SUMMARY REPORT

Analysis Information

Item name:	NEG_SCREENING POLAR_Phenol Tannin_Alia IIUM	Analysis Method Item name:	NEG_SCREENING POLAR_PDA
Version:	4	Analysis Method Version:	2
Modified date:	Sep 22, 2020 10:19:31 Malay Peninsula Standard Time	Sample Set Created date:	Sep 09, 2020 12:33:35 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 Selection A: A1

Comment:

Gradient start: At injection

2D Repeat Enabled: No

Low Pressure Limit: 0 psi

Solvent Name B: Acetonitrile

Solvent Selection B: B1

Seal Wash Period: 5.000 min

Pre-Injector Volume: 0 µL

High Pressure Limit: 18000 psi

Gradient Table

Time (min)	Flow Rate (mL/min)	Composition A (%)	Composition B (%)	Curve
0.00	0.600	99.0	1.0	Initial
0.50	0.600	99.0	1.0	6
16.00	0.600	65.0	35.0	6
18.00	0.600	0.0	100.0	1
20.00	0.600	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

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: Negative

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: 600 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	0.600	99.0	1.0	Initial
0.50	0.600	99.0	1.0	6
16.00	0.600	65.0	35.0	6
18.00	0.600	0.0	100.0	1
20.00	0.600	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: Negative

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: 600 L/h

Capillary voltage: 2.50 kV

Lock correction

Mode: Automatic

Automatic sampling interval: No

Interval: 0.50 min

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

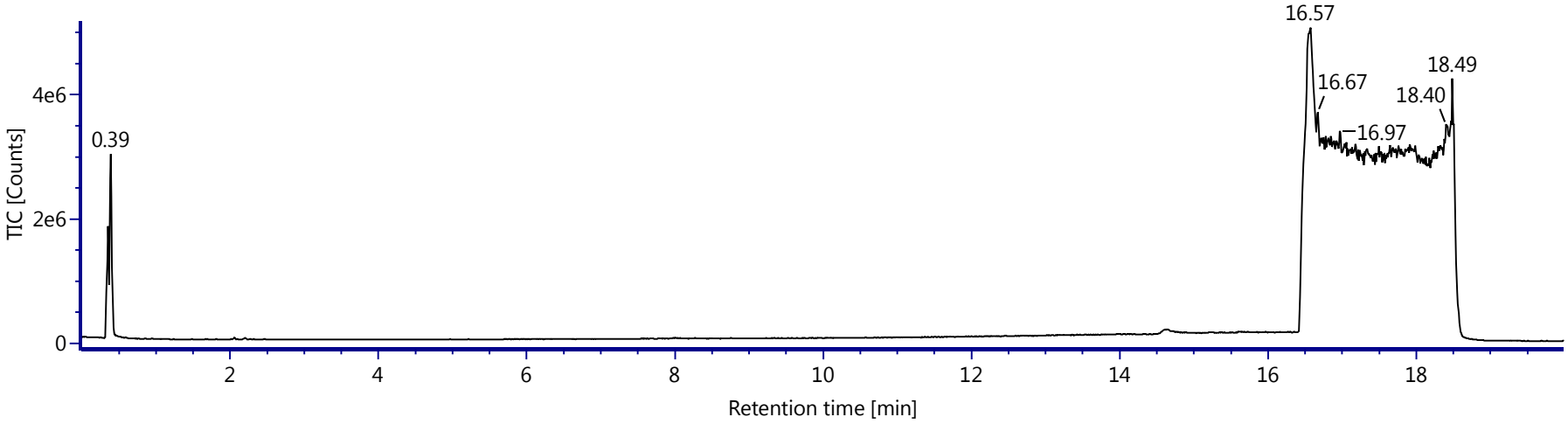
Trigger type: Network

Event input 1: Enabled

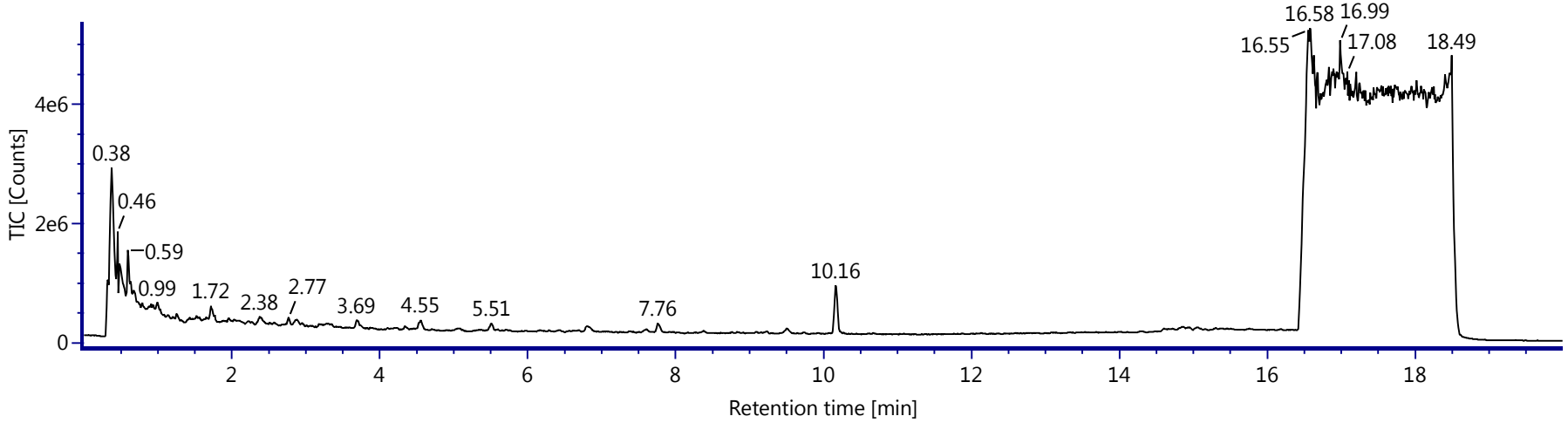
Event input 2: Disabled

TIC Plot

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

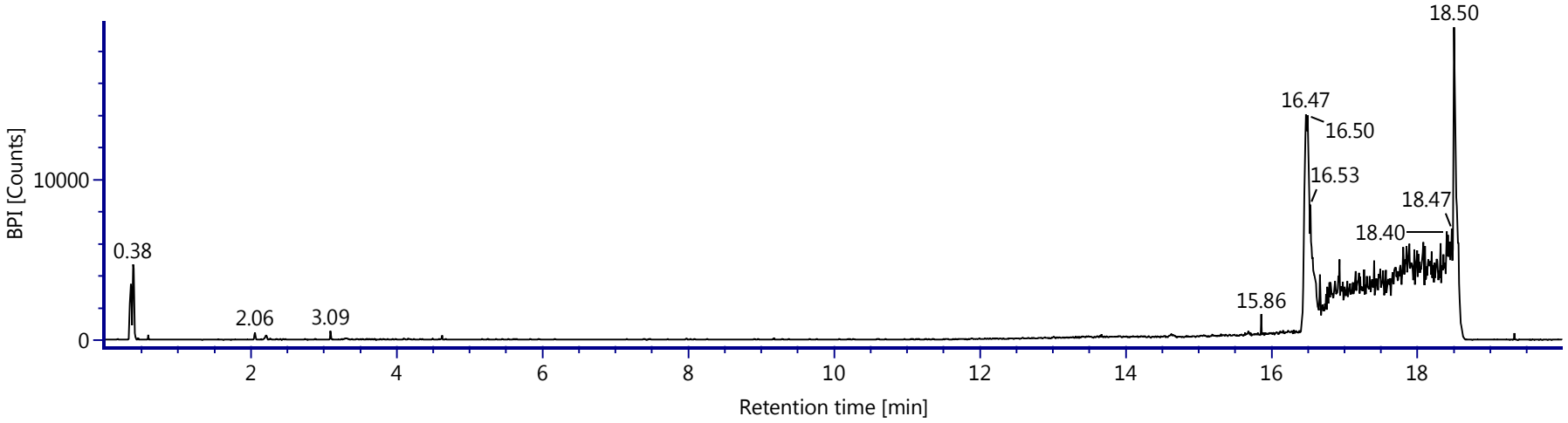


Item name: sample 2_01
Channel name: 2: HD TOF MSe (50-1000) -4eV ESI- (TIC)

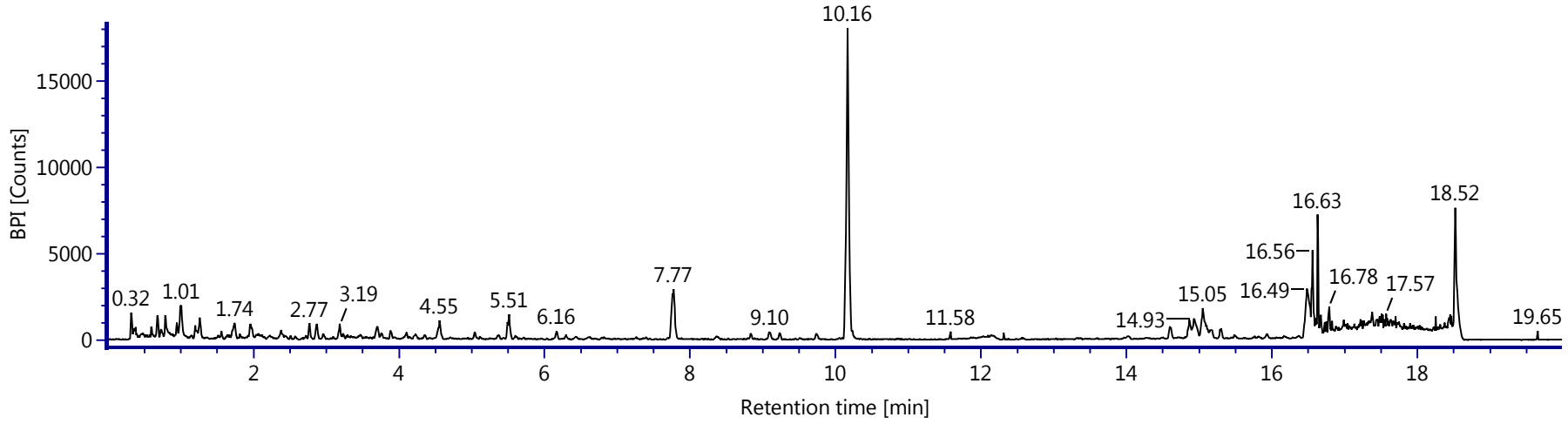


BPI Plot

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

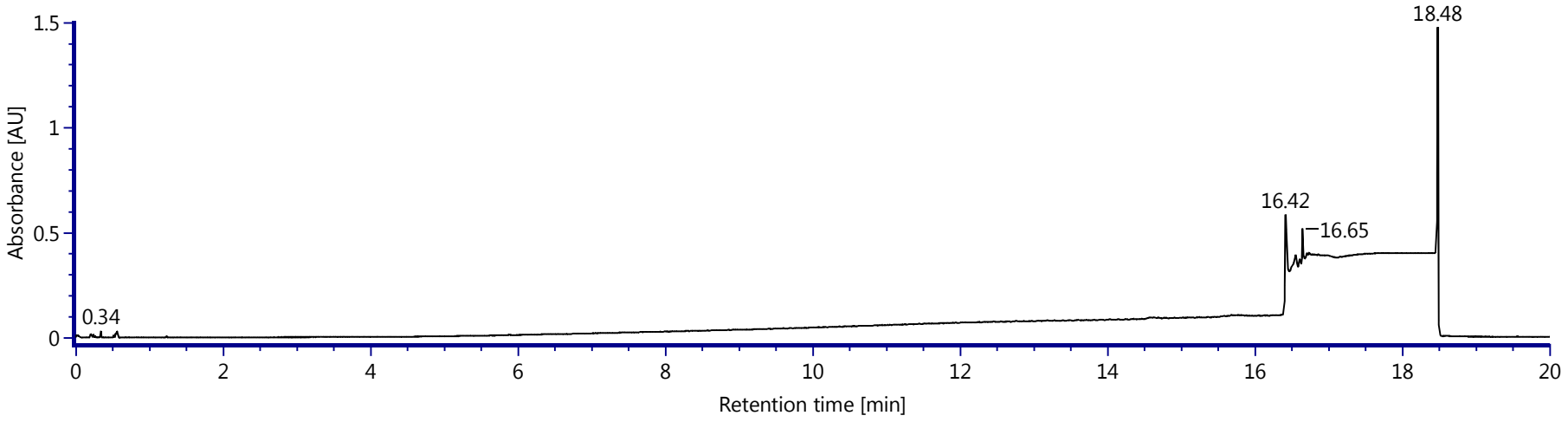


Item name: sample 2_01
Channel name: 2: HD TOF MSe (50-1000) -4eV ESI- (BPI)

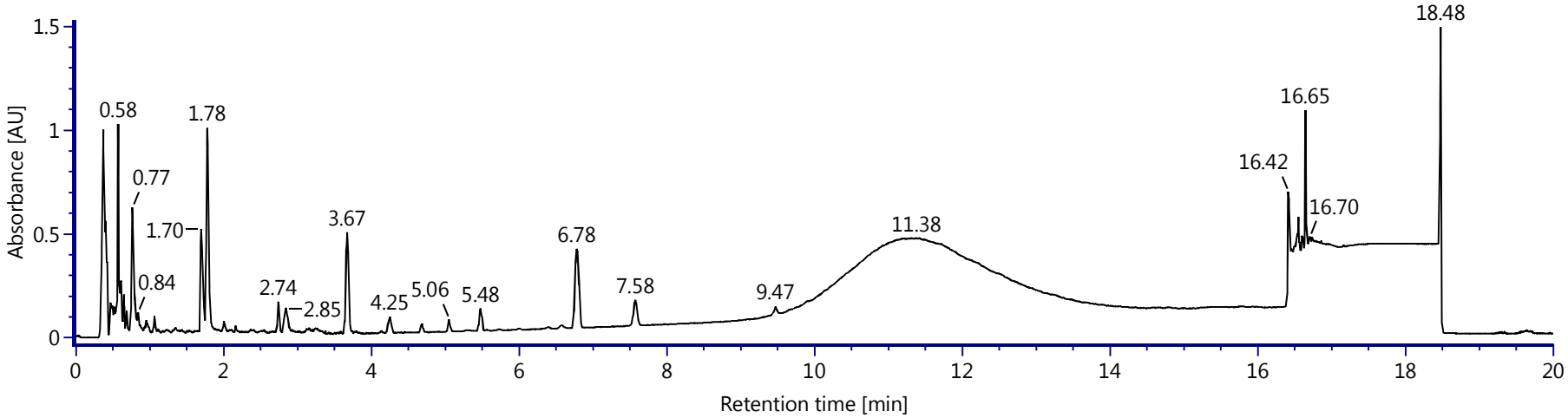


PDA Plot

Item name: blank water_01
Channel name: PDA MaxPlot (190-500)

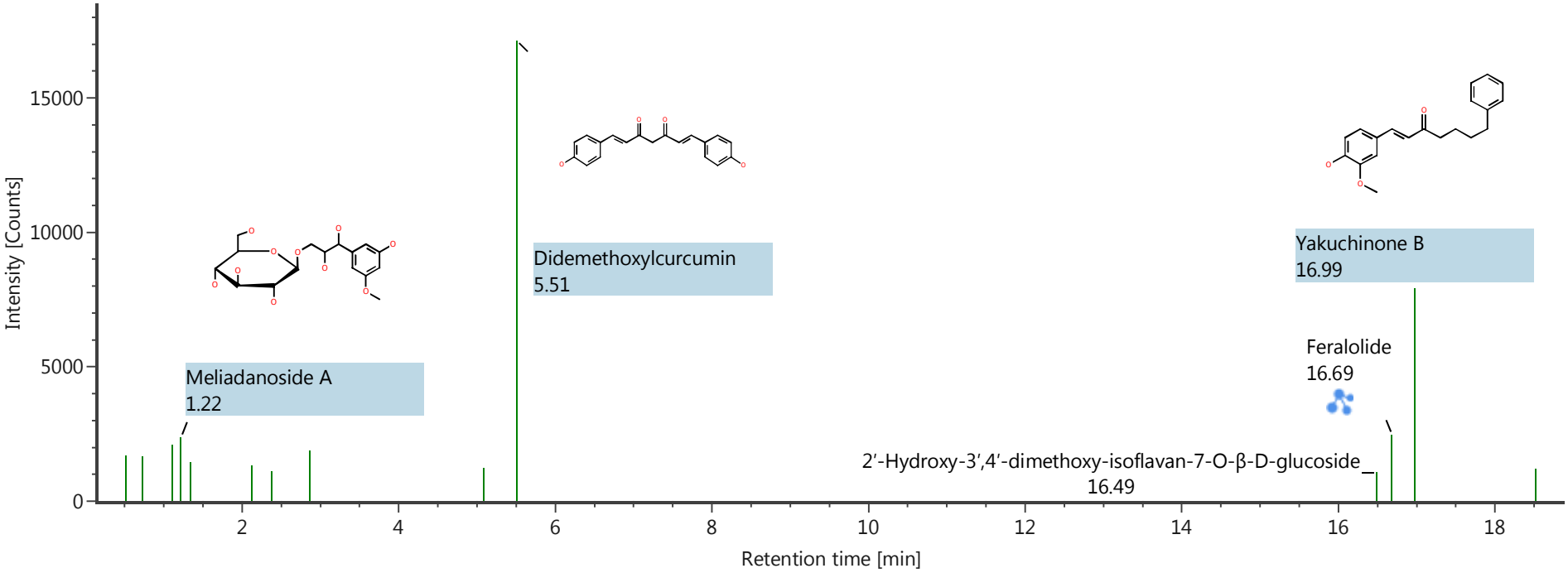


Item name: sample 2_01
Channel name: PDA MaxPlot (190-500)



Identified Compounds

Item name: sample 2_01



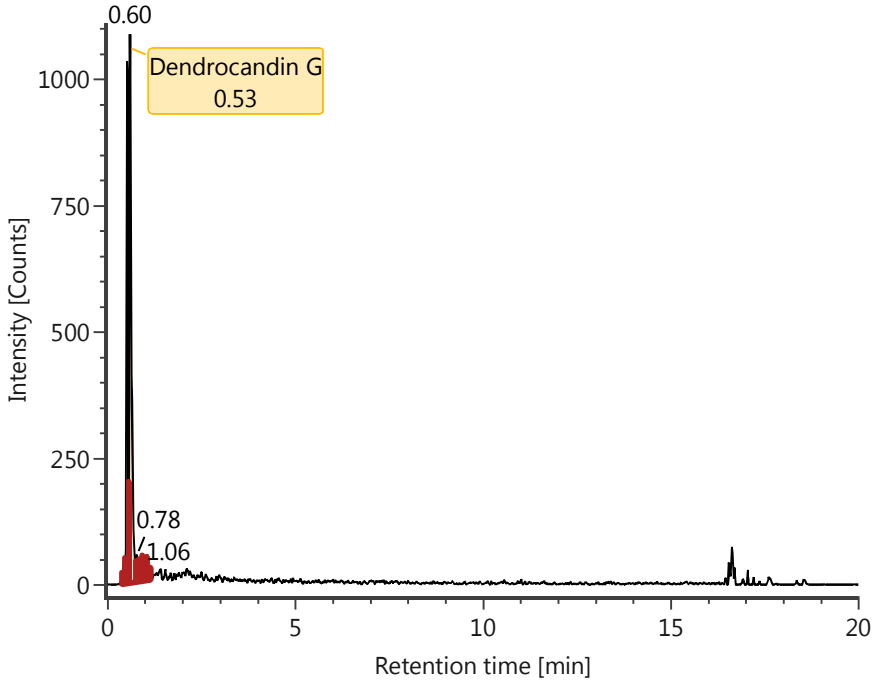
Item name: sample 2_01, Sample position: 1:B,3, Replicate number: 1

.	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	Dendrocandin G	C31H30O8	Identified	530.1984	575.1966	4.3	7.5	0.53	1680	+HCOO	220.36	0
2	Blestritin B	C30H30O6	Identified	486.2087	531.2069	4.5	8.5	0.74	1629	+HCOO	212.67	0
3	Benzopyran derivative Ⅱ	C32H30O7	Identified	526.2009	525.1936	1.7	3.3	1.11	2075	-H	213.32	0
4	Meliadanoside A	C16H24O10	Identified	376.1359	421.1341	-1.0	-2.4	1.22	2374	+HCOO	195.83	0
5	Dendrocandin F	C32H32O8	Identified	544.2133	543.2060	3.6	6.6	1.35	1433	-H	215.61	1
6	Octahydrocurcumin	C21H28O6	Identified	376.1859	421.1841	-2.6	-6.3	2.12	1304	+HCOO	198.21	0
7	3′,4′-Dimethoxy-isoflavan-7,2′-di-O-β-D-glucoside	C29H38O15	Identified	626.2216	671.2198	0.5	0.8	2.38	1090	+HCOO	254.40	0

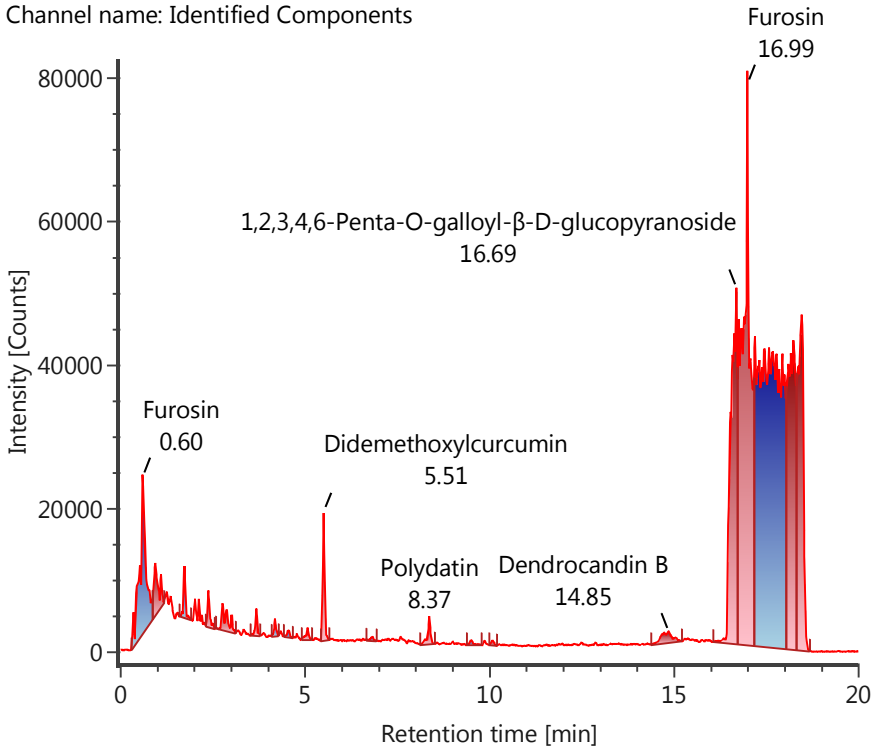
.	Component name	Formula	Identification status	Observed neutral mass (Da)	Observed m/z	Mass error (mDa)	Mass error (ppm)	Observed RT (min)	Response	Adducts	Observed CCS (Å^2)	Total Fragments Found
8	4-Hydroxyacetophenone	C8H8O2	Identified	136.0521	181.0503	-0.3	-1.8	2.87	1848	+HCOO, -H	144.29	1
9	Methyl-β-orsellinate	C9H10O4	Identified	182.0576	181.0503	-0.3	-1.8	2.87	1848	-H	144.29	3
10	Didemethoxylcurcumin	C19H16O4	Identified	308.1024	353.1006	-2.5	-7.0	5.08	1230	+HCOO	171.99	0
11	Moracin E	C19H16O4	Identified	308.1024	353.1006	-2.5	-7.0	5.08	1230	+HCOO	171.99	0
12	Moracin E	C19H16O4	Identified	308.1024	353.1006	-2.5	-6.9	5.51	4981	+HCOO	239.37	1
13	Didemethoxylcurcumin	C19H16O4	Identified	308.1024	353.1006	-2.5	-6.9	5.51	17118	+HCOO	196.06	3
14	Apocynin	C9H10O3	Identified	166.0627	165.0554	-0.3	-1.9	5.51	1099	-H	201.32	2
15	2′-Hydroxy-3′,4′-dimethoxy-isoflavan-7-O-β-D-glucoside	C23H28O10	Identified	464.1635	509.1617	-4.7	-9.3	16.49	1066	+HCOO	224.36	0
16	Feralolide	C18H16O7	Identified	344.0886	343.0813	-1.0	-2.9	16.69	2460	-H	179.09	1
17	Yakuchinone B	C20H22O3	Identified	310.1596	355.1578	2.7	7.7	16.99	7902	+HCOO	196.36	0
18	(3R,4R)-3,4-trans-7,2′-Dihydroxy-4′-methoxy-4-[(3R)-2′,7-dihydroxy-4′-methoxy-isoflavan-5′-yl]-isoflavan	C32H30O8	Identified	542.1936	587.1918	-0.5	-0.9	18.52	1177	+HCOO, -H	242.15	1

