



Knowledge that will change your world

Preparing data for upload to XCMSonline

Stephen Barnes, PhD

University of Alabama at Birmingham

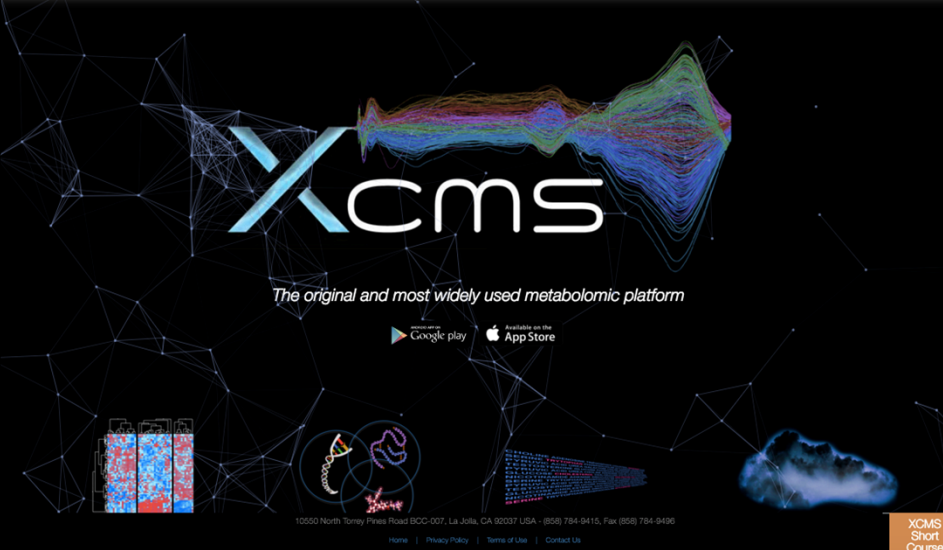
sbarnes@uab.edu

Synopsis

- LC-MS (and GC-MS) analysis generates a lot of data and requires **alignment** of individual data sets before statistical analysis can be performed
- We will discuss
 - Uploading data sets
 - Alignment principles

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XCMS Short Course

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You can check your system compatibility with our [System compatibility test](#)

N.B.: TSRI users already have accounts (via LDAP).

First Name

Last (Family) Name

Organization

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Password

Re-enter password

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)



Enter the code below password

Organization

Email

Password

Re-enter password

Participate in anonymous usage statistics ([View Details](#))

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)

Enter whatever appears here

Starting page for XCMSonline

Home  MRM Databases  Create Job  View Results  XCMS Public  XCMS Institute  Stored Datasets  Account  Toolbox  Help  Logout [empty1977]



The original and most widely used metabolomic and lipidomic platform

Latest News and Articles

Nature Methods "Systems Biology guided by XCMS Online Metabolomics"

Nature Methods 2018 "XCMS-MRM and METLIN-MRM: a cloud library and public resource for targeted analysis of small molecules"

View Public Shares page 3

Status	ID	Job Name	Biosource	Author(s)	Publication	Notes
VIEW	1270779	Asthma vs COPD (uncorrected mzML files)	HUMAN			
VIEW	1271289	Asthma vs COPD (corrected mzML files)	HUMAN			
VIEW	1197171	pair_2018-01-18T14:02:59	HUMAN			
VIEW	1275031	SGL_2018-12-02_23:14	HUMAN			
VIEW	1276381	P_2018-12-07_02:59	HUMAN			
VIEW	1181343	sazonalidade_fibra	HUMAN			
VIEW	1155786	agua	HUMAN			
VIEW	1155771	luz	HUMAN			
VIEW	1152766	temperature	HUMAN			
VIEW	1251319	Untargeted analysis of medicinal species: Maytenus ilicifolia, Maytenus aquifolium and their hybrid	HUMAN			

Showing 21 to 30 of 31 entries

First look at the results of the analysis

- [Citation Links](#)
- [Results Table](#)
- [Metabolomic Cloud Plot](#)
- [Interactive Heatmap](#)
- [iPCA](#)
- [Activity Network \(Connections\)](#)
- Multi-Omics Data**
- [Systems Biology Results](#)
- [Pathway Cloud Plot](#)

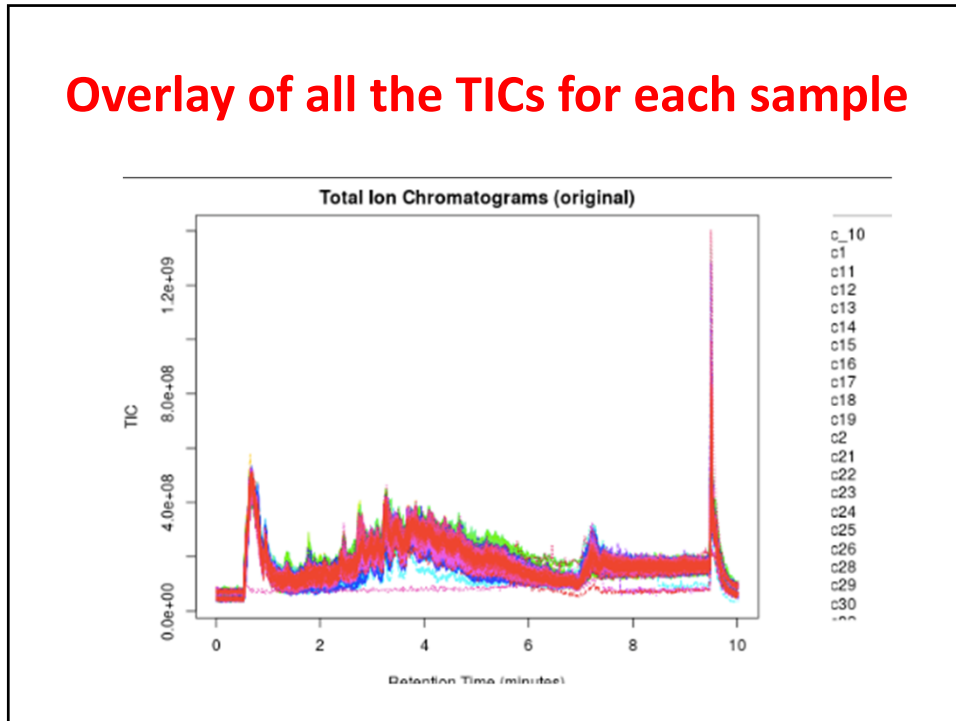
Datasets Used

- Qcs teste CWT (294864)
- Illicifolia Cwt (296098)
- Aquifolium Cwt (302567)
- Hibrida Cwt (303062)

