Knowledge that will change your world

Analyzing metabolomics data sets with MS-DIAL

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MS-DIAL

- A Windows-based program that can be used in discovery and quantitative analysis of metabolomics data
- Freely downloadable
- Requires the conversion of raw MS and MSMS data into .abf format
- Can be used with metabolites databases developed by the authors and/or constructed by users
  - has to be in .msp format

MS-DIAL project

http://prime.psc.riken.jp/Metabolomics_Software/MS-DIAL/index.html

Program download

Main program is available from here. MS-DIAL program.

MS-DIAL tutorial is downloadable from here. MS-DIAL tutorial.

File converter is downloadable from here. File converter.
*2015/5/1: now we are fixing the converter program for Waters-MS. The problem will be fixed as soon as possible.

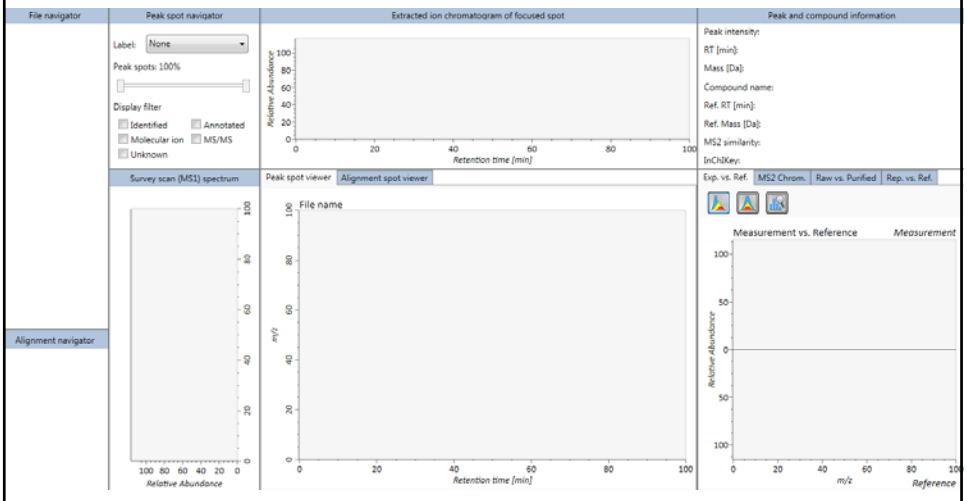
Demo files (.wiff and .wiff.scan, and the converted abf files) is available from here. data independent acquisition (SWATH) and data dependent acquisition (IDA) for algae lipidomics; Also see MSDIAL quick start

HILIC-SWATH-MS data (.wiff, .wiff.scan, and .abf) that we used for the explanation of mass spectral deconvolution is downloadable from here. HILIC(+)-SWATH-MS

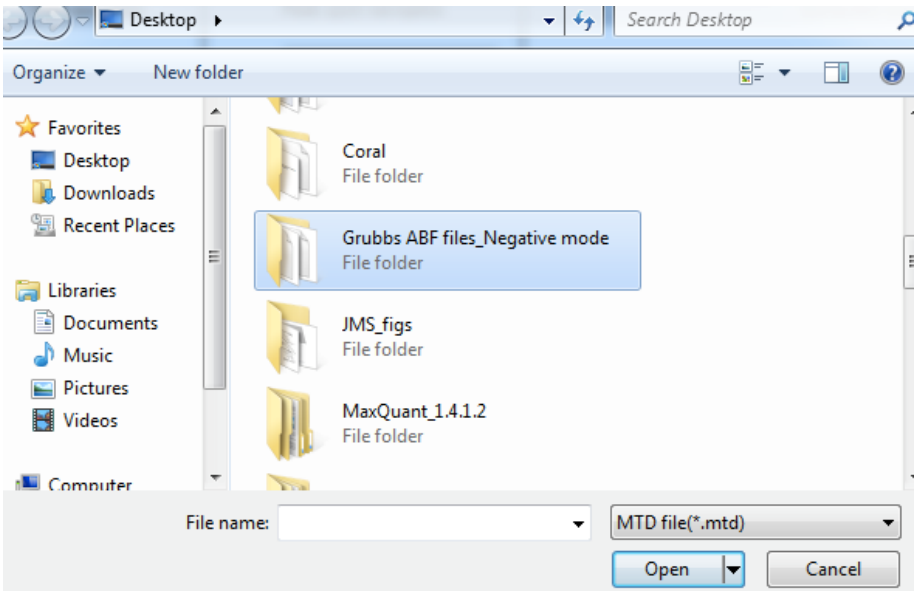
LipidBlast(fork version) excel macro that we used for the algae lipid profiling is downloadable from here.LipidBlast excel macro (fork version of) the original LipidBlast.

MS-DIAL mathematics is downloadable from here. MS-DIAL mathematics.

