GBSC 724
2-5-18

Processing data from XCMS

Stephen Barnes
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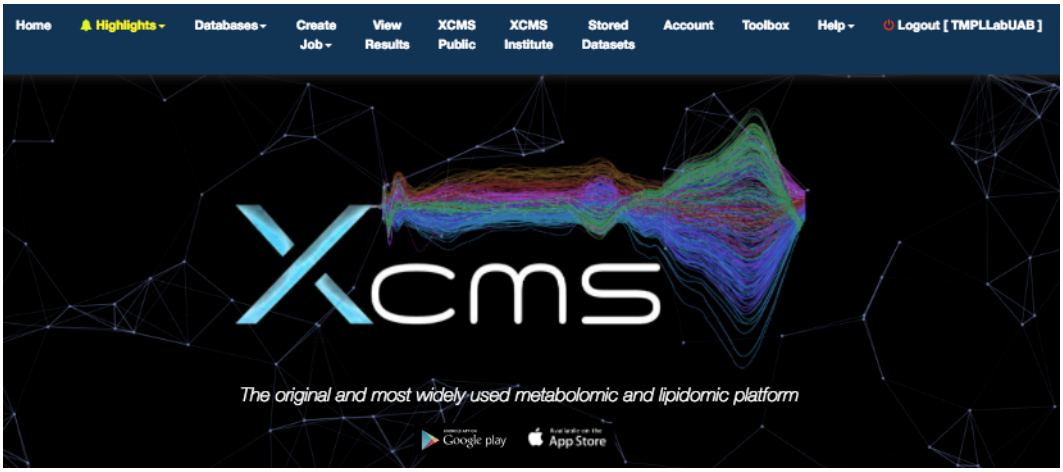
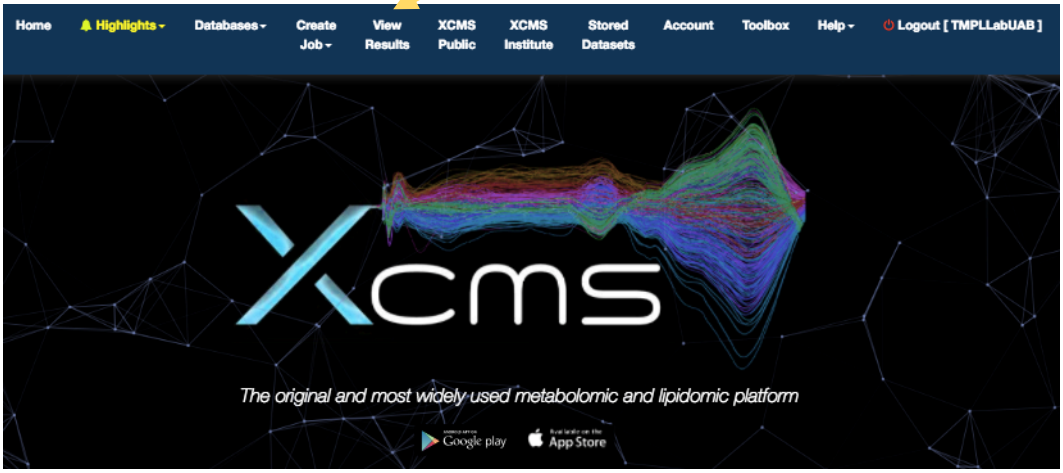
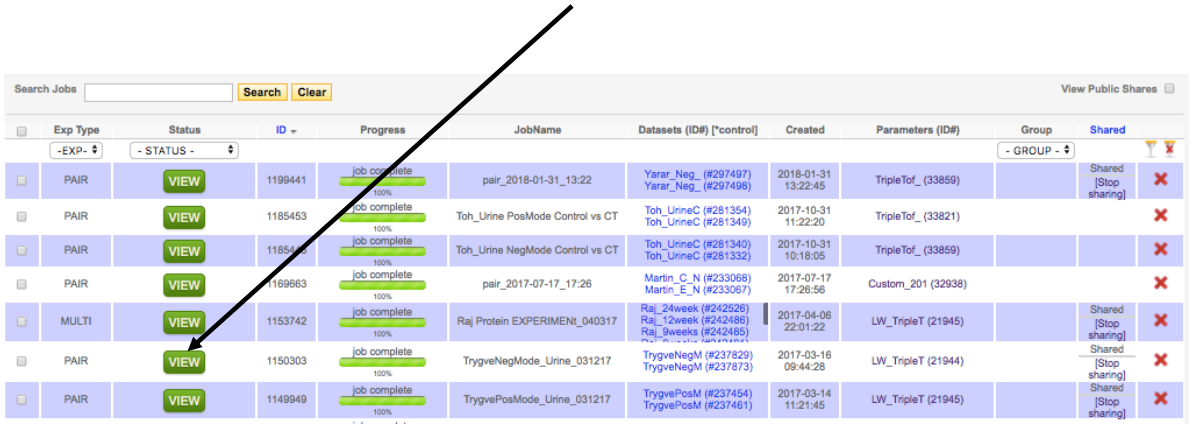
Logon to https://xcmsonline.scripps.edu/