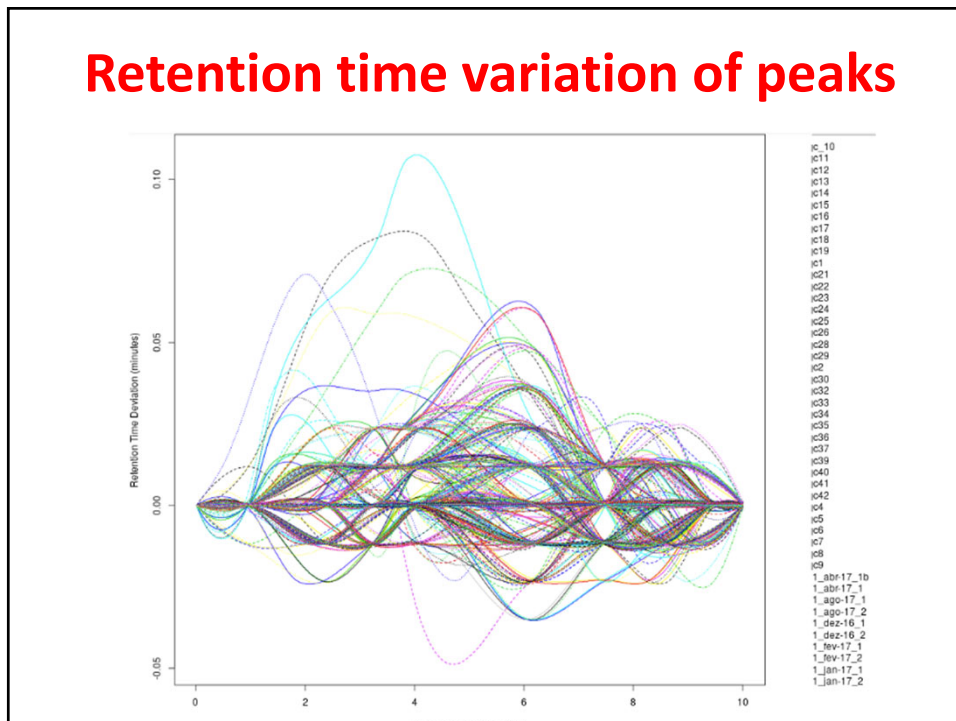
The figure displays six plots related to metabolomic data analysis:

- Total Ion Chromatograms (raw):** Shows intensity vs. retention time for multiple samples.
- Total Ion Chromatograms (processed):** Shows the same data after processing, with peaks more clearly defined.
- PCA Score Plot:** A scatter plot showing the separation of samples based on their chemical profiles.
- Non-Negative Matrix Factorization:** A heatmap showing the relationship between samples and identified metabolites.
- PCA Score Plot for pathway loading:** A scatter plot where the size and color of points represent the loading of metabolites on the principal components.

