

# USING AND UPLOADING TO XCMS ONLINE

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H. PAUL BENTON

## WHAT IS XCMS ONLINE?

- ▶ A Cloud based graphical interface to xcms
- ▶ Allows for multiple types of job analysis
- ▶ Multiple statistical analysis on the back end
- ▶ Additional tools to interact with data from just xcms

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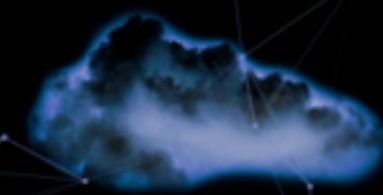
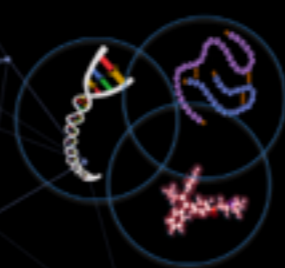
hpb

\*\*\*\*\*

[Login](#)

# XCMS

*The original and most widely used metabolomic platform*



## Statistics

XCMS has a unique graphical user interface that allows users to dig

## Systems Biology

XCMS allows users to perform pathway analyses directly from their

## Metlin

A goal for all metabolomic experiments is to identify metabolites,

## Your Personal Cloud

**XCMS<sup>plus</sup> is a personal cloud for high throughput metabolomics**

# 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).**



**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)

Participate in anonymous usage statistics ([View Details](#))

### View Jobs

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

Job Count: 43

Search Jobs

View Public Shares

<input type="checkbox"/>	Exp Type	Status	ID	Progress	JobName	Datasets (ID#) [*control]	Created	Parameters (ID#)	Group	Shared		
	-EXP-	-STATUS-										
<input type="checkbox"/>	MULTI	<a href="#">VIEW</a>	1110945	job complete 100%	MG_2016-05-17_10:52		2016-05-17 10:52:09	HPLC / Q-T (1)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<a href="#">VIEW</a>	1108694	job complete 100%	pair_2016-05-03_09:42		2016-05-03 09:42:26	HPLC / Q-T (1)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<a href="#">VIEW</a>	1103632	job complete 100%	MG_2016-04-01_10:55		2016-04-01 10:55:52	HPLC / Q-T (1)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<a href="#">VIEW</a>	1099046	job complete 100%	pair_2016-03-02_14:33	Pos-Pregna (#73122) Pos-Notpre (#73124)	2016-03-02 14:33:56	UPLC - Hig (11025)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<b>ERROR</b>	1097687	XCMS processing failed. 45%	MG_2016-02-24_16:41	0_QC4 (#77616) 0_QC3 (#77615) 0_QC2 (#77614)	2016-02-24 16:41:11	UPLC - Hig (14955)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<a href="#">VIEW</a>	1097668	job complete 100%	pair_2016-02-24_14:54	0_CAR-Symp (#77606) 0_CAR-Asym (#77605)	2016-02-24 14:54:24	HPLC / Q-T (1)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<a href="#">VIEW</a>	1096093	job complete 100%	MG_2016-02-17_00:13	servier_SU (#126053) servier_SU (#126052) servier_SU (#126051)	2016-02-17 00:13:26	HPLC / Q-T (1)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<a href="#">VIEW</a>	1096092	job complete 100%	pair_2016-02-17_00:12	servier_SU (#126053) servier_SU (#126050)	2016-02-17 00:12:33	HPLC / Q-T (1)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<a href="#">VIEW</a>	1095632	job complete 100%	MG_2016-02-12_19:07	Pos-Notpre (#73124) Pos-QC (#73123) Pos-Pregna (#73122)	2016-02-12 19:07:10	UPLC - Hig (14955)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<a href="#">VIEW</a>	1094304	job complete 100%	pair_2016-02-03_09:16	servier_SU (#126052) servier_SU (#126051)	2016-02-03 09:16:46	UPLC Water (9354)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<a href="#">VIEW</a>	1094204	job complete 100%	pair_2016-02-02_12:33	0_INT-CAR- (#77610) 0_INT-CAR- (#77611)	2016-02-02 18:19:54	HPLC / Q-T (1)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<a href="#">VIEW</a>	1089754	job complete 100%	MG_2015-12-28_10:58	servier_SU (#126053) servier_SU (#126052) servier_SU (#126051)	2015-12-28 10:58:21	HPLC / UHD (2)			<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<a href="#">VIEW</a>	1088498	job complete 100%	MG_2015-12-16_11:19	Pos-Notpre (#73124) Pos-QC (#73123) Pos-Pregna (#73122)	2015-12-16 11:19:11	Waters UPL (10669)		Shared [Stop sharing]	<input type="checkbox"/>	<input type="checkbox"/>

