H. Paul Benton

History of XCMS -> XCMS Online

- Development of Kernel density peak grouping and LOESS Retention time alignment - 2004 spring
- Checked into Bioconductor - Mid 2005 (Smith, C., Want, E. J., O'Maille, G., Abagyan, R., & Siuzdak, G. E. (2006). XCMS: Processing Mass Spectrometry Data for Metabolite Profiling Using Nonlinear Peak Alignment, Matching, and Identification. Analytical Chemistry, 78(3), 779–787. doi:10.1021/ac051437y)
- CentWave peak detection added - Late 2007 (Tautenhahn, R., Böttcher, C., & Neumann, S. (2008). Highly sensitive feature detection for high resolution LC/MS. BMC Bioinformatics, 9, 504. doi:10.1186/1471-2105-9-504)
- Tandem mass data - Mid/late 2007 (Benton, H. P., Wong, D. M., Trauger, S. A., & Siuzdak, G. E. (2008). XCMS2: processing tandem mass spectrometry data for metabolite identification and structural characterization. Analytical Chemistry, 80(16), 6382–6389. doi:10.1021/ac800795f)
- Parallel processing - Mid 2008
- OBI-Warp Retention time alignment added - Early 2009 (Prince, J. T., & Marcotte, E. M. (2006). Chromatographic Alignment of ESI-LC-MS Proteomics Data Sets by Ordered Bijective Interpolated Warping. Analytical Chemistry, 78(17), 6140–6152. doi:10.1021/ac0605344)
- XCMS Online Work started - Mid 2009 (Tautenhahn, R., Patti, G. J., Rinehart, D., & Siuzdak, G. E. (2012). XCMS Online: a web-based platform to process untargeted metabolomic data. Analytical Chemistry, 84(11), 5035–5039. doi:10.1021/ac300698c)
- Data correction algorithm built for XCMS (Benton, H. P., Want, E. J., & Ebbels, T. M. D. (2010). Correction of mass calibration gaps in liquid chromatography-mass spectrometry metabolomics data. Bioinformatics (Oxford, England), 26(19), 2488–2489. doi:10.1093/bioinformatics/btq441)
- meta-XCMS built into XCMS Online - 2012 (Tautenhahn, R., Patti, G. J., Kalisiak, E., Miyamoto, T., Schmidt, M., Lo, F. Y., et al. (2011). metaXCMS: Second-Order Analysis of Untargeted Metabolomics Data. Analytical Chemistry, 83(3), 696–700. doi:10.1021/ac102980g)
- Multiple class comparison & interactive PCA tools - Feb 2014

Different Jobs

- Pairwise - Performs a two class comparison - i.e. KO vs WT - univariate two class statistics + some multi-variate methods

- multi-group - Performs a multiple class comparison - univariate statistics with n classes (Anova, Kruskal–Wallis etc) + multi-variate methods

- metaXCMS - takes pairwise xcms reports and finds similar features between the pairwise (or mulitgroup) reports

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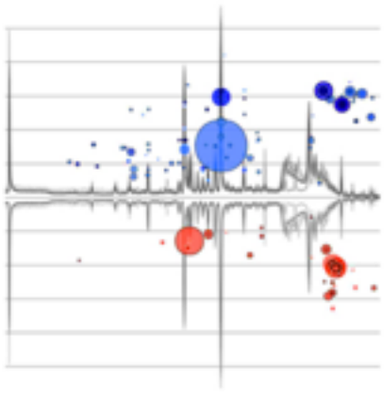
XCMS Online



Click here to view the new Interactive Cloud Plot!

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Do you want to hear about all of the latest XCMS Online news? Click here to get on our newsletter to keep informed about what we're doing to help you with your metabolomics data.

XCMS Online is a cloud-based metabolomic data processing platform that provides high-quality metabolomic analysis in an intuitive, web-based format. XCMS Online allows users to easily upload LC/MS metabolomic data that can then be processed with a few simple mouse clicks. You will need a user account to use the system. However user accounts are free and only require a valid e-mail address to register.

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METLIN

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Demo Dataset that can be used for testing

XCMS Server for your lab!

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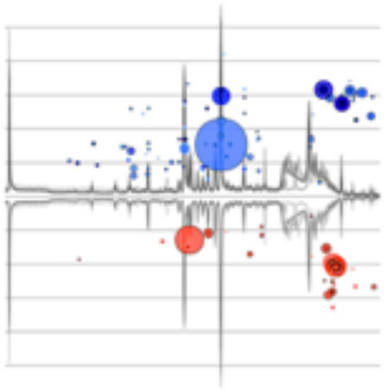
XCMS Online



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Demo Dataset that can be used for testing

XCMS Server for your lab!

masspec.scripps.edu

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Welcome.

Note: All new users require e-mail verification. A verification e-mail will be sent to the e-mail address your provide. Please add "scripps.edu" and "xcmsonline@gmail.com" to your whitelist.

You can check your system compatibility with our System compatibility test

Choose a username

First Name

Last Name

Organization/Affiliation

Enter your e-mail address

Pick a password

Note: Password must be at least 8 characters

Enter the password again

Verification - Please type letters you see in image

37EUVF

Participate in anonymous usage statistics (view detail)

This will be your permanent e-mail address to be used for:

- registration
- password resets
- job alerts (errors, completed)
- technical support
- system notifications (e.g. maintenance)

Scripps Center For Metabolomics XCMS Online

User: hpb Logout

Home | Create Job | View Results | Stored Datasets | Public Shares | XCMS Institute | Account | Contact

- Pairwise Job
- metaXCMS Job
- Multigroup Job

View Jobs

Share Job(s) | Job Grouping | Resubmit Job(s) | Delete Job(s)

Job Count: 16

Search Jobs [ ] Search Clear

View Public Shares [ ]

	Exp Type	Status	ID	Progress	JobName	Datasets (ID#) [*control]	Created	Parameters (ID#)	Group	Shared	
	-EXP-	- STATUS -							- GROUP -		
[ ]	MULTI	VIEW	1023248	job complete 100%	MG_2014-05-15_12:53	Pos-Notpre (#73124) Pos-QC (#73123) Pos-Pregna (#73122)	2014-05-15 12:53:24	Waters UPL (10669)			✖

Scripps Center For Metabolomics XCMS Online

User: hpb Logout

Home | Create Job | View Results | Stored Datasets | Public Shares | XCMS Institute | Account | Contact

Job Name | Dataset 1 (control) | Dataset 2 | Parameters | Submit Job | Reset Page

Job Name (1023391): hpbenton_2014-05-19_01:08:39

Dataset 1

Upload New Dataset OR Select Dataset

(See File Formats for more information)

Dataset 1 ID: Not Defined # Files: 0

Dataset 1 Name: Not Defined

Dataset 2

New Dataset OR Select Dataset

File Formats for more information)

Dataset 2 ID: Not Defined # Files: 0

Dataset 2 Name: Not Defined

Parameters Select Parameters

Submit Job

Upload new datasets as either raw data or open format data

Call you job something so you remember what it is

Upload Dataset 1

https://xcmsonline.scripps.edu/embed_upload_min.php?datasetorder=1&action=newjob&runuser=undefined&jobi

Storage Quota Usage (1.10 TB):

1 90%

1. Select only .mzXML, .mzData, mzData.XML, .netcdf, .cdf, .d, .wiff files (More info: File Formats)
2. After upload is complete (reassembled, md5 checked), this window will automatically close.

Dataset Name: Dataset_1 Save

file tree visible file list visible

Paste Remove... Retry failed 0 0 0 0

Drop Files Here

No files

Upload

Call your dataset something so you'll remember what it is

Loads - Upload window

Upload Dataset 1

https://xcmsonline.scripps.edu/embed_upload_min.php?datasetorder=1&action=newjob&runuser=undefined&jobi

Storage Quota Usage (1.10 TB):

1 90%

1. Select only .mzXML, .mzData, mzData.XML, .netcdf, .cdf, .d, .wiff files (More info: File Formats)
2. After upload is complete (reassembled, md5 checked), this window will automatically close.