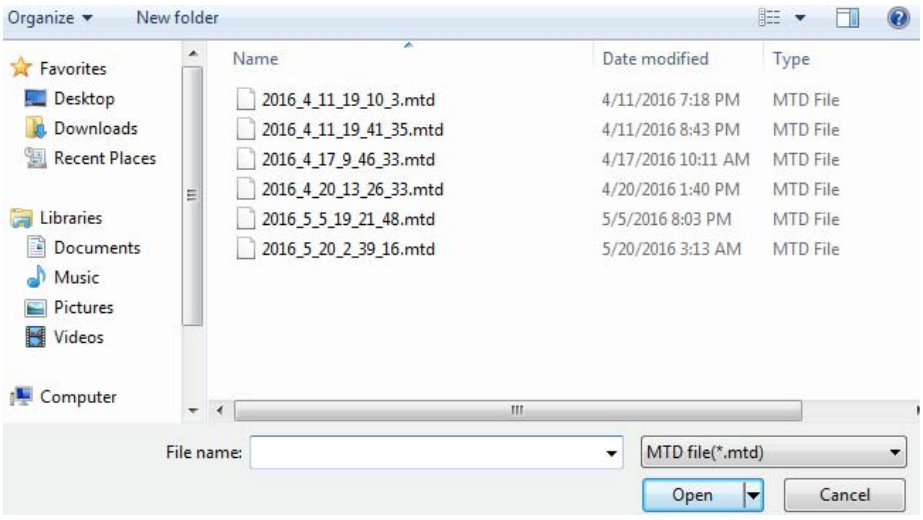
Basic page of MS-DIAL



You can open an existing file or a new one. Let's start with an existing one.

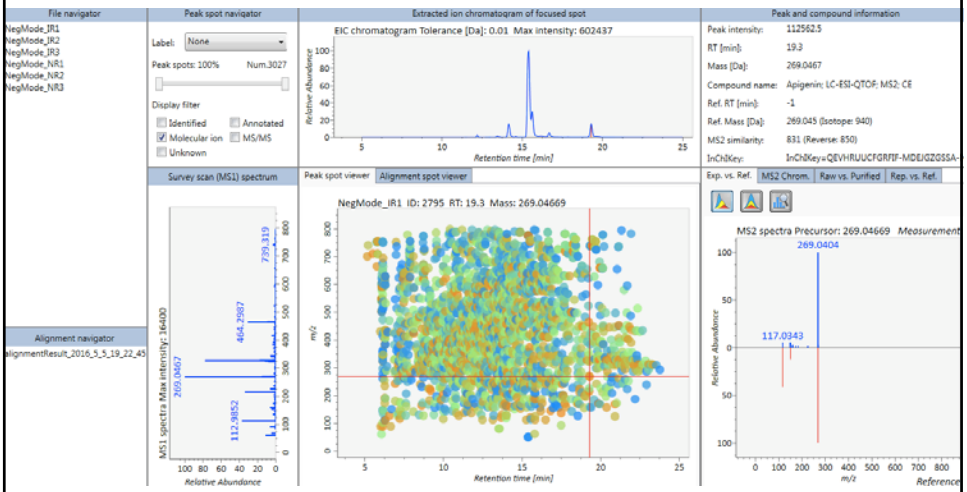


Previously saved files will be in .mtd format



The folder contains several .mtd files and one is selected

MS-DIAL output



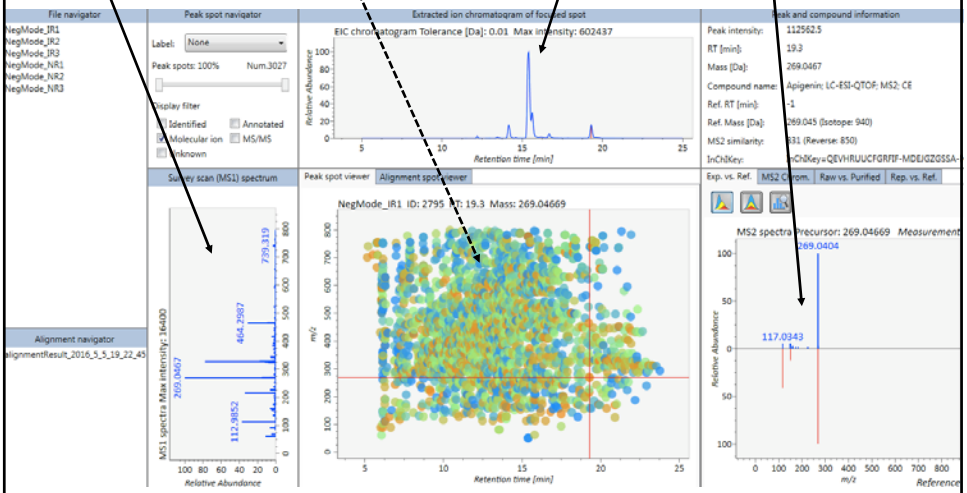
MS-DIAL output

XIC – selected ion chromatogram

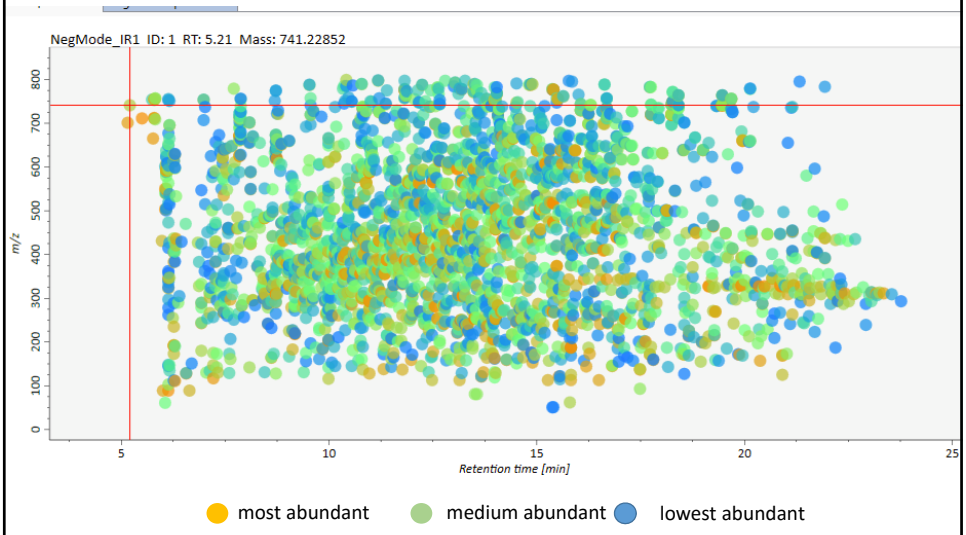
All detected peaks (*m/z* vs retention time)

