



Answers for Science.
Knowledge for Life.™



Solutions to Advance your Metabolomics Research

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Metabolomics & Lipidomics

SCIEX Metabolomics Portfolio

Discovery

Global Untargeted Screening

- 1000's of *features* in 10's of samples
- SWATH® / IDA Acquisition
- Brings data analysis from weeks to days



Global Targeted Screening

- Profile over 500 known *metabolites* in 10's of samples
- SWATH® / IDA Acquisition
- SCIEX Accurate Mass Spectral Library: processing to visualization in minutes



Translation/Validation



Targeted Profiling

- 100s of putative biomarkers on 100-1000s of samples
- QTRAP® Systems: Industry standard robustness
- Kits / reagents / existing methods:
 - aTRAQ™ Reagent for AAA
 - Amplifex reagents for enhanced sensitivity
- MRM assays for Vitamin D, Hormones/Steroids



Clinical Utilization



Validated Assays

- 10s of biomarkers and 100,000s of samples/yr.
- SCIEX Triple Quad™ 4500 MD
- MultiQuant™ Software MD
- Cliquant™ Software MD



Metabolomics Strategies – TripleTOF® System



**Single injection acquisition
MS and MS/MS data**

Non-targeted data acquisition
Generic MS setup

Targeted data acquisition
Target specific species 'MRM-like'

IDA SWATH®

Scheduled MRM^{HR} Workflow

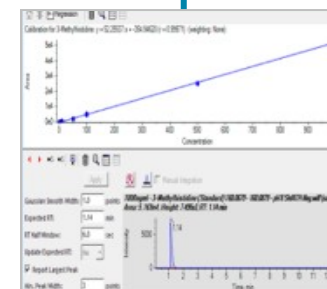
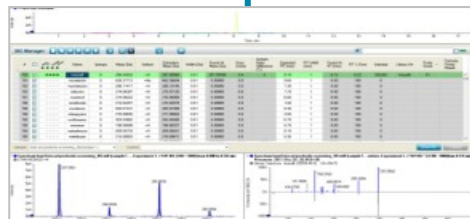
Global Untargeted Screening
Non-Targeted Global Metabolite Profile ID
1000s of metabolites

Database for 1000's of features

Global Targeted Screening
*Hypothesis Driven Biochemical
Pathway Approach*
ID 100s of metabolites