Dataset Name: Dataset_1 Save

file tree visible file list visible

Paste Remove... Retry failed 0 0 0 0

Upload

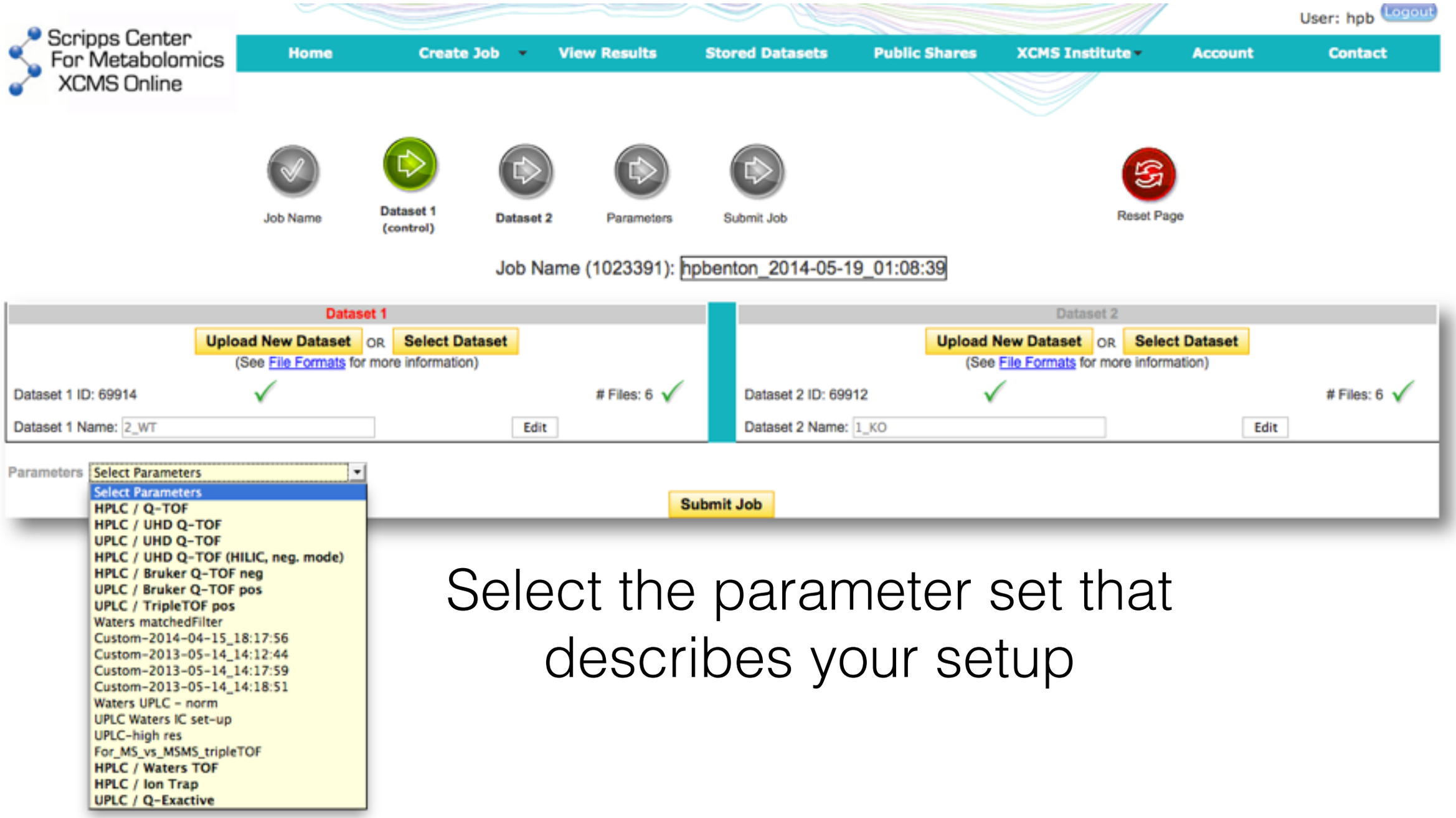
Open

EBC

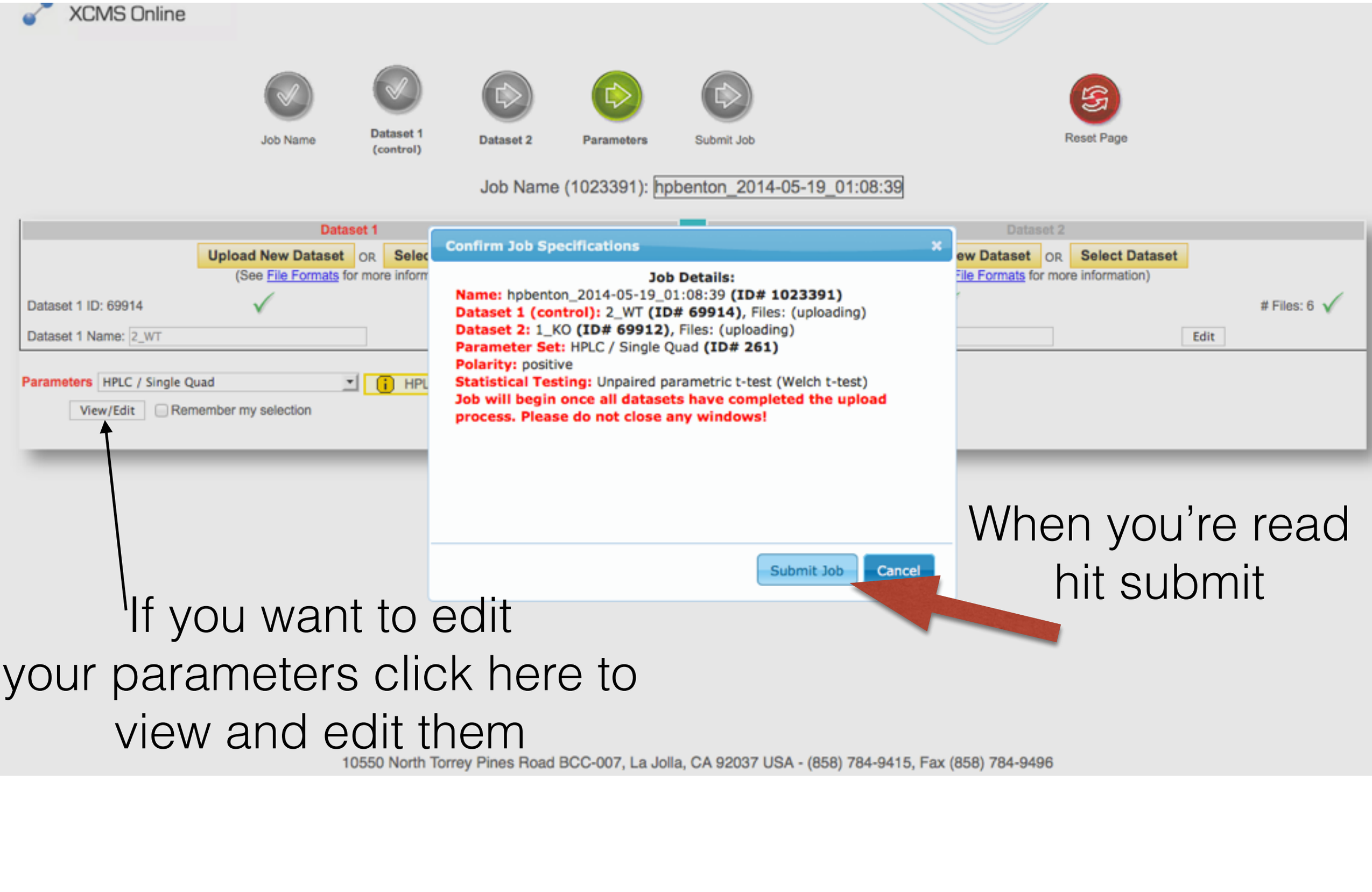
Name	Date Modified
EBC101.CDF	Tuesday, April 17, 2012 4:16 AM
EBC1A01.CDF	Tuesday, April 17, 2012 4:20 AM
EBC301.CDF	Tuesday, April 17, 2012 4:16 AM
EBC3A01.CDF	Tuesday, April 17, 2012 4:21 AM
EBC401.CDF	Tuesday, April 17, 2012 4:17 AM
EBC4A01.CDF	Tuesday, April 17, 2012 3:49 AM
EBC501.CDF	Tuesday, April 17, 2012 4:16 AM
EBC5A01.CDF	Tuesday, April 17, 2012 4:21 AM
EBC601.CDF	Tuesday, April 17, 2012 4:17 AM
EBC6A01.CDF	Tuesday, April 17, 2012 3:49 AM
EBC701.CDF	Tuesday, April 17, 2012 4:16 AM
EBC7A01.CDF	Tuesday, April 17, 2012 4:21 AM

