# SUMMARY REPORT

## Analysis Information

| | | | |
|---|---|---|---|
| Item name: | POS_SCREENING POLAR_Flavanoid Glycoside Tannin_Alia IIUM | Analysis Method Item name: | POS_SCREENING POLAR_PDA |
| Version: | 1 | Analysis Method Version: | 1 |
| Modified date: | Sep 21, 2020 16:46:46 Malay Peninsula Standard Time | Sample Set Created date: | Sep 09, 2020 10:31:41 Malay Peninsula Standard Time |
| Modified by: | Fashiha, Siti | Sample Set Instrument system name: | Vion_BSM_SMFTN_PDA |
| Folder: | Company/Central Lab/External/2020 | | |

## Sample Information

| | | | |
|---|---|---|---|
| Item name: | blank water_01 | Sample type: | Blank |
| Item description: | | Sample position: | 1:B,1 |
| Item name: | sample 2_01 | Sample type: | Unknown |
| Item description: | | Sample position: | 1:B,3 |

## Experimental Record : blank water_01

### I-Class Binary Solvent Manager

#### General

Solvent Name A: Water +0.1%Formic Acid

Solvent Name B: Acetonitrile

Solvent Selection A: A1

Solvent Selection B: B1

Comment:

Seal Wash Period: 5.000 min

Gradient start: At injection

Pre-Injector Volume: 0 µL

2D Repeat Enabled: No

High Pressure Limit: 18000 psi

Low Pressure Limit: 0 psi

Gradient Table

| Time (min) | Flow Rate (mL/min) | Composition A (%) | Composition B (%) | Curve |
|---|---|---|---|---|
| 0.00 | 0.500 | 99.0 | 1.0 | Initial |
| 0.50 | 0.500 | 99.0 | 1.0 | 6 |
| 16.00 | 0.500 | 65.0 | 35.0 | 6 |
| 18.00 | 0.500 | 0.0 | 100.0 | 1 |
| 20.00 | 0.500 | 99.0 | 1.0 | 1 |

### Data

System Pressure (psi) Channel Enabled: Yes

Flow Rate (mL/min) Channel Enabled: No

A Composition (%) Channel Enabled: No

B Composition (%) Channel Enabled: No

Primary A Pressure (psi) Channel Enabled: No

Accumulator A Pressure (psi) Channel Enabled: No

Primary B Pressure (psi) Channel Enabled: No

Accumulator B Pressure (psi) Channel Enabled: No

Degasser Pressure (psi) Channel Enabled: No

### Analog Out

Chart Out 1: Flow Rate

Chart Out 2: Flow Rate

### Events

Initial Switch 1: No Change

Initial Switch 2: No Change

Initial Switch 3: No Change

Pre-Analysis mode: No

Run Events: No

## PDA Detector

## General

Lamp state: On

Sampling rate: 10 points/sec

Filter Time Constant Mode: No filter

Filter Time Constant: N/A

Exposure Time: Auto

Interpolate 2nd Order Filter (340 nm) Region: No

Use UV Blocking Filter: No

Negative absorbance margin: -0.07 AU

### 3D Channel

Start Wavelength: 190 nm

End Wavelength: 500 nm

Resolution: 1.2 nm

Comment:

## 2D Channel Table

| Channel | Data mode | Spectral channel resolution | Wavelength 1 (nm) | Wavelength 2 (nm) | Minimum channel ratio |
|---|---|---|---|---|---|
| Channel 1 | Absorbance | 1.2 | 254 | | |

## Analog Out

### Output 1

Channel: 1: Absorbance : 254 nm

Ratio Full Scale: 100

Voltage Offset: 0 mV

Full Scale Range: 4.000 units

Full Scale Voltage: 2000 mV

## Events

### Switch 1

Initial Switch 1: No Change

Threshold State: On

Pulse width: 1 sec

Run Events: No

Threshold event: Channel: 1: Absorbance : 254 nm

Threshold Level: 1.000 AU

Rect wave period: 0.2 sec

## Sample Manager FTN

### General

Wash Solvent: H2O:MEOH:ACN:IPA 1:1:1:1

Wash Solvent Post Inject: 5 s

Load Ahead: Disabled

Column Temperature Enable: Yes

Column Temperature Alarm: No

Sample Temperature: 20.0 °C

Comment:

Wash Solvent Pre Inject: 0 s

Purge Solvent: 90:10 Water/MeOH

Loop Offline: Disabled

Column Temperature: 40.0 °C

Sample Temperature Enable: Yes

Sample Temperature Alarm Enable: No

### Data

Sample Temperature (°C) Channel Enabled: Yes

Ambient Temperature (°C) Channel Enabled: Yes

Seal Force (%) Channel Enabled: No

Column Temperature (°C) Channel Enabled: No

Sample Pressure (psi) Channel Enabled: No

Pre Heater Temperature (°C) Channel Enabled: No

### Dilution

Dilution Enable: Disabled

Dilution Dispense Purge Solvent: Disabled

Needle Placement (from bottom): Disabled

Post Dilution Delay: Disabled

### Events

Run Events: No

### Advanced

Syringe Draw Rate: Automatic

Pre Aspirate Air: Automatic

Mix Stroke Cycles: Automatic

Needle Placement (from bottom): 2.0 mm

Post Aspirate Air: Automatic

Mix Stroke Volume: Automatic

## Vion IMS QTof

Instrument software build: 2.0.0

## Method

Polarity: Positive

Analyzer mode: Sensitivity

## Function 1 : MS$^{E}$

Mode: High Definition MS$^{E}$

End time: 20.00 min

High mass: 1000 m/z

Low collision energy: 4.00 eV

High collision energy ramp end: 40.00 eV

Intensity threshold: 10000 counts

Start time: 0.00 min

Low mass: 50 m/z

Scan time: 0.200 s

High collision energy ramp start: 10.00 eV

Enable Tof data reduction on acquired data: Yes

## Source parameters

Source type: ESI

Desolvation temperature: 550 °C

Desolvation gas: 800 L/h

Source temperature: 120 °C

Cone gas: 50 L/h

Capillary voltage: 2.50 kV

## Lock correction

Mode: Automatic

Automatic sampling interval: Yes

## Options

Acquisition check failure: Stop acquisition

Automatic detector check: Disabled

## Events

| Time (min) | Event | Parameters |
|---|---|---|
| Initial | Flow state | LC, Sample |
| Initial | Infusion | Start, Reference |
| Initial | Refill | Refill always, Reference |
| Initial | Reservoir | B, Reference |

### Method trigger

Trigger type: Network

Event input 1: Enabled

Event input 2: Disabled

## Experimental Record : sample 2_01

### I-Class Binary Solvent Manager

#### General

Solvent Name A: Water +0.1%Formic Acid

Solvent Name B: Acetonitrile

Solvent Selection A: A1

Solvent Selection B: B1

Comment:

Seal Wash Period: 5.000 min

Gradient start: At injection

Pre-Injector Volume: 0 µL

2D Repeat Enabled: No

High Pressure Limit: 18000 psi

Low Pressure Limit: 0 psi

Gradient Table

| Time (min) | Flow Rate (mL/min) | Composition A (%) | Composition B (%) | Curve |
|---|---|---|---|---|
| 0.00 | 0.500 | 99.0 | 1.0 | Initial |
| 0.50 | 0.500 | 99.0 | 1.0 | 6 |
| 16.00 | 0.500 | 65.0 | 35.0 | 6 |
| 18.00 | 0.500 | 0.0 | 100.0 | 1 |
| 20.00 | 0.500 | 99.0 | 1.0 | 1 |

#### Data

System Pressure (psi) Channel Enabled: Yes

Flow Rate (mL/min) Channel Enabled: No

A Composition (%) Channel Enabled: No

B Composition (%) Channel Enabled: No

Primary A Pressure (psi) Channel Enabled: No

Accumulator A Pressure (psi) Channel Enabled: No

Primary B Pressure (psi) Channel Enabled: No

Accumulator B Pressure (psi) Channel Enabled: No

Degasser Pressure (psi) Channel Enabled: No

### Analog Out

Chart Out 1: Flow Rate

Chart Out 2: Flow Rate

### Events

Initial Switch 1: No Change

Initial Switch 2: No Change

Initial Switch 3: No Change

Pre-Analysis mode: No

Run Events: No

## PDA Detector

## General

Lamp state: On

Sampling rate: 10 points/sec

Filter Time Constant Mode: No filter

Filter Time Constant: N/A

Exposure Time: Auto

Interpolate 2nd Order Filter (340 nm) Region: No

Use UV Blocking Filter: No

Negative absorbance margin: -0.07 AU

### 3D Channel

Start Wavelength: 190 nm

End Wavelength: 500 nm

Resolution: 1.2 nm

Comment:

## 2D Channel Table

| Channel | Data mode | Spectral channel resolution | Wavelength 1 (nm) | Wavelength 2 (nm) | Minimum channel ratio |
|---|---|---|---|---|---|
| Channel 1 | Absorbance | 1.2 | 254 | | |

## Analog Out

### Output 1

Channel: 1: Absorbance : 254 nm

Full Scale Range: 4.000 units

Ratio Full Scale: 100

Full Scale Voltage: 2000 mV

Voltage Offset: 0 mV

## Events

### Switch 1

Initial Switch 1: No Change

Threshold event: Channel: 1: Absorbance : 254 nm

Threshold State: On

Threshold Level: 1.000 AU

Pulse width: 1 sec

Rect wave period: 0.2 sec

Run Events: No

## Sample Manager FTN

### General

Wash Solvent: H2O:MEOH:ACN:IPA 1:1:1:1

Wash Solvent Pre Inject: 0 s

Wash Solvent Post Inject: 5 s

Purge Solvent: 90:10 Water/MeOH

Load Ahead: Disabled

Loop Offline: Disabled

Column Temperature Enable: Yes

Column Temperature: 40.0 °C

Column Temperature Alarm: No

Sample Temperature Enable: Yes

Sample Temperature: 20.0 °C

Sample Temperature Alarm Enable: No

Comment:

### Data

Sample Temperature (°C) Channel Enabled: Yes

Column Temperature (°C) Channel Enabled: No

Ambient Temperature (°C) Channel Enabled: Yes

Sample Pressure (psi) Channel Enabled: No

Seal Force (%) Channel Enabled: No

Pre Heater Temperature (°C) Channel Enabled: No

### Dilution

Dilution Enable: Disabled

Needle Placement (from bottom): Disabled

Dilution Dispense Purge Solvent: Disabled

Post Dilution Delay: Disabled

### Events

Run Events: No

### Advanced

Syringe Draw Rate: Automatic

Needle Placement (from bottom): 2.0 mm

Pre Aspirate Air: Automatic

Post Aspirate Air: Automatic

Mix Stroke Cycles: Automatic

Mix Stroke Volume: Automatic

## Vion IMS QTof

Instrument software build: 2.0.0

## Method

Polarity: Positive

Analyzer mode: Sensitivity

## Function 1 : MS$^{E}$

Mode: High Definition MS$^{E}$

Start time: 0.00 min

End time: 20.00 min

Low mass: 50 m/z

High mass: 1000 m/z

Scan time: 0.200 s

Low collision energy: 4.00 eV

High collision energy ramp start: 10.00 eV

High collision energy ramp end: 40.00 eV

Enable Tof data reduction on acquired data: Yes

Intensity threshold: 10000 counts

## Source parameters

Source type: ESI

Source temperature: 120 °C

Desolvation temperature: 550 °C

Cone gas: 50 L/h

Desolvation gas: 800 L/h

Capillary voltage: 2.50 kV

## Lock correction

Mode: Automatic

Automatic sampling interval: Yes

## Options

Acquisition check failure: Stop acquisition

Automatic detector check: Disabled

## Events

| Time (min) | Event | Parameters |
|---|---|---|
| Initial | Flow state | LC, Sample |
| Initial | Infusion | Start, Reference |
| Initial | Refill | Refill always, Reference |
| Initial | Reservoir | B, Reference |

## Method trigger

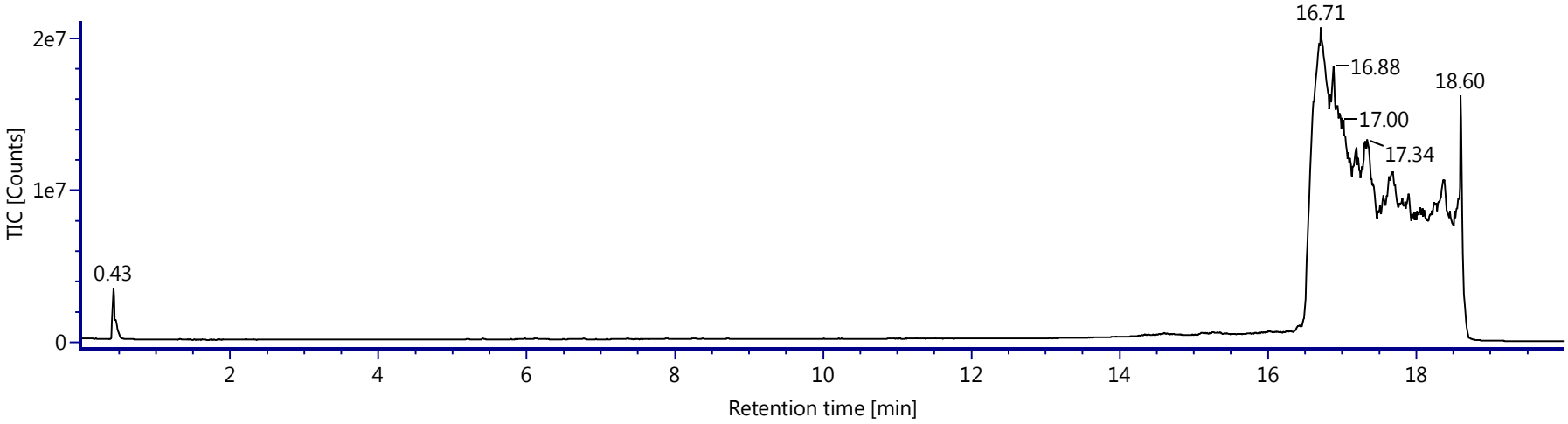
Trigger type: Network

Event input 1: Enabled

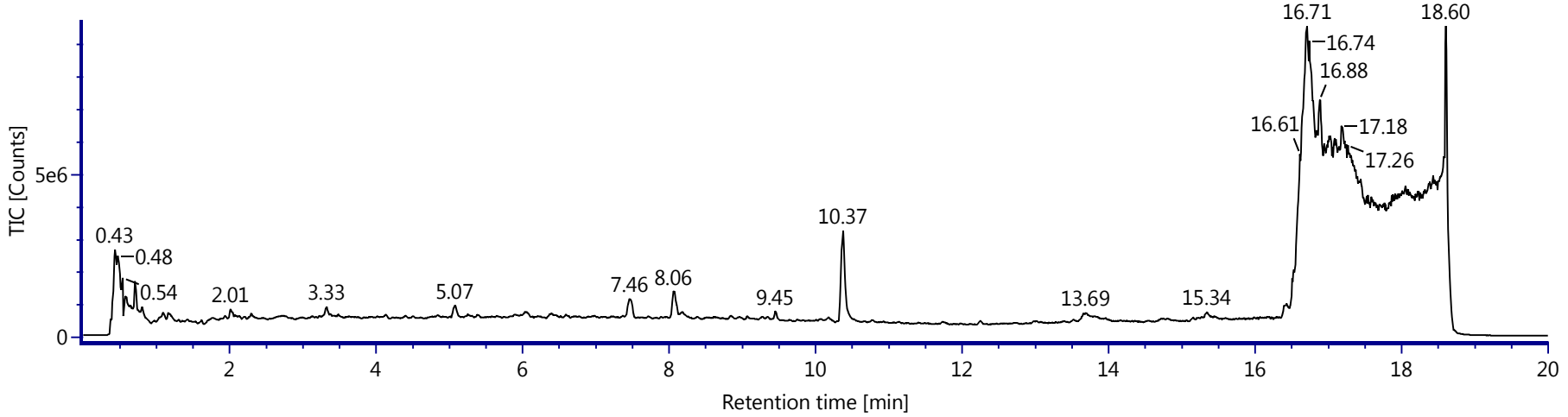
Event input 2: Disabled

# TIC Plot

**Item name: blank water_01**
**Channel name: 2: HD TOF MSe (50-1000) 4eV ESI+ (TIC)**

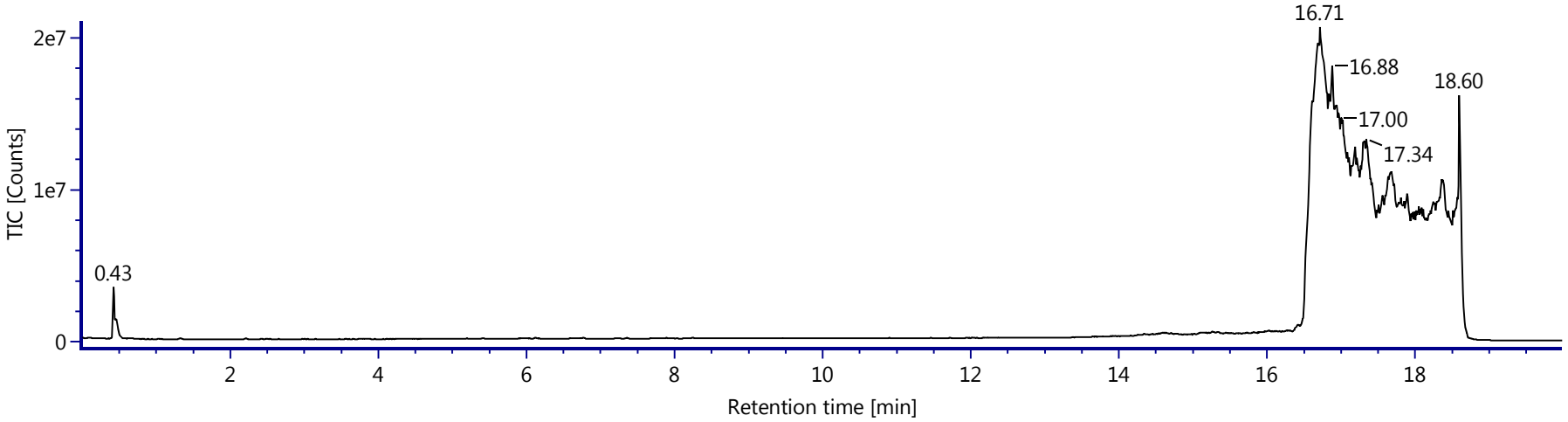



**Item name: sample 2_01**
**Channel name: 2: HD TOF MSe (50-1000) 4eV ESI+ (TIC)**

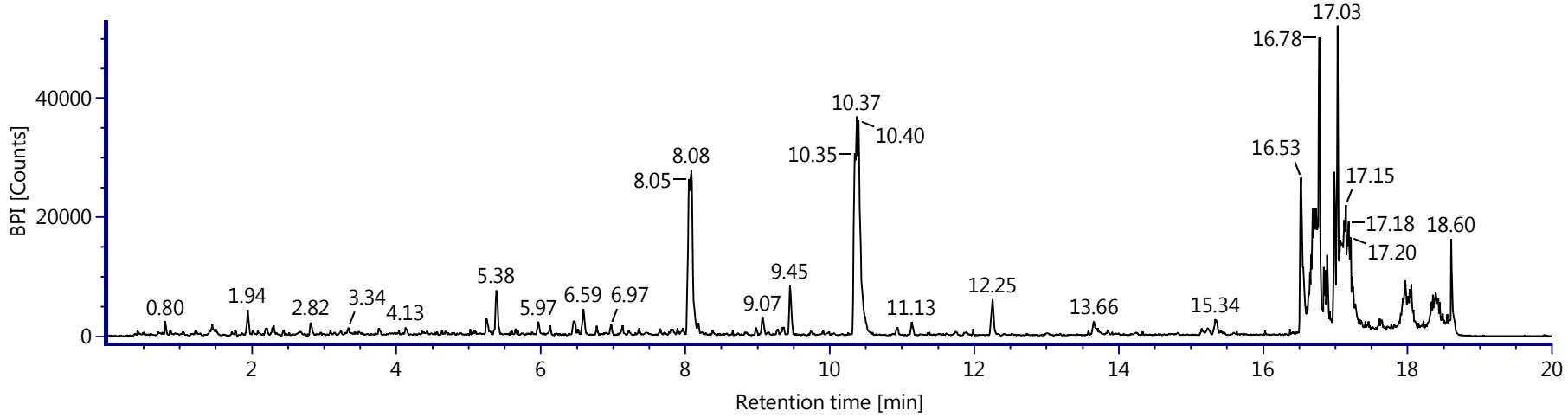


# BPI Plot

**Item name: blank water_01**
**Channel name: 2: HD TOF MSe (50-1000) 4eV ESI+ (TIC)**

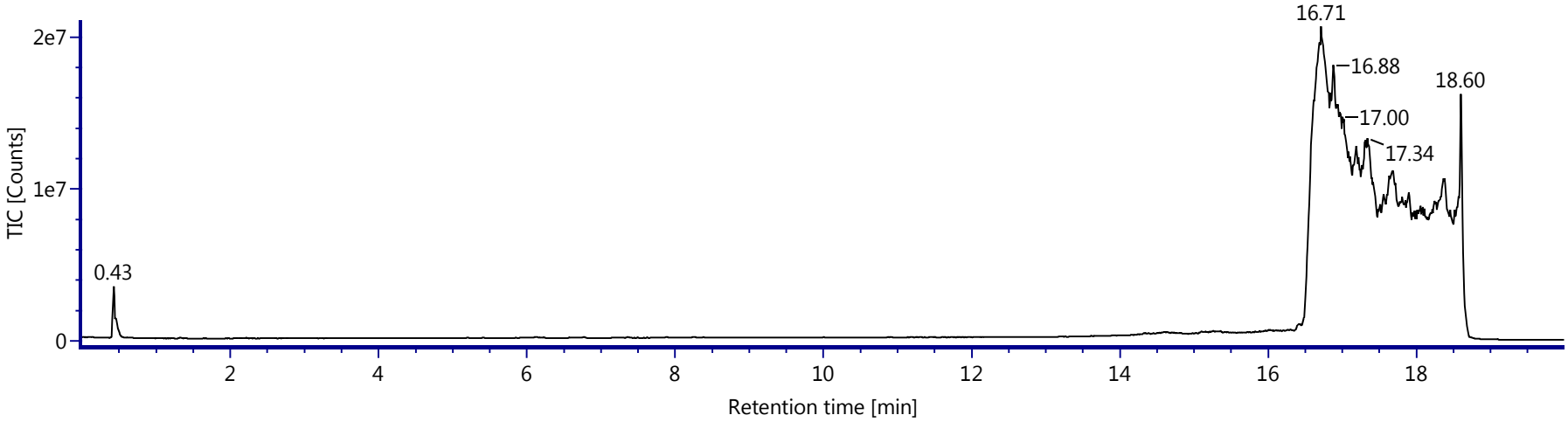



**Item name: sample 2_01**
**Channel name: 2: HD TOF MSe (50-1000) 4eV ESI+ (BPI)**

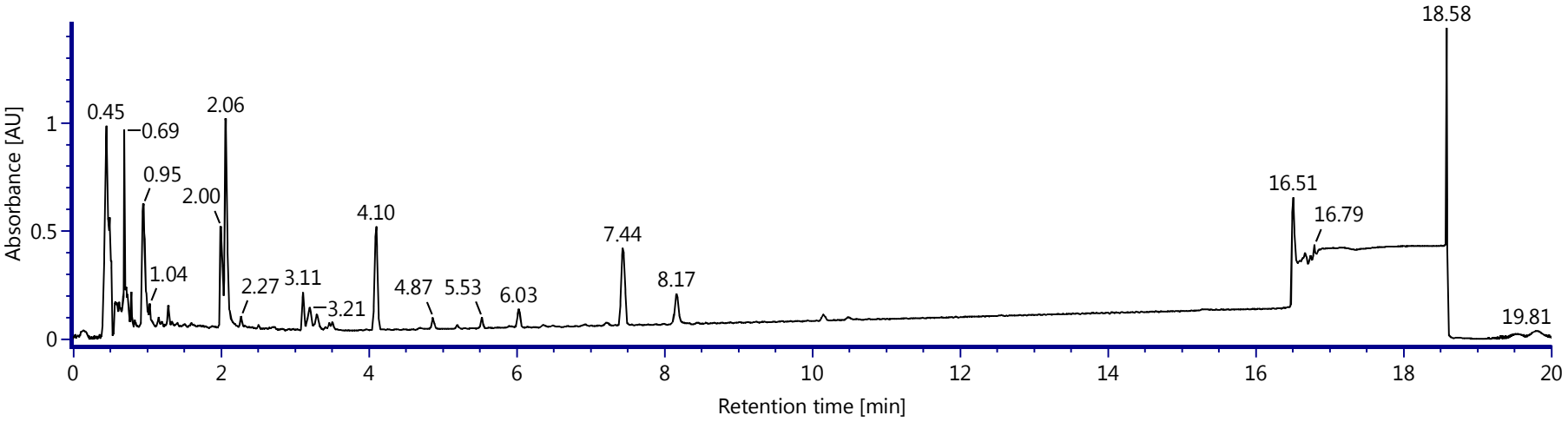


# PDA Plot

**Item name: blank water_01**
**Channel name: 2: HD TOF MSe (50-1000) 4eV ESI+ (TIC)**

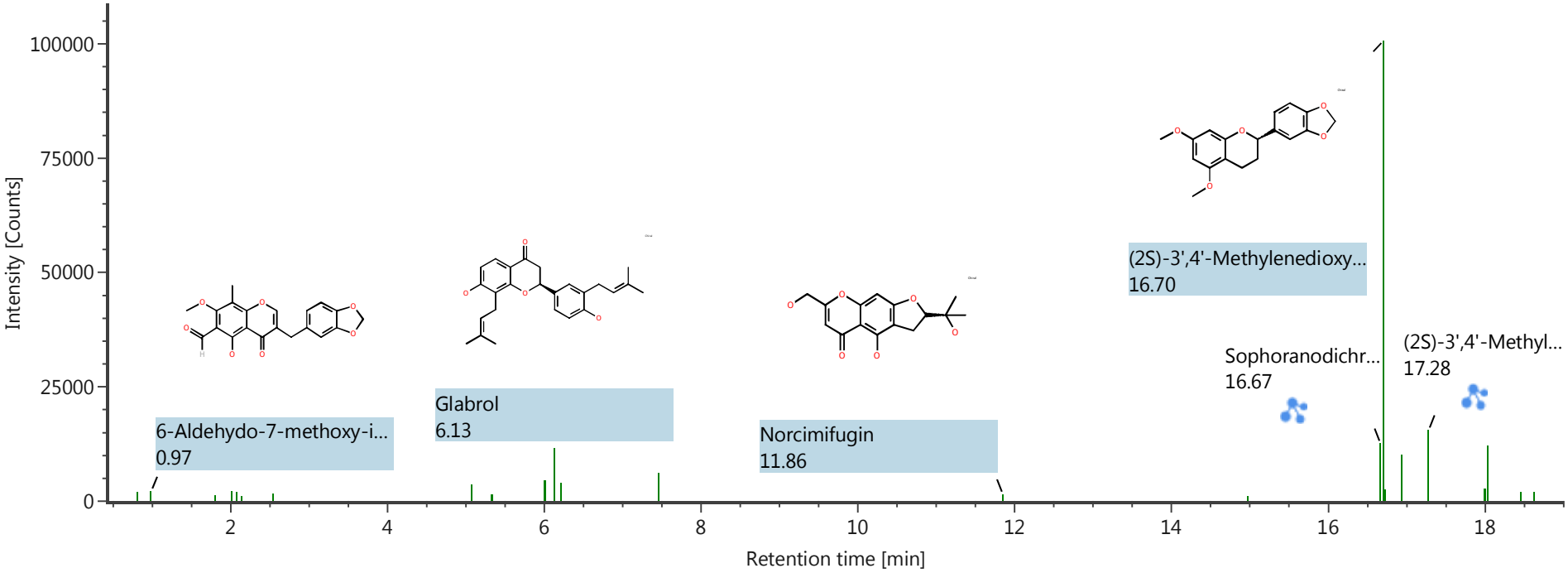



**Item name: sample 2_01**
**Channel name: PDA MaxPlot (190-500)**



# Identified Compounds (Good & Poor match)

Item name: sample 2_01




Item name: sample 2_01, Sample position: 1:B,3, Replicate number: 1

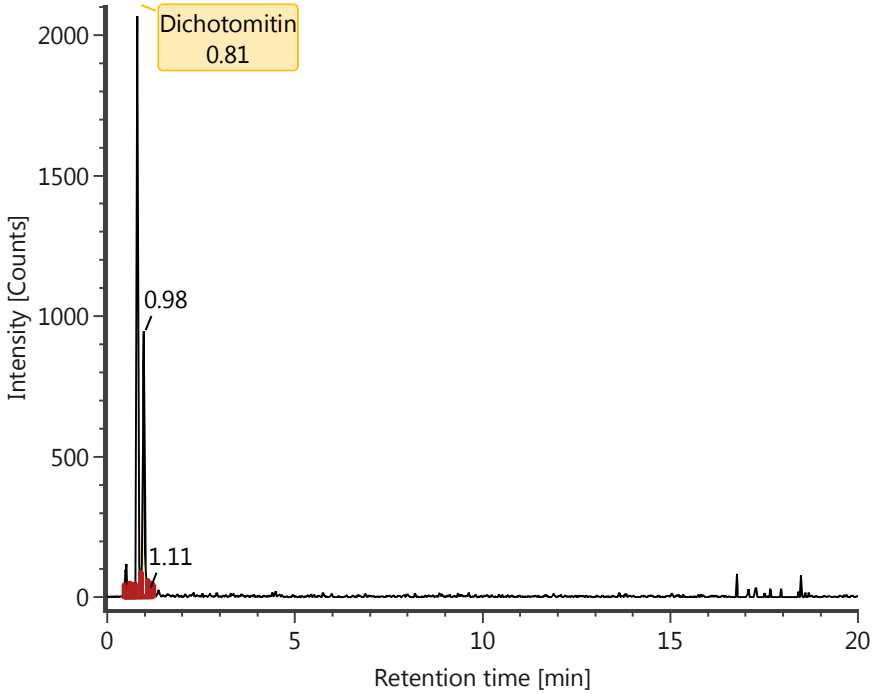
| . | Component name | Formula | Identification status | Observed neutral mass (Da) | Observed m/z | Mass error (mDa) | Mass error (ppm) | Observed RT (min) | Response | Adducts | Observed CCS (Å²) | Total Fragments Found |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Dichotomitin | C18H14O8 | Identified | 358.0708 | 381.0600 | 2.0 | 5.1 | 0.81 | 2004 | +Na, +K | 183.78 | 1 |
| 2 | Kurarinone | C26H30O6 | Identified | 438.2086 | 477.1717 | 4.3 | 9.1 | 0.82 | 1147 | +K | 207.77 | 1 |
| 3 | 6-Aldehydo-7-methoxy-isoophiopogonone A | C20H16O7 | Identified | 368.0919 | 391.0811 | 2.3 | 5.9 | 0.97 | 2090 | +Na | 181.97 | 2 |
| 4 | Irisflorentin | C20H18O8 | Identified | 386.1029 | 409.0921 | 2.7 | 6.7 | 0.97 | 1856 | +Na | 182.29 | 1 |
| 5 | Dichotomitin | C18H14O8 | Identified | 358.0710 | 381.0603 | 2.2 | 5.7 | 0.98 | 1279 | +Na | 184.29 | 0 |
| 6 | Bavachinin | C21H22O4 | Identified | 338.1506 | 361.1398 | -1.2 | -3.3 | 1.81 | 1161 | +Na | 181.66 | 0 |
| 7 | Mirificin | C26H28O13 | Identified | 548.1485 | 549.1557 | -4.5 | -8.3 | 2.02 | 2036 | +H, +Na | 258.43 | 0 |

| . | Component name | Formula | Identification status | Observed neutral mass (Da) | Observed m/z | Mass error (mDa) | Mass error (ppm) | Observed RT (min) | Response | Adducts | Observed CCS (Å$^2$) | Total Fragments Found |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 8 | Naringenin-4′-glucoside-7-rutinoside | C33H42O19 | Identified | 742.2294 | 765.2186 | -2.7 | -3.5 | 2.02 | 1049 | +Na | 260.68 | 1 |
| 9 | 6-Methoxy-2-(2-phenylethyl)chromone | C18H16O3 | Identified | 280.1122 | 303.1014 | 2.2 | 7.4 | 2.08 | 2014 | +Na | 198.61 | 0 |
| 10 | Kosamol A | C30H38O8 | Identified | 526.2611 | 565.2243 | 4.5 | 7.9 | 2.15 | 1059 | +K | 216.63 | 1 |
| 11 | 5-Hydroxyauranetin | C20H20O8 | Identified | 388.1159 | 395.1313 | 0.1 | 0.2 | 2.54 | 1504 | +Li | 194.15 | 0 |
| 12 | (-)-Epiafzelechin-3-O-(6"-O-acetyl)-β-D-allosepyranoside | C23H26O11 | Identified | 478.1467 | 479.1539 | -0.9 | -1.8 | 5.07 | 3463 | +H | 225.46 | 1 |
| 13 | Silymonin | C25H22O9 | Identified | 466.1220 | 473.1375 | -4.3 | -9.2 | 5.07 | 2073 | +Li | 224.21 | 0 |
| 14 | Daidzin_1 | C21H20O9 | Identified | 416.1114 | 439.1006 | 0.7 | 1.6 | 5.33 | 1112 | +Na | 196.30 | 0 |
| 15 | 3,4,2'-Trihydroxychal-cone-4'-O-β-D-glucopyranoside | C21H22O10 | Identified | 434.1225 | 457.1118 | 1.2 | 2.7 | 5.33 | 1272 | +Na | 199.28 | 0 |
| 16 | Pinnatifinoside B | C23H20O10 | Identified | 456.1045 | 457.1118 | -1.2 | -2.5 | 5.33 | 1272 | +H | 199.28 | 1 |
| 17 | Bavachalcone | C20H20O4 | Identified | 324.1343 | 347.1235 | -1.9 | -5.5 | 6.01 | 4354 | +Na | 182.22 | 0 |
| 18 | Corylifolinin | C20H20O4 | Identified | 324.1343 | 347.1235 | -1.9 | -5.5 | 6.01 | 4354 | +Na | 182.22 | 0 |
| 19 | Glabrol | C25H28O4 | Identified | 392.2017 | 393.2089 | 2.9 | 7.4 | 6.13 | 11513 | +H | 179.88 | 0 |
| 20 | Lupinifolin | C25H26O5 | Identified | 406.1813 | 407.1886 | 3.3 | 8.0 | 6.22 | 3843 | +H, +Na | 182.49 | 1 |
| 21 | Hibiscetin-3-O-glucoside | C21H20O14 | Identified | 496.0851 | 497.0923 | -0.2 | -0.5 | 7.47 | 6132 | +H | 217.13 | 0 |
| 22 | Norcimifugin | C15H16O6 | Identified | 292.0940 | 299.1094 | -0.7 | -2.4 | 11.86 | 1429 | +Li | 167.93 | 0 |
| 23 | 5-Hydroxy-7,8-dimethoxy-6-methyl-3-(3',4'-dihydroxybenzyl) chroman-4-one | C19H20O7 | Identified | 360.1207 | 367.1362 | -0.2 | -0.5 | 14.98 | 1037 | +Li | 177.93 | 0 |
| 24 | Sophoranodichromane D | C25H28O5 | Identified | 408.1961 | 415.2115 | 2.4 | 5.7 | 16.67 | 12569 | +Li, +H | 205.99 | 17 |
| 25 | (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane | C18H18O5 | Identified | 314.1151 | 337.1043 | -0.3 | -0.9 | 16.70 | 100608 | +Na, +Li | 179.50 | 5 |
| 26 | Ophiopogonanone B | C18H18O5 | Identified | 314.1151 | 337.1043 | -0.3 | -0.9 | 16.70 | 100608 | +Na, +Li | 179.50 | 6 |
| 27 | Kuwanon S | C25H26O5 | Identified | 406.1777 | 407.1850 | -0.3 | -0.8 | 16.71 | 1296 | +H, +Li, +Na | 209.90 | 42 |
| 28 | Neokurarinol | C27H34O7 | Identified | 470.2297 | 471.2370 | -0.8 | -1.6 | 16.72 | 1267 | +H | 219.52 | 31 |
| 29 | Glabrol | C25H28O4 | Identified | 392.1994 | 393.2067 | 0.6 | 1.6 | 16.72 | 2413 | +H, +Li | 195.67 | 34 |

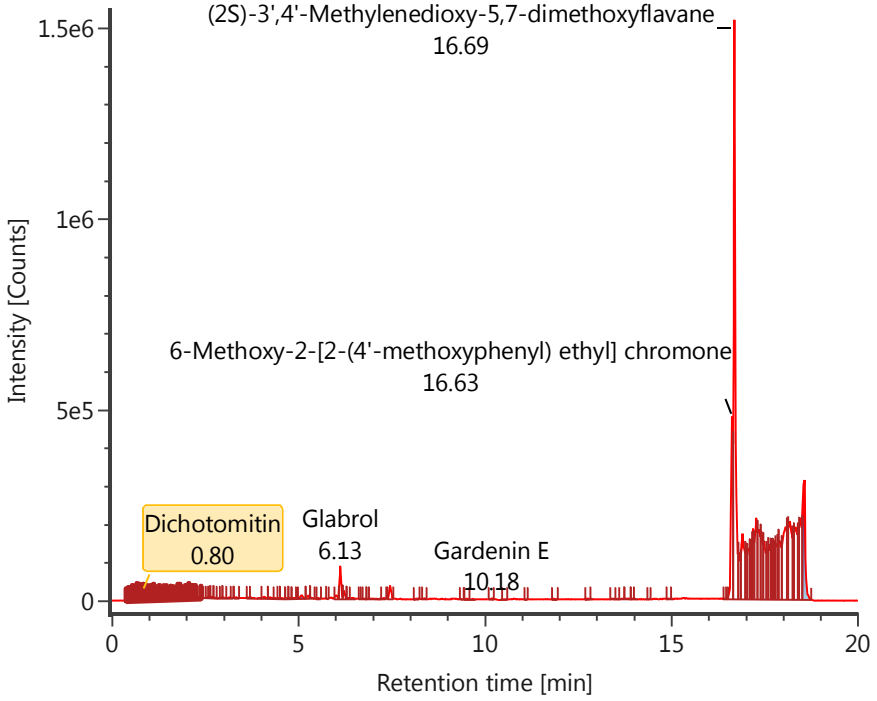
| . | Component name | Formula | Identification status | Observed neutral mass (Da) | Observed m/z | Mass error (mDa) | Mass error (ppm) | Observed RT (min) | Response | Adducts | Observed CCS (Å$^2$) | Total Fragments Found |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 30 | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one | C18H18O5 | Identified | 314.1147 | 337.1039 | -0.8 | -2.3 | 16.95 | 10015 | +Na | 178.84 | 0 |
| 31 | (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane | C18H18O5 | Identified | 314.1150 | 337.1043 | -0.4 | -1.2 | 17.28 | 15479 | +Na | 179.31 | 0 |
| 32 | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one | C18H18O5 | Identified | 314.1150 | 337.1043 | -0.4 | -1.2 | 17.28 | 15479 | +Na | 179.31 | 0 |
| 33 | Glabrol | C25H28O4 | Identified | 392.2017 | 393.2090 | 2.9 | 7.4 | 18.00 | 2633 | +H | 181.39 | 1 |
| 34 | (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane | C18H18O5 | Identified | 314.1153 | 337.1045 | -0.1 | -0.3 | 18.03 | 12092 | +Na | 179.64 | 0 |
| 35 | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one | C18H18O5 | Identified | 314.1153 | 337.1045 | -0.1 | -0.3 | 18.03 | 12092 | +Na | 179.64 | 0 |
| 36 | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one | C18H18O5 | Identified | 314.1173 | 321.1327 | 1.8 | 5.7 | 18.46 | 1800 | +Li | 181.35 | 1 |
| 37 | 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one | C18H18O5 | Identified | 314.1154 | 321.1309 | 0.0 | 0.0 | 18.60 | 1458 | +Li | 178.40 | 0 |
| 38 | Kuraridinol | C26H32O7 | Identified | 456.2185 | 457.2257 | 3.7 | 8.0 | 18.63 | 1903 | +H | 164.66 | 3 |

# Details of Identified Components

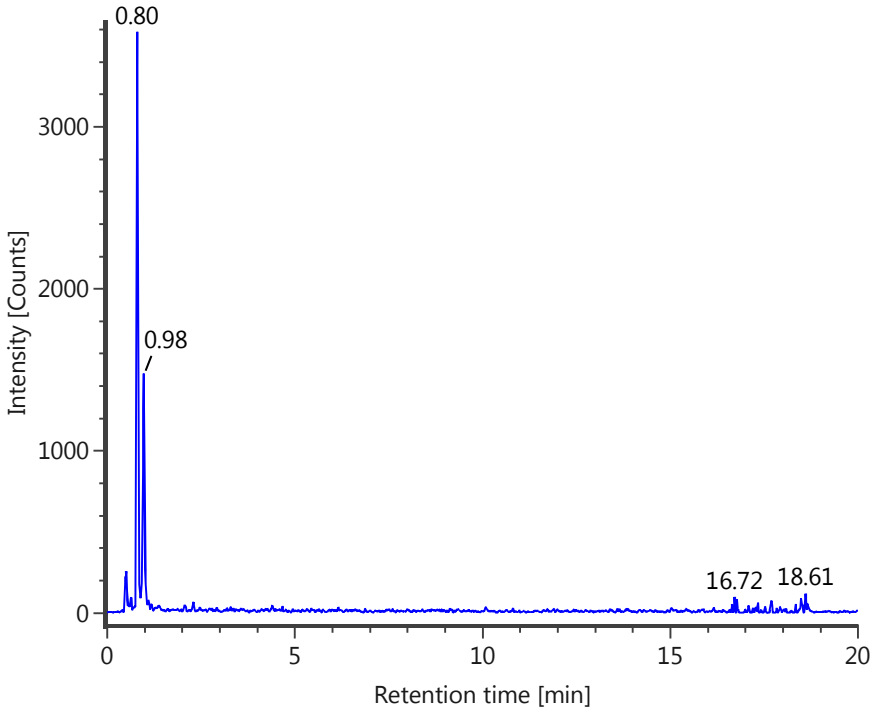
Item name: sample 2_01
Channel name: Dichotomitin [+Na] : (18.8 PPM) 381.0600 : DT=5.10 to 5.63 ms



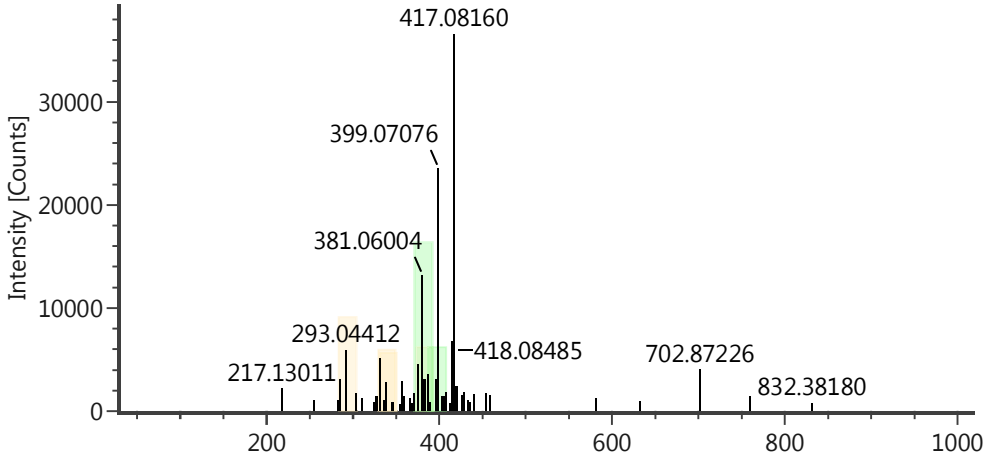
Item name: sample 2_01
Channel name: Identified Components



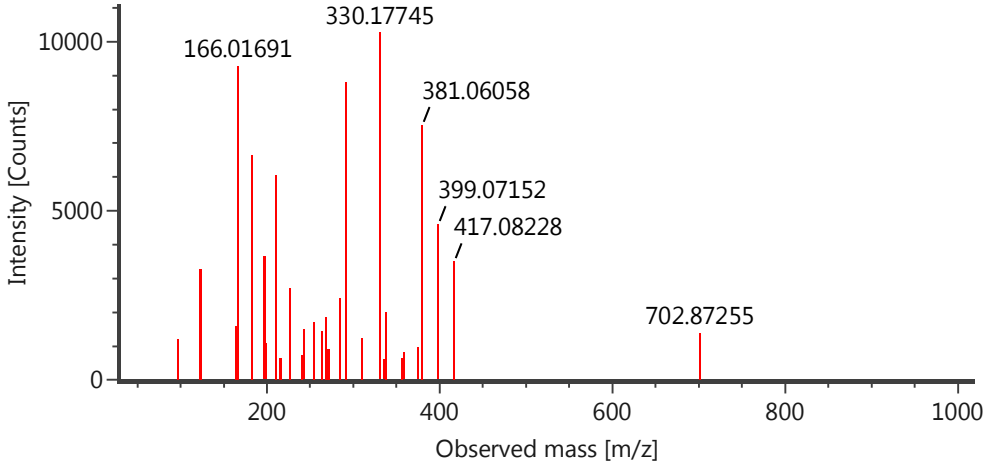
Item name: sample 2_01
Channel name: Dichotomitin [+Na] : (18.8 PPM) 381.0600



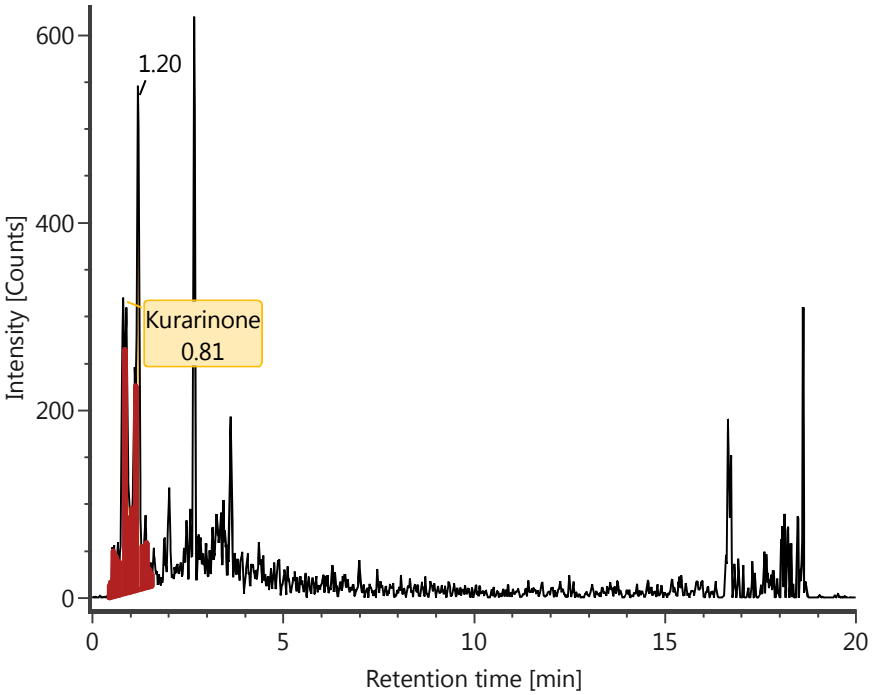

Item name: sample 2_01
Component name: Dichotomitin
Channel name: Low energy : Time 0.8082 +/- 0.0231 minutes : Drift Times: 5.36 +/- 0.26, 5.54 +/- 0.27 ms



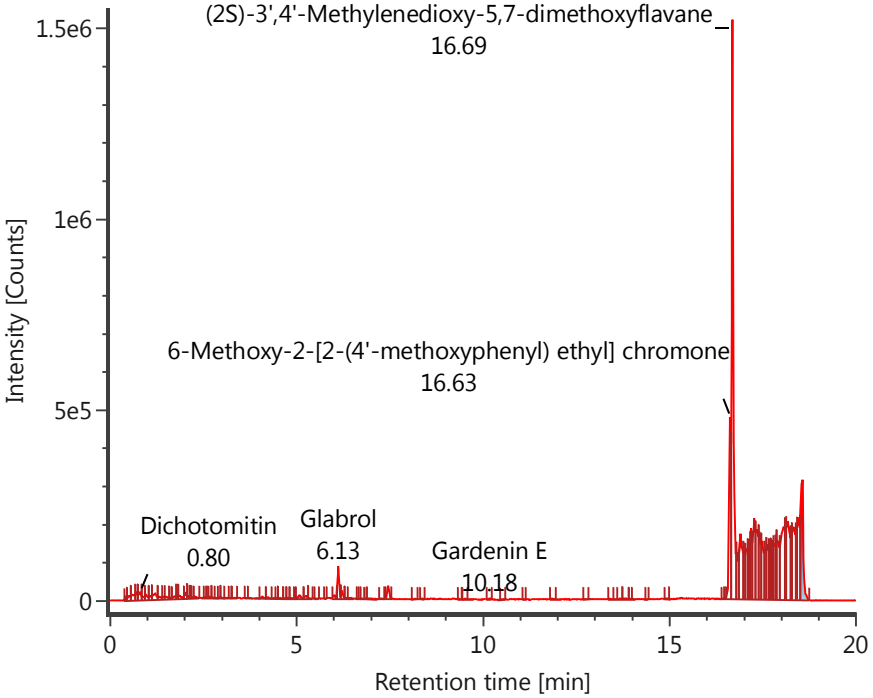

Item name: sample 2_01
Component name: Dichotomitin
Channel name: High energy : Time 0.8082 +/- 0.0231 minutes : Drift Times: 5.23 +/- 0.26, 5.41 +/- 0.27 ms



