

15

## Mass Spectrum SmartFormula Report

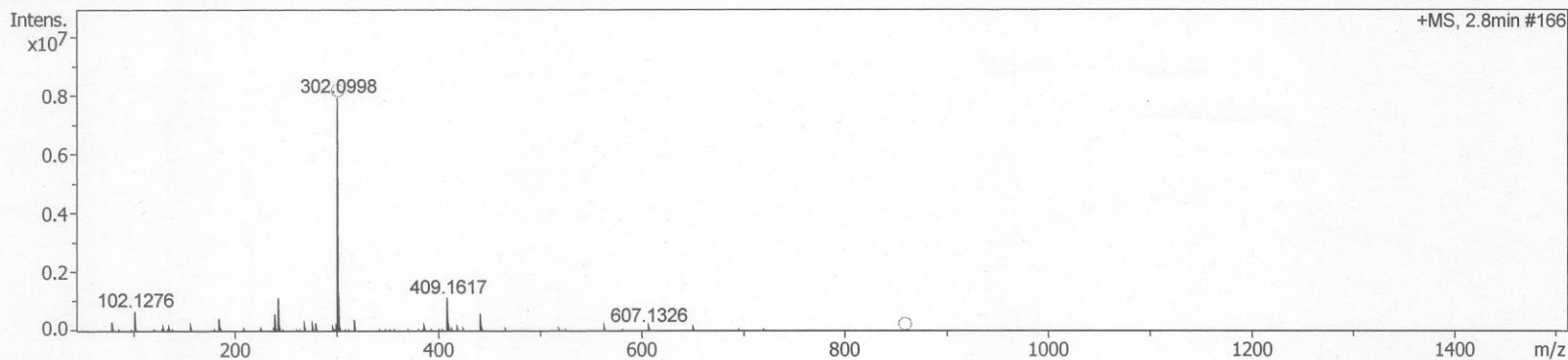
### Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01165.d  
Method esi\_pos\_low.m  
Sample Name SK01165  
Comment

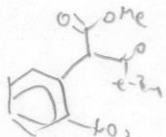
Acquisition Date 2/24/2022 3:45:36 PM  
Operator Demo User  
Instrument compact 8255754.20198

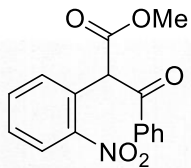
### Acquisition Parameter

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	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
302.0998	1	C <sub>14</sub> H <sub>17</sub> NNaO <sub>5</sub>	302.0999	0.2	3.2	1	100.00	7.0	even	ok





S1 (keto:enol = 3:4)

## Mass Spectrum SmartFormula Report

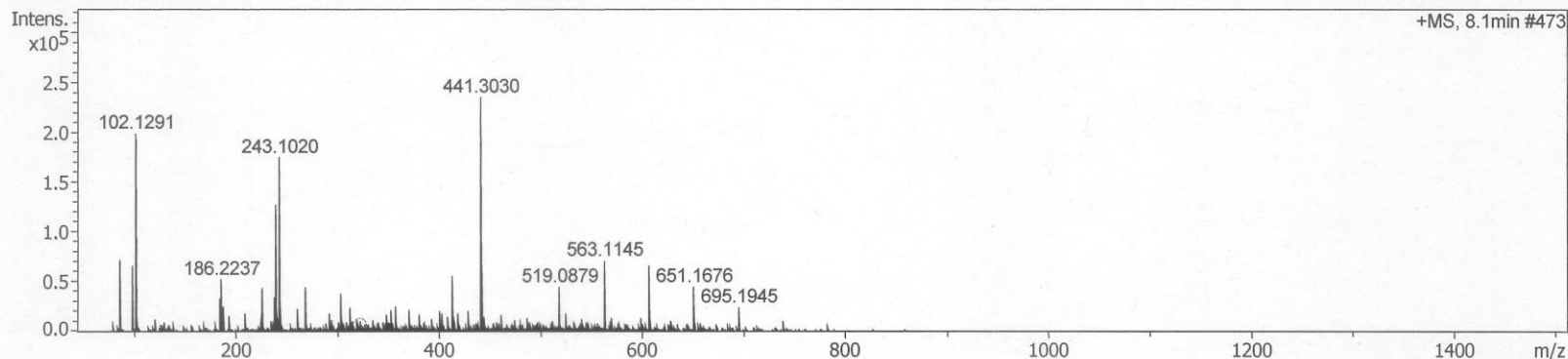
### Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01169.d  
 Method esi\_pos\_low.m  
 Sample Name SK01169  
 Comment

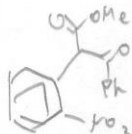
Acquisition Date 2/24/2022 4:42:23 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

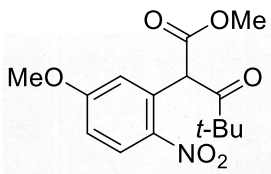
### Acquisition Parameter

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	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
322.0686	1	C <sub>16</sub> H <sub>13</sub> NNaO <sub>5</sub>	322.0686	-0.1	n.a.	1	100.00	11.0	even	ok





S2

# Mass Spectrum SmartFormula Report

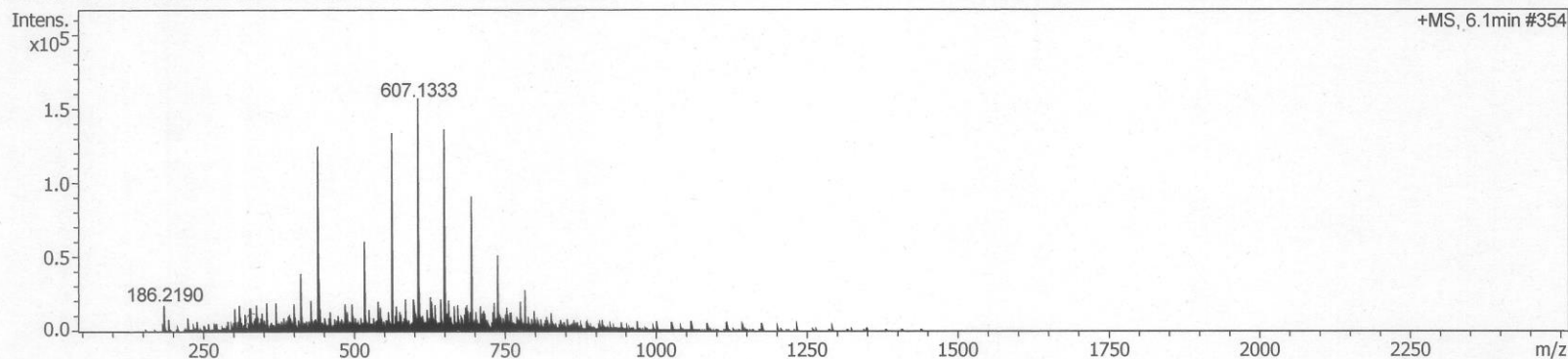
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01167.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK01167  
 Comment

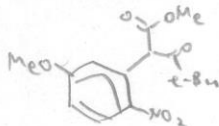
Acquisition Date 3/2/2022 2:42:47 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

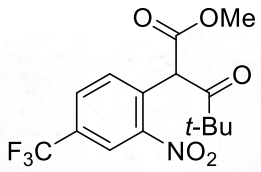
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
332.1105	1	C <sub>15</sub> H <sub>19</sub> NNaO <sub>6</sub>	332.1105	-0.3	n.a.	1	100.00	7.0	even	ok