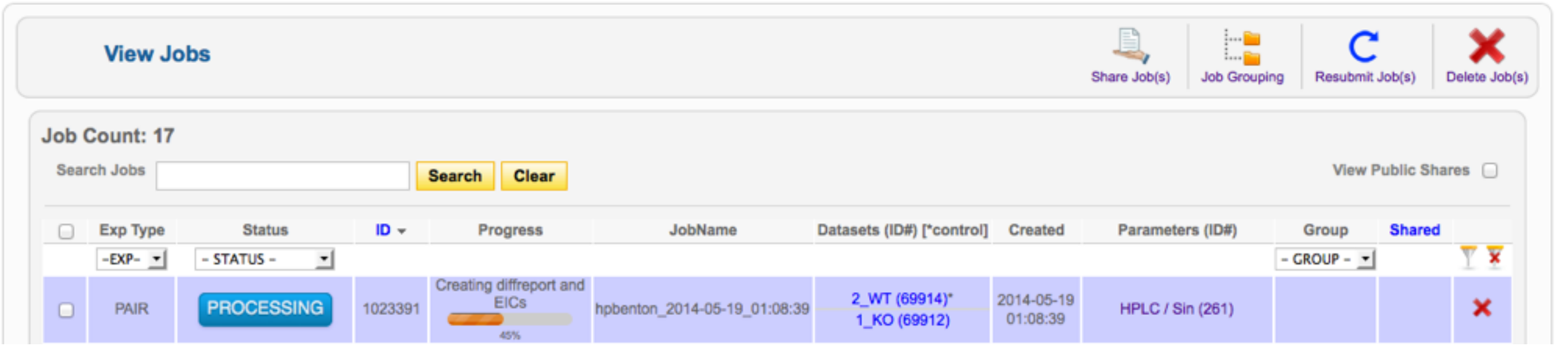
File Format: All Files

Cancel Choose



Select the parameter set that describes your setup


XCMS Online
Job Name
Dataset 1 (control)
Dataset 2
Parameters
Submit Job
Reset Page
Job Name (1023391): hpbenton_2014-05-19_01:08:39
Dataset 1
Upload New Dataset
OR
Select Dataset
(See File Formats for more information)
Dataset 1 ID: 69914
Dataset 1 Name: 2_WT
Dataset 2
Select Dataset
File Formats for more information)
Files: 6
Edit
Parameters HPLC / Single Quad
View/Edit
Remember my selection
Confirm Job Specifications
Job Details:
Name: hpbenton_2014-05-19_01:08:39 (ID# 1023391)
Dataset 1 (control): 2_WT (ID# 69914), Files: (uploading)
Dataset 2: 1_KO (ID# 69912), Files: (uploading)
Parameter Set: HPLC / Single Quad (ID# 261)
Polarity: positive
Statistical Testing: Unpaired parametric t-test (Welch t-test)
Job will begin once all datasets have completed the upload process. Please do not close any windows!
Submit Job
Cancel
If you want to edit your parameters click here to view and edit them
When you're read hit submit
10550 North Torrey Pines Road BCC-007, La Jolla, CA 92037 USA - (858) 784-9415, Fax (858) 784-9496



The job processes and reports where it is in the process
NB: not always linear time depending on number of features

- Once the job is finished you can click on the view button and see the results.

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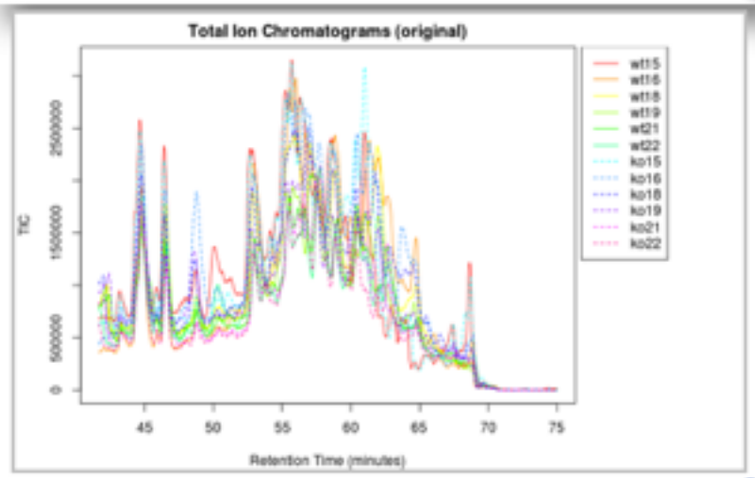
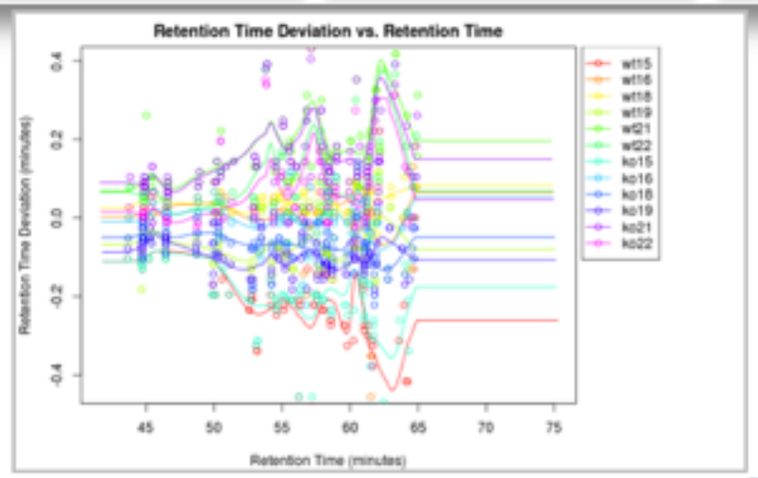
Home | Create Job | View Results | Stored Datasets | Public Shares | XCMS Institute | Account | Contact

Job ID:	1023391	**Job Name:**	hpbenton_2014-05-19_01:08:39	**Create Date:**	2014-05-19 01:08:39
Parameter (ID#)	HPLC / Single Quad (261)	**Log:**	View Log	**Finish Date:**	2014-05-19 01:27:33
Status:	job complete	**Total Aligned Features:**	387	**Experiment Type:**	Pairwise
Datasets Used:	2_WT(ID#69914) * vs. 1_KO(ID#69912)	**Paired Samples:**	False	**Share Status:**	Not Shared

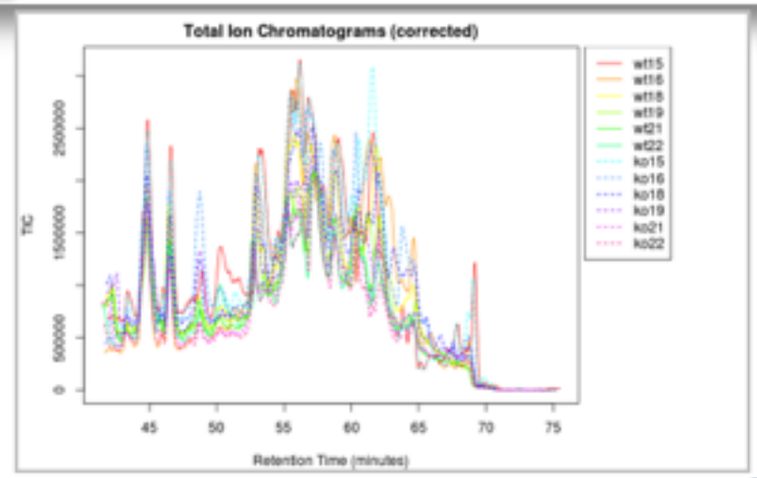
BROWSE RESULT TABLE | INTERACTIVE CLOUD PLOT | iPCA



