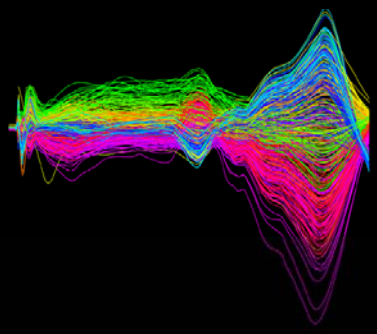
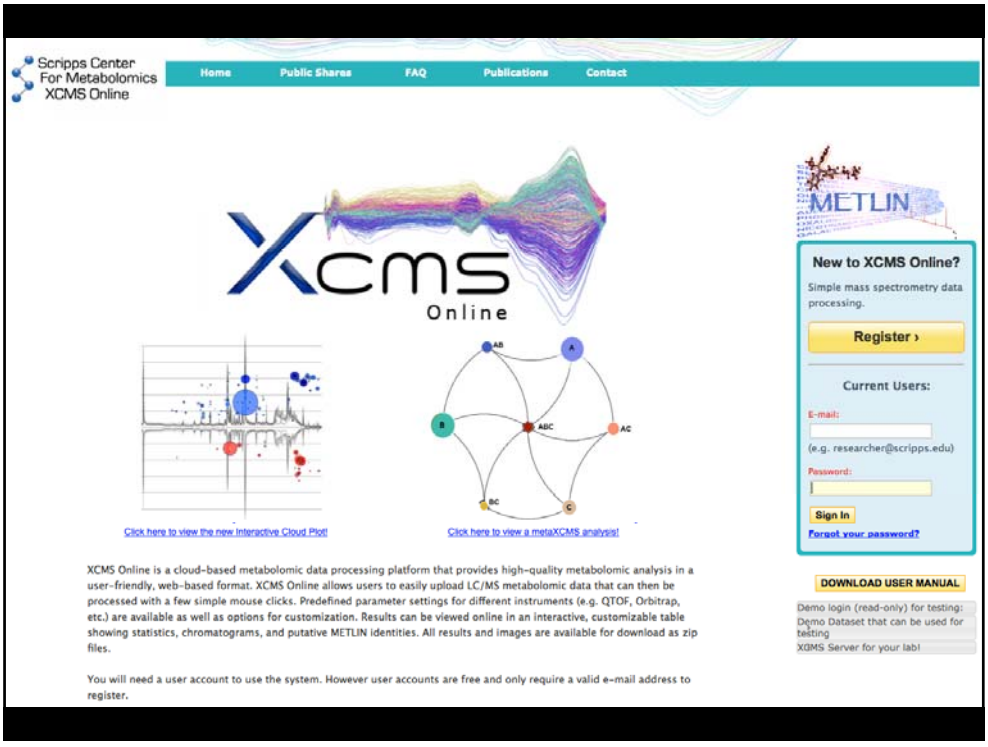
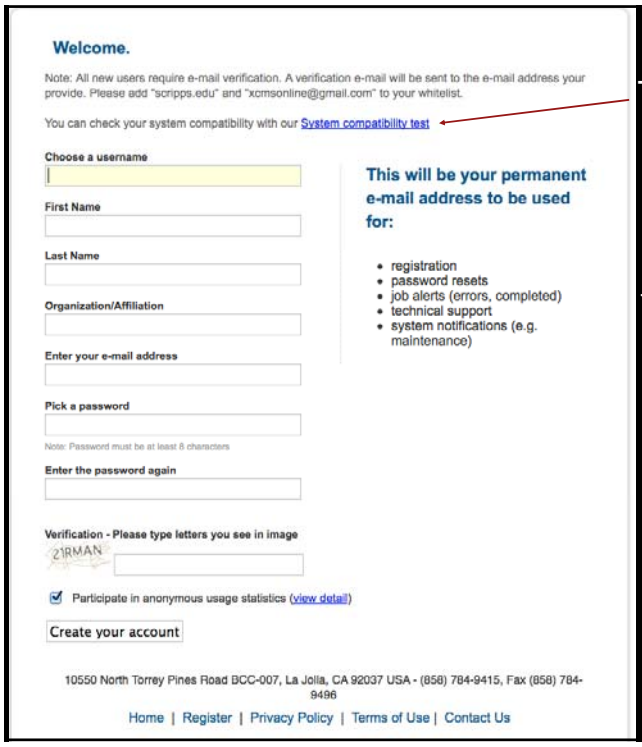
XCMS Online