S3

# Mass Spectrum SmartFormula Report

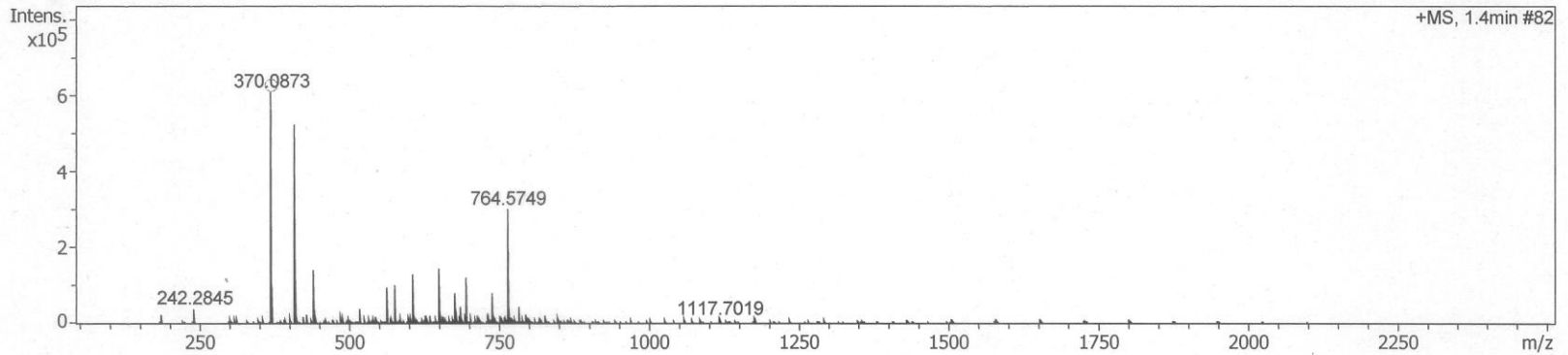
## Analysis Info

Analysis Name: D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01168.d  
 Method: esi\_pos\_low\_150to2500.m  
 Sample Name: SK01168  
 Comment:

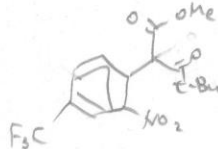
Acquisition Date: 3/2/2022 1:46:40 PM  
 Operator: Demo User  
 Instrument: compact  
 8255754.20198

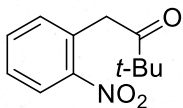
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
370.0873	1	C <sub>15</sub> H <sub>16</sub> F <sub>3</sub> NNaO <sub>5</sub>	370.0873	-0.1	2.8	1	100.00	7.0	even	ok





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# Mass Spectrum SmartFormula Report

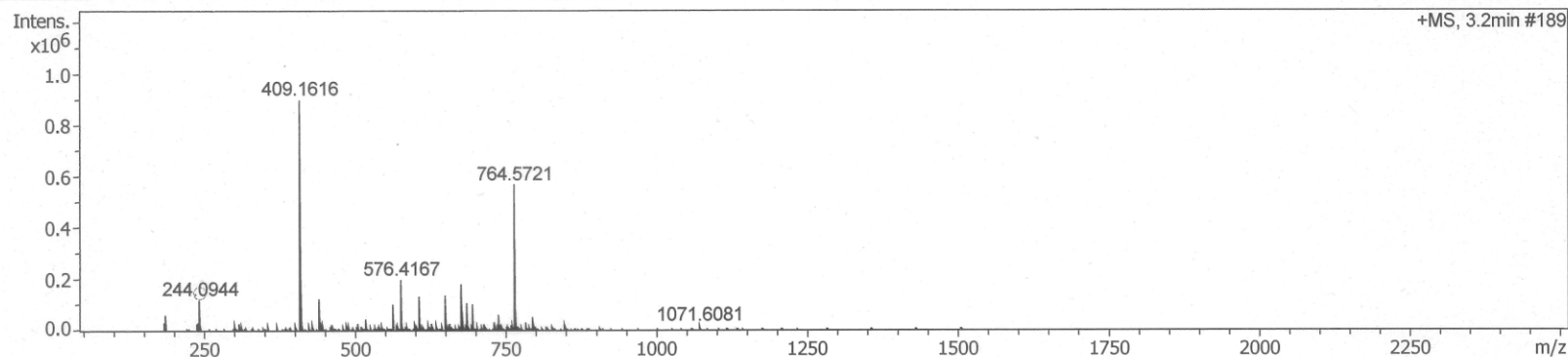
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01129.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK01129  
 Comment

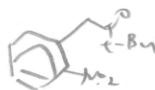
Acquisition Date 3/2/2022 4:08:52 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

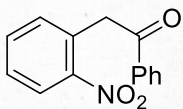
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
244.0944	1	C <sub>12</sub> H <sub>15</sub> NNaO <sub>3</sub>	244.0944	0.3	5.0	1	100.00	6.0	even	ok





S4

# Compound Spectrum SmartFormula Report

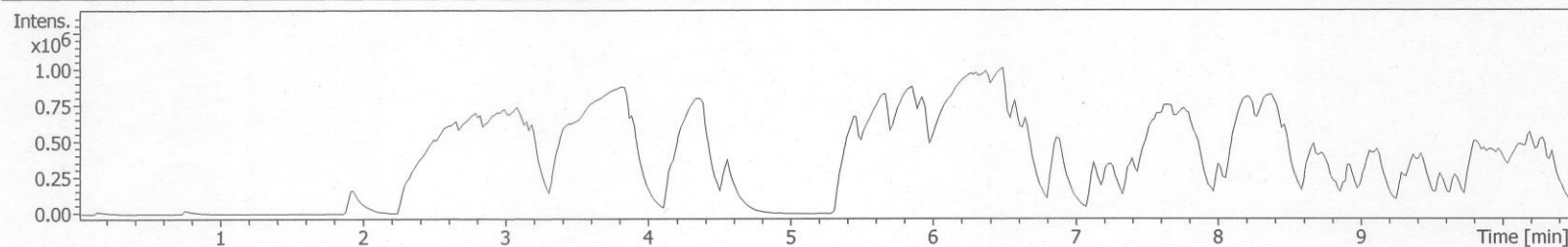
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01171.d  
 Method esi\_pos\_low.m  
 Sample Name SK01171  
 Comment

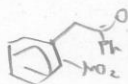
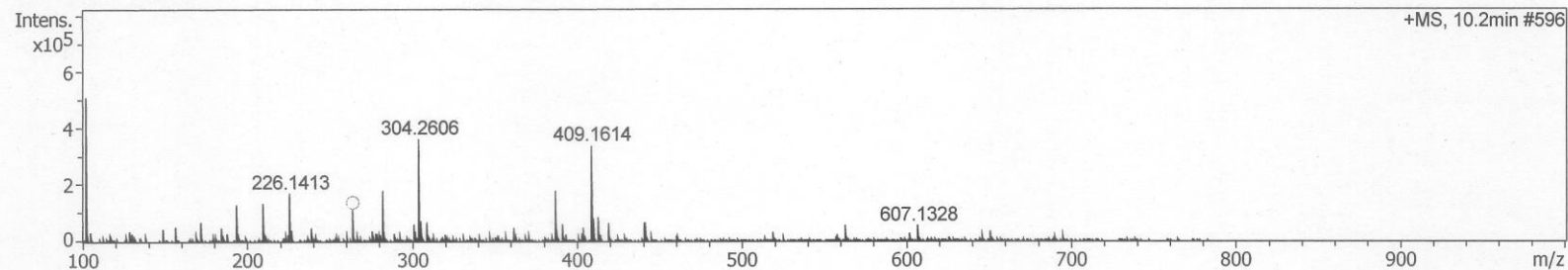
Acquisition Date 2/14/2022 3:43:51 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

## Acquisition Parameter

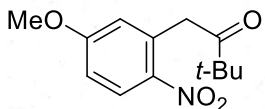
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



## +MS, 10.2min #596



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
264.0631	1	C14H11NNaO3	264.0631	-0.1	3.4	1	100.00	10.0	even	ok



S5

# Compound Spectrum SmartFormula Report

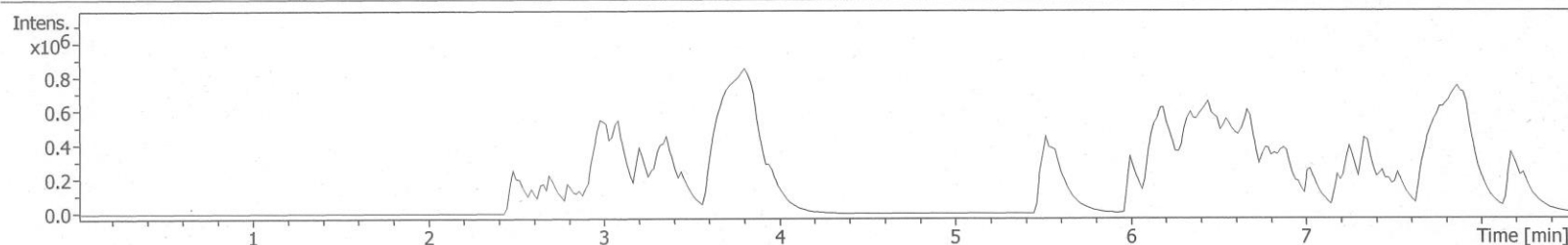
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01172.d  
 Method esi\_pos\_low.m  
 Sample Name SK01172  
 Comment