MS1 spectrum

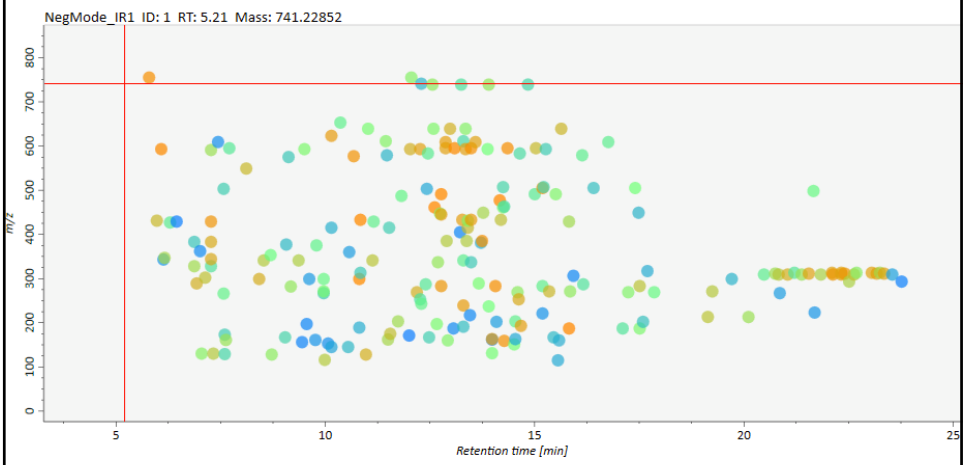
MSMS spectrum of target and database hit



