

a rtMS

Analytical R Tools
for Mass Spectrometry

<http://artms.org>



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Analytical R Tools
for Mass Spectrometry

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Goals

- 1** Facilitate the analysis of Mass-Spectrometry based **Proteomics** data using the programming language

- 2** Provide different levels of analysis to ensure **data quality, quantification**, and frame results in a **biological context**.

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Quantification Methods

Label Free
SILAC (+/- Fractionation)

Analysis of

+Global Proteome
+AP-MS
+PostTranslational Modifications

Phosphorylation (PH)
Ubiquitination (UB)
Acetylation (AC)
(and any MaxQuant supported PTM)



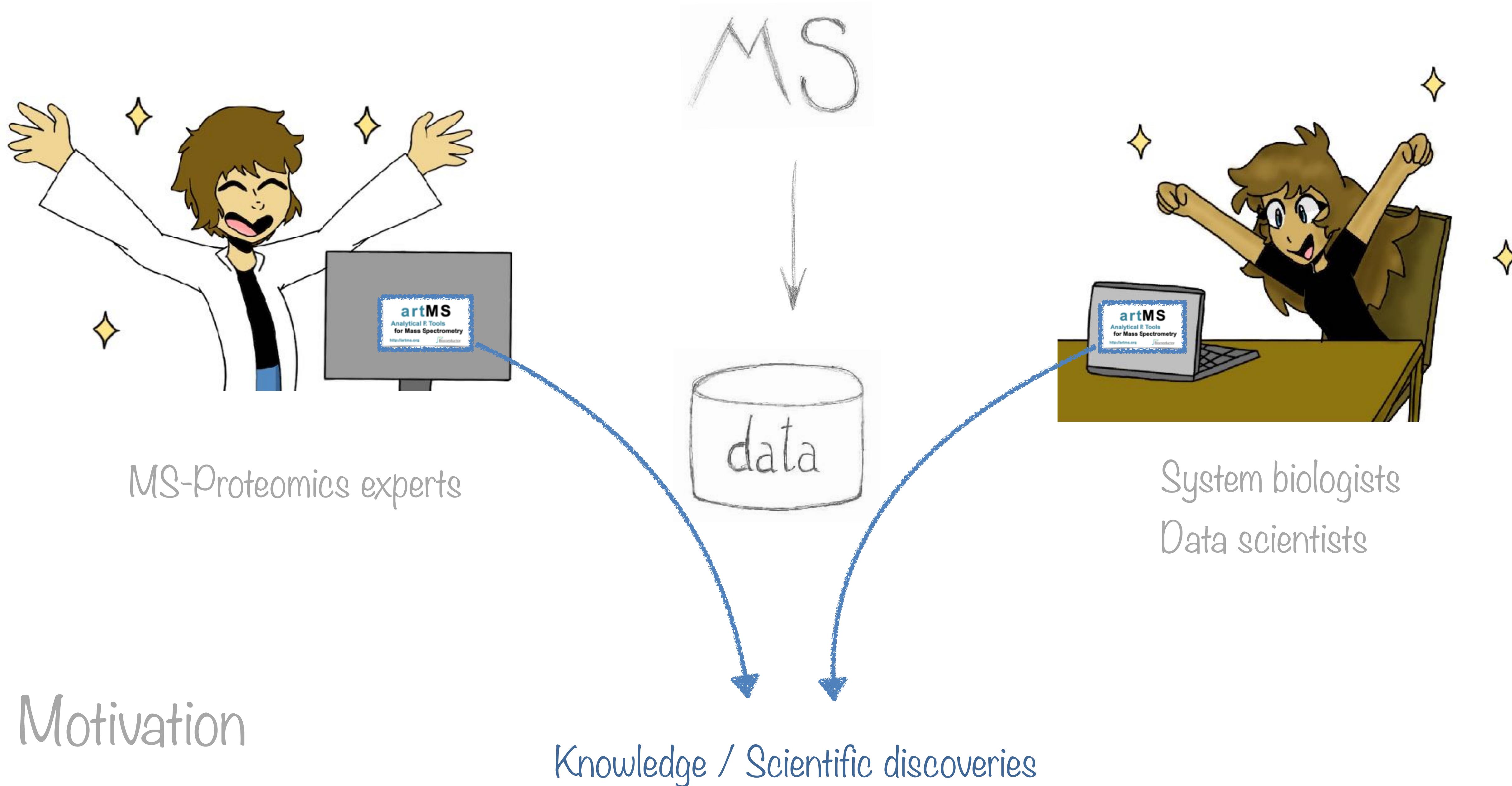
MS-Proteomics experts

Motivation



System biologists
Data scientists

Knowledge / Scientific discoveries

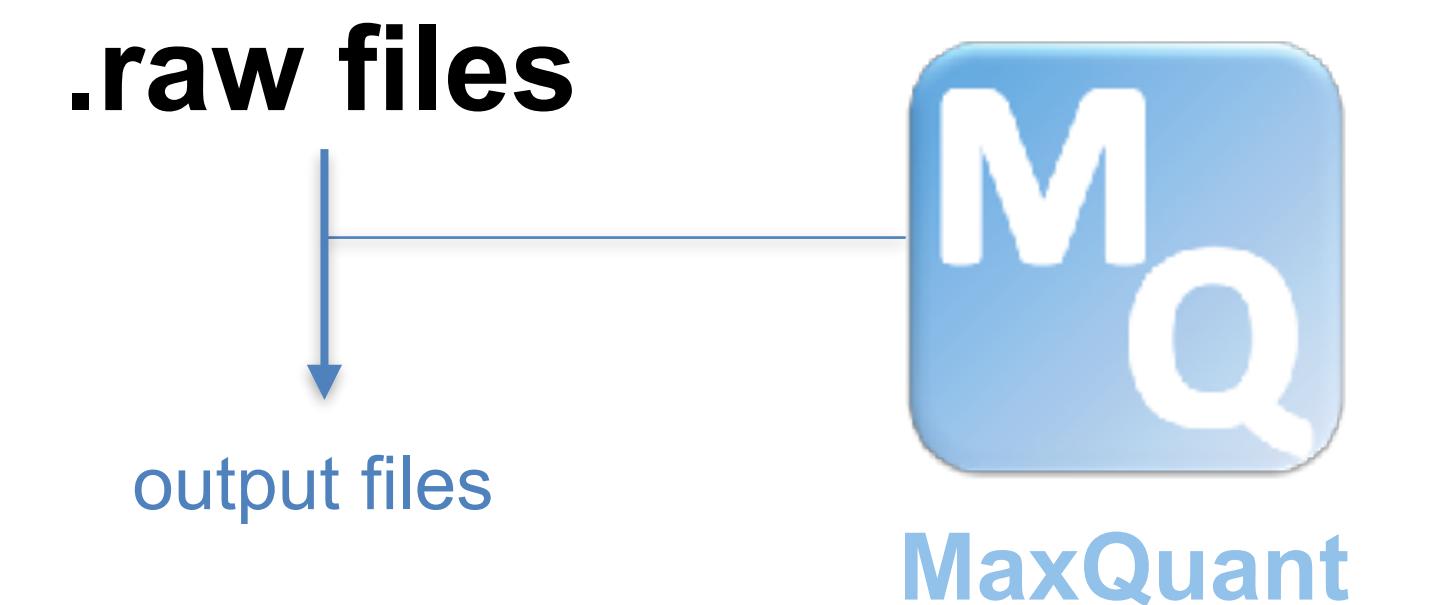


Experimental

Computational



Proteomics pipeline
PH, UB, AB, APMS...



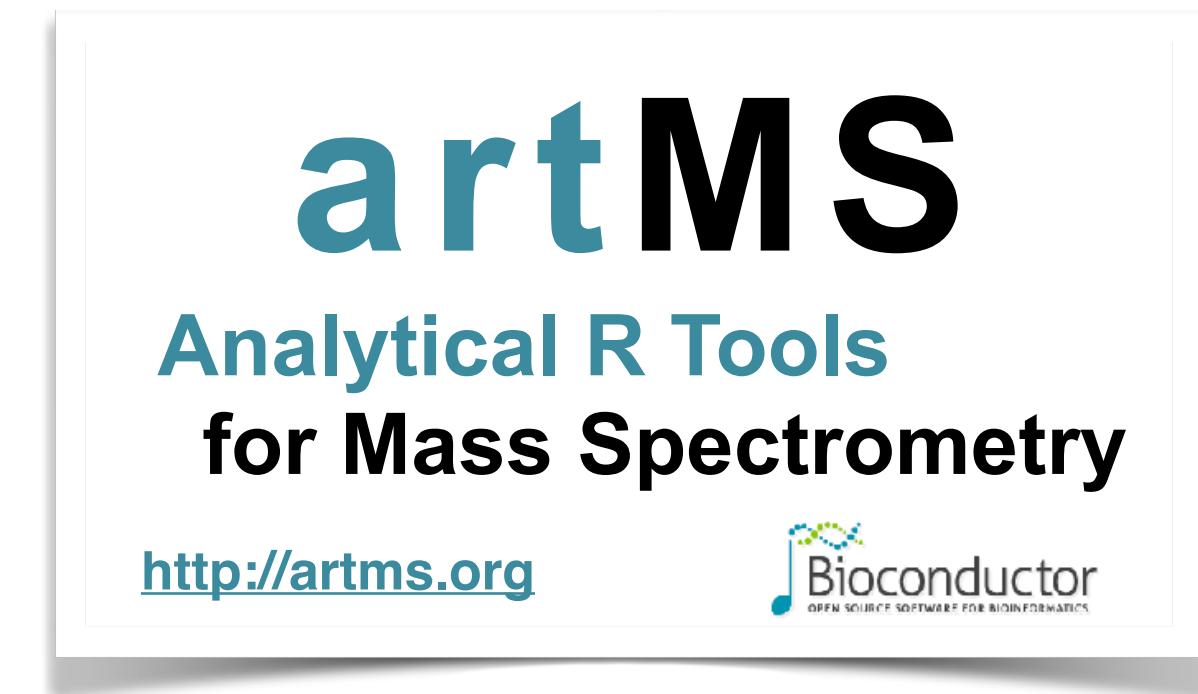
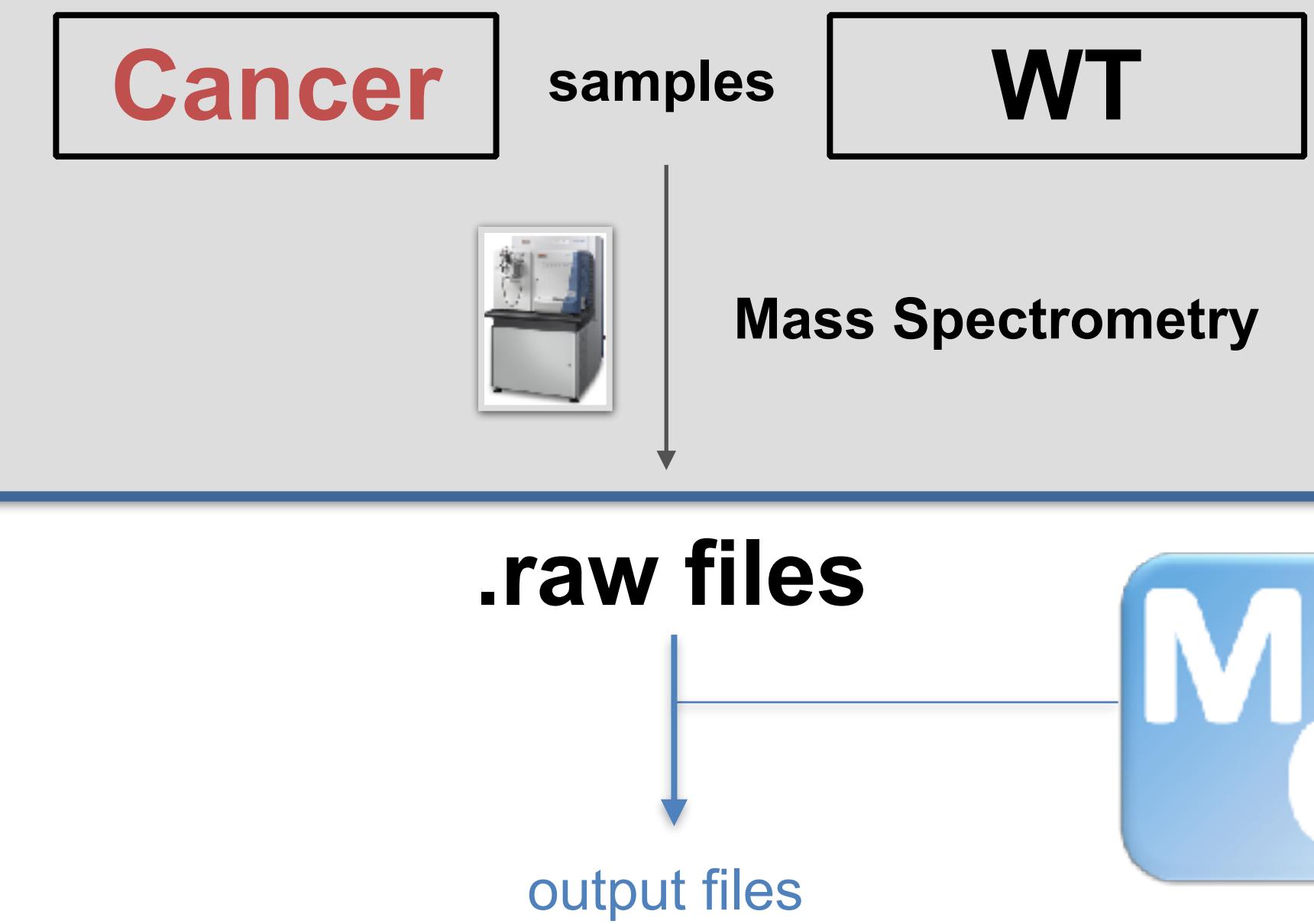
- Tool widely used
- Algorithms yield high mass accuracy and precision
- It covers a wide variety of proteomics experiments
- Simplified user interface
- It can now run on **Linux** (improved performance)