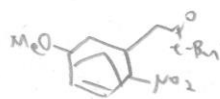
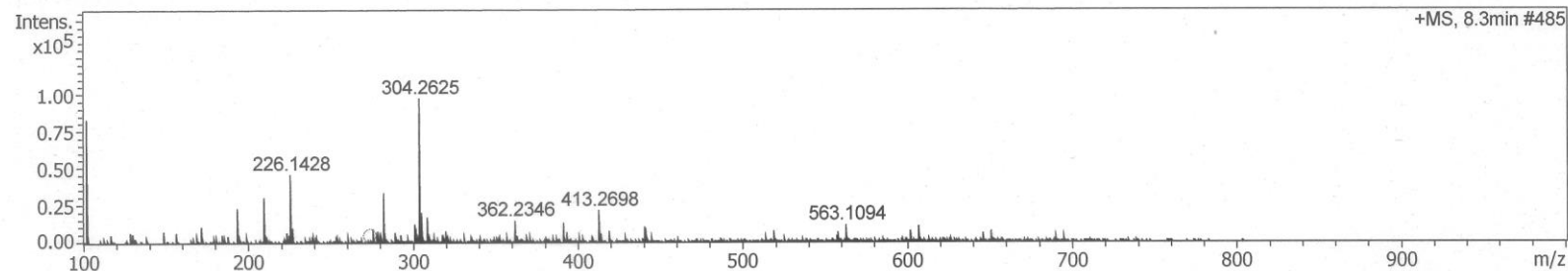
Acquisition Date 2/14/2022 4:03:33 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

## Acquisition Parameter

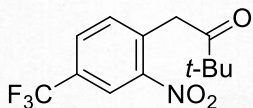
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



## +MS, 8.3min #485



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
274.1050	1	C13H17NNaO4	274.1050	-0.2	467.4	1	100.00	6.0	even	ok



S6

# Mass Spectrum SmartFormula Report

## Analysis Info

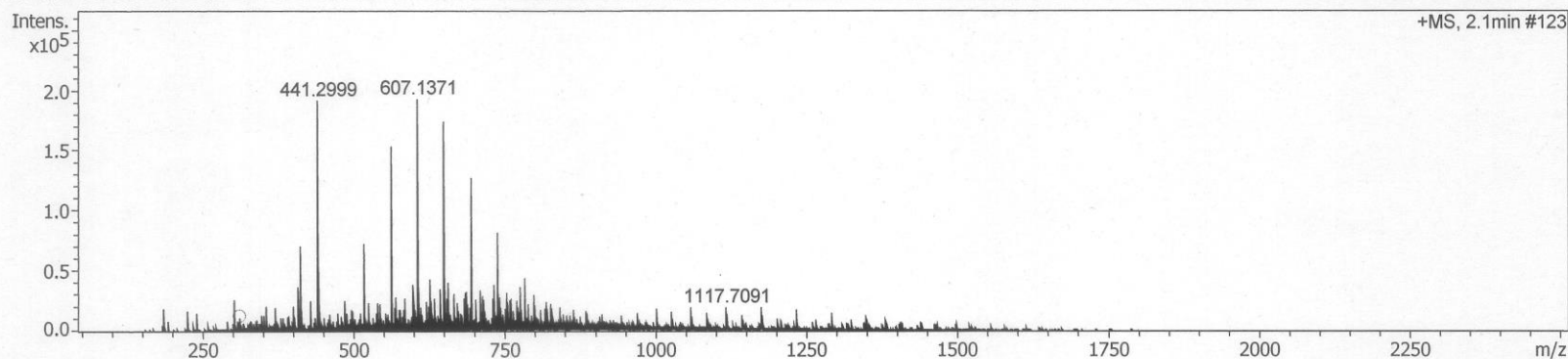
Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01170.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK01170  
 Comment

Acquisition Date 3/2/2022 1:54:03 PM

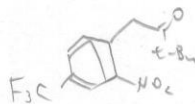
Operator Demo User  
 Instrument compact 8255754.20198

## Acquisition Parameter

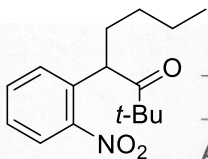
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
312.0818	1	C13H14F3NNaO3	312.0818	-0.2	31.3	1	100.00	6.0	even	ok







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# Mass Spectrum SmartFormula Report

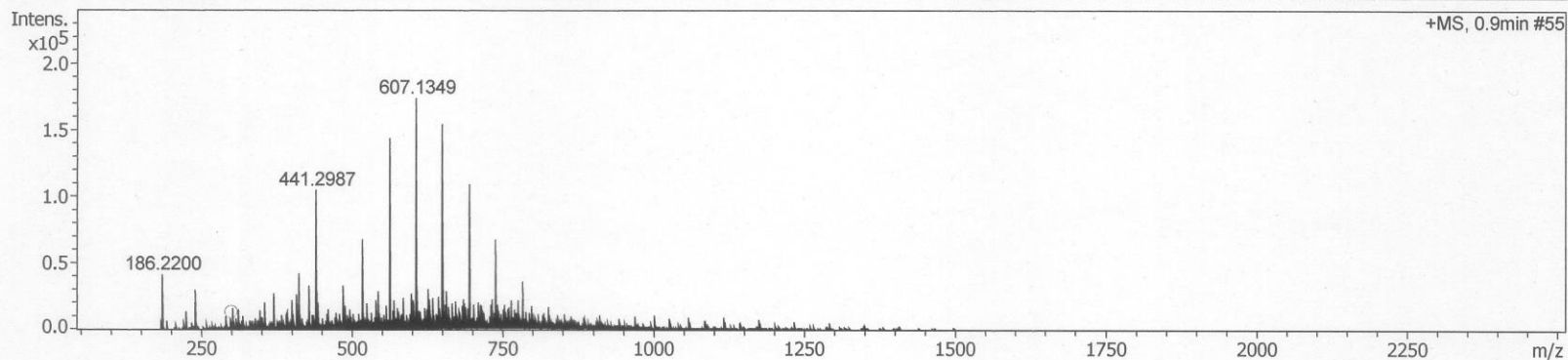
## Analysis Info

Analysis Name: D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01032.d  
 Method: esi\_pos\_low\_150to2500.m  
 Sample Name: SK01032  
 Comment:

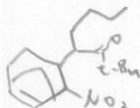
Acquisition Date: 3/2/2022 4:15:44 PM  
 Operator: Demo User  
 Instrument: compact  
 8255754.20198

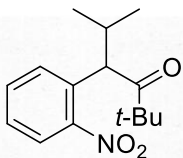
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
300.1570	1	C <sub>16</sub> H <sub>23</sub> NNaO <sub>3</sub>	300.1570	-0.0	n.a.	1	100.00	6.0	even	ok





S7

# Compound Spectrum SmartFormula Report

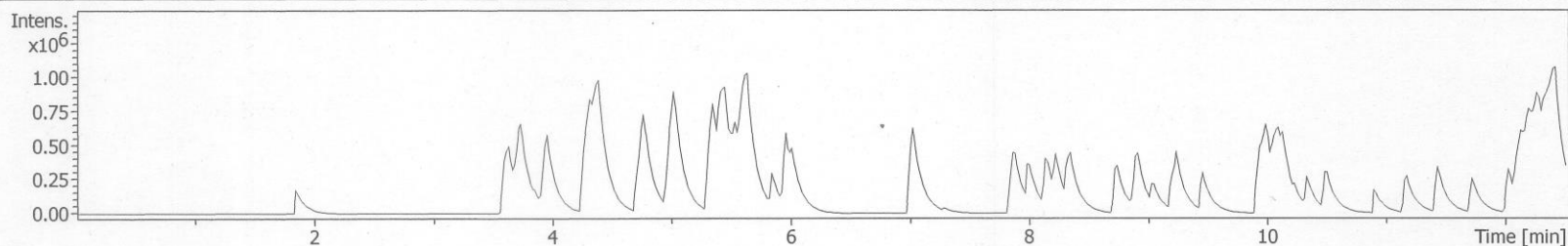
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01149.d  
 Method esi\_pos\_low.m  
 Sample Name SK01149  
 Comment

