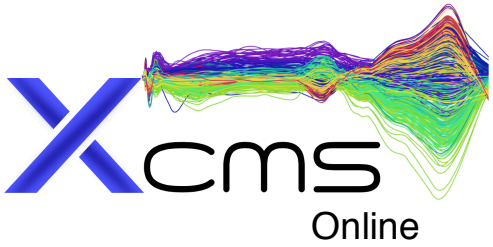
THE UNIVERSITY OF ALABAMA AT BIRMINGHAM

THE SCRIPPS RESEARCH INSTITUTE®

5th UAB Metabolomics Workshop



Xavier Domingo-Almenara

Outline

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

Introduction

XCMS Online

2006 — XCMS

2008 — centWave

2009

XCMS Online production

2011

2012 — Public release

Today

- More than 14,000 users
- Average of 50 jobs per day
- 75 users logging in per day
- More than 250,000 experiments processed

3

Introduction

XCMS vs XCMS

XCMS

Requires (some) R knowledge

Review of results: manual and tiresome

Processing speed: depending on N# samples and computer

Xcms Online

Easy-to-use

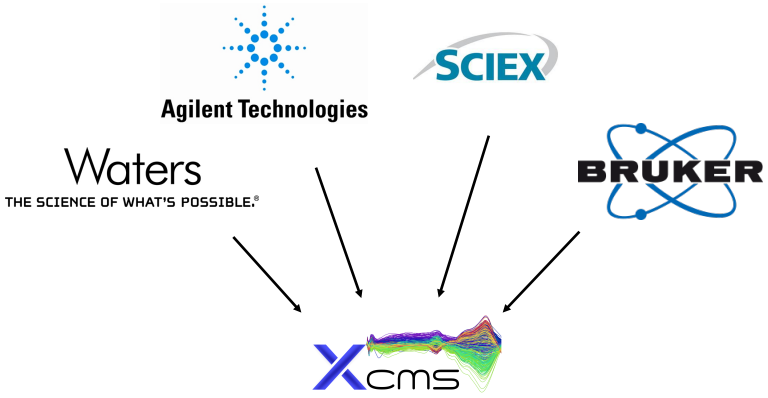
Review of results: fast and easy

Processing speed: fast

Cloud-based benefits: data sharing and streamline analysis

XCMS Online

Uploading samples



5

XCMS Online

Data processing

Peak detection — MatchedFilter, CentWave

Peak grouping

Retention time alignment

CAMERA *via* **Annotation**

Statistical Analysis

6

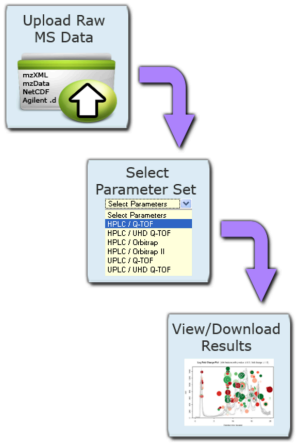
XCMS Online

Job types in XCMS Online

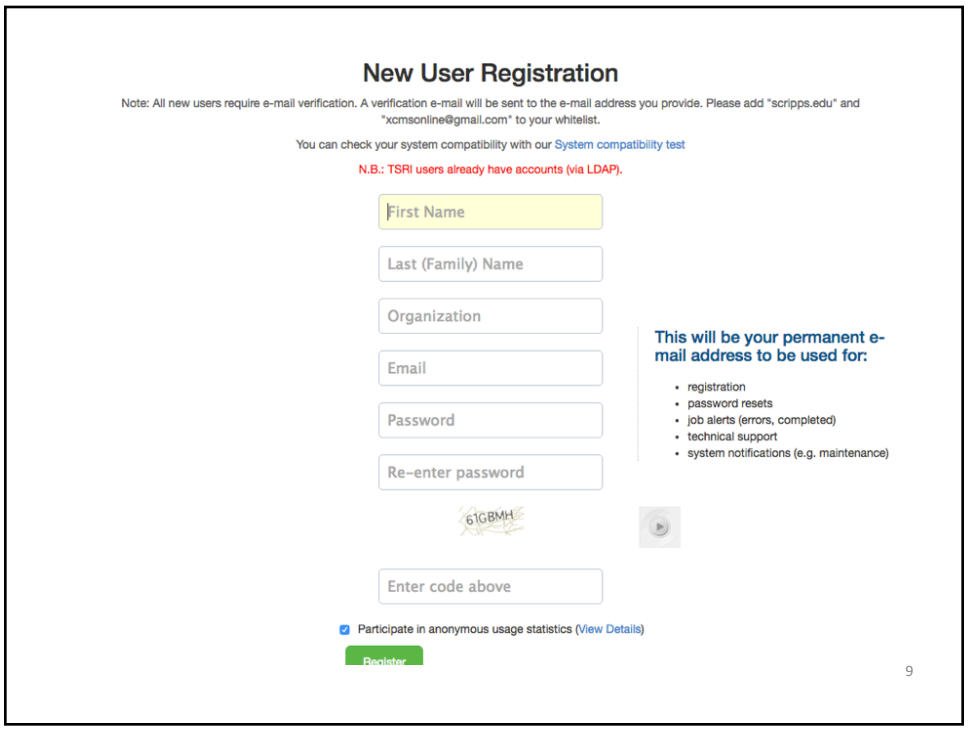
- Single Class Jobs – Either single file or single dataset (class or unknown classes)
- Pairwise analysis Jobs – Two class comparison, works best with KO –vs- WT type experiments
- Multigroup/class Jobs – Multiple classes including Quality control samples. Great for Time series jobs or multiple knockouts
- meta-XCMS- Finds the overlap between many pairwise jobs. (Must have same control samples)