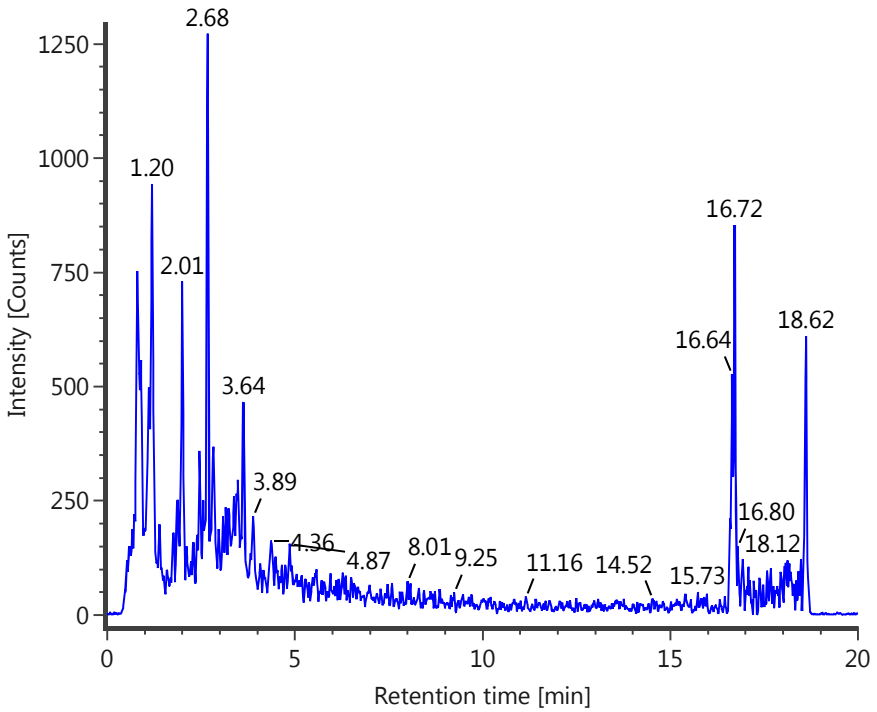
Item name: sample 2_01
Channel name: Kurarinone [+K] : (18.8 PPM) 477.1717 : DT=5.98 to 6.54 ms



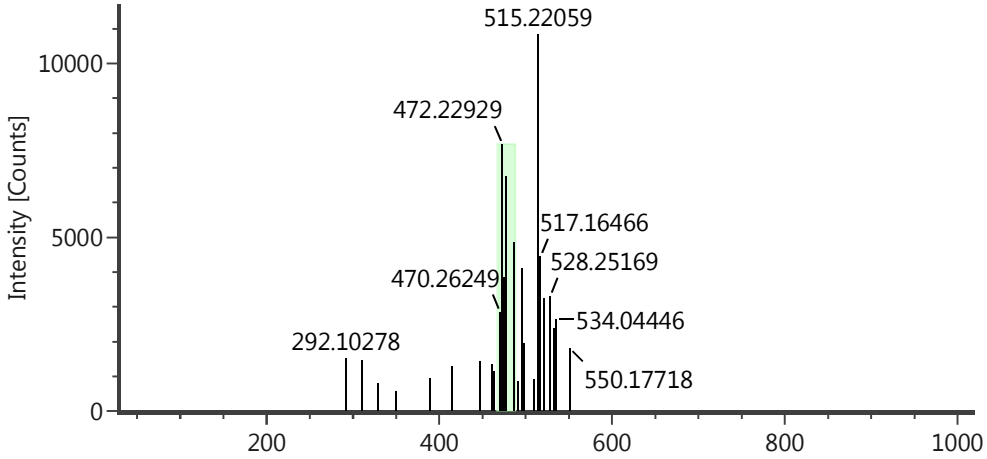
Item name: sample 2_01
Channel name: Identified Components



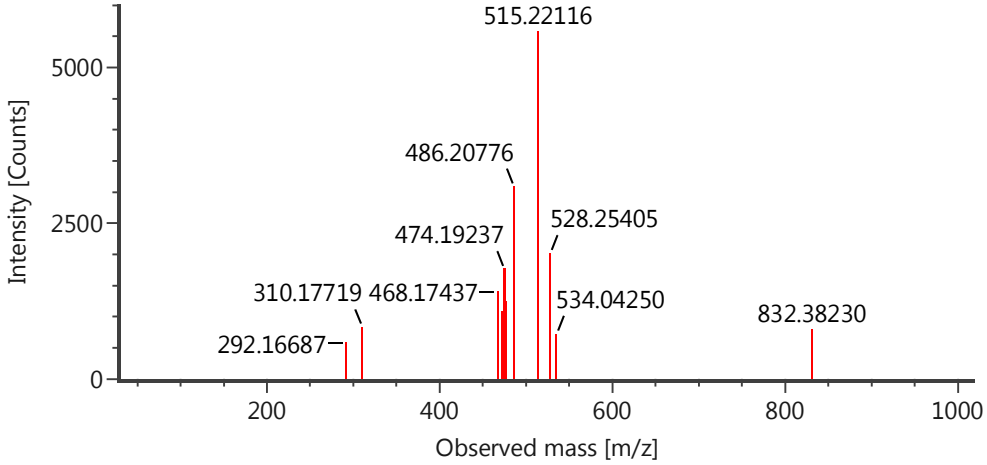
Item name: sample 2_01
Channel name: Kurarinone [+K] : (18.8 PPM) 477.1717



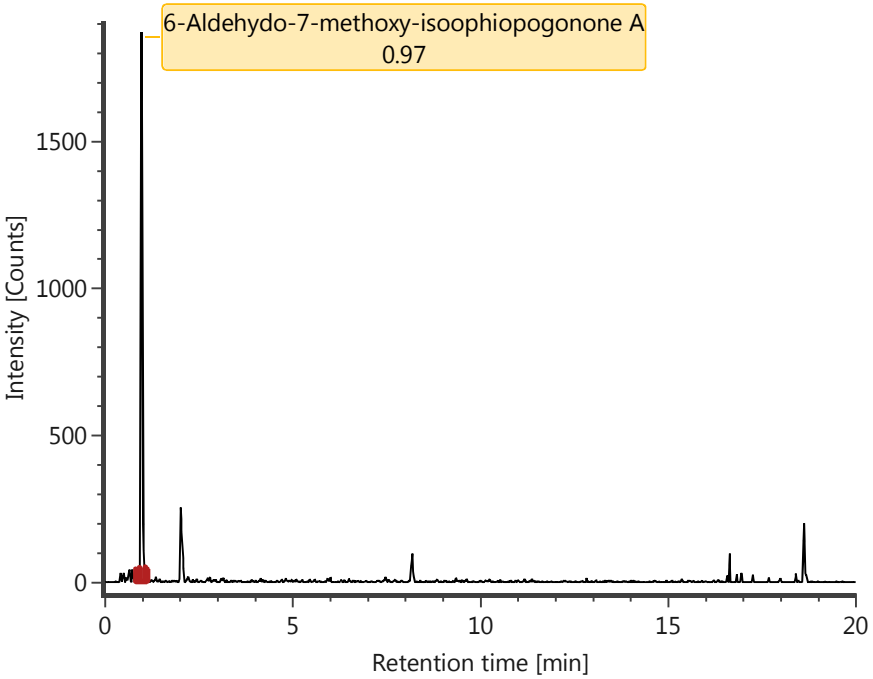

Item name: sample 2_01
Component name: Kurarinone
Channel name: Low energy : Time 0.8175 +/- 0.0231 minutes :
Drift Times: 6.25 +/- 0.28 ms



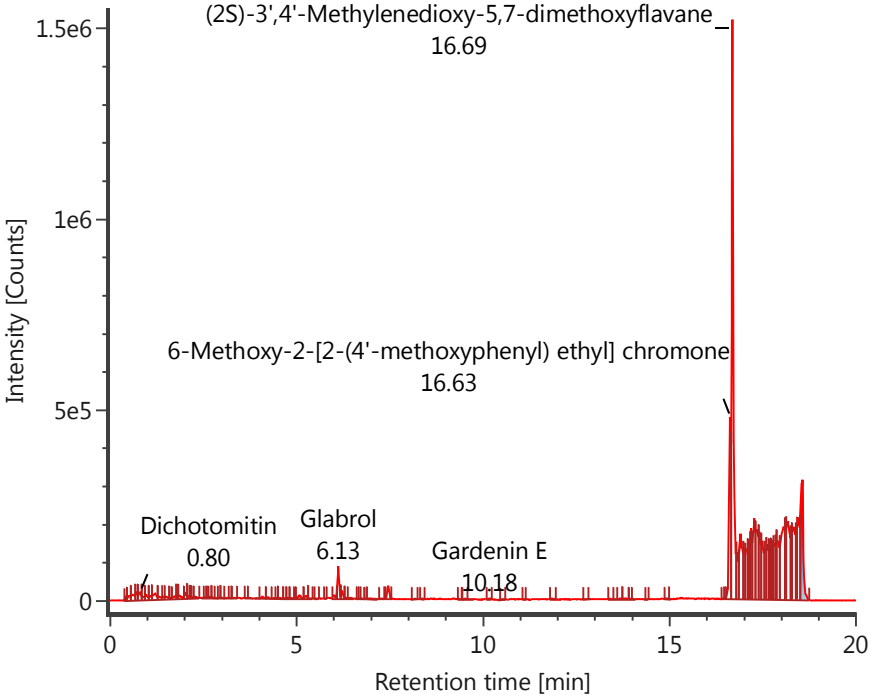

Item name: sample 2_01
Component name: Kurarinone
Channel name: High energy : Time 0.8175 +/- 0.0231 minutes :
Drift Times: 6.11 +/- 0.28 ms



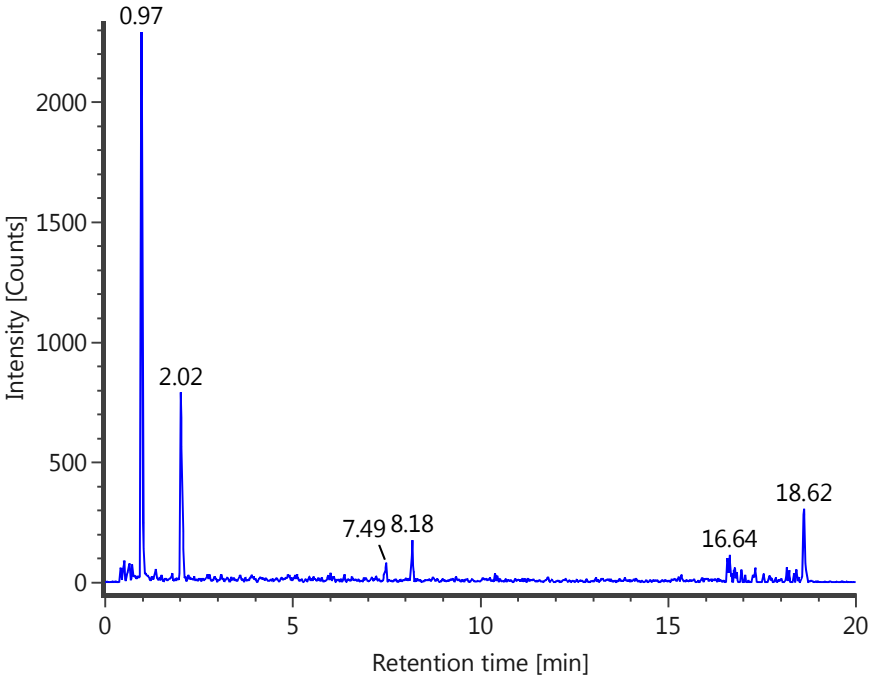
Item name: sample 2_01
Channel name: 6-Aldehydo-7-methoxy-isoophiopogonone A [+Na] : (18.8 PPM)
391.0811 : DT=5.03 to 5.56 ms



Item name: sample 2_01
Channel name: Identified Components

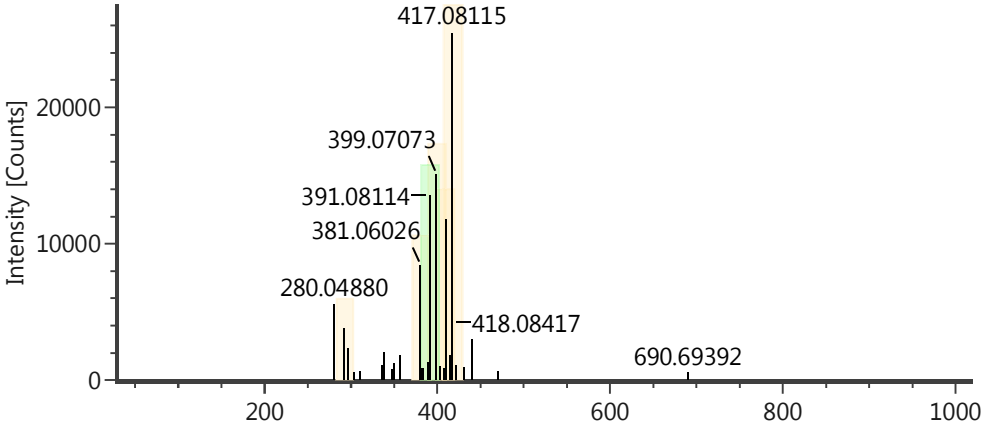


Item name: sample 2_01
Channel name: 6-Aldehydo-7-methoxy-isoophiopogonone A [+Na] : (18.8 PPM) 391.0811



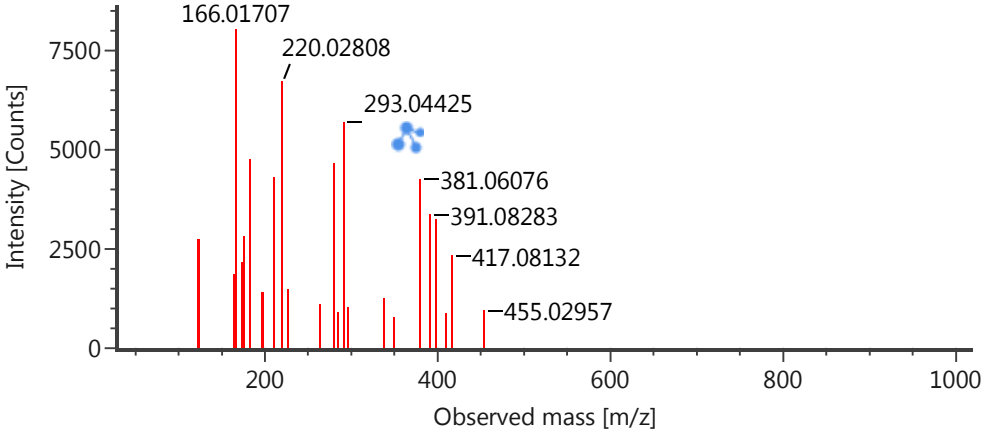

Item name: sample 2_01
Component name: 6-Aldehydo-7-methoxy-isoophiopogonone A

Channel name: Low energy : Time 0.9739 +/- 0.0231 minutes : Drift Times: 5.30 +/- 0.26 ms

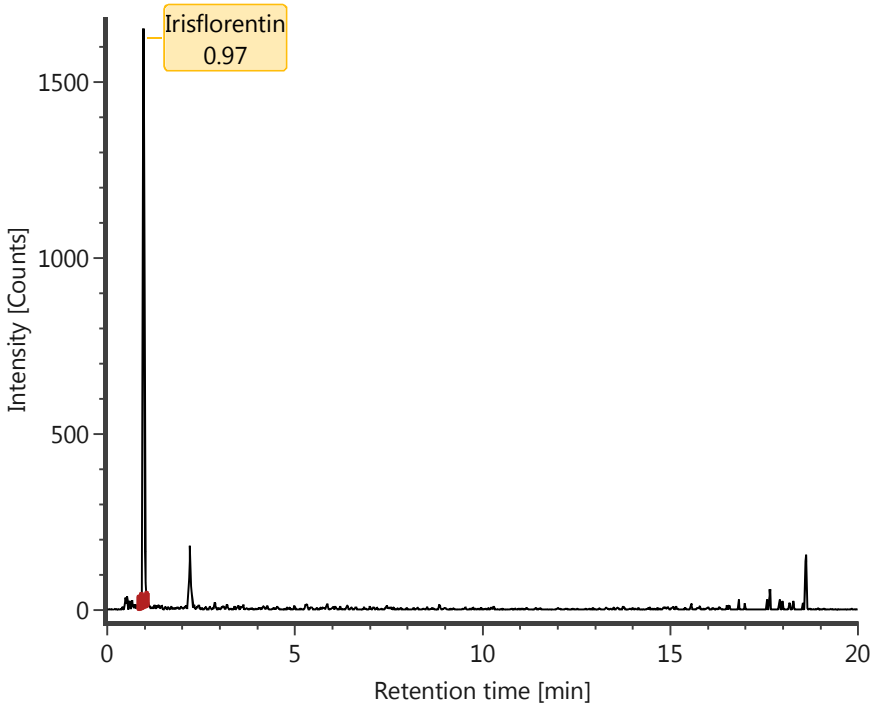



Item name: sample 2_01
Component name: 6-Aldehydo-7-methoxy-isoophiopogonone A

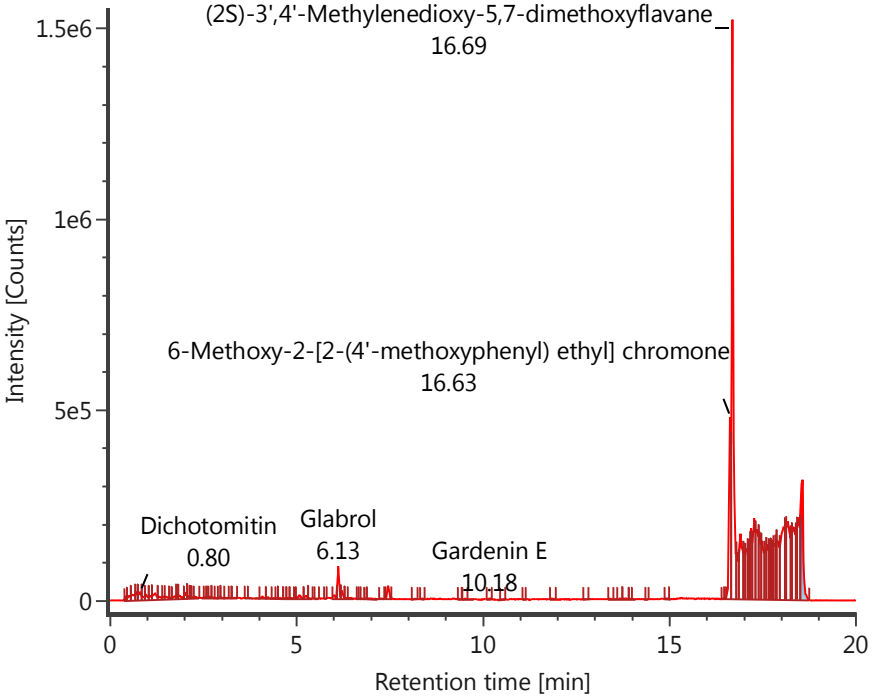
Channel name: High energy : Time 0.9739 +/- 0.0231 minutes : Drift Times: 5.16 +/- 0.26 ms



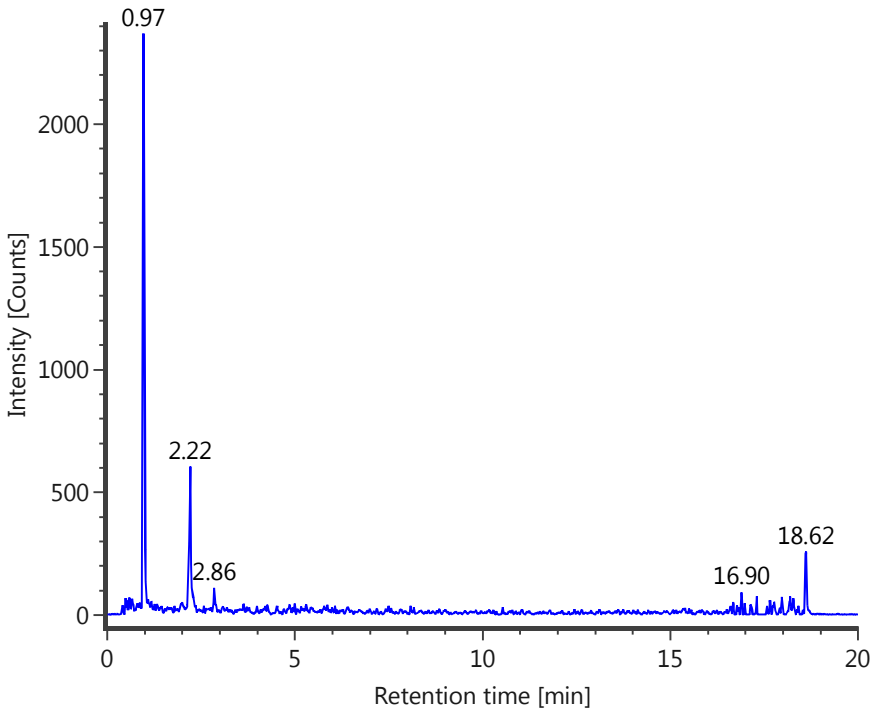
Item name: sample 2_01
Channel name: Irisflorentin [+Na] : (18.8 PPM) 409.0921 : DT=5.04 to 5.56 ms



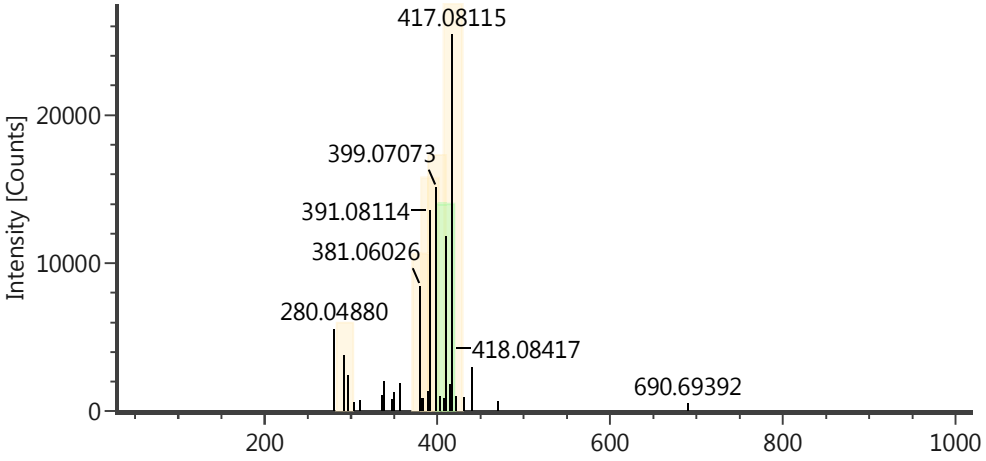
Item name: sample 2_01
Channel name: Identified Components



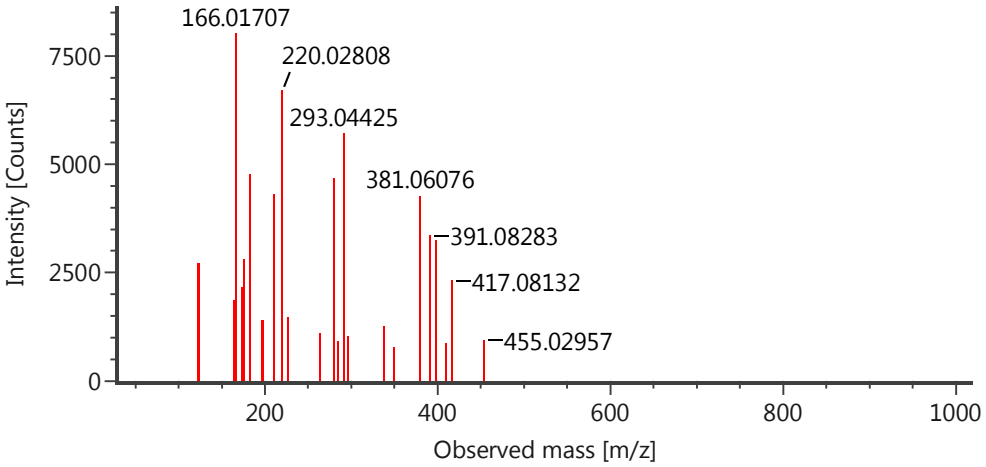
Item name: sample 2_01
Channel name: Irisflorentin [+Na] : (18.8 PPM) 409.0921



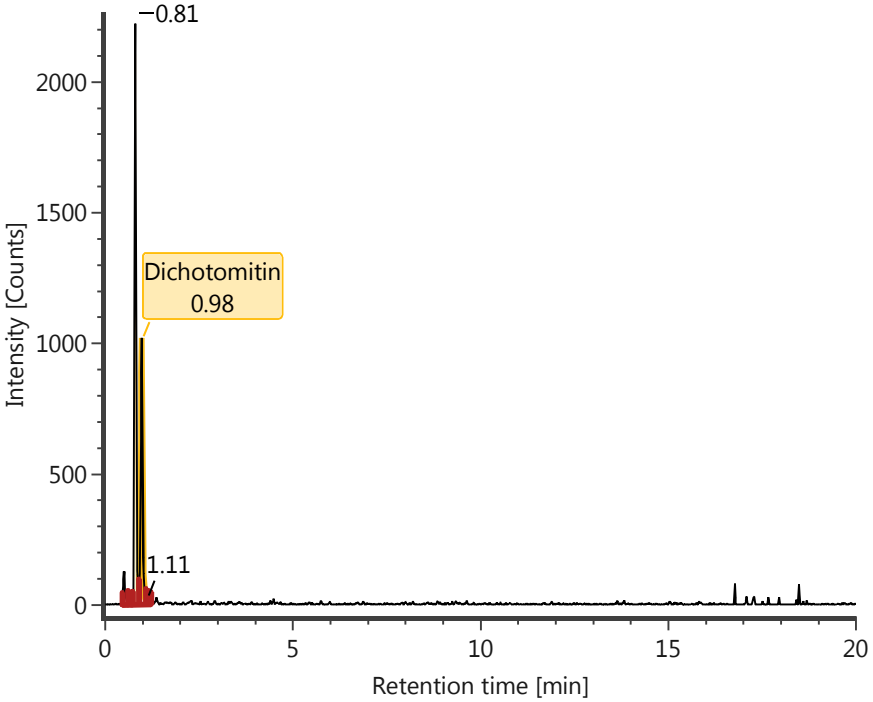

Item name: sample 2_01
Component name: Irisflorentin
Channel name: Low energy : Time 0.9743 +/- 0.0231 minutes :
Drift Times: 5.31 +/- 0.26 ms



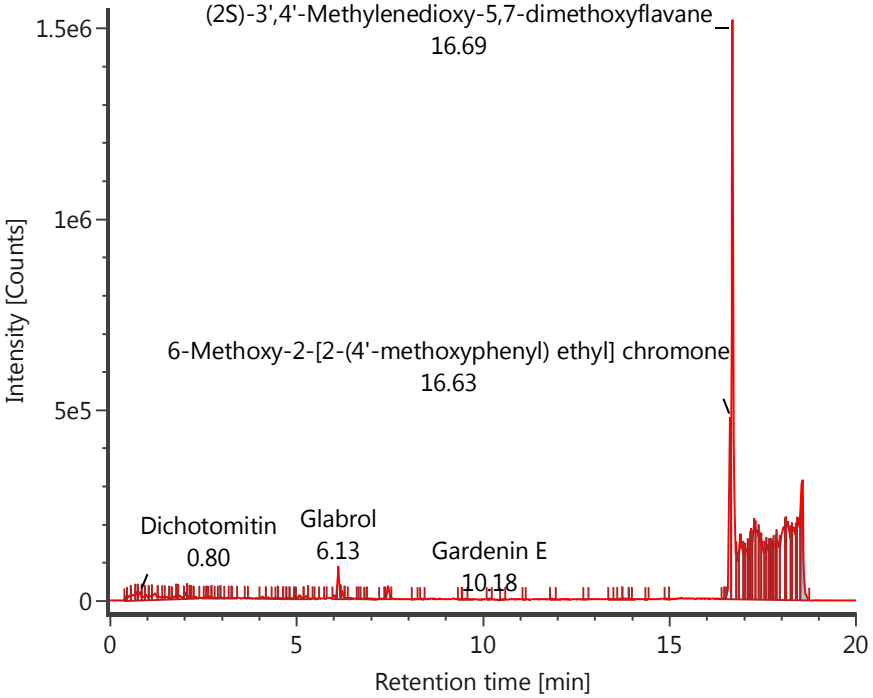

Item name: sample 2_01
Component name: Irisflorentin
Channel name: High energy : Time 0.9743 +/- 0.0231 minutes :
Drift Times: 5.18 +/- 0.26 ms



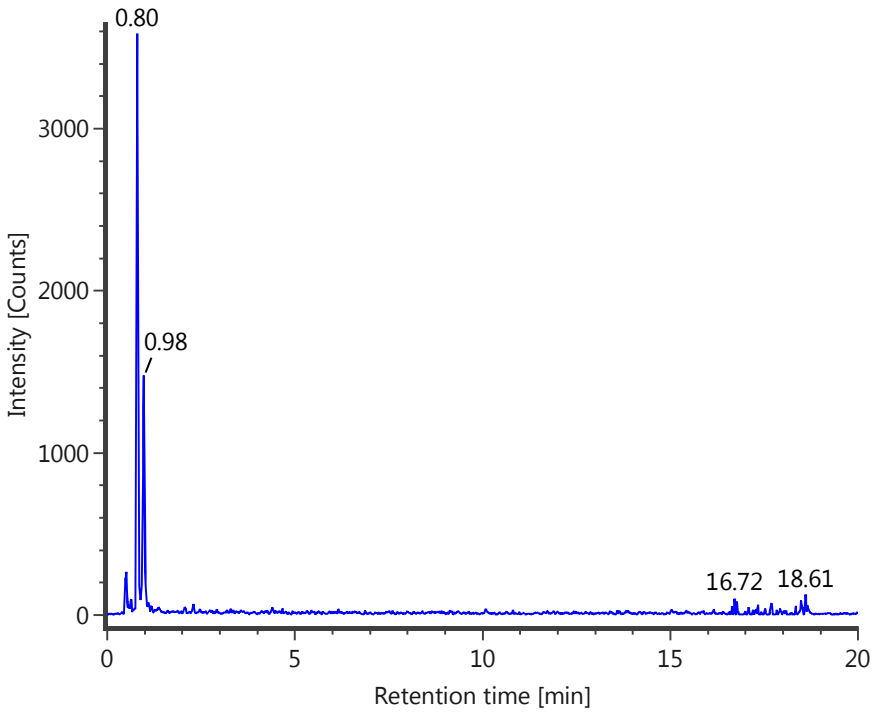
Item name: sample 2_01
Channel name: Dichotomitin [+Na] : (18.8 PPM) 381.0603 : DT=5.12 to 5.65 ms



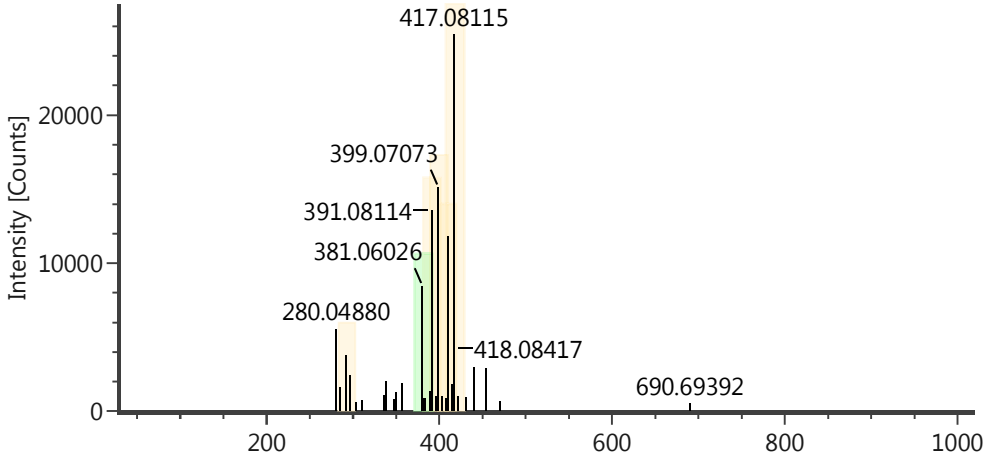
Item name: sample 2_01
Channel name: Identified Components



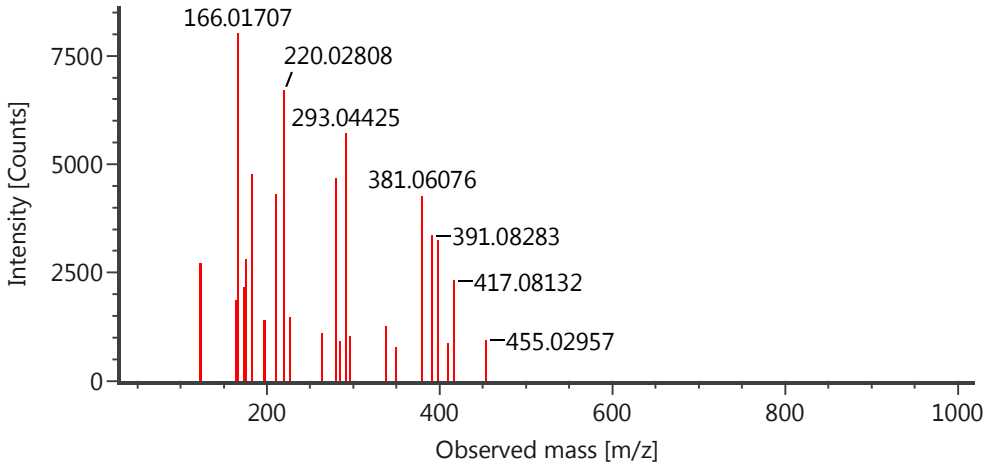
Item name: sample 2_01
Channel name: Dichotomitin [+Na] : (18.8 PPM) 381.0603



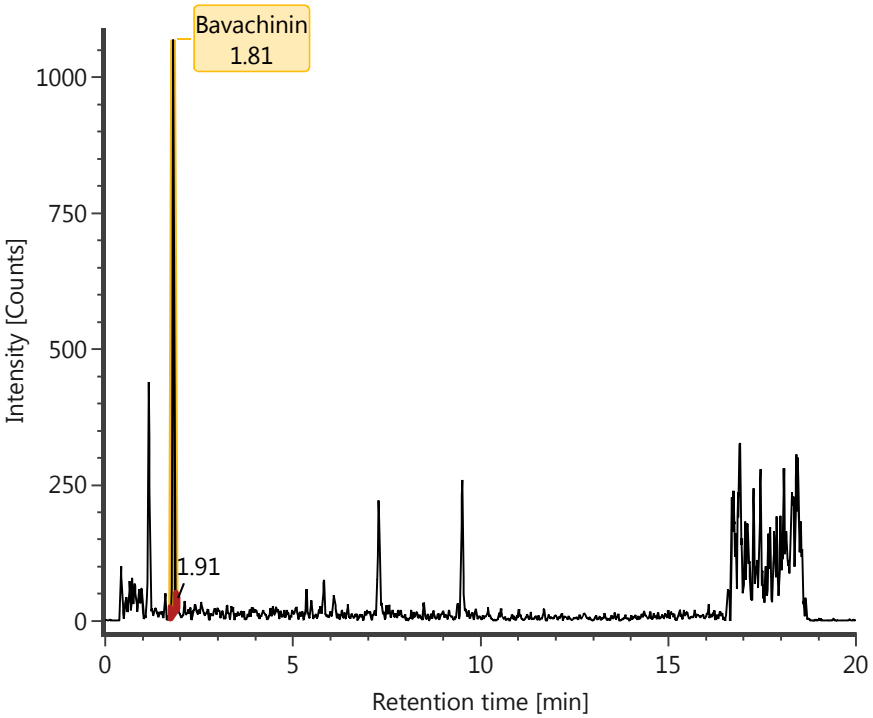

Item name: sample 2_01
Component name: Dichotomitin
Channel name: Low energy : Time 0.9801 +/- 0.0231 minutes : Drift Times: 5.38 +/- 0.26 ms



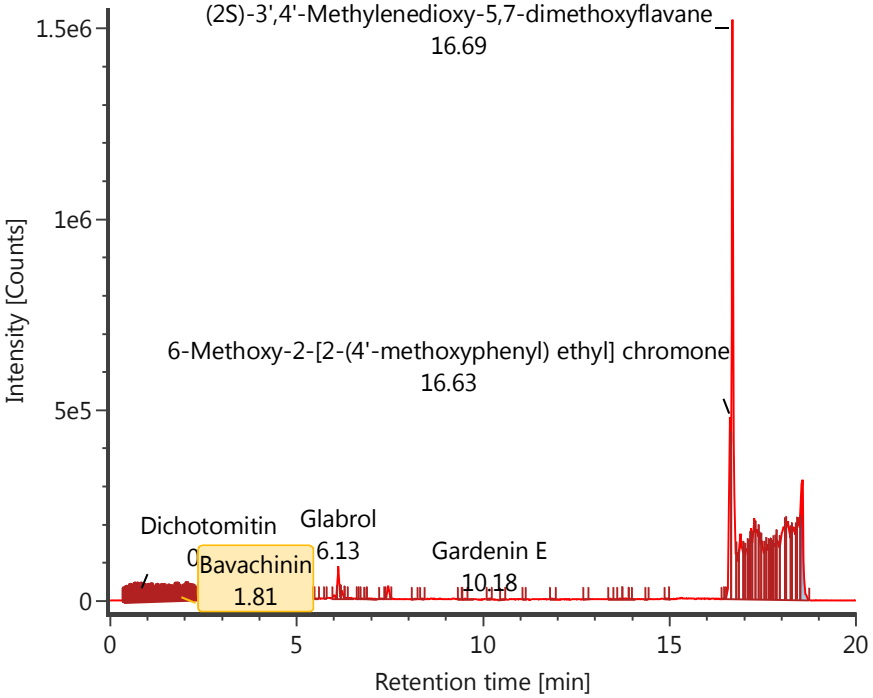

Item name: sample 2_01
Component name: Dichotomitin
Channel name: High energy : Time 0.9801 +/- 0.0231 minutes : Drift Times: 5.25 +/- 0.26 ms



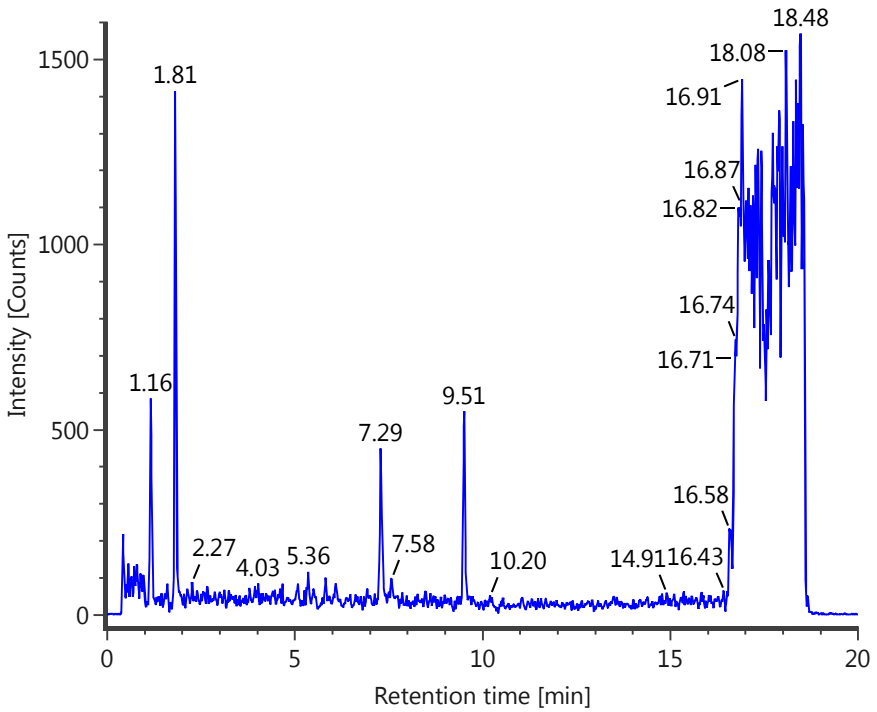
Item name: sample 2_01
Channel name: Bavachinin [+Na] : (18.8 PPM) 361.1398 : DT=5.03 to 5.56 ms



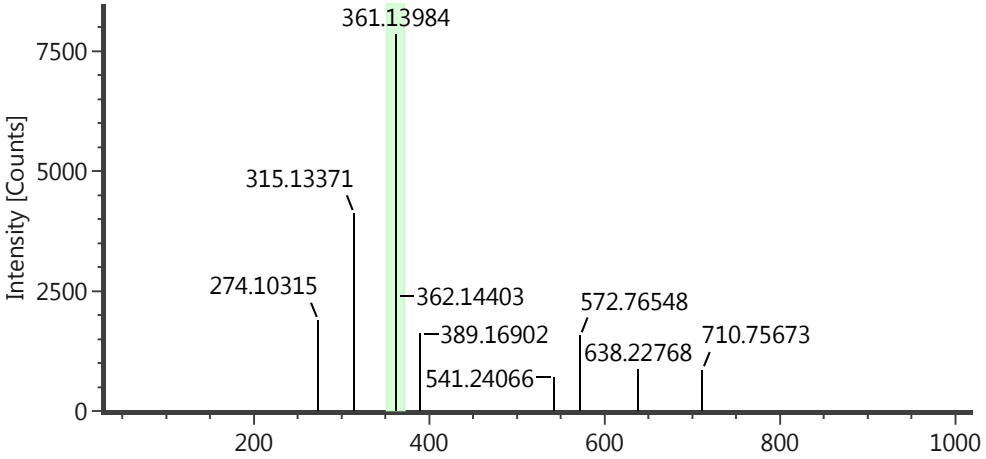
Item name: sample 2_01
Channel name: Identified Components



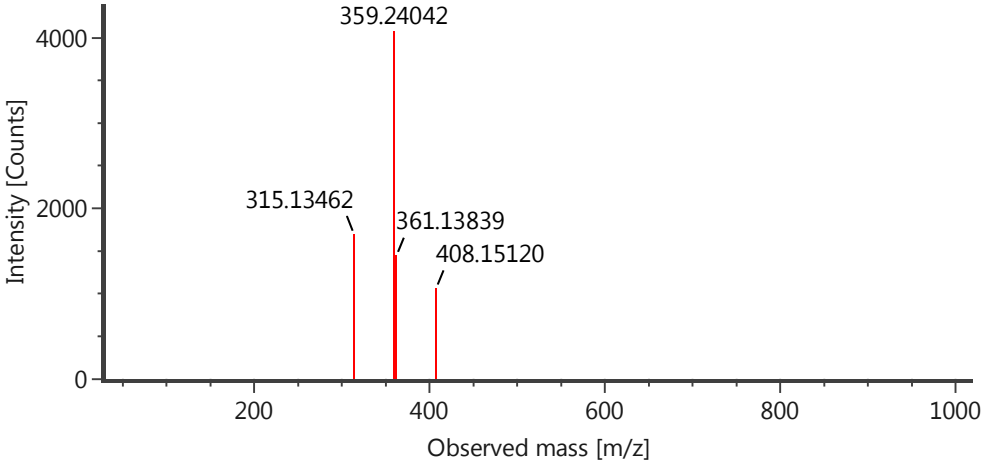
Item name: sample 2_01
Channel name: Bavachinin [+Na] : (18.8 PPM) 361.1398



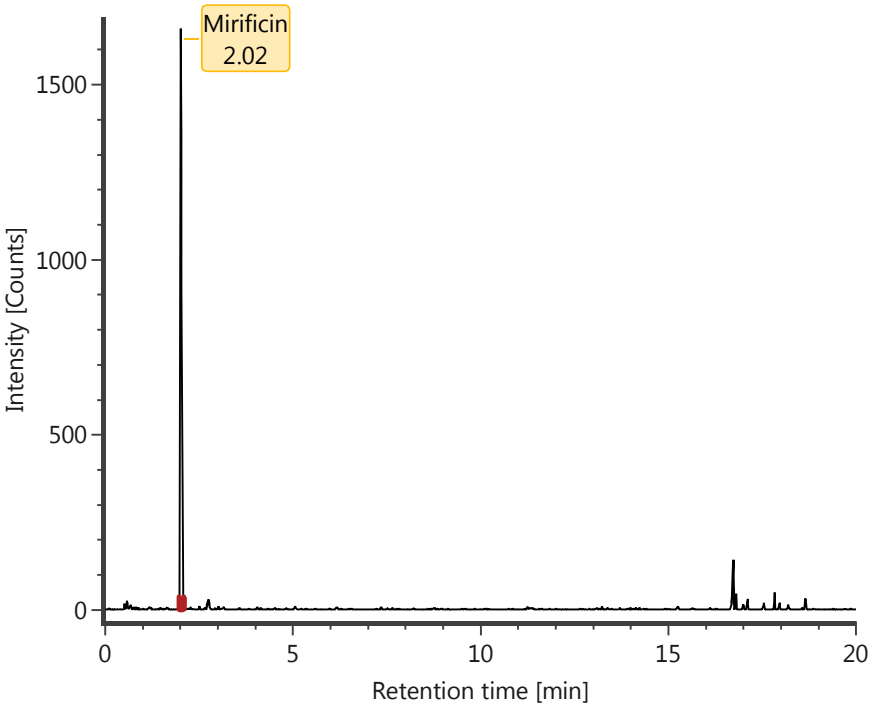

Item name: sample 2_01
Component name: Bavachinin
Channel name: Low energy : Time 1.8131 +/- 0.0231 minutes :
Drift Times: 5.28 +/- 0.26 ms



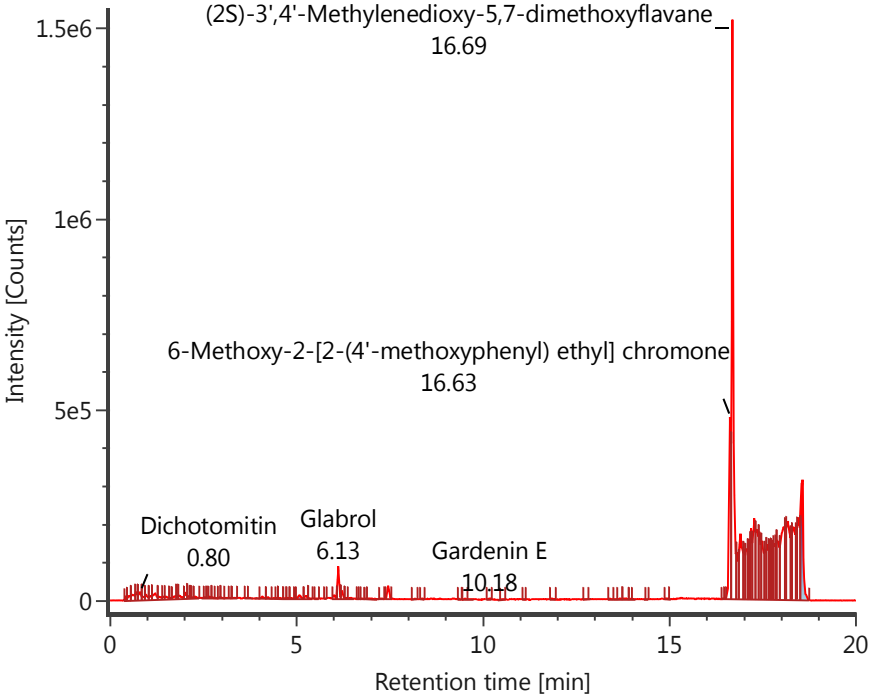

Item name: sample 2_01
Component name: Bavachinin
Channel name: High energy : Time 1.8131 +/- 0.0231 minutes :
Drift Times: 5.15 +/- 0.26 ms



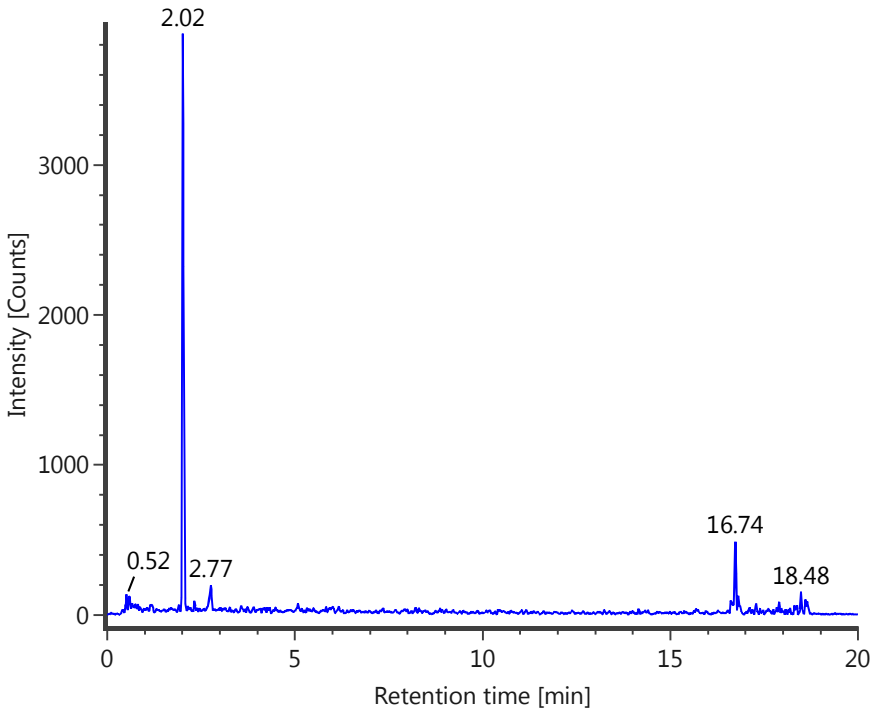
Item name: sample 2_01
Channel name: Mirificin [+H] : (18.8 PPM) 549.1557 : DT=7.65 to 8.26 ms



