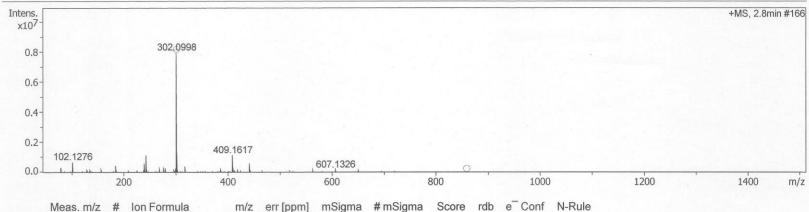
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

This journal is a The Royal Society of Chemistry 2022

15

## Mass Spectrum SmartFormula Report

**Analysis Info Acquisition Date** 2/24/2022 3:45:36 PM Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01165.d Method Operator Demo User esi pos low.m SK01165 Instrument 8255754.20198 Sample Name compact Comment **Acquisition Parameter** ESI Positive Set Nebulizer 0.3 Bar Source Type Ion Polarity Set Capillary 4500 V Set Dry Heater 200 °C Focus Not active 3.0 l/min Set End Plate Offset -500 V Set Dry Gas Scan Begin 50 m/z Set Charging Voltage 2000 V Set Divert Valve Scan End 1500 m/z Source Set Corona 0 nA Set APCI Heater 0°C



100.00

7.0

even

302.0999

C14H17NNaO5

302.0998

0.2

**S1** (keto:enol = 3:4)

## Mass Spectrum SmartFormula Report

**Analysis Info** Acquisition Date 2/24/2022 4:42:23 PM Analysis Name D:\Data\Data Lab\S. Yokoshima. Lab\Kitayama\SK01169.d Method esi pos low.m Operator Demo User Sample Name SK01169 Instrument compact 8255754.20198 Comment **Acquisition Parameter** Source Type ESI Positive Set Nebulizer Ion Polarity 0.3 Bar Focus Not active Set Capillary 4500 V Set Dry Heater 200 °C Scan Begin Set End Plate Offset -500 V Set Dry Gas 3.0 I/min 50 m/z Set Divert Valve Scan End Set Charging Voltage 2000 V 1500 m/z Source Set Corona 0 nA Set APCI Heater 0°C Intens. +MS, 8.1min #473 x105 2.5-441.3030 102.1291 2.0 243.1020 1.5-1.0 563.1145 186.2237 519.0879 651.1676 0.5 695.1945 0.0 200 400 600 800 1000 1200 1400 m/z

# mSigma

Score

100.00

rdb

11.0

even

C16H13NNaO5

Meas. m/z # Ion Formula

1

322.0686

m/z

322.0686

err [ppm]

-0.1

mSigma

n.a.

e Conf N-Rule

## Mass Spectrum SmartFormula Report

Analysis Info

D:\Data\Data Lab\S. Yokoshima. Lab\Kitayama\SK01167.d Analysis Name

Method esi pos low 150to2500.m Sample Name

Comment

SK01167

**Acquisition Date** 

3/2/2022 2:42:47 PM

Operator Instrument

Demo User compact

8255754.20198

**Acquisition Parameter** 

Source Type Focus Scan Begin Scan End

ESI Not active 50 m/z 2500 m/z

Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

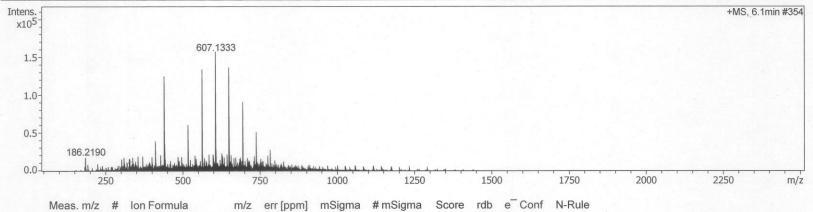
Positive 4500 V -500 V 2000 V 0 nA

100.00

7.0

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 l/min Source 0°C



332.1105

1 C15H19NNaO6

332.1105

-0.3

n.a.

## Mass Spectrum SmartFormula Report

### Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01168.d

Method esi\_pos\_low\_150to2500.m Sample Name SK01168

Comment

Acquisition Date

3/2/2022 1:46:40 PM

Operator Instrument

Demo User compact

8255754.20198

#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End ESI Not active 50 m/z 2500 m/z Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

-0.1

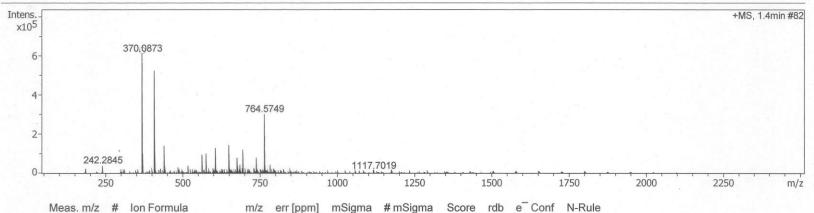
Positive 4500 V -500 V 2000 V 0 nA

100.00

7.0

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 I/min Source 0 °C



C15H16F3NNaO5

370.0873

370.0873

1

## Mass Spectrum SmartFormula Report

Analysis Info Acquisition Date

Analysis Name

Method Sample Name

esi\_pos\_low\_150to2500.m SK01129

Comment

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01129.d

Operator Instrument Demo User

3/2/2022 4:08:52 PM

compact

8255754.20198

**Acquisition Parameter** 

Source Type Focus Scan Begin Scan End

ESI Not active 50 m/z 2500 m/z

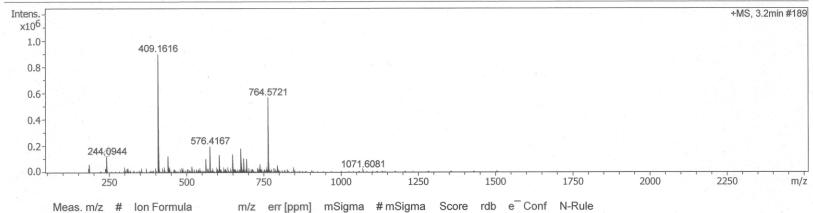
Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