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

### View Jobs

View Public Shares

Search Jobs

<input type="checkbox"/>	Exp Type	Status	ID	Progress	JobName	Parameters (ID#)	Group	Shared				
	-EXP-	-STATUS-					- GROUP -					
<input type="checkbox"/>	MULTI	<b>ERROR</b>	1097687	XCMS processing failed. 45%	MG_2016-02-24_16:41	0_QC3 (#77615) 0_QC2 (#77614)	2016-02-24 16:41:11	UPLC - Hig (14955)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<b>VIEW</b>	1097668	job complete 100%	pair_2016-02-24_14:54	0_CAR-Symp (#77606) 0_CAR-Asym (#77605)	2016-02-24 14:54:24	HPLC / Q-T (1)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<b>VIEW</b>	1096093	job complete 100%	MG_2016-02-17_00:13	servier_SU (#126053) servier_SU (#126052) servier_SU (#126051)	2016-02-17 00:13:26	HPLC / Q-T (1)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<b>VIEW</b>	1096092	job complete 100%	pair_2016-02-17_00:12	servier_SU (#126053) servier_SU (#126050)	2016-02-17 00:12:33	HPLC / Q-T (1)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<b>VIEW</b>	1095632	job complete 100%	MG_2016-02-12_19:07	Pos-Notpre (#73124) Pos-QC (#73123) Pos-Pregna (#73122)	2016-02-12 19:07:10	UPLC - Hig (14955)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<b>VIEW</b>	1094304	job complete 100%	pair_2016-02-03_09:16	servier_SU (#126052) servier_SU (#126051)	2016-02-03 09:16:46	UPLC Water (9354)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	PAIR	<b>VIEW</b>	1094204	job complete 100%	pair_2016-02-02_12:33	0_INT-CAR- (#77610) 0_INT-CAR- (#77611)	2016-02-02 18:19:54	HPLC / Q-T (1)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<b>VIEW</b>	1089754	job complete 100%	MG_2015-12-28_10:58	servier_SU (#126053) servier_SU (#126052) servier_SU (#126051)	2015-12-28 10:58:21	HPLC / UHD (2)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	MULTI	<b>VIEW</b>	1088498	job complete 100%	MG_2015-12-16_11:19	Pos-Notpre (#73124) Pos-QC (#73123) Pos-Pregna (#73122)	2015-12-16 11:19:11	Waters UPL (10669)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Shared [Stop sharing] <input type="checkbox"/>



**1 Dataset 1**

Load New Dataset OR Select Dataset  
(See [File Formats](#) for more information)

Dataset 1 ID: **Not Defined**  
Dataset 1 no. of files: **0**  
Dataset 1 Name:

**2 Dataset 2**

Load New Dataset OR Select Dataset  
(See [File Formats](#) for more information)

Dataset 2 ID: **Not Defined**  
Dataset 2 no. of files: **0**  
Dataset 2 Name:

**3 Parameters**

Select Parameters

**Job Summary**

Job ID: 1116917  
User: hpb (42)  
Job Name:    
Dataset 1:  (control)  
Dataset 2:   
Parameter Set: 0

**4 Submit**

Click here to complete your job



## Upload Dataset 1

<https://xcmsonline.scripps.edu/upload/index.php?datasetorder=1&action=newjob&runuser=undefined&jobid=1116...>

ID:198709

### Save Dataset & Proceed

Storage Quota Usage (2.86 TB):

1.10%

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:

**Save**

DROP HERE

**BROWSE**

1

Load New Data

(See [File Form](#))

Dataset 1

Dataset

Dat

Not Defined

04 Edit

(control)

Submit Job



ID:198709

**Save Dataset & Proceed**

Storage Quota Usage (2.86 TB):

1.10%

- 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: Dataset\_1

**Save**

**DROP HERE** **BROWSE**

	coke_x_10_a.mzXML 246.18 MB	✗
	coke_x_10_b.mzXML 245.05 MB	✗
	coke_x_10_c.mzXML 245.63 MB	✗

1 Data

Load New Dataset

(See [File Formats](#))

Dataset 1 ID

Dataset 1

Datas

Not Defined

4. Edit

(control)

Submit Job



1 Dataset 1

Load New Dataset OR Select Dataset  
(See [File Formats](#) for more information)

2 Dataset 2

Load New Dataset OR Select Dataset  
(See [File Formats](#) for more information)