H. Paul Benton

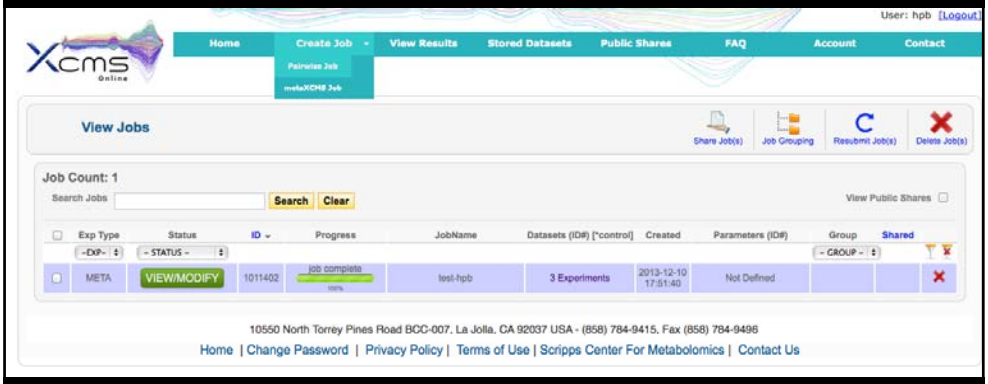


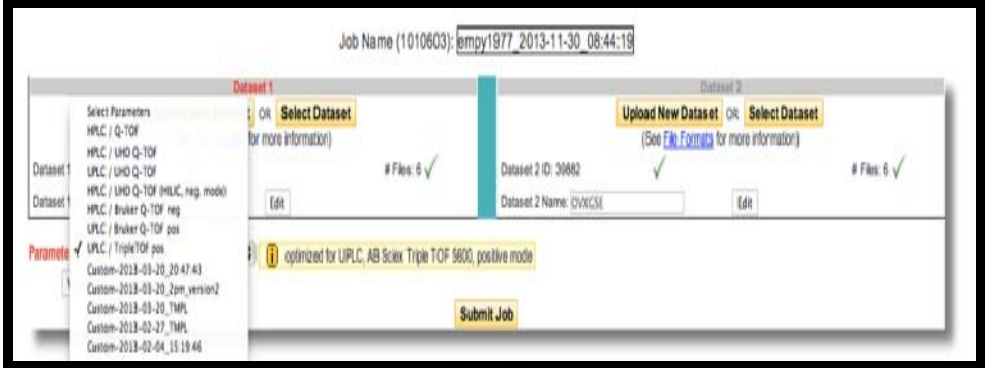


Test your browser

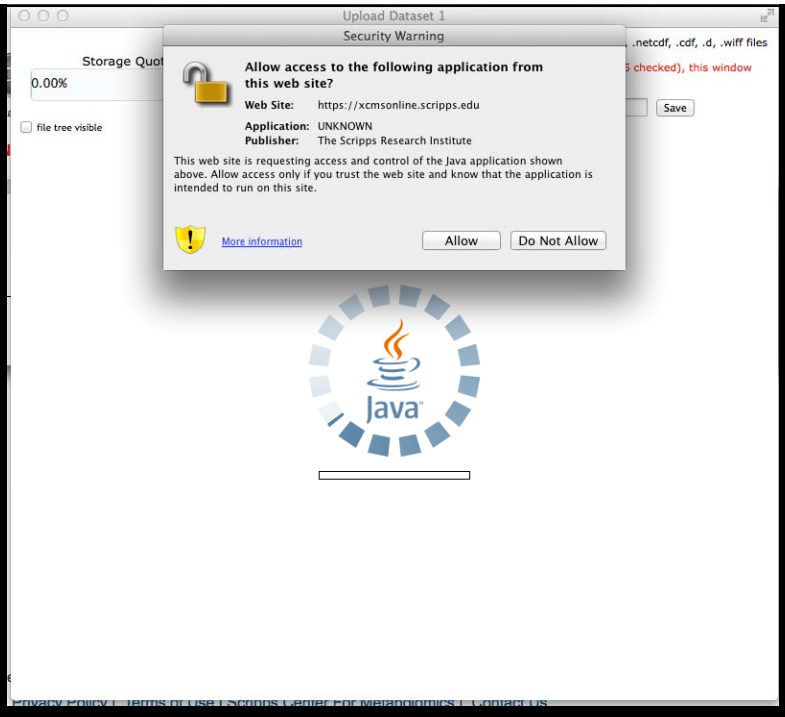