Sciex Curated library

Targeted Profiling
Quantitative Analysis
ID 10s of metabolites

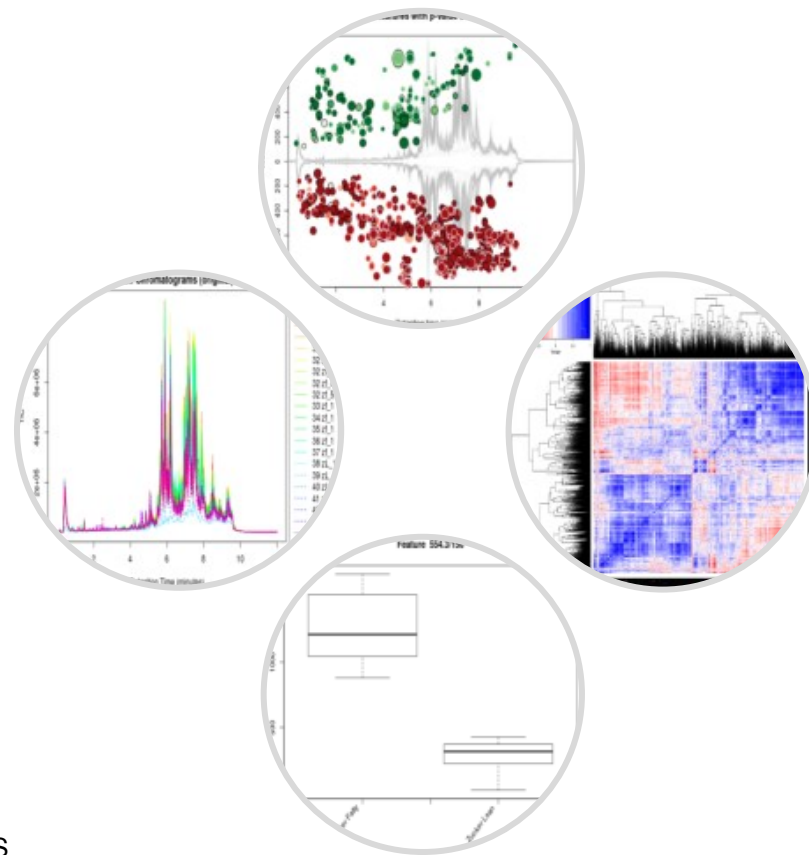


Metabolomics Simplified: XCMS^{Plus}

Most cited Metabolomics Software in the World!



- More than 6000 unique users worldwide
- Developed with Gary Siuzdak at Scripps Research Institute
- Load, process and review your data
- Statistics, identification and KEGG pathways
- Link your data to the Composite database
 - 240,546 metabolites, 62,192 HR-MSMS, 12,127 Metabolites with HR-MSMS



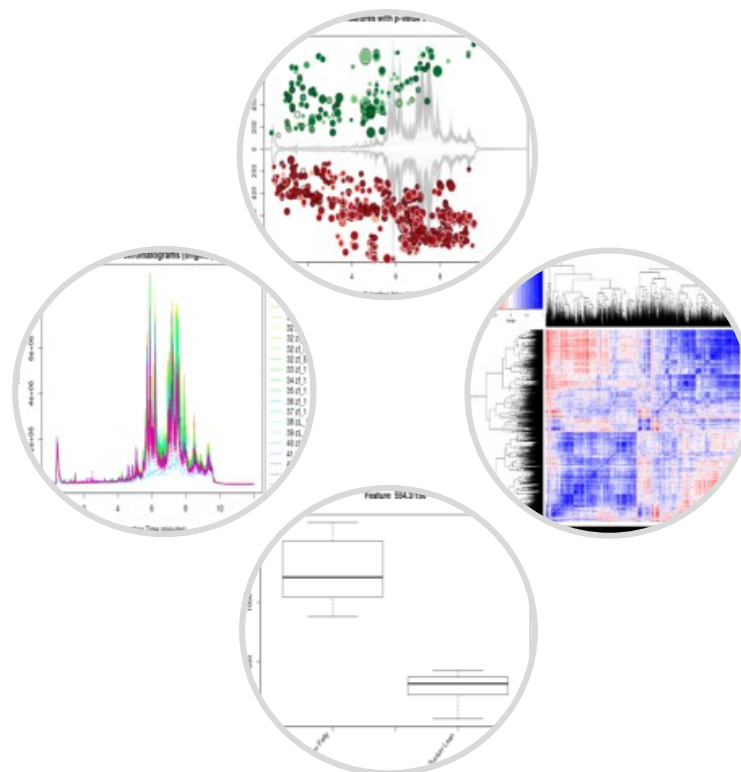
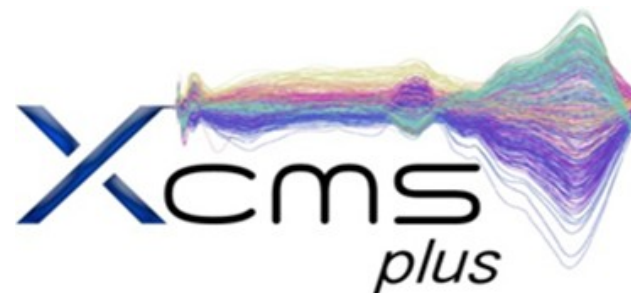
Metabolomics Simplified: XCMS^{plus}

Benefits over Online

- Upload time for XCMS Online: ~4-6 hours*
- Processing time for XCMS Online: ~16-18 hours (**total ~ 24 hours**)
- Upload time for XCMS^{plus}: ~1 minute
- Processing time for XCMS^{plus}: ~45 minutes (**total ~ 1 hour**)
- Unlimited data storage capabilities#
- Unlimited data sharing capabilities
- Secure data storage on private network
- Technical and installation support