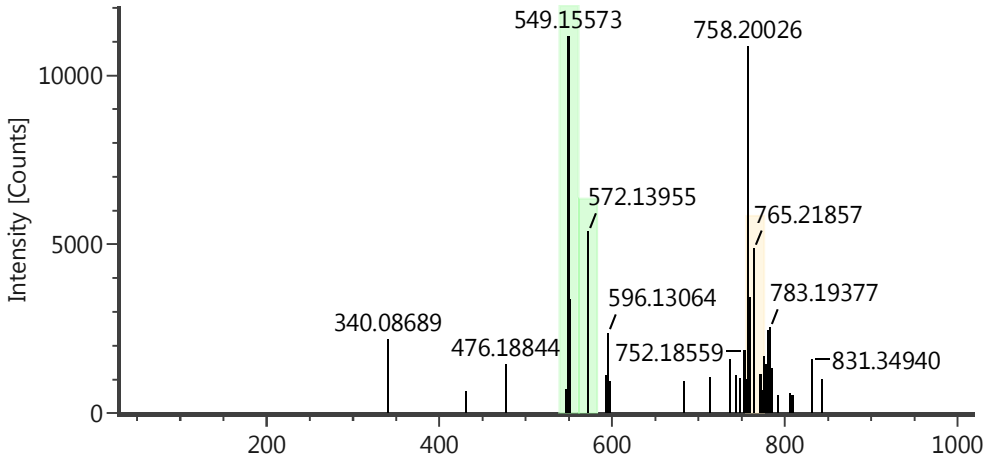
Item name: sample 2_01
Channel name: Identified Components



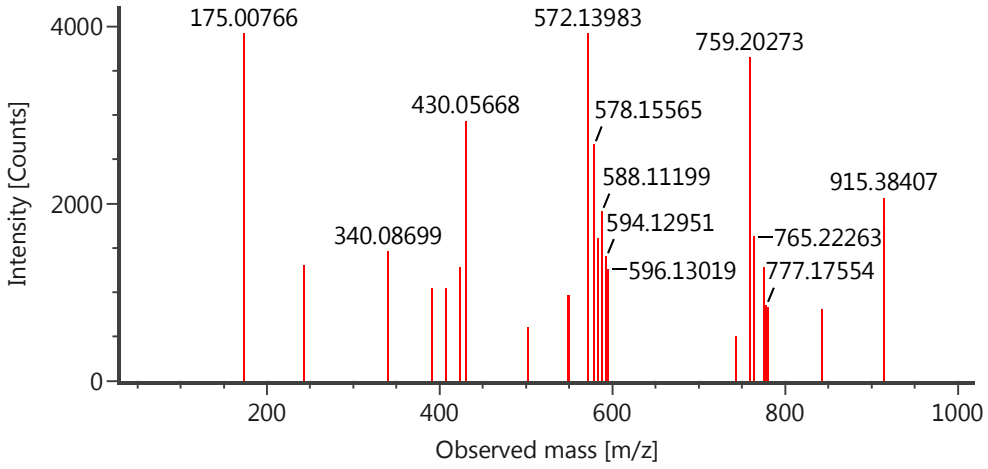
Item name: sample 2_01
Channel name: Mirificin [+H] : (18.8 PPM) 549.1557



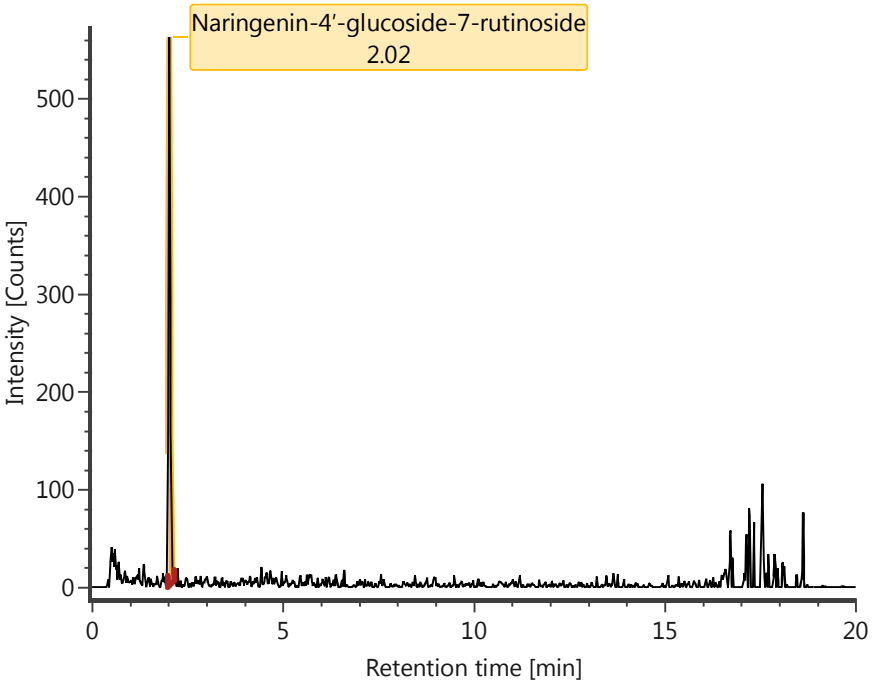

Item name: sample 2_01
Component name: Mirificin
Channel name: Low energy : Time 2.0233 +/- 0.0231 minutes :
Drift Times: 7.96 +/- 0.31, 8.03 +/- 0.31 ms



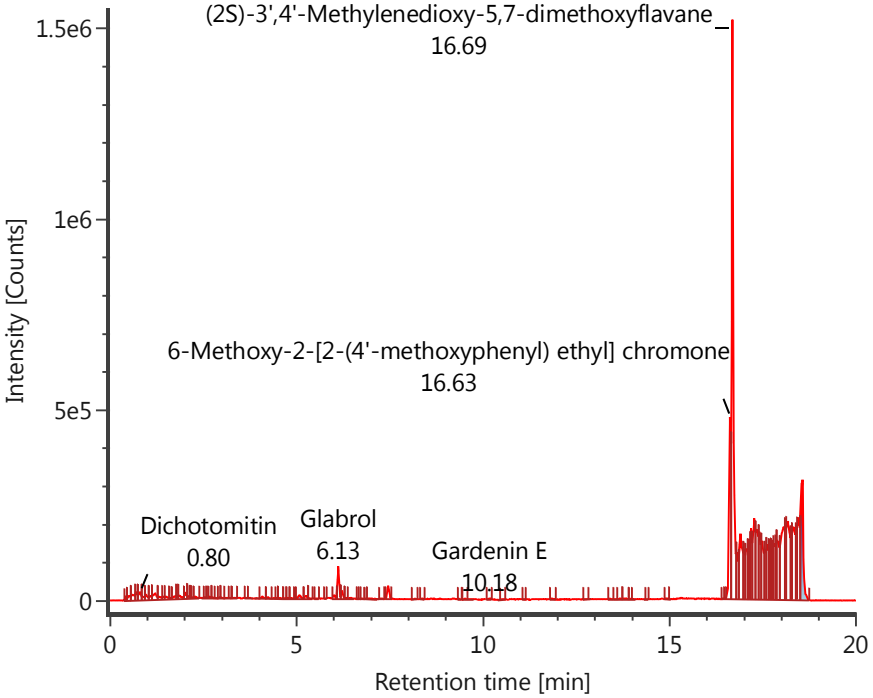

Item name: sample 2_01
Component name: Mirificin
Channel name: High energy : Time 2.0233 +/- 0.0231 minutes :
Drift Times: 7.82 +/- 0.31, 7.90 +/- 0.31 ms



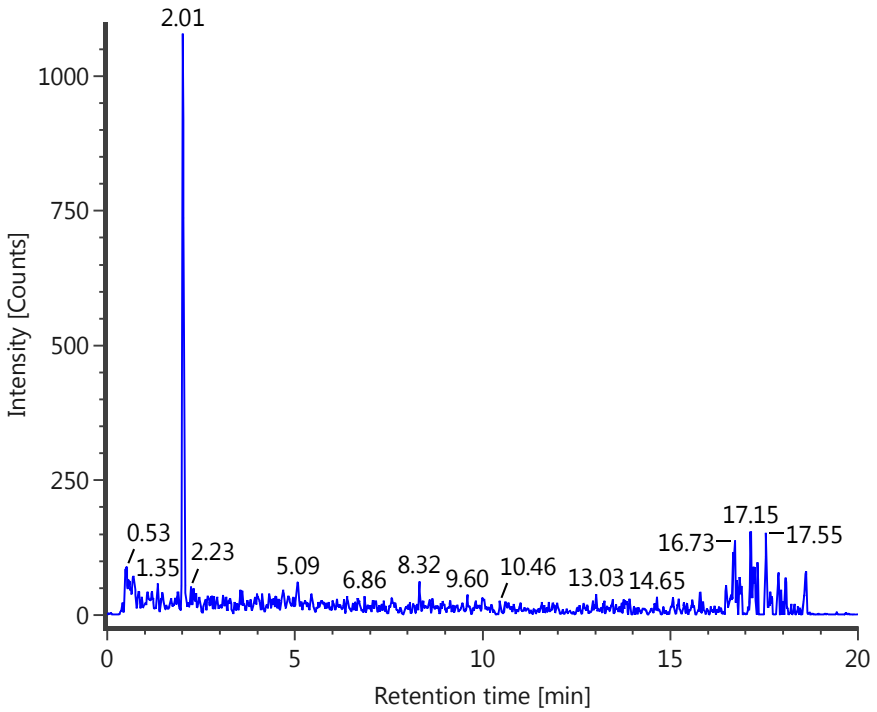
Item name: sample 2_01
Channel name: Naringenin-4′-glucoside-7-rutinoside [+Na] : (18.8 PPM) 765.2186 :
DT=7.66 to 8.28 ms



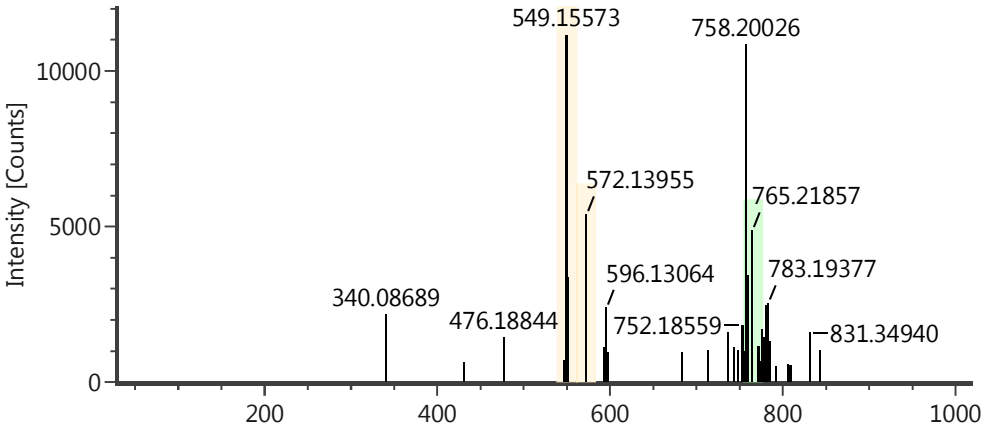
Item name: sample 2_01
Channel name: Identified Components



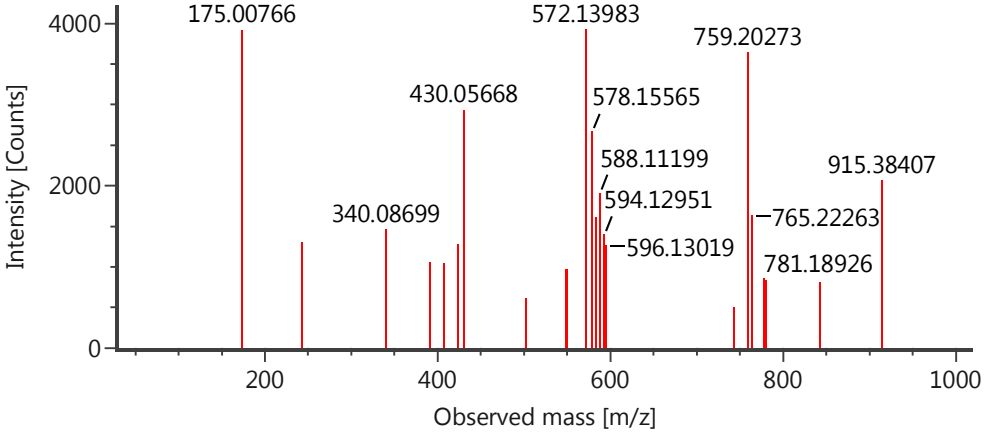
Item name: sample 2_01
Channel name: Naringenin-4′-glucoside-7-rutinoside [+Na] : (18.8 PPM) 765.2186



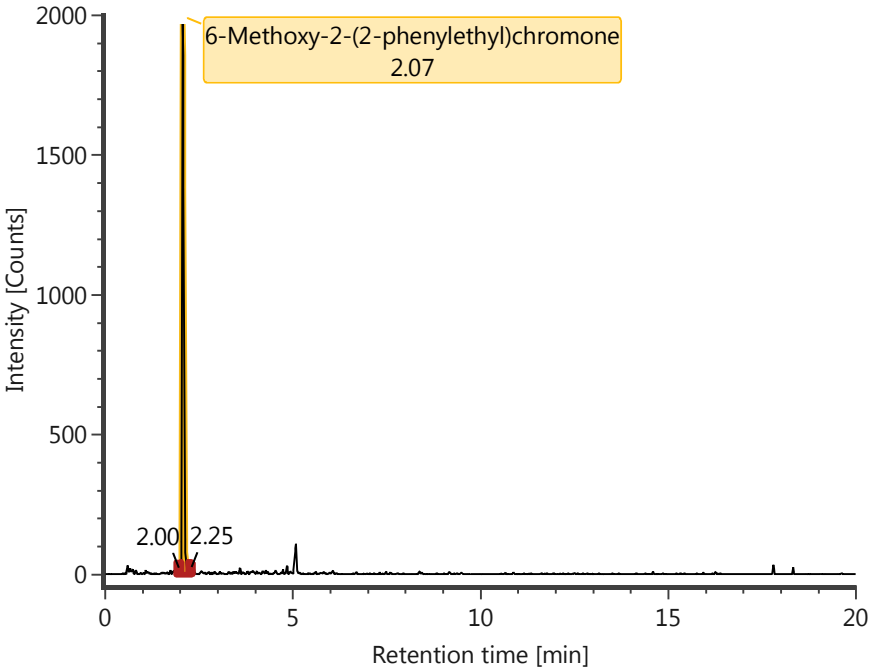

Item name: sample 2_01
Component name: Naringenin-4′-glucoside-7-rutinoside
Channel name: Low energy : Time 2.0247 +/- 0.0231 minutes : Drift Times: 8.00 +/- 0.31 ms



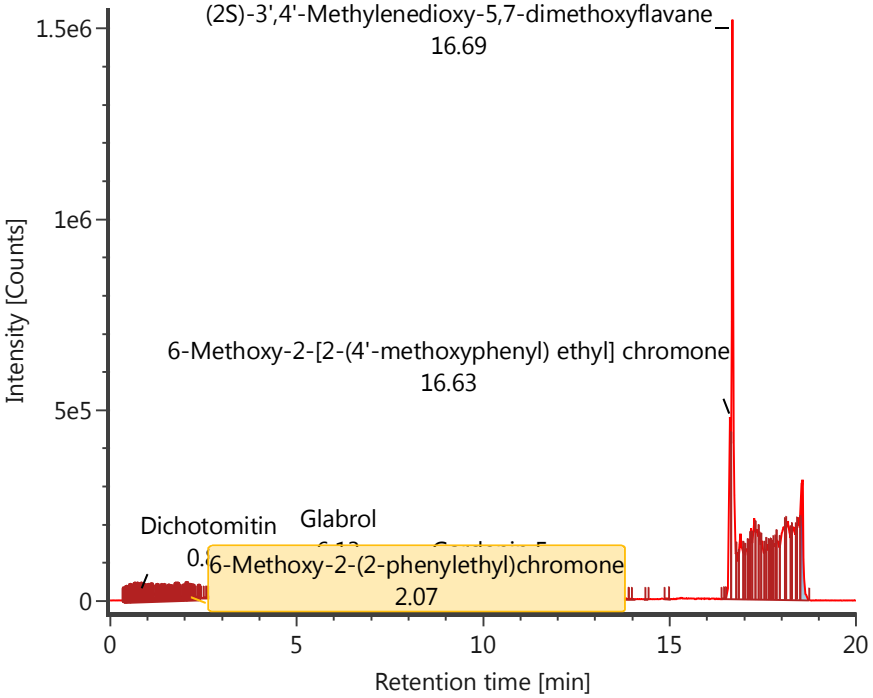

Item name: sample 2_01
Component name: Naringenin-4′-glucoside-7-rutinoside
Channel name: High energy : Time 2.0247 +/- 0.0231 minutes : Drift Times: 7.87 +/- 0.31 ms



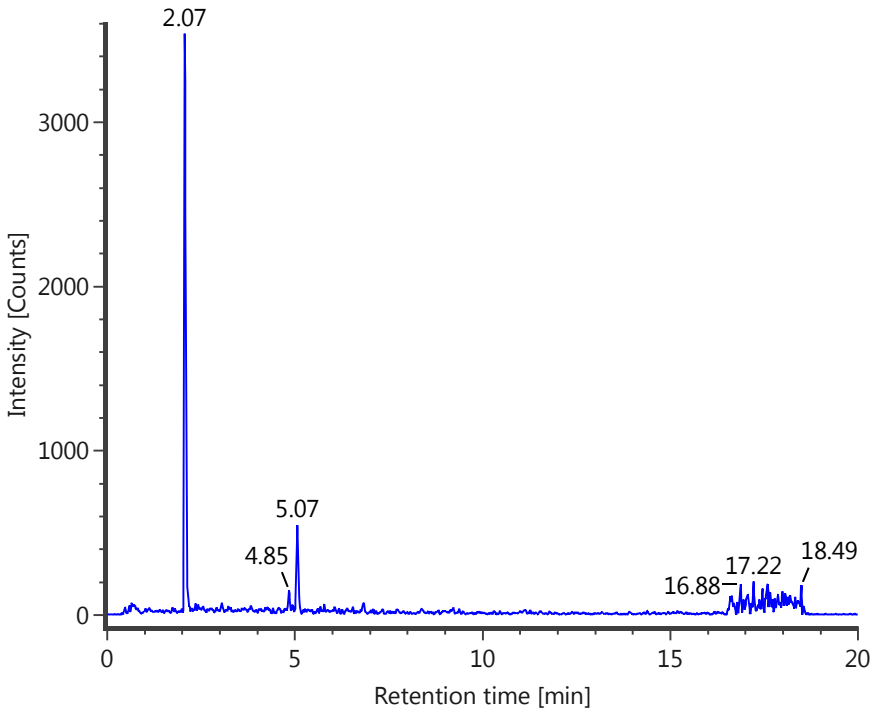
Item name: sample 2_01
Channel name: 6-Methoxy-2-(2-phenylethyl)chromone [+Na] : (18.8 PPM)
303.1014 : DT=5.62 to 6.17 ms



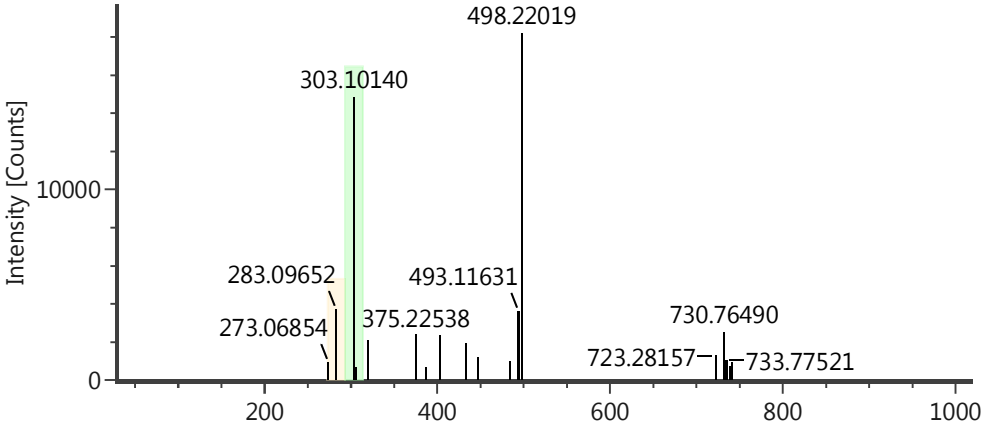
Item name: sample 2_01
Channel name: Identified Components



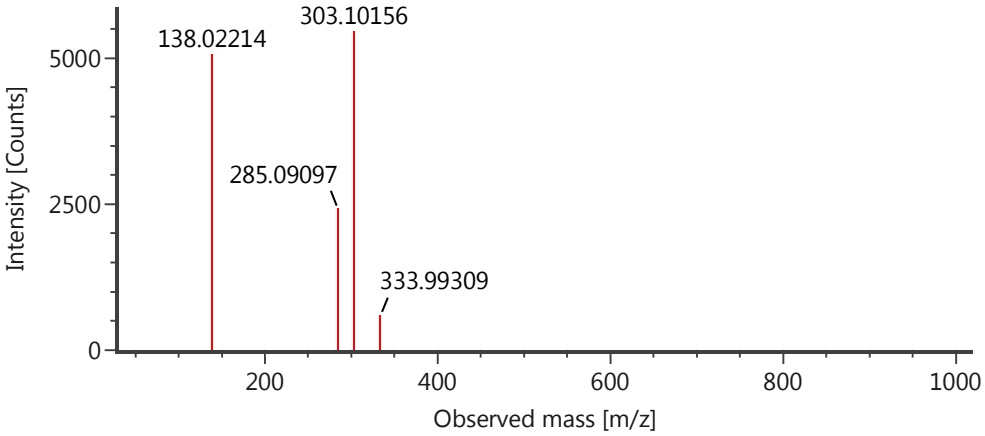
Item name: sample 2_01
Channel name: 6-Methoxy-2-(2-phenylethyl)chromone [+Na] : (18.8 PPM) 303.1014



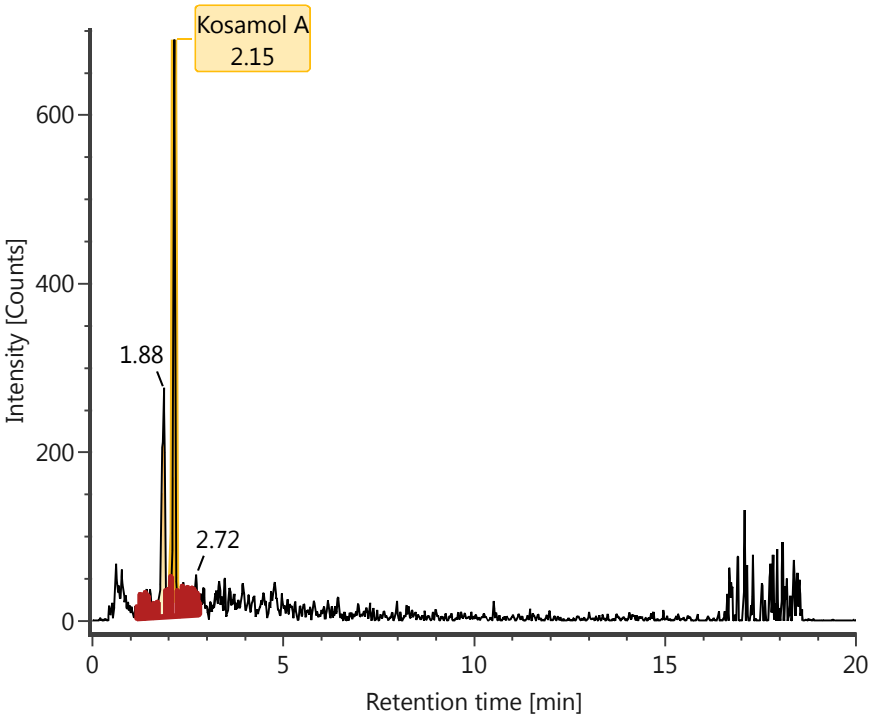

Item name: sample 2_01
Component name: 6-Methoxy-2-(2-phenylethyl)chromone
Channel name: Low energy : Time 2.0790 +/- 0.0231 minutes : Drift Times: 5.89 +/- 0.27 ms



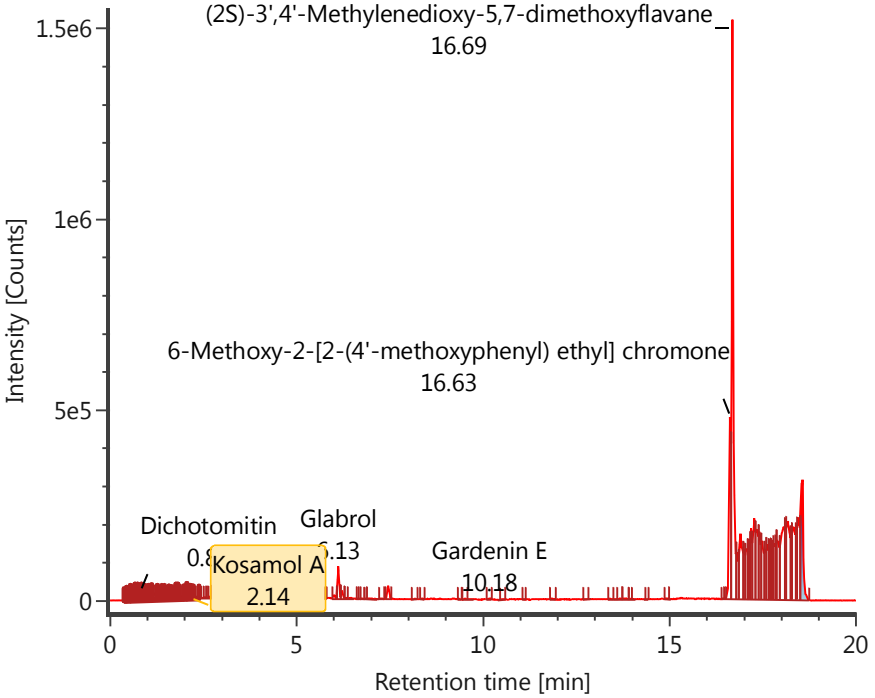

Item name: sample 2_01
Component name: 6-Methoxy-2-(2-phenylethyl)chromone
Channel name: High energy : Time 2.0790 +/- 0.0231 minutes : Drift Times: 5.76 +/- 0.27 ms



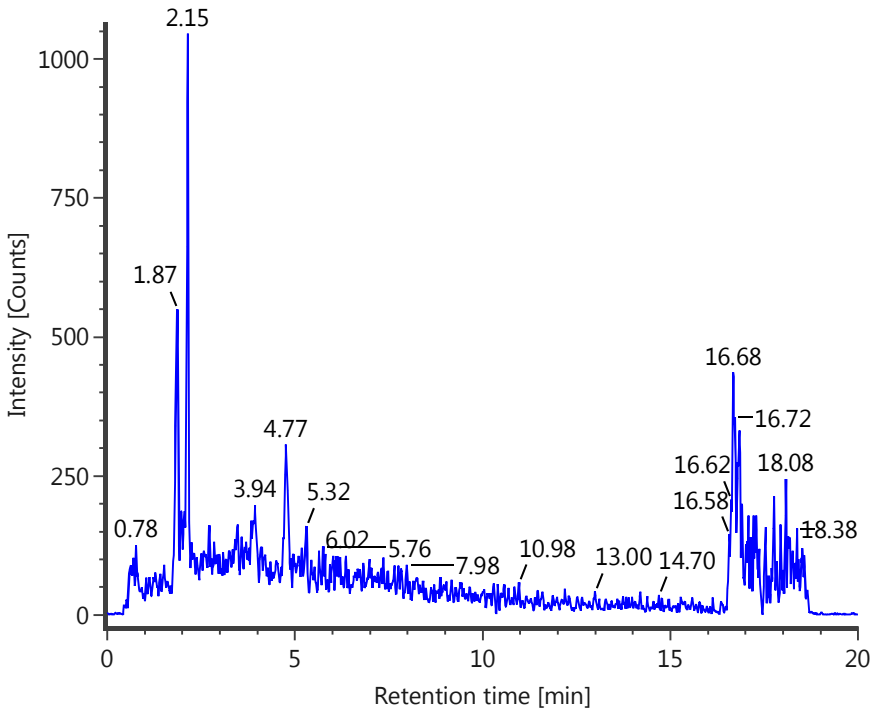
Item name: sample 2_01
Channel name: Kosamol A [+K] : (18.8 PPM) 565.2243 : DT=6.26 to 6.82 ms



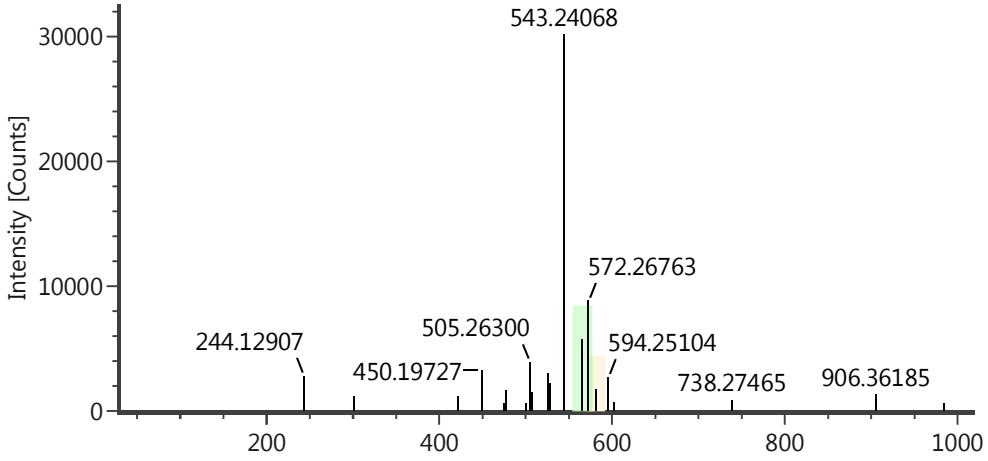
Item name: sample 2_01
Channel name: Identified Components



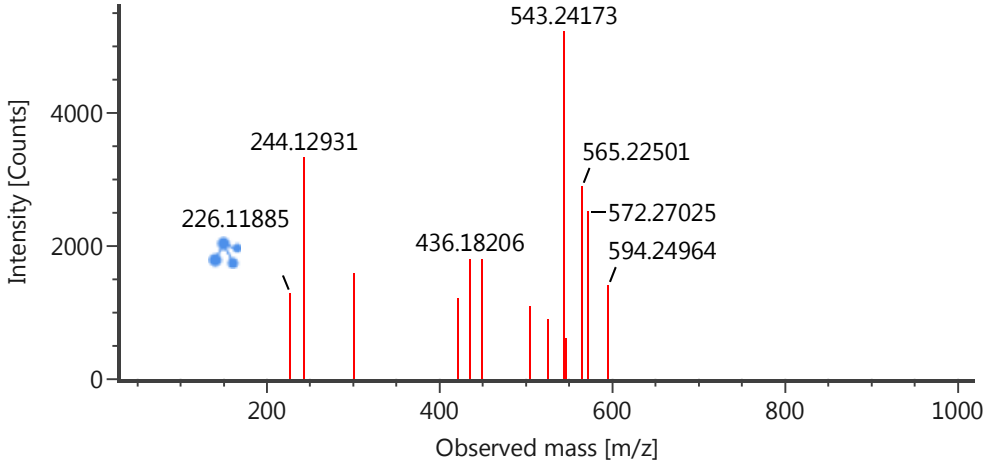
Item name: sample 2_01
Channel name: Kosamol A [+K] : (18.8 PPM) 565.2243



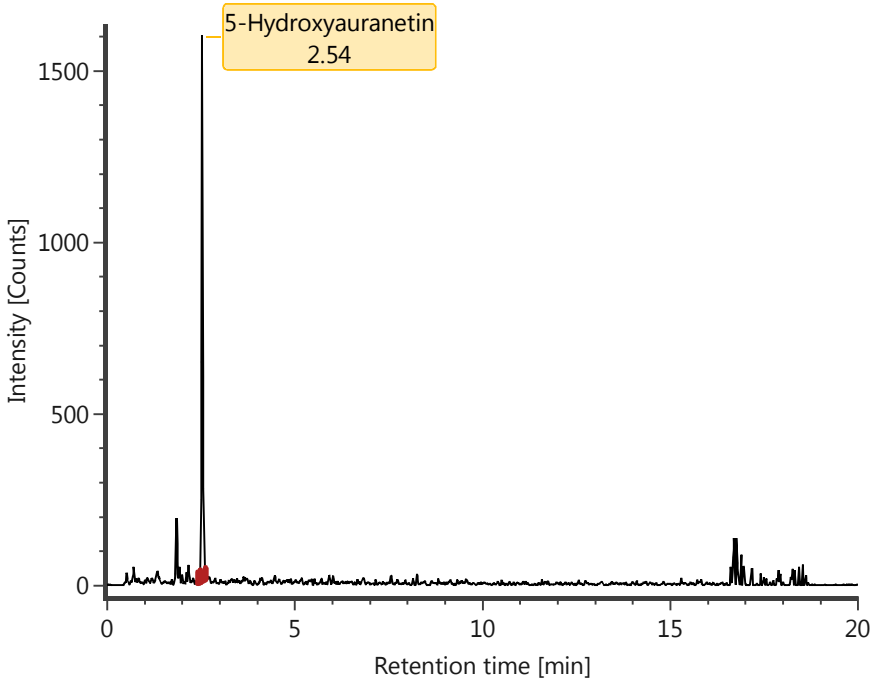

Item name: sample 2_01
Component name: Kosamol A
Channel name: Low energy : Time 2.1519 +/- 0.0231 minutes :
Drift Times: 6.55 +/- 0.28 ms



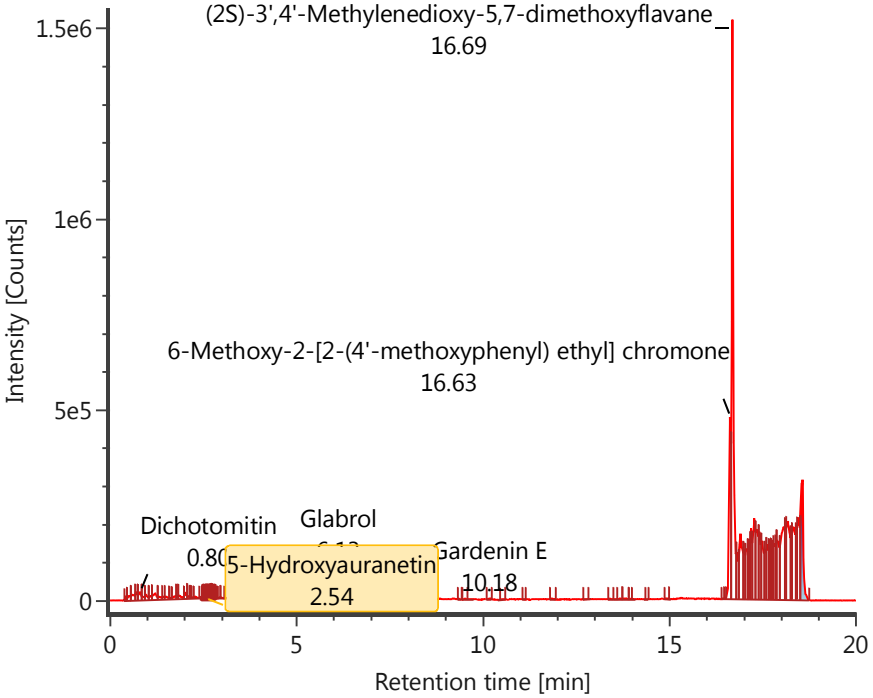

Item name: sample 2_01
Component name: Kosamol A
Channel name: High energy : Time 2.1519 +/- 0.0231 minutes :
Drift Times: 6.42 +/- 0.28 ms



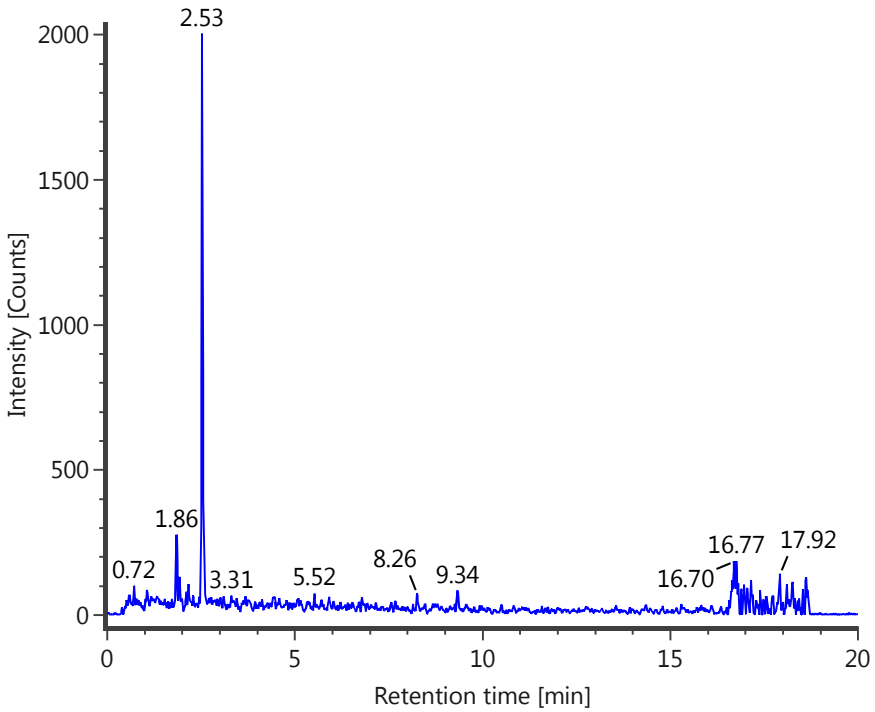
Item name: sample 2_01
Channel name: 5-Hydroxyauranetin [+Li] : (18.8 PPM) 395.1313 : DT=5.47 to 6.01 ms



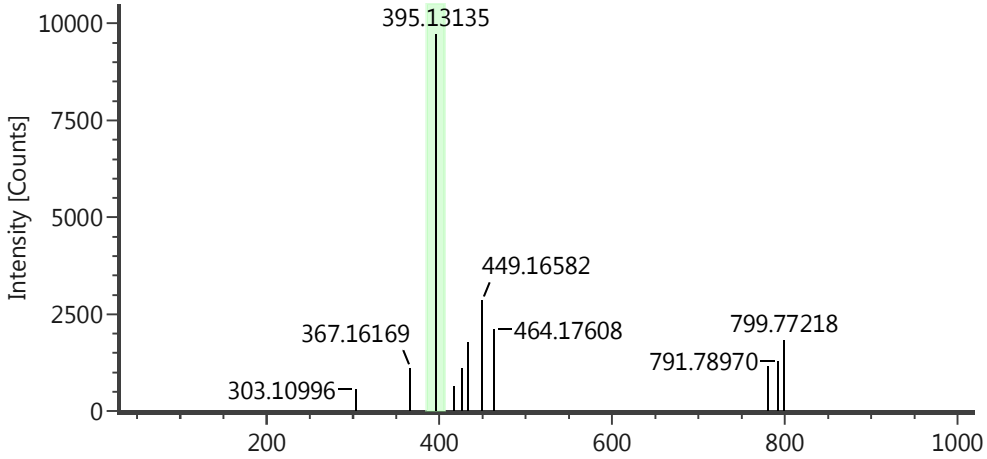
Item name: sample 2_01
Channel name: Identified Components



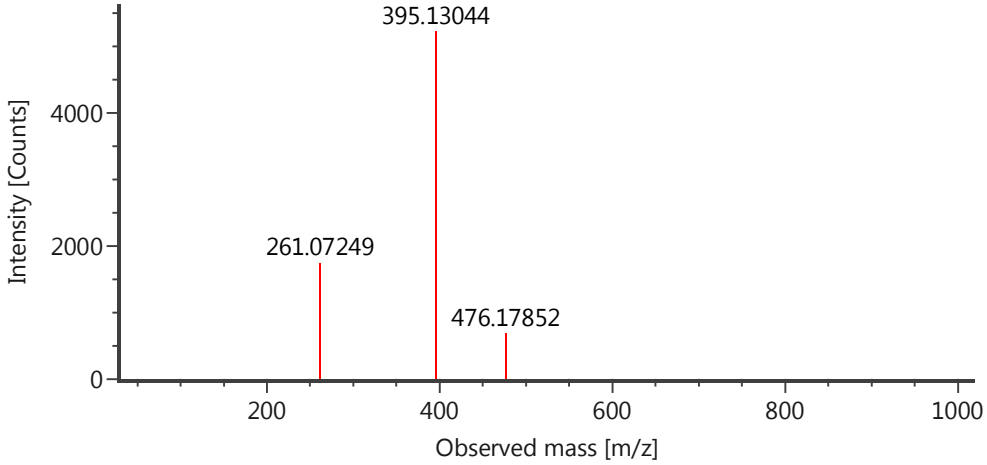
Item name: sample 2_01
Channel name: 5-Hydroxyauranetin [+Li] : (18.8 PPM) 395.1313



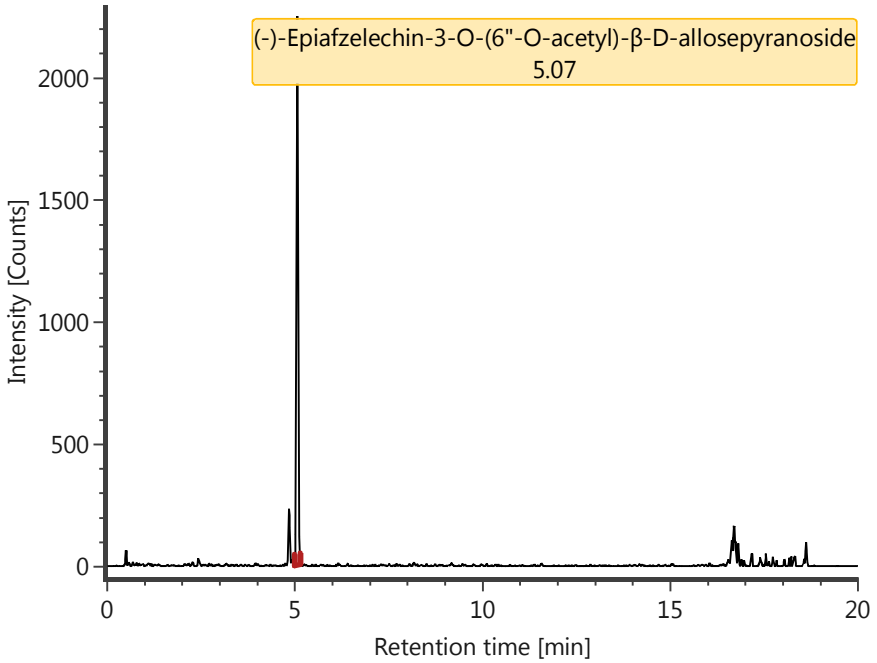

Item name: sample 2_01
Component name: 5-Hydroxyauranetin
Channel name: Low energy : Time 2.5381 +/- 0.0231 minutes : Drift Times: 5.75 +/- 0.27 ms



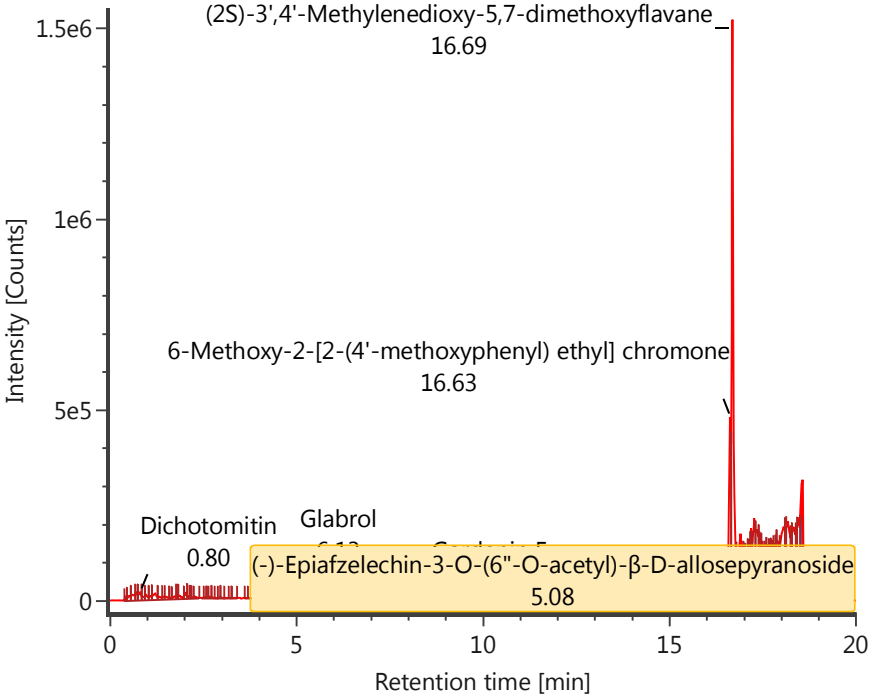

Item name: sample 2_01
Component name: 5-Hydroxyauranetin
Channel name: High energy : Time 2.5381 +/- 0.0231 minutes : Drift Times: 5.62 +/- 0.27 ms



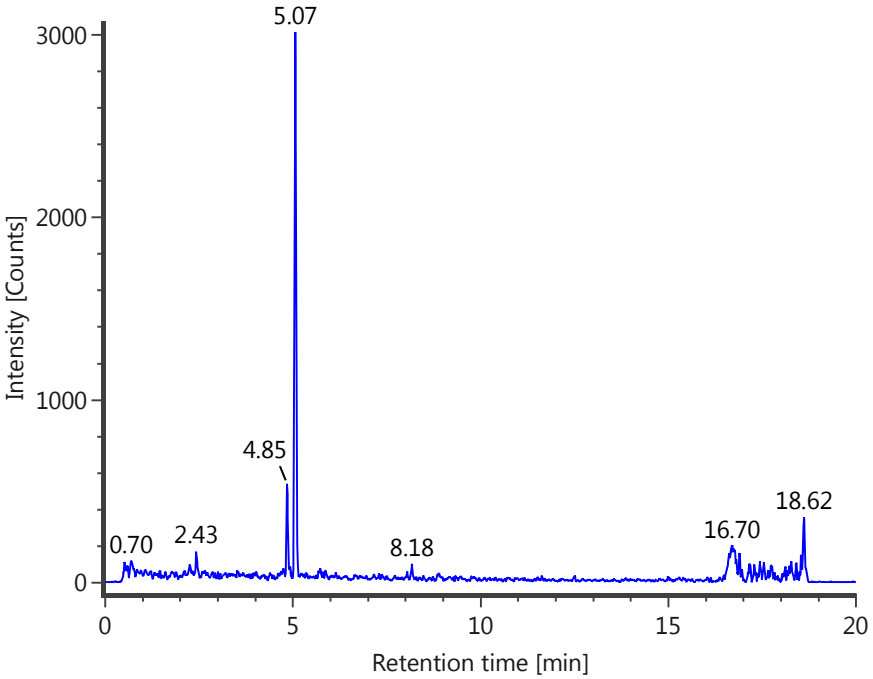
Item name: sample 2_01
Channel name: (-)-Epiafzelechin-3-O-(6"-O-acetyl)-β-D-allosepyranoside [+H] :
(18.8 PPM) 479.1539 : DT=6.57 to 7.15 ms



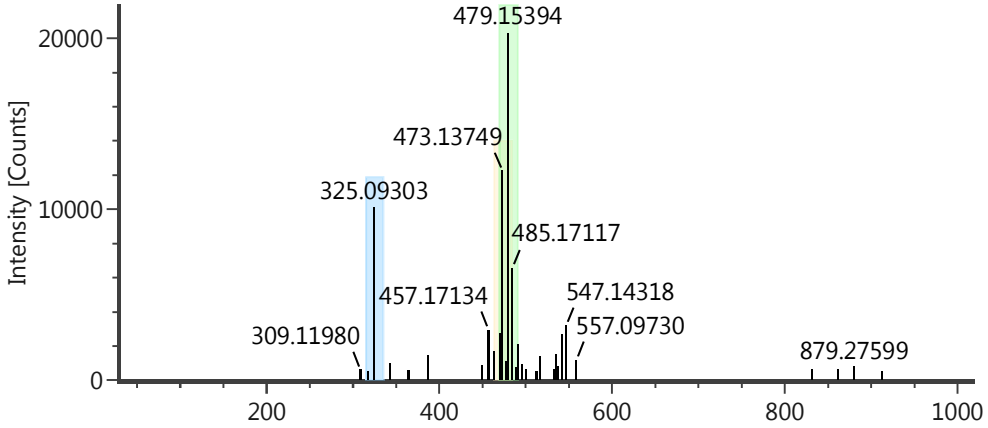
Item name: sample 2_01
Channel name: Identified Components



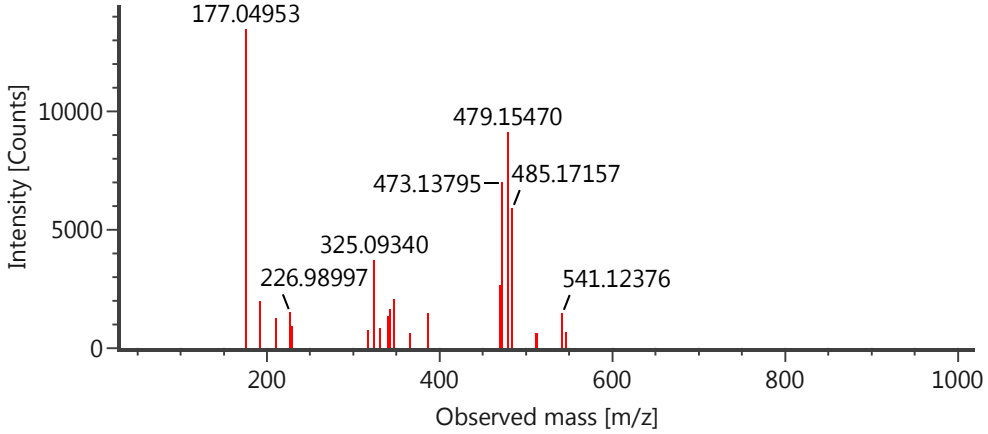
Item name: sample 2_01
Channel name: (-)-Epiafzelechin-3-O-(6"-O-acetyl)-β-D-allosepyranoside [+H] : (18.8 PPM) 479.1539



