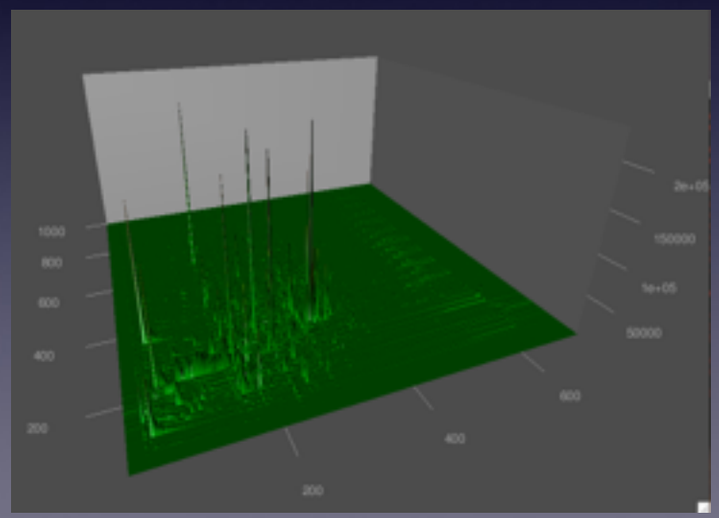
Data Processing with XCMS Online

H. Paul Benton

Wednesday June 17, 2015
10:30-11;15 All Attendees (LRC 249)
XCMS online (introduction and XCMS processed data sets)

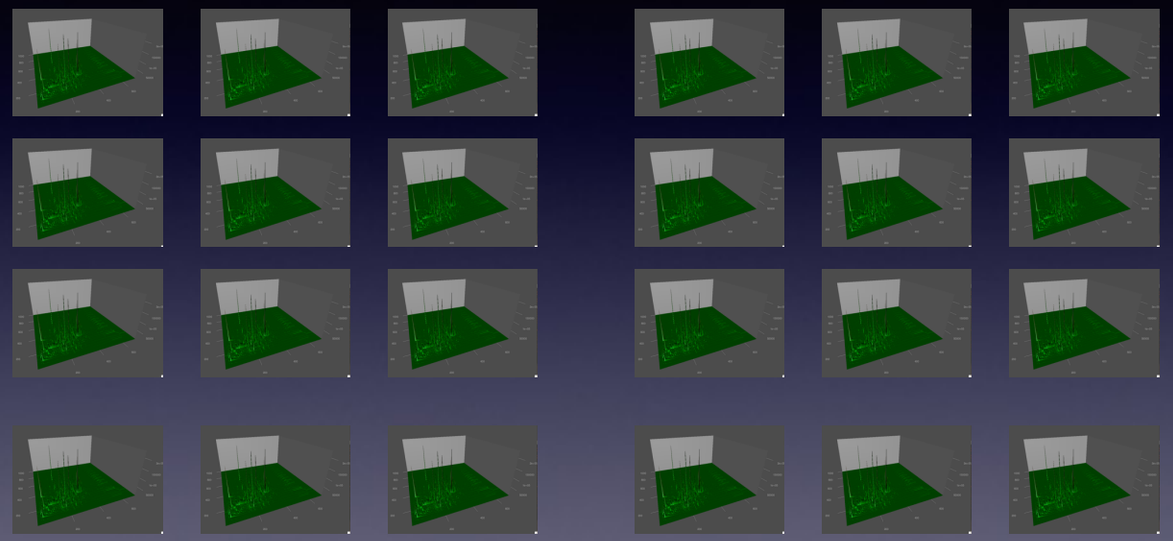
What do we have

- What is the data that we have and what does it look like?



Urine Grubb
Group 1

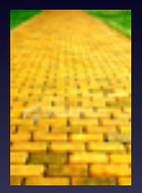
Urine Grubb
Group 2



What do we need

1. Statistic results from data
2. List of Features - (prefer identified metabolites)
3. Characterisation - adducts / isotopes