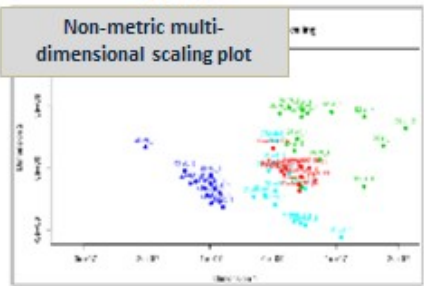
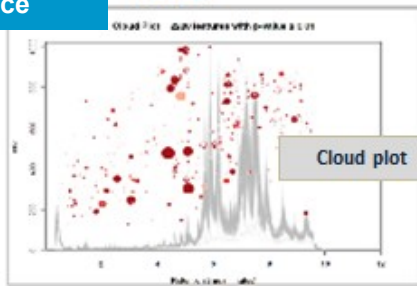
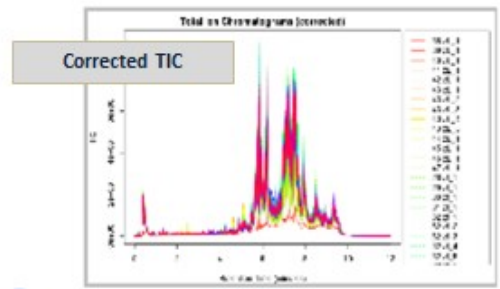
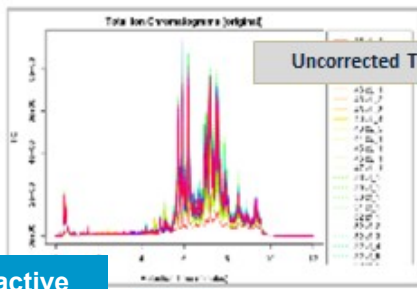
* For 40 IDA TripleTOF® data files totaling ~3.23GB

Dependent on HD on OS



Metabolomics Simplified: XCMS^{plus}

Single Interactive Workspace



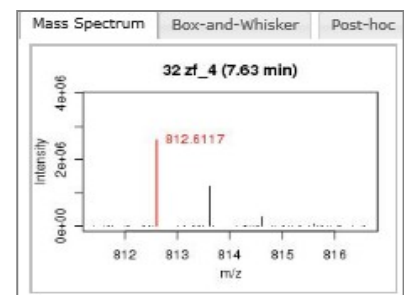
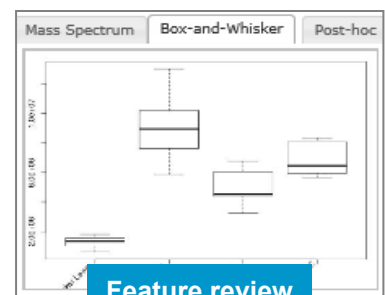
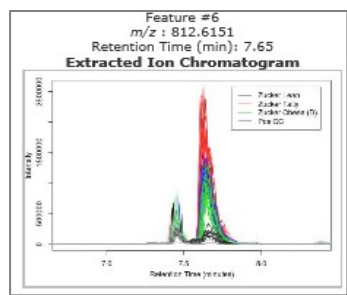
Feature	P Value	Q Value	M/Z	RT	Max Int	Isotope	Feature Gp
4	7.03423e-20	2.37150e-17	0.000	814.6228	7.65	637,769	[1033][M+2]+
5	1.84345e-19	4.97197e-17	0.000	824.1060	7.65	5,147	
6	3.54467e-19	7.08693e-17	0.000	812.6151	7.65	2,580,065	[1033][M]+
7	1.12151e-17	1.74949e-15	0.000	831.5555	7.07	25,431	[704][M+1]+
8	1.13189e-17	1.74949e-15			7.35	2,840,831	[1084][M]+
9	1.16758e-17	1.74949e-15			7.45	3,721,689	[1028][M]+