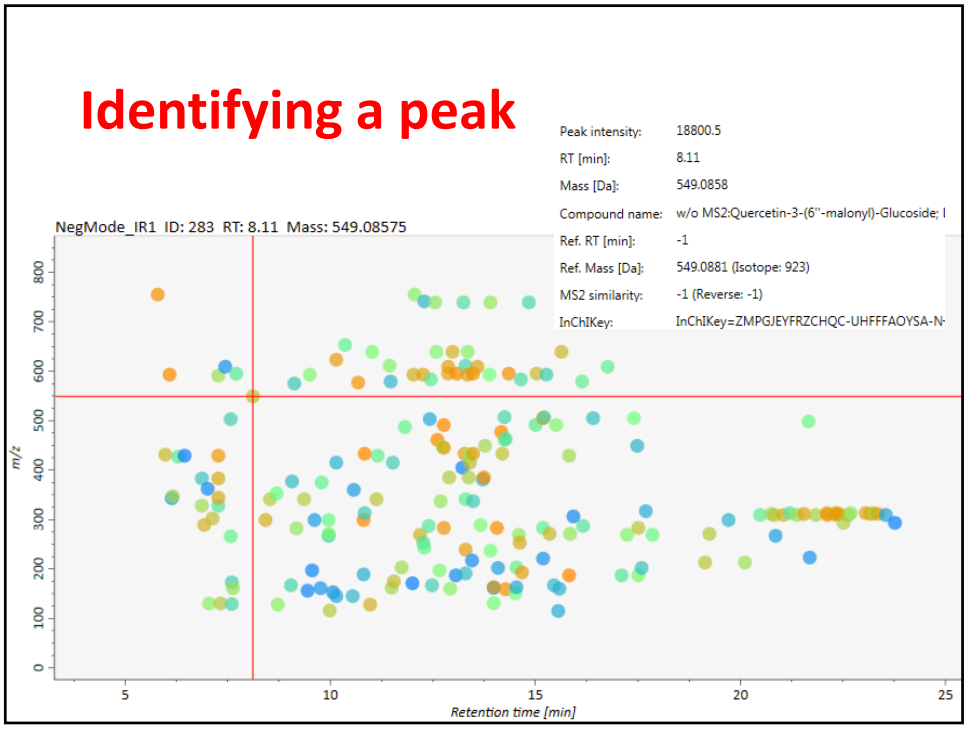
Contour plot of all the data



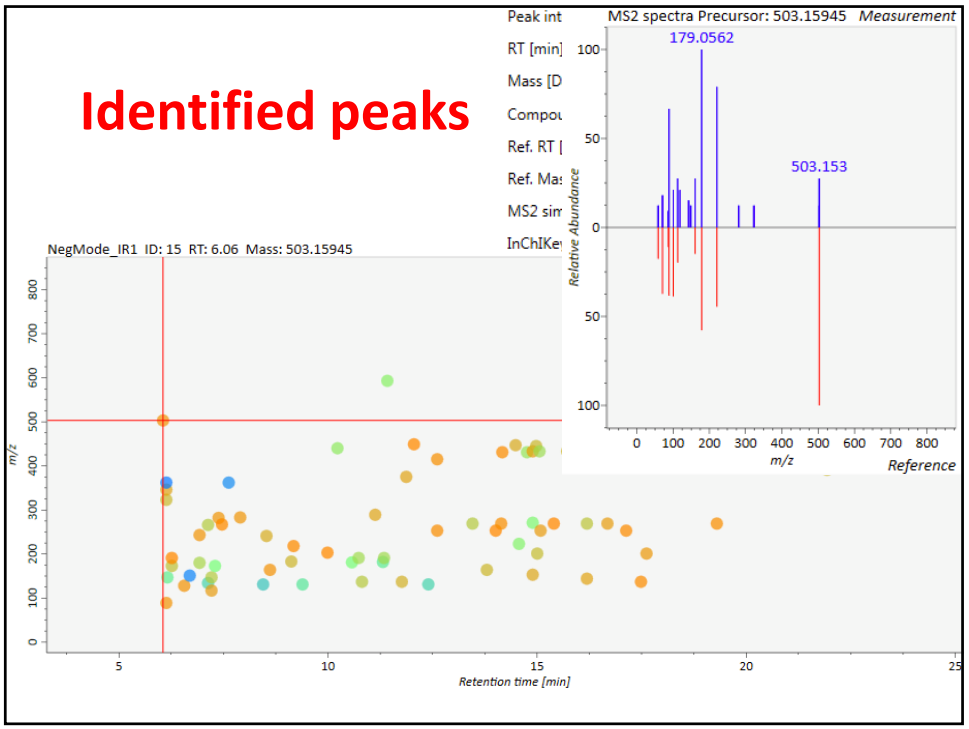
Annotated peaks



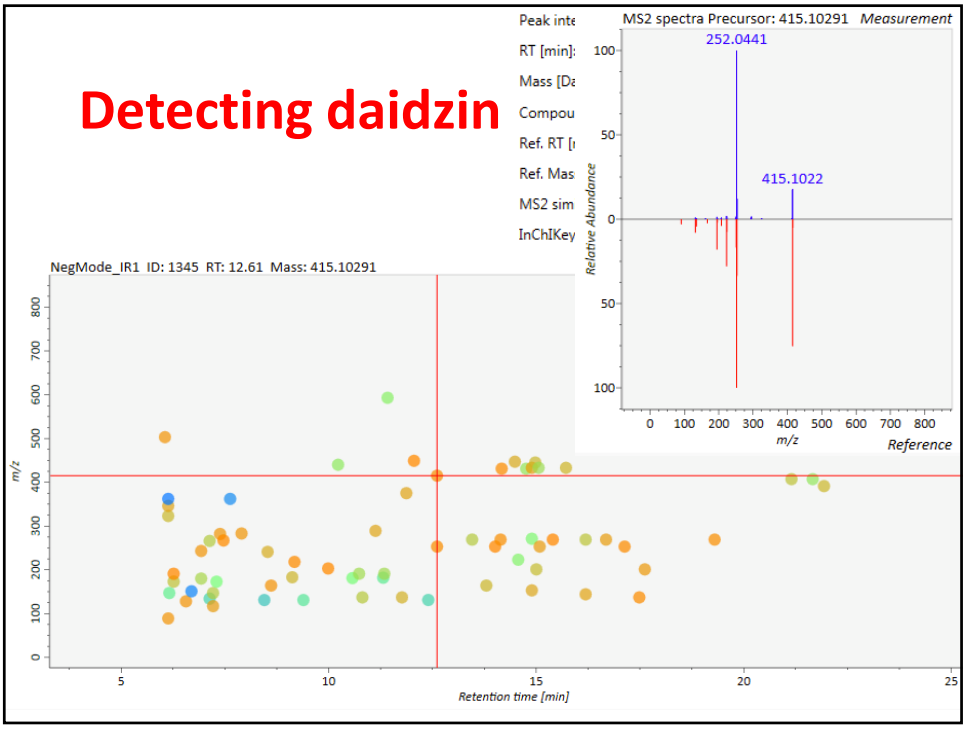
Identifying a peak



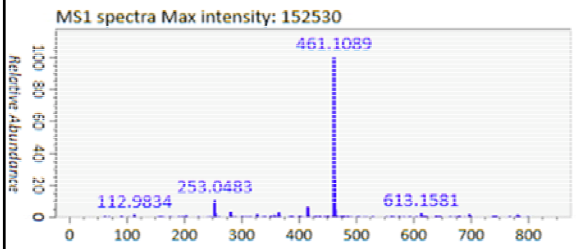
Identified peaks



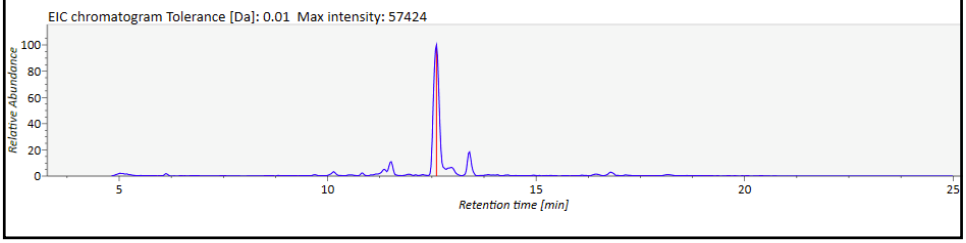
