ASMS 2022 Minneapolis

Visualization of Mass Spectrometry Related Data

ASMS Bioinformatics Interest Group

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Agenda

- Overview
- Visualization tools
- Metabolomics study examples
- Interactive discussion

Two different worlds?

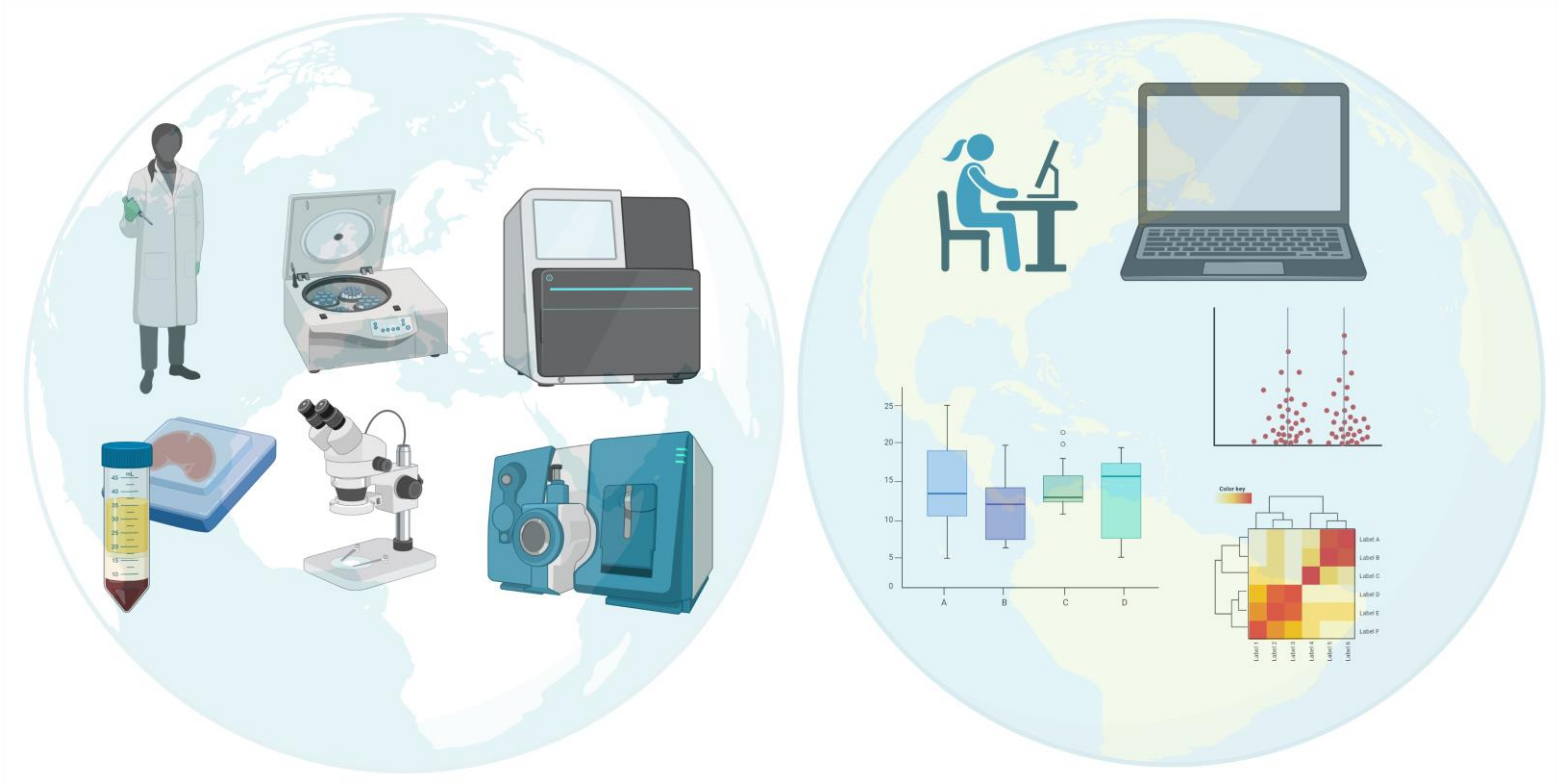
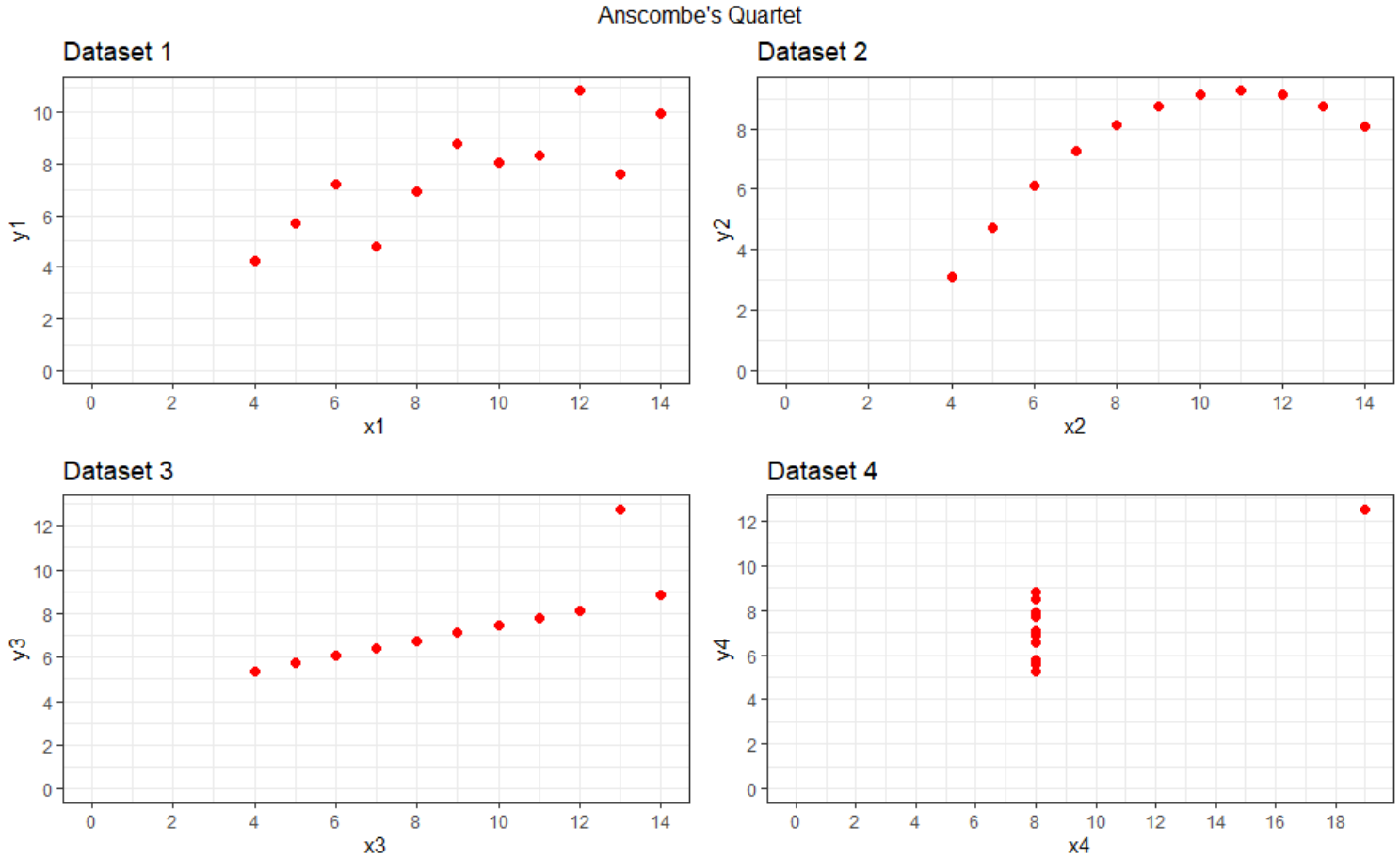


Figure made by Arzu Tugce Guler
created with Biorender.com

A picture is worth a thousand words

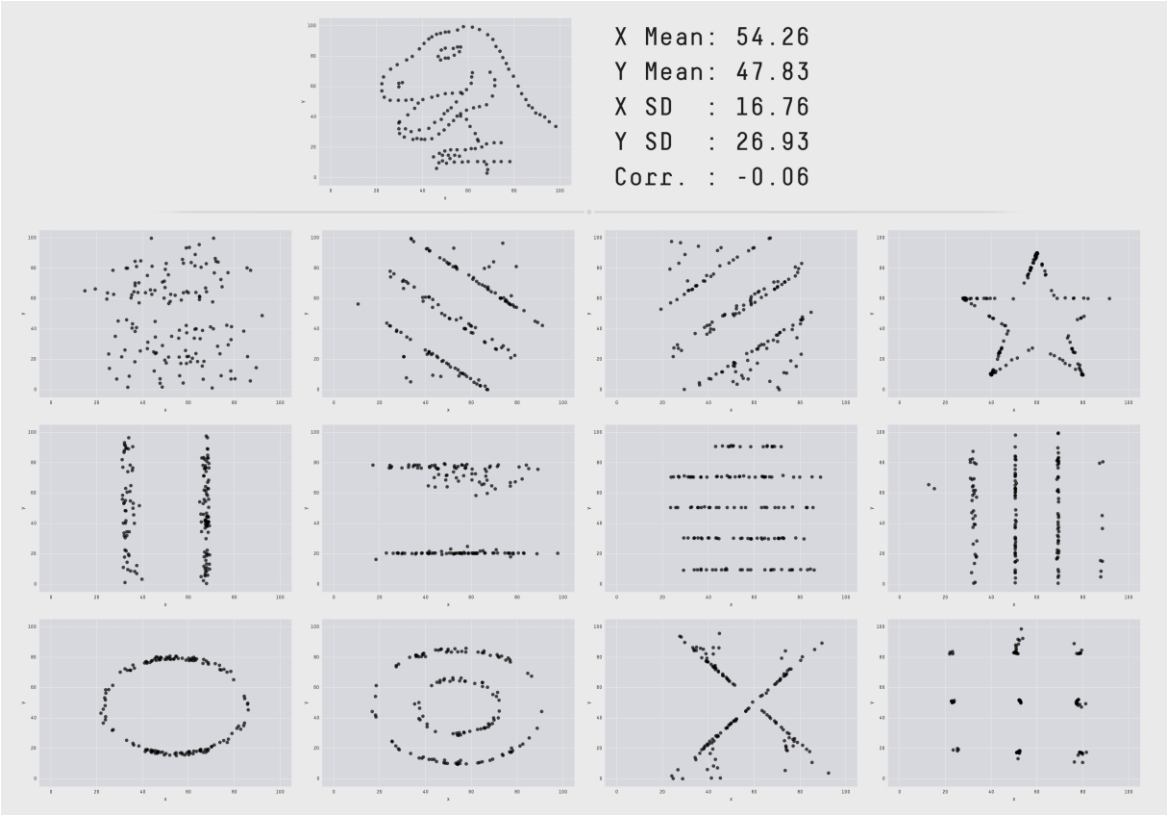
Anscombe's Quartet

```
> datasets::anscombe
   x1 x2 x3 x4    y1   y2    y3    y4
1  10 10 10  8  8.04 9.14  7.46  6.58
2   8  8  8  8  6.95 8.14  6.77  5.76
3  13 13 13  8  7.58 8.74 12.74  7.71
4   9  9  9  8  8.81 8.77  7.11  8.84
5  11 11 11  8  8.33 9.26  7.81  8.47
6  14 14 14  8  9.96 8.10  8.84  7.04
7   6  6  6  8  7.24 6.13  6.08  5.25
8   4  4  4 19  4.26 3.10  5.39 12.50
9  12 12 12  8 10.84 9.13  8.15  5.56
10  7  7  7  8  4.82 7.26  6.42  7.91
11  5  5  5  8  5.68 4.74  5.73  6.89
> fBasics::basicStats(anscombe)
                   x1        x2        x3        x4        y1        y2        y3        y4
nobs       11.000000 11.000000 11.000000 11.000000 11.000000 11.000000 11.000000 11.000000
NAs         0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
Minimum     4.000000  4.000000  4.000000  8.000000  4.260000  3.100000  5.390000  5.250000
Maximum    14.000000 14.000000 14.000000 19.000000 10.840000  9.260000 12.740000 12.500000
1. Quartile 6.500000  6.500000  6.500000  8.000000  6.315000  6.695000  6.250000  6.170000
3. Quartile 11.500000 11.500000 11.500000 8.000000  8.570000  8.950000  7.980000  8.190000
Mean        9.000000  9.000000  9.000000  9.000000  7.500909  7.500909  7.500000  7.500909
Median      9.000000  9.000000  9.000000  8.000000  7.580000  8.140000  7.110000  7.040000
Sum        99.000000 99.000000 99.000000 99.000000 82.510000 82.510000 82.500000 82.510000
SE Mean     1.000000  1.000000  1.000000  1.000000  0.612541  0.612568  0.612196  0.612242
LCL Mean    6.771861  6.771861  6.771861  6.771861  6.136083  6.136024  6.135943  6.136748
UCL Mean   11.228139 11.228139 11.228139 11.228139  8.865735  8.865795  8.864057  8.865070
Variance   11.000000 11.000000 11.000000 11.000000  4.127269  4.127629  4.122620  4.123249
Stdev       3.316625  3.316625  3.316625  3.316625  2.031568  2.031657  2.030424  2.030579
Skewness    0.000000  0.000000  0.000000  2.466911 -0.048374 -0.978693  1.380120  1.120774
Kurtosis   -1.528926 -1.528926 -1.528926  4.520661 -1.199123 -0.514319  1.240044  0.628751
```



Take home lesson: never trust summary statistics alone; always visualize your data!

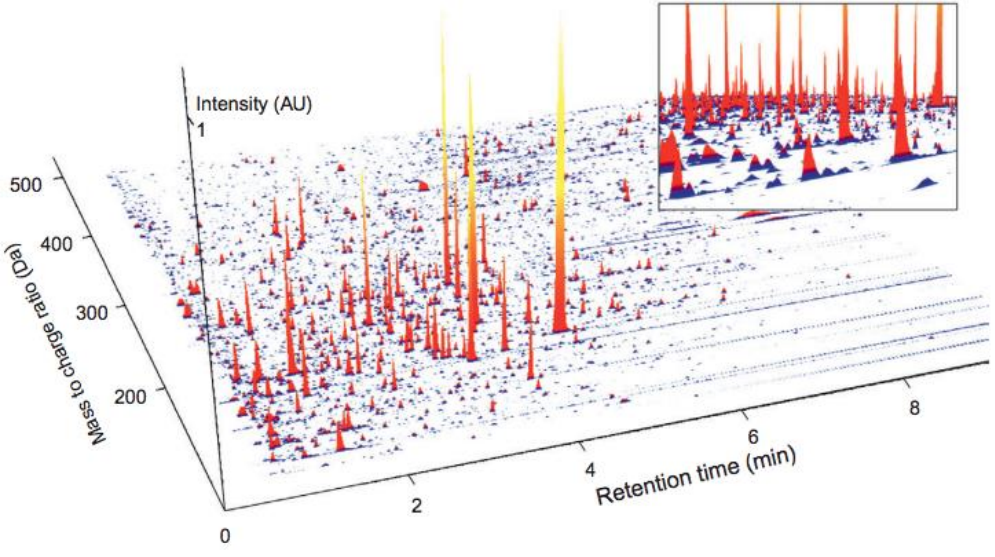
Datasaurus (aka Anscombosaurus)

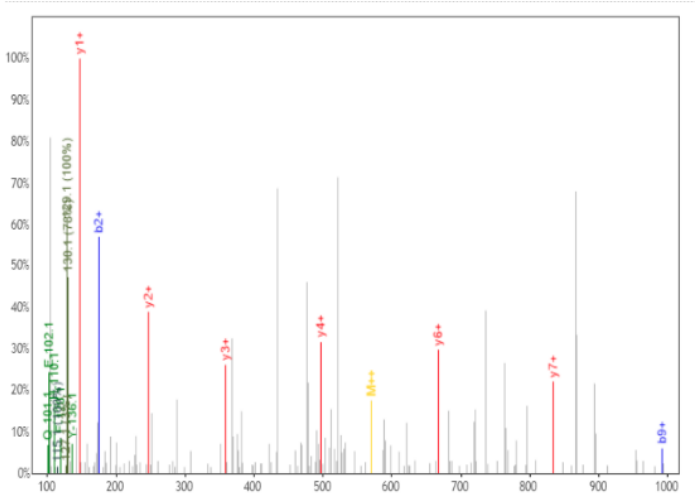


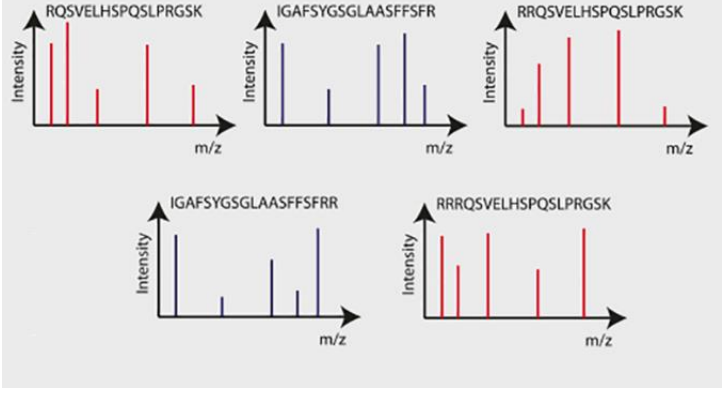
Take home lesson: *“never trust summary statistics alone; always visualize your data!”*

Albert Cairo: http://www.thefunctionalart.com/2016/08/download-datasaurus-never-trust-summary.html