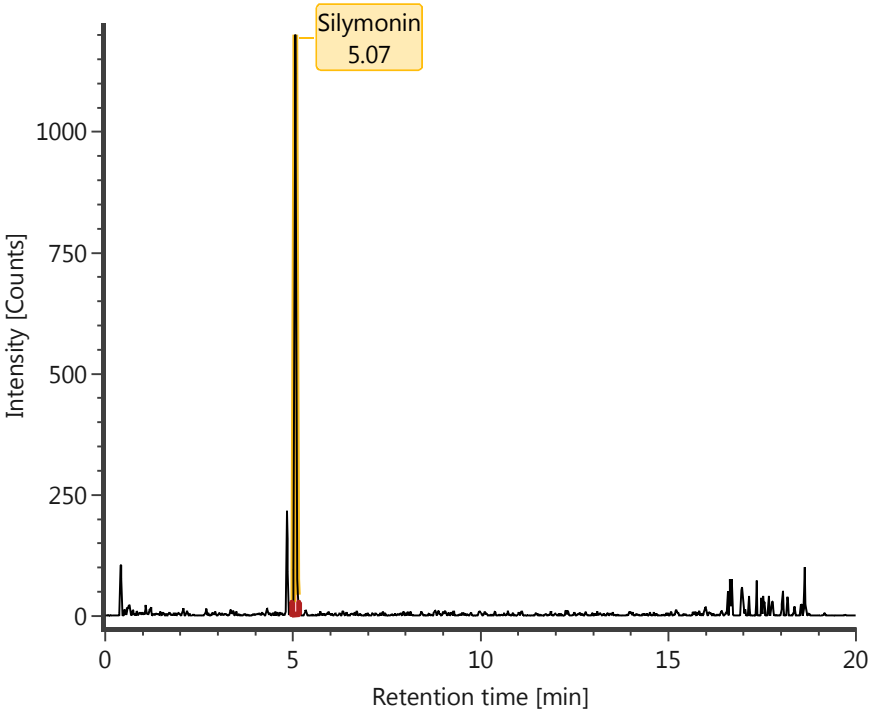

Item name: sample 2_01
Component name: (-)-Epiafzelechin-3-O-(6"-O-acetyl)-β-D-allosepyranoside
Channel name: Low energy : Time 5.0737 +/- 0.0231 minutes : Drift Times: 6.86 +/- 0.29 ms



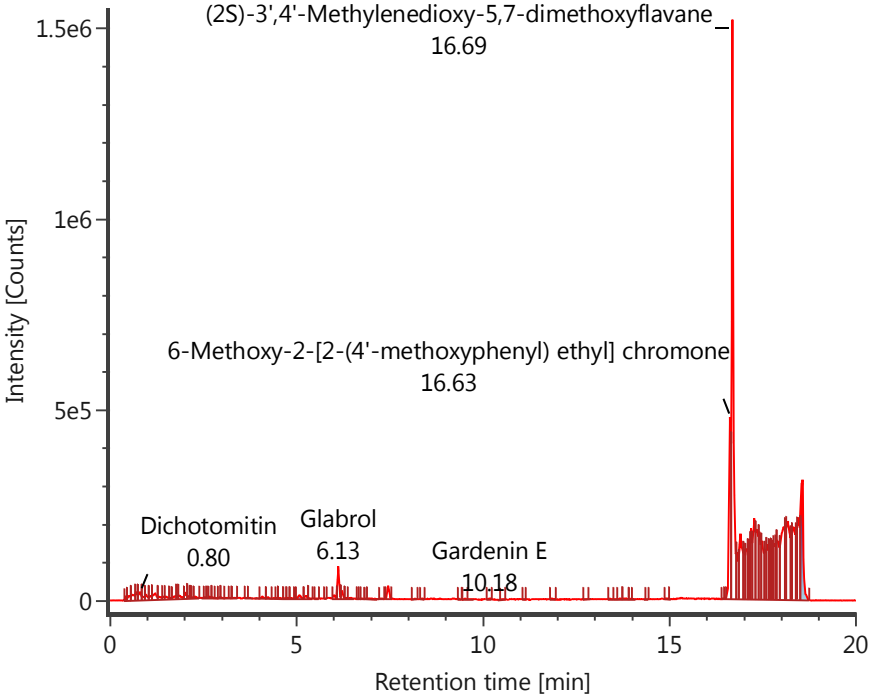

Item name: sample 2_01
Component name: (-)-Epiafzelechin-3-O-(6"-O-acetyl)-β-D-allosepyranoside
Channel name: High energy : Time 5.0737 +/- 0.0231 minutes : Drift Times: 6.73 +/- 0.29 ms



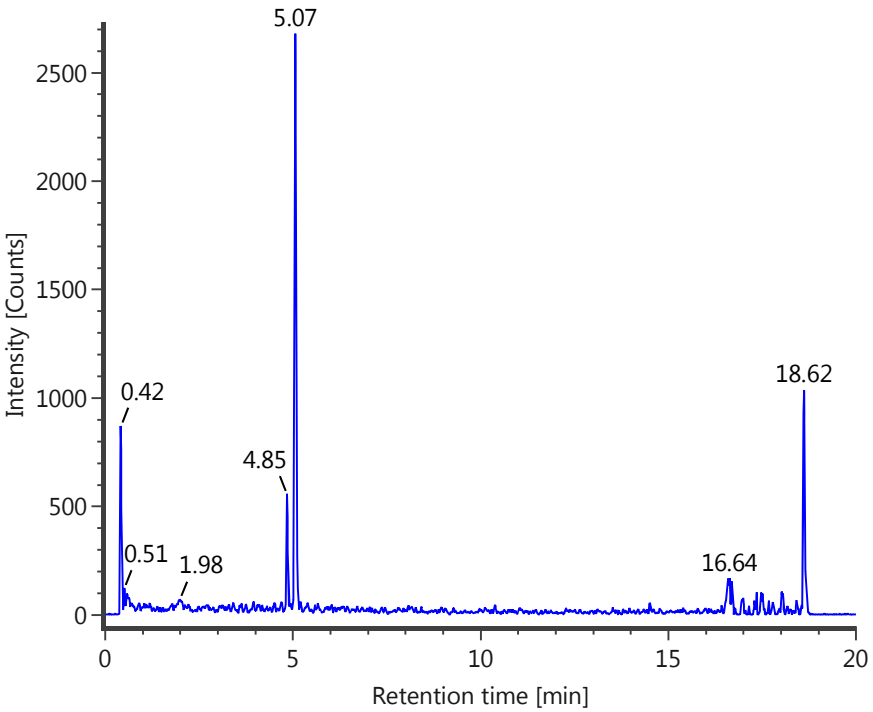
Item name: sample 2_01
Channel name: Silymonin [+Li] : (18.8 PPM) 473.1375 : DT=6.53 to 7.11 ms



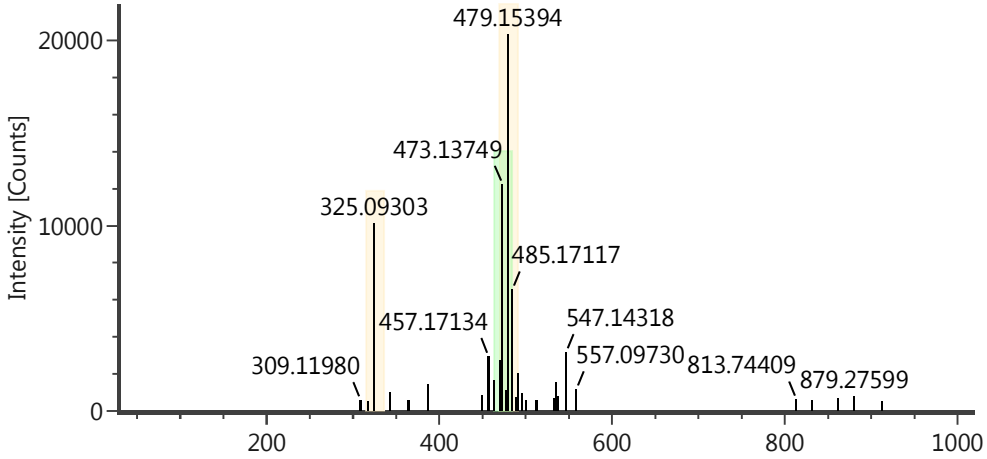
Item name: sample 2_01
Channel name: Identified Components



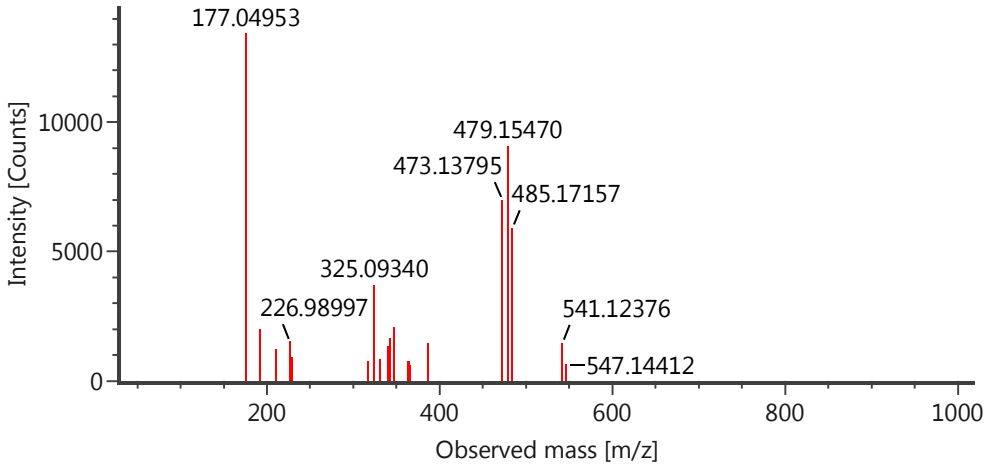
Item name: sample 2_01
Channel name: Silymonin [+Li] : (18.8 PPM) 473.1375



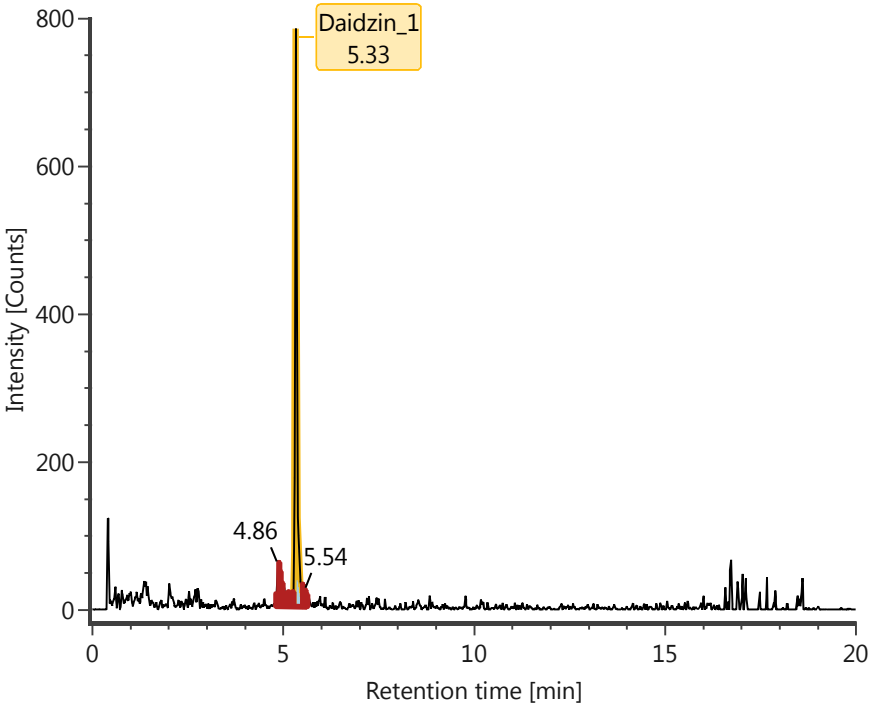

Item name: sample 2_01
Component name: Silymonin
Channel name: Low energy : Time 5.0749 +/- 0.0231 minutes :
Drift Times: 6.82 +/- 0.29 ms



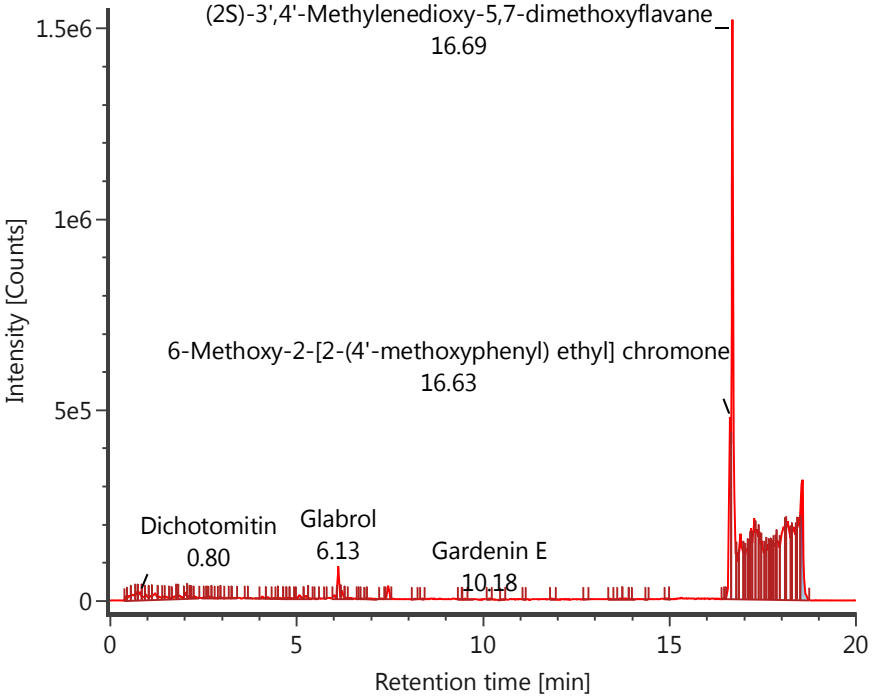

Item name: sample 2_01
Component name: Silymonin
Channel name: High energy : Time 5.0749 +/- 0.0231 minutes :
Drift Times: 6.69 +/- 0.29 ms



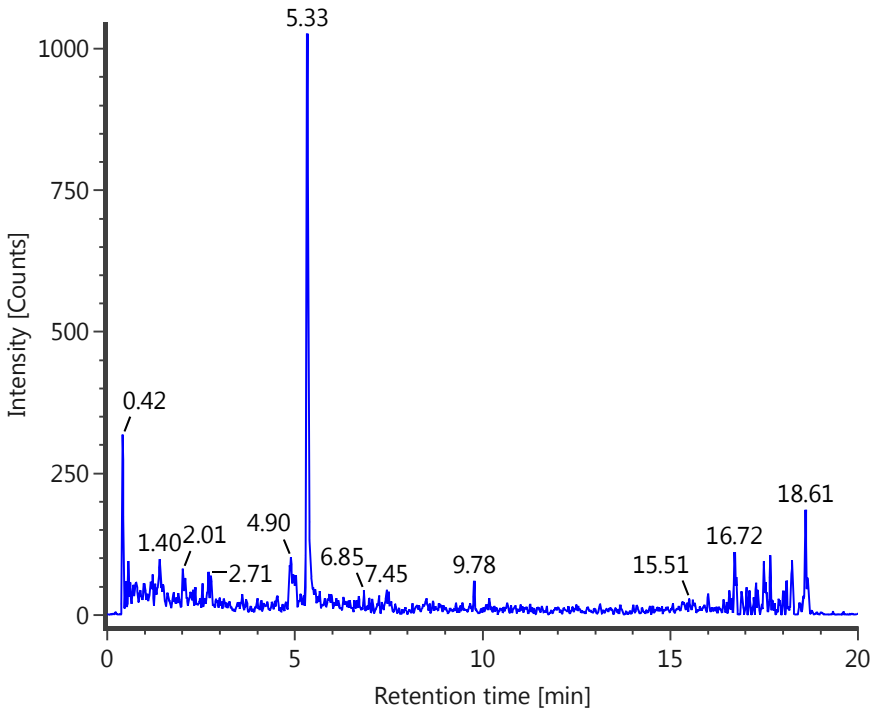
Item name: sample 2_01
Channel name: Daidzin_1 [+Na] : (18.8 PPM) 439.1006 : DT=5.55 to 6.09 ms



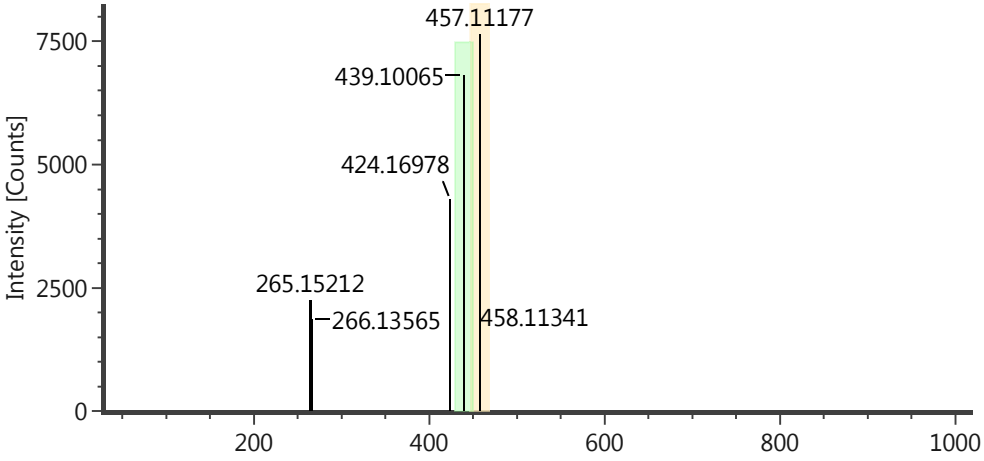
Item name: sample 2_01
Channel name: Identified Components



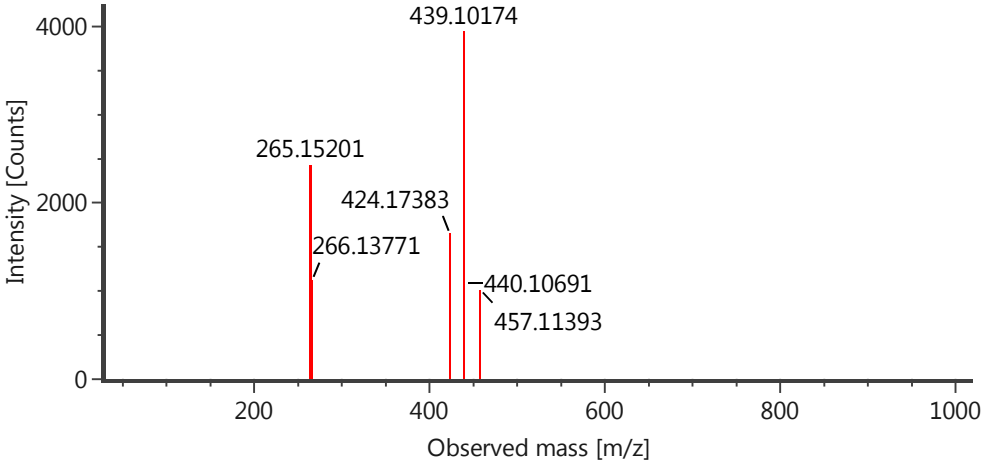
Item name: sample 2_01
Channel name: Daidzin_1 [+Na] : (18.8 PPM) 439.1006



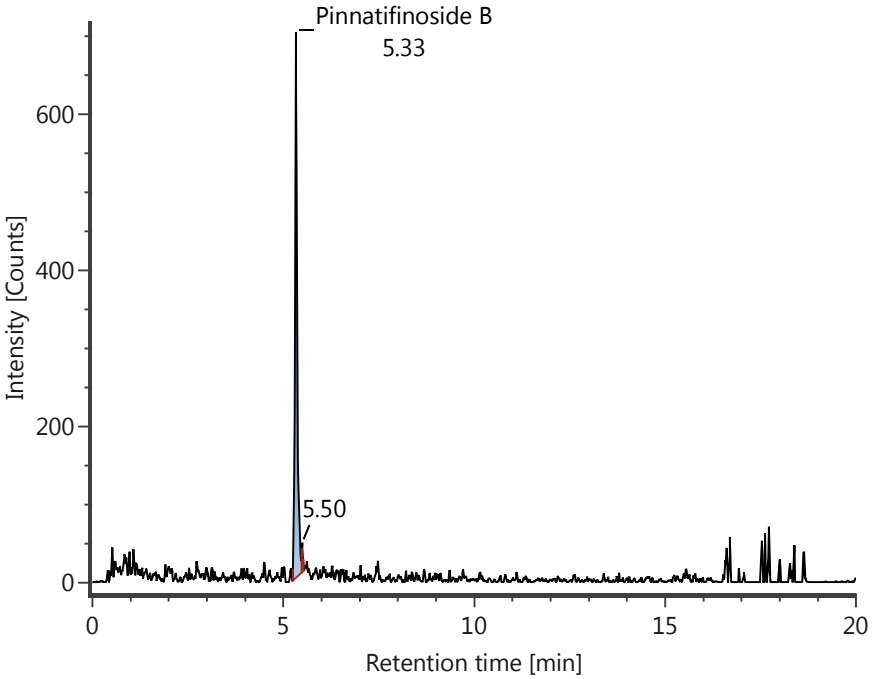

Item name: sample 2_01
Component name: Daidzin_1
Channel name: Low energy : Time 5.3335 +/- 0.0231 minutes :
Drift Times: 5.83 +/- 0.27 ms



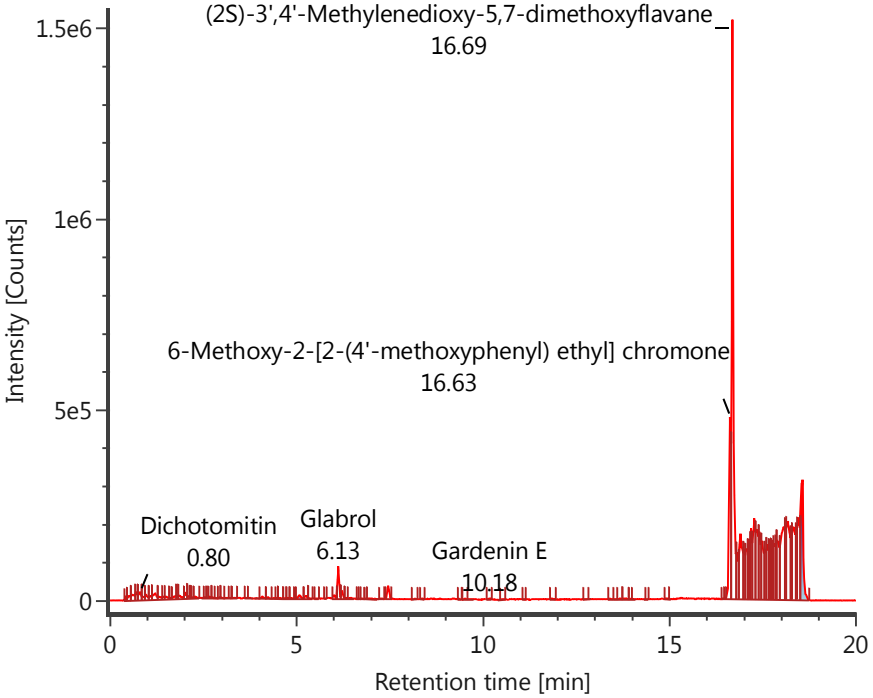

Item name: sample 2_01
Component name: Daidzin_1
Channel name: High energy : Time 5.3335 +/- 0.0231 minutes :
Drift Times: 5.70 +/- 0.27 ms



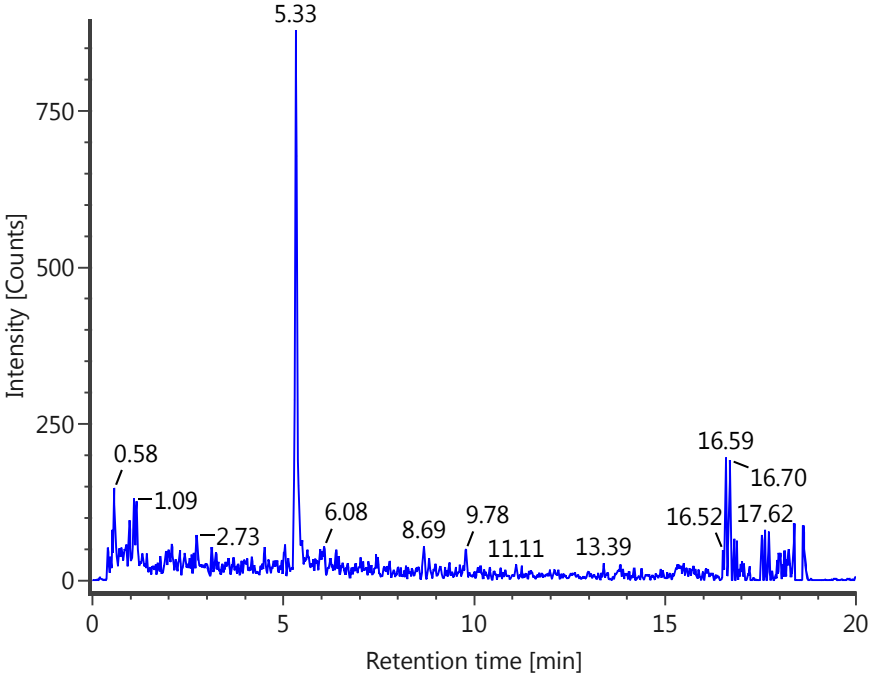
Item name: sample 2_01
Channel name: 3,4,2'-Trihydroxychal-cone-4'-O-β-D-glucopyranoside [+Na] :
Pinnatifinoside B [+H] : (18.8 PPM) 457.1118 : DT=5.68 to 6.22 ms



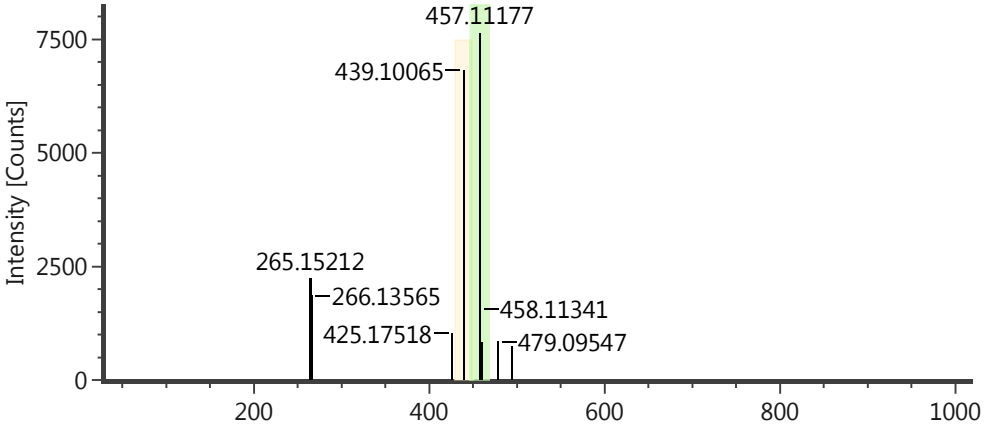
Item name: sample 2_01
Channel name: Identified Components



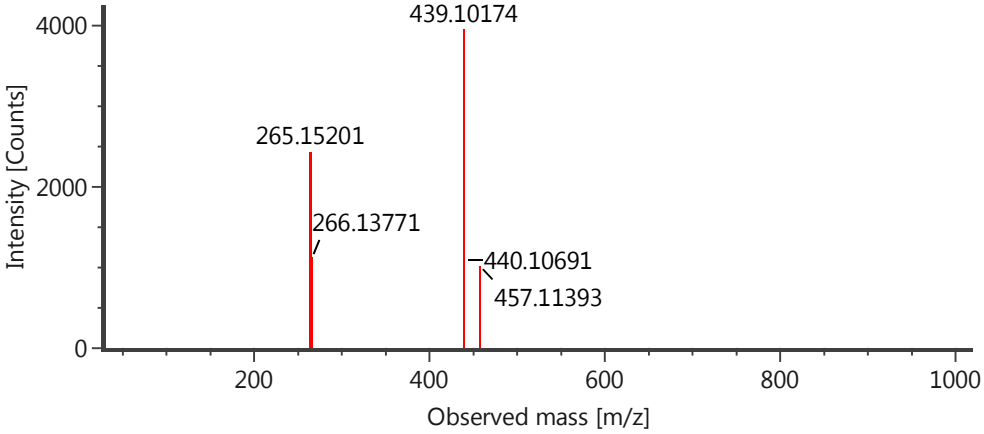
Item name: sample 2_01
Channel name: 3,4,2'-Trihydroxychal-cone-4'-O-β-D-glucopyranoside [+Na] : Pinnatifinoside B [+H] : (18.8 PPM) 457.1118



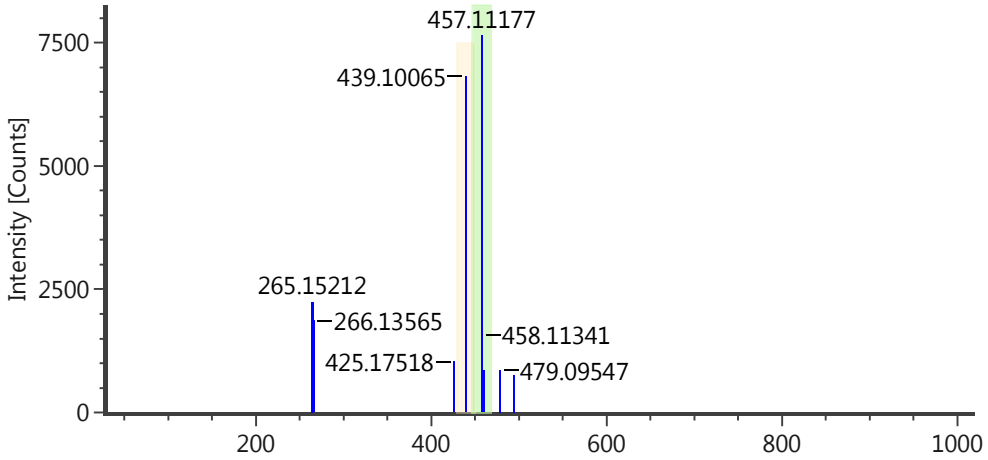

Item name: sample 2_01
Component name: 3,4,2'-Trihydroxychal-cone-4'-O-β-D-glucopyranoside
Channel name: Low energy : Time 5.3340 +/- 0.0231 minutes : Drift Times: 5.94 +/- 0.27 ms



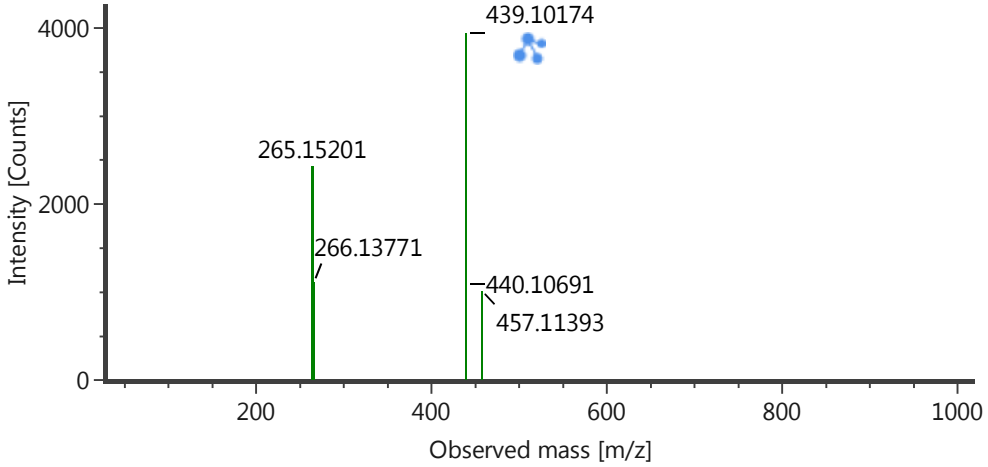

Item name: sample 2_01
Component name: 3,4,2'-Trihydroxychal-cone-4'-O-β-D-glucopyranoside
Channel name: High energy : Time 5.3340 +/- 0.0231 minutes : Drift Times: 5.81 +/- 0.27 ms



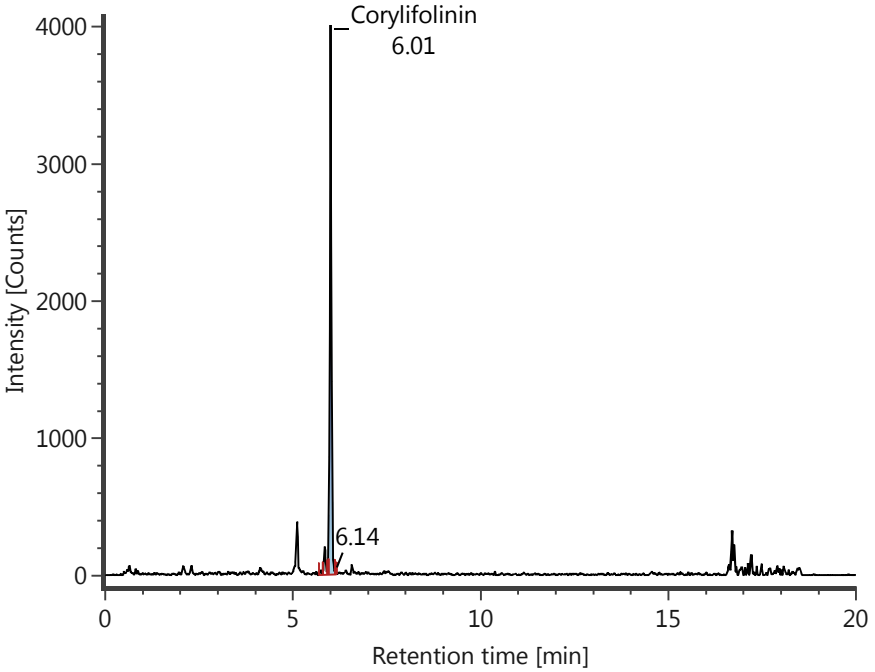
Item name: sample 2_01
Component name: Pinnatifinoside B
Channel name: Low energy : Time 5.3340 +/- 0.0231 minutes : Drift Times: 5.94 +/- 0.27 ms



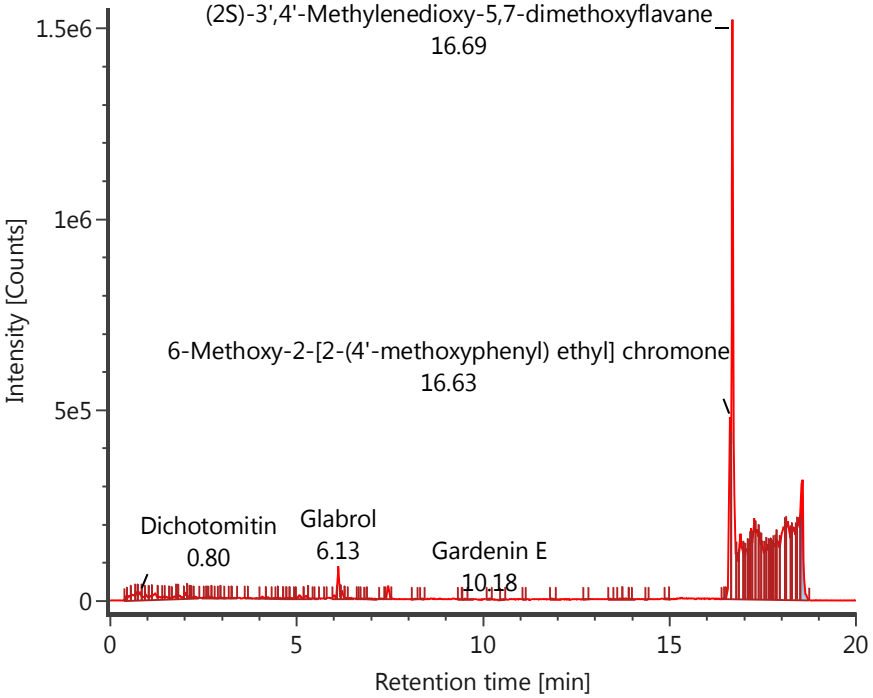

Item name: sample 2_01
Component name: Pinnatifinoside B
Channel name: High energy : Time 5.3340 +/- 0.0231 minutes : Drift Times: 5.81 +/- 0.27 ms



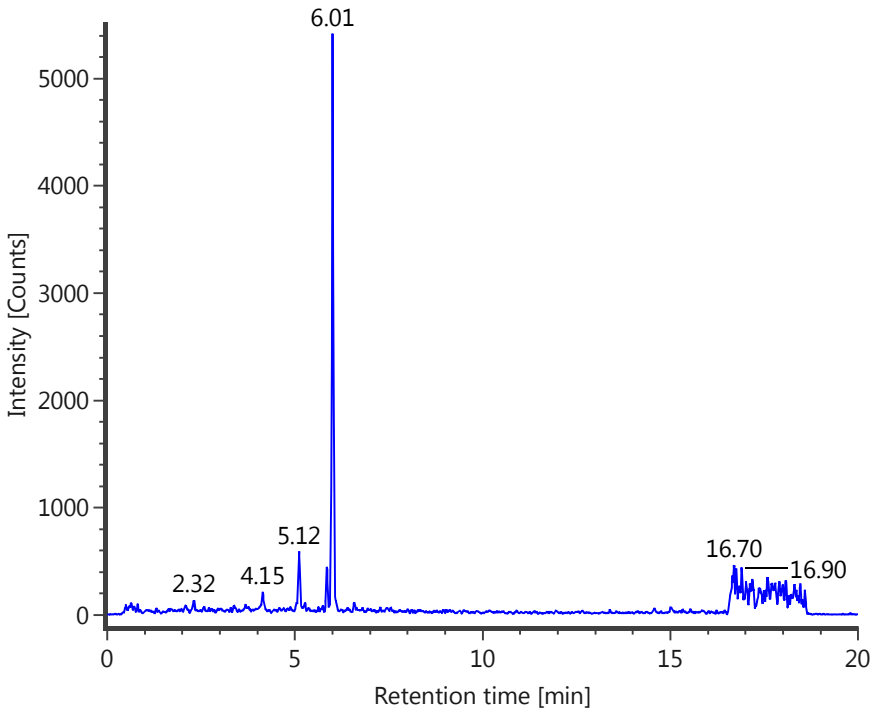
Item name: sample 2_01
Channel name: Bavachalcone [+Na] : Corylifolinin [+Na] : (18.8 PPM) 347.1235 :
DT=5.04 to 5.56 ms



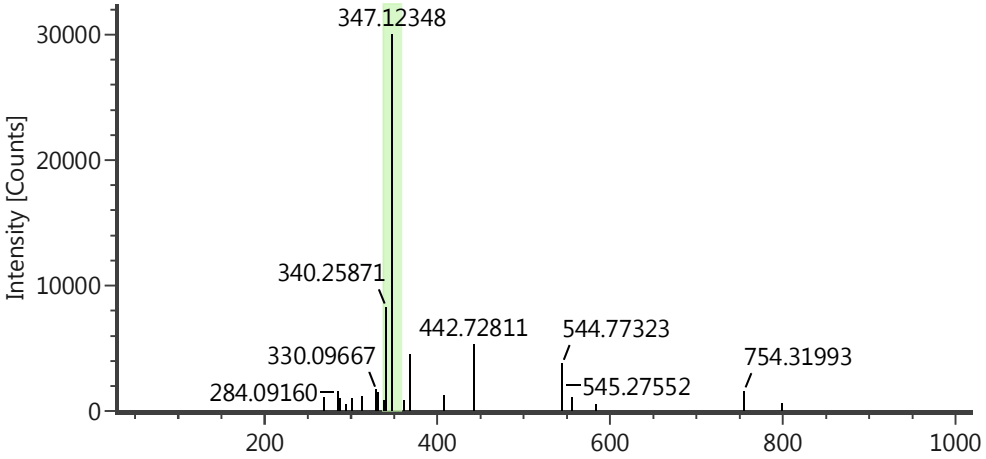
Item name: sample 2_01
Channel name: Identified Components



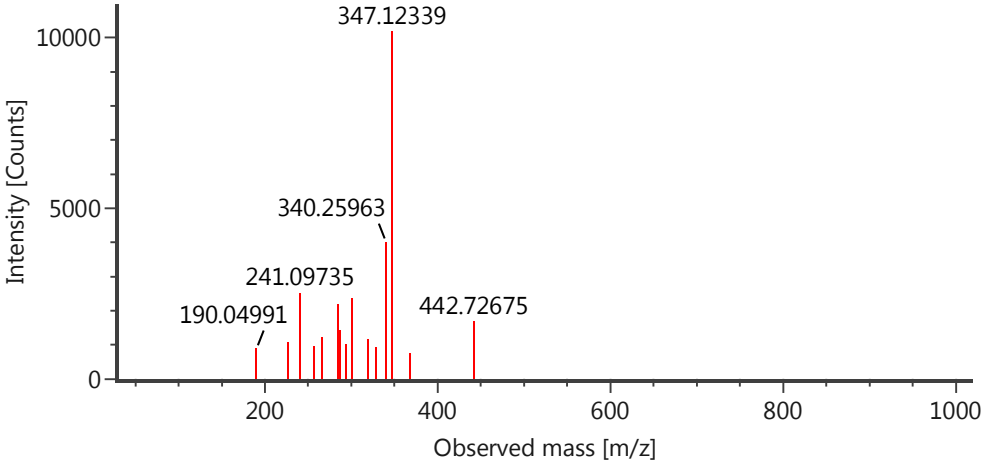
Item name: sample 2_01
Channel name: Bavachalcone [+Na] : Corylifolinin [+Na] : (18.8 PPM) 347.1235



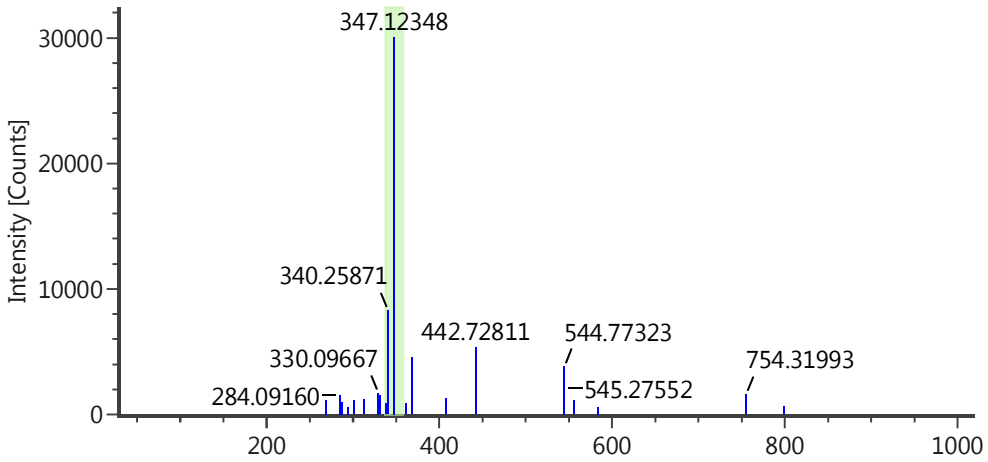

Item name: sample 2_01
Component name: Bavachalcone
Channel name: Low energy : Time 6.0097 +/- 0.0231
minutes : Drift Times: 5.30 +/- 0.26 ms



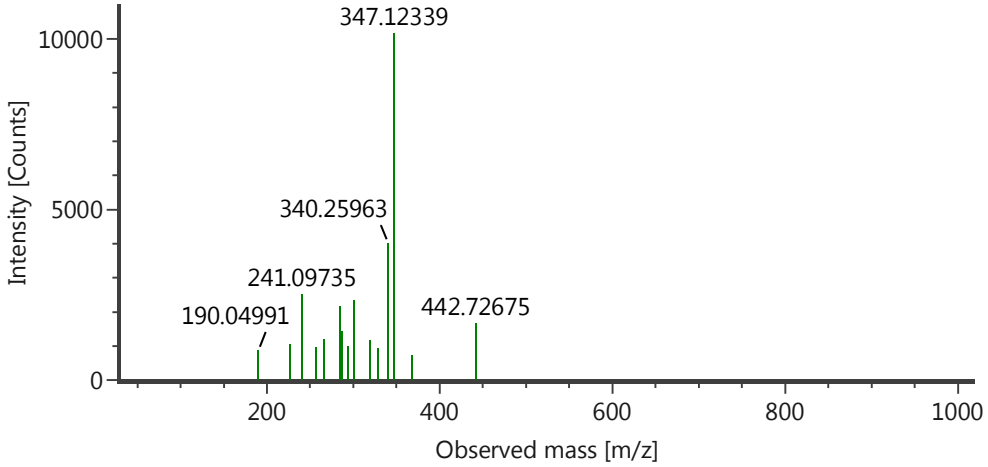

Item name: sample 2_01
Component name: Bavachalcone
Channel name: High energy : Time 6.0097 +/- 0.0231
minutes : Drift Times: 5.17 +/- 0.26 ms



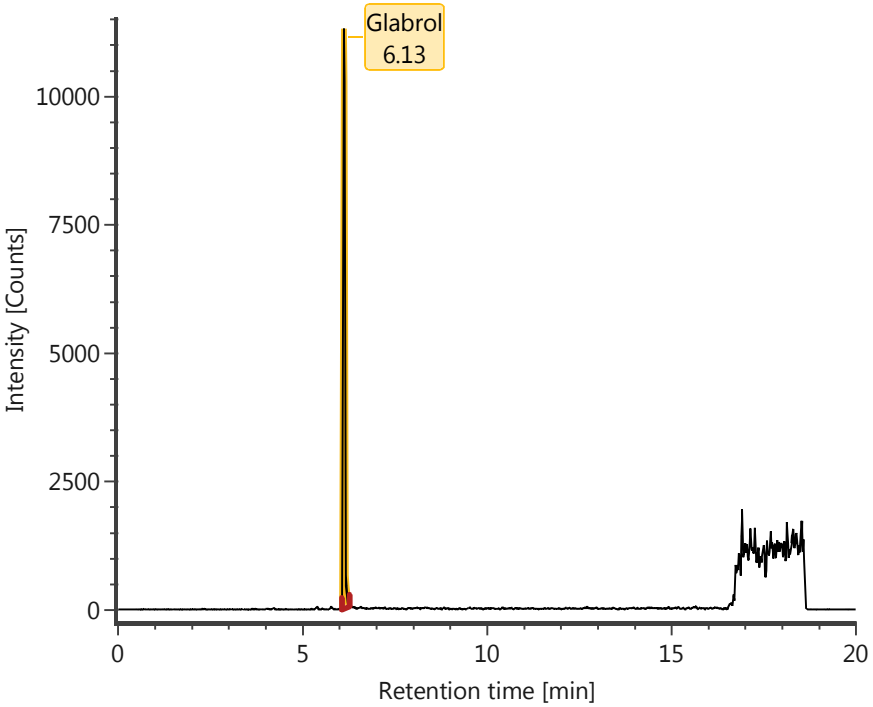
Item name: sample 2_01 Channel name: Low energy : Time 6.0097 +/- 0.0231 minutes :
Component name: Corylifolinin Drift Times: 5.30 +/- 0.26 ms



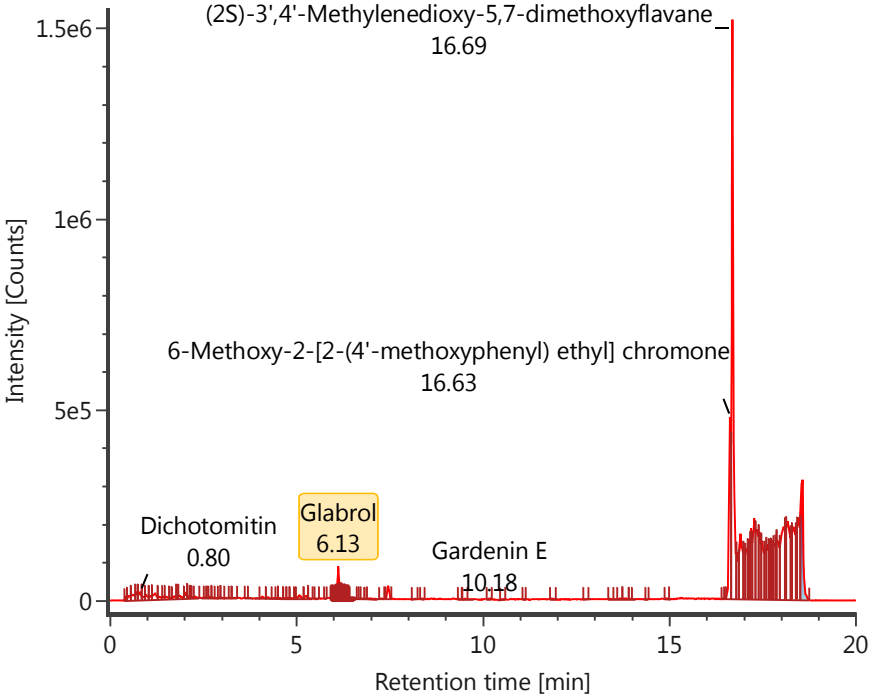

Item name: sample 2_01 Channel name: High energy : Time 6.0097 +/- 0.0231 minutes :
Component name: Corylifolinin Drift Times: 5.17 +/- 0.26 ms



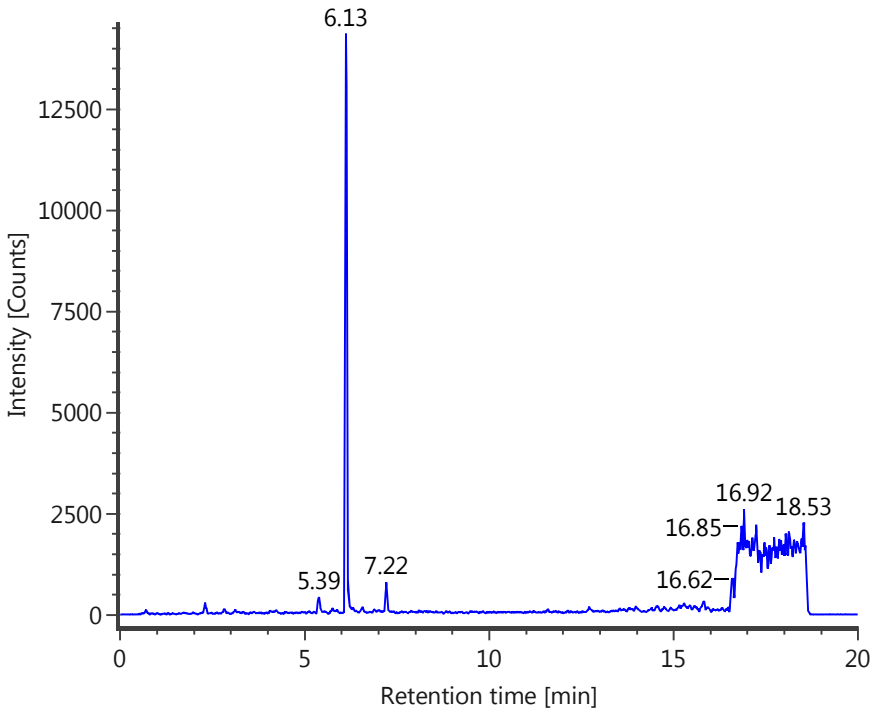
Item name: sample 2_01
Channel name: Glabrol [+H] : (18.8 PPM) 393.2089 : DT=4.96 to 5.48 ms