Details of Identified Components

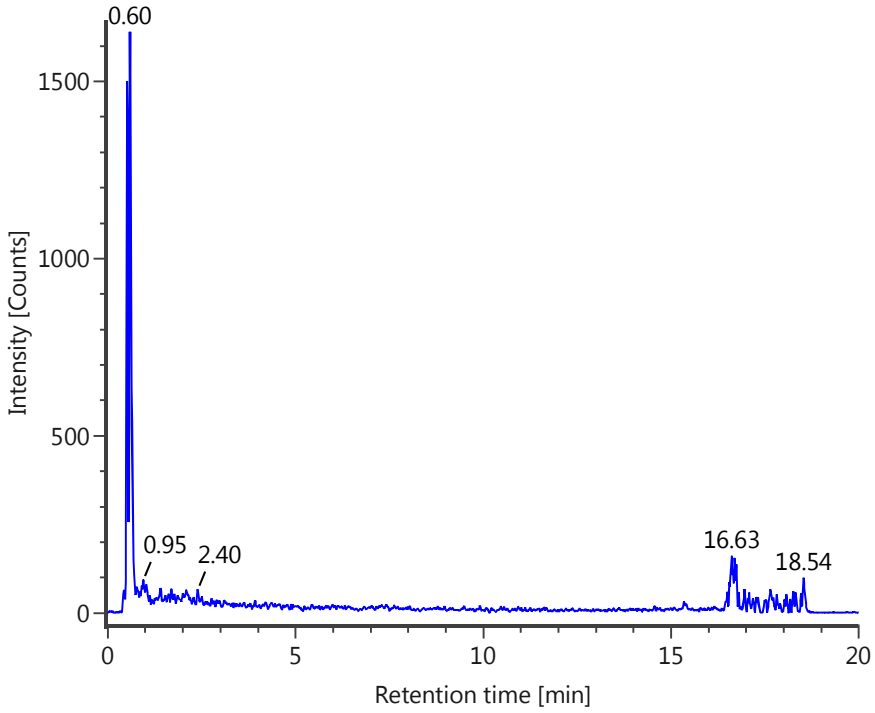
Item name: sample 2_01
Channel name: Dendrocandin G [+HCOO] : (16.3 PPM) 575.1966 : DT=6.60 to 7.22 ms



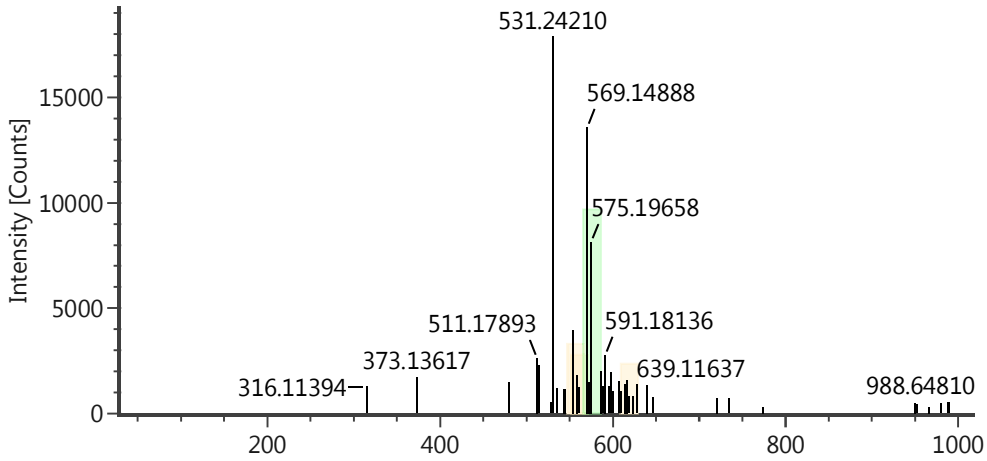
Item name: sample 2_01
Channel name: Identified Components



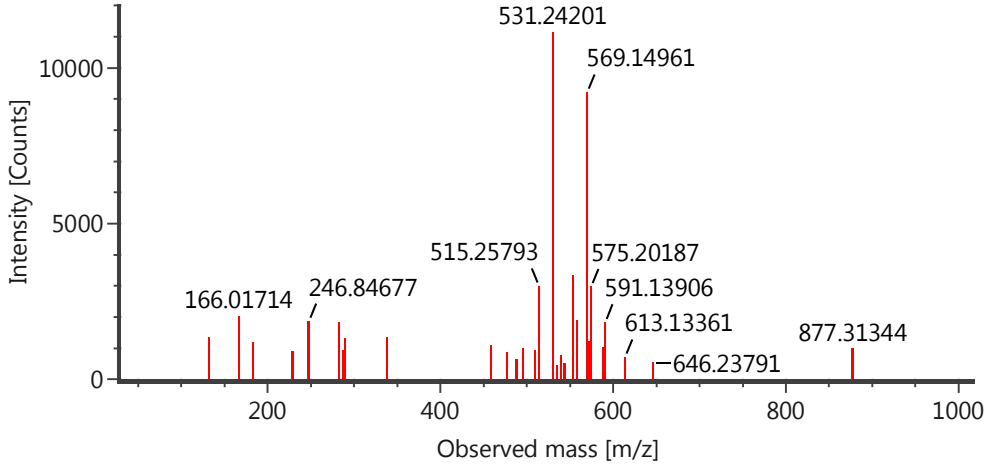
Item name: sample 2_01
Channel name: Dendrocandin G [+HCOO] : (16.3 PPM) 575.1966



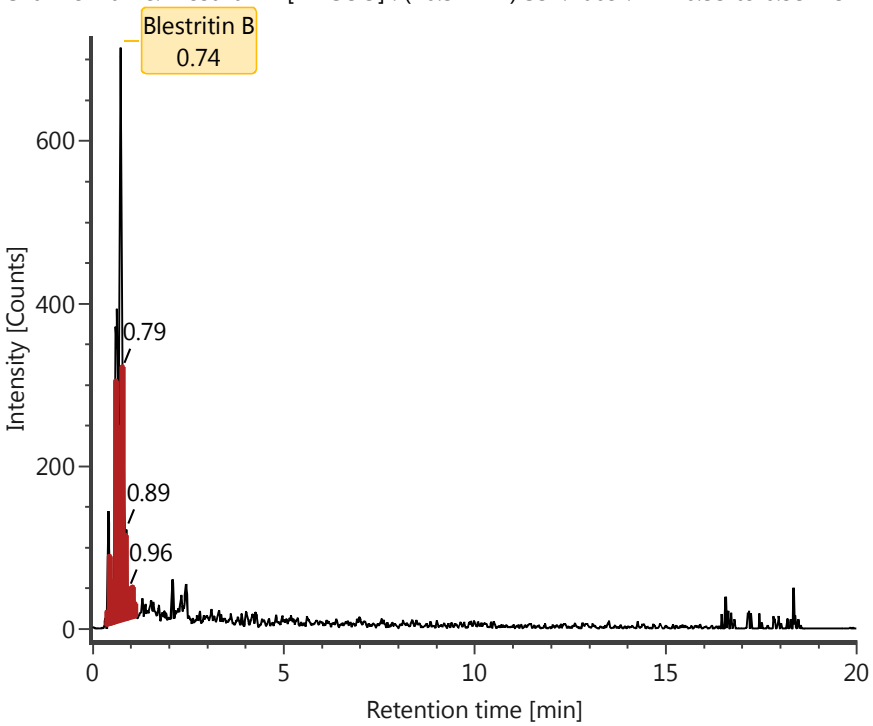
Item name: sample 2_01
Component name: Dendrocandin G
Channel name: Low energy : Time 0.5279 +/- 0.0245 minutes : Drift Times: 6.92 +/- 0.31 ms



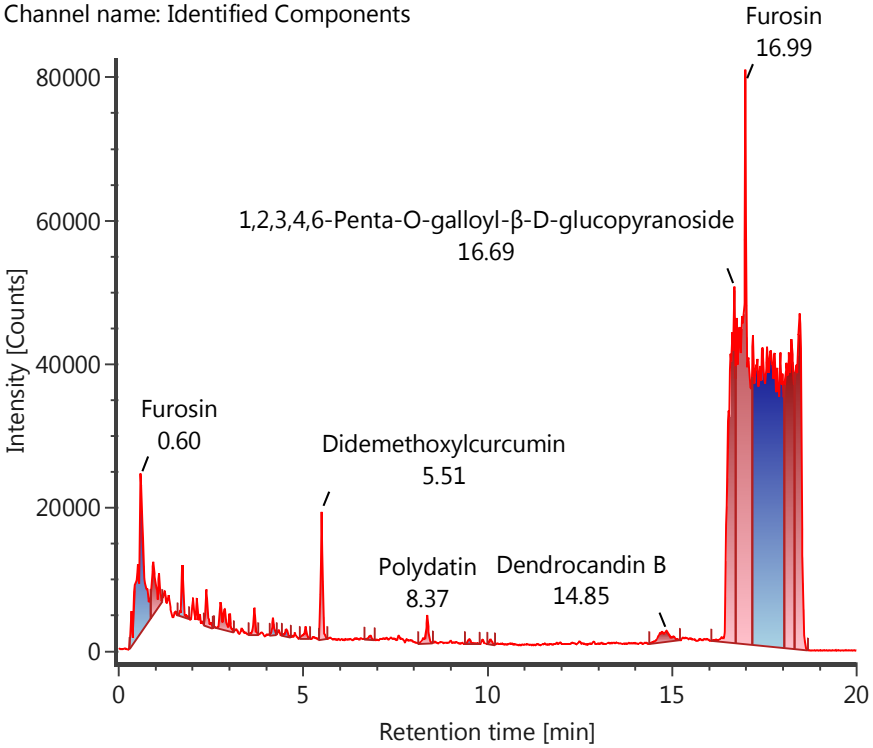
Item name: sample 2_01
Component name: Dendrocandin G
Channel name: High energy : Time 0.5279 +/- 0.0245 minutes : Drift Times: 6.84 +/- 0.31 ms



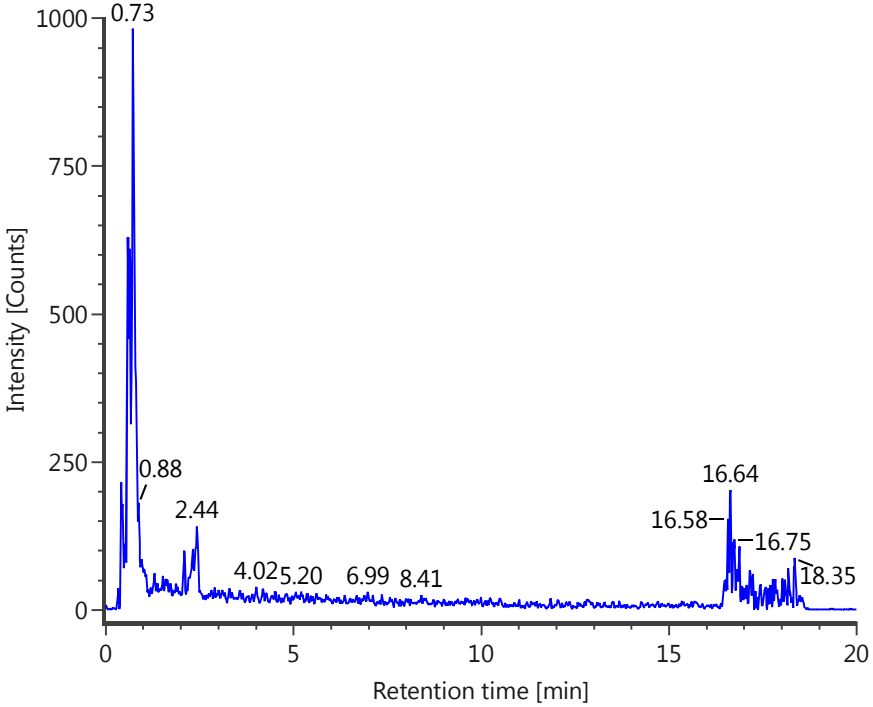
Item name: sample 2_01
Channel name: Blestritin B [+HCOO] : (16.3 PPM) 531.2069 : DT=6.33 to 6.93 ms



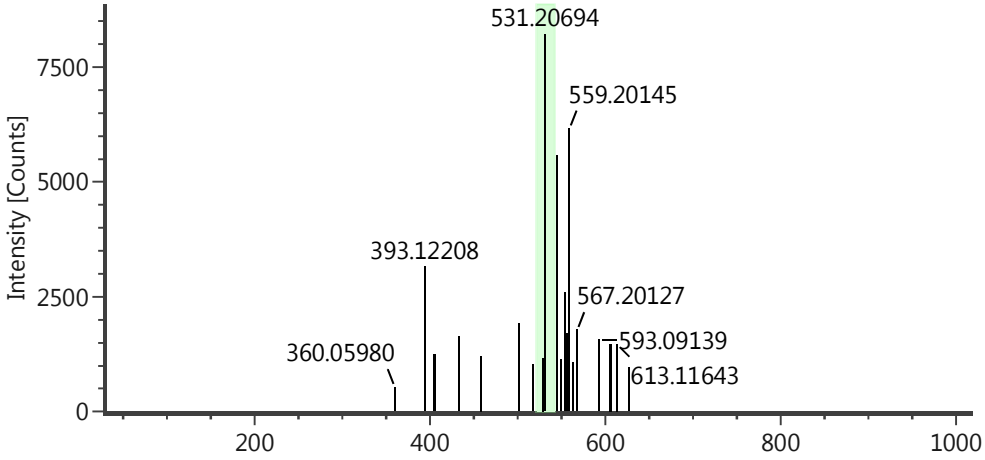
Item name: sample 2_01
Channel name: Identified Components



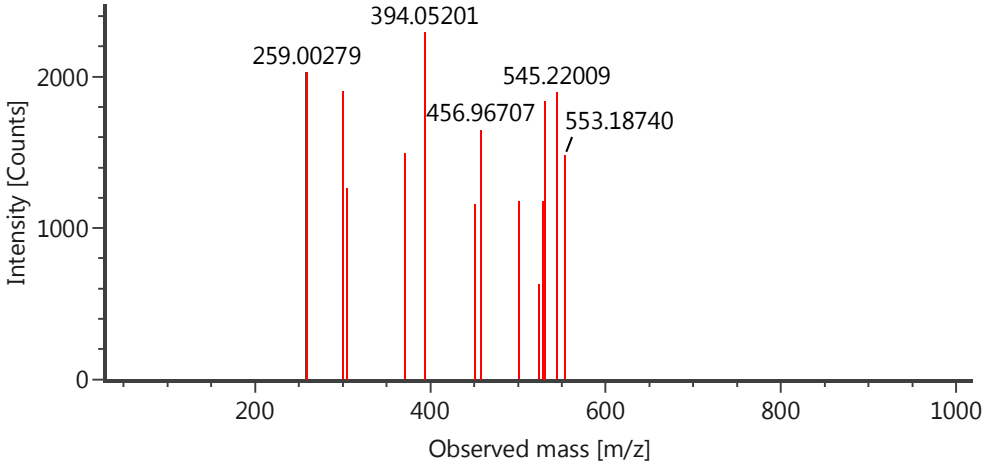
Item name: sample 2_01
Channel name: Blestritin B [+HCOO] : (16.3 PPM) 531.2069



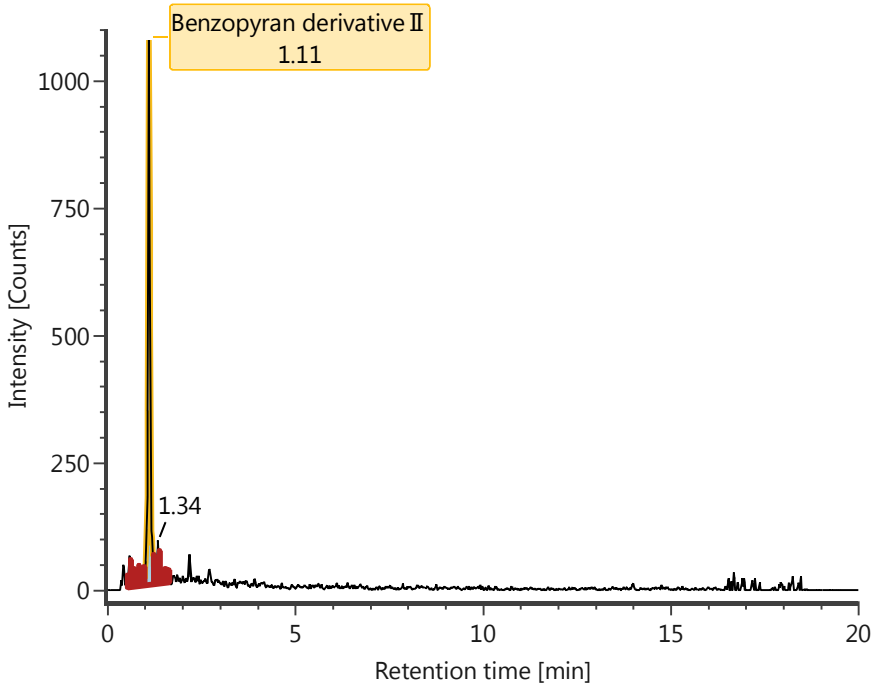
Item name: sample 2_01
Component name: Blestritin B
Channel name: Low energy : Time 0.7425 +/- 0.0245 minutes :
Drift Times: 6.63 +/- 0.30 ms



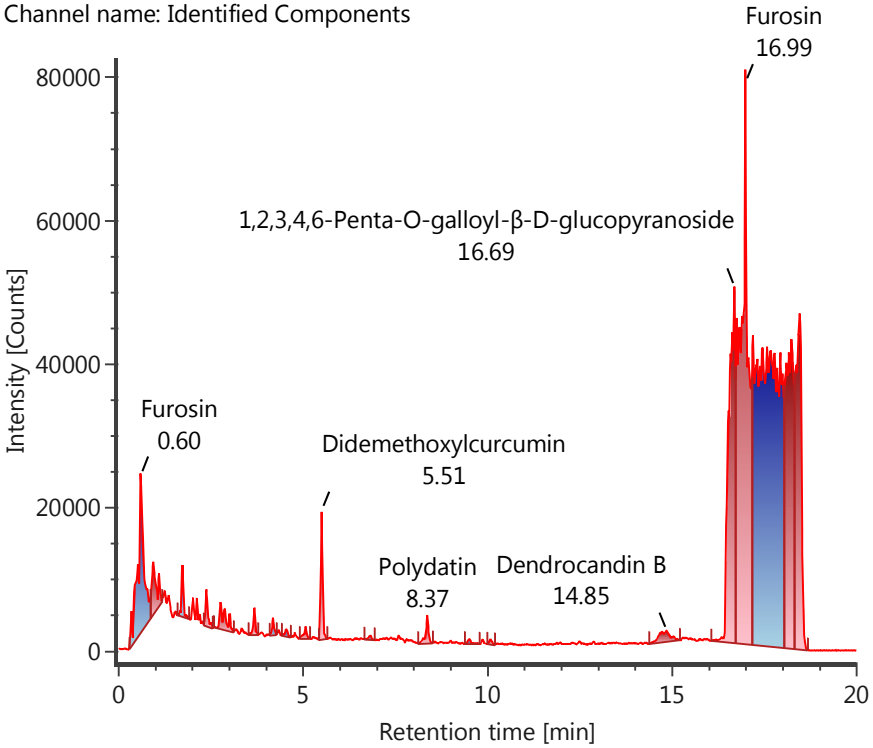
Item name: sample 2_01
Component name: Blestritin B
Channel name: High energy : Time 0.7425 +/- 0.0245 minutes :
Drift Times: 6.55 +/- 0.30 ms



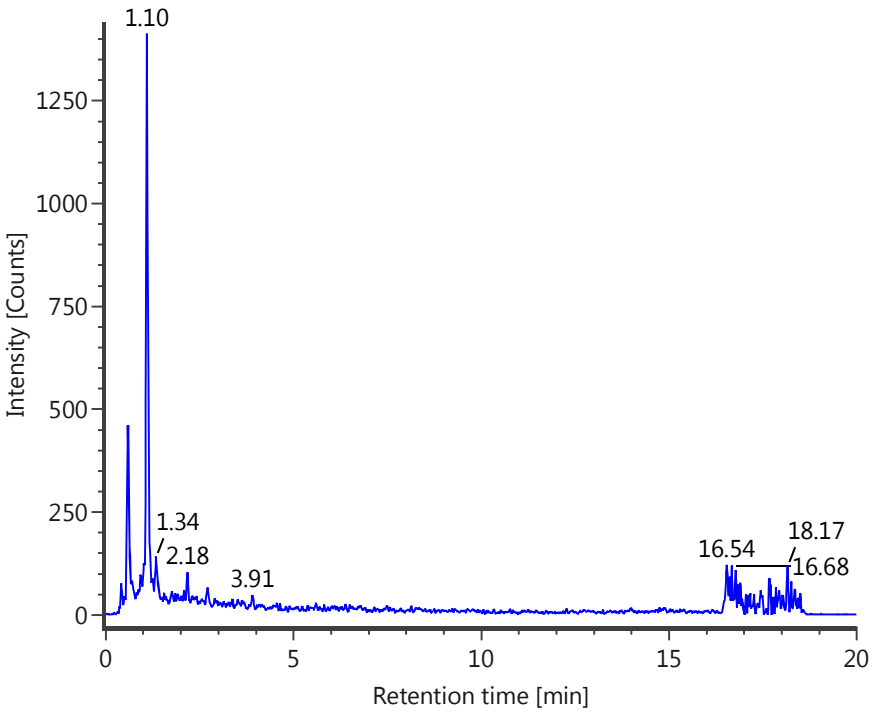
Item name: sample 2_01
Channel name: Benzopyran derivative Ⅱ [-H] : (16.3 PPM) 525.1936 : DT=6.36 to 6.97 ms



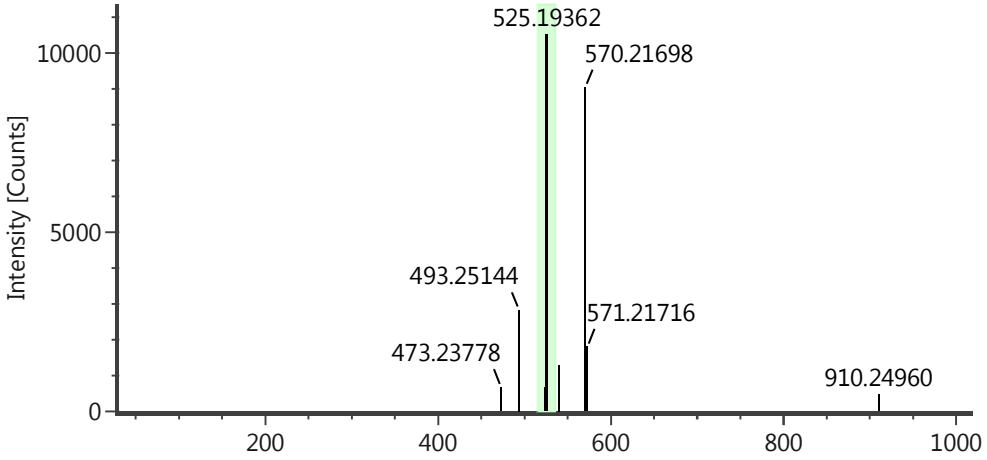
Item name: sample 2_01
Channel name: Identified Components