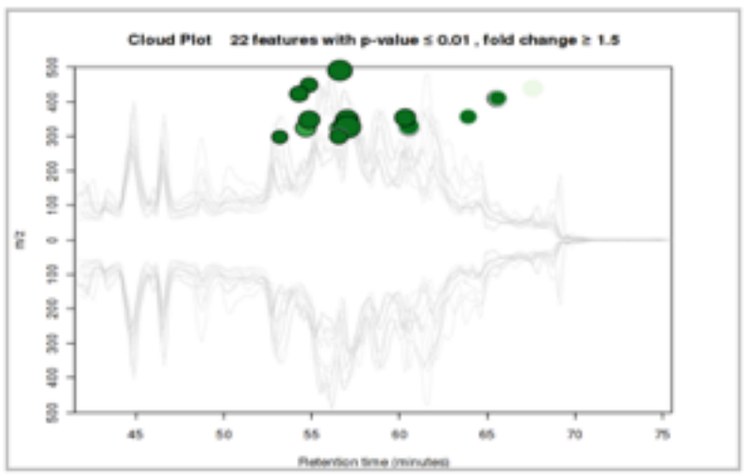
PNG PDF



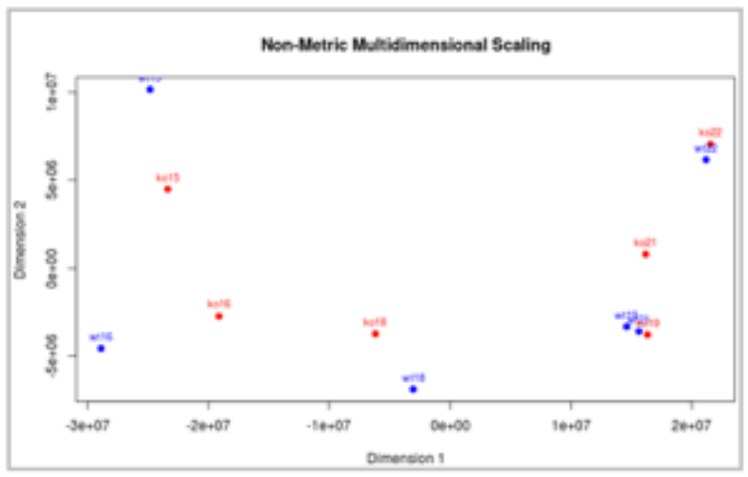
PNG PDF



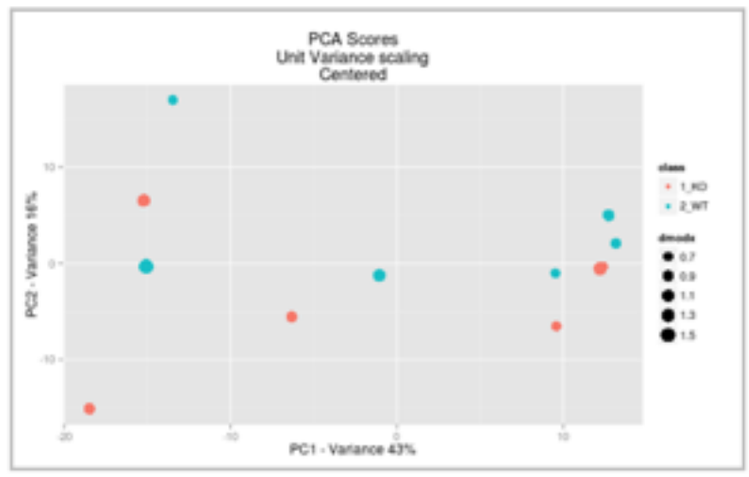
PNG PDF



PNG PDF SVG ▶ Interactive Version



PNG PDF



PNG PDF ▶ More

Complete Downloadable Results (including diffreport, EIC's, boxplots, etc.) : results.zip

Return to Job List

Download the results to you local machine

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User: hpb Logout

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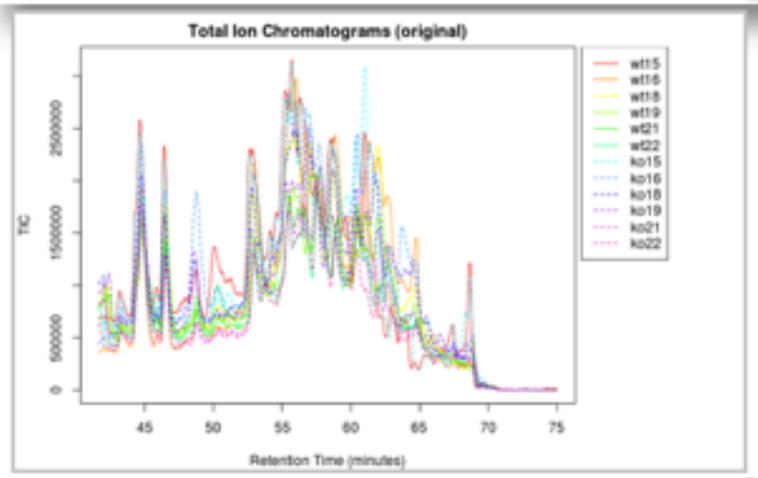
Job ID:	1023391	**Job Name:**	hpbenton_2014-05-19_01:08:39	**Create Date:**	2014-05-19 01:08:39
Parameter (ID#)	HPLC / Single Quad (261)	**Log:**	View Log	**Finish Date:**	2014-05-19 01:27:33
Status:	job complete	**Total Aligned Features:**	387	**Experiment Type:**	Pairwise
Datasets Used:	2_WT(ID#69914) * vs. 1_KO(ID#69912)	**Paired Samples:**	False	**Share Status:**	Not Shared

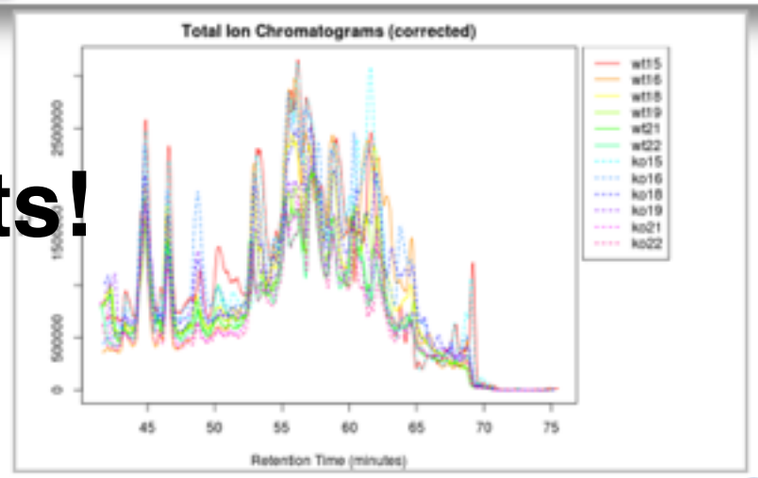
BROWSE RESULT TABLE | INTERACTIVE CLOUD PLOT | iPCA

Table of results!



PNG PDF

PNG PDF



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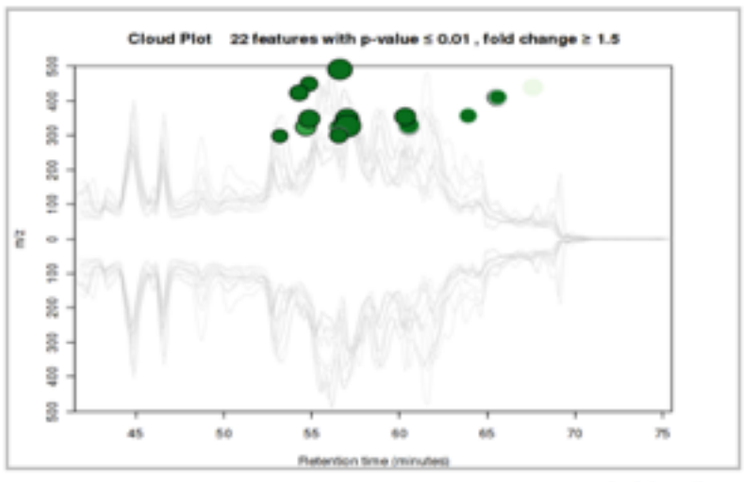
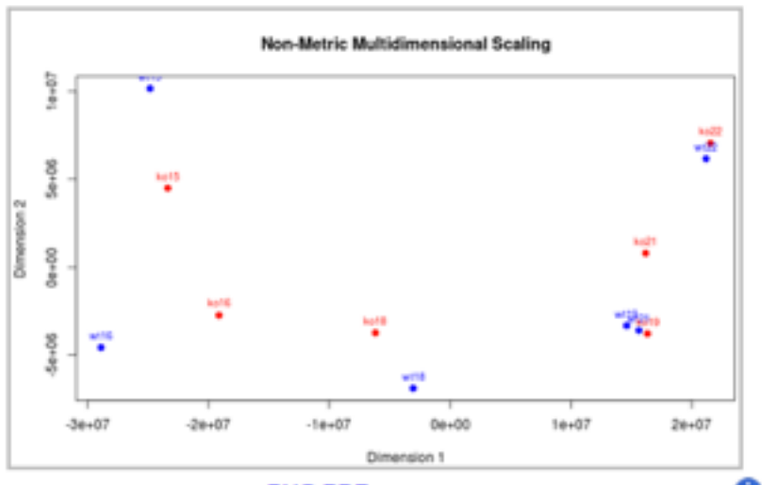


