





			V	'iew	ing the	e dat	ase	ets		
	PAIR	VIEW	1052098	job complete	MCF10AT_NTVec vs KD1_NegMode	MCF10AT_NT (#89883) MCF10AT_KD (#89884)	2015-03-19 16:22:46	NanoLc Neg (10374)	Shared [Stop sharing]	×
	PAIR	VIEW	1052085	job complete	MCF10AT_NTVec vs KD1_PosMode	MCF10AT_NT (#89683) MCF10AT_KD (#89684)	2015-03-19 14:10:30	nanoLC_560 (9920)	Shared [Stop sharing]	×
	PAIR	VIEW	1051960	job complete	PAIR_2015-03-18_17:24	Sham_Cutts (#115973) GSE_Cutts_ (#115883)	2015-03-18 17:24:58	nanoLC_560 (9920)		×
	PAIR	VIEW	1051941	job complete	SUM159VMP_VS_NF2c16_N egMode	SUM159_VMP (#89938) SUM159_NF2 (#89955)	2015-03-18 13:24:52	NanoLc Neg (10374)	Shared [Stop sharing]	×
0	PAIR	VIEW	1051935	job complete	SUM159VMP_VS_NF2c16_Po sMode	SUM159_VMP (#89688) SUM159_NF2 (#89689)	2015-03-18 12:07:33	nanoLC_560 (9920)	Shared [Stop sharing]	×
	PAIR	VIEW	1051415	job complete	Grubbs_urine_pos_mmchg	Grubbs_Uri (#107301) Grubbs_Uri (#107315)	2015-03-12 19:11:09	nanoLC_560 (9920)	Shared [Stop sharing]	×
	PAIR	VIEW	1051379	job complete	Aman Set 3 Comparison	Aman_Set3_ (#115309) Aman_Set3- (#115234)	2015-03-12 13:21:25	nanoLC_560 (9920)	Shared [Stop sharing]	×
	PAIR	VIEW	1051373	job complete	Grubbs_urine_neg_mmchg	Grubbs_Uri (#107534) Grubbs_Uri (#107626)	2015-03-12 12:19:17	NanoLC5600 (10377)		×
	PAIR	VIEW	1051324	job complete	Grubbs_diet_neg_mmchg	Grubbs_Non (#108897) Grubbs_Irr (#108890)	2015-03-12 05:55:12	NanoLc Neg (10374)	Shared [Stop sharing]	×
	PAIR		1051271	job complete	Grubbs_diet_pos_mmchg	Grubbs_Non (#109003) Grubbs_Irr (#108990)	2015-03-11 22:05:58	nanoLC_560 (9920)	Shared [Stop sharing]	×
	PAIR	VIEV	1050983	job complete	Sera Positive Mode	McLean_Har (#114812) McLean_Har (#114794)	2015-03-09 22:30:49	nanoLC_560 (9920)		×
0	PAIR	VIEW	1047227	job complete	Grubbs_Diet_PosMode	Grubbs_Irr (#108990) Grubbs_Non (#109003)	2015-02-05 17:51:27	nanoLC_560 (9920)	Shared [Stop sharing]	×









►		boxplot	Mar 12, 2015, 6:19 AM		Folder
	0	CloudPlot-svg.svg Ion chromatograms	Mar 12, 2015, 6:52 AM	968 KB	SVG document
		CloudPlot.pdf	Mar 12, 2015, 6:52 AM	366 KB	PDF Document
		CloudPlot.png	Mar 12, 2015, 6:52 AM	99 KB	PNG image
►		EIC	Mar 12, 2015, 6:21 AM		Folder
	-	Heatmap_1051324.png	Mar 12, 2015, 6:22 AM	45 KB	PNG image
	28	Heatmap_Cor_1051324.png	Mar 12, 2015, 6:51 AM	356 KB	PNG image
		MDS.pdf	Mar 12, 2015, 6:51 AM	5 KB	PDF Document
		MDS.png	Mar 12, 2015, 6:51 AM	15 KB	PNG image
►		mummichog	Mar 12, 2015, 6:24 AM		Folder
		MVstats_ScalingPlot_1051324.pdf	Mar 12, 2015, 6:51 AM	105 KB	PDF Document
	-	PCA-diagnostics.pdf	Mar 12, 2015, 6:51 AM	5 KB	PDF Document
		PCA-diagnostics.png	Mar 12, 2015, 6:51 AM	5 KB	PNG image
	-	PCA-loadings-all.pdf	Mar 12, 2015, 6:51 AM	35 KB	PDF Document
	-	PCA-loadings-all.png	Mar 12, 2015, 6:51 AM	20 KB	PNG image
	-	PCA.pdf	Mar 12, 2015, 6:51 AM	5 KB	PDF Document
		PCA.png	Mar 12, 2015, 6:51 AM	18 KB	PNG image
		result.tsv	Mar 12, 2015, 6:52 AM	1.4 MB	Plain Text
	-	rtcor.pdf	Mar 12, 2015, 6:17 AM	61 KB	PDF Document
		rtcor.png	Mar 12, 2015, 6:17 AM	40 KB	PNG image
		TICs_rtcor.pdf	Mar 12, 2015, 6:17 AM	70 KB	PDF Document
		TICs_rtcor.png	Mar 12, 2015, 6:17 AM	63 KB	PNG image
		TICs.pdf	Mar 12, 2015, 6:13 AM	71 KB	PDF Document
		TICs.png	Mar 12, 2015, 6:13 AM	62 KB	PNG image
		XCMS.annotated.diffreiatedDiet_NegMode.tsv	Mar 12, 2015, 6:52 AM	1.5 MB	Plain Text
		XCMS.diffreportGrubiatedDiet_NegMode.tsv	Mar 12, 2015, 6:21 AM	1.5 MB	Plain Text
	X	XCMS.diffreportGrubatedDiet_NegMode.xlsx	Mar 12, 2015, 6:22 AM	1.2 MB	Micros(.xlsx)
		XCMSOnline_log.txt	Mar 12, 2015, 6:52 AM	2 KB	Plain Text





►		boxplot		Mar 12, 2015, 6:19 AM	**	Folder
	0	CloudPlot-svg.svg		Mar 12, 2015, 6:52 AM	968 KB	SVG document
	-	CloudPlot.pdf		Mar 12, 2015, 6:52 AM	366 KB	PDF Document
		CloudPlot.png		Mar 12, 2015, 6:52 AM	99 KB	PNG image
►		EIC		Mar 12, 2015, 6:21 AM		Folder
	00	Heatmap_1051324.png		Mar 12, 2015, 6:22 AM	45 KB	PNG image
	25	Heatmap_Cor_1051324.png		Mar 12, 2015, 6:51 AM	356 KB	PNG image
	-	MDS.pdf		Mar 12, 2015, 6:51 AM	5 KB	PDF Document
		MDS.png		Mar 12, 2015, 6:51 AM	15 KB	PNG image
►		mummichog		Mar 12, 2015, 6:24 AM		Folder
	-	MVstats_ScalingPlot_1051324.pdf	F.	Mar 12, 2015, 6:51 AM	105 KB	PDF Document
	-	PCA-diagnostics.pdf		Mar 12, 2015, 6:51 AM	5 KB	PDF Document
		PCA-diagnostics.png		Mar 12, 2015, 6:51 AM	5 KB	PNG image
	-	PCA-loadings-all.pdf		Mar 12, 2015, 6:51 AM	35 KB	PDF Document
	-	PCA-loadings-all.png D	ouble click	Mar 12, 2015, 6:51 AM	20 KB	PNG image
	-	PCA.pdf O	n this file	Mar 12, 2015, 6:51 AM	5 KB	PDF Document
		PCA.png		Mar 12, 2015, 6:51 AM	18 KB	PNG image
		result.tsv		Mar 12, 2015, 6:52 AM	1.4 MB	Plain Text
	-	rtcor.pdf		Mar 12, 2015, 6:17 AM	61 KB	PDF Document
		rtcor.png		Mar 12, 2015, 6:17 AM	40 KB	PNG image
		TICs_rtcor.pdf		Mar 12, 2015, 6:17 AM	70 KB	PDF Document
		TICs_rtcor.png		Mar 12, 2015, 6:17 AM	63 KB	PNG image
	-	TICs.pdf		Mar 12, 2015, 6:13 AM	71 KB	PDF Document
		TICs.png		Mar 12, 2015, 6:13 AM	62 KB	PNG image
		XCMS:annotated.diffreiatedDiet_	NegMode.tsv	Mar 12, 2015, 6:52 AM	1.5 MB	Plain Text
		XCMS.diffreportGrubiatedDiet_N	legMode.tsv	Mar 12, 2015, 6:21 AM	1.5 MB	Plain Text
	X	CMS.diffreportGrubatedDiet_N	egMode.xlsx	Mar 12, 2015, 6:22 AM	1.2 MB	Micros(.xlsx)
		XCMSOnline_log.txt		Mar 12, 2015, 6:52 AM	2 KB	Plain Text