3 Parameters

✓ Select Parameters

- HPLC / Q-TOF
- HPLC / UHD Q-TOF
- UPLC / UHD Q-TOF
- HPLC / UHD Q-TOF (HILIC, neg. mode)
- HPLC / Bruker Q-TOF neg
- UPLC / Bruker Q-TOF pos
- UPLC / TripleTOF pos
- UPLC / Orbitrap
- UPLC-high res
- UPLC Waters IC set-up
- Waters matchedFilter
- Waters UPLC - norm
- For\_MS\_vs\_MSMS\_tripleTOF
- Water\_IC neg
- hv test
- HPLC / TripleTOF pos- HPB
- UPLC - High Res POS (Waters) -with mummi
- UPLC - High Res POS (Waters)
- HPLC - UHD Qtof pairs
- HPLC / Single Quad
- UPLC / Q-Exactive
- HPLC / Ion Trap
- HPLC / Waters TOF
- HPLC / Orbitrap II
- HPLC / Orbitrap
- Custom-2015-06-17\_08:31:53
- GC / Single Quad (centWave)
- GC / Single Quad (matchedFilter)
- GC / TOF

Job Summary

Job ID: 1116917  
User: hpb (42)  
Job Name: pair\_2016-07-04 [Edit]  
Dataset 1: 1\_KO (control)  
Dataset 2: 2\_WT  
Parameter Set: 0

Dataset 1 ID: 69912  
Dataset 1 no. of files: 6  
Dataset 1 Name:  
1\_KO [Edit]

Dataset 2 ID: 69914  
Dataset 2 no. of files: 6  
Dataset 2 Name:  
2\_WT [Edit]

4 Submit

Click here to complete your job [Submit Job]



1 Dataset 1

OR

(See [File Formats](#) for more information)

Dataset 1 ID: **69912**

Dataset 1 no. of files: **6**

Dataset 1 Name:

2 Dataset 2

OR

(See [File Formats](#) for more information)

3 Parameters

HPLC / Q-TOF

optimized for HPLC with ~60 min gradient, ESI-QTOF-MS (e.g. Agilent Q-

**Confirm Job Specifications** ✕

**Job Details:**

**Name:** pair\_2016-07-04\_20:57 (ID# 1116917)

**Dataset 1 (control):** 1\_KO (ID# 69912), Files: 6

**Dataset 2:** 2\_WT (ID# 69914), 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!**

Job Summary

Job ID: 1116917

User: hpb (42)

Job Name: pair\_2016-07-04

Dataset 1: 1\_KO (control)

Dataset 2: 2\_WT

Parameter Set: 1

4 Submit

[Click here to complete your job](#)


## View Jobs

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

Job Count: 44

Search Jobs

View Public Shares

<input type="checkbox"/>	Exp Type	Status	ID ▾	Progress	JobName	Datasets (ID#) [*control]	Created	Parameters (ID#)	Group	Shared	
	-EXP- ▾	- STATUS - ▾							- GROUP - ▾		 
<input type="checkbox"/>	PAIR	<b>PROCESSING</b>	1116917	SUBMITTED  0%	pair_2016-07-04_20:57	1_KO (#69912) 2_WT (#69914)	2016-07-04 20:57:31	HPLC / Q-T (1)			

## You recently submitted job (#1116917) on XCMS Online.

Hi Hpb,

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

Job Name: pair\_2016-07-04\_20:57  
Create Date: 2016-07-04 20:57:31 (Server Timezone)  
Experiment Type: Pairwise Comparison  
Parameter Name: HPLC / Q-TOF (#1)  
Polarity: positive  
Datasets: 1\_KO (control)  
2\_WT

**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](mailto: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)

Download Results  
hash: Not Available

# Pairwise Results Summary: Coke vs. Pepsi (#114247)

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)	<a href="#">View Log</a>	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