Mac users should use Firefox as it lets you use java

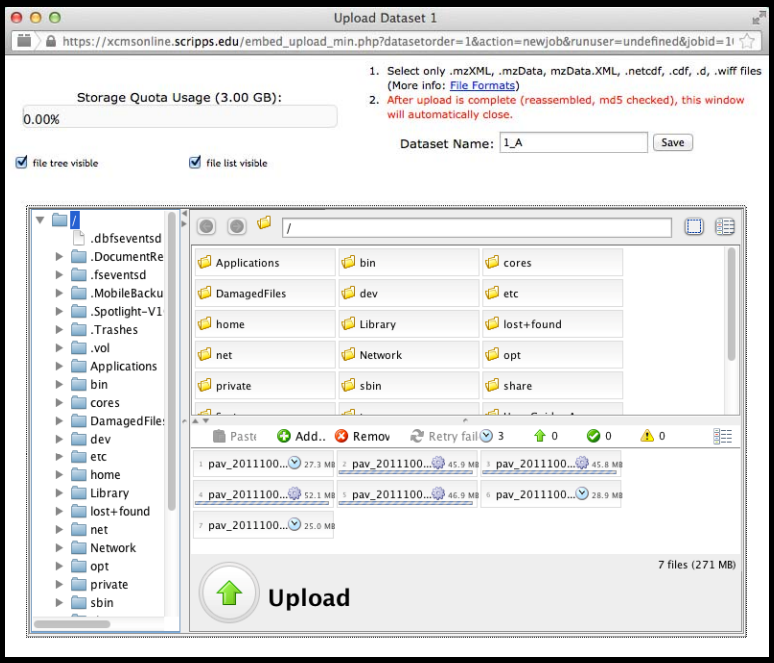
Windows users are recommend to use IE or Firefox

