CTG Data”
    - Action: Exports a .xlsx version of the prepared CTG data
    - Take the name of the imported CTG file and append “prep” to it:
      * e.g. “CPDM\_1279X\_Incucyte\_Confluency\_prep.xlsx”
* TabPanel: “Joined Data”
  + Display: joined\_data data frame as a DT interactive table
  + Display: "Select Location of Control Variables" - Radio Button
    - Button 1: "Treatment Name" (Default If Tecan Drugging Data = "Yes")
    - Button 2: "Well Annotation" (Default If Tecan Drugging Data = "No")
  + Display: "Please Select the Media Control" - Drop Down Menu
    - Drop-down menu of unique values from variable treatment\_name or well\_anotation of joined\_data, data frame depending on "Select Location of Control Variables", please include a value for "None" within the list as well
    - If str\_detect("Media") in treatment\_name or well\_anotation then make the default value "Media", otherwise make the default value "None"
  + Display: "Please Select the Negative Control" - Drop Down Menu
    - Drop-down menu of unique values from variable treatment\_name or well\_anotation of joined\_data, data frame depending on "Select Location of Control Variables", please include a value for "None" within the list as well
    - If str\_detect("DMSO 0.5%") in treatment\_name or well\_anotation then make the default value "DMSO 0.5%", otherwise make the default value "None"
  + Display: "Please Select the Positive Control" - Drop Down Menu
    - Drop-down menu of unique values from variable treatment\_name or well\_anotation of joined\_data, data frame depending on "Select Location of Control Variables", please include a value for "None" within the list as well
    - If str\_detect("DMSO 10%") in treatment\_name or well\_anotation then make the default value "DMSO 10%", otherwise make the default value "None"
  + Action: Based on the selections of the control variables please update the variable treatment\_type of the joined\_data data frame with the following criteria:
    - If [treatment\_name/well\_annotation] is equal to [Selected Media Control] then treatment\_type = "Media Control"
    - If [treatment\_name/well\_annotation] is equal to [Selected Negative Control] then treatment\_type = "Negative Control"
    - If [treatment\_name/well\_annotation] is equal to [Selected Positive Control] then treatment\_type = "Positive Control"
    - All other values would be the default output, either "Monotherapy" or "Combination Therapy"
  + "Export Data" - Click Button (Only Shown after Joined Data is Clicked)
    - Exports the joined\_data (sheet 1) and a wide dataset of meta-data file based on the user metrics (e.g. filtering metrics, growth metric units, time units, R version, date: sheet 2) to excel using the write\_xlsx function using the following naming convention:
      * Extract the "Plate\_##" from the Labguru Plate File Name and make lower case (var = plate\_num):
        + e.g. "plate\_01"
      * If the button "Labguru Model Name" is selected, use that selected value as all lower case (var = labguru\_name):
        + e.g. "cpdm\_2951"
      * If the button "Well Range" use that selected value as all lower case (var = labguru\_name):
        + e.g. "custom\_labguru\_name"
      * Finally create the name based on the following selections (append “joined” to end of all outputs):
        + If Labguru Plate Map Present:

If Tecan Drugging Data = "Yes", "Drugging Type" = "Monotherapy", Data Type = "Imaging"

"plate\_num\_labguru\_name\_growth.xlsx" (e.g. plate\_01\_cpdm\_2951\_growth\_joined.xlsx")

If Tecan Drugging Data = "Yes", "Drugging Type" = "Synergy", Data Type = "Imaging"

"plate\_num\_labguru\_name\_growth\_syn.xlsx" (e.g. plate\_01\_cpdm\_2951\_growth\_syn\_joined.xlsx")

If Tecan Drugging Data = "No", Data Type = "Imaging"

"plate\_num\_labguru\_name\_growth.xlsx" (e.g. plate\_01\_cpdm\_2951\_growth\_joined.xlsx")

If Tecan Drugging Data = "Yes", "Drugging Type" = "Monotherapy", Data Type = "CTG"

"plate\_num\_labguru\_name\_ctg.xlsx" (e.g. plate\_01\_cpdm\_2951\_ctg\_joined.xlsx")

If Tecan Drugging Data = "Yes", "Drugging Type" = "Synergy", Data Type = "CTG"

"plate\_num\_labguru\_name\_ctg\_syn.xlsx" (e.g. plate\_01\_cpdm\_2951\_ctg\_syn\_joined.xlsx")

If Tecan Drugging Data = "No", Data Type = "CTG"

"plate\_num\_labguru\_name\_ctg.xlsx" (e.g. plate\_01\_cpdm\_2951\_ctg\_joined.xlsx")

* + - * + If NO Labguru Plate Map Present:

If Tecan Drugging Data = "Yes", "Drugging Type" = "Monotherapy", Data Type = "Imaging"

“tecan\_growth\_joined.xlsx”

If Tecan Drugging Data = "Yes", "Drugging Type" = "Synergy", Data Type = "Imaging"

“tecan\_growth\_syn\_joined.xlsx”

If Tecan Drugging Data = "Yes", "Drugging Type" = "Monotherapy", Data Type = "CTG"

"tecan\_ctg\_joined.xlsx"

If Tecan Drugging Data = "Yes", "Drugging Type" = "Synergy", Data Type = "CTG"

"tecan\_ctg\_syn\_joined.xlsx"

* + "Transfer Data to QC RShiny” - Click Button
    - Transfers the dataset the QC RShiny (Pending design of QC RShiny)

Sample Datasets (Located In “Test Folder”)

* tecan\_incucyte\_ctg\_monotherapy – Folder, test set 1
  + Plate\_01\_CPDM\_2951\_CSM\_7549\_Patient\_Sample\_20230803.xlsx – a sample Labguru plate map
  + DT-24.0001\_Tecan\_Report\_20230804.xlsx – a sample Tecan Report file
    - Set Drugging Type to “Monotherapy”
  + CPDM\_2951\_CSM\_7549\_Patient\_Sample\_Incucyte\_Confluency.txt – a sample Growth file
    - Set Data File Type to “Imaging”
    - Set Imaging Equipment to “Incucyte”
    - Set Growth Metric Tupe to “Confluency”
    - Set Time Units to “Hours”
  + Plate\_01\_CTG\_20230811.xlsx – a sample CTG file
    - Set Data File Type to “CTG”
* tecan\_incucyte\_ctg\_monotherapy – Folder, test set 2
  + Plate\_01\_CPDM\_1279X\_PDCL\_3DS\_M01\_P20\_20240417.xlsx – a sample Labguru plate map
  + DT-24.0022\_Tecan\_Report\_20240418.xlsx – a sample Tecan Report file
    - Set Drugging Type to “Synergy”
  + CPDM\_1279X\_Incucyte\_Confluency.txt – a sample Growth file
    - Set Data File Type to “Imaging”
    - Set Imaging Equipment to “Incucyte”
    - Set Growth Metric Tupe to “Object Sum Area”
    - Set Time Units to “Hours”
  + Plate\_01\_CTG\_20230811.xlsx – a sample CTG file
    - Set Data File Type to “CTG”
* cytation\_file\_example.txt – a sample Growth file
  + Set Data File Type to “Imaging”
  + Set Imaging Equipment to “Cytation”