Visualization of mass spectrometry data

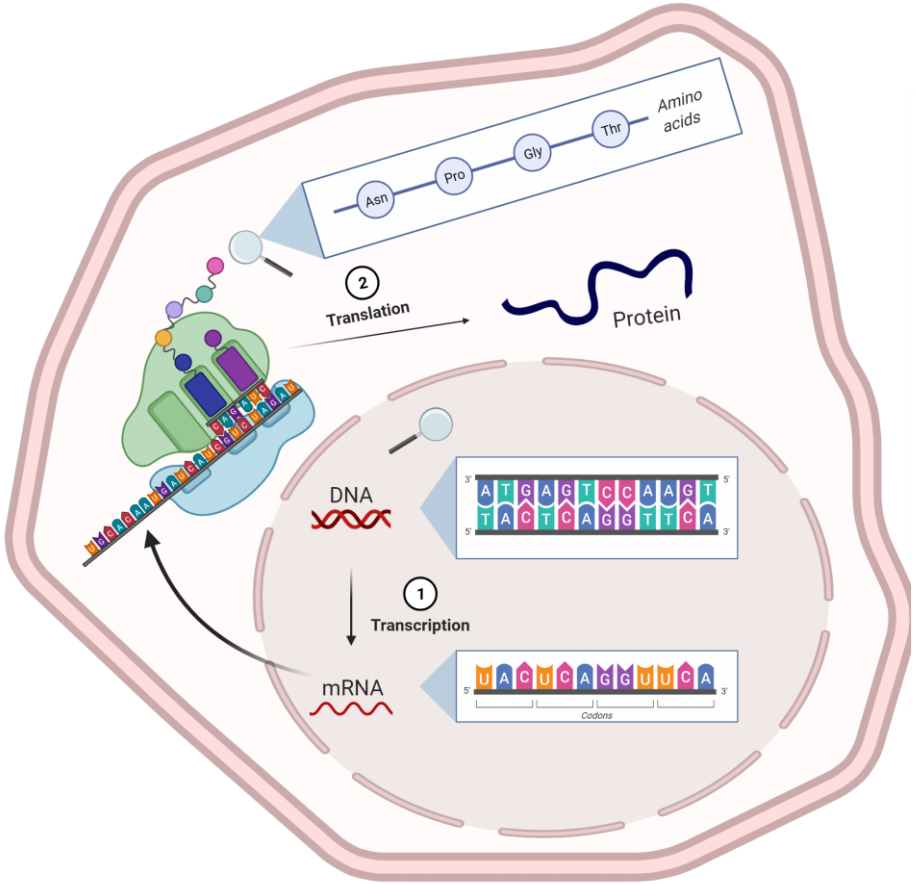






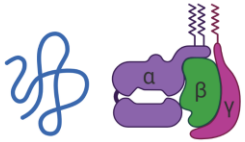
1.Doana. *Metabolic Phenotyping in Personalized and Public Healthcare* 2016
2.https://phosphopedia.gs.washington.edu/PhosphoproteomicsAssay/index.xhtml
3.Saeed et. al IE*EE/ACM Trans Comput Biol Bionform* 2018

The -omics

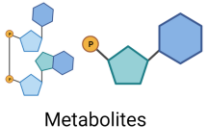


GENOMICS

TRANSCRIPTOMICS



PROTEOMICS



METABOLOMICS

Figure made by Arzu Tugce Guler
created with Biorender.com

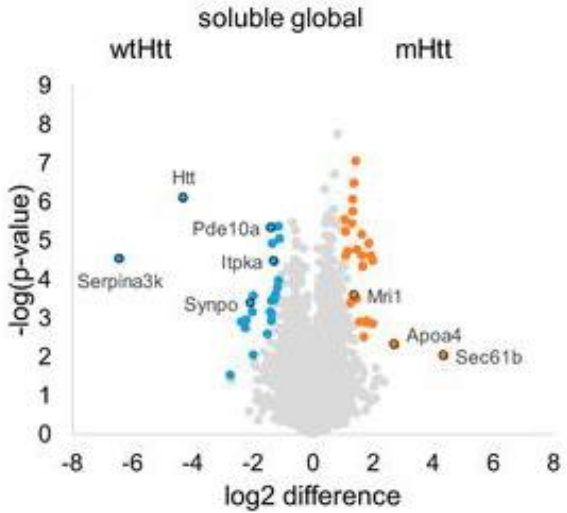
Visualizations for mass spectrometry-based proteomics data

- Numeric data (with or without labels)
  e.g. volcano plots, heatmaps, boxplots, PCAs etc.

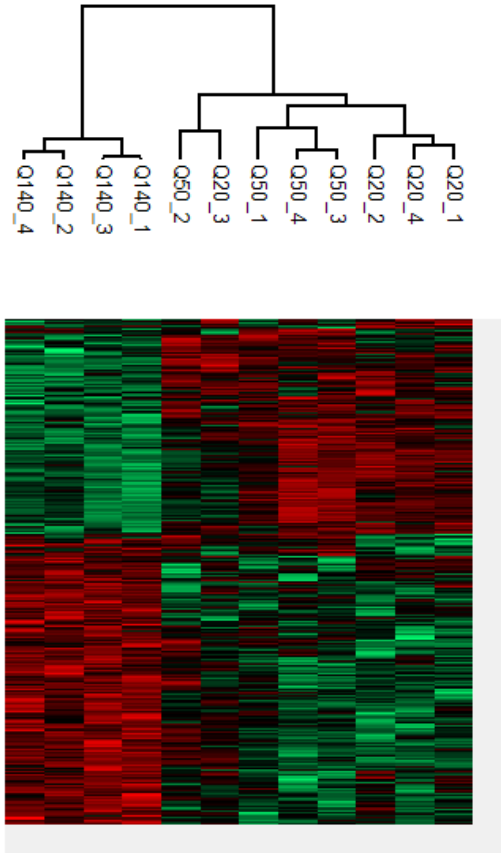
- Trees / networks
  e.g. ontologies, gene ontology enrichments, protein interaction networks etc.

- Images
  e.g. experiment workflows, anatomical visualizations, western blots etc.

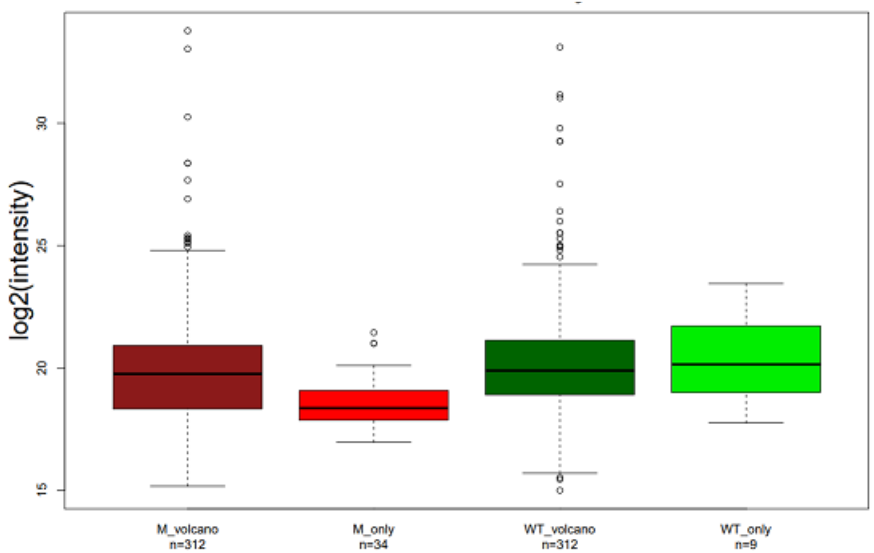
Volcano plots



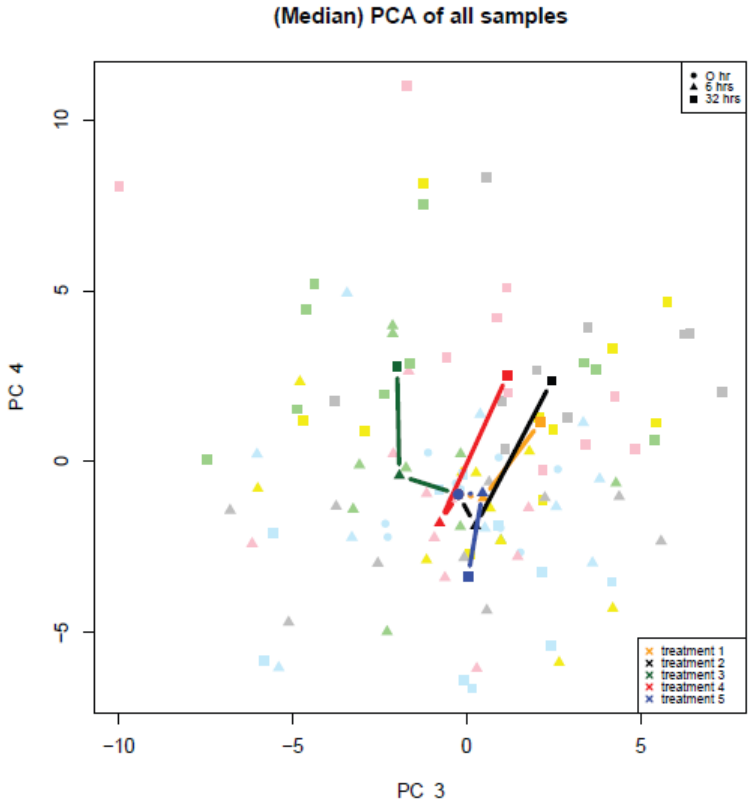
Heatmap


Q20_1
Q20_4
Q20_2
Q50_3
Q50_4
Q50_1
Q20_3
Q50_2
Q140_1
Q140_3
Q140_2
Q140_4

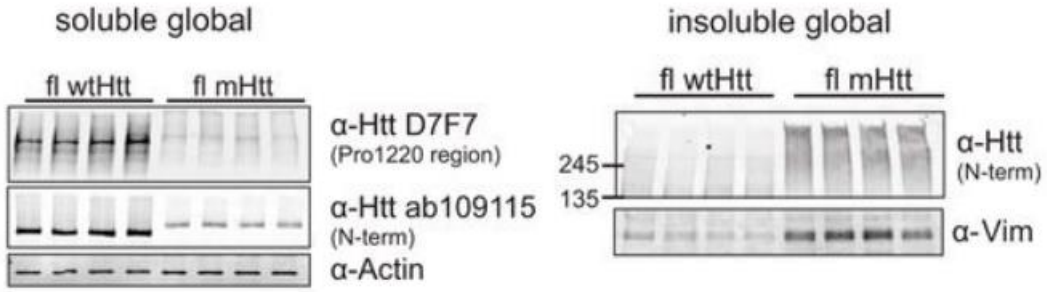
Boxplot


log2(intensity)
15
20
25
30
M_volcano
n=312
M_only
n=34
WT_volcano
n=312
WT_only
n=9

PCA

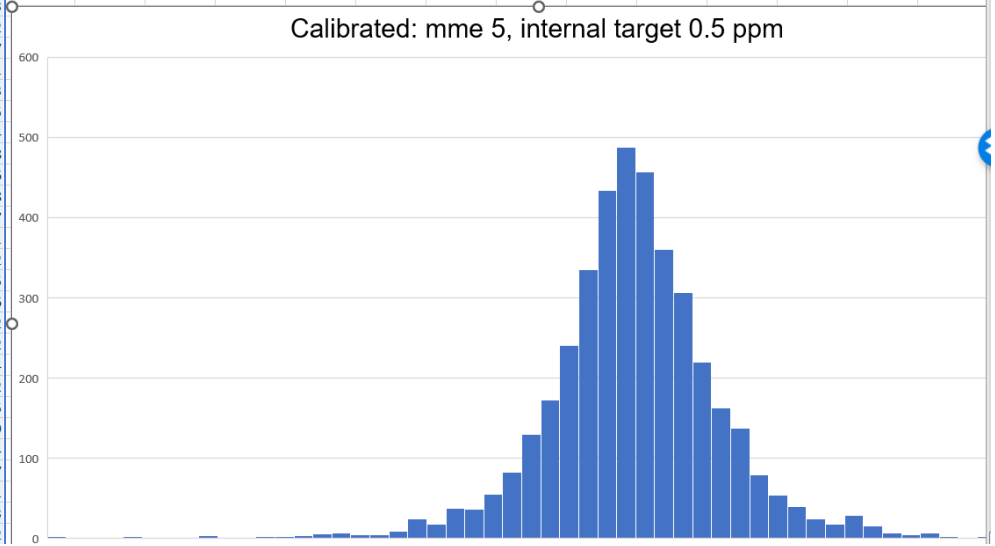

(Median) PCA of all samples
0 hr
6 hrs
32 hrs
treatment 1
treatment 2
treatment 3
treatment 4
treatment 5
PC 4
PC 3
10
5
0
−5
−10
−5
0
5

Western blots / gels, microscope images



Tools for visualizing numeric data

	A	B	C	D	E	F	G	H
1	probability	spectrum	expect	ions	peptide	protein	calc_neutral_pep_mass	ppm
2	0,9996	calibrated	0,00013	okt-22	K.EALGIPA	sp|P31939	1173,6394	7,9633
3	0,9957	calibrated	0,0181	sep-22	K.QITQSAL	sp|P78527	1299,7147	7,3962
4	1	calibrated	0,000161	sep-68	K.EKAPSIIF	sp|P1798(	1959,0565	6,9717
5	0,9985	calibrated	0,000429	sep-20	K.DAYQVIL	sp|Q9BZZ5	1219,6449	6,9061
6	1	calibrated	9,29E-05	nov-20	K.HLSVND	sp|P30048	1205,6517	6,5533
7	0,9996	calibrated	1,23E-06	aug-18	K.LASDLLE	sp|P12814	1214,6659	6,5425
8	1	calibrated	0,000526	aug-30	R.IGNVEIS	sp|P15927	1710,004	6,224
9	0,9977	calibrated	0,00076	okt-18	R.DLIVATI	sp|P31939	1041,6434	6,1518
10	1	calibrated	3,50E-06	dec-84	K.SGYHQS	sp|P10768	2307,1244	6,1046
11	0,9917	calibrated	0,0084	jul-28	R.TINLYPL	sp|O43809	1744,9036	6,1018
12	1	calibrated	8,88E-05	15/34	K.VSHVST(	sp|P00558	1739,9054	6,0417
13	0,996	calibrated	0,000578	nov-24	K.ASSAAGL	sp|Q1456(	1172,6513	5,9881
14	0,9988	calibrated	0,00306	okt-20	K.VDATAE	sp|P13667	1132,5612	5,952
15	0,997	calibrated	5,15	2/240	K.GPRGSQ	sp|Q6ZN1	3417,465	5,7625
16	1	calibrated	0,000106	okt-24	R.VTWDSS	sp|Q9ULV	1537,6984	5,6546
17	0,9981	calibrated	0,364	okt-60	K.EGKPTIV	sp|O7593	1844,9044	5,6252
18	1	calibrated	0,00664	nov-72	R.KPLVLC[	sp|P27695	2190,1467	5,5782
19	0,9942	calibrated	0,00695	jun-26	K.VWQLQI	sp|Q9NYU	1661,8526	5,3964
20	1	calibrated	2,21E-05	dec-22	K.TGQAAE	sp|O0023	1156,6452	5,3292
21	1	calibrated	0,00201	15/52	K.AHGGYS	sp|P06576	1405,6739	5,3035
22	0,9976	calibrated	0,0109	nov-18	K.ALGDLIS	sp|Q9Y49(	987,5601	5,2979
23	1	calibrated	5,52E-06	13/56	K.TVAGQD	sp|P30043	1511,8671	5,2174
24	0,9966	calibrated	0,000705	sep-18	K.VLDIIATI	sp|P07686	1098,6649	5,2127
25	1	calibrated	6,88E-05	sep-80	K.VIAVYDL	sp|P38646	2250,2148	5,2031
26	0,9991	calibrated	0,265	sep-44	R.FIFEDQII	sp|P02730	1562,7841	5,1363
27	0,9971	calibrated	0,000224	sep-18	K.VNTPTT	sp|P26639	1150,5982	5,1182



Excel*

- Quick and adaptable
- Especially good for internal sanity checks

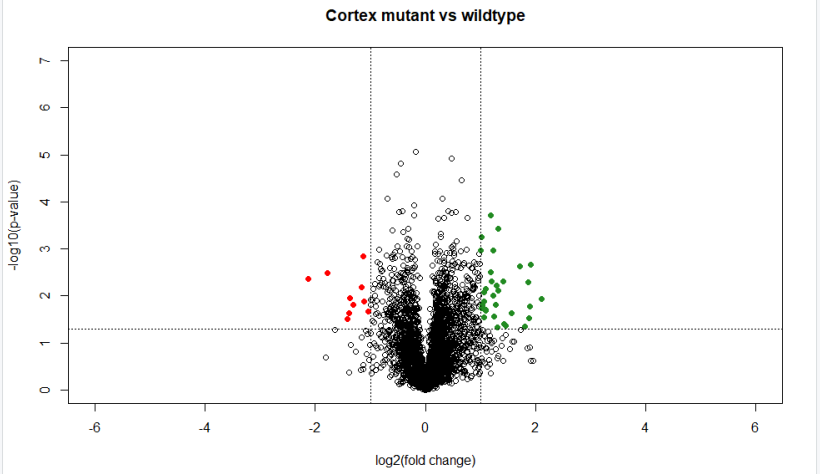
** commercial*

RStudio

File Edit Code View Plots Session Build Debug Profile Tools Help

```
+     }
+     else if( (fold_change[i]>min_log2_fold_change) && (pval[i,1]<max_pval) )
+     {
+         points(fold_change[i],-log10(pval[i,1]), pch=19, col="forestgreen");
+         #text(fold_change[i]+0.20,-log10(pval[i])+0.20, labels[i,1], col="forestgreen");
+         changes[i] <- "+"
+         print(c("up",labels[i,1]))
+         no_up <- no_up + 1
+     }
+ }
[1] "up"   "Agrn"
[1] "up"   "Kalrn"
[1] "down" "Tomm5"
[1] "up"   "Kpna4"
[1] "up"   "Lgmn"
[1] "up"   "Pde4a"
[1] "up"   "Srp54"
[1] "down" "Cox7c"
[1] "down" "Ptma"
[1] "up"   "Crat"
[1] "up"   "Pcbp3"
[1] "up"   "Abce1"
[1] "down" "Rpl37a"
[1] "up"   "Kifap3"
[1] "up"   "Hsd12"
[1] "up"   "Cul4a"
[1] "up"   "Hp1bp3"
[1] "up"   "Ttll12"
[1] "down" "Cdkl5"
[1] "up"   "Unc13a"
[1] "up"   "Raly"
[1] "down" "Cox8a"
[1] "up"   "Srm"
[1] "down" "Cbarp"
[1] "up"   "Plcxd3"
[1] "down" "Gprin3"
[1] "up"   "Uba6"
[1] "up"   "Ttc19"
[1] "up"   "Pitrm1"
[1] "down" "Ccdc9"
[1] "up"   "Dcaf11"
[1] "up"   "Fbxl15"
[1] "up"   "Wan2c1"
[1] "up"   "Scgn"
[1] "up"   "Xpo5"
[1] "up"   "Pacsin3"
[1] "up"   "Prpf8"
[1] "up"   "Acsl3"
[1] "up"   "Ttpal"
[1] "up"   "Lamtor2"
[1] "up"   "Cyth1"
[1] "down" "Golga5"
[1] "up"   "Mtmr1"
>
> abline(v=min_log2_fold_change, lty=3);
> abline(v=-min_log2_fold_change, lty=3);
> abline(h=-log10(max_fdr), lty=3);
>
```

no_up	33
non_na_intensities	Large numeric (42030 elements, 4.7 MB)
protein	chr [1:4011] "Cullin-4B" "Brefeldin A-inhibited guanine nucleotide-exchange protein …
Q140_1	3687L
Q140_2	3495L
Q140_3	3608L
Q140_4	3642L
Q20_1	3491L
Q20_2	3416L
Q20_3	3518L
Q20_4	3374L