Proteomics pipeline

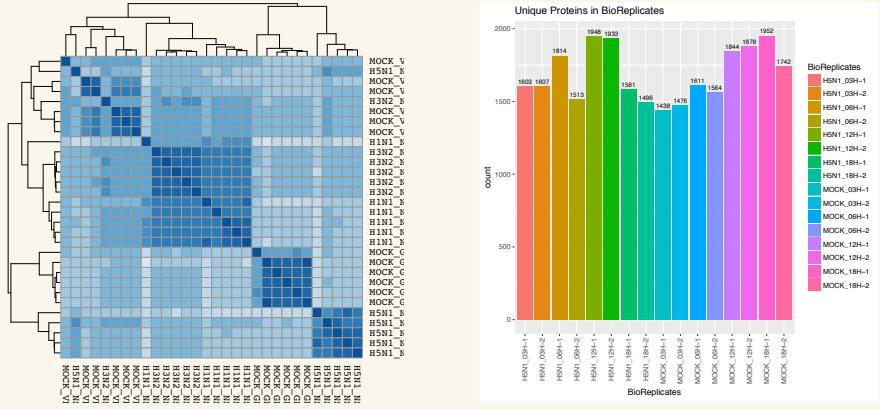
PH, UB, AB, APMS...

Experimental

Computational



Quality control



Relative quantification



evidence + keys + contrast
log2FC / p-value / adj.pvalues

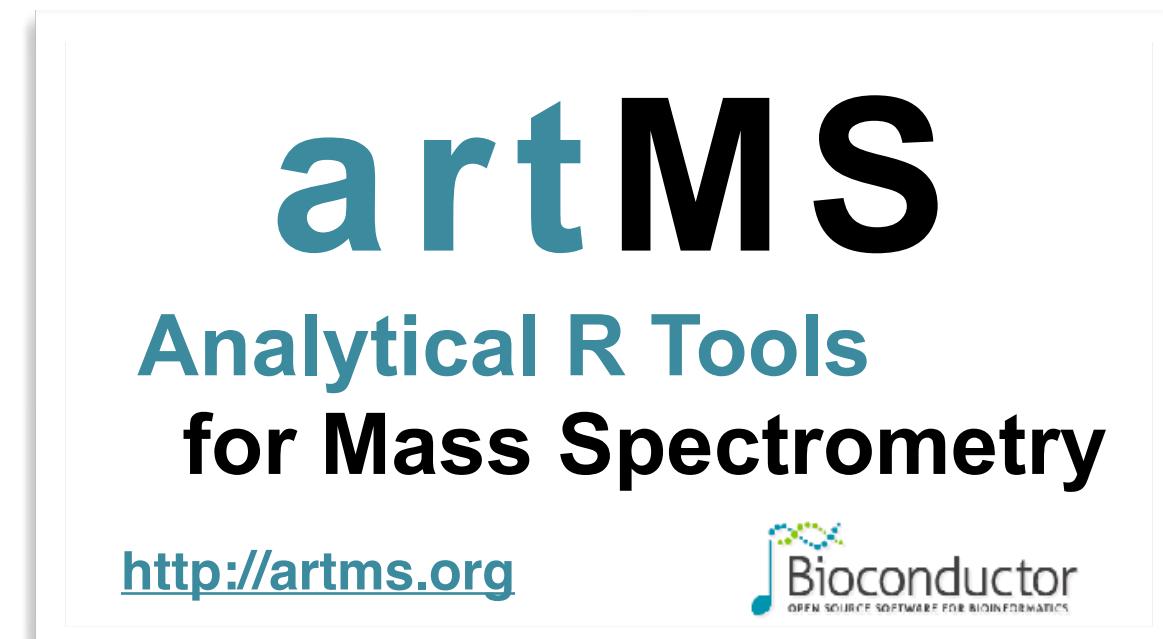
Functional analysis

Data integration
Imputation
Enrichment analysis
Pathway analysis
Network generation

Miscellaneous

SAINTq
SAINTexpress
PHOTON
Phosphate

How does it work?



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Installation

Installation

To install this package, start R (version "4.0") and enter:

```
if (!requireNamespace("BiocManager", quietly = TRUE))
  install.packages("BiocManager")

BiocManager::install("artMS")
```

For older versions of R, please refer to the appropriate [Bioconductor release](#).



(Recommended, stable)



(Development, less stable)

```
install.packages("devtools")
library(devtools)
install_github("biodavidjm/artMS")
```

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Input Files

evidence.txt

+

keys.txt

+

contrast.txt

Configuration

config.yaml

Quality control

artmsQualityControlEvidenceBasic()
artmsQualityControlEvidenceExtended()
artmsQualityControlSummaryExtended()

artmsQuantification()

Basic Functions

artmsAnalysisQuantifications()

Miscellaneous

artmsEvidenceToSAINTq()
artmsEvidenceToSaintExpress()
artmsPhosphateOutput()
artmsPhotonOutput()
etc

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Input Files

evidence.txt

keys.txt

contrast.txt

Configuration

config.yaml

Experimental design

Quality control

Relative quantification

Functional analysis

Miscellaneous

| | A | B | C | D | E |
|----|----------|------------------|-----------|--------------|-----|
| 1 | RawFile | IsotopeLabelType | Condition | BioReplicate | Run |
| 2 | qx006145 | L | Cal33 | Cal33-1 | 1 |
| 3 | qx006146 | L | Cal33 | Cal33-2 | 2 |
| 4 | qx006147 | L | Cal33 | Cal33-3 | 3 |
| 5 | qx006148 | L | Cal33 | Cal33-4 | 4 |
| 6 | qx006154 | L | HSC6 | HSC6-1 | 5 |
| 7 | qx006151 | L | HSC6 | HSC6-2 | 6 |
| 8 | qx006152 | L | HSC6 | HSC6-3 | 7 |
| 9 | qx006153 | L | HSC6 | HSC6-4 | 8 |
| 10 | | | | | |