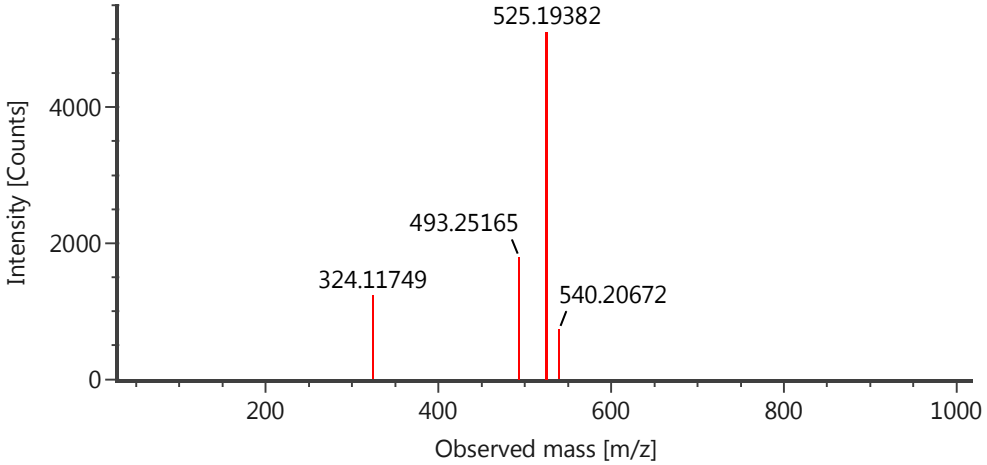
Item name: sample 2_01
Channel name: Benzopyran derivative Ⅱ [-H] : (16.3 PPM) 525.1936



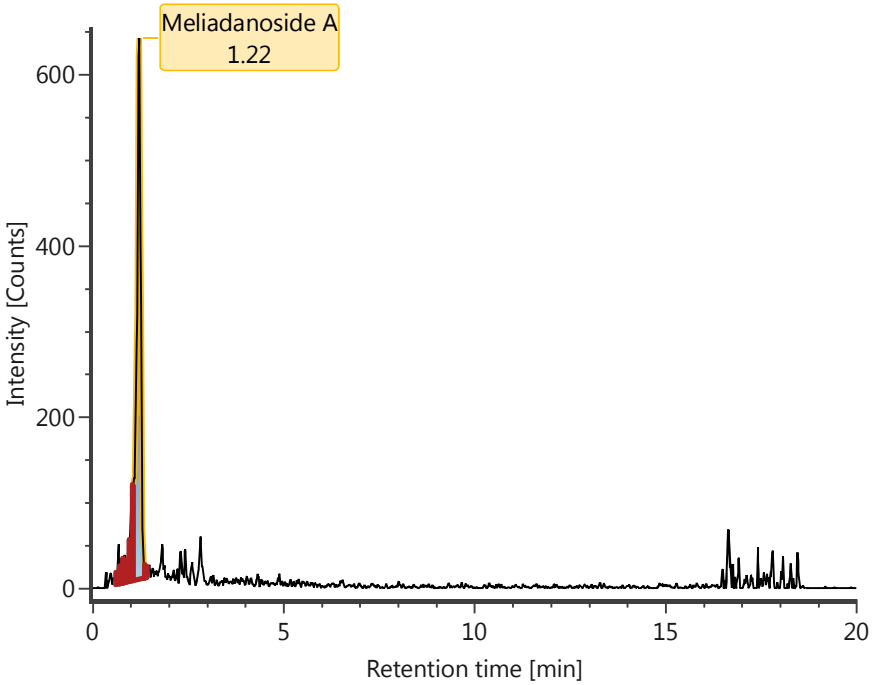
Item name: sample 2_01
Component name: Benzopyran derivative Ⅱ
Channel name: Low energy : Time 1.1076 +/- 0.0245 minutes : Drift Times: 6.65 +/- 0.30 ms



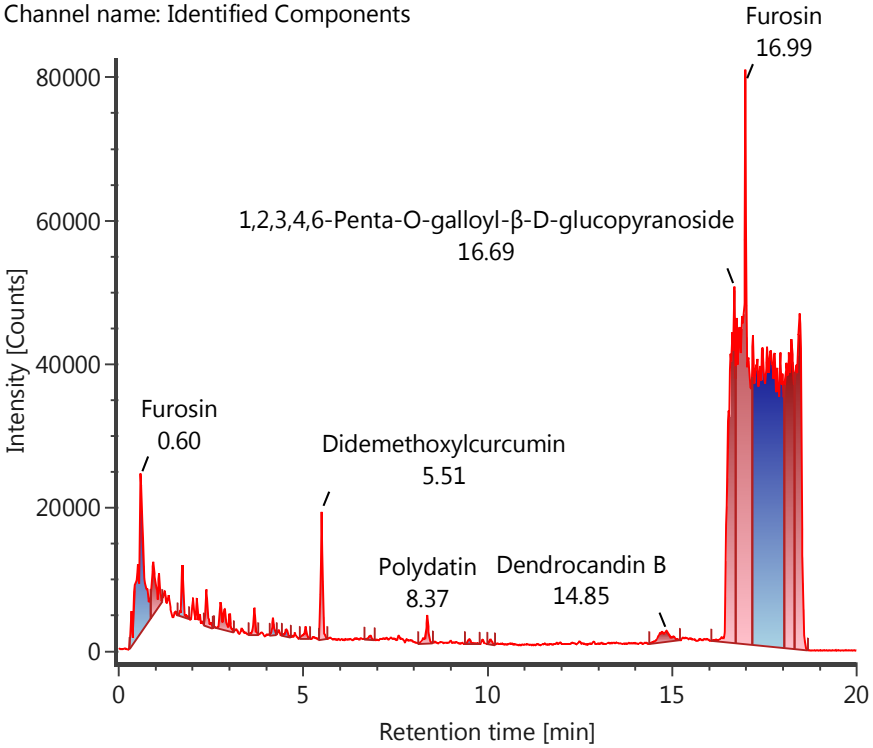
Item name: sample 2_01
Component name: Benzopyran derivative Ⅱ
Channel name: High energy : Time 1.1076 +/- 0.0245 minutes : Drift Times: 6.57 +/- 0.30 ms



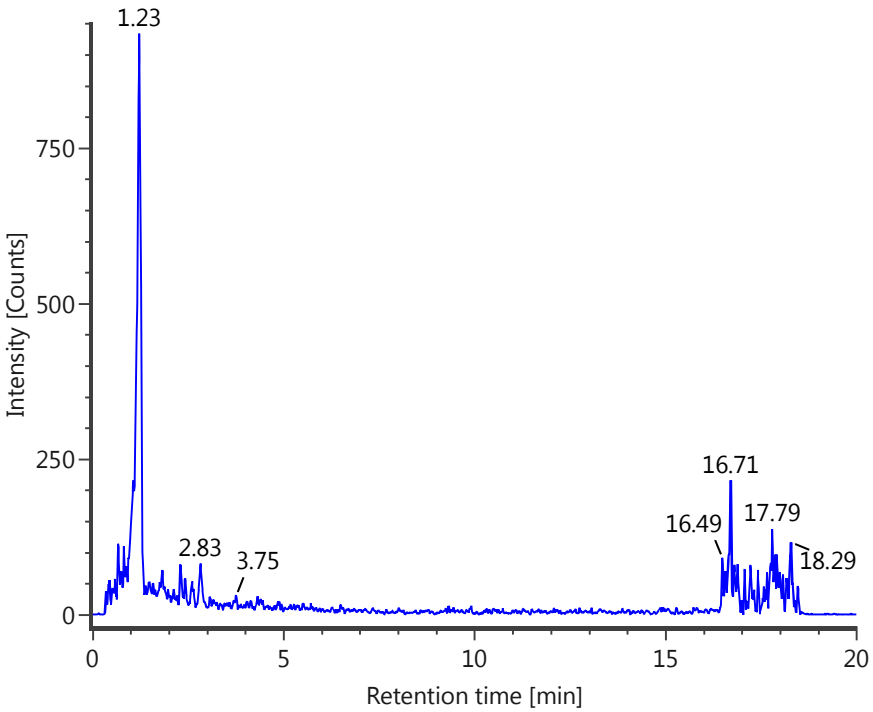
Item name: sample 2_01
Channel name: Meliadanoside A [+HCOO] : (16.3 PPM) 421.1341 : DT=5.69 to 6.27 ms



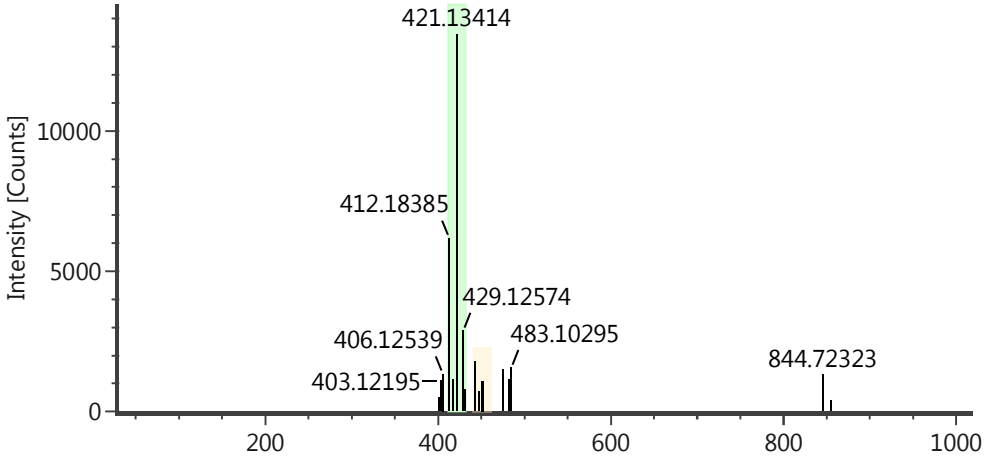
Item name: sample 2_01
Channel name: Identified Components



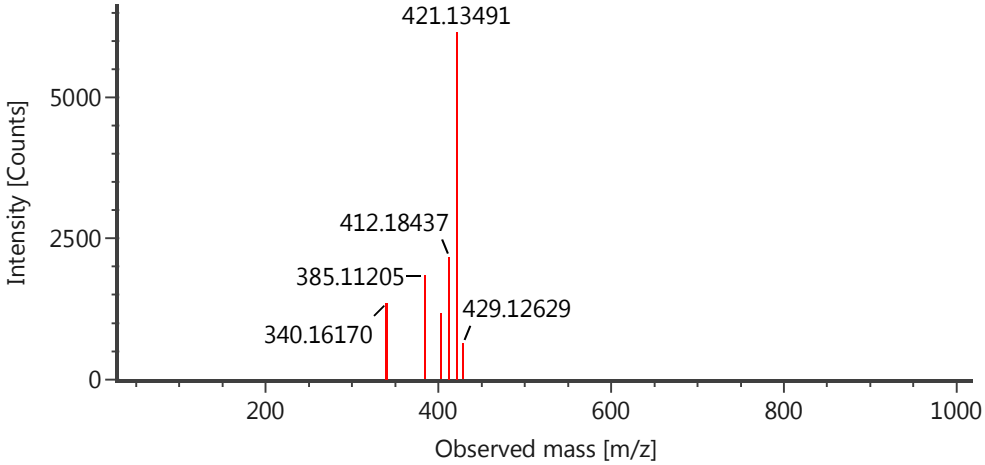
Item name: sample 2_01
Channel name: Meliadanoside A [+HCOO] : (16.3 PPM) 421.1341



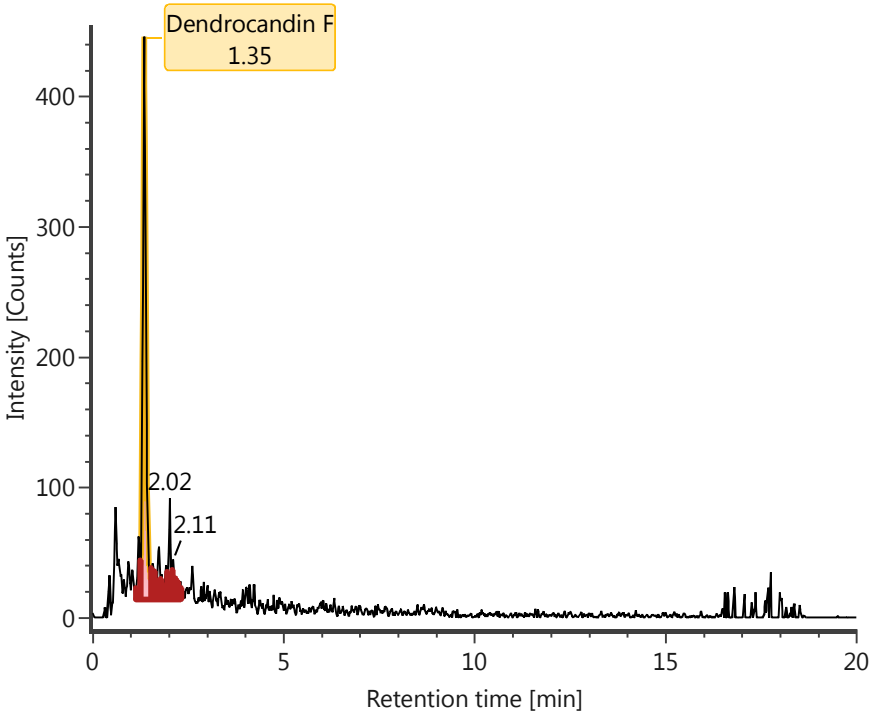
Item name: sample 2_01
Component name: Meliadanoside A
Channel name: Low energy : Time 1.2230 +/- 0.0245
minutes : Drift Times: 5.98 +/- 0.29 ms



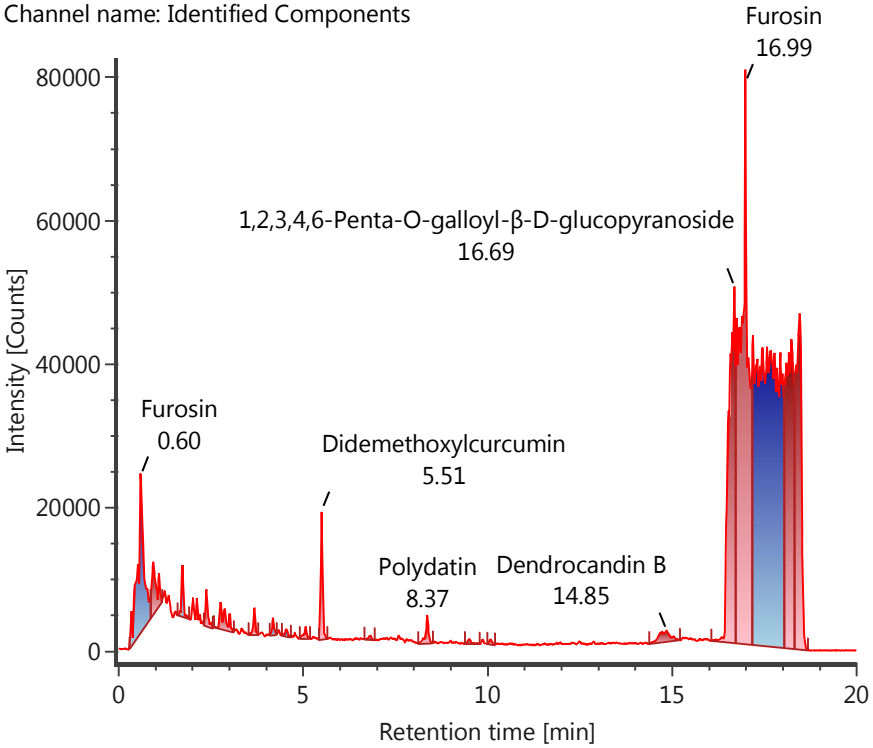
Item name: sample 2_01
Component name: Meliadanoside A
Channel name: High energy : Time 1.2230 +/- 0.0245
minutes : Drift Times: 5.90 +/- 0.29 ms



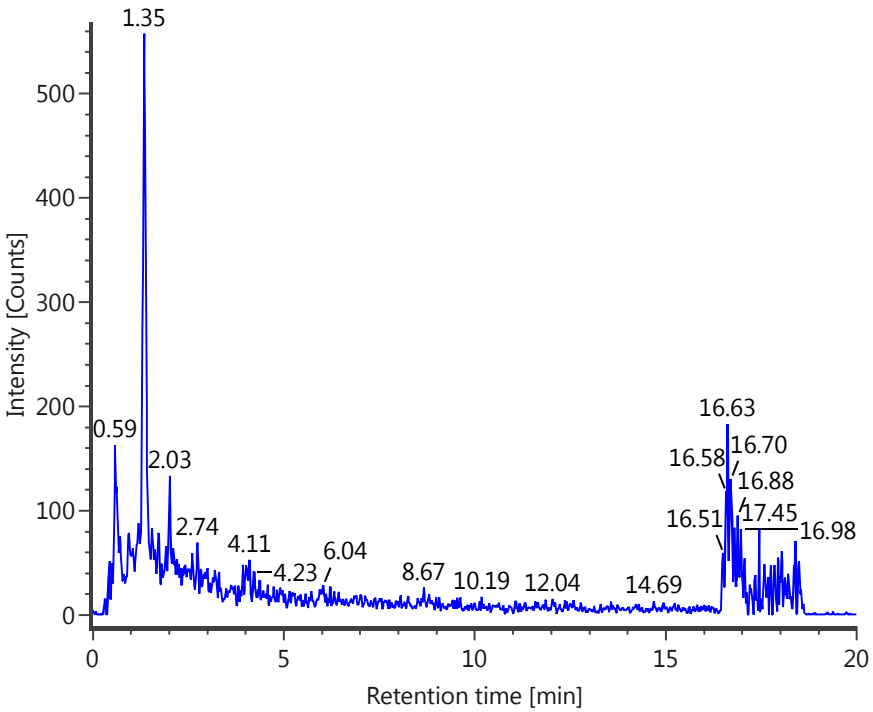
Item name: sample 2_01
Channel name: Dendrocandin F [-H] : (16.3 PPM) 543.2060 : DT=6.43 to 7.04 ms



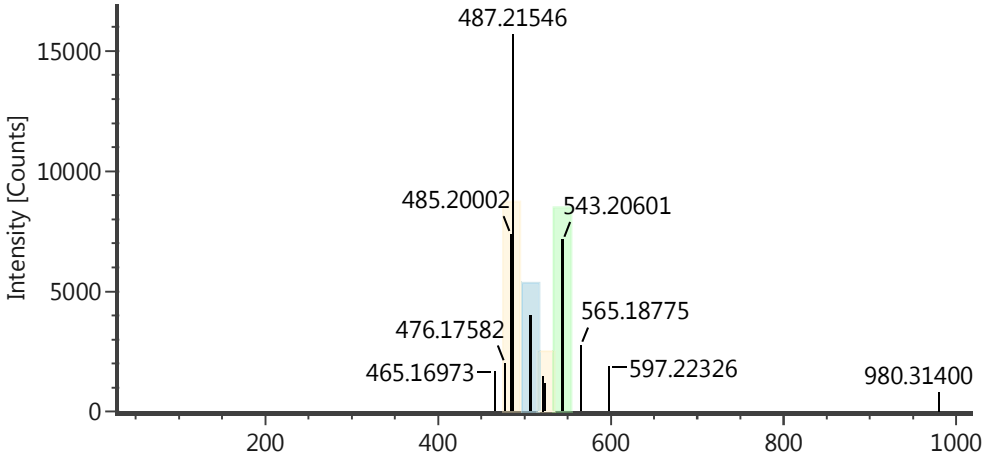
Item name: sample 2_01
Channel name: Identified Components



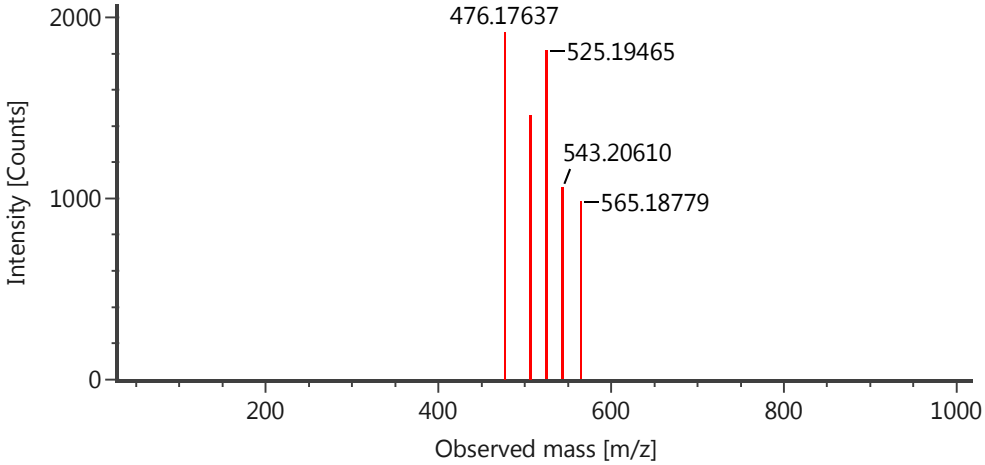
Item name: sample 2_01
Channel name: Dendrocandin F [-H] : (16.3 PPM) 543.2060



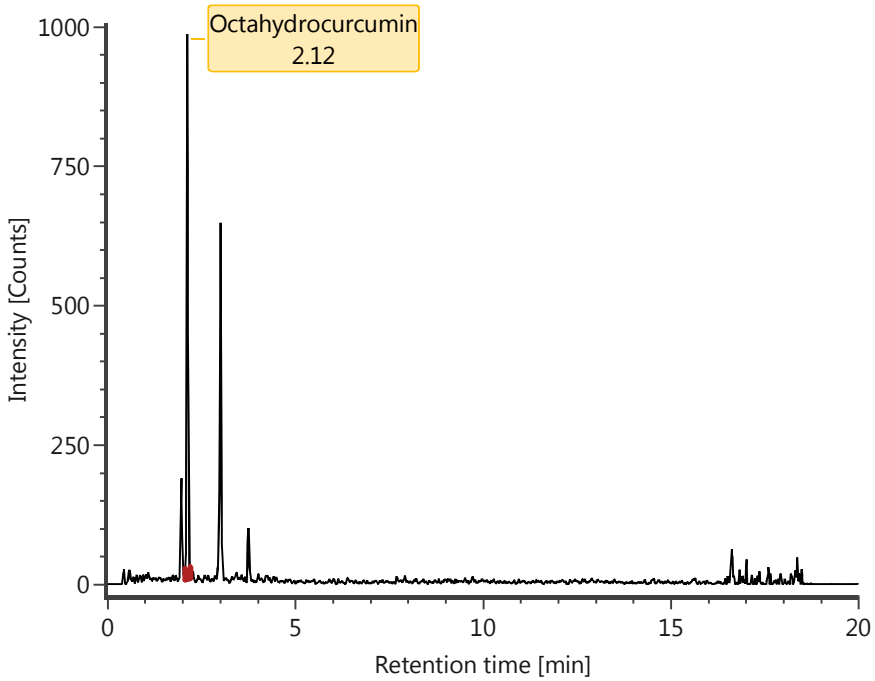
Item name: sample 2_01
Component name: Dendrocandin F
Channel name: Low energy : Time 1.3530 +/- 0.0245 minutes : Drift Times: 6.74 +/- 0.31 ms