R

Useful R libraries for more advanced, publication quality visualizations

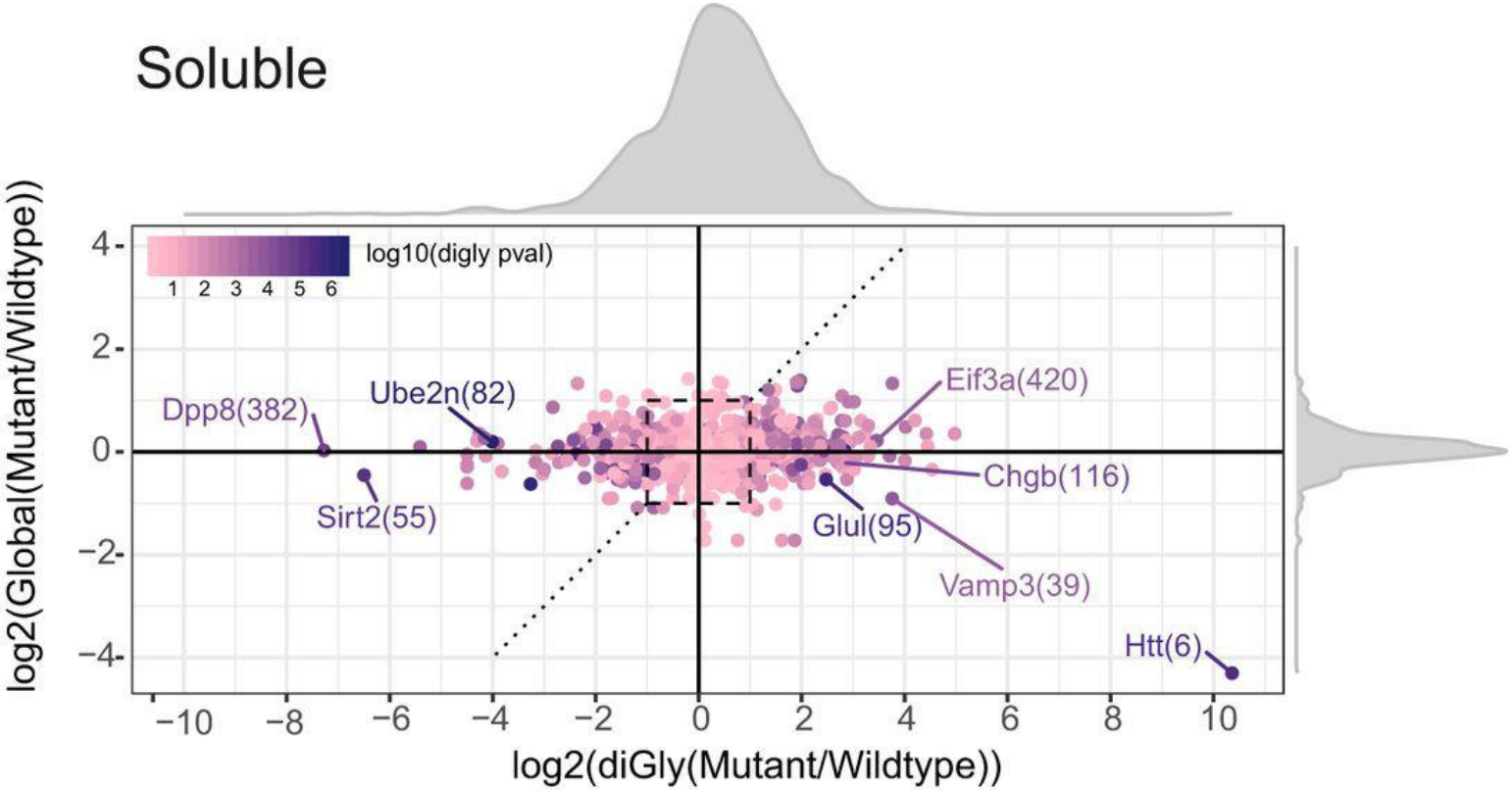
There are currently 161 Proteomics and 118 Mass Spectrometry packages in Bioconductor version 3.15.

- ggplot2
- lattice
- shiny*
- plotly*

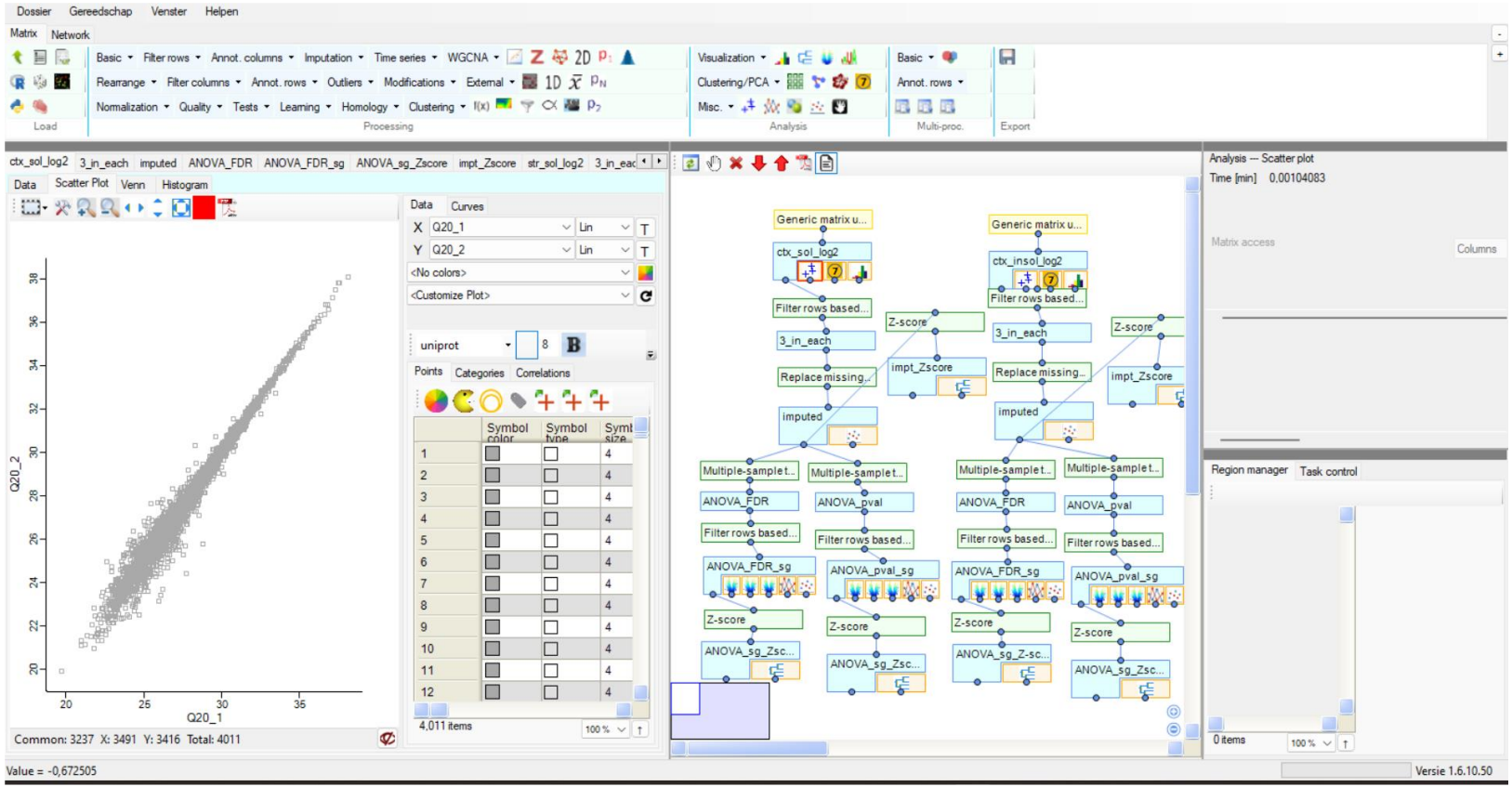
- MSstats
- protViz

** commercial*

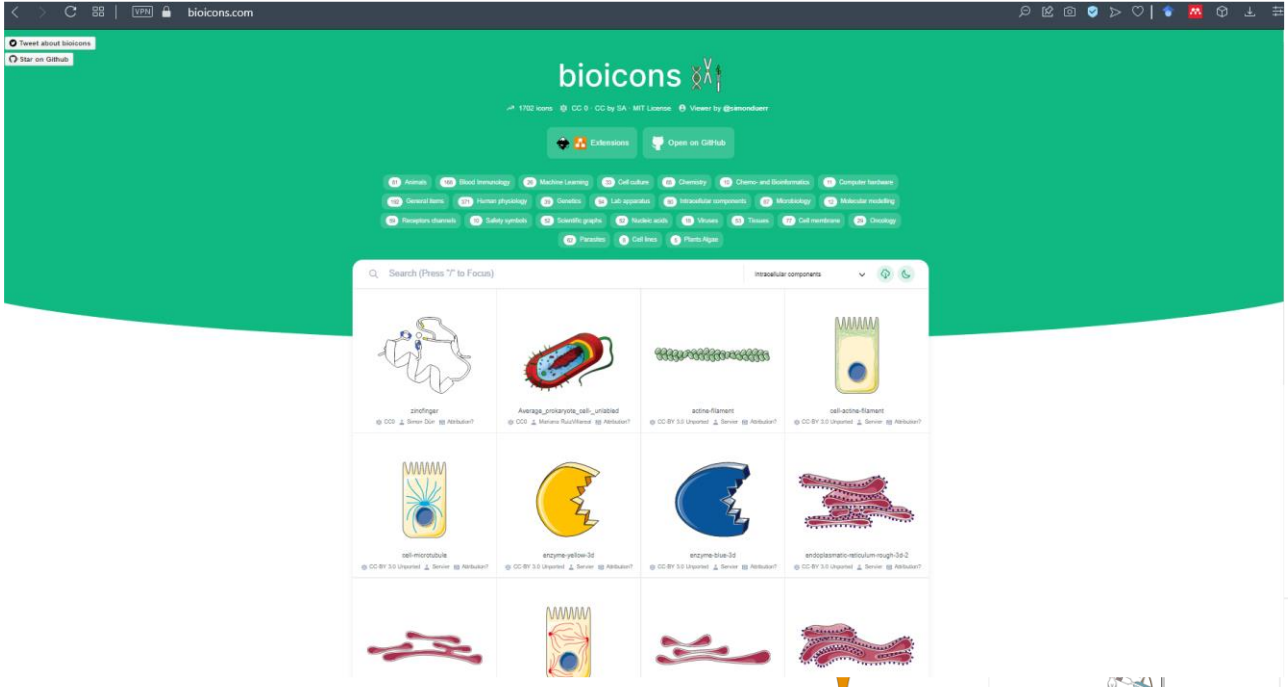
ggplot2


Soluble
log10(digly pval)
1 2 3 4 5 6
Dpp8(382)
Ube2n(82)
Sirt2(55)
Eif3a(420)
Chgb(116)
Glul(95)
Vamp3(39)
Htt(6)
log2(Global(Mutant/Wildtype))
log2(diGly(Mutant/Wildtype))
4
2
0
−2
−4
−10
−8
−6
−4
−2
0
2
4
6
8
10

Perseus


Dossier
Gereedschap
Venster
Helpen
Matrix
Network
Load
Processing
Analysis
Multi-proc.
Export
Data
Scatter Plot
Venn
Histogram
Curves
Points
Categories
Correlations
Common: 3237 X: 3491 Y: 3416 Total: 4011
4,011 items
Generic matrix u...
ctx_sol_log2
ctx_insol_log2
Filter rows based...
3_in_each
Z-score
impt_Zscore
Replace missing...
imputed
Multiple-samplet...
ANOVA_FDR
ANOVA_pval
ANOVA_FDR_sg
ANOVA_pval_sg
ANOVA_sg_Zsc...
Analysis -- Scatter plot
Time [min] 0,00104083
Matrix access
Columns
Region manager
Task control
0 items
Value = -0,672505
Versie 1.6.10.50

Tools for icons / anatomical visualizations



- bioicons

dropper

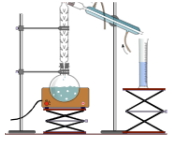
CC0 OpenClipart Attribution?

glass-rod

CC0 OpenClipart Attribution?

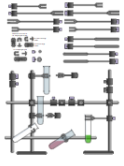
dropper-glas

CC0 OpenClipart Attribution?



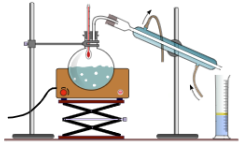
fractional-distillation

CC0 OpenClipart Attribution?



laboratory-stands

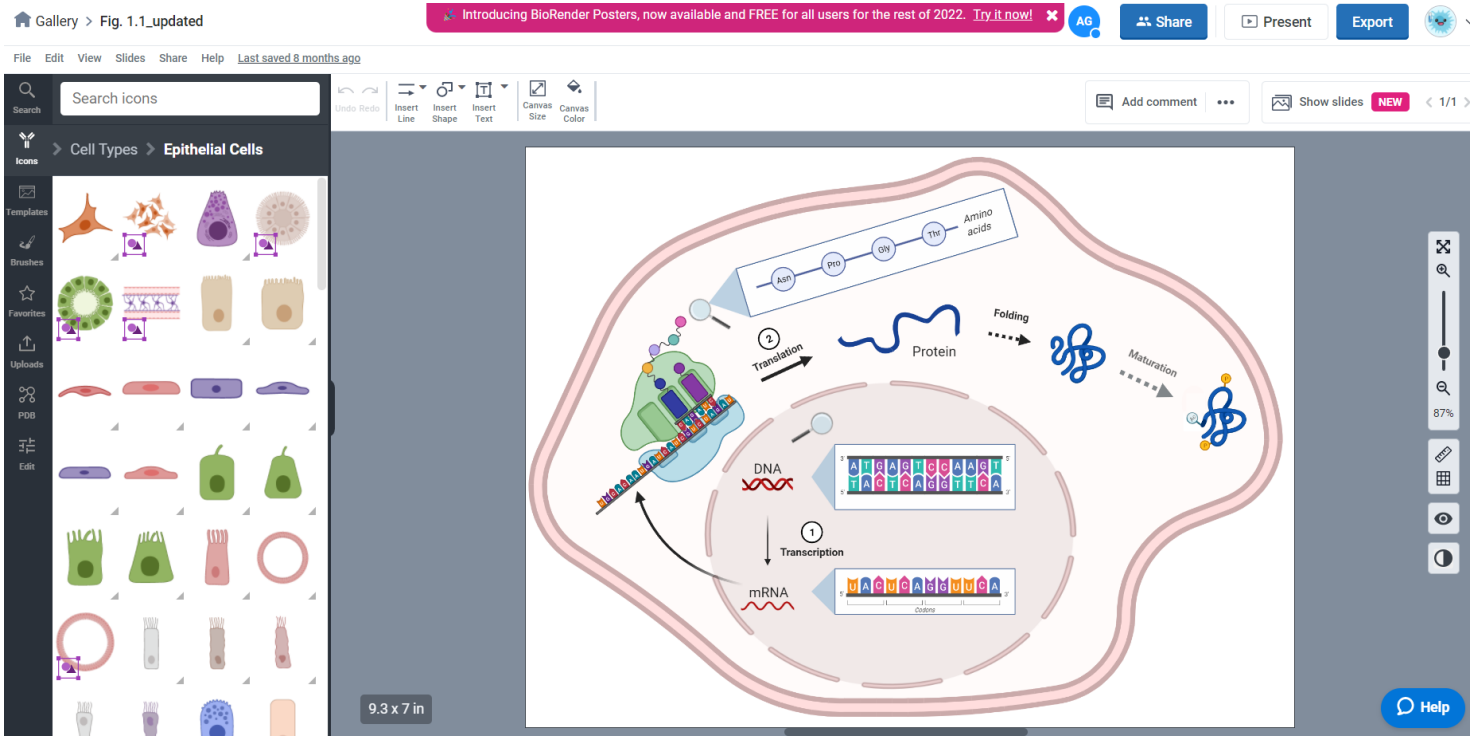
CC0 OpenClipart Attribution?



distillation

CC0 OpenClipart Attribution?