PNG PDF SVG ▶ Interactive Version



PNG PDF

PNG PDF ▶ More

Complete Downloadable Results (including diffreport, EIC's, boxplots, etc.) : results.zip

Return to Job List

Quick Compound Search: Search Clear

Job#1023394 : hpbenton_2014-05-19_01:36:33

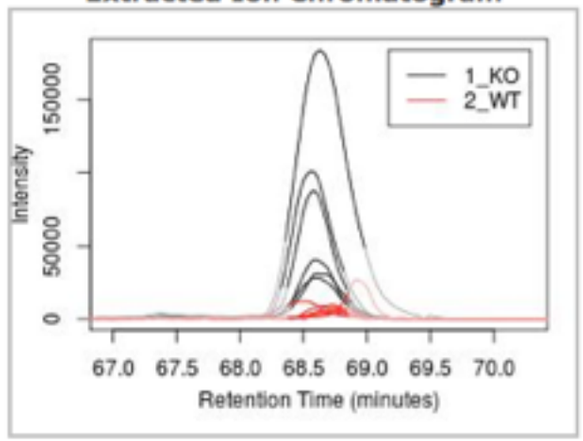
Columns Hide isotopic peaks Page 1 of 4 100 View 1 - 100 of 382

Feature	UP/DOWN	fold change	p-value	m/z	retention time	MaxInt	Ctrl(x̄)	Exp(x̄)	isotopes	adducts	feature g	Notes
1	DOWN	3.5	0.00216	298.1508	53.09	10,300	187,827	53,422			94	
2	DOWN	4.8	0.00216	300.1898	56.51	284,800	4,563,459	952,529	[5][M]+		11	
3	DOWN	5.4	0.00216	301.1879	56.52	58,696	951,475	175,317	[5][M+1]+		11	
4	DOWN	6.9	0.00216	322.1212	56.52	21,160	254,781	36,673			11	
5	DOWN	7.1	0.00216	324.1584	54.59	19,424	199,736	28,038			98	
6	DOWN	14.3	0.00216	326.2000	56.96	232,896	3,603,052	251,102	[12][M]+		27	
7	DOWN	27.8	0.00216	327.1989	57.00	50,504	847,011	30,505	[12][M+1]+		27	
8	DOWN	11.6	0.00216	328.2000	60.55	320,704	2,964,612	256,107		[M+H]+ 32	18	
9	DOWN	11.6	0.00216	329.2000	60.26	53,912	534,358	45,948			69	
10	UP	1.1	0.00216	339.1878	55.33	120,544	2,743,211	3,025,075			1	
11	DOWN	9.2	0.00216	348.1620	54.78	9,212	152,313	16,491			112	
12	DOWN	12.7	0.00216	348.1431	56.99	21,528	319,112	25,093			27	
13	DOWN	3.1	0.00216	352.1384	58.26	15,272	136,749	44,226			39	
14	DOWN	4.7	0.00216	356.2000	63.87	106,776	1,226,923	259,393	[19][M]+	[M+H]+ 35	49	
15	DOWN	4.2	0.00216	357.2062	63.89	26,896	320,038	76,340	[19][M+1]+		49	
16	DOWN	8.5	0.00216	376.1857	57.66	9,595	113,435	13,320		[M+Na]+ 3	16	
17	DOWN	13.8	0.00216	382.2000	63.24	41,568	311,083	22,558			80	
18	DOWN	5.7	0.00216	384.2298	66.62	80,272	713,301	124,071			59	
19	DOWN	15.1	0.00216	398.3000	67.64	22,112	128,117	7,306		[M+H-H20]	51	
20	DOWN	8.3	0.00216	410.2658	65.69	71,648	1,003,465	120,888			64	
21	DOWN	5.4	0.00216	411.2339	65.69	22,480	323,826	59,475			64	
22	DOWN	9.1	0.00216	412.2919	68.61	183,936	1,330,017	146,398	[26][M]+		32	
23	DOWN	9.2	0.00216	413.2918	68.61	52,216	394,274	42,852	[26][M+1]+		32	
24	DOWN	5.4	0.00216	423.1499	54.27	11,119	195,641	36,493			108	
25	DOWN	17.3	0.00216	438.2991	67.64	101,424	747,935	43,241	[31][M]+	[M+Na]+ 4	51	
26	DOWN	11.0	0.00216	439.2984	67.64	32,200	237,979	21,686	[31][M+1]+		51	
27	DOWN	4.9	0.00216	449.1321	54.85	6,725	129,330	26,612			14	
28	DOWN	5.0	0.00216	493.2000	61.08	22,840	356,093	71,591	[39][M+1]+		21	

Please click on a row to view feature details

Feature #22
m/z : 412.2919
Retention Time (min): 68.61

Extracted Ion Chromatogram



Box-and-Whisker Plot

Image not available

Original Settings | Add New View | Remove Current View | Toggle Help Box | Shrink | Reset Size | Magnify

