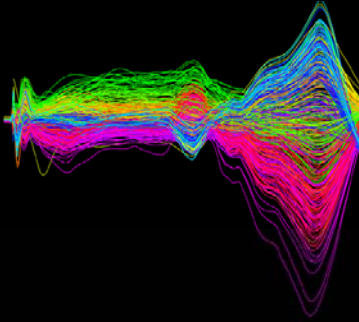


XCMS Online



H. Paul Benton

Scripps Center
For Metabolomics
XCMS Online

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XCMS Online

Click here to view the new Interactive Clout Plot

Click here to view a metaXCMS analysis!

XCMS Online is a cloud-based metabolomic data processing platform that provides high-quality metabolomic analysis in a user-friendly, web-based format. XCMS Online allows users to easily upload LC/MS metabolomic data that can then be processed with a few simple mouse clicks. Predefined parameter settings for different instruments (e.g. QTOF, Orbitrap, etc.) are available as well as options for customization. Results can be viewed online in an interactive, customizable table showing statistics, chromatograms, and putative METLIN identities. All results and images are available for download as zip files.

You will need a user account to use the system. However user accounts are free and only require a valid e-mail address to register.

NEW TO XCMS ONLINE?
Simple mass spectrometry data processing.

Register >

Current Users:

E-mail:
(e.g., researcher@scripps.edu)

Password:

Sign In

[Forgot your password?](#)

DOWNLOAD USER MANUAL

Demo login (read-only) for testing:
Demo Dataset that can be used for testing
XCMS Server for your lab!

Welcome.

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

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

Choose a username

First Name

Last Name

Organization/Affiliation


Enter your e-mail address

Pick a password

Note: Password must be at least 8 characters

Enter the password again

Verification - Please type letters you see in image



Participate in anonymous usage statistics ([view detail](#))

Create your account

10550 North Torrey Pines Road BCC-007, La Jolla, CA 92037 USA - (858) 784-9415, Fax (858) 784-9496

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Test your browser

Mac users should use Firefox as it lets you use java

Windows users are recommend to use IE or Firefox

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Xcms Online Home **Create Job** View Results Stored Datasets Public Shares FAQ Account Contact

Pairwise Job testXCMF Job

View Jobs [Share Job\(s\)](#) [Job Grouping](#) [Resubmit Job\(s\)](#) [Delete Job\(s\)](#)

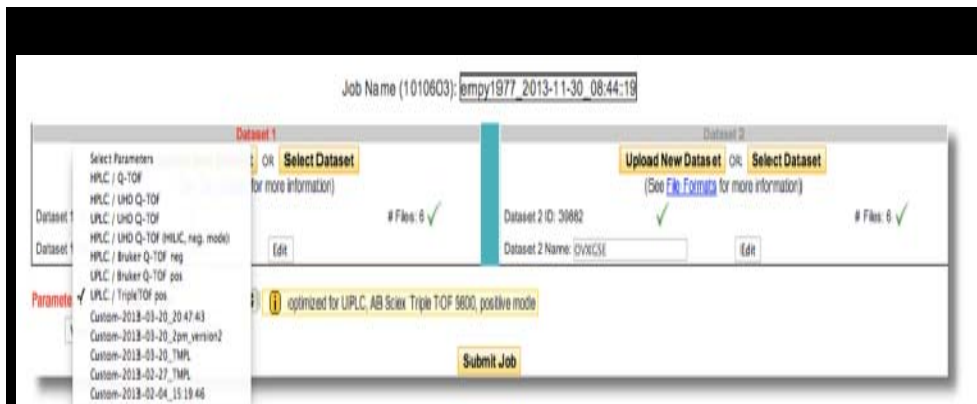
Job Count: 1

Search Jobs [Search](#) [Clear](#) [View Public Shares](#)