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			LAU			Inc	μu	1	101				
A	В	С	D	E	F	G	н	I	J	K	L	М	N
	name	fold	log2fold	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
	M500T18_	3.177186	-1.66775	-69.9353	4.25E-07	0.000591	DOWN	499.7199	499.7144	499.721	17.9395	17.8955	17.9438
2	M251T15	2.538102	1.34375	57.295	7.07E-07	0.000591	UP	251.0044	251.0023	251.0067	14.64618	14.62393	14.66083
1	M417T18	2.457688	1.297302	55.09394	1.17E-06	0.000651	UP	417.2121	417.2091	417.2133	17.85967	17.82967	17.8865
	M199T19	2.493736	1.318309	40.96574	2.92E-06	0.001223	UP	199.1334	199.1321	199.1345	18.99725	18.97583	19.0271
;	M537T14_	1.778737	0.830853	31.72212	1.16E-05	0.003885	UP	537.1257	537.1252	537.1263	13.75913	13.74583	13.7724
5	M325T11	1.695199	0.761455	49.07387	1.61E-05	0.003885	UP	325.0931	325.0922	325.0951	11.21367	11.20732	11.2524
1	M144T16	2.012298	1.008844	33.20396	1.69E-05	0.003885	UP	144.0457	144.0453	144.0465	16.20212	16.19118	16.21943
3	M357T13_	2.594144	1.375258	32.88002	1.92E-05	0.003885	UP	357.0822	357.082	357.0837	12.66457	12.65622	12.6886
)	M426T8	6.841469	2.774306	22.7141	2.37E-05	0.003885	UP	426.0323	426.0321	426.0345	8.13925	8.13335	8.15796
0	M347T13	1.995841	0.996997	22.19083	2.44E-05	0.003885	UP	347.168	347.1634	347.172	13.05983	13.00283	13.1152
1	M591T15_	2.88852	1.530331	31.66855	2.55E-05	0.003885	UP	591.1369	591.135	591.1397	14.92045	14.89628	14.96255
2	M630T16	2.300034	1.201655	23.19857	3E-05	0.004174	UP	629.784	629.7792	629.7876	16.32718	16.27417	16.34668
3	M438T12_	1.608298	0.685535	24.90868	3.44E-05	0.004174	UP	438.1711	438.1709	438.1714	12.30179	12.27012	12.3334
4	M425T8	4.383821	2.132189	20.21984	3.77E-05	0.004174	UP	425.045	425.0435	425.0457	8.13335	8.112117	8.15796
.5	M151T15	2.067456	1.047856	20.92318	4.47E-05	0.004174	UP	151.0399	151.0366	151.0405	14.53876	14.51367	14.5699
.6	M506T15	1.435551	0.521604	20.18947	4.83E-05	0.004174	UP	506.1093	506.1066	506.1145	15.21824	15.18848	15.2506
7	M789T15	2.016565	1.0119	18.58276	5.06E-05	0.004174	UP	789.2271	789.2264	789.2278	14.96682	14.95903	14.9746
8	M315T16	3.633561	1.861384	25.13321	5.14E-05	0.004174	UP	315.143	315.1425	315.1436	16.35723	16.35473	16.38143
9	M641T16_	3.070745	1.618589	24.93903	5.26E-05	0.004174	UP	640.7743	640.774	640.7759	16.35723	16.35473	16.3814
20	M582T16_3	1.484257	0.569741	18.25259	5.37E-05	0.004174	UP	582.278	582.2752	582.2823	15.50497	15.47808	15.5102

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M N min rtmax													
M N min rtmax													
min rtmax		L	К	J		н	G	F	E		C	В	A
	i rt	rtmed	mzmax	mzmin	mzmed	updown	qvalue	pvalue	tstat	log2fold	fold	name	
17.8955 17.943	9395	17.9395	499.721	499.7144	499.7199	DOWN	0.000591	4.255-07	-69.9353	1.66775	3.177186	M500T18_	
14.62393 14.660	4618	14.64618	251.0067	251.0023	251.0044	UP	0.000591	7.078-07	57.295	1.34375	2.538102	M251T15	2
17.82967 17.88	5967	17.85967	417.2133	417.2091	417.2121	UP	0.000651	1.178-06	55.09394	1.297302	2.457688	M417T18	8
18.97583 19.027	9725	18.99725	199.1345	199.1321	199.1334	UP	0.001223	2.928-06	40.96574	1.318309	2.493736	M199T19	1
13.74583 13.772	5913	13.75913	537.1263	537.1252	537.1257	UP	0.003885	1.168-05	31.72212	0.830853	1.778737	M537T14_	5
11.20732 11.252	1367	11.21367	325.0951	325.0922	325.0931	UP	0.003885	1.61E-05	49.07387	0.761455	1.695199	M325T11	5
16.19118 16.219	0212	16.20212	144.0465	144.0453	144.0457	UP	0.003885	1.698-05	33.20396	1.008844	2.012298	M144T16	7
12.65622 12.688	6457	12.66457	357.0837	357.082	357.0822	UP	0.003885	1.928-05	32.88002	1.375258	2.594144	M357T13_	8
8.13335 8.1579	3925	8.13925	426.0345	426.0321	426.0323	UP	0.003885	2.378-05	22.7141	2.774306	6.841469	M426T8	9
13.00283 13.115	5983	13.05983	347.172	347.1634	347.168	UP	0.003885	2.448-05	22.19083	0.996997	1.995841	M347T13	10
14.89628 14.962	2045	14.92045	591.1397	591.135	591.1369	UP	0.003885	2.555-05	31.66855	1.530331	2.88852	M591T15_	11
16.27417 16.346	2718	16.32718	629.7876	629.7792	629.784	UP	0.004174	3E-05	23.19857	1.201655	2.300034	M630T16	12
12.27012 12.333	0179	12.30179	438.1714	438.1709	438.1711	UP	0.004174	3.448-05	24.90868	0.685535	1.608298	M438T12_	13
8.112117 8.1579	3335	8.13335	425.0457	425.0435	425.045	UP	0.004174	3.778-05	20.21984	2.132189	4.383821	M425T8	14
14.51367 14.569	3876	14.53876	151.0405	151.0366	151.0399	UP	0.004174	4.47E-05	20.92318	1.047856	2.067456	M151T15	15
15.18848 15.250	1824	15.21824	506.1145	506.1066	506.1093	UP	0.004174	4.83E-05	20.18947	0.521604	1.435551	M506T15	16
14.95903 14.974	6682	14.96682	789.2278	789.2264	789.2271	UP	0.004174	5.068-05	18.58276	1,0119	2.016565	M789T15	17
16.35473 16.381	5723	16.35723	315.1436	315.1425	315.143	UP	0.004174	5.148-05	25.13321	1.861384	3.633561	M315T16	18
16.35473 16.381	5723	16.35723	640.7759	640.774	640.7743	UP	0.004174	5.268-05	24.93903	1.618589	3.070745	M641T16_	19
15.47808 15.510	0497	15.50497	582.2823	582.2752	582.278	UP	0.004174	5.378-05	18.25259	0.569741	1.484257	M582T16_	20
	15723 15723 10497	16.35723 16.35723 15.50497	315.1436 640.7759 582.2823	315.1425 640.774 582.2752	315.143 640.7743 582.278	UP UP UP	0.004174 0.004174 0.004174	5:148:05 5:268:05 5:378:05	25.13321 24.93903 18.25259	1.014589 0.569741	3.033561 3.070745 1.484257	M315T16 M641T16_ M582T16_	19

	name	fold	log2fold	tstat	pvalue	gvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
1208	M209T3	1.369143	0.453273	2.709012	0.055919	0.077433	UP	208.9602	208.9598	208.9611	3.28215	3.265233	3.3416
378	M323T3	1.434411	0.520459	5.353103	0.006801	0.030027	UP	322.938	322.9359	322.9407	3.32005	3.295083	3.361817
549	M271T3	1.186928	0.247232	5.44988	0.01248	0.038025	UP	270.9417	270.9411	270.9425	3.32005	3.295083	3.361817
895	M387T3	1.394198	0.479436	4.649027	0.031911	0.059621	UP	386.9358	386.9344	386.9368	3.32005	3.295083	3.361817
1689	M272T3	1.088879	0.122844	2.524051	0.111581	0.110419	UP	271.941	271.9398	271.9434	3.326167	3.29085	3.361817
892	M325T3	1.375868	0.460342	3.79855	0.031801	0.059554	UP	324.9303	324.929	324.9401	3.32705	3.30445	3.361817
1378	M391T3	1.312616	0.392445	3.507716	0.071514	0.086812	UP	390.9101	390.9064	390.9131	3.32705	3.30445	3.367883
1623	M291T3	1.256324	-0.32921	-2.50694	0.102207	0.105294	DOWN	290.9445	290.9436	290.9464	3.327583	3.295083	3.361817
749	M324T3	1.275929	0.351548	3.759227	0.022331	0.049864	UP	323.9378	323.9374	323.9399	3.331108	3.298017	3.361817
2099	M154T3	1.037093	0.052546	1.655429	0.189385	0.150928	UP	154.0059	154.0023	154.0117	3.331492	3.30095	3.361817
1845	M387T5	1.154483	0.207247	2.022386	0.135817	0.123138	UP	387.114	387.113	387.1145	4.978417	4.97	4.9968
2204	M388T5	1.139738	0.188702	1.768345	0.215874	0.163842	UP	388.1168	388.115	388.1176	4.978417	4.970667	4.9961
1315	M404T5	1.345221	-0.42784	-2.9703	0.065723	0.083602	DOWN	404.1036	404.1014	404.1047	4.983425	4.945983	5.01041
1128	M564T5	1.522219	0.606175	3.224519	0.049554	0.073486	UP	564.0012	563.9964	564.0092	4.984925	4.917883	5.026
2862	M772T5_2	1.106141	-0.14554	-0.84381	0.44698	0.26116	DOWN	772.2342	772.227	772.2367	4.992317	4.97	5.03
3327	M643T5_1	1.122221	-0.16636	-0.46213	0.67351	0.338631	DOWN	642.6763	642.6715	642.6794	4.992317	4.930767	4.9968
1060	M419T5	1.160736	-0.21504	-3.76575	0.042847	0.067616	DOWN	419.1222	419.1178	419.1251	4.998867	4.97	5.03
3479	M418T5	1.009913	0.01423	0.343979	0.752961	0.362038	UP	418.1259	418.1251	418.1274	4.999242	4.99615	5.03
805	M534T5	2.270077	1.182742	4.124107	0.02608	0.054177	UP	534.0049	533.9957	534.0074	4.999617	4.99685	5.0956
2042	M768T5	1.190096	-0.25108	-1.66652	0.174057	0.142584	DOWN	768.2396	768.2371	768.241	4.999617	4.992317	5.02216
1207	M446T5	1.377175	0.461712	2.687478	0.055893	0.077433	UP	446.1187	446.1181	446.1194	5.003833	4.970667	5.03