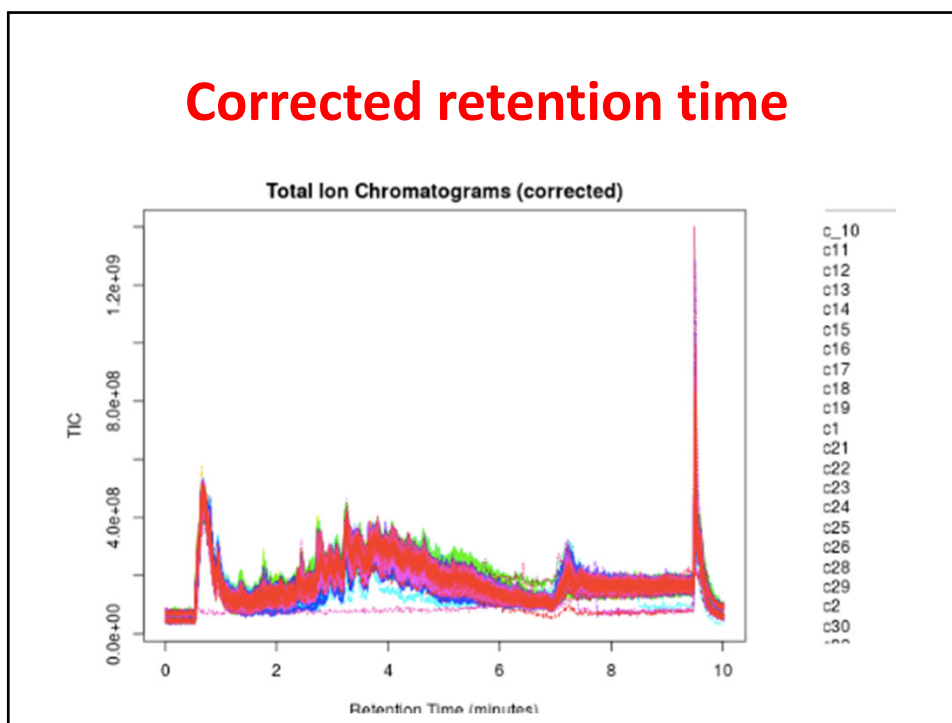
Overlay of all the TICs for each sample



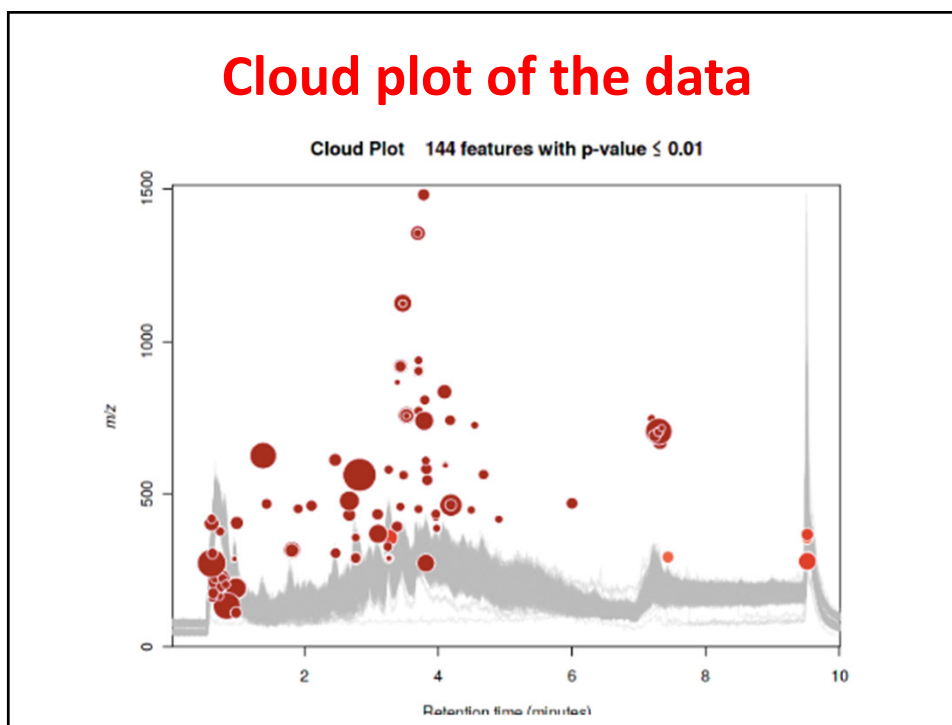
Retention time variation of peaks



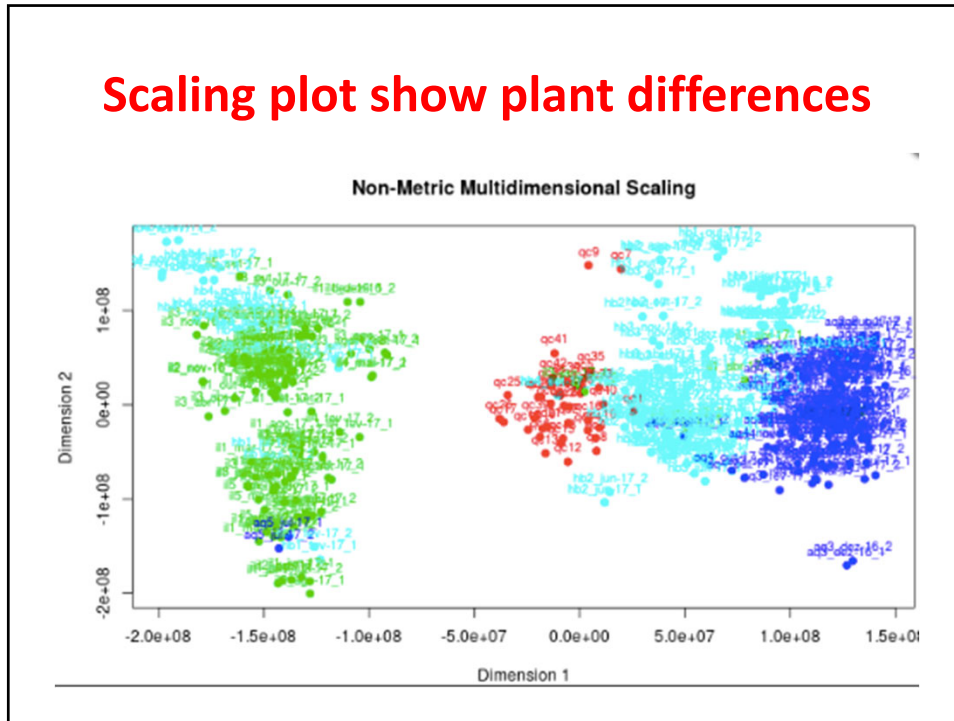
Corrected retention time



Cloud plot of the data



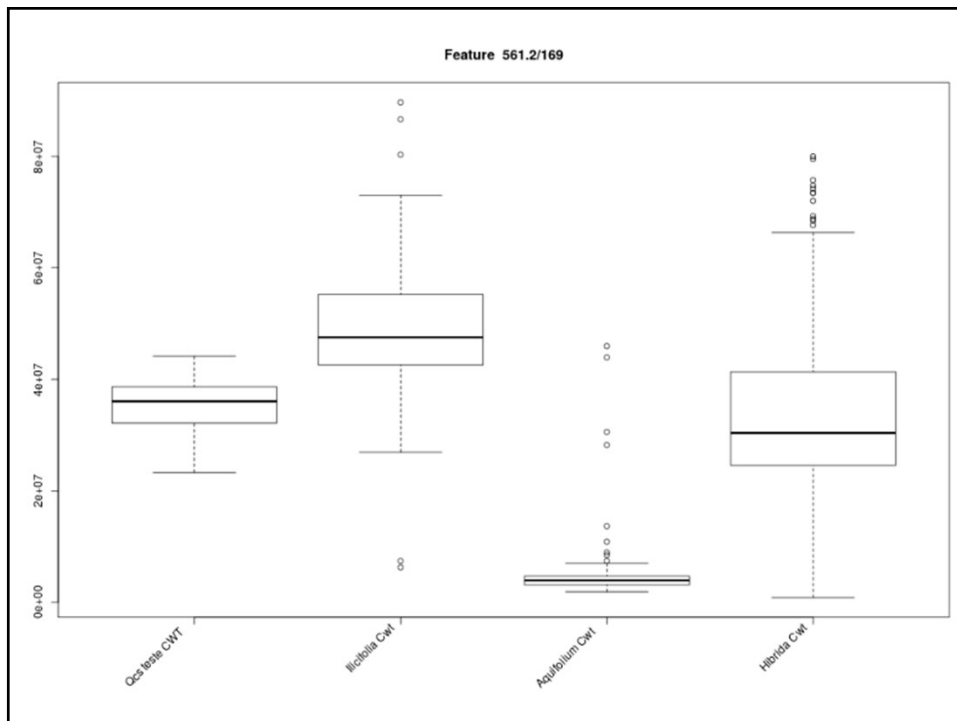
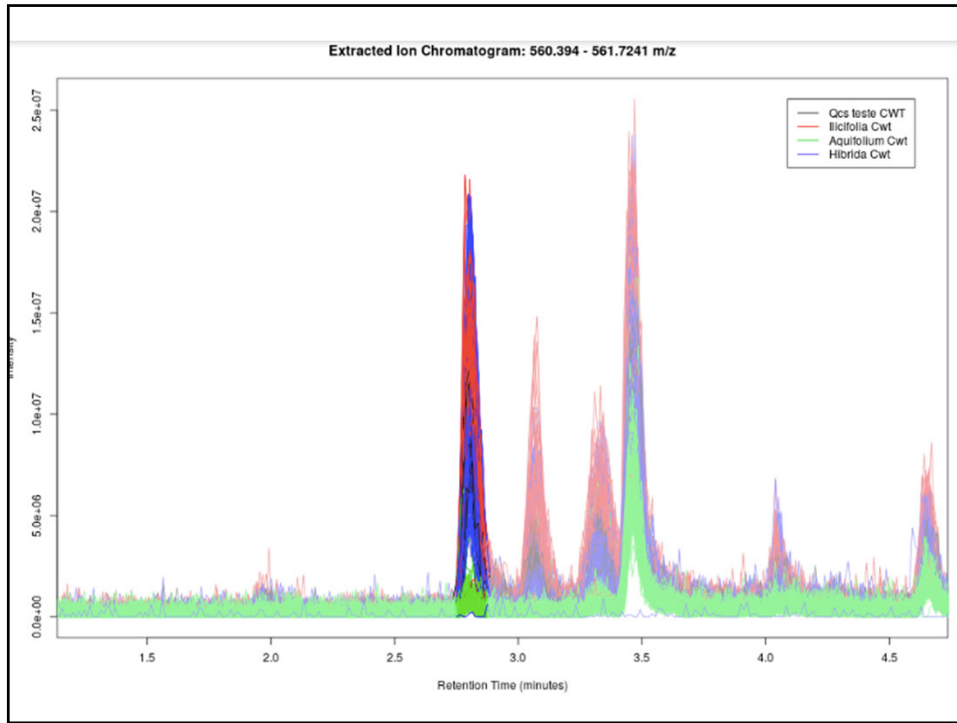
Scaling plot show plant differences



Results – most significant ions

JOB#1251319 : UNTARGETED ANALYSIS OF MEDICINAL SPECIES: MAYTENUS ILICIFOLIA, MAYTENUS AQUIFOLIA

featureidx	pvalue	qvalue	CV	mzmed	rtmed	maxint
1	6.03291e-56	9.36519e-56	0.149	545.2159	3.83	8,510,464
2	8.82338e-56	9.36519e-56	0.143	273.1025	3.81	6,872,576
3	5.84188e-54	3.29595e-54	0.142	562.1447	2.81	12,175,360
4	6.61697e-54	3.51164e-54	0.135	561.1901	2.81	21,801,984