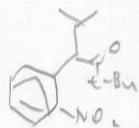
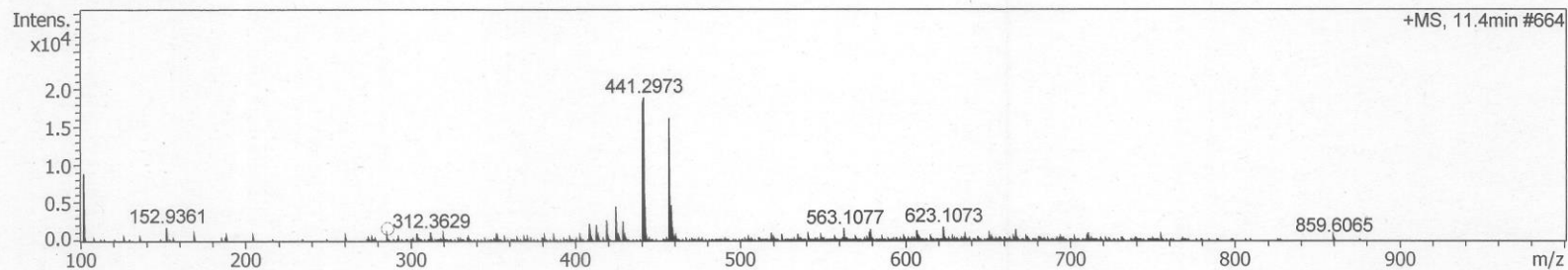
Acquisition Date 2/14/2022 4:19:13 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

## Acquisition Parameter

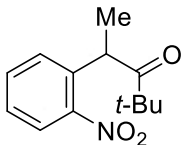
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



## +MS, 11.4min #664



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
286.1414	1	C <sub>15</sub> H <sub>21</sub> NNaO <sub>3</sub>	286.1414	-0.3	48.2	1	100.00	6.0	even	ok



S8

# Compound Spectrum SmartFormula Report

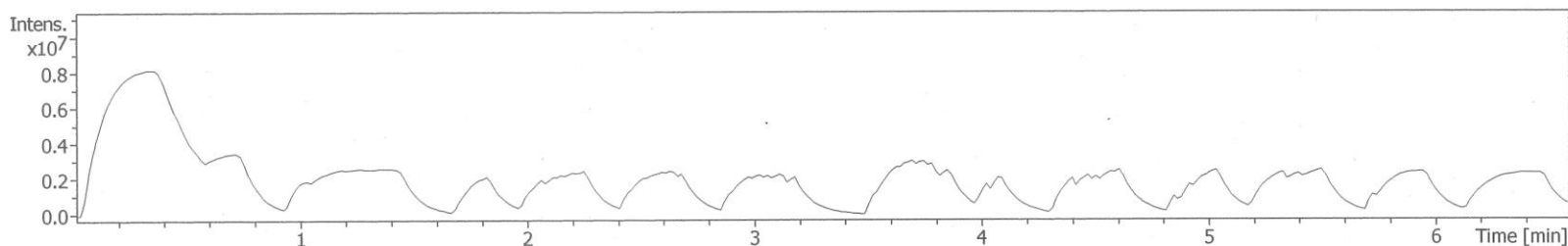
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK03023 P.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK03023 P  
 Comment

Acquisition Date 9/11/2022 7:05:52 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

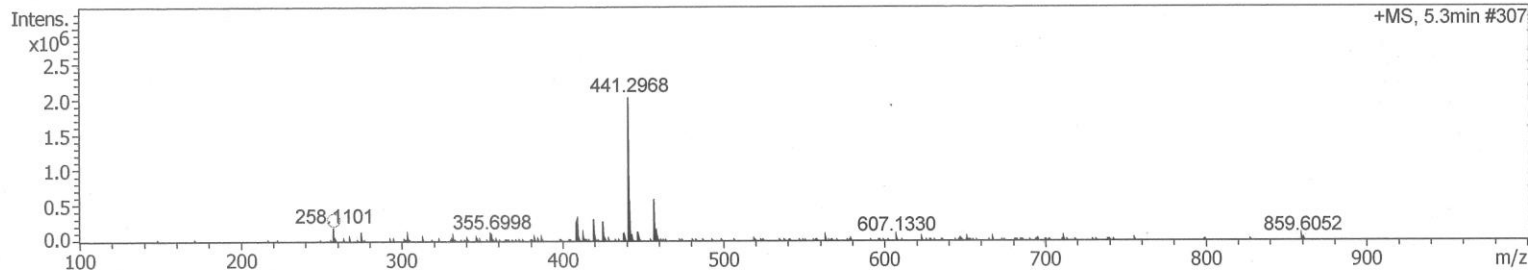
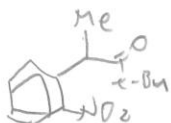
## Acquisition Parameter

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	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	1300.0 Vpp	Set Divert Valve	Source

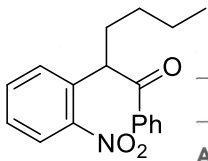


#	RT [min]	Area	Int. Type	I	S/N	Trace	Max. m/z	FWHM [min]
1	5.3	0		2034477		BPC +All MS	441.2968	

## Cmpd 1, 5.3 min



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
258.1101	1	C13H17NNaO3	258.1101	-0.3	10.3	1	100.00	6.0	even	ok



S9

# Mass Spectrum SmartFormula Report

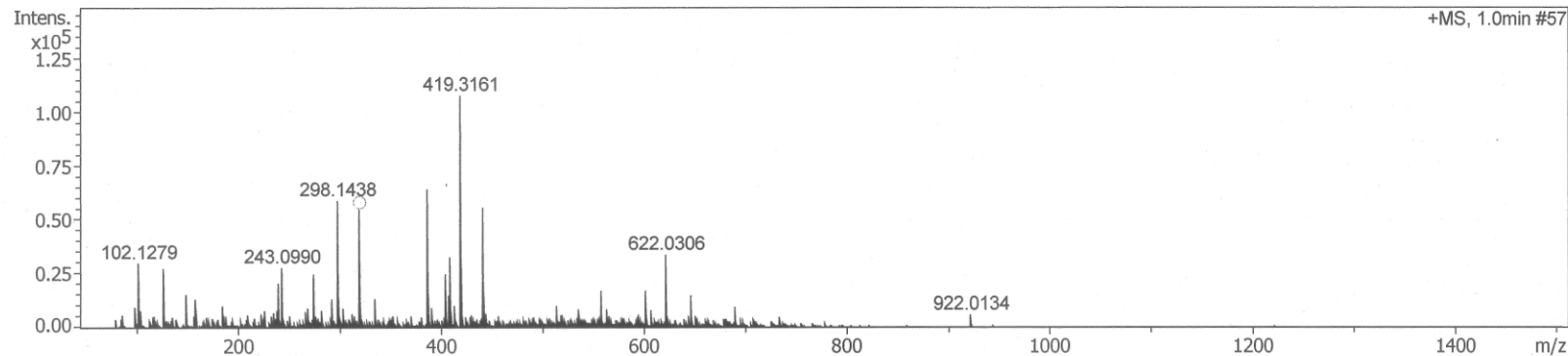
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01067.d  
 Method esi\_pos\_low.m  
 Sample Name SK01067  
 Comment

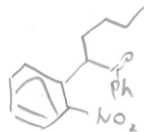
Acquisition Date 2/24/2022 5:07:28 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

## 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	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
320.1257	1	C18H19NNaO3	320.1257	-0.1	7.0	1	100.00	10.0	even	ok