Detecting daidzin



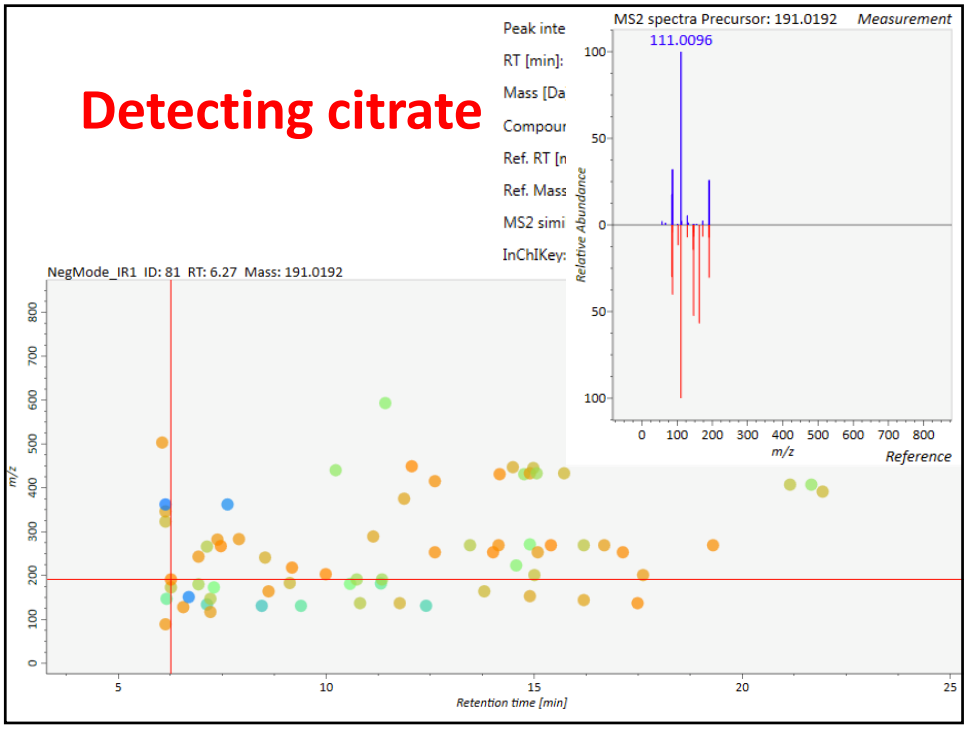
Additional data for daidzin



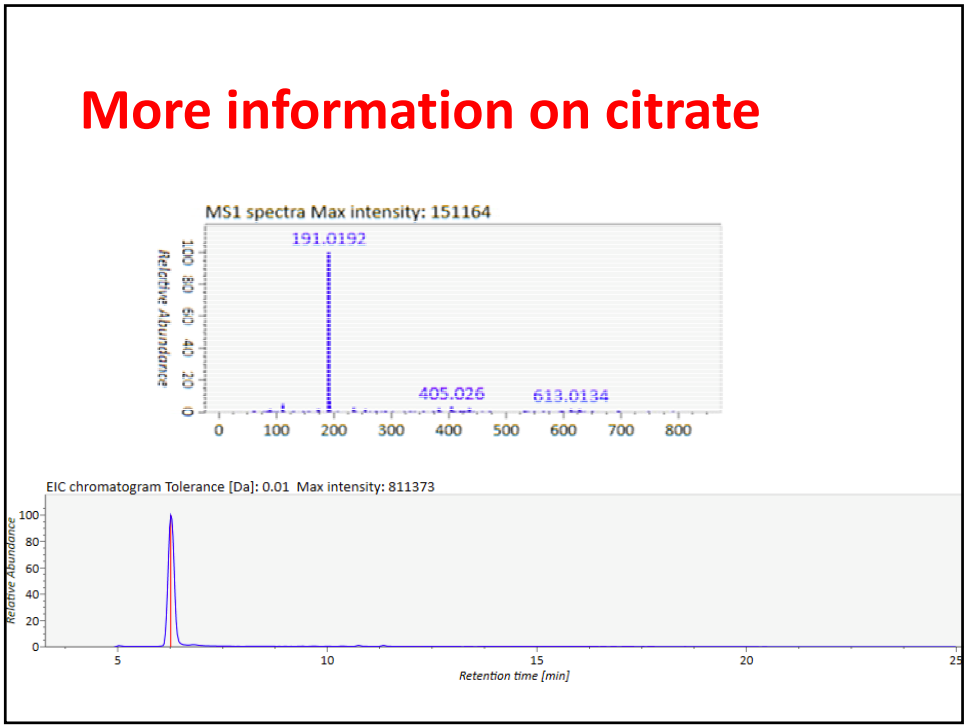
This is the mass spectrum collected at the top of the EIC peak. The major ion is *m/z* 461.1089 and is the formic acid adduct $[M+FA-H]^-$