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	name	fold	log2fold	-log P-value	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
i	M500T18_1	3.17718625	-1.6677497	6.37194281	-69.935309	4.2468E-07	0.00059116	DOWN	499.71989	499.714381	499.721035	17.9395	17.8955	17.943833
96	M165T15	1.66018323	-0.7313425	3 24367484	-36.133032	0.00057059	0.00994236	DOWN	165.055502	165.054308	165.056684	14.6864667	14.6478333	14.7180
47	M574T18	2.13905717	-1.096975	3.78771429	-29.64074	0.00016304	0.00569183	DOWN	574.266065	574.263028	574.272462	17.7115	17.6941667	17.736833
38	M517T15_2	1.75943722	-0.815114	3.93600908	-27.522969	0.00011588	0.00501453	DOWN	517.194812	517.191996	517.198037	14.6337667	14.59155	14.664316
42	M574T17_2	1.59552933	-0.6740351	3.89904915	-23.534148	0.00012617	0.00502501	DOWN	573.751404	573.745446	573.752077	17.0508333	17.0495	17.1253333
69	M567T12_1	1.21578562	-0.2818889	3.50811164	-22.910965	0.00031038	0.00742882	DOWN	567.214555	567.212376	567.21642	12.4962667	12.4584667	12.523583
206	M504T10	2.04744309	-1.0338234	2.65836289	-18.693823	0.00219602	0.01783223	DOWN	504.138121	504.136349	504.14049	10.1241	10.1203667	10.144133
21	M175T15_2	1.75024008	-0.8075528	4.26057989	-18.65345	5.4881E-05	0.00417379	DOWN	175.097496	175.096898	175.098239	14.8694333	14.8666333	14.8793
30	M529T12	1.20815162	-0.2728015	4.06091097	-18.56302	8.6914E-05	0.0046548	DOWN	529.193978	529.191284	529.195264	11.8747	11.8619333	11.902983
177	M231T16_2	3.00517465	-1.5874488	2.79422291	-16.956079	0.00160612	0.01517888	DOWN	231.15918	231.158231	231.160844	15.6376667	15.5836667	15.6379
46	M493T18_2	2.09585981	-1.0675422	3.80434853	-16.138394	0.00015691	0.00569183	DOWN	493.237441	493.235949	493.237575	18.1235	18.1161667	18.1653333
56	M287T12	1.49870741	-0.5837188	-3.63982195	-14.759869	0.00022918	0.00684582	DOWN	287.077916	287.073836	287.083574	12.4962667	12.40445	12.5506
124	M565T12_1	1.40852493	-0.4941851	3.08759847	-14.151015	0.00081734	0.01094051	DOWN	565.215654	565.215406	565.217814	12.4962667	12.4853	12.523583
67	M175T15_1	1.65329893	-0.7253476	3.54719875	-14.110635	0.00028366	0.0070821	DOWN	175.076333	175.075715	175.077592	14.8742	14.8672667	14.882916
57	M490T14_1	2.28133744	-1.1898799	3.62228199	-13.866683	0.00023863	0.00700292	DOWN	490.13636	490.134832	490.13757	14.1682333	14.1636833	14.168983
170	M490T14_2	2.64201512	-1.4016387	2.82058063	-13.640201	0.00151154	0.01487326	DOWN	490.150671	490.14958	490.151411	14.2480333	14.2477833	14.2697
55	M187T17	1.65717691	-0.7287276	3.64858184	-13.139663	0.0002246	0.00683111	DOWN	187.097276	187.096754	187.098391	17.4558333	17.4535	17.484166
327	M587T12	1.21922912	-0.2859693	2.27459764	-12.965168	0.00531377	0.02715163	DOWN	587.234503	587.233346	587.23698	12.2213833	12.1999667	12.252533
324	M289T11	1.803374	-0.8506986	2.28411244	-12.840128	0.00519861	0.02682321	DOWN	289.082598	289.076863	289.086635	11.1201167	11.10205	11.144033
74	M317T11	1.18992599	-0.2508718	3.44500584	-12.785979	0.00035892	0.00808092	DOWN	317.082663	317.080868	317.083426	11.208525	11.1920667	11.2338

A	В	С	D	E	F	G	н	1	1	к	L	м	N	0
	name	fold	log2fold	-log P-value	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
	M500118_1	3.1//18625	-1.66//49/	6.3/194281	-69.935309	4.2468E-07	0.00059116	DOWN	499.71989	499.714381	499.721035	17.9395	17.8955	17.943833
70	M103113	1.00018323	-0./313425	3.2430/484	-30.133032	0.00057059	0.00994230	DOWN	165.055502	165.054308	165.050684	14.0804007	14.64/8333	14./180
18	M517T15 2	1 75943722	-0.815114	3 93600908	.27 522969	0.00011588	0.00501453	DOWN	517 194812	517 191996	517 198037	14 6337667	14 59155	14 664316
17	M574T17 2	1 59552933	-0.6740351	3,89904915	-23 534148	0.00012617	0.00502501	DOWN	573 751404	573 745446	573 752077	17 0508333	17.0495	17 125333
59	M567T12 1	1.21578562	-0.2818889	3.50811164	-22,910965	0.00031038	0.00742882	DOWN	567,214555	567.212376	567.21642	12,4962667	12.4584667	12.523583
206	M504T10	2.04744309	-1.0338234	2.65836289	-18.693823	0.00219602	0.01783223	DOWN	504,138121	504.136349	504.14049	10.1241	10.1203667	10.144133
21	M175T15 2	1.75024008	-0.8075528	4.26057989	-18.65345	5.4881E-05	0.00417379	DOWN	175.097496	175.096898	175.098239	14.8694333	14.8666333	14.879
30	M529T12	1.20815162	-0.2728015	4.06091097	-18.56302	8.6914E-05	0.0046548	DOWN	529.193978	529.191284	529.195264	11.8747	11.8619333	11.902983
77	M231T16_2	3.00517465	-1.5874488	2.79422291	-16.956079	0.00160612	0.01517888	DOWN	231.15918	231.158231	231.160844	15.6376667	15.5836667	15.6379
16	M493T18_2	2.09585981	-1.0675422	3.80434853	-16.138394	0.00015691	0.00569183	DOWN	493.237441	493.235949	493.237575	18.1235	18.1161667	18.165333
56	M287T12	1.49870741	-0.5837188	3.63982195	-14.759869	0.00022918	0.00684582	DOWN	287.077916	287.073836	287.083574	12.4962667	12.40445	12.5506
24	M565T12_1	1.40852493	-0.4941851	3.08759847	-14.151015	0.00081734	0.01094051	DOWN	565.215654	565.215406	565.217814	12.4962667	12.4853	12.523583
57	M175T15_1	1.65329893	-0.7253476	3.54719875	-14.110635	0.00028366	0.0070821	DOWN	175.076333	175.075715	175.077592	14.8742	14.8672667	14.882916
57	M490T14_1	2.28133744	-1.1898799	3.62228199	-13.866683	0.00023863	0.00700292	DOWN	490.13636	490.134832	490.13757	14.1682333	14.1636833	14.168983
170	M490T14_2	2.64201512	-1.4016387	2.82058063	-13.640201	0.00151154	0.01487326	DOWN	490.150671	490.14958	490.151411	14.2480333	14.2477833	14.2697
55	M187T17	1.65717691	-0.7287276	3.64858184	-13.139663	0.0002246	0.00683111	DOWN	187.097276	187.096754	187.098391	17.4558333	17.4535	17.484166
327	M587T12	1.21922912	-0.2859693	2.27459764	-12.965168	0.00531377	0.02715163	DOWN	587.234503	587.233346	587.23698	12.2213833	12.1999667	12.252533
324	M289T11	1.803374	-0.8506986	2.28411244	-12.840128	0.00519861	0.02682321	DOWN	289.082598	289.076863	289.086635	11.1201167	11.10205	11.144033
74	M317T11	1.18992599	-0.2508718	3.44500584	-12.785979	0.00035892	0.00808092	2 DOWN	317.082663	317.080868	317.083426	11.208525	11.1920667	11.233





