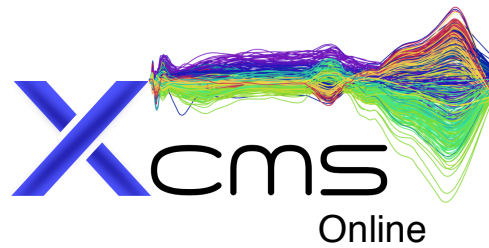


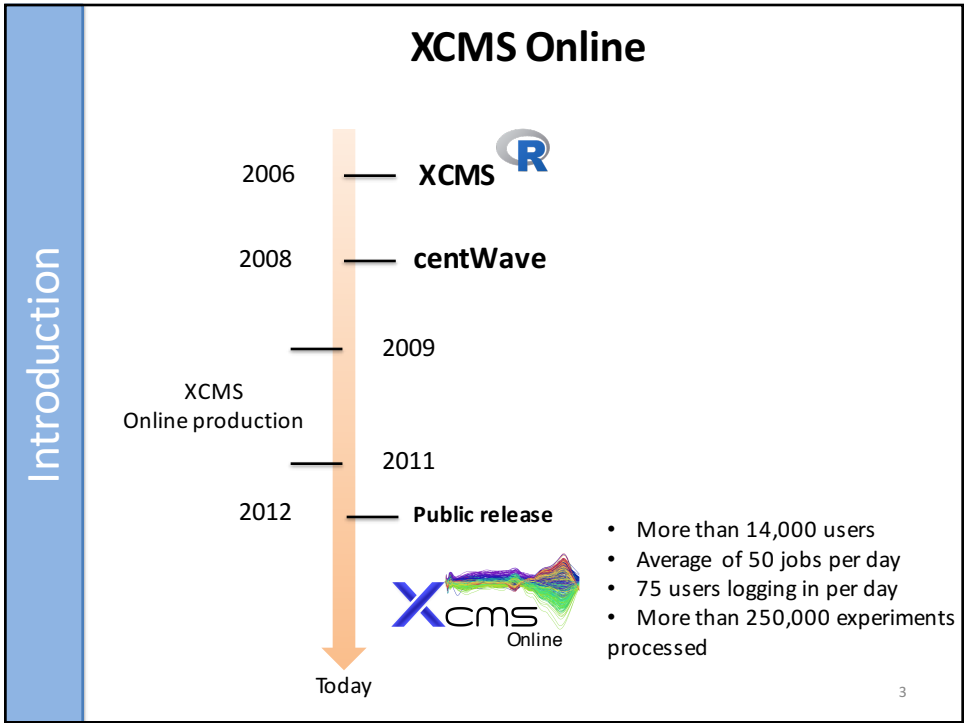
## 5th UAB Metabolomics Workshop



Xavier Domingo-Almenara

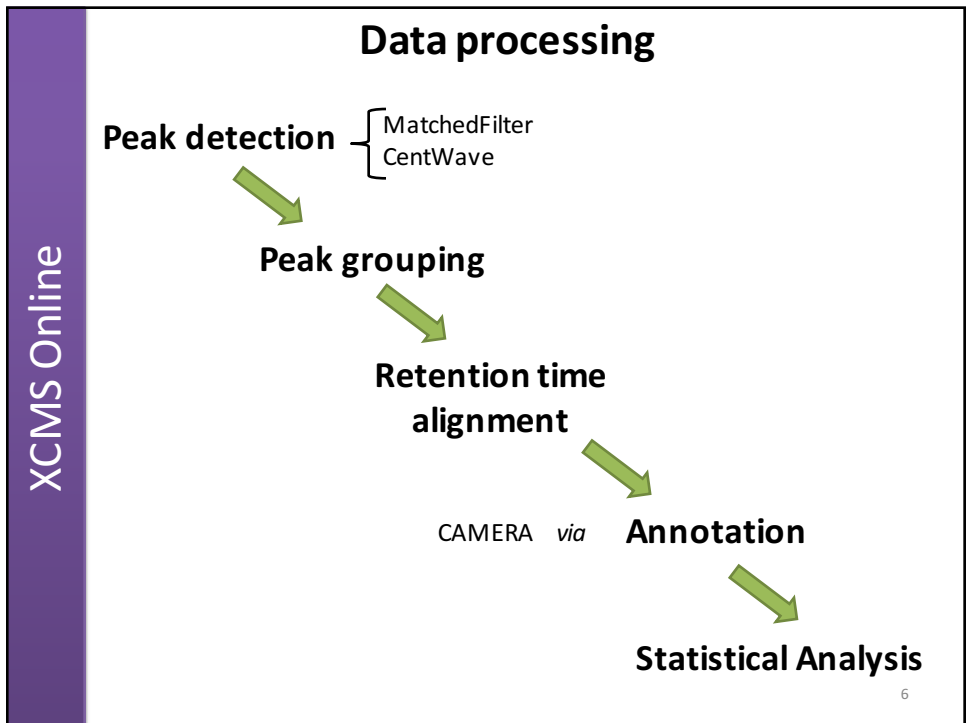
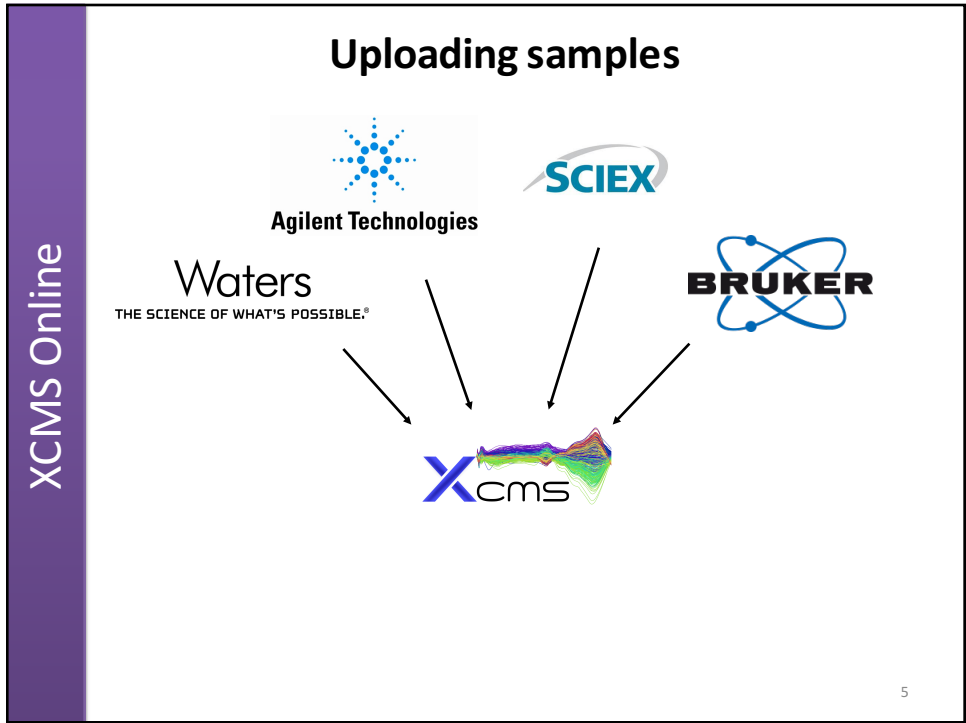
### *Outline*