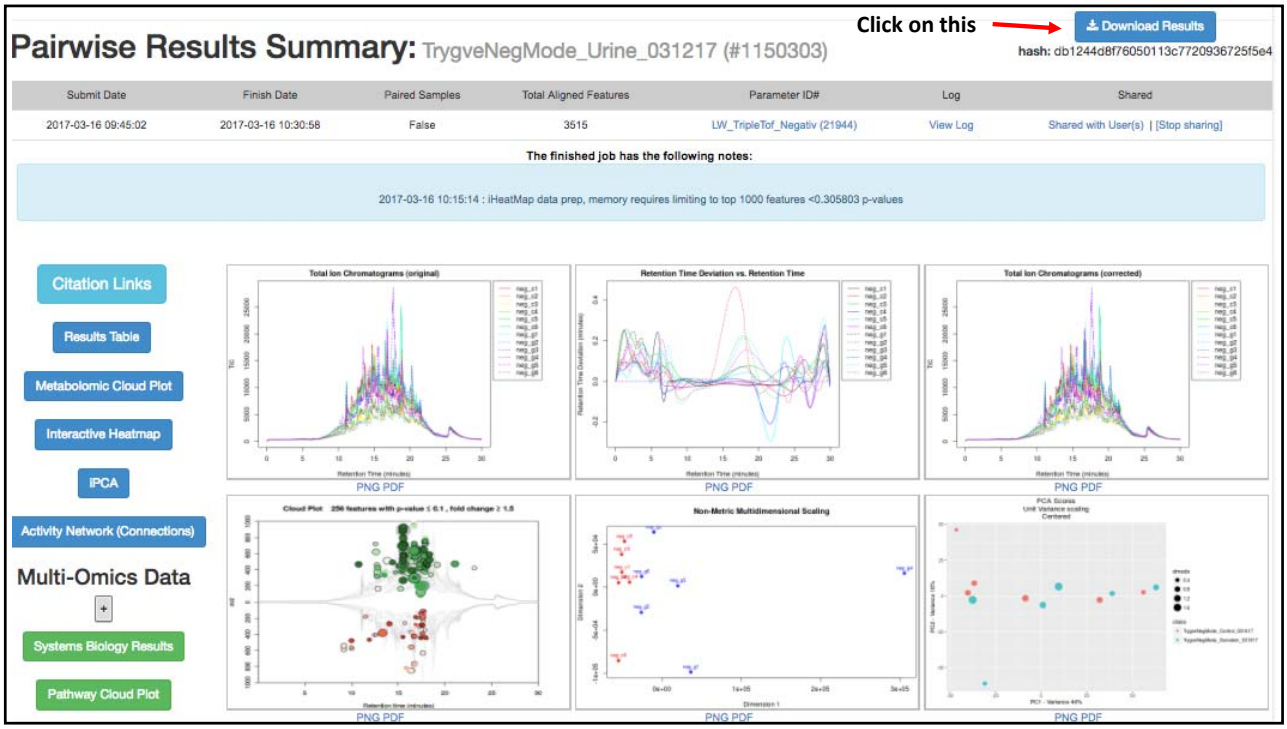


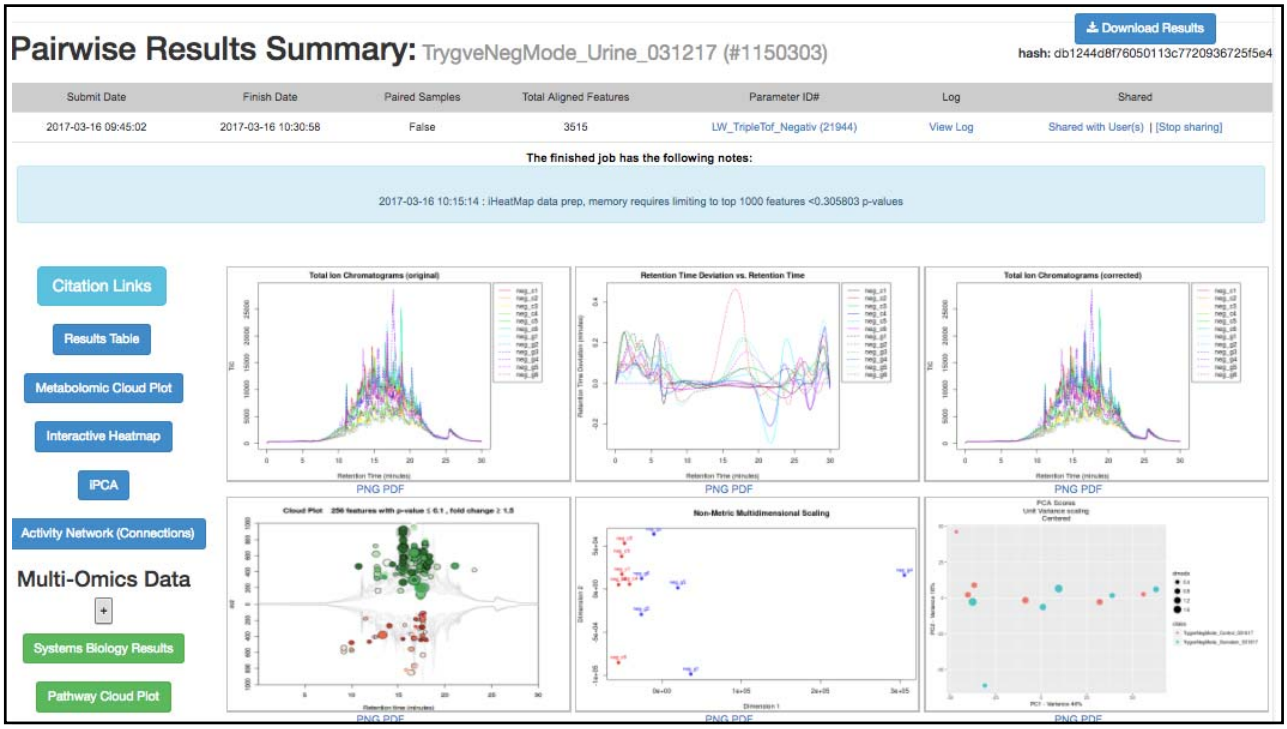
Go to View Results

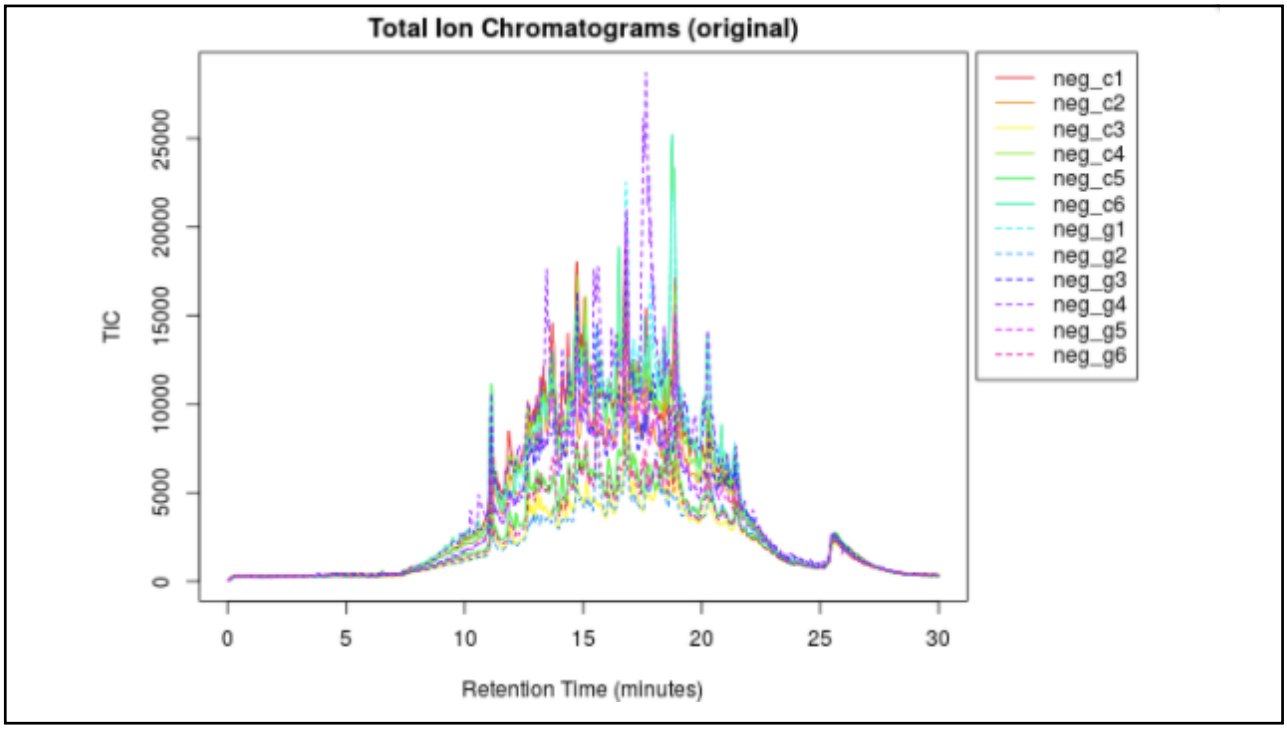


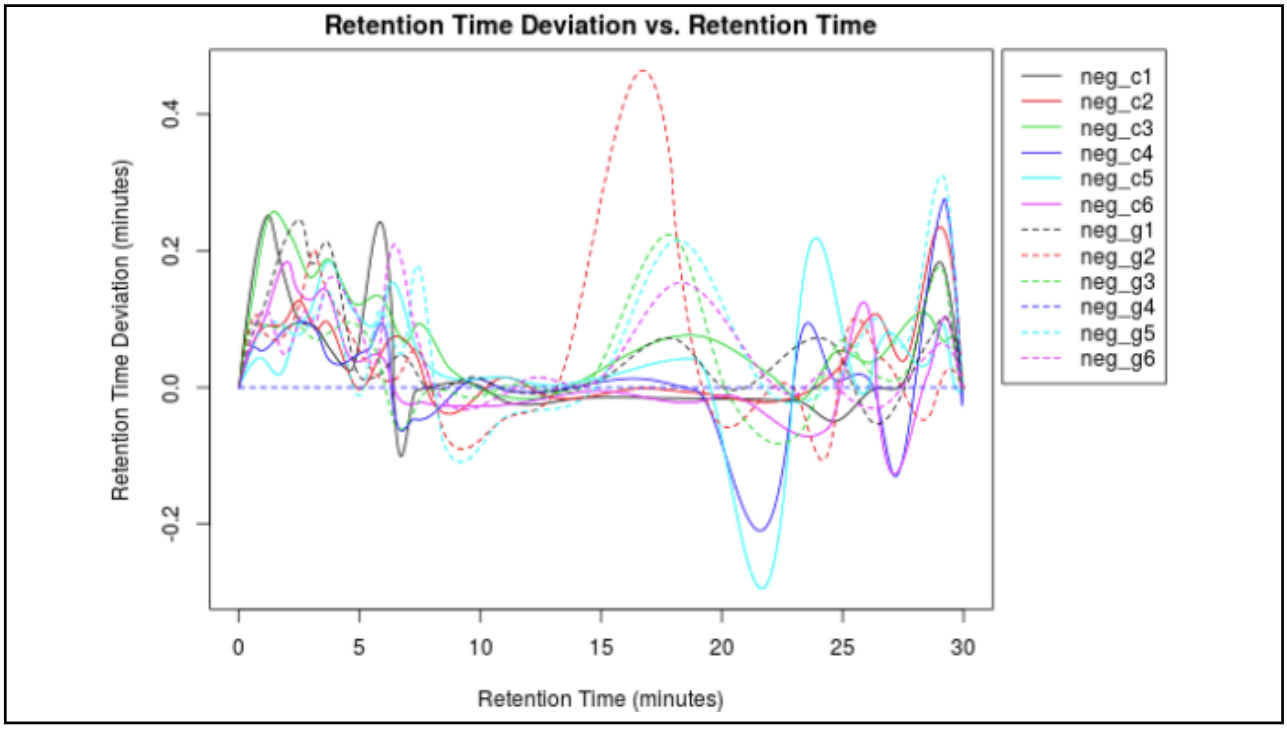
Select the file to view

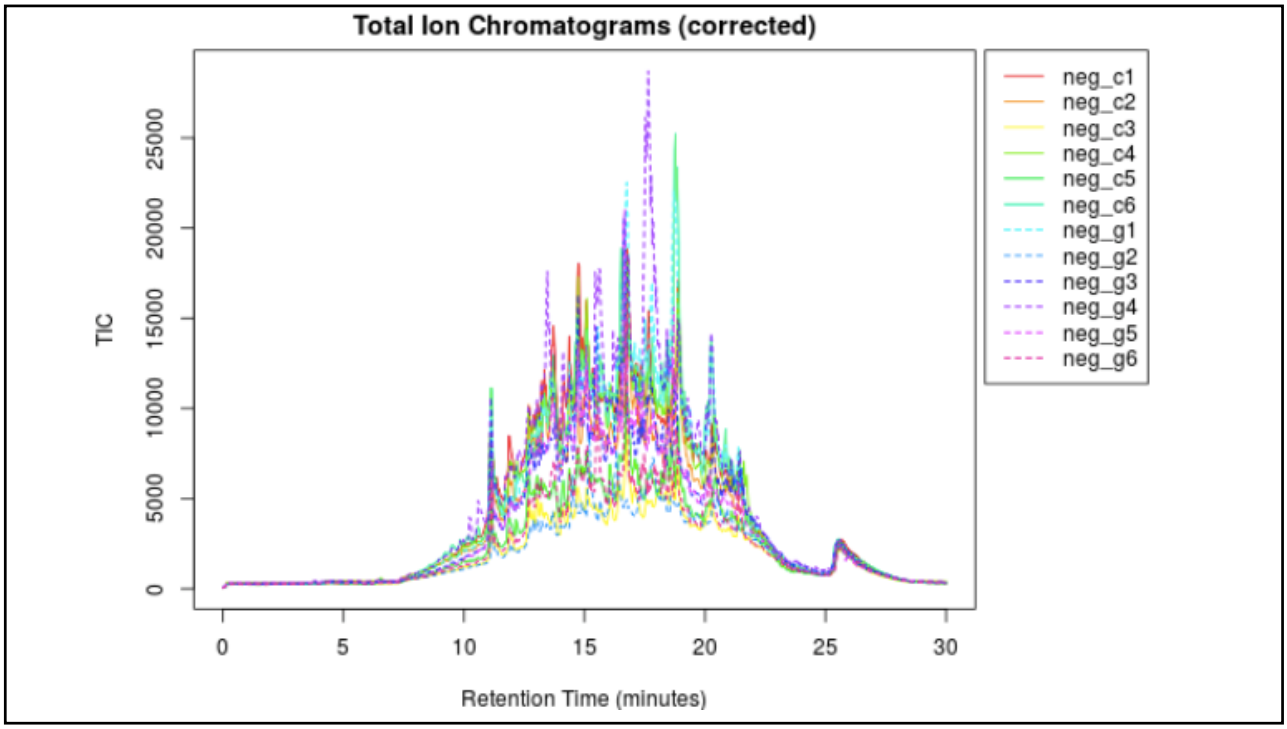


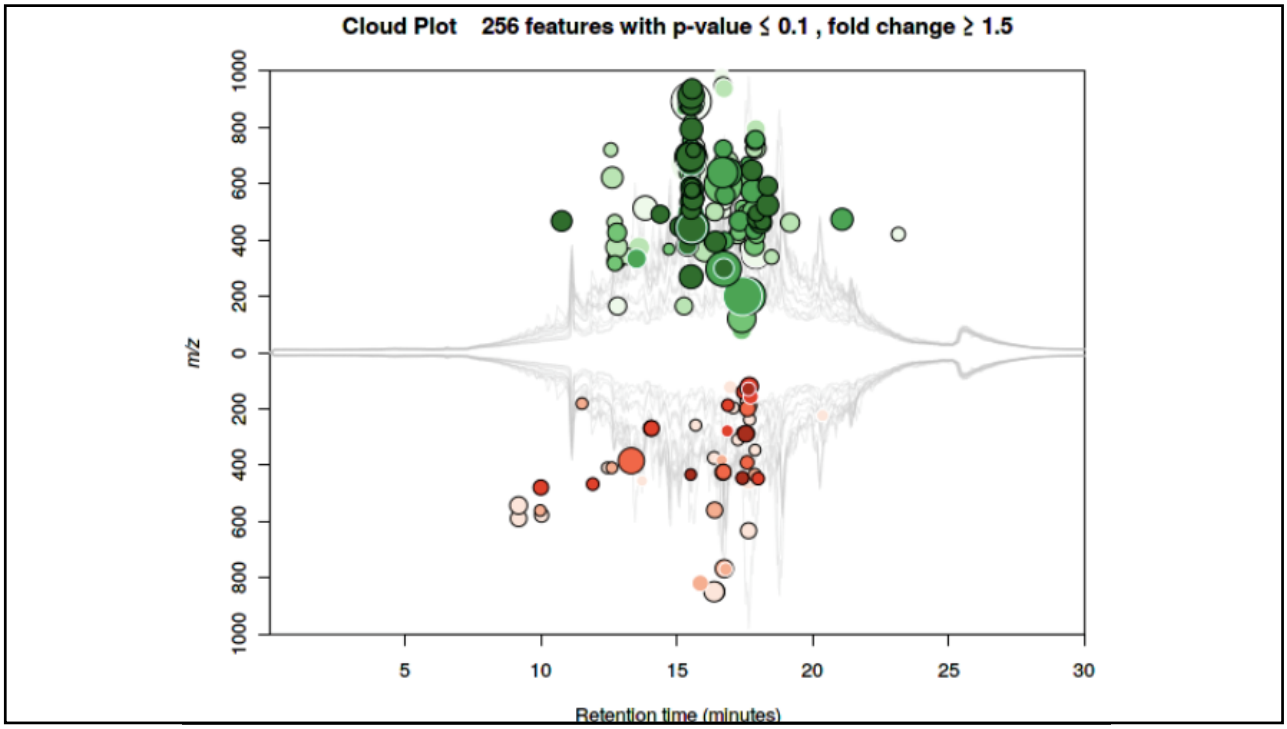

Click on this
Download Results
Pairwise Results Summary: TrygveNegMode_Urine_031217 (#1150303)
hash: db1244d8f76050113c7720936725f5e4
Submit Date
Finish Date
Paired Samples
Total Aligned Features
Parameter ID#
Log
Shared
2017-03-16 09:45:02
2017-03-16 10:30:58
False
3515
LW_TripleTof_Negativ (21944)
View Log
Shared with User(s) | [Stop sharing]
The finished job has the following notes:
2017-03-16 10:15:14 : iHeatMap data prep, memory requires limiting to top 1000 features <0.305803 p-values
Citation Links
Results Table
Metabolomic Cloud Plot
Interactive Heatmap
IPCA
Activity Network (Connections)
Multi-Omics Data
Systems Biology Results
Pathway Cloud Plot
Total Ion Chromatograms (original)
Retention Time Deviation vs. Retention Time
Total Ion Chromatograms (corrected)
Cloud Plot
Non-Metric Multidimensional Scaling
PCA Scores
PNG PDF


Download Results
Pairwise Results Summary: TrygveNegMode_Urine_031217 (#1150303)
hash: db1244d8f76050113c7720936725f5e4
Submit Date
Finish Date
Paired Samples
Total Aligned Features
Parameter ID#
Log
Shared
2017-03-16 09:45:02
2017-03-16 10:30:58
False
3515
LW_TripleTof_Negativ (21944)
View Log
Shared with User(s) | [Stop sharing]
The finished job has the following notes:
2017-03-16 10:15:14 : iHeatMap data prep, memory requires limiting to top 1000 features <0.305803 p-values
Citation Links
Results Table
Metabolomic Cloud Plot
Interactive Heatmap
IPCA
Activity Network (Connections)
Multi-Omics Data
Systems Biology Results
Pathway Cloud Plot
Total Ion Chromatograms (original)
Retention Time Deviation vs. Retention Time
Total Ion Chromatograms (corrected)
Cloud Plot