Basic pipeline of data processing



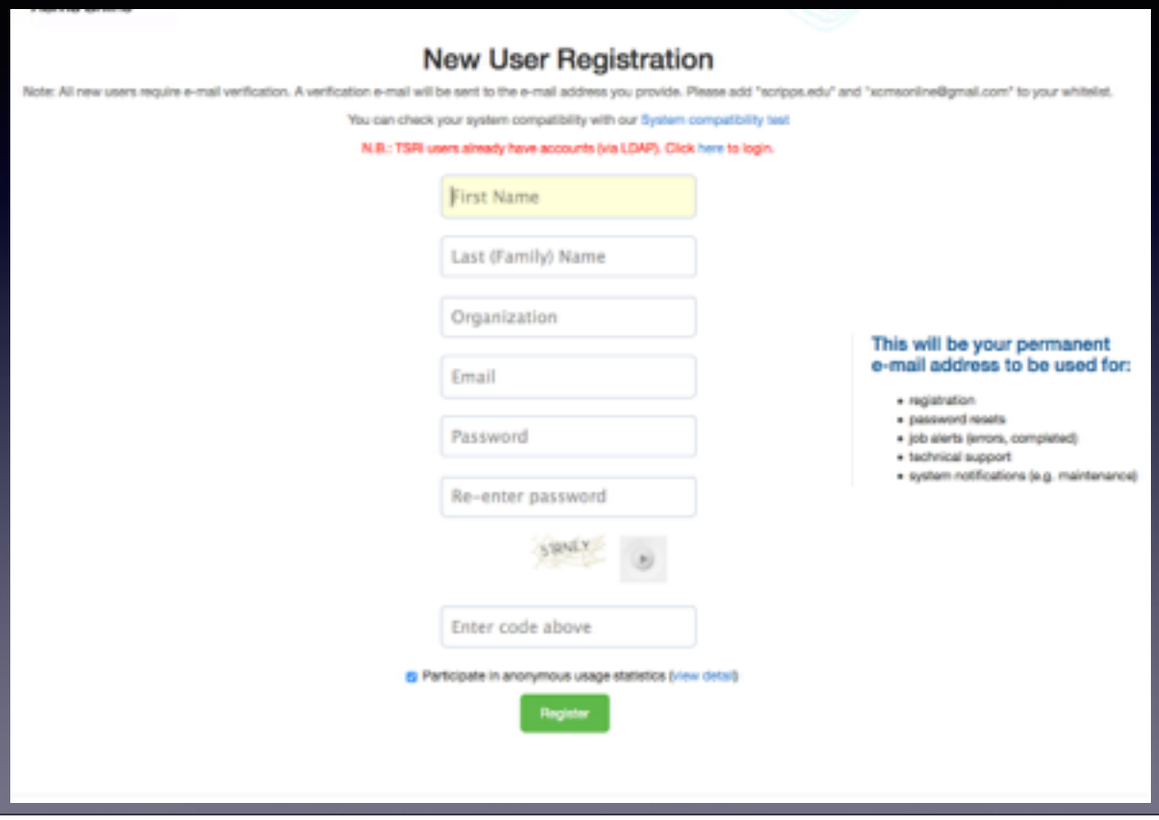
Peak Detection

Grouping
Groups similar Peaks

Retention Time

Statistical Analysis of Classes

Intro to XO


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 "xomsonline@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). Click here to login.
First Name
Last (Family) Name
Organization
Email
Password
Re-enter password
Enter code above
Participate in anonymous usage statistics (view detail)
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)

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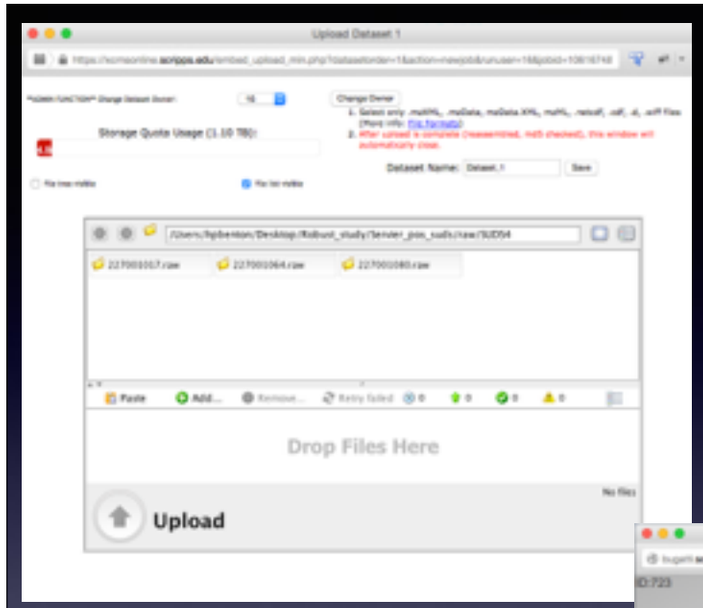
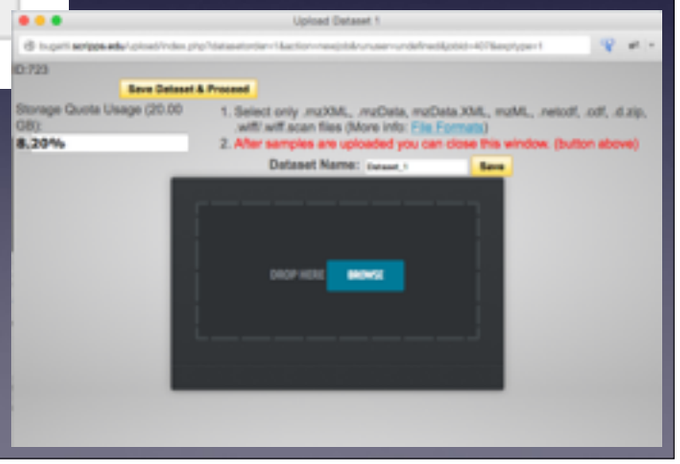
Dataset 1
Dataset 2
Parameters
Select Parameters
Dataset 1 ID: Not Defined
Dataset 1 no. of files: 0
Dataset 1 Name:
Not Defined
Dataset 2 ID: Not Defined