- Two cell cancer cell lines: **Cal33, HSC6**
- 4 biological replicates each

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Input Files

evidence.txt

+

keys.txt

+

contrast.txt

Configuration

config.yaml

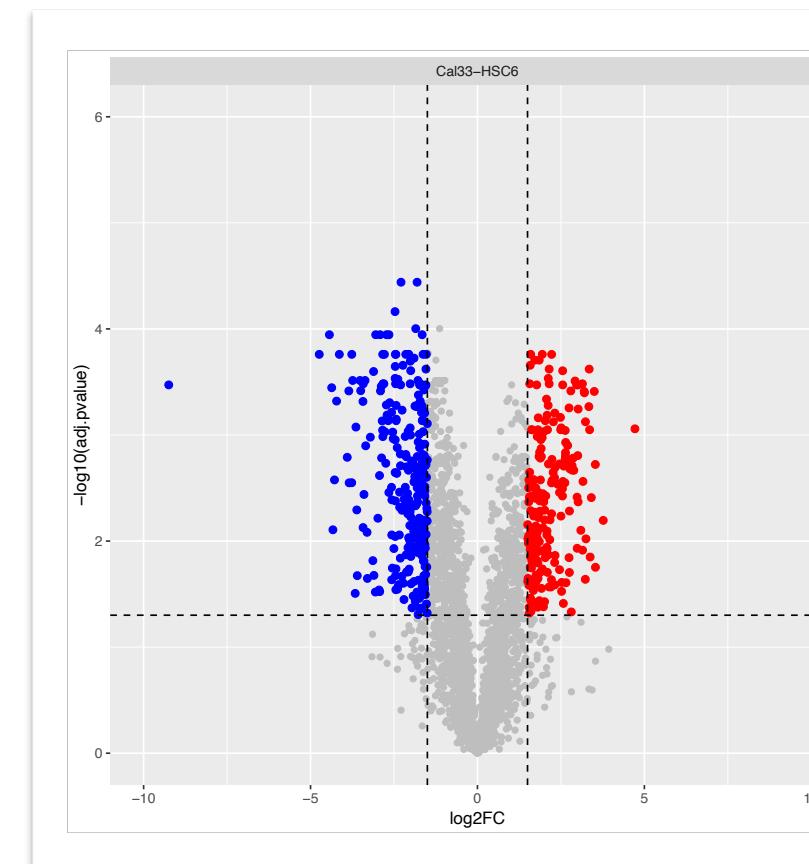
Quality control

Relative quantification

Functional analysis

Miscellaneous

Relative quantification between conditions



Cal33-HSC6

- Two cell cancer cell lines: **Cal33, HSC6**
- 4 biological replicates each

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Input Files

evidence.txt

keys.txt

contrast.txt

Configuration

config.yaml

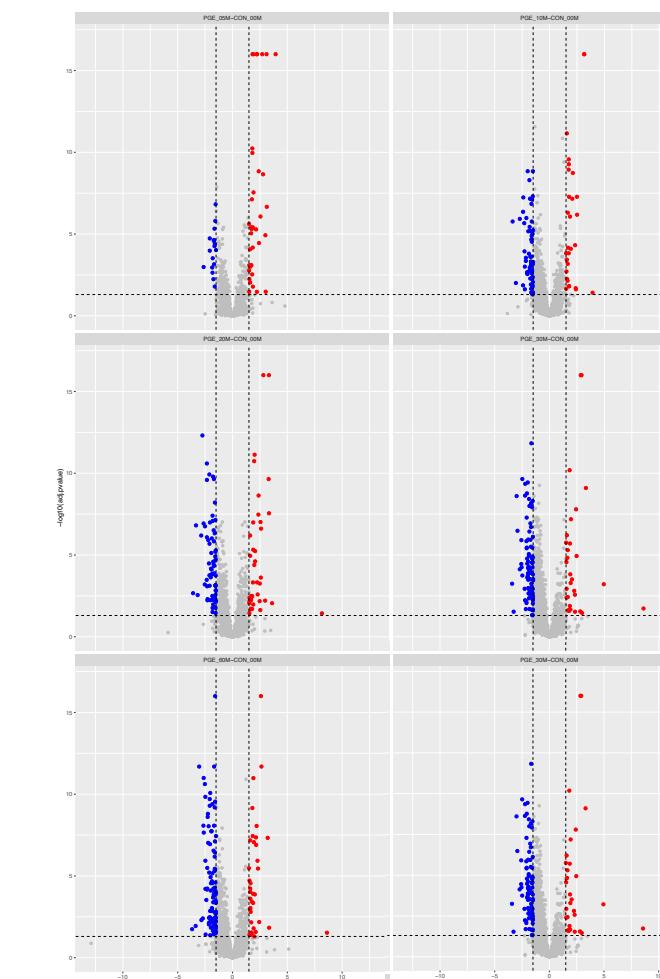
Quality control

MS stats
Relative quantification

Functional analysis

Miscellaneous

Relative quantification between conditions



A-B
A-C
A-D
D-E
D-F
D-G
etc

- Several conditions: **A, B, C, D, E, F, G**
- 4 biological replicates each

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Quality control



Relative quantification

Functional analysis

Miscellaneous

```
config-phglobal.yaml x
1 files:
2   evidence: evidence.txt
3   keys: keys.txt
4   contrasts: contrast.txt
5   summary: summary.txt
6   output: phglobal_results/phglobal-results.txt
7 qc:
8   basic: 1
9   extended: 1
10  extendedSummary: 1
11 data:
12  enabled: 1
13  fractions:
14    enabled: 0
15  silac:
16    enabled: 0
17  filters:
18    enabled: 1
19    contaminants: 1
20    protein_groups: remove
21    modifications: PH
22    sample_plots: 1
23 msstats:
24  enabled: 1
25  msstats_input:
26  profilePlots: none
27  normalization_method: equalizeMedians
28  normalization_reference:
29  summaryMethod: TMP
30  censoredInt: NA
31  cutoffCensored: minFeature
32  MBimpute: 1
33  feature_subset: all
34  output_extras:
35  enabled: 1
36  annotate:
37    enabled: 1
38    species: HUMAN
39  plots:
40    volcano: 1
41    heatmap: 1
42    LFC: -0.58 0.58
43    FDR: 0.05
44    heatmap_cluster_cols: 0
45    heatmap_display: log2FC
```

Files

Configuration

config.yaml

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Quality control



Relative quantification

Functional analysis

Miscellaneous

```
config-phglobal.yaml x
1 files:
2   evidence: evidence.txt
3   keys: keys.txt
4   contrasts: contrast.txt
5   summary: summary.txt
6   output: phglobal_results/phglobal-results.txt
7 qc:
8   basic: 1
9   extended: 1
10  extendedSummary: 1
11 data:
12   enabled: 1
13   fractions:
14     enabled: 0
15   silac:
16     enabled: 0
17   filters:
18     enabled: 1
19     contaminants: 1
20     protein_groups: remove
21     modifications: PH
22     sample_plots: 1
23 msstats:
24   enabled: 1
25   msstats_input:
26   profilePlots: none
27   normalization_method: equalizeMedians
28   normalization_reference:
29   summaryMethod: TMP
30   censoredInt: NA
31   cutoffCensored: minFeature
32   MBimpute: 1
33   feature_subset: all
34   output_extras:
35     enabled: 1
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38     species: HUMAN
39   plots:
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44     heatmap_cluster_cols: 0
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```

Configuration

config.yaml

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Quality control



Relative quantification

Functional analysis

Miscellaneous

```
config-phglobal.yaml x
1 files:
2   evidence: evidence.txt
3   keys: keys.txt
4   contrasts: contrast.txt
5   summary: summary.txt
6   output: phglobal_results/phglobal-results.txt
7 qc:
8   basic: 1
9   extended: 1
10  extendedSummary: 1
11 data:
12   enabled: 1
13   fractions:
14     enabled: 0
15   silac:
16     enabled: 0
17   filters:
18     enabled: 1
19     contaminants: 1
20     protein_groups: remove
21     modifications: PH
22     sample_plots: 1
23 msstats:
24   enabled: 1
25   msstats_input:
26   profilePlots: none
27   normalization_method: equalizeMedians
28   normalization_reference:
29   summaryMethod: TMP
30   censoredInt: NA
31   cutoffCensored: minFeature
32   MBimpute: 1
33   feature_subset: all
34   output_extras:
35     enabled: 1
36   annotate:
37     enabled: 1
38     species: HUMAN
39   plots:
40     volcano: 1
41     heatmap: 1
42     LFC: -0.58 0.58
43     FDR: 0.05
44     heatmap_cluster_cols: 0
45     heatmap_display: log2FC
```

Proteomics details

Configuration

config.yaml

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Quality control



Relative quantification

Functional analysis

Miscellaneous

Configuration

config.yaml

```
config-phglobal.yaml x
1 files:
2   evidence: evidence.txt
3   keys: keys.txt
4   contrasts: contrast.txt
5   summary: summary.txt
6   output: phglobal_results/phglobal-results.txt
7 qc:
8   basic: 1
9   extended: 1
10  extendedSummary: 1
11 data:
12   enabled: 1
13   fractions:
14     enabled: 0
15   silac:
16     enabled: 0
17   filters:
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19     contaminants: 1
20     protein_groups: remove
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25   msstats_input:
26     profilePlots: none
27     normalization_method: equalizeMedians
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32     MBimpute: 1
33     feature_subset: all
34     output_extras:
35       enabled: 1
36       annotate:
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39       plots:
40         volcano: 1
41         heatmap: 1
42         LFC: -0.58 0.58
43         FDR: 0.05
44         heatmap_cluster_cols: 0
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```

Relative Quantification
(MSstats)

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Quality control



Relative quantification

Functional analysis

Miscellaneous

```
config-phglobal.yaml x
1 files:
2   evidence: evidence.txt
3   keys: keys.txt
4   contrasts: contrast.txt
5   summary: summary.txt
6   output: phglobal_results/phglobal-results.txt
7 qc:
8   basic: 1
9   extended: 1
10  extendedSummary: 1
11 data:
12  enabled: 1
13  fractions:
14    enabled: 0
15  silac:
16    enabled: 0
17  filters:
18    enabled: 1
19    contaminants: 1
20    protein_groups: remove
21    modifications: PH
22    sample_plots: 1
23 msstats:
24  enabled: 1
25  msstats_input:
26  profilePlots: none
27  normalization_method: equalizeMedians
28  normalization_reference:
29  summaryMethod: TMP
30  censoredInt: NA
31  cutoffCensored: minFeature
32  MBimpute: 1
33  feature_subset: all
34 output_extras:
35  enabled: 1
36  annotate:
37    enabled: 1
38    species: HUMAN
39  plots:
40    volcano: 1
41    heatmap: 1
42    LFC: -0.58 0.58
43    FDR: 0.05
44    heatmap_cluster_cols: 0
45    heatmap_display: log2FC
```

Outputs / extras

Configuration
config.yaml

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Input Files

| | |
|--|--------------|
| | evidence.txt |
| | keys.txt |

Quality control

artmsQualityControlEvidenceBasic()
artmsQualityControlEvidenceExtended()
artmsQualityControlSummaryExtended()



Relative quantification

Functional analysis

Miscellaneous

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<http://artms.org>



Quality control

artmsQualityControlEvidenceBasic()

artmsQualityControlEvidenceExtended()

artmsQualityControlSummaryExtended()

artmsQuantification()

artmsAnalysisQuantifications()

artmsEvidenceToSAINTq()

artmsEvidenceToSaintExpress()

artmsPhosphateOutput()

artmsPhotonOutput()

etc

Input Files

evidence.txt
keys.txt

Console

Terminal

~ /

```
> library(artMS)
> artmsQualityControlEvidenceBasic(evidence_file = "evidence.txt",
+                                     keys_file = "keys.txt")
```

artMS: BASIC QUALITY CONTROL (evidence.txt based)

>> MERGING FILES

-- Plot: correlation matrices

---- by Biological replicates

---- by Conditions

-- Plot: intensity stats

---- PH PROCESSED

-- Plot: PTM PH stats

<< Basic quality control analysis completed!

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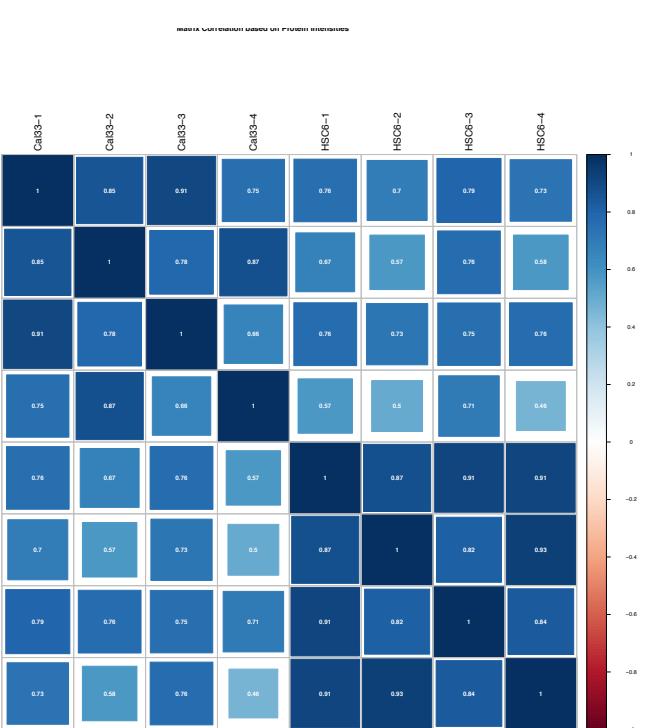
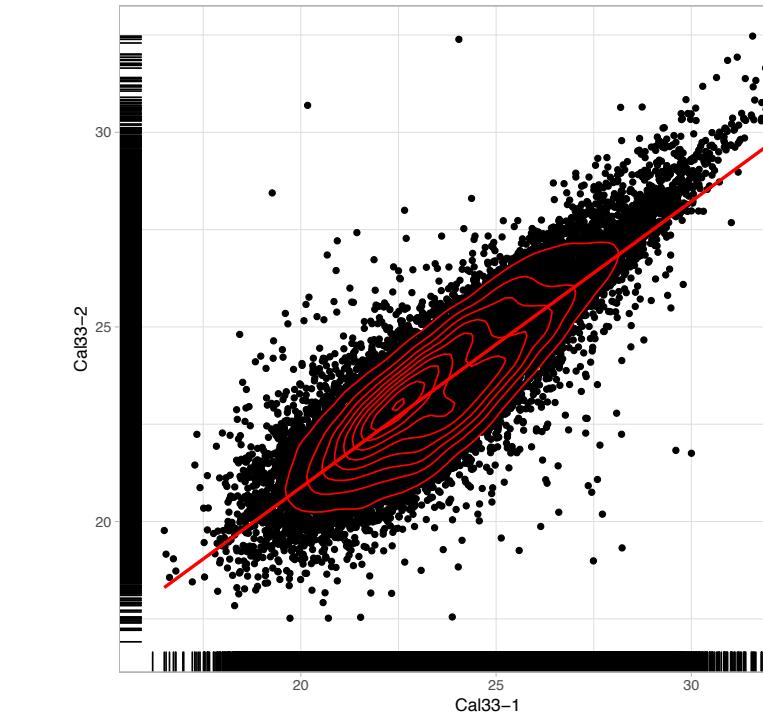
<http://artms.org>