Non-Metric Multidimensional Scaling
PCA Scores
PNG PDF


Total Ion Chromatograms (original)
TIC
0
5000
10000
15000
20000
25000
0
5
10
15
20
25
30
Retention Time (minutes)
neg_c1
neg_c2
neg_c3
neg_c4
neg_c5
neg_c6
neg_g1
neg_g2
neg_g3
neg_g4
neg_g5
neg_g6

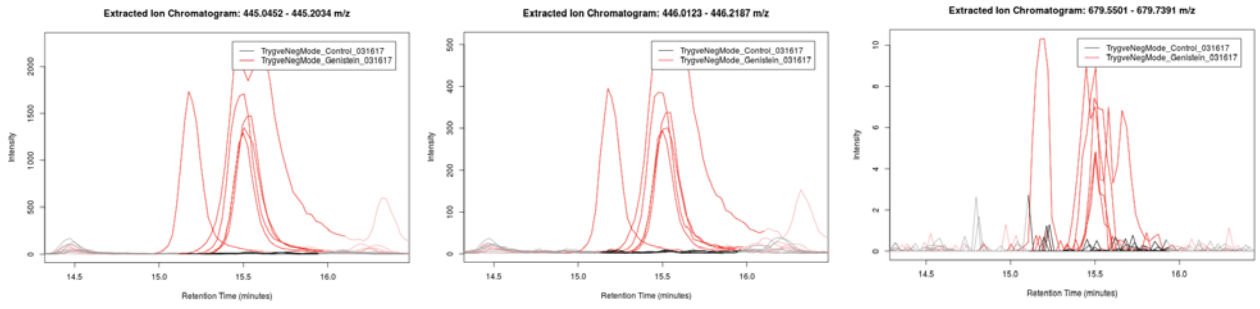

Retention Time Deviation vs. Retention Time
Retention Time Deviation (minutes)
-0.2
0.0
0.2
0.4
0
5
10
15
20
25
30
Retention Time (minutes)
neg_c1
neg_c2
neg_c3
neg_c4
neg_c5
neg_c6
neg_g1
neg_g2
neg_g3
neg_g4
neg_g5
neg_g6


Total Ion Chromatograms (corrected)
TIC
0
5000
10000
15000
20000
25000
0
5
10
15
20
25
30
Retention Time (minutes)
neg_c1
neg_c2
neg_c3
neg_c4
neg_c5
neg_c6
neg_g1
neg_g2
neg_g3
neg_g4
neg_g5
neg_g6


Cloud Plot 256 features with p-value ≤ 0.1 , fold change ≥ 1.5
m/z
1000
800
600
400
200
0
200
400
600
800
1000
5
10
15
20
25
30
Retention time (minutes)

Go to your download folder and unzip the Results file. Then open it.

Open the EIC folder



These are uncorrected for retention time variation between samples

Name	Date Modified	Size	Kind
boxplot	Mar 16, 2017, 10:59 AM	--	Folder
CloudPlot-svg.svg	Mar 16, 2017, 11:06 AM	1.4 MB	SVG Document
CloudPlot.pdf	Mar 16, 2017, 11:05 AM	509 KB	PDF Document
CloudPlot.png	Mar 16, 2017, 11:05 AM	70 KB	PNG image
EIC	Mar 16, 2017, 11:03 AM	--	Folder
MDS.pdf	Mar 16, 2017, 11:03 AM	5 KB	PDF Document
MDS.png	Mar 16, 2017, 11:03 AM	17 KB	PNG image
ms2_spectra	Mar 16, 2017, 11:18 AM	--	Folder
mummichog	Mar 16, 2017, 11:18 AM	--	Folder
MVstats_ScalingPlot_1150303.pdf	Mar 16, 2017, 11:03 AM	94 KB	PDF Document
PCA-diagnostics.pdf	Mar 16, 2017, 11:03 AM	5 KB	PDF Document
PCA-diagnostics.png	Mar 16, 2017, 11:03 AM	5 KB	PNG image
PCA-loadings-all.pdf	Mar 16, 2017, 11:03 AM	32 KB	PDF Document
PCA-loadings-all.png	Mar 16, 2017, 11:03 AM	38 KB	PNG image
PCA.pdf	Mar 16, 2017, 11:03 AM	5 KB	PDF Document
PCA.png	Mar 16, 2017, 11:03 AM	22 KB	PNG image