Main Panel | Advanced

p-value

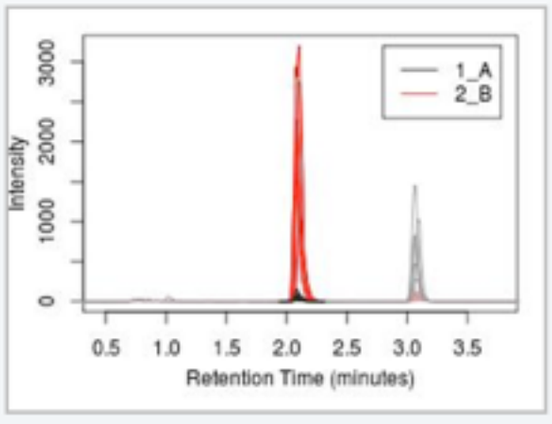
0 | 0-0.01 | 1

fold change

0 | 1.5 - 4123.356 | 4123.356

Regenerate Cloud Plot

EIC | Box and Whisker | Spectrum

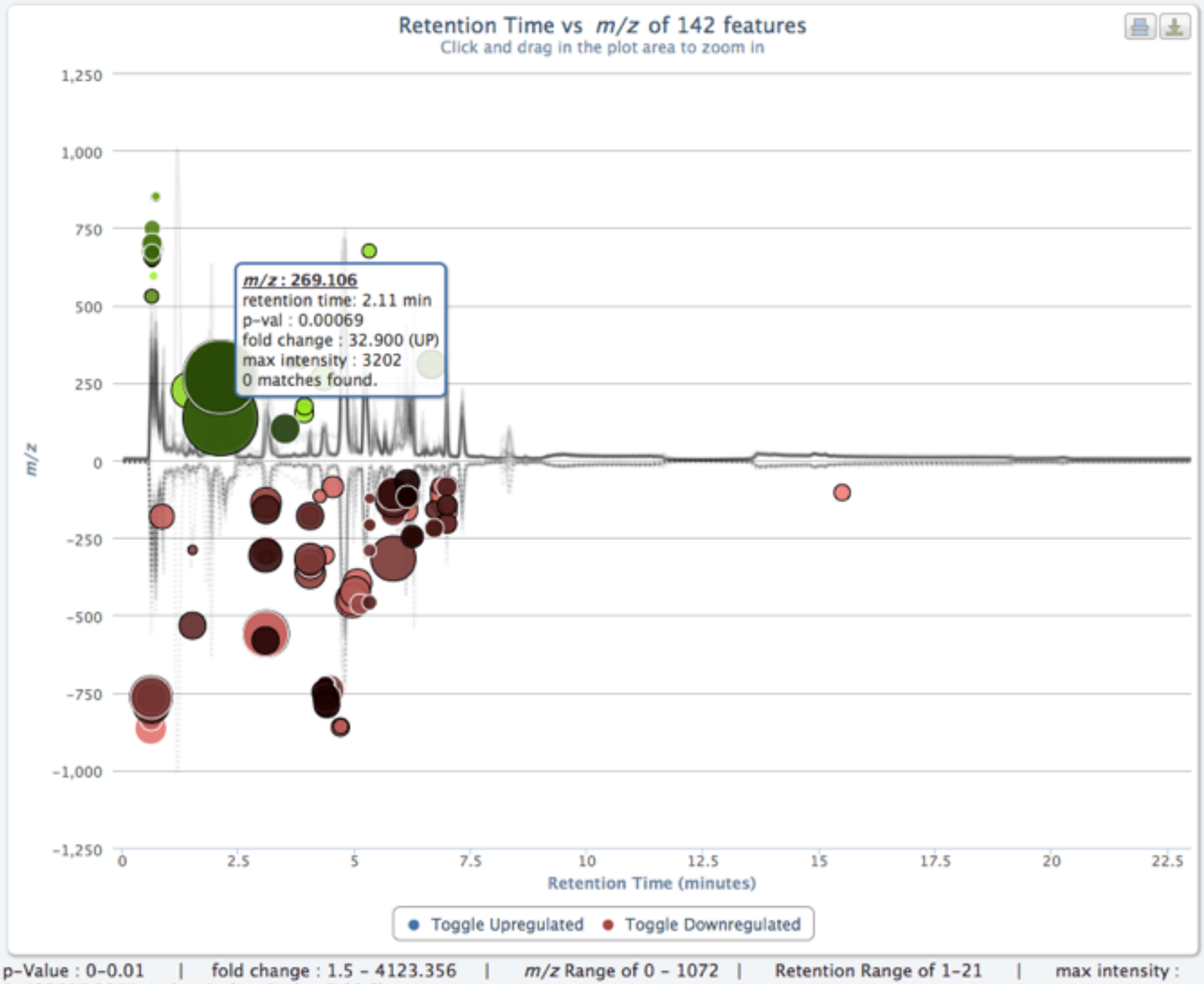


Bubble Size Multiplier

22

Download Cloud Plot Manual

View 1



p-Value : 0-0.01 | fold change : 1.5 - 4123.356 | *m/z* Range of 0 - 1072 | Retention Range of 1-21 | max intensity : 0-122607.2375 | Radius Scale : Fold Change

Table View

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User: hpb Logout

Home | Create Job | View Results | Stored Datasets | Public Shares | XCMS Institute | Account | Contact

1 → 2 → 3 → 4 Reset

1 Select Datasets

Upload New Dataset OR Select Dataset

(See File Formats for more information)

2 Define QC Dataset (optional)

-No QC Selected-

3 Parameters

Select Parameters

ID	Dataset Name	Number of Files

Job Summary

Job ID: 1023396

User: hpb (42)

Job Name: MG_2014-05-19_02:0 Edit

Datasets: 0

Parameter Set: Select Parameters

4 Submit

Click here to complete your job Submit Job

Multigroup Results Summary: MG_2014-05-15_12:53 (#1023248)

Submit Date	Finish Date	Total Aligned Features	Parameters	Log	Shared
2014-05-15 13:18:00	2014-05-15 14:07:38	2056	Waters UPLC - norm (10669)	View Log	NOT SHARED

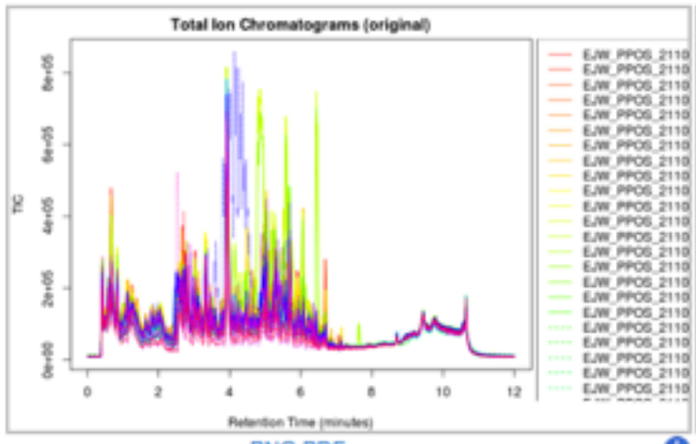
View Results Table

View iCloud Plot

View iPCA

Datasets Used

- Pos-Notpregnant (73124)
- Pos-QC (73123)
- Pos-Pregnant (73122)



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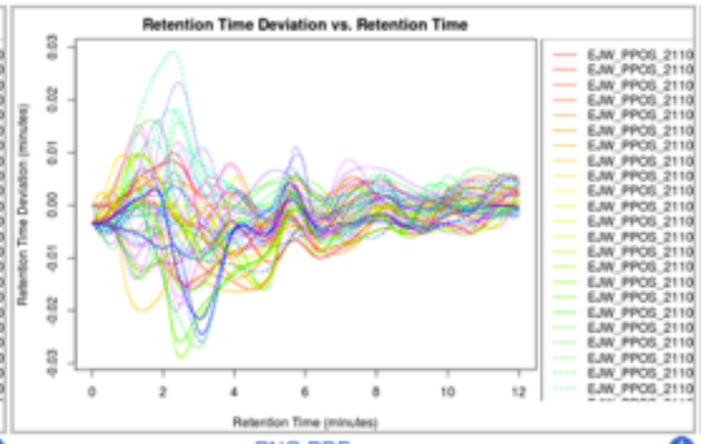

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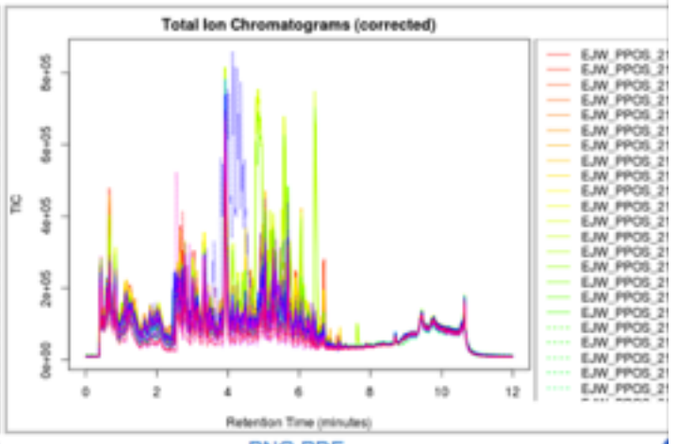

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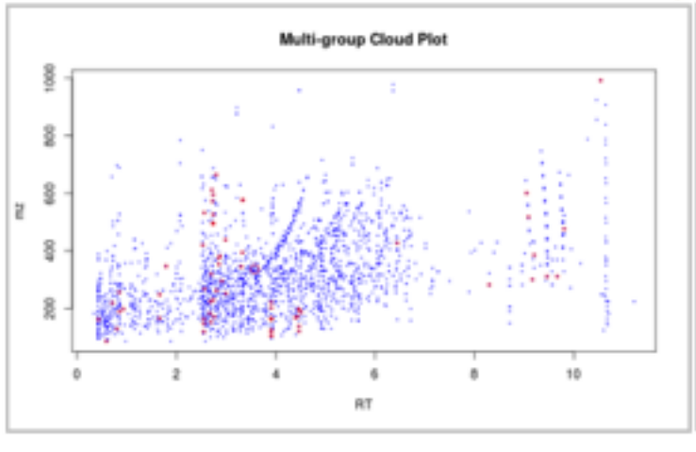

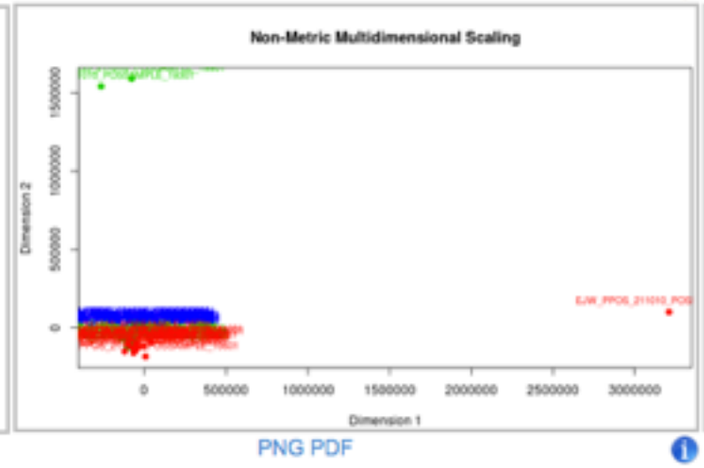

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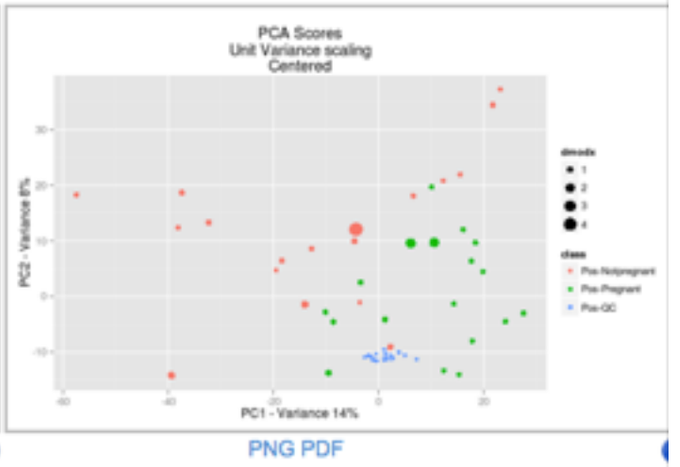