- *Introduction*
- *XCMS Online*
- *XCMS Online Demo*
- *Additional features*



### XCMS vs XCMS

XCMS	
Requires (some) R knowledge	Easy-to-use
Review of results: manual and tiresome	Review of results: fast and easy
Processing speed: depending on N# samples and computer	Processing speed: fast
	Cloud-based benefits: data sharing and streamline analysis







## New User Registration

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

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

Email

Password

Re-enter password



Enter code above


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)

9

Home ▲ Highlights - Databases - Create Job - View Results XCMS Public XCMS Institute Stored Datasets Account Toolbox Help - Logout [ xdomingo ]

- Single Job
- Pairwise Job
- Meta XCMS Job
- Multigroup Job 

Home **Highlights** Databases - Create Job - View Results XCMS Public XCMS Institute Stored Datasets Account Toolbox Help - Logout [ xdomingo ]

1 Select Datasets  OR  (See File Formats for more information)

2 Define QC Dataset (optional)

3 Parameters

4 Submit

Job Summary  
Job ID: 1167191  
User: xdomingo (14683)  
Job Name:    
Datasets: 0  
Parameter Set: 0

ID	Dataset Name	Number of Files
----	--------------	-----------------

ID:258523 **Save Dataset & Proceed**

Storage Quota Usage (25.04 GB):

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 ABCIox files, please upload the both the wiff and the wiff.scan

Dataset Name:

DROP HERE

Save Dataset & Proceed

Storage Quota Usage (25.04 GB): 1.40%


Dataset Name: KO\_M Save

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

DROP HERE BROWSE

KO\_F

Name	
B645_retina_L_F_KO_aq_C18POS_acid.mzXML	J
B645_retina_R_F_KO_aq_C18POS_acid.mzXML	J
B693_retina_L_F_KO_aq_C18POS_acid.mzXML	J
B693_retina_R_F_KO_aq_C18POS_acid.mzXML	J
B696_retina_L_F_KO_aq_C18POS_acid.mzXML	J
B696_retina_R_F_KO_aq_C18POS_acid.mzXML	J



Loading folders is not allowed in OSX

Save Dataset & Proceed

Storage Quota Usage (25.04 GB): 9.50%

Dataset Name: KO\_F Save

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

DROP HERE BROWSE

B645_retina_L_F_KO_aq_C18POS_acid.mzXML	81.47 MB	✓
B645_retina_R_F_KO_aq_C18POS_acid.mzXML	81.54 MB	✓
B693_retina_L_F_KO_aq_C18POS_acid.mzXML	81.00 MB	✓
B693_retina_R_F_KO_aq_C18POS_acid.mzXML	82.74 MB	✓
B696_retina_L_F_KO_aq_C18POS_acid.mzXML	80.92 MB	✓
B696_retina_R_F_KO_aq_C18POS_acid.mzXML	82.87 MB	✓

**1 Select Datasets**  
 OR   
(See File Formats for more information)

ID	Dataset Name	Number of Files
<input type="checkbox"/> 258532	KO_F	8
<input type="checkbox"/> 258534	KO_M	8
<input type="checkbox"/> 258535	QC	5
<input type="checkbox"/> 258537	WT_F	5
<input type="checkbox"/> 258538	WT_M	14

**2 Define QC Dataset (optional)**  
 ? -No QC Selected-

**3 Parameters**  
 Select Parameters

**4 Submit**  
 Click here to complete your job

Job ID: 1167202  
 User: xdomingo (14683)  
 Job Name: MG\_2017-06-29\_16:31   
 Datasets: 5  
 Parameter Set: 0

**1 Select Datasets**  
 OR   
(See File Formats for more information)

ID	Dataset Name	Number of Files
<input type="checkbox"/> 258532	KO_F	8
<input type="checkbox"/> 258534	KO_M	8
<input type="checkbox"/> 258535	QC	5
<input type="checkbox"/> 258537	WT_F	5
<input type="checkbox"/> 258538	WT_M	14