Input Files

evidence.txt
keys.txt

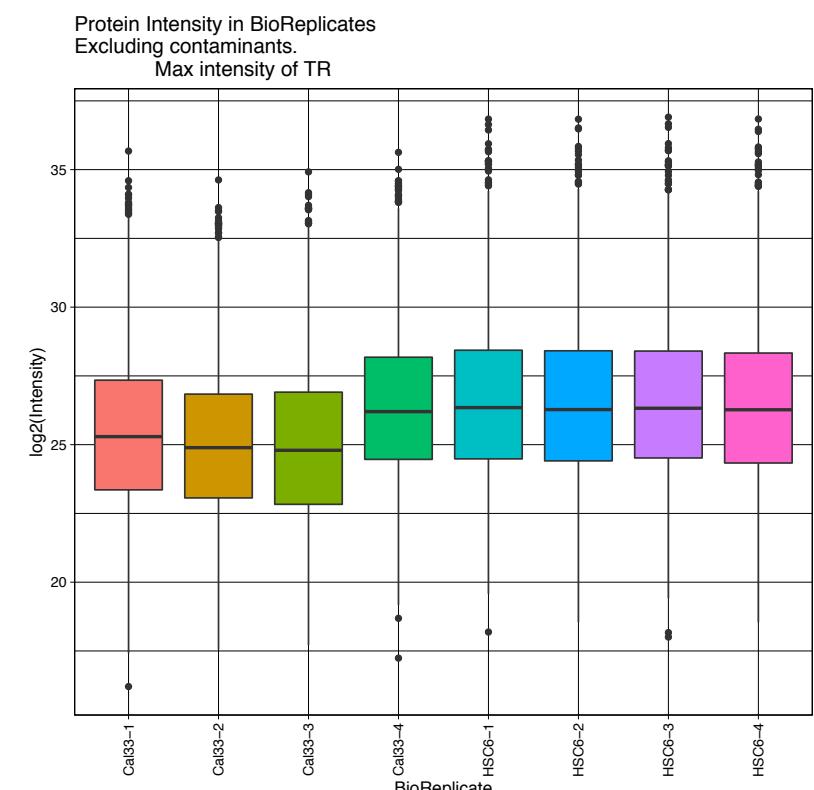
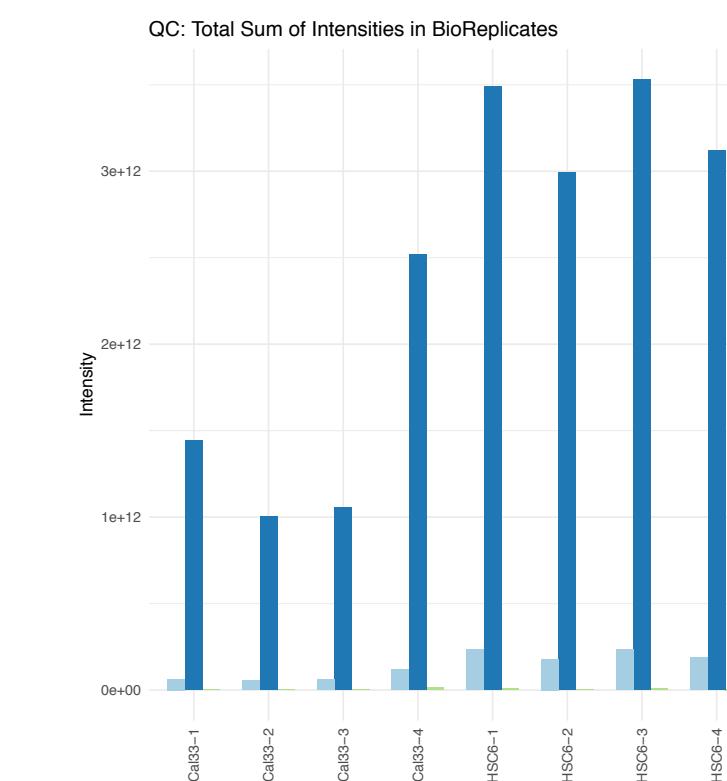
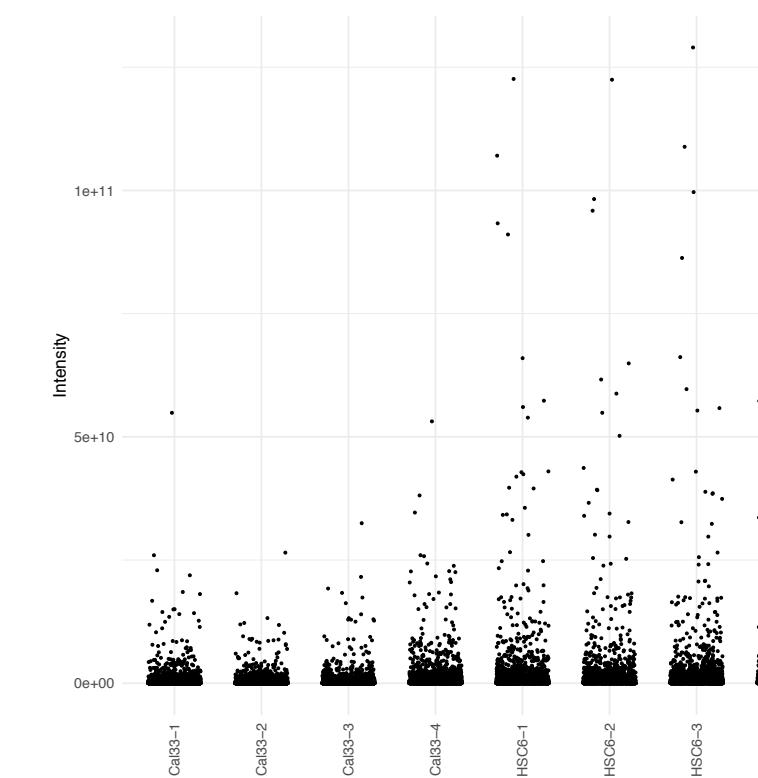
Peptide Reproducibility between Bioreplicas
(condition: Cal33) Cal33-1 vs Cal33-2
(n = 43691 r = 0.85)



Quality control

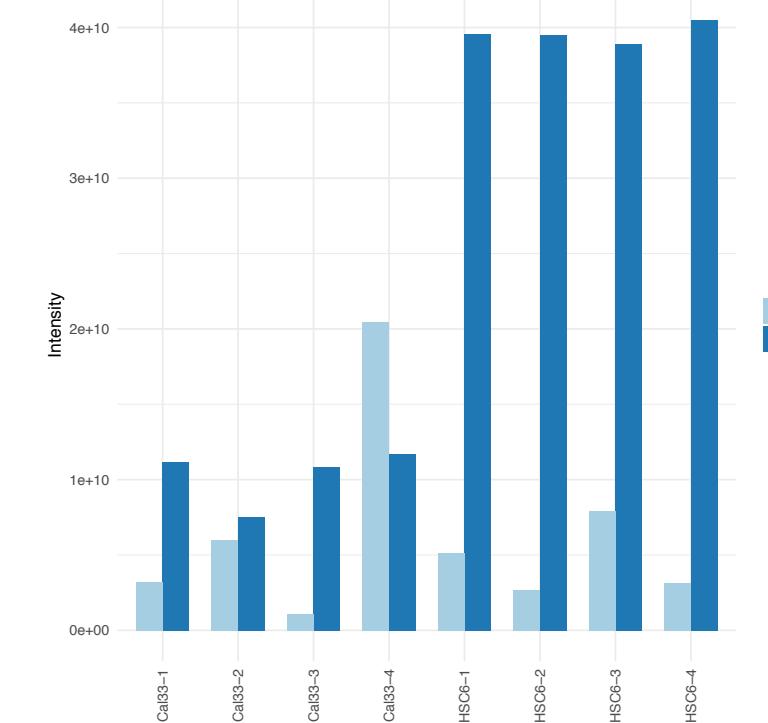
artmsQualityControlEvidenceBasic()

- Reproducibly
- MS Intensity
- Spectral Counts
- Contaminants
- PTMs

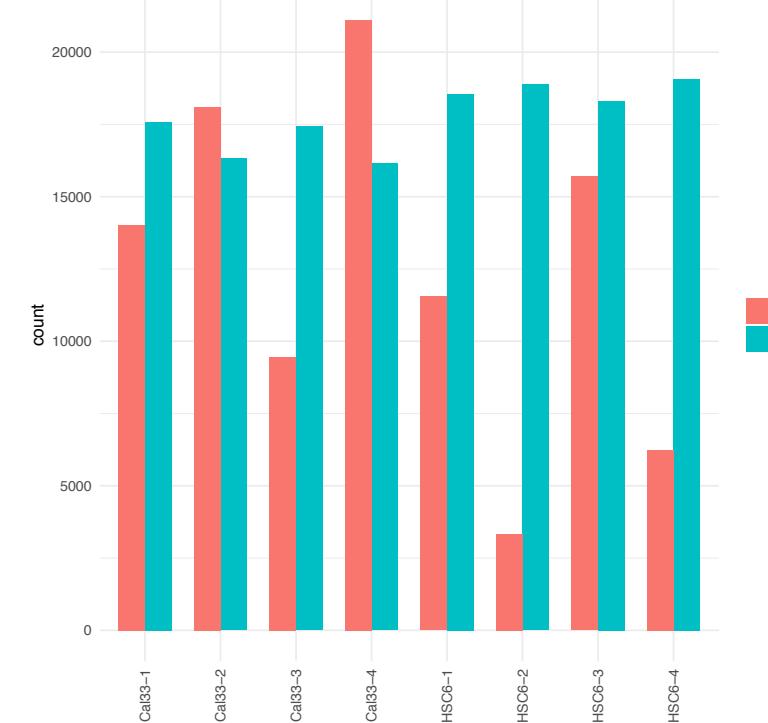


Functional analysis

Total Peptide Intensity in Biological Replicas



Peptide Count in Biological Replicas



Miscellaneous

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<http://artms.org>



Input Files

evidence.txt
keys.txt

Quality control

artmsQualityControlEvidenceBasic()
artmsQualityControlEvidenceExtended()

artmsQuantification()

artmsAnalysisQuantifications()

artmsEvidenceToSAINTq()
artmsEvidenceToSaintExpress()
artmsPhosphateOutput()
artmsPhotonOutput()
etc

Relative quantification

Functional analysis

Miscellaneous

```
Console Terminal ~ / ~> artmsQualityControlEvidenceExtended(evidence_file = "evidence.txt",
+ keys_file = "keys.txt")
-----
artMS: EXTENDED QUALITY CONTROL (-evidence.txt based)
-----
>> MERGING FILES
>> GENERATING QC PLOTS
--- Plot PSM done
--- Plot IONS done
--- Plot TYPE done
--- Plot PEPTIDES done
--- Plot PEPTIDE OVERLAP done
--- Plot PROTEINS done
--- Plot PROTEIN OVERLAP done
--- Plot Plot Ion Oversampling done
--- Plot Charge State done
--- Plot Mass Error done
--- Plot Mass-over-Charge distribution done
--- Plot Peptide Intensity CV done
--- Plot Peptide Detection (using modified.sequence) done
--- Plot Protein Intensity CV done
--- Plot Protein Detection done
--- Plot ID overlap done
--- Plot PCA and Inter-Correlation (WARNING: it might take a long time.
Please, be patient)
--- Plot Sample Preparation... done
>> QC extended completed
```

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Analytical R Tools for Mass Spectrometry

