



Knowledge that will change your world

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MS-DIAL 2.0

A comprehensive metabolomics package

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Download the program and file converter

- This is PC-based software and does not have a Mac or Linux equivalent
- It can, however, be run in Windows 7 on a Mac using VMWare Fusion emulation
- Go to http://prime.psc.riken.jp/Metabolomics_Software/MS-DIAL/ to download the program
- Unzip MS-DIAL and place the folder on the desktop
- Also download the file converter program to make .abf files at the same website

Download demonstration files

- Scroll down on the MS-DIAL homepage to “Demonstration files”
- Click on the link below to get LC/MS/MS data sets (.wiff and .wiff.scan, and the converted abf files) for lipid profiling of algae.
 - [data independent acquisition \(SWATH\) and data dependent acquisition \(IDA\) for algae lipidomics](#)
- Then scroll down until you see this file

ABF files of the raw data set, SWATH, Negative ion mode.



20140809_MS-DIAL_DemoFiles_Swath zip archive:
(abf)

1,833MB

Starting MS-DIAL

Name	Date modified	Type	Size
MonaRestApi.dll.config	8/23/2017 12:29 PM	CONFIG File	3 KB
MonaRestApiTests.dll	7/17/2017 6:27 PM	Application extens...	10 KB
MonaRestApiTests.dll.config	6/13/2017 4:40 PM	CONFIG File	3 KB
MSDIAL	2/4/2018 12:24 AM	Application	4,645 KB
MSDIAL.exe.config	7/29/2017 10:48 PM	CONFIG File	2 KB
MSDIAL	2/2/2018 5:11 PM	Configuration sett...	1 KB
MSDIAL.vshost.exe.config	7/29/2017 10:48 PM	CONFIG File	2 KB
MsdialConsoleApp	2/3/2018 6:10 PM	Application	114 KB
MsdialConsoleApp.exe.config	7/1/2016 12:39 PM	CONFIG File	1 KB
MsdialConsoleApp.vshost.exe.config	7/1/2016 12:39 PM	CONFIG File	1 KB
MsdialGcmsProcess.dll	2/3/2018 6:47 PM	Application extens...	141 KB
MsdialLcmsProcess.dll	2/3/2018 6:10 PM	Application extens...	180 KB
MSDIAL-LipidDBs-VS32-FiehnO.lbm	2/2/2018 4:19 PM	LBM File	280,560 KB
MSMS-AllPublic-Curated-PosNeg	2/17/2018 10:06 AM	Windows Installer ...	94,690 KB
MzmlDataHandler.dll	2/3/2018 6:10 PM	Application extens...	33 KB
NetCdfDataHandler.dll	2/3/2018 6:10 PM	Application extens...	22 KB
Newtonsoft.Json.dll	7/1/2016 12:53 PM	Application extens...	478 KB
PairwisePlot.dll	2/3/2018 6:47 PM	Application extens...	85 KB
RawDataHandler.dll	2/3/2018 6:10 PM	Application extens...	7 KB

Click on File

Entering MS-DIAL

The screenshot displays the MS-DIAL software interface. At the top left, an arrow points to the 'File' menu. The interface is divided into several sections:

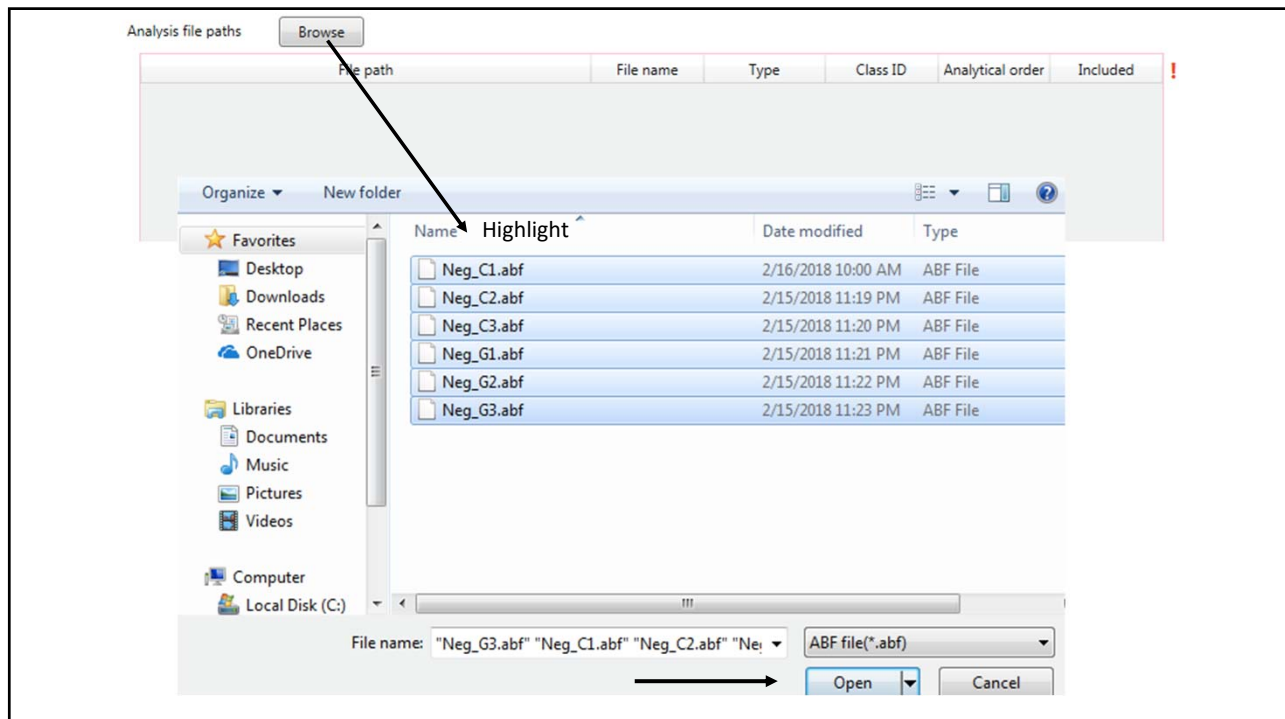
- File navigator:** Includes a 'Label' dropdown (set to 'None'), a 'Scan #' field (set to '-1'), and a 'Peak spots: 100%' slider.
- Display filter:** Contains checkboxes for 'Identified', 'Molecular ion', 'Unknown', 'Annotated', 'MS/MS', and 'Unique ions'.
- Extracted ion chromatogram of focused spot:** A plot of 'Relative Abundance' vs 'Retention time [min]'.
- Bar chart of aligned spots:** A bar chart showing aligned spots.
- Peak and compound information:** Fields for 'Peak intensity', 'RT [min]', 'Mass [Da]', 'Compound name', 'Ref. RT [min]', 'Ref. Mass [Da]', 'MS2 similarity', and 'InChIKey'.
- Survey scan (MS1) spectrum:** A plot of 'Relative Abundance' vs 'm/z'.
- Peak spot viewer:** A plot of 'File name' vs 'Retention time [min]'.
- Alignment spot viewer:** A plot of 'm/z' vs 'Retention time [min]'.
- Measurement vs. Reference:** A plot of 'Relative Abundance' vs 'm/z' comparing 'Measurement' and 'Reference'.
- Alignment navigator:** A vertical bar on the left side.

Loading the files and defining type

The screenshot shows the 'Loading the files and defining type' configuration screen. It includes the following fields and options:

- Project file path:** A text box containing 'C:\Users\Admin\Desktop\ABF_files\2018_2_17_20_21_58.mtd' and a 'Browse' button. An arrow points to the 'Browse' button with the text 'Choose the files'.
- Ionization type:** Radio buttons for 'Soft ionization (LC/MS, LC/MS/MS, or precursor-oriented GC/MS/MS)' (selected) and 'Hard ionization (GC/MS)'.
- Method type:** Radio buttons for 'Conventional LC/MS or data dependent MS/MS' (selected) and 'Data independent MS/MS'. An arrow points to the 'Conventional LC/MS or data dependent MS/MS' option.
- Experiment file:** A text box and a 'Browse' button.
- Data type (MS1):** Radio buttons for 'Profile data' (selected) and 'Centroid data'.
- Data type (MS/MS):** Radio buttons for 'Profile data' (selected) and 'Centroid data'. A note states 'SCIEX data are in the profile mode'.
- Ion mode:** Radio buttons for 'Positive ion mode' and 'Negative ion mode' (selected). An arrow points to the 'Negative ion mode' option.
- Target omics:** Radio buttons for 'Metabolomics' (selected) and 'Lipidomics'. An arrow points to the 'Metabolomics' option.
- Advanced:** A dropdown menu labeled 'Advanced: add further meta data'.
- Next:** A button at the bottom right.