Dataset 2 no. of files: 0
Dataset 2 Name:
Not Defined
Job ID: 1061674
Job Name:
Edit
Dataset 1: Not Defined
Dataset 2: Not Defined
Parameter Set1: Select Parameters
Click here to complete your job
Submit Job



Java uploader:
Good for folder RAW files
ie : Agilent, Waters etc



HTML uploader:
Good for speed
parallel upload

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Dataset 1
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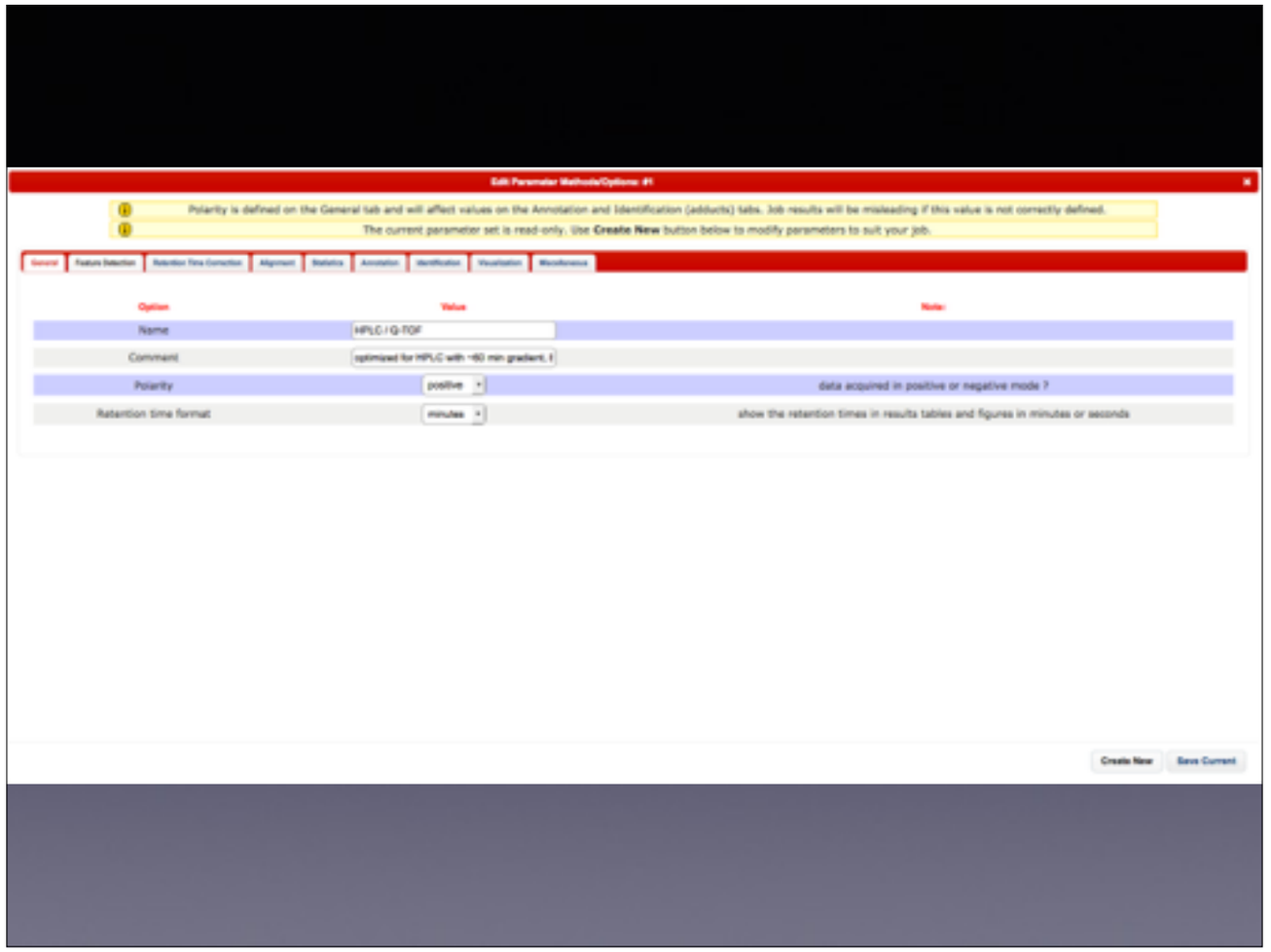
Parameters
Select Parameters
Dataset 1 ID: Not Defined
Dataset 1 no. of files: 0
Dataset 1 Name:
Not Defined
Dataset 2 ID: Not Defined
Dataset 2 no. of files: 0
Dataset 2 Name:
Not Defined
Job ID: 1061674
Job Name:
Edit
Dataset 1: Not Defined
Dataset 2: Not Defined
Parameter Set1: Select Parameters
Click here to complete your job
Submit Job