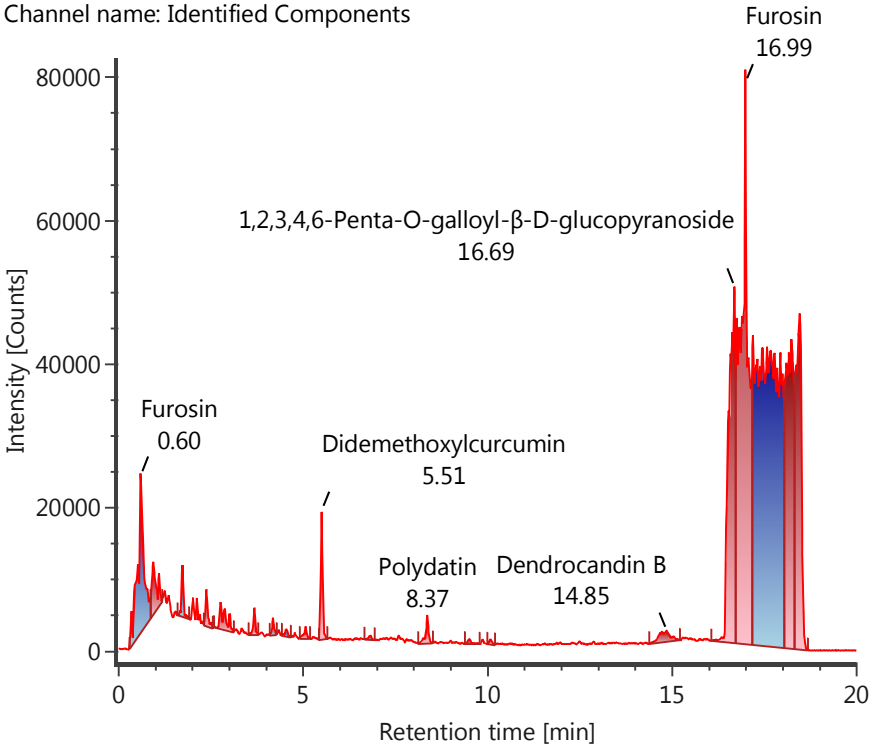
Item name: sample 2_01
Component name: Dendrocandin F
Channel name: High energy : Time 1.3530 +/- 0.0245 minutes : Drift Times: 6.66 +/- 0.31 ms



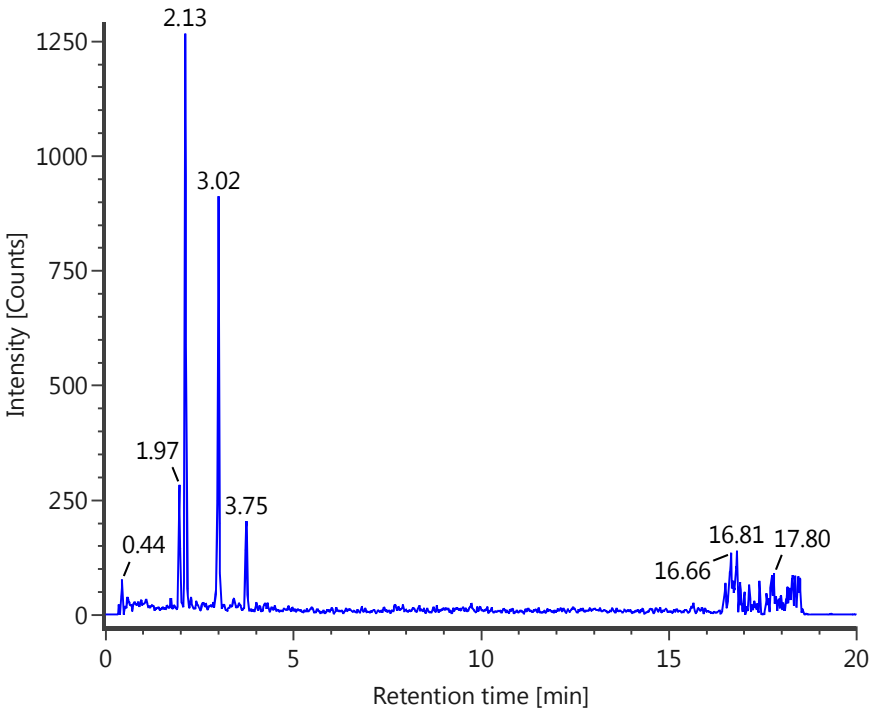
Item name: sample 2_01
Channel name: Octahydrocurcumin [+HCOO] : (16.3 PPM) 421.1841 : DT=5.77 to 6.36 ms



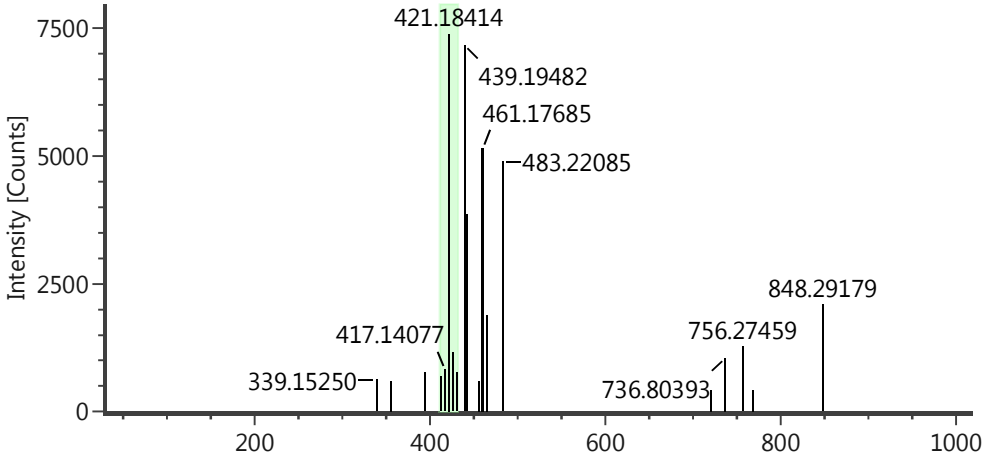
Item name: sample 2_01
Channel name: Identified Components



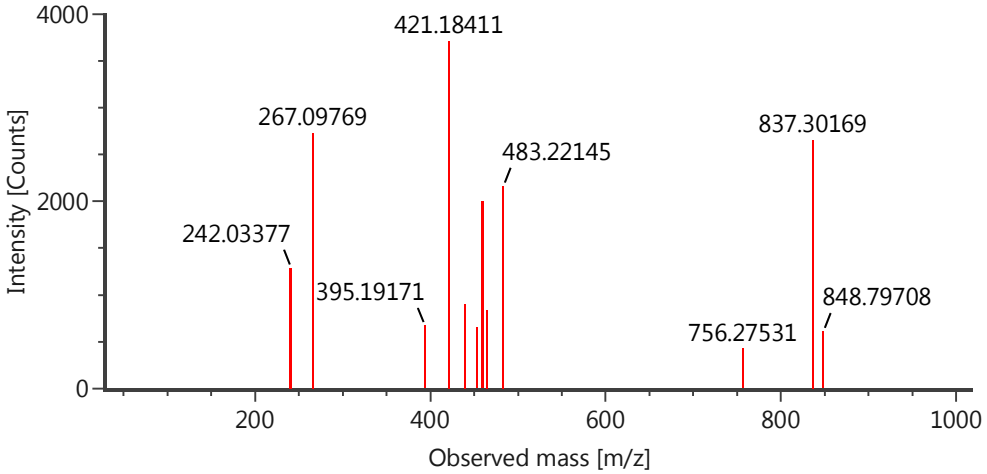
Item name: sample 2_01
Channel name: Octahydrocurcumin [+HCOO] : (16.3 PPM) 421.1841



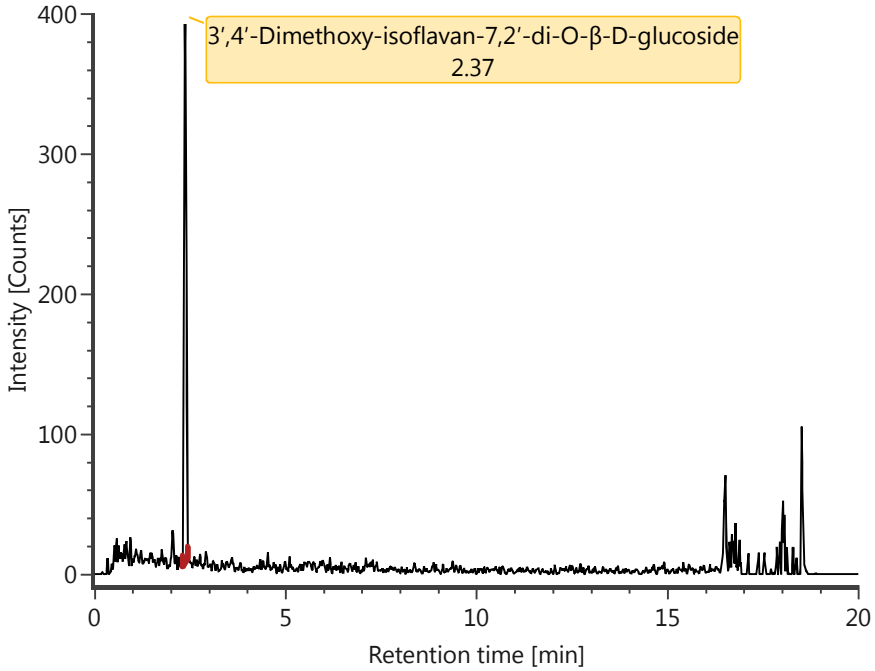
Item name: sample 2_01
Component name: Octahydrocurcumin
Channel name: Low energy : Time 2.1242 +/- 0.0245 minutes : Drift Times: 6.07 +/- 0.29 ms



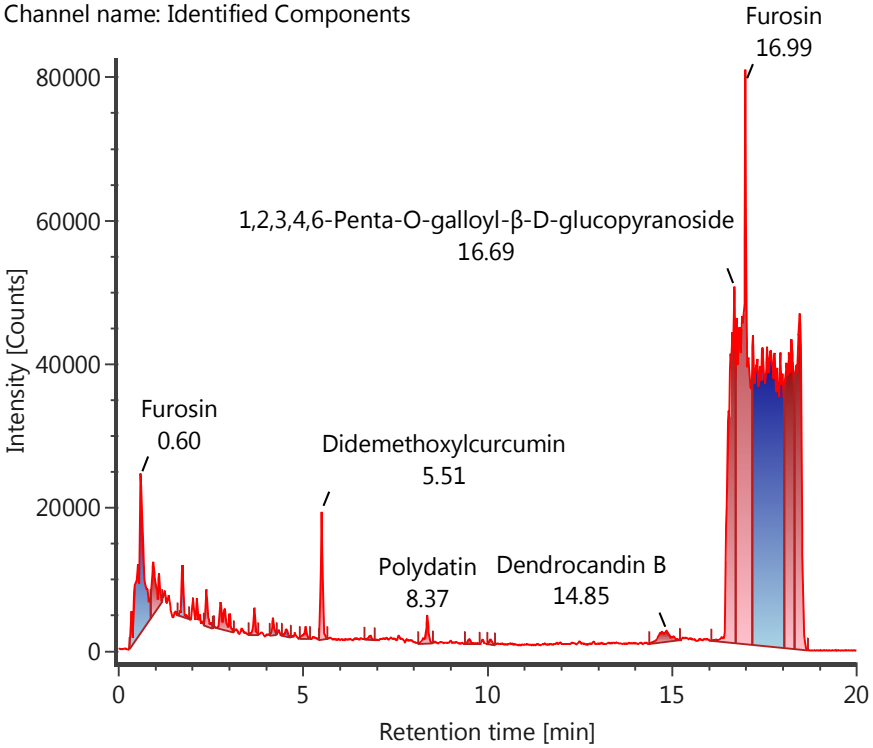
Item name: sample 2_01
Component name: Octahydrocurcumin
Channel name: High energy : Time 2.1242 +/- 0.0245 minutes : Drift Times: 5.99 +/- 0.29 ms



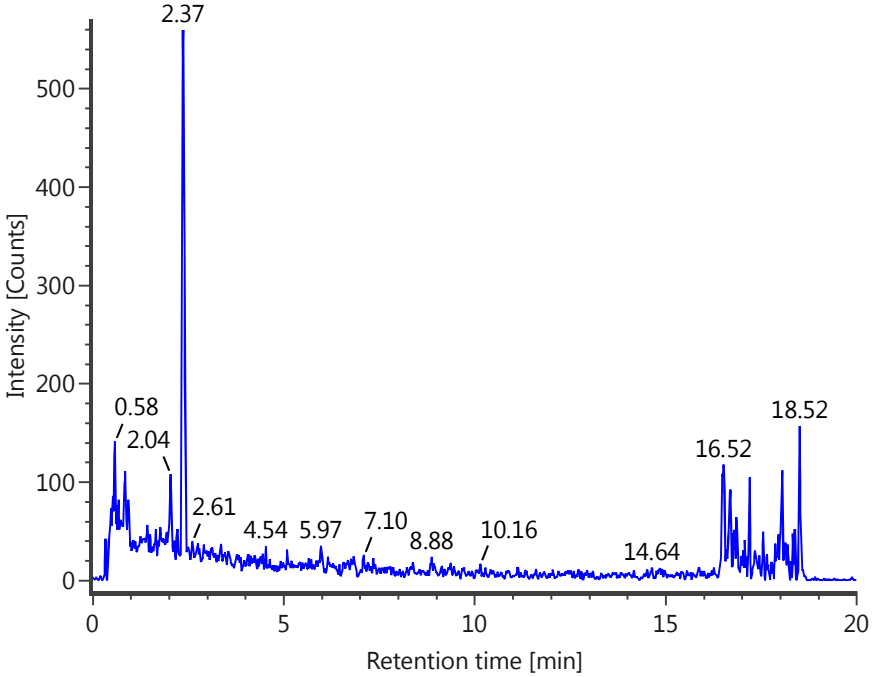
Item name: sample 2_01
Channel name: 3′,4′-Dimethoxy-isoflavan-7,2′-di-O-β-D-glucoside [+HCOO] : (16.3 PPM) 671.2198 : DT=7.78 to 8.45 ms



Item name: sample 2_01
Channel name: Identified Components

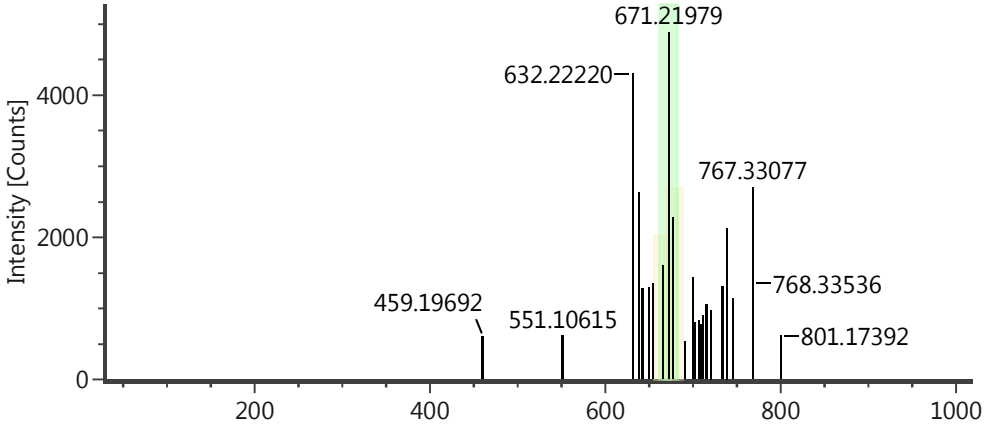


Item name: sample 2_01
Channel name: 3′,4′-Dimethoxy-isoflavan-7,2′-di-O-β-D-glucoside [+HCOO] : (16.3 PPM) 671.2198



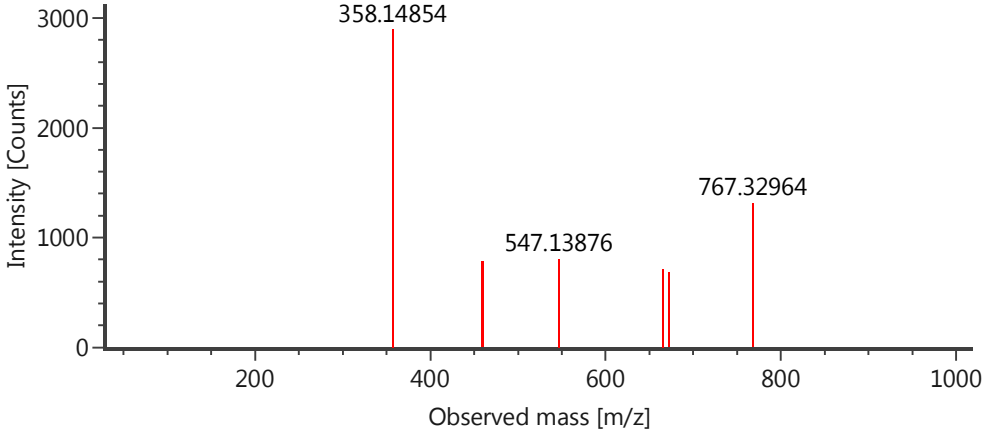
Item name: sample 2_01
Component name: 3′,4′-Dimethoxy-isoflavan-7,2′-di-O-β-D-glucoside

Channel name: Low energy : Time 2.3810 +/- 0.0245 minutes : Drift Times: 8.11 +/- 0.33 ms

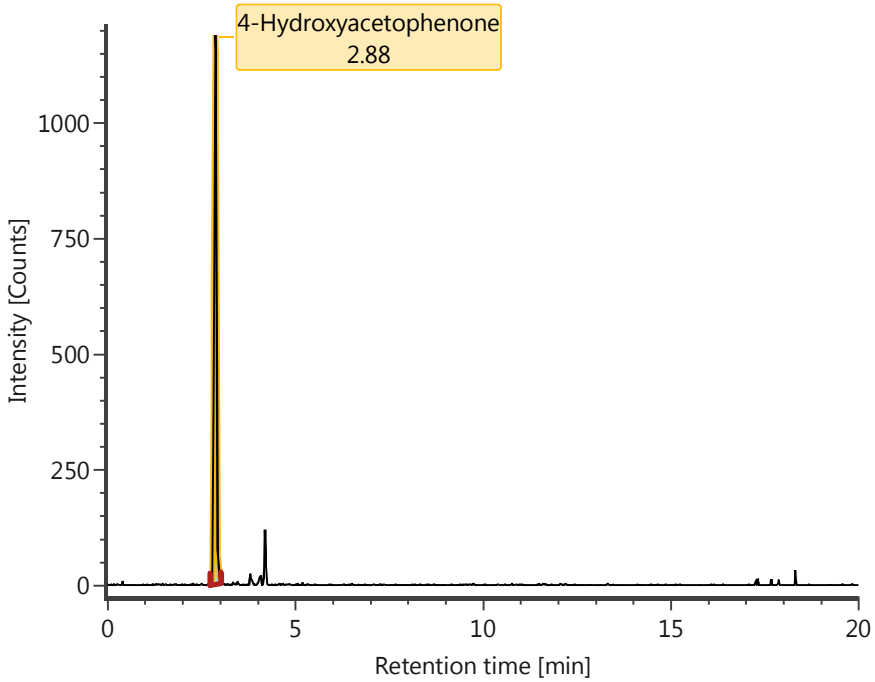


Item name: sample 2_01
Component name: 3′,4′-Dimethoxy-isoflavan-7,2′-di-O-β-D-glucoside

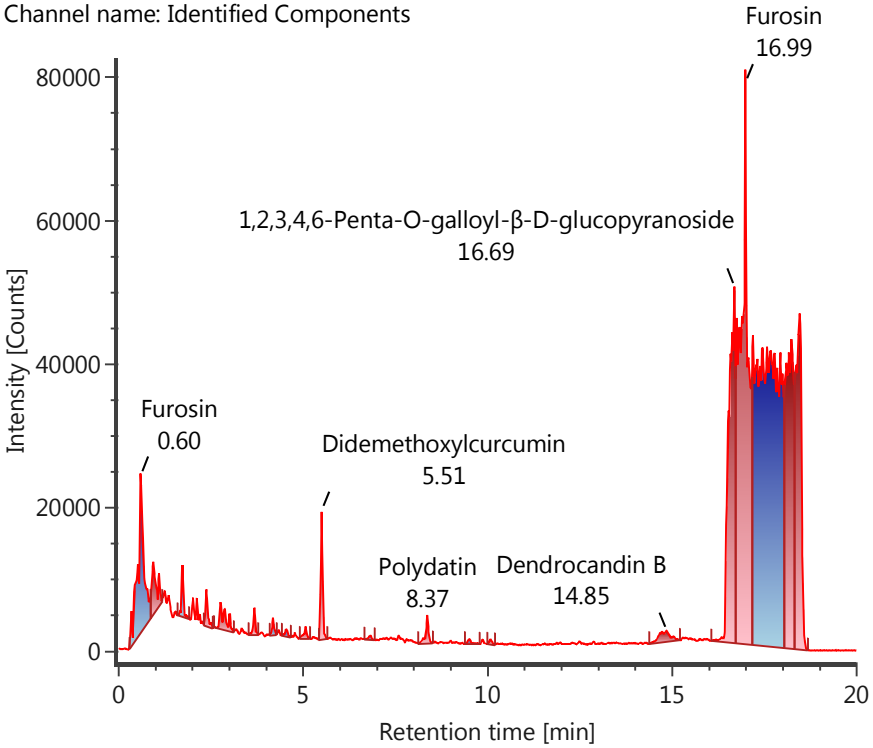
Channel name: High energy : Time 2.3810 +/- 0.0245 minutes : Drift Times: 8.03 +/- 0.33 ms



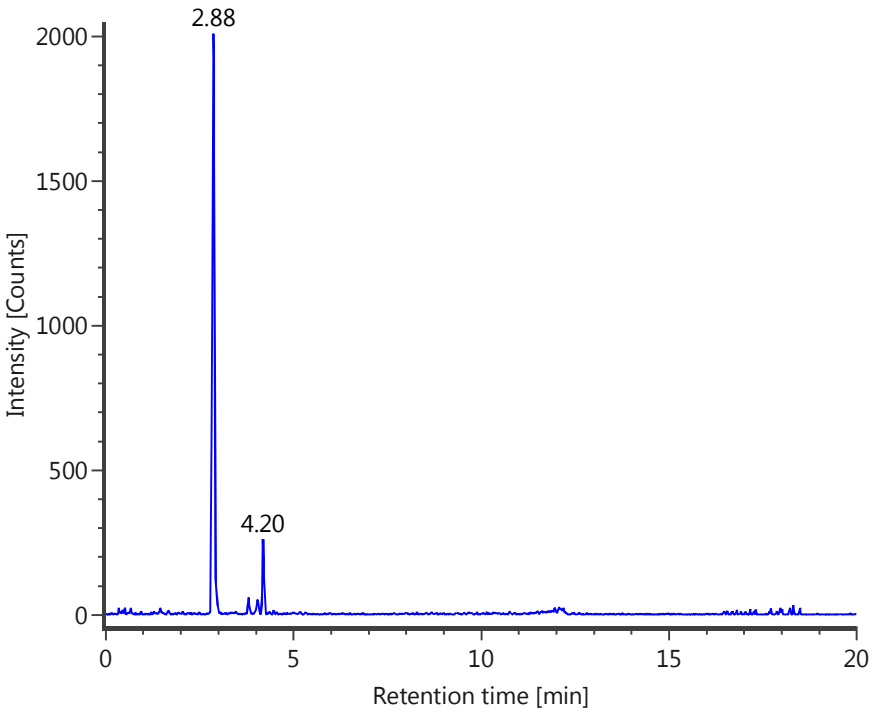
Item name: sample 2_01
Channel name: 4-Hydroxyacetophenone [+HCOO] : (16.3 PPM) 181.0503 : DT=3.56 to 4.06 ms