Selecting the mouse urine data



Set the groups

Analysis file paths

File path	File name	Type	Class ID	Analytical order	Included
C:\Users\Admin\Desktop\ABF_files\Neg_C1.abf	Neg_C1	Sample	1	1	<input checked="" type="checkbox"/>
C:\Users\Admin\Desktop\ABF_files\Neg_C2.abf	Neg_C2	Sample	1	2	<input checked="" type="checkbox"/>
C:\Users\Admin\Desktop\ABF_files\Neg_C3.abf	Neg_C3	Sample	1	3	<input checked="" type="checkbox"/>
C:\Users\Admin\Desktop\ABF_files\Neg_G1.abf	Neg_G1	Sample	2	4	<input checked="" type="checkbox"/>
C:\Users\Admin\Desktop\ABF_files\Neg_G2.abf	Neg_G2	Sample	2	5	<input checked="" type="checkbox"/>
C:\Users\Admin\Desktop\ABF_files\Neg_G3.abf	Neg_G3	Sample	2	6	<input checked="" type="checkbox"/>



Setting up the parameters for MS-DIAL

Data collection **Peak detection** MS2Dec Identification Adduct Alignment Isotope tracking

Data collection parameters

Retention time begin: min

Retention time end: min

Mass range begin: Da

Mass range end: Da

Centroid parameters

MS1 tolerance: Da

MS2 tolerance: Da

Isotope recognition

Maximum charged number:

Data collection Peak detection **MS2Dec** Identification Adduct Alignment Isotope tracking

Peak detection parameters

Smoothing method: ▼

Smoothing level: scan

Minimum peak width: scan

Minimum peak height: amplitude

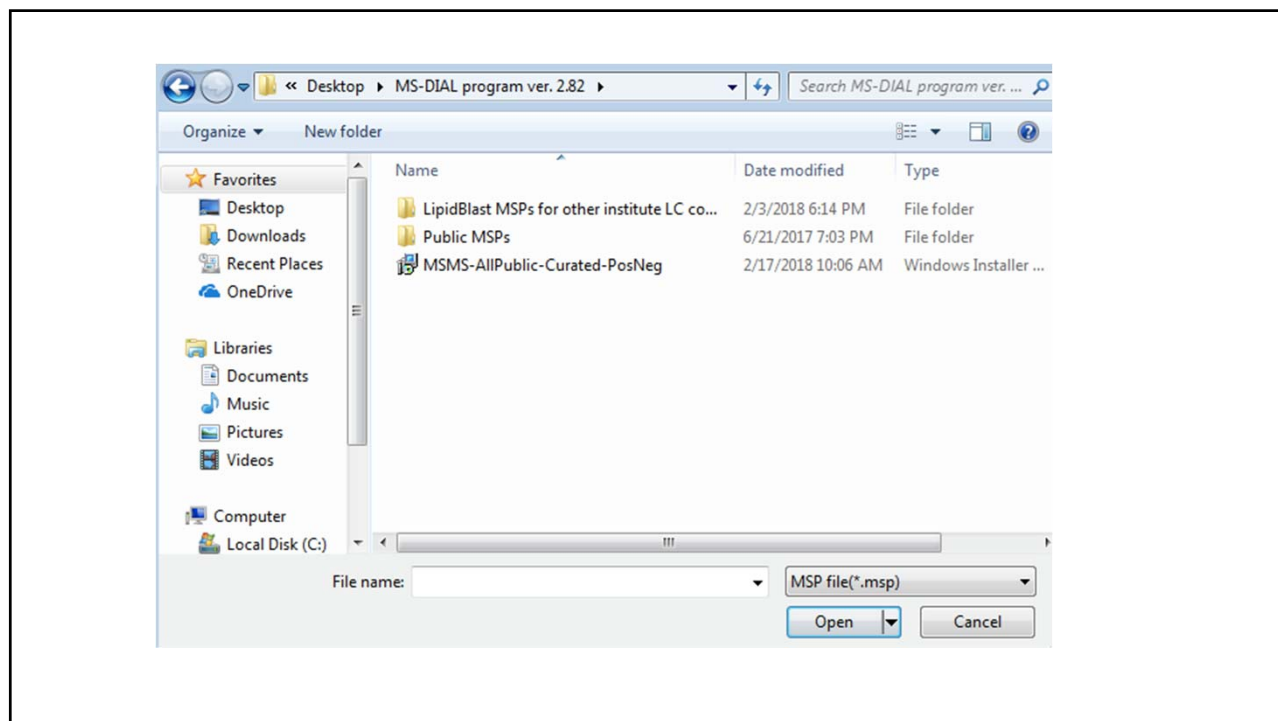
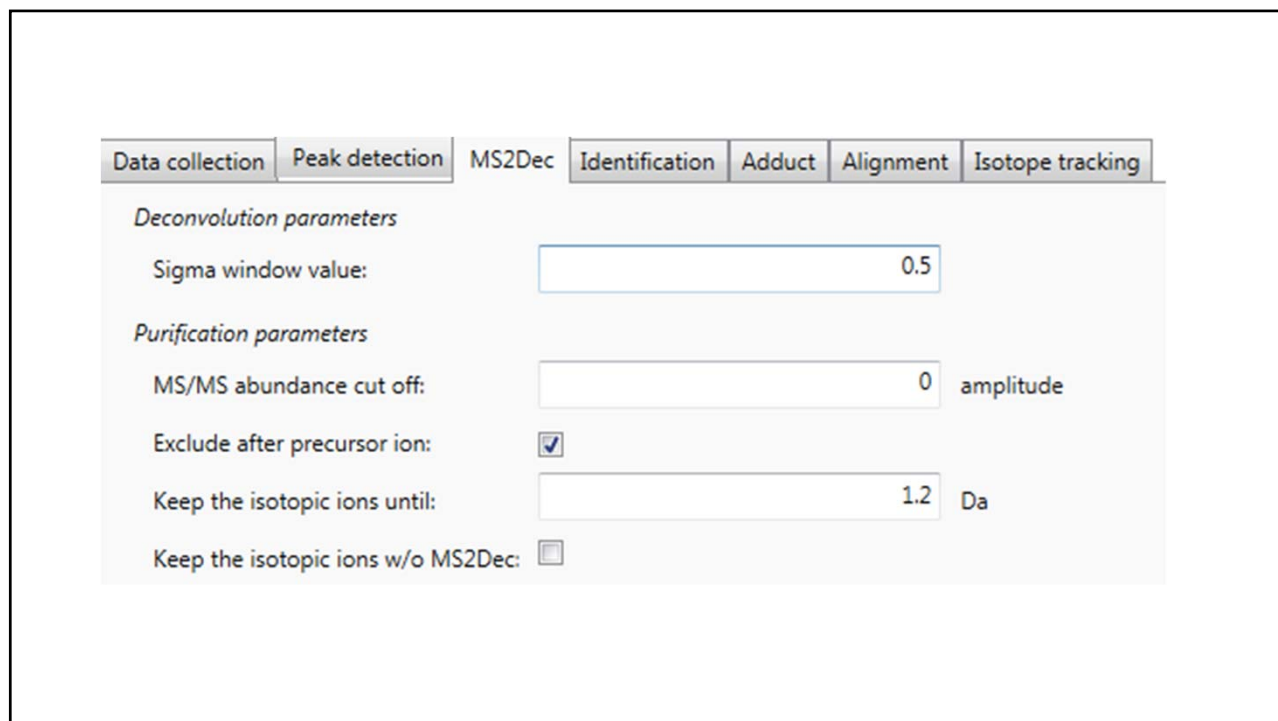
Peak spotting parameters

Mass slice width: Da

Exclusion mass list:

Accurate mass [Da]	Mass tolerance [Da]

Together with Alignment



Data collection Peak detection MS2Dec Identification Adduct Alignment Isotope tracking

MSP file and MS/MS identification setting

MSP file: C:\Users\Admin\Desktop\MS-DIAL program ver. 2.82\MSMS-AllPublic-C

Retention time tolerance: min

Accurate mass tolerance (MS1): Da

Accurate mass tolerance (MS2): Da

Identification score cut off: %

Use retention information for scoring:

Text file and post identification (retention time and accurate mass based) setting

Text file:

Retention time tolerance: min

Accurate mass tolerance: Da

Identification score cut off: %

Data collection Peak detection MS2Dec Identification Adduct Alignment Isotope tracking

Adduct ion setting

Molecular species	Charge	Accurate mass [Da]	Included
[M-H]-	1	-1.00782503207	<input checked="" type="checkbox"/>
[M-H ₂ O-H]-	1	-19.01838971207	<input type="checkbox"/>
[M+Na-2H]-	1	20.97411921676	<input type="checkbox"/>
[M+Cl]-	1	34.96885268	<input type="checkbox"/>
[M+K-2H]-	1	36.94805661586	<input type="checkbox"/>
[M+FA-H]-	1	44.99765396793	<input checked="" type="checkbox"/>
[M+Hac-H]-	1	59.01330396793	<input type="checkbox"/>
[M+Br]-	1	78.9183371	<input type="checkbox"/>
[M+TFA-H]-	1	112.98503896793	<input type="checkbox"/>
[M-C ₆ H ₁₀ O ₄]-	1	-146.05790879894	<input type="checkbox"/>
[M-C ₆ H ₁₀ O ₅]-	1	-162.0528234185	<input type="checkbox"/>
[M-C ₆ H ₈ O ₆]-	1	-176.03208797392	<input type="checkbox"/>
[2M-H]-	1	-1.00782503207	<input checked="" type="checkbox"/>
[2M+FA-H]-	1	44.99765396793	<input checked="" type="checkbox"/>
[2M+Hac-H]-	1	59.01330396793	<input type="checkbox"/>
[3M-H]-	1	-1.00782503207	<input type="checkbox"/>
[M-2H]2-	2	-2.01565006414	<input type="checkbox"/>
[M-3H]3-	3	-3.02347509621	<input type="checkbox"/>

Data collection | Peak detection | MS2Dec | Identification | Adduct | Alignment | **Isotope tracking**

Alignment parameters setting

Result name: alignmentResult_2018_2_17_20_49_29

Reference file: Neg_C1

Retention time tolerance: 0.2 min

MS1 tolerance: 0.01 Da

Retention time factor: 0.5 (0-1)

MS1 factor: 0.5 (0-1)

Peak count filter: 0 %

N% detected in at least one group: 0 %

Detected in all QCs

Data collection | **Peak detection** | MS2Dec | Identification | Adduct | Alignment | **Isotope tracking**