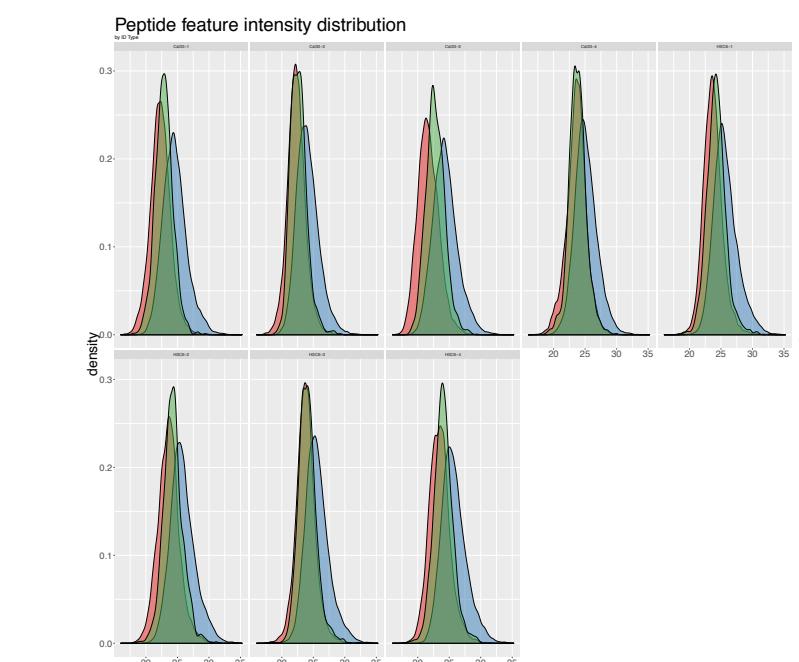
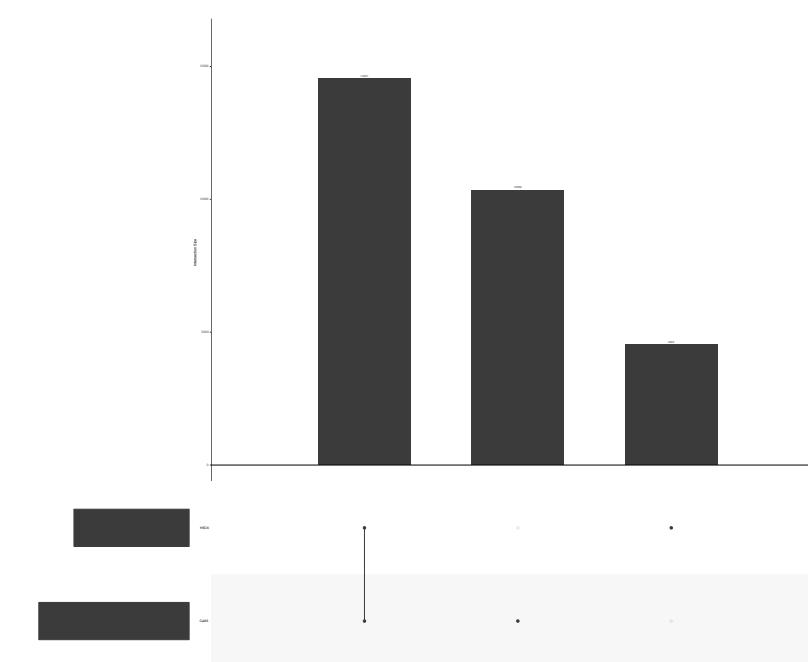
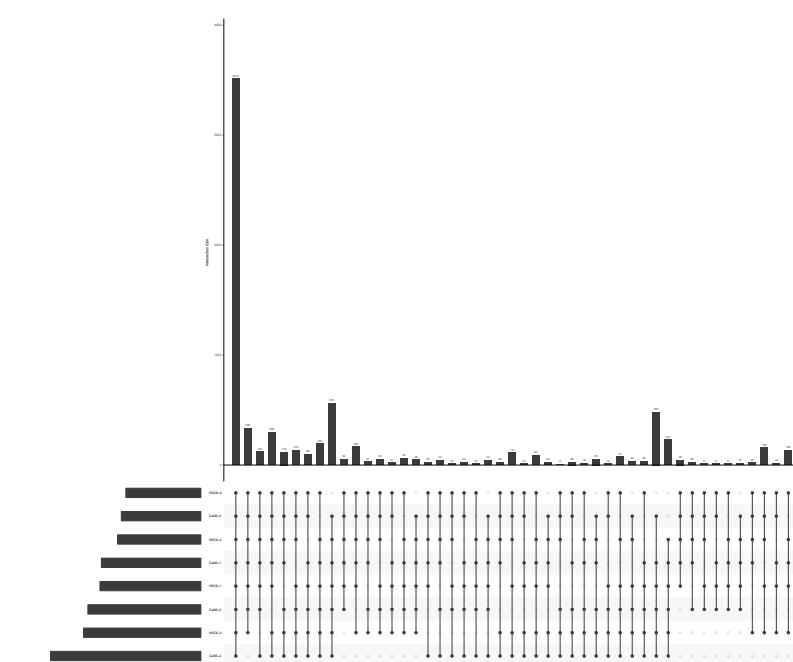
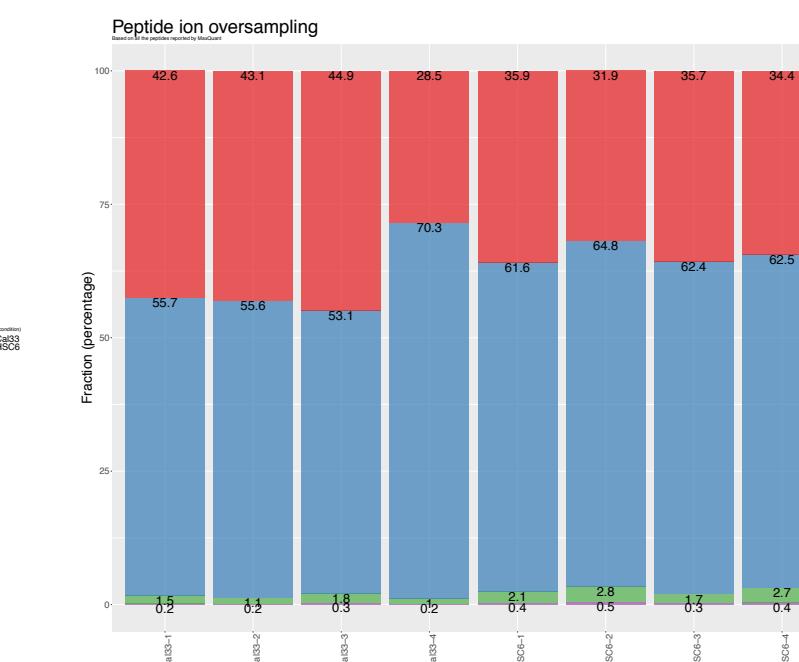
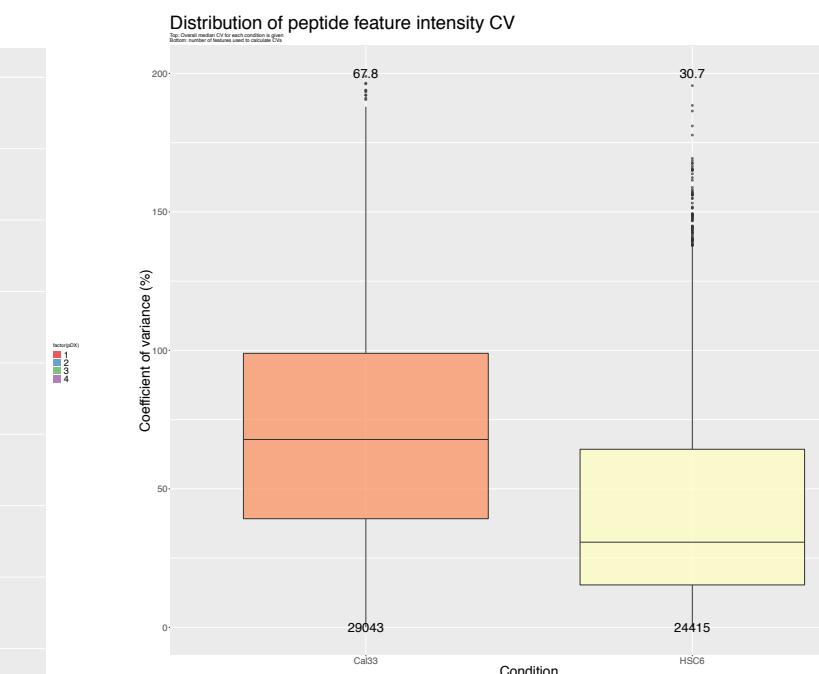
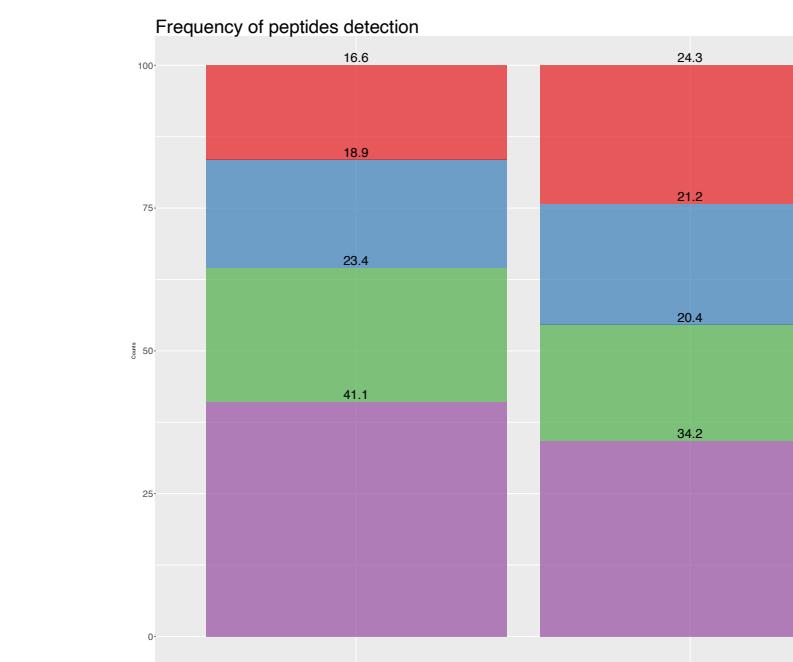
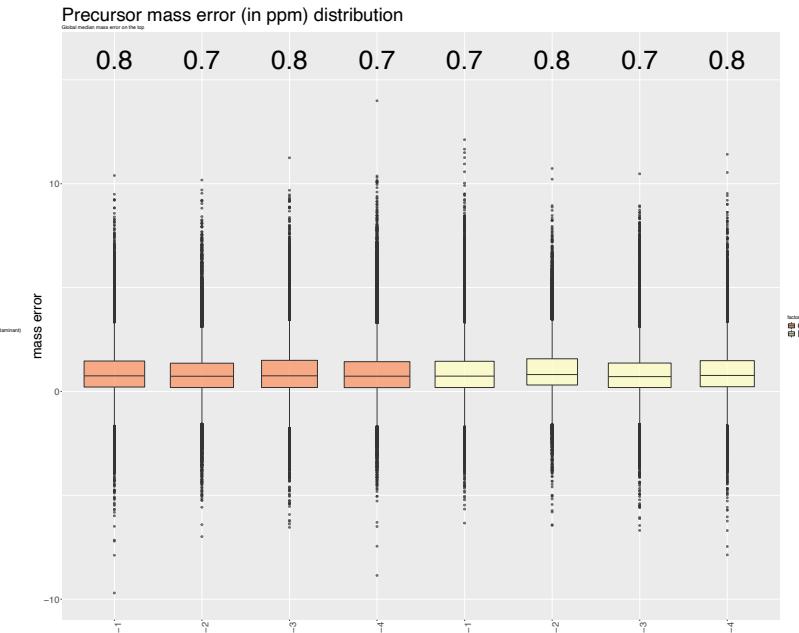
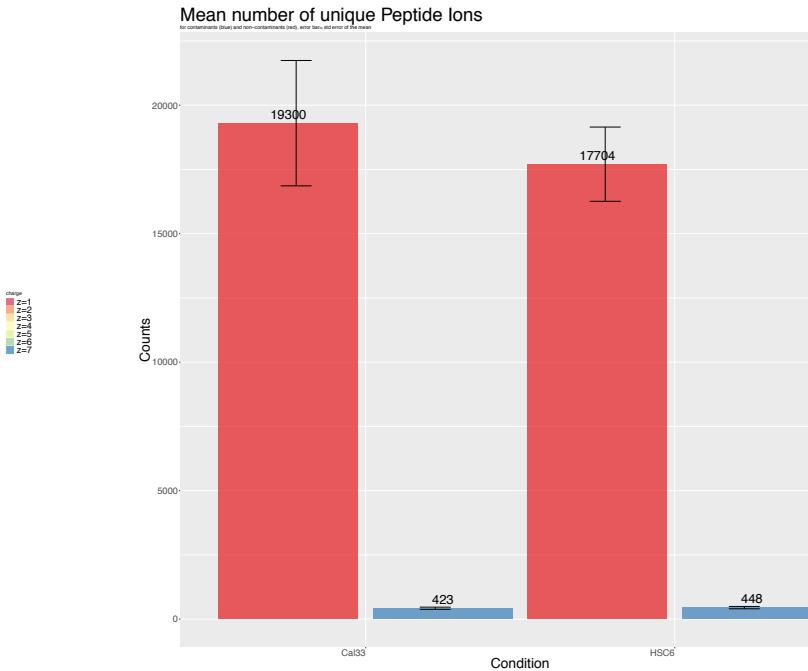
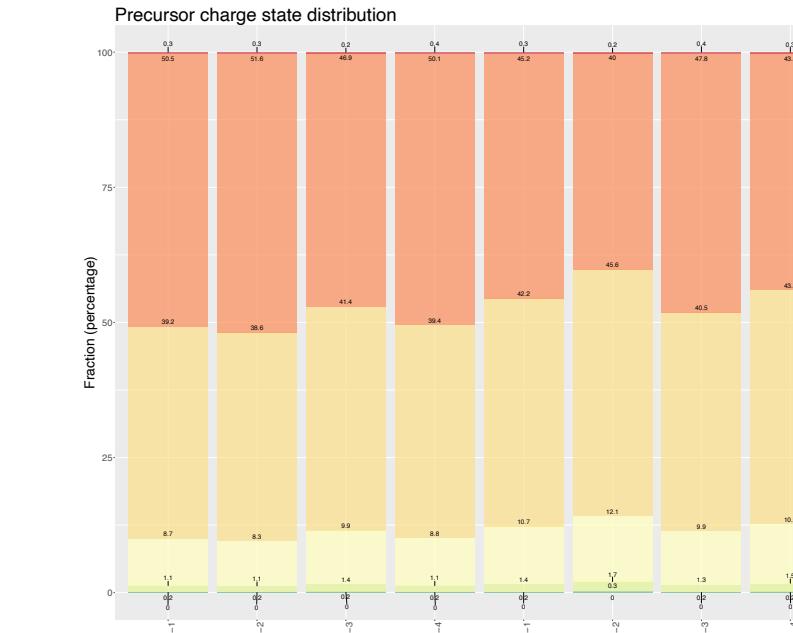
<http://artms.org>