Positive 4500 V -500 V 2000 V 0 nA

100.00

6.0

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater 0.3 Bar 200 °C 3.0 I/min Source 0°C



C12H15NNaO3 244.0944

244.0944

1

0.3

## Compound Spectrum SmartFormula Report

#### Analysis Info

Analysis Name

D:\Data\Data Lab\S. Yokoshima. Lab\Kitayama\SK01171.d

Method Sample Name Comment

esi pos low.m SK01171

Acquisition Date

2/14/2022 3:43:51 PM

Operator Instrument Demo User compact

8255754.20198

#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End

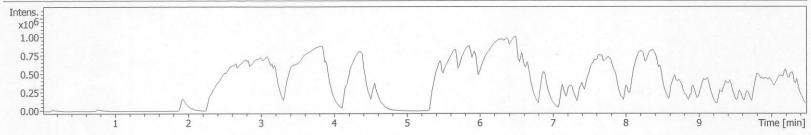
ESI Not active 50 m/z 2500 m/z

C14H11NNaO3 264.0631

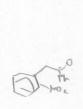
Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

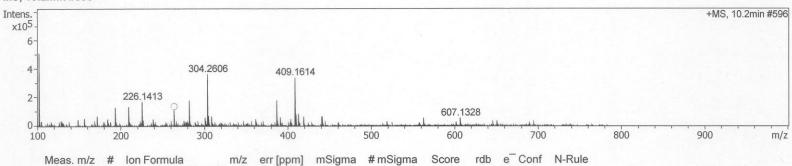
Positive 4500 V -500 V 2000 V 0 nA

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater 0.3 Bar 200 °C 3.0 l/min Source 0°C



#### +MS, 10.2min #596





100.00

10.0

even

SK01171.d

Bruker Compass DataAnalysis 5.1

printed:

-0.1

2/14/2022 4:01:31 PM

3.4

demo by:

Page 1 of 1

## Compound Spectrum SmartFormula Report

#### Analysis Info

Acquisition Date

2/14/2022 4:03:33 PM

Analysis Name Method Sample Name

Comment

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01172.d

Operator

Demo User

Instrument

compact

8255754.20198

#### **Acquisition Parameter**

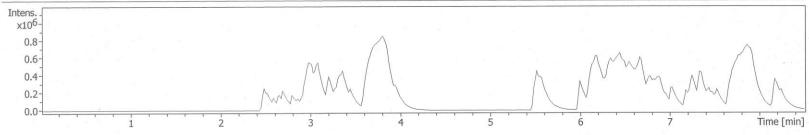
Source Type Focus Scan Begin Scan End ESI Not active 50 m/z 2500 m/z

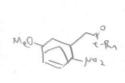
esi\_pos\_low.m

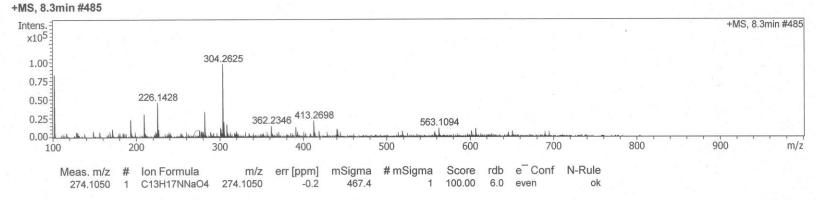
SK01172

lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona Positive 4500 V -500 V 2000 V 0 nA Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 l/min Source 0 °C







SK01172.d

Bruker Compass DataAnalysis 5.1

printed:

2/14/2022 4:17:20 PM

by: demo

Page 1 of 1

## Mass Spectrum SmartFormula Report

Analysis Info

Acquisition Date

3/2/2022 1:54:03 PM

Analysis Name Method Sample Name

Comment

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01170.d

Operator Instrument Demo User compact

8255754.20198

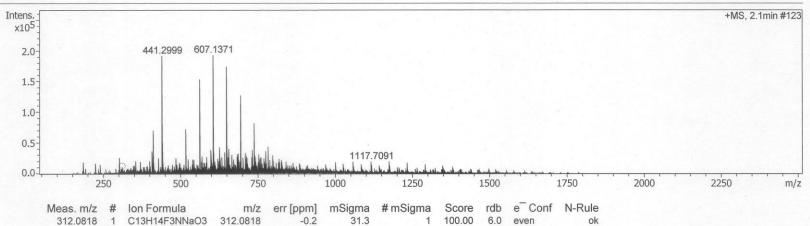
**Acquisition Parameter** 

Source Type Focus Scan Begin Scan End ESI Not active 50 m/z 2500 m/z

SK01170

esi pos low 150to2500.m

Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona Positive 4500 V -500 V 2000 V 0 nA Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater 0.3 Bar 200 °C 3.0 I/min Source 0 °C