Edit Parameter Methods/Options: #1
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
HPLC / Q-TOF
Comment
optimized for HPLC with ~60 min gradient, f
Polarity
positive
data acquired in positive or negative mode ?
Retention time format
minutes
show the retention times in results tables and figures in minutes or seconds
Create New
Save Current

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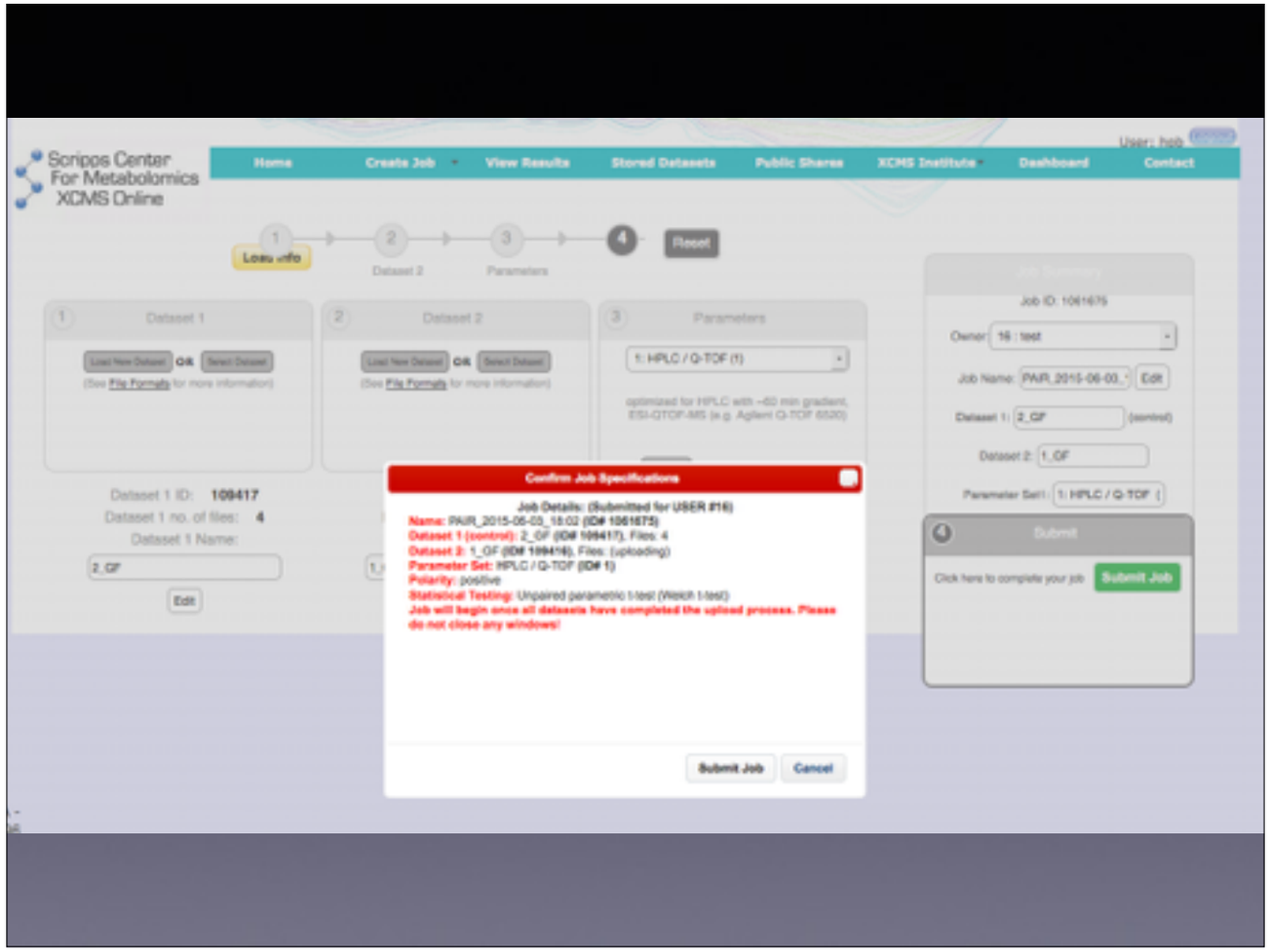
Dataset 1
Dataset 2
Parameters
Select Parameters
Dataset 1 ID: Not Defined
Dataset 1 no. of files: 0
Dataset 1 Name:
Not Defined
Dataset 2 ID: Not Defined
Dataset 2 no. of files: 0
Dataset 2 Name:
Not Defined
Job ID: 1061674
Job Name:
Edit
Dataset 1: Not Defined
Dataset 2: Not Defined
Parameter Set1: Select Parameters
Click here to complete your job
Submit Job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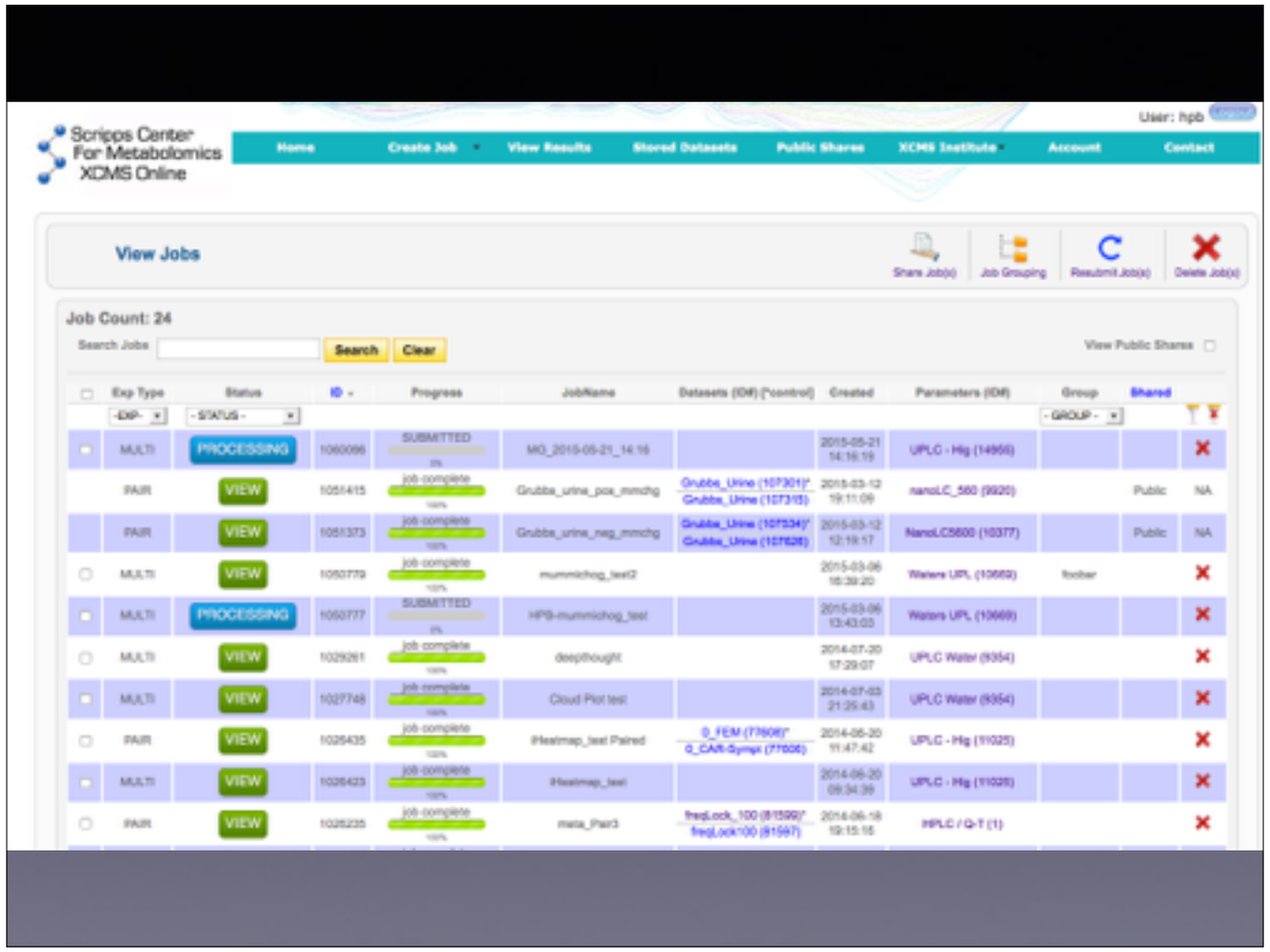
Reset
Dataset 1
Dataset 2
Parameters
Dataset 1 ID: 109417
Dataset 1 no. of files: 4
Dataset 1 Name:
2_CF
Edit
1: HPLC / Q-TOF (1)
Confirm Job Specifications
Job Details: (Submitted for USER #16)
Name: PAIR_2015-06-03_18:02 (ID# 1061675)
Dataset 1 (control): 2_CF (ID# 109417). Files: 4
Dataset 2: 1_CF (ID# 109416). Files: (uploading)
Parameter Set: HPLC / Q-TOF (ID# 1)
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
Job ID: 1061675
Owner: 16 : test
Job Name: PAIR_2015-06-03_
Edit
Dataset 1: 2_CF
(control)
Dataset 2: 1_CF
Parameter Set: 1: HPLC / Q-TOF (
Submit
Click here to complete your job
Submit Job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Job Count: 24
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Exp Type
Status
ID
Progress
JobName
Datasets (DB) ["control]
Created
Parameters (DB)
Group
Shared
-EXP-
- STATUS -
- GROUP -
MULTI
PROCESSING
SUBMITTED
VIEW
PAIR
job complete
Grubbs_urine_pos_mmchg
Grubbs_urine_neg_mmchg
mummichog_test2
HPB-mummichog_test
deepthought
Cloud Plot test
Heatmap_test Paired
Heatmap_test
meta_Pair3
UPLC - Hg (14966)
nanoLC_560 (9920)
NanoLC5600 (10377)
Waters UPL (10669)
UPLC Water (9354)
UPLC - Hg (11025)
HPLC / Q-T (1)
Public
NA