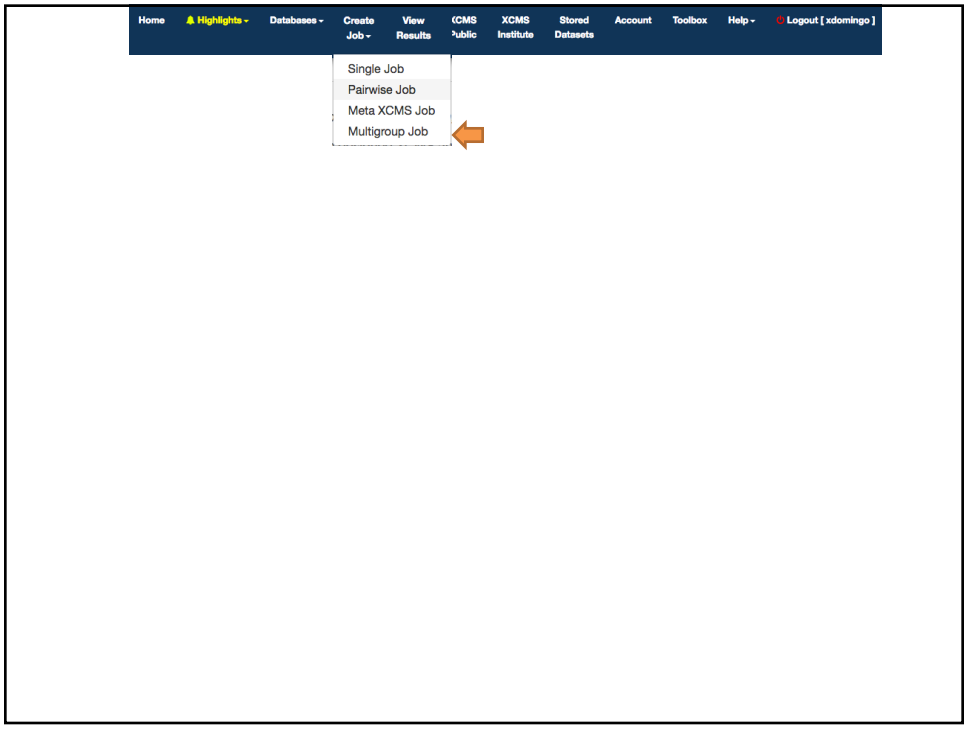
7

(pseudo-) Live XCMS demo



8


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
61GBMH
Enter code above
Participate in anonymous usage statistics (View Details)
Register
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
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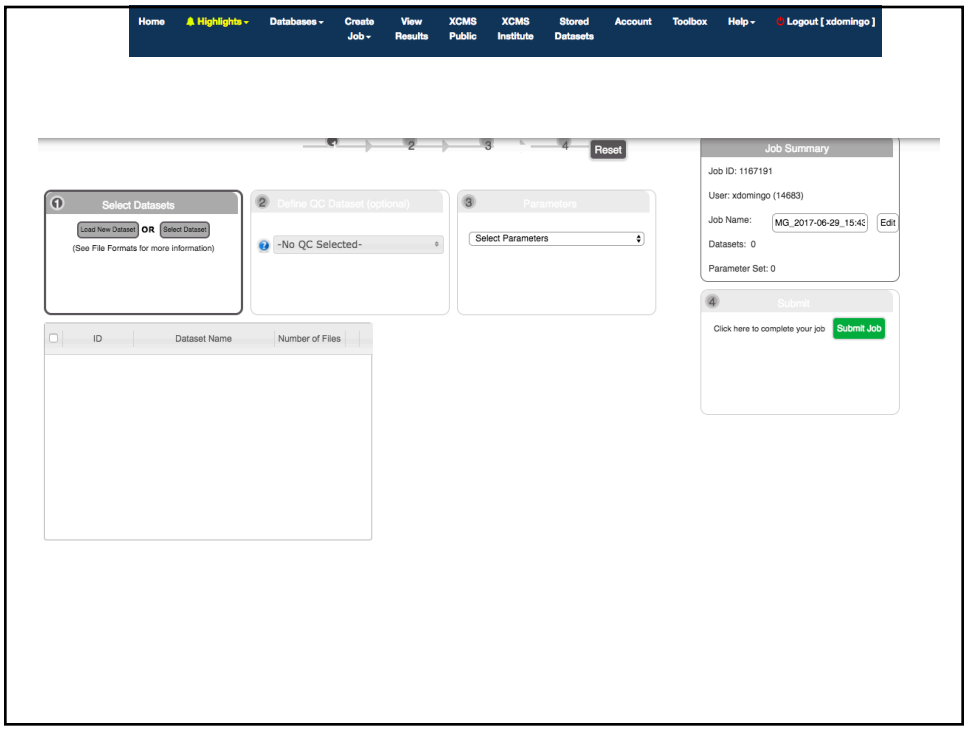
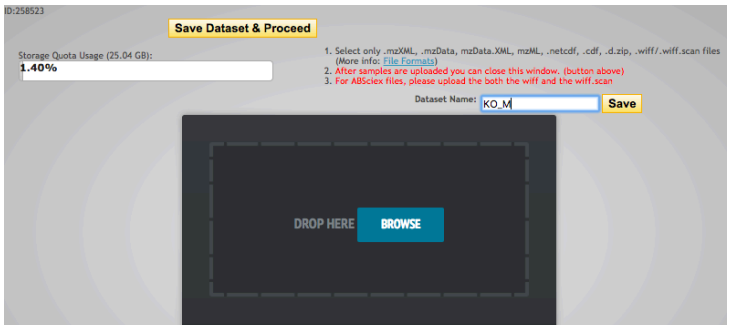
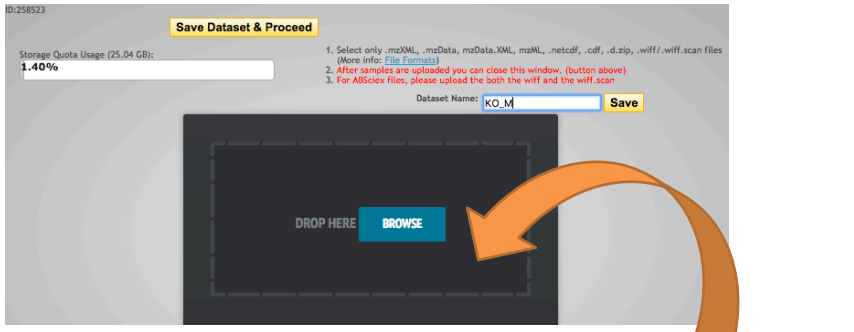
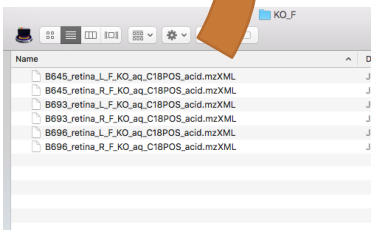
XCMS Public
XCMS Institute
Stored Datasets
Account
Toolbox
Help
Logout [xdomingo]
Single Job
Pairwise Job
Meta XCMS Job
Multigroup Job

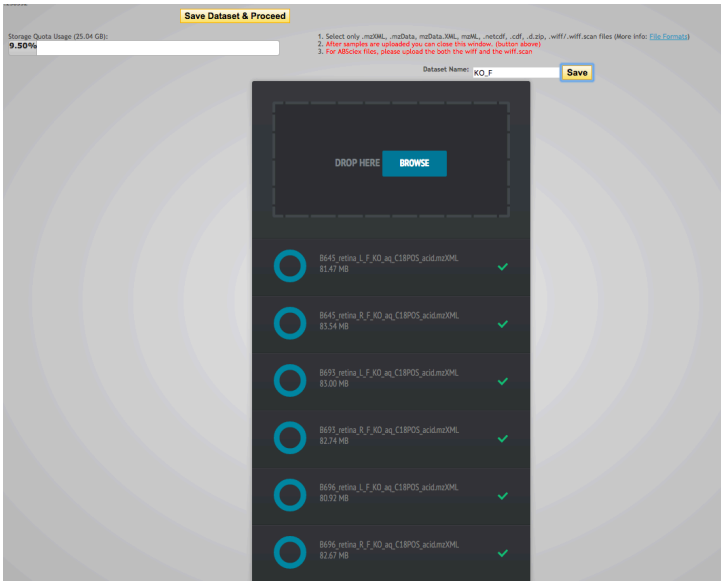

Home
Highlights
Databases
Create Job
View Results
XCMS Public
XCMS Institute
Stored Datasets
Account
Toolbox
Help
Logout [xdomingo]
Reset
Job Summary
Job ID: 1167191
User: xdomingo (14683)
Job Name:
MG_2017-06-29_15:43
Edit
Datasets: 0
Parameter Set: 0
Select Datasets
Load New Dataset
OR
Select Dataset
(See File Formats for more information)
Define QC Dataset (optional)
-No QC Selected-
Parameters
Select Parameters
Submit
Click here to complete your job
Submit Job
ID
Dataset Name
Number of Files

