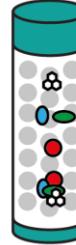


Getting Started with **PROMISed**



v.1.0.2

Dennis Schlossarek

AG Skirycz - Small-Molecule Signalling

Max Planck Institute of Molecular Plant Physiology

schlossarek@mpimp-golm.mpg.de

This instruction will give a short overview of how to start and navigate through PROMISed. For a detailed description of the application, please refer to:
[Schlossarek et al, 2021, PROMISed: A novel web-based tool to facilitate analysis and visualization of the molecular interaction networks from co-fractionation mass spectrometry experiments.]

RStudio

File Edit Code View Session Build Debug Profile Tools Help

Go to file/function Addins

Project: (None)

app.R Functions_PROMISEd_v1.0.0.R app.R

Welcome to PROMISEd: A PROtein Metabolite Interaction using Size-Separation Data analysis tool

List of Required packages:

require(shiny) # For the App to run

require(shinyBS) # Shiny meeting bootstrap? Allows hovering Tooltips

require(shinyCSSloaders) #

require(shinybusy) #

require(DT) # To render interactive Data-Tables

require(stringr) # Data handling and organization

require(stats) # General Statistics

require(MESS) # Used for MESS::auc (area under the curve)

require(dplyr) #

require(RColorBrewer) # Nice Color pallettes

require(ggsci) # pal_startrek color-pallete

require(ggplot2) # For proper Plotting

require(multcompview) # For plotting (here, significance-indices in boxplot)

require(gridExtra) # Organisation of ggplots

require(grid) # Organisation of ggplots

require(igraph) # For Network creation and analysis

require(visNetwork) # AWESOME interactive network

require(pheatmap) # AWESOME pretty heatmaps

require(tidyverse)

require(pastecs)

require(zip)

require(eulerr)

require(VennDiagram)

Load functions from outside R-scripts

source("./Functions_PROMISEd_v.1.0.0.R")

source("./publication_list_HTML.R")

Load Example Data Files

metabolite_demo_data <- read.delim("./dummy_metabolite_data.txt", row.names = 1)

protein_demo_data <- read.delim("./dummy_protein_data.txt", row.names = 1)

Create Graphical User Interface

ui <- fluidPage(# Start of USER-INTERFACE

br(),

tags\$head(

tags\$style(HTML('#select_previous{background-color:lightgrey}')),

tags\$style(HTML('#select_next{background-color:lightgrey}')))

),

Load a rotating SEC-column gif as loading icon

add_busy_gif(

timeout = 1000,

src = "PROMIS rotating.gif".

52

1:1 (Top Level) R Script

Console Jobs

R 4.0.3 - H:/Phd Projects/11.ShinyApps/PROMIS/PROMISEd-main3 ↵

Loading required package: futile.logger

Warning: package 'futile.logger' was built under R version 4.0.4

Listening on http://127.0.0.1:6805

Warning: The select input "select_rows_b" contains a large number of options; consider using server-side selectize for massively improved performance. See the Details section of the ?selectizeInput help topic.

Warning in <observer>(...): NAs introduced by coercion

Warning in dir.create("promised_tmp") : 'promised_tmp' already exists

> runApp()

Listening on http://127.0.0.1:6805

Warning in dir.create("promised_tmp") : 'promised_tmp' already exists

Warning in dir.create("promised_tmp") : 'promised_tmp' already exists

> |

Environment History Connections Tutorial

Import Dataset 486 MiB

Global Environment

deconvolute.array deconvolute.new deconvoluted.list disclaimer_HTML filterPeaksSpanFraction_ get_peak_names GetIntersections ListCoelutions loessDS manhattan.anova.boxplot manhattan.anova.shiny manhattan.row maxNormalizeML namesCombn Plot2selections PlotBestHit PlotDeconvoluted PlotMyArray.row PlotMyArray.shiny publication_list_HTML scale_coreness

function (x, var_min_peak, var_limit_small, var_limit_larg...) function (my_data, var_min_peak, var_limit_small, var_limit_larg...) function () function (z) function (x) function (x) function (data1, data2, selector, pcc_threshold, method, names_t...) function (y, span, normalization) function (manhattan_distances, name_panel, names_treatments, j) function (x, names_treatments, pvalue) function (x, names_treatments, select_rows, j) function () function (x) function () function (data1, data2, selector1, selector2) function (decon_data1, decon_data2, selector, pcc_threshold, met...) function (rep_comb, deconvoluted, my_row_name, treatment) function (x, my_row_name, names_treatments, titel_name, plot_wh...) function (x, names_treatments) function () function (x)

Files Plots Packages Help Viewer

Click on the small white arrow

Getting Started with PROMISEd

2

RStudio

File Edit Code View Session Build Debug Profile Tools Help

Go to file/function Addins

Project: (None)

app.R Functions_PROMISEd_v1.0.0.R app.R

Welcome to PROMISed: A PROtein Metabolite Interaction using Size-Separation Data analysis tool

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require(pheatmap) # AWESOME pretty heatmaps

require(tidyverse)

require(pastecs) # for local maxima

require(zip)

require(eulerr) # for venn diagrams

require(VennDiagram)

Load functions from outside R-scripts

source("./Functions_PROMISEd_v.1.0.0.R")

source("./publication_list_HTML.R")

Load Example Data Files

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Create Graphical User Interface

ui <- fluidPage(# Start of USER-INTERFACE

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tags\$style(HTML('#select_next{background-color:lightgrey}')))

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src = "PROMIS rotating.gif".