Table of features

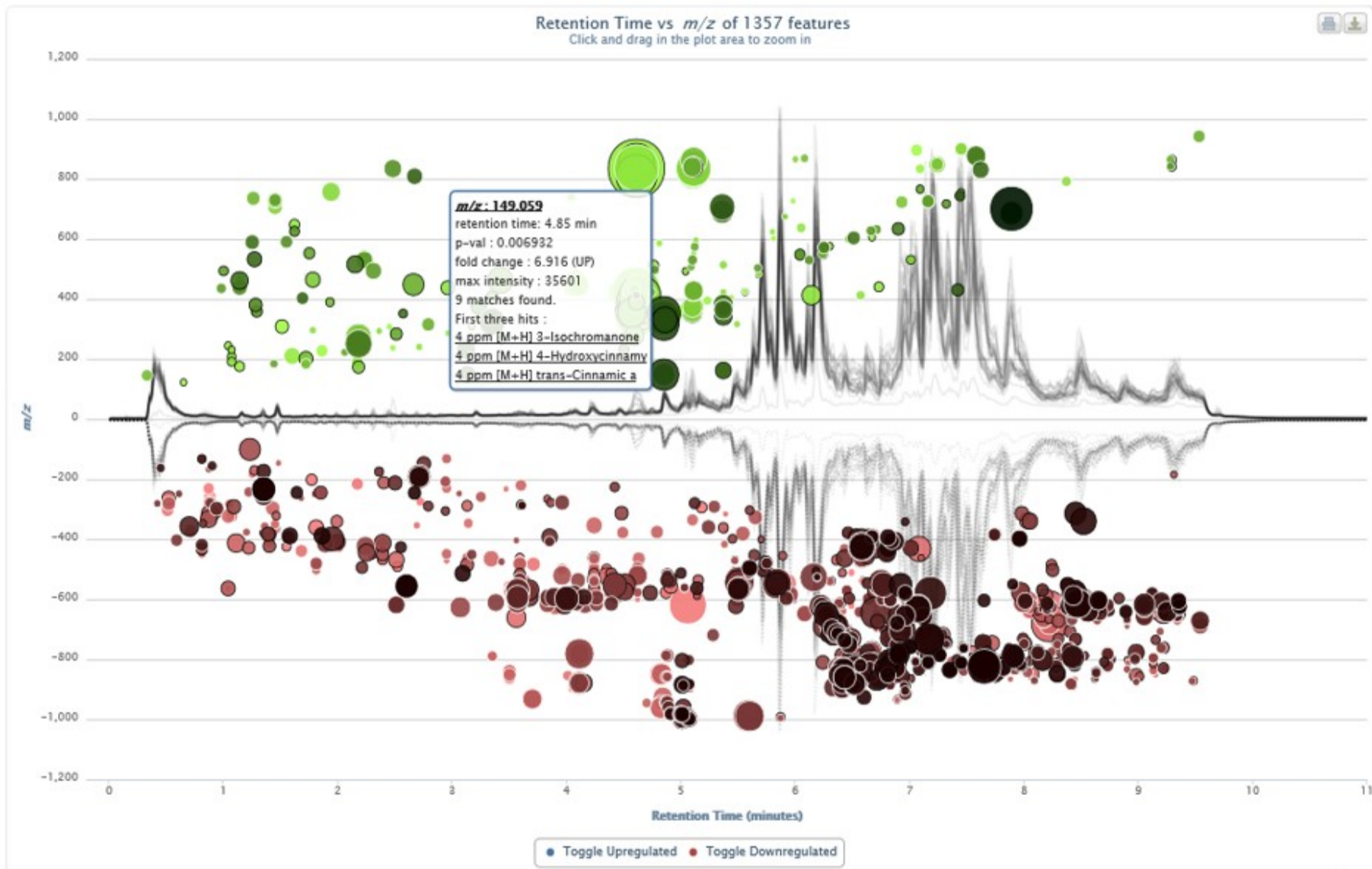


PPM	Name	Adduct
2	PC(18:0/22:3(13Z,16	M+H
2	PC(18:0/20:3(5E,8E,	M+H
2	PC(18:0/20:3(5Z,11Z	M+H
2	PC(18:0/20:3(5Z,8Z,	M+H
2	PC(18:0/20:3(5Z,8Z,	M+H
2	PC(18:0/20:3(8Z,11Z	M+H
2	PC(18:2(9Z,12Z)/20:	M+H
2	PC(18:1(9Z)/22:2(13:	M+H
2	PC(18:0/20:3(5Z,8Z,	M+H

Identification from Composite Database



Metabolomics Simplified: XCMS^{plus}





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