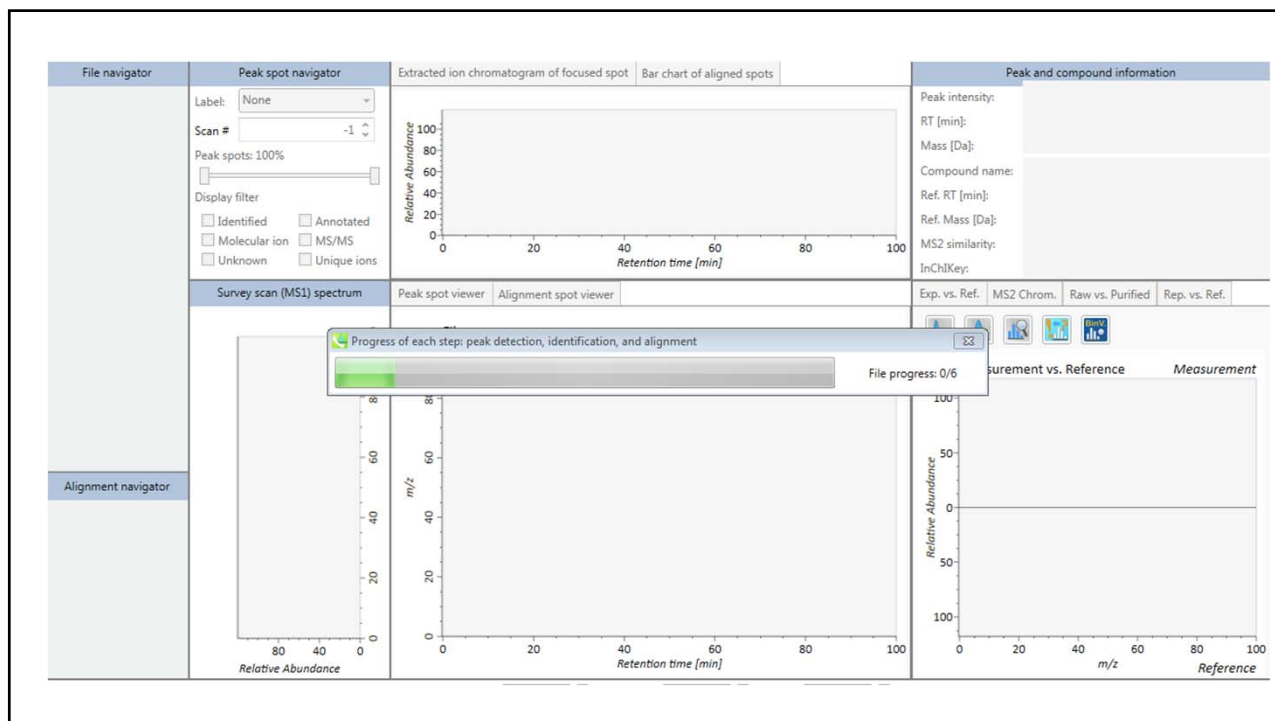
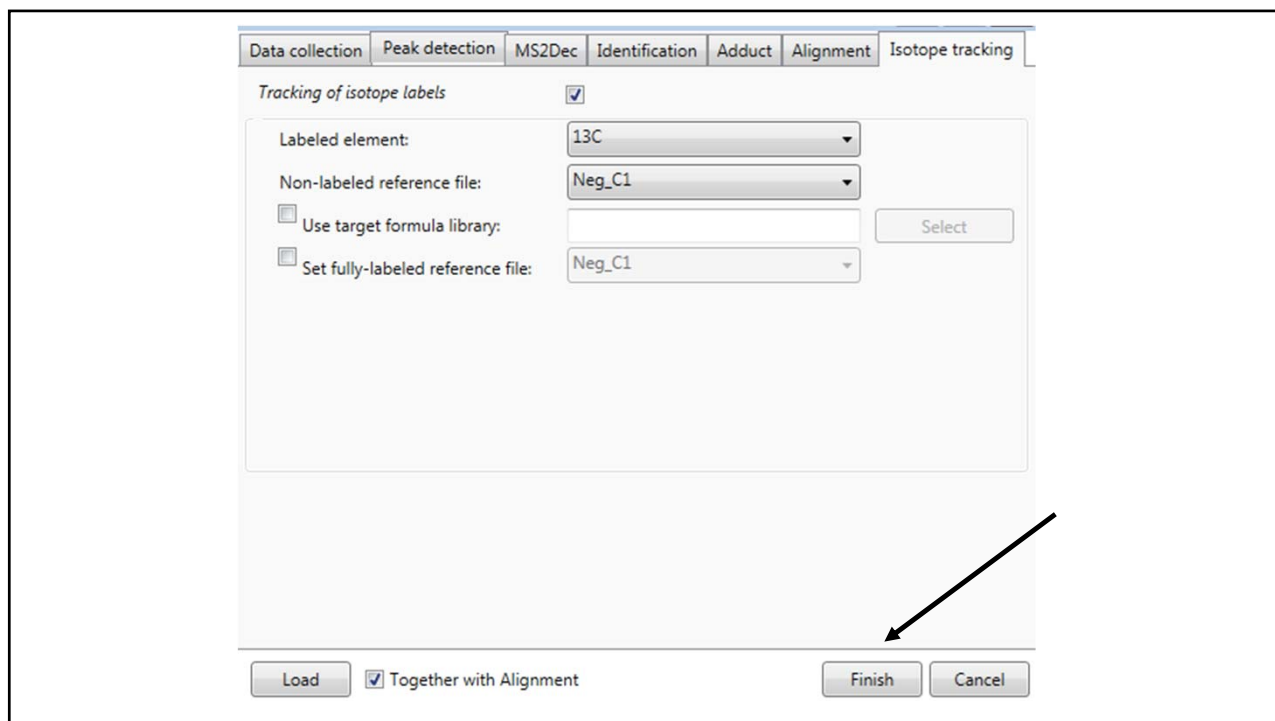
Tracking of isotope labels