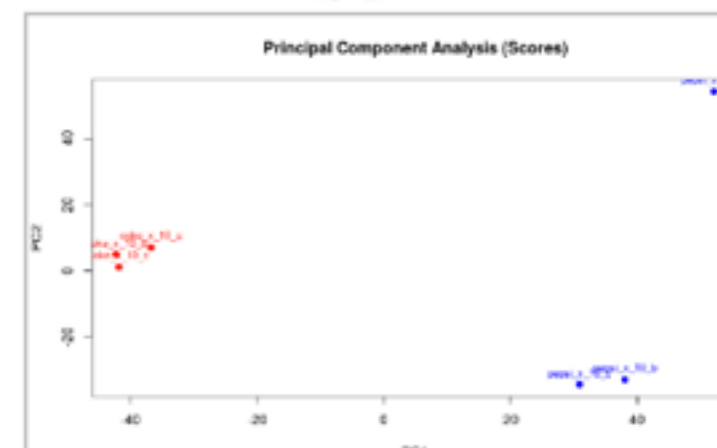
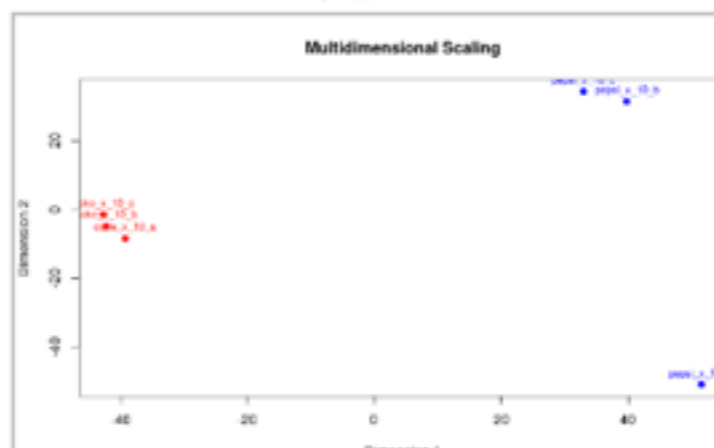
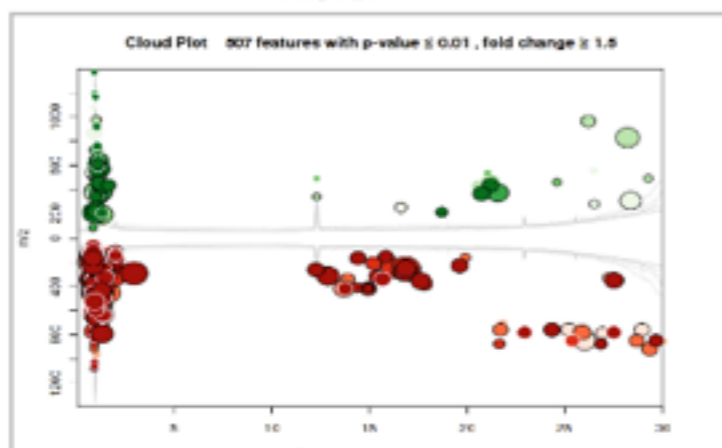
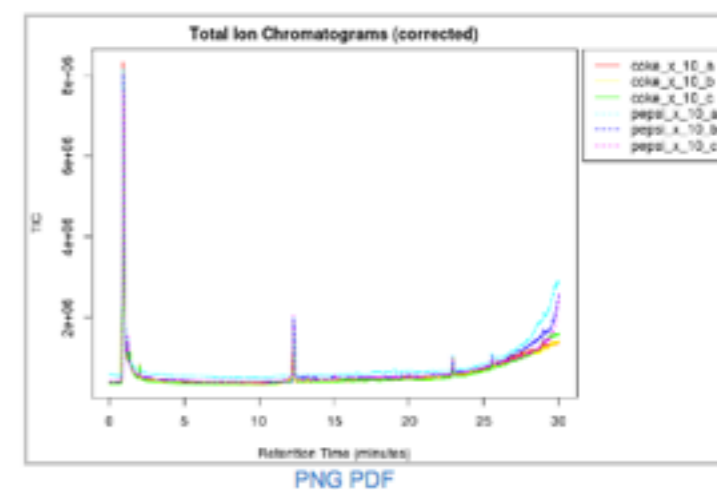
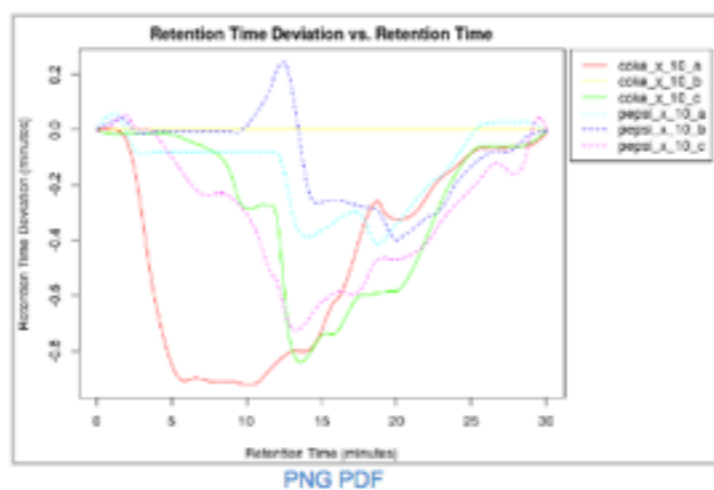
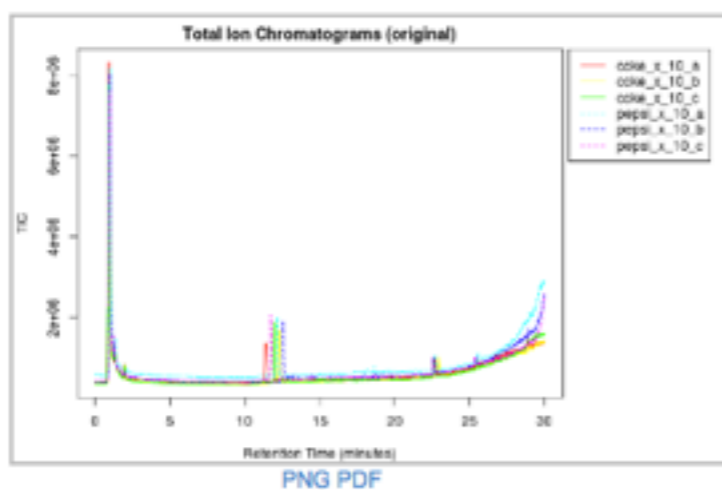
View Interactive Cloud Plot