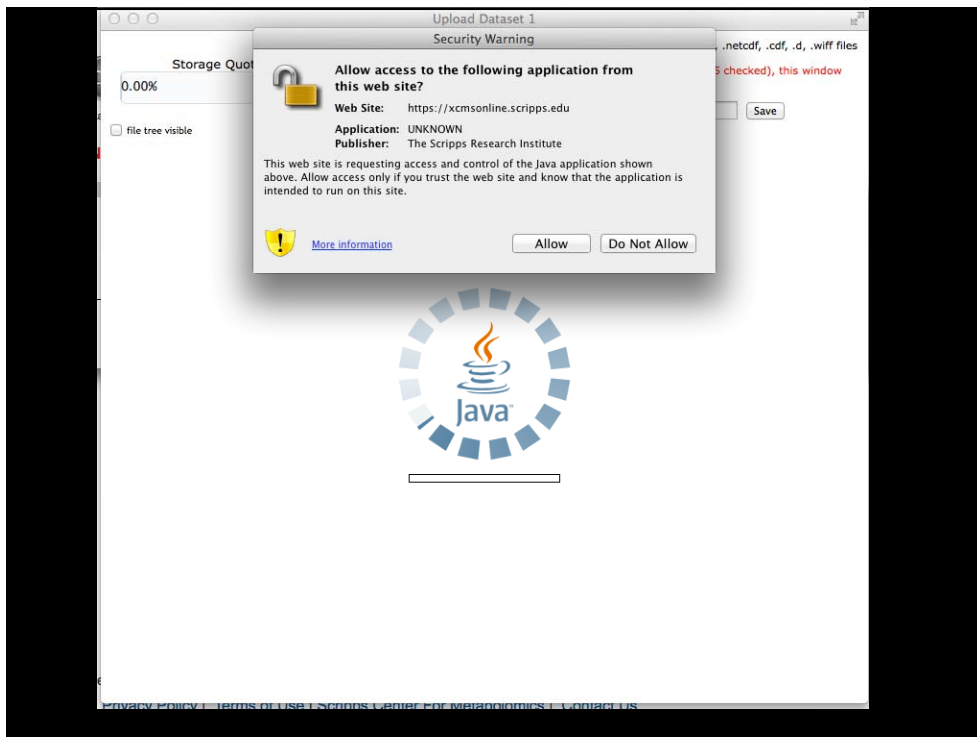
<input type="checkbox"/>	Exp Type	Status	ID	Progress	JobName	Datasets (ID#) [control]	Created	Parameters (ID#)	Group	Shared
<input type="checkbox"/>	META	VIEW/MODIFY	1011402	Job complete 100%	test-hpb	3 Experiments	2013-12-10 17:31:40	Not Defined		<input checked="" type="checkbox"/>

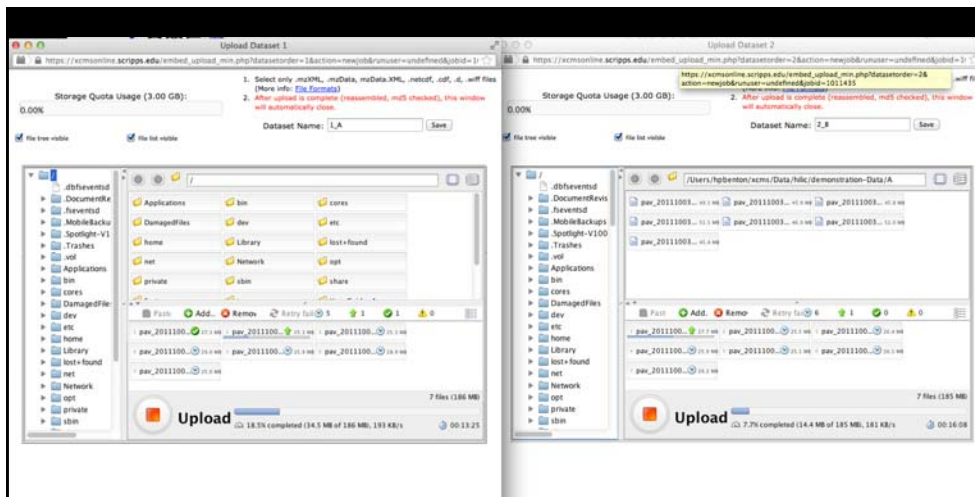
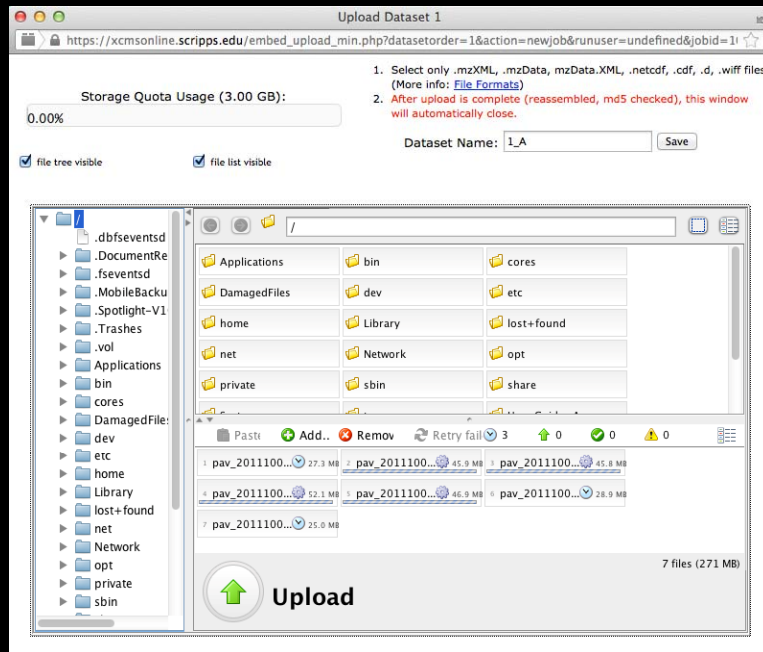
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- This lets you do a pair wise analysis where you have 2 classes
- Parameter setting are fully customisable