Labeled element: 13C

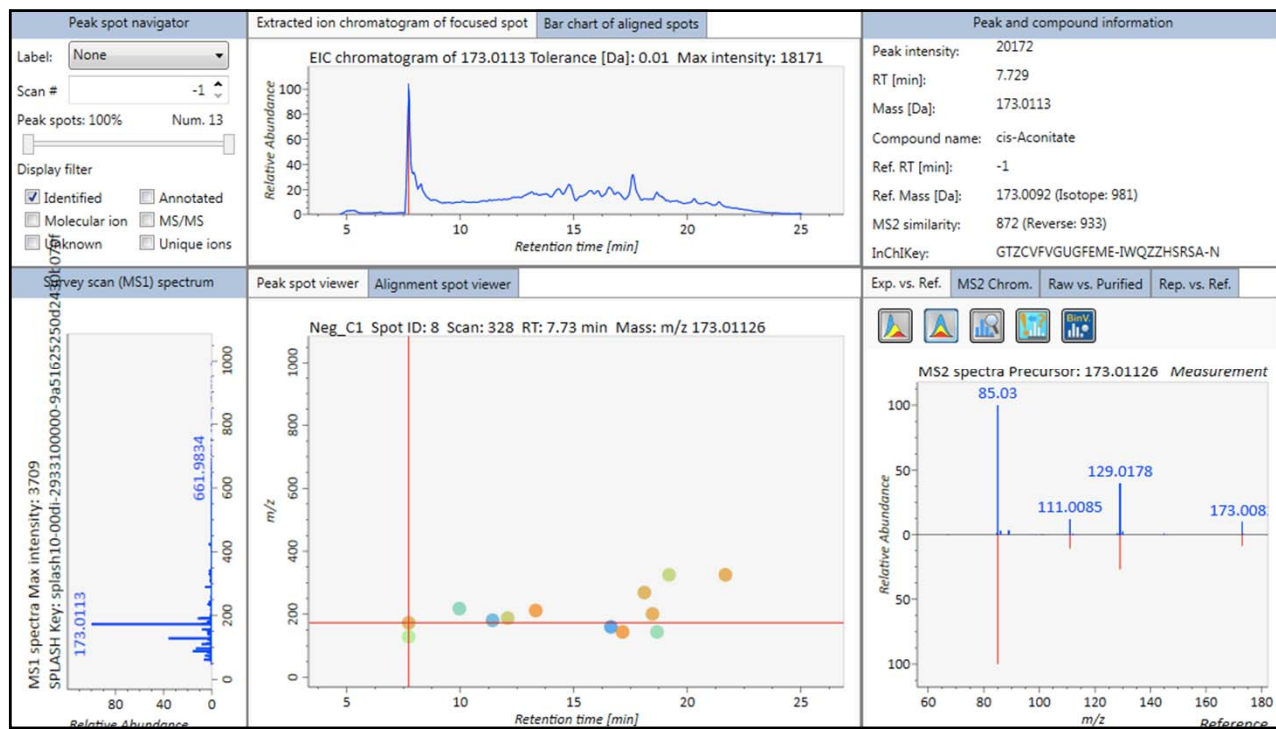
Non-labeled reference file: Neg_C1

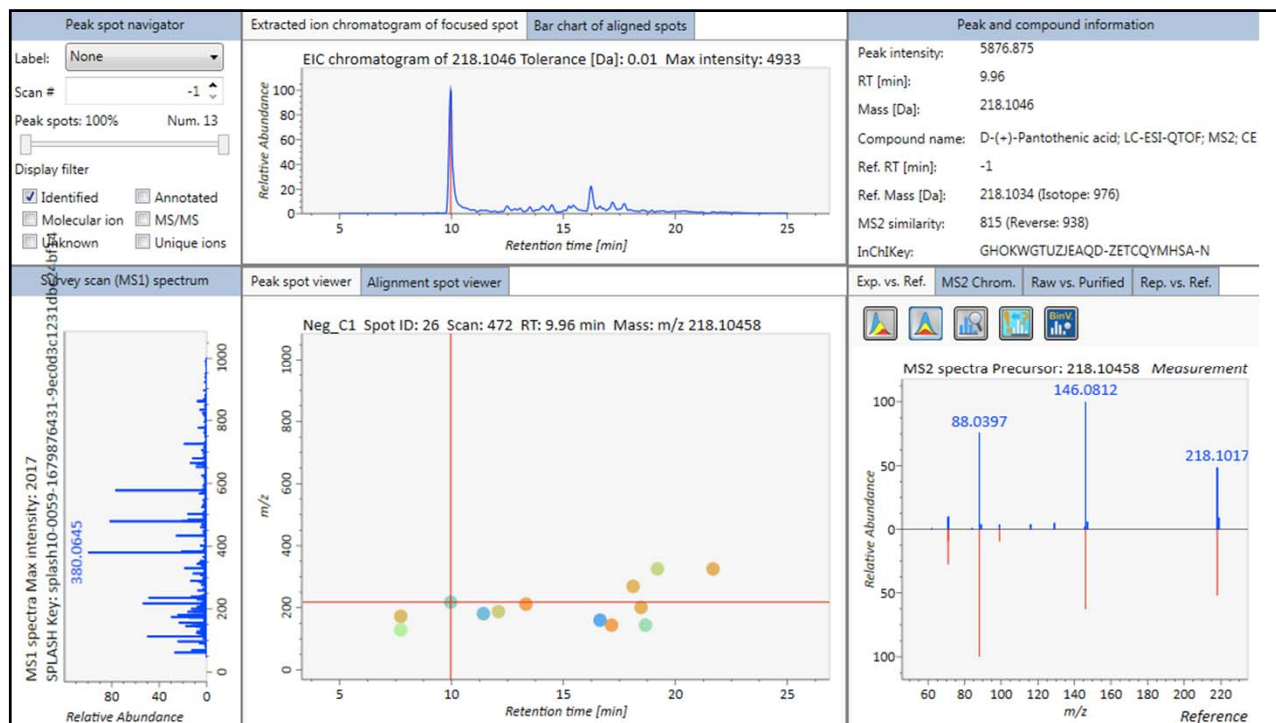
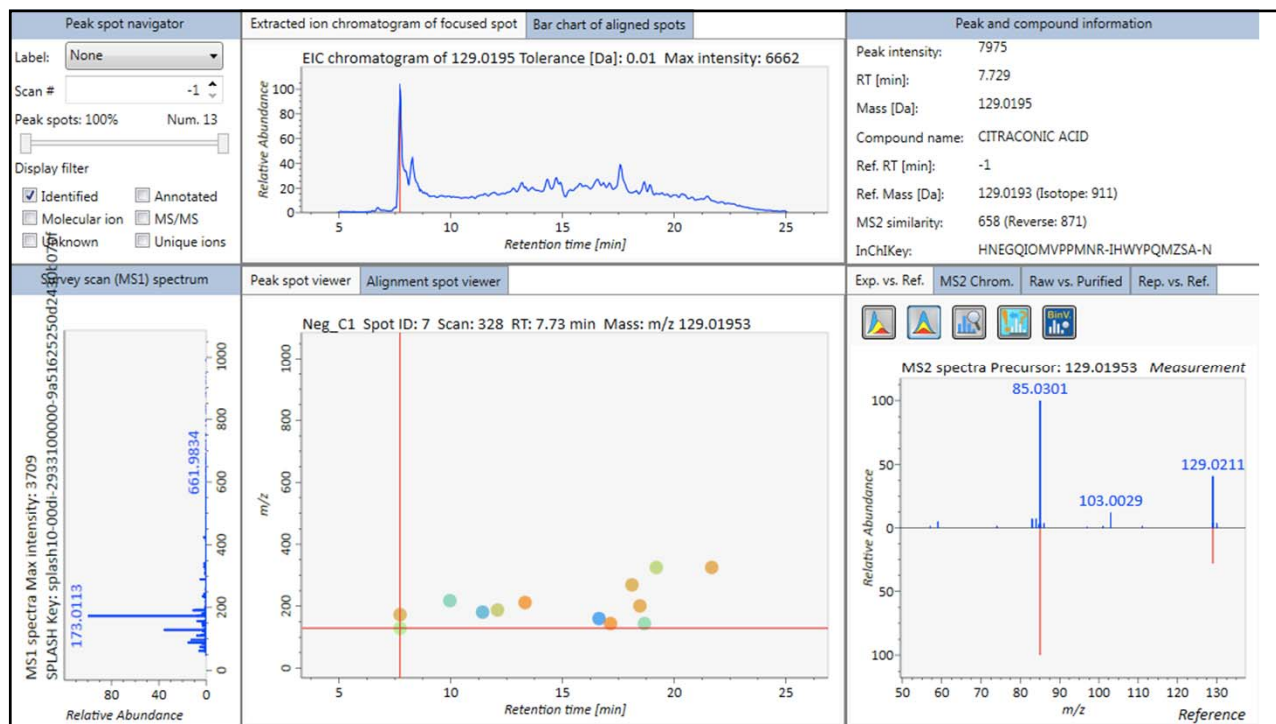
Use target formula library:

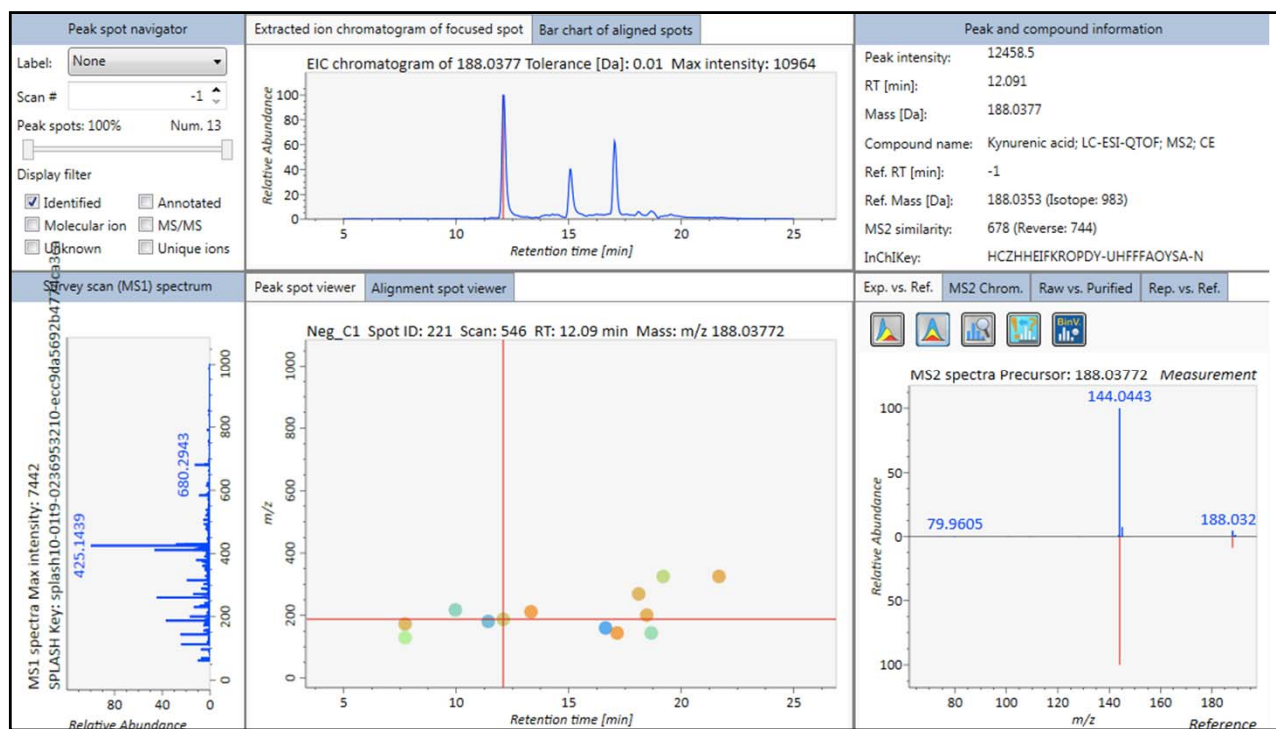
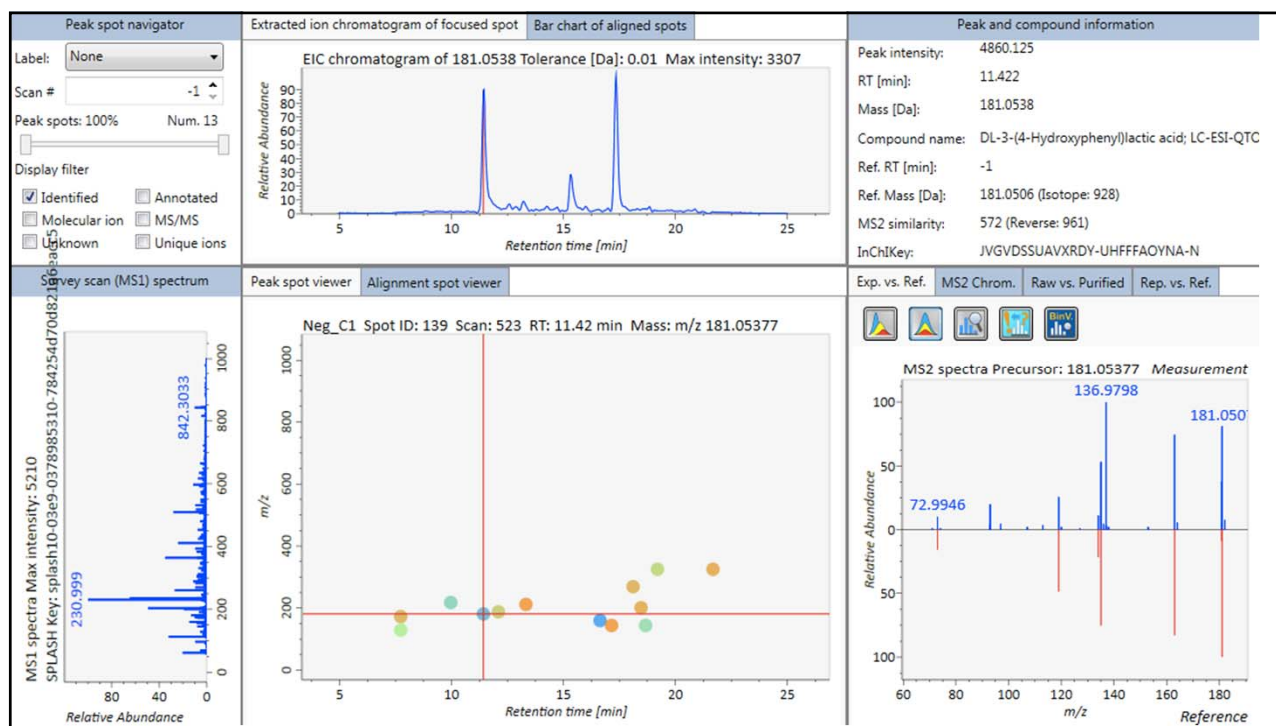
Set fully-labeled reference file: Neg_C1