View Interactive Heatmap

View IPCA

## Datasets Used

- Coke (1505) \*
- Pepsi (1507)

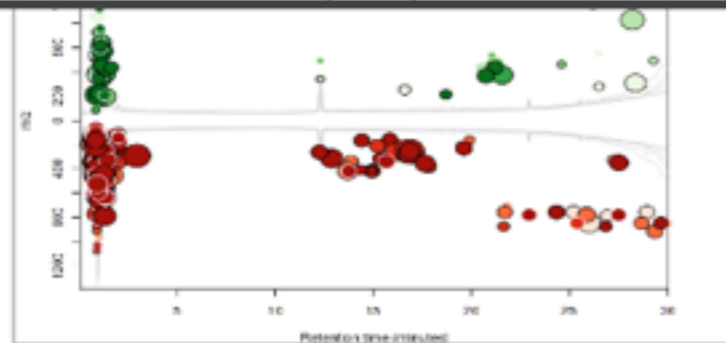
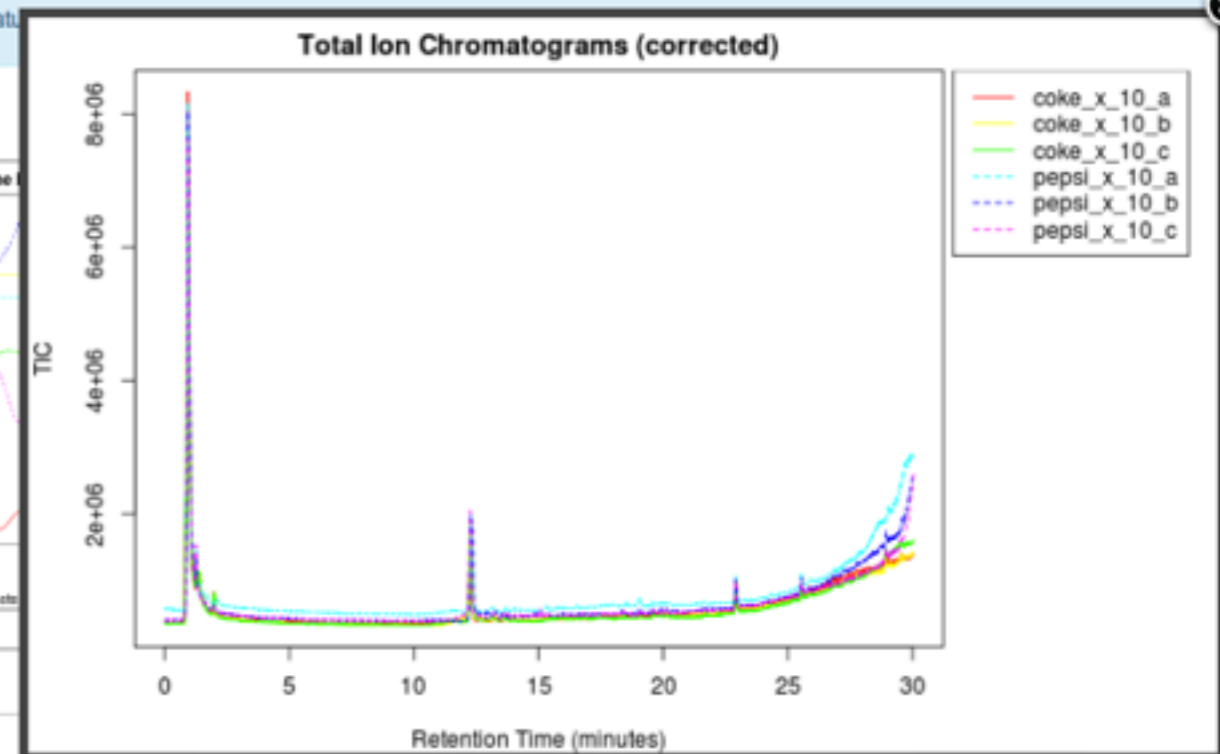
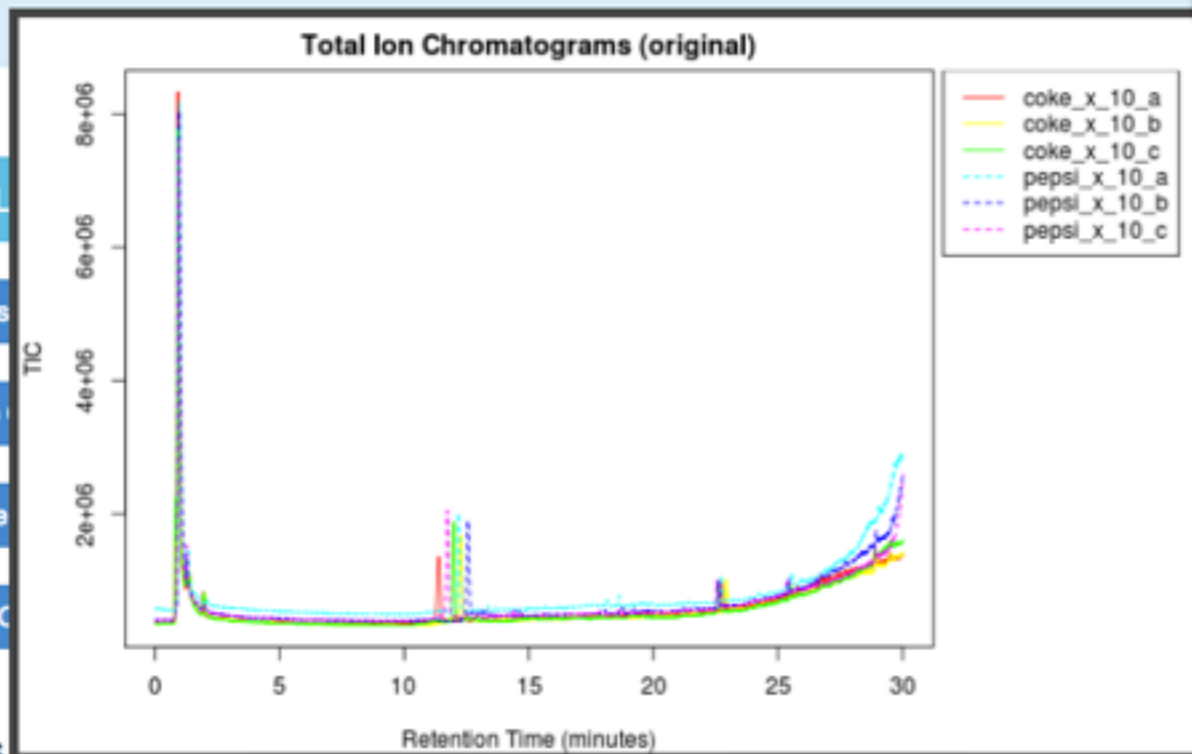


# Pairwise Results Summary: Coke vs. Pepsi (#114247)

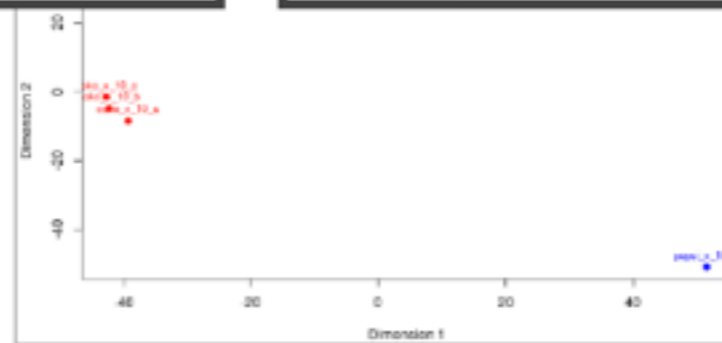
hash: Not Available

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)	<a href="#">View Log</a>	NOT SHARED