## Mass Spectrum SmartFormula Report

#### Analysis Info

Analysis Name Method

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01032.d

esi\_pos\_low\_150to2500.m me SK01032

Sample Name Comment Acquisition Date

3/2/2022 4:15:44 PM

Operator Instrument

Demo User compact

8255754.20198

#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End ESI Not active 50 m/z 2500 m/z Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona Positive 4500 V -500 V 2000 V 0 nA

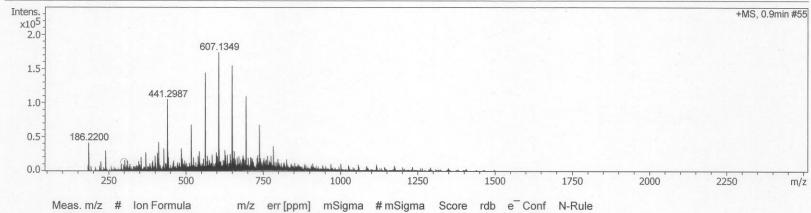
100.00

6.0

even

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 I/min Source 0 °C



C. E. B.

C16H23NNaO3

300.1570

300.1570

-0.0

n.a.

## Compound Spectrum SmartFormula Report

#### Analysis Info

Analysis Name

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01149.d

Method Sample Name

Comment

SK01149

esi\_pos\_low.m

Instrument

**Acquisition Date** 

2/14/2022 4:19:13 PM

Operator

Demo User compact

8255754.20198

#### **Acquisition Parameter**

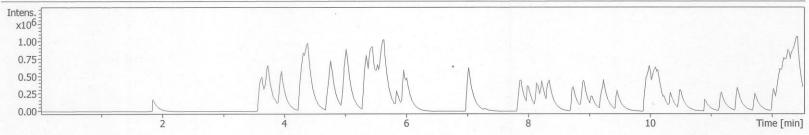
Source Type Scan Begin Scan End

ESI Not active 50 m/z 2500 m/z

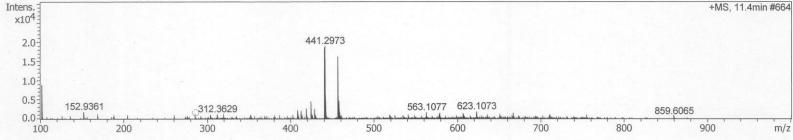
Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

Positive 4500 V -500 V 2000 V 0 nA

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater 0.3 Bar 200 °C 3.0 I/min Source 0°C



#### +MS, 11.4min #664



# mSigma Score rdb e Conf N-Rule Meas. m/z # Ion Formula m/z err [ppm] mSigma 1 C15H21NNaO3 286.1414 -0.3 48.2 100.00 6.0 even

### Compound Spectrum SmartFormula Report

#### Analysis Info

Analysis Name Method Sample Name

Comment

D:\Data\Data Lab\S. Yokoshima. Lab\Kitayama\SK03023 P.d

esi\_pos\_low\_150to2500.m

SK03023 P

Acquisition Date

9/11/2022 7:05:52 PM

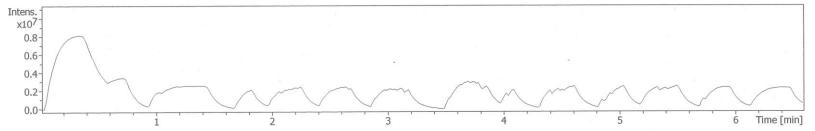
Operator Instrument Demo User compact

8255754.20198

#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End ESI Not active 50 m/z 2500 m/z lon Polarity Set Capillary Set End Plate Offset Set Collision Cell RF

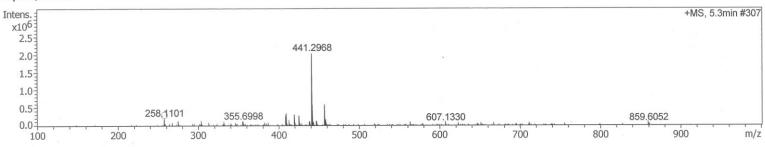
Positive 4500 V -500 V 1300.0 Vpp Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve 0.3 Bar 200 °C 3.0 I/min Source



#	RT [min]	Area	Int. Type	I	S/N	Trace	Max. m/z	FWHM [min]
1	5.3	0		2034477		BPC +All MS	441.2968	

#### Cmpd 1, 5.3 min





e Conf N-Rule mSigma # mSigma Meas. m/z # Ion Formula Score rdb m/z err [ppm] -0.3 10.3 100.00 6.0 even ok C13H17NNaO3 258.1101 258.1101

#### **Analysis Info**

Analysis Name

D:\Data\Data Lab\S. Yokoshima. Lab\Kitayama\SK01067.d

Method

Sample Name Comment

esi pos low.m SK01067

m/z

320.1257

err [ppm] -0.1

Operator Instrument

Acquisition Date

Demo User

compact

8255754.20198

#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End

ESI Not active 50 m/z 1500 m/z

Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

mSigma

7.0

Positive 4500 V -500 V 2000 V 0 nA

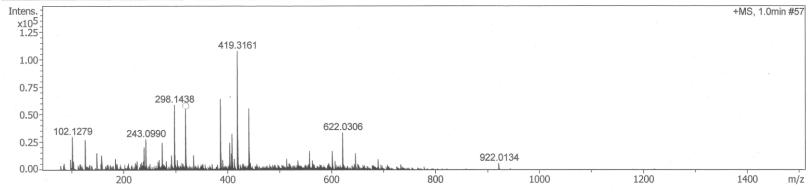
Score

100.00

10.0

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater 0.3 Bar 200 °C 3.0 l/min Source 0°C