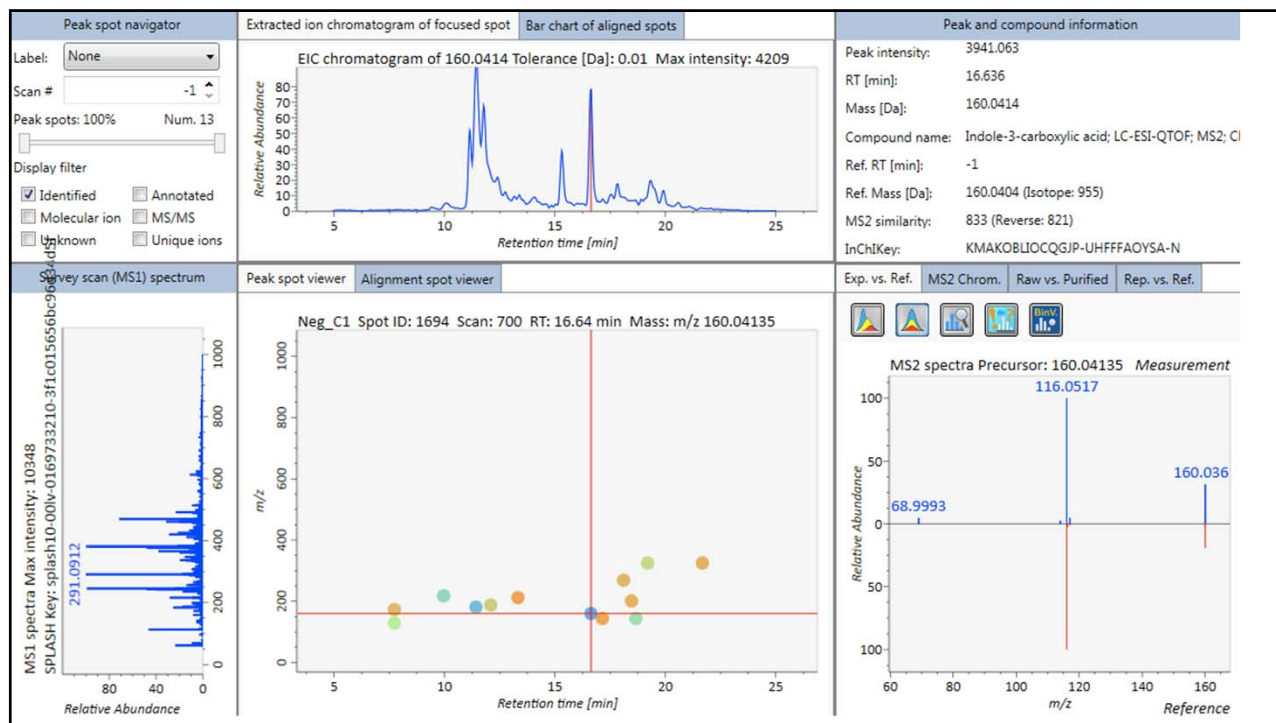
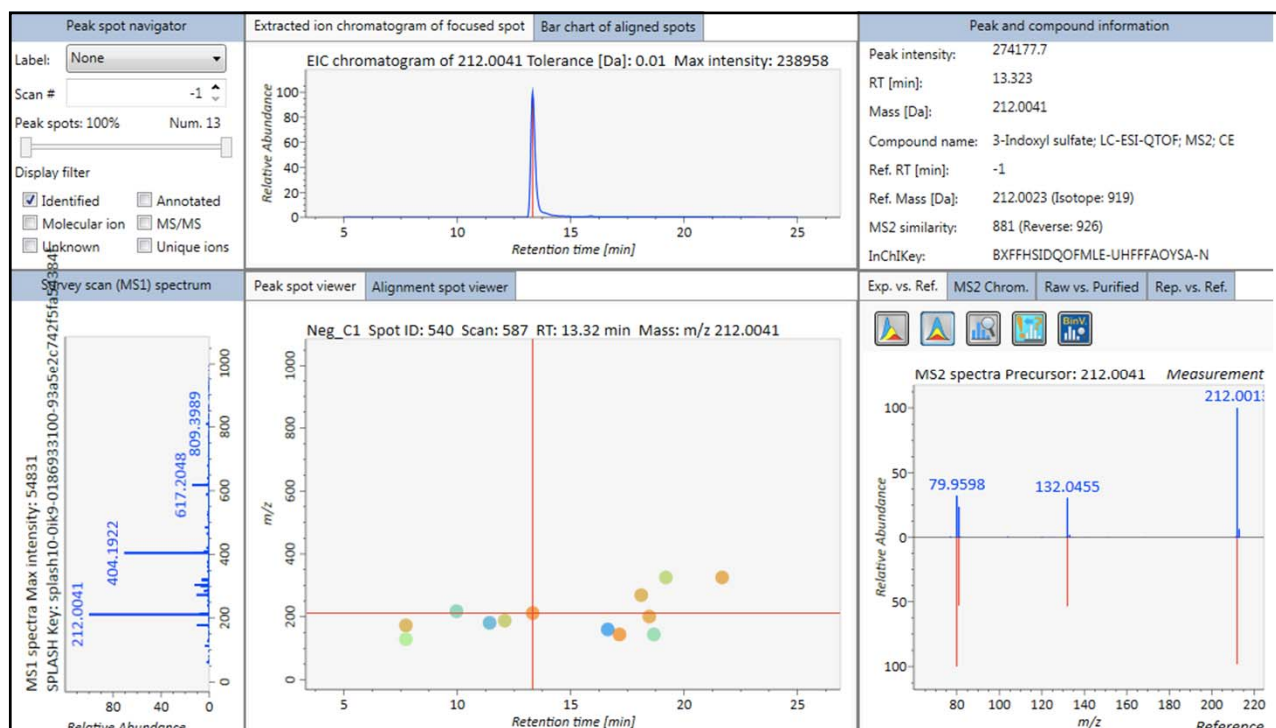


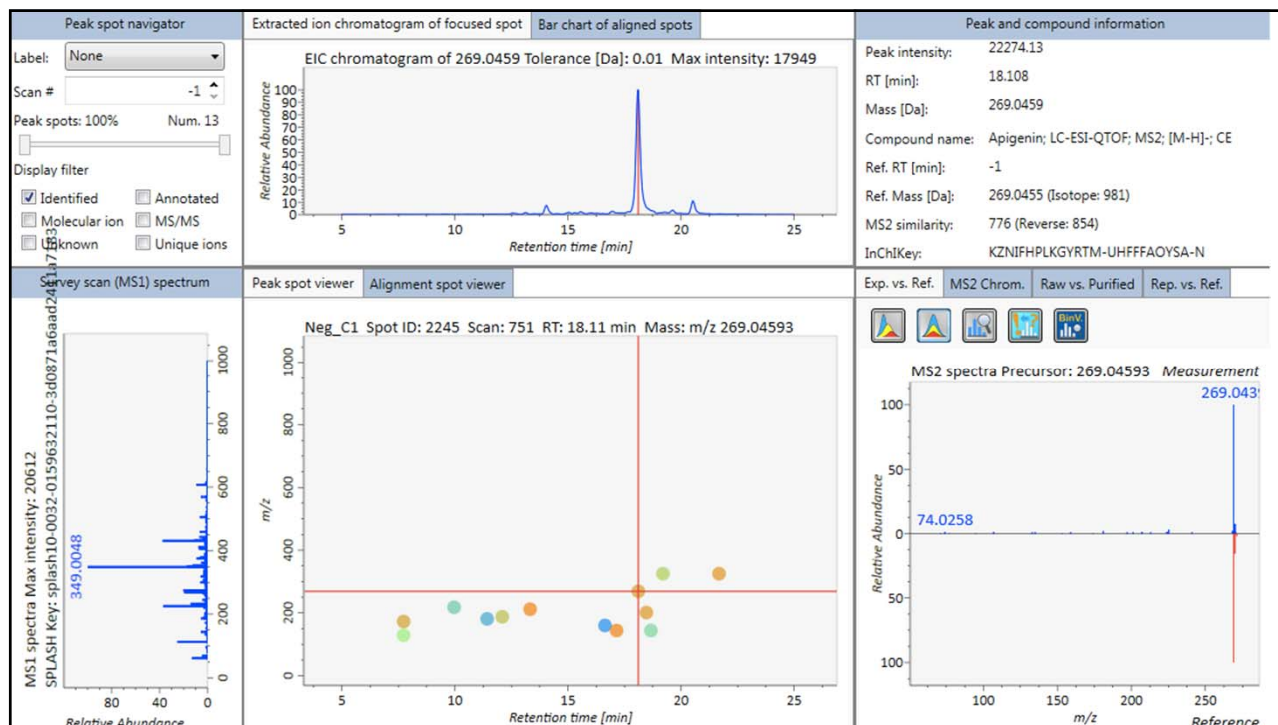
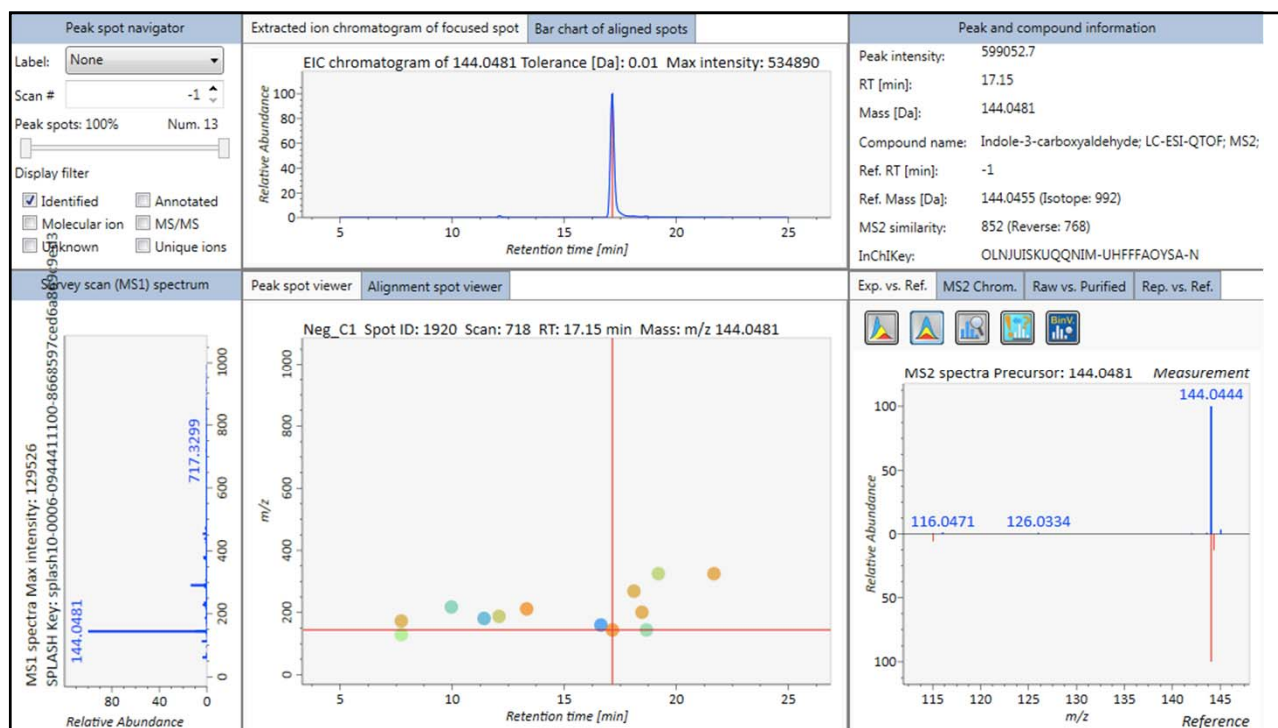
Ions identified in neg_c1