**2 Define QC Dataset (optional)**  
 ? 1 selected

**3 Parameters**  
 ✓ Select Parameters  
 GC / Single Quad (centWave)  
 GC / Single Quad (matchedFilter)  
 GC / TOF  
 HPLC - UHD Qtof pairs  
 HPLC / Bruker Q-TOF neg  
 HPLC / Ion Trap  
 HPLC / Orbitrap  
 HPLC / Orbitrap II  
 HPLC / Q-TOF  
 HPLC / Single Quad  
 HPLC / UHD Q-TOF  
 HPLC / UHD Q-TOF (HILIC, neg. mode)  
 HPLC / Waters TOF  
 UPLC - High Res POS (Waters)  
 UPLC / Bruker Q-TOF pos  
**UPLC / Orbitrap**  
 UPLC / Q-Exactive  
 UPLC / TripleTOF pos  
 UPLC / UHD Q-TOF  
 Custom\_2017-06-29

**4 Submit**  
 Click here to complete your job

Job ID: 1167202  
 User: xdomingo (14683)  
 Job Name: MG\_2017-06-29\_16:31   
 Datasets: 5  
 Parameter Set: 0

The screenshot shows a multi-step configuration process:

- 1 Select Datasets:** Includes buttons for 'Load New Dataset' and 'Select Dataset'. A note below says '(See File Formats for more information)'.
- 2 Define QC Dataset (optional):** A dropdown menu currently shows '-No QC Selected-'.
- 3 Parameters:** A dropdown menu is set to 'UPLC / UHD Q-TOF'. Below it is a descriptive text: 'optimized for UPLC with ~15 min gradient, high resolution ESI-QTOF-MS (e.g. Agilent UHD Q-TOF 6538)'. At the bottom of this section is a 'View/Edit' button and a checkbox for 'Remember my selection'. A blue arrow points to the 'View/Edit' button.
- 4 Submit:** A 'Submit Job' button and a link 'Click here to complete your job'.

Job summary information on the right:

- Job ID: 1167202
- User: xdomingo (14683)
- Job Name: MG\_2017-06-29\_1630 (with an 'Edit' button)
- Datasets: 5
- Parameter Set: 0

A table of selected datasets is shown below the 'Select Datasets' step:

ID	Dataset Name	Number of Files
<input type="checkbox"/> 258532	KO_F	8
<input type="checkbox"/> 258534	KO_M	8
<input type="checkbox"/> 258535	QC	5
<input type="checkbox"/> 258537	WT_F	5
<input type="checkbox"/> 258538	WT_M	14

Watch pop-up blockers!

Browser address bar: <https://xcmsonline.scripps.edu/parameters2.php?action=edit&edit=0&base=155&runuser=undefined&context=1&jobid=1167202>

### 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
<b>Option</b>		<b>Value</b>		<b>Note:</b>				
Name	UPLC / UHD Q-TOF							
Comment	optimized for UPLC with ~15 min gradient, hi							
Retention time format	minutes		show the retention times in results tables and figures in minutes or seconds					
Polarity	positive		data acquired in positive or negative mode ?					
<input type="button" value="Create New"/> <input type="button" value="Cancel"/>								

**1 Select Datasets**

OR

(See File Formats for more information)

**2 Define QC Dataset (optional)**

1 selected

**3 Parameters**

Custom\_2017-06-29

Remember my selection

User: xdomingo (14683)

Job Name: MG\_2017-06-29\_16:35

Datasets: 5

Parameter Set: 32488

<input type="checkbox"/>	ID	Dataset Name	Number of Files	<input type="button" value=""/>
<input type="checkbox"/>	258532	KO_F	6	<input type="button" value=""/>
<input type="checkbox"/>	258534	KO_M	8	<input type="button" value=""/>
<input type="checkbox"/>	258535	QC	5	<input type="button" value=""/>
<input type="checkbox"/>	258537	WT_F	5	<input type="button" value=""/>
<input type="checkbox"/>	258538	WT_M	14	<input type="button" value=""/>

**4 Submit**

Click here to complete your job

[%FORMS\_RETURN\_URL%]

**You recently submitted job (#1167191) on XCMS Online.**

Hi Xdomingo,

We started processing your recently submitted job with the following details:

Job Name: DEB  
 Create Date: 2017-06-29 15:43:54 (Server Timezone)  
 Experiment Type:  
 Parameter Name: Custom\_2017-06-29 (#32482)  
 Polarity: positive  
 Datasets: KO\_F (control)  
           KO\_M  
           WT\_M  
           QC

If these are not the correct parameters for this job, please log in to XCMS Online [%FORMS\_RETURN\_URL%] to cancel this job. Otherwise you do not have to take any other action; the system will continue processing.

We will send another e-mail if an error occurs or when this job is finished.  
 If you have any questions about this job you may contact the system administrator at xcmsonline@gmail.com.