2/24/2022 5:07:28 PM



# mSigma

Ion Formula

C18H19NNaO3

Meas. m/z

320.1257

#

e Conf N-Rule

## Mass Spectrum SmartFormula Report

#### Analysis Info

Analysis Name

D:\Data\Data Lab\S. Yokoshima. Lab\Kitayama\SK01145.d

esi pos low 150to2500.m

Sample Name Comment

Method

SK01145

Operator Instrument

**Acquisition Date** 

Demo User

compact

3/2/2022 2:55:50 PM

8255754.20198

#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End

ESI Not active 50 m/z 2500 m/z

Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

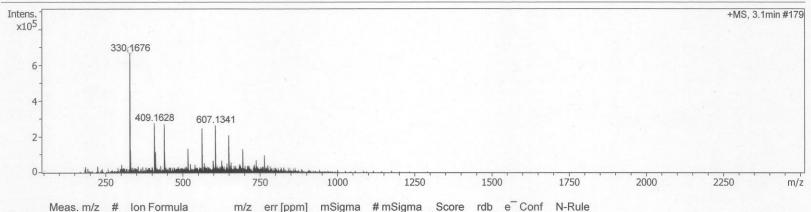
Positive 4500 V -500 V 2000 V 0 nA

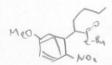
100.00

6.0

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 l/min Source 0°C





330.1676

C17H25NNaO4

-0.2

Analysis Info

Acquisition Date

3/2/2022 2:32:08 PM

Analysis Name Method D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01139 again.d

Operator

Demo User

Sample Name Comment esi\_pos\_low\_150to2500.m SK01139 again

Instrument

compact

8255754.20198

#### **Acquisition Parameter**

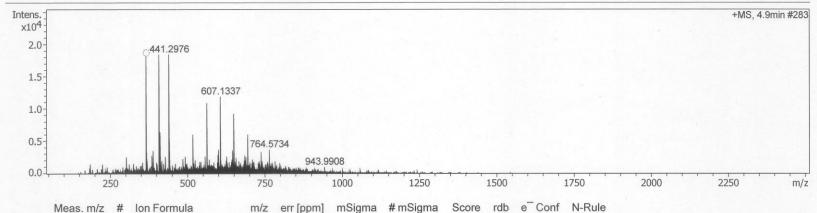
Source Type Focus Scan Begin Scan End ESI Not active 50 m/z 2500 m/z lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

0.1

1.5

Positive 4500 V -500 V 2000 V 0 nA

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater 0.3 Bar 200 °C 3.0 I/min Source 0 °C



368.1444

C17H22F3NNaO3

368.1444

1

6.0

S12b

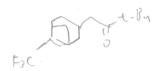
## Mass Spectrum SmartFormula Report

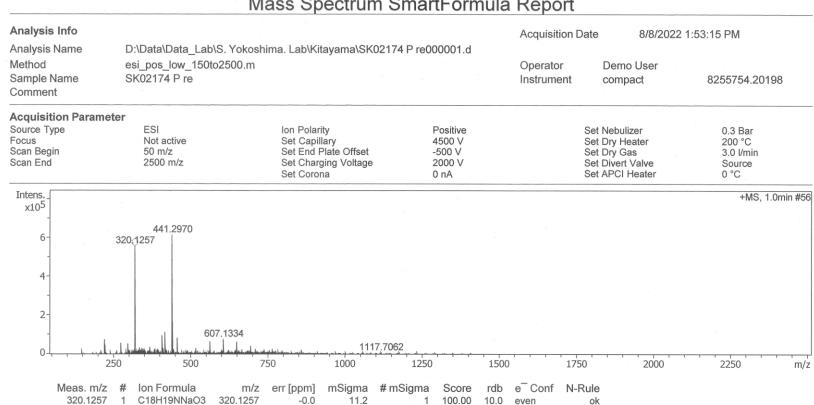
Analysis Info				Acquisition D	ate 8/8/2022	2 2:03:38 PM	
Analysis Name Method Sample Name Comment	D:\Data\Data_Lab\S. Yolesi_pos_low_150to2500. SK02170 P re	oshima. Lab\Kitayama\SK02170 F m	re000001.d	Operator Instrument	Demo User compact	8255754.201	198
Acquisition Paramet Source Type Focus Scan Begin Scan End	ESI Not active 50 m/z 2500 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	0.3 Bar 200 °C 3.0 l/min Source 0 °C	
Intens. x105 2.0-1.5-1.0-1.0-1.0-1.0-1.0-1.0-1.0-1.0-1.0-1.0	441.2960 99 607.1324					+MS, 1	1.7min #

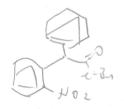


S12c

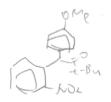
Analysis Info Acquisition Date 8/8/2022 2:09:25 PM D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02161 P000001.d **Analysis Name** Method esi pos low 150to2500.m Operator Demo User Sample Name SK02161 P Instrument compact 8255754.20198 Comment **Acquisition Parameter** Source Type ESI Ion Polarity Positive Set Nebulizer 0.3 Bar Focus Not active Set Capillary 4500 V Set Dry Heater 200 °C Scan Begin Set End Plate Offset -500 V Set Dry Gas 3.0 l/min 50 m/z Scan End 2500 m/z Set Charging Voltage 2000 V Set Divert Valve Source Set APCI Heater Set Corona 0 nA 0°C Intens. +MS, 2.1min #122 x10<sup>5</sup> 441.2962 267:0968 607.1325 1001.6261 500 1250 1500 1750 2000 2250 250 750 1000 m/z err [ppm] mSigma #mSigma Score rdb e Conf N-Rule Meas. m/z # Ion Formula m/z 267.0968 1 C13H15F3NaO 267.0967 -0.42.2 100.00 5.0 even