PNG PDF

Complete Downloadable Results (including diffreport, EIC's, boxplots, etc.) : results.zip

Interactive PCA

Main Panel | Advanced

X- axis PC options
1

Y-Axis PC options
2

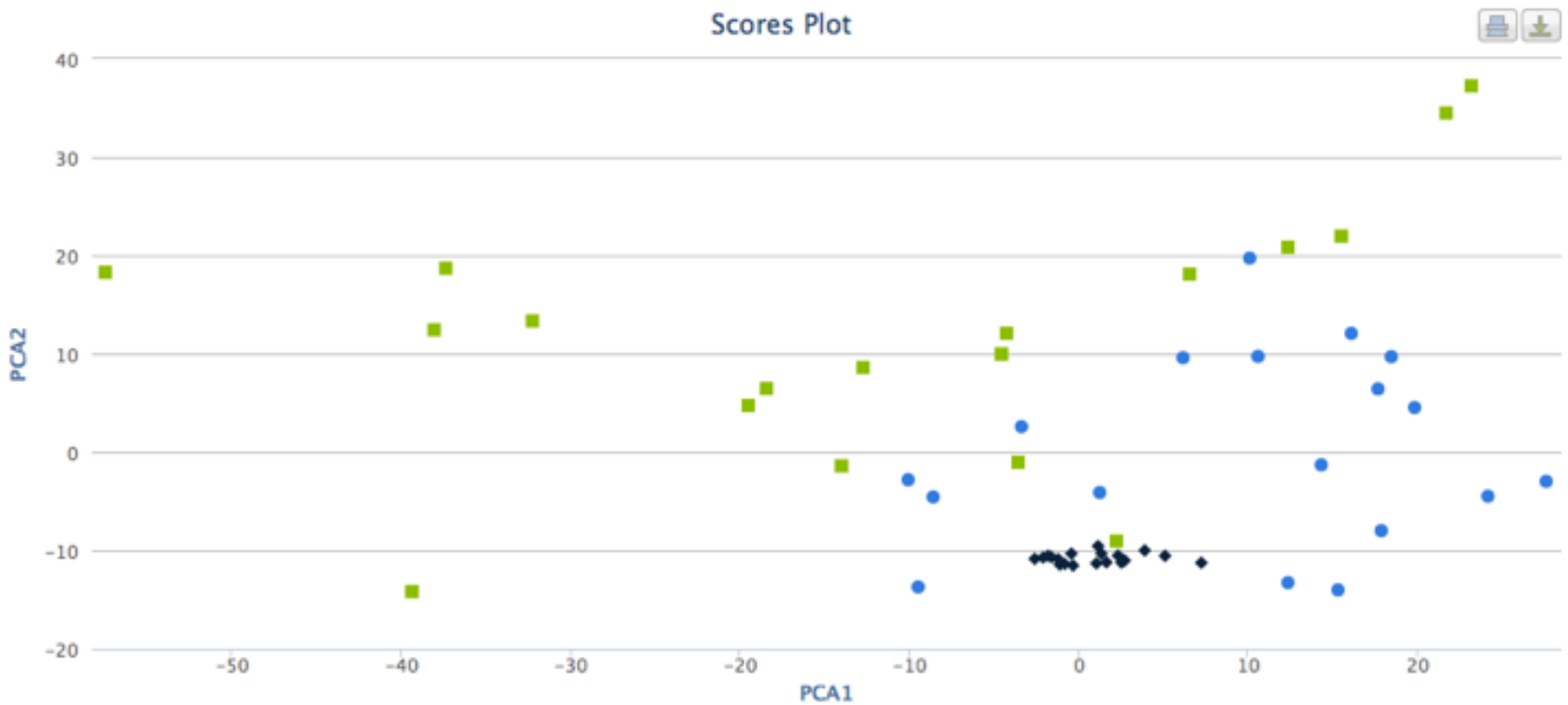
Modify loadings threshold (how many are shown)
1000