Selecting all ions with p < 0.01 and making a new sheet

1	M500T18_1	3.17718625	-1.6677497	6.37194281	-69.935309	4.2468E-07	0.00059116 DOV	WN 499.71989	499.714381	499.721035	17.9395	17.8955	17.943833
2	M251T15	2.5381022	1.34375016	6.15069974	57.2949952	7.0681E-07	0.00059116 UP	251.004448	251.00233	251.006679	14.646175	14.6239333	14.660833
В	M417T18	2.45768759	1.29730154	5.93242838	55.093938	1.1683E-06	0.00065146 UP	417.212131	417.209144	417.213252	17.8596667	17.8296667	17.886
4	M199T19	2.49373586	1.31830866	5.53403205	40.9657391	2.9239E-06	0.00122277 UP	199.133402	199.132069	199.134536	18.99725	18.9758333	19.027166
5	M537T14_2	1.77873662	0.83085291	4.93437072	31.7221237	1.1631E-05	0.00388536 UP	537.125737	537.125207	537.126266	13.7591333	13.7458333	13.772433
6	M325T11	1.69519907	0.7614547	4.79236518	49.0738693	1.613E-05	0.00388536 UP	325.093116	325.092202	325.095085	11.2136667	11.2073167	11.2524
7	M144T16	2.01229805	1.00884401	4.77150826	33.2039585	1.6924E-05	0.00388536 UP	144.045677	144.045279	144.046454	16.2021167	16.1911833	16.219433
в	M357T13_2	2.59414359	1.37525834	4.71777294	32.8800228	1.9153E-05	0.00388536 UP	357.082227	357.081993	357.083674	12.6645667	12.6562167	12.688666
9	M426T8	6.84146926	2.77430619	4.6257974	22.7140999	2.367E-05	0.00388536 UP	426.03226	426.032122	426.034541	8.13925	8.13335	8.1579666
10	M347T13	1.99584111	0.99699687	4.61237735	22.1908286	2.4413E-05	0.00388536 UP	347.167955	347.163411	347.172006	13.059825	13.0028333	13.1152
480	M611T16_2	1.17035124	-0.2269416	2.00908774	-5.3602012	0.00979292	0.03401502 DOV	WN 611.278173	611.27616	611.284794	15.8765083	15.8224333	15.954433
480	M611T16_2 M711T18	1.17035124 1.26827471	-0.2269416 -0.3428673	2.00908774 2.00794425	-5.3602012 -7.6797212	0.00979292 0.00981874	0.03401502 DOV 0.03401502 DOV	WN 611.278173 WN 711.31911	611.27616 711.31715	611.284794 711.322138	15.8765083 18.05925	15.8224333 17.9893333	15.954433
480 482 483	M611T16_2 M711T18 M576T17_2	1.17035124 1.26827471 1.13201205	-0.2269416 -0.3428673 0.17888932	2.00908774 2.00794425 2.00693443	-5.3602012 -7.6797212 5.45812005	0.00979292 0.00981874 0.0098416	0.03401502 DOV 0.03401502 DOV 0.03401502 DO	WN 611.278173 WN 711.31911 576.245602	611.27616 711.31715 576.244742	611.284794 711.322138 576.249542	15.8765083 18.05925 17.081	15.8224333 17.9893333 16.9721667	15.954433 18.133333 17.237
480 482 483 484	M611T16_2 M711T18 M576T17_2 M115T16	1.17035124 1.26827471 1.13201205 1.41760411	-0.2269416 -0.3428673 0.17888932 0.5034547	2.00908774 2.00794425 2.00693443 2.00604191	-5.3602012 -7.6797212 5.45812005 4.72201644	0.00979292 0.00981874 0.0098416 0.00986184	0.03401502 DOV 0.03401502 DOV 0.03401502 DV 0.03401502 UP	WN 611.278173 WN 711.31911 576.245602 115.004417	611.27616 711.31715 576.244742 115.001493	611.284794 711.322138 576.249542 115.006234	15.8765083 18.05925 17.081 15.5579167	15.8224333 17.9893333 16.9721667 15.5327833	15.954433 18.133333 17.237 15.5616
480 482 483 484 485	M611T16_2 M711T18 M576T17_2 M115T16 M342T9	1.17035124 1.26827471 1.13201205 1.41760411 1.47951495	-0.2269416 -0.3428673 0.17888932 0.5034547 0.56512427	2.00908774 2.00794425 2.00693443 2.00604191 2.00572431	-5.3602012 -7.6797212 5.45812005 4.72201644 6.37522916	0.00979292 0.00981874 0.00986184 0.00986184 0.00986906	0.03401502 DOV 0.03401502 DOV 0.03401502 UP 0.03401502 UP 0.03401502 UP	WN 611.278173 WN 711.31911 576.245602 115.004417 342.090705	611.27616 711.31715 576.244742 115.001493 342.087875	611.284794 711.322138 576.249542 115.006234 342.09202	15.8765083 18.05925 17.081 15.5579167 9.3506	15.8224333 17.9893333 16.9721667 15.5327833 9.30873333	15.954433 18.133333 17.237 15.5616 9.3755
480 482 483 484 485 486	M611716_2 M711718 M57617_2 M115716 M34279 M197710	1.17035124 1.26827471 1.13201205 1.41760411 1.47951495 1.26666403	-0.2269416 -0.3428673 0.17888932 0.5034547 0.56512427 0.34103392	2.00908774 2.00794425 2.00693443 2.00604191 2.00572431 2.0030799	-5.3602012 -7.6797212 5.45812005 4.72201644 6.37522916 6.82066584	0.00979292 0.00981874 0.0098416 0.00986184 0.00986906 0.0092933	0.03401502 DOV 0.03401502 DOV 0.03401502 UP 0.03401502 UP 0.03401502 UP 0.03401502 UP	WN 611.278173 WN 711.31911 576.245602 115.004417 342.090705 197.025861	611.27616 711.31715 576.244742 115.001493 342.087875 197.023886	611.284794 711.322138 576.249542 115.006234 342.09202 197.027836	15.8765083 18.05925 17.081 15.5579167 9.3506 9.56196667	15.8224333 17.9893333 16.9721667 15.5327833 9.30873333 9.55711667	15.954433 18.133333 17.237 15.5616 9.3755 9.568166
480 482 483 484 485 486 487	M611716_2 M711718 M576TJ7_2 M115716 M342T9 M397710 M201718	1.17035124 1.26827471 1.13201205 1.41760411 1.47951495 1.26666403 1.31936278	-0.2269416 0.3428673 0.5034547 0.5034547 0.350512427 0.34103392 0.39984133	2.00908774 2.00794425 2.0069443 2.00604191 2.00527431 2.0028376	-5.3602012 -7.6797212 5.45812005 4.72201644 6.37522916 6.82066584 4.70021934	0.00979292 0.00981874 0.00986187 0.00986186 0.00986906 0.00992933 0.00992933	0.03401502 DOV 0.03401502 DOV 0.03401502 DV 0.03401502 UP 0.03401502 UP 0.03401502 UP 0.03401502 UP	WN 611.278173 WN 711.31911 576.245602 115.00417 342.090705 197.025861 201.105988	611.27616 711.31715 576.244742 115.001493 342.087875 197.023886 201.103323	611.284794 711.322138 576.249542 115.006234 342.09202 197.027836 201.107267	15.8765083 18.05925 17.081 15.5579167 9.56196667 17.615583	15.8224333 17.9893333 16.9721667 15.5327833 9.30873333 9.55711667 17.5908333	15.954433 18.13333 17.237 15.5616 9.3755 9.5668166 17.625833
480 482 483 484 485 486 487 488	M611T16_2 M7J1T18 M576T17_2 M115T16 M342T9 M197T10 M201T18 M162T11	1.17035124 1.26827471 1.13201205 1.47951495 1.26666403 1.31936278 1.09119523	-0.2269416 -0.3428673 0.3034587 0.50512427 0.36512427 0.39984131 0.12590925	2.00908774 2.00794425 2.00693443 2.00572431 2.0037799 2.00283676 2.00273294	-5.3602012 -7.6797212 5.45812005 4.7220164 6.32052916 6.82066584 4.70021934 6.75086139	0.00979292 0.00981874 0.0098616 0.00986206 0.00992933 0.00993489 0.00938489	0.03401502 DO 0.03401502 DO 0.03401502 UP 0.03401502 UP 0.03401502 UP 0.03401502 UP 0.03401502 UP 0.03401502 UP	WN 611.278173 WN 711.31911 576.2450 115.00417 342.09070 197.025861 201.05598 162.05598	611.27616 711.31715 576.244742 115.001493 342.087875 197.023886 201.10323 162.052952	611.284794 711.322138 576.249542 115.006234 342.09202 197.027836 201.107267 162.054782	15.8765083 18.05925 17.081 15.5579167 9.56196667 17.6155833 11.4542	15.8224333 17.989333 16.9721667 15.532783 9.30873333 9.55711667 17.5908333 11.45454167	15.954433 18.13333 17.237 15.5616 9.3755 9.5668166 17.625833 11.496366
480 482 483 484 485 486 486 487 488 489	M611T16_2 M711T18 M576T17_2 M115T16 M342T9 M197T10 M201T18 M167T11 M131T14_1	1.17035124 1.26827471 1.13201205 1.41760411 1.47951495 1.26666403 1.31936278 1.09119523 1.31291812	-0.2269416 -0.3428673 0.5034547 0.50512427 0.34103392 0.34103392 0.39984131 0.1250925 -0.3927769	2.00908774 2.00794425 2.00693443 2.006794435 2.0027831 2.0027839 2.00288676 2.0027894	-5.3602012 5.45812005 4.72201644 6.37522916 6.82066584 4.70021934 6.75086139 5.53314033	0.00979292 0.0098184 0.00986184 0.00986184 0.00992489 0.00993489 0.00993489	0.03401502 DOV 0.03401502 DOV 0.03401502 DOV 0.03401502 UP 0.03401502 UP 0.03401502 UP 0.03401502 UP 0.03401502 DOV	WN 611.278.173 WN 71.1.31911 578.2450 115.00417 342.009705 197.02566 201.105598 126.035951 W1 311.00559	611.27616 711.31715 576.244742 115.001493 342.087875 197.02386 201.103323 162.052952 131.048953	611.284794 711.322138 576.249542 115.006234 342.09202 197.027836 201.107267 162.054782 133.056393	15.8765083 18.05925 17.081 15.5579167 9.3509 9.5619667 17.6155833 11.4542 13.7197	15.8224333 17.9893333 16.9721667 15.5327833 9.3087333 9.55711667 17.5508333 11.4454167 13.6594667	15.954433 18.133333 17.237 15.5616 9.3755 9.5668166 17.625833 11.496366 13.719766