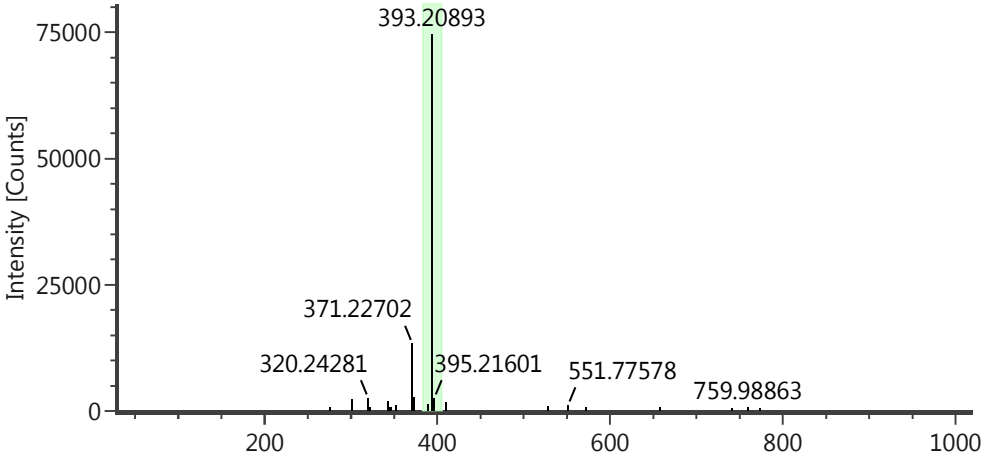
Item name: sample 2_01
Channel name: Identified Components



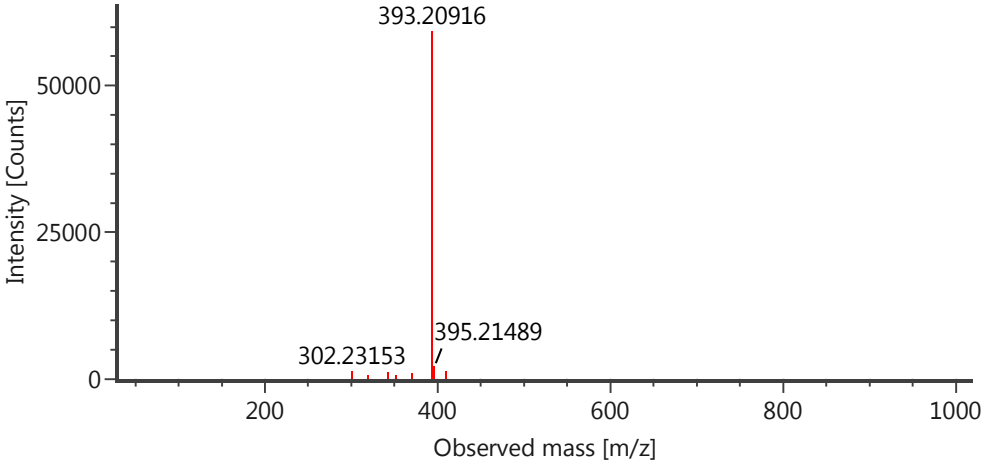
Item name: sample 2_01
Channel name: Glabrol [+H] : (18.8 PPM) 393.2089



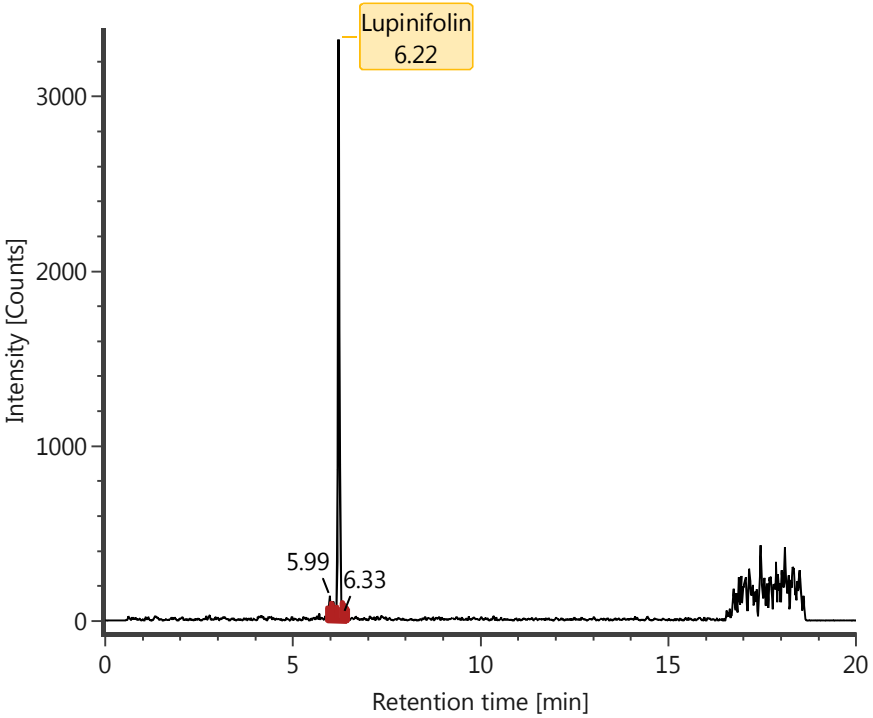

Item name: sample 2_01
Component name: Glabrol
Channel name: Low energy : Time 6.1301 +/- 0.0231 minutes : Drift Times: 5.22 +/- 0.26 ms



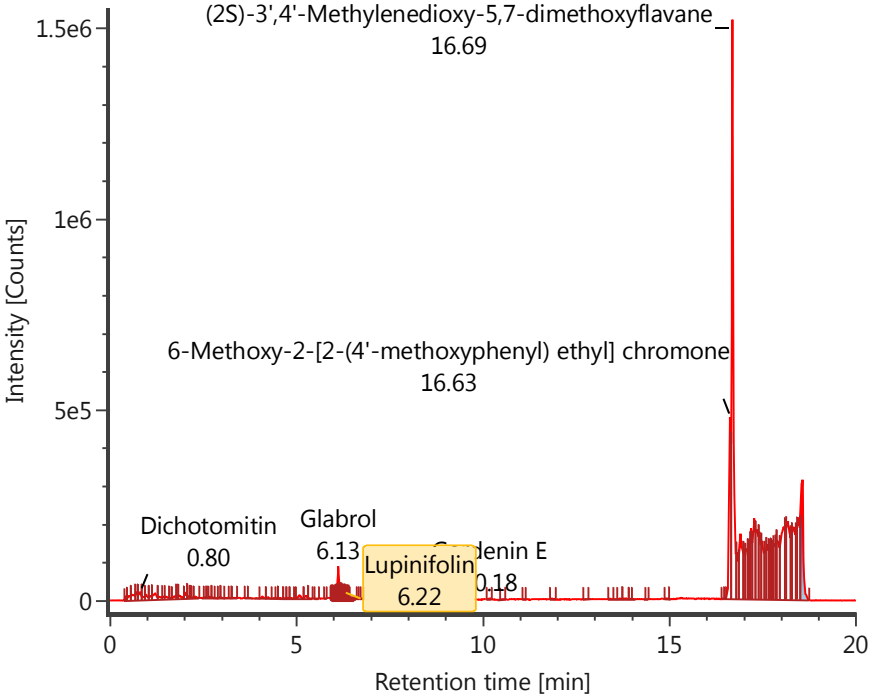

Item name: sample 2_01
Component name: Glabrol
Channel name: High energy : Time 6.1301 +/- 0.0231 minutes : Drift Times: 5.08 +/- 0.26 ms



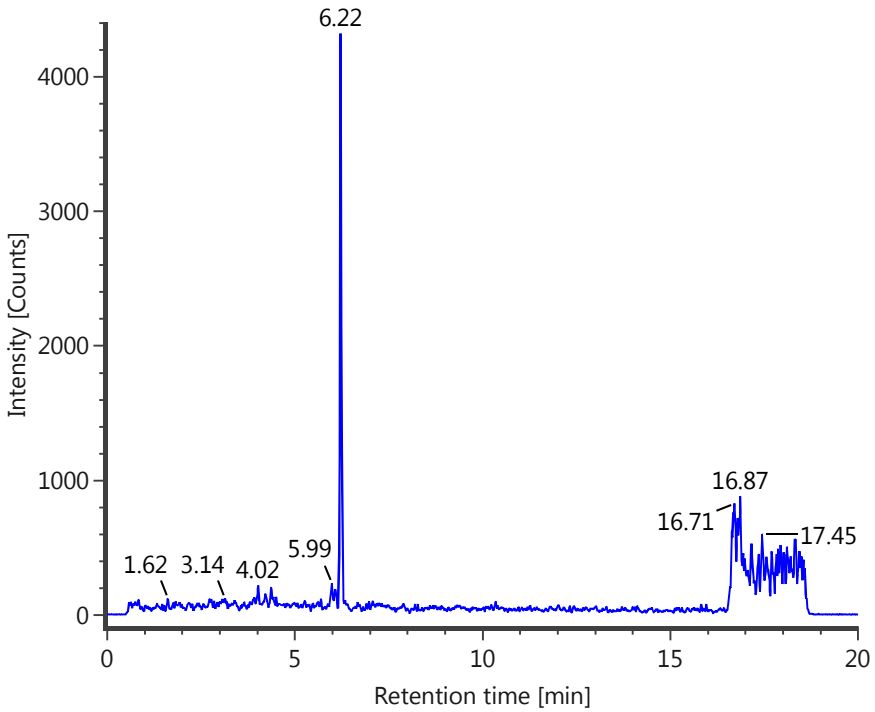
Item name: sample 2_01
Channel name: Lupinifolin [+H] : (18.8 PPM) 407.1886 : DT=5.06 to 5.58 ms



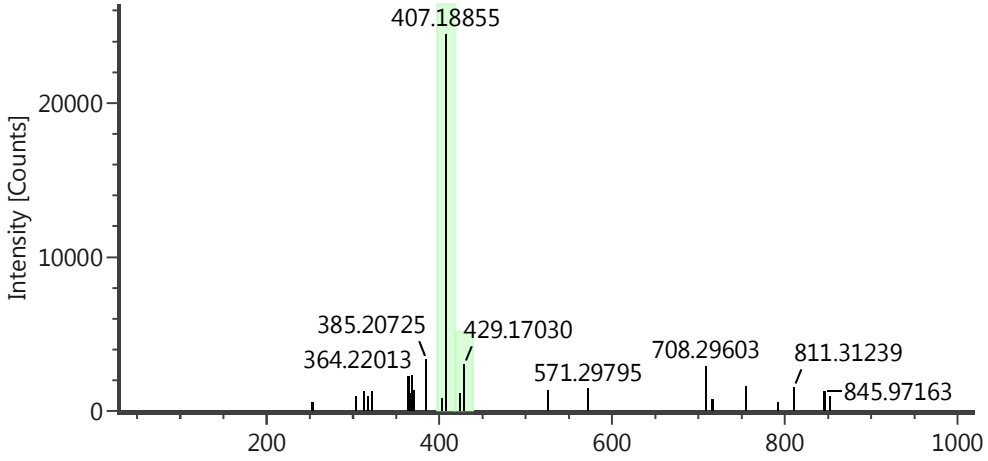
Item name: sample 2_01
Channel name: Identified Components



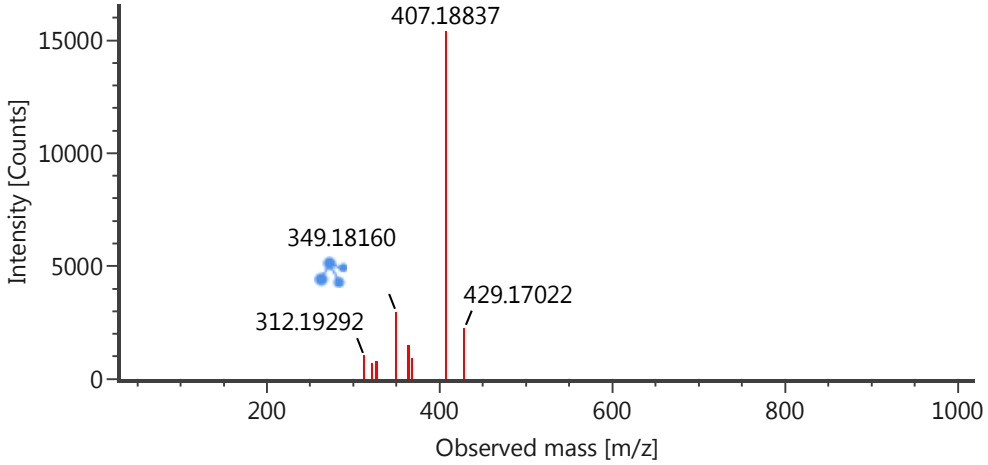
Item name: sample 2_01
Channel name: Lupinifolin [+H] : (18.8 PPM) 407.1886



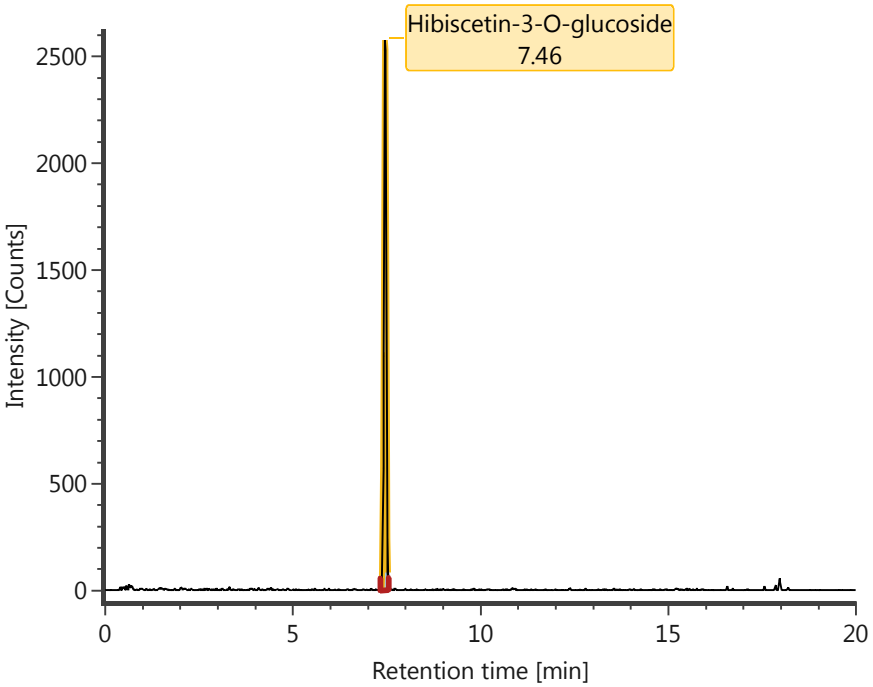

Item name: sample 2_01
Component name: Lupinifolin
Channel name: Low energy : Time 6.2247 +/- 0.0231 minutes :
Drift Times: 5.32 +/- 0.26, 5.73 +/- 0.27 ms



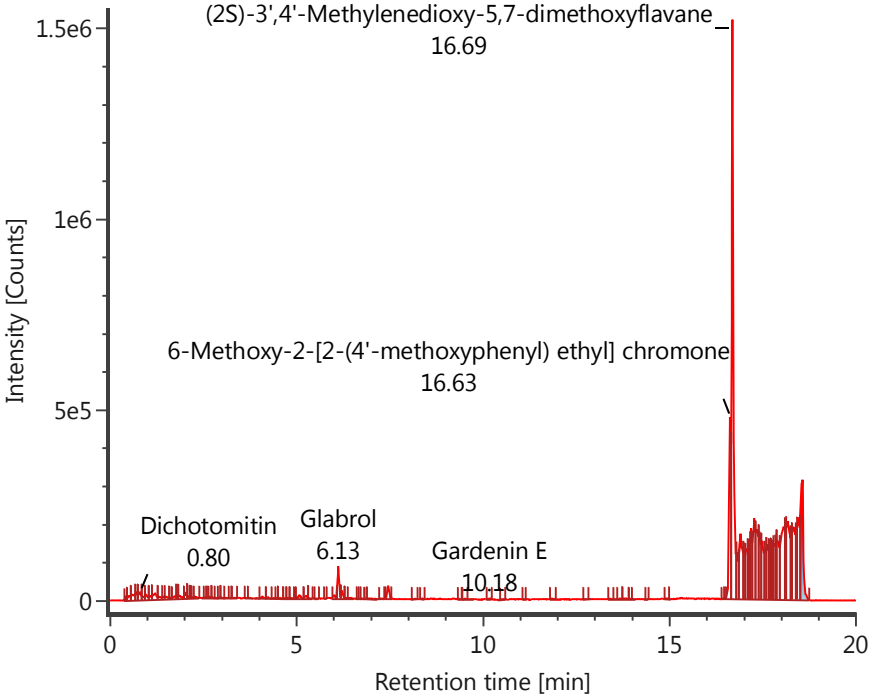

Item name: sample 2_01
Component name: Lupinifolin
Channel name: High energy : Time 6.2247 +/- 0.0231 minutes :
Drift Times: 5.18 +/- 0.26, 5.59 +/- 0.27 ms



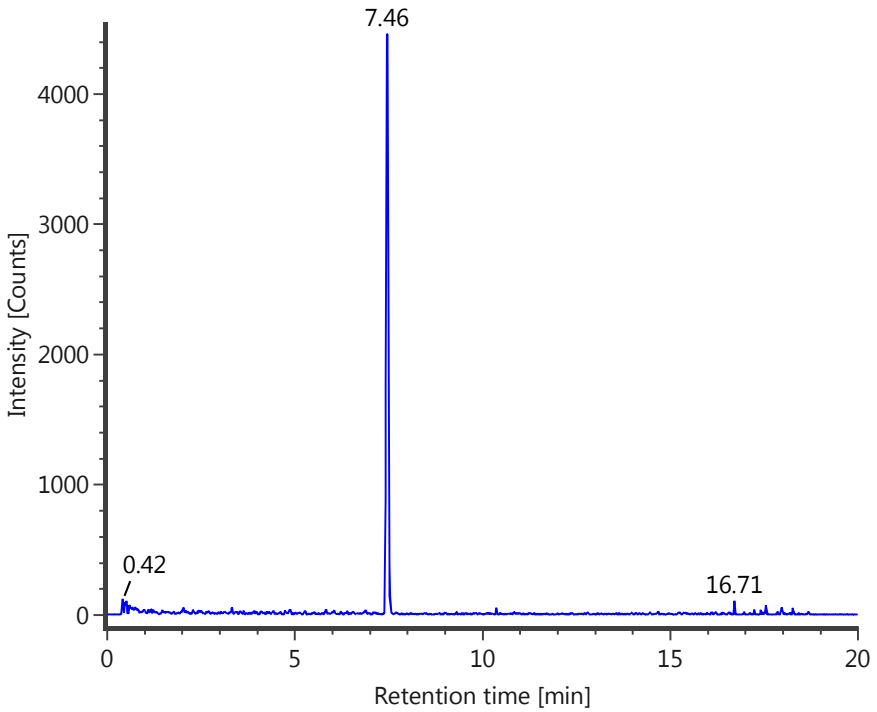
Item name: sample 2_01
Channel name: Hibiscetin-3-O-glucoside [+H] : (18.8 PPM) 497.0923 : DT=6.30 to 6.87 ms



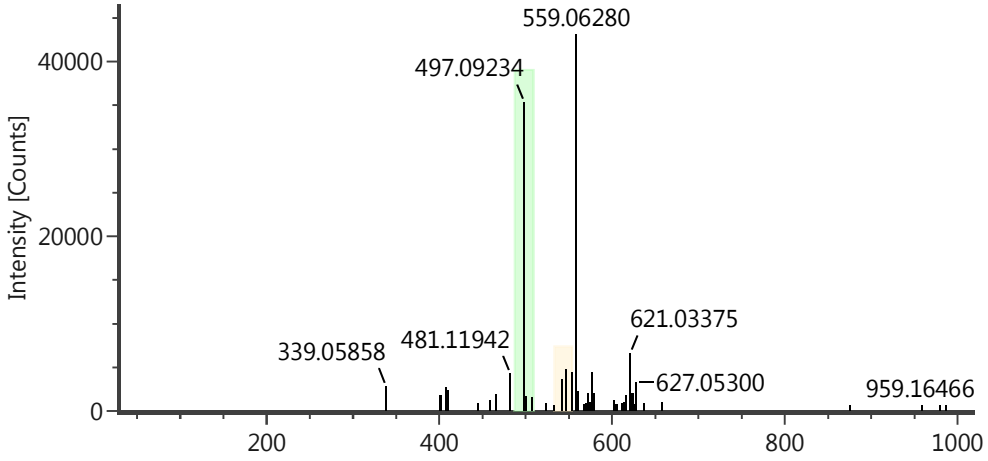
Item name: sample 2_01
Channel name: Identified Components



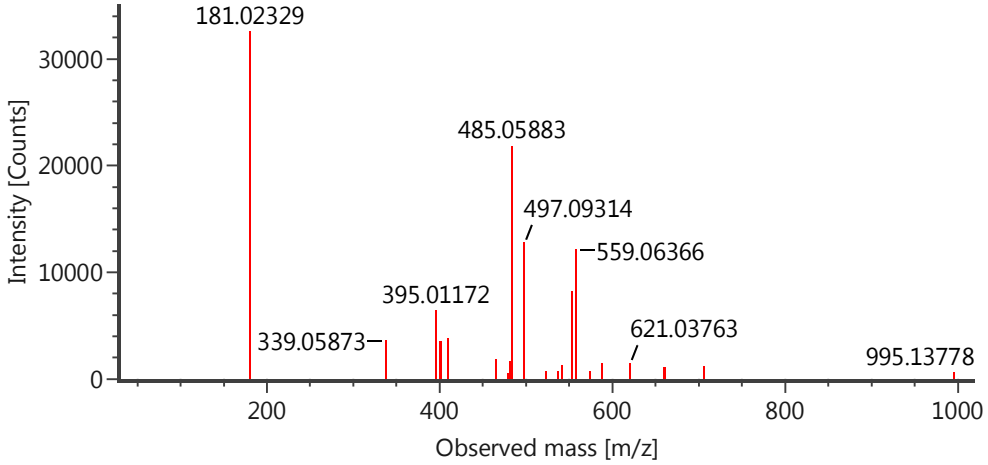
Item name: sample 2_01
Channel name: Hibiscetin-3-O-glucoside [+H] : (18.8 PPM) 497.0923



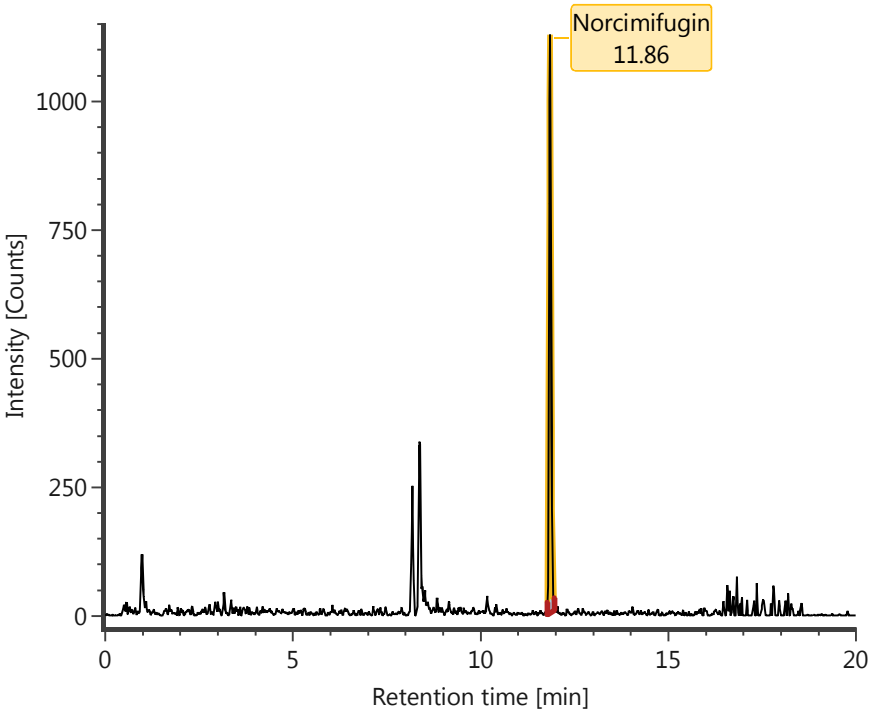

Item name: sample 2_01
Component name: Hibiscetin-3-O-glucoside
Channel name: Low energy : Time 7.4660 +/- 0.0231 minutes : Drift Times: 6.57 +/- 0.28 ms



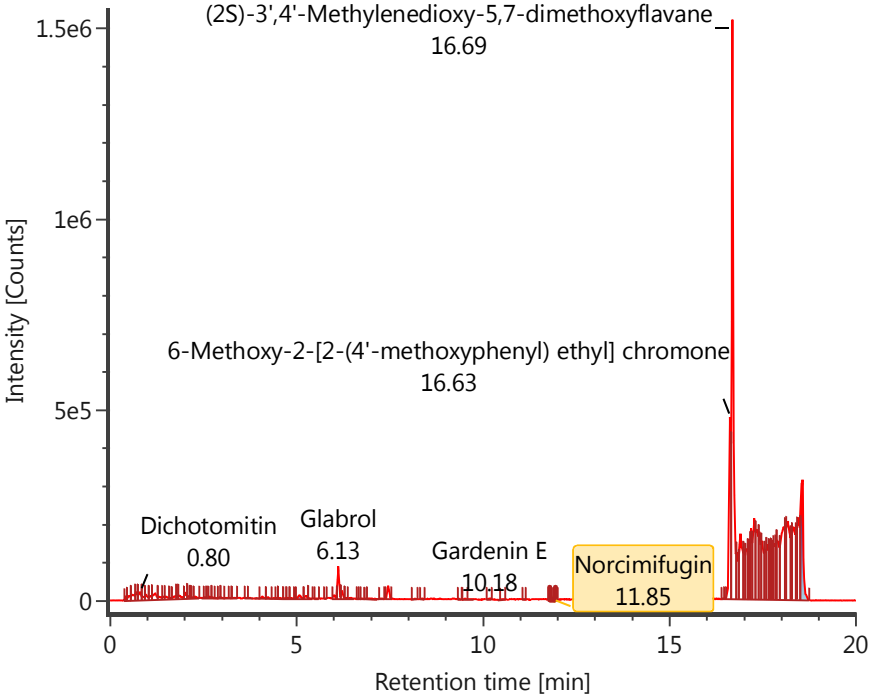

Item name: sample 2_01
Component name: Hibiscetin-3-O-glucoside
Channel name: High energy : Time 7.4660 +/- 0.0231 minutes : Drift Times: 6.44 +/- 0.28 ms



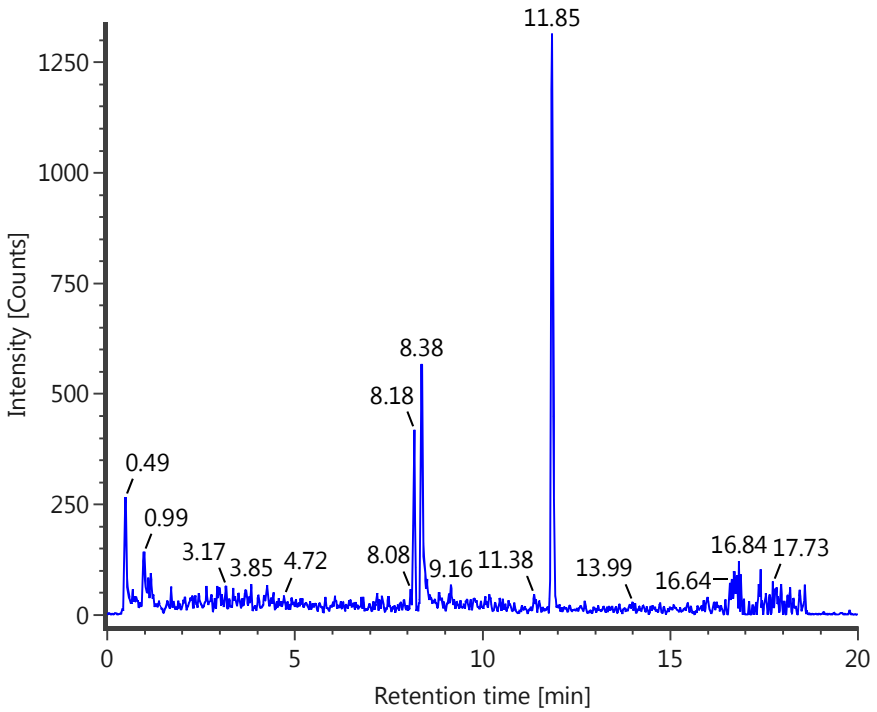
Item name: sample 2_01
Channel name: Norcimifugin [+Li] : (18.8 PPM) 299.1094 : DT=4.49 to 4.99 ms



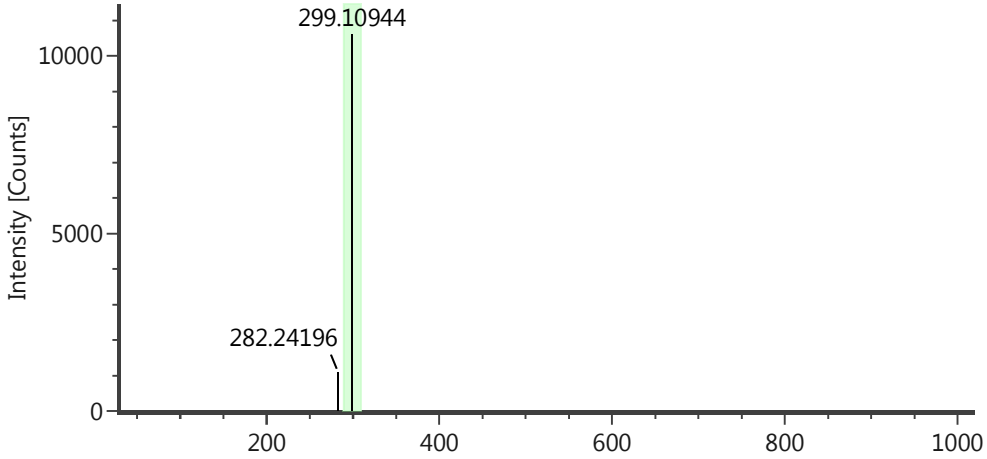
Item name: sample 2_01
Channel name: Identified Components



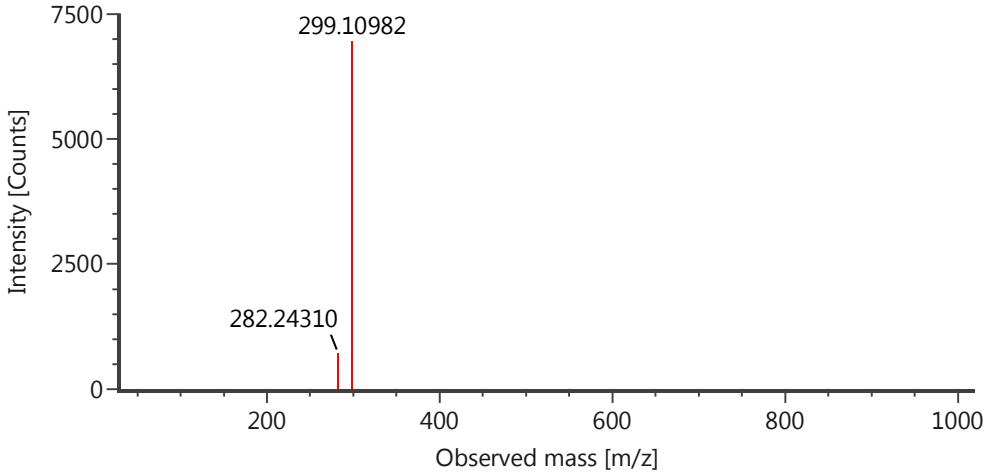
Item name: sample 2_01
Channel name: Norcimifugin [+Li] : (18.8 PPM) 299.1094



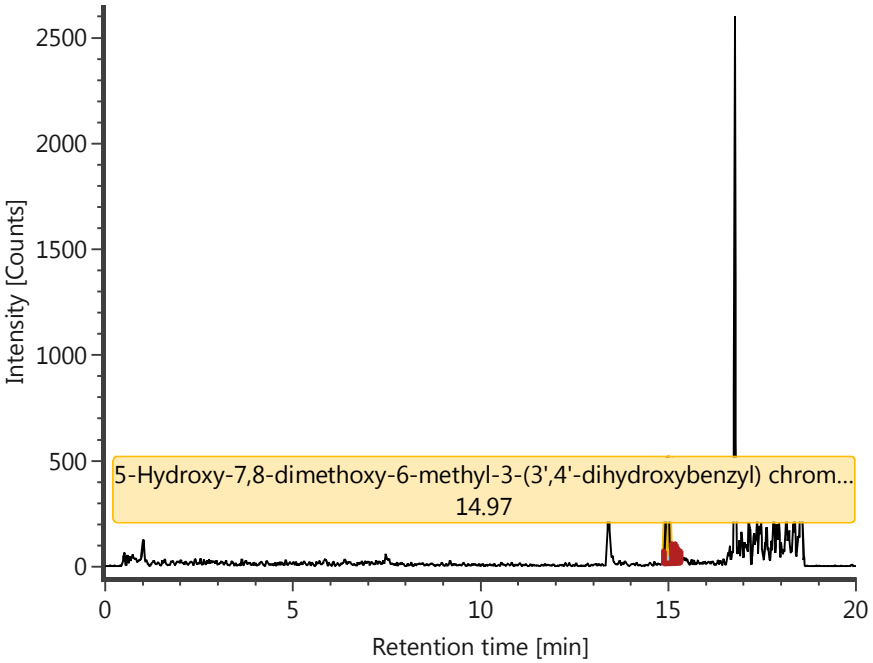

Item name: sample 2_01
Component name: Norcimifugin
Channel name: Low energy : Time 11.8575 +/- 0.0231 minutes : Drift Times: 4.74 +/- 0.25 ms



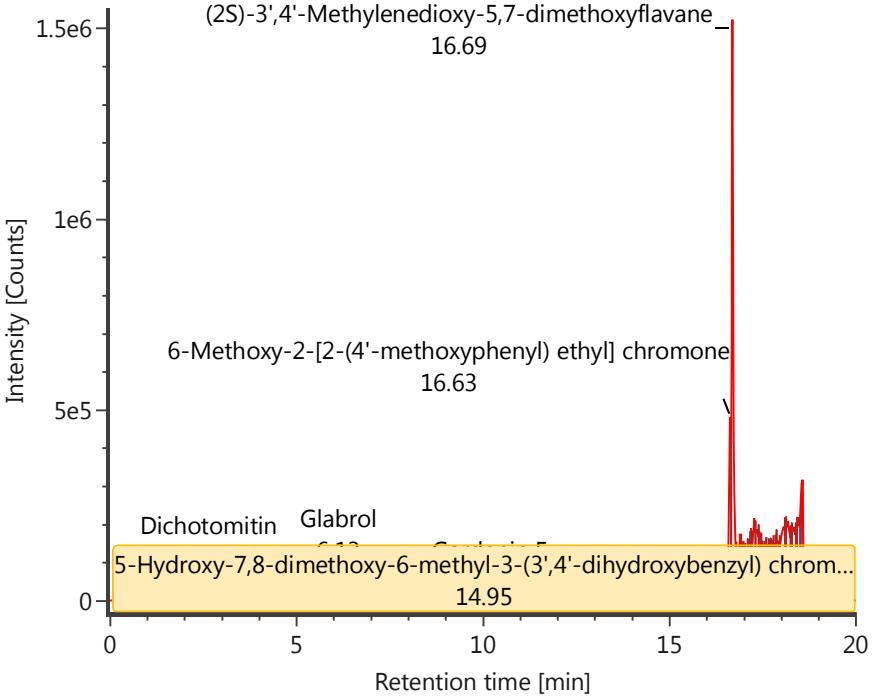

Item name: sample 2_01
Component name: Norcimifugin
Channel name: High energy : Time 11.8575 +/- 0.0231 minutes : Drift Times: 4.61 +/- 0.25 ms



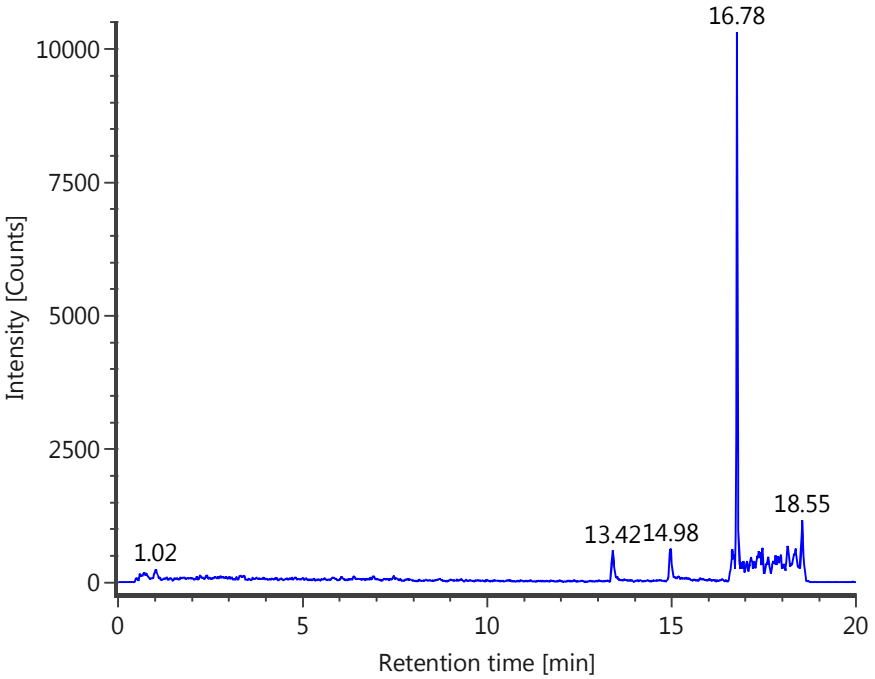
Item name: sample 2_01
Channel name: 5-Hydroxy-7,8-dimethoxy-6-methyl-3-(3',4'-dihydroxybenzyl) chroman-4-one [+Li] : (18.8 PPM) 367.1362 : DT=4.88 to 5.39 ms



Item name: sample 2_01
Channel name: Identified Components

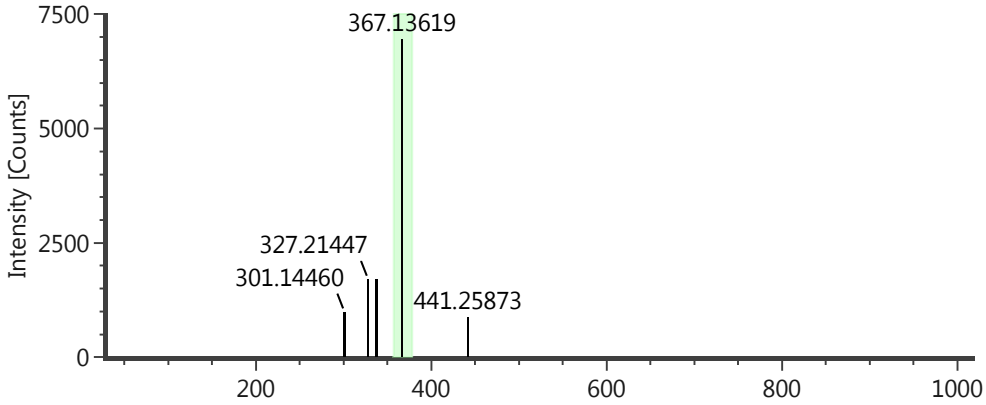


Item name: sample 2_01
Channel name: 5-Hydroxy-7,8-dimethoxy-6-methyl-3-(3',4'-dihydroxybenzyl) chroman-4-one [+Li] : (18.8 PPM) 367.1362



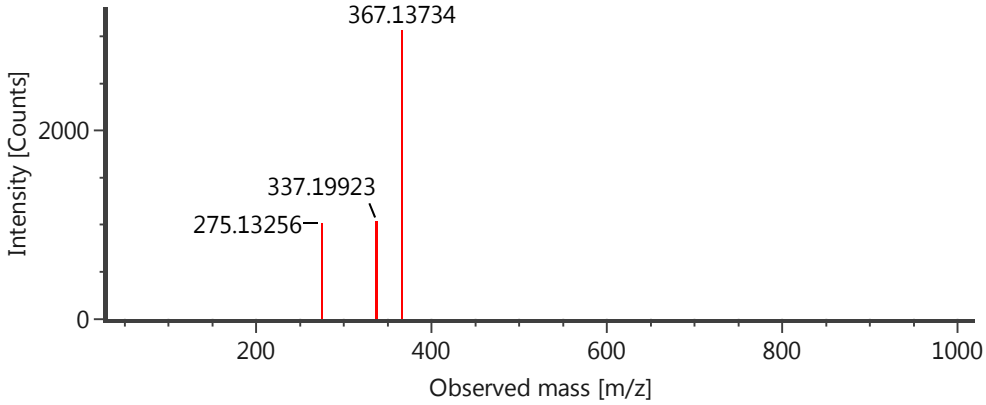

Item name: sample 2_01
Component name: 5-Hydroxy-7,8-dimethoxy-6-methyl-3-(3',4'-dihydroxybenzyl) chroman-4-one

Channel name: Low energy : Time 14.9807 +/- 0.0231 minutes : Drift Times: 5.14 +/- 0.26 ms

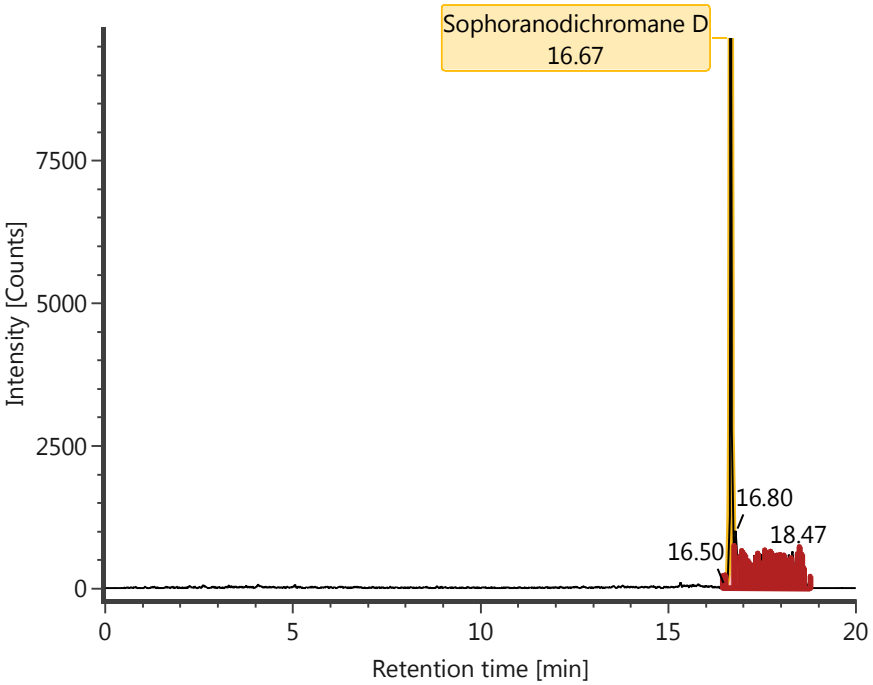



Item name: sample 2_01
Component name: 5-Hydroxy-7,8-dimethoxy-6-methyl-3-(3',4'-dihydroxybenzyl) chroman-4-one

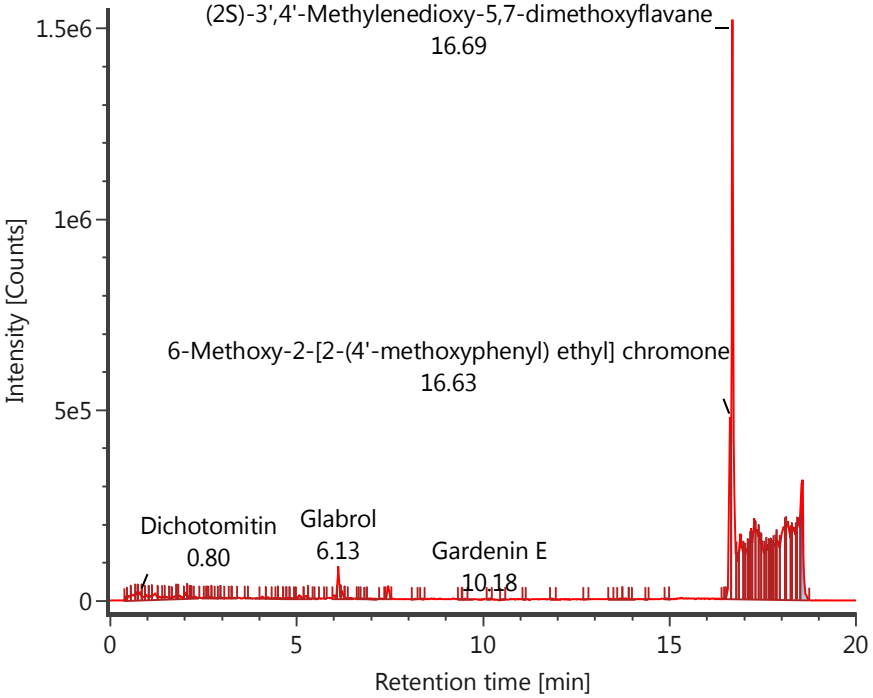
Channel name: High energy : Time 14.9807 +/- 0.0231 minutes : Drift Times: 5.01 +/- 0.26 ms



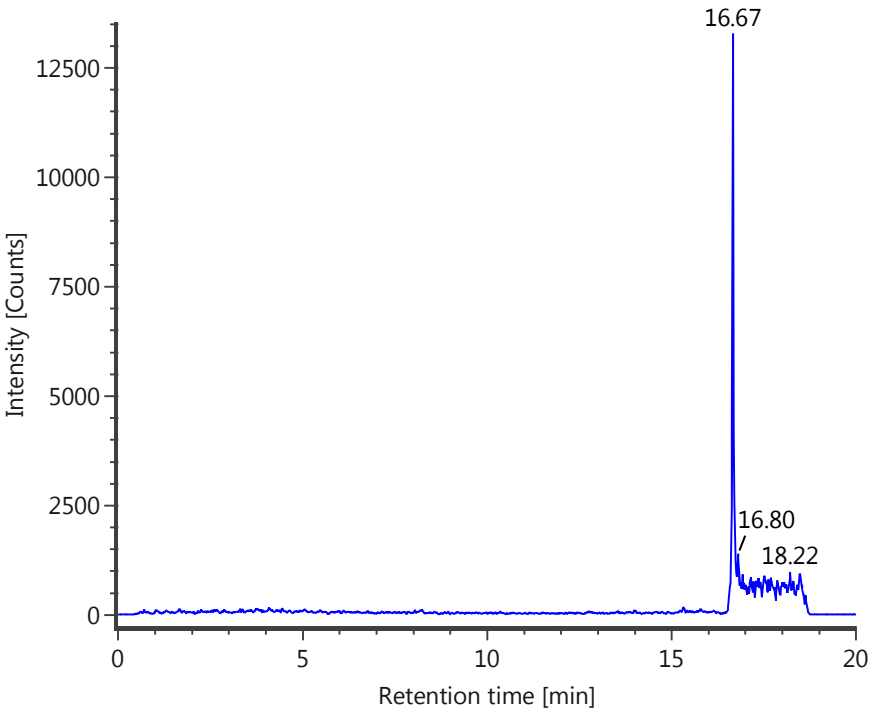
Item name: sample 2_01
Channel name: Sophoranodichromane D [+Li] : (18.8 PPM) 415.2115 : DT=5.91 to 6.47 ms



Item name: sample 2_01
Channel name: Identified Components

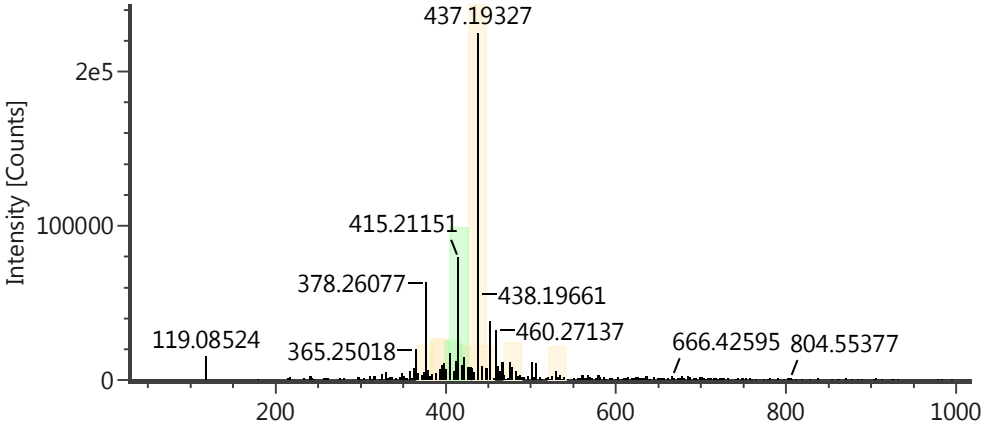


Item name: sample 2_01
Channel name: Sophoranodichromane D [+Li] : (18.8 PPM) 415.2115