XCMS Online Administrators say:  
 Computer Source IP: 137.131.17.212

Regards,  
 XCMS Online Administrator  
[xcmsonline@scripps.edu](mailto:xcmsonline@scripps.edu)

10550 North Torrey Pines Road  
 BCC-007,  
 La Jolla, CA 92037  
 Phone (858) 784-9415  
 Fax (858) 784-9498

Home **Highlights** - Databases - Create Job - View Results - XCMS Public - XCMS Institute - Stored Datasets - Account - Toolbox - Help - Logout [ xdomingo ]

Job Count: 2

Search Jobs  Search Clear View Public Shares

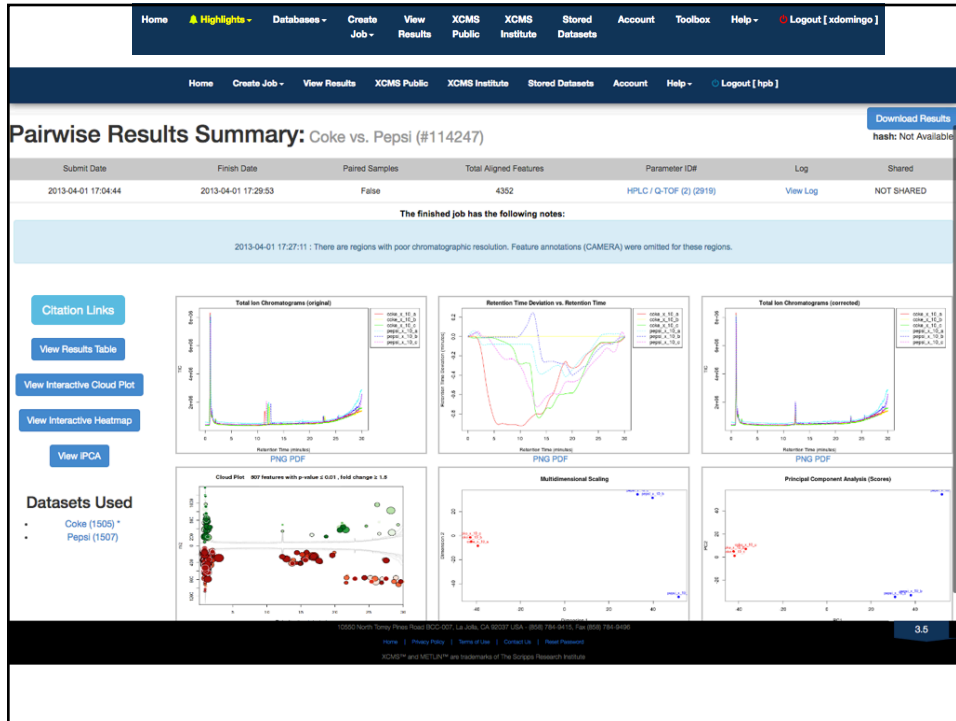
Exp Type	Status	ID	Progress	JobName	Datasets (DB) [control]	Created	Parameters (DB)	Group	Shared
MULTI	PROCESSING	1187202	<div style="width: 100%; height: 10px; background-color: #ccc; position: relative;"> <span style="position: absolute; left: 0; top: -10px; font-size: 8px;">SUBMITTED</span> <span style="position: absolute; left: 50%; top: -10px; font-size: 8px;">%</span> </div>	MS_2017-05-29_16:35	KO_F (#258532) KO_M (#258534) CO_ (#258535) W#_ (#258536)	2017-05-29 16:25:27	Custom_201 (24488)		<input checked="" type="checkbox"/>

Home **Highlights** - Databases - Create Job - View Results - XCMS Public - XCMS Institute - Stored Datasets - Account - Toolbox - Help - Logout [ xdomingo ]

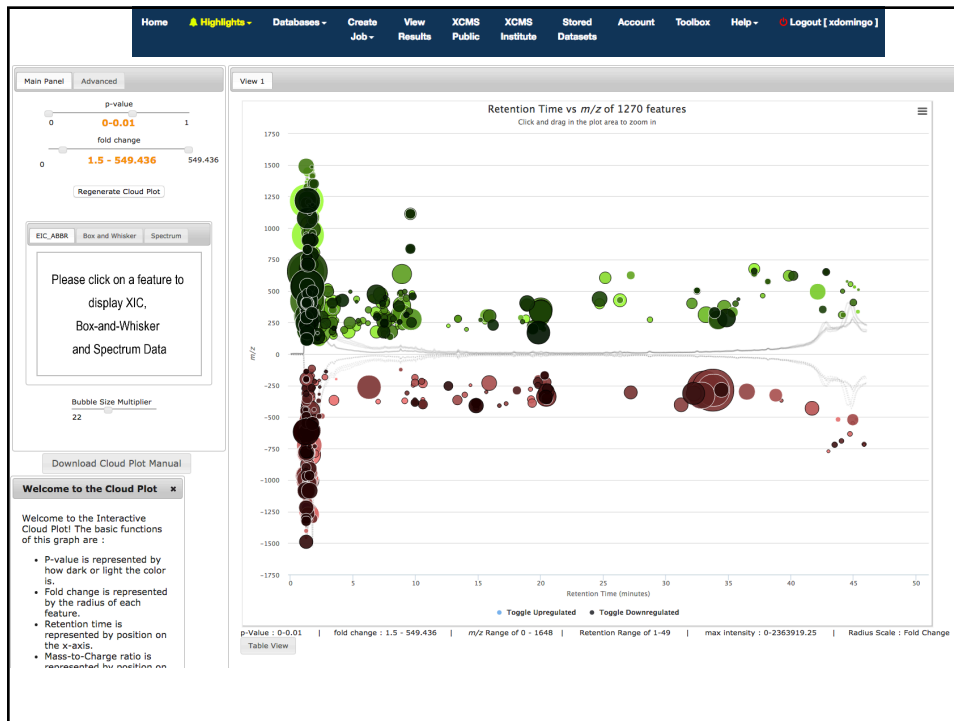
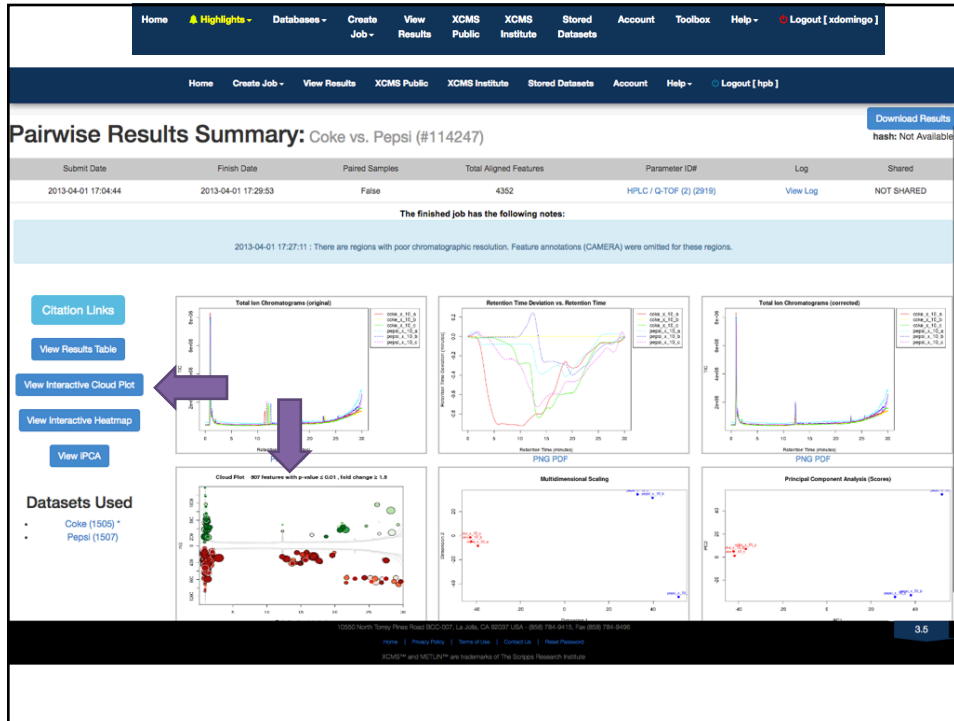
Job Count: 229