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A241T18_1	27.4045917	4.77634573	3.30532767	40.46059	0.00049508	0.00920165	UP	241.108312	241.107471	241.109437	17.59125	17.5871667	17.6198333
A240T18	16.4294376	4.03821119	2.05479101	10.0229195	0.00881473	0.03293413	UP	240.359872	240.356187	240.361536	17.5906667	17.5871667	17.5916667
M242T18	16.3870912	4.03448789	2.91477253	27.6130715	0.00121682	0.013362	UP	242.110341	242.109733	242.111274	17.5906667	17.5871667	17.5916667
M424T8_1	13.0179292	3.70242807	3.83389494	30.5724419	0.00014659	0.00557299	UP	424.028175	424.026455	424.029895	8.12178333	8.11845	8.12511667
M424T8_2	11.1363641	3.47720638	3.61174395	29.8423152	0.00024449	0.00703395	UP	424.0396	424.036272	424.044862	8.1363	8.12225	8.15796667
VI227T16	7.16213011	2.84038873	2.75564323	19.5959381	0.00175532	0.01604506	UP	227.092249	227.090325	227.093361	15.8502167	15.8489333	15.8756833
M426T8	6.84146926	2.77430619	4.6257974	22.7140999	2.367E-05	0.00388536	UP	426.03226	426.032122	426.034541	8.13925	8.13335	8.15796667
M171T18_2	6.77813538	2.76088845	2.21189773	12.4050347	0.00613907	0.0288409	UP	171.102926	171.102581	171.103387	17.6959167	17.6403333	17.698
M278T15	6.10860512	2.61084298	2.49625447	16.1413878	0.00318967	0.02084209	UP	278.101274	278.100858	278.105129	14.64535	14.6205333	14.6608333
	1												
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M184T9	1.53161283	-0.6150517	2.95136904	-8.3891049	0.00111849	0.01290324	DOWN	184.01267	184.009146	184.016193	9.12173333	9.12105	9.12241667
M184T9 M655T19	1.53161283	-0.6150517 -0.6122145	2.95136904 3.17714123	-8.3891049 -10.355352	0.00111849	0.01290324 0.01049515	DOWN	184.01267 655.441309	184.009146 655.431657	184.016193 655.442502	9.12173333 19.139	9.12105 19.1328333	9.12241667 19.1483333
M184T9 M655T19 M605T13	1.53161283 1.52860376 1.52721469	-0.6150517 -0.6122145 0.61090289	2.95136904 3.17714123 2.83316714	-8.3891049 -10.355352 7.78489386	0.00111849 0.00066506 0.00146836	0.01290324 0.01049515 0.01470795	DOWN DOWN UP	184.01267 655.441309 605.241635	184.009146 655.431657 605.240209	184.016193 655.442502 605.245899	9.12173333 19.139 12.844175	9.12105 19.1328333 12.83055	9.12241667 19.1483333 12.8973
M184T9 M655T19 M605T13 M505T10_2	1.53161283 1.52860376 1.52721469 1.52573259	-0.6150517 -0.6122145 0.61090289 -0.6095021	2.95136904 3.17714123 2.83316714 2.88092563	-8.3891049 -10.355352 7.78489386 -8.1460738	0.00111849 0.00066506 0.00146836 0.00131545	0.01290324 0.01049515 0.01470795 0.01358432	DOWN DOWN UP DOWN	184.01267 655.441309 605.241635 505.142079	184.009146 655.431657 605.240209 505.139106	184.016193 655.442502 605.245899 505.14635	9.12173333 19.139 12.844175 10.1496833	9.12105 19.1328333 12.83055 10.14745	9.12241667 19.1483333 12.8973 10.1714167
V184T9 V1655T19 V1605T13 V1505T10_2 V148T10_2	1.53161283 1.52860376 1.52721469 1.52573259 1.52445007	-0.6150517 -0.6122145 0.61090289 -0.6095021 0.6082889	2.95136904 3.17714123 2.83316714 2.88092563 2.03801647	-8.3891049 -10.355352 7.78489386 -8.1460738 9.29372235	0.00111849 0.00066506 0.00146836 0.00131545 0.00916186	0.01290324 0.01049515 0.01470795 0.01358432 0.03356554	DOWN DOWN UP DOWN UP	184.01267 655.441309 605.241635 505.142079 448.137373	184.009146 655.431657 605.240209 505.139106 448.128591	184.016193 655.442502 605.245899 505.14635 448.139353	9.12173333 19.139 12.844175 10.1496833 9.63695	9.12105 19.1328333 12.83055 10.14745 9.6166	9.12241667 19.1483333 12.8973 10.1714167 9.68833333
M184T9 M655T19 M605T13 M505T10_2 M448T10_2 M519T15	1.53161283 1.52860376 1.52721469 1.52573259 1.52445007 1.52108123	-0.6150517 -0.6122145 0.61090289 -0.6095021 0.6082889 -0.6050972	2.95136904 3.17714123 2.83316714 2.88092563 2.03801647 2.40027776	-8.3891049 -10.355352 7.78489386 -8.1460738 9.29372235 -6.5189034	0.00111849 0.00066506 0.00146836 0.00131545 0.00916186 0.00397853	0.01290324 0.01049515 0.01470795 0.01358432 0.03356554 0.02302821	DOWN DOWN UP DOWN UP DOWN	184.01267 655.441309 605.241635 505.142079 448.137373 518.614618	184.009146 655.431657 605.240209 505.139106 448.128591 518.611173	184.016193 655.442502 605.245899 505.14635 448.139353 518.618064	9.12173333 19.139 12.844175 10.1496833 9.63695 15.481275	9.12105 19.1328333 12.83055 10.14745 9.6166 15.4780833	9.12241667 19.1483333 12.8973 10.1714167 9.68833333 15.4844667
M184T9 M655T19 M605T13 M505T10_2 M488T10_2 M519T15 M243T17	1.53161283 1.52860376 1.52721469 1.52573259 1.52445007 1.52108123 1.5163421	-0.6150517 -0.6122145 0.61990289 -0.6095021 0.6082889 -0.6050972 0.60059527	2.95136904 3.17714123 2.83316714 2.88092563 2.03801647 2.40027776 2.76595921	-8.3891049 -10.355352 7.78489386 -8.1460738 9.29372235 -6.5189034 7.7550418	0.00111849 0.00066506 0.00146836 0.00131545 0.00916186 0.00397853 0.00171412	0.01290324 0.01049515 0.01470795 0.01358432 0.03356554 0.02302821 0.01584156	DOWN DOWN UP DOWN UP DOWN UP	184.01267 655.441309 605.241635 505.142079 448.137373 518.614618 243.123357	184.009146 655.431657 605.240209 505.139106 448.128591 518.611173 243.122711	184.016193 655.442502 605.245899 505.14635 548.139333 518.618064 243.124292	9.12173333 19.139 12.844175 10.1496833 9.63695 15.481275 16.7584167	9.12105 19.1328333 12.83055 9.6166 15.4780833 16.7355	9.12241667 19.1483333 12.8973 10.1714167 9.68833333 15.4844667 16.7886667
M184T9 M655T19 M605T13 M505T10_2 M448T10_2 M519T15 M243T17 M761T16	1.53161283 1.52860376 1.52721469 1.52573259 1.52445007 1.52108123 1.5163421 1.51582446	-0.6150517 -0.6122145 0.61090289 -0.6095021 0.6082889 -0.6050972 0.60059527 0.60010269	2.95136904 3.17714123 2.83316714 2.88092563 2.03801647 2.40027776 2.76595921 3.7779874	-8.3891049 -10.355352 7.78489386 -8.1460738 9.29372235 -6.5189034 7.7550418 15.3680847	0.00111849 0.00066506 0.00146836 0.00131545 0.00916186 0.00397853 0.00171412 0.00016673	0.01290324 0.01049515 0.01470795 0.01358432 0.03356554 0.02302821 0.01584156 0.00569183	DOWN DOWN UP DOWN UP DOWN UP UP	184.01267 655.441309 605.241635 505.142079 448.137373 518.614618 243.12357 761.225784	184.009146 655.431657 605.240209 505.139106 448.128591 518.611173 243.122711 761.219871	184.016193 655.442502 605.245899 505.14635 448.139353 518.618064 243.124292 761.226168	9.12173333 19.139 12.844175 10.1496833 9.63695 15.481275 16.7584167 15.56165	9.12105 19.1328333 12.83055 10.14745 9.6166 15.4780833 16.7355 15.4844667	9.12241667 19.1483333 12.8973 10.1714167 9.68833333 15.4844667 16.7886667 15.6112333
M184T9 M655T19 M605T13 M505T10_2 W448T10_2 W519T15 W243T17 W761T16 M290T18	1.53161283 1.52860376 1.52721469 1.5273259 1.52445007 1.52108123 1.5163421 1.51582466 1.51586402	-0.6150517 -0.6122145 0.61090289 -0.6095021 0.6082889 -0.6059527 0.60059527 0.60010269 0.59995474	2.95136904 3.17714123 2.83316714 2.88092563 2.03801647 2.40027776 2.76595921 3.7779874 2.3382065	-8.3891049 -10.355352 -7.78489386 -8.1460738 9.29372235 -6.5189034 7.7550418 15.3660847 6.0786388	0.00111849 0.00066506 0.00146836 0.00131545 0.00916186 0.00397853 0.00171412 0.00016673 0.0045898	0.01290324 0.01049515 0.01470795 0.01358432 0.03356554 0.02302821 0.01584156 0.00569183 0.02509041	DOWN DOWN UP DOWN UP UP UP UP	184.01267 655.441309 605.241635 505.142079 448.137373 518.614618 243.123357 761.225784 290.172463	184.009146 655.431657 605.240209 505.139106 448.128591 518.651173 243.122711 761.219871 290.168635	184.016193 655.442502 605.245899 505.14635 448.139353 518.618064 243.124292 761.226168 290.173506	9.12173333 19.139 12.844175 10.1496833 9.63695 15.481275 16.7584167 15.56165 17.940333	9.12105 19.1328333 12.83055 10.14745 9.6166 15.4780833 16.7355 15.4844667 17.8955	9.12241667 19.148333 12.8973 10.1714167 9.68833333 15.4844667 16.7886667 15.6112333 17.9438333