Open this Excel file

XCMS-diffreport-MultiClass.xlsx	Mar 16, 2017, 11:03 AM	1.5 MB	Micros...(.xlsx)
XCMS.annotated.diffreport..TrygveNegMode_Co...031617.vs.TrygveNegMode_Genistein_031617.tsv	Mar 16, 2017, 11:04 AM	1.7 MB	Plain Text
XCMS.diffreport..TrygveNegMode_Control_031617.vs.TrygveNegMode_Genistein_031617.tsv	Mar 16, 2017, 11:03 AM	1.7 MB	Plain Text
XCMSOnline_log.txt	Mar 16, 2017, 11:06 AM	2 KB	Plain Text

name	fold	log2fold	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
M576T16	2.140863	1.098192	6.471971	0.000187	1	UP	576.0311	576.0295	576.0343	15.55267	15.50438	15.57185
M588T16	2.503567	1.323985	5.924246	0.000274	1	UP	588.0089	588.0058	588.0124	15.53854	15.4518	15.55267
M586T16	4.399275	2.137266	7.286641	0.000405	1	UP	586.0128	586.0107	586.0144	15.52853	15.50395	15.57185
M936T16	3.705296	1.889589	7.288022	0.000524	1	UP	936.1249	936.1182	936.1251	15.55267	15.52048	15.58452
M544T16	4.175901	2.062087	6.676605	0.000975	1	UP	544.038	544.0277	544.0401	15.58208	15.17577	15.63362
M565T16	2.499698	1.321754	5.367571	0.001252	1	UP	565.0197	565.0178	565.023	15.52993	15.19867	15.54638
M587T16	2.684865	1.42485	5.027966	0.001384	1	UP	587.0171	587.0103	587.0213	15.52993	15.19867	16.12952
M400T26	1.206201	-0.27047	-4.35801	0.001426	1	DOWN	399.8719	399.8648	399.8725	25.9475	25.92167	25.9885
M445T17	1.717576	-0.78037	-4.22913	0.001766	1	DOWN	445.2424	445.2296	445.2437	17.4055	17.33333	17.50667
M508T16	3.277203	1.712465	5.257903	0.001788	1	UP	508.0811	508.0762	508.0856	15.51506	15.19867	15.5307
M591T16	4.838643	2.274602	5.525247	0.002122	1	UP	591.0061	591.0034	591.0077	15.50438	15.19867	15.58045
M591T18	3.32535	1.733506	4.647917	0.002695	1	UP	591.0354	591.0306	591.0429	18.338	18.219	18.42767
M513T16_	2.55776	1.354881	4.319248	0.002796	1	UP	513.0706	513.0693	513.0715	15.54638	15.19867	15.55518
M718T16	1.978588	0.984471	4.341172	0.002799	1	UP	718.111	718.1045	718.1116	15.59753	15.52993	15.69347
M535T16	4.812779	2.26687	5.262474	0.002836	1	UP	535.0422	535.0415	535.0425	15.52517	15.4769	15.66007
M575T16	5.225725	2.385631	5.278349	0.002963	1	UP	575.0318	575.0301	575.0334	15.55745	15.52993	15.74043
M590T16	3.467603	1.793939	4.749198	0.003298	1	UP	590.0077	590.0032	590.0143	15.5038	15.19867	15.54638
M696T16	13.97159	3.804424	4.93442	0.00403	1	UP	695.5807	695.5769	695.5827	15.50177	15.17577	15.54638
M546T16_	4.050259	2.018014	4.91106	0.004103	1	UP	546.0116	546.0095	546.0118	15.55745	15.55267	15.98707
M467T11	3.852899	1.945944	4.526655	0.00416	1	UP	467.0841	467.0819	467.0859	10.74827	10.6722	10.77068
M913T16_	9.23821	3.207613	4.951031	0.004201	1	UP	913.1462	913.1407	913.1483	15.51164	15.19867	15.58045
M585T16	3.085587	1.625545	4.322821	0.004476	1	UP	585.0249	585.0209	585.0259	15.52993	15.52573	15.54638

Insert a new column

Create a new value - negative log p and copy this to the rest of the file

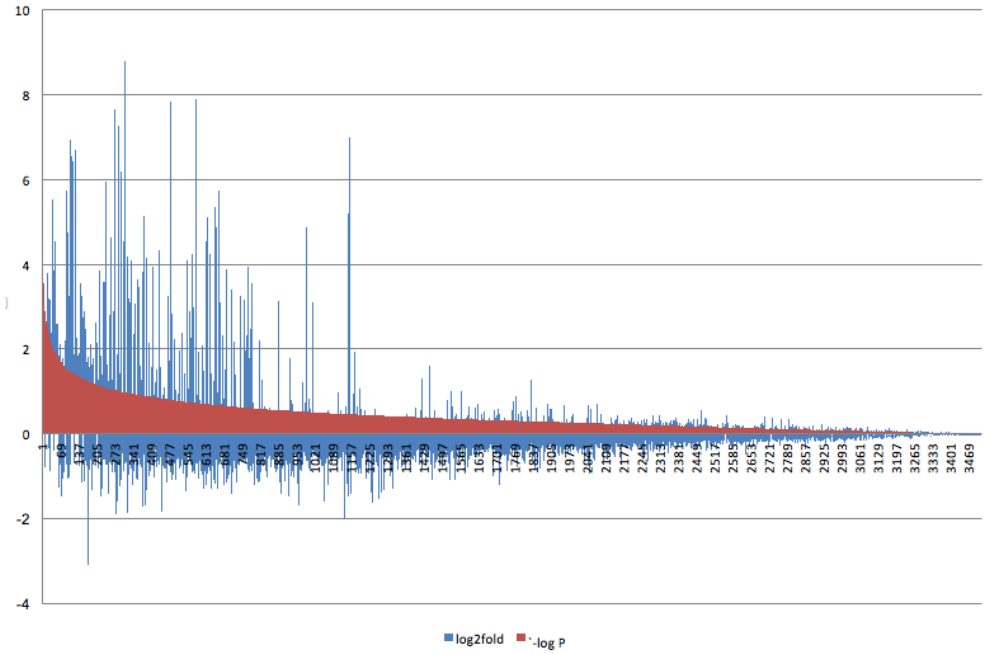
name	fold	log2fold	`-log P	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
M576T16	2.140863	1.098192	=-log(f2)	6.471971	0.000187	1	UP	576.0311	576.0295	576.0343	15.55267	15.50438	15.57185
M588T16	2.503567	1.323985		5.924246	0.000274	1	UP	588.0089	588.0058	588.0124	15.53854	15.4518	15.55267
M586T16	4.399275	2.137266		7.286641	0.000405	1	UP	586.0128	586.0107	586.0144	15.52853	15.50395	15.57185
M936T16	3.705296	1.889589		7.288022	0.000524	1	UP	936.1249	936.1182	936.1251	15.55267	15.52048	15.58452
M544T16	4.175901	2.062087		6.676605	0.000975	1	UP	544.038	544.0277	544.0401	15.58208	15.17577	15.63362
M565T16	2.499698	1.321754		5.367571	0.001252	1	UP	565.0197	565.0178	565.023	15.52993	15.19867	15.54638
M587T16	2.684865	1.42485		5.027966	0.001384	1	UP	587.0171	587.0103	587.0213	15.52993	15.19867	16.12952
M400T26	1.206201	-0.27047		-4.35801	0.001426	1	DOWN	399.8719	399.8648	399.8725	25.9475	25.92167	25.9885
M445T17	1.717576	-0.78037		-4.22913	0.001766	1	DOWN	445.2424	445.2296	445.2437	17.4055	17.33333	17.50667
M508T16	3.277203	1.712465		5.257903	0.001788	1	UP	508.0811	508.0762	508.0856	15.51506	15.19867	15.5307
M591T16	4.838643	2.274602		5.525247	0.002122	1	UP	591.0061	591.0034	591.0077	15.50438	15.19867	15.58045
M591T18	3.32535	1.733506		4.647917	0.002695	1	UP	591.0354	591.0306	591.0429	18.338	18.219	18.42767
M513T16_	2.55776	1.354881		4.319248	0.002796	1	UP	513.0706	513.0693	513.0715	15.54638	15.19867	15.55518
M718T16	1.978588	0.984471		4.341172	0.002799	1	UP	718.111	718.1045	718.1116	15.59753	15.52993	15.69347
M535T16	4.812779	2.26687		5.262474	0.002836	1	UP	535.0422	535.0415	535.0425	15.52517	15.4769	15.66007
M575T16	5.225725	2.385631		5.278349	0.002963	1	UP	575.0318	575.0301	575.0334	15.55745	15.52993	15.74043
M590T16	3.467603	1.793939		4.749198	0.003298	1	UP	590.0077	590.0032	590.0143	15.5038	15.19867	15.54638
M696T16	13.97159	3.804424		4.93442	0.00403	1	UP	695.5807	695.5769	695.5827	15.50177	15.17577	15.54638