Search Jobs  Search Clear View Public Shares

Exp Type	Status	ID	Progress	JobName	Datasets (DB) [control]	Created	Parameters (DB)	Group	Shared
PAIR	VIEW	1129560	<div style="width: 100%; height: 10px; background-color: #ccc; position: relative;"> <span style="position: absolute; left: 0; top: -10px; font-size: 8px;">job complete</span> </div>			2017-05-13 08:37:45	UPLC1 (8676)		<input checked="" type="checkbox"/>
PAIR	VIEW	1129558	<div style="width: 100%; height: 10px; background-color: #ccc; position: relative;"> <span style="position: absolute; left: 0; top: -10px; font-size: 8px;">job complete</span> </div>			2017-05-13 08:47:40	Custom_201 (24371)		<input checked="" type="checkbox"/>
PAIR	VIEW	1129548	<div style="width: 100%; height: 10px; background-color: #ccc; position: relative;"> <span style="position: absolute; left: 0; top: -10px; font-size: 8px;">job complete</span> </div>			2017-05-30 08:02:25	Custom_201 (24276)		<input checked="" type="checkbox"/>
SINGLE	VIEW	1129546	<div style="width: 100%; height: 10px; background-color: #ccc; position: relative;"> <span style="position: absolute; left: 0; top: -10px; font-size: 8px;">job complete</span> </div>			2017-05-26 16:30:15	HPLC1 UHPLD (8674)		<input checked="" type="checkbox"/>
SINGLE	VIEW	1129544	<div style="width: 100%; height: 10px; background-color: #ccc; position: relative;"> <span style="position: absolute; left: 0; top: -10px; font-size: 8px;">job complete</span> </div>			2017-05-25 13:43:27	HPLC1 (DB) (136)		<input checked="" type="checkbox"/>
PAIR	VIEW	1129542	<div style="width: 100%; height: 10px; background-color: #ccc; position: relative;"> <span style="position: absolute; left: 0; top: -10px; font-size: 8px;">job complete</span> </div>			2017-05-26 09:59:55	Enos Fun (24275)		<input checked="" type="checkbox"/>
PAIR	VIEW	1129539	<div style="width: 100%; height: 10px; background-color: #ccc; position: relative;"> <span style="position: absolute; left: 0; top: -10px; font-size: 8px;">job complete</span> </div>			2017-05-25 12:27:01	Custom_201 (24266)		<input checked="" type="checkbox"/>
MULTI	ERROR	1129536	<div style="width: 100%; height: 10px; background-color: #ccc; position: relative;"> <span style="position: absolute; left: 0; top: -10px; font-size: 8px;">File check &amp; TICs level</span> </div>			2017-05-25 12:20:30	HPLC-Bruker (787)		<input checked="" type="checkbox"/>







Home **Highlights** Databases Create Job View Results XCMS Public XCMS Institute Stored Datasets Account Toolbox Help Logout [ xdoming ]

Home Create Job View Results XCMS Public XCMS Institute Stored Datasets Account Help Logout [ hpb ]