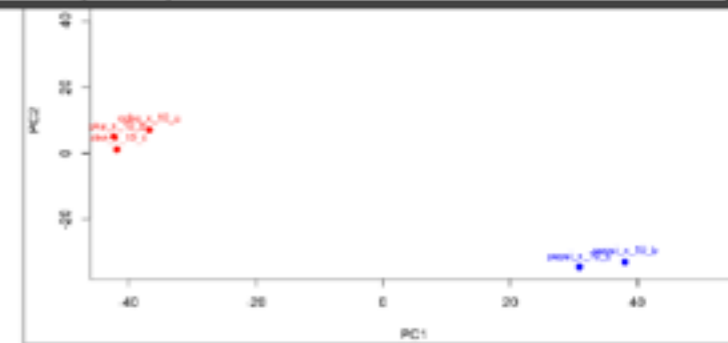
The finished job has the following notes:



[PNG](#) [PDF](#)



[PNG](#) [PDF](#)



[PNG](#) [PDF](#)

- [Citation L](#)
- [View Results](#)
- [View Interactive](#)
- [View Interactive](#)
- [View IPC](#)

- Datasets**
- Coke (1505) \*
  - Pepsi (1507)

Quick Compound Search:  Search Clear

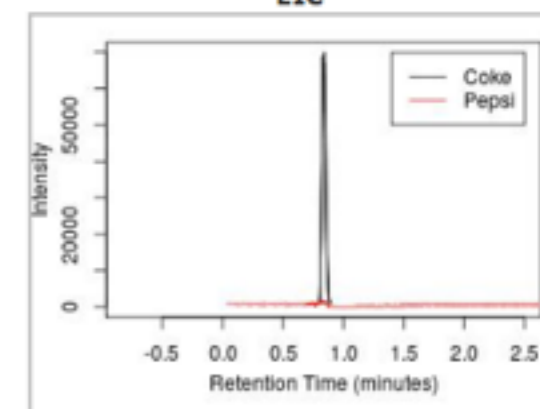
JOB#114247 : COKE VS. PEPSI

Columns Hide isotopic peaks Page 1 of 44 View 1 - 100 of 4,352

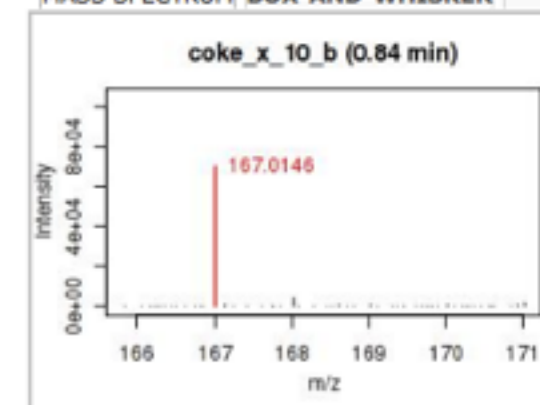
featureidx	fold	pvalue	updown	mzmed	rtmed	maxint	dataset1_mz	dataset2_mz	isotopes	adducts	peakgroup	usernotes
1	14.0	2.43784e-7	DOWN	167.0146	0.84	69,785	161,156	11,532	[30][M] <sup>+</sup>	[M+Na] <sup>+</sup> 144.13		
2	19.8	5.63165e-7	DOWN	252.0896	16.84	5,293	19,516	985		[M+NH <sub>4</sub> ] <sup>+</sup> 234.55		
3	19.6	6.91957e-7	DOWN	526.1777	0.91	4,835	15,747	804	[389][M+3] <sup>2+</sup>		1	
4	27.5	1.34235e-6	DOWN	229.9443	0.84	1,546	3,436	125		[3M+H+K] <sup>2+</sup> 13		
5	5.4	1.87943e-6	DOWN	233.9691	0.84	2,791	7,352	1,373		[3M+Na+K+Ni] <sup>3</sup>		
6	4.1	3.91793e-6	DOWN	92.4751	0.84	823	1,874	454			3	
7	13.1	6.38014e-6	DOWN	434.1698	1.27	2,361	4,953	379		[M+H-CH <sub>3</sub> ] <sup>+</sup> 416		
8	6.6	7.30438e-6	DOWN	467.1917	0.95	45,408	199,306	30,350	[333][M] <sup>+</sup>		1	
9	9.9	8.20524e-6	DOWN	452.1933	0.88	924	2,371	239	[318][M+1] <sup>+</sup>		70	
10	15.8	8.68738e-6	DOWN	192.9431	0.84	3,012	7,612	481			3	
11	7.9	0.00001	DOWN	594.2191	0.97	2,705	8,028	1,022			1	
12	5.9	0.00001	DOWN	494.1221	1.41	390	1,665	282	[363][M+1] <sup>+</sup>		6	
13	8.8	0.00001	DOWN	493.2003	0.89	667	1,810	205			26	
14	1.8	0.00001	DOWN	113.0715	0.91	6,807	13,653	7,591			1	
15	10.7	0.00002	DOWN	328.0565	1.45	1,164	9,056	845	[176][M+1] <sup>+</sup>		6	
16	8.2	0.00002	DOWN	637.1889	1.32	1,018	4,160	510	[471][M+2] <sup>+</sup>		24	
17	5.5	0.00002	DOWN	245.5550	1.38	677	5,344	976	[95][M+1] <sup>2+</sup>		6	
18	17.0	0.00002	DOWN	473.1798	0.89	1,860	4,768	281			26	