		Se	eleo	ctin	g tl	hos	se v	vit	h fo	ld-	cha	nge	9	
			in	crea	ase	>1	.5 a	ano	d ne	w	oag	e		
		Sort	by U	P/DC	WN									
1	name	fold	log2fold	-log P-value	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
2	M241T18 1	27.4045917	4.77634573	3.30532767	40.46059	0.00049508	0.00920165	UP	241.108312	241.107471	241.109437	17.59125	17.5871667	17.6198333
3	M240T18	16.4294376	4.03821119	2.05479101	10.0229195	0.00881473	0.03293413	UP	240.359872	240.356187	240.361536	17.5906667	17.5871667	17.5916667
4	M242T18	16.3870912	4.03448789	2.91477253	27.6130715	0.00121682	0.013362	UP	242.110341	242.109733	242.111274	17.5906667	17.5871667	17.5916667
5	M424T8_1	13.0179292	3.70242807	3.83389494	30.5724419	0.00014659	0.00557299	UP	424.028175	424.026455	424.029895	8.12178333	8.11845	8.12511667
6	M424T8_2	11.1363641	3.47720638	3.61174395	29.8423152	0.00024449	0.00703395	UP	424.0396	424.036272	424.044862	8.1363	8.12225	8.15796667
7	M227T16	7.16213011	2.84038873	2.75564323	19.5959381	0.00175532	0.01604506	UP	227.092249	227.090325	227.093361	15.8502167	15.8489333	15.8756833
8	M426T8	6.84146926	2.77430619	4.6257974	22.7140999	2.367E-05	0.00388536	UP	426.03226	426.032122	426.034541	8.13925	8.13335	8.15796667
9	M171T18_2	6.77813538	2.76088845	2.21189773	12.4050347	0.00613907	0.0288409	UP	171.102926	171.102581	171.103387	17.6959167	17.6403333	17.698
10	M278T15	6.10860512	2.61084298	2.49625447	16.1413878	0.00318967	0.02084209	UP	278.101274	278.100858	278.105129	14.64535	14.6205333	14.6608333
38	M587T8	1.17946394	0.23813131	2,24949465	5.44286982	0.00562996	0.02794546	UP	587.123047	587.120063	587.129497	7.51885	7.49283333	7.5402
39	M431T12 3	1.17183289	0.22876684	2.10375786	6.61525602	0.00787485	0.03165926	UP	431,191141	431,190612	431,191451	12.1466167	12.1357167	12.15485
340	M403T19	1.14660846	0.19737283	2.04169228	4.81730337	0.00908464	0.03347246	UP	403.269495	403.268237	403.270058	18.9244167	18.9113333	18.973
841	M545T10	1.14353987	0.19350666	2.73436639	7.36957773	0.00184346	0.01631577	UP	545.172989	545.170135	545.175188	9.96228333	9.93963333	9.98838333
342	M295T14	1.13866277	0.18734054	2.2077779	7.17433484	0.00619758	0.0288409	UP	295.058287	295.057779	295.059344	14.0641	14.0602	14.0875333
343	M383T12 1	1.1348121	0.18245344	2.17530962	5.61475903	0.00667868	0.03002729	UP	383.077906	383.077749	383.080144	12.4962667	12.4313833	12.49645
844	M635T11_2	1.13366549	0.180995	2.12820167	7.22587127	0.00744386	0.03105201	UP	635.23033	635.226956	635.231231	11.0496833	10.9833667	11.0760167
845	M576T17_2	1.13201205	0.17888932	2.00693443	5.45812005	0.0098416	0.03401502	UP	576.245602	576.244742	576.249542	17.081	16.9721667	17.2375
846	M231T16_1	1.13052077	0.1769875	2.66711209	13.5258148	0.00215223	0.01773485	UP	231.138481	231.13648	231.139489	15.6399167	15.6359833	15.64
47	M162T11	1.09119523	0.12590925	2.00277294	6.75086139	0.00993635	0.03401502	UP	162.053951	162.052952	162.054782	11.4542	11.4454167	11.4963667

Selecting those with fold-change decrease >1.5 and new page

-	name	1010	logzfold	-log P-value	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
2	M377T18	3.72924023	-1.8988817	2.59661412	-9.9493137	0.00253155	0.01916149	DOWN	377.280273	377.279809	377.280485	18.2675	18.2525	18.29
3	M500T18_1	3.17718625	-1.6677497	6.37194281	-69.935309	4.2468E-07	0.00059116	DOWN	499.71989	499.714381	499.721035	17.9395	17.8955	17.943833
4	M424T18	3.15396982	-1.6571689	2.30821987	-8.465829	0.0049179	0.02644019	DOWN	424.286919	424.285903	424.288206	18.2798333	18.2675	18.29
5	M493T18_1	3.14854207	-1.6546839	2.61484641	-12.339822	0.00242747	0.01871241	DOWN	492.732075	492.731096	492.733053	17.9241667	17.908	17.940333
6	M251T17	3.12450783	-1.643629	2.34919635	-11.996006	0.00447511	0.02464783	DOWN	251.059425	251.059206	251.060194	16.6583333	16.6248	16.670783
7	M231T16_2	3.00517465	-1.5874488	2.79422291	-16.956079	0.00160612	0.01517888	DOWN	231.15918	231.158231	231.160844	15.6376667	15.5836667	15.6379
8	M768T12	2.84825797	-1.5100798	2.07827637	-5.0543868	0.00835071	0.03256133	DOWN	767.829662	767.826195	767.833128	11.6209083	11.60575	11.636066
9	M525T14_2	2.6848561	-1.4248448	2.30517791	-6.0601844	0.00495247	0.02646754	DOWN	525.284116	525.27453	525.287438	13.6901417	13.6671667	13.718
10	M490T14_2	2.64201512	-1.4016387	2.82058063	-13.640201	0.00151154	0.01487326	DOWN	490.150671	490.14958	490.151411	14.2480333	14.2477833	14.2697
								+						
117	M419T11_1	1.17810985	-0.2364741	2.41792855	-7.9513274	0.00382007	0.02265429	DOWN	419.035272	419.033926	419.03625	11.3799333	11.3681333	11.388166
117	7 M419T11_1 3 M611T16_2	1.17810985	-0.2364741 4 -0.2269416	2.41792855 2.00908774	-7.9513274 -5.3602012	0.00382007	0.02265429	DOWN 2 DOWN	419.035272 611.278173	419.033926 611.27616	419.03625 611.284794	11.3799333 15.8765083	11.3681333 15.8224333	11.388166 15.954433
1117	7 M419T11_1 3 M611T16_2 9 M565T15	1.17810985 1.17035124 1.16633313	9 -0.2364741 4 -0.2269416 3 -0.2219799	2.41792855 2.00908774 2.23155622	-7.9513274 -5.3602012 -6.7354962	0.00382007 0.00979292 0.00586737	0.02265425 0.03401502 0.02853127	DOWN DOWN DOWN	419.035272 611.278173 565.120094	419.033926 611.27616 565.119191	419.03625 611.284794 565.121328	11.3799333 15.8765083 14.6141	11.3681333 15.8224333 14.59155	11.388166 15.954433 14.664316
117	7 M419T11_1 8 M611T16_2 9 M565T15 9 M535T14	1.17810985 1.17035124 1.16633313 1.16407717	-0.2364741 -0.2269416 -0.2219799 -0.2191867	2.41792855 2.00908774 2.23155622 2.26682318	-7.9513274 -5.3602012 -6.7354962 6.1061825	0.00382007 0.00979292 0.00586737 0.00540975	0.02265425 0.03401502 0.02853127 0.02737525	DOWN DOWN DOWN DOWN	419.035272 611.278173 565.120094 535.110262	419.033926 611.27616 565.119191 535.106754	419.03625 611.284794 565.121328 535.111276	11.3799333 15.8765083 14.6141 13.5184917	11.3681333 15.8224333 14.59155 13.4834667	11.388166 15.954433 14.664316 13.562266
1117 118 119 120	<pre>/ M419T11_1 / M611T16_2 / M565T15 / M565T15 / M535T14 / M221T19</pre>	1.17810985 1.17035124 1.16633313 1.16407717 1.15855517	9 -0.2364741 4 -0.2269416 3 -0.2219799 7 -0.2191867 7 -0.2123267	2.41792855 2.00908774 2.23155622 2.26682318 2.15628902	-7.9513274 -5.3602012 -6.7354962 -6.1061825 -5.6641662	0.00382007 0.00979292 0.00586737 0.00540975 0.00697768	0.02265429 0.03401502 0.02853127 0.02737525 0.03031695	DOWN DOWN DOWN DOWN DOWN	419.035272 611.278173 565.120094 535.110262 221.084846	419.033926 611.27616 565.119191 535.106754 221.08127	419.03625 611.284794 565.121328 535.111276 221.085397	11.3799333 15.8765083 14.6141 13.5184917 19.0063333	11.3681333 15.8224333 14.59155 13.4834667 18.9436667	11.388166 15.954433 14.664316 13.562266 19.030666
117	<pre>/ M419T11_1 8 M611T16_2 9 M565T15 9 M553T14 1 M221T19 2 M119T14</pre>	1.17810985 1.17035124 1.1663331 1.16407713 1.15855517 1.1541478	9 -0.2364741 -0.2269416 -0.2219799 -0.2191867 -0.2123267 -0.206828	2.41792855 2.00908774 2.23155622 2.26682318 2.15628902 2.25839361	-7.9513274 -5.3602012 -6.7354962 -6.1061829 -5.6641662 -9.9584077	0.00382007 0.00979292 0.00586733 0.00540975 0.00697768 0.00551577	0.02265425 0.03401502 0.02853127 0.02737525 0.03031695 0.02758935	DOWN DOWN DOWN DOWN DOWN DOWN DOWN	419.035272 611.278173 565.120094 535.110262 221.084846 119.039425	419.033926 611.27616 565.119191 535.106754 221.08127 119.033334	419.03625 611.284794 565.121328 535.111276 221.085397 119.042616	11.3799333 15.8765083 14.6141 13.5184917 19.0063333 14.0117333	11.3681333 15.8224333 14.59155 13.4834667 18.9436667 14.0084	11.388166 15.954433 14.664316 13.562266 19.030666 14.038183
1117 118 120 121 122	<pre>7 M419T11_1 8 M611T16_2 9 M565T15 9 M565T15 1 M221T19 2 M119T14 8 M621T15 </pre>	1.17810985 1.17035124 1.16633313 1.16407117 1.15855517 1.1541478 1.14909666	9 -0.2364741 -0.2269416 3 -0.2219799 -0.2123267 -0.205828 5 -0.2005002	2.41792855 2.00908774 2.23155622 2.26682318 2.15628900 2.25839361 2.13061065	-7.9513274 -5.3602012 -6.7354962 -6.1061829 -5.6641662 -9.9584077 -5.1113482	0.00382007 0.00979292 0.00586737 0.00540975 0.00697768 0.00551577 0.00740269	0.02265429 0.03401502 0.02853127 0.02737525 0.03031699 0.02758935 0.03095745	DOWN DOWN DOWN DOWN DOWN DOWN DOWN DOWN	419.035272 611.278173 565.120094 535.110262 221.08486 119.039425 621.206427	419.033926 611.27616 565.119191 525.106754 221.08127 119.033334 621.205274	419.03625 611.284794 565.121328 535.111276 221.085397 119.042616 621.20758	11.3799333 15.8765083 14.6141 13.5184917 19.0063333 14.0117333 15.1936583	11.3681333 15.8224333 14.59155 13.4834667 14.0084 15.1884833	11.388166 15.954433 14.664316 13.562266 19.030666 14.038183 15.198833
111 118 120 121 123 123	7 M419T11_1 8 M611T16_2 9 M565T15 9 M535T14 M221T19 M19T14 9 M621T15 4 M607T16	1.17810988 1.17035124 1.16633312 1.16407717 1.15855517 1.1541478 1.14909666 1.11674864	9 -0.2364741 4 -0.2269416 3 -0.2219799 7 -0.2123267 -0.2123267 -0.205828 -0.2005002 4 -0.1593045	2.41792855 2.00908774 2.23155622 2.26682318 2.15628903 2.25839361 2.13061062 2.01321577	-7.9513274 -5.3602012 -6.7354962 -6.1051829 -5.6641662 -9.9584077 -5.1113482 -5.863233	0.00382007 0.00979292 0.00586737 0.00540975 0.0069768 0.00551577 0.00740269 0.00970028	0.02265425 0.03401502 0.02853127 0.02737525 0.03031695 0.02758935 0.03095745 0.03401502	DOWN DOWN DOWN DOWN DOWN DOWN DOWN	419.035272 611.278173 565.120094 535.110262 221.084846 119.039425 621.206427 607.130977	419.033926 611.27616 565.119191 535.106754 221.08127 119.03334 621.205274 607.129251	419.03625 611.284794 565.121328 535.111276 221.085397 119.042616 621.20758 607.131787	11.3799333 15.8765083 14.6141 13.5184917 19.0063333 14.0117333 15.1936583 15.9016833	11.3681333 15.8224333 14.59155 13.4834667 18.9436667 14.0084 15.1884833 15.87635	11.388166 15.954433 14.664316 19.030666 14.038183 15.198833 15.902666
111 118 120 121 123 124 125	7 M419T11_1 8 M611T16_2 9 M565T15 9 M535T14 1 M221T19 2 M119T14 8 M621T15 5 M621T16 5 M517T12_1	1.17810985 1.17035124 1.1663313 1.16407717 1.15855517 1.1541478 1.14909660 1.11674864 1.08641083	-0.2364741 -0.2269416 -0.2219799 -0.2121867 -0.2123267 -0.206828 -0.2005002 -0.2005002 -0.1593045 1-0.1195697	2.41792855 2.00908774 2.23155622 2.26682318 2.15628902 2.25839361 2.13061065 2.13061065 2.01321577 2.06759188	 -7.9513274 -5.3602012 -6.7354962 -6.1051825 -5.6641662 -9.9584077 -5.1113482 -5.863233 -5.3916682 	0.00382007 0.00979292 0.00586737 0.00540975 0.00551577 0.00740265 0.00970028 0.00855871	0.02265425 0.03401502 0.02853127 0.02737525 0.03031695 0.032758935 0.03401502 0.03280741	DOWN DOWN DOWN DOWN DOWN DOWN DOWN DOWN	419.035272 611.278173 565.120094 535.110262 221.084846 119.039425 621.206427 607.130977 517.213031	419.033926 611.27616 565.119191 535.106754 221.08127 119.03334 621.205274 607.129251 517.208377	419.03625 611.284794 565.121328 535.111276 221.085397 119.042616 621.20758 607.131787 517.213509	11.3799333 15.8765083 14.6141 13.5184917 19.0063333 14.0117333 15.1936583 15.9016833 12.1466167	11.3681333 15.8224333 14.59155 13.4834667 18.9436667 14.0084 15.1884833 15.87635 12.1357167	11.388166 15.954433 14.664316 13.562266 14.038183 15.198833 15.902666 12.198633