S10

# Mass Spectrum SmartFormula Report

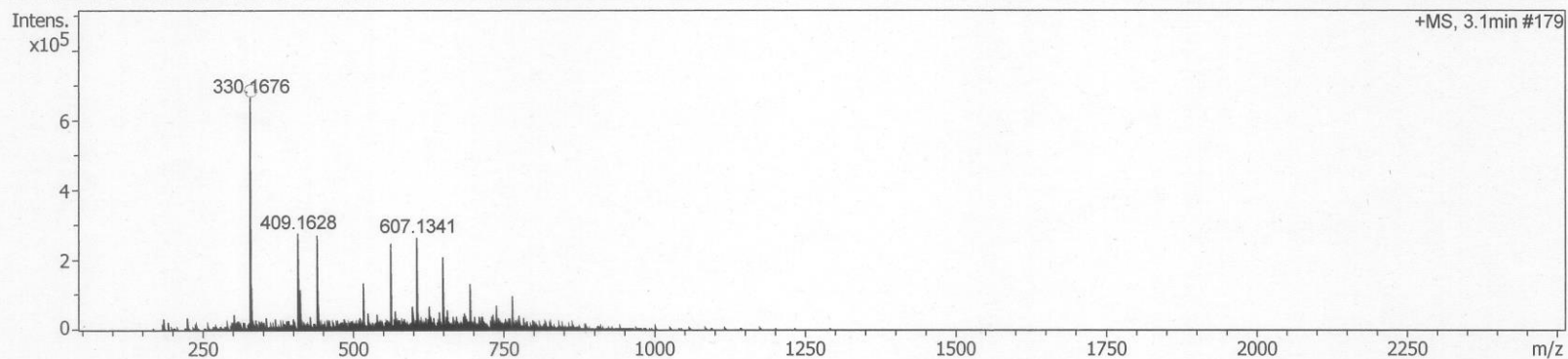
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01145.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK01145  
 Comment

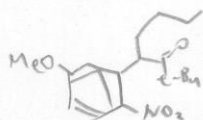
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 Operator Demo User  
 Instrument compact 8255754.20198

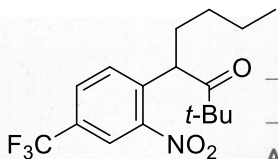
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
330.1676	1	C17H25NNaO4	330.1676	-0.2	5.8	1	100.00	6.0	even	ok





S11

# Mass Spectrum SmartFormula Report

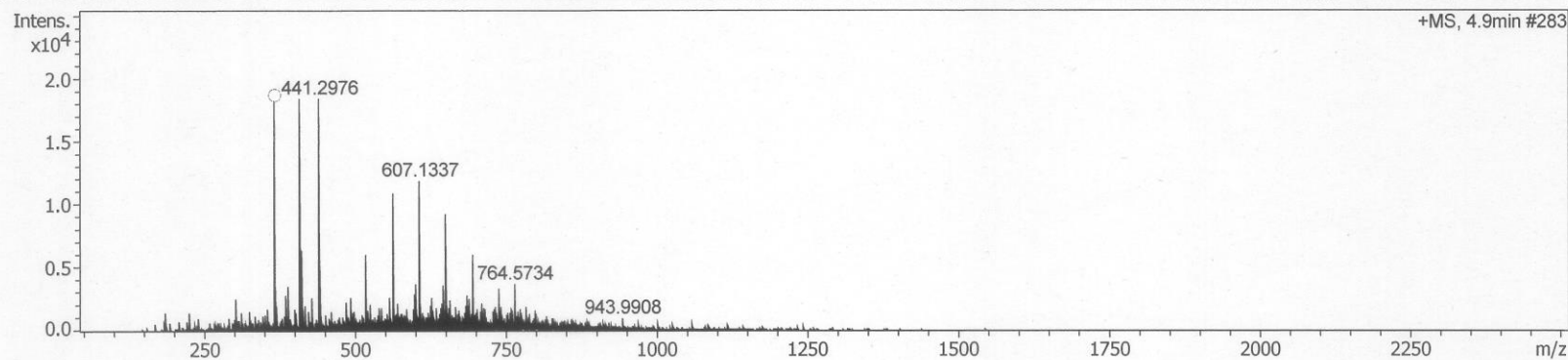
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01139 again.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK01139 again  
 Comment

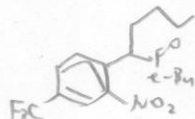
Acquisition Date 3/2/2022 2:32:08 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

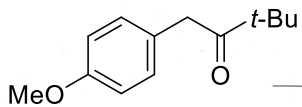
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
368.1444	1	C17H22F3NNaO3	368.1444	0.1	1.5	1	100.00	6.0	even	ok





S12b

# Mass Spectrum SmartFormula Report

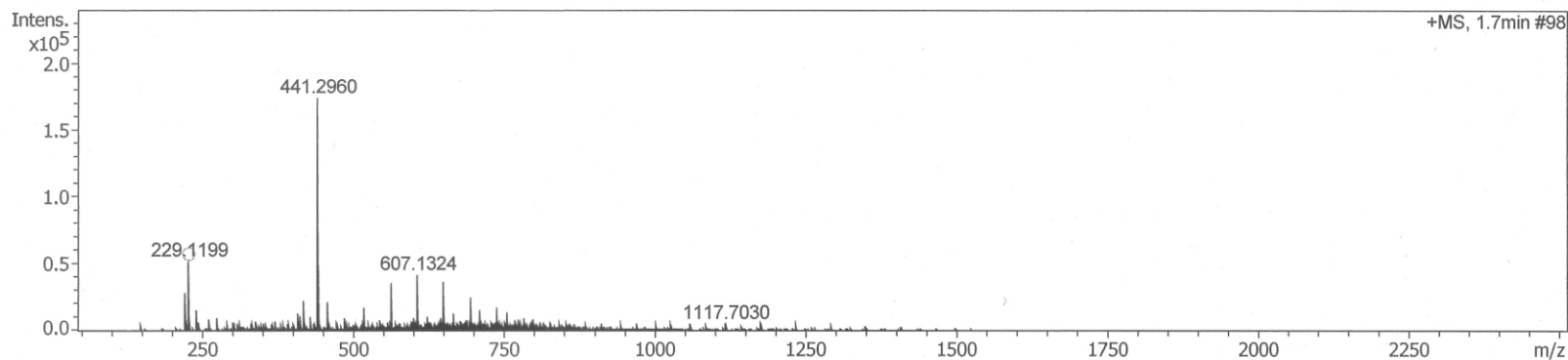
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02170 P re000001.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02170 P re  
 Comment

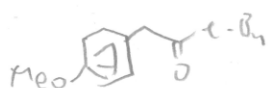
Acquisition Date 8/8/2022 2:03:38 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

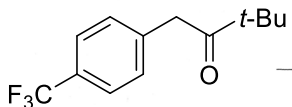
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
229.1199	1	C13H18NaO2	229.1199	-0.2	17.8	1	100.00	5.0	even	ok





**S12c**

# Mass Spectrum SmartFormula Report

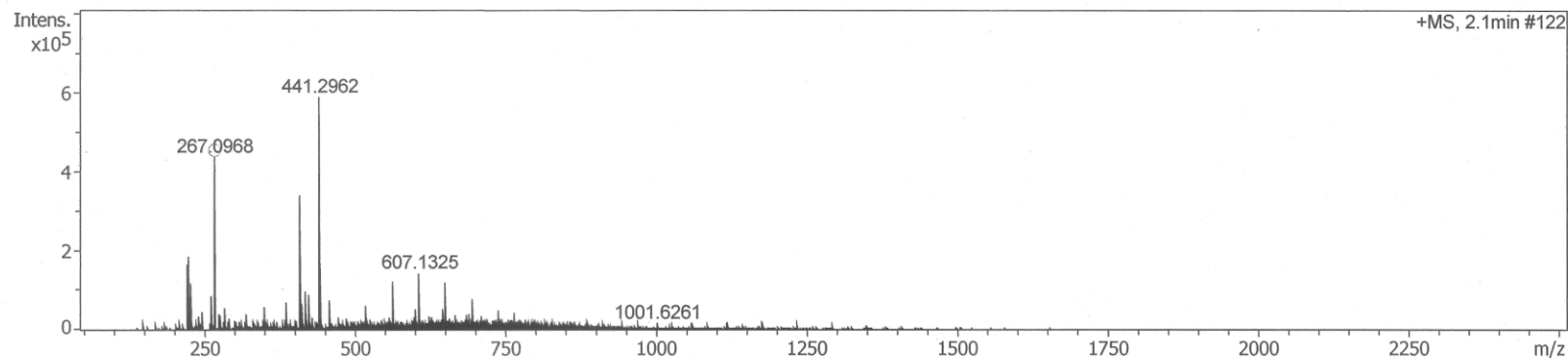
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02161 P000001.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02161 P  
 Comment