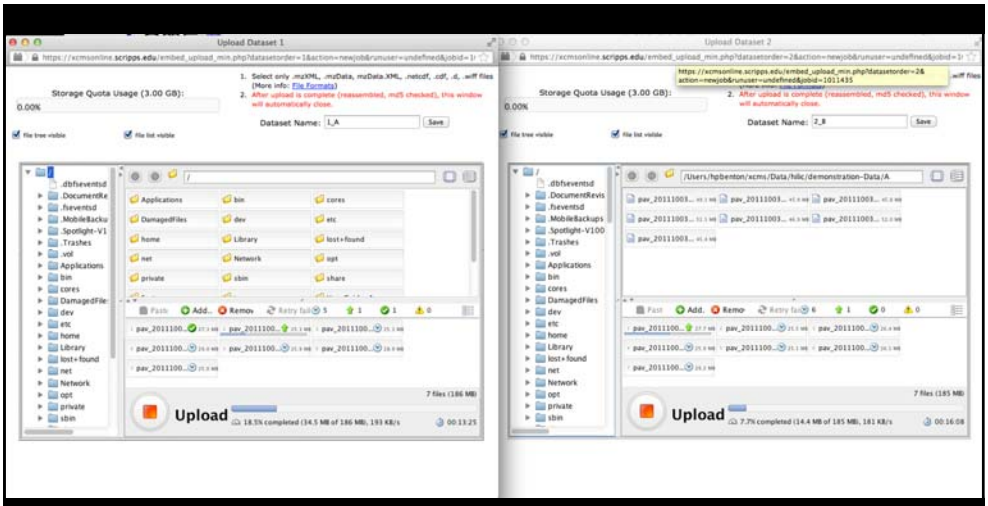




- This lets you do a pair wise analysis where you have 2 classes
- Parameter setting are fully customisable

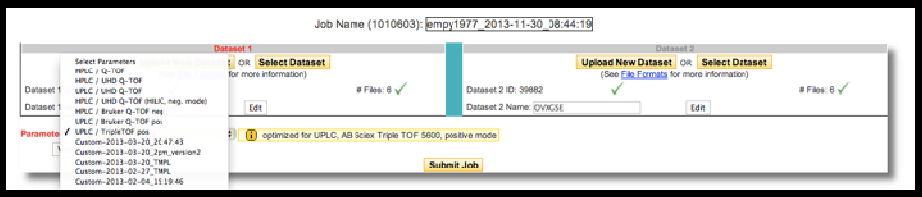




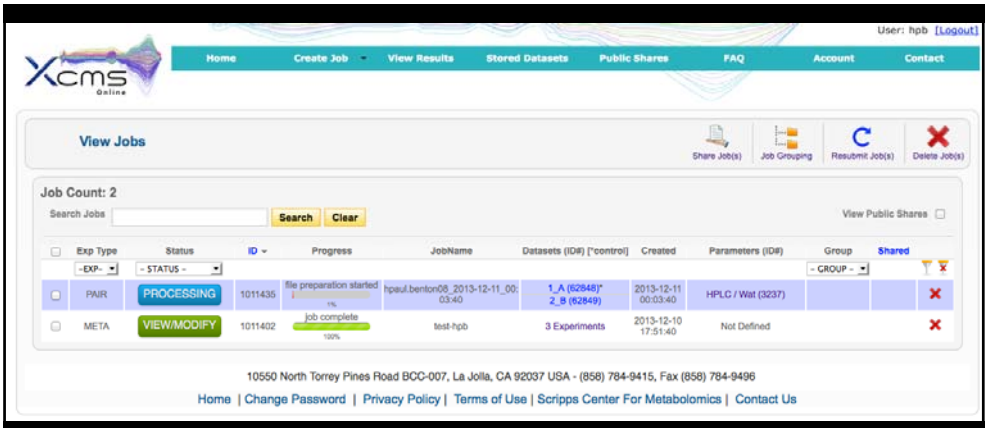


- Have 2 running at once to speed things up
- Increased speed is around the corner
  - Using an Aspera licence to stream data
- Check out xcms Server as well for local server support