Reducing the number of ions

Metaboanalyst will filter ions if you don't

1	A	В	С	D	E	F	G	н	1	J	к	L	м	N
1		name	fold	log2fold	tstat	pvalue	qvalue	updown	mzmed	mzmin	mzmax	rtmed	rtmin	rtmax
2	1207	M446T5	1.377175	0.461712	2.687478	0.055893	0.077433	UP	446.1187	446.1181	446.1194	5.003833	4.970667	5.037
3	40	M149T5	1.90913	0.932916	18.0073	0.00012	0.005015	UP	149.0452	149.0443	149.0455	5.004642	4.99615	5.09565
4	1904	M428T5	1.113881	-0.1556	-1.82025	0.145891	0.128174	DOWN	428.1189	428.1158	428.122	5.006933	4.97	5.043867
5	2305	M415T5	1.10218	-0.14036	-1.37875	0.24297	0.176326	DOWN	415.1069	415.106	415.1077	5.007133	4.99615	5.018117
6	3204	M431T5	1.088047	0.121741	0.55343	0.614273	0.320704	UP	431.0058	430.9997	431.0088	5.008492	4.97	5.0903
7	2951	M417T5	1.026591	-0.03786	-0.79944	0.484807	0.274812	DOWN	417.1238	417.122	417.1243	5.022617	4.999617	5.043867
8	2828	M461T5	1.211062	0.276273	0.875784	0.436068	0.257935	UP	461.0385	461.0379	461.0397	5.0238	5.010417	5.079233
9	1603	M737T5	1.461053	0.547009	2.301815	0.100029	0.10421	UP	737.1304	737.1269	737.1334	5.0261	4.970667	5.043867
10	2473	M430T5	1.09405	-0.12968	-1.19016	0.304376	0.205884	DOWN	430.118	430.1169	430.119	5.03155	5.022167	5.049267
11	620	M445T5	1.637928	0.711872	4.193747	0.015944	0.04293	UP	445.1174	445.1162	445.1178	5.03155	4.99685	5.0698
12	934	M134T5	1.160373	0.214588	3.212711	0.033865	0.060651	UP	134.0173	134.0161	134.0181	5.052367	4.992317	5.204667
13	647	M59T5	1.557694	0.639411	4.258795	0.017423	0.045047	UP	59.01358	59.01234	59.01613	5.063733	4.972833	5.09565
14	1919	M528T5	1.266863	0.341261	2.016901	0.14872	0.129638	UP	528.0399	528.0329	528.0433	5.078825	5.018117	5.116783
15	1091	M498T5	1.984819	0.989007	4.038585	0.046207	0.07082	UP	498.0279	498.0252	498.0327	5.087442	5.023067	5.131433
	-			30	087 ion	s – too	many	– nee	d to red	uce to	2000			
8077	1706	M253T23	1.416906	-0.50274	-2.06326	0.114028	0.11168	DOWN	253.1829	253.1801	253.1839	23.30983	23.2595	23.36067
8078	2067	M515T24	1.091546	0.126373	1.903596	0.18148	0.146867	UP	514.9764	514.9749	514.9768	23.57683	23.5595	23.59583
8079	3049	M316T24	1.126937	0.172406	0.704824	0.528703	0.289953	UP	316.257	316.2568	316.2576	23.67358	23.66283	23.695
3080	3307	M315T24	1.069737	0.097255	0.469644	0.665489	0.336622	UP	315.2532	315.253	315.2548	23.67517	23.66217	23.69017
3081	606	M239T24	1.528422	-0.61204	-4.80953	0.015381	0.042457	DOWN	239.1648	239.1641	239.1658	23.74325	23.731	23.77283
8082	497	M415T24	1.750608	0.807856	4.712873	0.010264	0.034546	UP	415.2702	415.2695	415.271	23.82217	23.8215	23.82283
8083	3454	M293T24	1.035401	-0.05019	-0.38613	0.735035	0.355976	DOWN	293.2115	293.2107	293.2126	23.82742	23.79517	23.85517
8084	3810	M315T24_	1.010898	0.015637	0.076505	0.944836	0.414735	UP	315.2533	315.253	315.2539	24.01042	23.99983	24.0295
8085	3630	M316T24_	1.029368	-0.04176	-0.22468	0.84074	0.387428	DOWN	316.2574	316.2568	316.2581	24.01042	23.99983	24.0245
8086	1617	M661T24	1.103245	-0.14175	-2.1225	0.101419	0.104917	DOWN	660.9736	660.973	660.9755	24.471	24.44683	24.48183
8087	3726	M295T25	1.048568	-0.06842	-0.14967	0.892584	0.400688	DOWN	295.2277	295.2274	295.2282	24.54858	24.508	24.58
8088	3905	M296T25	1.00045	0.000649	0.001523	0.99891	0.427899	UP	296.2314	296.231	296.2319	24.56108	24.55383	24.56833