Quick Compound Search:  Search Clear

JOB#114247 : COKE VS. PEPSI

featureid#	fold	prvalue	updown	mumad	rtimed	maxhit	dataset_mri	isotopes	adducts	peakgroup	usernotes
1	14.0	2.4376e-7	DOWN	167.0148	0.84	69.785	161.156	11.532 [90]M+	[M+Na]+ 144.13		
2	19.8	8.4316e-7	DOWN	252.0898	16.84	5.293	19.516	985	[M+NH4]+ 234.05		
3	19.8	6.9195e-7	DOWN	526.1777	0.91	4.835	15.747	804 [889]M+32+			
4	27.6	1.3423e-6	DOWN	229.8443	0.84	1.546	3.436	128	[M+H+H2]+ 13		
5	5.4	1.8793e-6	DOWN	233.9691	0.84	2.791	7.352	1.373	[M+Na+K+Ni]3		
6	4.1	3.9179e-6	DOWN	92.4751	0.84	823	1.674	454			
7	13.1	6.3801e-6	DOWN	434.1698	1.27	2.361	4.953	379	[M+H+CH3]+ 4.16		
8	6.6	7.3043e-6	DOWN	467.1917	0.95	45.408	199.306	30.350 [333]M+			
9	9.9	8.2052e-6	DOWN	452.1933	0.88	924	2.371	239 [318]M+1+			
10	15.8	8.6878e-6	DOWN	192.9431	0.84	3.012	7.612	481			
11	7.9	0.00001	DOWN	594.2191	0.97	2.705	8.028	1.022			
12	5.9	0.00001	DOWN	484.1221	1.41	390	1.895	262 [363]M+1+			
13	8.8	0.00001	DOWN	493.2003	0.89	607	1.810	208			
14	1.8	0.00001	DOWN	113.0715	0.91	6.507	13.653	7.591			
15	10.7	0.00002	DOWN	328.0565	1.45	1.164	9.056	845 [170]M+1+			
16	8.2	0.00002	DOWN	637.1889	1.32	1.018	4.160	510 [471]M+2+			
17	5.5	0.00002	DOWN	245.5550	1.38	677	5.344	976 [89]M+12+			
18	17.0	0.00002	DOWN	473.1798	0.89	1.860	4.768	281			
19	11.5	0.00002	DOWN	351.1643	27.51	1.175	3.024	0	[M+2K+H]+ 27.84		
20	2.0	0.00003	DOWN	414.1427	14.92	358	1.397	685	[M+NH4]+ 398.82		
21	10.1	0.00004	DOWN	379.1736	0.88	1.403	2.670	88			
22	2.8	0.00004	DOWN	216.0657	0.94	30.294	61.136	21.789 [67]M+			
23	7.0	0.00004	DOWN	263.0550	12.24	1.583	9.740	1.400 [113]M+			
24	2.9	0.00004	UP	611.0654	1.06	2.748	3.010	8.817 [633]M+			
25	3.2	0.00004	DOWN	431.1704	1.26	19.706	31.930	9.933	[M+H+H2]+ 4.16		
26	2.6	0.00004	DOWN	287.0763	1.55	785	2.733	1.047			
27	9.0	0.00005	DOWN	490.8187	0.84	919	1.482	164	[M+K]+ 451.83		
28	5.7	0.00005	DOWN	156.0148	0.84	5.335	12.340	2.147	[M+NH4]+ 453		
29	5.7	0.00006	DOWN	463.1478	1.29	7.236	23.925	4.222			
30	2.0	0.00006	DOWN	535.0933	1.14	385	1.895	379			

View 1 - 100 of 4,352

Feature #1  
m/z: 147.0146  
Retention Time (min): 0.84  
EIC

MASS SPECTRUM BOX-AND-WHISKER  
coke\_x\_10\_b (0.84 min)

PPM	Name	Adduct	COMPOSI
2	N,N'-bis(2-chloroethyl)M+H+H2O	648	
20	3,4-Dihydroxy-2-butylM+H+H2O	63660	

3.5

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

### Connection Report

Showing: Module 1 Node size: Medium Visual style: Drag

Top pathways

Pathways	overlap_size
degradation of purine ribonucleosides	2
D-mannose degradation	0
CDP-acylglycerol biosynthesis	0
alanine degradation III	0

**nature methods**  
Techniques for life scientists and chemists

Home Current issue Comment Research Archive Authors & referees About the journal

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NATURE METHODS | CORRESPONDENCE

### Systems biology guided by XCMS Online metabolomics

Tao Huan, Erica M Forsberg, Duane Rinehart, Caroline H Johnson, Julijana Ivanisevic, H Paul Benton, Minglang Fang, Aries Aisporna, Brian Hilmers, Farris L Poole, Michael P Thorgersen, Michael W W Adams, Gregory Krantz, Matthew W Fields, Paul D Robbins, Laura J Niederhofer, Trey Ideker, Erica L Majumder, Judy D Wall, Nicholas J W Ratray, Royston Goodacre, Luke L Lalson & Gary Sluzdak

The XCMS Institute faculty

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- 3.0 Data Analysis
  - 3.1 Data Upload Preparation
  - 3.2 Uploading Datasets
  - 3.3 Pairwise Job Creation
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  - 3.5 Multigroup Job Creation
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- 4.0 Results
  - 4.1 View Results Table
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- 5.0 Account Management
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- 7.0 Parameter Management
- 8.0 Job Sharing
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  - Appendix I: Java Issues
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**Other Resources**