Parameter selection

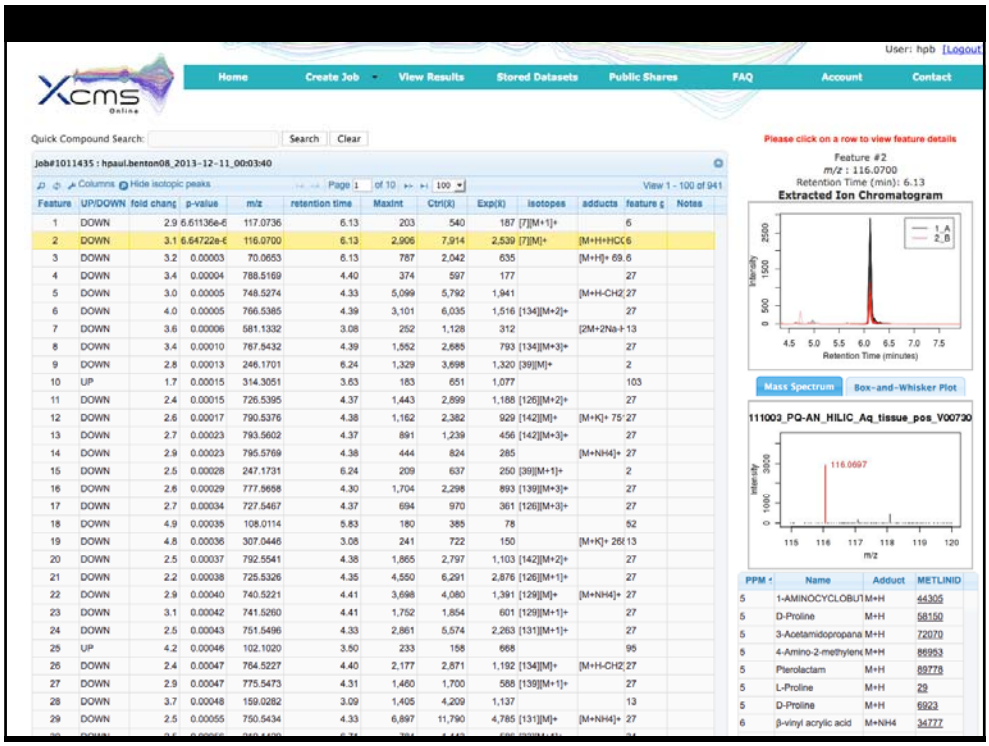


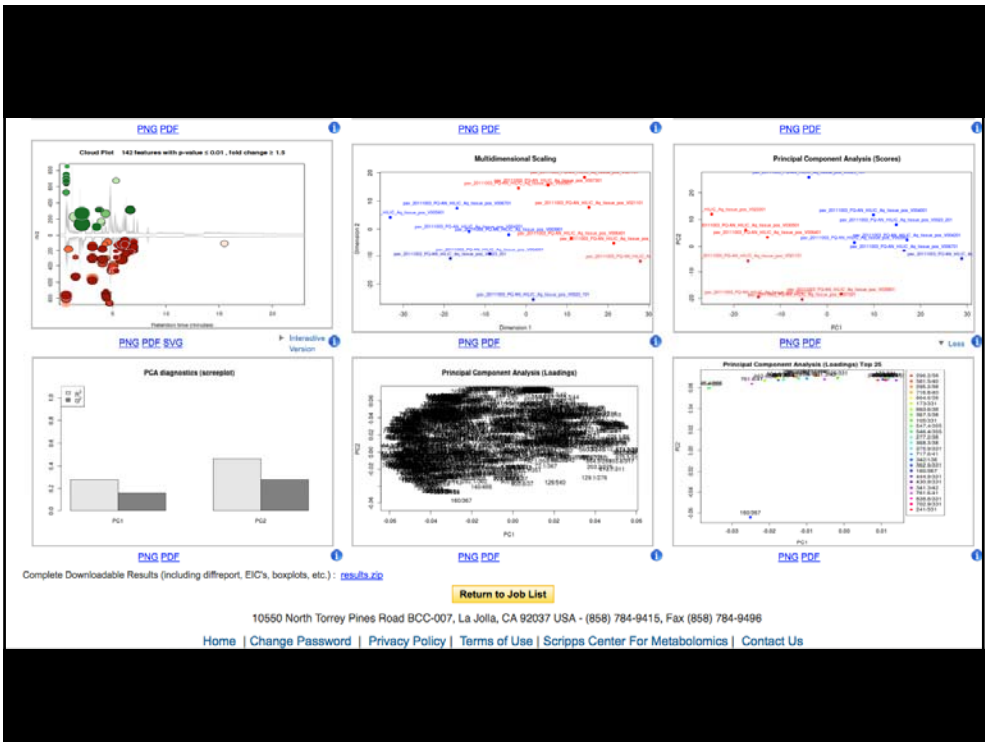
- Use drop down box under “Parameters”
- Select “UPLC/TripleTOF” - or preferred setting
- Make sure you get the parameter settings you want
  - Check the parameter setting by clicking custom