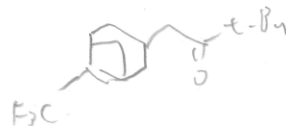
Acquisition Date 8/8/2022 2:09:25 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

## Acquisition Parameter

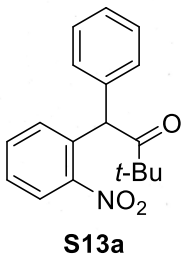
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
267.0968	1	C13H15F3NaO	267.0967	-0.4	2.2	1	100.00	5.0	even	ok







# Mass Spectrum SmartFormula Report

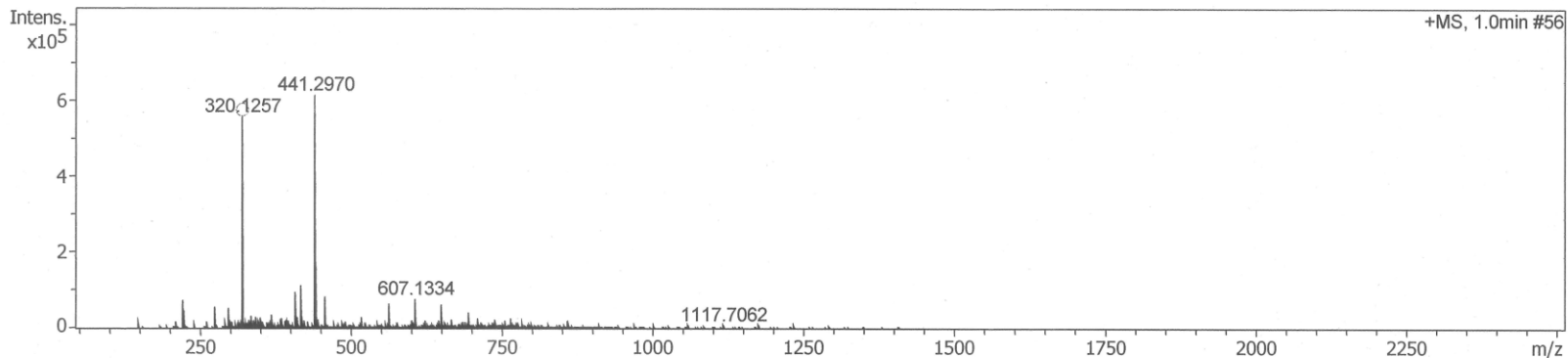
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02174 P re000001.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02174 P re  
 Comment

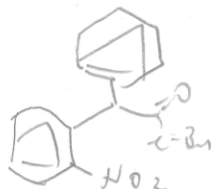
Acquisition Date 8/8/2022 1:53:15 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

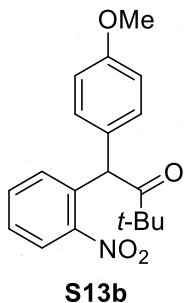
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
320.1257	1	C <sub>18</sub> H <sub>19</sub> NNaO <sub>3</sub>	320.1257	-0.0	11.2	1	100.00	10.0	even	ok





# Mass Spectrum SmartFormula Report

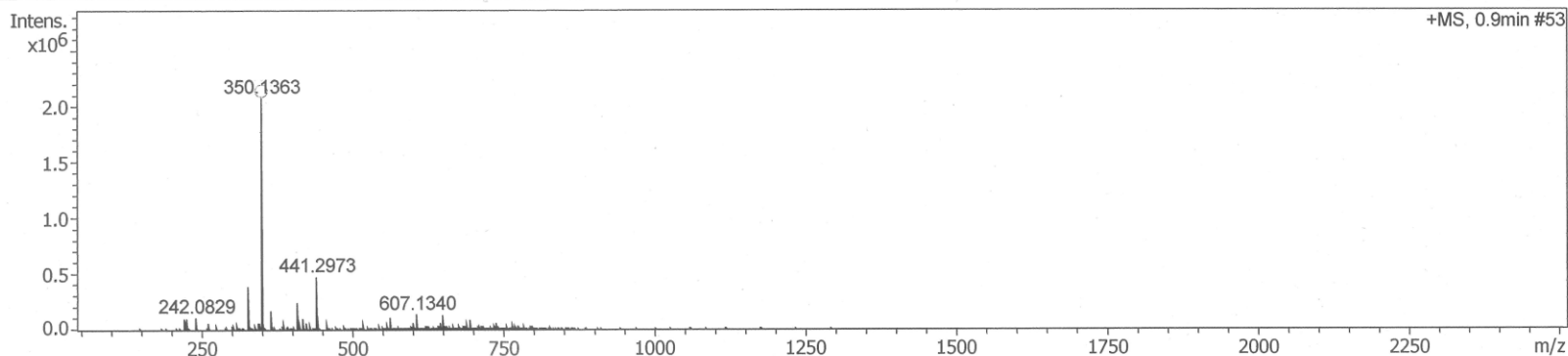
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02173 P000001.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02173 P  
 Comment

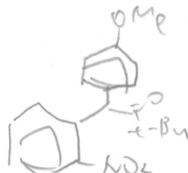
Acquisition Date 8/8/2022 2:24:58 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

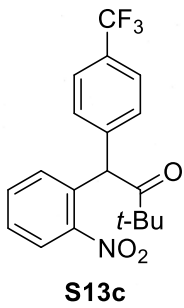
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
350.1363	1	C <sub>19</sub> H <sub>21</sub> NNaO <sub>4</sub>	350.1363	-0.1	2.0	1	100.00	10.0	even	ok





# Mass Spectrum SmartFormula Report

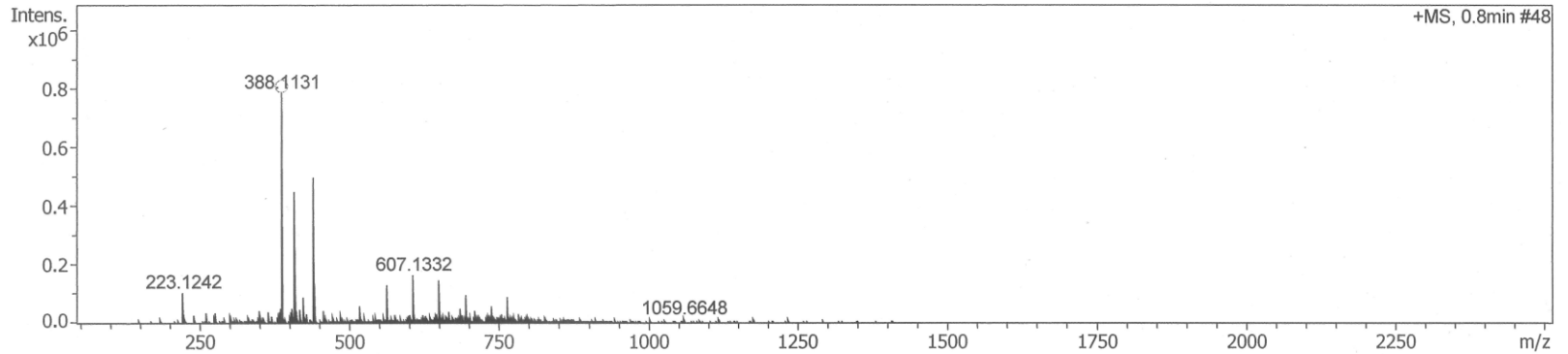
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02163 P000001.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02163 P  
 Comment

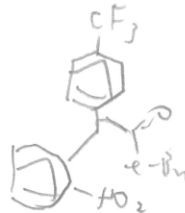
Acquisition Date 8/8/2022 2:29:19 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