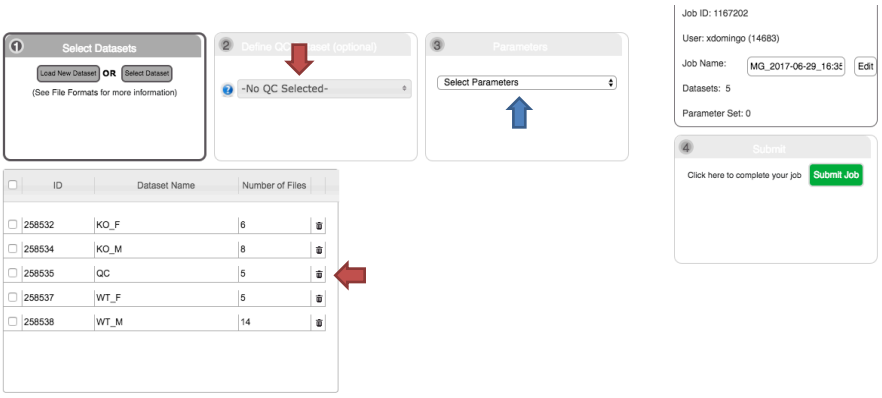

ID:258523
Save Dataset & Proceed
Storage Quota Usage (25.04 GB):
1.40%
1. Select only .mzXML, .mzData, mzData.XML, mzML, .netcdf, .cdf, .d.zip, .wiff/.wiff.scan files
(More info: File Formats)
2. After samples are uploaded you can close this window. (button above)
3. For ABSciex files, please upload the both the wiff and the wiff.scan
Dataset Name:
KO_M
Save
DROP HERE
BROWSE