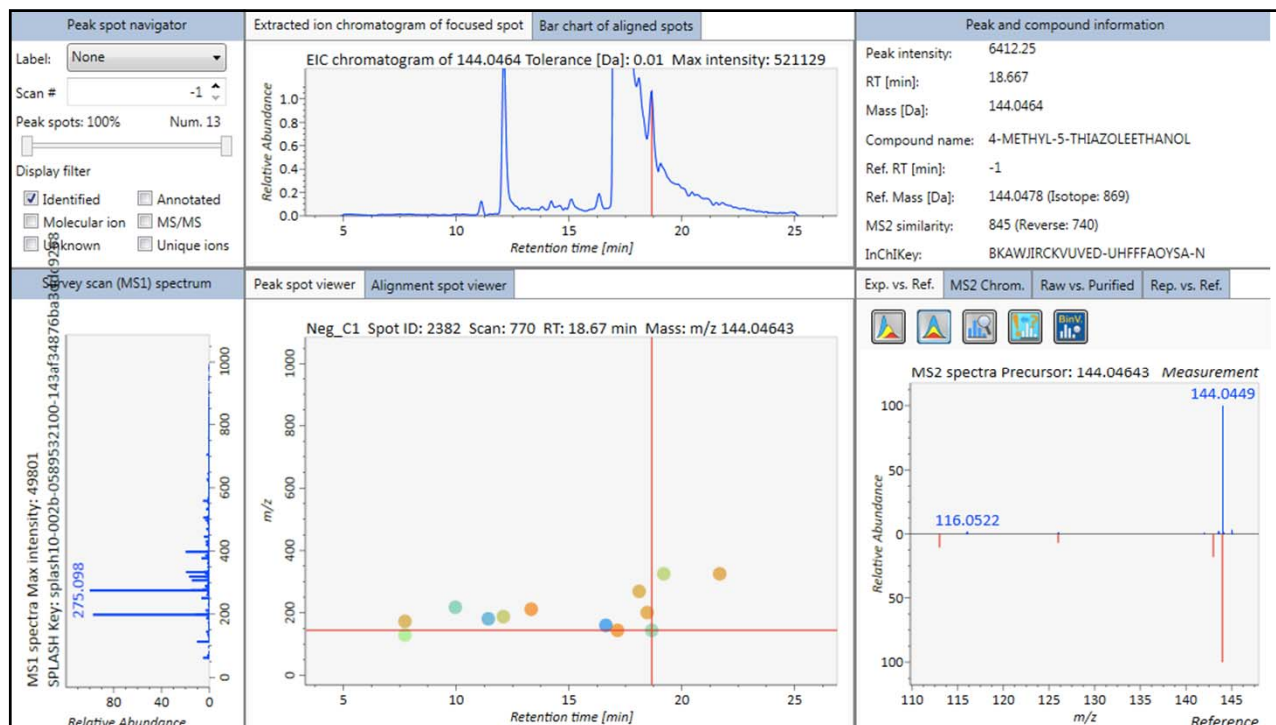
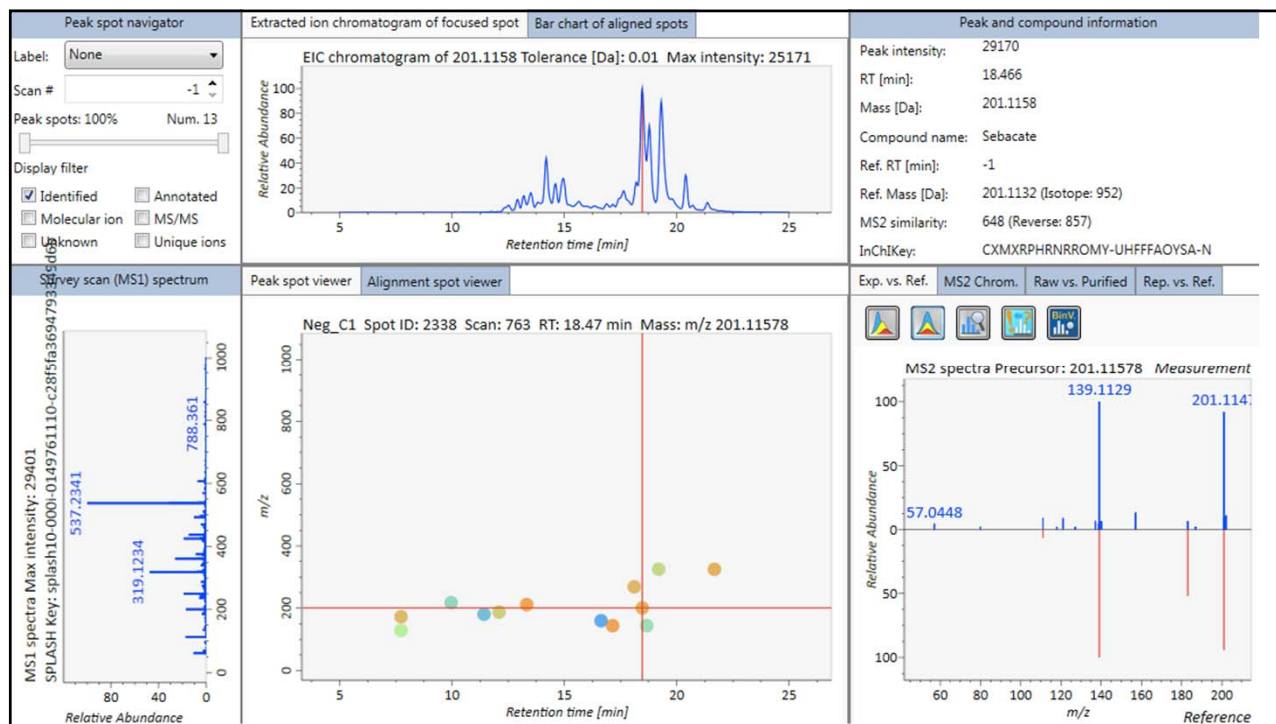


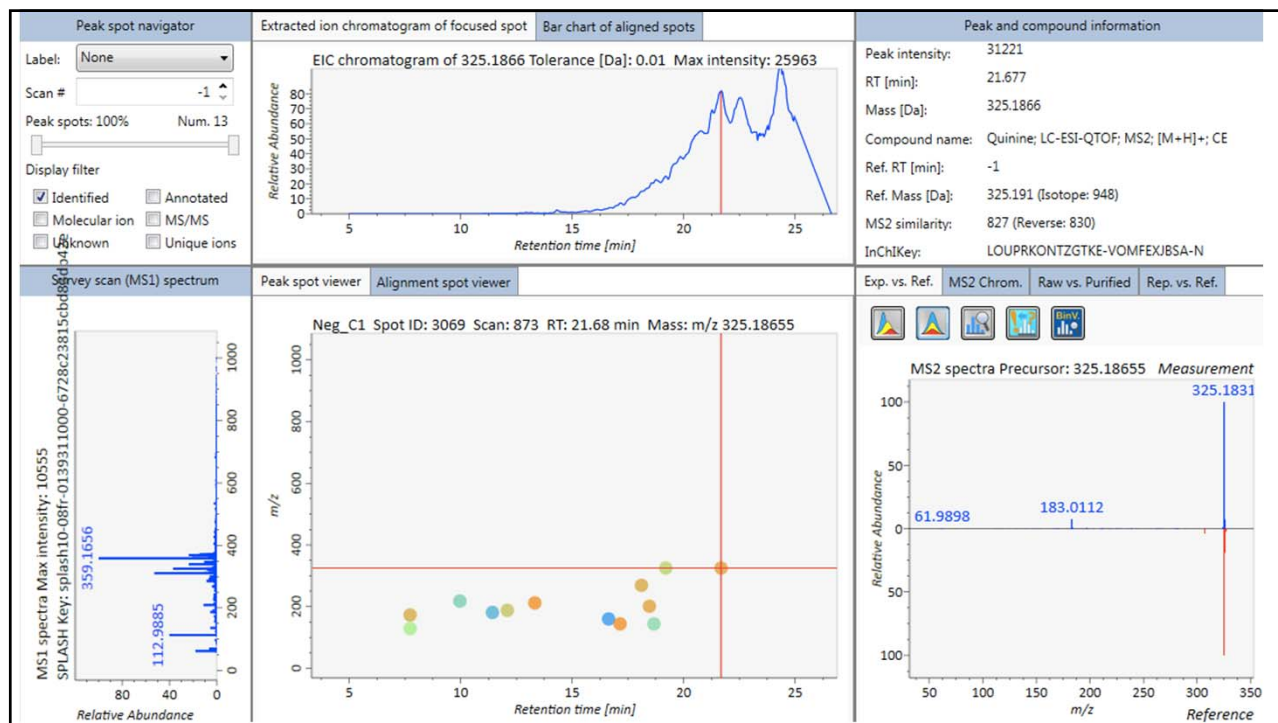
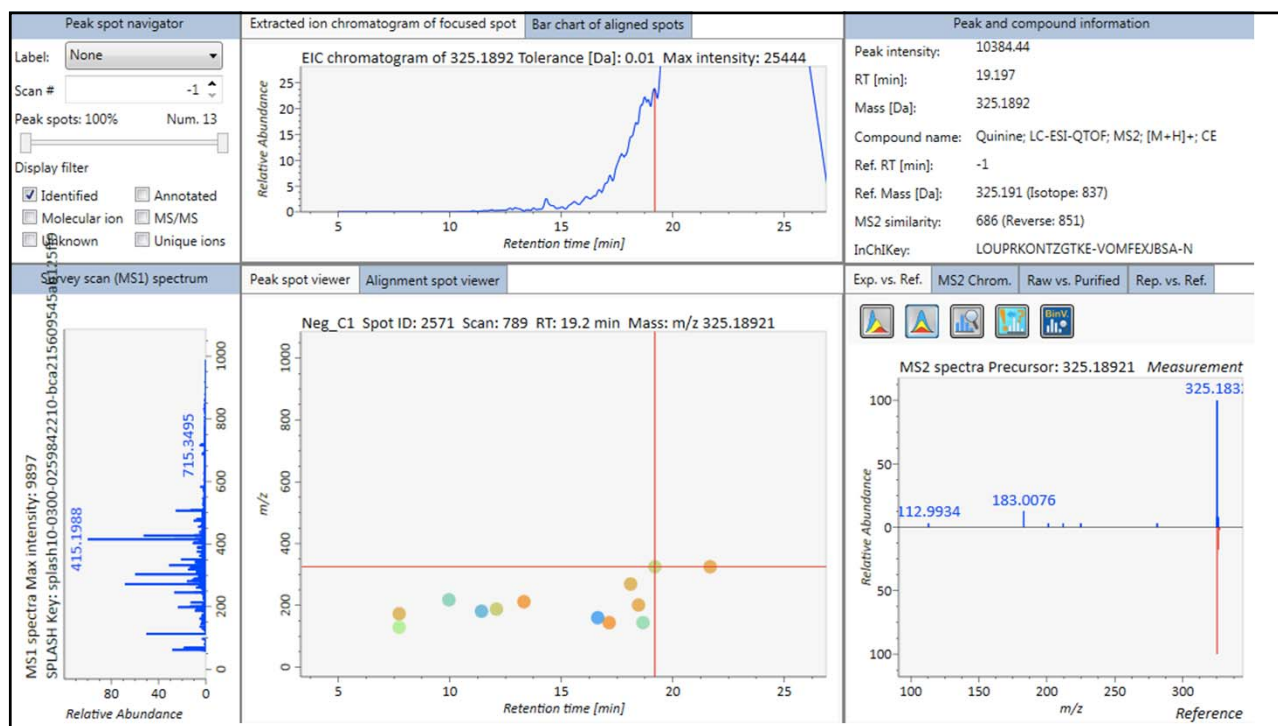