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Listening on http://127.0.0.1:6805

Warning in dir.create("promised_tmp") : 'promised_tmp' already exists

Warning in dir.create("promised_tmp") : 'promised_tmp' already exists

Run in Window

Run in Viewer Pane

Run External (selected)

In R Console

In Background Job

Record Test

Run Tests

Select “Run External”

Environment History Connections Tutorial

Import Dataset 486 MiB

Global Environment

deconvolute.array function (x, var_min_peak, var_limit_small, var_limit_larg...
deconvolute.new function (my_data, var_min_peak, var_limit_small, var_limit_larg...
deconvoluted.list function ()
disclaimer_HTML function ()
filterPeaksSpanFraction_ function (z)
get_peak_names function (x)
GetIntersections function (x)
ListCoelutions function (data1, data2, selector, pcc_threshold, method, names_t...
loessDS function (y, span, normalization)
manhattan.anova.boxplot function (manhattan_distances, name_panel, names_treatments, j)
manhattan.anova.shiny function (x, names_treatments, pvalue)
manhattan.row function (x, names_treatments, select_rows, j)
maxNormalizeML function (x)
namesCombn function (x)
Plot2selections function (data1, data2, selector1, selector2)
PlotBestHit function (decon_data1, decon_data2, selector, pcc_threshold, met...
PlotDeconvoluted function (rep_comb, deconvoluted, my_row_name, treatment)
PlotMyArray.row function (x, my_row_name, names_treatments, titel_name, plot_wh...
PlotMyArray.shiny function (x, names_treatments)
publication_list_HTML function ()
scale_coreness function (x)

Files Plots Packages Help Viewer

3

RStudio

File Edit Code View Session Build Debug Profile Tools Help

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Listening on http://127.0.0.1:6805

Warning in dir.create("promised_tmp") : 'promised_tmp' already exists

Warning in dir.create("promised_tmp") : 'promised_tmp' already exists

Getting Started with PROMISEd

Run App

Start the App by Clicking „RunApp“

Environment History Connections Tutorial

Import Dataset 486 MiB

Global Environment

deconvolutearray deconvolute.new deconvoluted.list disclaimer_HTML filterPeaksSpanFraction_ get_peak_names GetIntersections ListCoelutions loessDS manhattan.anova.boxplot manhattan.anova.shiny manhattan.row maxNormalizeML namesCombn Plot2selections PlotBestHit PlotDeconvoluted PlotMyArray.row PlotMyArray.shiny publication_list_HTML scale_coreness

Files Plots Packages Help Viewer

4

**Dataset displayed** Dataset A Dataset B

PROMISed review Version: 1.0.2

Data Upload

1. Pre-Processing

2. Replicate Pooling

3. Deconvolution

4. Data Integration

5. Network Analysis

6. Differential Fractionation

About

Disclaimer

Upload Dataset A Browse... No file selected
Upload Dataset B Browse... No file selected
Confirm Data Upload

Download Demo-Datasets:

 Metabolites**This is PROMISed start page**

Getting Started with PROMISed

127.0.0.1:6805 x + 127.0.0.1:6805

Apps Managed bookmarks dict.cc | Wörterbuc... Internal pages - Ne... Mail - schlossarek... Rakete MAX - das Intranet Mail.UP uni-potsda... Home - PubMed -... visOptions function... igraph R manual pa... 25 items (Saccharo... myshiny.mpimp-go... Reading list

PROMISed review Version: 1.0.2

Data Upload 1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration 5. Network Analysis 6. Differential Fractionation About Disclaimer

Upload Dataset A

Browse... No file selected

Upload Dataset B

Browse... No file selected

Confirm Data Upload

Download Demo-Datasets:

Metabolites

Proteins

For a quick start, scroll down and download the Demo-Datasets

PROMISed 2021
Privacy policy | Imprint | Getting Started with PROMISed 6

127.0.0.1:6805 x + 127.0.0.1:6805

Apps Managed bookmarks dict.cc | Wörterbuc... Internal pages - Ne... Mail - schlossarek... Rakete MAX - das Intranet Mail.UP uni-potsda... Home - PubMed -... visOptions function... igraph R manual pa... 25 items (Saccharo... myshiny.mpimp-go... Reading list

PROMISed review Version: 1.0.2

Data Upload 1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration 5. Network Analysis 6. Differential Fractionation About Disclaimer

Upload Dataset A

Browse... No file selected 1

Upload Dataset B

Browse... No file selected 2

Confirm Data Upload

Download Demo-Datasets:

 Metabolites

 Proteins

Upload the data here using drag-and-drop, or browse for the files on your computer.