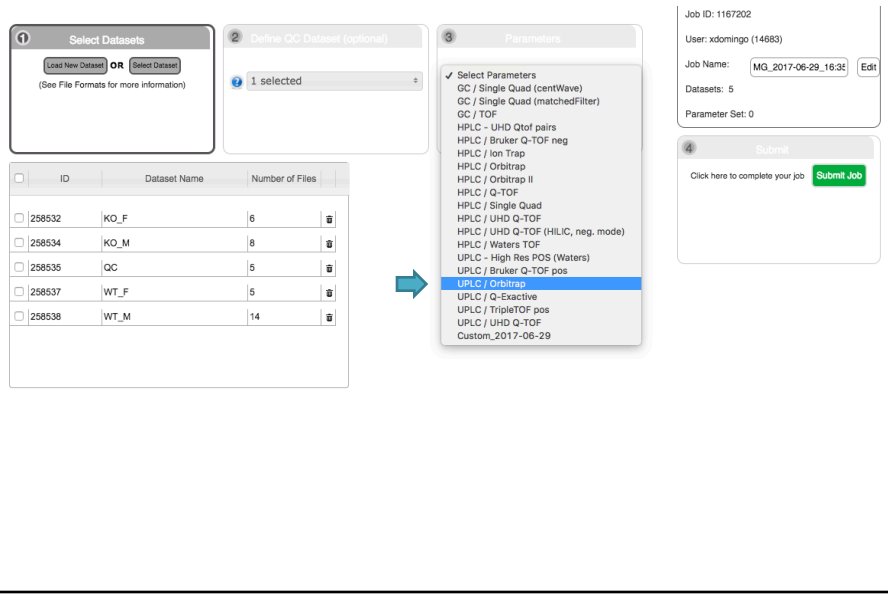


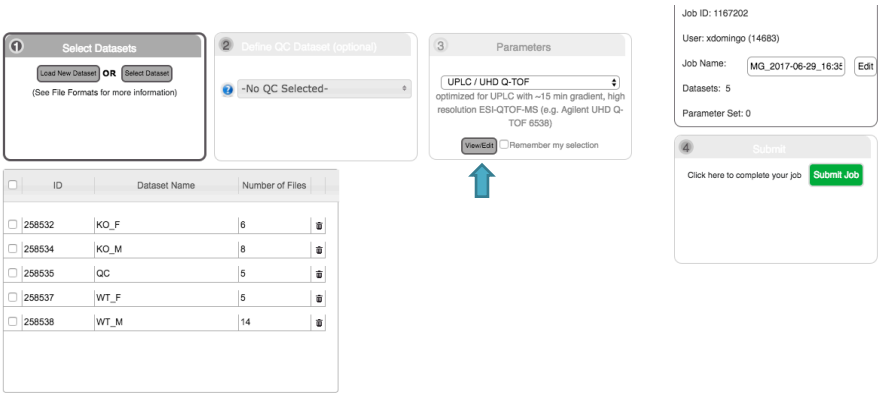


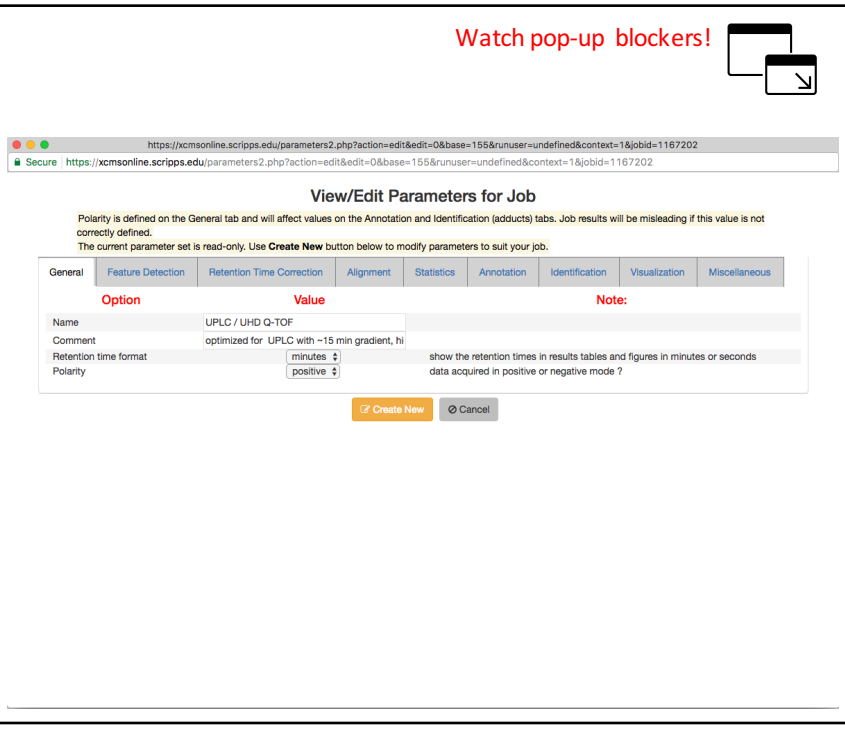
Loading folders is not allowed in OSX

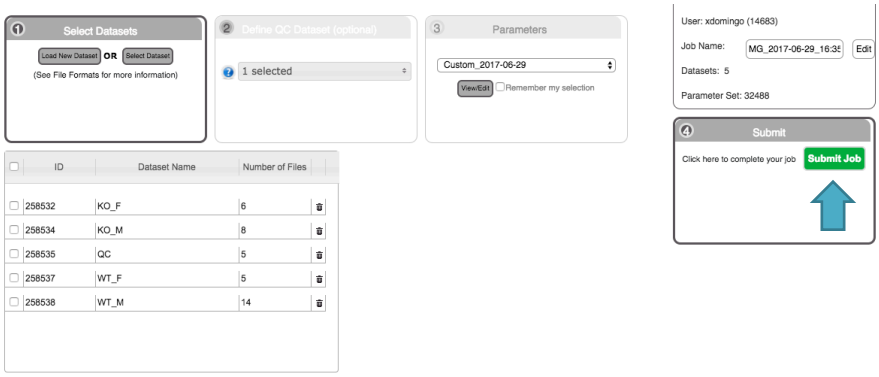


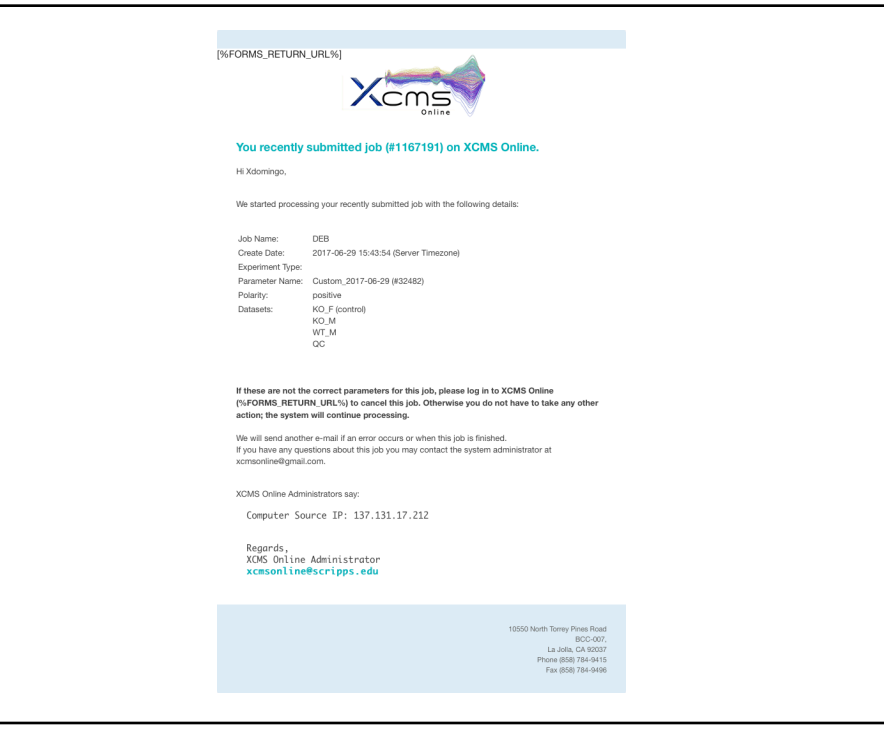

Select Datasets
Load New Dataset
OR
Select Dataset
(See File Formats for more information)
-No QC Selected-
Select Parameters
Job ID: 1167202
User: xdomingo (14683)
Job Name:
MG_2017-06-29_16:3
Edit
Datasets: 5
Parameter Set: 0
Submit
Click here to complete your job
Submit Job
ID
Dataset Name
Number of Files
258532 KO_F 6
258534 KO_M 8
258535 QC 5
258537 WT_F 5
258538 WT_M 14


Select Datasets
Load New Dataset
OR
Select Dataset
(See File Formats for more information)
1 selected
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
Job ID: 1167202
User: xdomingo (14683)
Job Name:
MG_2017-06-29_16:3
Edit
Datasets: 5
Parameter Set: 0
Submit
Click here to complete your job
Submit Job
ID
Dataset Name
Number of Files
258532 KO_F 6
258534 KO_M 8
258535 QC 5
258537 WT_F 5
258538 WT_M 14


Select Datasets
Load New Dataset
OR
Select Dataset
(See File Formats for more information)
2 Define QC Dataset (optional)
-No QC Selected-
3 Parameters
UPLC / UHD Q-TOF
optimized for UPLC with ~15 min gradient, high resolution ESI-QTOF-MS (e.g. Agilent UHD Q-TOF 6538)
View/Edit
Remember my selection
Job ID: 1167202
User: xdomingo (14683)
Job Name:
MG_2017-06-29_16:3
Edit
Datasets: 5
Parameter Set: 0
4 Submit
Click here to complete your job
Submit Job
ID
Dataset Name
Number of Files
258532 KO_F 6
258534 KO_M 8
258535 QC 5
258537 WT_F 5
258538 WT_M 14


Watch pop-up blockers!
https://xcmsonline.scripps.edu/parameters2.php?action=edit&edit=0&base=155&runuser=undefined&context=1&jobid=1167202
Secure 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
Option
Value
Note:
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 ?
Create New
Cancel





[%FORMS_RETURN_URL%]

XCMS Online

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.

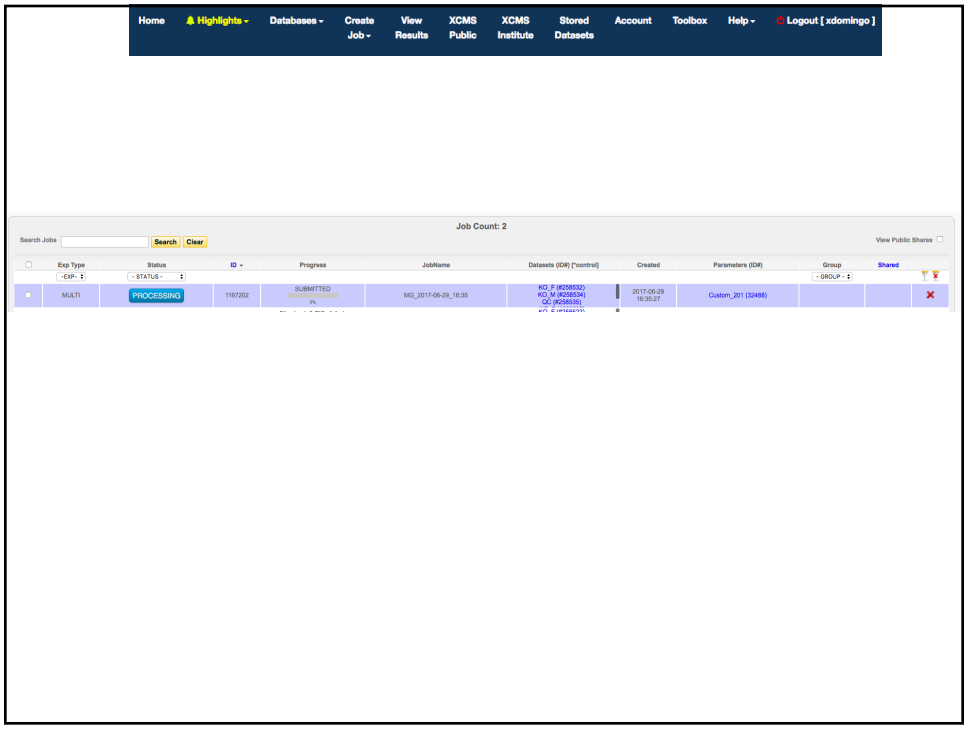
We will send another e-mail if an error occurs or when this job is finished.
If you have any questions about this job you may contact the system administrator at xcmsonline@gmail.com.