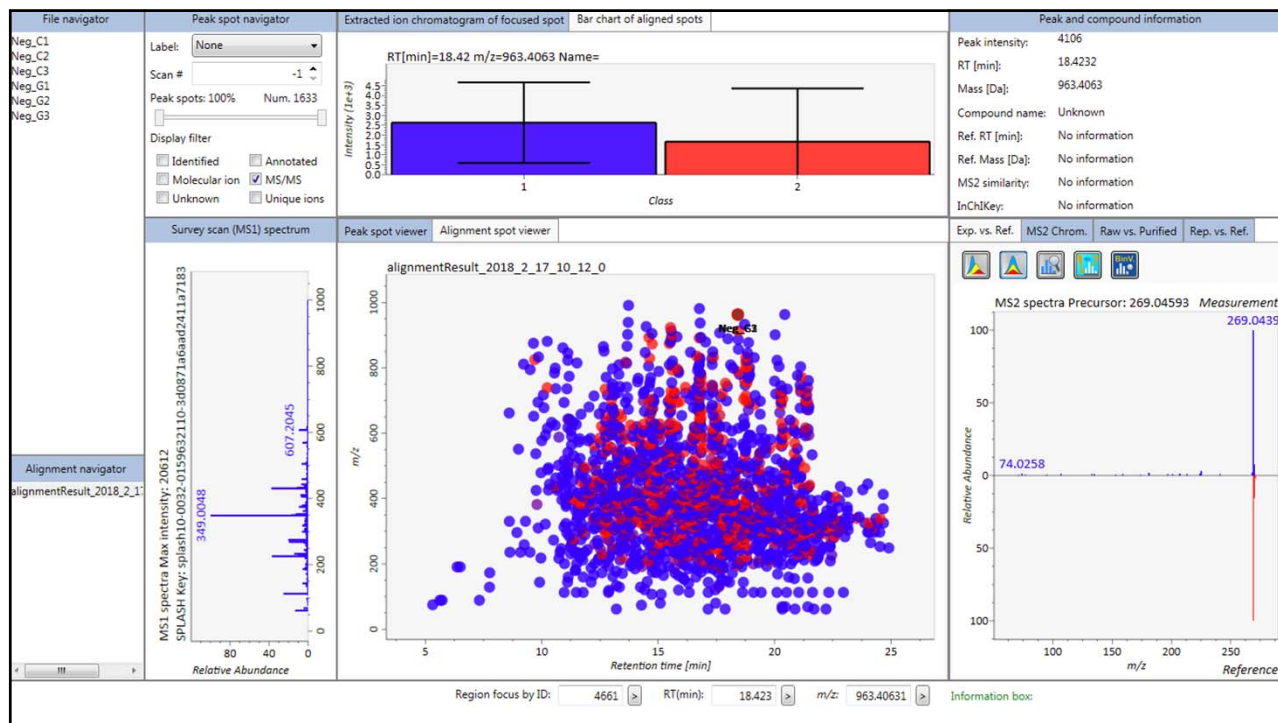
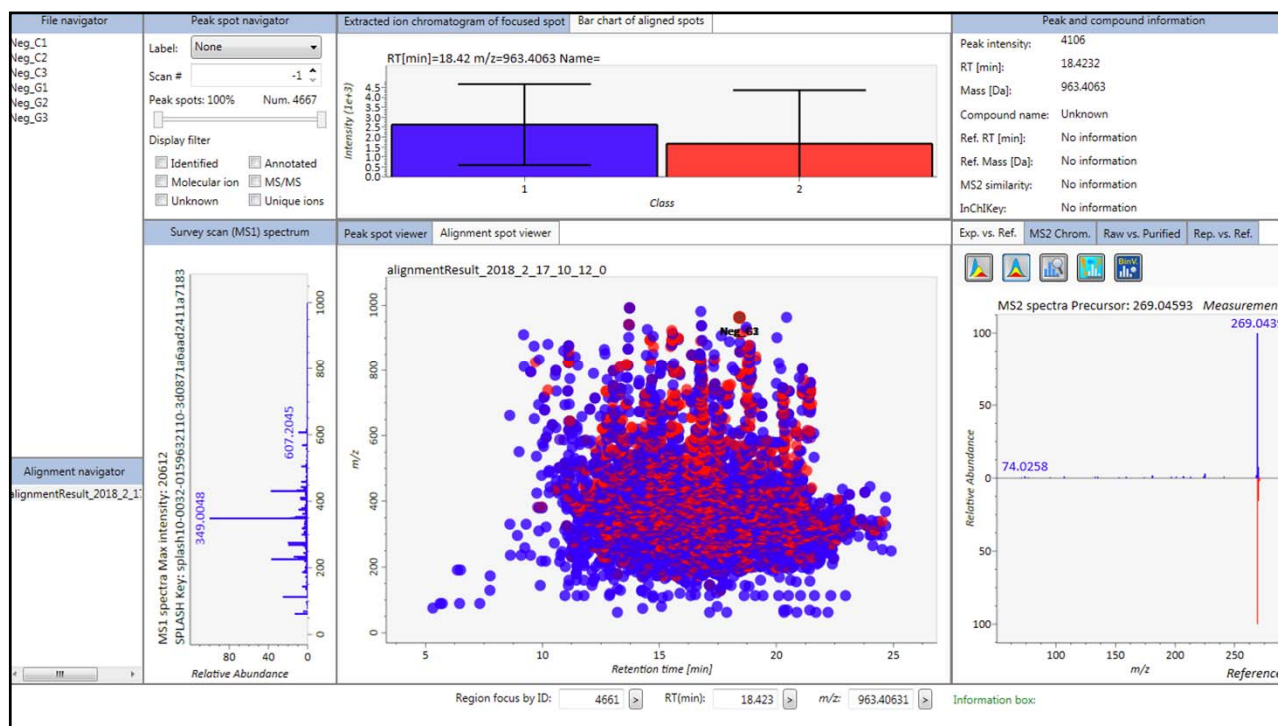