- Login to see XCMS Institute
- XCMS FAQ
- Contact Us

**XCMS Online Usage Instructions**

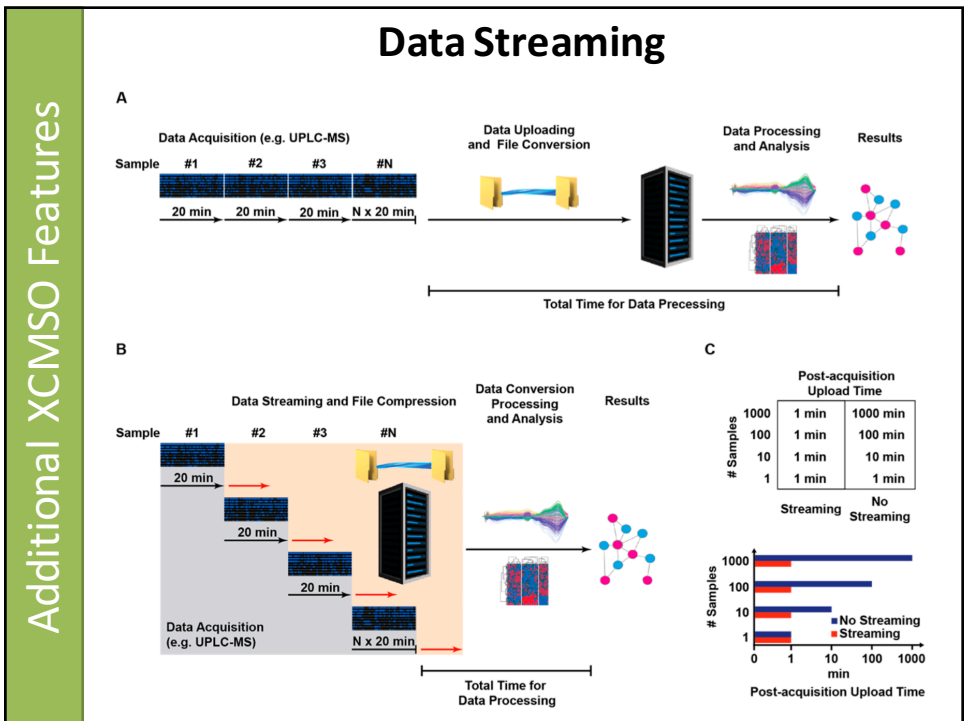
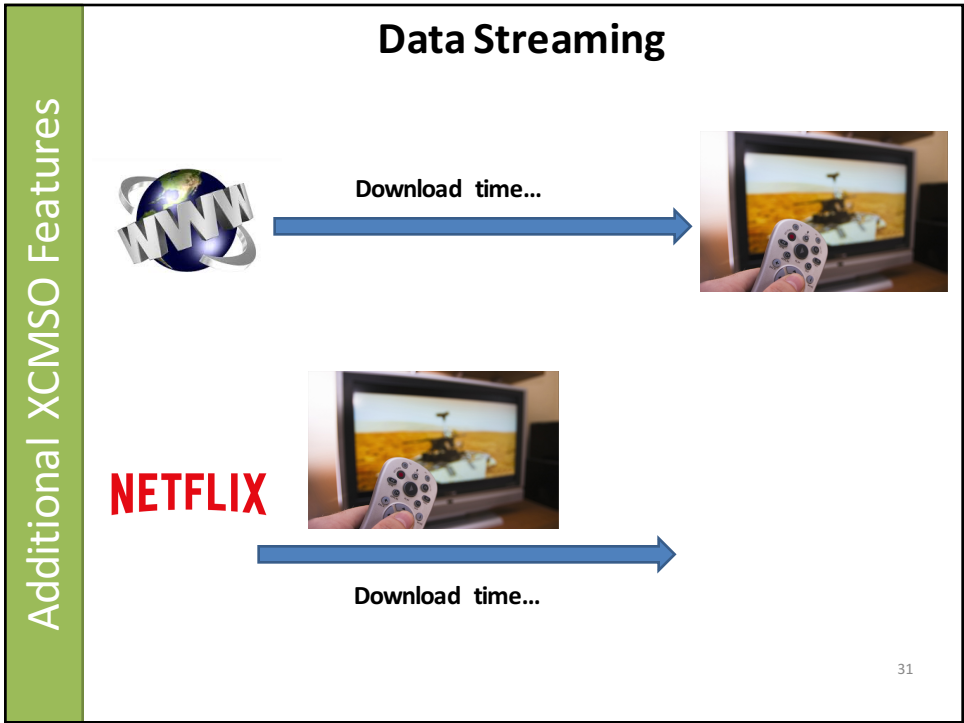
Version 03.03  
Revised March 2016

**Overview**

XCMS Online is an innovative platform with an intuitive graphical interface which allows users to easily upload and process LC/MS data for untargeted metabolomics profiling. XCMS Online provides a complete metabolomics workflow including feature detection, retention time correction, alignment, annotation and statistical analysis. To facilitate the usage, predefined parameter sets for different instrument setups (e.g. HPLC/QTOF, UPLC/QTOF, HPLC/Orbitrap) can be selected. Customized settings can be created from these templates. Results can be browsed online in an interactive, customizable table that shows feature statistics, EICs, box plots, and putative METLIN ID's for each metabolite. All results including the images may also be downloaded as a zip file for offline analysis.


Initially, the platform was developed for two-group comparisons to match the independent, "control" versus "disease" experimental design. It now enables users to perform dependent (paired) two-group comparisons, meta-analysis, and multigroup comparisons, with comprehensive statistical output and interactive visualization tools. Newly incorporated statistical tests cover a wide array of univariate analyses. Multigroup comparison allows for the identification of differentially expressed metabolite features across multiple classes of data while higher order meta-analysis facilitates the identification of shared metabolic patterns across multiple two-group comparisons. Given the complexity of these data sets, we have developed an interactive platform where users can monitor the statistical output of univariate (cloud plots) and multivariate (PCA plots) data analysis in real time by adjusting the threshold and range of various parameters. On the interactive cloud plot, metabolite features can be filtered out by their significance level (p-value), fold change, mass-to-charge ratio, retention time, and intensity. The variation pattern of each feature can be visualized on both extracted-ion chromatograms and box plots. The interactive principal component analysis includes scores, loadings, and score plots that can be adjusted depending on scaling criteria.