XCMS Online Administrators say:

Computer Source IP: 137.131.17.212

Regards,
XCMS Online Administrator
xcmsonline@scripps.edu

10550 North Torrey Pines Road
BCC-007,
La Jolla, CA 92037
Phone (858) 784-9415
Fax (858) 784-9496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XCMS Institute
Stored Datasets
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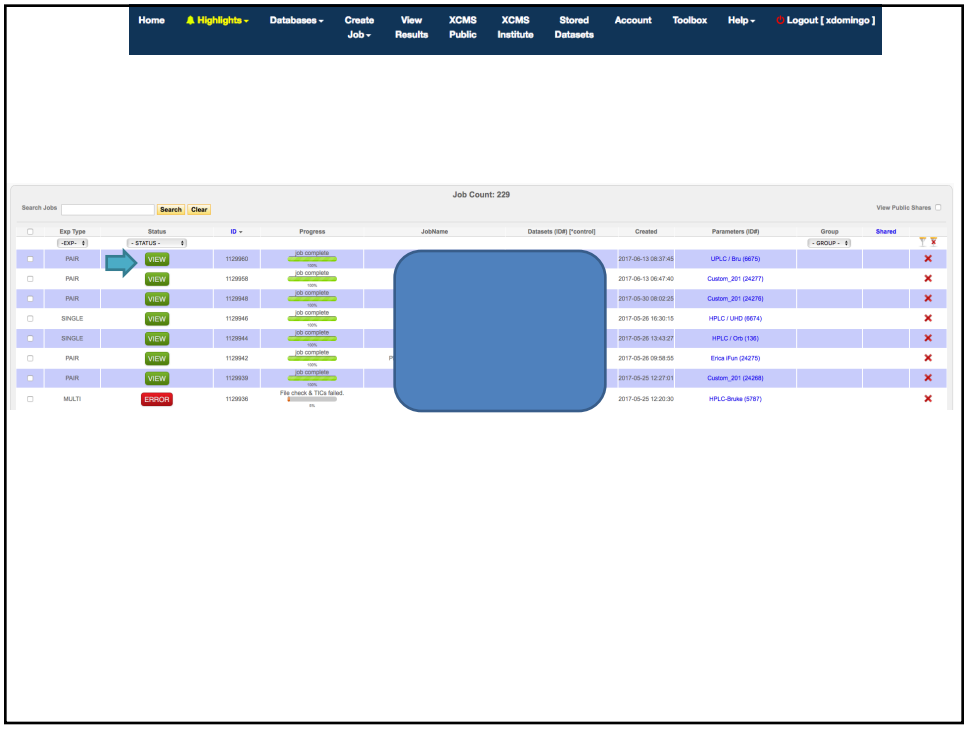
Help
Logout [xdomingo]
Job Count: 2
Search Jobs
Search
Clear
View Public Shares
Exp Type
Status
ID
Progress
JobName
Datasets (ID#) [*control]
Created
Parameters (ID#)
Group
Shared
MULTI
PROCESSING
1167202
SUBMITTED
MG_2017-06-29_16:35
2017-06-29 16:35:27
Custom_201 (32488)


Home
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XCMS Institute
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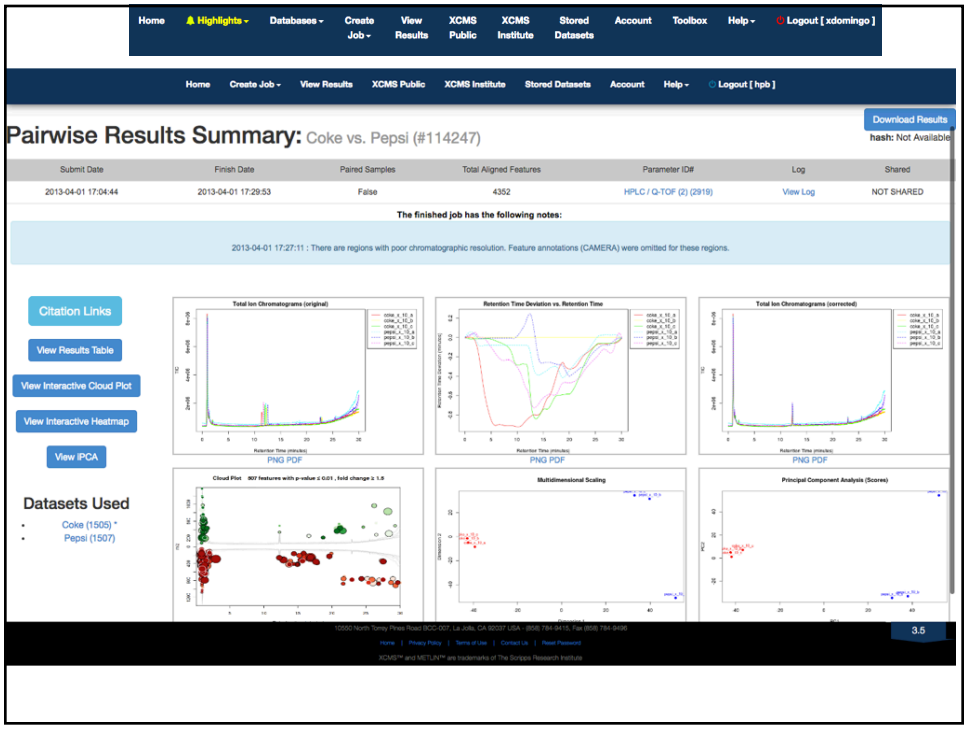
Help
Logout [xdomingo]
Job Count: 229
Search Jobs
Search
Clear
View Public Shares
Exp Type
Status
ID
Progress
JobName
Datasets (ID#) [*control]
Created
Parameters (ID#)
Group
Shared
PAIR
VIEW
1129960
job complete
2017-06-13 08:37:45
UPLC / Bru (6675)
PAIR
VIEW
1129958
job complete
2017-06-13 06:47:40
Custom_201 (24277)
PAIR
VIEW
1129948
job complete
2017-05-30 08:02:23
Custom_201 (24276)
SINGLE
VIEW
1129946
job complete
2017-05-26 16:30:15
HPLC / UHD (6674)
SINGLE
VIEW
1129944
job complete
2017-05-26 13:43:27
HPLC / Orb (136)
PAIR
VIEW
1129942
job complete
2017-05-26 09:58:55
Erica iFun (24275)
PAIR
VIEW
1129939
job complete
2017-05-25 12:27:01
Custom_201 (24268)
MULTI
ERROR
1129936
File check & TICs failed.
2017-05-25 12:20:30
HPLC-Bruke (5787)


Home
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XCMS Public
XCMS Institute
Stored Datasets
Account
Toolbox
Help
Logout [xdomingo]
Home
Create Job
View Results
XCMS Public
XCMS Institute
Stored Datasets
Account
Help
Logout [hpb]
Pairwise Results Summary: Coke vs. Pepsi (#114247)
Download Results
hash: Not Available
Submit Date
Finish Date
Paired Samples
Total Aligned Features
Parameter ID#
Log
Shared
2013-04-01 17:04:44
2013-04-01 17:29:53
False
4352
HPLC / Q-TOF (2) (2919)
View Log
NOT SHARED
The finished job has the following notes:
2013-04-01 17:27:11 : There are regions with poor chromatographic resolution. Feature annotations (CAMERA) were omitted for these regions.
Citation Links
View Results Table
View Interactive Cloud Plot
View Interactive Heatmap
View iPCA
Datasets Used
Coke (1505) *
Pepsi (1507)
Total Ion Chromatograms (original)
Retention Time Deviation vs. Retention Time
Total Ion Chromatograms (corrected)
PNG PDF
PNG PDF
PNG PDF
Cloud Plot
Multidimensional Scaling
Principal Component Analysis (Scores)
3.5