Note that you have to start with Dataset A before uploading Dataset B.

Protein_Demodata....txt Metabolite_Demodata....txt

Getting Started with PROMISed 7 Show all

127.0.0.1:6805 x + 127.0.0.1:6805

Apps Managed bookmarks dict.cc | Wörterbuc... Internal pages - Ne... Mail - schlossarek... Rakete MAX - das Intranet Mail.UP uni-potsda... Home - PubMed -... visOptions function... igraph R manual pa... 25 items (Saccharo... myshiny.mpimp-go... Reading list

PROMISed review Version: 1.0.2

Data Upload 1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration 5. Network Analysis 6. Differential Fractionation About Disclaimer

Upload Dataset A

Browse... Metabolite_Demodata_PROMISed (3).txt Upload complete

First Column to Analyse 1 Condition1_Rep_1_Frac1

Last Column to Analyse 360 Condition3_Rep_3_Frac40

If your files contains additional information, specify here where your fractionation profiles start and end

Upload Dataset B

Browse... Protein_Demodata_PROMISed (2).txt Upload complete

First Column to Analyse 1 Condition1_Rep_1_Frac1

Last Column to Analyse 120 Condition3_Rep_1_Frac40

Confirm Data Upload

Confirm your Data

Download Demo-Datasets:

Metabolites

Proteins

Protein_Demodata_.txt Metabolite_Demod...txt

Getting Started with PROMISed 8 Show all

127.0.0.1:6805 x +

127.0.0.1:6805

Apps Managed bookmarks dict.cc | Wörterbuc... Internal pages - Ne... Mail - schlossarek... Rakete MAX - das Intranet Mail.UP uni-potsda... Home - PubMed -... visOptions function... igraph R manual pa... 25 items (Saccharo... myshiny.mpimp-go... Reading list

PROMISed

Dataset displayed
 Dataset A
 Dataset B

Max Planck Institute of Molecular Plant Physiology

Max Planck Institute of Molecular Plant Physiology

PROMISed review Version: 1.0.2

1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration 5. Network Analysis 6. Differential Fractionation About Disclaimer

Pre-Processing

Remove Single Peaks
 Normalize
Minimum Relative Intensity
0.1
 Profile Smoothing
Span-Value
0.15

Raw Profiles

You can now change the Pre-Processing Parameters here before starting with the analysis

If you want to change this parameters later on, click „Start Analysis“ again to confirm your changes.

Start Analysis

PROMISed

Dataset displayed
 Dataset A
 Dataset B



PROMISed review Version: 1.0.2

1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration 5. Network Analysis 6. Differential Fractionation About Disclaimer

Pre-Processing

Remove Single Peaks

Normalize

Minimum Relative Intensity

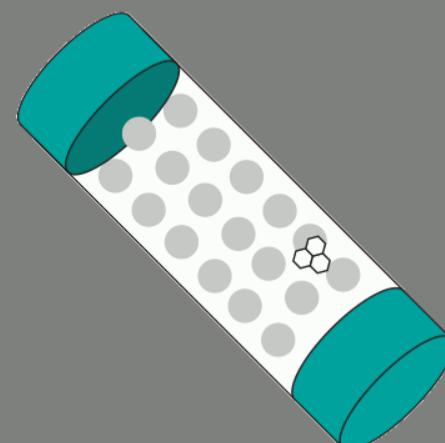
0.1

Profile Smoothing

Span-Value

0.15

Start Analysis



Some steps require loading time. As long as the column is spinning and white, the app is calculating.

PROMISed

Dataset displayed
 Dataset A
 Dataset B

Metabolite01

Protein0001

Max Planck Institute of Molecular Plant Physiology

Max Planck Institute of Molecular Plant Physiology

PROMISed review Version: 1.0.2

1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration 5. Network Analysis 6. Differential Fractionation About Disclaimer