Analysis Info Acquisition Date 8/8/2022 2:24:58 PM D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02173 P000001.d Analysis Name Method esi\_pos\_low\_150to2500.m Operator Demo User SK02173 P Instrument compact 8255754.20198 Sample Name Comment **Acquisition Parameter** ESI Ion Polarity Positive Set Nebulizer 0.3 Bar Source Type 200 °C Not active Set Capillary 4500 V Set Dry Heater Focus Set End Plate Offset 3.0 I/min -500 V Set Dry Gas Scan Begin 50 m/z 2000 V Set Divert Valve Source Scan End 2500 m/z Set Charging Voltage 0°C Set APCI Heater Set Corona 0 nA +MS, 0.9min #53 Intens. x106 350.1363 2.0 1.5-1.0-441.2973 0.5 607.1340 242.0829 1000 1750 2000 2250 750 1250 1500 m/z 250 500 mSigma rdb e Conf N-Rule err [ppm] # mSigma Score Meas. m/z # Ion Formula m/z 100.00 350.1363 C19H21NNaO4 350.1363 -0.1 2.0 10.0 even



#### Analysis Info Acquisition Date 8/8/2022 2:29:19 PM D:\Data\Data Lab\S. Yokoshima. Lab\Kitayama\SK02163 P000001.d Analysis Name Method esi pos low 150to2500.m Operator Demo User Sample Name SK02163 P Instrument 8255754.20198 compact Comment **Acquisition Parameter** Source Type ESI Ion Polarity Positive Set Nebulizer 0.3 Bar Focus Not active Set Capillary 4500 V Set Dry Heater 200 °C Scan Begin Set End Plate Offset -500 V Set Dry Gas 3.0 I/min 50 m/z 2500 m/z 2000 V Set Divert Valve Scan End Set Charging Voltage Source 0°C Set Corona 0 nA Set APCI Heater Intens. +MS, 0.8min #48 x106 388,1131 0.8 0.6-0.4 0.2 607.1332 223.1242 1059.6648 250 500 750 1000 1250 1500 1750 2000 2250 m/z mSigma #mSigma e Conf N-Rule Meas. m/z # Ion Formula m/z err [ppm] Score rdb 388.1131 3.1 100.00 C19H18F3NNaO3 388.1131 0.0 10.0 ok

#### Analysis Info

Analysis Name

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02063 P.d

esi\_pos\_low\_150to2500.m

Sample Name Comment

Method

Operator Instrument

**Acquisition Date** 

Demo User

compact

5/25/2022 4:11:17 PM

8255754.20198

#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End

ESI Not active 50 m/z 2500 m/z

SK02063 P

Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

Positive 4500 V -500 V 2000 V 0 nA

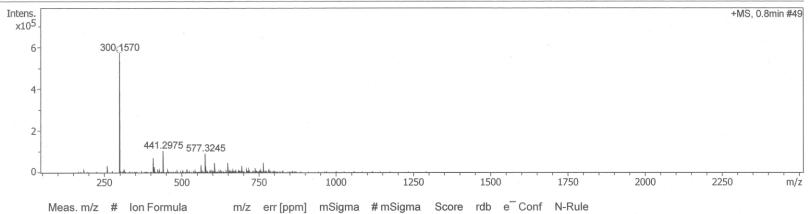
rdb

6.0

even

100.00

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater 0.3 Bar 200 °C 3.0 I/min Source 0°C





C16H23NNaO3

Meas. m/z #

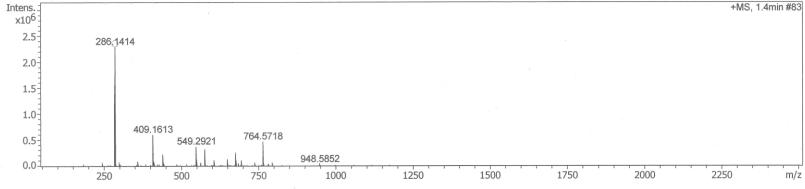
300.1570

m/z err [ppm]

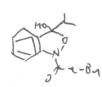
0.0

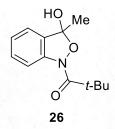
0.4

Analysis Info				Acquisition D	ate 5/25/202	2 3:09:33 PM
Analysis Name	D:\Data\Data_Lab\S. Yol	koshima. Lab\Kitayama\SK02093	Prere.d			
Method Sample Name Comment	esi_pos_low_150to2500. SK02093 Prere	m		Operator Instrument	Demo User compact	8255754.20198
cquisition Paran	neter					
ource Type	ESI	Ion Polarity	Positive		Set Nebulizer	0.3 Bar
ocus	Not active	Set Capillary	4500 V		Set Dry Heater	200 °C
can Begin	50 m/z	Set End Plate Offset	-500 V		Set Dry Gas	3.0 l/min
can End	2500 m/z	Set Charging Voltage	2000 V		Set Divert Valve	Source
		Set Corona	0 nA		Set APCI Heater	0 °C









### Compound Spectrum SmartFormula Report

#### Analysis Info

Comment

Analysis Name Method Sample Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK03025 P2.d

esi\_pos\_low\_150to2500.m

SK03025 P2

Acquisition Date

9/11/2022 7:17:22 PM

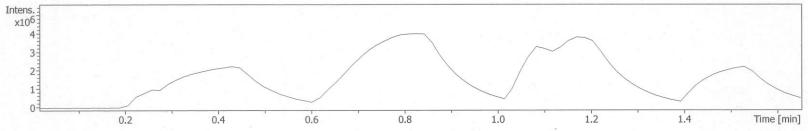
Operator Instrument Demo User compact

8255754.20198

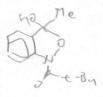
#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End ESI Not active 50 m/z 2500 m/z lon Polarity Set Capillary Set End Plate Offset Set Collision Cell RF