5	5.62525e-53	2.38827e-53	0.159	563.1780	4.67	10,763,264
6	1.98850e-52	7.03534e-53	0.106	561.1982	3.47	23,953,408
7	7.51842e-52	1.82616e-52	0.129	834.2289	4.09	9,391,104
8	7.53218e-52	1.82807e-52	0.137	833.3131	4.09	13,384,704
9	8.04366e-52	1.89724e-52	0.104	739.2925	3.78	29,903,872
10	2.90585e-51	6.16858e-52	0.111	740.2017	3.78	16,901,120
11	6.20722e-51	1.19789e-51	0.194	715.4036	7.34	4,780,288
12	4.37856e-50	7.62488e-51	0.107	562.1453	3.47	11,867,136
13	1.11941e-49	1.65610e-50	0.222	1,123.4251	3.46	26,100,736
14	1.31254e-49	1.86243e-50	0.169	564.1507	4.67	5,573,376
15	1.32503e-49	1.87519e-50	0.129	741.0460	3.78	8,337,408
16	1.83722e-49	2.43754e-50	0.183	834.4048	4.09	8,310,272
17	3.37369e-49	4.10225e-50	0.208	1,124.2938	3.46	10,603,520
18	3.94484e-49	4.65230e-50	0.219	1,123.6221	3.46	11,350,016