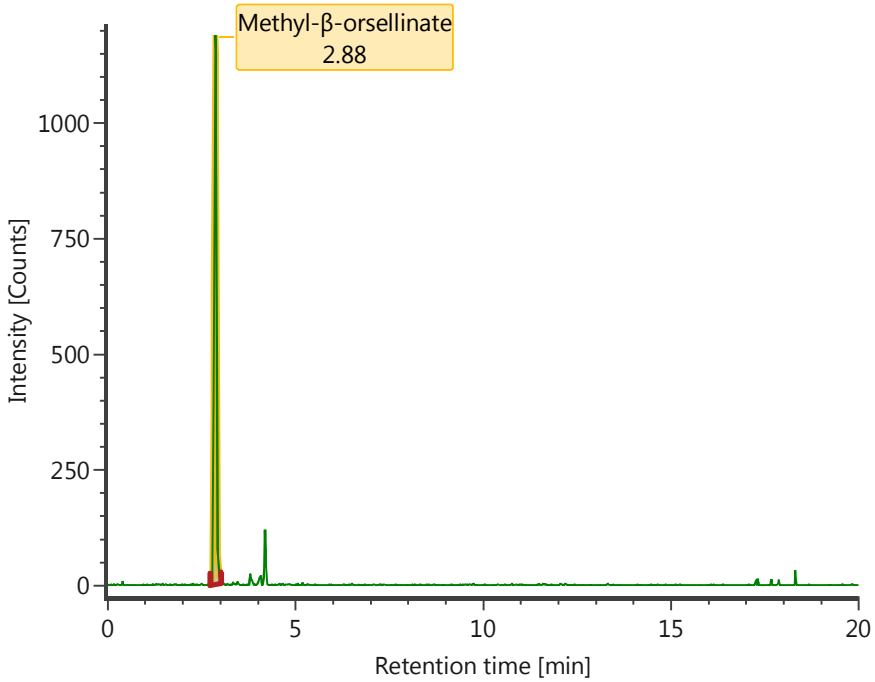
Item name: sample 2_01
Channel name: Identified Components



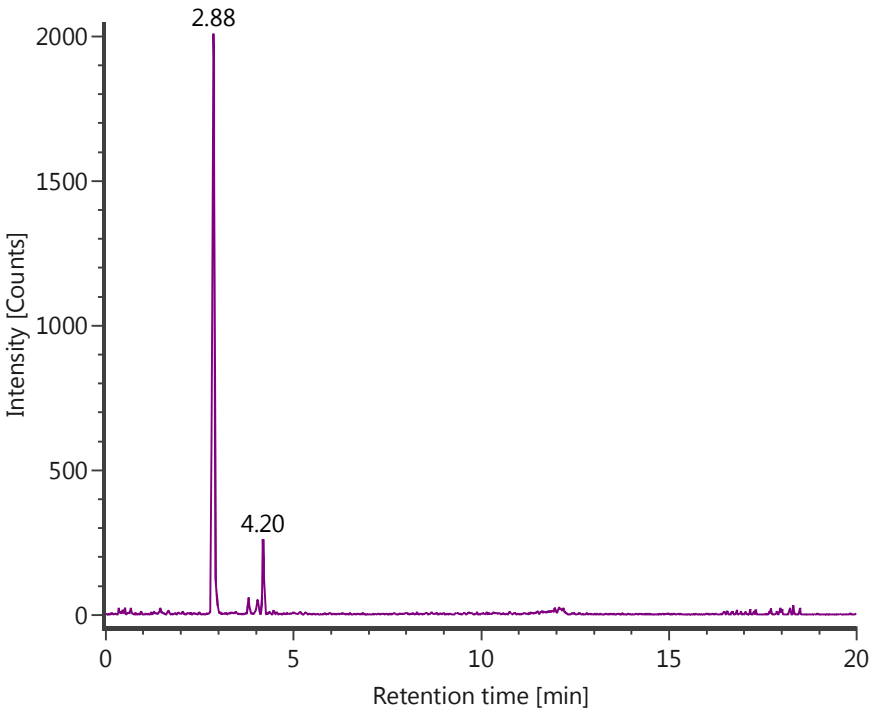
Item name: sample 2_01
Channel name: 4-Hydroxyacetophenone [+HCOO] : (16.3 PPM) 181.0503



Item name: sample 2_01
Channel name: Methyl-β-orsellinate [-H] : (16.3 PPM) 181.0503 : DT=3.56 to 4.06 ms

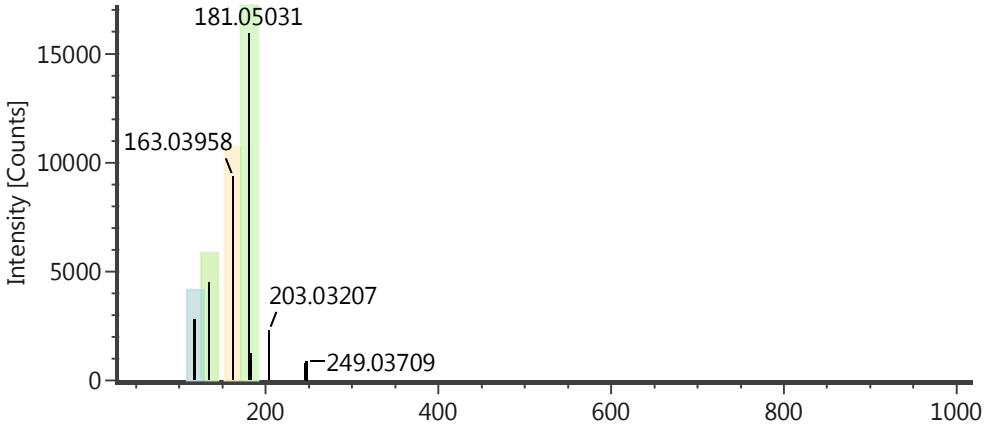


Item name: sample 2_01
Channel name: Methyl-β-orsellinate [-H] : (16.3 PPM) 181.0503



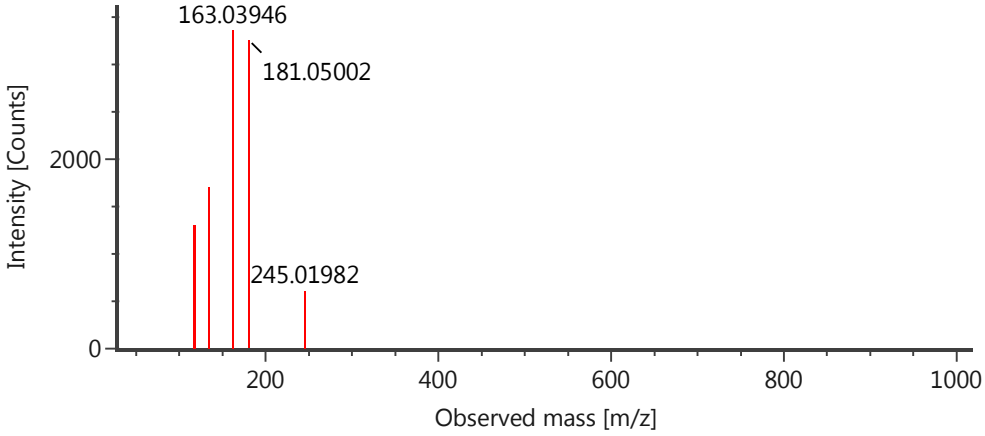
Item name: sample 2_01
Component name: 4-Hydroxyacetophenone

Channel name: Low energy : Time 2.8727 +/- 0.0245 minutes : Drift Times: 3.81 +/- 0.25, 3.69 +/- 0.25 ms

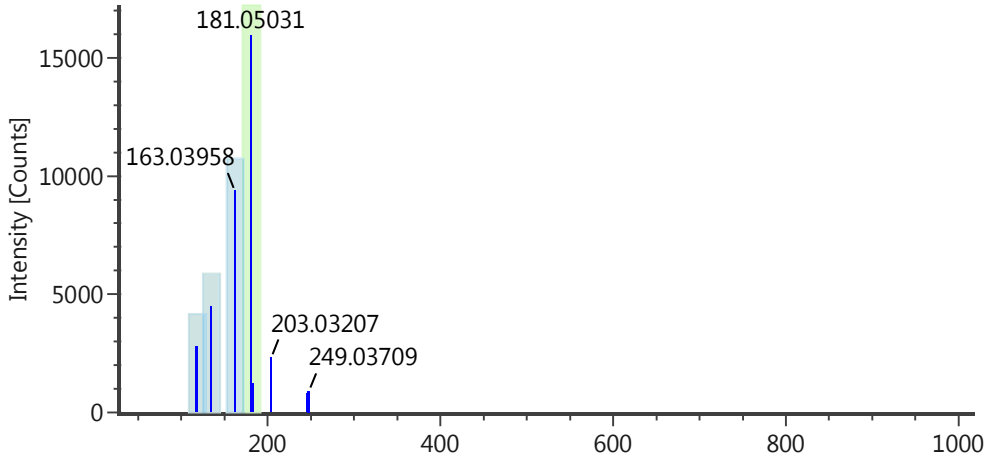


Item name: sample 2_01
Component name: 4-Hydroxyacetophenone

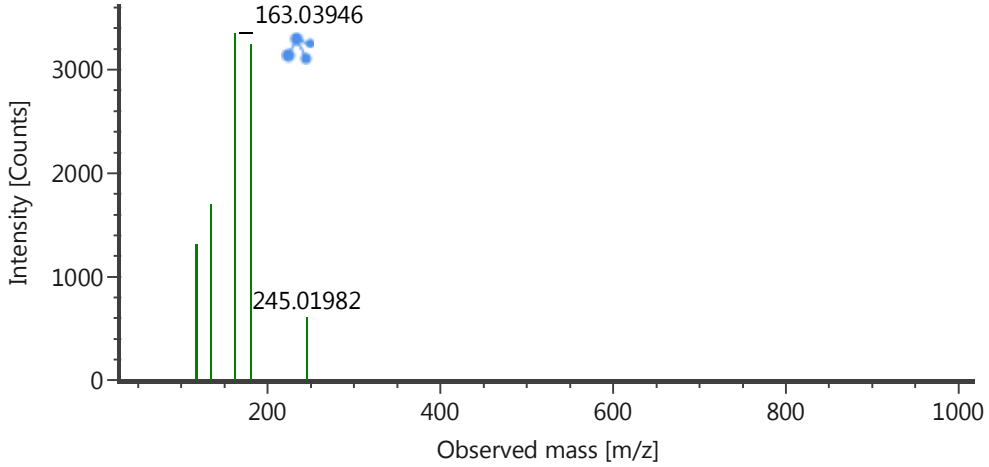
Channel name: High energy : Time 2.8727 +/- 0.0245 minutes : Drift Times: 3.73 +/- 0.25, 3.60 +/- 0.25 ms



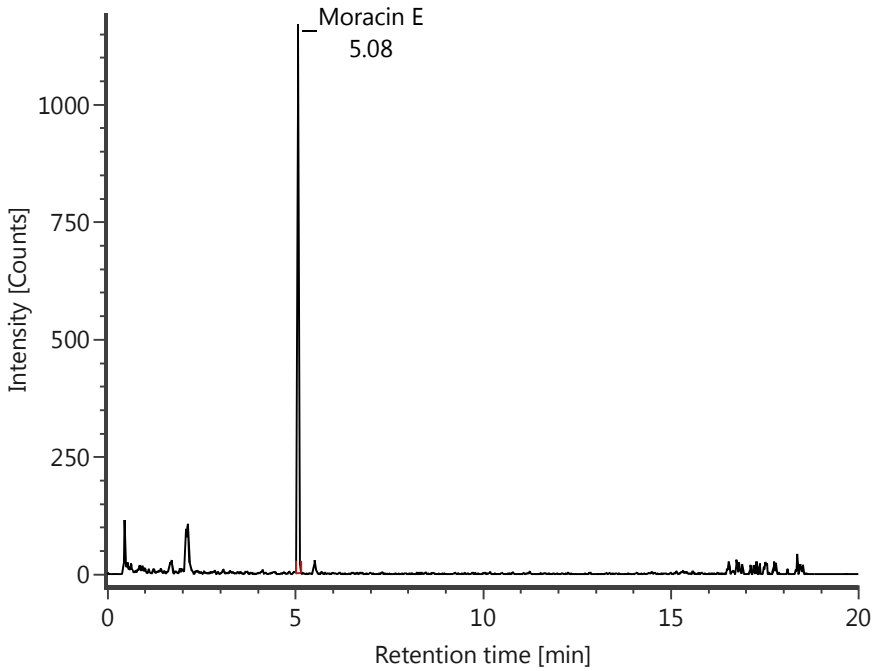
Item name: sample 2_01
Component name: Methyl-β-orsellinate
Channel name: Low energy : Time 2.8727 +/- 0.0245 minutes : Drift Times: 3.81 +/- 0.25 ms



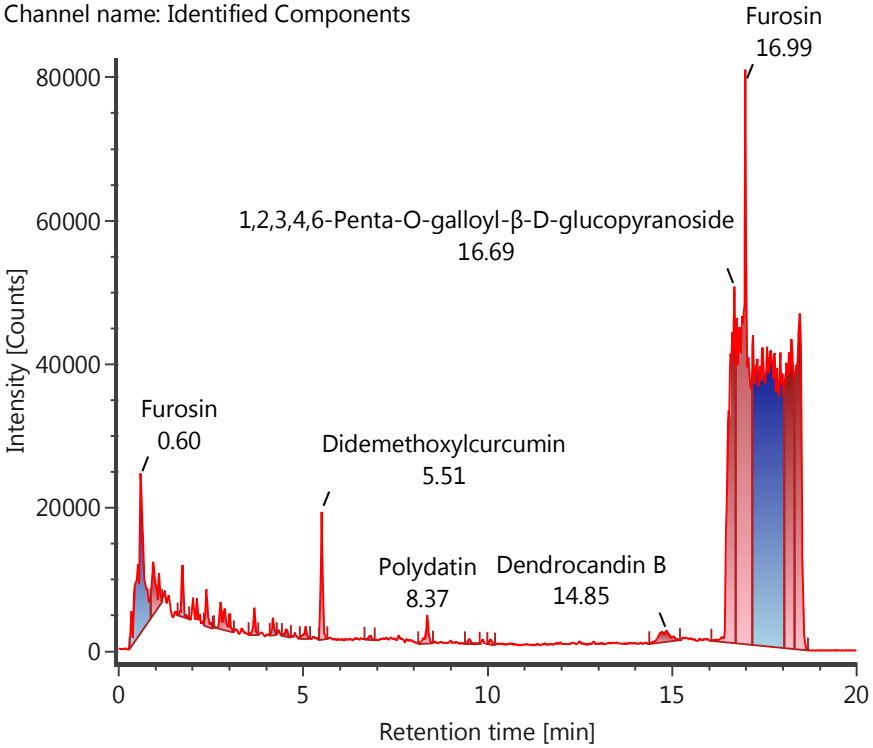
Item name: sample 2_01
Component name: Methyl-β-orsellinate
Channel name: High energy : Time 2.8727 +/- 0.0245 minutes : Drift Times: 3.73 +/- 0.25 ms



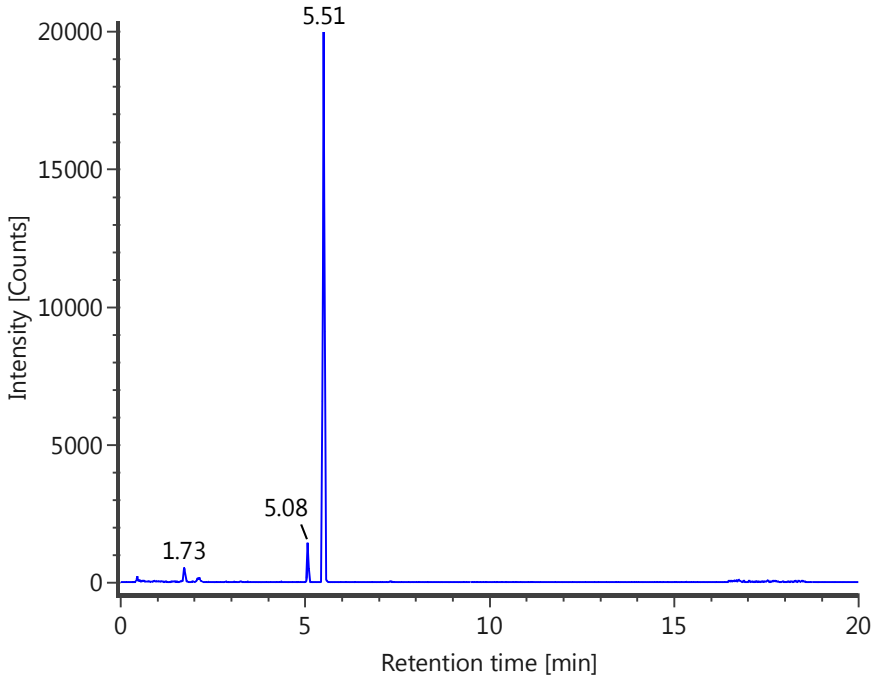
Item name: sample 2_01
Channel name: Didemethoxylcurcumin [+HCOO] : Moracin E [+HCOO] : (16.3 PPM)
353.1006 : DT=4.79 to 5.34 ms



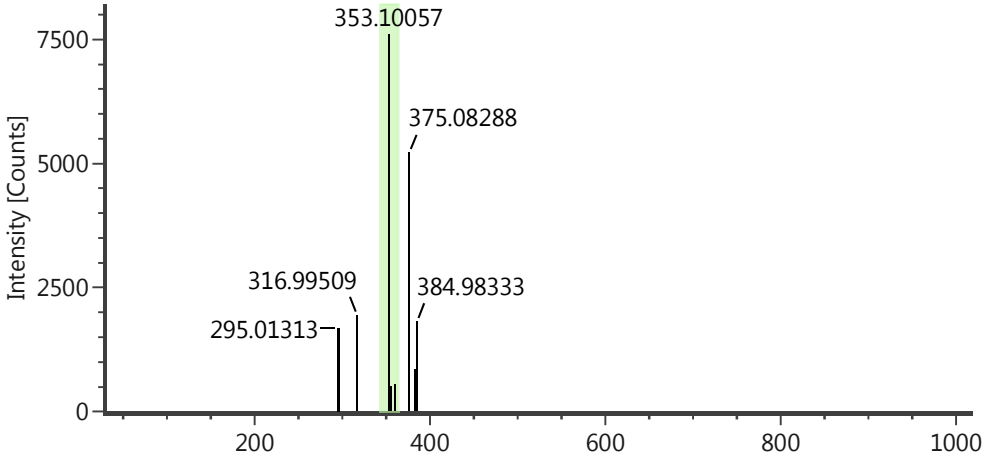
Item name: sample 2_01
Channel name: Identified Components



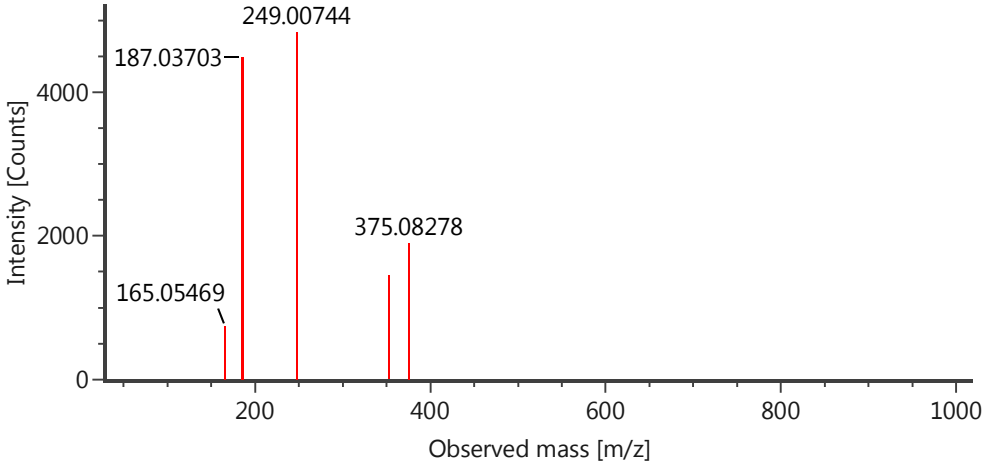
Item name: sample 2_01
Channel name: Didemethoxylcurcumin [+HCOO] : Moracin E [+HCOO] : (16.3 PPM) 353.1006



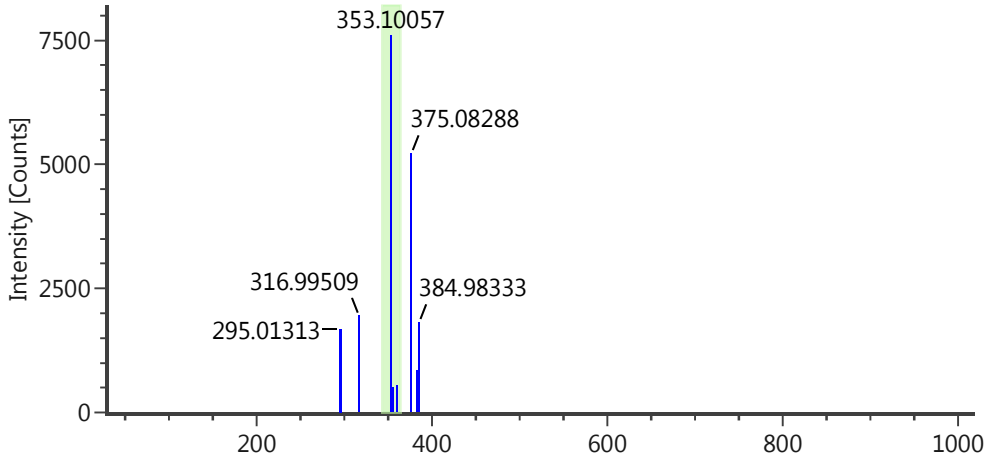
Item name: sample 2_01
Component name: Didemethoxylcurcumin
Channel name: Low energy : Time 5.0819 +/- 0.0245 minutes : Drift Times: 5.06 +/- 0.27 ms



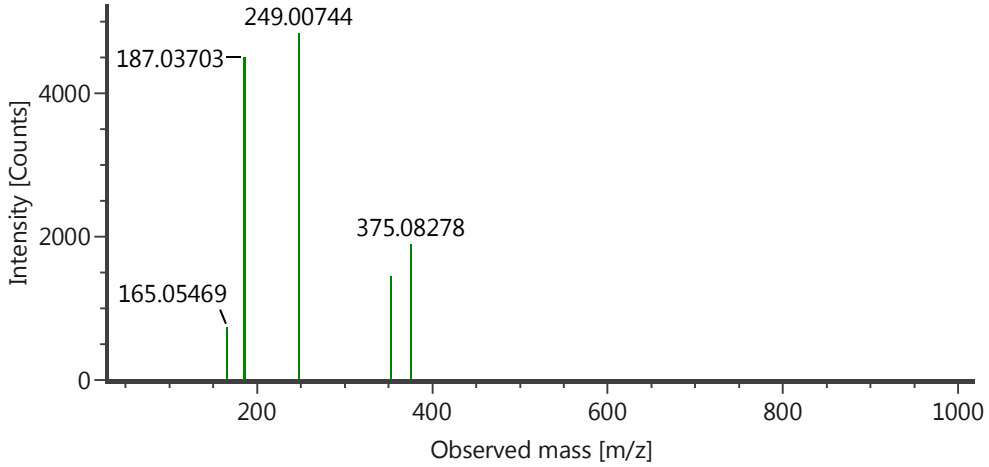
Item name: sample 2_01
Component name: Didemethoxylcurcumin
Channel name: High energy : Time 5.0819 +/- 0.0245 minutes : Drift Times: 4.98 +/- 0.27 ms