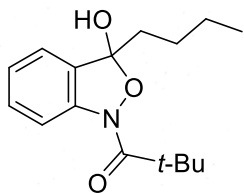
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
388.1131	1	C19H18F3NNaO3	388.1131	0.0	3.1	1	100.00	10.0	even	ok





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# Mass Spectrum SmartFormula Report

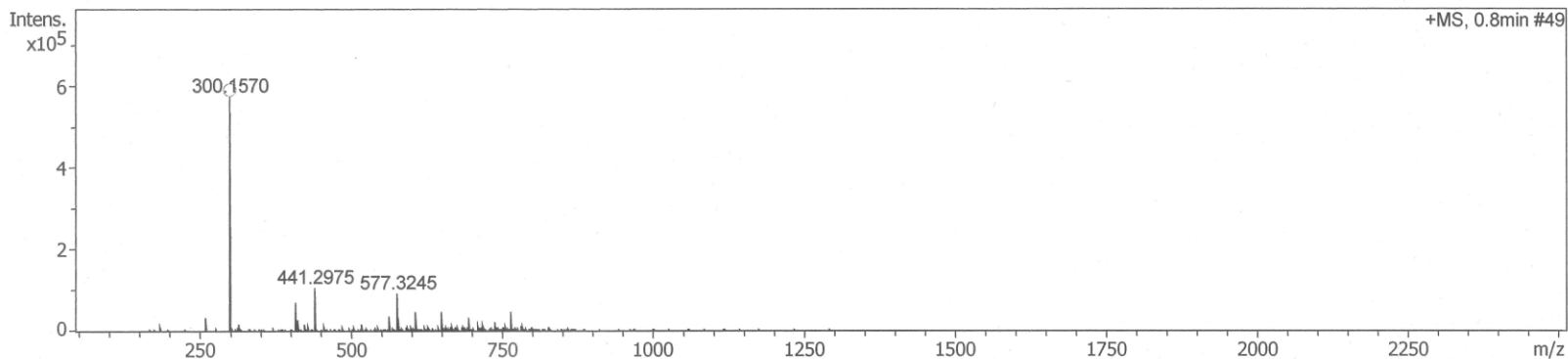
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02063 P.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02063 P  
 Comment

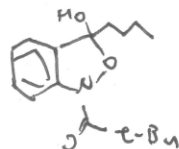
Acquisition Date 5/25/2022 4:11:17 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

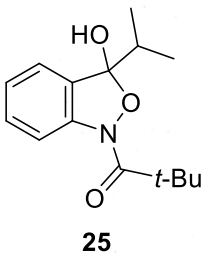
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
300.1570	1	C <sub>16</sub> H <sub>23</sub> NNaO <sub>3</sub>	300.1570	0.0	0.4	1	100.00	6.0	even	ok





# Mass Spectrum SmartFormula Report

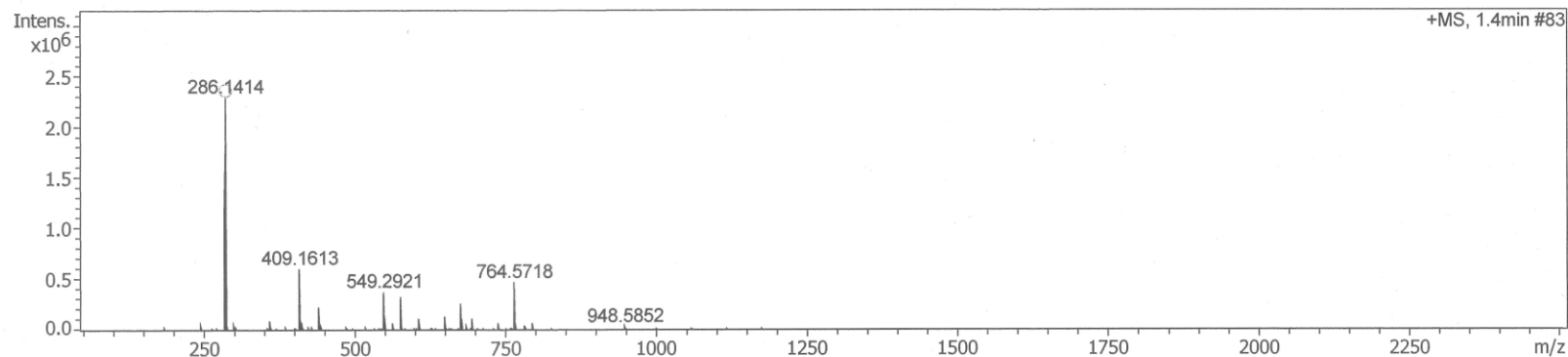
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02093 Prere.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02093 Prere  
 Comment

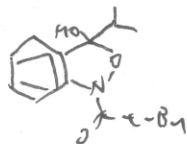
Acquisition Date 5/25/2022 3:09:33 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

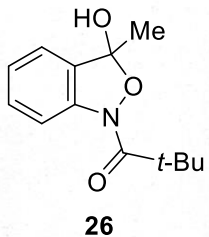
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
286.1414	1	C <sub>15</sub> H <sub>21</sub> NNaO <sub>3</sub>	286.1414	-0.1	3.1	1	100.00	6.0	even	ok





# Compound Spectrum SmartFormula Report

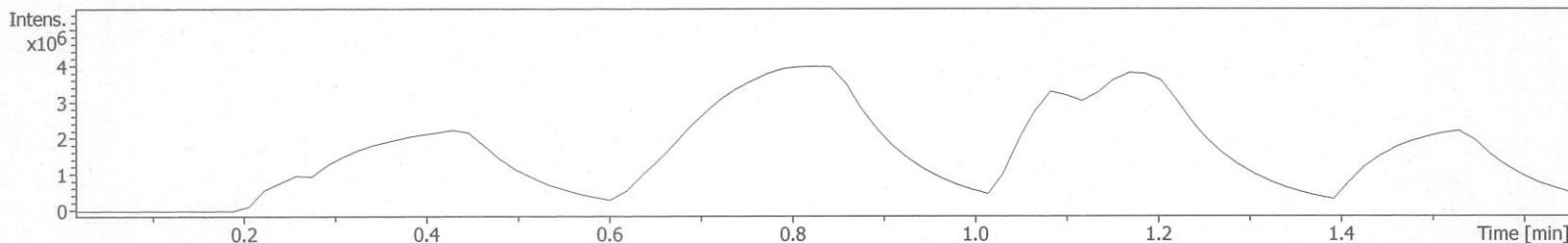
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK03025 P2.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK03025 P2  
 Comment

Acquisition Date 9/11/2022 7:17:22 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

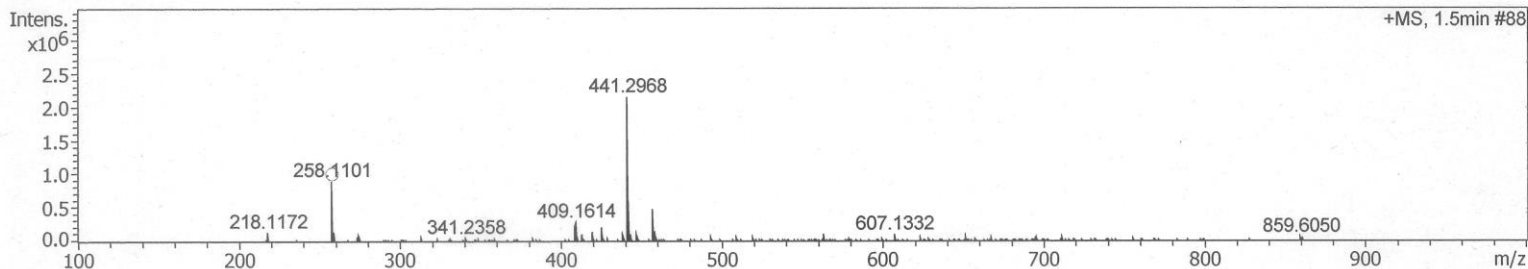
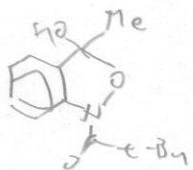
## Acquisition Parameter

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	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	1300.0 Vpp	Set Divert Valve	Source