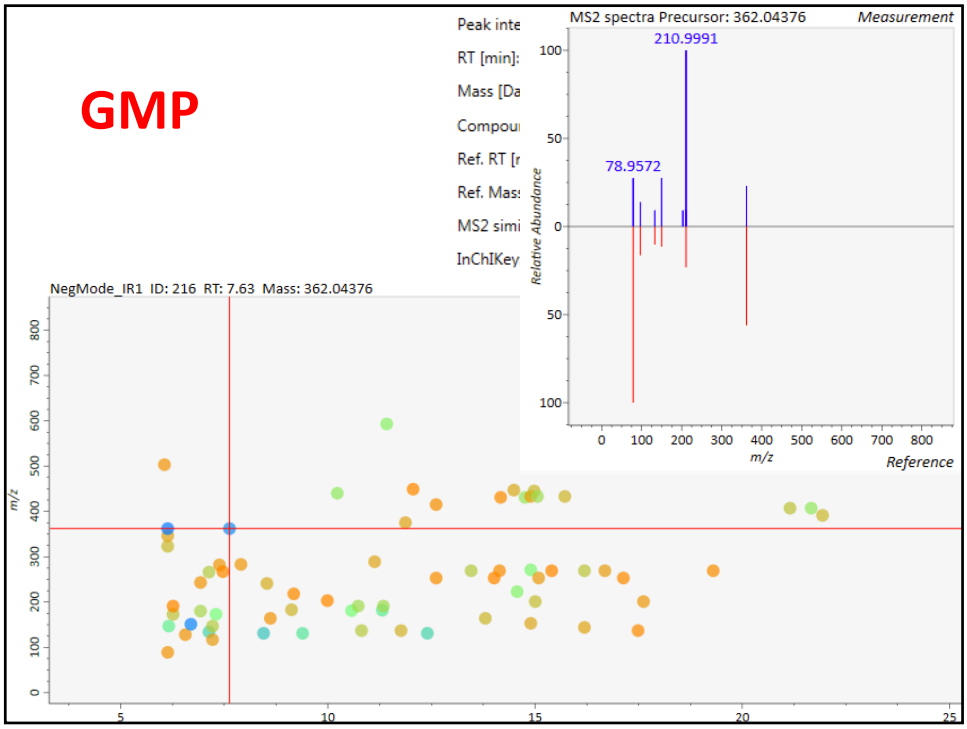
Detecting citrate



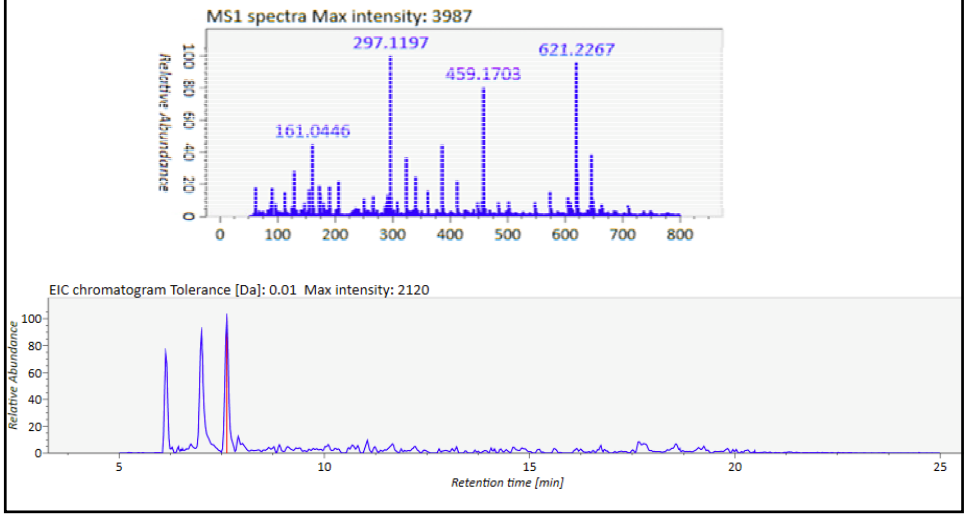
More information on citrate



GMP



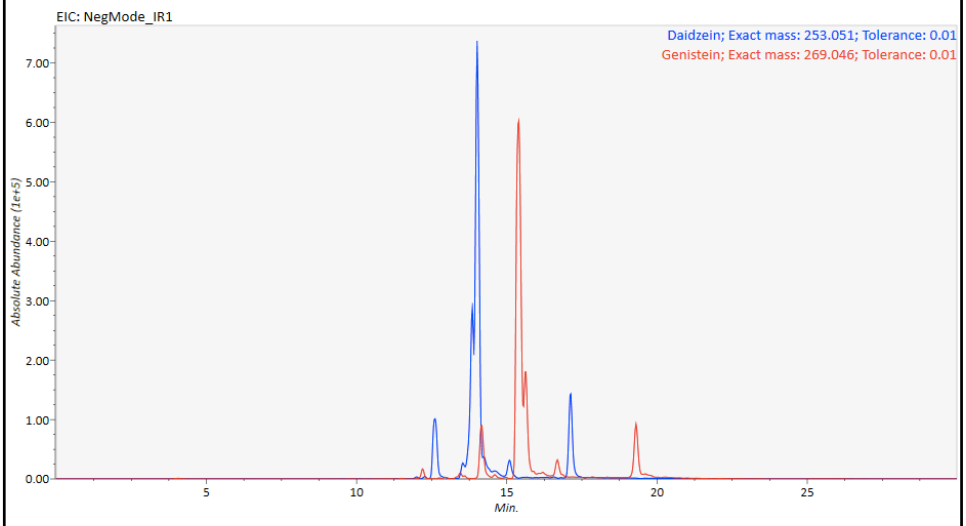
More info on GMP



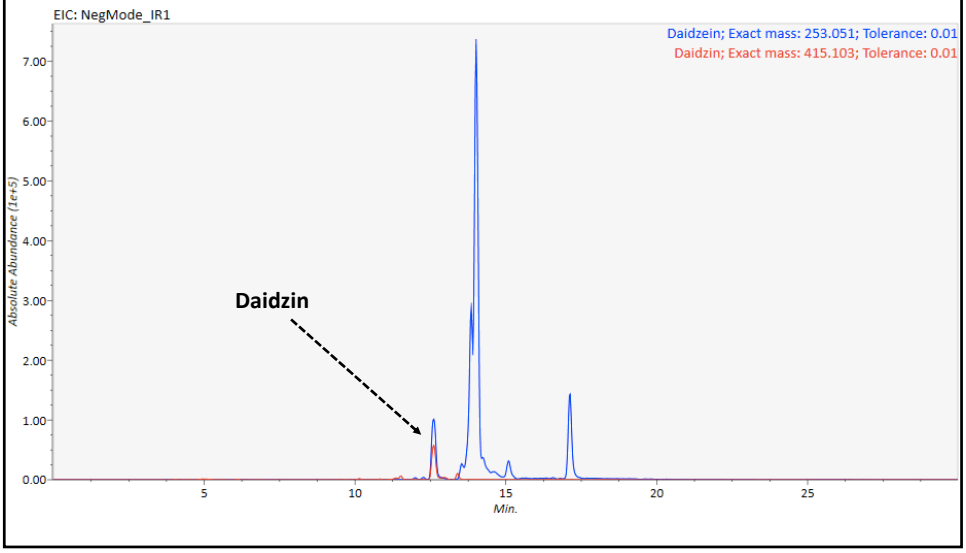
Selecting ions for known metabolites

• Daidzein	253.051
• Daidzin	415.103
• Genistein	269.046
• Genistin	431.099
• Folic acid	440.132
• Pantothenate	218.103
• Riboflavin	375.131
• Cholic acid	407.280
• Taurocholate	514.285
• Glycocholate	465.302
• Deoxycholate	391.285