You will need a user account to use the system however user accounts only require a valid e-mail address to register. To process datasets using XCMS Online you will need to create a job which involves uploading the datasets, defining parameters and submitting the job. You will be notified of your job status, including errors/warnings that you can correct prior to resubmitting a job. After processing is complete, you will be notified via e-mail that your results are ready for review.



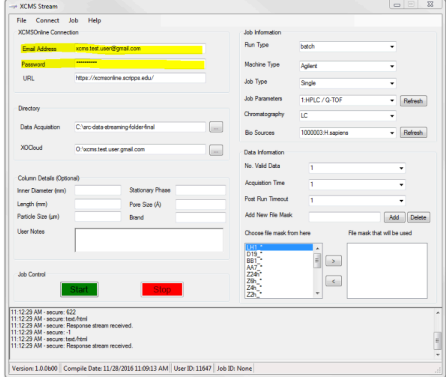
## Data Streaming

Additional XCMSO Features





↑

- (1) Download XCMS Stream into your computer
- (2) Set the parameters
- (3) Do not worry about uploading samples or waiting

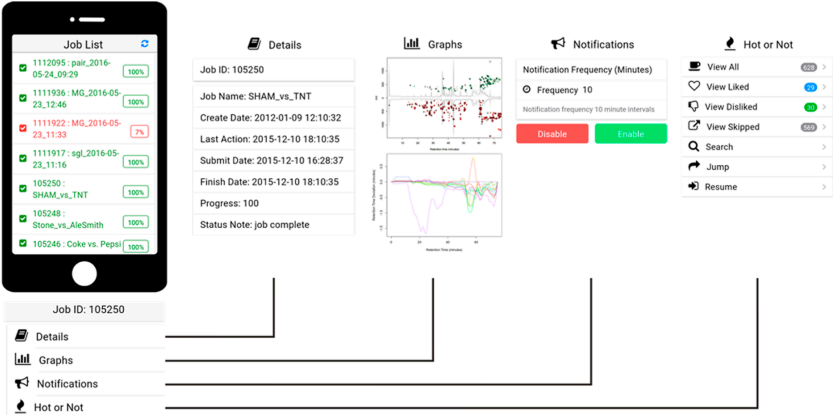


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## XCMS Mobile App

Additional XCMSO Features



34

Additional XCMSO Features

### Hot or Not

35

Additional XCMSO Features

### Hot or Not

**EIC DETAILED INFO**

Fold	2.05
log2fold	1.04
tstat	10
pvalue	0.0000124
qvalue	0.00102
mzmed	525.3940
rtmed	66.10
maxint	13284
dataset1_mean	82653
dataset1_sd	18838
dataset2_mean	169431
dataset2_sd	10480

## References

analytical  
chemistry

Article

pubs.acs.org/ac

### Data Streaming for Metabolomics: Accelerating Data Processing and Analysis from Days to Minutes

J. Rafael Montenegro-Burke,<sup>†,△,○</sup> Aries E. Aisporna,<sup>†,△</sup> H. Paul Benton,<sup>†</sup> Duane Rinehart,<sup>†</sup> Mingliang Fang,<sup>†</sup> Tao Huan,<sup>†</sup> Benedikt Warth,<sup>○</sup> Erica Forsberg,<sup>○</sup> Brian T. Abe,<sup>‡</sup> Julijana Ivanisevic,<sup>#</sup> Dennis W. Wolan,<sup>||</sup> Luc Teyton,<sup>‡</sup> Luke Lairson,<sup>§</sup> and Gary Siuzdak<sup>\*,†,‡</sup>

analytical  
chemistry

Article

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### Smartphone Analytics: Mobilizing the Lab into the Cloud for Omic-Scale Analyses

J. Rafael Montenegro-Burke,<sup>†</sup> Thiery Phommavongsay,<sup>†</sup> Aries E. Aisporna,<sup>†</sup> Tao Huan,<sup>†</sup> Duane Rinehart,<sup>†</sup> Erica Forsberg,<sup>†</sup> Farris L. Poole,<sup>§</sup> Michael P. Thorgersen,<sup>‡</sup> Michael W. W. Adams,<sup>‡</sup> Gregory Krantz,<sup>§</sup> Matthew W. Fields,<sup>§</sup> Trent R. Northen,<sup>||</sup> Paul D. Robbins,<sup>‡</sup> Laura J. Niedernhofer,<sup>‡</sup> Luke Lairson,<sup>#</sup> H. Paul Benton,<sup>†</sup> and Gary Siuzdak<sup>\*,†,‡</sup>

## The XCMS Online Team



Prof. Gary  
Siuzdak



Dr. Paul  
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### Senior Developers



Aries  
Aisporna



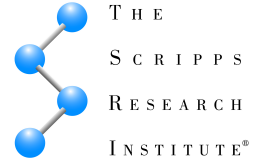
Duane  
Rinehart

### Intern

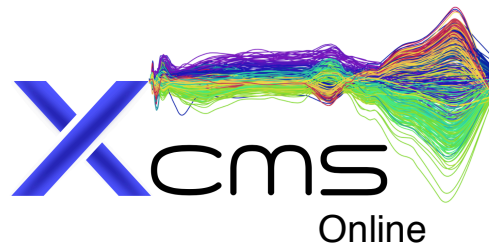


Thiery  
Phommavongsay

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## 5th UAB Metabolomics Workshop



Xavier Domingo-Almenara