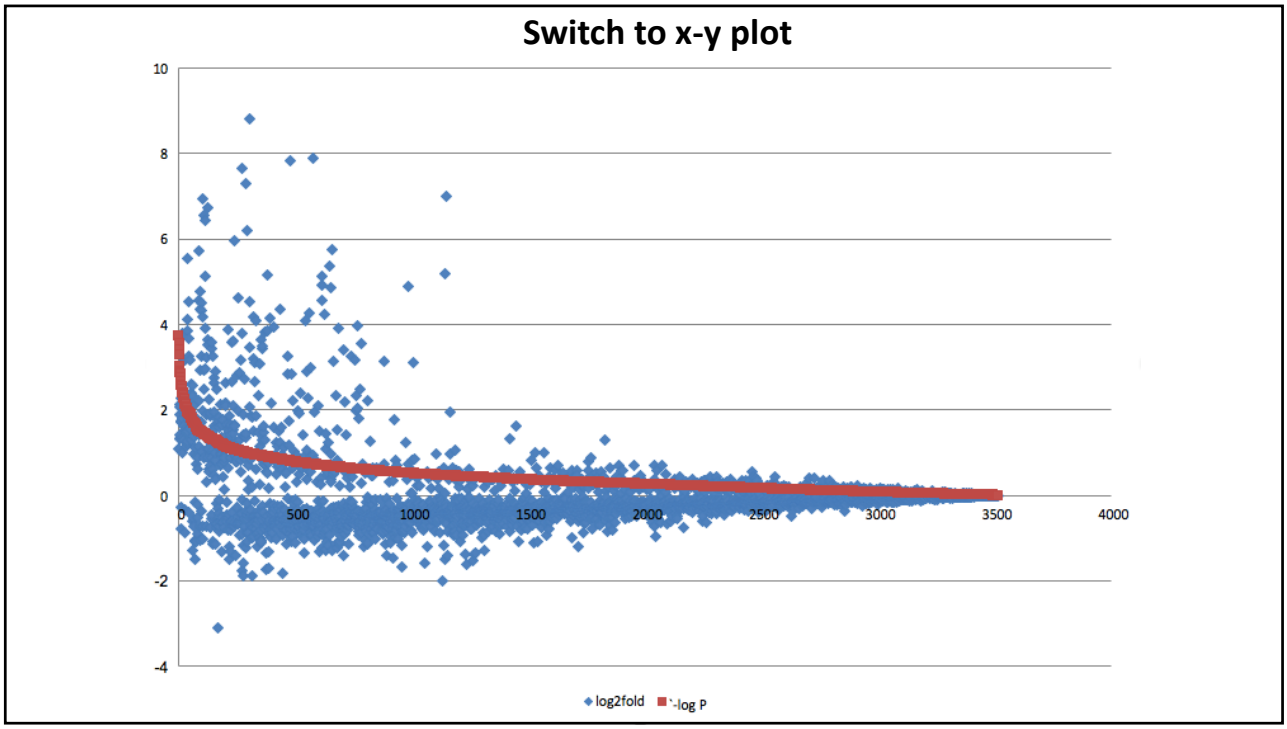
A	B	C	D	E	F	G	H	I	J	K	L	M	N
name	fold	log2fold	`-log P	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
M576T16	2.140863	1.098192	3.72813	6.471971	0.000187	1	UP	576.0311	576.0295	576.0343	15.55267	15.50438	15.57185
M588T16	2.503567	1	3.56171	5.924246	0.000274	1	UP	588.0089	588.0058	588.0124	15.53854	15.4518	15.55267
M586T16	4.399275	2.137266	3.392011	7.286641	0.000405	1	UP	586.0128	586.0107	586.0144	15.52853	15.50395	15.57185
M936T16	3.705296	1.889589	3.280374	7.288022	0.000524	1	UP	936.1249	936.1182	936.1251	15.55267	15.52048	15.58452
M544T16	4.175901	2.062087	3.010867	6.676605	0.000975	1	UP	544.038	544.0277	544.0401	15.58208	15.17577	15.63362
M565T16	2.499698	1.321754	2.902373	5.367571	0.001252	1	UP	565.0197	565.0178	565.023	15.52993	15.19867	15.54638
M587T16	2.684865	1.42485	2.858756	5.027966	0.001384	1	UP	587.0171	587.0103	587.0213	15.52993	15.19867	16.12952
M400T26	1.206201	-0.27047	2.845799	-4.35801	0.001426	1	DOWN	399.8719	399.8648	399.8725	25.9475	25.92167	25.9885
M445T17	1.717576	-0.78037	2.752906	-4.22913	0.001766	1	DOWN	445.2424	445.2296	445.2437	17.4055	17.33333	17.50667
M508T16	3.277203	1.712465	2.747717	5.257903	0.001788	1	UP	508.0811	508.0762	508.0856	15.51506	15.19867	15.5307
M591T16	4.838643	2.274602	2.673233	5.525247	0.002122	1	UP	591.0061	591.0034	591.0077	15.50438	15.19867	15.58045
M591T18	3.32535	1.733506	2.569403	4.647917	0.002695	1	UP	591.0354	591.0306	591.0429	18.338	18.219	18.42767
M513T16_	2.55776	1.354881	2.553523	4.319248	0.002796	1	UP	513.0706	513.0693	513.0715	15.54638	15.19867	15.55518
M718T16	1.978588	0.984471	2.553014	4.341172	0.002799	1	UP	718.111	718.1045	718.1116	15.59753	15.52993	15.69347
M535T16	4.812779	2.26687	2.547325	5.262474	0.002836	1	UP	535.0422	535.0415	535.0425	15.52517	15.4769	15.66007
M575T16	5.225725	2.385631	2.528257	5.278349	0.002963	1	UP	575.0318	575.0301	575.0334	15.55745	15.52993	15.74043
M590T16	3.467603	1.793939	2.48179	4.749198	0.003298	1	UP	590.0077	590.0032	590.0143	15.5038	15.19867	15.54638
M696T16	13.97159	3.804424	2.394695	4.93442	0.00403	1	UP	695.5807	695.5769	695.5827	15.50177	15.17577	15.54638
M546T16_	4.050259	2.018014	2.38694	4.91106	0.004103	1	UP	546.0116	546.0095	546.0118	15.55745	15.55267	15.98707
M467T11	3.852899	1.945944	2.380881	4.526655	0.00416	1	UP	467.0841	467.0819	467.0859	10.74827	10.6722	10.77068
M913T16_	9.23821	3.207613	2.376639	4.951031	0.004201	1	UP	913.1462	913.1407	913.1483	15.51164	15.19867	15.58045
M585T16	3.085587	1.625545	2.349125	4.322821	0.004476	1	UP	585.0249	585.0209	585.0259	15.52993	15.52573	15.54638
M592T16	2.466057	1.302206	2.288373	4.206206	0.005148	1	UP	592.014	592.0085	592.016	15.57845	15.50438	15.59753
M708T16	2.894059	1.533094	2.238925	4.110799	0.005769	1	UP	708.1911	708.1893	708.1943	15.54638	15.22163	15.68688