Quality control

artmsQualityControlEvidenceExtended()

- Charge State Distribution
 - ID overlap
 - Peptide Ion Statistics
 - Precursor Mass Error
 - Precursor m/z error
 - Frequency Peptide Detection
 - Peptide Intensity CV
 - Peptide Statistics
 - Peptide Ion oversampling
 - Protein detection frequency
 - Protein Statistics / CV
 - PCA
 - Peptide-spectrum matches
 - MaxQuant Type statistics



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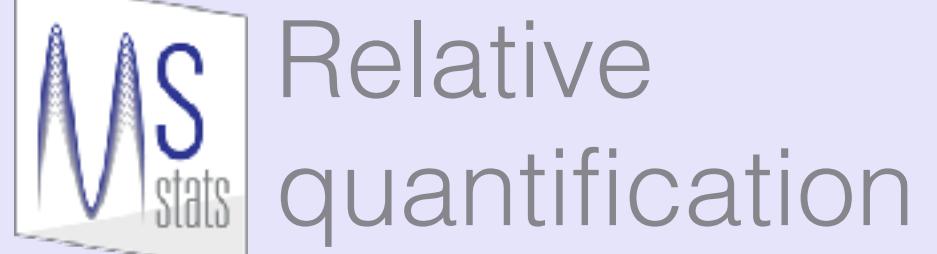
<http://artms.org>



Quality control

artmsQualityControlEvidenceBasic()
artmsQualityControlEvidenceExtended()
artmsQualityControlSummaryExtended()

- MS1 scan counts
- MS2 scan counts
- MS2 identification rate
- Isotope Pattern counts



Functional analysis

Miscellaneous

Input Files

summary.txt
keys.txt

```
> artmsQualityControlSummaryExtended(summary_file = "summary.txt",
+                                     keys_file = "keys.txt")
```

artMS: EXTENDED QUALITY CONTROL (-evidence.txt based)

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<http://artms.org>



Input Files

evidence.txt
keys.txt

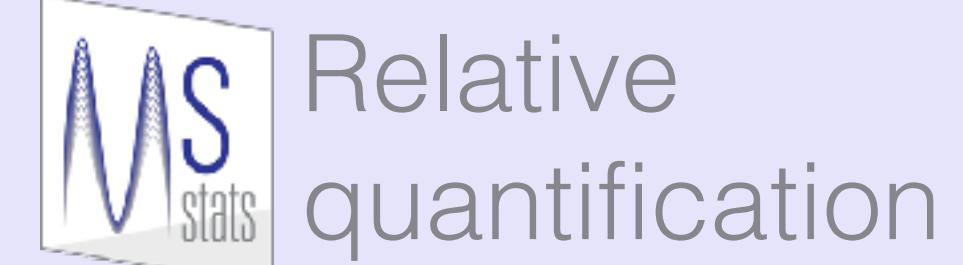
Quality control

artmsQualityControlEvidenceBasic()
artmsQualityControlEvidenceExtended()
artmsQualityControlSummaryExtended()

artmsQuantification()

artmsAnalysisQuantifications()

artmsEvidenceToSAINTq()
artmsEvidenceToSaintExpress()
artmsPhosphateOutput()
artmsPhotonOutput()
etc



Functional analysis

Miscellaneous

artMS

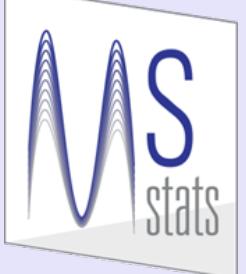
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Input Files
MQ evidence.txt
keys.txt

Quality control



Relative
quantification

artmsQuantification()

Functional analysis

Miscellaneous



<http://msstats.org/>

MSstats is an open-source R package for **statistical relative quantification of proteins** and peptides in global, targeted, and data-independent proteomics.

It uses a family of **linear mixed models** that attempts to:

- minimize bias and inefficiencies in spectrometry-based proteomics,
- distinguish the systematic variation from random artifacts,
- maximize the reproducibility of the results

Developed by **Meena Choi** from **Olga Vitek lab**

Used in



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Input Files

evidence.txt
keys.txt
contrast.txt
config.yaml

Quality control



Relative quantification

Functional analysis

Miscellaneous

artmsQuantification("config.yaml")

```
Console Terminal ~ / ~> artmsQuantification(yaml_config_file = "config-phglobal.yaml")
-----
artMS: Relative Quantification using MSstats
-----
>> Reading the configuration file
-- Folder: [quant-phglobal-pre] created
>> LOADING DATA
>> MERGING FILES
>> FILTERING
-- Contaminants CON__IREV__ removed
-- Removing protein groups
---- Use <Leading.razor.protein> as Protein ID
>> CONVERTING THE DATA TO MSSTATS FORMAT
-- Selecting Sequence Type: MaxQuant 'Modified.sequence' column
-- Adding NA values for missing values (required by MSstats)
-- Write out the MSstats input file (-mss.txt)
>> RUNNING MSstats (it usually takes a 'long' time: please, be patient)
    (MSstats messages are turned off.
     Select <display_msstats = TRUE> to activate MSstats outputs)
>> MSstats done
>> ANNOTATING THE RESULTS (adding gene symbols and protein names)
-- Selected hits for plots with LFC between -0.58 and 0.58 at 0.05 FDR:1207
>> PLOTTING HEATMAP FOR SIGNIFICANT CHANGES
>> PLOTTING VOLCANO PLOT
quant-phglobal-pre/phglobal-results-volcano.pdf is ready
>> ANALYSIS COMPLETED
```

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Input Files

evidence.txt
keys.txt
contrast.txt
config.yaml

Quality control



Relative quantification

Functional analysis

Miscellaneous

artmsQuantification("config.yaml")

TXT FILES

- quantification-results.txt
- quantification-results-annotated.txt
- Normalized abundance
 - * results_ModelQC.txt
 - * results_RunlevelData.txt
 - * results-mss-groupQuant.txt
 - * results-mss-normalized.txt
 - * results-mss-sampleQuant.txt
- results_sampleSize.txt
- results_experimentPower.txt

PDF FILES

- results-heatmap.pdf
- results-peptidecounts-perBait.pdf
- results-peptidecounts.pdf
- results-sign.pdf
- results-volcano.pdf

artMS

Analytical R Tools
for Mass Spectrometry

<http://artms.org>



Input Files

evidence.txt
keys.txt
contrast.txt
config.yaml

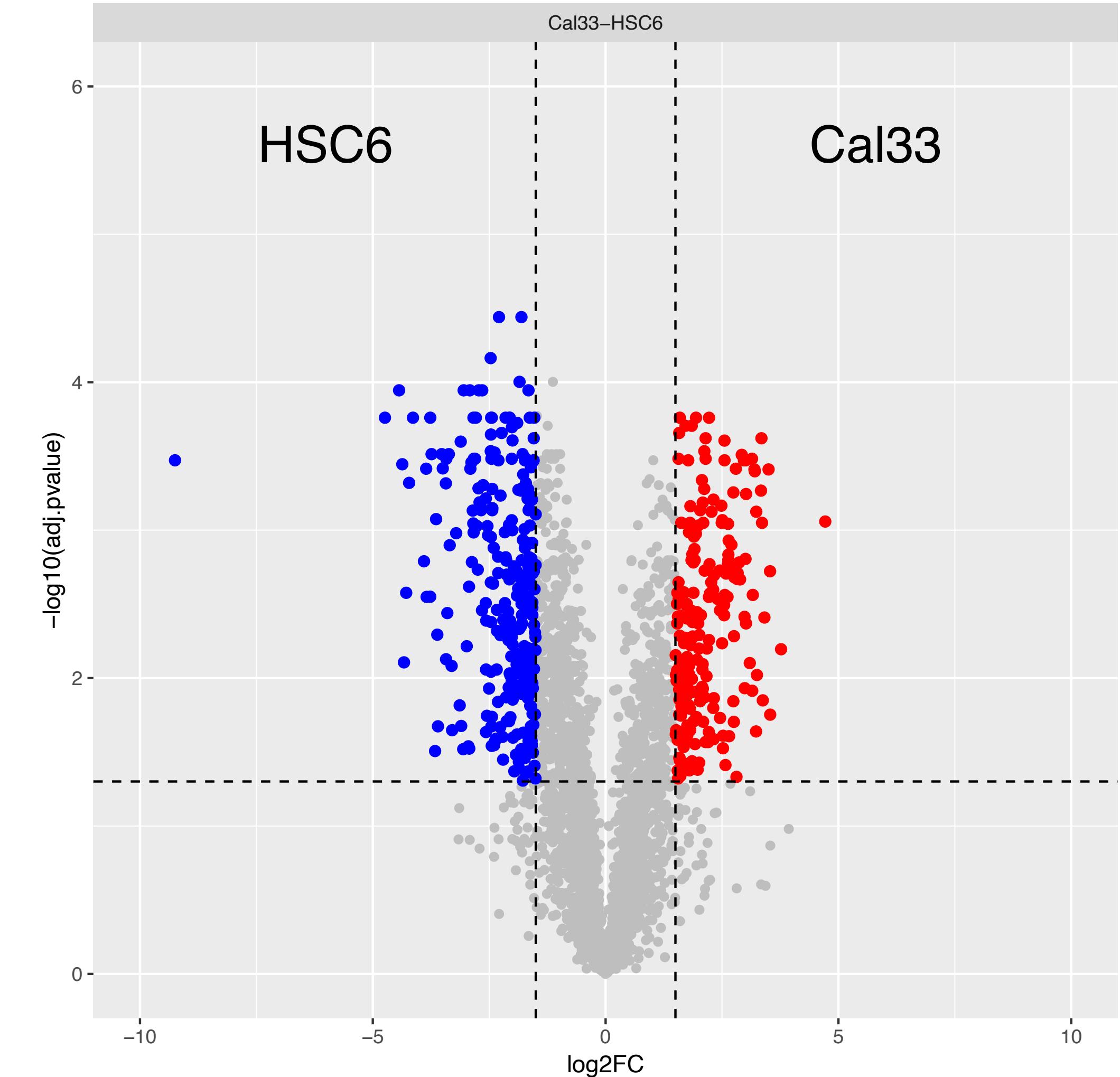
Quality control

Relative quantification

Functional analysis

Miscellaneous

artmsQuantification("config.yaml")