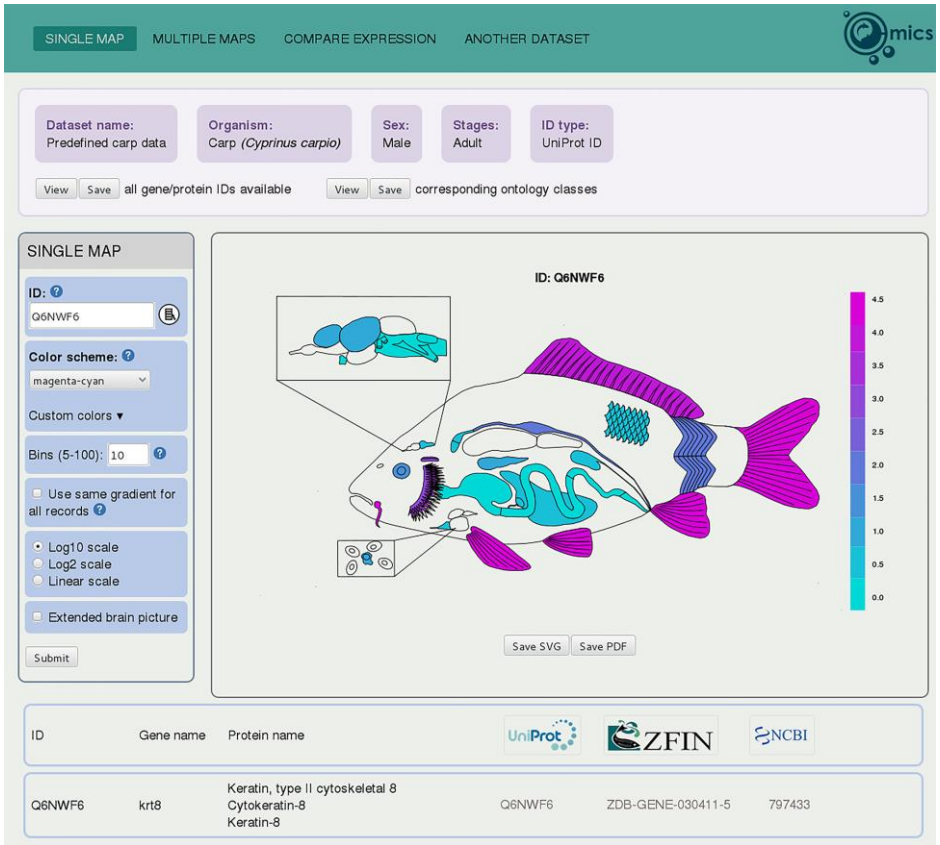
Tools for icons / anatomical visualizations



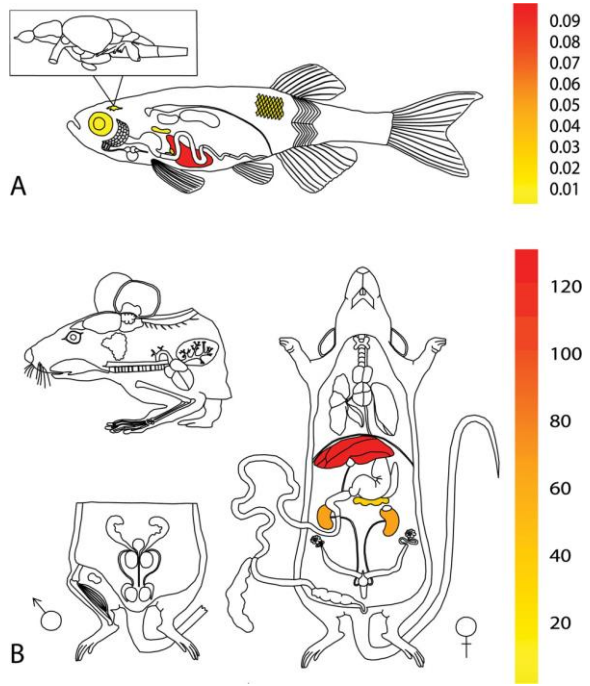
- BioRender*

* *commercial*

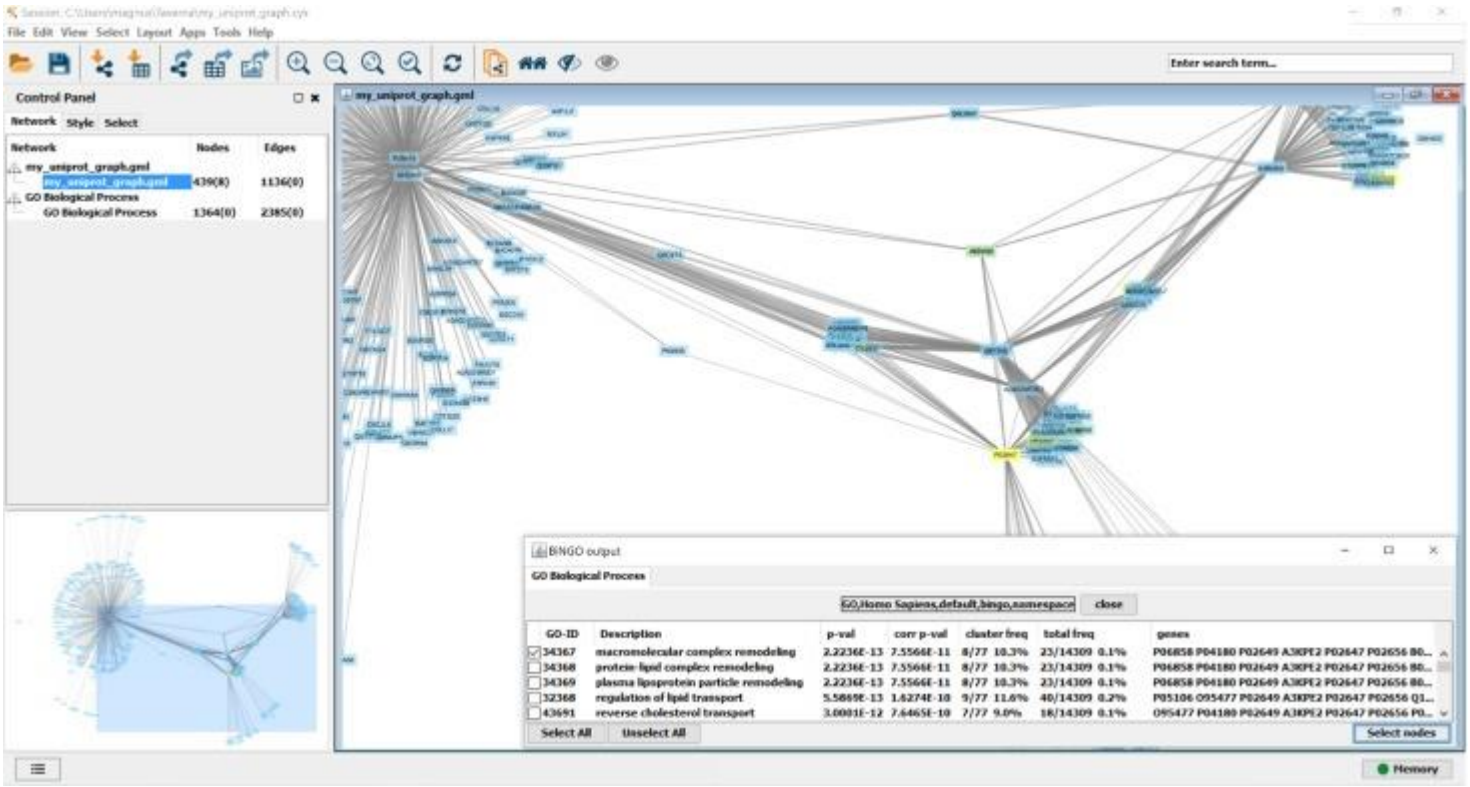
Tools for icons / anatomical visualizations



- COMICS

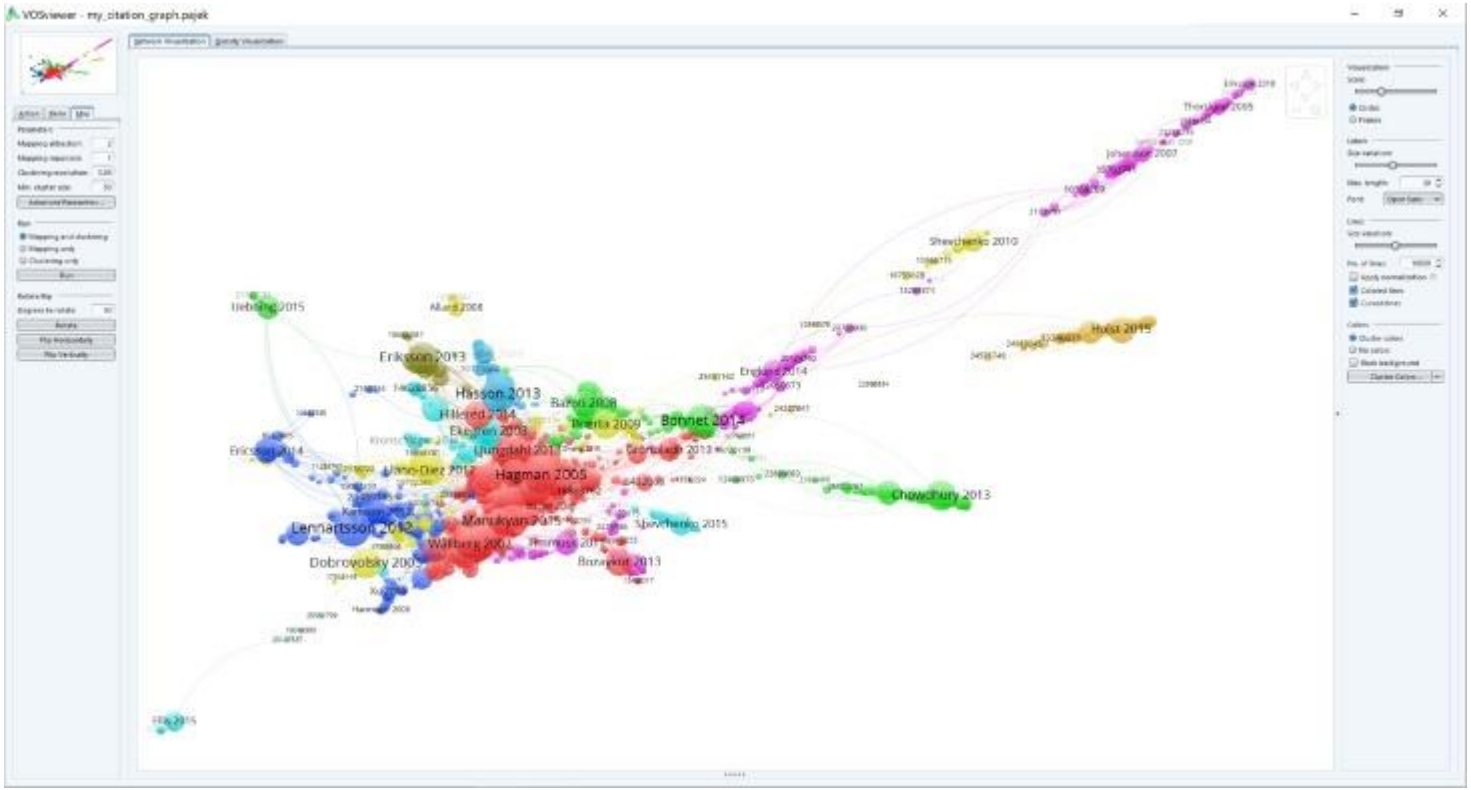


Tools for network visualizations



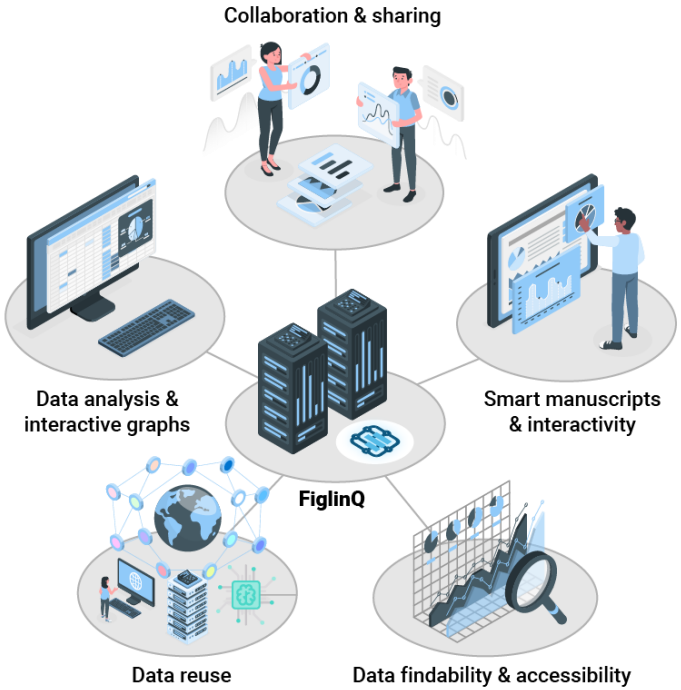
- Cytoscape

Tools for network visualizations

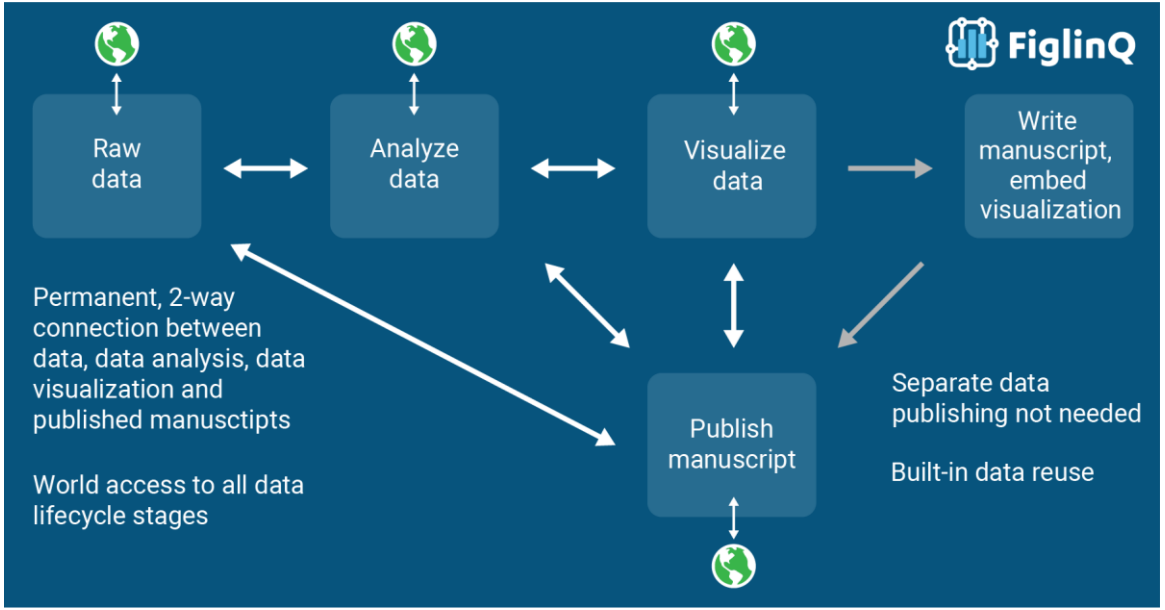


- VOSviewer

Interactive plots



- FiglinQ*



** commercial / paid subscription*

FiglinQ

+ Trace

Import

atguler

Structure
Traces
Subplots
Theme
Style
Annotate
Analyze
Export
JSON

Save

Share

trace 0

Type: Heatmap

X: O

Y: B

Z: C D E F G H I J K L M N

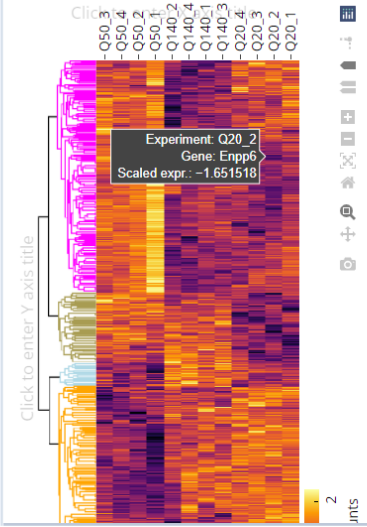
Options

Transpose: No | Yes

Verdana

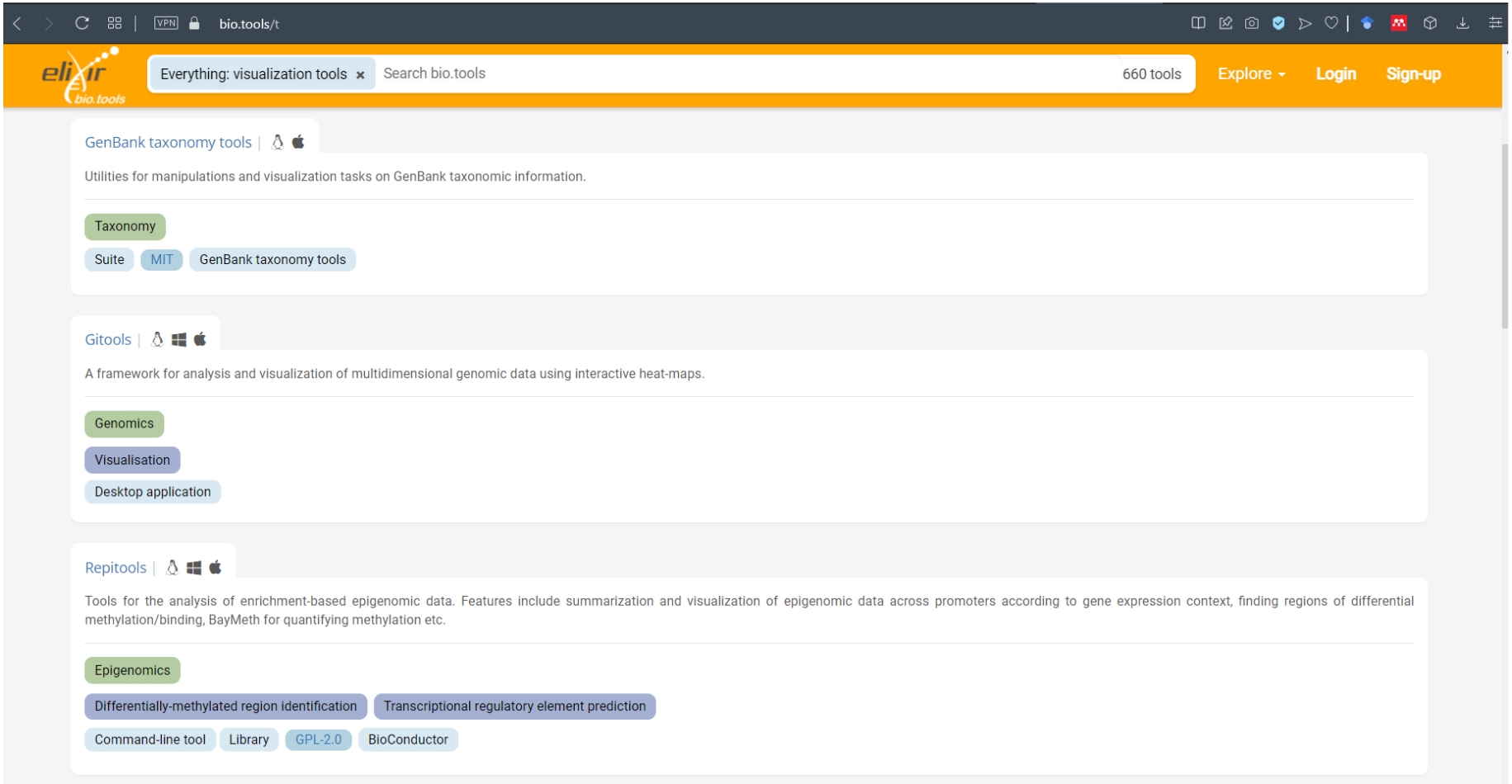
	A	B	C	D	E	F	G	H	I	J	K	L	M
1	1	Nampt	0.215198204	0.298555106	0.452983439	0.839390337	0.328380436	-1.574401259	-1.55439043	-1.675691485	0.492631763	0.949865162	0.964351356
2	2	Actr3	0.052884884	-0.432632983	0.443350881	1.353461981	0.107286558	-1.084760666	-1.380514383	-1.896587133	0.531504989	0.719460905	0.667079151
3	3	Add1	0.198700041	-0.016361643	0.040212072	0.758406579	-0.233907223	-1.302159309	-1.38063097	-1.088271618	-0.533631742	1.187776089	1.9056741
4	4	Cdk5	0.03537906	-0.776342154	0.374365509	0.962719321	-1.003786564	-0.605718374	-1.678633332	-0.268917114	-0.013393712	0.293967843	2.172554255
5	5	Rpl9	0.727042794	-0.953475177	-0.081508435	1.052151918	-0.345692635	-1.121615767	-1.85233593	-0.614684105	0.554352283	0.243497774	1.326607227
6	6	Erh	0.376109749	-0.505896509	-0.168753669	0.848609746	-0.409587651	-2.162545919	-1.431761503	0.322642356	1.076853275	0.27465266	0.753981233
7	7	Mvp	-0.933950245	-0.813658237	0.580756485	1.300670505	-0.854547679	-0.713124335	-1.241092205	-0.788911879	0.886659861	1.467129707	0.064919449
8	8	Cacnb4	-0.247023597	0.264265597	1.223759294	0.792339027	-0.476846278	-1.638639212	-1.205763578	-0.688996553	0.807108283	1.749877453	-0.187789887