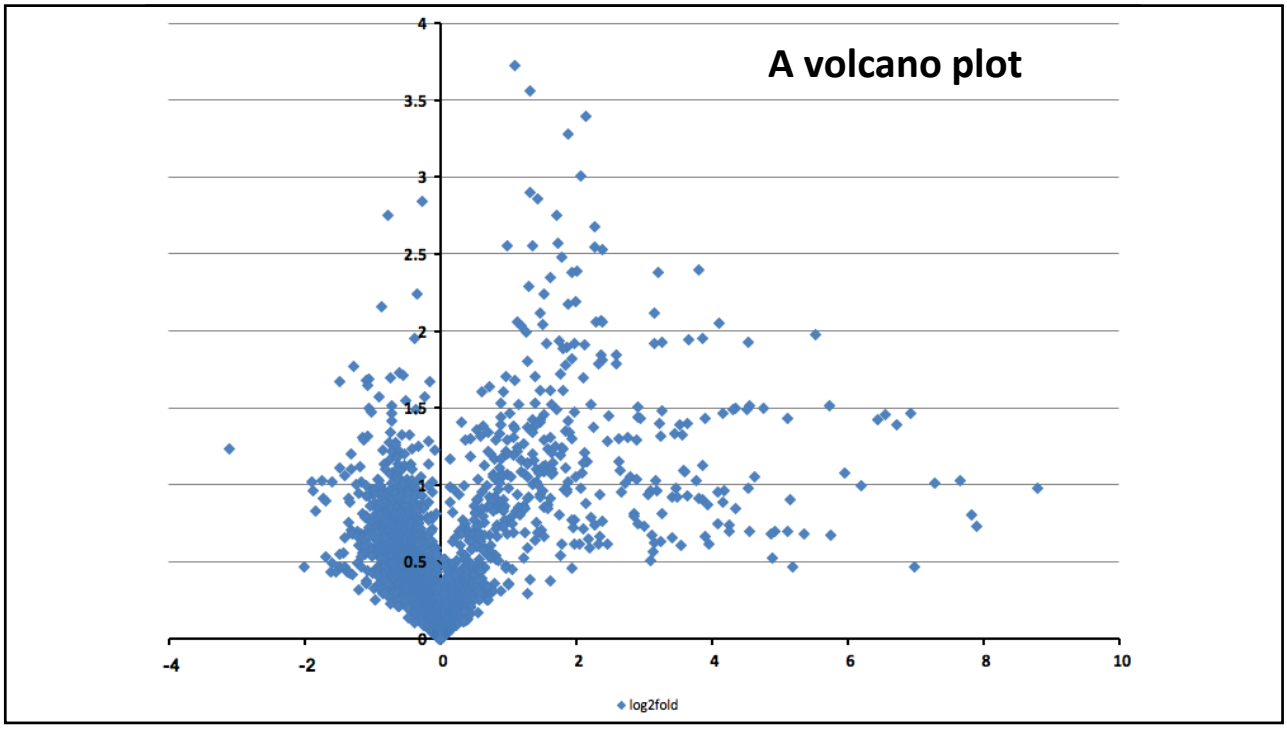
Select the log_2fold and –logP columns

name	fold	log2fold	-log P	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
M576T16	2.140863	1.098192	3.72813	6.471971	0.000187	1	UP	576.0311	576.0295	576.0343	15.55267	15.50438	15.57185
M588T16	2.503567	1.323985	3.56171	5.924246	0.000274	1	UP	588.0089	588.0058	588.0124	15.53854	15.4518	15.55267
M586T16	4.399275	2.137266	3.392011	7.286641	0.000405	1	UP	586.0128	586.0107	586.0144	15.52853	15.50395	15.57185
M936T16	3.705296	1.889589	3.280374	7.288022	0.000524	1	UP	936.1249	936.1182	936.1251	15.55267	15.52048	15.58452
M544T16	4.175901	2.062087	3.010867	6.676605	0.000975	1	UP	544.038	544.0277	544.0401	15.58208	15.17577	15.63362
M565T16	2.499698	1.321754	2.902373	5.367571	0.001252	1	UP	565.0197	565.0178	565.023	15.52993	15.19867	15.54638
M587T16	2.684865	1.42485	2.858756	5.027966	0.001384	1	UP	587.0171	587.0103	587.0213	15.52993	15.19867	16.12952
M400T26	1.206201	-0.27047	2.845799	-4.35801	0.001426	1	DOWN	399.8719	399.8648	399.8725	25.9475	25.92167	25.9885
M445T17	1.717576	-0.78037	2.752906	-4.22913	0.001766	1	DOWN	445.2424	445.2296	445.2437	17.4055	17.33333	17.50667
M508T16	3.277203	1.712465	2.747717	5.257903	0.001788	1	UP	508.0811	508.0762	508.0856	15.51506	15.19867	15.5307
M591T16	4.838643	2.274602	2.673233	5.525247	0.002122	1	UP	591.0061	591.0034	591.0077	15.50438	15.19867	15.58045
M591T18	3.32535	1.733506	2.569403	4.647917	0.002695	1	UP	591.0354	591.0306	591.0429	18.338	18.219	18.42767
M513T16_	2.55776	1.354881	2.553523	4.319248	0.002796	1	UP	513.0706	513.0693	513.0715	15.54638	15.19867	15.55518
M718T16	1.978588	0.984471	2.553014	4.341172	0.002799	1	UP	718.111	718.1045	718.1116	15.59753	15.52993	15.69347
M535T16	4.812779	2.26687	2.547325	5.262474	0.002836	1	UP	535.0422	535.0415	535.0425	15.52517	15.4769	15.66007
M575T16	5.225725	2.385631	2.528257	5.278349	0.002963	1	UP	575.0318	575.0301	575.0334	15.55745	15.52993	15.74043
M590T16	3.467603	1.793939	2.48179	4.749198	0.003298	1	UP	590.0077	590.0032	590.0143	15.5038	15.19867	15.54638
M696T16	13.97159	3.804424	2.394695	4.93442	0.00403	1	UP	695.5807	695.5769	695.5827	15.50177	15.17577	15.54638

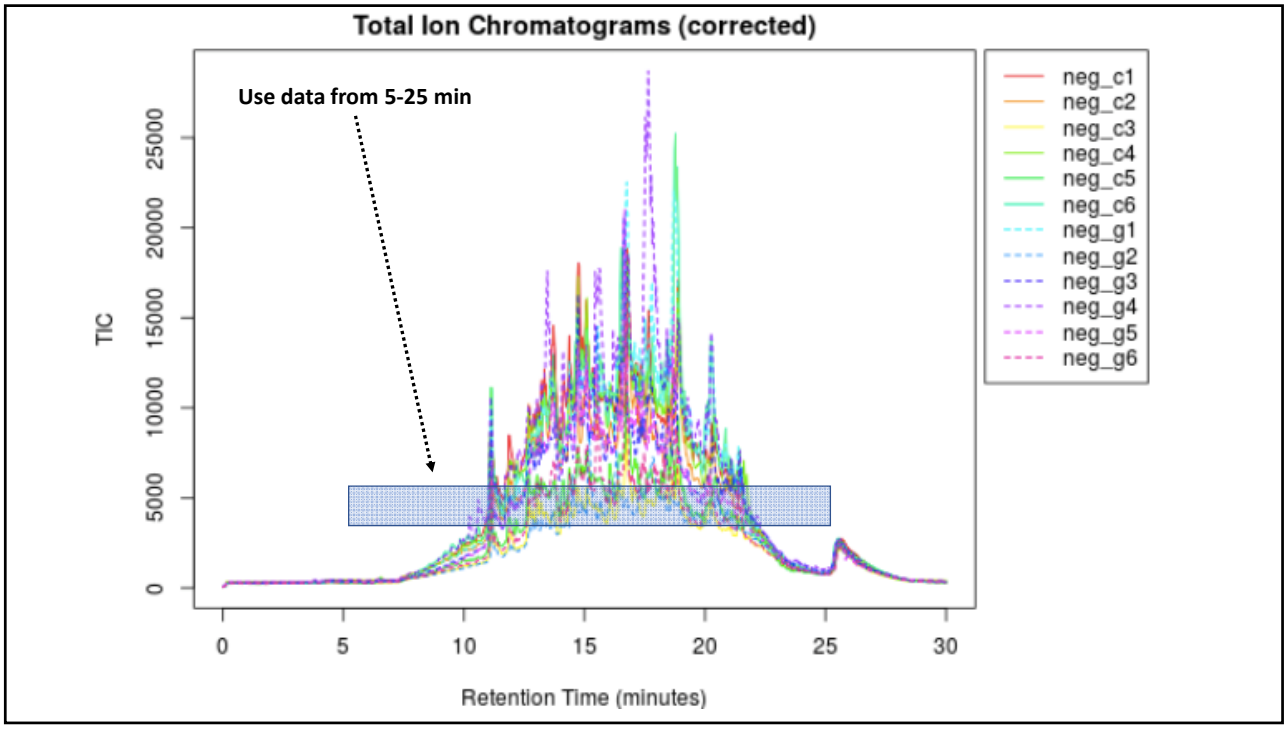
Select the Insert Chart Sheet



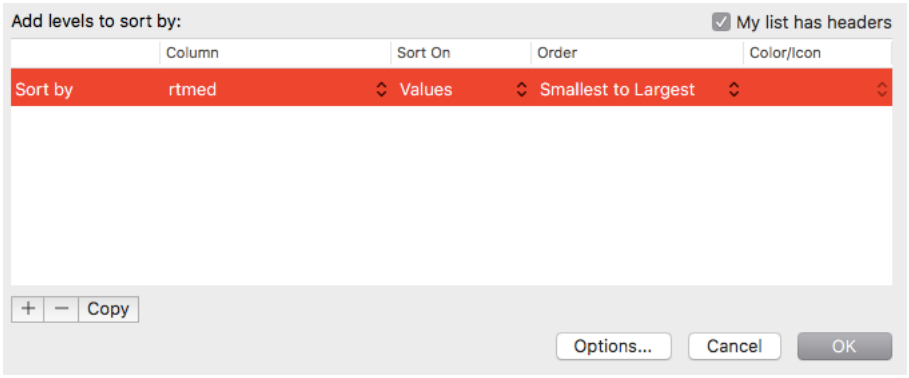

Switch to x-y plot
10
8
6
4
2
0
-2
-4
0
500
1000
1500
2000
2500
3000
3500
4000
log2fold
-log p


A volcano plot
4
3.5
3
2.5
2
1.5
1
0.5
0
-4
-2
0
2
4
6
8
10
log2fold

Let's think about data clean up



Highlight all the values and sort by RT



name	fold	log2fold	-log P	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
M105T5	1.050711	0.071366	0.120742	0.319106	0.757283	1	UP	105.0217	105.0194	105.0222	5.1857	4.888033	5.2445
M334T6	1.222371	-0.28968	0.253912	-0.61151	0.557298	1	DOWN	333.9268	333.9251	333.9274	6.371983	6.162383	7.366083
M224T6	1.177229	-0.2354	0.142043	-0.37222	0.721036	1	DOWN	224.0226	224.0194	224.0244	6.493717	6.309783	6.61305
M147T7	1.426047	-0.51202	0.459834	-1.00539	0.34687	1	DOWN	147.0316	147.0316	147.0317	6.820717	6.751233	6.844433
M167T7	1.057884	-0.08118	0.047643	-0.13401	0.896101	1	DOWN	167.0227	167.0201	167.023	7.151567	6.973867	7.51065
M424T7	1.332956	-0.41463	0.373322	-0.83593	0.423329	1	DOWN	424.0473	424.0454	424.0485	7.463533	7.3086	7.527617
M164T7	1.340476	-0.42275	0.425099	-0.9307	0.375752	1	DOWN	164.0579	164.0569	164.059	7.498233	7.429017	7.53495
M85T8	1.407615	-0.49325	0.605089	-1.23368	0.248262	1	DOWN	85.03211	85.0298	85.03233	7.791883	7.778733	7.820667
M174T8	1.334217	-0.41599	0.559818	-1.15586	0.275538	1	DOWN	174.0145	174.0126	174.0153	7.797617	7.778733	7.820667
M129T8	1.489987	-0.5753	0.772405	-1.49275	0.168887	1	DOWN	129.0213	129.0193	129.0219	7.802633	7.6612	7.840333
M173T8	1.504456	-0.58924	0.72658	-1.42012	0.187681	1	DOWN	173.0107	173.0088	173.0113	7.802825	7.6612	7.8707
M496T25	1.139357	0.18822	0.633331	1.288399	0.232632	1	UP	495.9715	495.9689	495.9738	25.00017	24.95883	25.00983
M431T25	1.021877	0.031222	0.115077	0.305121	0.767226	1	UP	430.9727	430.9708	430.9741	25.00217	24.95883	25.058
M385T25	1.003144	0.004529	0.01087	0.032382	0.975282	1	UP	384.9347	384.9331	384.9361	25.00292	24.9335	25.0965
M495T25	1.005987	0.008612	0.025032	0.072042	0.943991	1	UP	494.9683	494.9659	494.9699	25.00833	24.95883	25.06417
M249T25	1.023991	-0.0342	0.126218	-0.33107	0.747794	1	DOWN	248.9613	248.96	248.9622	25.03975	24.9625	25.12867
M519T25	1.003697	0.005323	0.014164	0.041253	0.967913	1	UP	519.2764	519.2725	519.2778	25.176	25.09467	25.2295
M233T25	1.006647	-0.00956	0.040171	-0.1154	0.911652	1	DOWN	233.1558	233.1549	233.1571	25.20558	25.12967	25.333
M305T25	1.07437	-0.10349	0.414531	-0.92756	0.385008	1	DOWN	304.914	304.9128	304.916	25.38167	25.30683	26.71133
M289T27	1.071558	-0.09971	0.477152	-1.02136	0.33331	1	DOWN	288.9097	288.9086	288.9103	26.6255	26.4825	26.72217
M269T27	1.124123	-0.1688	1.132054	-2.02451	0.073781	1	DOWN	268.9276	268.9266	268.9282	26.641	26.54625	26.731
M205T27	1.079969	-0.11099	1.021354	-1.8455	0.095202	1	DOWN	204.958	204.9564	204.9585	26.68458	26.59933	26.873
M159T27	1.006981	0.010036	0.037471	0.106593	0.917336	1	UP	158.9528	158.9509	158.9531	26.71267	26.62933	26.81467
M340T27	1.190511	-0.25158	0.303642	-0.7089	0.497002	1	DOWN	339.9193	339.9179	339.9199	26.725	26.641	26.93983
M255T27	1.110606	-0.15135	1.668296	-3.06324	0.021464	1	DOWN	254.9397	254.9386	254.9404	26.92492	26.83833	27.06083