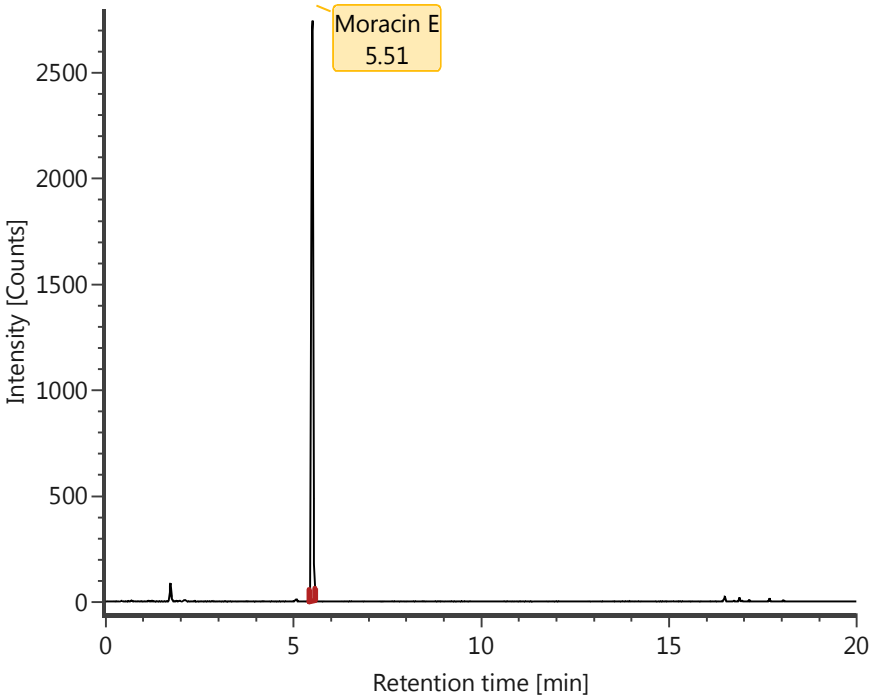
Item name: sample 2_01 Channel name: Low energy : Time 5.0819 +/- 0.0245 minutes :
Component name: Moracin E Drift Times: 5.06 +/- 0.27 ms



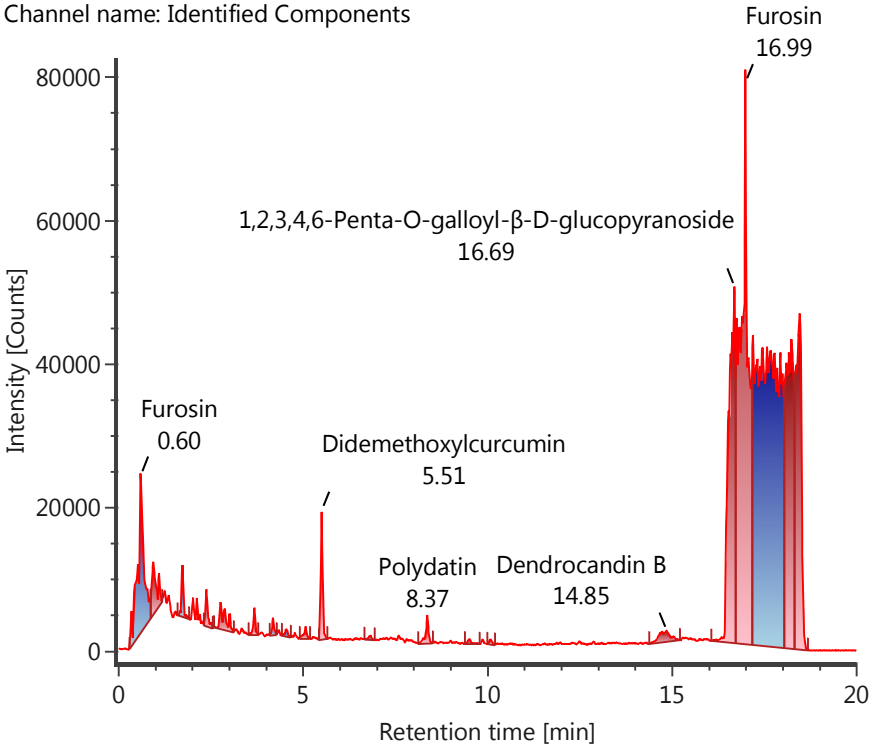
Item name: sample 2_01 Channel name: High energy : Time 5.0819 +/- 0.0245 minutes :
Component name: Moracin E Drift Times: 4.98 +/- 0.27 ms



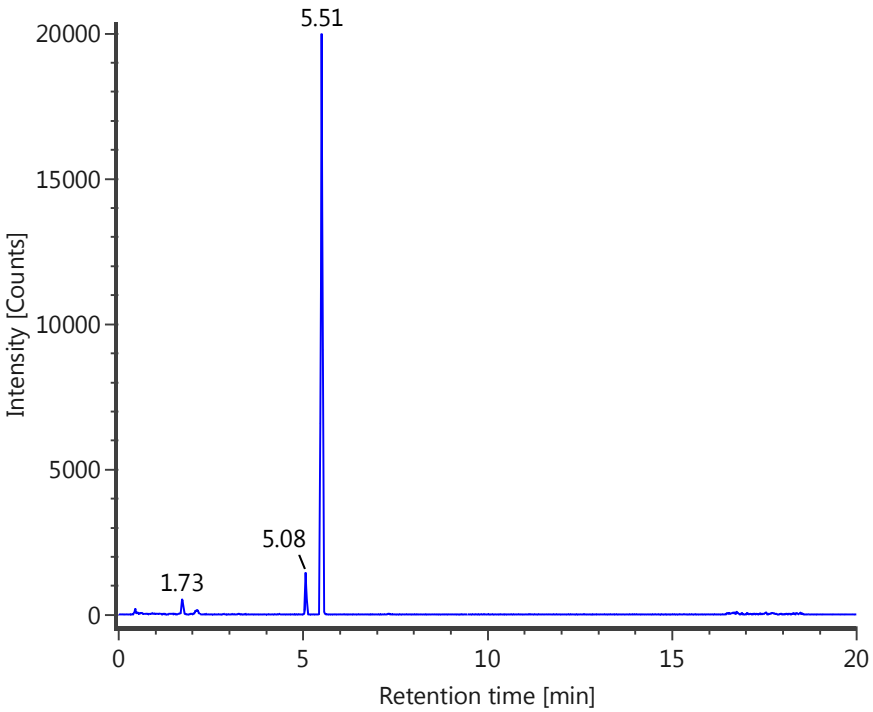
Item name: sample 2_01
Channel name: Moracin E [+HCOO] : (16.3 PPM) 353.1006 : DT=7.15 to 7.79 ms



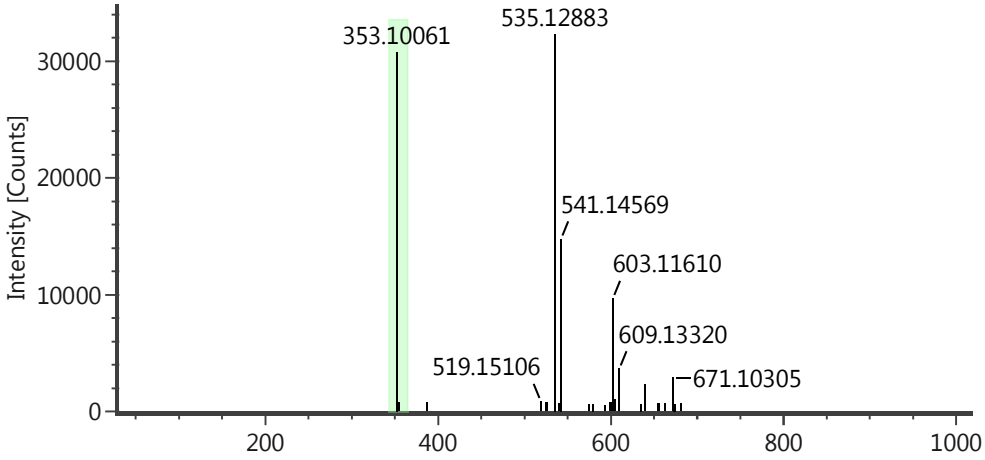
Item name: sample 2_01
Channel name: Identified Components



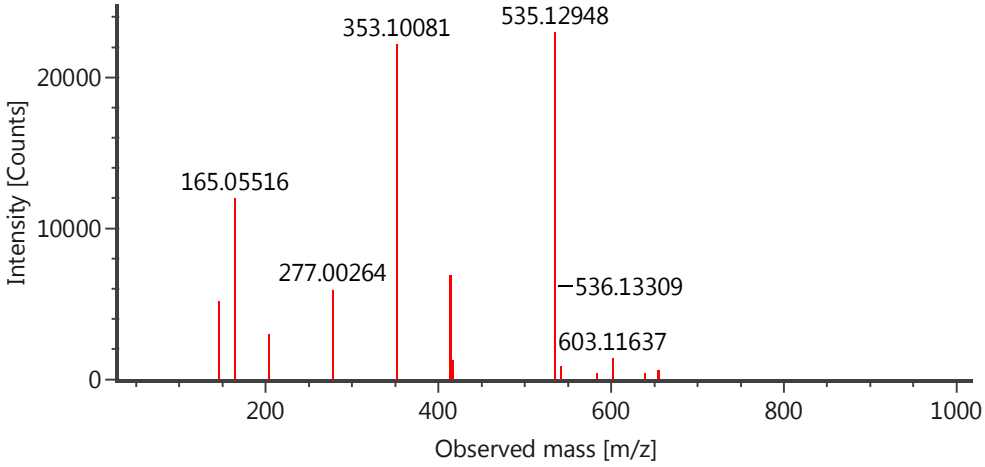
Item name: sample 2_01
Channel name: Moracin E [+HCOO] : (16.3 PPM) 353.1006



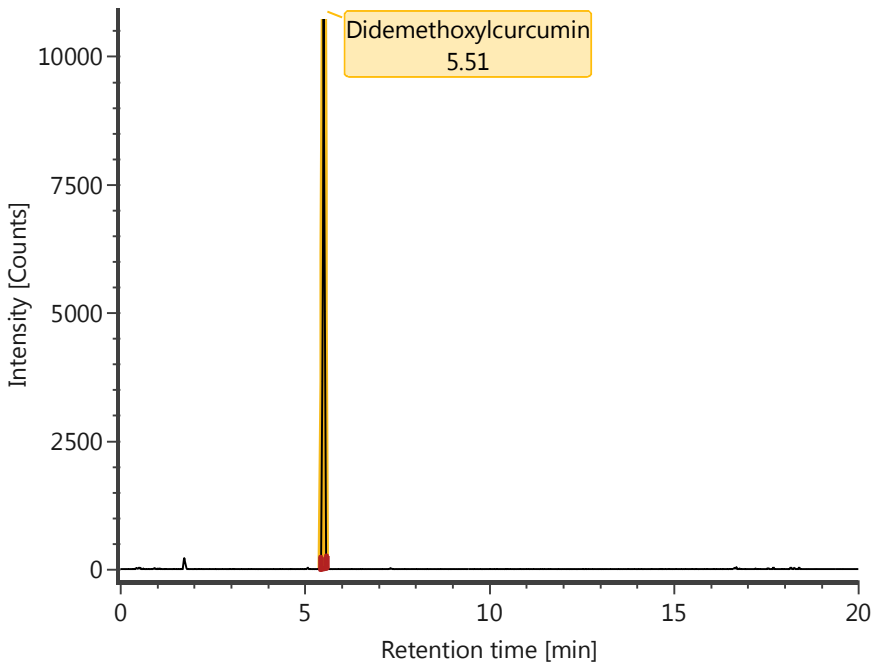
Item name: sample 2_01
Component name: Moracin E
Channel name: Low energy : Time 5.5075 +/- 0.0245 minutes :
Drift Times: 7.47 +/- 0.32 ms



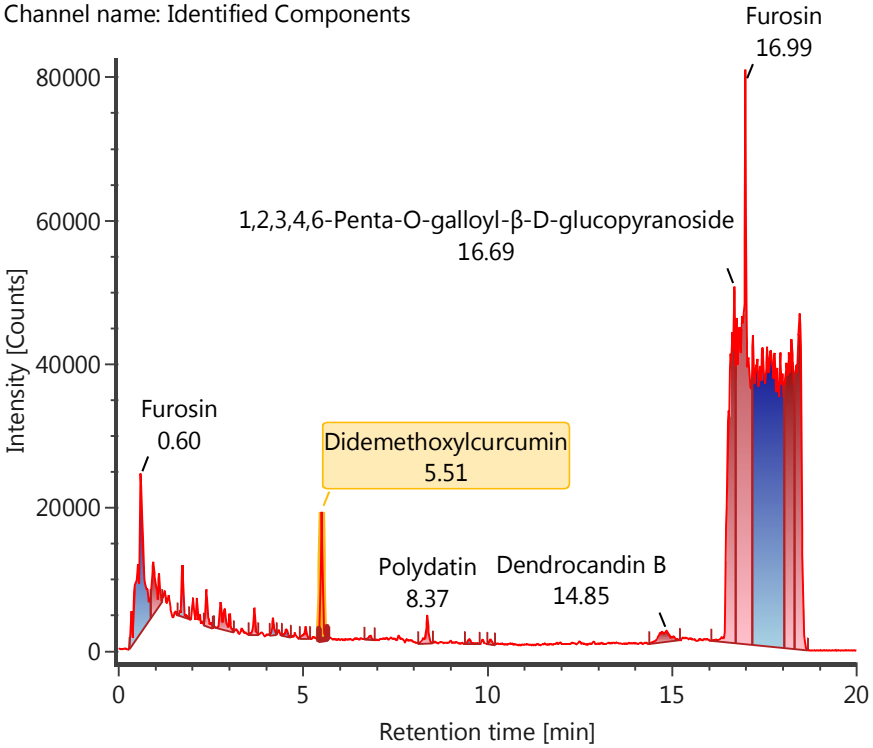
Item name: sample 2_01
Component name: Moracin E
Channel name: High energy : Time 5.5075 +/- 0.0245 minutes :
Drift Times: 7.39 +/- 0.32 ms



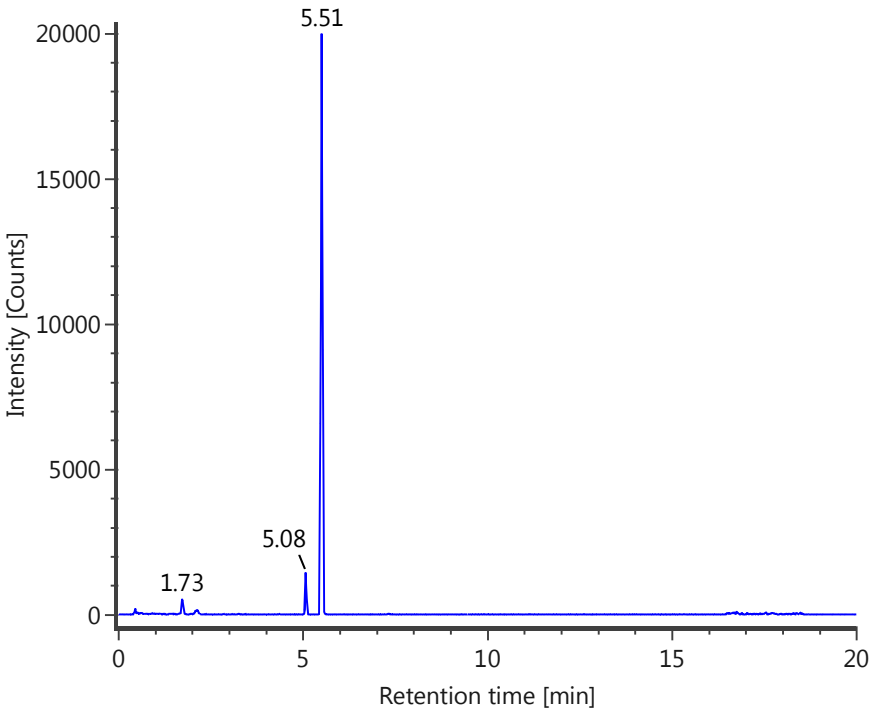
Item name: sample 2_01
Channel name: Didemethoxylcurcumin [+HCOO] : (16.3 PPM) 353.1006 : DT=5.66 to 6.24 ms



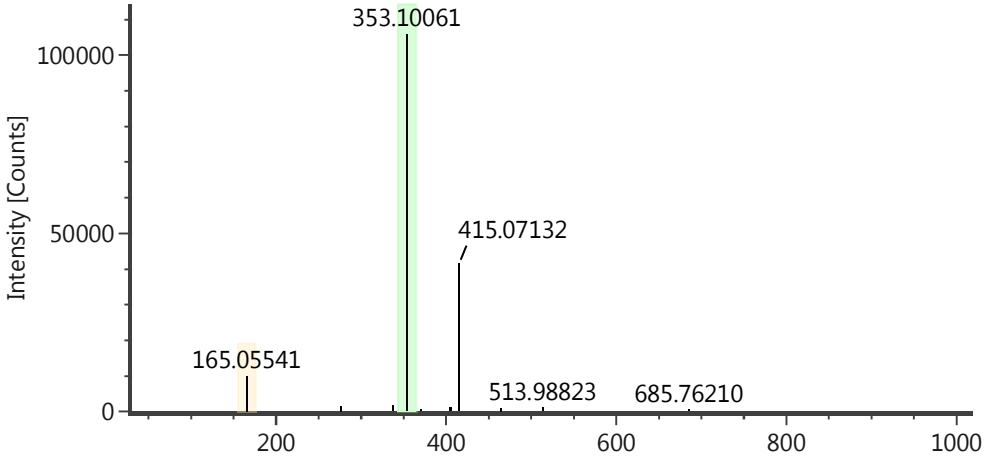
Item name: sample 2_01
Channel name: Identified Components



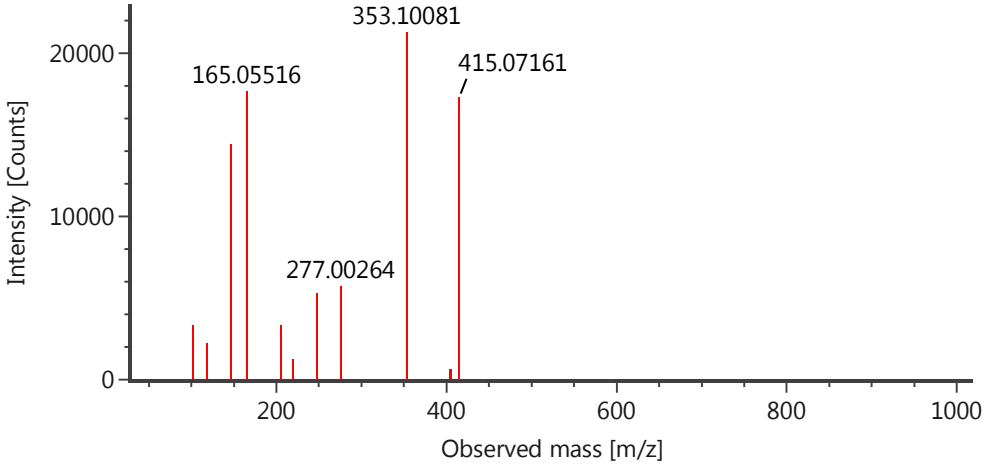
Item name: sample 2_01
Channel name: Didemethoxylcurcumin [+HCOO] : (16.3 PPM) 353.1006



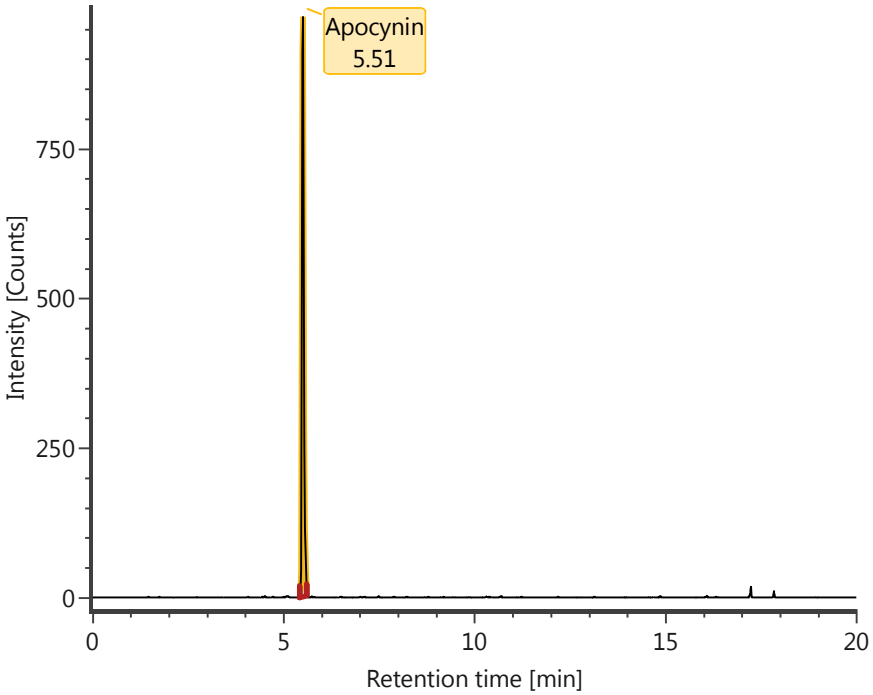
Item name: sample 2_01
Component name: Didemethoxylcurcumin
Channel name: Low energy : Time 5.5086 +/- 0.0245 minutes : Drift Times: 5.96 +/- 0.29 ms



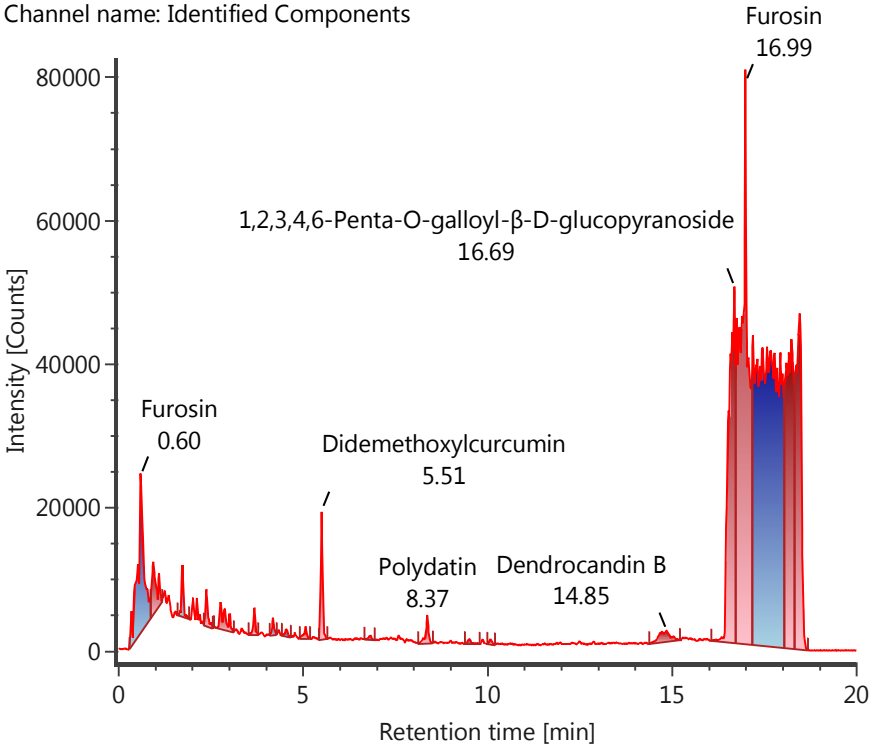
Item name: sample 2_01
Component name: Didemethoxylcurcumin
Channel name: High energy : Time 5.5086 +/- 0.0245 minutes : Drift Times: 5.87 +/- 0.29 ms



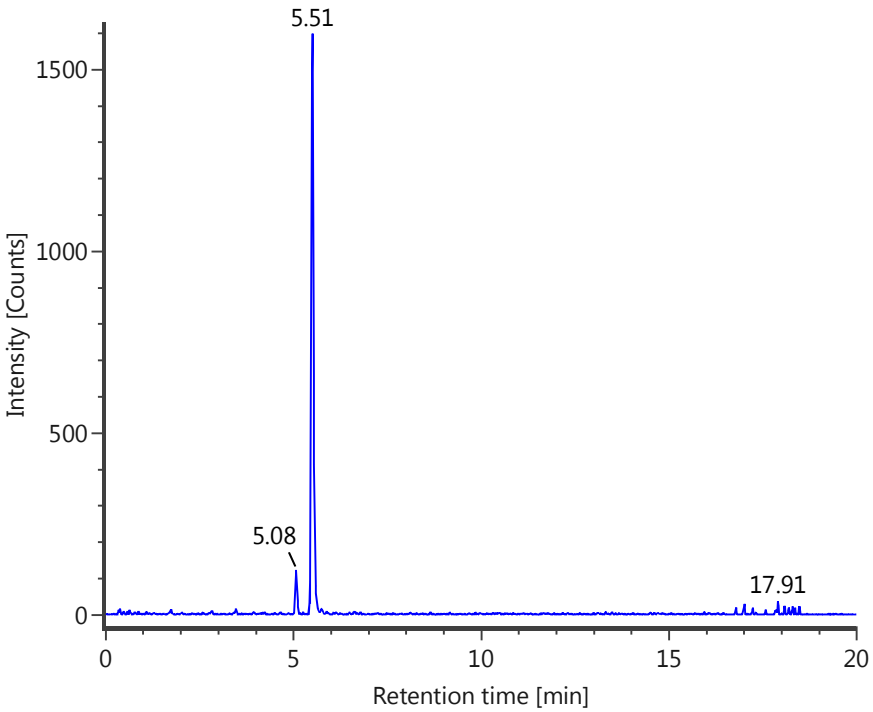
Item name: sample 2_01
Channel name: Apocynin [-H] : (16.3 PPM) 165.0554 : DT=5.58 to 6.16 ms