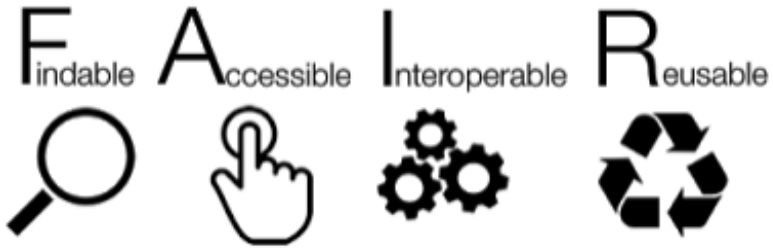
cerebellum_insol_data



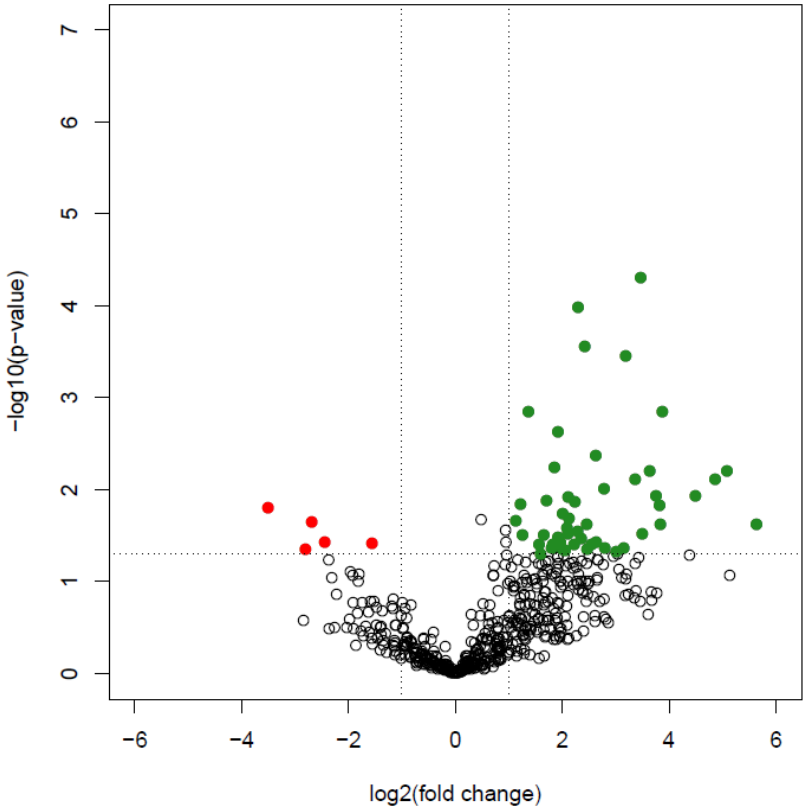
Searching for (visualization) tools

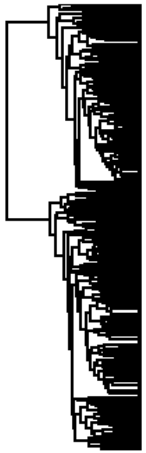
- Essential scientific and technical information about software tools, databases and services for bioinformatics and the life sciences.

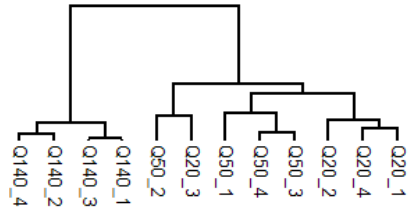

bio.tools/t
elixir bio.tools
Everything: visualization tools ×
Search bio.tools
660 tools
Explore
Login
Sign-up
GenBank taxonomy tools |
Utilities for manipulations and visualization tasks on GenBank taxonomic information.
Taxonomy
Suite
MIT
GenBank taxonomy tools
Gitools |
A framework for analysis and visualization of multidimensional genomic data using interactive heat-maps.
Genomics
Visualisation
Desktop application
Repitools |
Tools for the analysis of enrichment-based epigenomic data. Features include summarization and visualization of epigenomic data across promoters according to gene expression context, finding regions of differential methylation/binding, BayMeth for quantifying methylation etc.
Epigenomics
Differentially-methylated region identification
Transcriptional regulatory element prediction
Command-line tool
Library
GPL-2.0
BioConductor

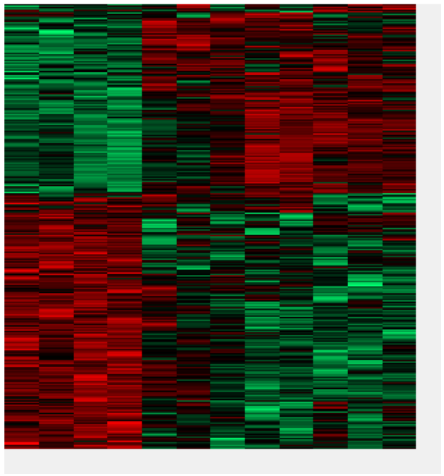

Findable
Accessible
Interoperable
Reusable

Colors & ambiguity

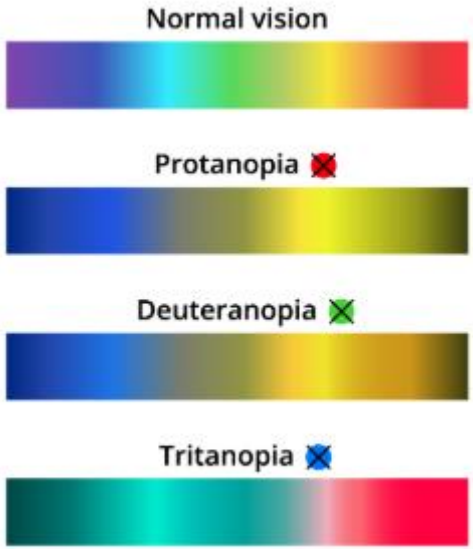


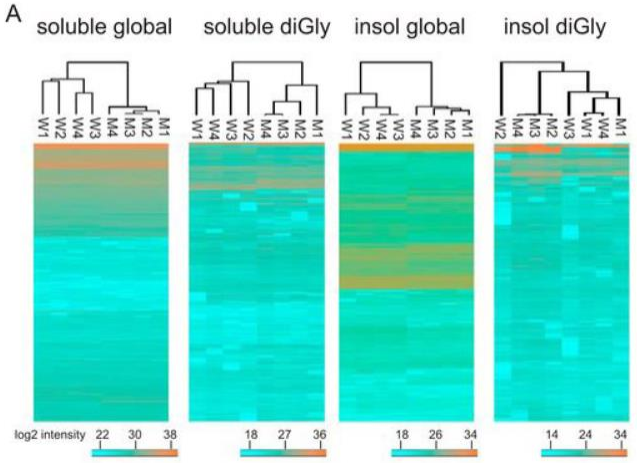


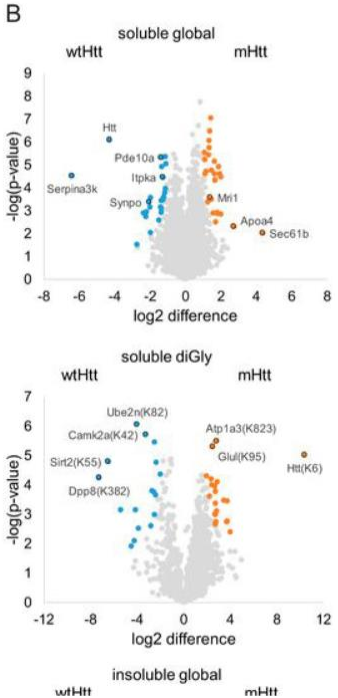




Colors & ambiguity







Mass spectrometry data in MetaboLights

the home for metabolomics experiments and derived information

Claire O'Donovan
EMBL-EBI Metabolomics Team

www.ebi.ac.uk

EMBL-EBI

MetaboLights

FAIR Guiding Principles

Provide a guideline for data producers and publishers to enhance the reusability of scientific data

Findable

Accessible

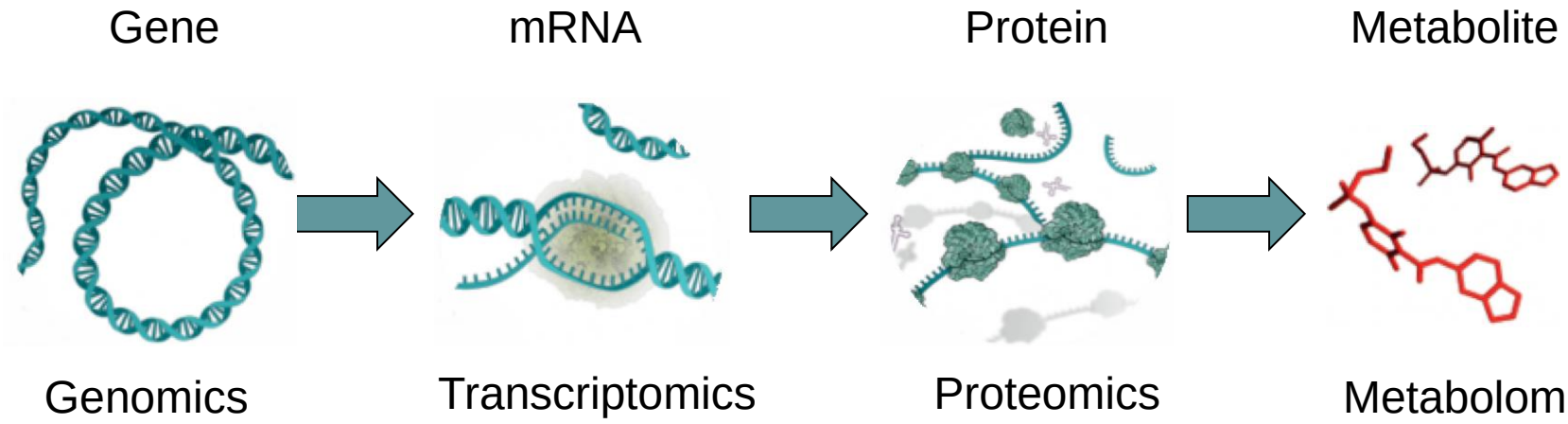
Interoperable

Re-useable

Good research data management is not a goal in itself, but rather the key conduit leading to knowledge discovery and innovation, and to subsequent data and knowledge integration and reuse.

Metabolomics: data management

MetaboLights



Can metabolomics learn from the other omic techniques and not repeat many of the same mistakes that have been made in which a lot of data were collected but little information was gleaned?

Metabolomics: the final frontier?

Timothy D Veenstra

Genome Medicine 2012 4:40

https://doi.org/10.1186/gm339

The Metabolomics Standards Initiative (MSI)

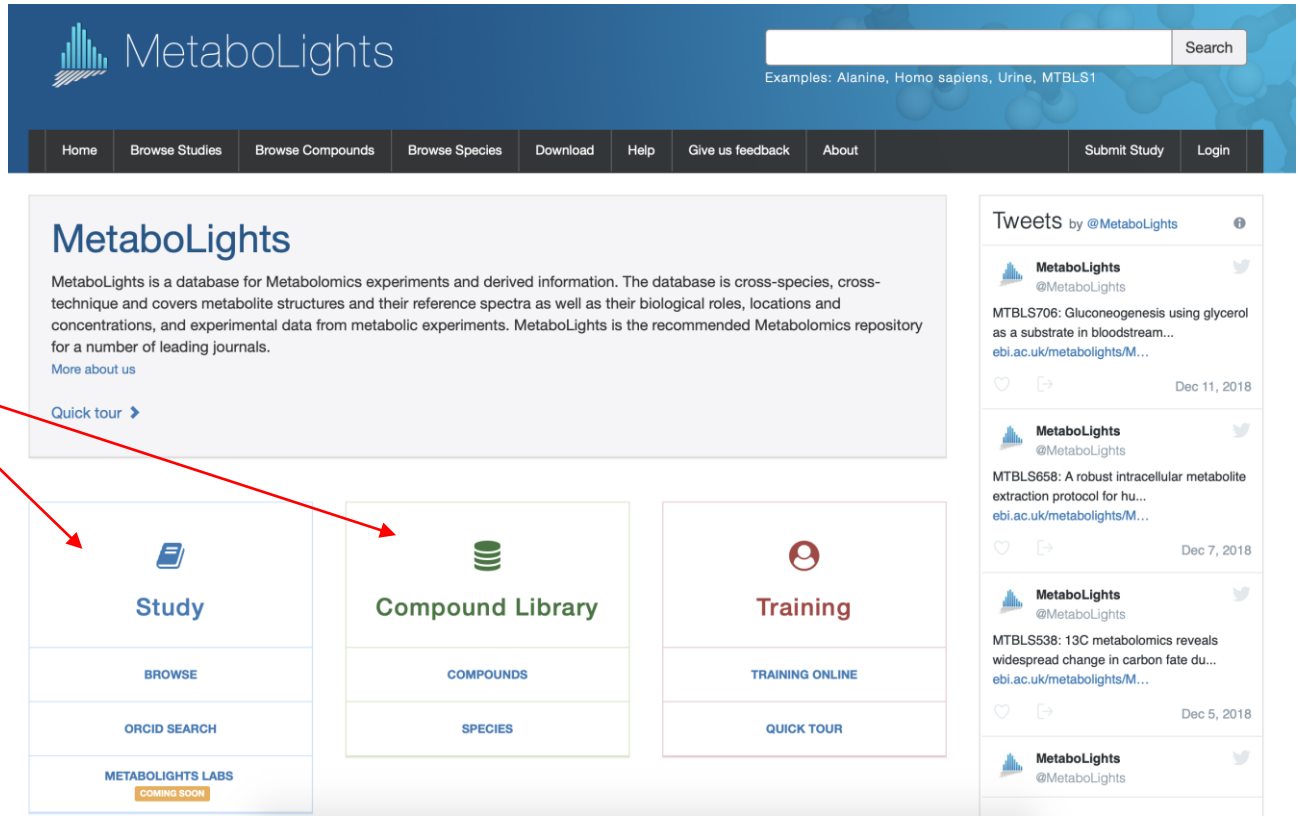
The MSI is an academic policy provider, to support the development of open data and metadata formats for metabolomics.

- community-agreed reporting standards
- minimal information (MI) checklists
- data exchange formats to support
  the MIs reporting standards,
  allow data to be efficiently applied,
  shared and reused

METABOLOMICS SOCIETY

MetaboLights

Open Source Study Repository & Metabolite Knowledgebase



https://www.ebi.ac.uk/metabolights

EMBL-EBI

MetaboLights user base

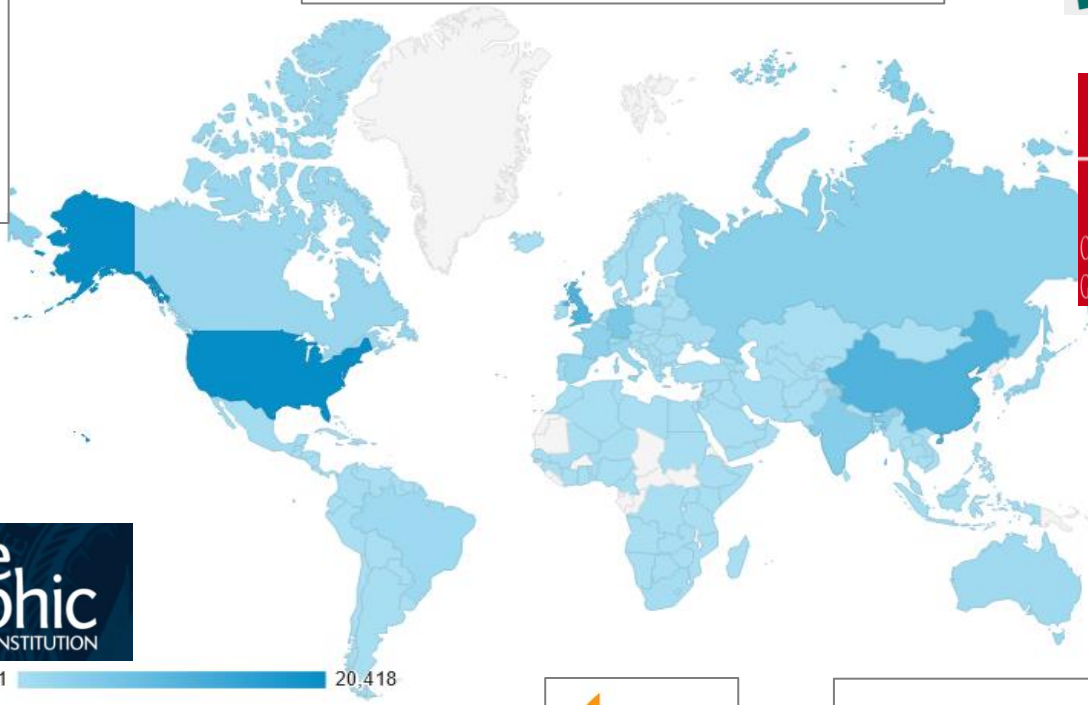
MaHPIC

Malaria Host-Pathogen Interaction Center (NIH)