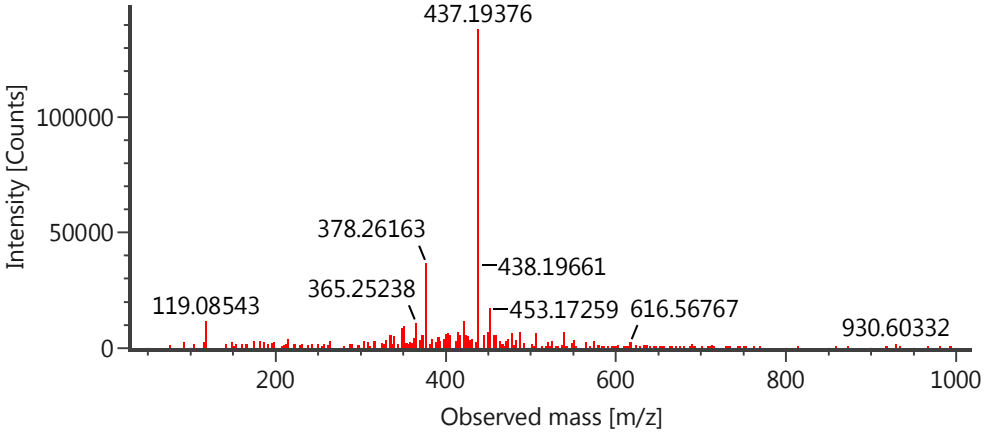

Item name: sample 2_01
Component name: Sophoranodichromane D

Channel name: Low energy : Time 16.6707 +/- 0.0231 minutes : Drift Times: 6.18 +/- 0.28, 6.24 +/- 0.28 ms

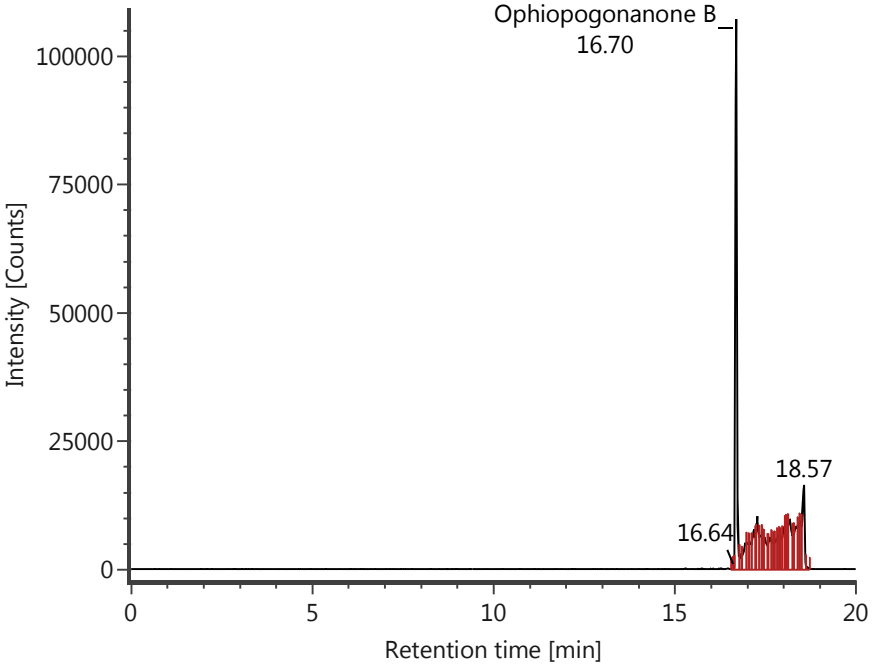



Item name: sample 2_01
Component name: Sophoranodichromane D

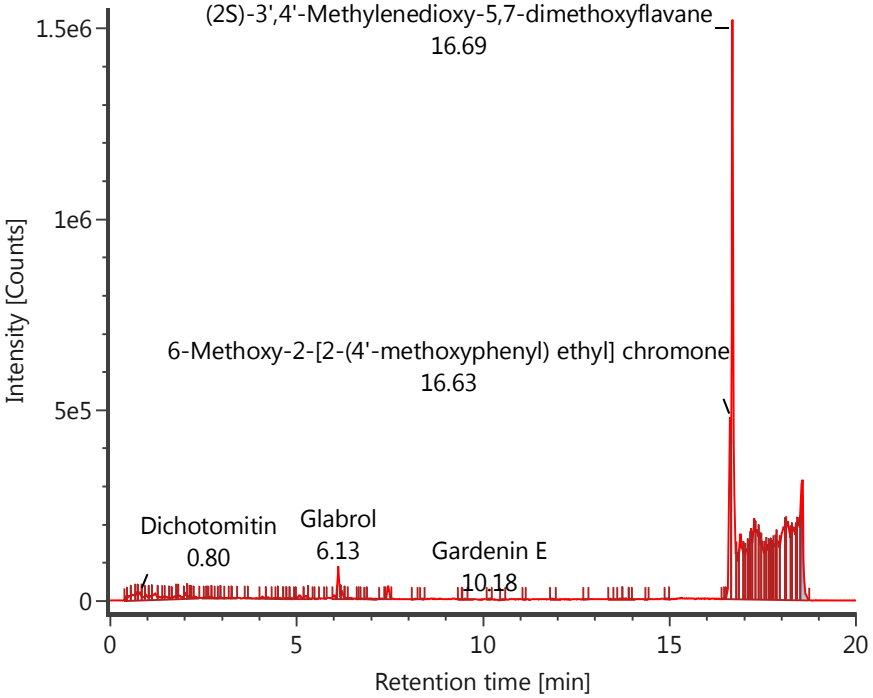
Channel name: High energy : Time 16.6707 +/- 0.0231 minutes : Drift Times: 6.05 +/- 0.28, 6.10 +/- 0.28 ms



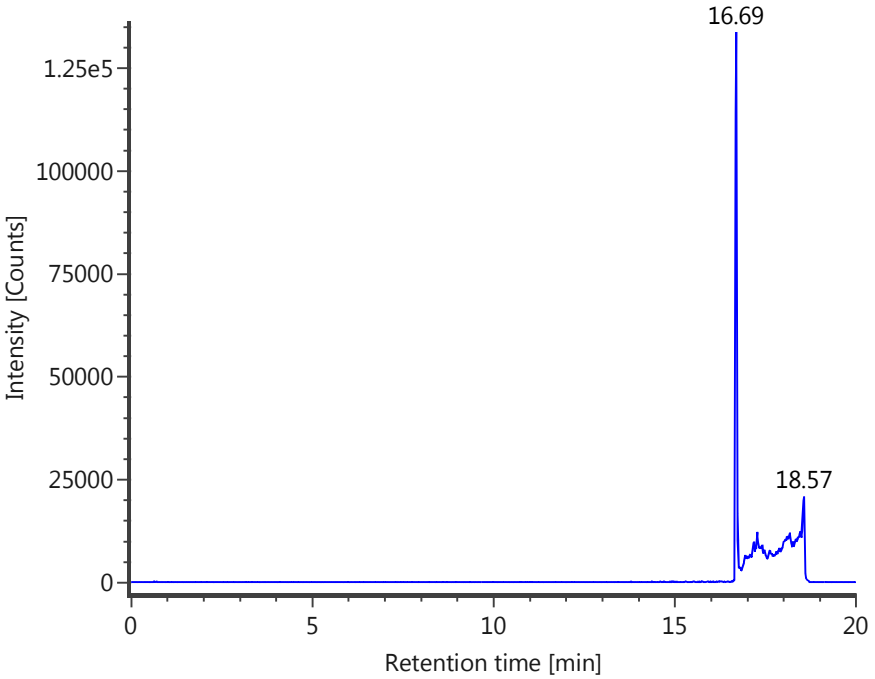
Item name: sample 2_01
Channel name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane [+Na] :
Ophiopogonanone B [+Na] : (18.8 PPM) 337.1043 : DT=4.94 to 5.45 ms



Item name: sample 2_01
Channel name: Identified Components

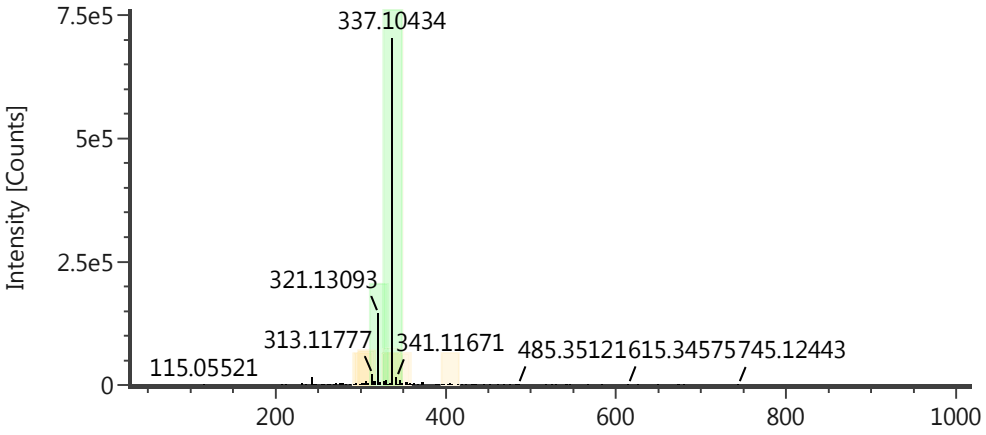


Item name: sample 2_01
Channel name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane [+Na] : Ophiopogonanone B [+Na] : (18.8 PPM) 337.1043



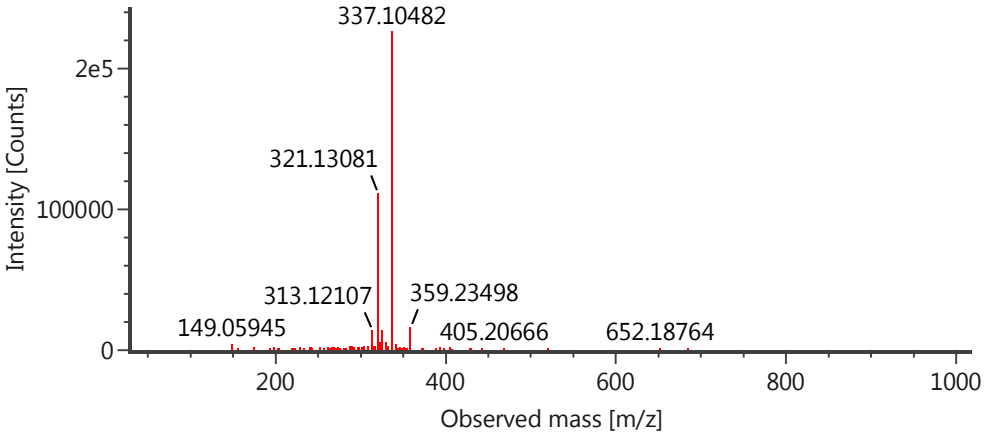

Item name: sample 2_01
Component name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane

Channel name: Low energy : Time 16.6982 +/- 0.0231 minutes : Drift Times: 5.20 +/- 0.26, 5.18 +/- 0.26 ms

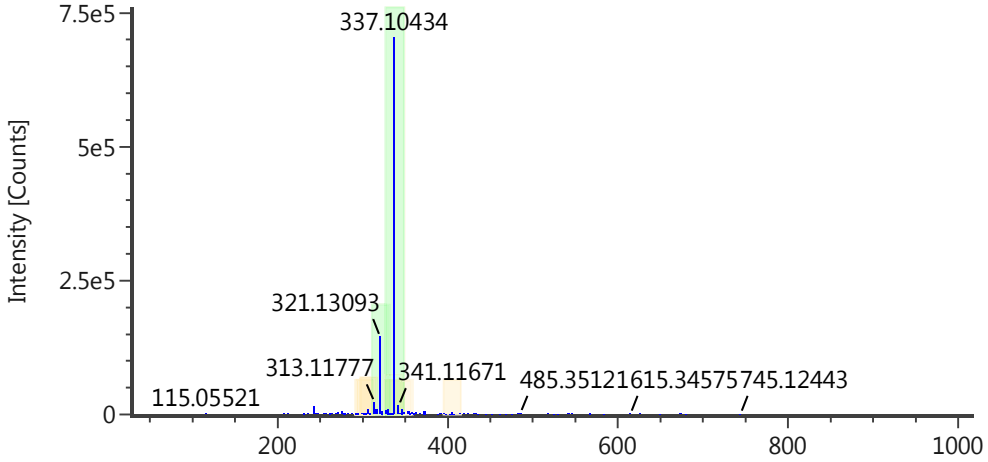



Item name: sample 2_01
Component name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane

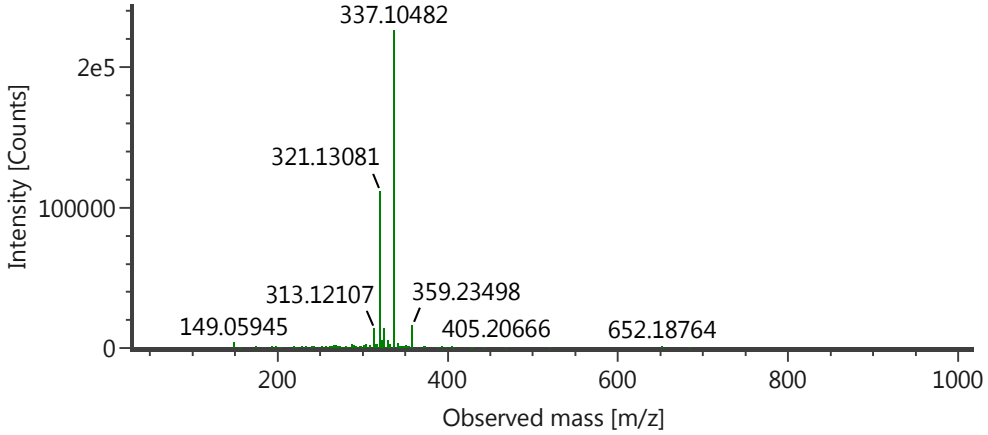
Channel name: High energy : Time 16.6982 +/- 0.0231 minutes : Drift Times: 5.06 +/- 0.26, 5.04 +/- 0.26 ms



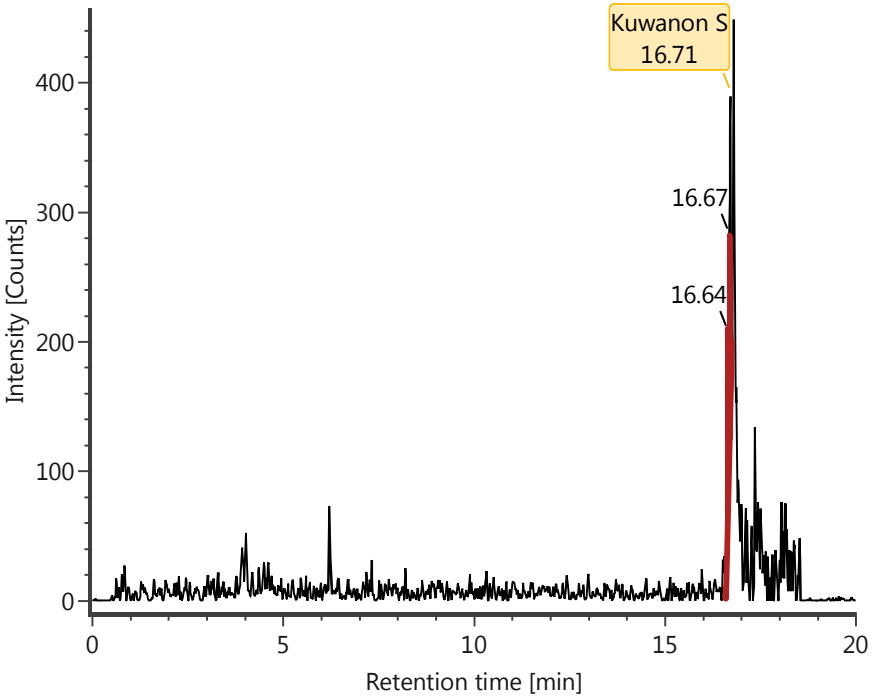
Item name: sample 2_01 Channel name: Low energy : Time 16.6982 +/- 0.0231
Component name: Ophiopogonanone B minutes : Drift Times: 5.20 +/- 0.26, 5.18 +/- 0.26 ms



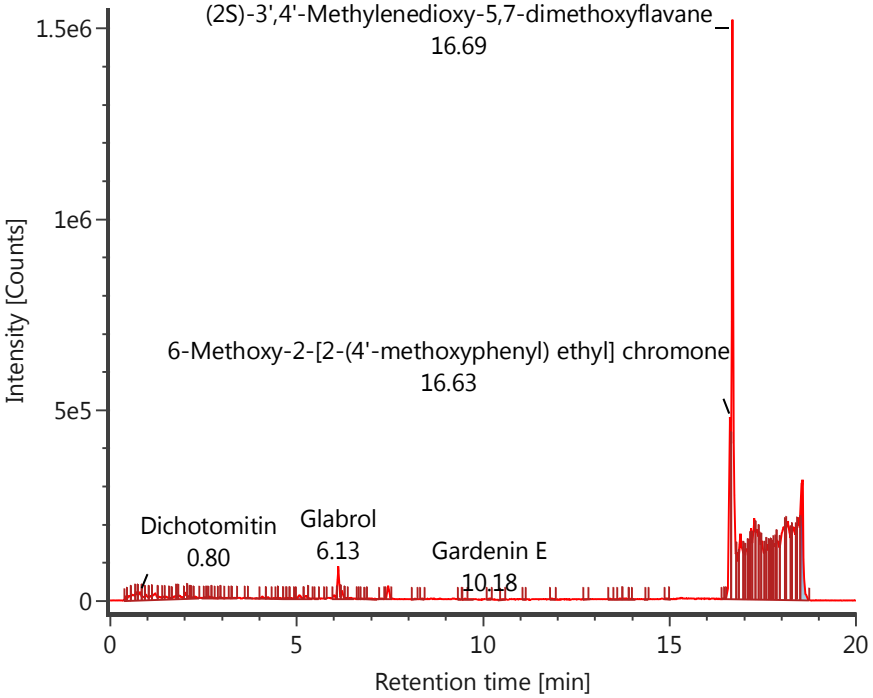

Item name: sample 2_01 Channel name: High energy : Time 16.6982 +/- 0.0231 minutes : Drift Times: 5.06 +/- 0.26, 5.04 +/- 0.26 ms
Component name: Ophiopogonanone B



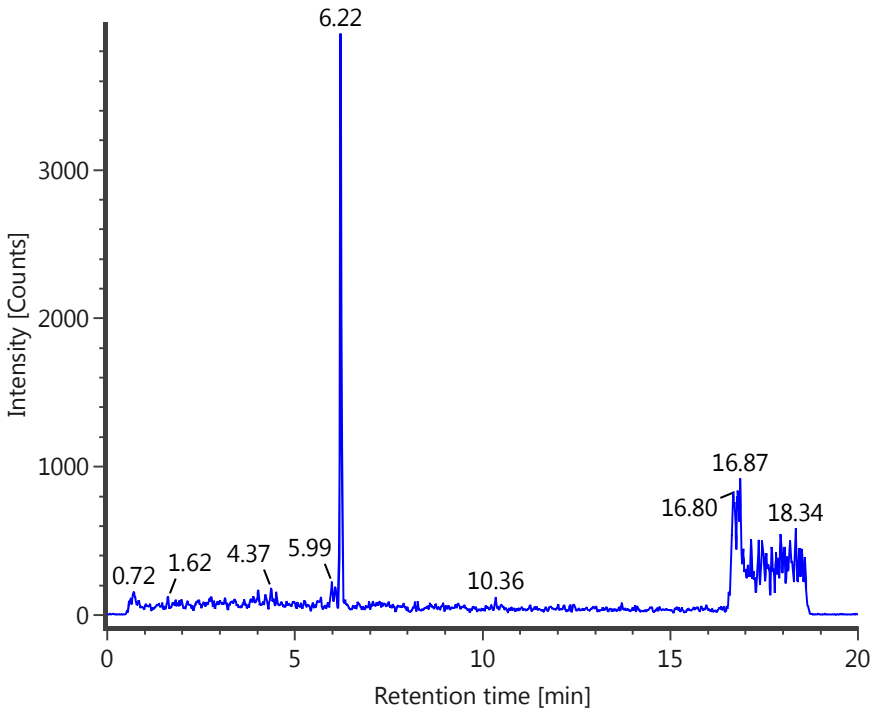
Item name: sample 2_01
Channel name: Kuwanon S [+H] : (18.8 PPM) 407.1850 : DT=6.05 to 6.60 ms



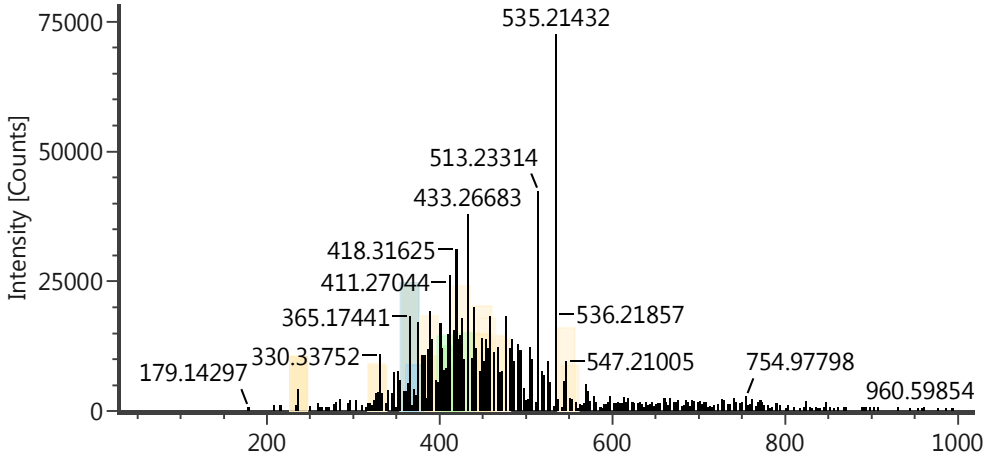
Item name: sample 2_01
Channel name: Identified Components



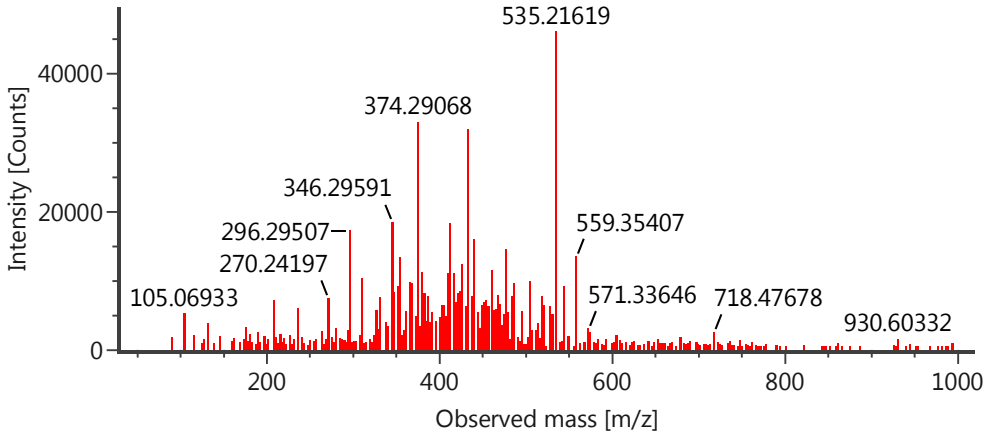
Item name: sample 2_01
Channel name: Kuwanon S [+H] : (18.8 PPM) 407.1850



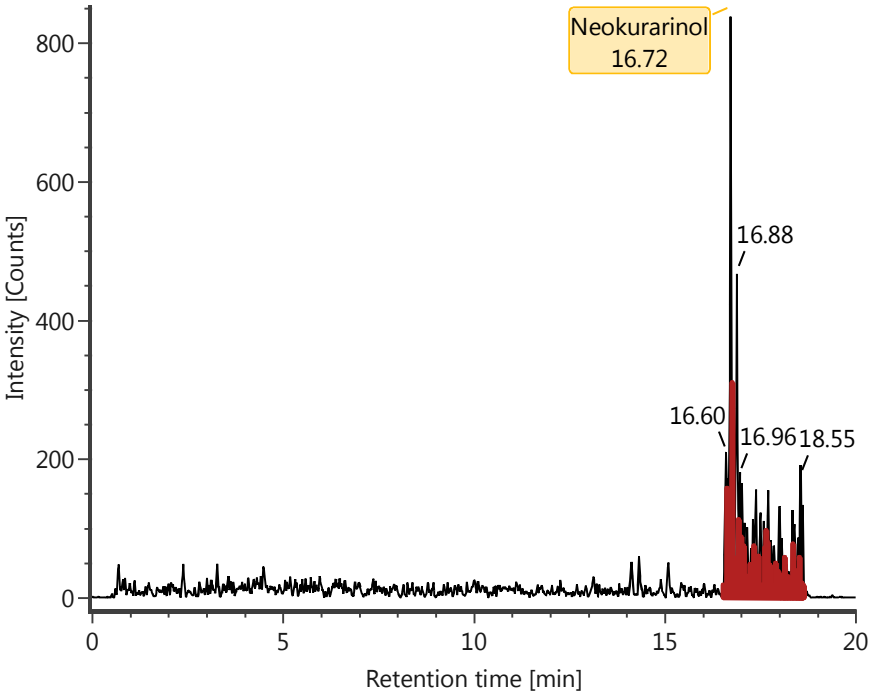

Item name: sample 2_01 Channel name: Low energy : Time 16.7078 +/- 0.0231 minutes :
Component name: Kuwanon S Drift Times: 6.32 +/- 0.28, 6.10 +/- 0.28, 6.45 +/- 0.28 ms



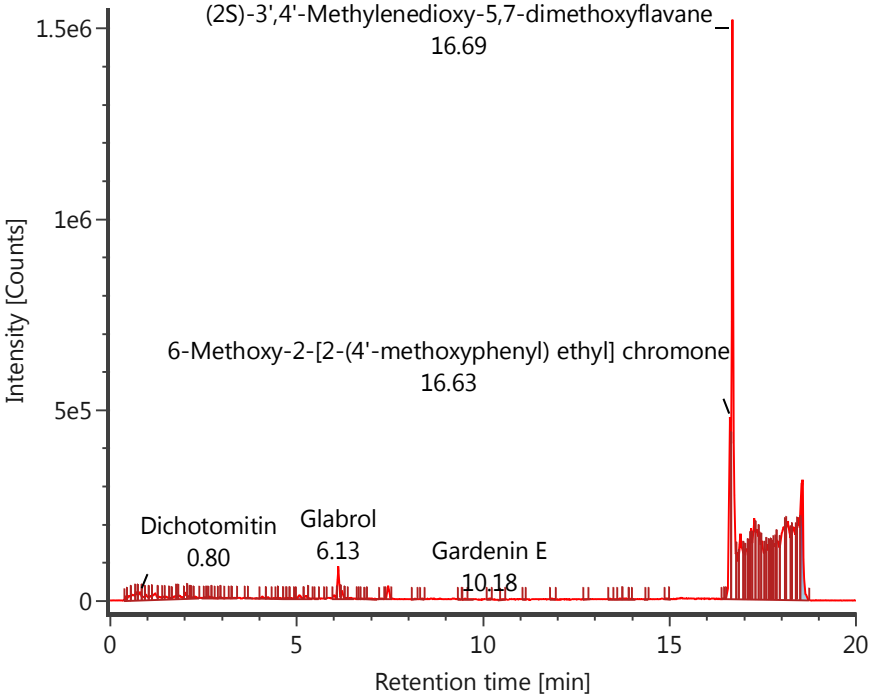

Item name: sample 2_01 Channel name: High energy : Time 16.7078 +/- 0.0231
Component name: Kuwanon S minutes : Drift Times: 6.19 +/- 0.28, 5.97 +/- 0.28, 6.32 +/- 0.28 ms



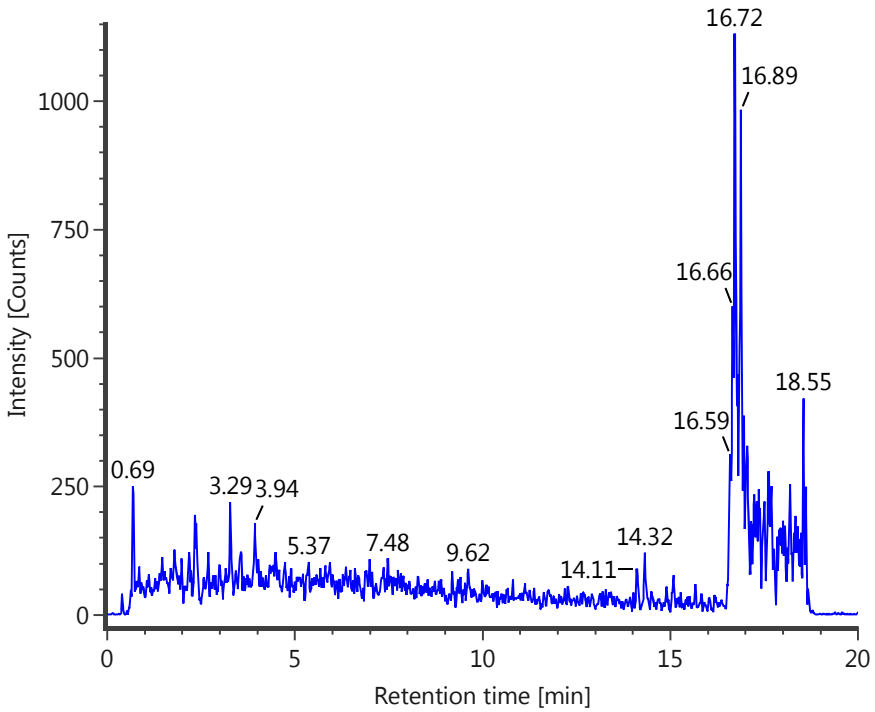
Item name: sample 2_01
Channel name: Neokurarinol [+H] : (18.8 PPM) 471.2370 : DT=6.36 to 6.93 ms



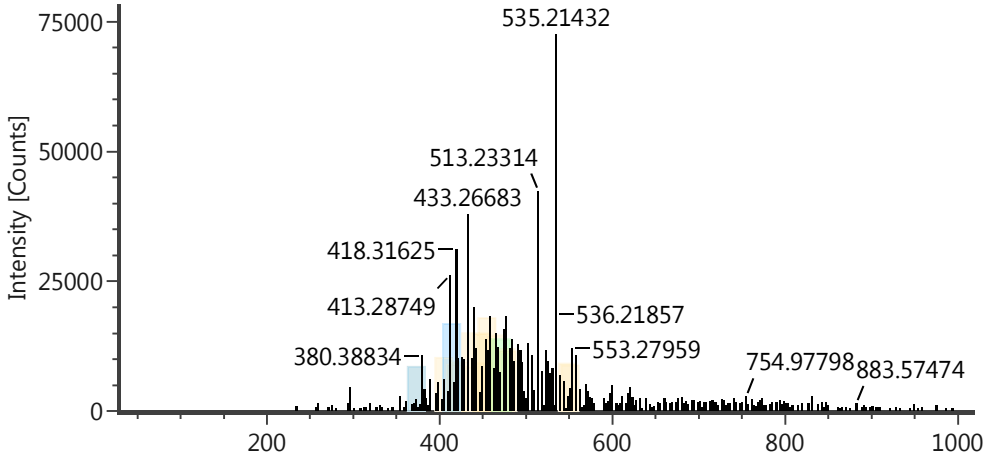
Item name: sample 2_01
Channel name: Identified Components



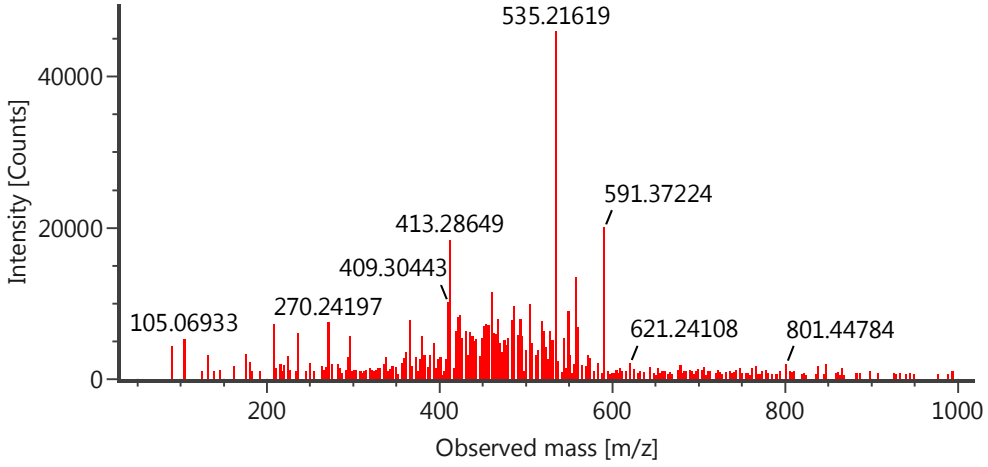
Item name: sample 2_01
Channel name: Neokurarinol [+H] : (18.8 PPM) 471.2370



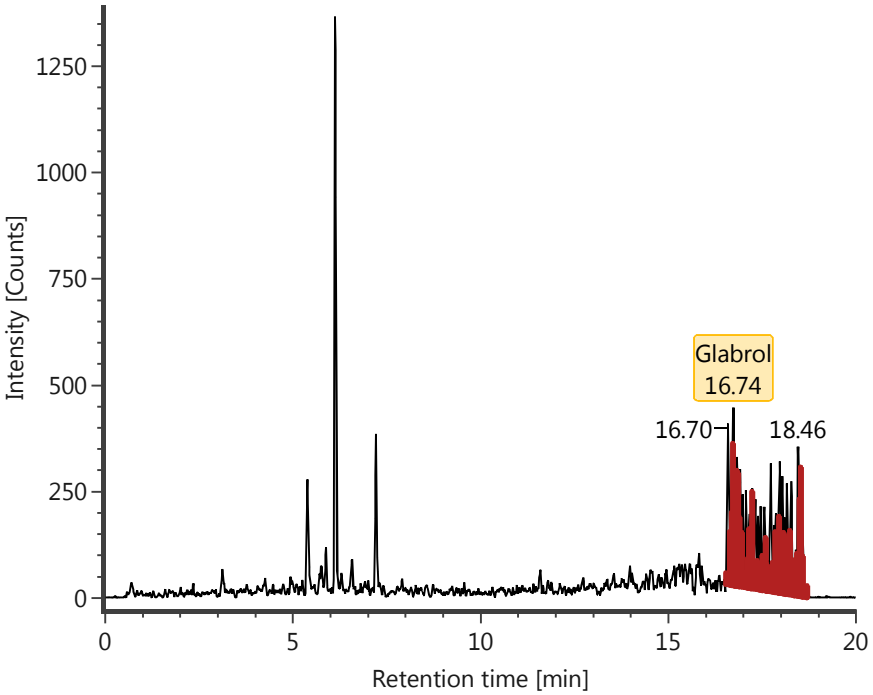

Item name: sample 2_01
Component name: Neokurarinol
Channel name: Low energy : Time 16.7165 +/- 0.0231 minutes : Drift Times: 6.66 +/- 0.28 ms



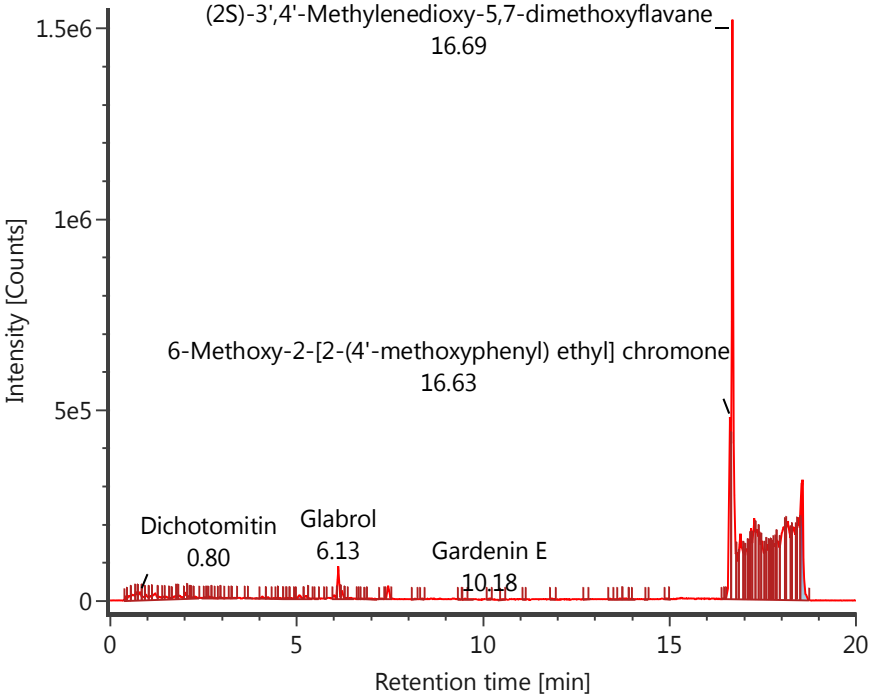

Item name: sample 2_01
Component name: Neokurarinol
Channel name: High energy : Time 16.7165 +/- 0.0231 minutes : Drift Times: 6.53 +/- 0.28 ms



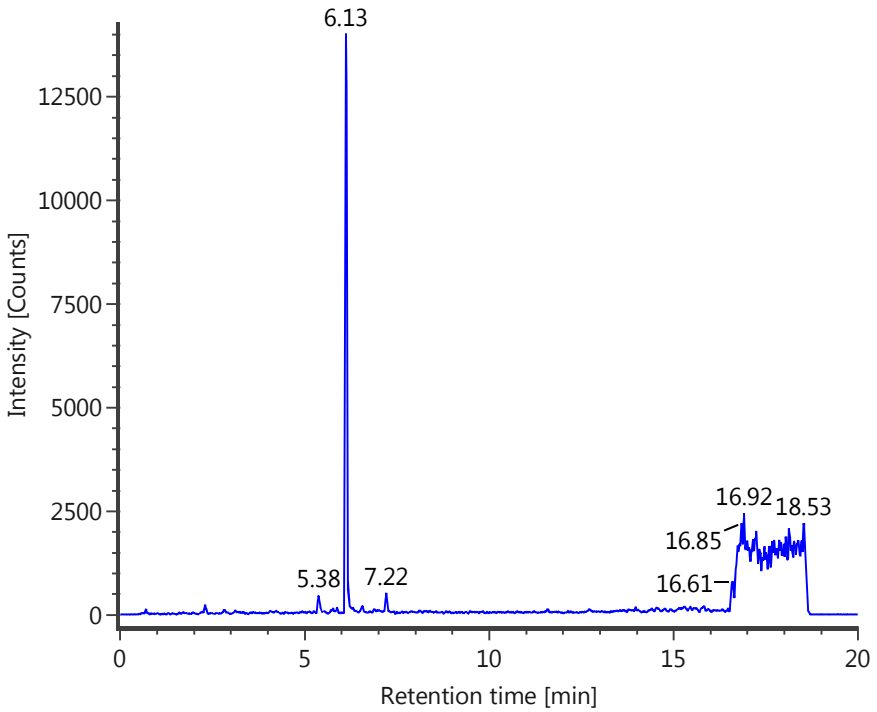
Item name: sample 2_01
Channel name: Glabrol [+H] : (18.8 PPM) 393.2067 : DT=5.50 to 6.04 ms



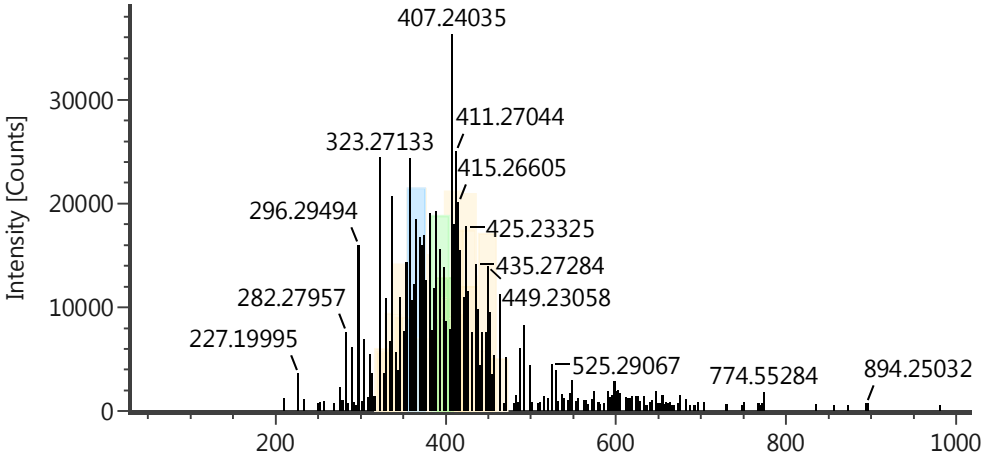
Item name: sample 2_01
Channel name: Identified Components



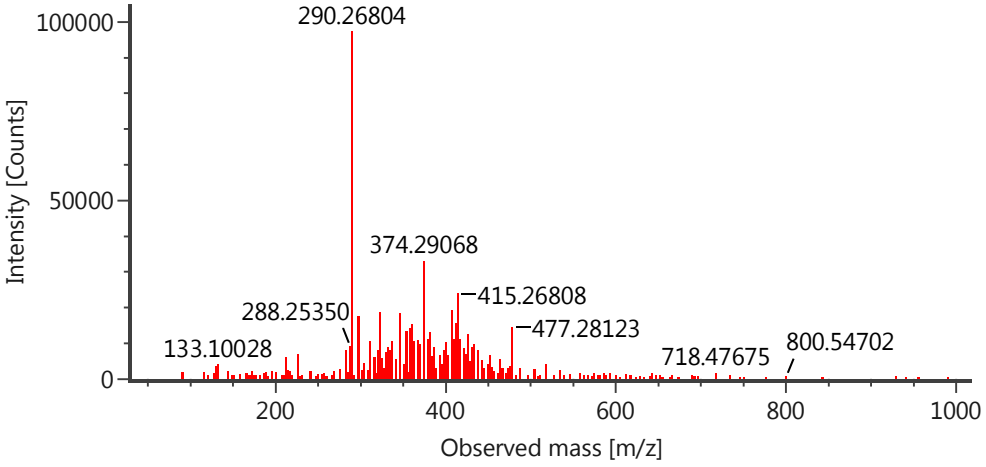
Item name: sample 2_01
Channel name: Glabrol [+H] : (18.8 PPM) 393.2067



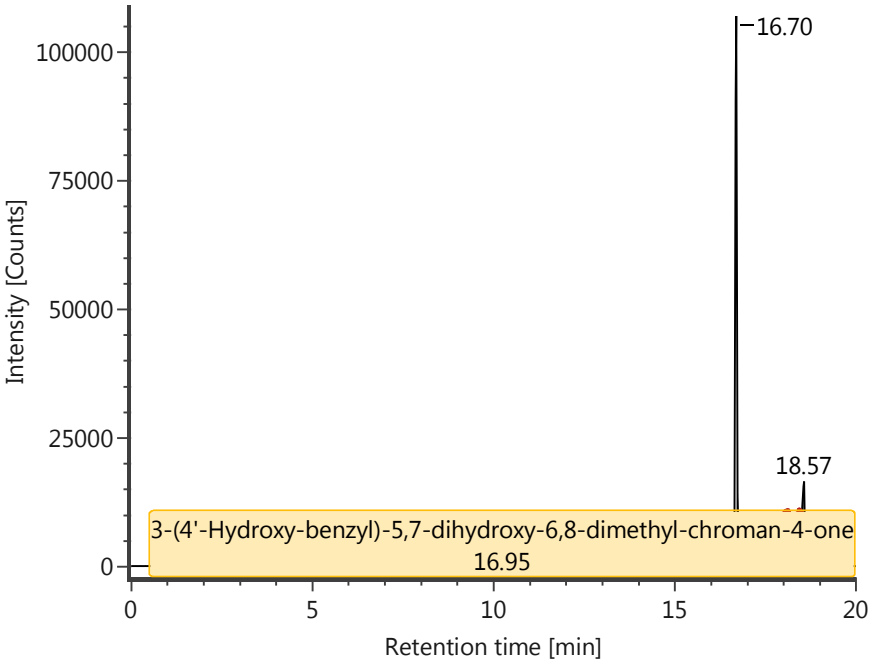

Item name: sample 2_01
Component name: Glabrol
Channel name: Low energy : Time 16.7237 +/- 0.0231 minutes :
Drift Times: 5.81 +/- 0.27, 6.03 +/- 0.27 ms



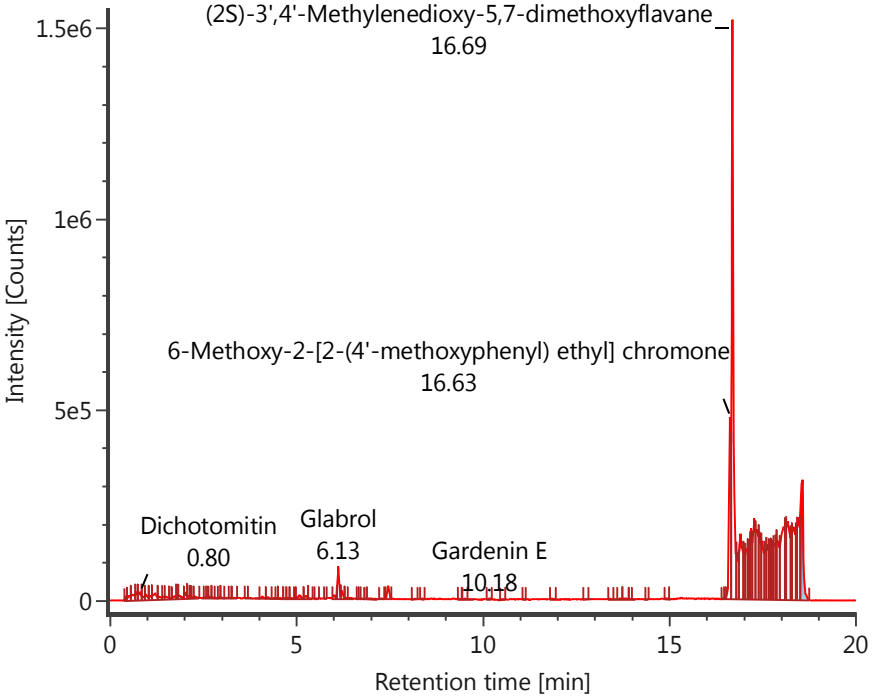

Item name: sample 2_01
Component name: Glabrol
Channel name: High energy : Time 16.7237 +/- 0.0231 minutes :
Drift Times: 5.67 +/- 0.27, 5.90 +/- 0.27 ms



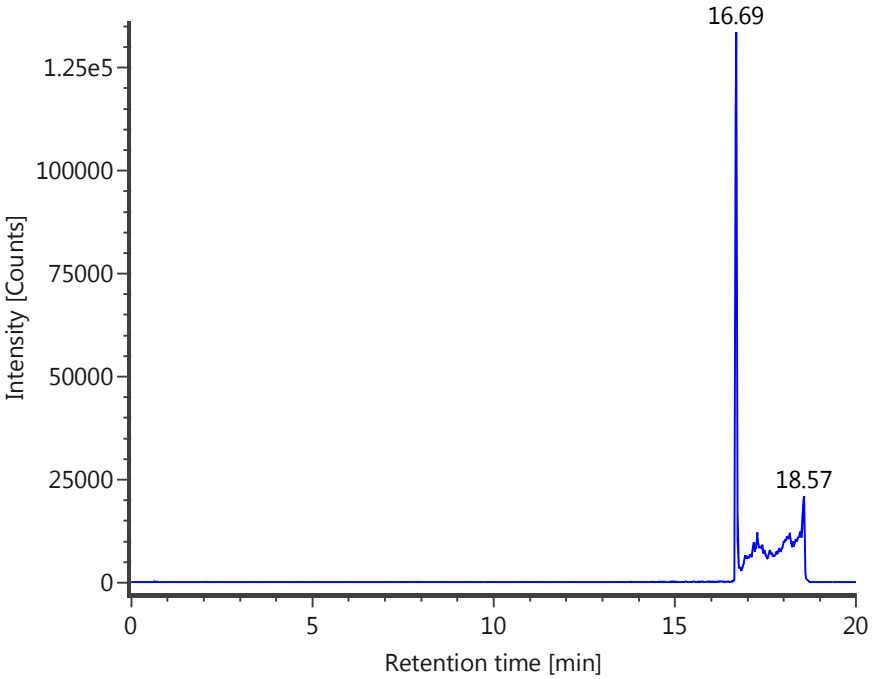
Item name: sample 2_01
Channel name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one
[+Na] : (18.8 PPM) 337.1039 : DT=4.91 to 5.43 ms



Item name: sample 2_01
Channel name: Identified Components

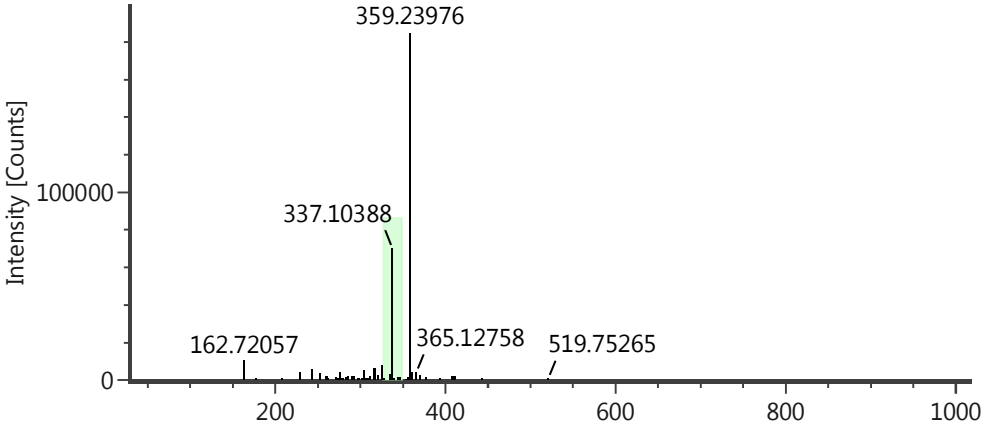


Item name: sample 2_01
Channel name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one [+Na] : (18.8 PPM) 337.1039