Pre-Processing

Raw Profiles

Remove Single Peaks

Normalize

Minimum Relative Intensity
0.1

Profile Smoothing

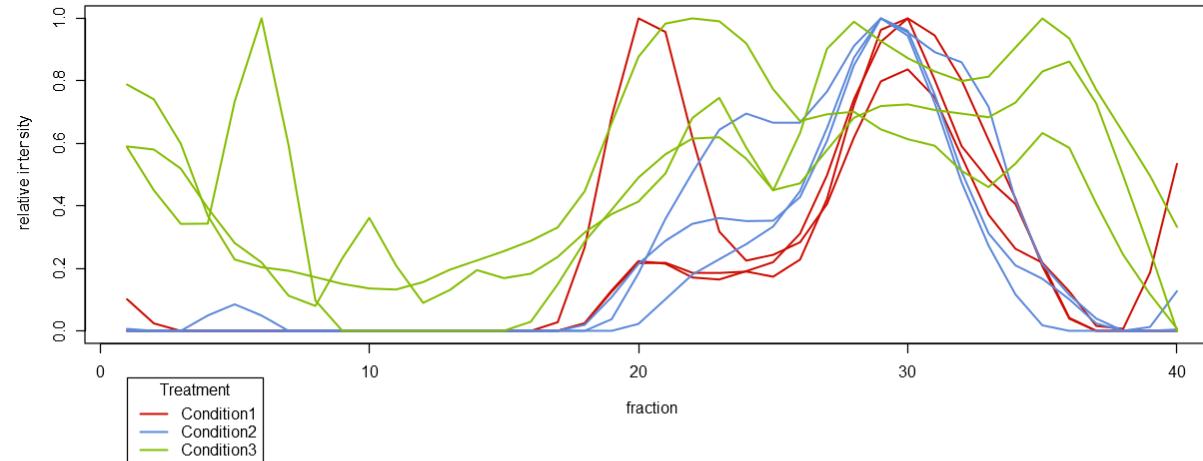
Span-Value
0.15

Start Analysis

Download Pre-Processed Data

Replicates to Plot

- Condition1_Rep_1
- Condition1_Rep_2
- Condition1_Rep_3
- Condition2_Rep_1
- Condition2_Rep_2
- Condition2_Rep_3
- Condition3_Rep_1
- Condition3_Rep_2
- Condition3_Rep_3



The data is now loaded and pre-processed!



Dataset displayed
 Dataset A
 Dataset B

Metabolite01
Protein0001



PROMISed review Version: 1.0.2

[1. Pre-Processing](#) [2. Replicate Pooling](#) [3. Deconvolution](#) [4. Data Integration](#) [5. Network Analysis](#) [6. Differential Fractionation](#) [About](#) [Disclaimer](#)

Navigate through the data analysis steps using the different tabs.

Pre-Processing

 Remove Single Peaks Normalize**Minimum Relative Intensity**

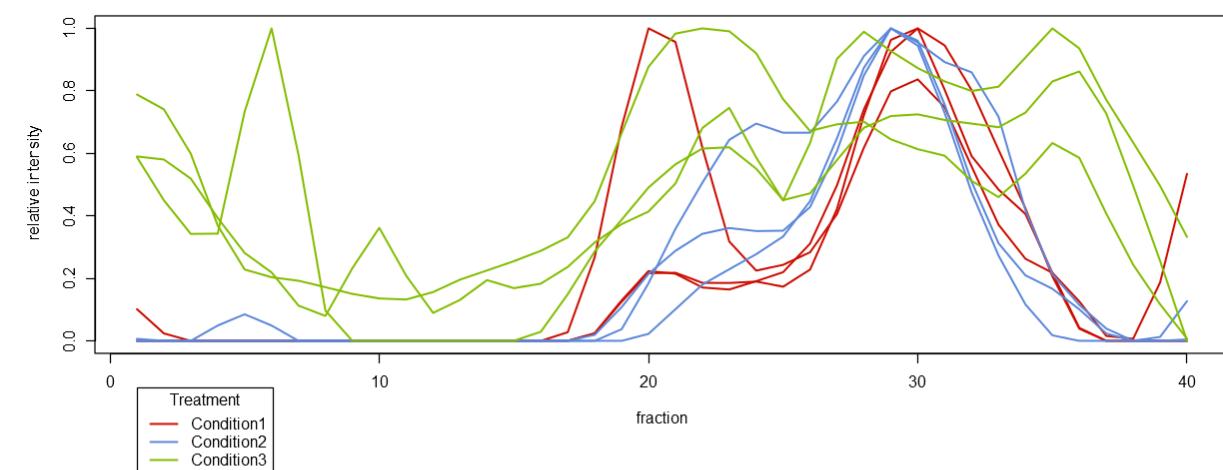
0.1

 Profile Smoothing**Span-Value**

0.15

[Start Analysis](#) [Download Pre-Processed Data](#)

Raw Profiles

**Replicates to Plot**

- Condition1_Rep_1
- Condition1_Rep_2
- Condition1_Rep_3
- Condition2_Rep_1
- Condition2_Rep_2
- Condition2_Rep_3
- Condition3_Rep_1
- Condition3_Rep_2
- Condition3_Rep_3

PROMISed

Dataset displayed: Metabolite01
Dataset A

Dataset displayed: Protein0001
Dataset B

Max Planck Institute of Molecular Plant Physiology

PROMISed review Version: 1.0.2

1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration 5. Network Analysis 6. Differential Fractionation About Disclaimer

Replicate Pooling

Correlation Method: Pearson

Reproducibility Threshold: 0.7

Keep Single Replicates?