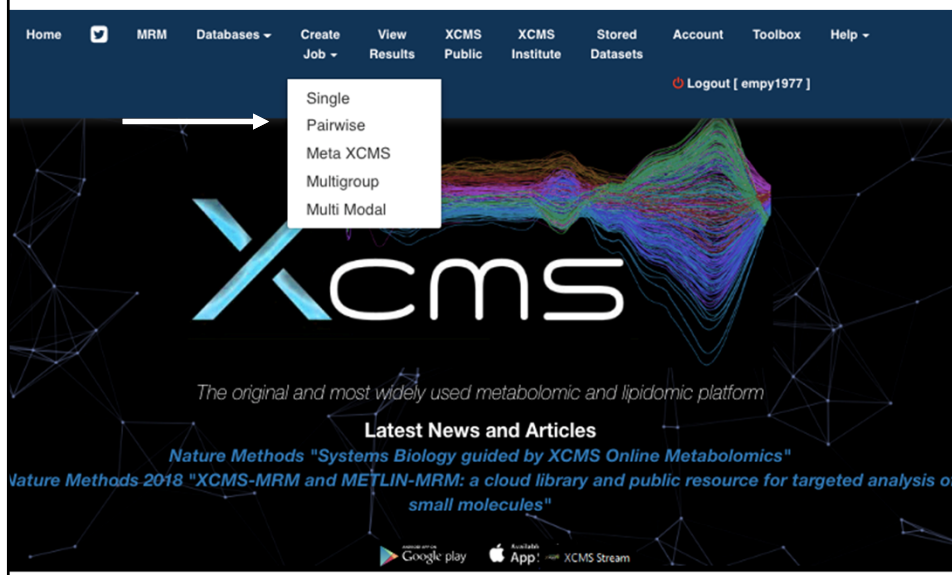


Go back to home page and create a job



The screenshot shows the XCMS homepage. The navigation menu at the top includes: Home, MRM, Databases, Create Job, View Results, XCMS Public, XCMS Institute, Stored Datasets, Account, Toolbox, and Help. A white arrow points to the 'Create Job' dropdown menu, which is open, showing options: Single, Pairwise, Meta XCMS, Multigroup, and Multi Modal. The main content area features the XCMS logo, the tagline 'The original and most widely used metabolomic and lipidomic platform', and a section for 'Latest News and Articles' with links to Nature Methods articles. At the bottom, there are logos for Google Play, the App Store, and XCMS Stream.

Select pairwise



This screenshot is identical to the one above, but with the 'Pairwise' option selected in the 'Create Job' dropdown menu. A white arrow points to the 'Pairwise' option. The rest of the page content, including the navigation menu, logo, tagline, news section, and footer, remains the same.

Let's load the control dataset

1 SELECT DATASET 1 2 SELECT DATASET 2 3 SELECT PARAMETERS 4 REVIEW & SUBMIT

SELECT DATASET 1
(See [File Formats](#) for more information)

ID ▲	Dataset Name ▼	File Count ▼
Please upload or select dataset(s)		

Name the control_neg data set

Save Dataset & Proceed

Storage Quota Usage (100.00 GB):
32.6%

1. Select only .mzXML, .mzData, mzData.XML, mzML, .netcdf, .cdf, .d.zip, .wiff / .wiff.scan files (More info: [File Formats](#))
2. After samples are uploaded you can close this window. (button above)
3. For ABSciex files, please upload the both the wiff and the wiff.scan

Dataset Name:

DROP HERE













Locate the control files

Files for uploading 1-28-19			Today at 9:35 PM	--
	Neg_G3.wiff.scan	January 29, 2018 at 1:24 PM	122.4 MB	
	Neg_G3.wiff	January 29, 2018 at 1:24 PM	6 MB	
	Neg_G2.wiff.scan	January 29, 2018 at 1:24 PM	130.3 MB	
	Neg_G2.wiff	January 29, 2018 at 1:23 PM	6.5 MB	
	Neg_G1.wiff.scan	January 29, 2018 at 10:14 AM	118.7 MB	
	Neg_G1.wiff	January 29, 2018 at 10:12 AM	6 MB	
	Neg_C3.wiff.scan	January 27, 2018 at 1:16 PM	119.3 MB	
	Neg_C3.wiff	January 27, 2018 at 1:15 PM	6.1 MB	
	Neg_C2.wiff.scan	January 27, 2018 at 1:15 PM	124.6 MB	
	Neg_C2.wiff	January 27, 2018 at 1:14 PM	5.9 MB	
	Neg_C1.wiff.scan	January 27, 2018 at 1:13 PM	126.9 MB	
	Neg_C1.wiff	January 27, 2018 at 1:12 PM	5.9 MB	

Showing progress of uploading

The image displays two panels of upload progress indicators. Each indicator consists of a circular progress bar, the file name, and its size. The left panel shows progress for four files: Neg_C3.wiff.scan (119.28 MB), Neg_C3.wiff (6.14 MB), Neg_C2.wiff.scan (124.57 MB), and Neg_C2.wiff (5.87 MB). The right panel shows progress for the same four files, but with status indicators: a red 'X' for Neg_C3.wiff.scan and Neg_C2.wiff.scan, and a green checkmark for Neg_C3.wiff and Neg_C2.wiff.


.wiffscan goes green once uploaded

 Neg_C3.wiffscan 119.28 MB	 Neg_C3.wiffscan 119.28 MB
 Neg_C3.wiff 6.14 MB	 Neg_C3.wiff 6.14 MB
 Neg_C2.wiffscan 124.57 MB	 Neg_C2.wiffscan 124.57 MB
 Neg_C2.wiff 5.87 MB	 Neg_C2.wiff 5.87 MB
 Neg_C1.wiffscan 126.95 MB	 Neg_C1.wiffscan 126.95 MB
 Neg_C1.wiff 5.92 MB	 Neg_C1.wiff 5.92 MB

Moving on to the next dataset

SELECT DATASET 1
(See [File Formats](#) for more information)

[Load New Dataset](#) [Select Dataset](#)

ID ▲	Dataset Name	File Count	
378284	Control_neg	6	

[Next](#)

Load the second set of data

SELECT DATASET 2
(See [File Formats](#) for more information)

ID	Dataset Name	File Count
Please upload or select dataset(s)		

Name the Gen_neg data set

Save Dataset & Proceed

Storage Quota Usage (100.00 GB): 83.0%

1. Select only .mzXML, .mzData, mzData.XML, mzML, .netcdf, .cdf, .d.zip, .wiff/.wiff.scan files
 (More info: [File Formats](#))
 2. After samples are uploaded you can close this window. (button above)
 3. For ABSciex files, please upload the both the wiff and the wiff.scan