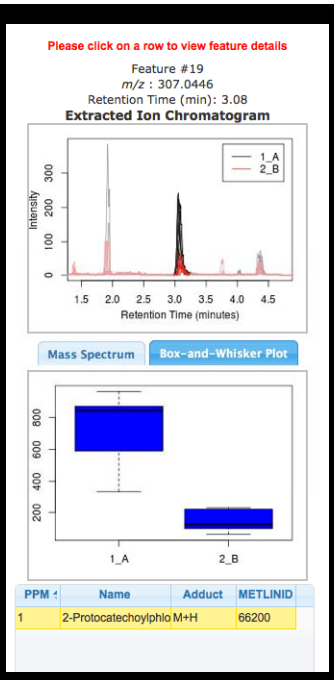
- File types:
- Converted - mzXML, mzData, netCDF (CDF), mzML (new)
- Vendors - Agilent, Waters, Thermo, AB Sciex, Bruker
  - Online does the converting for you!


User: hpb [Logout]
Home
Create Job
View Results
Stored Datasets
Public Shares
FAQ
Account
Contact
Job ID: 1011435
Job Name: hpaul.benton08_2013-12-11_00:03:40
Create Date: 2013-12-11 00:03:40
Parameter (ID#) HPLC / Waters TOF (3237)
Log: View Log
Finish Date: 2013-12-11 00:45:22
Status: job complete (See Warnings)
Total Aligned Features: 941
Experiment Type: Pairwise
Datasets Used: 1_A(ID#62846) * vs. 2_B(ID#62849)
Paired Samples: False
Share Status: Not Shared
2013-12-11 00:33:47 : Correction of mass calibration gaps failed (stitch). Processing data without correction.
BROWSE RESULT TABLE
INTERACTIVE CLOUD PLOT
Total Ion Chromatograms (original)
Retention Time Deviation vs. Retention Time
Total Ion Chromatograms (corrected)
PNG PDF
PNG PDF
PNG PDF
Cloud Plot 142 features with p-value ≤ 0.01 , fold change ≥ 1.5
Multidimensional Scaling
Principal Component Analysis (Scores)
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