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Job ID: 1051415
Job Name: Grubbs_urine_pos_mnchg
Create Date: 2015-03-12 19:11:09
Parameter (ID#) nanoLC_5600_TripleTOF (9920)
Log: View Log
Finish Date: 2015-03-12 20:06:48
Status: job complete (See Warnings)
Total Aligned Features: 2,058
Experiment Type: Pairwise
Datasets Used: Grubbs_UrineGroup1_PosMode(ID#1073431) * vs. Grubbs_UrineGroup2_PosMode(ID#1073115)
Paired Samples: False
Share Status: Shared with 1 User(s) | Stop sharing!
2015-03-12 20:03:42 : HeatMap data prep, memory requires limiting to top 1000 features <0.293796 p-values
VIEW RESULTS TABLE
INTERACTIVE CLOUD PLOT
PCA
INTERACTIVE HEATMAP
CONNECTIONS
DOWNLOAD RESULTS
hash: 5f5897a444b54f10a7ac933a886f1a77c
Total Ion Chromatograms (original)
Retention Time Deviation vs. Retention Time
Total Ion Chromatograms (corrected)
PNG PDF
PNG PDF
PNG PDF
PNG PDF SVG
Interactive Version
PNG PDF
PNG PDF
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Quick Compound Search: Search Clear

JobID1551415 : Grubba_urine_pos_mmchg

Columns | Hide isotopic peaks | Page 1 of 21 | 100 | View 1 - 100 of 2,058

Feature	fold chang	p-value	UP/DOWN	m/z	retention time	MaxInt	Ctrl(E)	Exp(E)	isotopes	adducts	feature g	Notes
1	3.0	5.33087e-(	DOWN	204.1446	11.55	8,367	61,606	20,590			38	
2	1.5	6.94626e-(	UP	567.2266	13.99	3,858	21,603	31,736		[M+Na]+	9	
3	6.5	2.04304e-(	DOWN	257.1582	8.75	13,544	108,889	12,876		[M+H-H2O]	53	
4	3.8	2.44253e-(	DOWN	234.1553	11.74	8,264	71,894	19,157		[M+H-CH3	57	
5	2.2	6.72076e-(	DOWN	345.1104	10.74	5,082	44,308	20,112			33	
6	1.8	1.03879e-(	UP	377.1435	11.91	160,143	501,472	909,410	[69][M]+		16	
7	1.3	2.79905e-(	DOWN	181.0589	11.24	148,137	925,013	715,125			14	
8	1.5	4.09600e-(	UP	193.4786	13.99	4,468	20,927	32,018			4	
9	2.5	4.56496e-(	DOWN	249.1814	19.42	3,787	68,040	26,914			136	
10	1.8	5.57117e-(	DOWN	390.1744	12.87	3,108	43,753	23,898		[M+K+NH	148	
11	1.6	6.06996e-(	UP	425.1022	13.61	2,843	16,840	27,629		[2M+K]+	11	
12	2.3	6.40652e-(	DOWN	549.3642	16.16	2,285	14,390	6,283	[134][M]+	[3M+2Na-(	24	
13	12.0	6.81485e-(	DOWN	264.1574	20.80	13,532	78,586	6,567			71	
14	12.8	7.42942e-(	DOWN	216.1570	19.07	14,665	190,443	14,860			112	
15	1.7	8.21184e-(	DOWN	60.0598	4.07	3,251	24,935	14,491			55	
16	14.1	8.97905e-(	DOWN	248.1283	18.35	9,604	80,675	5,712		[M+2H-NH	120	
17	1.9	0.00001	DOWN	303.2159	12.42	29,542	149,101	76,604		[M+K]+	26	78
18	1.4	0.00001	UP	218.0802	13.64	9,404	61,598	86,497			43	
19	2.0	0.00001	UP	387.1564	13.59	97,540	314,443	626,870	[73][M]+	[2M+H]+	114	
20	1.8	0.00001	UP	388.1631	13.59	24,007	87,967	158,940	[73][M+1]+		4	
21	6.9	0.00001	DOWN	185.1617	11.11	12,691	65,866	9,478			41	
22	1.4	0.00002	DOWN	337.1529	11.68	6,223	66,295	63,571		[M+K]+	29	100
23	1.5	0.00002	UP	79.0393	13.99	19,510	97,724	148,525			4	
24	1.3	0.00002	UP	411.1241	13.59	2,843	19,391	25,843	[83][M+1]+		4	
25	1.3	0.00002	DOWN	263.1011	12.14	101,023	840,335	634,440	[36][M]+	[M+Na]+	2	34
26	1.5	0.00002	DOWN	445.2751	15.94	3,149	25,110	16,276			11	
27	1.3	0.00002	DOWN	264.1037	12.16	15,074	131,618	102,419	[36][M+1]+		34	
28	1.8	0.00002	DOWN	466.0050	7.27	1,318	11,278	6,279		[M+H-NH3	10	
29	1.9	0.00002	DOWN	325.2067	17.02	21,176	139,795	73,202			99	
30	23.2	0.00002	DOWN	230.1724	20.64	17,858	153,667	8,623			105	

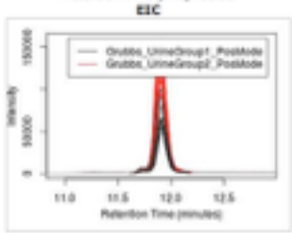
Columns | Export | Page 1 of 21 | 100 | View 1 - 100 of 2,058

Return to Job Summary

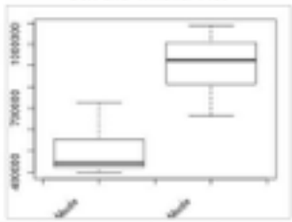
Please click on a row to view feature details