Dataset Name:

DROP HERE

Selecting genistein files

Name	Size	Kind	Date Modified	Date Added
<input checked="" type="checkbox"/> Neg_G3.wiff.scan	122.4 MB	Document	Jan 29, 2018 at 1:24 PM	Today at 9:11 PM
<input checked="" type="checkbox"/> Neg_G3.wiff	6 MB	Document	Jan 29, 2018 at 1:24 PM	Today at 9:11 PM
<input checked="" type="checkbox"/> Neg_G2.wiff.scan	130.3 MB	Document	Jan 29, 2018 at 1:24 PM	Today at 9:11 PM
<input checked="" type="checkbox"/> Neg_G2.wiff	6.5 MB	Document	Jan 29, 2018 at 1:23 PM	Today at 9:11 PM
<input checked="" type="checkbox"/> Neg_G1.wiff.scan	118.7 MB	Document	Jan 29, 2018 at 10:14 AM	Today at 9:11 PM
<input checked="" type="checkbox"/> Neg_G1.wiff	6 MB	Document	Jan 29, 2018 at 10:12 AM	Today at 9:11 PM
<input type="checkbox"/> Neg_C3.wiff.scan	119.3 MB	Document	Jan 27, 2018 at 1:16 PM	Today at 9:10 PM
<input type="checkbox"/> Neg_C3.wiff	6.1 MB	Document	Jan 27, 2018 at 1:15 PM	Today at 9:10 PM
<input type="checkbox"/> Neg_C2.wiff.scan	124.6 MB	Document	Jan 27, 2018 at 1:15 PM	Today at 9:10 PM
<input type="checkbox"/> Neg_C2.wiff	5.9 MB	Document	Jan 27, 2018 at 1:14 PM	Today at 9:10 PM
<input type="checkbox"/> Neg_C1.wiff.scan	126.9 MB	Document	Jan 27, 2018 at 1:13 PM	Today at 9:10 PM
<input type="checkbox"/> Neg_C1.wiff	5.9 MB	Document	Jan 27, 2018 at 1:12 PM	Today at 9:10 PM

Gen_neg files uploaded

<input checked="" type="checkbox"/>	Neg_G3.wiff.scan 122.40 MB	✓
<input checked="" type="checkbox"/>	Neg_G3.wiff 6.05 MB	✓
<input checked="" type="checkbox"/>	Neg_G2.wiff.scan 130.25 MB	✓
<input checked="" type="checkbox"/>	Neg_G2.wiff 6.51 MB	✓
<input checked="" type="checkbox"/>	Neg_G1.wiff.scan 118.66 MB	✓
<input checked="" type="checkbox"/>	Neg_G1.wiff 5.98 MB	✓

Go to stored datasets

<input type="checkbox"/>	DatasetName	Active	Status	Comment	Upload Date	Files	Size	ID	Owner
<input type="checkbox"/>	Gen_neg	✓	UPLOAD_COMPLETE		2019-01-27 20:31:09	6	371.8 MB	378285	1664
<input type="checkbox"/>	Control_neg	✓	UPLOAD_COMPLETE		2019-01-27 20:09:22	6	370.7 MB	378284	1664

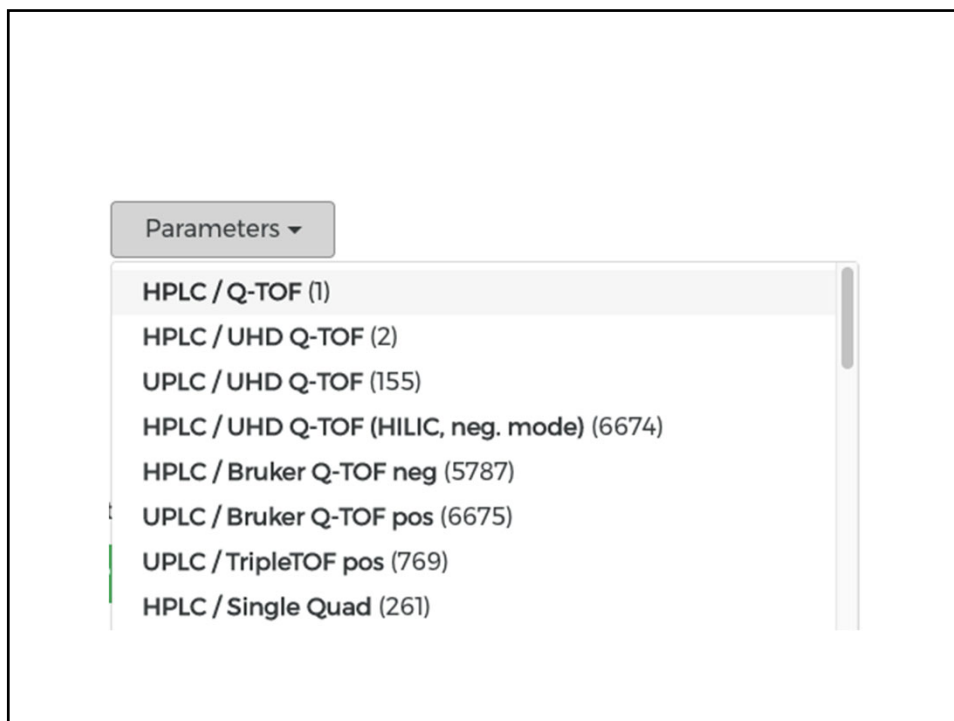
SELECT PARAMETERS

Parameters ▾

None

Save as Default


Note: You may need to allow popup windows in your browser



SELECT PARAMETERS

TripleTof_LandonWilsonNEGATIVE_use only ▾

[View/Edit](#)

 No Notes Available

Save as Default

Note: You may need to allow popup windows in your browser

[Previous](#) [Next](#)

View/Edit Parameters for Job

Click to go back, hold to see history

Polarity is defined on the General tab and will affect values on the Annotation and Identification (adducts) tabs. Job results will be misleading if this value is not correctly defined.