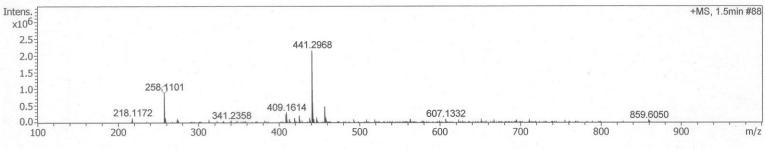
Positive 4500 V -500 V 1300.0 Vpp Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve 0.3 Bar 200 °C 3.0 I/min Source



# RT [min] Area Int. Type I S/N Trace Max. m/z FWHM [min]
1 1.5 0 2141378 BPC +All MS 441.2968

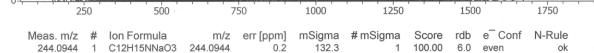


#### Cmpd 1, 1.5 min



Meas. m/z # Ion Formula m/z err [ppm] mSigma #mSigma Score rdb e Conf N-Rule 258.1101 1 C13H17NNaO3 258.1101 -0.2 3.7 1 100.00 6.0 even ok

Analysis Info				Acquisition D	oto	2 4:37:37 PM
•	DiData Data Lable Value	ahima LahliftanamaleK02000	) amainO d	Acquisition D	2 4.37.37 PIVI	
Analysis Name D:\Data\Data_Lab\S. Yokos  Method esi_pos_low_150to2500.m  Sample Name SK02098 again2  Comment		iima. Lab\Kitayama\SK02098 again2.d		Operator Instrument	Demo User compact	8255754.20198
Acquisition Param	neter					
Source Type Focus Scan Begin Scan End	ESI Not active 50 m/z 2500 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	0.3 Bar 200 °C 3.0 l/min Source 0 °C
Intens. x10 <sup>4</sup> -						+MS, 1.8min
6-	441.2972					
07	607.1338					



186.2202

2000

2250

m/z

#### 28a (keto:hemiacetal = 1:2

## Mass Spectrum SmartFormula Report

#### Analysis Info Analysis Name

Method

D:\Data\Data Lab\S. Yokoshima. Lab\Kitayama\SK02177 P000001.d

esi\_pos\_low\_150to2500.m

Sample Name Comment

Operator Instrument

**Acquisition Date** 

Demo User

compact

8/8/2022 2:37:52 PM

8255754.20198

#### **Acquisition Parameter**

Source Type
Focus
Scan Begin
Scan End

**ESI** Not active 50 m/z 2500 m/z

C18H19NNaO3

SK02177 P

Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

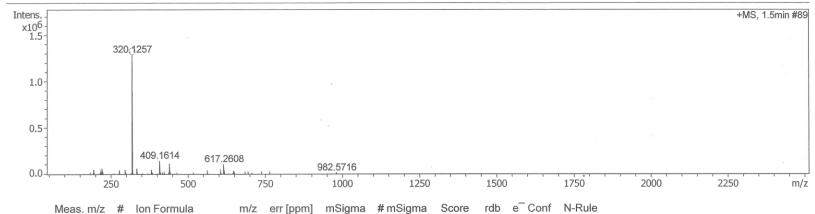
Positive 4500 V -500 V 2000 V 0 nA

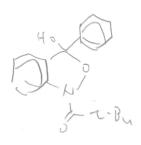
100.00

10.0

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 l/min Source 0°C



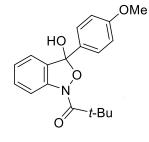


320.1257

320.1257

3.3

ok



#### **Analysis Info**

Analysis Name

Method Sample Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02176 P6000001.d

esi\_pos\_low\_150to2500.m

SK02176 P6

Acquisition Date

8/8/2022 1:19:53 PM

Operator Instrument

e Conf

even

N-Rule

ok

Demo User

compact

8255754.20198

### 28b (keto:hemiacetal = 3:1)Comment

#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End

ESI Not active 50 m/z 2500 m/z

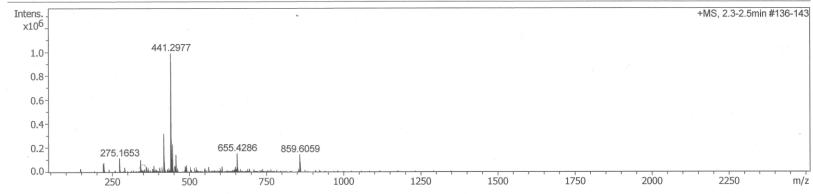
Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

mSigma

45.7

Positive 4500 V -500 V 2000 V 0 nA

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater 0.3 Bar 200 °C 3.0 l/min Source 0 °C



# mSigma

Score

100.00

rdb

10.0

m/z

350.1363

Ion Formula

C19H21NNaO4

Meas. m/z #

350.1363

err [ppm]