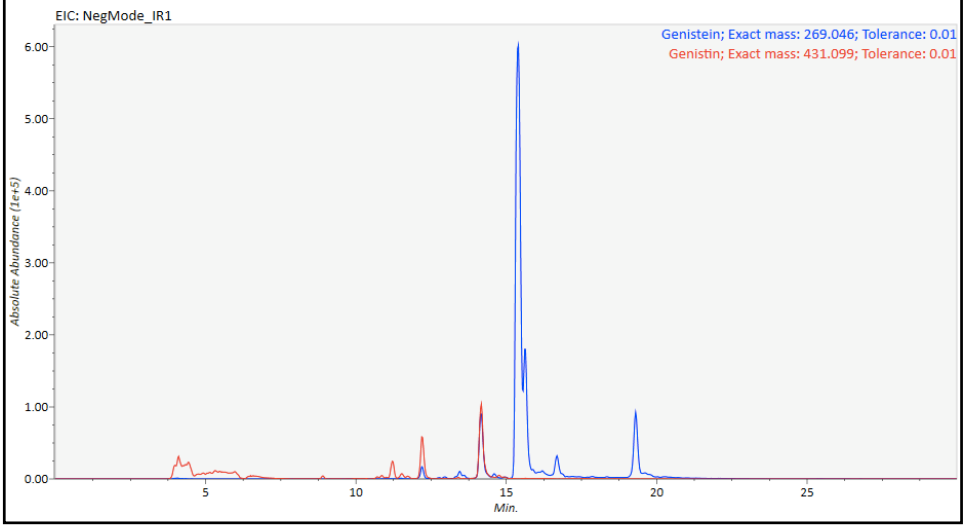
Two isoflavones as aglycones



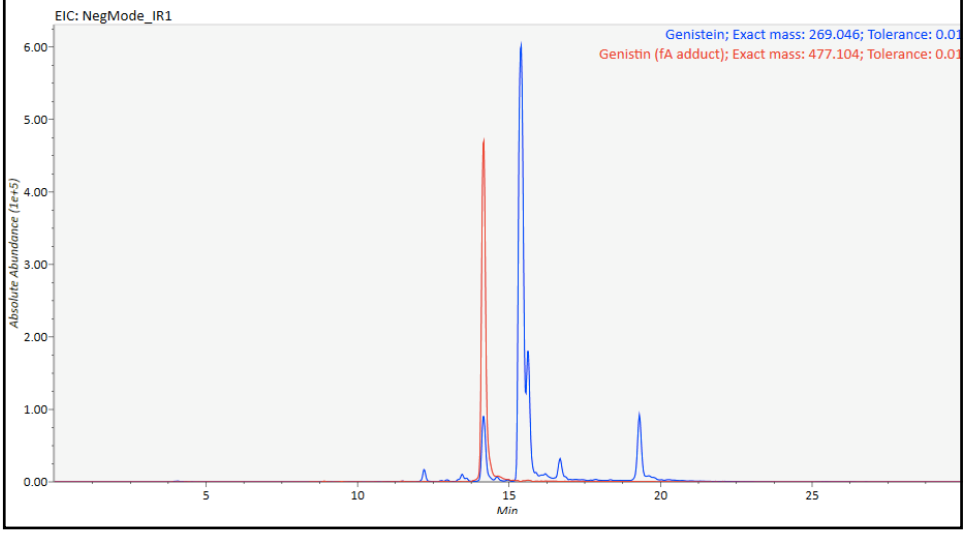
Localizing the daidzin peak



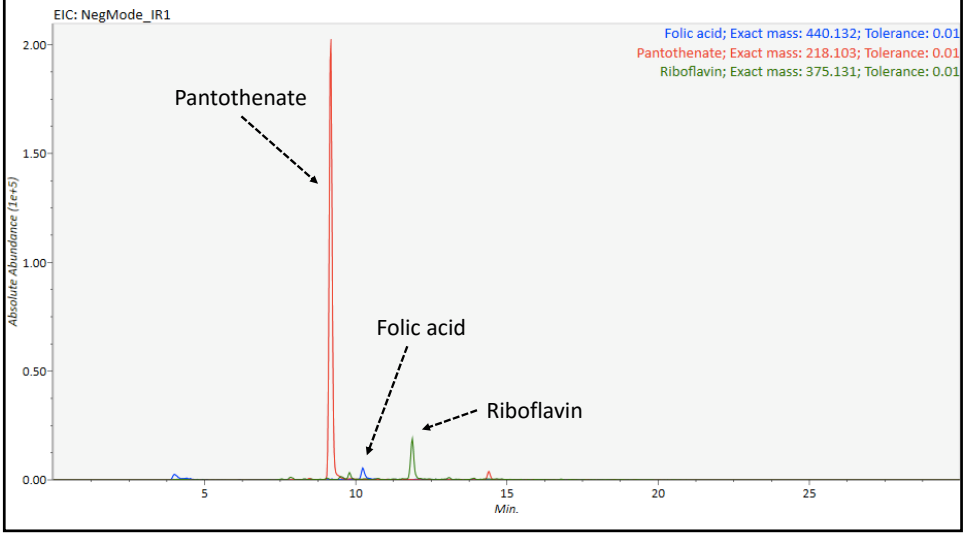
Genistin and genistein peaks



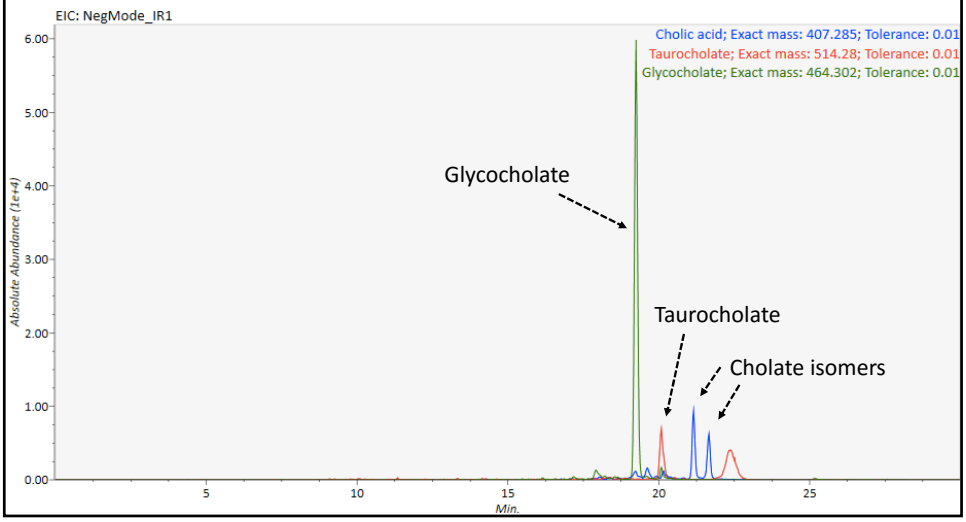
Genistin forms a FA adduct



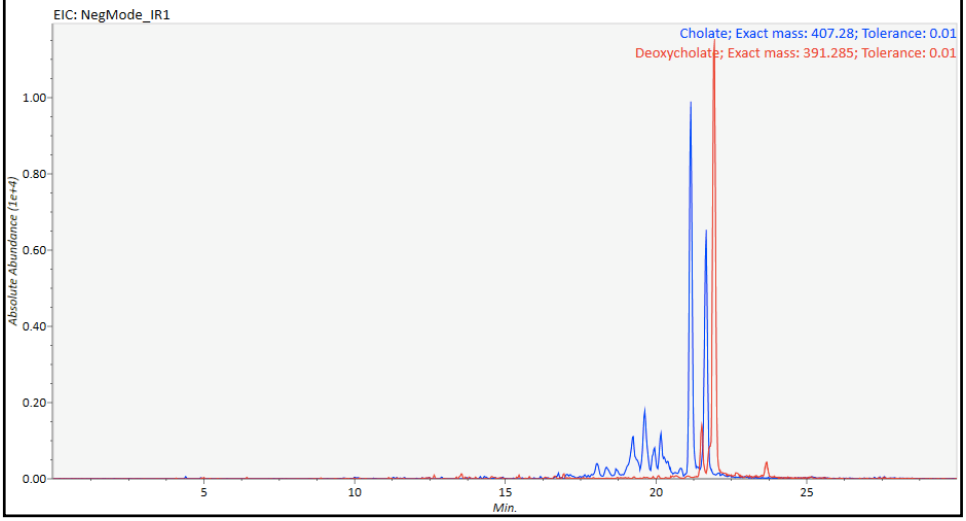
Vitamins



Bile acids



Cholate and deoxycholate isomers



Access to data files at Riken

- http://prime.psc.riken.jp/?action=drop_index

- **This website has a large number of downloadable data files, including those in .abf format**
- **Besides data-dependent data acquisition (DDA) data files, there are also SWATH-MS files where data-independent data acquisition (IDA)**
- **The latter allow for quantitative data collection (poly MRM-MS).**