Feature #6
m/z : 377.1435
Retention Time (min): 11.91

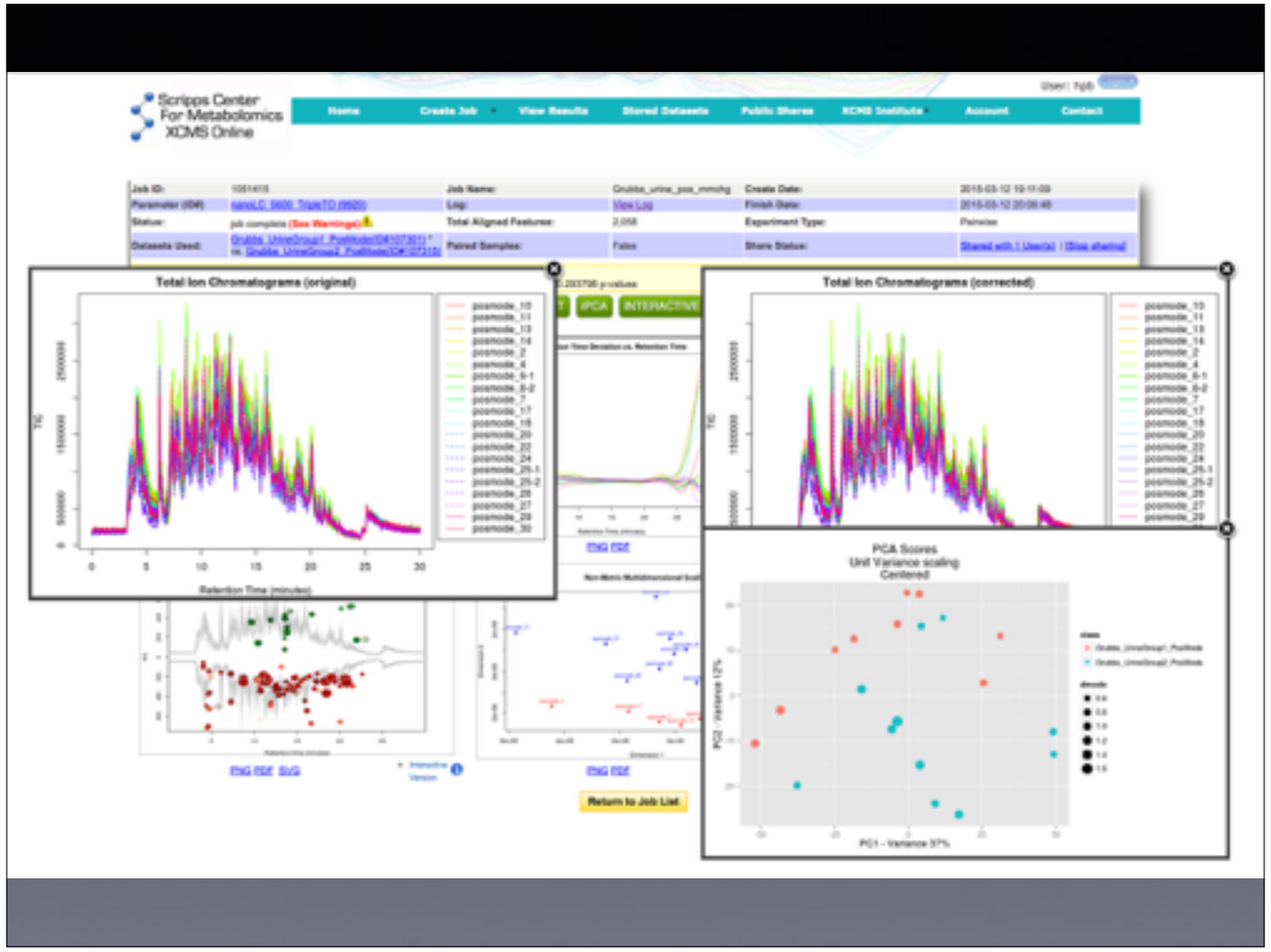
EIC



Box-and-Whisker Plot



PPM	Name	Adduct	COMPOSI
2	Loganate	M+H	44647
2	(1R5,2R5)-Guaiacyl(	M+H	89156
2	(1x,2x)-Guaiacylglyox	M+H	89157
2	(1x,2x)-Guaiacylglyox	M+H	95080
4	Propiomazine hydroc	M+H	88637
5	Ethynylestradiol 3-su	M+H	1171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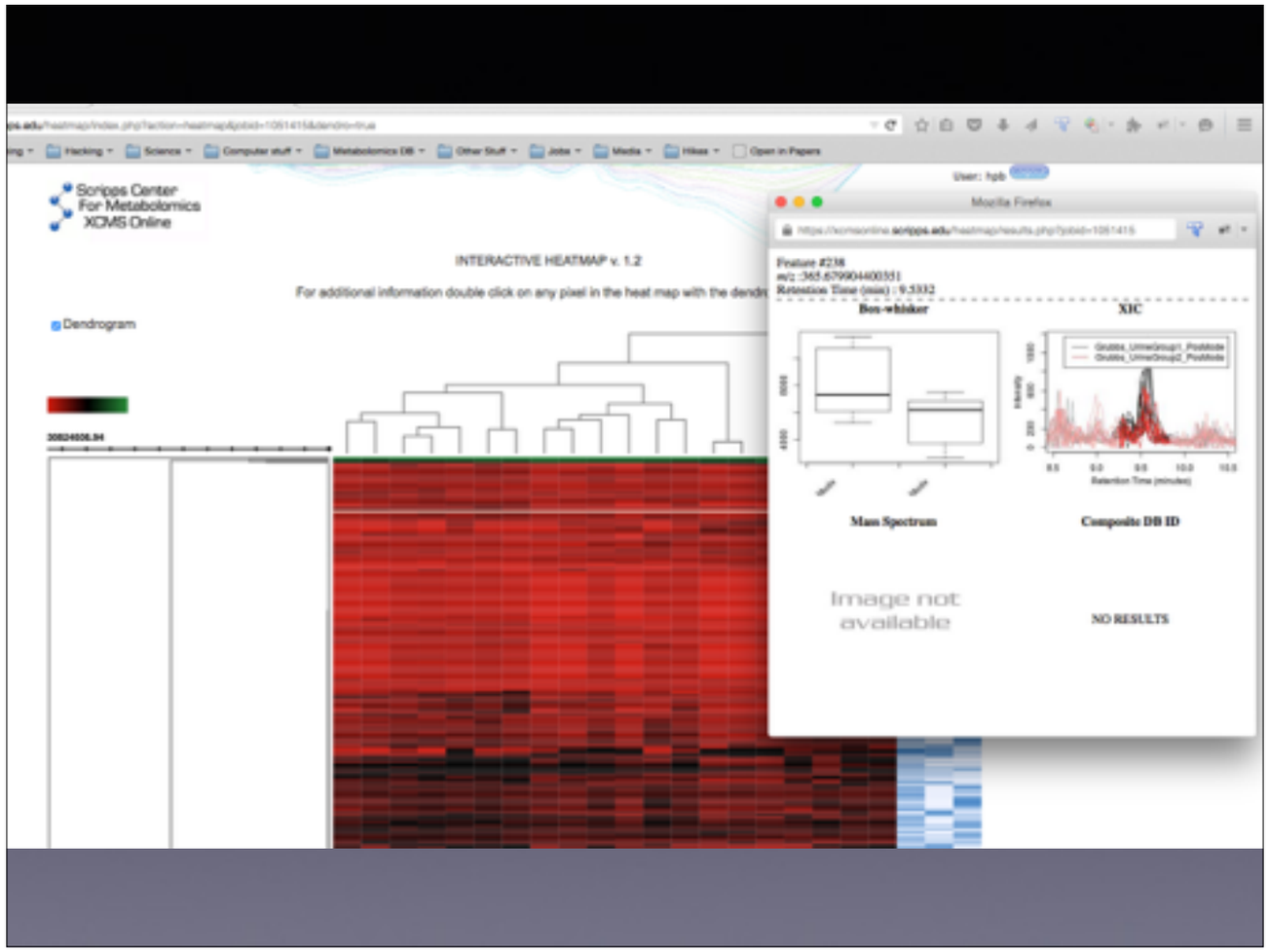
Total Ion Chromatograms (original)