19	11.5	0.00002	DOWN	351.1643	27.51	1,175	3,024	0		[M+2K-H] <sup>+</sup> 27.84		
20	2.0	0.00003	DOWN	414.1427	14.92	358	1,397	685		[M+NH <sub>4</sub> ] <sup>+</sup> 396.82		
21	10.1	0.00004	DOWN	379.1736	0.88	1,403	2,670	88			70	
22	2.8	0.00004	DOWN	216.0667	0.94	30,294	61,136	21,789	[67][M] <sup>+</sup>		1	
23	7.0	0.00004	DOWN	263.0550	12.24	1,583	9,740	1,400	[113][M] <sup>+</sup>		216	
24	2.9	0.00004	UP	611.0654	1.08	2,748	3,010	8,817	[453][M] <sup>+</sup>	[M+K] <sup>+</sup> 572.1	5	
25	3.2	0.00004	DOWN	431.1704	1.26	19,705	31,930	9,933		[M+H-H <sub>2</sub> O] <sup>+</sup> 416		
26	2.6	0.00004	DOWN	287.0783	1.55	785	2,733	1,047			258	
27	9.0	0.00005	DOWN	490.8187	0.84	919	1,482	164		[M+K] <sup>+</sup> 451.8	3	
28	5.7	0.00005	DOWN	156.0148	0.84	5,335	12,340	2,147		[3M+NH <sub>4</sub> ] <sup>+</sup> 453		
29	5.7	0.00006	DOWN	463.1478	1.29	7,236	23,925	4,222			16	
30	2.0	0.00006	DOWN	535.0031	1.14	495	1,955	987		[M+K] <sup>+</sup> 495.0	50	

Please click on a row to view feature details

Feature #1  
m/z : 167.0146  
Retention Time (min): 0.84  
EIC



MASS SPECTRUM BOX-AND-WHISKER



PPM	Name	Adduct	COMPOSI
2	N,N'-bis(2-chloroethyl)	M+H-H <sub>2</sub> O	648
20	3,4-Dihydroxy-2-butar	M+H-H <sub>2</sub> O	63860



# NEW STREAMING SOFTWARE

XCMS Cascade

File Connect Job Help

Email Address

Password

URL

Local Directory  ...

XOCloud Directory  ...

Run Type

Machine Type

Job Type

Job Parameters  Refresh

# Valid Data

File Check Timeout

Post Run Timeout

Add New File Mask  Add

Choose file mask from here

- G1G\_\*
- URA\_\*
- VNG\_\*
- C1C\_\*
- B1B\_\*
- A1A\_\*

File mask that will be used

10:54:20 AM - json: 7297--7  
10:54:20 AM - json: 7298--8  
10:54:20 AM - json: 7299--9  
10:54:20 AM - json: 7301--10  
10:54:20 AM - json: 7302--11  
10:54:20 AM - json: 7303--12  
10:54:20 AM - json: 4573--aa1

Version: 1.0.0b00 || Compile Date: 6/13/2016 10:54:10 AM || User ID: 16 || Job ID || Status: Logged In

# THE NEW UPLOADER