Download Pooled Replicates

Pooled Replicates Global Fractionation Profile

Metabolite01

The graph displays the relative intensity of metabolites across 40 fractions for three different conditions. Condition 1 (red) shows a sharp peak at fraction 30. Condition 2 (blue) has a broader peak around fraction 25. Condition 3 (green) shows a more gradual increase peaking around fraction 35. The y-axis represents relative intensity from 0.0 to 1.0, and the x-axis represents the fraction number.

fraction	Condition1 (red)	Condition2 (blue)	Condition3 (green)
0	0.05	0.05	0.65
10	0.05	0.05	0.15
20	0.50	0.15	0.35
30	0.95	0.90	0.85
40	0.05	0.05	0.20

Treatment: Condition1, Condition2, Condition3

PROMISed 2021
Privacy policy | Imprint |

PROMISed

Dataset displayed
 Dataset A
 Dataset B

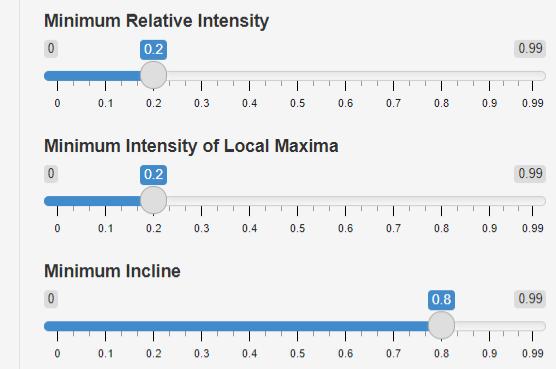
Metabolite01
Protein0001



PROMISed review Version: 1.0.2

1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration 5. Network Analysis 6. Differential Fractionation About Disclaimer