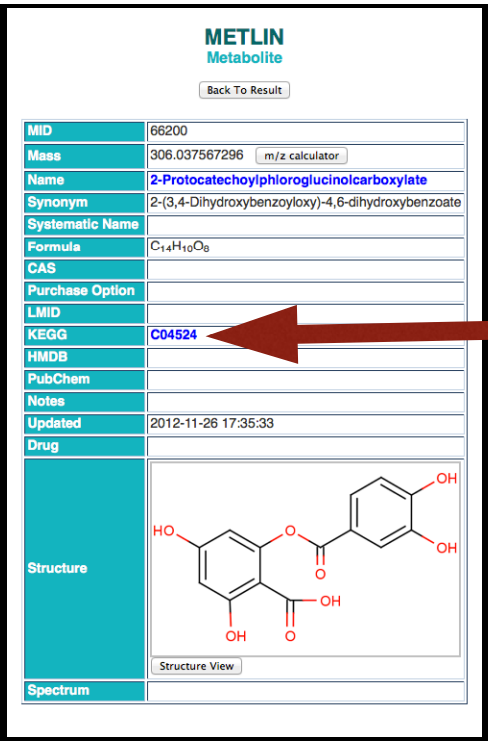

User: hpb [Logout]
Home
Create Job
View Results
Stored Datasets
Public Shares
FAQ
Account
Contact
Quick Compound Search:
Search
Clear
Job#1011435 : hpaul.benton08_2013-12-11_00:03:40
Columns
Hide isotopic peaks
Page 1 of 10
100
View 1 - 100 of 941
Feature | UP/DOWN | fold chang | p-value | m/z | retention time | MaxInt | Ctrl(k) | Exp(k) | isotopes | adducts | feature g | Notes
1 DOWN 2.9 6.61136e-6 117.0736 6.13 203 540 187 [7][M+1]+ 6
2 DOWN 3.1 6.64722e-6 116.0700 6.13 2,906 7,914 2,539 [7][M]+ [M+H+HCO 6
3 DOWN 3.2 0.00003 70.0653 6.13 787 2,042 635 [M+H]+ 69.6
4 DOWN 3.4 0.00004 788.5169 4.40 374 597 177 27
5 DOWN 3.0 0.00005 748.5274 4.33 5,099 5,792 1,941 [M+H-CH2 27
6 DOWN 4.0 0.00005 766.5385 4.39 3,101 6,035 1,516 [134][M+2]+ 27
7 DOWN 3.6 0.00006 581.1332 3.08 252 1,128 312 [2M+2Na-H 13
8 DOWN 3.4 0.00010 767.5432 4.39 1,552 2,685 793 [134][M+3]+ 27
9 DOWN 2.8 0.00013 246.1701 6.24 1,329 3,698 1,320 [39][M]+ 2
10 UP 1.7 0.00015 314.3051 3.63 183 651 1,077 103
11 DOWN 2.4 0.00015 726.5395 4.37 1,443 2,899 1,188 [126][M+2]+ 27
12 DOWN 2.6 0.00017 790.5376 4.38 1,162 2,382 929 [142][M]+ [M+K]+ 75 27
13 DOWN 2.7 0.00023 793.5602 4.37 891 1,239 456 [142][M+3]+ 27
14 DOWN 2.9 0.00023 795.5769 4.38 444 824 285 [M+NH4]+ 27
15 DOWN 2.5 0.00028 247.1731 6.24 209 637 250 [39][M+1]+ 2
16 DOWN 2.6 0.00029 777.5658 4.30 1,704 2,298 893 [139][M+3]+ 27
17 DOWN 2.7 0.00034 727.5467 4.37 694 970 361 [126][M+3]+ 27
18 DOWN 4.9 0.00035 108.0114 5.83 180 385 78 52
19 DOWN 4.8 0.00036 307.0446 3.08 241 722 150 [M+K]+ 26 13
20 DOWN 2.5 0.00037 792.5541 4.38 1,865 2,797 1,103 [142][M+2]+ 27
21 DOWN 2.2 0.00038 725.5326 4.35 4,550 6,291 2,876 [126][M+1]+ 27
22 DOWN 2.9 0.00040 740.5221 4.41 3,698 4,080 1,391 [129][M]+ [M+NH4]+ 27
23 DOWN 3.1 0.00042 741.5260 4.41 1,752 1,854 601 [129][M+1]+ 27
24 DOWN 2.5 0.00043 751.5496 4.33 2,861 5,574 2,263 [131][M+1]+ 27
25 UP 4.2 0.00046 102.1020 3.50 233 158 668 95
26 DOWN 2.4 0.00047 764.5227 4.40 2,177 2,871 1,192 [134][M]+ [M+H-CH2 27
27 DOWN 2.9 0.00047 775.5473 4.31 1,460 1,700 588 [139][M+1]+ 27
28 DOWN 3.7 0.00048 159.0282 3.09 1,405 4,209 1,137 13
29 DOWN 2.5 0.00055 750.5434 4.33 6,897 11,790 4,785 [131][M]+ [M+NH4]+ 27
Please click on a row to view feature details
Feature #2
m/z : 116.0700
Retention Time (min): 6.13
Extracted Ion Chromatogram
Intensity
Retention Time (minutes)
1_A
2_B
Mass Spectrum
Box-and-Whisker Plot
111003_PQ-AN_HILIC_Aq_tissue_pos_V00730
116.0697
Intensity
m/z
PPM | Name | Adduct | METLINID
5 1-AMINOCYCLOBUT M+H 44305
5 D-Proline M+H 58150
5 3-Acetamidopropana M+H 72070
5 4-Amino-2-methylene M+H 86953
5 Pterolactam M+H 89778
5 L-Proline M+H 29
5 D-Proline M+H 6923
6 β-vinyl acrylic acid M+NH4 34777

