**Workflow of the second Shiny app.**

**Name ? DRomics\_multilevels**

**Examples :**

* Scenedesmus, triclosan
* Nicolas Creusot data ? PB because it was not aimed to do metabolomics
* PICT study when it will be published
* Another data with metabolomics time (Mechthild)
* IRSN data zebra fish at different times

**Page 1**

First input : the number of experimental levels e.g. different molecular levels (transcriptomics, metabolomis, …) , different experimental time points or different biological models (different species, different experimental settings), …

Step to repeat (+ button or numerical input with the number of results ):

Merge for each results data frame form the workflow, corresponding to a condition (PICT or not), a molecular level (metabolo or transcripto), a time, … -> identified by an **experimental level**

Input :

* the name of the experimental level (string)
* the results data frame from the DRomics workflow (DRomics\_output ?) : .txt
* the annotation data frame that may be longer (one item with more than one annotation) or shorter (items without any annotation) than DRomics\_output : .txt

Action :

* merge on id + add of a column named “label” with the label -> extendedres\_ith
* At the end -> rbind of all the extendedres\_ith -> extendedres

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Numerical input : minimal number of items (default 3, from 1 to 10 ?) to keep the item for one factor level

Do we keep the item in the other factor levels if it appears more than min\_nb\_of\_items in another factor level ? YES because if you have 9 and 10 with two levels

PB with quantiles – write a message to say that quantiles on low number of items are not reliable

Radio- button : Ordering of the annotations : alphabetic order, or order of apparition (chosen by the user) in the input, ordered by total number of items in all the experimental levels

Action :

* Filtering of annotations to plot
* Trendplot and sensitivity

trendplot()

* (extendedres)
* (group = annotation)
* (facetby = label)
* add.color = TRUE

sensitivityplot()

* (extendedres)
* BMD type = (“zSD”, “xfold”)
* BMD summary = c(“first.quartile”, “median”, “median.and.IQR”)
* (group = annotation)
* colorby = label or nothing
* if no colorby ECDF\_plot = TRUE
* BMD\_log\_transfo = FALSE

Each with possible exportation of the plot

**Page 3**

Put again the input of page 2 with the last value proposed by the user as the default value

Optional focus on some annotations : mark the chosen annotations (by default none are marked) with a button to mark all

Common arguments so only one question for both functions, except add.CI and colorby

bmdplot()

* **(Extendedres)**
* **BMD type = (“zSD”, “xfold”)**
* add.CI = FALSE
* **facetby (for columns) = annotation or label or none**
* **facetby2 (for rows) = label or annotation or none (conditioned by facetby)**
* colorby and shapeby (select input in the columns of extendedres)
* **BMD\_log\_transfo = FALSE**
* **add.label = FALSE**

bmdplotwithgradient()

* **(extendedres)**
* **BMD type = (“zSD”, “xfold”)**
* **facetby (for columns) = annotation or label or none**
* **facetby2 (for rows) = label or annotation or none (conditioned by facetby)**
* **BMD\_log\_transfo = FALSE**
* **add.label = FALSE**
* shapeby (select input in the columns of extendedres) (not proposed if add.label = TRUE)

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Put again the input of page 3 with the last value proposed by the user as the default value

Optional focus on some annotations : mark the chosen annotations (by default the ones marked on page 3) with a button to mark all

curvesplot()

* (extendedres)
* Min and max doses to define the range for DR curves
* facetby (for columns) = annotation or label or none (by default the one in page 3)
* facetby2 (for rows) = label or annotation or none (conditioned by facetby) (by default the one in page 3)
* colorby (select input in the columns of extendedres)
* dose\_log\_transfo = (by default the one in page 3 for BMD\_log\_transfo)

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The script