METABOLON

Precision Metabolomics

MAX-PLANCK



OIST

OKINAWA INSTITUTE OF SCIENCE AND TECHNOLOGY GRADUATE UNIVERSITY

Pacific Northwest NATIONAL LABORATORY

NHS National Institute for Health Research BioResource

Woods Hole Oceanographic INSTITUTION

CHEAR Children's Health Exposure Analysis Resource

NIH

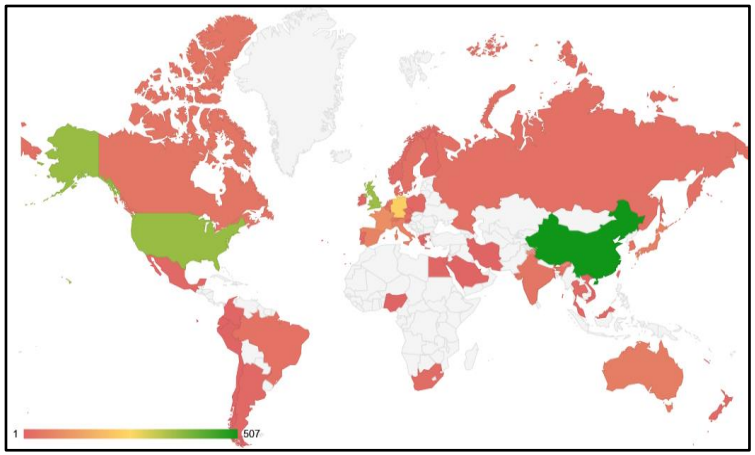
PHENOME CENTRE BIRMINGHAM

UNIVERSITY OF CAMBRIDGE

National Phenome Centre

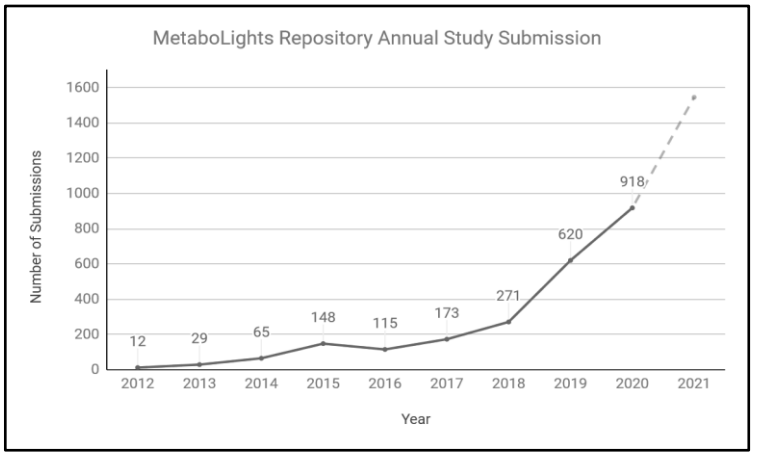
embric

EUROPEAN MARINE BIOLOGICAL RESEARCH INFRASTRUCTURE CLUSTER

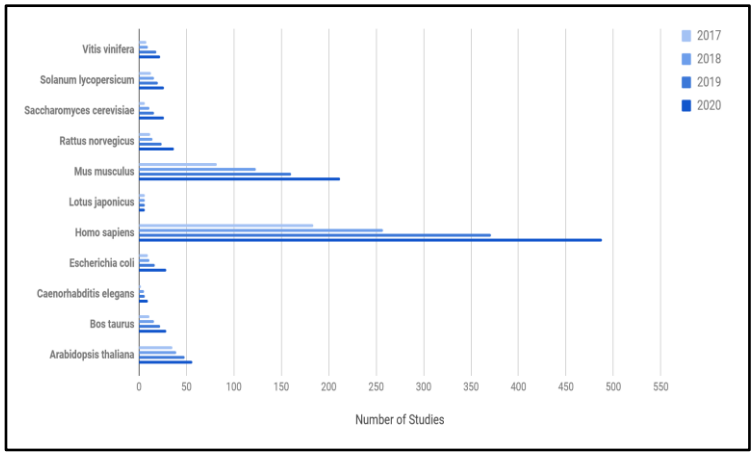


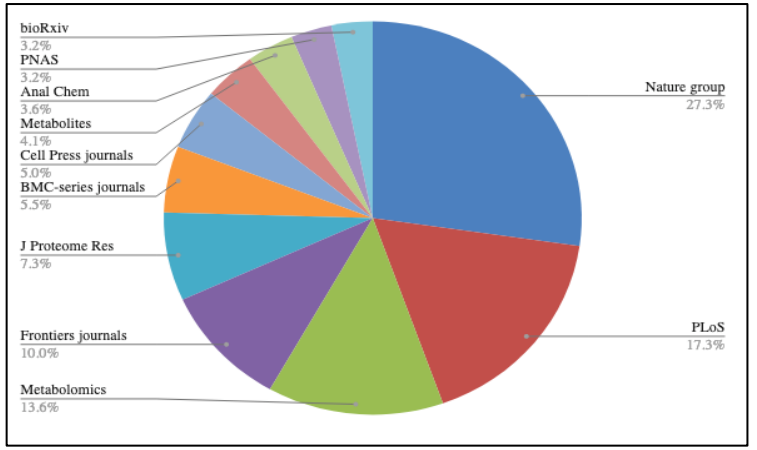
Geographical distribution of submitted studies

(Top 10: China: 507, USA: 362, UK: 356, Germany: 235, France: 94, Japan: 68, Spain: 66, Italy: 64, Australia: 53, Netherlands: 39)

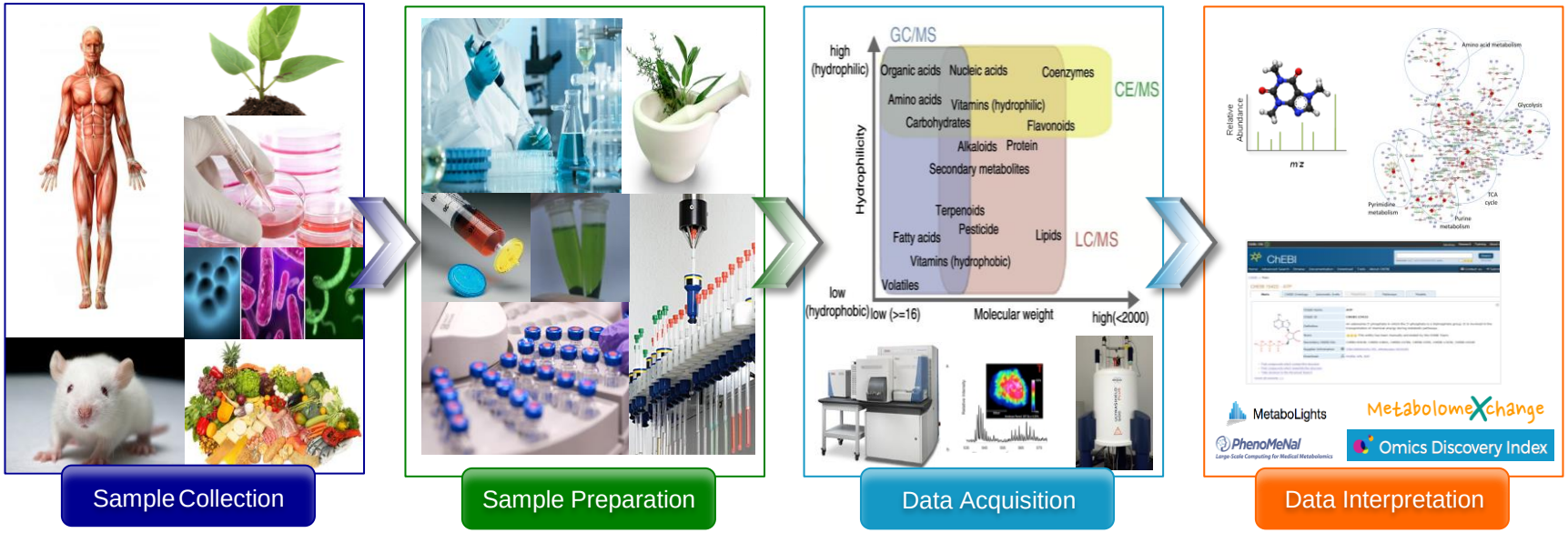


MetaboLights study submission rates per year





MetaboLights Database

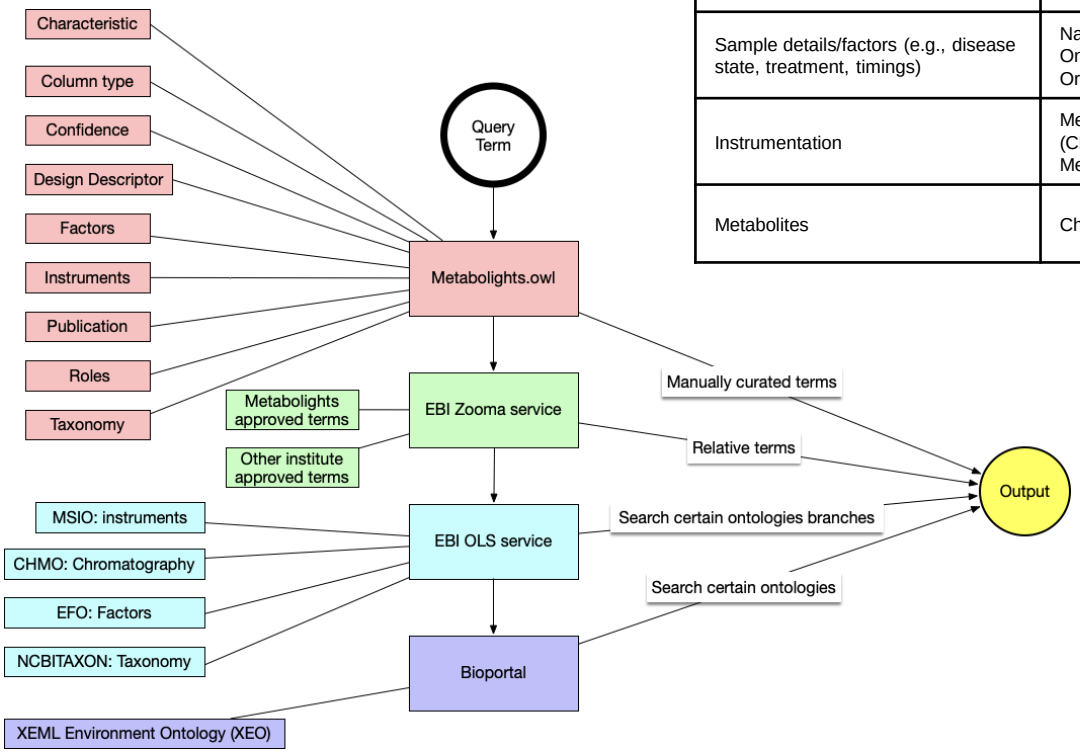


- Cross species, cross technique
- Comprehensive information collection
- Open access, discoverable through various portals

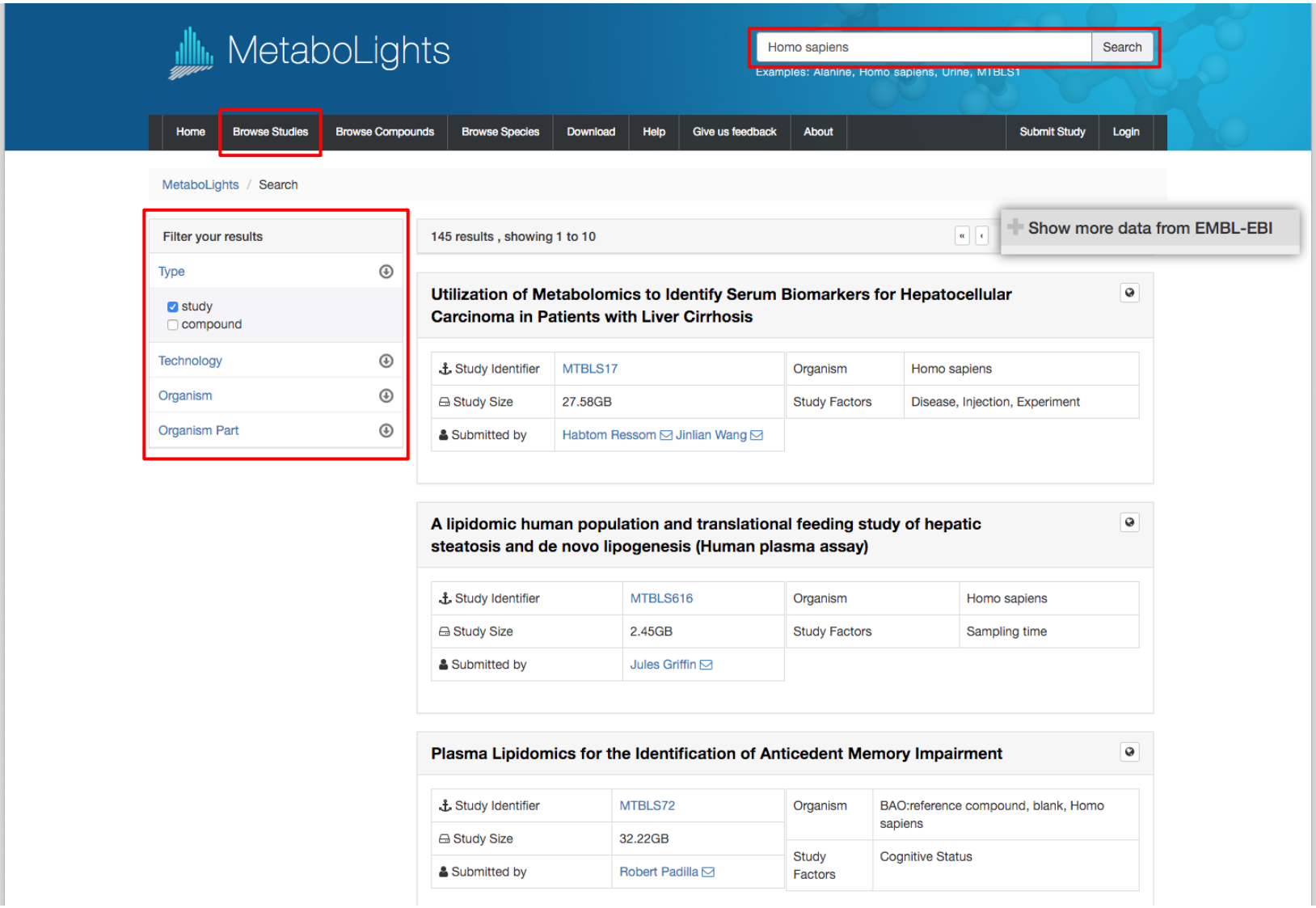
MetaboLights: Ontology mapping

Ontologies: Controlled vocabulary

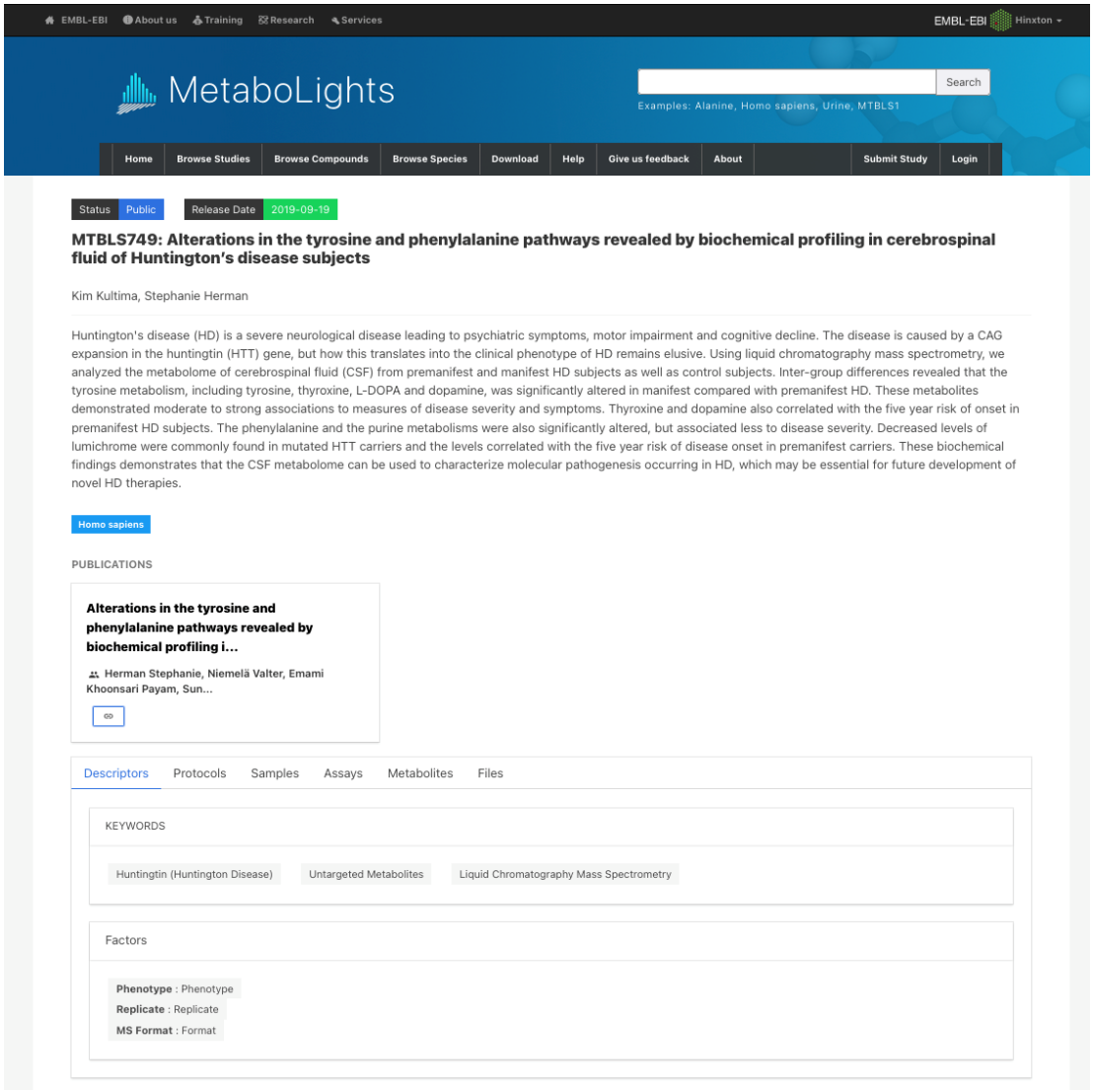
Area	Ontology
Species/Organism, Organism part	National Center for Biotechnology Information Organismal Classification (NCBITAXON), World Register of Marine Species (WoRMS), National Cancer Institute Thesaurus (NCIT), Environment Ontology (ENVO), Brenda Tissue and Enzyme Source Ontology (BTO)
Sample details/factors (e.g., disease state, treatment, timings)	National Cancer Institute Thesaurus (NCIT), Experimental Factor Ontology (EFO), Plant Ontology (PO), Unit of Measurement Ontology (UO), Human Phenotype Ontology (HP), Orphanet Rare Disease ontology (ORDO)
Instrumentation	Metabolomics Standards Initiative Ontology (MSIO), Chemical Methods Ontology (CHMO), Mass Spectrometry Ontology (MS), Unit of Measurement Ontology (UO) MetaboLights (MTBLS) …
Metabolites	Chemical Entities of Biological Interest (ChEBI) … cross ref to other databases