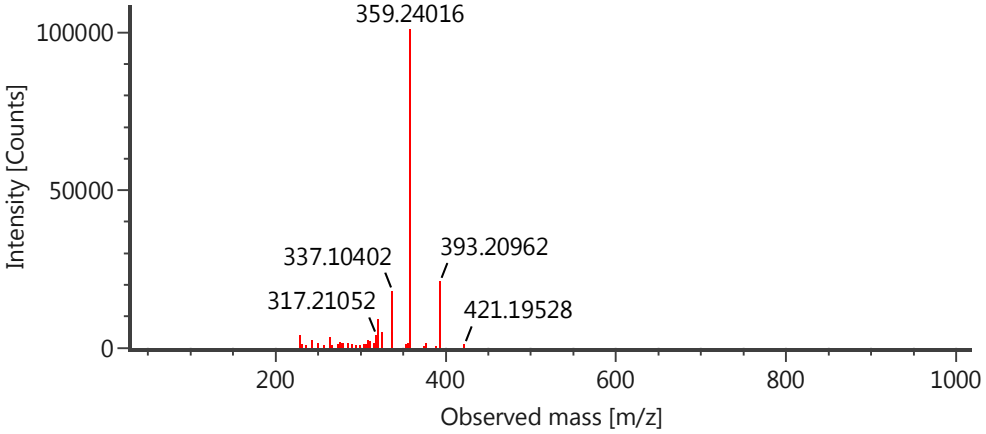

Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one

Channel name: Low energy : Time 16.9504 +/- 0.0231 minutes : Drift Times: 5.17 +/- 0.26 ms

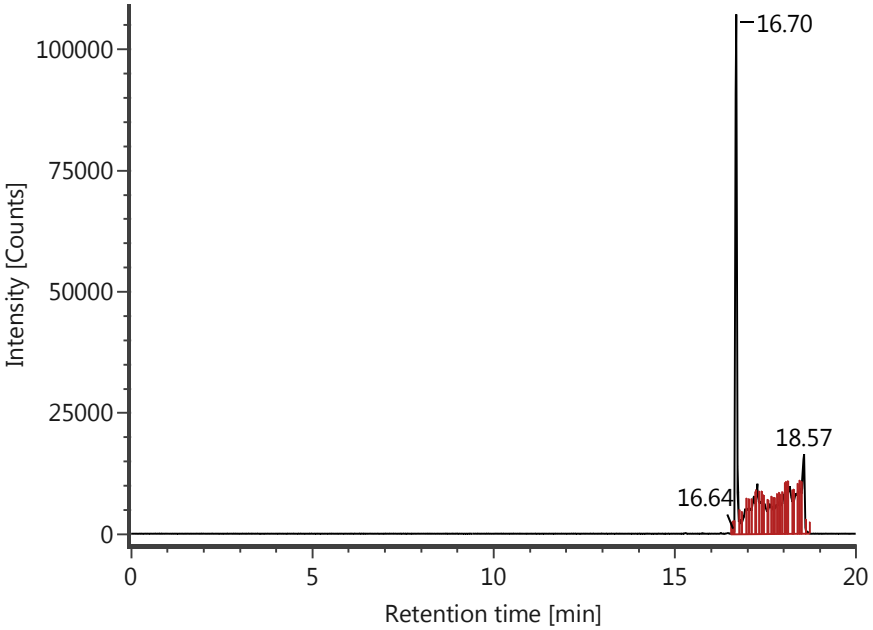



Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one

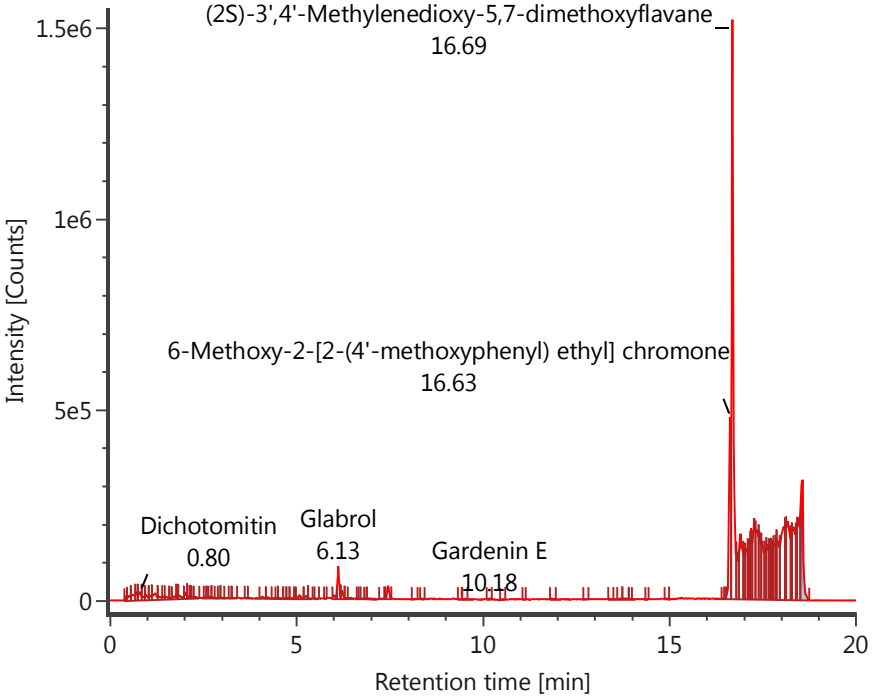
Channel name: High energy : Time 16.9504 +/- 0.0231 minutes : Drift Times: 5.04 +/- 0.26 ms



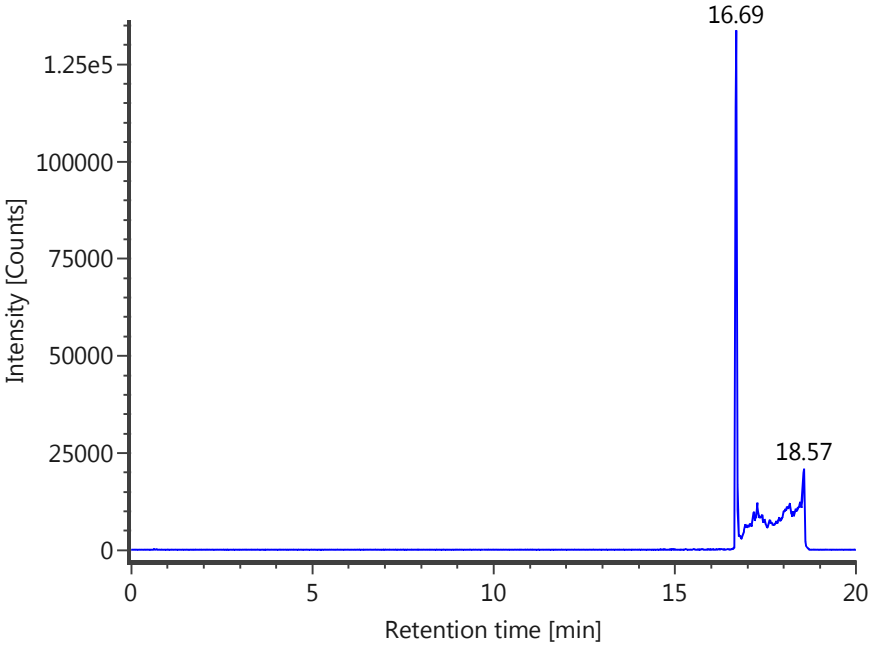
Item name: sample 2_01
Channel name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane [+Na] : 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one [+Na] : (18.8 PPM)
337.1043 : DT=4.92 to 5.44 ms



Item name: sample 2_01
Channel name: Identified Components

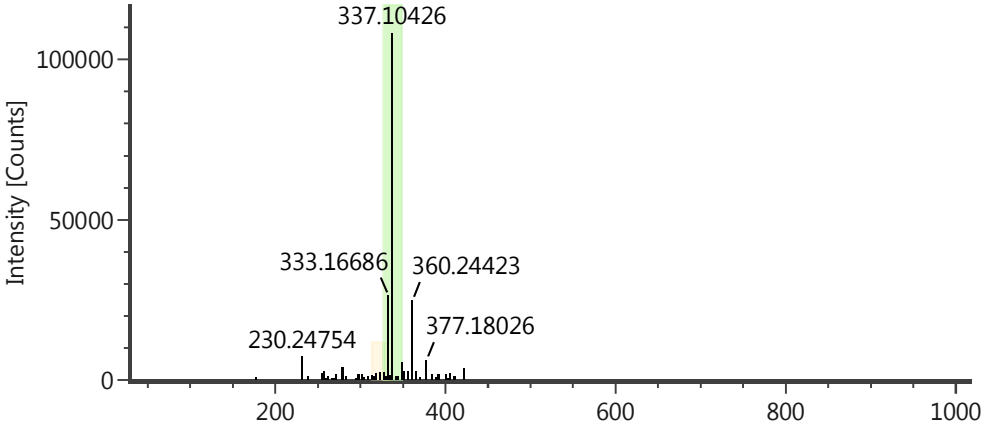


Item name: sample 2_01
Channel name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane [+Na] : 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one [+Na] : (18.8 PPM) 337.1043



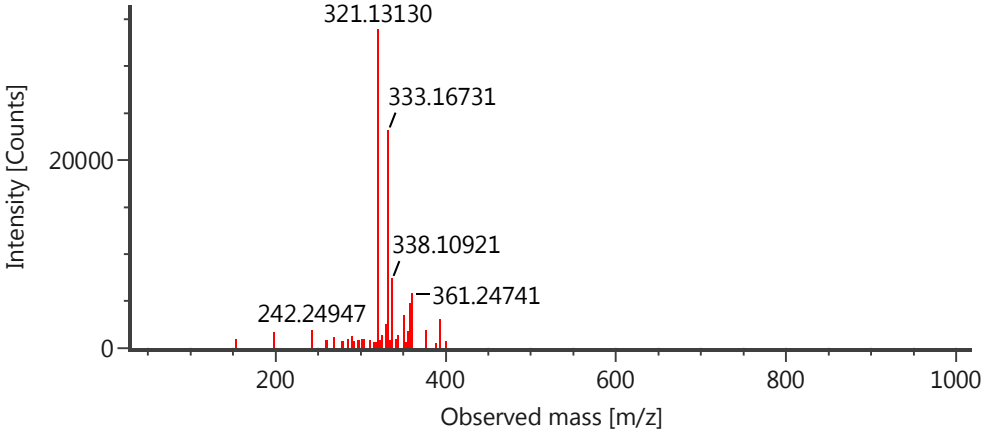

Item name: sample 2_01
Component name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane

Channel name: Low energy : Time 17.2816 +/- 0.0231 minutes : Drift Times: 5.19 +/- 0.26 ms



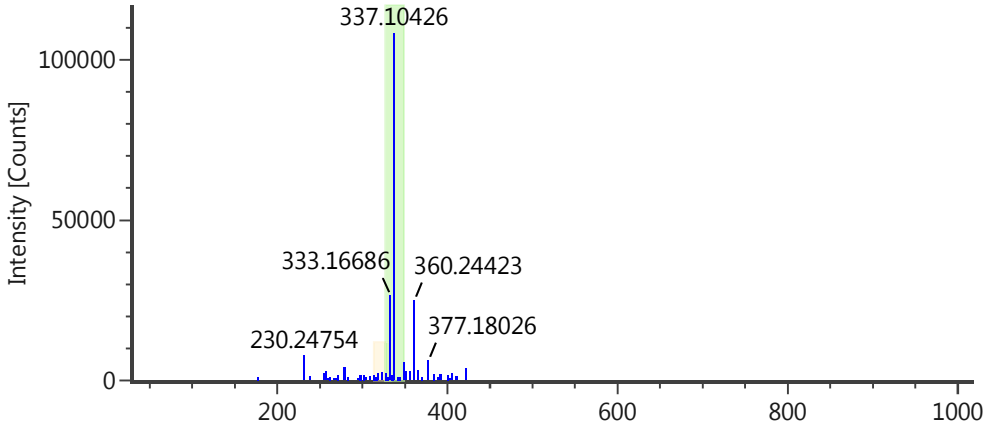

Item name: sample 2_01
Component name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane

Channel name: High energy : Time 17.2816 +/- 0.0231 minutes : Drift Times: 5.06 +/- 0.26 ms



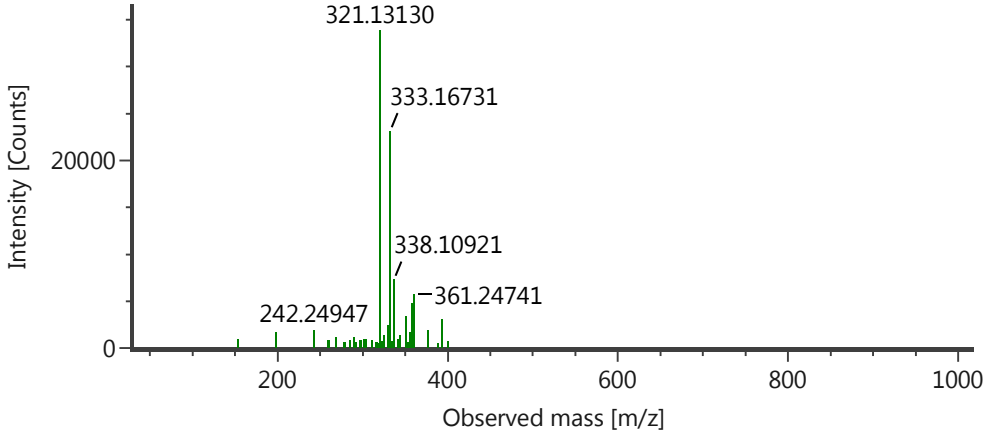
Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one

Channel name: Low energy : Time 17.2816 +/- 0.0231 minutes : Drift Times: 5.19 +/- 0.26 ms

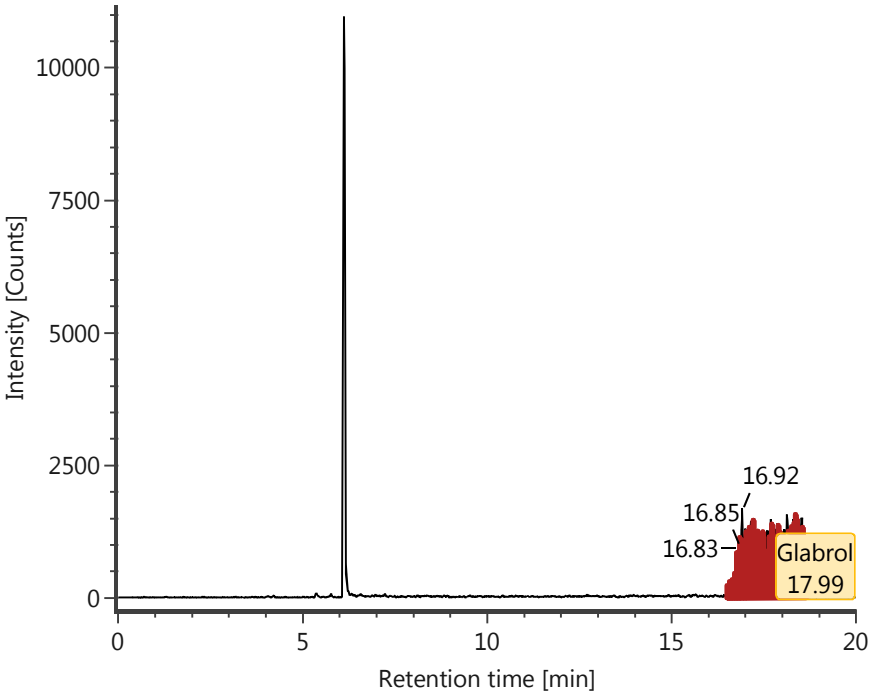



Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one

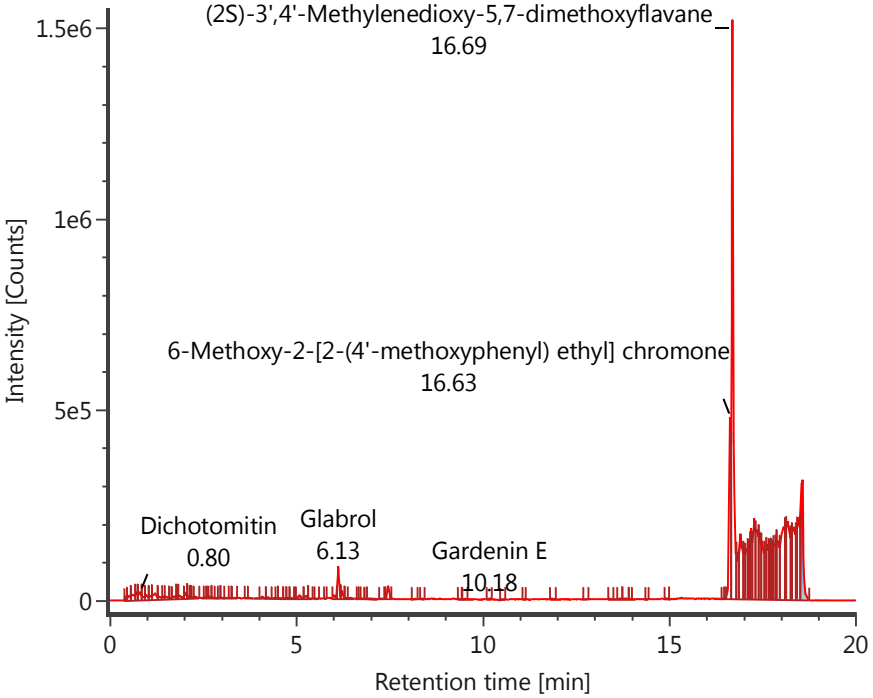
Channel name: High energy : Time 17.2816 +/- 0.0231 minutes : Drift Times: 5.06 +/- 0.26 ms



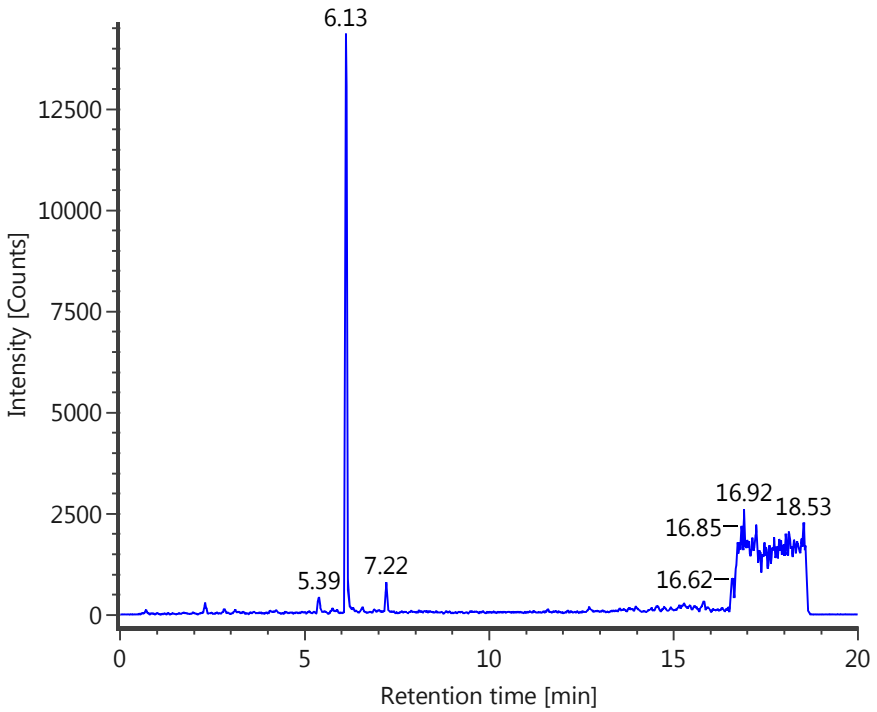
Item name: sample 2_01
Channel name: Glabrol [+H] : (18.8 PPM) 393.2090 : DT=5.03 to 5.55 ms



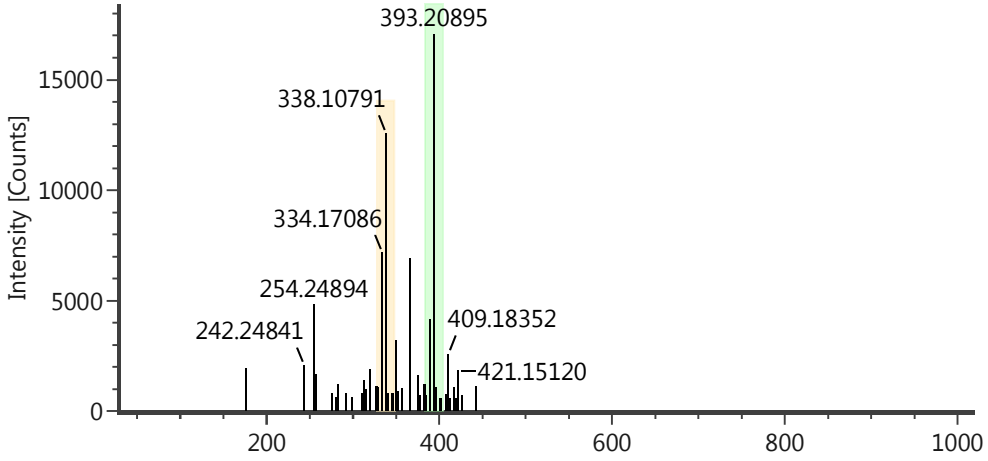
Item name: sample 2_01
Channel name: Identified Components



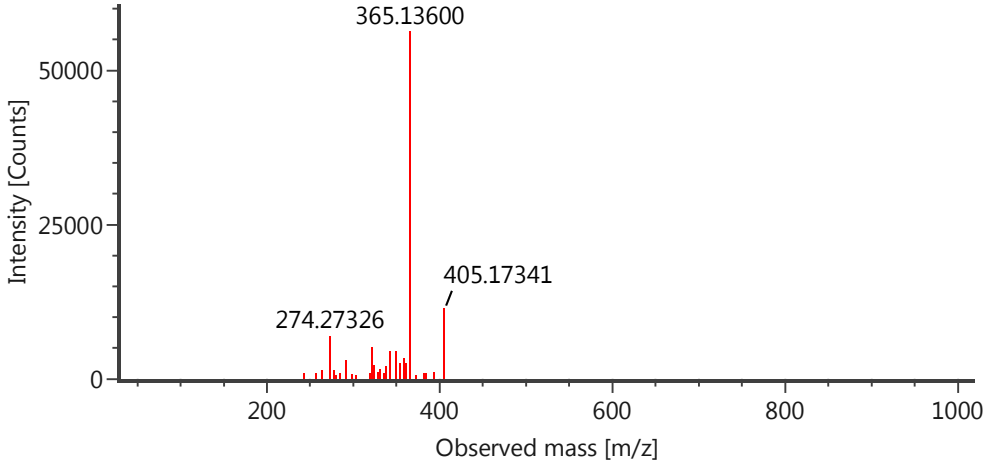
Item name: sample 2_01
Channel name: Glabrol [+H] : (18.8 PPM) 393.2090



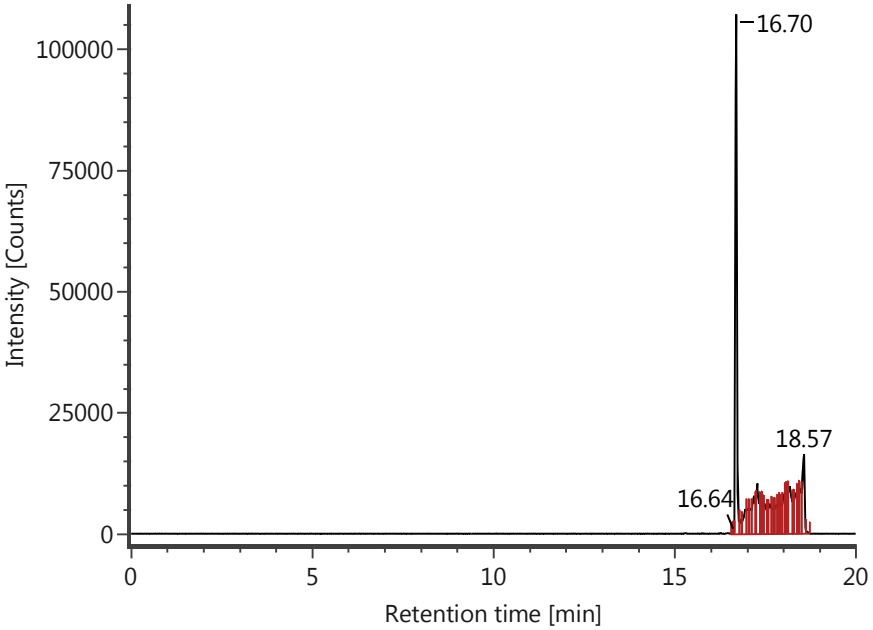

Item name: sample 2_01
Component name: Glabrol
Channel name: Low energy : Time 18.0033 +/- 0.0231 minutes :
Drift Times: 5.27 +/- 0.26 ms



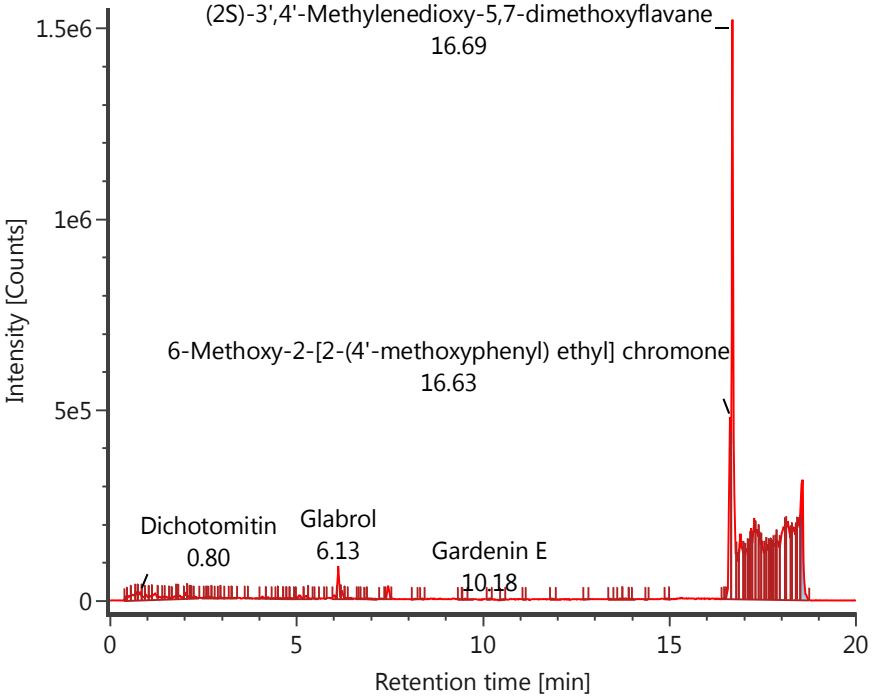

Item name: sample 2_01
Component name: Glabrol
Channel name: High energy : Time 18.0033 +/- 0.0231 minutes :
Drift Times: 5.14 +/- 0.26 ms



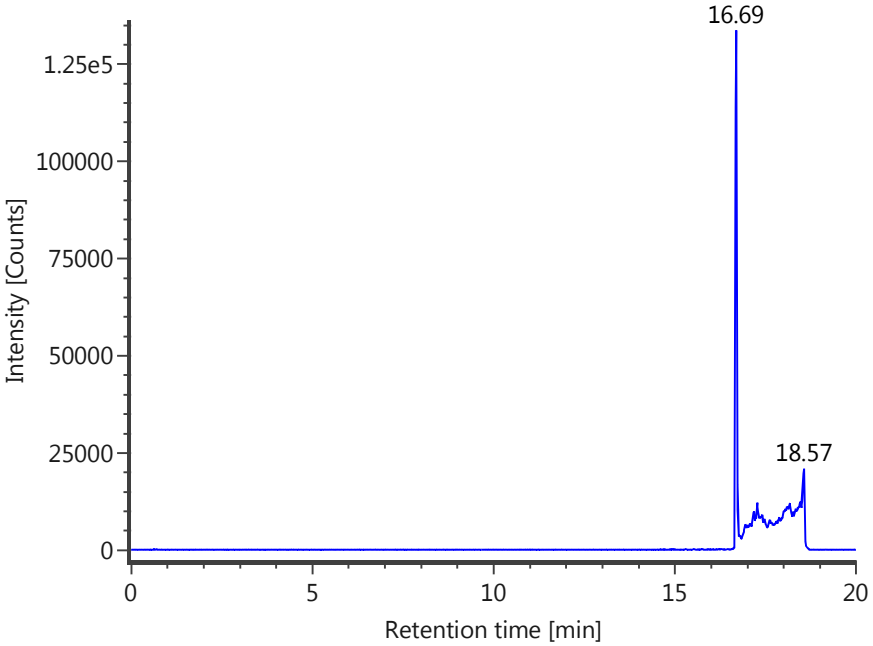
Item name: sample 2_01
Channel name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane [+Na] : 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one [+Na] : (18.8 PPM)
337.1045 : DT=4.94 to 5.46 ms



Item name: sample 2_01
Channel name: Identified Components

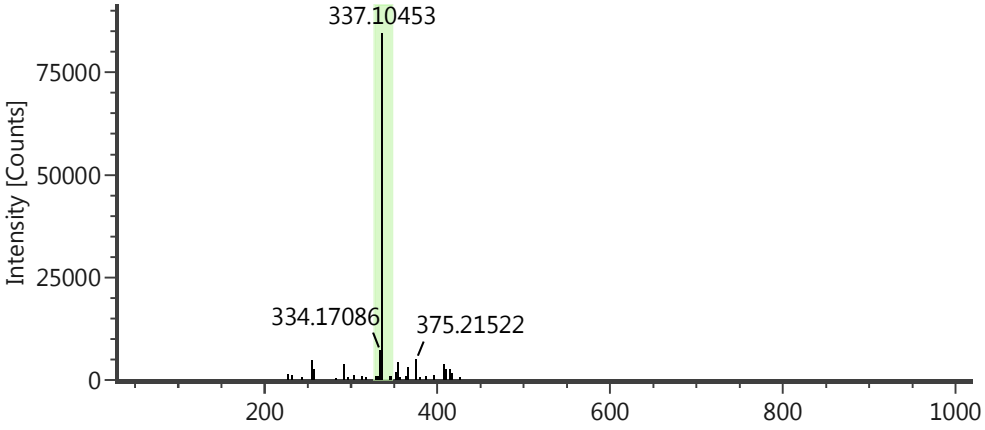


Item name: sample 2_01
Channel name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane [+Na] : 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one [+Na] : (18.8 PPM) 337.1045



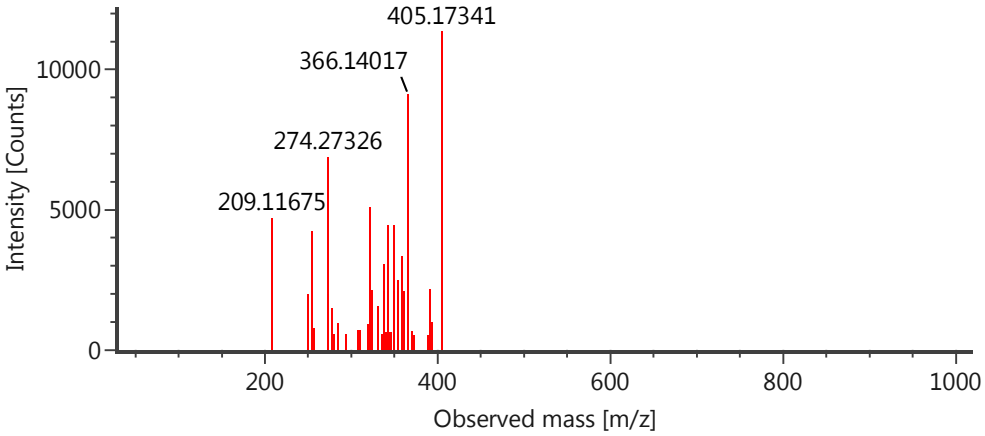

Item name: sample 2_01
Component name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane

Channel name: Low energy : Time 18.0290 +/- 0.0231 minutes : Drift Times: 5.20 +/- 0.26 ms



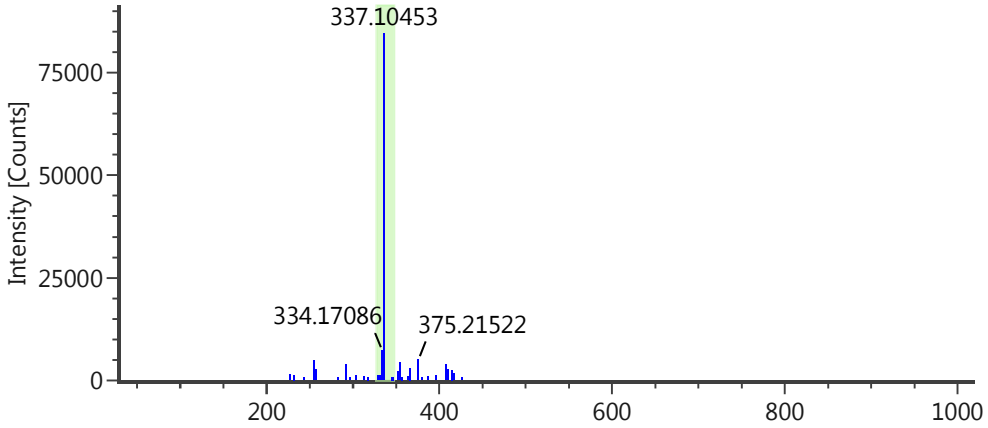

Item name: sample 2_01
Component name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane

Channel name: High energy : Time 18.0290 +/- 0.0231 minutes : Drift Times: 5.07 +/- 0.26 ms



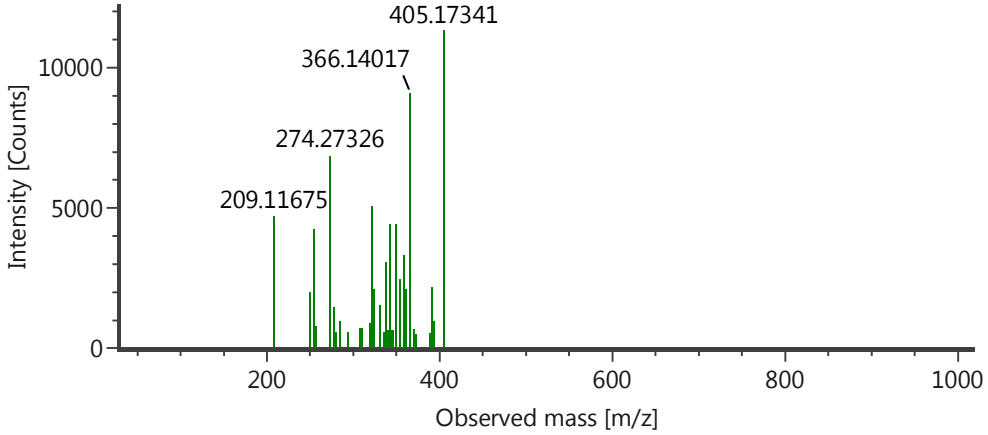
Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one

Channel name: Low energy : Time 18.0290 +/- 0.0231 minutes : Drift Times: 5.20 +/- 0.26 ms

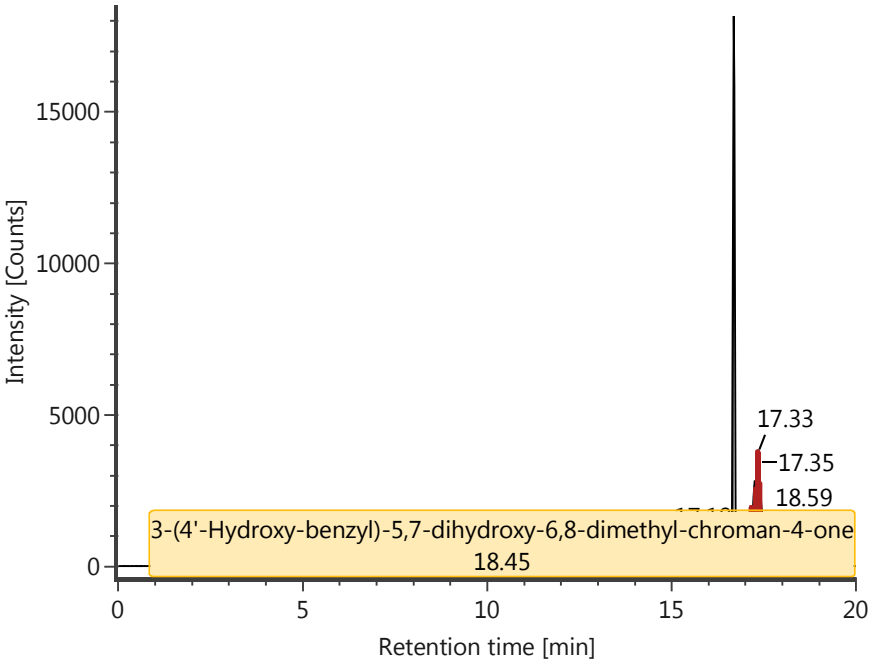



Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one

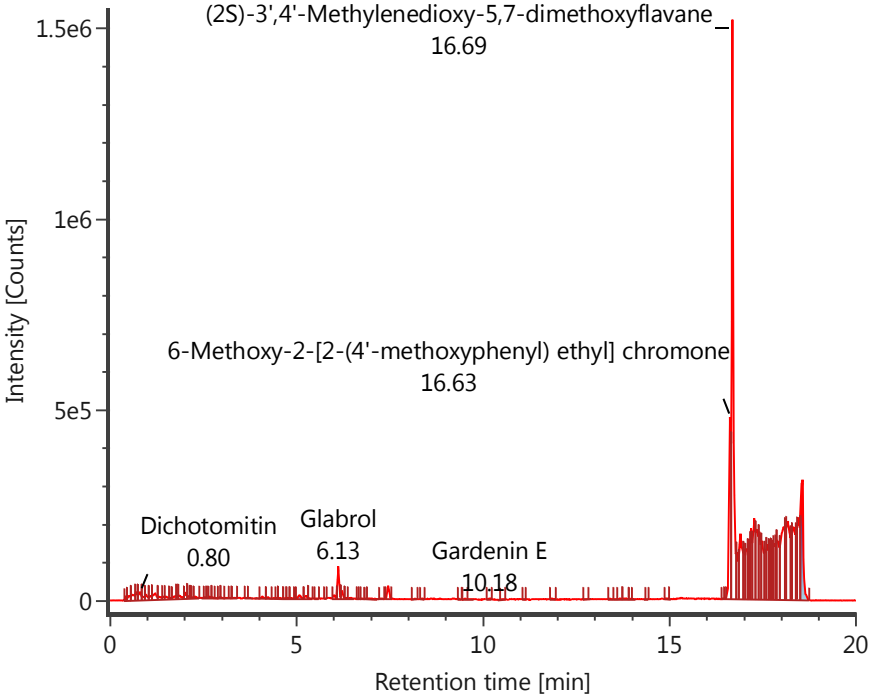
Channel name: High energy : Time 18.0290 +/- 0.0231 minutes : Drift Times: 5.07 +/- 0.26 ms



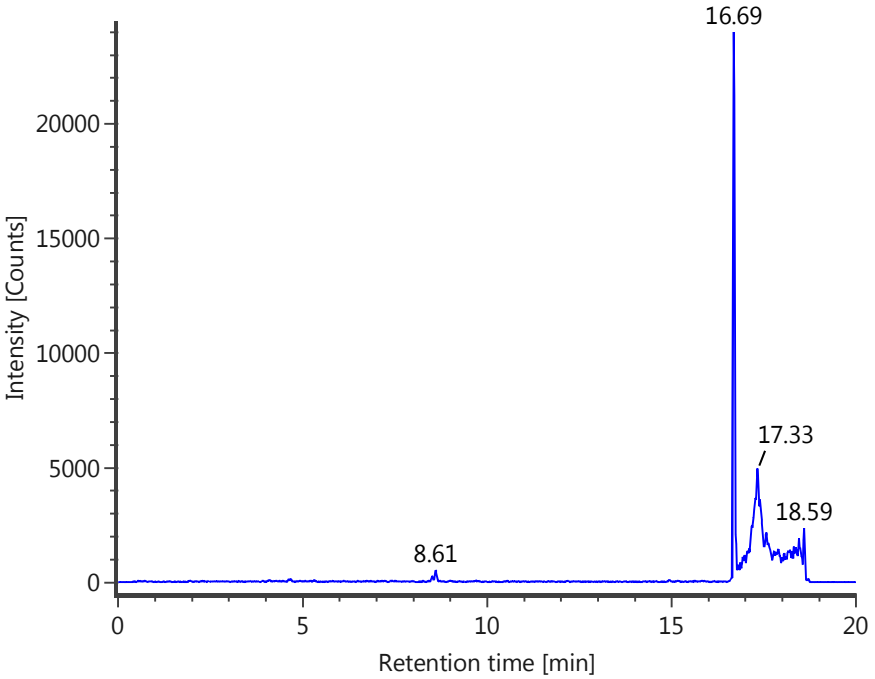
Item name: sample 2_01
Channel name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one
[+Li] : (18.8 PPM) 321.1327 : DT=5.03 to 5.55 ms



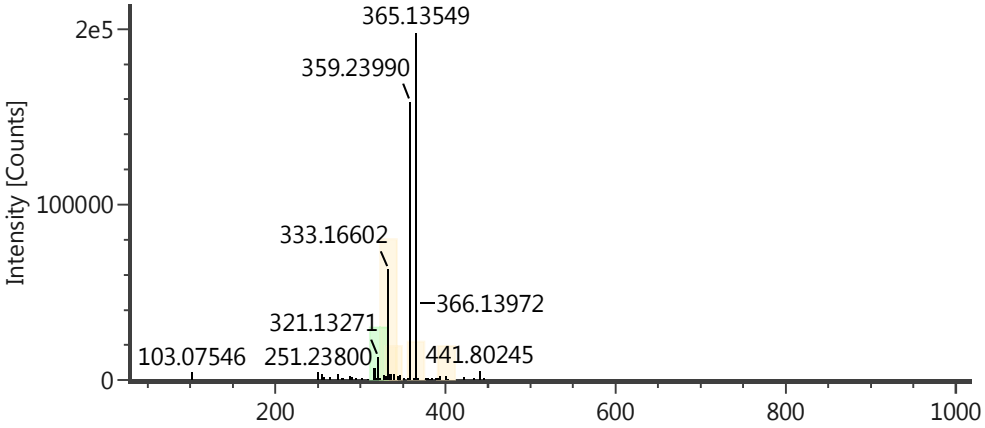
Item name: sample 2_01
Channel name: Identified Components



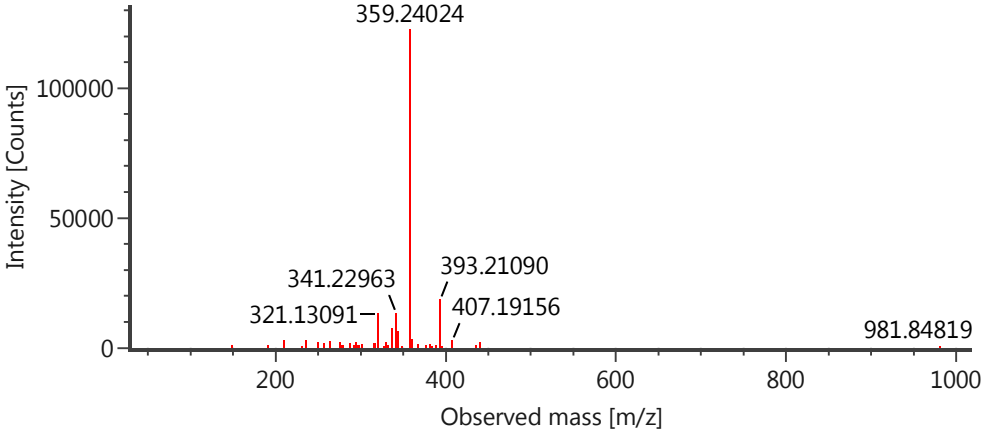
Item name: sample 2_01
Channel name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one [+Li] : (18.8 PPM) 321.1327



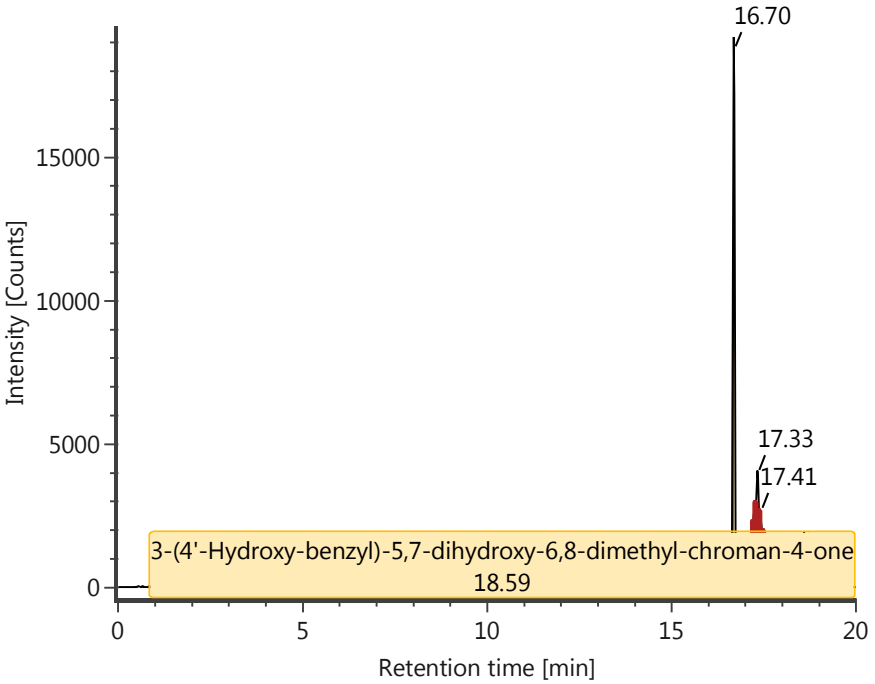

Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one
Channel name: Low energy : Time 18.4565 +/- 0.0231 minutes : Drift Times: 5.26 +/- 0.26 ms



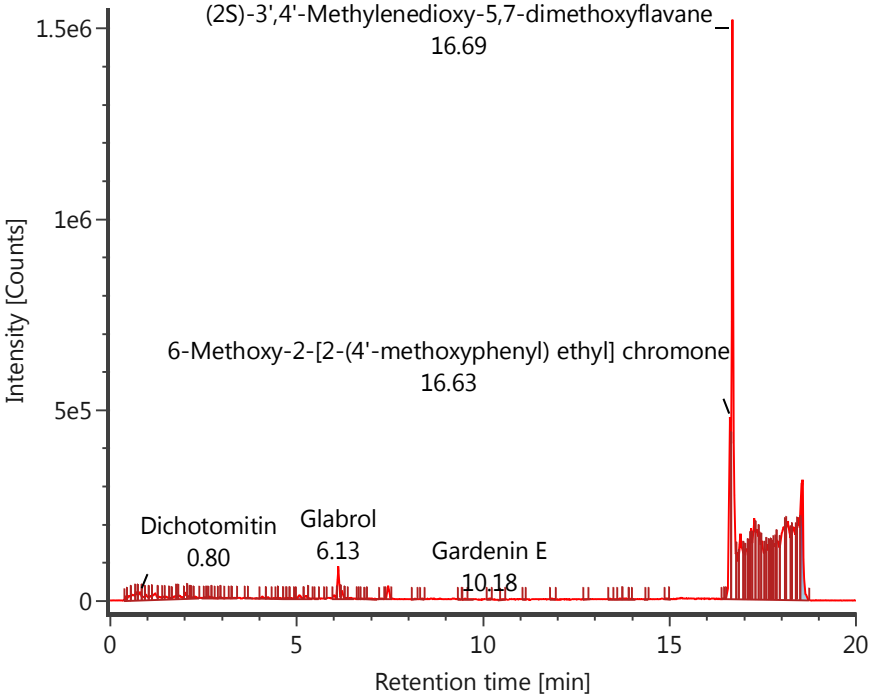

Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one
Channel name: High energy : Time 18.4565 +/- 0.0231 minutes : Drift Times: 5.13 +/- 0.26 ms



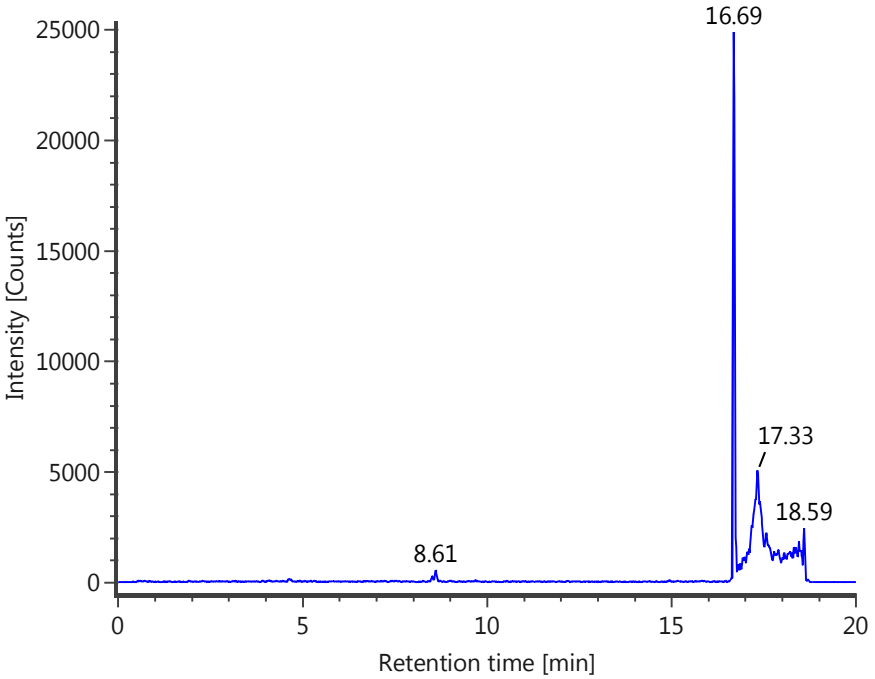
Item name: sample 2_01
Channel name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one
[+Li] : (18.8 PPM) 321.1309 : DT=4.87 to 5.39 ms