Total Ion Chromatograms (corrected)
Retention Time (minutes)
TIC
PCA Scores
Unit Variance scaling
Centered
PC1 - Variance 57%
PC2 - Variance 12%
PNG PDF SVG
Return to Job List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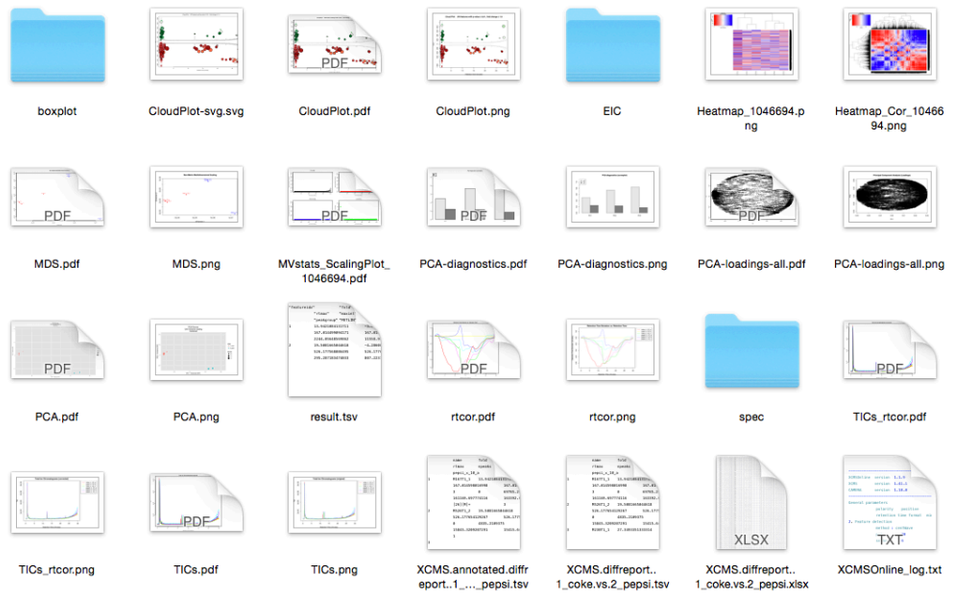
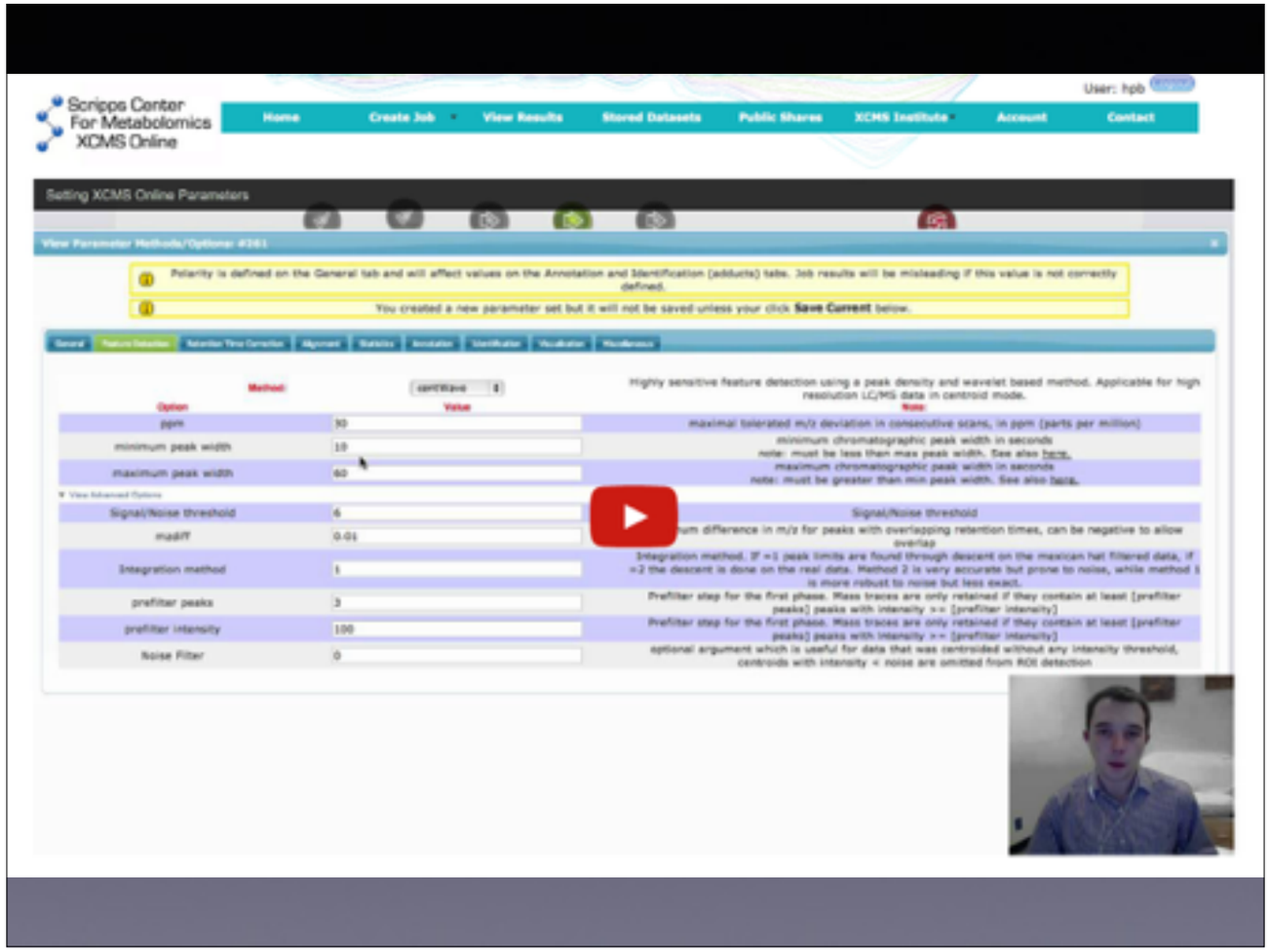
INTERACTIVE HEATMAP v. 1.2
Dendrogram
Mozilla Firefox
Feature #238
Retention Time (min) : 9.5332
Box-whisker
XIC
Mass Spectrum
Composite DB ID
Image not
available
NO RESULTS