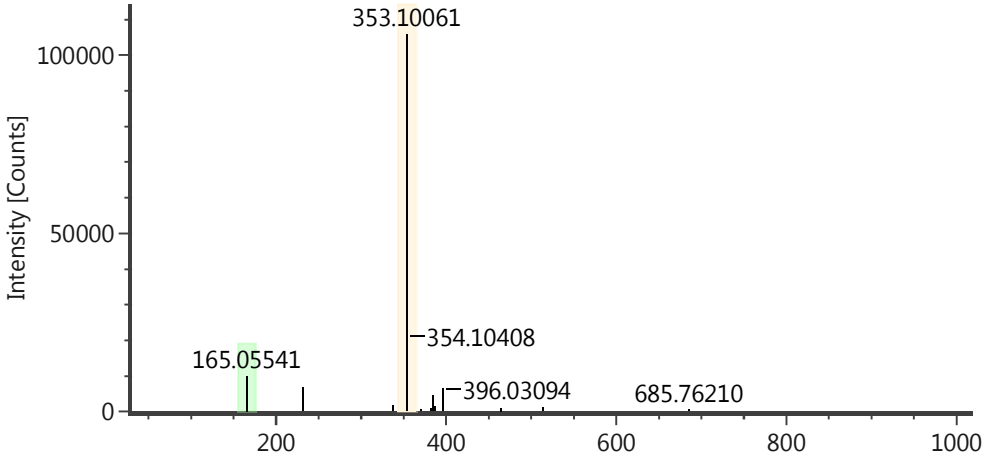
Item name: sample 2_01
Channel name: Identified Components



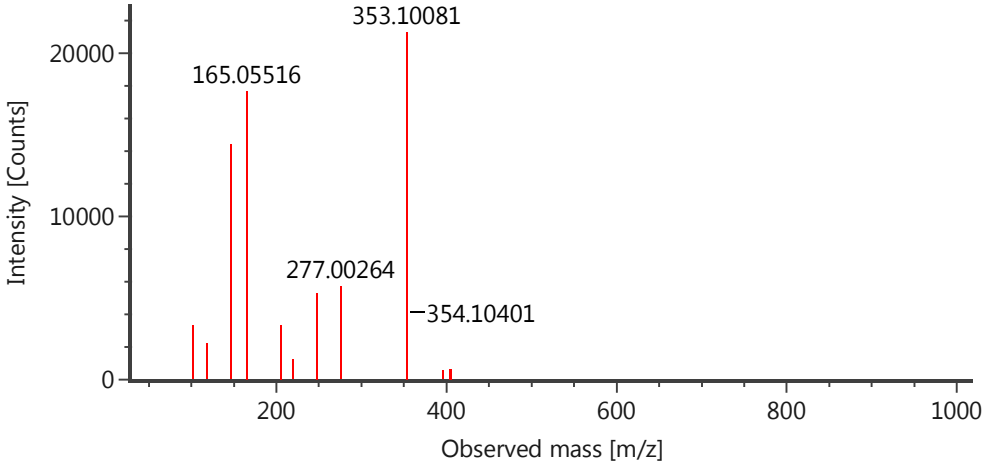
Item name: sample 2_01
Channel name: Apocynin [-H] : (16.3 PPM) 165.0554



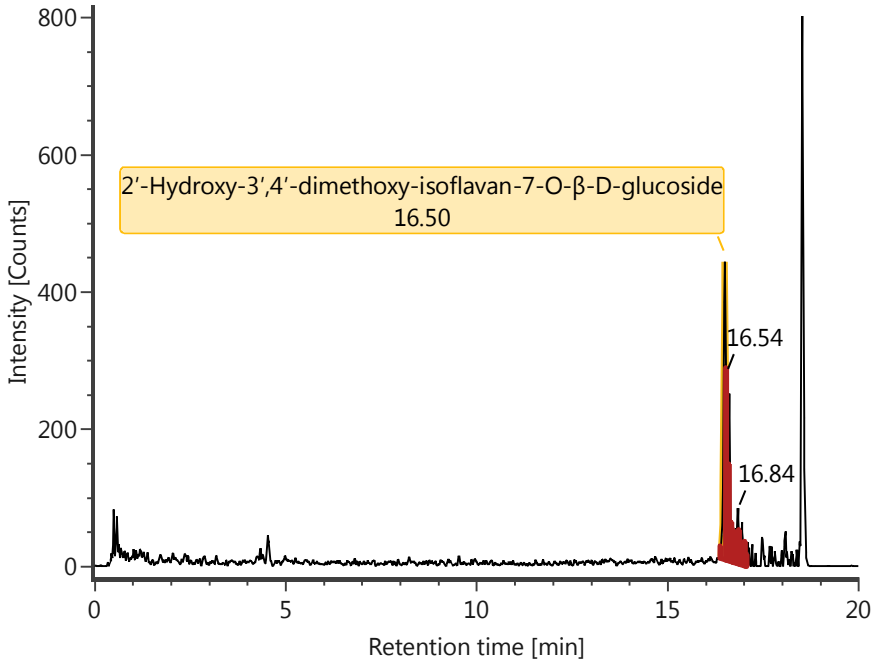
Item name: sample 2_01
Component name: Apocynin
Channel name: Low energy : Time 5.5096 +/- 0.0245 minutes :
Drift Times: 5.87 +/- 0.29 ms



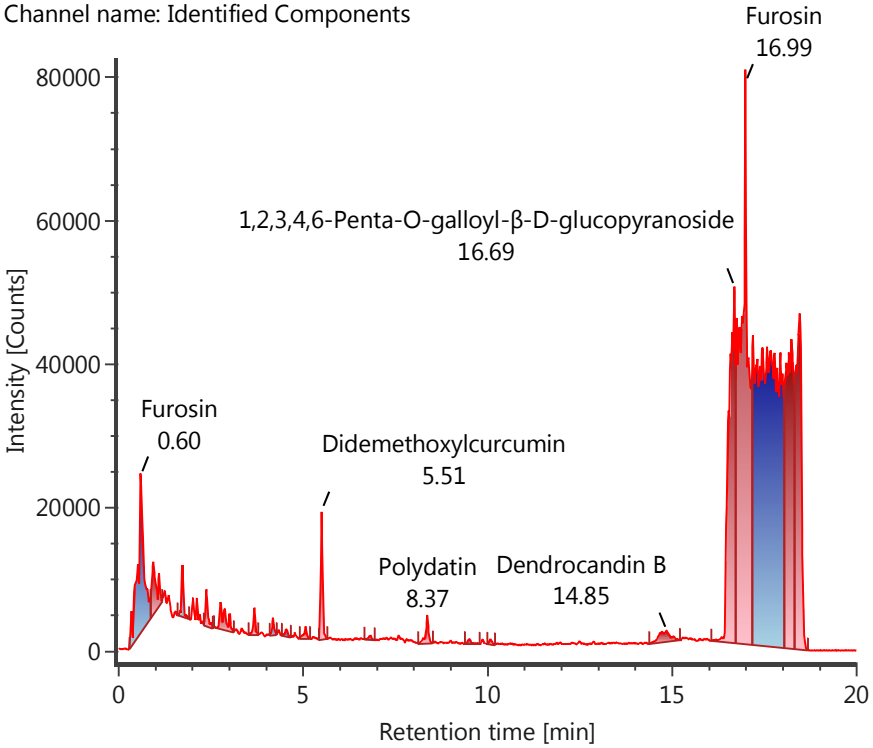
Item name: sample 2_01
Component name: Apocynin
Channel name: High energy : Time 5.5096 +/- 0.0245 minutes :
Drift Times: 5.79 +/- 0.29 ms



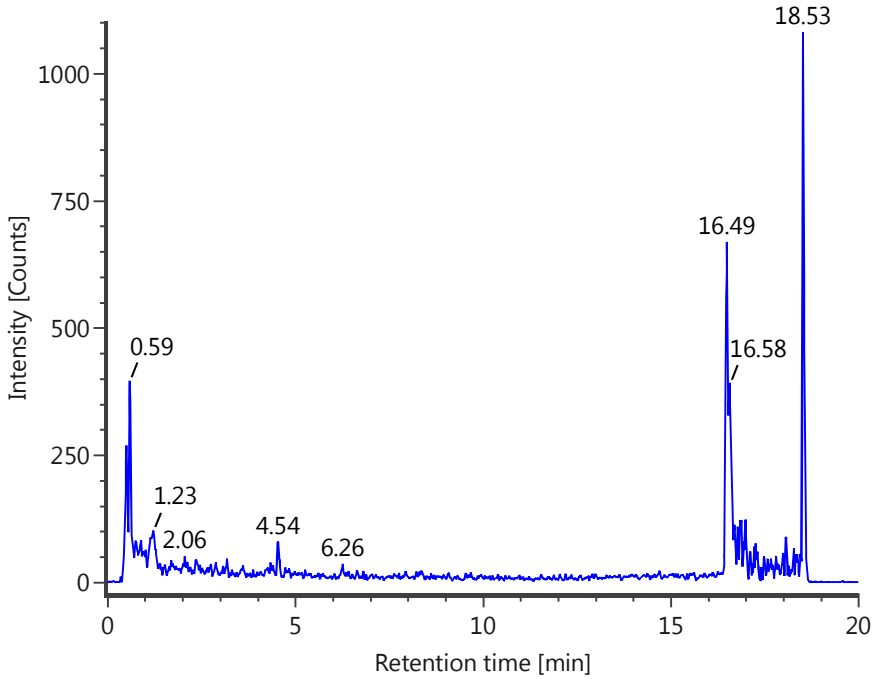
Item name: sample 2_01
Channel name: 2′-Hydroxy-3′,4′-dimethoxy-isoflavan-7-O-β-D-glucoside [+HCOO] :
(16.3 PPM) 509.1617 : DT=6.72 to 7.34 ms



Item name: sample 2_01
Channel name: Identified Components

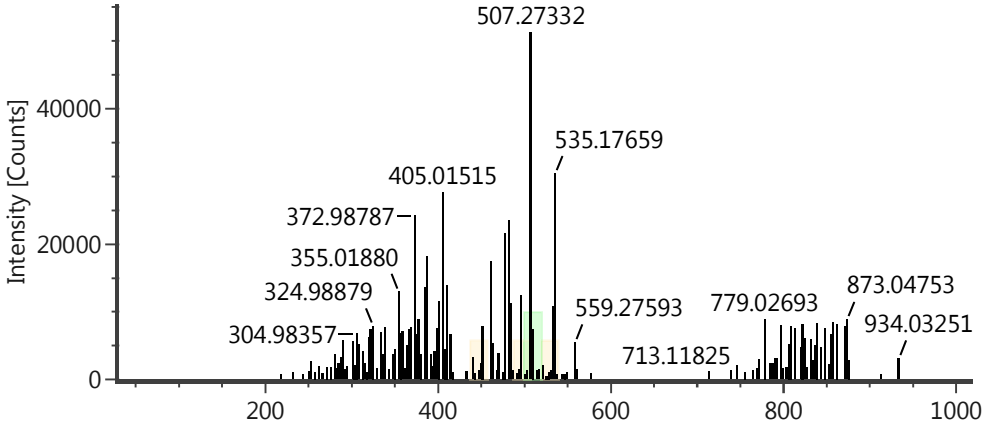


Item name: sample 2_01
Channel name: 2′-Hydroxy-3′,4′-dimethoxy-isoflavan-7-O-β-D-glucoside [+HCOO] : (16.3 PPM) 509.1617



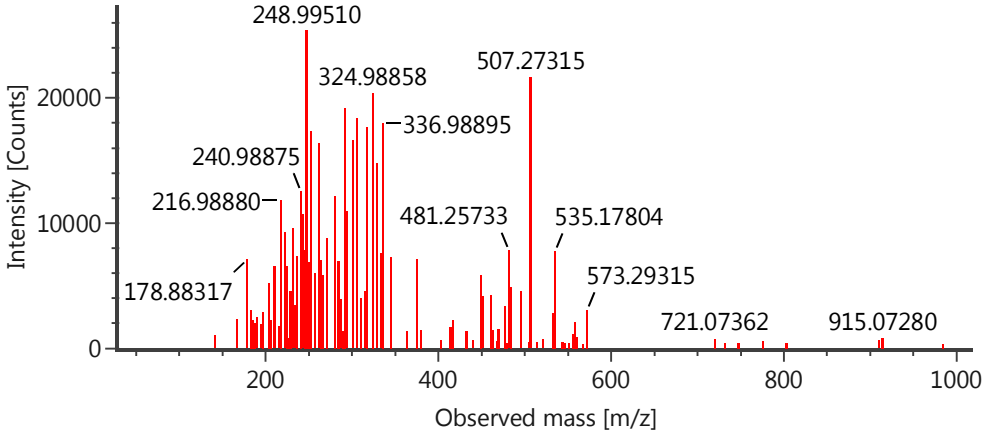
Item name: sample 2_01
Component name: 2′-Hydroxy-3′,4′-dimethoxy-isoflavan-7-O-β-D-glucoside

Channel name: Low energy : Time 16.4937 +/- 0.0245 minutes : Drift Times: 7.04 +/- 0.31 ms

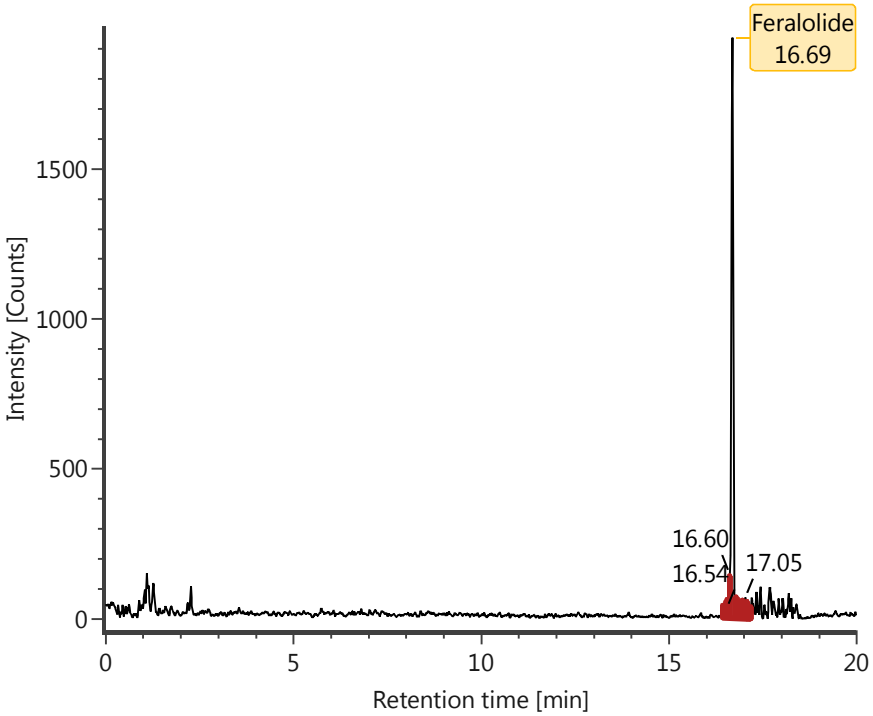


Item name: sample 2_01
Component name: 2′-Hydroxy-3′,4′-dimethoxy-isoflavan-7-O-β-D-glucoside

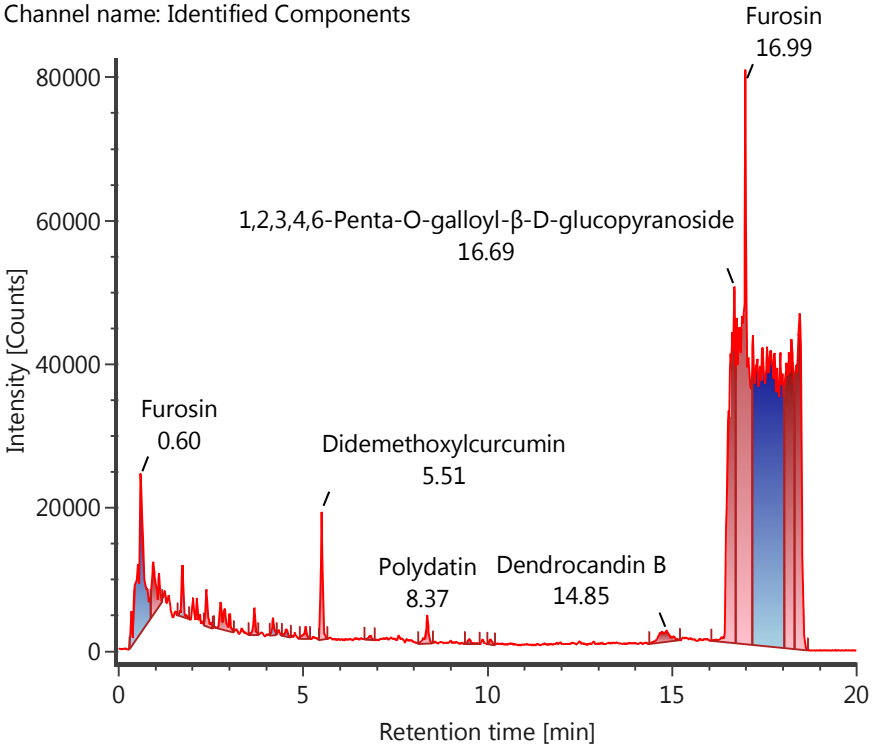
Channel name: High energy : Time 16.4937 +/- 0.0245 minutes : Drift Times: 6.96 +/- 0.31 ms



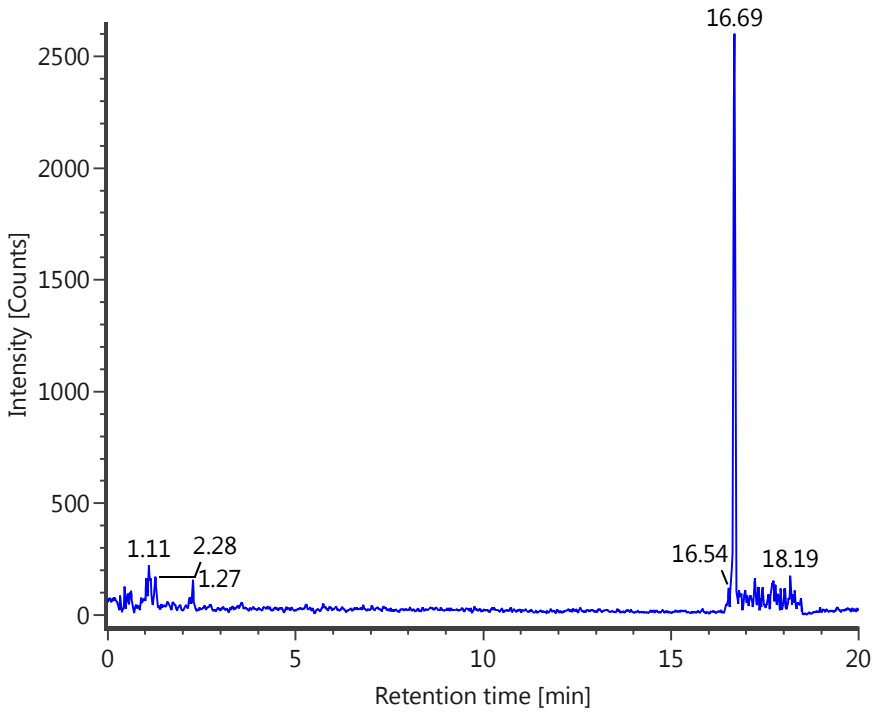
Item name: sample 2_01
Channel name: Feralolide [-H] : (16.3 PPM) 343.0813 : DT=5.06 to 5.62 ms



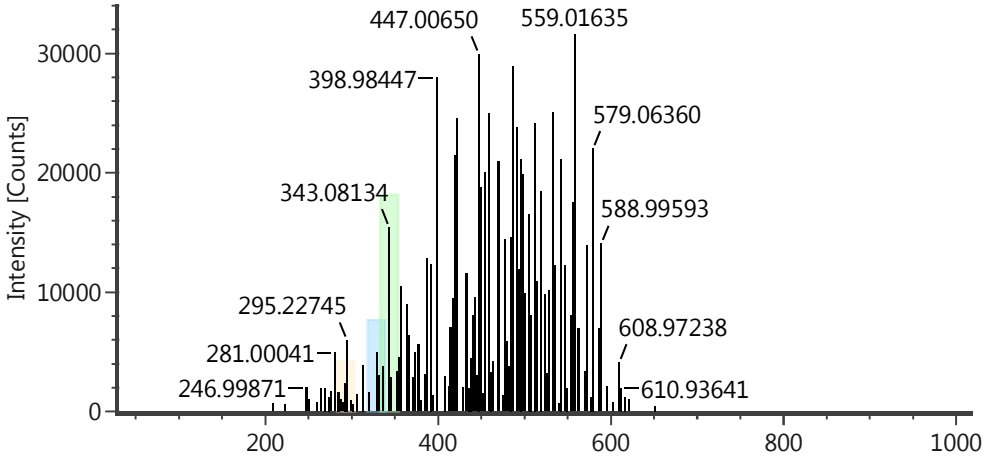
Item name: sample 2_01
Channel name: Identified Components



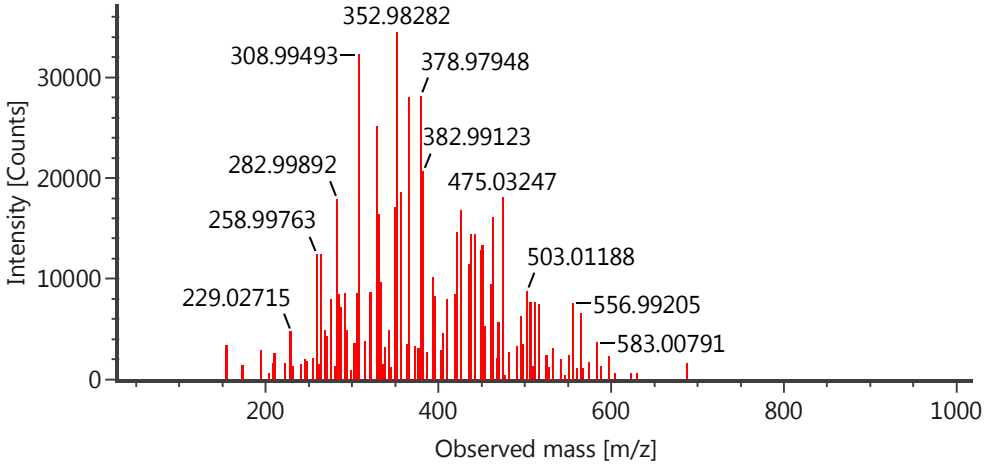
Item name: sample 2_01
Channel name: Feralolide [-H] : (16.3 PPM) 343.0813