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XCMS Public
XCMS Institute
Stored Datasets
Account
Help
Logout [hpb]
Pairwise Results Summary: Coke vs. Pepsi (#114247)
hash: Not Available
Submit Date
Finish Date
Paired Samples
Total Aligned Features
Parameter ID#
Log
Shared
2013-04-01 17:04:44
2013-04-01 17:29:53
False
4352
HPLC / Q-TOF (2) (2919)
View Log
NOT SHARED
The finished job has the following notes:
Total Ion Chromatograms (original)
Total Ion Chromatograms (corrected)
coke_x_10_a
coke_x_10_b
coke_x_10_c
pepsi_x_10_a
pepsi_x_10_b
pepsi_x_10_c
TIC
Retention Time (minutes)
Datasets
Coke (1505) *
Pepsi (1507)
PNG PDF
PNG PDF
PNG PDF
3.5


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XCMS Public
XCMS Institute
Stored Datasets
Account
Help
Logout [hpb]
Pairwise Results Summary: Coke vs. Pepsi (#114247)
Download Results
hash: Not Available
Submit Date
Finish Date
Paired Samples
Total Aligned Features
Parameter ID#
Log
Shared
2013-04-01 17:04:44
2013-04-01 17:29:53
False
4352
HPLC / Q-TOF (2) (2919)
View Log
NOT SHARED
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Citation Links
View Results Table
View Interactive Cloud Plot
View Interactive Heatmap
View iPCA
Datasets Used
Coke (1505) *
Pepsi (1507)
Total Ion Chromatograms (original)
Retention Time Deviation vs. Retention Time
Total Ion Chromatograms (corrected)
PNG PDF
PNG PDF
Cloud Plot
Multidimensional Scaling
Principal Component Analysis (Scores)
3.5


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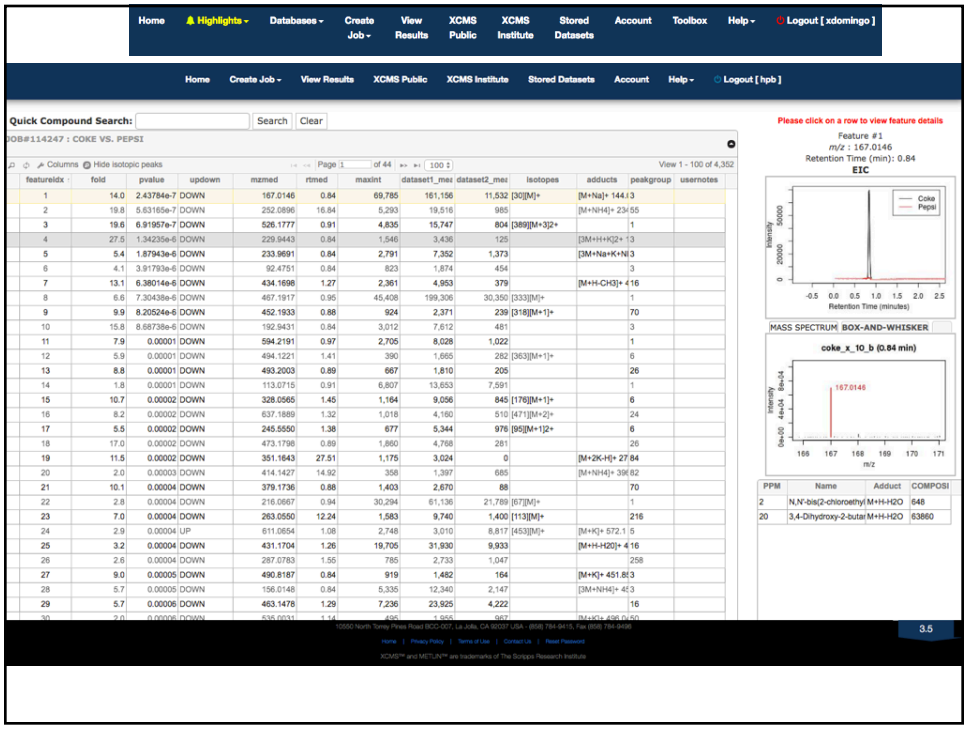
Main Panel
Advanced
p-value
0
0-0.01
1
fold change
0
1.5 - 549.436
549.436
Regenerate Cloud Plot
EIC_ABBR
Box and Whisker
Spectrum
Please click on a feature to display XIC, Box-and-Whisker and Spectrum Data
Bubble Size Multiplier
22
Download Cloud Plot Manual
Welcome to the Cloud Plot
Welcome to the Interactive Cloud Plot! The basic functions of this graph are :
P-value is represented by how dark or light the color is.
Fold change is represented by the radius of each feature.
Retention time is represented by position on the x-axis.
Mass-to-Charge ratio is
View 1
Retention Time vs m/z of 1270 features
Click and drag in the plot area to zoom in
m/z
Retention Time (minutes)
Toggle Upregulated
Toggle Downregulated
p-Value : 0-0.01 | fold change : 1.5 - 549.436 | m/z Range of 0 - 1648 | Retention Range of 1-49 | max intensity : 0-2363919.25 | Radius Scale : Fold Change
Table View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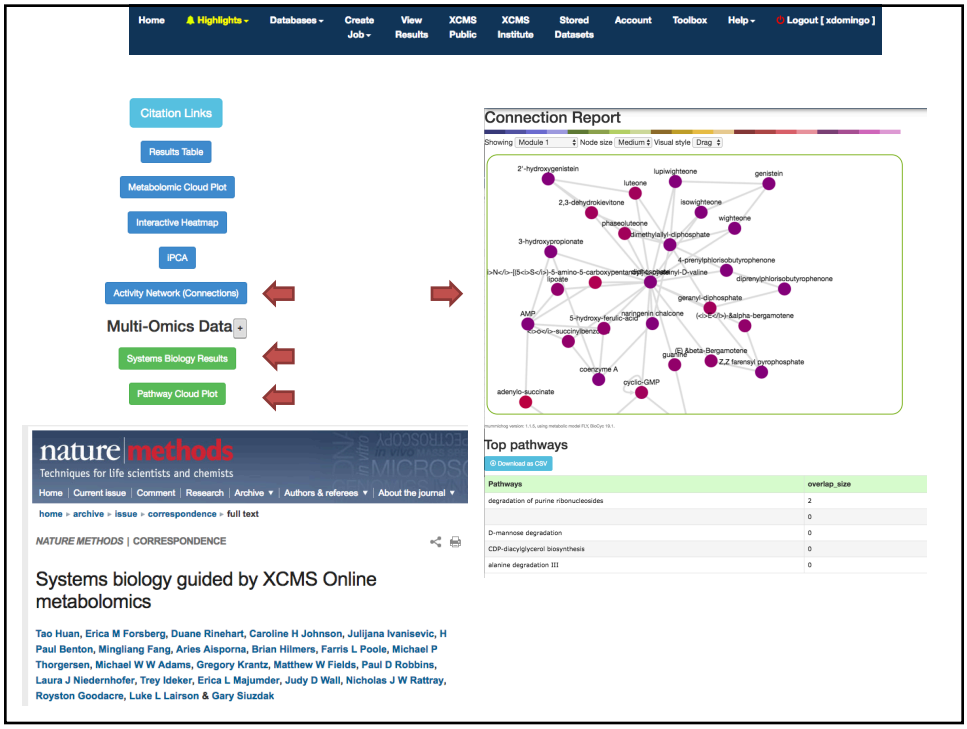
Logout [xdomingo]
Home
Create Job
View Results
XCMS Public
XCMS Institute
Stored Datasets
Account
Help
Logout [hpb]
Quick Compound Search:
Search
Clear
JOB#114247 : COKE VS. PEPSI
Please click on a row to view feature details
Feature #1
m/z : 167.0146
Retention Time (min): 0.84
EIC
Coke
Pepsi
Retention Time (minutes)
MASS SPECTRUM BOX-AND-WHISKER
coke_x_10_b (0.84 min)
167.0146
m/z
PPM
Name
Adduct
COMPOSI
2
N,N'-bis(2-chloroethyl
M+H-H2O
648
20
3,4-Dihydroxy-2-butar
M+H-H2O
63860
3.5