Delete these rows

Further filtering

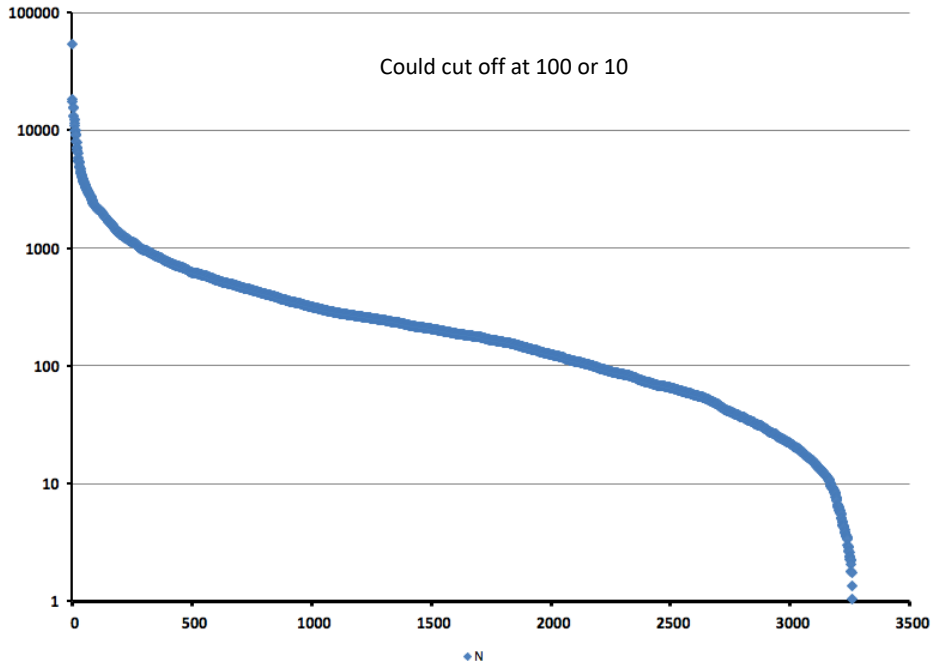
npeaks	TrygveNegMo	TrygveNegMo	maxint	mean1	sd1	mean2	sd2
12	6	6	3.9481508	78.9094857	16.7131056	82.9110786	25.771763
13	5	6	9.44552755	126.968236	48.1737646	103.870479	78.9900664
9	4	5	12.3016678	12.7295116	11.5712936	10.8131116	5.01535392
3	3	0	2.81247811	14.752113	9.62930528	10.3447617	4.75162395
7	3	2	1.77701455	8.99689686	5.9311881	8.50461298	6.76702648
10	5	5	4.5349935	49.9239188	28.0611904	37.4535515	23.4056952
8	4	4	0.96557111	6.39327491	3.43520826	4.7694047	2.54264818
5	3	2	1.66889827	9.25189259	4.31521183	6.57274156	3.11059733
5	3	2	3.39486906	22.5835622	9.24370059	16.9264581	7.63395379
10	5	5	14.9457158	101.425265	43.9497323	68.0712464	32.6180976
12	6	6	43.7795186	299.312351	136.252632	198.950541	106.779792
9	6	3	5.97004374	63.5537292	37.6056533	46.5565446	24.5921515
4	1	3	0.9169914	4.33886308	2.6572228	3.95130184	1.74293841
9	5	4	1.74138452	9.15309247	5.78062828	7.77448948	3.91714233
9	5	4	5.44174685	30.4690828	14.3219784	24.6519792	13.7883399
5	3	2	4.08796153	11.4250686	13.1041826	8.62546339	9.73833698
5	3	2	11.2416273	15.2033055	26.5169106	6.63705609	7.85268256
3	3	0	7.52435681	11.2952303	16.2320351	3.52514656	1.056735
11	6	5	4.37547922	81.8886496	35.7221773	64.509303	23.5169926
10	5	5	26.6051098	64.710185	67.5815473	33.7580415	35.0310099
5	3	2	8.43573476	17.8571222	20.4223134	7.94362795	4.70324952
3	3	0	3.01761924	9.26971358	7.49155625	5.14986019	1.91670266

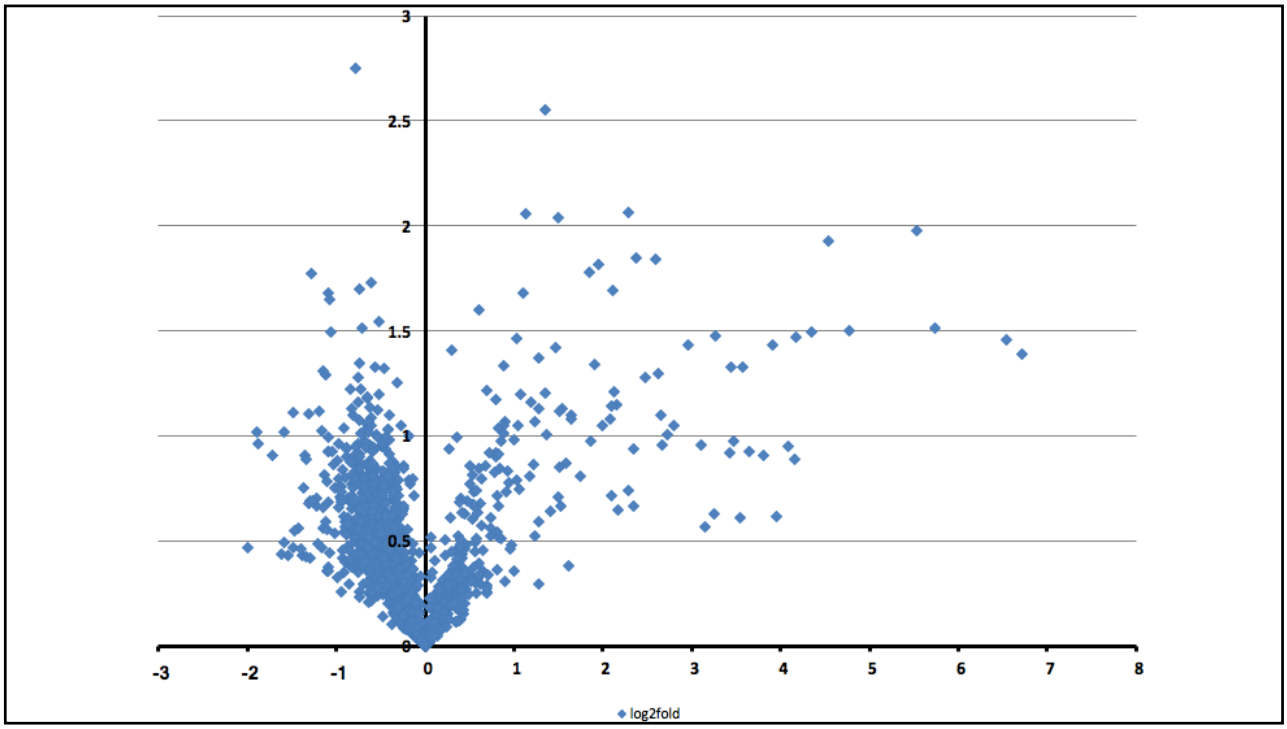
Order by "npeaks" – delete those with <6

Order by mean1 – high to low

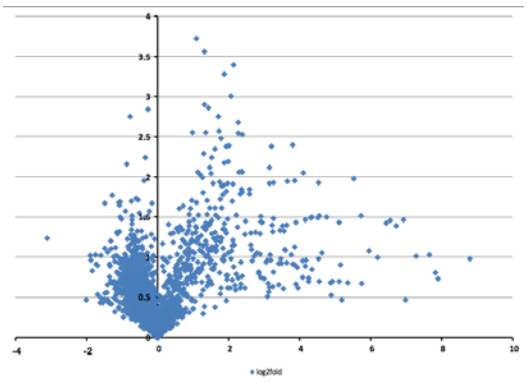
Copy "Mean1" to a new sheet and add numbers to column A

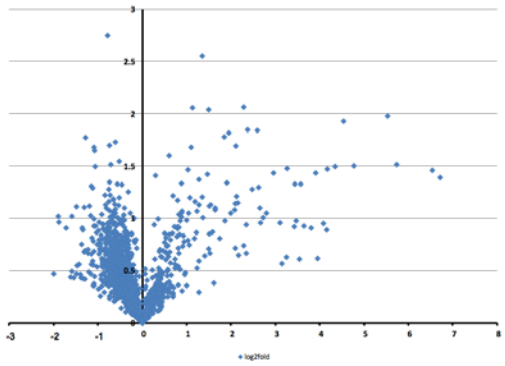
N	mean1
1	53679.6231
2	18370.82
3	17353.8765
4	15633.4487
5	15586.7788
6	15474.6495
7	13299.5466
8	13248.6918
9	12398.9935
10	12379.0473
11	11531.4527
12	10878.652
13	10045.869
14	10034.3588
15	9240.04201
16	9167.63798
17	9086.15151
18	8086.17968
19	7827.71298
20	7215.50625
21	6933.31371
22	6714.43152
23	6615.06798
24	6446.55975
25	5842.27992
26	5819.35538