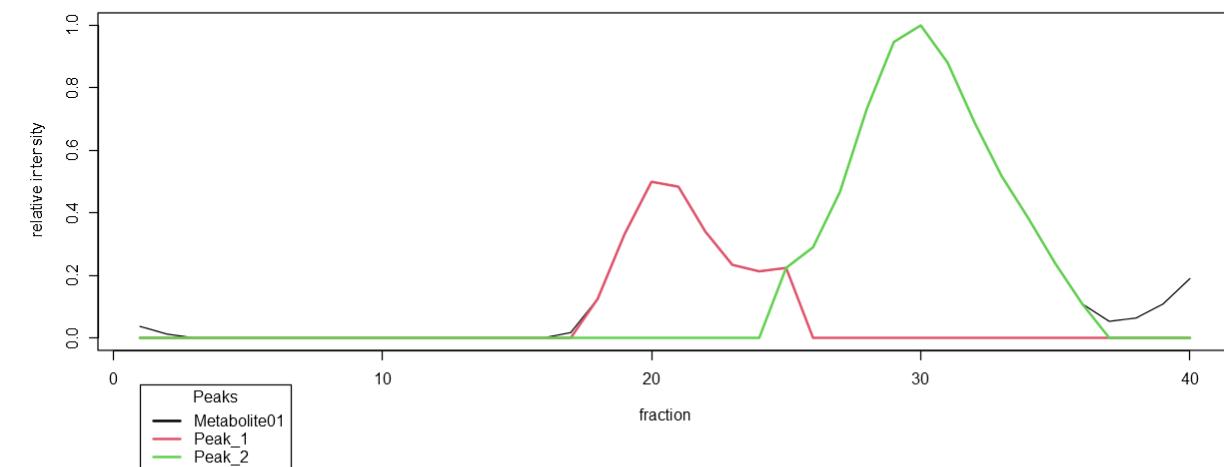
Deconvolutuion Settings



No Deconvolution

 Download Deconvoluted Data

Condition1 Condition2 Condition3



PROMISed review Version: 1.0.2

Dataset displayed
 Dataset A
 Dataset B

Metabolite01

Protein0001

Max Planck Institute of Molecular Plant Physiology

Correlation

Correlation Method
 Pearson Kendall-tau Spearman

Correlation Threshold
0 0.7 0.99

Confirm Correlation Settings

Layout
 Venn Diagram Euler Diagram

Correlation Tables Intersection Table

Intersections of Conditions Condition1 Condition2 Condition3

625

106

9

12

257

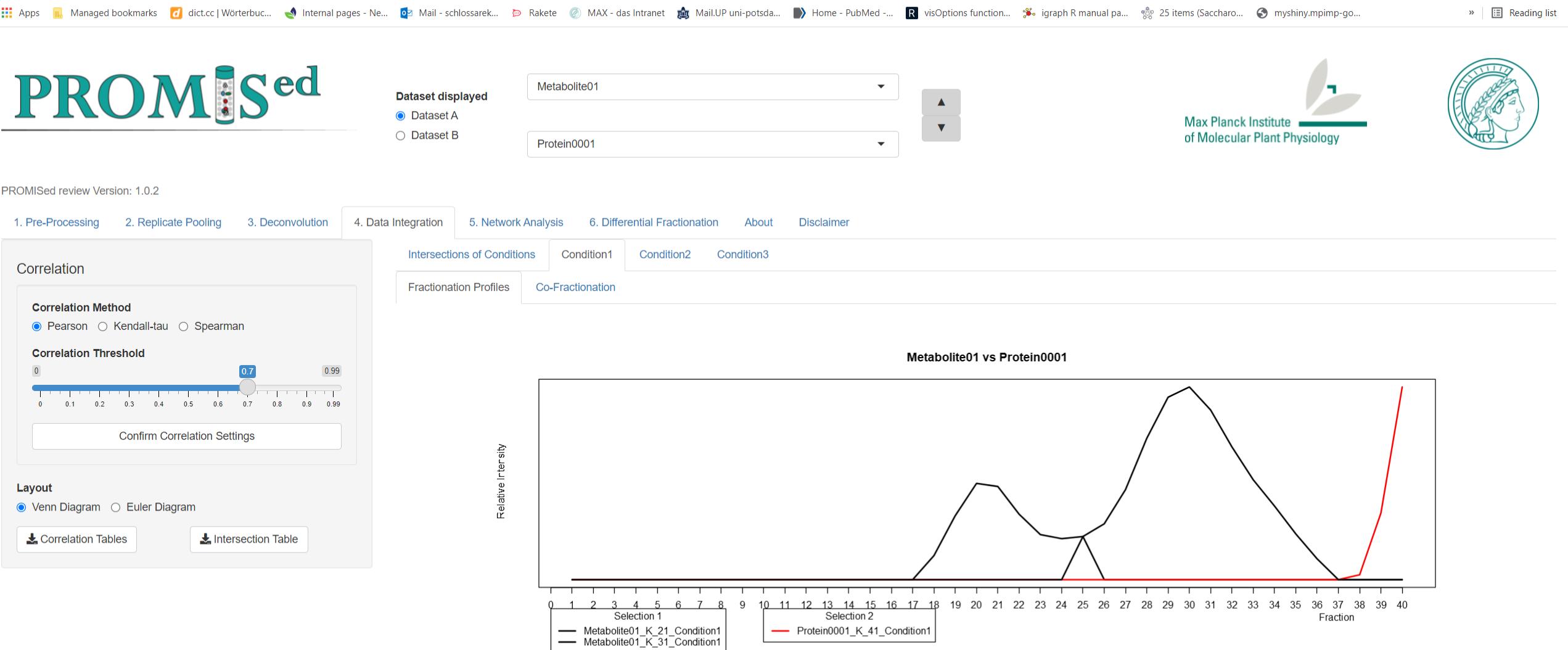
35

43

Condition1 Condition2 Condition3

Make sure to confirm the correlation settings before checking for co-fractionations or creating networks

Getting Started with PROMISed





Dataset displayed
 Dataset A
 Dataset B

Metabolite01

Protein0001



PROMISed review Version: 1.0.2

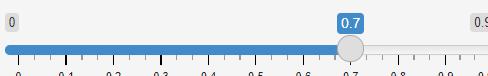
[1. Pre-Processing](#) [2. Replicate Pooling](#) [3. Deconvolution](#) [4. Data Integration](#) [5. Network Analysis](#) [6. Differential Fractionation](#) [About](#) [Disclaimer](#)

Intersections of Conditions [Condition1](#) [Condition2](#) [Condition3](#)
[Fractionation Profiles](#) [Co-Fractionation](#)