The current parameter set is read-only. Use **Create New** button below to modify parameters to suit your job.

General Feature Detection Retention Time Correction Alignment Statistics Annotation Identification Visualization Miscellaneous

Option	Value	Note:
Name	TripleTof_LandonWilsonNEGATIVE_use only	
Comment		
Polarity	negative ▾	data acquired in positive or negative mode ?
Retention time format	minutes ▾	show the retention times in results tables and figures in minutes or seconds

[Save](#) [Create New](#) [Delete](#) [Cancel](#)

View/Edit Parameters for Job

Polarity is defined on the General tab and will affect values on the Annotation and Identification (adducts) tabs. Job results will be misleading if this value is not correctly defined.

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General Feature Detection Retention Time Correction Alignment Statistics Annotation Identification Visualization Miscellaneous

Method: centWave

Option	Value	Note:
ppm	15	maximal tolerated m/z deviation in consecutive scans, in ppm (parts per million)
minimum peak width	5	minimum chromatographic peak width in seconds note: must be less than max peak width. See also here .
maximum peak width	30	maximum chromatographic peak width in seconds note: must be greater than min peak width. See also here .
View Advanced Options		
mzdiff	0.01	minimum difference in m/z for peaks with overlapping retention times, can be negative to allow overlap
Signal/Noise threshold	3	Signal/Noise threshold
Integration method	1	Integration method. If =1 peak limits are found through descent on the mexican hat filtered data. If =2 the descent is done on the real data. Method 2 is very accurate but prone to noise, while method 1 is more robust to noise but less exact.
prefilter peaks	3	Prefilter step for the first phase. Mass traces are only retained if they contain at least [prefilter peaks] peaks with intensity >= [prefilter intensity]
prefilter intensity	2	Prefilter step for the first phase. Mass traces are only retained if they contain at least [prefilter peaks] peaks with intensity >= [prefilter intensity]
Noise Filter	0	optional argument which is useful for data that was centroided without any intensity threshold, centroids with intensity < noise are omitted from ROI detection

View/Edit Parameters for Job

Polarity is defined on the General tab and will affect values on the Annotation and Identification (adducts) tabs. Job results will be misleading if this value is not correctly defined.

The current parameter set is read-only. Use **Create New** button below to modify parameters to suit your job.

General Feature Detection Retention Time Correction Alignment Statistics Annotation Identification Visualization Miscellaneous

Method: obl warp

Option	Value	Note:
profStep	1	step size (in m/z) to use for profile generation from the raw data files

View/Edit Parameters for Job

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[Miscellaneous](#)

Option	Value	Note:
bw	<input type="text" value="5"/>	Allowable retention time deviations, in seconds. In more detail: bandwidth (standard deviation or half width at half maximum) of gaussian smoothing kernel to apply to the peak density chromatogram
minfrac	<input type="text" value="0.5"/>	minimum fraction of samples necessary in at least one of the sample groups for it to be a valid group
mzwid	<input type="text" value="0.015"/>	width of overlapping m/z slices to use for creating peak density chromatograms and grouping peaks across samples
View Advanced Options		
minsamp	<input type="text" value="1"/>	minimum number of samples necessary in at least one of the sample groups for it to be a valid group
max	<input type="text" value="100"/>	maximum number of groups to identify in a single m/z slice

View/Edit Parameters for Job

Polarity is defined on the General tab and will affect values on the Annotation and Identification (adducts) tabs. Job results will be misleading if this value is not correctly defined.
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Option	Value	Note:
Statistical test	<input type="text" value="Unpaired parametric t-test (Welch t-test)"/>	Statistical test method: Welch t-test (unequal variances) or Wilcoxon Rank Sum test
Perform paired test	<input type="button" value="VIEW PAIRS"/>	The selected statistical test is performed as a paired test. The sample pairs need to be specified.
Perform post-hoc analysis	<input type="text" value="True"/>	Perform post-hoc analysis [multigroup only]
p-value threshold (highly significant features)	<input type="text" value="0.01"/>	Features with a p-value less than this threshold are considered highly significant. Some statistical figures (e.g. Mirror plot) are generated using only the dysregulated features according to this threshold.
fold change threshold (highly significant features)	<input type="text" value="1.5"/>	Features with a fold change greater than this threshold are considered highly significant. Some statistical figures (e.g. Mirror plot) are generated using only the dysregulated features according to this threshold.
p-value threshold (significant features)	<input type="text" value="0.05"/>	Features with a p-value less than this threshold are not considered significant and are omitted from some calculations to save time and space. EIC's, annotations and database ID's are not generated for features with p-values above this threshold.
View Advanced Options		
value	<input type="text" value="into"/>	intensity values to be used for the diffreport. If value="into", integrated peak intensities are used. If value="maxo", maximum peak intensities are used.
Normalization	<input type="text" value="None"/>	Normalize the intensity values by either probabilistic quotient or cyclic loess normalization.