-0.1

## 28c

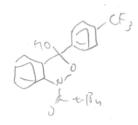
Mass Spectrum SmartFormula Report **Analysis Info** Acquisition Date 8/8/2022 2:58:39 PM D:\Data\Data Lab\S. Yokoshima. Lab\Kitayama\SK02180 P rere000001.d Analysis Name Method esi\_pos\_low\_150to2500.m Operator Demo User Sample Name SK02180 P rere Instrument 8255754.20198 compact Comment **Acquisition Parameter** Source Type ESI Ion Polarity Positive Set Nebulizer 0.3 Bar 4500 V Focus Not active Set Capillary Set Dry Heater 200 °C Set End Plate Offset -500 V 3.0 I/min Scan Begin 50 m/z Set Dry Gas Scan End 2500 m/z Set Charging Voltage 2000 V Set Divert Valve Source Set APCI Heater 0°C Set Corona 0 nA Intens. +MS, 1.7min #99 x10<sup>5</sup> 1.5-388,1131 1.0 607.1339 0.5 223.1256

1250

1500

Meas. m/z # Ion Formula m/z err [ppm] mSigma #mSigma Score rdb e Conf N-Rule 388.1131 1 C19H18F3NNaO3 388.1131 0.0 2.2 1 100.00 10.0 even ok

1000



750

500

250

1750

2000

2250

m/z

## Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name

Method Sample Name esi\_pos\_low\_150to2500.m

Comment

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02059 P.d

SK02059 P

Acquisition Date

5/25/2022 4:15:17 PM

Operator Instrument Demo User compact

8255754.20198

**Acquisition Parameter** 

Source Type Focus Scan Begin Scan End

ESI Not active 50 m/z 2500 m/z

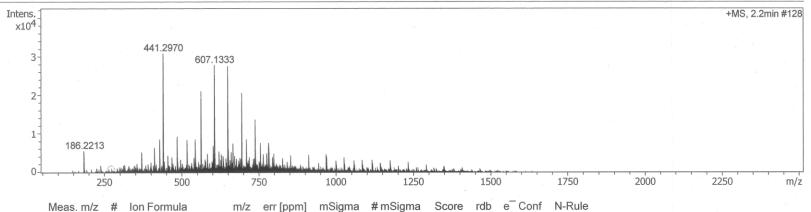
Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

Positive 4500 V -500 V 2000 V 0 nA

100.00

6.0

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater 0.3 Bar 200 °C 3.0 l/min Source 0°C





1 C14H19NNaO3

272.1257

272.1257

-0.0

n.a.

Analysis Info

Acquisition Date

5/25/2022 3:54:29 PM

Analysis Name Method

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02062 P.d

Operator Instrument Demo User

compact

8255754.20198

Sample Name Comment

**Acquisition Parameter** 

Source Type Focus Scan Begin Scan End

ESI Not active 50 m/z 2500 m/z

SK02062 P

esi\_pos\_low\_150to2500.m

Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

Positive 4500 V -500 V 2000 V 0 nA

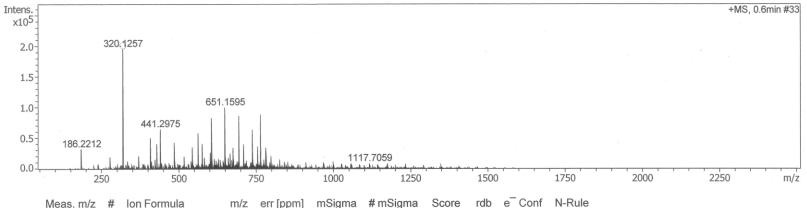
100.00

10.0

even

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 l/min Source 0°C



C18H19NNaO3 320.1257

320.1257

1

0.2

## Mass Spectrum SmartFormula Report

Analysis Info *t*-Bu

Analysis Name

Method esi pos low 150to2500.m

Sample Name Comment

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02070 P.d

SK02070 P

Acquisition Date

5/25/2022 3:22:26 PM

Operator Instrument

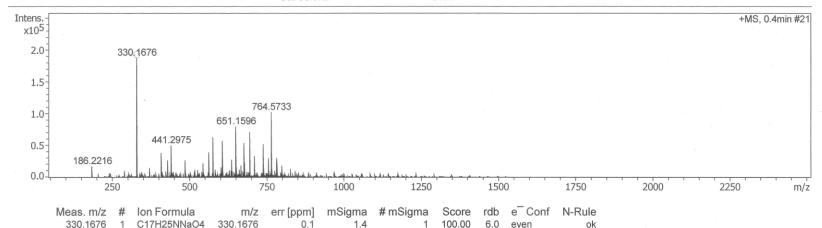
Demo User

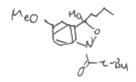
compact

8255754.20198

#### **Acquisition Parameter**

Source Type ESI Ion Polarity Positive Set Nebulizer 0.3 Bar Not active Set Capillary 4500 V Set Dry Heater 200 °C Focus Set End Plate Offset -500 V Set Dry Gas 3.0 l/min Scan Begin 50 m/z Scan End 2500 m/z Set Charging Voltage 2000 V Set Divert Valve Source Set APCI Heater 0°C Set Corona 0 nA