Correlation

Correlation Method
 Pearson Kendall-tau Spearman

Correlation Threshold



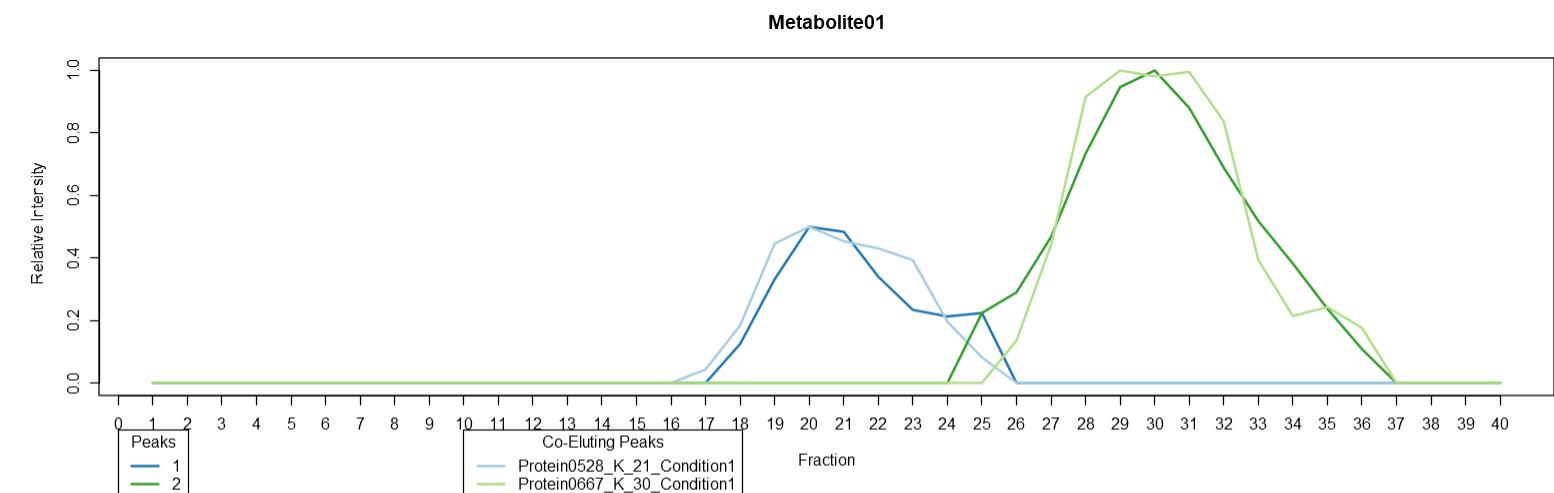
Confirm Correlation Settings

Layout

Venn Diagram Euler Diagram

[Correlation Tables](#)

[Intersection Table](#)



Show 10 entries

Search:

Protein0001 K 41 Condition1

Getting Started with PROMISed

Metabolite01_K_21_Condition1

-0.095

Metabolite01_K_31_Condition1

-0.115

17



Dataset displayed

 Dataset A Dataset B

Protein0001

Max Planck Institute
of Molecular Plant Physiology

PROMISed review Version: 1.0.2

1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration

5. Network Analysis

6. Differential Fractionation

About

Disclaimer

Network

Filter Network on

 No Filter Selection 1 Selection 2

Node Colors

 Cluster k-Coreness

Layout

 Force-directed Circles

Condition1

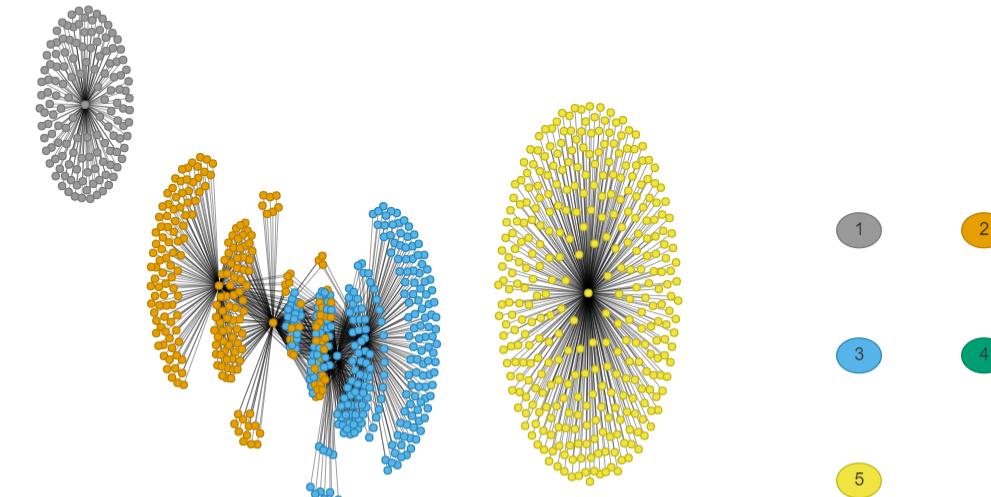
Condition2

Condition3

Select by id

Select by cluster

Community



Get Network Files

Getting Started with PROMISed



Dataset displayed

 Dataset A Dataset B

Protein0001



PROMISed review Version: 1.0.2

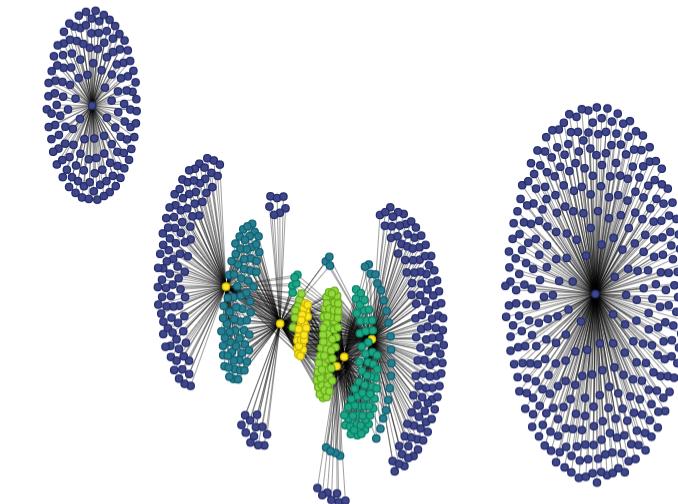
1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration

5. Network Analysis

6. Differential Fractionation

About

Disclaimer

Network**Filter Network on** No Filter Selection 1 Selection 2**Node Colors** Cluster k-Coreness**Layout** Force-directed Circles**k-coreness**[Get Network Files](#)

Dataset A
 Dataset B

Protein0001



PROMISe review Version: 1.0.2

[1. Pre-Processing](#) [2. Replicate Pooling](#) [3. Deconvolution](#) [4. Data Integration](#) [5. Network Analysis](#) [6. Differential Fractionation](#) [About](#) [Disclaimer](#)

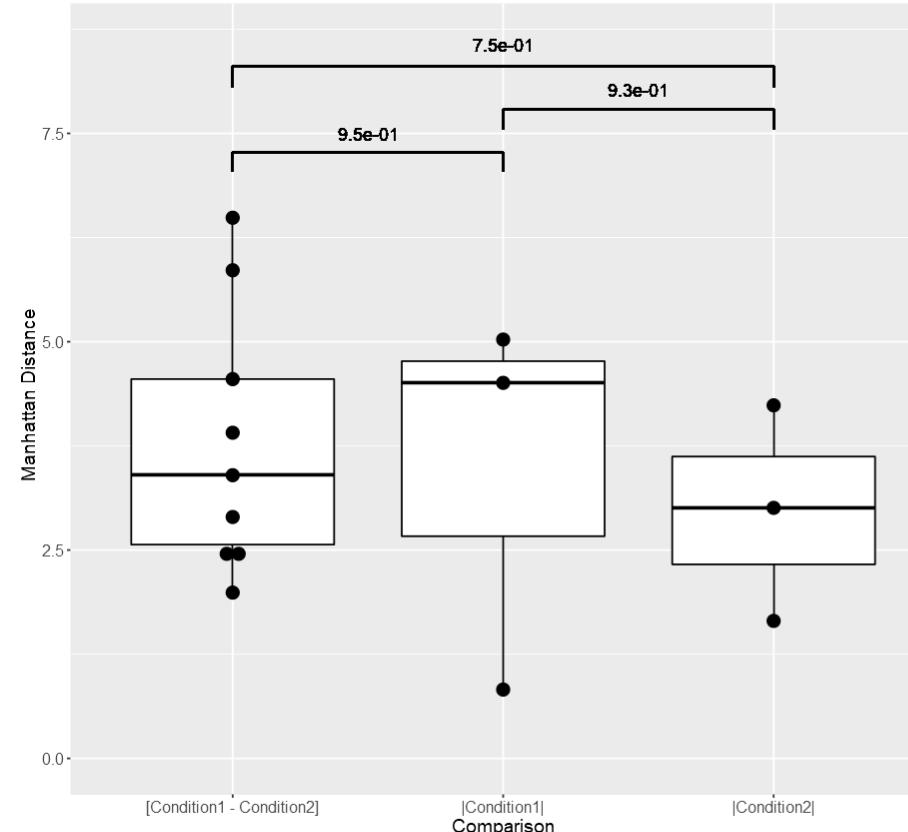
Differential Fractionation

p-Value Threshold

0.05

 [Download Dis-Elution-Score Results](#)
[\[Condition1 - Condition2\]](#) [\[Condition1 - Condition3\]](#) [\[Condition2 - Condition3\]](#)

Comparing Manhattan Distances between Treatments and Replicates



	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Combinations	2	1.5e+00	7.6e-01	2.7e-01	7.7e-01
Residuals	12	3.4e+01	2.8e+00	NA	NA

	diff	lwr	upr	p adj
Condition1 -[Condition1 - Condition2]	-3.249e-01	-3.308e+00	2.658e+00	9.547e-0
Condition2 -[Condition1 - Condition2]	-8.133e-01	-3.797e+00	2.170e+00	7.525e-0
Condition2 - Condition1	-4.884e-01	-4.142e+00	3.165e+00	9.327e-0



Dataset displayed
 Dataset A
 Dataset B



PROMISed review Version: 1.0.2

1. Pre-Processing 2. Replicate Pooling 3. Deconvolution 4. Data Integration 5. Network Analysis 6. Differential Fractionation About Disclaimer

Pre-Processing

Remove Single Peaks

Normalize

Minimum Relative Intensity

0.1

Profile Smoothing

Span-Value

0.15

Start Analysis

Raw Profiles



If the app crashed it appears grey.
Please check if your uploaded data fulfills
the requirements and format.

A common reason for crashes are wrong
column-names or duplicate row-names.
Also, make sure your fractionation
profiles only contain numbers.