Home
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Stored Datasets
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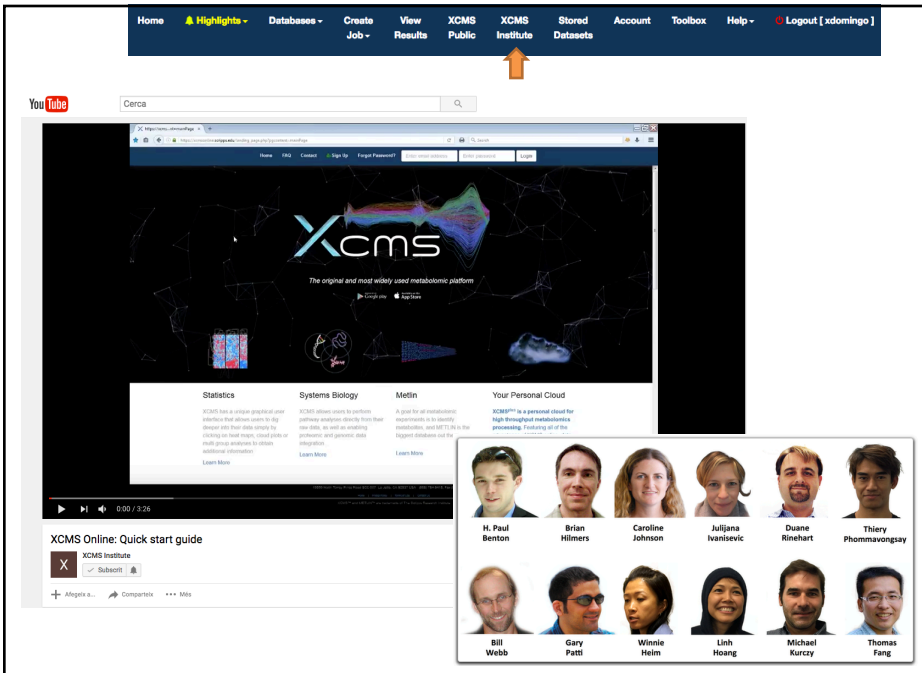
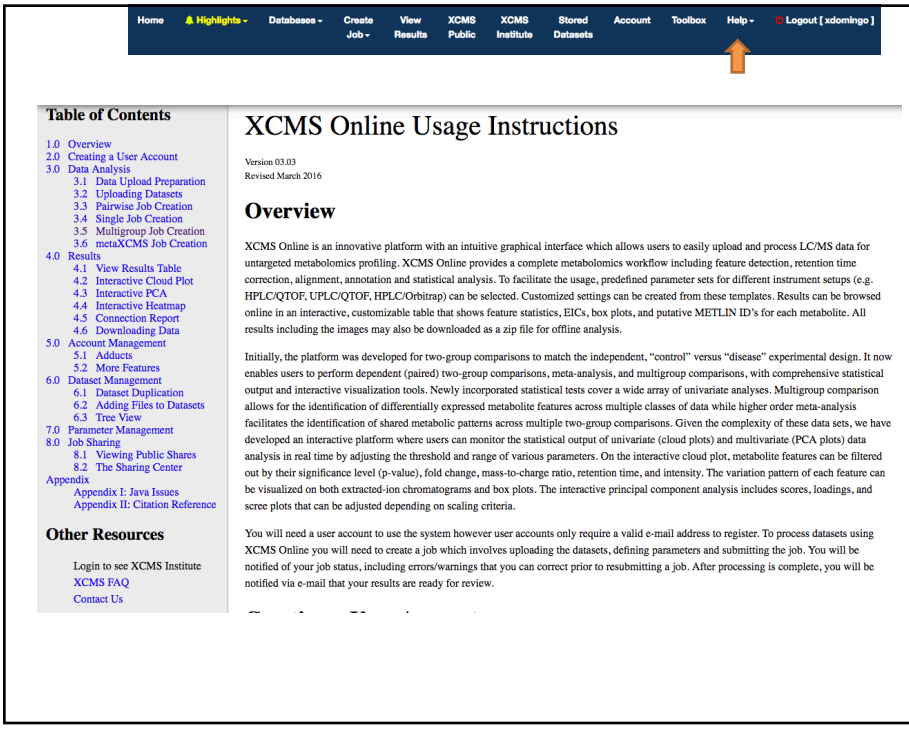
Help
Logout [xdomingo]
Citation Links
Results Table
Metabolomic Cloud Plot
Interactive Heatmap
IPCA
Activity Network (Connections)
Multi-Omics Data
Systems Biology Results
Pathway Cloud Plot
Connection Report
Top pathways
Download as CSV
Pathways
overlap_size
degradation of purine ribonucleosides
2
D-mannose degradation
0
CDP-diacylglycerol 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
home ▸ archive ▸ issue ▸ correspondence ▸ full text
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, Mingliang 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 Niedernhofer, Trey Ideker, Erica L Majumder, Judy D Wall, Nicholas J W Rattray, Royston Goodacre, Luke L Lairson & Gary Siuzdak