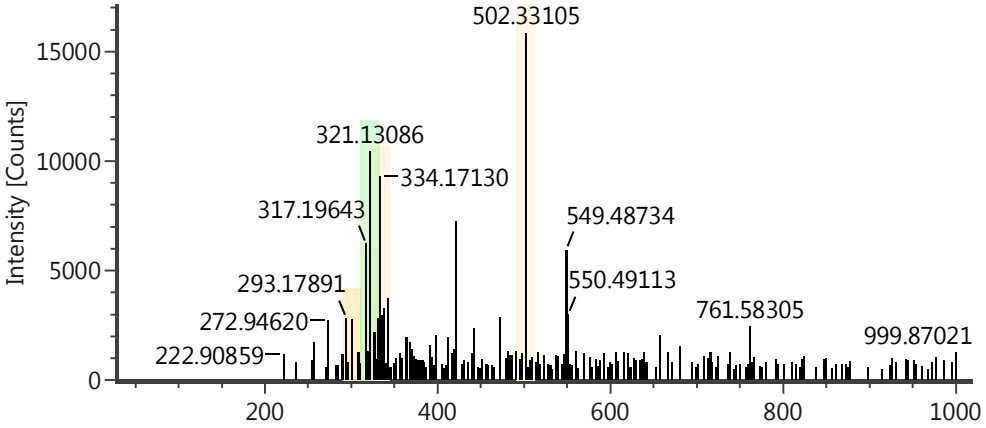
Item name: sample 2_01
Channel name: Identified Components



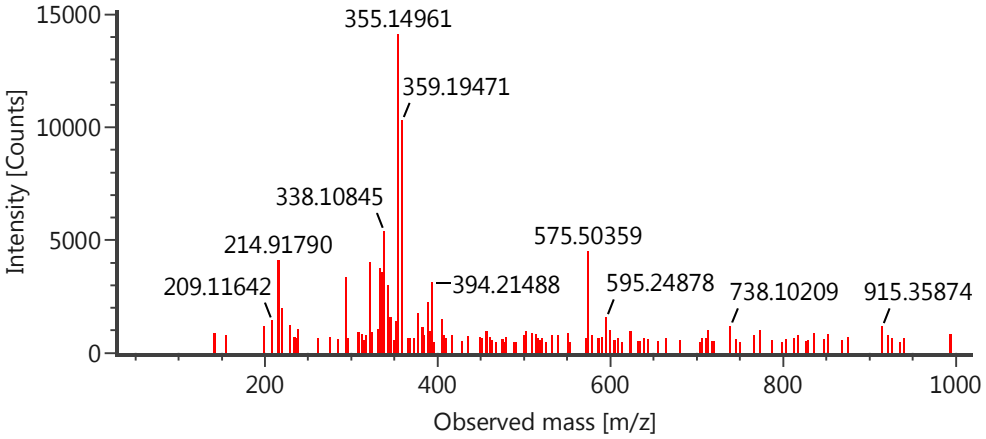
Item name: sample 2_01
Channel name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one [+Li] : (18.8 PPM) 321.1309



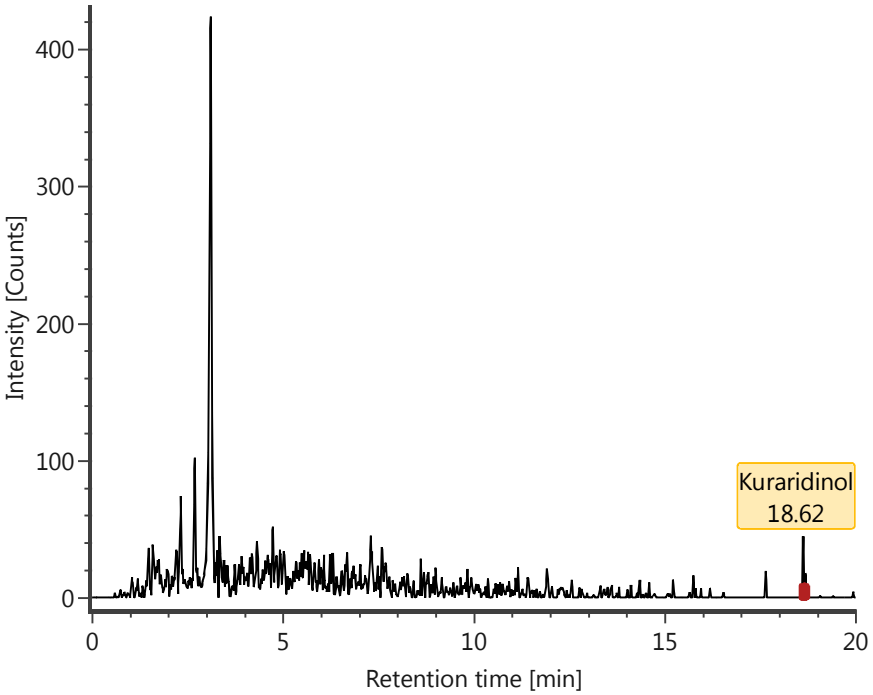

Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one
Channel name: Low energy : Time 18.5964 +/- 0.0231 minutes : Drift Times: 5.15 +/- 0.26 ms



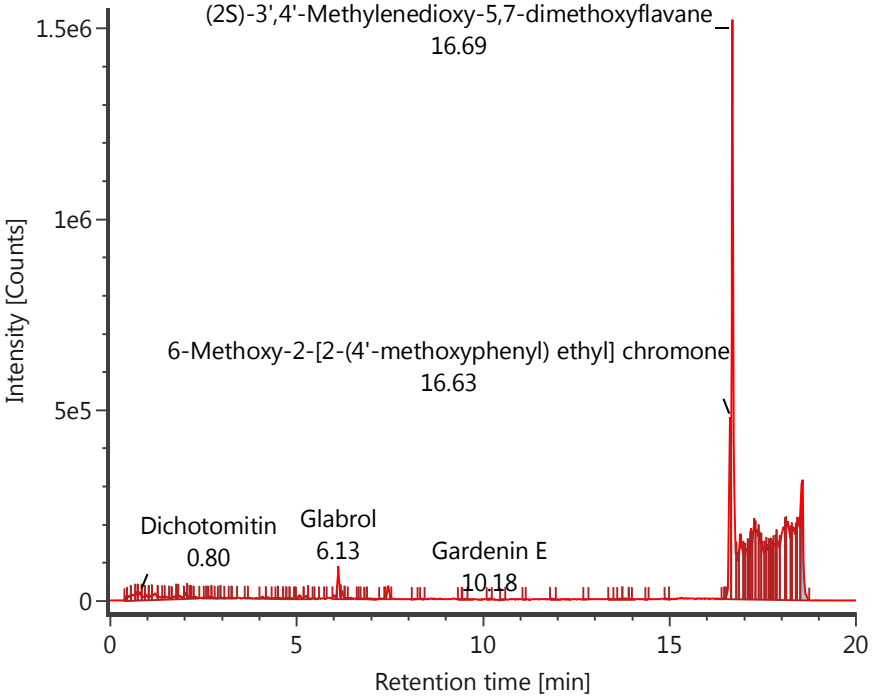

Item name: sample 2_01
Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one
Channel name: High energy : Time 18.5964 +/- 0.0231 minutes : Drift Times: 5.02 +/- 0.26 ms



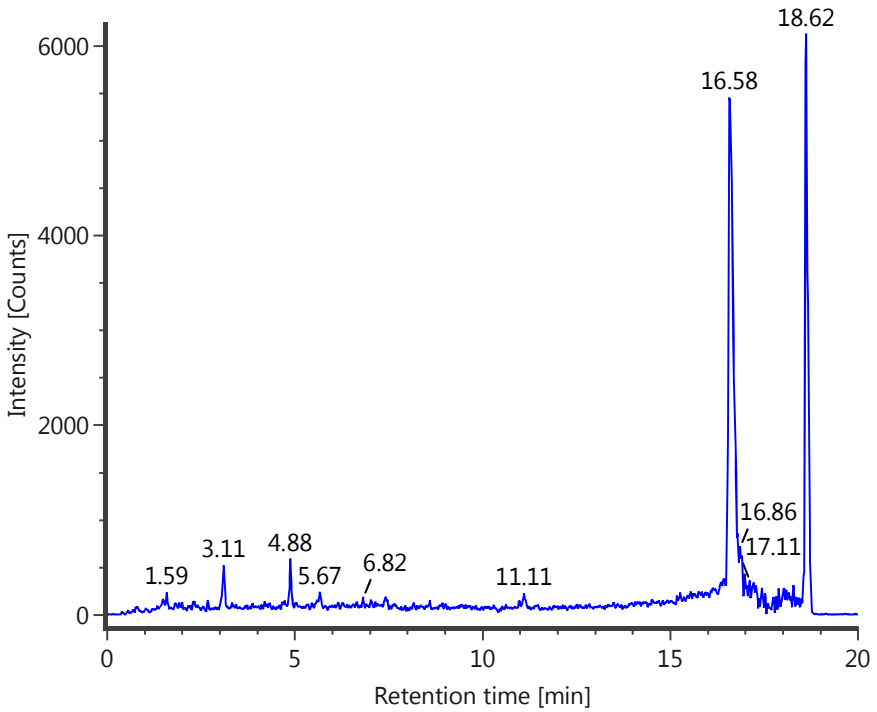
Item name: sample 2_01
Channel name: Kuraridinol [+H] : (18.8 PPM) 457.2257 : DT=4.36 to 4.85 ms



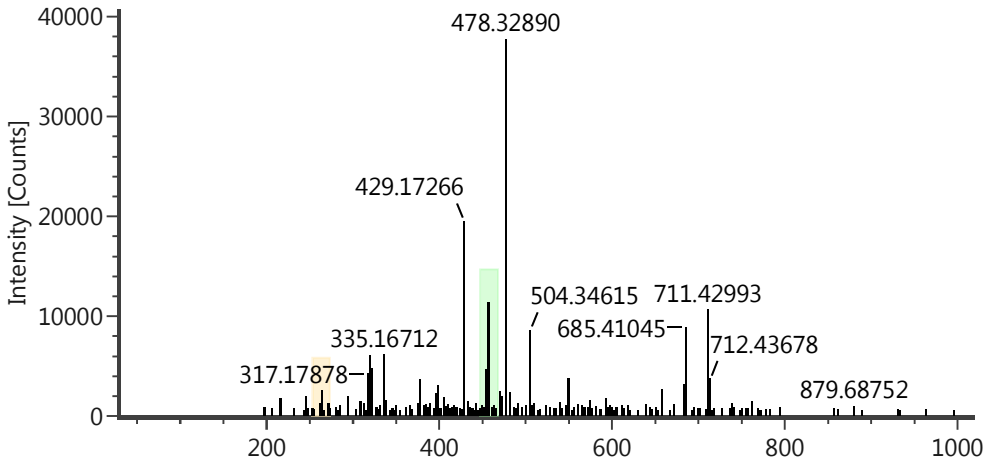
Item name: sample 2_01
Channel name: Identified Components



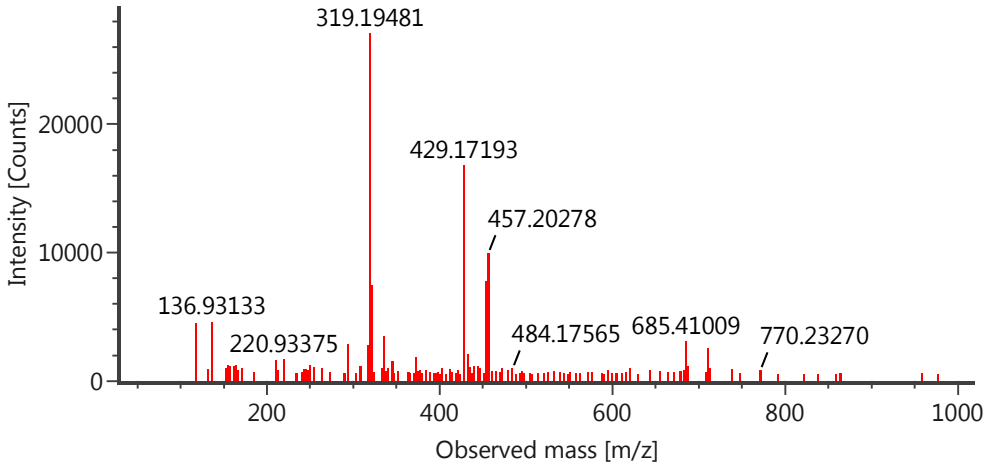
Item name: sample 2_01
Channel name: Kuraridinol [+H] : (18.8 PPM) 457.2257




Item name: sample 2_01
Component name: Kuraridinol
Channel name: Low energy : Time 18.6315 +/- 0.0231 minutes :
Drift Times: 4.62 +/- 0.25 ms

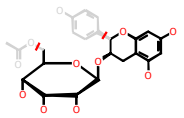



Item name: sample 2_01
Component name: Kuraridinol
Channel name: High energy : Time 18.6315 +/- 0.0231 minutes : Drift Times: 4.49 +/- 0.25 ms

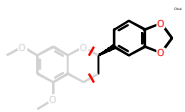
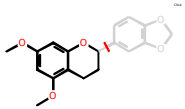


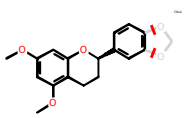
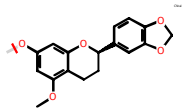
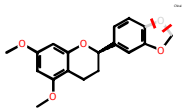
# Fragmentation (high energy)

Item name: sample 2_01, Component name: (-)-Epiafzelechin-3-O-(6"-O-acetyl)-β-D-allosepyranoside

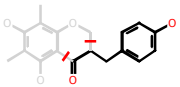
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 325.09179 | Theoretical | 325.09340 | 1.6 | 4.925 | 518 | 5.07549 | 6.49592 | C15H17O8 |  |

Item name: sample 2_01, Component name: (2S)-3',4'-Methylenedioxy-5,7-dimethoxyflavane

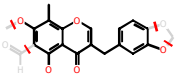
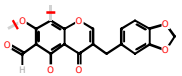
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 149.05971 | Theoretical | 149.05945 | -0.3 | -1.736 | 353 | 16.69991 | 4.95762 | C9H9O2 |  |
| 2 | 193.08592 | Theoretical | 193.08477 | -1.2 | -5.974 | 119 | 16.71985 | 5.23272 | C11H13O3 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 269.11722 | Theoretical | 269.11827 | 1.1 | 3.914 | 227 | 16.70070 | 4.95948 | C17H17O3 |  |
| 4 | 301.10705 | Theoretical | 301.10752 | 0.5 | 1.564 | 196 | 16.69238 | 5.15310 | C17H17O5 |  |
| 5 | 301.14344 | Theoretical | 301.14325 | -0.2 | -0.624 | 245 | 16.71026 | 5.08853 | C18H21O4 |  |

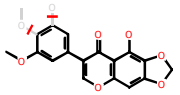
Item name: sample 2_01, Component name: 3-(4'-Hydroxy-benzyl)-5,7-dihydroxy-6,8-dimethyl-chroman-4-one

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 149.05971 | Theoretical | 149.05980 | 0.1 | 0.642 | 84 | 18.45279 | 5.04647 | C9H9O2 |  |

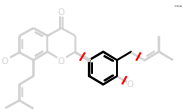
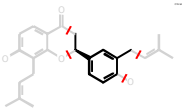
Item name: sample 2_01, Component name: 6-Aldehydo-7-methoxy-isoophiopogonone A

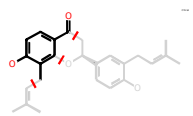
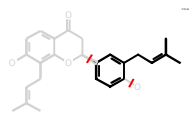
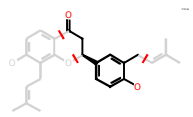
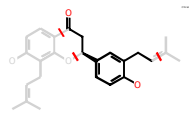
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 293.04445 | Theoretical | 293.04425 | -0.2 | -0.696 | 862 | 0.98487 | 5.20858 | C17H9O5 |  |
| 2 | 339.04993 | Theoretical | 339.05127 | 1.3 | 3.957 | 178 | 0.98076 | 5.16858 | C18H11O7 |  |

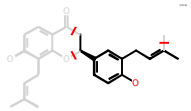
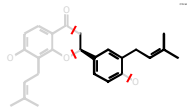
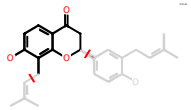
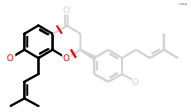
Item name: sample 2_01, Component name: Dichotomitin

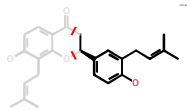
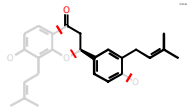
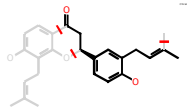
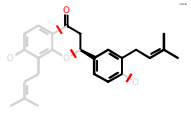
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 311.05501 | Theoretical | 311.05585 | 0.8 | 2.672 | 170 | 0.81037 | 5.20696 | C17H11O6 |  |

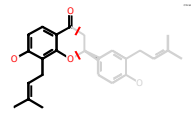
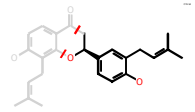
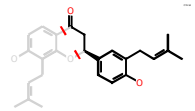
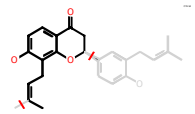
Item name: sample 2_01, Component name: Glabrol

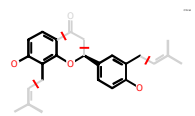
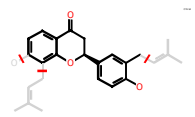
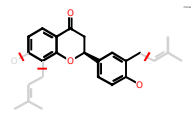
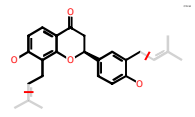
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 91.05423 | Theoretical | 91.05351 | -0.7 | -7.829 | 133 | 16.71064 | 5.74367 | C7H7 |  |
| 2 | 117.06988 | Theoretical | 117.06984 | 0.0 | -0.312 | 147 | 16.71092 | 5.52579 | C9H9 |  |

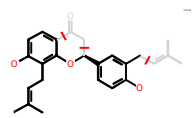
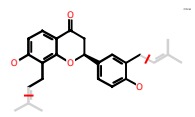
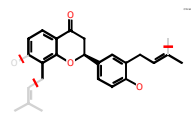
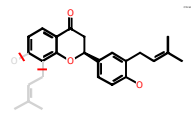
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 137.05971 | Theoretical | 137.05929 | -0.4 | -3.031 | 105 | 16.74915 | 5.82354 | C8H9O2 |  |
| 4 | 145.10118 | Theoretical | 145.10013 | -1.1 | -7.244 | 175 | 16.72772 | 5.72995 | C11H13 |  |
| 5 | 165.09101 | Theoretical | 165.09053 | -0.5 | -2.903 | 147 | 16.72416 | 5.84504 | C10H13O2 |  |
| 6 | 173.05971 | Theoretical | 173.05913 | -0.6 | -3.352 | 96 | 16.73462 | 5.43273 | C11H9O2 |  |

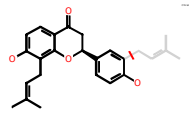
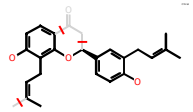
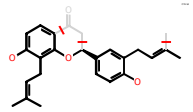
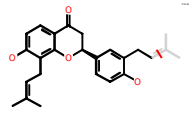
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | 173.09609 | Theoretical | 173.09537 | -0.7 | -4.146 | 191 | 16.71382 | 5.55181 | C12H13O |  |
| 8 | 173.13248 | Theoretical | 173.13186 | -0.6 | -3.572 | 153 | 16.72056 | 6.00457 | C13H17 |  |
| 9 | 179.07027 | Theoretical | 179.07132 | 1.0 | 5.856 | 112 | 16.75015 | 6.03023 | C10H11O3 |  |
| 10 | 179.10666 | Theoretical | 179.10604 | -0.6 | -3.447 | 118 | 16.75156 | 5.70085 | C11H15O2 |  |

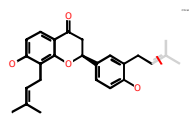
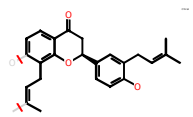
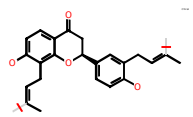
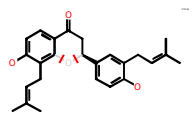
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | 187.11174 | Theoretical | 187.11073 | -1.0 | -5.416 | 139 | 16.72410 | 5.50883 | C13H15O |  |
| 12 | 197.09609 | Theoretical | 197.09595 | -0.1 | -0.727 | 212 | 16.72194 | 6.03756 | C14H13O |  |
| 13 | 201.09101 | Theoretical | 201.09084 | -0.2 | -0.835 | 197 | 16.73888 | 6.05635 | C13H13O2 |  |
| 14 | 201.12739 | Theoretical | 201.12690 | -0.5 | -2.436 | 148 | 16.75557 | 6.10806 | C14H17O |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | 207.10157 | Theoretical | 207.10092 | -0.6 | -3.129 | 115 | 16.74277 | 5.95345 | C12H15O3 |  |
| 16 | 207.13796 | Theoretical | 207.13782 | -0.1 | -0.666 | 85 | 16.72747 | 6.09913 | C13H19O2 |  |
| 17 | 215.10666 | Theoretical | 215.10688 | 0.2 | 1.031 | 250 | 16.72668 | 6.01731 | C14H15O2 |  |
| 18 | 217.08592 | Theoretical | 217.08672 | 0.8 | 3.700 | 115 | 16.72479 | 5.44403 | C13H13O3 |  |

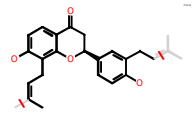
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | 241.08592 | Theoretical | 241.08735 | 1.4 | 5.909 | 228 | 16.70690 | 5.66113 | C15H13O3 |  |
| 20 | 254.09375 | Theoretical | 254.09194 | -1.8 | -7.123 | 93 | 16.71854 | 5.81587 | C16H14O3 |  |
| 21 | 255.10157 | Theoretical | 255.10049 | -1.1 | -4.251 | 194 | 16.71765 | 5.99933 | C16H15O3 |  |
| 22 | 293.08084 | Theoretical | 293.07993 | -0.9 | -3.083 | 143 | 16.73625 | 5.93854 | C18H13O4 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | 293.11722 | Theoretical | 293.11593 | -1.3 | -4.395 | 99 | 16.74471 | 5.58783 | C19H17O3 |  |
| 24 | 294.08866 | Theoretical | 294.08773 | -0.9 | -3.163 | 137 | 16.72028 | 6.11014 | C18H14O4 |  |
| 25 | 303.10157 | Theoretical | 303.09992 | -1.6 | -5.434 | 89 | 16.71848 | 5.55540 | C20H15O3 |  |
| 26 | 305.11722 | Theoretical | 305.11853 | 1.3 | 4.300 | 210 | 16.70713 | 5.48962 | C20H17O3 |  |

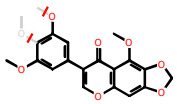
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 325.14344 | Theoretical | 325.14386 | 0.4 | 1.308 | 249 | 16.73804 | 5.76178 | C20H21O4 |  |
| 28 | 335.16417 | Theoretical | 335.16326 | -0.9 | -2.708 | 168 | 16.73160 | 6.04566 | C22H23O3 |  |
| 29 | 337.17982 | Theoretical | 337.18139 | 1.6 | 4.643 | 386 | 16.73138 | 5.60753 | C22H25O3 |  |
| 30 | 350.15126 | Theoretical | 350.15208 | 0.8 | 2.340 | 211 | 16.71994 | 5.57317 | C22H22O4 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | 352.16691 | Theoretical | 352.16660 | -0.3 | -0.871 | 197 | 16.70207 | 5.58031 | C22H24O4 |  |
| 32 | 359.16417 | Theoretical | 359.16481 | 0.6 | 1.766 | 508 | 16.70908 | 5.64326 | C24H23O3 |  |
| 33 | 365.17474 | Theoretical | 365.17411 | -0.6 | -1.716 | 1777 | 16.71896 | 5.75354 | C23H25O4 |  |
| 34 | 379.22677 | Theoretical | 379.22648 | -0.3 | -0.766 | 353 | 16.75270 | 5.81296 | C25H31O3 |  |

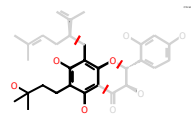
Item name: sample 2_01, Component name: Glabrol

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 335.12779 | Theoretical | 335.12918 | 1.4 | 4.148 | 78 | 18.01743 | 5.21671 | C21H19O4 |  |

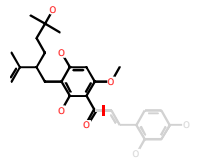
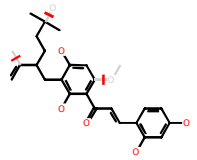
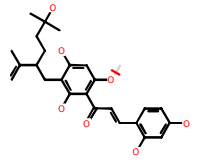
Item name: sample 2_01, Component name: Irisflorentin

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 339.04993 | Theoretical | 339.05127 | 1.3 | 3.957 | 178 | 0.98076 | 5.16858 | C18H11O7 |  |

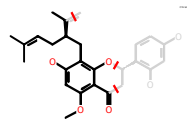
Item name: sample 2_01, Component name: Kosamol A

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 226.11996 | Theoretical | 226.11885 | -1.1 | -4.914 | 151 | 2.14382 | 6.34233 | C12H18O4 |  |

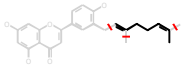
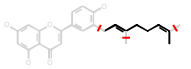
Item name: sample 2_01, Component name: Kuraridinol

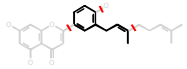
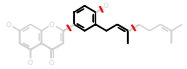
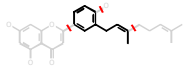
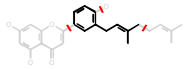
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 321.16965 | Theoretical | 321.16832 | -1.3 | -4.139 | 101 | 18.62443 | 4.50042 | C18H25O5 |  |
| 2 | 393.16965 | Theoretical | 393.16913 | -0.5 | -1.313 | 88 | 18.62562 | 4.55561 | C24H25O5 |  |
| 3 | 443.20643 | Theoretical | 443.20596 | -0.5 | -1.055 | 171 | 18.61694 | 4.24735 | C25H31O7 |  |

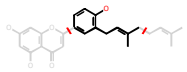
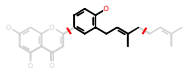
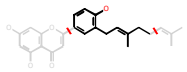
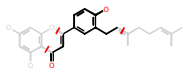
Item name: sample 2_01, Component name: Kurarinone

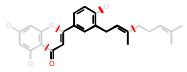
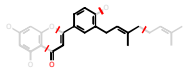
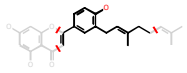
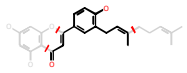
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 292.16691 | Theoretical | 292.16687 | 0.0 | -0.155 | 77 | 0.83771 | 6.04744 | C17H24O4 |  |

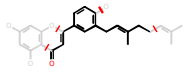
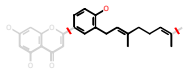
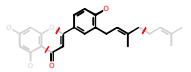
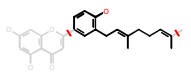
Item name: sample 2_01, Component name: Kuwanon S

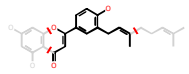
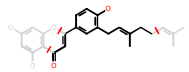
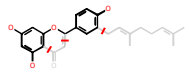
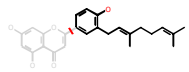
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 91.05423 | Theoretical | 91.05351 | -0.7 | -7.829 | 133 | 16.71064 | 5.74367 | C7H7 |  |
| 2 | 105.06988 | Theoretical | 105.06933 | -0.6 | -5.246 | 417 | 16.72412 | 6.48702 | C8H9 |  |

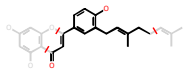
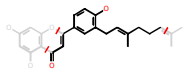
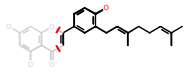
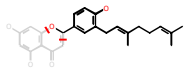
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 128.06205 | Theoretical | 128.06136 | -0.7 | -5.420 | 138 | 16.70183 | 5.88192 | C10H8 |  |
| 4 | 131.08553 | Theoretical | 131.08533 | -0.2 | -1.466 | 319 | 16.70219 | 6.01032 | C10H11 |  |
| 5 | 133.10118 | Theoretical | 133.10028 | -0.9 | -6.732 | 342 | 16.70373 | 6.15077 | C10H13 |  |
| 6 | 145.10118 | Theoretical | 145.10013 | -1.1 | -7.243 | 175 | 16.72772 | 5.72995 | C11H13 |  |

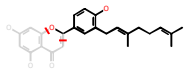
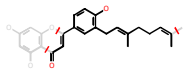
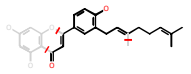
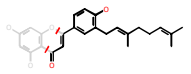
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | 161.09609 | Theoretical | 161.09555 | -0.5 | -3.352 | 115 | 16.69928 | 6.05502 | C11H13O |  |
| 8 | 163.11174 | Theoretical | 163.11061 | -1.1 | -6.963 | 160 | 16.72797 | 6.58643 | C11H15O |  |
| 9 | 173.09609 | Theoretical | 173.09589 | -0.2 | -1.171 | 85 | 16.70959 | 6.19109 | C12H13O |  |
| 10 | 175.07536 | Theoretical | 175.07586 | 0.5 | 2.868 | 334 | 16.70000 | 6.39180 | C11H11O2 |  |

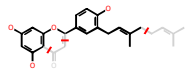
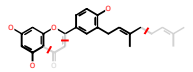
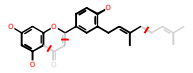
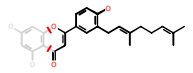
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | 181.06479 | Theoretical | 181.06438 | -0.4 | -2.272 | 93 | 16.70158 | 5.76557 | C13H9O |  |
| 12 | 194.07262 | Theoretical | 194.07318 | 0.6 | 2.901 | 73 | 16.70141 | 6.34186 | C14H10O |  |
| 13 | 197.09609 | Theoretical | 197.09595 | -0.1 | -0.727 | 212 | 16.72194 | 6.03756 | C14H13O |  |
| 14 | 201.09101 | Theoretical | 201.09084 | -0.2 | -0.835 | 197 | 16.73888 | 6.05635 | C13H13O2 |  |

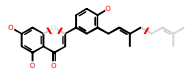
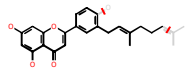
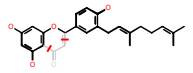
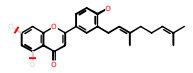
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | 211.11174 | Theoretical | 211.11273 | 1.0 | 4.690 | 199 | 16.69936 | 5.77489 | C15H15O |  |
| 16 | 213.12739 | Theoretical | 213.12608 | -1.3 | -6.160 | 100 | 16.69456 | 5.99408 | C15H17O |  |
| 17 | 215.10666 | Theoretical | 215.10688 | 0.2 | 1.031 | 250 | 16.72668 | 6.01731 | C14H15O2 |  |
| 18 | 217.15869 | Theoretical | 217.15978 | 1.1 | 5.013 | 112 | 16.69885 | 6.36351 | C15H21O |  |

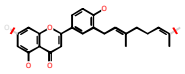
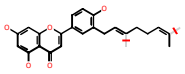
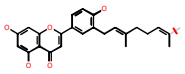
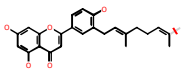
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | 219.10157 | Theoretical | 219.10202 | 0.4 | 2.032 | 185 | 16.70390 | 6.14521 | C13H15O3 |  |
| 20 | 227.10666 | Theoretical | 227.10695 | 0.3 | 1.313 | 230 | 16.70070 | 6.11960 | C15H15O2 |  |
| 21 | 229.04954 | Theoretical | 229.04871 | -0.8 | -3.591 | 74 | 16.70137 | 6.12615 | C13H9O4 |  |
| 22 | 229.15869 | Theoretical | 229.15950 | 0.8 | 3.534 | 83 | 16.68704 | 6.01026 | C16H21O |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | 231.13796 | Theoretical | 231.13800 | 0.0 | 0.190 | 180 | 16.68578 | 6.27554 | C15H19O2 |  |
| 24 | 241.12231 | Theoretical | 241.12171 | -0.6 | -2.460 | 207 | 16.72017 | 6.19162 | C16H17O2 |  |
| 25 | 253.15869 | Theoretical | 253.15900 | 0.3 | 1.220 | 81 | 16.71092 | 6.12460 | C18H21O |  |
| 26 | 255.13796 | Theoretical | 255.13727 | -0.7 | -2.689 | 139 | 16.73314 | 5.98228 | C17H19O2 |  |

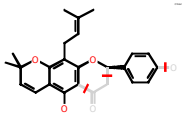
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | 257.15361 | Theoretical | 257.15416 | 0.6 | 2.160 | 140 | 16.69902 | 5.84910 | C17H21O2 |  |
| 28 | 266.13013 | Theoretical | 266.12828 | -1.9 | -6.963 | 105 | 16.71159 | 6.09609 | C18H18O2 |  |
| 29 | 271.16926 | Theoretical | 271.16936 | 0.1 | 0.399 | 163 | 16.69982 | 5.72004 | C18H23O2 |  |
| 30 | 281.15361 | Theoretical | 281.15420 | 0.6 | 2.101 | 206 | 16.70094 | 6.00915 | C19H21O2 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | 293.08084 | Theoretical | 293.07993 | -0.9 | -3.083 | 143 | 16.73625 | 5.93854 | C18H13O4 |  |
| 32 | 294.08866 | Theoretical | 294.08773 | -0.9 | -3.162 | 137 | 16.72028 | 6.11014 | C18H14O4 |  |
| 33 | 300.13561 | Theoretical | 300.13602 | 0.4 | 1.376 | 138 | 16.72910 | 6.15238 | C18H20O4 |  |
| 34 | 301.17982 | Theoretical | 301.18116 | 1.3 | 4.455 | 87 | 16.69799 | 6.38923 | C19H25O3 |  |

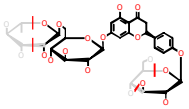
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | 325.14344 | Theoretical | 325.14386 | 0.4 | 1.308 | 249 | 16.73804 | 5.76178 | C20H21O4 |  |
| 36 | 350.15126 | Theoretical | 350.15208 | 0.8 | 2.340 | 217 | 16.71353 | 6.28372 | C22H22O4 |  |
| 37 | 365.17474 | Theoretical | 365.17411 | -0.6 | -1.715 | 1777 | 16.71896 | 5.75354 | C23H25O4 |  |
| 38 | 371.16417 | Theoretical | 371.16388 | -0.3 | -0.791 | 658 | 16.71899 | 5.74984 | C25H23O3 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 39 | 373.14344 | Theoretical | 373.14318 | -0.3 | -0.689 | 336 | 16.70270 | 5.98495 | C24H21O4 |  |
| 40 | 379.15400 | Theoretical | 379.15465 | 0.7 | 1.715 | 183 | 16.70138 | 6.53113 | C23H23O5 |  |
| 41 | 391.15400 | Theoretical | 391.15483 | 0.8 | 2.111 | 332 | 16.69019 | 6.44969 | C24H23O5 |  |
| 42 | 393.16965 | Theoretical | 393.17051 | 0.9 | 2.191 | 711 | 16.71929 | 5.72868 | C24H25O5 |  |

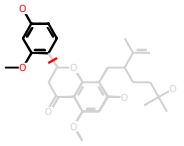
Item name: sample 2_01, Component name: Lupinifolin

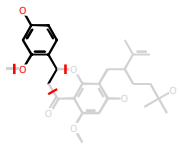
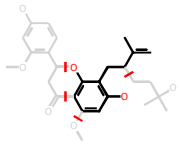
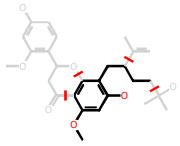
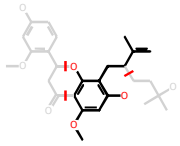
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 349.17982 | Theoretical | 349.18160 | 1.8 | 5.094 | 429 | 6.22465 | 5.10610 | C23H25O3 |  |

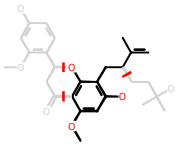
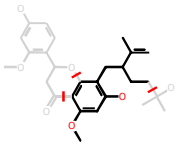
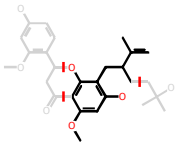
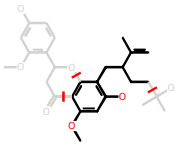
Item name: sample 2_01, Component name: Naringenin-4′-glucoside-7-rutinoside

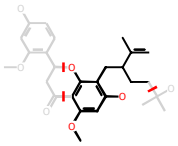
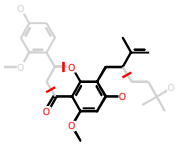
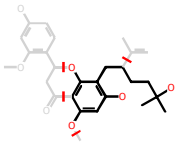
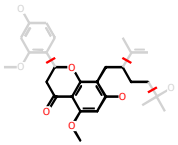
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 584.17357 | Theoretical | 584.17378 | 0.2 | 0.365 | 302 | 2.02046 | 7.59535 | C26H32O15 |  |

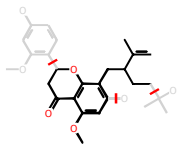
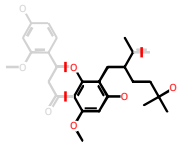
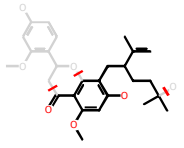
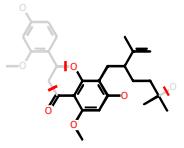
Item name: sample 2_01, Component name: Neokurarinol

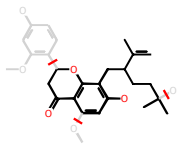
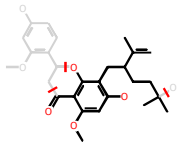
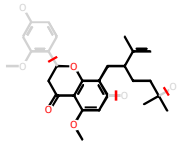
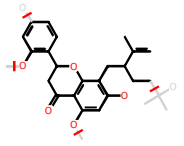
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 125.05971 | Theoretical | 125.05961 | -0.1 | -0.748 | 81 | 16.69556 | 6.39431 | C7H9O2 |  |

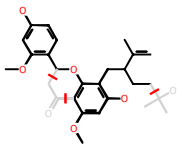
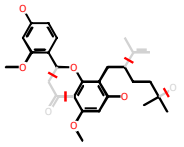
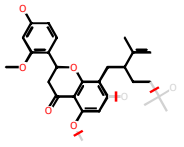
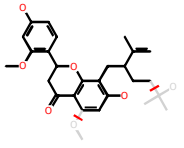
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 139.07536 | Theoretical | 139.07464 | -0.7 | -5.119 | 85 | 16.70366 | 6.36758 | C8H11O2 |  |
| 3 | 175.07536 | Theoretical | 175.07586 | 0.5 | 2.869 | 334 | 16.70000 | 6.39180 | C11H11O2 |  |
| 4 | 181.12231 | Theoretical | 181.12249 | 0.2 | 1.039 | 225 | 16.69540 | 6.32980 | C11H17O2 |  |
| 5 | 207.10157 | Theoretical | 207.10089 | -0.7 | -3.276 | 96 | 16.73812 | 6.57387 | C12H15O3 |  |

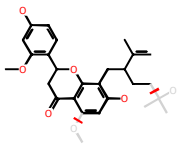
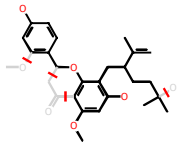
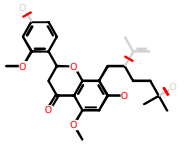
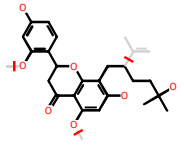
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 209.11722 | Theoretical | 209.11664 | -0.6 | -2.764 | 972 | 16.70066 | 6.37103 | C12H17O3 |  |
| 7 | 215.10666 | Theoretical | 215.10742 | 0.8 | 3.552 | 211 | 16.72319 | 6.59458 | C14H15O2 |  |
| 8 | 217.08592 | Theoretical | 217.08504 | -0.9 | -4.038 | 76 | 16.73867 | 6.70329 | C13H13O3 |  |
| 9 | 221.15361 | Theoretical | 221.15448 | 0.9 | 3.958 | 87 | 16.69774 | 6.31908 | C14H21O2 |  |

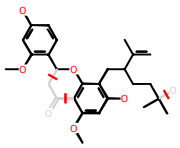
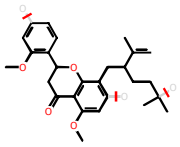
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 233.11722 | Theoretical | 233.11722 | 0.0 | -0.019 | 111 | 16.69594 | 6.69018 | C14H17O3 |  |
| 11 | 237.11214 | Theoretical | 237.11133 | -0.8 | -3.379 | 719 | 16.69938 | 6.34994 | C13H17O4 |  |
| 12 | 238.11996 | Theoretical | 238.12001 | 0.1 | 0.210 | 255 | 16.69930 | 6.70486 | C13H18O4 |  |
| 13 | 249.11214 | Theoretical | 249.11134 | -0.8 | -3.194 | 251 | 16.73315 | 6.44637 | C14H17O4 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | 269.11722 | Theoretical | 269.11831 | 1.1 | 4.032 | 187 | 16.72964 | 6.27341 | C17H17O3 |  |
| 15 | 282.18256 | Theoretical | 282.18337 | 0.8 | 2.856 | 105 | 16.71748 | 6.51250 | C16H26O4 |  |
| 16 | 285.14852 | Theoretical | 285.14709 | -1.4 | -5.020 | 189 | 16.71397 | 6.50214 | C18H21O3 |  |
| 17 | 301.14344 | Theoretical | 301.14344 | 0.0 | 0.004 | 162 | 16.71010 | 6.66238 | C18H21O4 |  |

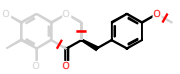
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 18 | 301.17982 | Theoretical | 301.18116 | 1.3 | 4.455 | 87 | 16.69799 | 6.38923 | C19H25O3 |  |
| 19 | 307.19039 | Theoretical | 307.19108 | 0.7 | 2.258 | 124 | 16.70688 | 6.65337 | C18H27O4 |  |
| 20 | 311.16417 | Theoretical | 311.16276 | -1.4 | -4.549 | 97 | 16.72968 | 6.68828 | C20H23O3 |  |
| 21 | 360.09923 | Theoretical | 360.09984 | 0.6 | 1.706 | 81 | 16.71026 | 6.63323 | C22H16O5 |  |

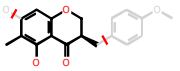
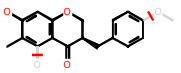
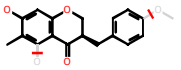
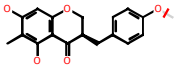
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | 373.20095 | Theoretical | 373.20016 | -0.8 | -2.110 | 417 | 16.71517 | 6.50775 | C22H29O5 |  |
| 23 | 374.20878 | Theoretical | 374.20859 | -0.2 | -0.486 | 137 | 16.72792 | 6.59592 | C22H30O5 |  |
| 24 | 377.13835 | Theoretical | 377.13809 | -0.3 | -0.700 | 360 | 16.72349 | 6.66375 | C23H21O5 |  |
| 25 | 379.15400 | Theoretical | 379.15465 | 0.7 | 1.715 | 183 | 16.70138 | 6.53113 | C23H23O5 |  |

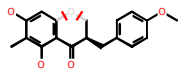
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | 381.16965 | Theoretical | 381.16819 | -1.5 | -3.819 | 470 | 16.72042 | 6.58667 | C23H25O5 |  |
| 27 | 383.22169 | Theoretical | 383.22208 | 0.4 | 1.023 | 190 | 16.70834 | 6.71396 | C24H31O4 |  |
| 28 | 399.21660 | Theoretical | 399.21755 | 1.0 | 2.390 | 324 | 16.73440 | 6.38983 | C24H31O5 |  |
| 29 | 400.15165 | Theoretical | 400.14977 | -1.9 | -4.722 | 140 | 16.71013 | 6.48502 | C22H24O7 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | 414.24008 | Theoretical | 414.24019 | 0.1 | 0.276 | 1505 | 16.72047 | 6.67476 | C25H34O5 |  |
| 31 | 416.19821 | Theoretical | 416.19953 | 1.3 | 3.172 | 150 | 16.69907 | 6.65566 | C27H28O4 |  |

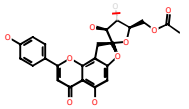
Item name: sample 2_01, Component name: Ophiopogonanone B

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 149.05971 | Theoretical | 149.05945 | -0.3 | -1.736 | 353 | 16.69991 | 4.95762 | C9H9O2 |  |

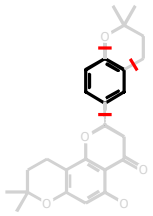
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 193.08592 | Theoretical | 193.08477 | -1.2 | -5.975 | 119 | 16.71985 | 5.23272 | C11H13O3 |  |
| 3 | 264.07810 | Theoretical | 264.07833 | 0.2 | 0.882 | 163 | 16.70098 | 5.20353 | C17H12O3 |  |
| 4 | 269.11722 | Theoretical | 269.11827 | 1.1 | 3.914 | 227 | 16.70070 | 4.95948 | C17H17O3 |  |
| 5 | 301.10705 | Theoretical | 301.10752 | 0.5 | 1.564 | 196 | 16.69238 | 5.15310 | C17H17O5 |  |

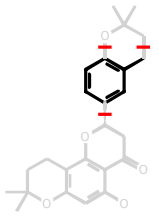
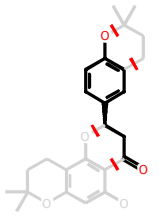
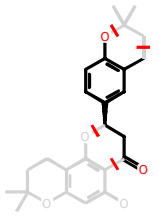
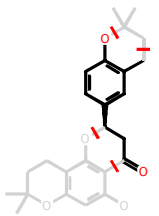
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 301.14344 | Theoretical | 301.14325 | -0.2 | -0.624 | 245 | 16.71026 | 5.08853 | C18H21O4 |  |

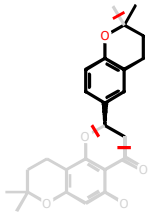
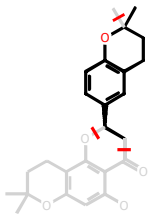
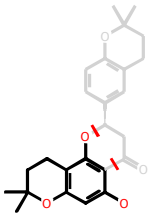
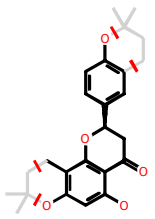
Item name: sample 2_01, Component name: Pinnatifinoside B

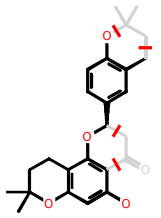
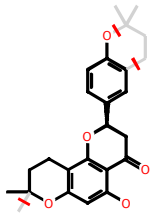
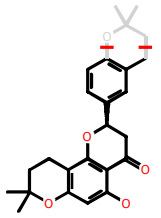
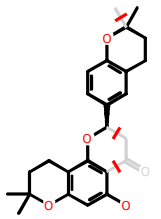
| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 439.10236 | Theoretical | 439.10174 | -0.6 | -1.407 | 822 | 5.33405 | 5.66513 | C23H19O9 |  |

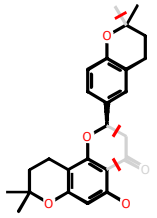
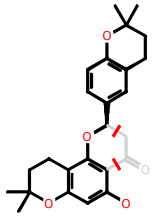
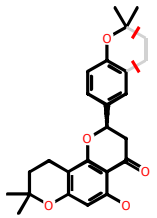
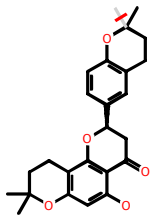
Item name: sample 2_01, Component name: Sophoranodichromane D

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 77.03858 | Theoretical | 77.03826 | -0.3 | -4.141 | 73 | 16.66722 | 5.91206 | C6H5 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 93.06988 | Theoretical | 93.06907 | -0.8 | -8.690 | 182 | 16.66421 | 5.80962 | C7H9 |  |
| 3 | 149.05971 | Theoretical | 149.05916 | -0.5 | -3.675 | 193 | 16.68387 | 6.22656 | C9H9O2 |  |
| 4 | 161.05971 | Theoretical | 161.05903 | -0.7 | -4.172 | 144 | 16.67854 | 6.05828 | C10H9O2 |  |
| 5 | 165.09101 | Theoretical | 165.09299 | 2.0 | 12.037 | 134 | 16.69155 | 6.26091 | C10H13O2 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 173.09609 | Theoretical | 173.09720 | 1.1 | 6.393 | 129 | 16.64396 | 6.14710 | C12H13O |  |
| 7 | 175.11174 | Theoretical | 175.11185 | 0.1 | 0.625 | 270 | 16.67450 | 6.26336 | C12H15O |  |
| 8 | 191.07027 | Theoretical | 191.07133 | 1.1 | 5.527 | 126 | 16.67611 | 6.03543 | C11H11O3 |  |
| 9 | 281.04445 | Theoretical | 281.04517 | 0.7 | 2.564 | 80 | 16.69169 | 6.06873 | C16H9O5 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 309.11214 | Theoretical | 309.11222 | 0.1 | 0.263 | 261 | 16.66222 | 5.85747 | C19H17O4 |  |
| 11 | 324.09923 | Theoretical | 324.09761 | -1.6 | -4.998 | 218 | 16.67668 | 6.20862 | C19H16O5 |  |
| 12 | 337.14344 | Theoretical | 337.14221 | -1.2 | -3.640 | 195 | 16.67123 | 6.11246 | C21H21O4 |  |
| 13 | 354.18256 | Theoretical | 354.18406 | 1.5 | 4.239 | 474 | 16.68355 | 5.89594 | C22H26O4 |  |

| | Expected m/z | Status | Observed m/z | Mass error (mDa) | Mass error (ppm) | Detector counts | Observed RT (min) | Observed drift (ms) | Formula | Structure |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | 355.19039 | Theoretical | 355.19061 | 0.2 | 0.625 | 233 | 16.64532 | 5.83967 | C22H27O4 |  |
| 15 | 369.20604 | Theoretical | 369.20562 | -0.4 | -1.135 | 493 | 16.68451 | 5.81825 | C23H29O4 |  |
| 16 | 383.18530 | Theoretical | 383.18540 | 0.1 | 0.273 | 524 | 16.69132 | 5.96583 | C23H27O5 |  |
| 17 | 395.18530 | Theoretical | 395.18728 | 2.0 | 5.003 | 445 | 16.64598 | 5.96076 | C24H27O5 |  |