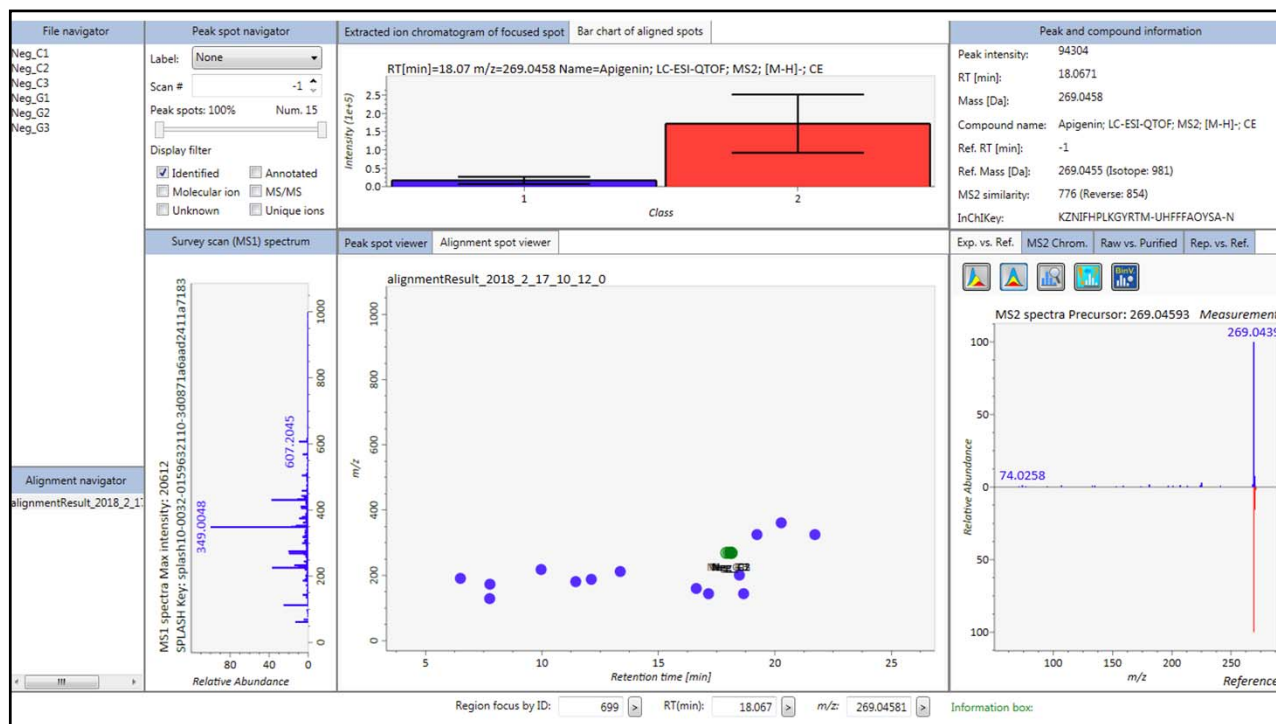




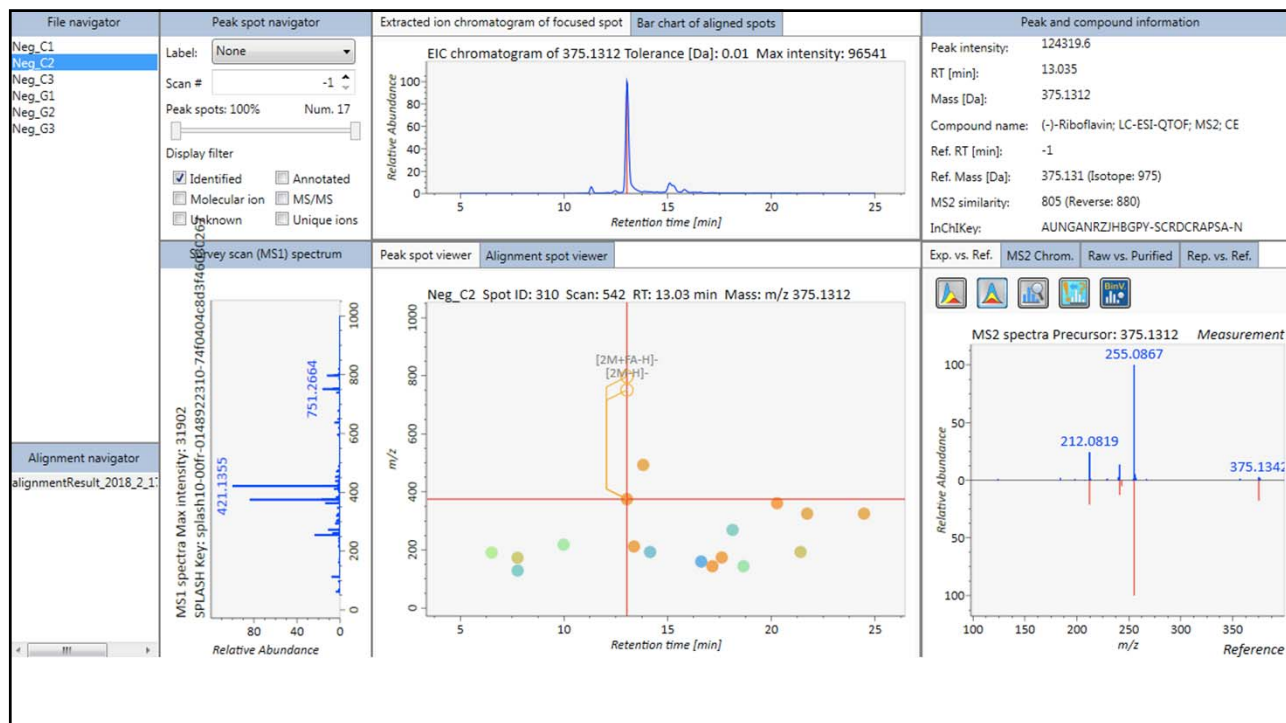
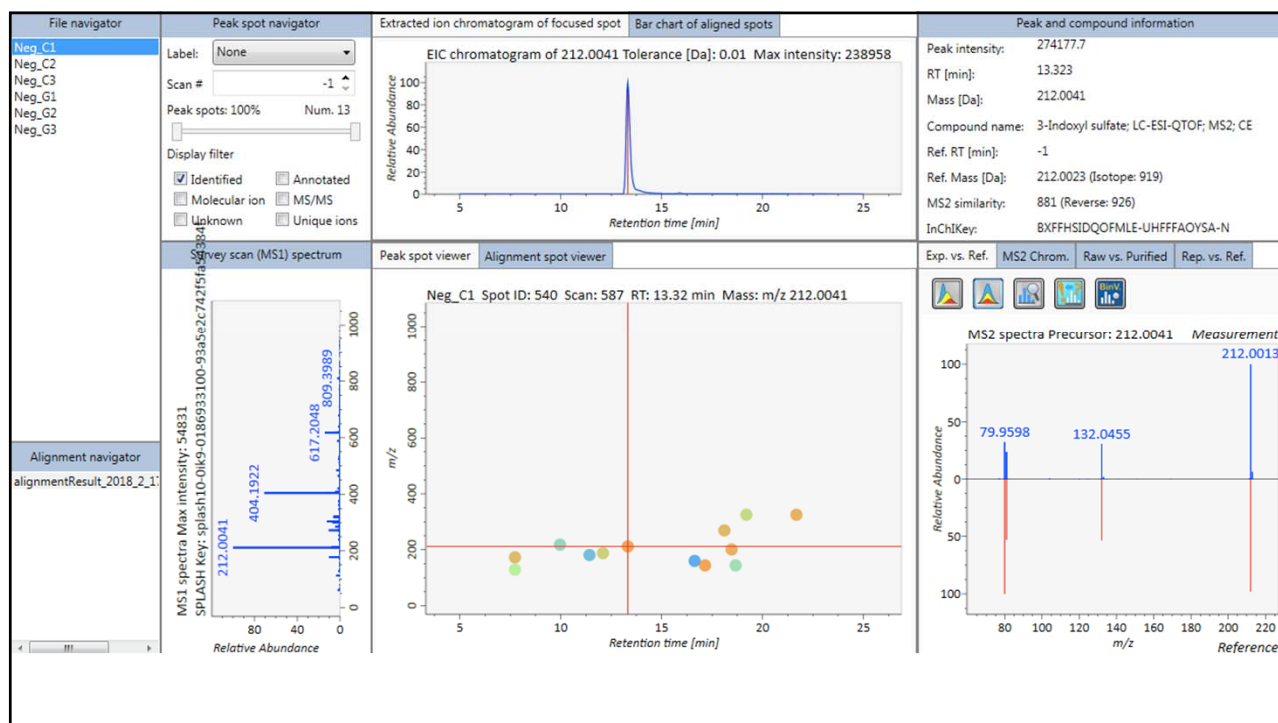


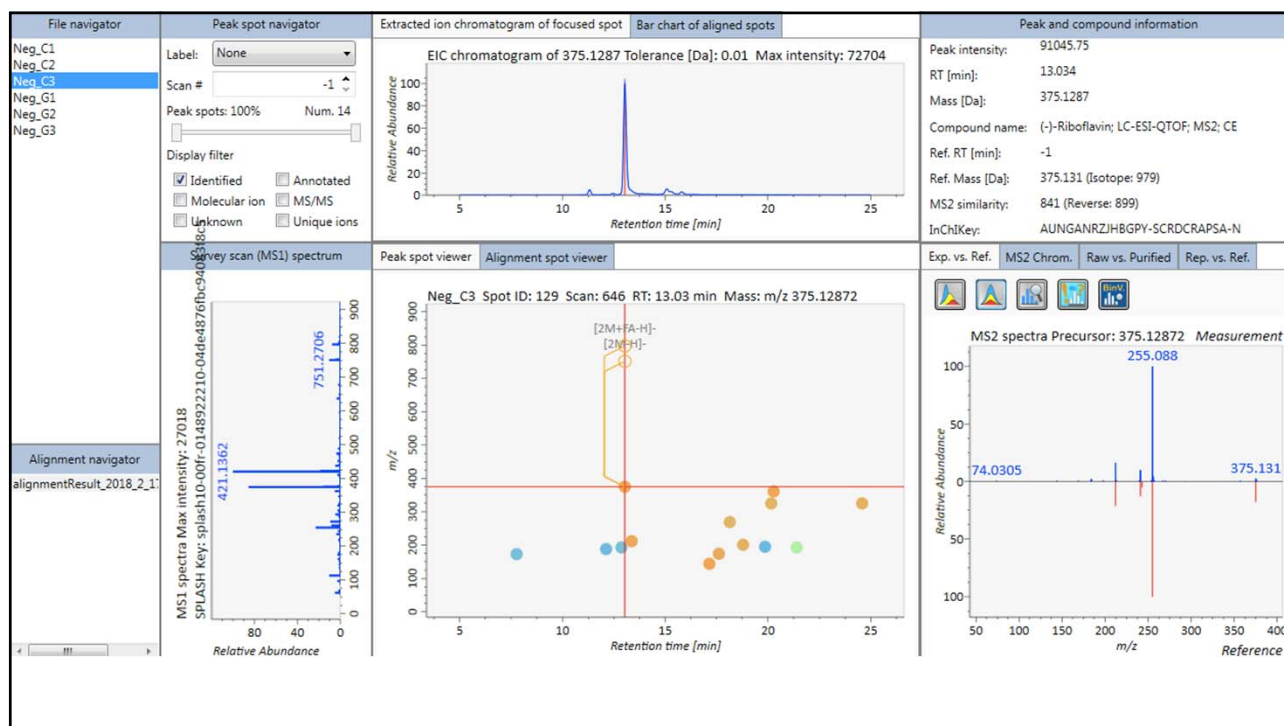






Mice on the control diet





Mice on the genistein diet