	A	В	С	D	E	F	G	Н	1	J
1		fold	log2fold	tstat	pvalue	qvalue	mzmed	Rt_med	Mean_NR	Mean_IR
2	2642	1.02133818	-0.0304606	-1.0167497	0.3679932	0.23299293	253.032519	13.693675	3306740.23	3237655
3	2050	1.06546213	0.09147932	1.64240724	0.1769922	0.14436164	305.070478	13.2466667	1696194.92	1807233
4	2363	1.03350529	0.04754577	1.31253109	0.26364298	0.18663292	293.114861	10.9970917	1498747.05	1548963
5	2062	1.06204886	0.08685014	1.83471727	0.17924862	0.14541289	387.165616	11.766275	1381508.16	1467229
6	219	1.56524555	0.646389	8.04462309	0.00249317	0.01904335	329.231644	19.98	908081.785	1421371
7	906	1.05982475	-0.0838257	-3.2232179	0.03249886	0.06000338	269.045847	15.4403833	1446007.76	1364384
8	3584	1.00772798	-0.0111063	-0.2483095	0.81740307	0.38137667	461.109237	12.6152917	1342598.38	1332302
9	3514	1.02524051	-0.0359624	-0.3227556	0.77687837	0.36981714	191.019737	6.29196667	1330544.62	1297788
10	262	2.10952508	1.07691824	17.1166071	0.00332954	0.0212578	187.097625	15.8236583	466760.497	984643
11	1204	1.04541773	-0.0640795	-3.3960413	0.05562863	0.07728721	477.103942	14.181775	949647.413	908390
12	3603	1.01149995	0.01649625	0.24489561	0.82505665	0.38304982	503.119673	15.1001833	837553.526	847185
13	2744	1.04975796	0.07005672	0.9921432	0.40313583	0.24569897	309.109607	8.73341667	730056.217	766382
14	3686	1.00585021	-0.0084155	-0.1880312	0.86797629	0.39388838	519.115262	16.6849167	750027.76	745665
15	3722	1.00579783	0.00834035	0.15323255	0.89011985	0.4000441	467.213875	16.0323333	696267.638	700304
	F									
				S	elect the	e top 200	0 ions			
990	2401	1.36338159	-0.4471894	-1.4532346	0.27812273	0.19376712	630.313619	17.0609167	7976.77407	585
991	1663	1.17585328	0.23370805	2.17623743	0.10786161	0.10849518	285.038382	14.1529083	4974.98016	5850
992	3226	1.05094952	0.07169337	0.53776289	0.6215183	0.32227403	253.240184	13.6925833	5551.67508	5835
993	331	1.71149617	0.77525806	6.8723704	0.00541689	0.02737525	165.05593	11.56685	3408.55073	5834
994	3445	1.04068237	-0.0575298	-0.3728769	0.73078619	0.35479787	555.083177	15.2506667	6069.97147	583
995	711	1.18215249	-0.2414161	-4.2605693	0.02073158	0.04877515	582.082969	15.4834167	6872.78357	5814
996	296	1.46569412	-0.5515841	-7.7272252	0.00427027	0.02413235	339.070163	14.5664833	8516.5468	5811
997	349	1.28161543	-0.3579634	-6.5367788	0.00601293	0.02874864	624.267431	11.6629	7446.25062	5810
998	2974	1.11100076	-0.1518598	-0.8069474	0.49568244	0.27880357	603.285239	13.2274	6453.07992	5808
999	1022	1.58584765	0.66525418	4.24548217	0.04075359	0.06657426	517.298822	20.1105	3662.08997	5808
000	3137	1.07937018	0.11018974	0.61520781	0.57876407	0.30857698	337.002039	15.6117667	5366,47259	5792

Areas of aligned metabolites by sample

negmode_nr1 negmode_nr 3320701 321128 1650544 165250 1502083 153754	2 negmode_nr3 5 3388235 7 1785534	negmode_ir1 3247804	negmode_ir2 3308733	negmode_ir3 3156426
3320701 321128 1650544 165250 1502083 153754	5 3388235 7 1785534	3247804	3308733	3156426
1650544 165250 1502083 153754	7 1785534	1009024		
1502083 153754		1900024	1746573	1767097
	9 1456609	1602389	1497667	1546834
1348351 139673	1399435	1538662	1387977	1475049
942173 83927	5 942798	1519979	1335058	1409076
1476742 144382	1417457	1401542	1343338	1348272
1389740 132633	1311725	1399942	1301020	1295945
1395260 146372	7 1132647	1307379	1276028	1309956
469492 46464	466149	1044107	964298	945524
963917 95798	8 927037	903994	904583	916594
846739 81098	4 854938	919809	799096	822651
751388 73445	B 704322	833628	740626	724893
757382 70682	5 785876	744625	749518	742854
685156 71192	5 691722	750467	674733	675713
804585 76022	1 750478	726812	609044	647972
717398 70988	739525	670560	613870	640035
513949 58595	582984	543410	498409	586219
22783 1791	5 17732	557699	528582	514971
501645 50785	464691	515378	475918	482951
477094 48274	490705	495190	477892	475722
non-irradiate	d diet	irr	adiated c	liet

	Cr	oatir		v files for each sample
	CI	catii	18.03	
1	mzmed	rtmed	negmode nr1	
2	499.71989	17.9395	9846	 Copy the median <i>m/z</i> and median Rt
3	251.004448	14.646175	28534	values into a new Excel file. Then copy
4	417.212131	17.8596667	6340	the column of energy from the first
5	199.133402	18.99725	18534	the column of areas from the first
6	537.125737	13.7591333	17847	sample in Group 1. Save as an Excel
7	325.093116	11.2136667	23162	file
8	144.045677	16.2021167	26142	.CSV file.
9	357.082227	12.6645667	12999	 Note that the file name must not have
10	426.03226	8.13925	893	snaces – use an underscore instead of a
11	347.167955	13.059825	10415	spaces use an underscore instead of a
12	591.136922	14.92045	26263	space.
13	629.783983	16.3271833	3051	 Leave the file open and replace the
14	438.171148	12.3017917	15492	
15	425.045022	8.13335	3088	yellow column with the areas from the
16	151.039947	14.5387583	7302	next Group 1 sample. Save as a second
17	506.109327	15.2182417	23595	
18	789.227085	14.9668167	10301	.CSV THE.
19	315.142993	16.3572333	6312	Continue until all Group 1 and Group 2
20	640.774334	16.3572333	3677	
21	582.278039	15.5049667	13805	samples have a corresponding .csv file.







) Upload you	ır data	
Tab-delimiter Data Type: Format: Data File:	text (.txt) or comma-separated values (.csv) file: Concentrations Spectral bins Peak intensity table Samples in rows (unpaired) Choose File No file chosen	Submit
Zipped Files	(.zip) :	
Data Type: Data File: Pair File:	NMR peak list MS peak list MS spectra Choose File Diet_negroode.zip Choose File No file chosen	Submit



Processing M5 peak list data :	
Peaks need to be matched across samples	in order to be compared. For two-column format (mass and intensities), peaks are grouped by
heir m/z values. For three column data (ma	ss, retention time, and intensities), the program will further group peaks based on their retention
ime. Users need to supply tolerance values	in order to proceed. Here are some suggested values: mass tolerance - 0.25 (m/z); retention time
30 (seconds) for LC-MS peak, and 5 (seco	nds) for GC-MS peaks. Please note, If a sample has more than one peak in a group, they will be
eplaced by their sum; some groups will be	excluded if none of the classes has at least half its samples represented. Finally, the program
create a peak intensity table in which each s	sample occupies a row and each column represents a peak group identified by the median values
of its position (m/z and/or retention time).	
Mass tolerance (m/z):	0.001
Retention time tolerance:	.01
MS peak processing int	formation
The uploaded files are peak lists and intens	sities data.
A total of 6 samples were found.	
These samples contain a total of 18522 per	aks.
with an average of 3087 peaks per sample	
A total of 3087 peak groups were formed.	
Peaks of the same group were summed if t	hey are from one sample.
Peaks appear in less than half of samples i	n each group were ignored.
	Next



Non-informative variables can be characterized in two groups: variables of very small values - these variables can be detected using mean or
median; variables that are near-constant throughout the experiment conditions - these variables can be detected using standard deviation
(SD); or the robust estimate such as interquantile range (IQR). The relative standard deviation(RSD = SD/mean) is another useful variance
measure independent of the mean. The following empirical rules are applied during data filtering:
Less than 250 variables: 5% will be filtered;
Between 250 - 500 variables: 10% will be filtered;
Between 500 - 1000 variables: 25% will be filtered;
Over 1000 variables: 40% will be filtered;
Please note, in order to reduce the computational burden to the server, the None option is only for less than 2000 features. Over that, if you
choose None, the IQR filter will still be applied. In addition, the maximum allowed number of variables is 5000. If over 5000 variables were left
after filtering, only the top 5000 will be used in the subsequent analysis.
Interguantile range (IQR)
Median absolute deviation (MAD)
Relative standard deviation (RSD = SD/mean)
Non-parametric relative standard deviation (MAD/median)
Mean intensity value
Median intensity value
None (less than 2000 features)
Process

San	pple normalization			
	None Sample specific normalization (i. Normalization by sum Normalization by median Normalization by reference sample Specify a reference sample	e. dry weight, volume)	e_ir1 v	Click here to specify
0	Normalization by reference feature	50.12842/14.09	-	

Data transform	nation
None	
Log trans	formation (generalized logarithm transformation or glog)
Cube roo	t transformation (take cube root of data values)
Data scaling	
None	
Auto scal	ing (mean-centered and divided by the standard deviation of each variable)
Pareto sc	aling (mean-centered and divided by the square root of standard deviation of each variable)
Range sc	aling (mean-centered and divided by the range of each variable)