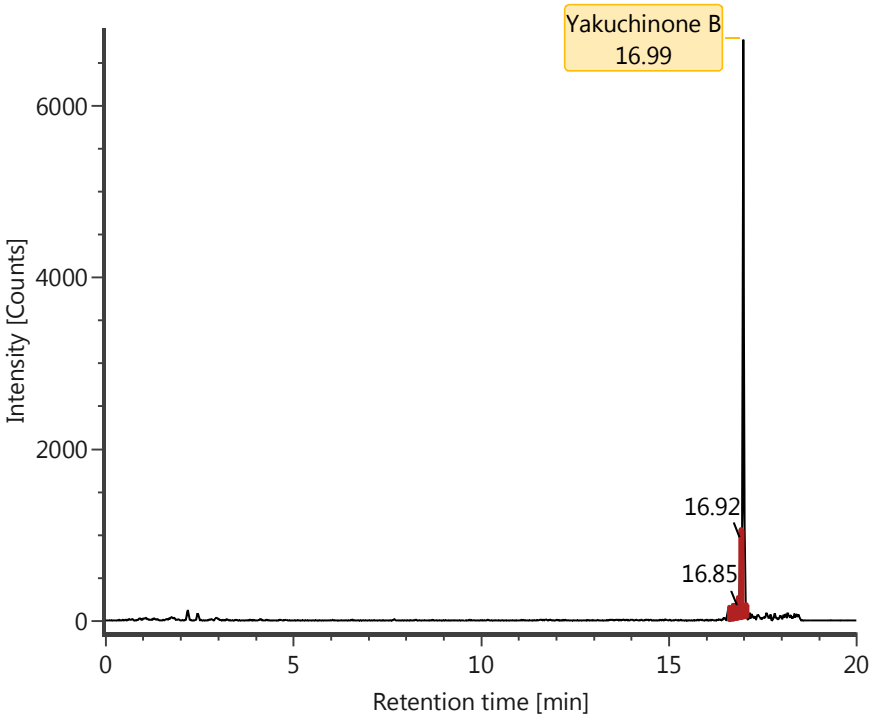
Item name: sample 2_01 Channel name: Low energy : Time 16.6918 +/- 0.0245 minutes :
Component name: Feralolide Drift Times: 5.32 +/- 0.28 ms



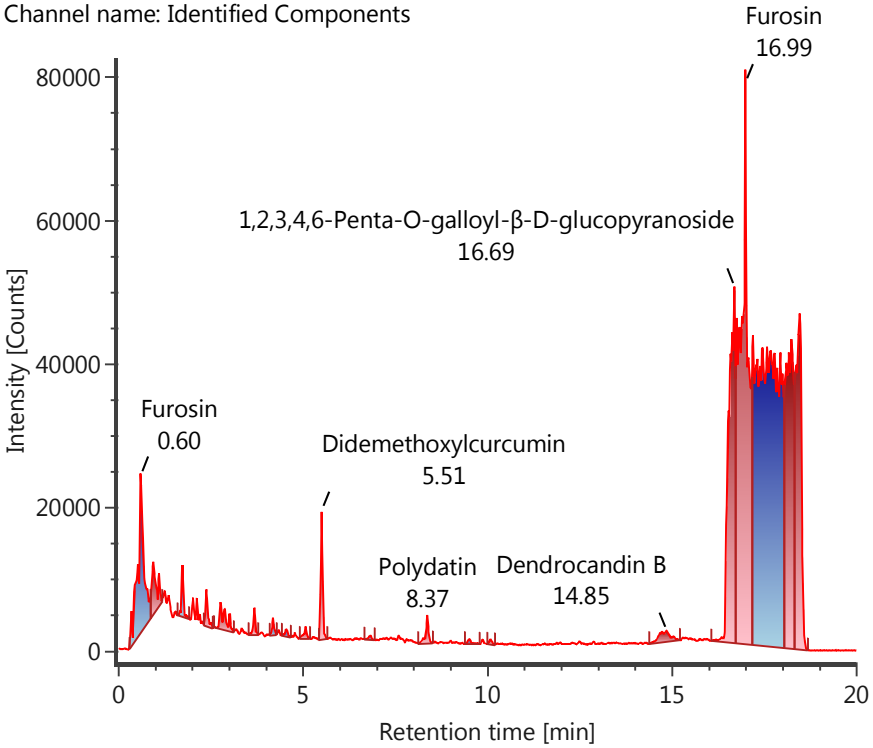
Item name: sample 2_01 Channel name: High energy : Time 16.6918 +/- 0.0245 minutes :
Component name: Feralolide Drift Times: 5.24 +/- 0.28 ms



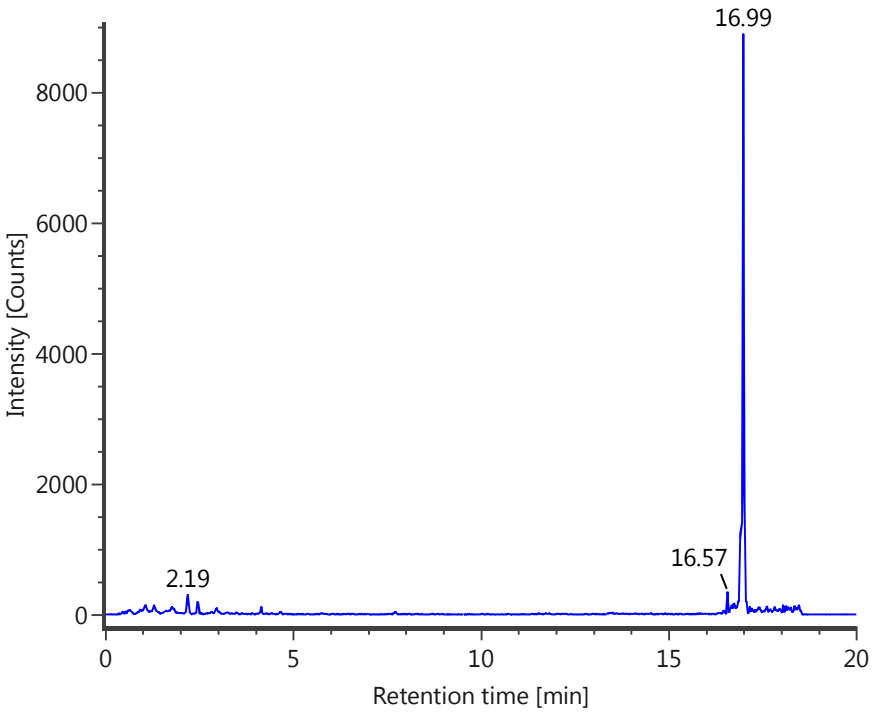
Item name: sample 2_01
Channel name: Yakuchinone B [+HCOO] : (16.3 PPM) 355.1578 : DT=5.69 to 6.27 ms



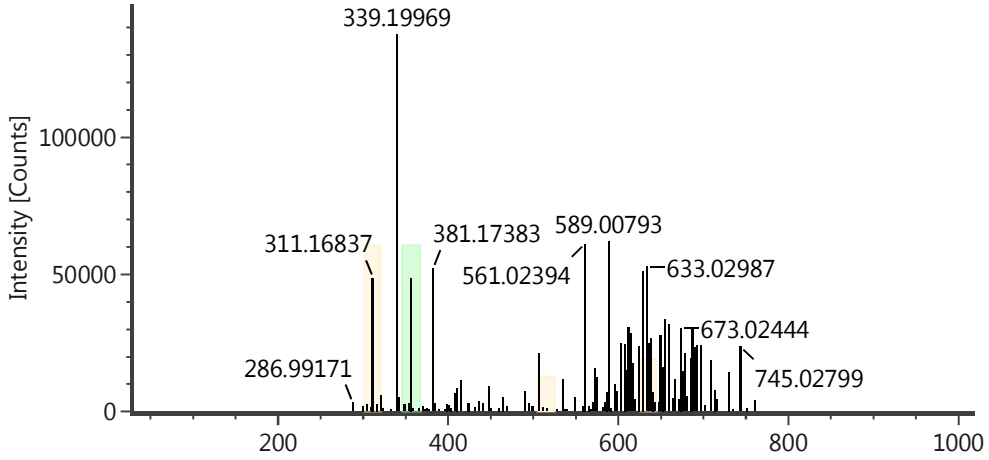
Item name: sample 2_01
Channel name: Identified Components



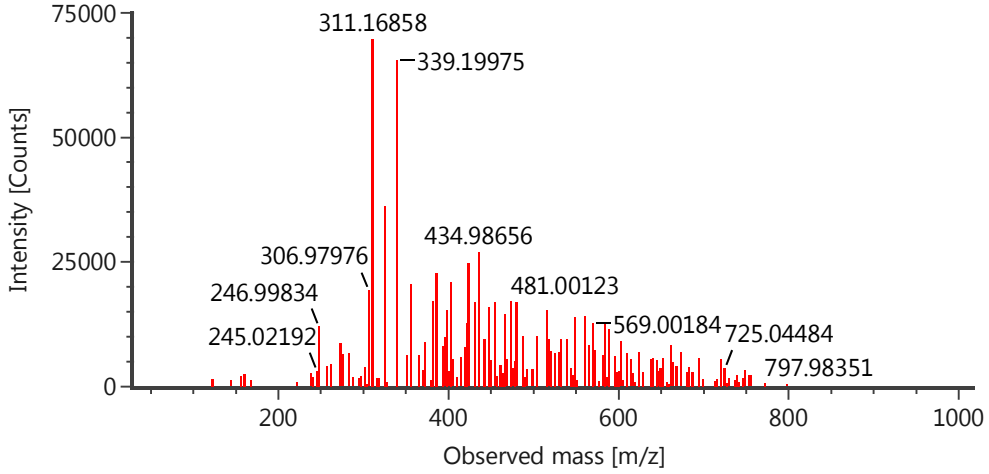
Item name: sample 2_01
Channel name: Yakuchinone B [+HCOO] : (16.3 PPM) 355.1578



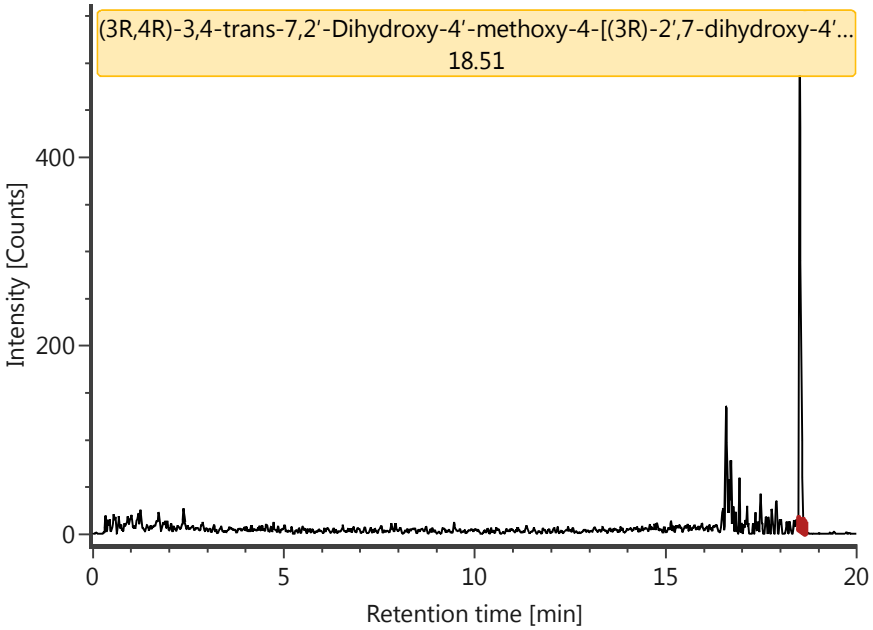
Item name: sample 2_01
Component name: Yakuchinone B
Channel name: Low energy : Time 16.9874 +/- 0.0245 minutes : Drift Times: 5.97 +/- 0.29 ms



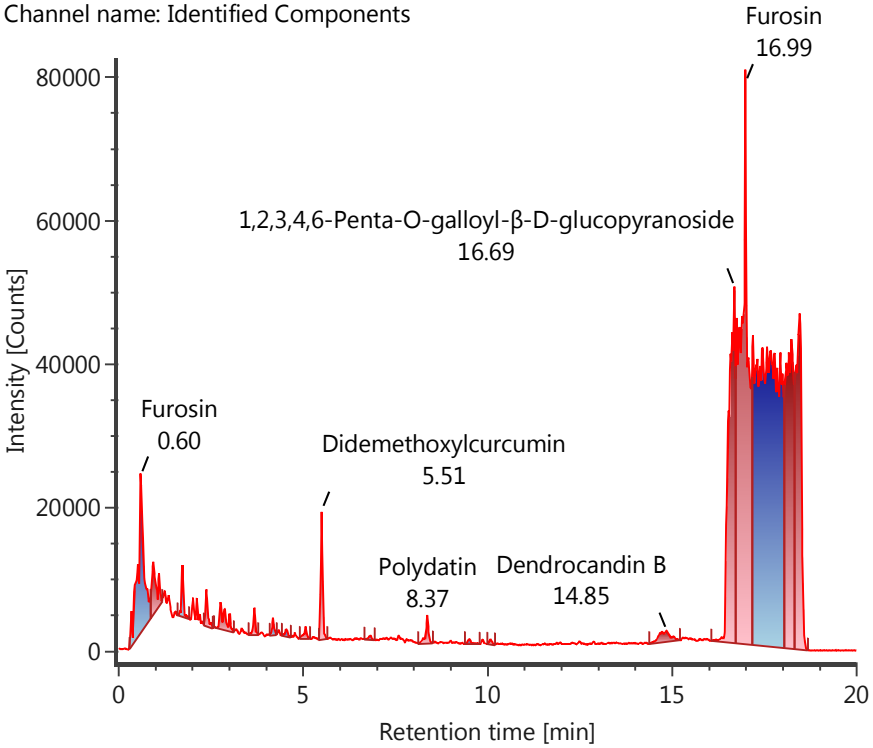
Item name: sample 2_01
Component name: Yakuchinone B
Channel name: High energy : Time 16.9874 +/- 0.0245 minutes : Drift Times: 5.89 +/- 0.29 ms



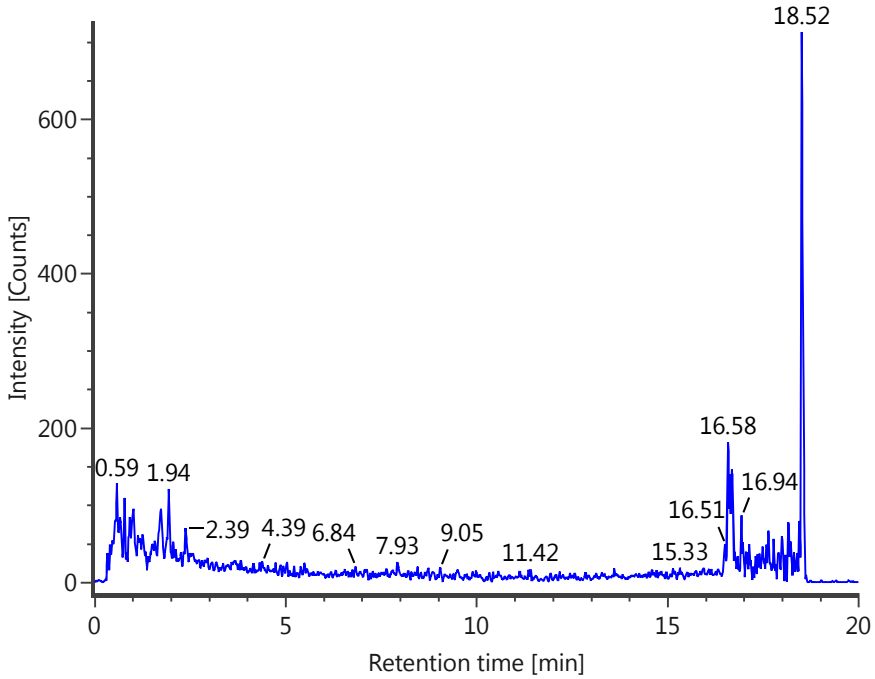
Item name: sample 2_01
Channel name: (3R,4R)-3,4-trans-7,2′-Dihydroxy-4′-methoxy-4-[(3R)-2′,7-dihydroxy-4′-methoxy-isoflavan-5′-yl]-isoflavan [+HCOO] : (16.3 PPM) 587.1918 : DT=7.37 to 8.02 ms



Item name: sample 2_01
Channel name: Identified Components

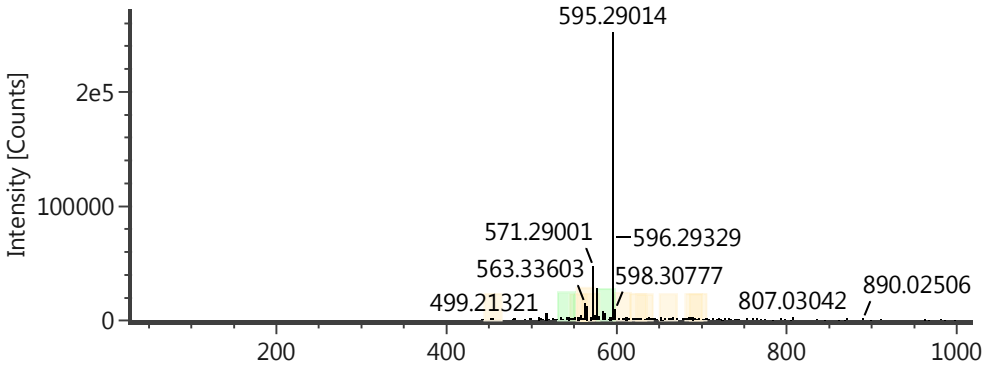


Item name: sample 2_01
Channel name: (3R,4R)-3,4-trans-7,2′-Dihydroxy-4′-methoxy-4-[(3R)-2′,7-dihydroxy-4′-methoxy-isoflavan-5′-yl]-isoflavan [+HCOO] : (16.3 PPM) 587.1918



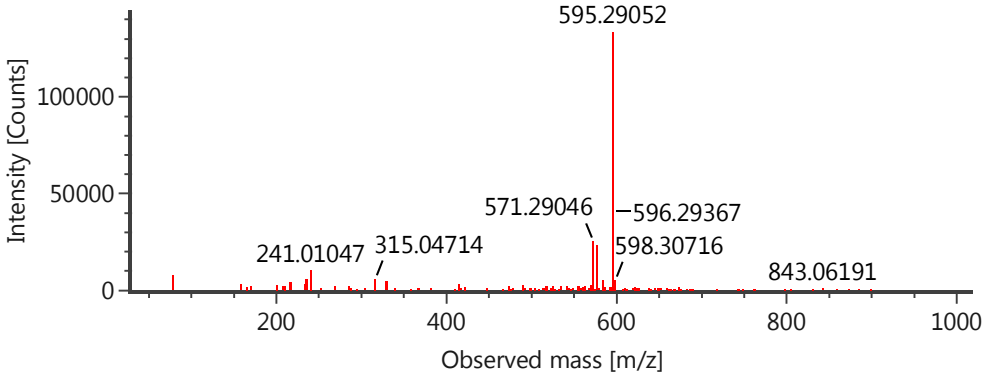
Item name: sample 2_01
Component name: (3R,4R)-3,4-trans-7,2′-Dihydroxy-4′-methoxy-4-[(3R)-2′,7-dihydroxy-4′-methoxy-isoflavan-5′-yl]-isoflavan

Channel name: Low energy : Time 18.5241 +/- 0.0245 minutes : Drift Times: 7.68 +/- 0.32, 7.68 +/- 0.32 ms



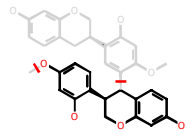
Item name: sample 2_01
Component name: (3R,4R)-3,4-trans-7,2′-Dihydroxy-4′-methoxy-4-[(3R)-2′,7-dihydroxy-4′-methoxy-isoflavan-5′-yl]-isoflavan

Channel name: High energy : Time 18.5241 +/- 0.0245 minutes : Drift Times: 7.59 +/- 0.32, 7.59 +/- 0.32 ms

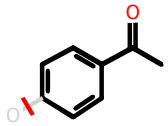


Fragmentation (high energy)

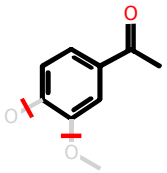
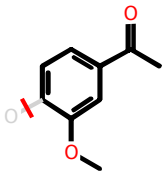
Item name: sample 2_01, Component name: (3R,4R)-3,4-trans-7,2′-Dihydroxy-4′-methoxy-4-[(3R)-2′,7-dihydroxy-4′-methoxy-isoflavan-5′-yl]-isoflavan

	Expected m/z	Status	Observed m/z	Mass error (mDa)	Mass error (ppm)	Detector counts	Observed RT (min)	Observed drift (ms)	Formula	Structure
1	253.05063	Theoretical	253.04936	-1.3	-5.043	111	18.50397	7.30854	C15H9O4	

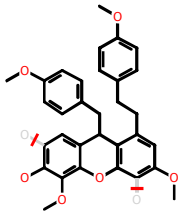
Item name: sample 2_01, Component name: 4-Hydroxyacetophenone

	Expected m/z	Status	Observed m/z	Mass error (mDa)	Mass error (ppm)	Detector counts	Observed RT (min)	Observed drift (ms)	Formula	Structure
1	119.05024	Theoretical	119.04989	-0.3	-2.889	123	2.87323	3.58951	C8H7O	

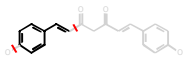
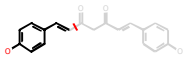
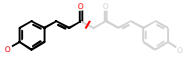
Item name: sample 2_01, Component name: Apocynin

	Expected m/z	Status	Observed m/z	Mass error (mDa)	Mass error (ppm)	Detector counts	Observed RT (min)	Observed drift (ms)	Formula	Structure
1	119.05024	Theoretical	119.04996	-0.3	-2.303	204	5.50998	5.77180	C8H7O	
2	147.04515	Theoretical	147.04470	-0.4	-3.051	1651	5.50901	5.77852	C9H7O2	

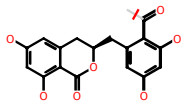
Item name: sample 2_01, Component name: Dendrocandin F

	Expected m/z	Status	Observed m/z	Mass error (mDa)	Mass error (ppm)	Detector counts	Observed RT (min)	Observed drift (ms)	Formula	Structure
1	507.18131	Theoretical	507.18202	0.7	1.397	283	1.35202	6.44646	C32H27O6	

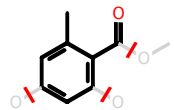
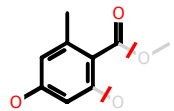
Item name: sample 2_01, Component name: Didemethoxylcurcumin

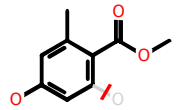
	Expected m/z	Status	Observed m/z	Mass error (mDa)	Mass error (ppm)	Detector counts	Observed RT (min)	Observed drift (ms)	Formula	Structure
1	103.05532	Theoretical	103.05518	-0.1	-1.348	287	5.50609	5.79067	C8H7	
2	119.05024	Theoretical	119.04996	-0.3	-2.303	204	5.50998	5.77180	C8H7O	
3	147.04515	Theoretical	147.04470	-0.4	-3.051	1651	5.50901	5.77852	C9H7O2	

Item name: sample 2_01, Component name: Feralolide

	Expected m/z	Status	Observed m/z	Mass error (mDa)	Mass error (ppm)	Detector counts	Observed RT (min)	Observed drift (ms)	Formula	Structure
1	328.05885	Theoretical	328.05758	-1.3	-3.883	955	16.69045	4.99620	C17H12O7	

Item name: sample 2_01, Component name: Methyl-β-orsellinate

	Expected m/z	Status	Observed m/z	Mass error (mDa)	Mass error (ppm)	Detector counts	Observed RT (min)	Observed drift (ms)	Formula	Structure
1	119.05024	Theoretical	119.04989	-0.3	-2.888	123	2.87323	3.58951	C8H7O	
2	135.04515	Theoretical	135.04466	-0.5	-3.621	170	2.87136	3.63555	C8H7O2	

	Expected m/z	Status	Observed m/z	Mass error (mDa)	Mass error (ppm)	Detector counts	Observed RT (min)	Observed drift (ms)	Formula	Structure
3	163.04007	Theoretical	163.03946	-0.6	-3.729	369	2.87034	3.65287	C9H7O3	

Item name: sample 2_01, Component name: Moracin E

	Expected m/z	Status	Observed m/z	Mass error (mDa)	Mass error (ppm)	Detector counts	Observed RT (min)	Observed drift (ms)	Formula	Structure
1	147.04515	Theoretical	147.04470	-0.5	-3.077	540	5.50823	7.25256	C9H7O2