Contents of results.zip file
XCMS.diffreport. And XCMS.annotated.diffreport are the data tables with all the intensity values associated with them not results.tsv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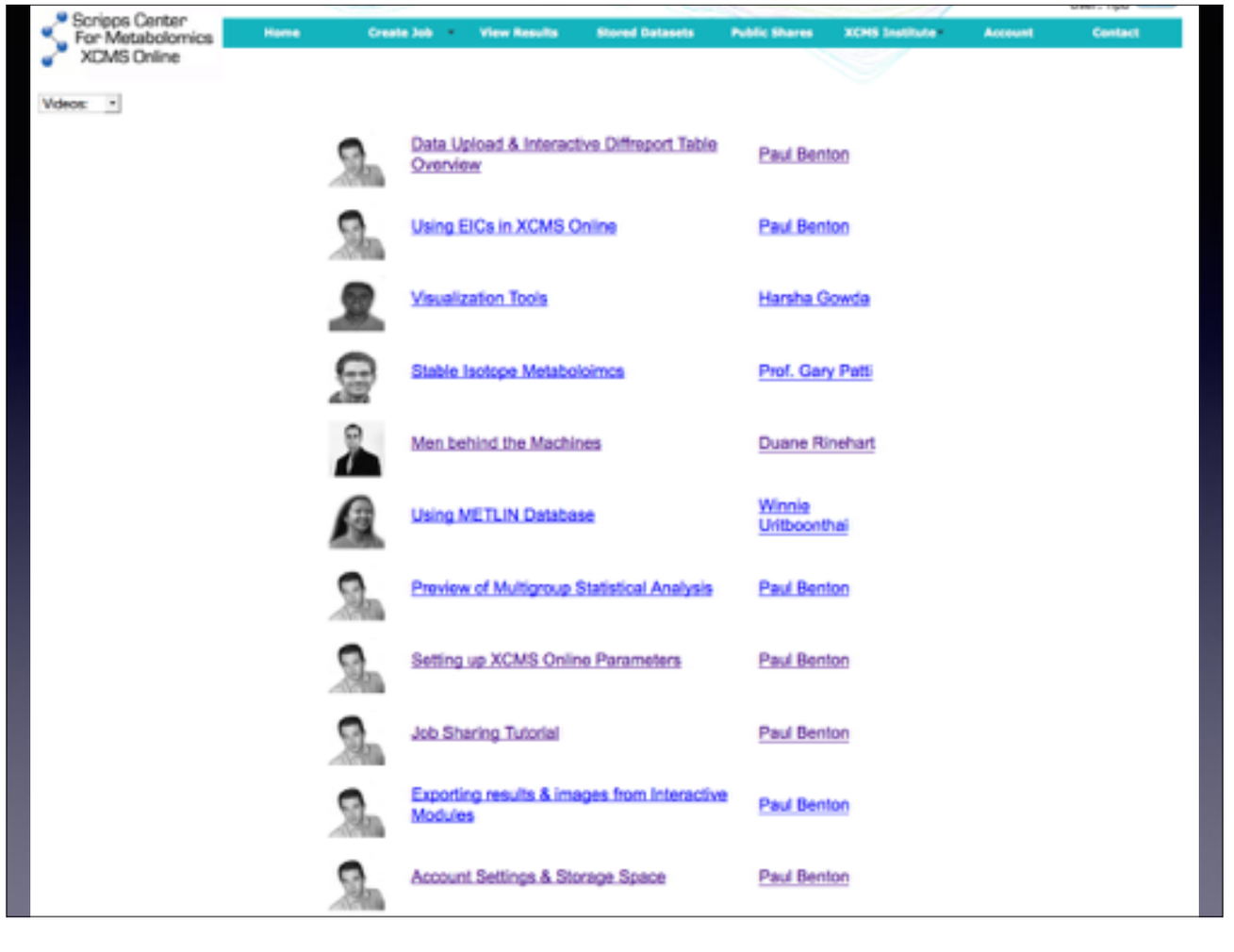
Setting XCMS Online Parameters
Polarity is defined on the General tab and will affect values on the Annotation and Identification (adducts) tabs. Job results will be misleading if this value is not correctly defined.
You created a new parameter set but it will not be saved unless your click Save Current below.
Highly sensitive feature detection using a peak density and wavelet based method. Applicable for high resolution LC/MS data in centroid mode.
Option
Value
Note
ppm
30
maximal tolerated m/z deviation in consecutive scans, in ppm (parts per million)
minimum peak width
10
minimum chromatographic peak width in seconds
note: must be less than max peak width. See also here.
maximum peak width
60
maximum chromatographic peak width in seconds
note: must be greater than min peak width. See also here.
Signal/Noise threshold
6
Signal/Noise threshold
mzdiff
0.01
Integration method
1
prefilter peaks
3
prefilter intensity
100
Noise Filter
0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Stable Isotope Metaboloimcs
Prof. Gary Patti
Men behind the Machines
Duane Rinehart
Using METLIN Database
Winnie Uritboonthai
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Setting up XCMS Online Parameters
Paul Benton
Job Sharing Tutorial
Paul Benton
Exporting results & images from Interactive Modules
Paul Benton
Account Settings & Storage Space
Paul Benton

Thank you :)

- Questions?

Gary Siuzdak

Duane Rinehart

Aries
Aisporna

The whole
xcms team