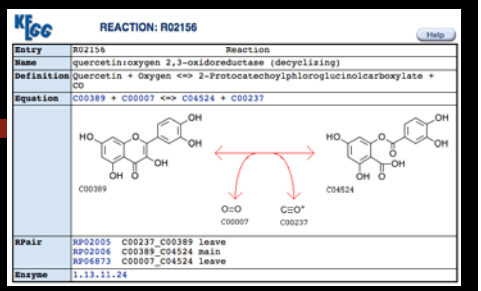

PNG PDF
Cloud Plot 142 features with p-value ≤ 0.01 , fold change ≥ 1.5
PNG PDF SVG
Interactive Version
PNG PDF
Multidimensional Scaling
PNG PDF
PNG PDF
Principal Component Analysis (Scores)
PNG PDF
Loss
PCA diagnostics (screeplot)
PNG PDF
PNG PDF
Principal Component Analysis (Loadings)
PNG PDF
PNG PDF
Principal Component Analysis (Loadings) Top 25
PNG PDF
Complete Downloadable Results (including diffreport, EIC's, boxplots, etc.) : results.zip
Return to Job List
10550 North Torrey Pines Road BCC-007, La Jolla, CA 92037 USA - (858) 784-9415, Fax (858) 784-9496
Home | Change Password | Privacy Policy | Terms of Use | Scripps Center For Metabolomics | Contact Us


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
Intensity
Retention Time (minutes)
Bubble Size Multiplier
22
Download Cloud Plot Manual
View 1
Retention Time vs m/z of 142 features
Click and drag in the plot area to zoom in
m/z : 269.106
retention time: 2.11 min
p-val : 0.00069
fold change : 32.900 (UP)
max intensity : 3202
0 matches found.
m/z
Retention Time (minutes)
Toggle Upregulated
Toggle Downregulated
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



- Clicking each feature gives an EIC with it's mass spectrum (highest intensity sample) and box plots.
- An automagicly generated METLIN link for the predicted mass within the ppm range specified in the parameter settings.

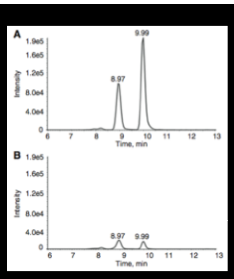




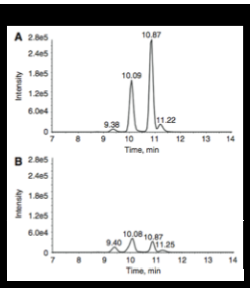
DE GRUYTER DOI 10.1515/hmbci-2013-0044 — Horm Mol Biol Clin Invest 2013; x(x): xxx–xxx

John K. Cutts, Thomas R. Peavy, Doyle R. Moore, Jeevan Prasain, Stephen Barnes and Helen Kim*

Ovariectomy lowers urine levels of unconjugated (+)-catechin, (–)-epicatechin, and their methylated metabolites in rats fed grape seed extract



Unconjugated catechins



Unconjugated 3-O-methyl catechins

Thank you :)

- Questions?
- 46 citations - http://pubs.acs.org/doi/abs/10.1021/ac300698c
- Many more updates coming soon including speed and more stats + Multi-class analysis

Duane Rinehart

Gary Siuzdak

The whole xcms team