View/Edit Parameters for Job

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Option	Value	Note:
ppm	<input type="text" value="5"/>	ppm error
m/z absolute error	<input type="text" value="0.01"/>	m/z absolute error
Search for	<input type="text" value="isotopes + adducts"/>	Search for 1.) just isotopic features or 2.) isotopic features and adducts formations, dimers, trimers, neutral losses, etc. WARNING: searching for all adducts can increase the total processing time by approximately 50 %

View/Edit Parameters for Job

Polarity is defined on the General tab and will affect values on the Annotation and Identification (adducts) tabs. Job results will be misleading if this value is not correctly defined.
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Option	Value	Note:
ppm	<input type="text" value="5"/>	tolerance for database search
adducts	<div style="border: 1px solid gray; padding: 2px;"> [M+H]- [M+H₂O+H]- [M+Na-2H]- [M+Cl]- [M+K-2H]- [M+FA-H]- [M-2H]2- [M-3H]3- [M+CH₃COO]- [M+F]- </div>	adducts to be considered for database search
sample biosource	<input type="button" value="SELECT BIOSOURCE"/> <input type="button" value="set default"/>	Select your species/cell line, etc. that correspond to your samples. Default human.
pathway ppm deviation	SELECTED: <input type="text" value="5"/>	metabolite pathway lookup
input intensity threshold	<input type="text"/>	minimum intensity cut-off for pathway analysis
significant list p-value cutoff	<input type="text" value="AUTO"/>	significant list p-value cut-off

View/Edit Parameters for Job

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Option	Value	Note:
EIC width	<input style="width: 150px;" type="text" value="100"/>	Default width for extracted ion chromatograms in seconds

Save
Create New
Delete
Cancel

View/Edit Parameters for Job

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Option	Value	Note:
Correct mass calibration gaps	<input type="checkbox"/>	Correction of mass calibration gaps - subtract LockMass scans from data. Only applicable for Waters instruments !
Bypass file sanity check	<input type="checkbox"/>	All uploaded files are normally checked for different types of errors and inconsistencies. This option disables the file sanity check. Unfortunately necessary for certain types of GC/MS data when used with centWave. Only disable this check if you know what you are doing!

Save
Create New
Delete
Cancel

1 SELECT DATASET 1 2 SELECT DATASET 2 3 SELECT PARAMETERS 4 REVIEW & SUBMIT

SELECT PARAMETERS

TripleTof_LandonWilsonNEGATIVE_use only ▾

[View/Edit](#)

⚠ No Notes Available

Save as Default

Note: You may need to allow popup windows in your browser

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REVIEW & SUBMIT

User ID

1664

Job ID

1286073

Job Name

P_2019-01-27_20.05

Dataset1

378284

Dataset2

378285

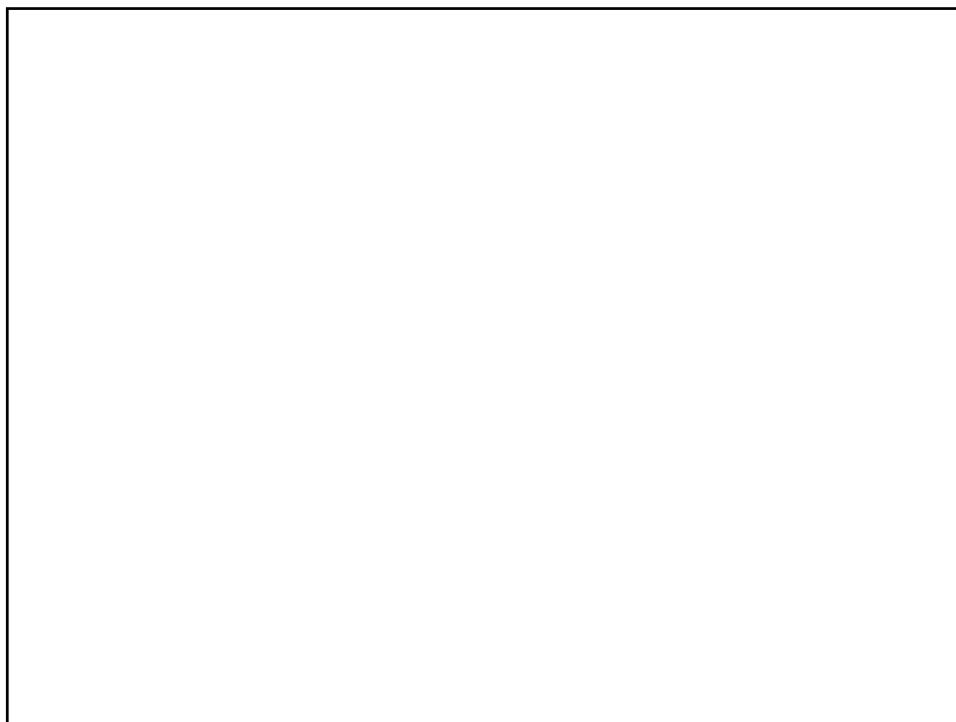
Parameter ID

TripleTof_LandonWilsonNEGATIVE_use only (33859)

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PAIR	PROCESSING	1286073	SUBMITTED 0%	P_2019-01-27_20.05	Control_ne (#378284) Cen_neg (#378285)	2019-01-27 20:05:51	33859		Share	Delete



Tips for naming files for upload to XCMS Online

- Before uploading, it is a good idea to create separate file folders on your hard drive to better organize your data into the groups you want to examine.
- Add enough description to discriminate between different samples and sample set names.
- Adding the ionization mode in the name is preferable, i.e. PosMode or NegMode.
- Eliminate open spaces in the data file name by using “_” (underscore) notation. Open spaces can cause upload errors in XCMS Online.

Example of DataSet Name: Control_Neg

What does a LC-MS data set consist of?

- A Q-TOF instrument during the LC run, for example, acquires data on a 2.25 second duty cycle
 - 0-250 msec
 - High resolution/mass accuracy MS spectrum
 - 250-2250 msec
 - A succession of selected MSMS spectra
 - If each MSMS spectrum is collected for 100 msec, then 20 precursor ions can be selected in the duty cycle
 - The precursor ions are selected from the MS spectrum observed in the current duty cycle
 - Once an ion has been selected for MSMS it can be placed on a “don’t observe” list for say 90 sec

What ions are observed in LC-MS data?

- Ions coming from the biological system being studied
- Ions from compounds introduced into the extract during storage and extraction
- Ions from the solvent used for the chromatography
- Ions from the column material
- Ions from the previous sample that was run