Sample Info

Sample:	JL-7.wiff (sample 1)
Sample Name:	JL-7
Sample ID:	N/A
Comment:	N/A

Acquisition Info

Method Path:	D:\Analyst Data\Projects\BA\2021_03_30\Acquisition Methods\20211029-FUFANG+DAIXIEZU-NEG.dam
Batch Path:	D:\Analyst Data\Projects\BA\2021_03_30\Batch\20211223-JL.dab
Acquisition Date:	2021年12月26日
Acquisition Time:	12:09:58
User Name:	5600-PC\5600
Acquisition Method:	20211029-FUFANG+DAIXIEZU-NEG.dam
Rack:	1
Plate:	1
Vial:	88
Injection Volume:	2.00

Quantitation Info

Sample Type:	Unknown
Dilution Factor:	1.0000

Log Info

ExionLC Binary Gradient AD Pump :	N/A
AD Pump:	N/A
Serial#:	AB3AD5571187|AB3AD5571186
ROM Version:	3.21
ExionLC Autosampler AD Autosampler:	N/A
Serial#:	AB3AC5570538
ROM Version:	3.15
ExionLC Column Oven AD Column Oven:	N/A
Serial#:	AB3CT5570435
ROM Version:	3.11
ExionLC System Controller Controller:	N/A
Serial#:	ABCBM5570937
ROM Version:	3.40
Injection Volume used:	2.00 µl

Mass Spectrometer:	TripleTOF 5600-1
Config Table Version:	02
Firmware Version:	MIA4000 ------- MIL4000 MIB4000
Component Name:	Hybrid Quadrupole-TOF LC/MS/MS Mass Spectrometer
Component ID:	TripleTOF 5600+
Manufacturer:	AB Sciex Instruments
Model:	5035153/S
Serial Number:	BN25481802
Source Housing:	DuoSpray Ion Source
Dynamic Accumulation (Constant Counts Approach):	N/A
Candidates Sort Type:	1
Peak Intensity High End:	2000 cps
Accumulation Time For High Intensity Peaks:	50 ms

Time (from start of run):	00:00:01
Mass Spectrometer:	TripleTOF 5600-1
Start of Run - Detailed Status:	N/A
Vacuum Status:	At Pressure
Vacuum Gauge (10e-5 Torr):	3.5
Backing Pump:	Ok
Q1 Turbo Pump:	Normal
Q2/TOF Turbo Pump:	Normal
Sample Introduction Status:	Ready
Source/Ion Path Electronics:	On
Source Type:	DuoSpray Ion Source
Source Temperature (at setpoint):	550.0 C
Source Exhaust Pump:	Ok
Interface Heater:	Ready

Time (from start of run):	00:34:30
Mass Spectrometer:	TripleTOF 5600-1
End of Run - Detailed Status:	N/A
Vacuum Status:	At Pressure
Vacuum Gauge (10e-5 Torr):	3.5
Backing Pump:	Ok
Q1 Turbo Pump:	Normal
Q2/TOF Turbo Pump:	Normal
Sample Introduction Status:	Ready

Source/Ion Path Electronics:	On
Source Type:	DuoSpray Ion Source
Source Temperature (at setpoint):	550.0 C
Source Exhaust Pump:	Ok
Interface Heater:	Ready

IDA

With intensity greater than:	10
Switch after:	12 spectra
Use advanced settings:	True
Always exclude:	True
Exclude for:	0 sec
Mass tolerance units:	mDa
Mass tolerance:	50
Use inclusion list:	False
Use exclusion list:	False
Ignore peaks within:	6 Da
Real time:	None
Spectrum file:	aaa
Dynamic background subtraction:	True
Fragment intensity multiplier:	2
Maximum accumulation:	2 sec
Allow standard filters for Smart IDA:	True
Never exclude former target ions:	True
Exclude isotopes window:	4 Da

Period 1, Experiment 1

Experiment Type:	TOF MS
Num. Cycles:	2719
Polarity:	Negative
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Intensity Threshold:	1.00 cps
Settling Time:	0.0000 msec

Accumulation Time (sec):	0.1000
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-10.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRDx	28287.600
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	140.155

Start Mass:	100.0000
End Mass:	1250.0000

RF Transmission

Mass	*Time (%)*
80.00	49.9
200.00	50.1

Period 1, Experiment 2

Experiment Type:	TOF MS^2
Num. Cycles:	2719
Polarity:	Negative
Product :	IDA
Duration:	33.998 mins

Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	70.160

Start Mass: 50.0000

End Mass: 1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 3

Experiment Type:	TOF MS^2
Num. Cycles:	2719
Polarity:	Negative
Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000

CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	70.320

Start Mass: 50.0000
End Mass: 1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 4

Experiment Type:	TOF MS^2
Num. Cycles:	2719
Polarity:	Negative
Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec

MCA: No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	70.480

Start Mass: 50.0000
End Mass: 1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 5

Experiment Type: TOF MS^2
Num. Cycles: 2719
Polarity: Negative
Product : IDA

Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	70.640

Start Mass:	50.0000
End Mass:	1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 6

Experiment Type:	TOF MS^2
Num. Cycles:	2719
Polarity:	Negative
Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*

CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	70.800

Start Mass:	50.0000
End Mass:	1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 7

Experiment Type:	TOF MS^2
Num. Cycles:	2719
Polarity:	Negative
Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500

MR Pause: 1.0221 msec
MCA: No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	70.960

Start Mass: 50.0000
End Mass: 1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 8

Experiment Type: TOF MS^2
Num. Cycles: 2719
Polarity: Negative

Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	71.120

Start Mass:	50.0000
End Mass:	1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 9

Experiment Type:	TOF MS^2
Num. Cycles:	2719
Polarity:	Negative
Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	71.280

Start Mass: 50.0000
End Mass: 1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 10

Experiment Type:	TOF MS^2
Num. Cycles:	2719
Polarity:	Negative
Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec

Accumulation Time (sec): 0.0500
MR Pause: 1.0221 msec
MCA: No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	71.440

Start Mass: 50.0000
End Mass: 1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 11

Experiment Type: TOF MS^2
Num. Cycles: 2719

Polarity:	Negative
Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000

XA1	71.600

Start Mass: 50.0000
End Mass: 1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 12

Experiment Type:	TOF MS^2
Num. Cycles:	2719
Polarity:	Negative
Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps
Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	71.760

Start Mass: 50.0000
End Mass: 1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Period 1, Experiment 13

Experiment Type:	TOF MS^2
Num. Cycles:	2719
Polarity:	Negative
Product :	IDA
Duration:	33.998 mins
Period Cycle Time:	0.750 secs
Period Delay:	0.00 secs
Relative Start Time:	0.00 msec
Experiments in Period:	13
Scan Mode:	None
Num. Time Bins to Sum:	4
Used TDC Channels:	1 2 3 4
Resolution Q1:	Unit
Intensity Threshold:	0.00 cps

Settling Time:	0.0000 msec
Accumulation Time (sec):	0.0500
MR Pause:	1.0221 msec
MCA:	No

Experiment Parameters

Parameter	*Value*
CUR	35.000
GS1	55.000
GS2	55.000
ISVF	4500.000
TEM	550.000

Mass Range Parameters

Parameter	*Value*
CE	-35.000
CES	15.000
DP	-50.000
IDIx	0.000
IDUx	5.000
IRD	66.633
IRDx	28287.600
IRW	24.917
IRWx	24917.311
IWIx	0.000
IWUx	5.000
XA1	71.920

Start Mass:	50.0000
End Mass:	1250.0000

RF Transmission

Mass	*Time (%)*
40.00	50.0
130.00	50.0

Instrument Tables and Parameters

Resolution Table, Quad 1, Negative, Unit, TOF Resolution Mode: High Resolution

Last Modification Date Time:	March 19, 2019 13:41:02
IE1:	-2.000
VS1:	0.319
HST:	0.000
VS2:	0.000

Mass (Da)	*Offset Value*
44.998	62.375
411.260	62.510
585.385	62.513
933.637	62.522
1165.804	62.525

Resolution Table, Quad 1, Negative, Unit, TOF Resolution Mode: High Sensitivity

Last Modification Date Time:	March 19, 2019 13:40:07
IE1:	-2.000
VS1:	-0.072
HST:	-1.164
VS2:	0.000

Mass (Da)	*Offset Value*
44.998	62.375
411.260	62.510
585.385	62.513
933.637	62.522
1165.804	62.525

Mass Calibration Table, Quad 1, Negative, Unit Resolution

Last Modification Date Time:	March 19, 2019 13:02:16

Mass (Da)	*Dac Value*
44.998	1855
411.260	17204
585.385	24501
933.637	39099
1165.804	48833

TOF Mass Calibration Parameters

Polarity	*Scan*	*Slope*	*Delay (nsec)*
Positive	TOFMS	7.035336142532576300e-004	7.698454565179516700e-001
Positive	MS/MS High Resolution	7.035842328723026500e-004	7.701766605329759500e-001
Positive	MS/MS High Sensitivity	7.035497128210093900e-004	7.809775824287201700e-001
Negative	TOFMS	7.035135526785305600e-004	6.646054171925938100e-001
Negative	MS/MS High Resolution	7.035391323346215500e-004	6.531979174834904300e-001
Negative	MS/MS High Sensitivity	7.035348418494880300e-004	7.380599846958644200e-001

Show TOF Resolution Parameters in Manual Tune: Yes

Keyed Text

File was created with the software version: Analyst TF 1.7.1