MetaboLights: Browse or search studies

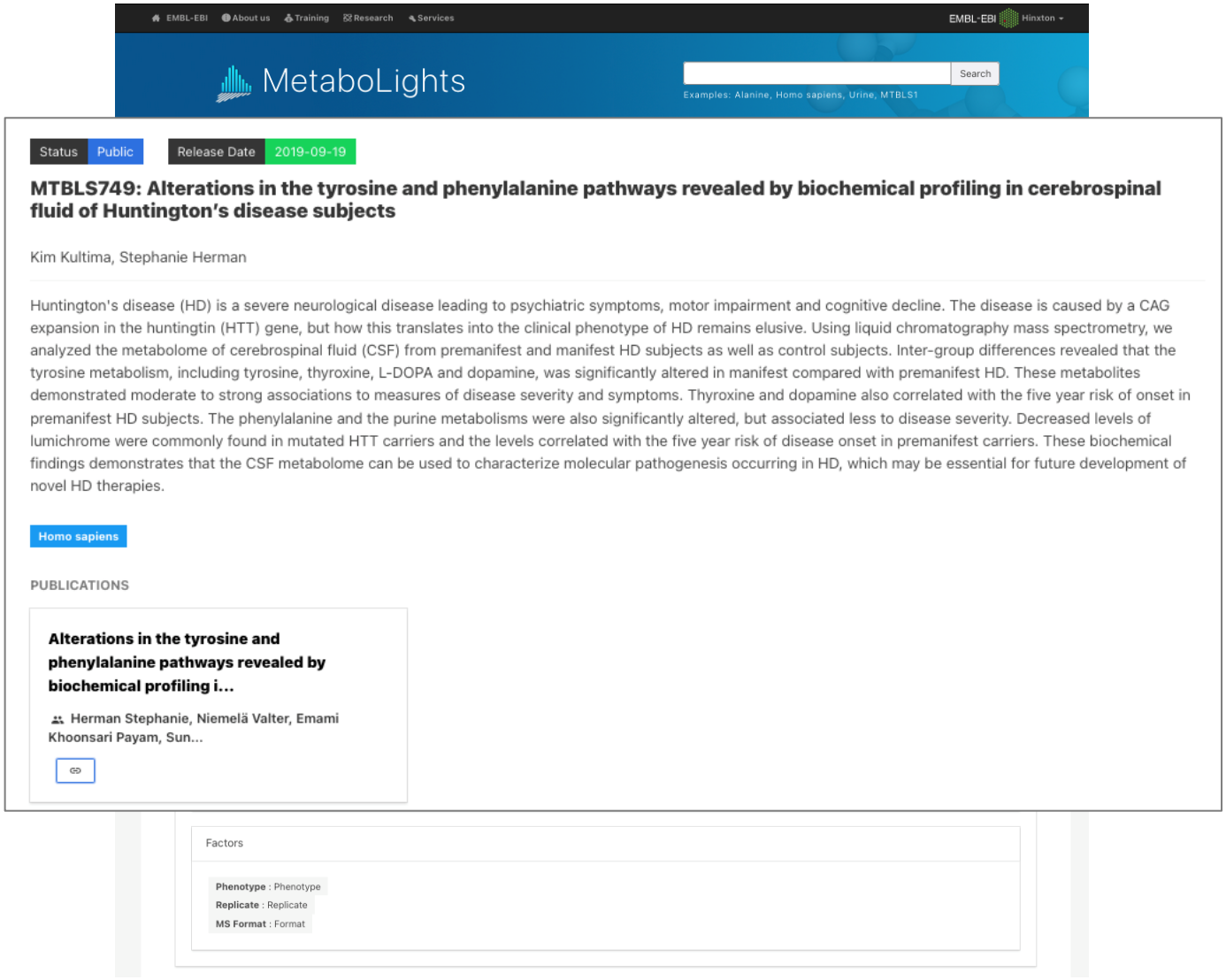


MetaboLights – Study information



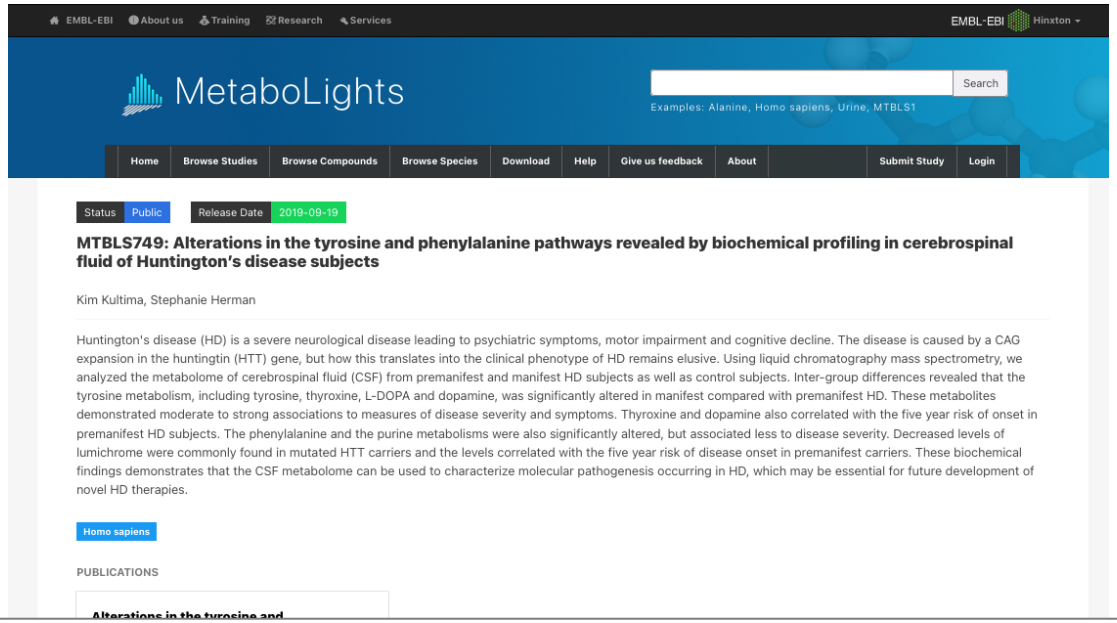
MTBLS749

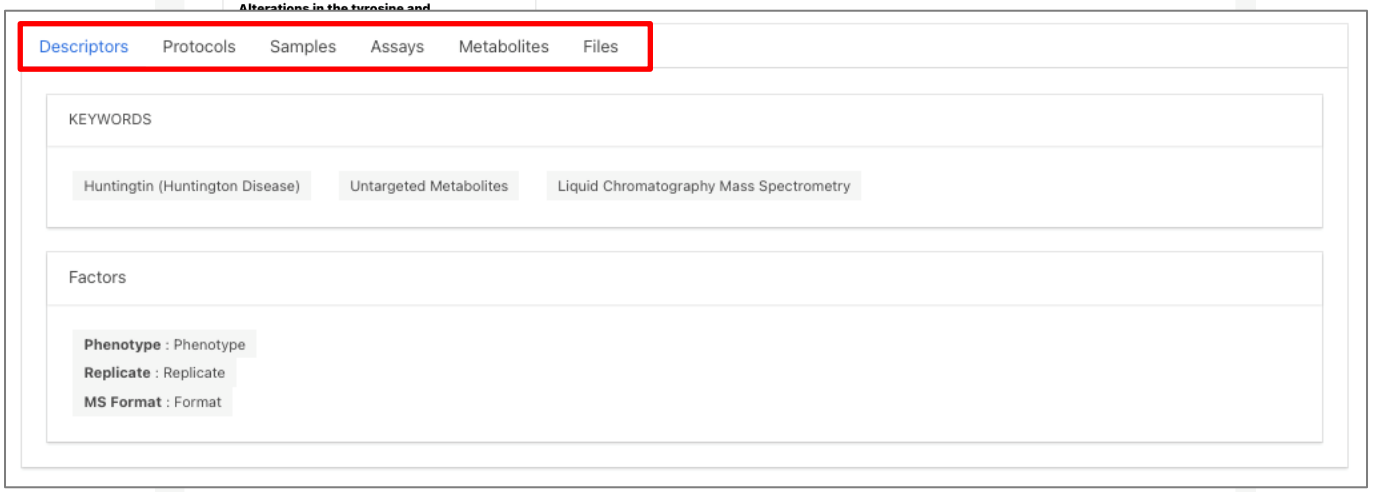
MetaboLights – Study information



MTBLS749

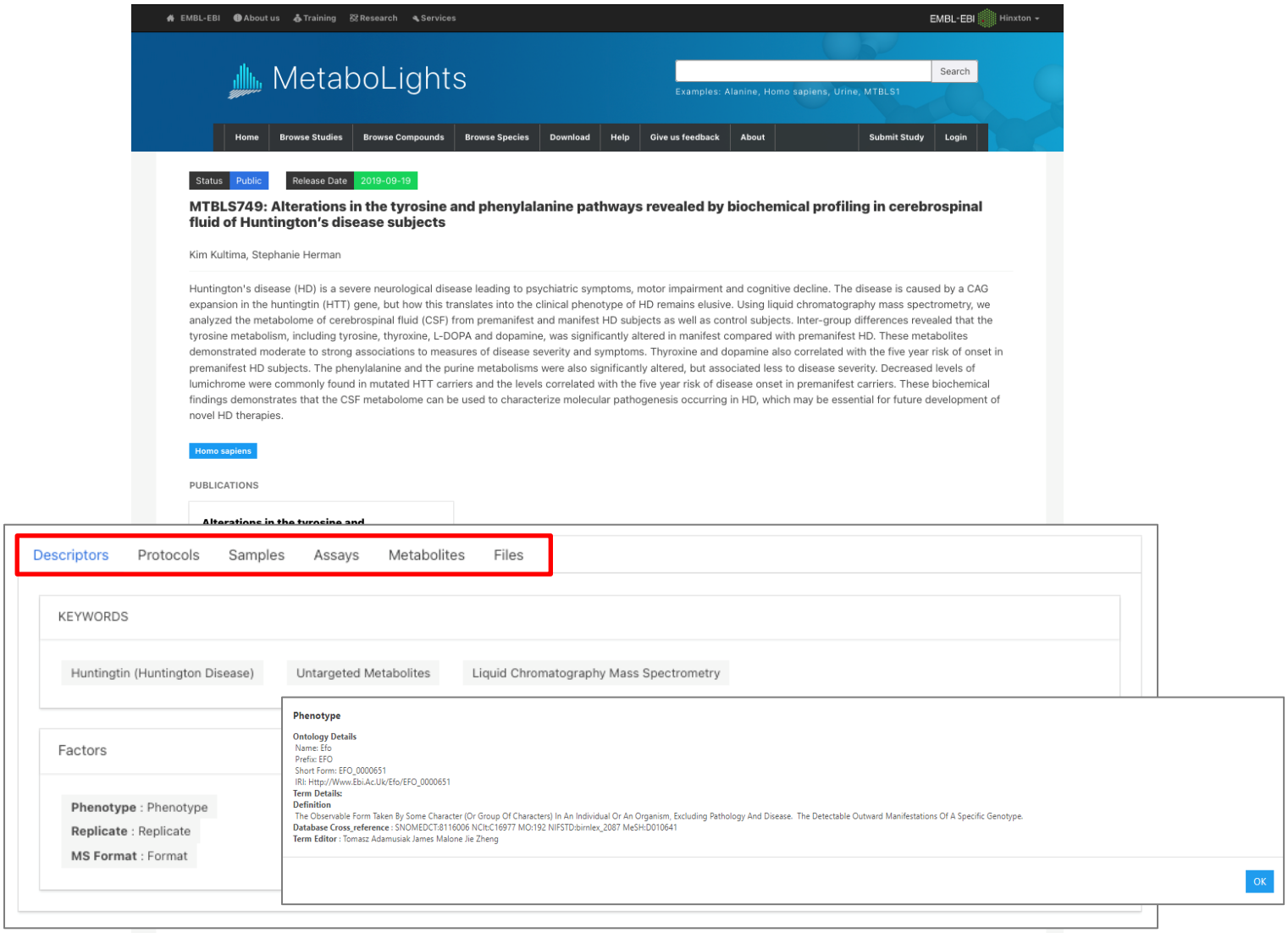
MetaboLights – Study information





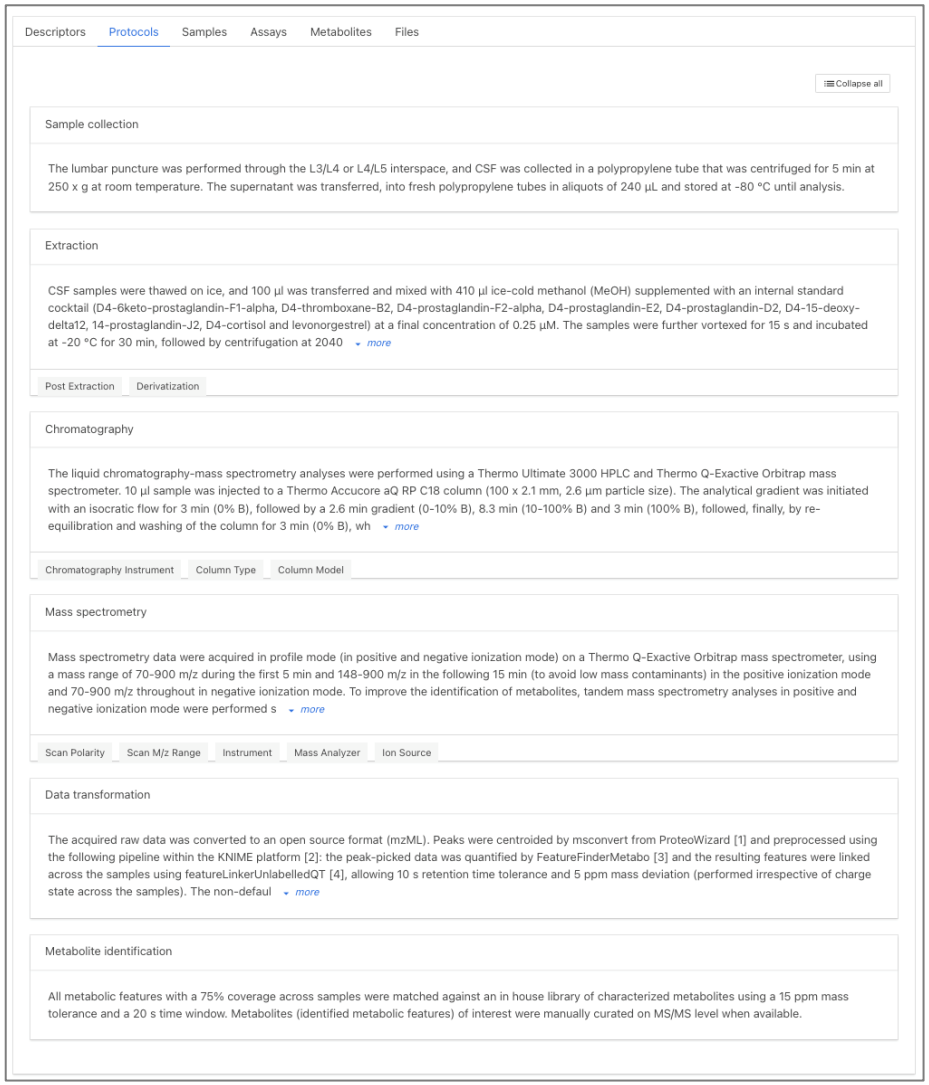
MTBLS749

MetaboLights – Study information



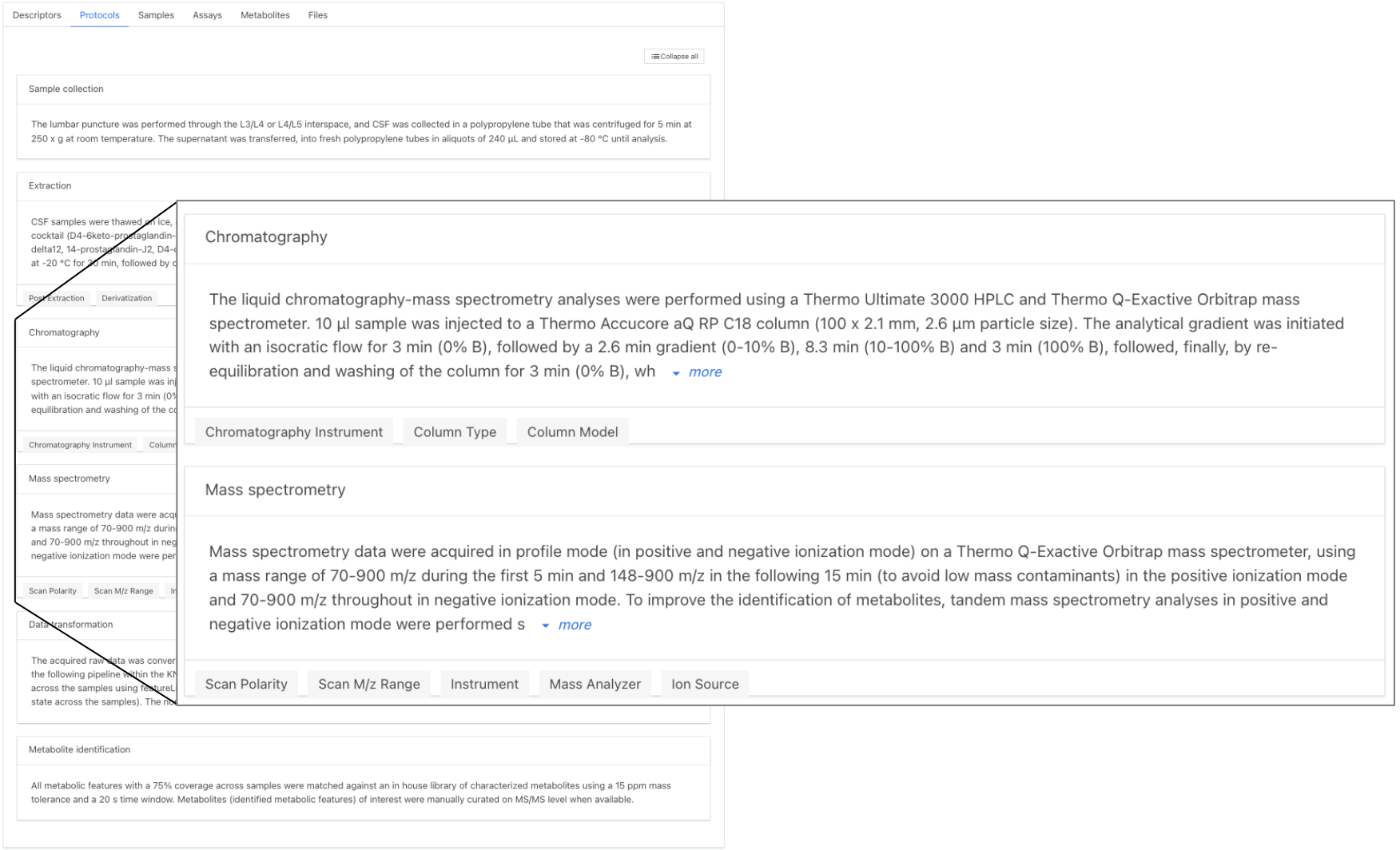
MTBLS749

MetaboLights – Study information



MTBLS749

MetaboLights – Study information



MTBLS749

MetaboLights – Study information

Descriptors | Protocols | Samples | Assays | Metabolites | Files

File: s_MTBLS749.txt

Items per page: 494 | 1 – 494 of 494

Filter

Protocol REF	Sample Name	Organism	Organism part	Phenotype	Replicate	MS format
Sample collection	1_Rep1_NEG	Homo sapiens	cerebrospinal fluid	control	1	MS1 format
Sample collection	1_Rep1_POS	Homo sapiens	cerebrospinal fluid	control	1	MS1 format
Sample collection	1_Rep2_NEG	Homo sapiens	cerebrospinal fluid	control	2	MS1 format
Sample collection	1_Rep2_POS	Homo sapiens	cerebrospinal fluid	control	2	MS1 format
Sample collection	10_Rep1_NEG	Homo sapiens	cerebrospinal fluid	control	1	MS1 format
Sample collection	10_Rep1_POS	Homo sapiens	cerebrospinal fluid	control	1	MS1 format
Sample collection	10_Rep2_NEG	Homo sapiens	cerebrospinal fluid	control	2	MS1 format
Sample collection	10_Rep2_POS	Homo sapiens	cerebrospinal fluid	control	2	MS1 format
Sample collection	11_Rep1_NEG	Homo sapiens	cerebrospinal fluid	control	1	MS1 format
Sample collection	11_Rep1_POS	Homo sapiens	cerebrospinal fluid	control	1	MS1 format
Sample collection	11_Rep2_NEG	Homo sapiens	cerebrospinal fluid	control	2	MS1 format
Sample collection	11_Rep2_POS	Homo sapiens	cerebrospinal fluid	control	2	MS1 format