- 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

Job Name (1010603): temp1977_2013-11-30_08:44:19

Dataset 1

Select Parameters
 HPLC / Q-TOF
 HPLC / LHD Q-TOF
 HPLC / LHD Q-TOF (HPLC, neg. mode)
 HPLC / Bruker Q-TOF neg.
 HPLC / Bruker Q-TOF pos.
 HPLC / TripleTOF pos.
 Custom-2013-03-29_21:47:43
 Custom-2013-03-29_21m_version2
 Custom-2013-03-29_TMP
 Custom-2013-02-27_TMP
 Custom-2013-02-04_11:19:45

Dataset 2

Dataset 2 ID: 39902
 Dataset 2 Name: (VXGJ)

Files: 0 ✓

optimized for UPLC, AB Sciex Triple TOF 5600, positive mode

- 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

xcms Online

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User: hpb [Logout]

View Jobs

Share Job(s) Job Grouping Resubmit Job(s) Delete Job(s)

Job Count: 2

Search Jobs Search Clear View Public Shares

Exp Type	Status	ID	Progress	JobName	Datasets (ID#) [control]	Created	Parameters (ID#)	Group	Shared
PAIR	PROCESSING	1011435	file preparation started 100%	tpaul_benton08_2013-12-11_00:03:40	1_A (52944)* 2_B (62949)	2013-12-11 00:03:40	HPLC / Wat (3237)		✗
META	VIEW/MODIFY	1011402	job complete 100%	test-hpb	3 Experiments	2013-12-10 17:51:40	Not Defined		✗

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- 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](#)

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Quick Compound Search:

Job#1011435 : hpaui_benton08_2013-12-11_00:03:40

Columns: Hide Isotopic peaks Page 1 of 10 View 1 - 100 of 941

Feature	UP/DOWN	fold chang	p-value	m/z	retention time	MaxInt	ChI(X)	Exp(X)	Isotopes	adducts	feature c	Notes
1	DOWN	2.9	6.611356e-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]+	69.6	
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+13]		
8	DOWN	3.4	0.00010	767.5432	4.39	1,852	2,685	793	[134]M+3+		27	
9	DOWN	2.8	0.00013	246.1701	6.24	1,329	3,898	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	777.5698	4.30	1,704	2,298	893	[139]M+3+		27	
17	DOWN	2.7	0.00034	727.5487	4.37	694	970	361	[126]M+3+		27	
18	DOWN	4.9	0.00035	108.0114	5.83	180	385	78			82	
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	2,676	[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+3+		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	3.90	233	188	668			96	
26	DOWN	2.4	0.00047	764.5227	4.40	2,177	2,671	1,192	[134]M+	[M+H-CH2]+	27	
27	DOWN	2.9	0.00047	775.5473	4.31	1,460	1,700	588	[138]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