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Functional analysis

artmsAnalysisQuantifications()

artmsEvidenceToSAINTq()
artmsEvidenceToSaintExpress()
artmsPhosphateOutput()
artmsPhotonOutput()
etc

```
Console Terminal ~ / ~

> artmsAnalysisQuantifications(
  log2fc_file = "quant-phglobal-pre/phglobal-results.txt",
  modelqc_file = "quant-phglobal-pre/phglobal-results_ModelQC.txt",
  species = "human")

-----  
artMS: ANALYSIS OF QUANTIFICATIONS  
-----  
--- No Pathogen extra in these samples  
>> LOADING QUANTIFICATIONS (-results.txt from MSstats)  
>> LOADING modelqc FILE (ABUNDANCE)  
--- Outliers kept (user selection)  
--- Total number of genes/proteins: 3526  
--- Removing log2fc outliers (-15 < log2fc < +15)  
>> IMPUTING MISSING VALUES  
--- Number of +/- INF values: 324  
--- Plotting distributions of log2fc and pvalues  
>> PLOTS: ABUNDANCE PLOTS  
>> PLOTS: REPRODUCIBILITY PLOTS  
>> PLOT: CORRELATION BETWEEN ALL COMPARISONS  
>> PLOT: CORRELATION BETWEEN QUANTIFICATIONS (based on log2fc values)  
--- Only one Comparison is available (correlation is not possible)  
>> PRINCIPAL COMPONENT ANALYSIS BASED ON ABUNDANCE  
>> ANNOTATIONS  
--- Abundance data  
--- Relative Quantifications (Log2fc)  
>> FILTERING CHANGES BEFORE PRINTING OUT  
--- Merging Changes with bioReplica Info  
--- Removing NA  
--- Add labeling of condition more abundant in the quantification  
--- Removing proteins not found in a minimal number (2) of biological replicates  
--- Filtering is done!  
>> GENERATING QC PLOTS ABOUT CHANGES (log2fc)  
--- Distribution of log2fc and pvalues  
--- Proportion imputed values  
>> HEATMAPS OF CHANGES (log2fc)  
--- All changes  
--- Only significant changes  
>> ENRICHMENT ANALYSIS OF SELECTED CHANGES USING GPROFILER  
1) Enrichment of ALL significant Changes  
---+ Enrichment analysis using gProfiler...done!  
--- No significant results from the enrichment analysis  
---+ Corum Protein Complex Enrichment Analysis  
2) Enrichment of selected POSITIVE significant changes  
---+ Enrichment analysis using gProfiler...done!  
---+ Corum Protein Complex Enrichment Analysis  
3) Enrichment of selected NEGATIVE significant changes  
---+ Enrichment analysis using gProfiler...done!  
---+ Corum Protein Complex Enrichment Analysis  
--- Annotating species(s) in files  
>> GENERATING FINAL OUTPUT FILES  
>> PLOT OUT: TOTAL NUMBER OF PROTEINS/SITES QUANTIFIED  
>> CLUSTERING ANALYSIS OF QUANTIFICATIONS  
>> WRITING THE OUTPUT FILES  
Folder <artms_cs_ph-cancer/quant-phglobal-pre/analysis_quant_adjpvale>
- EXCEL: artms_cs_ph-cancer/quant-phglobal-pre/analysis_quant_adjpvale/phglobal-results-summary.xlsx
- Log2fc Wide: artms_cs_ph-cancer/quant-phglobal-pre/analysis_quant_adjpvale/phglobal-results-log2fc-wide.txt
- Log2fc Impute: artms_cs_ph-cancer/quant-phglobal-pre/analysis_quant_adjpvale/phglobal-results-log2fc-wide.txt
- ENRICHMENT files should also be out
>> SUPER ANALYSIS COMPLETED
```

Miscellaneous

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EXCEL

TXT FILES

PDF FILES

- Annotations
- Summary files in different format (xls, txt) and shapes
- Numerous summary plots
- Enrichment analysis using Gprofiler
- PCA of protein abundance
- PCA of quantifications
- Clustering analysis

Functional analysis

artmsAnalysisQuantifications()

Miscellaneous

artmsEvidenceToSAINTq()
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-results-summary.xlsx

-results-abundance-long.txt
-results-abundance-wide.txt
-results-enrich-MAC-allsignificants-corum.txt
-results-enrich-MAC-allsignificants.txt
-results-enrich-MAC-negatives-corum.txt
-results-enrich-MAC-negatives.txt
-results-enrich-MAC-positives-corum.txt
-results-enrich-MAC-positives.txt
-results-log2fc-long.txt
-results-log2fc-wide.txt
-results.log2fc-clusterheatmap-enriched.txt
-results.log2fc-clusterheatmap.txt

-results-enrich-MAC-allsignificants-corum.pdf
-results-enrich-MAC-negatives-corum.pdf
-results-enrich-MAC-positives-corum.pdf
-results-pca-correlations.pdf
-results-pca-pca01.pdf
-results-pca-pca02.pdf
-results-pca-pca03.pdf
-results.clustering.abundance.all-overview.pdf
-results.clustering.abundance.all-zoom.pdf
-results.clustering.log2fc.all-overview.pdf
-results.clustering.log2fc.all-zoom.pdf
-results.clustering.log2fcSign.all-overview.pdf
-results.clustering.log2fcSign.all-zoom.pdf
-results.distributions.pdf
-results.distributionsFil.pdf
-results.imputation.pdf
-results.log2fc-clusterheatmap.pdf
-results.log2fc-clusters.pdf
-results.log2fc-corr.pdf
-results.log2fc-dendro.pdf
-results.log2fc-individuals-pca.pdf
-results.TotalQuantifications.pdf
-results.correlationConditions.pdf
-results.correlationQuantifications.pdf
-results.relativeABUNDANCE.pdf
-results.reproducibilityAbundance.pdf

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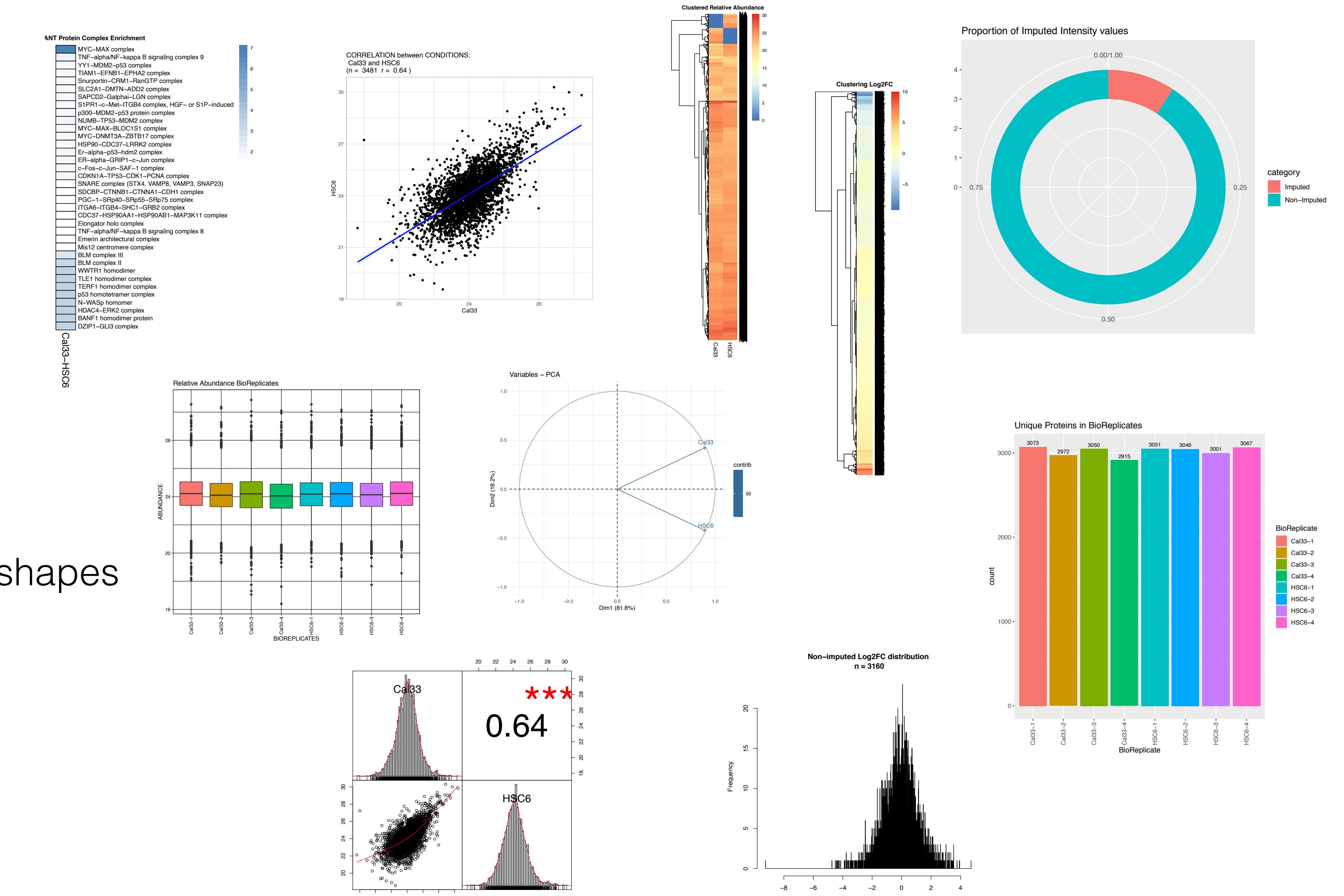
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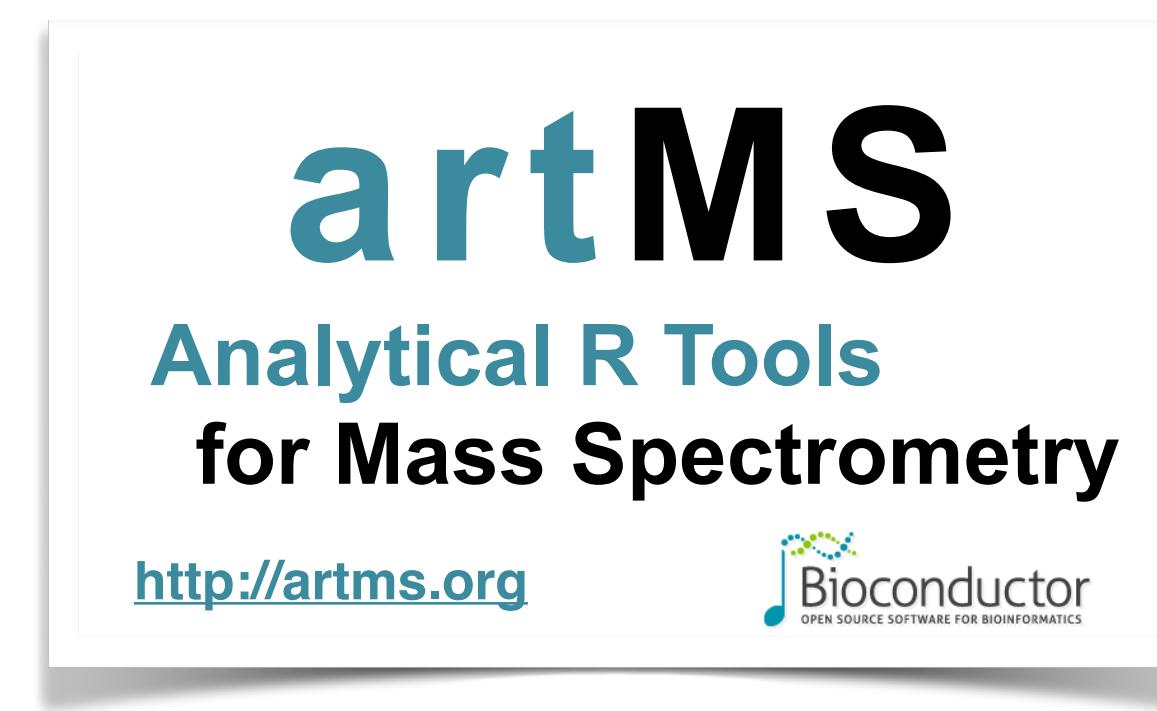
Functional analysis

artmsAnalysisQuantifications()