The XCMS Institute faculty



Additional XCMSO Features

Data Streaming

Download time…

NETFLIX

Download time…

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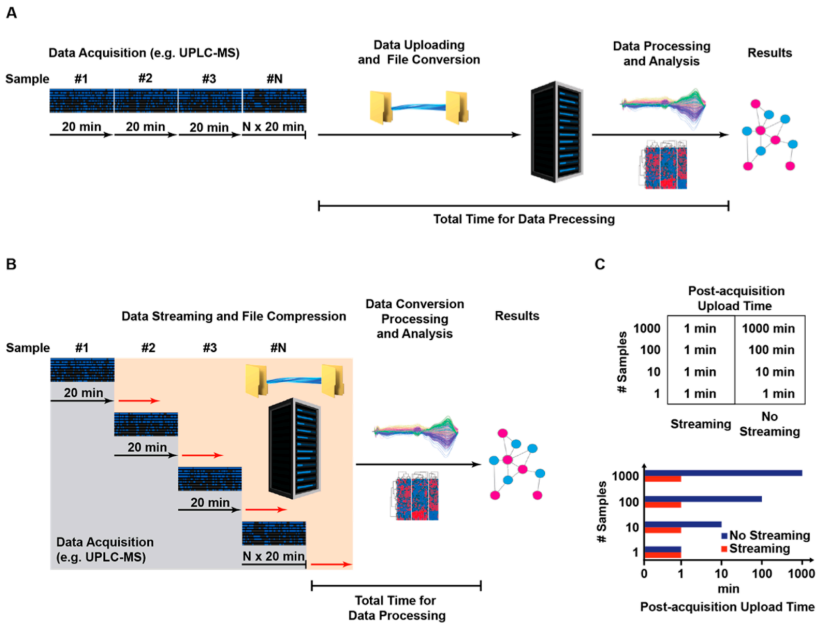
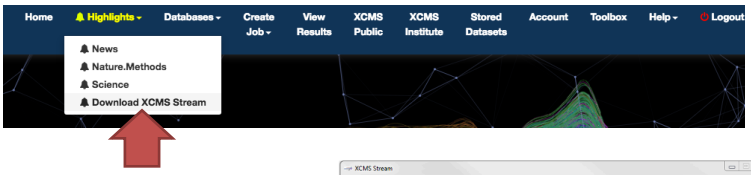
Additional XCMSO Features

Data Streaming



Additional XCMSO Features

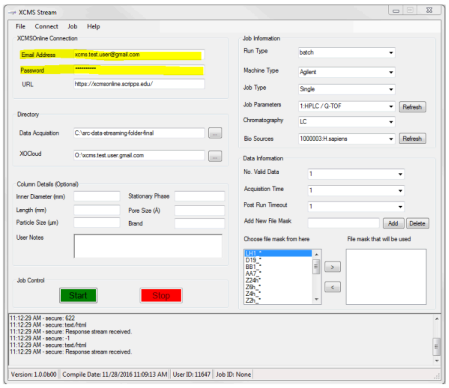
Data Streaming



(1) Download XCMS Stream into your computer

(2) Set the parameters

(3) Do not worry about uploading samples or waiting



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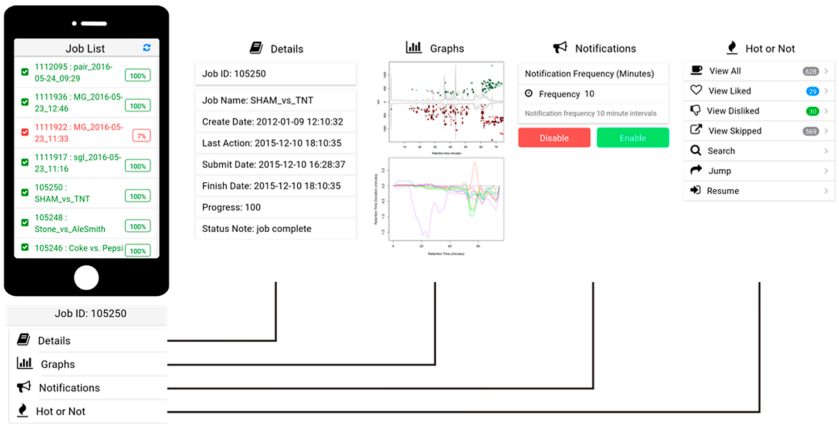
Additional XCMSO Features

XCMS Mobile App

GET IT ON Google Play

Available on the App Store



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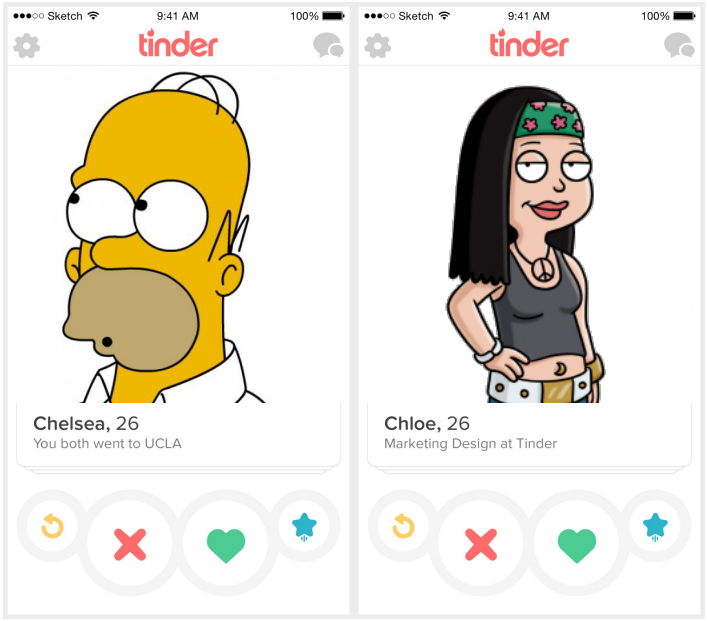
Additional XCMSO Features

Hot or Not



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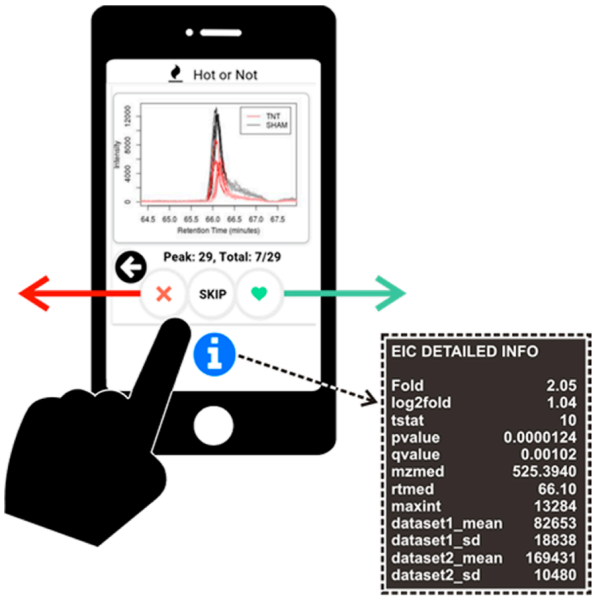
Additional XCMSO Features

Hot or Not



Additional XCMSO Features

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,[†,△] Aries E. Aisporna,[†,△] H. Paul Benton,[†] Duane Rinehart,[†] Mingliang Fang,[†] Tao Huan,[†] Benedikt Warth,[†] Erica Forsberg,[†] Brian T. Abe,[‡] Julijana Ivanisevic,[#] Dennis W. Wolan,[∥] Luc Teyton,[‡] Luke Lairson,[§] and Gary Siuzdak*[,†,⊥]

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

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

The XCMS Online Team

Prof. Gary Siuzdak

Dr. Paul Benton

Senior Developers

Aries Aisporna

Duane Rinehart

Intern

Thiery Phommavongsay

THE UNIVERSITY OF ALABAMA AT BIRMINGHAM

THE SCRIPPS RESEARCH INSTITUTE®

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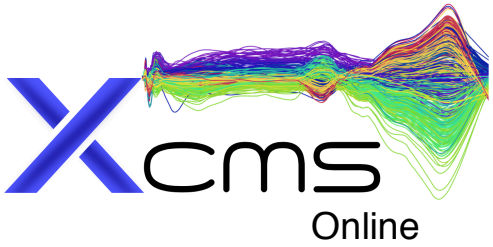

Xavier Domingo-Almenara