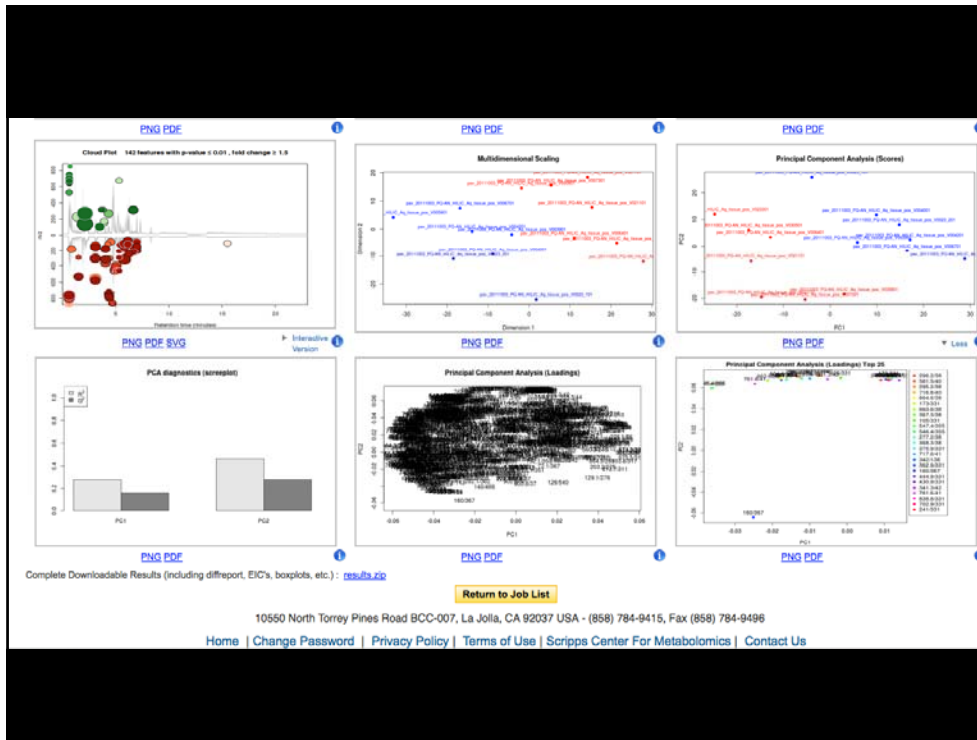
Extracted Ion Chromatogram

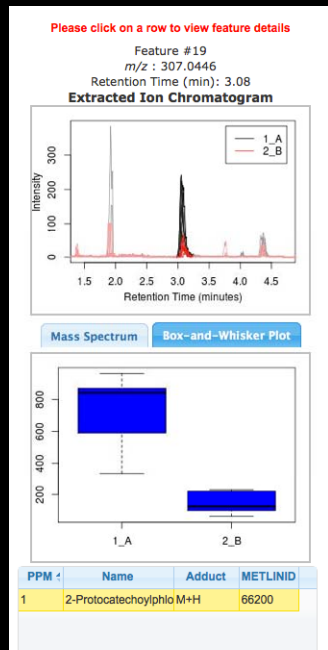
Mass Spectrum **Box-and-Whisker Plot**

111003_PQ-AN_HILIC_Aq_tissue_pos_V00730

PPM Name Adduct METLINID

5	1-AMINOCYCLOBUTM+H	M+H	44305
5	D-Proline	M+H	58150
5	3-Acetamidopropans M+H	M+H	72070
5	4-Amino-2-methylens M+H	M+H	86953
5	Pteridactam	M+H	89278
5	L-Proline	M+H	89
5	D-Proline	M+H	6923
6	β-vinyl acrylic acid	M+NH4	34772





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

METLIN
Metabolite

[Back To Result](#)

MID	66200
Mass	306.037567296 m/z calculator
Name	2-Protocatechylphloroglucinolcarboxylate
Synonym	2-(3,4-Dihydroxybenzoyloxy)-4,6-dihydroxybenzoate
Systematic Name	
Formula	C ₁₄ H ₁₀ O ₈
CAS	
Purchase Option	
LMID	
KEGG	C04524
HMDB	
PubChem	
Notes	
Updated	2012-11-26 17:35:33
Drug	
Structure	
Spectrum	

REACTION: R02156

Entry: R02156 Reaction

Name: quercetin:oxygen 2,3-oxidoreductase (decyclizing)

Definition: Quercetin + Oxygen <=> 2-Protocatechylphloroglucinolcarboxylate + CO

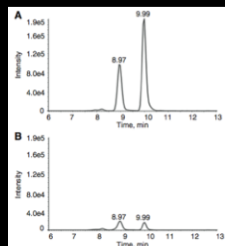
Equation: C00389 + C00007 <=> C04524 + C00237

HPair: RPO2005 C00237 C00389 leave
 RPO2006 C00389 C04524 main
 RPO6973 C00007 C04524 leave

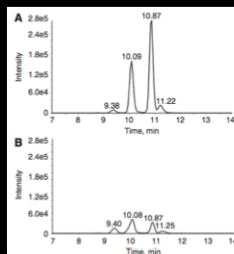
Enzyme: 1.13.11.34

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