MetaboLights – Study information

Descriptors | Protocols | Samples | Assays | Metabolites | Files

Assay Sheet 1 | Assay Sheet 2 | Assay Sheet 3 | Assay Sheet 4

File: a_MTBLS1987_LC-MS_positive_hilic_metabolite_profiling.txt

Items per page: 69 | 1 – 69 of 69

Filter

Protocol REF	Parameter Value - Chromatography Instrument	Parameter Value - Autosampler model	Parameter Value - Column model	Parameter Value - Column type	Parameter Value - Guard column	Labeled Extract Name	Label	Protocol REF	Parameter Value - Scan polarity	Parameter Value - Scan m/z range	Parameter Value - Instrument
Chromatography	Waters ACQUITY UPLC H-Class System		ACQUITY UPLC BEH Amide (1.7 µm, 2.1 mm x 100 mm; Waters)	HILIC				Mass spectrometry	Positive	50-1000	Waters Xevo G2-S QTof
Chromatography	Waters ACQUITY UPLC H-Class System		ACQUITY UPLC BEH Amide (1.7 µm, 2.1 mm x 100 mm; Waters)	HILIC				Mass spectrometry	Positive	50-1000	Waters Xevo G2-S QTof
Chromatography	Waters ACQUITY UPLC H-Class System		ACQUITY UPLC BEH Amide (1.7 µm, 2.1 mm x 100 mm; Waters)	HILIC				Mass spectrometry	Positive	50-1000	Waters Xevo G2-S QTof

MTBLS1987

MetaboLights – Study information

Descriptors | Protocols | Samples | **Assays** | Metabolites | Files | Validations

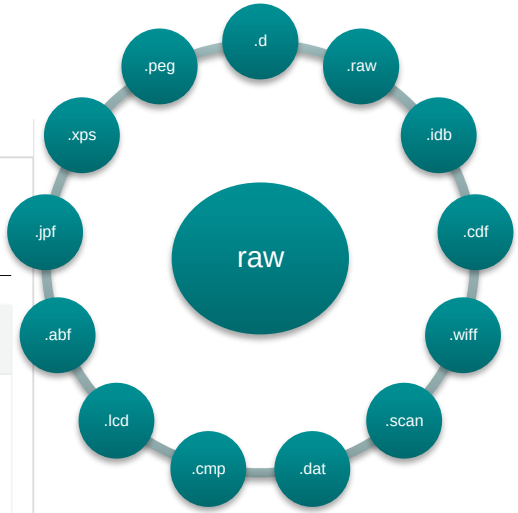
Assay Sheet 1 | Assay Sheet 2 | Assay Sheet 3 | Assay Sheet 4

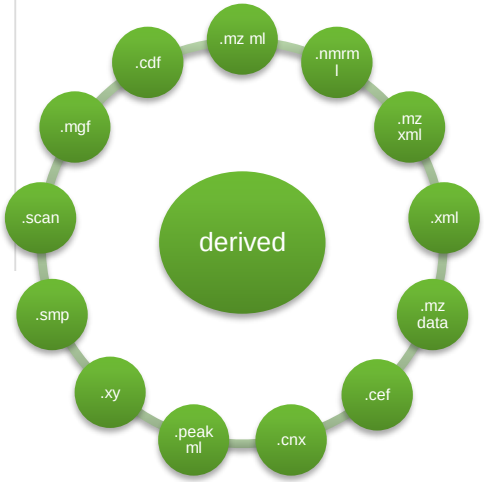
File: a_MTBLS1987_LC-MS_negative_hilic_metabolite_profiling.txt

Items per page: 69 1 – 69 of 69 69 1 – 69 of 69

Filter

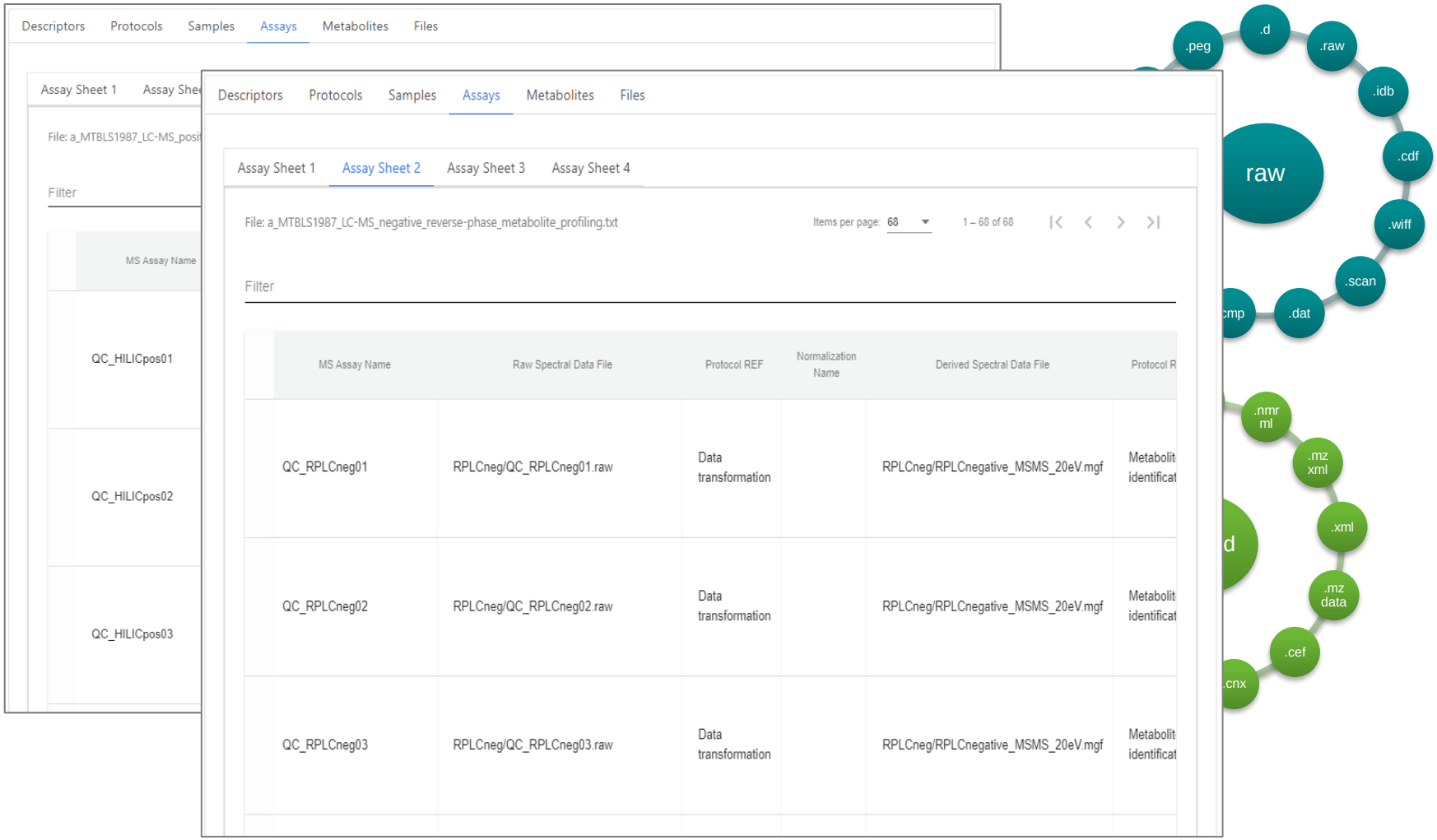
Raw Spectral Data File	Protocol REF	Normalization Name	Derived Spectral Data File	Protocol REF	Data Transformation Name	Metabolite Assignment File
HILICneg/QC_HILICneg01.raw	Data transformation		HILICneg/HILICnegative_MSMS_20eV.mgf	Metabolite identification		m_MTBLS1987_LC-MS_negative_hilic_metabolite_profiling_v2_maf.tsv
HILICneg/QC_HILICneg02.raw	Data transformation		HILICneg/HILICnegative_MSMS_20eV.mgf	Metabolite identification		m_MTBLS1987_LC-MS_negative_hilic_metabolite_profiling_v2_maf.tsv
HILICneg/QC_HILICneg03.raw	Data transformation		HILICneg/HILICnegative_MSMS_20eV.mgf	Metabolite identification		m_MTBLS1987_LC-MS_negative_hilic_metabolite_profiling_v2_maf.tsv





MTBLS1987

MetaboLights – Study information



MTBLS1987

EMBL-EBI

MetaboLights – Study information

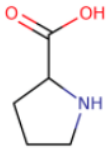
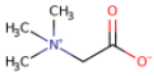
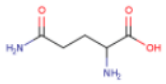
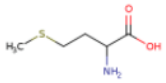
Descriptors | Protocols | Samples | Assays | Metabolites | Files

MAF Sheet 1 | MAF Sheet 2 | MAF Sheet 3 | MAF Sheet 4

File: m_MTBLS1987_LC-MS_positive_hilic_metabolite_profiling_v2_maf.tsv

Items per page: 13 1 – 13 of 13

Filter

Structure	Database identifier	Chemical formula	SMILES	InChI	Metabolite identification	Mass to charge
	CHEBI:26271		OC(=O)C1CCCN1	InChI=1S/C5H9NO2/c7-5(8)4-2-1-3-6-4/h4,6H,1-3H2,(H,7,8)	Proline	116.07029
	CHEBI:17750		C[N+](C)(C)CC([O-])=O	InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3	Betaine	118.08747
	CHEBI:28300		NC(CCC(N)=O)C(O)=O	InChI=1S/C5H10N2O3/c6-3(5(9)10)1-2-4(7)8/h3H,1-2,6H2,(H2,7,8)(H,9,10)	Glutamine	147.07607
	CHEBI:16811		CSCCC(N)C(O)=O	InChI=1S/C5H11NO2S/c1-9-3-2-4(6)5(7)8/h4H,2-3,6H2,1H3,(H,7,8)	Methionine	150.05818

MTBLS1987

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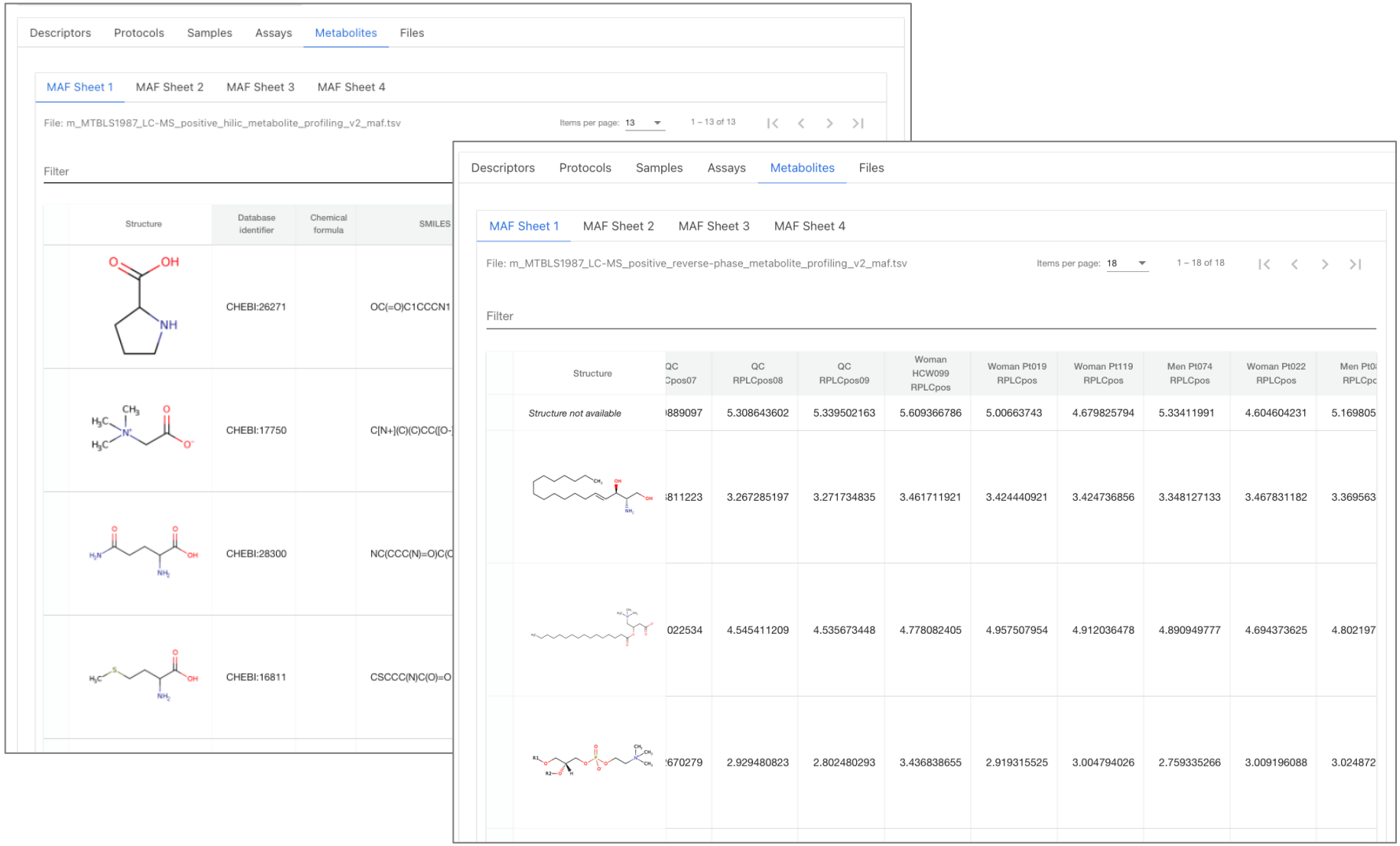
MetaboLights – Study information



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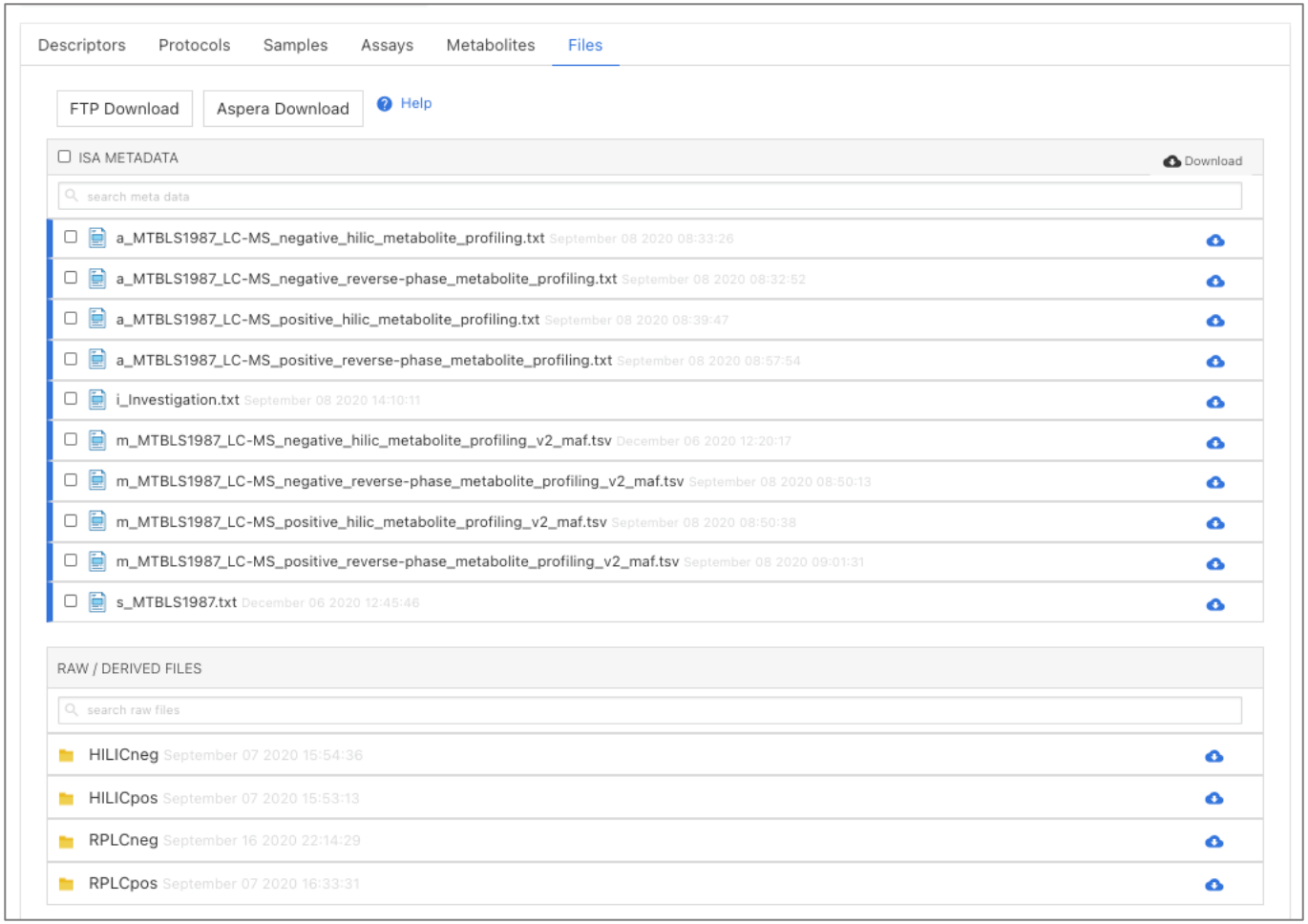
MetaboLights – Study information



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- Pamela Pruski
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- Felix Amaladoss
- Callum Martin
- Thomas Payne

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Questions:

- Do you submit your data to public repositories? MetaboLights/Metabolomics Workbench/MetaboBank (and PRIDE)

- Do you reuse public mass spectrometry studies?

a) Metadata

b) Raw data

c) Both

Questions:

- What data do you think we are missing?
- What tools do you use when manipulating/viewing the data? – either your internal data or the public data
- What tools would you like available with the repositories?