Effect of data clean up





Restricting to >100 cleaned up high fold changes with low p-values

Preparing for statistical analysis

Data for the individual urine samples

neg_c1	neg_c2	neg_c3	neg_c4	neg_c5	neg_c6	neg_g1	neg_g2	neg_g3	neg_g4	neg_g5	neg_g6
40108.6713	59975.0081	12493.5865	48408.3362	24307.6739	136784.463	121268.815	1798.85036	27801.3707	30026.8289	50152.5527	26989.1869
11800.0812	3687.9242	12674.2151	17473.0154	22323.9784	42265.7056	20655.8963	2993.6482	19541.5526	21503.2335	12761.3812	17981.8697
10605.1862	16509.689	14505.1051	26280.187	21081.0496	15142.0419	25282.2785	3032.72622	19582.367	30154.7717	7711.11059	9164.14869
15294.1991	13827.534	7058.50493	20562.2619	12447.0632	24611.1292	18506.882	4648.5004	16722.3128	20498.8636	9701.95075	10335.6156
20179.2207	25237.4428	11365.4755	17759.2326	17626.2779	1353.02329	8566.23371	7265.17353	8733.29388	22140.3781	5270.88327	8540.31692
19107.5341	20687.2477	3362.18366	17455.9182	5673.87308	26561.1406	15306.1461	817.97323	8390.26737	3101.61675	21902.4612	13000.4113
10051.866	14705.8879	3002.20415	12161.3571	5988.16122	33887.803	29748.9287	482.83231	6940.85338	7564.6735	12349.6928	6502.06622
26716.3293	2029.94527	5319.90018	20833.5463	8782.21363	15810.216	9473.79361	8736.55277	25682.6864	13129.3567	17656.4464	11377.7283
17320.1107	21544.96	4028.08522	15700.4543	6605.32931	9195.02147	6714.94811	645.733827	10546.1269	1445.34399	14564.3873	12757.319
7517.56134	8879.55236	4587.39506	14048.6826	7619.29374	31621.7986	24179.8711	4706.69962	10446.9647	32179.5292	4200.95061	8686.60196
15253.1527	10469.7465	4330.5906	15455.5443	6289.55847	17390.1238	15504.2599	3810.85418	10268.1122	5905.12764	10069.3987	9837.52168
5969.63146	10561.4083	7851.91828	17888.8542	12128.5999	10871.4996	13748.9189	1569.48359	9992.70525	18327.2186	4047.67876	6431.84234
7112.47831	6526.35242	1950.68618	9512.31281	5678.48838	29494.8961	11659.7285	1158.70184	3855.90855	20044.2904	3130.80371	5376.95117
13121.4963	14219.5815	4494.30258	12413.4768	6768.40885	9188.88677	17666.2276	4482.45998	8120.58709	4982.45671	8367.02041	6552.1173
26995.2478	179.84724	840.684661	15744.5834	2383.14793	9296.74104	3319.22912	2113.16724	23716.1375	5470.95061	10696.3593	4314.11922
22143.8068	638.964003	2580.98485	15116.386	4260.83314	10264.8532	7041.96146	3873.61641	12937.8095	4171.48653	10868.4369	5183.45726
9876.06282	12196.1746	5767.45377	12523.7796	8046.79264	6106.64566	9278.61248	4213.43042	8710.05301	10663.3207	7897.18798	6988.64851
7853.92191	7888.45117	8840.50979	8412.19764	8701.92631	6820.07127	7829.43591	8880.86794	8768.95437	7903.35442	8622.91763	8667.57827
7186.69537	5721.68255	1315.6735	11840.0847	4456.34174	16445.8	9670.23473	587.112472	6519.53566	11100.1892	2467.88388	2849.95906
4517.39182	6492.80158	5613.99657	11650.4023	8689.54899	6328.89621	10027.0427	1458.0806	7387.59185	10434.2819	3250.76678	3815.40354
7586.06852	8149.55526	1934.96827	9611.99622	4100.99654	10216.2974	9542.74119	1233.83597	3767.55226	4798.50905	3100.54869	3036.11322
10037.5731	11205.0449	3017.78793	8109.90389	5920.75112	1995.52823	9856.9007	1404.20882	7068.50107	9535.55215	5951.10288	6054.13671

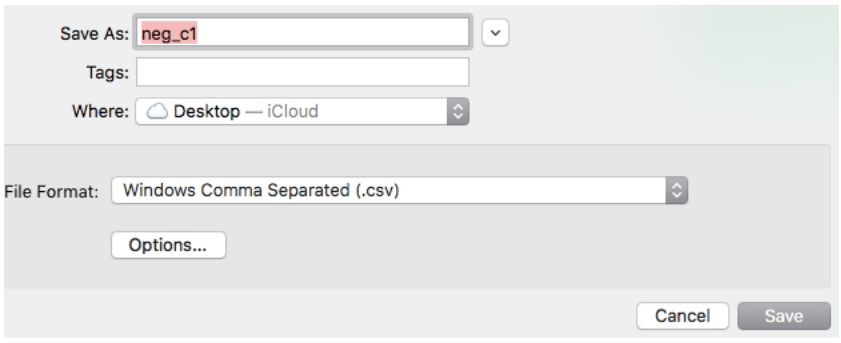
mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
427.179352	427.178095	427.181481	18.9075	18.7238333	18.9741667
275.096941	275.094306	275.097857	18.5358333	18.3706667	18.6298333
291.091565	291.090032	291.092346	16.8475	16.4415	17.071
411.126885	411.124417	411.128122	11.14365	11.1280667	11.1824167
341.124739	341.123427	341.126325	16.749	16.33	16.8451667
443.174191	443.167258	443.175216	13.70095	12.68755	13.7689167
428.182929	428.181389	428.184744	18.9075	18.7238333	18.9741667
283.083339	283.081957	283.085577	14.7544667	14.5198167	15.0729667
441.158755	441.156953	441.160012	15.0476417	14.76965	15.0953
361.202156	361.200842	361.204036	20.28525	20.1951667	20.4195
369.15603	369.154269	369.157345	21.4533333	21.4208333	21.7203333
319.123	319.121604	319.126127	18.5153333	18.3706667	18.6006667
537.233525	537.2305	537.235119	18.4066667	18.2481667	18.4825
144.047656	144.045737	144.048336	17.1201667	16.7375	17.1853333
567.170865	567.169426	567.172552	14.72745	14.5198167	14.7542333
187.008548	187.006968	187.00925	15.17885	14.9114333	15.2287
273.043043	273.03771	273.050438	13.0360167	12.9895833	13.19575
311.169348	311.16829	311.170372	21.87625	21.6735	22.201
823.260913	823.254937	823.263196	11.1297833	11.1033667	11.1561
309.10194	309.100489	309.102782	15.432975	15.0803667	15.4784833
404.19163	404.190416	404.193155	13.3802833	13.3484	13.42055

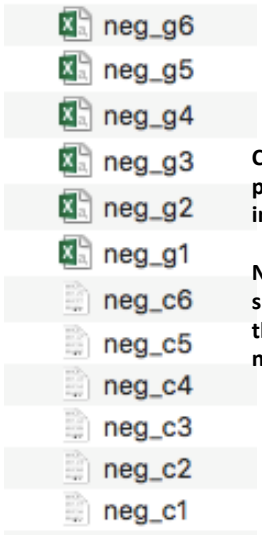
Transfer the mzmed and rtmed column data over to a new Excel file.

mzmed	rtmed
427.179352	18.9075
275.096941	18.5358333
291.091565	16.8475
411.126885	11.14365
341.124739	16.749
443.174191	13.70095
428.182929	18.9075
283.083339	14.7544667
441.158755	15.0476417
361.202156	20.28525
369.15603	21.4533333
319.123	18.5153333
537.233525	18.4066667
144.047656	17.1201667
567.170865	14.72745
187.008548	15.17885
273.043043	13.0360167
311.169348	21.87625
823.260913	11.1297833
309.10194	15.432975
404.19163	13.3802833
349.094511	14.3883
429.183945	18.8019167
407.1023	12.70755
377.195448	16.7926667

mzmed	rtmed	neg_c1
427.179352	18.9075	40108.6713
275.096941	18.5358333	11800.0812
291.091565	16.8475	10605.1862
411.126885	11.14365	15294.1991
341.124739	16.749	20179.2207
443.174191	13.70095	19107.5341
428.182929	18.9075	10051.866
283.083339	14.7544667	26716.3293
441.158755	15.0476417	17320.1107
361.202156	20.28525	7517.56134
369.15603	21.4533333	15253.1527
319.123	18.5153333	5969.63146
537.233525	18.4066667	7112.47831
144.047656	17.1201667	13121.4963
567.170865	14.72745	26995.2478
187.008548	15.17885	22143.8068
273.043043	13.0360167	9876.06282
311.169348	21.87625	7853.92191
823.260913	11.1297833	7186.69537
309.10194	15.432975	4517.39182
404.19163	13.3802833	7586.06852
349.094511	14.3883	10037.5731
429.183945	18.8019167	4967.60239

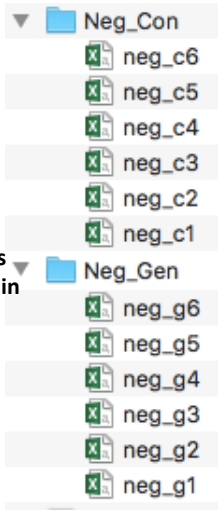
Add the values for neg_c1 and then save as a .csv file. Replace the third column for all the urine samples and save as .csv files (you don't need to transfer the mzmed and rtmed data).





Create two folders and put the individual files into them.

Note all files and folders should not have spaces in them. Use undersore as necessary.



Now "zip" up the two folders and give it a name.

Suggestion – Class_neg.zip

We're ready for stats analysis