Analy	212	Into
Alla!	1010	11110

Analysis Name

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02071 Prere.d

Method

Sample Name Comment

esi\_pos\_low\_150to2500.m

SK02071 Prere

Acquisition Date

5/25/2022 3:16:14 PM

Operator Instrument Demo User

compact

8255754.20198

#### **Acquisition Parameter**

Source Type Focus Scan Begin Scan End

ESI Not active 50 m/z 2500 m/z

C17H22F3NNaO3

368.1444

Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona

-0.1

19.7

Positive 4500 V -500 V 2000 V 0 nA

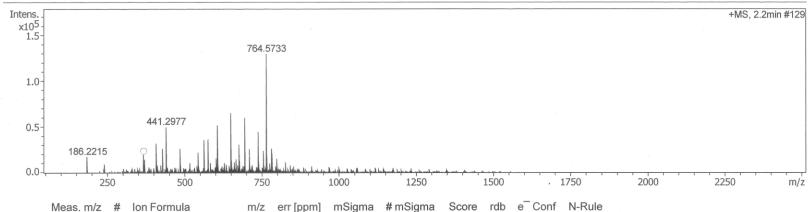
100.00

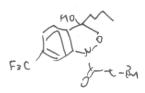
6.0

even

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 I/min Source 0°C





368.1444

1

## Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name Method D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01132 2.d

esi\_pos\_low\_150to2500.m SK01132 2

Sample Name Comment

Acquisition Date

3/3/2022 3:05:52 PM

Operator Instrument Demo User compact

8255754.20198

**Acquisition Parameter** 

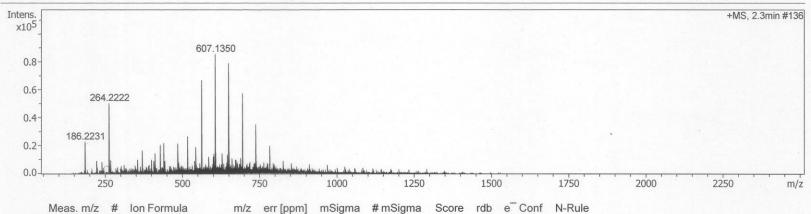
Source Type Focus Scan Begin Scan End ESI Not active 50 m/z 2500 m/z lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona Positive 4500 V -500 V 2000 V 0 nA

100.00

8.0

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 I/min Source 0 °C





256.0580

1 C12H11NNaO4

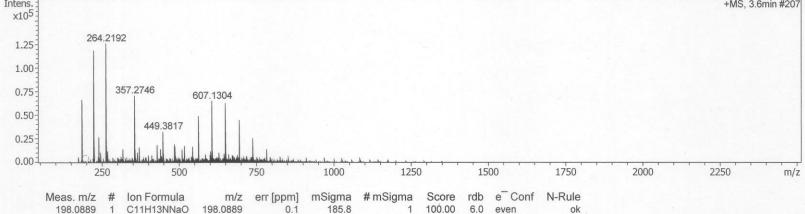
256.0580

0.2

n.a.

## Mass Spectrum SmartFormula Report

Analysis Info				Acquisition D	Date 3/3/2022	2:35:46 PM
Analysis Name	D:\Data\Data_Lab\S. Y	okoshima. Lab\Kitayama\SK01052	: 3.d			
Method Sample Name Comment	esi_pos_low_150to250 SK01052 3	0.m		Operator Instrument	Demo User compact	8255754.20198
Acquisition Param	neter					
Source Type	ESI	Ion Polarity	Positive		Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V		Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V		Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V		Set Divert Valve	Source
		Set Corona	0 nA		Set APCI Heater	0 °C





# Mass Spectrum SmartFormula Report

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Alla	IVSIS	IIIIO

Analysis Name D:

D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01212.d

Method esi\_pos\_low\_150to2500.m Sample Name SK01212

Comment

Acquisition Date

3/2/2022 3:34:42 PM

Operator Instrument Demo User compact

ct 8255754.20198

#### **Acquisition Parameter**

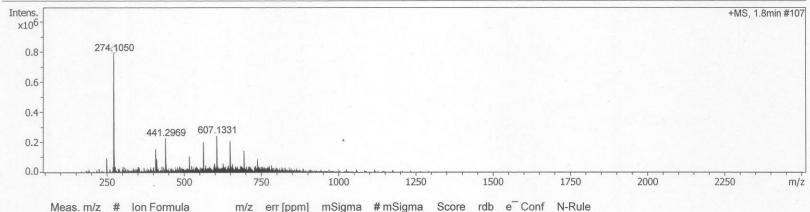
Source Type Focus Scan Begin Scan End ESI Not active 50 m/z 2500 m/z Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona Positive 4500 V -500 V 2000 V 0 nA

100.00

6.0 even

Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater

0.3 Bar 200 °C 3.0 l/min Source 0 °C





274.1050

C13H17NNaO4

274.1050 1

-0.2

1.3

ok

nalysis Info				Acquisition D	ate 3/3/2022	2:42:57 PM
nalysis Name	D:\Data\Data_Lab\S. Y					
ethod ample Name omment	esi_pos_low_150to250 SK01213	Operator Instrument	Demo User compact	8255754.20198		
cquisition Par	ameter					
ource Type ocus can Begin can End	ESI Not active 50 m/z 2500 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	0.3 Bar 200°C 3.0 l/min Source 0°C
Intens. 1						+MS, 2.0min #
	225.1968					
	25.1500					
4-						
2-						
	318.1421 607.13	33				



Mass Spectrum SmartFormula Report

Analysis Info				Acquisition	Date 3/3/2022	3:21:14 PM
Analysis Name	D:\Data\Data_Lab\S. Yo	okoshima. Lab\Kitayama\SK01214	3.d	, ioquious.		
Method Sample Name Comment	esi_pos_low_150to2500 SK01214 3	Operator Instrument	Demo User compact	8255754.20198		
Acquisition Paran	neter					
Source Type Focus Scan Begin Scan End	ESI Not active 50 m/z 2500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	0.3 Bar 200 °C 3.0 l/min Source 0 °C
Intens. x106						+MS, 4.1min
0.8-	409.1599					
0.6-						
0.4	607.131	3				
0.2-	264.2199	764.5714				

1250

1500



1000

250

1750

2000

2250

m/z