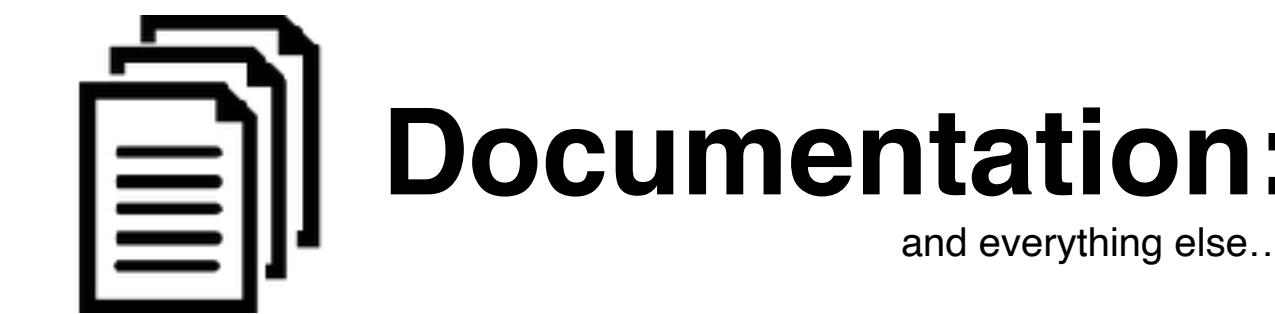
Miscellaneous

| A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q |
|---------|-------|----------------------------|----------|-------------------------|------------|--------------|-------------|-------------|---------|--------------|-------------|-------|------|-------|--------------|---------|
| Protein | Gene | ProteinName | EntrezID | Uniprot_PTM | Comparison | log2FC | pvalue | adj.pvalue | imputed | iLog2FC | iPValue | Cal33 | HSC6 | CMA | UniprotIDRef | Species |
| A0AVK6 | E2F8 | E2F transcription factor 8 | 19733 | ADAVK6_S538 | Cal33-HSC6 | 0.714864541 | 0.068971677 | 0.144027182 | no | 0.714864541 | 0.144027182 | 3 | 4 | Cal33 | A0AVK6 | human |
| A0AVK6 | F7F8 | F2F transcription factor 8 | 19733 | ANAVK6_S417 | Cal33-HSC6 | -1.643170638 | 0.020905156 | 0.063210769 | no | -1.643170638 | 0.063210769 | 3 | 4 | HSC6 | A0AVK6 | human |
| A0AVK6 | E2F8 | E2F transcription factor 8 | 19733 | ADAVK6_S71 | Cal33-HSC6 | -0.692523032 | 0.740104187 | 0.8C9434278 | no | -0.692523032 | 0.809434278 | 2 | 2 | HSC6 | A0AVK6 | human |
| A0FGRR | F5Y7 | extended synaptotagmin 7 | 57188 | ADFGR8_S676 | Cal33-HSC6 | -2.4575905 | 0.352698385 | 0.4E8321468 | no | -2.4575905 | 0.468371968 | 1 | 2 | HSC6 | A0FGRR | human |
| A0FGRR | E5Y2 | extended synaptotagmin 2 | 57488 | ADFGR8_S651 | Cal33-HSC6 | -0.198128315 | 0.405278123 | 0.518470215 | no | -0.198128315 | 0.518470215 | 3 | 3 | HSC6 | A0FGRR | human |
| A0FGRR | F5Y7 | extended synaptotagmin 7 | 57188 | ANFGR8_S641;A0FGRR_S693 | Cal33-HSC6 | #NIIIMI | | 0 | yes | 3.66610745 | 0.0198345 | 2 | 0 | Cal33 | A0FGRR | human |
| A0FGRR | E5Y2 | extended synaptotagmin 2 | 57488 | ADFGR8_S653 | Cal33-HSC6 | 0.950304175 | 0.15494643 | 0.254530287 | no | 0.950304175 | 0.254530287 | 4 | 4 | Cal33 | A0FGRR | human |
| A0FGRR | F5Y7 | extended synaptotagmin 7 | 57188 | ANFGR8_S716 | Cal33-HSC6 | -0.019383937 | 0.937856734 | 0.952376477 | no | -0.019383937 | 0.952376477 | 4 | 3 | HSC6 | A0FGRR | human |
| A0FGRR | E5Y2 | extended synaptotagmin 2 | 57488 | ADFGR8_S743 | Cal33-HSC6 | #NUM! | | 0 | yes | -7.793852072 | 0.0244517 | 0 | 4 | HSC6 | A0FGRR | human |
| A0FGRR | F5Y7 | extended synaptotagmin 7 | 57188 | ANFGR8_S758;ANFGR8_S761 | Cal33-HSC6 | -0.388729605 | 0.90F40R4R6 | 0.934755075 | no | -0.388729605 | 0.934755075 | 1 | 3 | HSC6 | A0FGRR | human |
| A0FGRR | E5Y2 | extended synaptotagmin 2 | 57488 | ADFGR8_S761 | Cal33-HSC6 | -0.710786851 | 0.02631059 | 0.016113125 | no | -0.710786851 | 0.016113125 | 2 | 4 | HSC6 | A0FGRR | human |
| A0FGRR | F5Y7 | extended synaptotagmin 7 | 57188 | ANFGR8_T701;ANFGR8_T705 | Cal33-HSC6 | -1.205399144 | 0.017277448 | 0.055442631 | no | -1.205399144 | 0.055442631 | 4 | 4 | HSC6 | A0FGRR | human |
| A0JLT2 | MEC19 | mediator complex subunit 1 | 219541 | ADJLT2_S5226 | Cal33-HSC6 | -0.628516166 | 0.213593755 | 0.32335184 | no | -0.628516166 | 0.32335184 | 4 | 4 | HSC6 | A0JLT2 | human |





<https://bioconductor.org/packages/release/bioc/html/artMS.html>



Documentation: <http://artms.org>
and everything else...



artMS: Analytical R Tools for Mass Spectrometry-based Proteomics

David Jimenez-Morales^{1*}, Alexandre Rosa Campos², Jeff Johnson, John Von Dollen³,

Matthew T Wheeler¹, Euan A Ashley¹, Nevan J. Krogan³, Danielle L. Swaney^{3*}

In preparation

¹. Stanford

². SBP

³. UCSF

Conditions: A and B

“protein-level”relative quantification

| protein_id | log2fc(A/B) | adj-value |
|------------|-------------|-----------|
| UGH2020 | 1.2 | 0.001 |

Case Studies

PH

Protein Phosphorylation

Example Protein: UGH2020

UGH2020 S45: _AAAAAAATAPP**S(ph)**PGPAQPGPR_

UGH2020 S134: _AAAPPQP**S(ph)**PPPTK_

UGH2020 S272: _AAATGNA**S(ph)**PGKLEHSK_

“site-specific” relative quantification

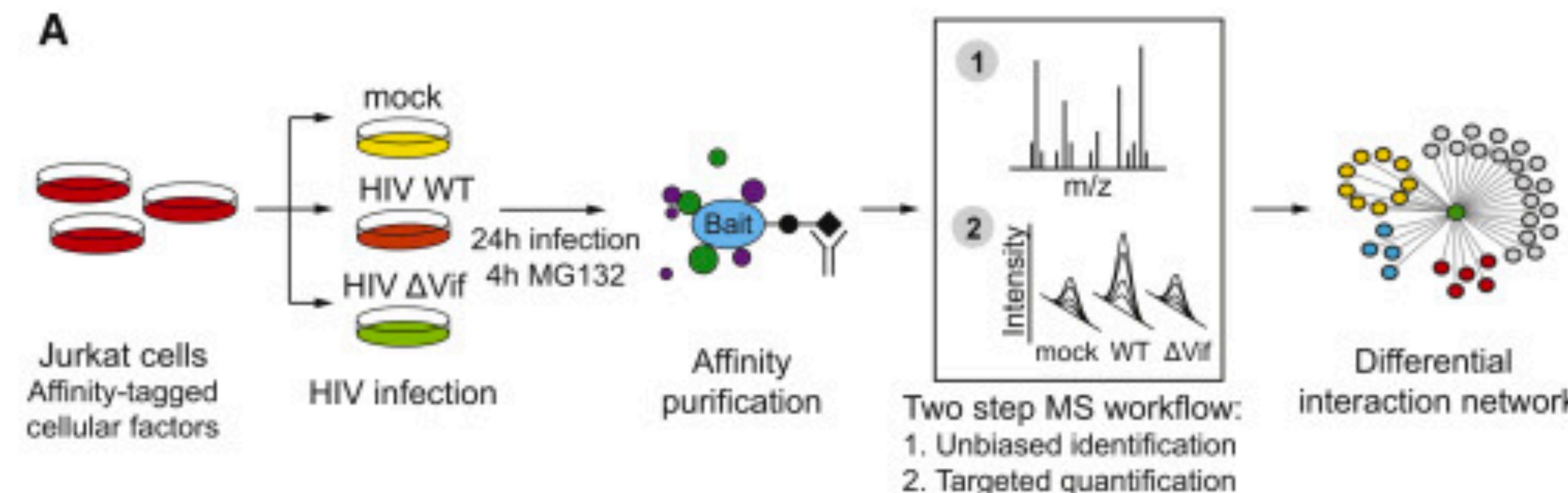
| protein_id | log2fc(A/B) | adj-value |
|--------------|-------------|-----------|
| UGH2020_S45 | 1.63 | 0.0001 |
| UGH2020_S134 | 0.15 | 0.23 |
| UGH2020_S272 | 0.72 | 0.04 |

Case Studies

APMS

Affinity Purification Mass Spectrometry

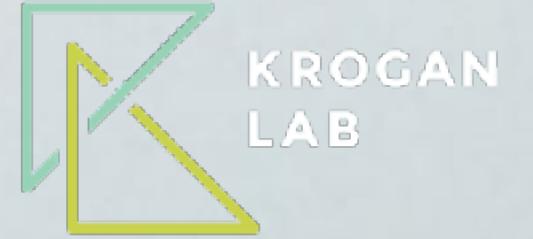
Bait protein: CUL5



acknowledgements



University California San Francisco



Nevan Krogan
Danielle Swaney
Ben Polacco
Ruth Huttenthal
John Von Dollen



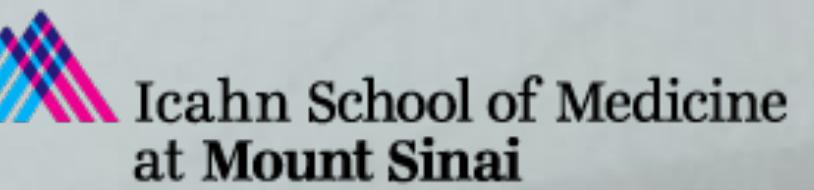
Euan Ashley
Matthew Wheeler



Alex Campos



Alex Pico



Jeff Johnson



Sara Jimenez-Lopez