Scaling options unit_variance

Center ☑

Regenerate Graph

Scree Plot | Scores Plot | Loadings Plot



Interactive PCA

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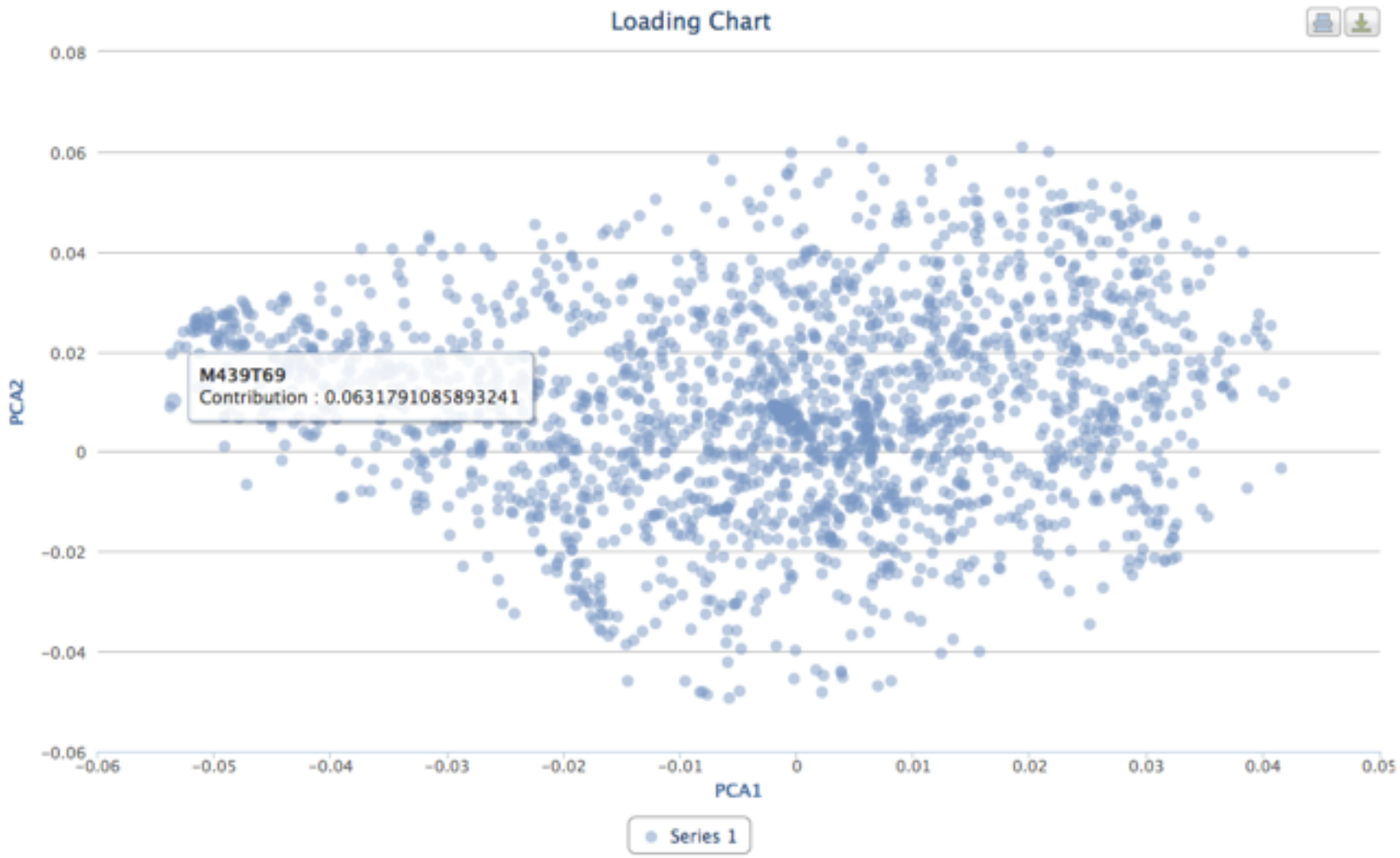
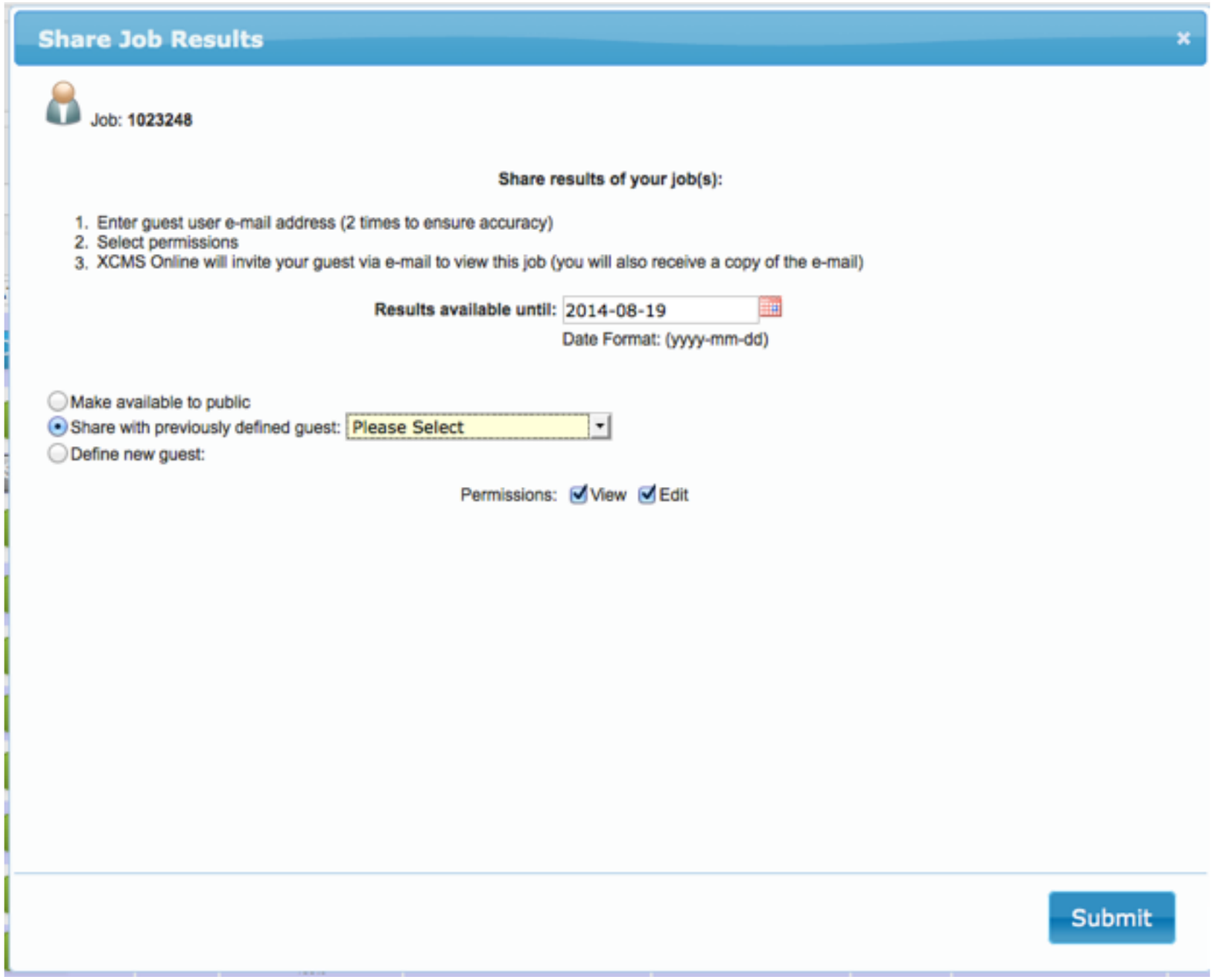
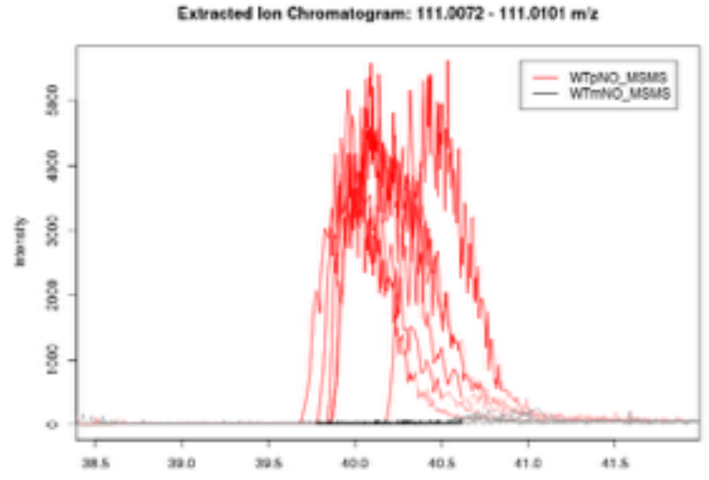


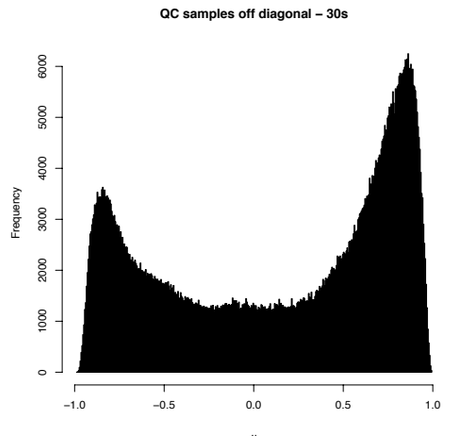


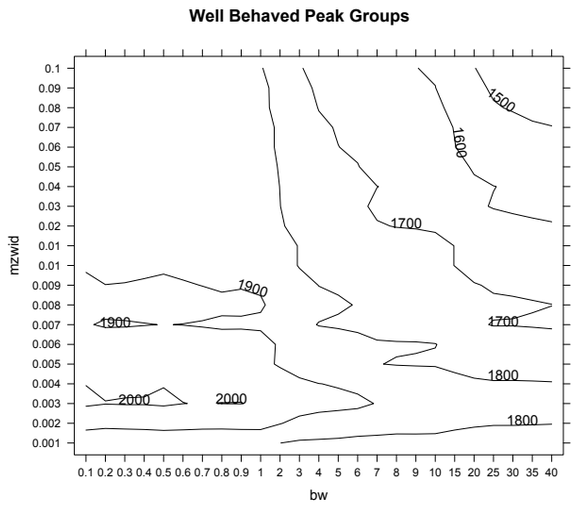
- You can share your results globally or locally with a colleague, collaborator, boss etc.

Interactive analysis of LC-MS datasets

- Bad retention time corrections
- Poor experimental parameters
- Poor experimental design







Developments

- Streaming - From MS -> data analysis in Real time
    - Allows iterative analysis to perform parameter correction/ learning
    - Check on instrument settings from last run
        - background
        - retention time shifts
        - etc
- Full online MS/MS selection, queuing and acquisition
    - Check other metabolites ID which are in regions of interest based on biological pathways & matrix type

* Rinehart D. . Metabolomic Data Streaming Enables Biological Dependent Data Acquisition Nature Biotechnology 2014

Developments

- isoXCMS -
  - Untargeted Stable isotope labele profiling !
    - Understand dynamics of all labeled metabolites
    - Tracing of metabolites from different pathway with isotope label

* Huang, X13CMS: global tracking of isotopic labels in untargeted metabolomics. Analytical Chemistry 2014 Feb 24;86(3): 1632-9

Summary

- XCMS Online allows eases XCMS use
- Full visual platform
- Data analysis platform - more in-depth statistical results and analysis plots
- XCMS Server allows Real Time MS data streaming
- IsoXCMS is a the next generation of untargeted metabolite profiling

Thank You!

- Questions?
- Many more updates coming soon including speed and more stats

Prof. Gary Siuzdak

Duane Rinehart

Dr. Colin Smith

Chinmay Gandhi

The whole xcms team