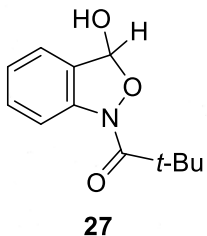


#	RT [min]	Area	Int. Type	I	S/N	Trace	Max. m/z	FWHM [min]
1	1.5	0		2141378		BPC +All MS	441.2968	

## Cmpd 1, 1.5 min



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



# Mass Spectrum SmartFormula Report

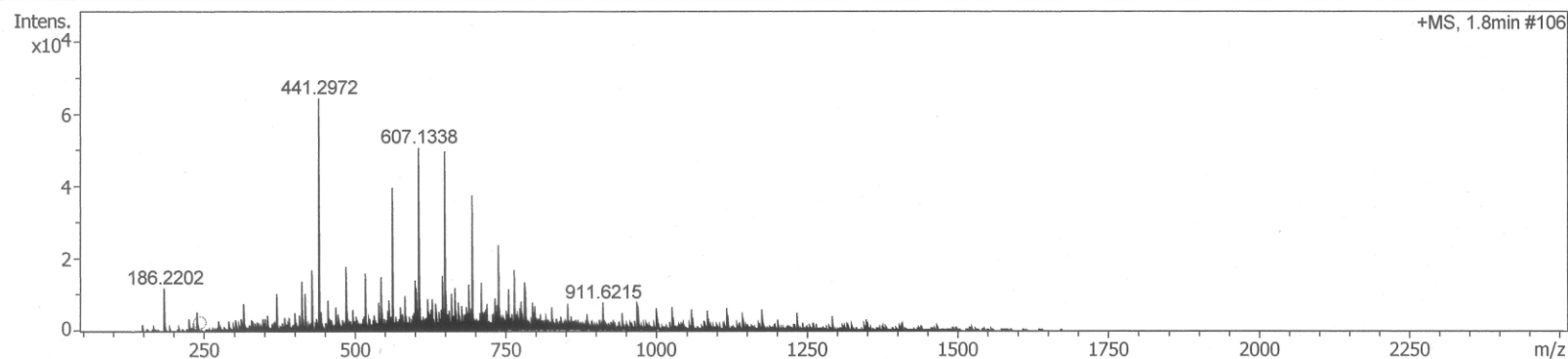
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02098 again2.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02098 again2  
 Comment

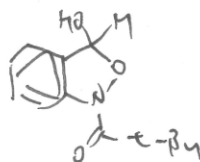
Acquisition Date 5/25/2022 4:37:37 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

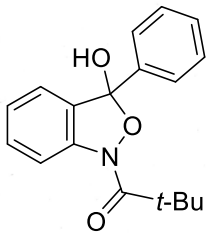
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
244.0944	1	C <sub>12</sub> H <sub>15</sub> NNaO <sub>3</sub>	244.0944	0.2	132.3	1	100.00	6.0	even	ok





28a (keto:hemiacetal = 1:2)

# Mass Spectrum SmartFormula Report

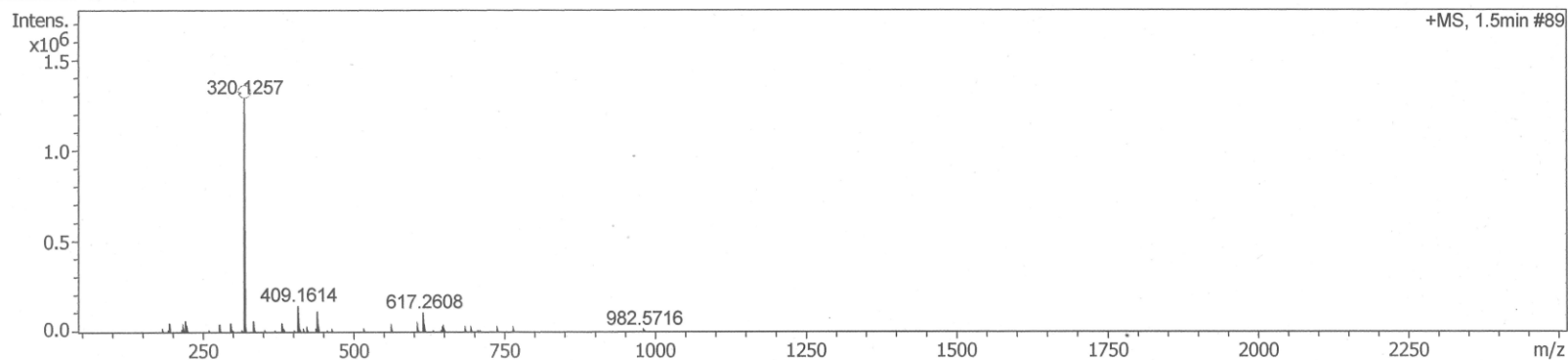
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02177 P000001.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02177 P  
 Comment

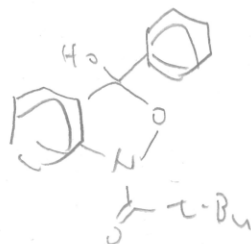
Acquisition Date 8/8/2022 2:37:52 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

## Acquisition Parameter

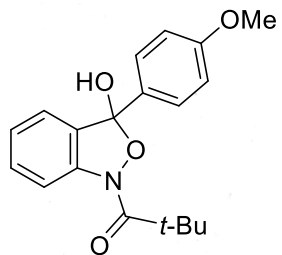
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
320.1257	1	C <sub>18</sub> H <sub>19</sub> NNaO <sub>3</sub>	320.1257	0.1	3.3	1	100.00	10.0	even	ok







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

# Mass Spectrum SmartFormula Report

## Analysis Info

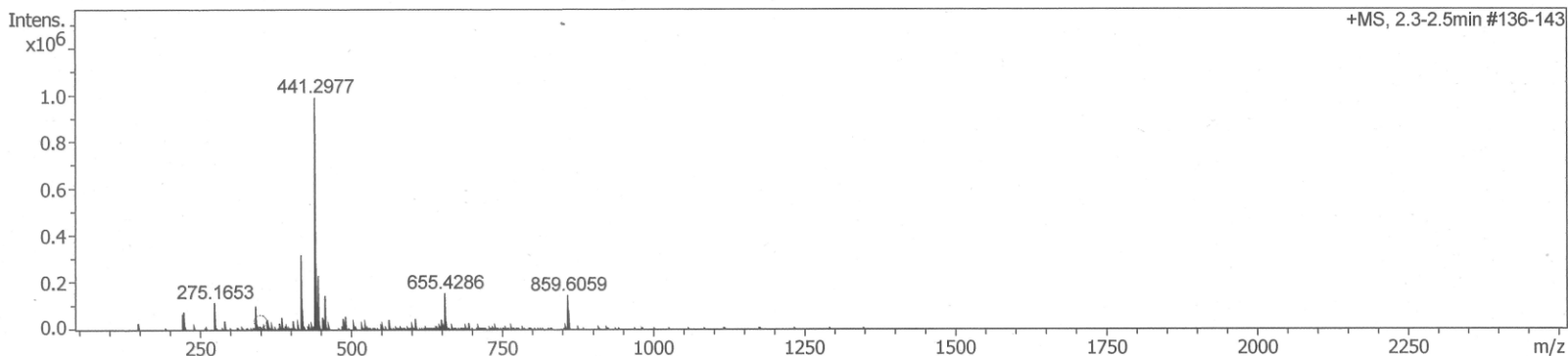
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 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02176 P6

Acquisition Date 8/8/2022 1:19:53 PM

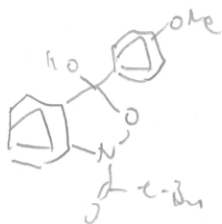
Operator Demo User  
 Instrument compact 8255754.20198

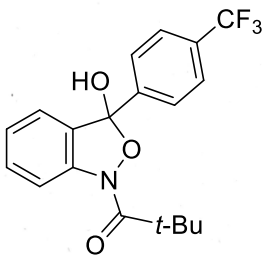
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
350.1363	1	C <sub>19</sub> H <sub>21</sub> NNaO <sub>4</sub>	350.1363	-0.1	45.7	1	100.00	10.0	even	ok





28c

# Mass Spectrum SmartFormula Report

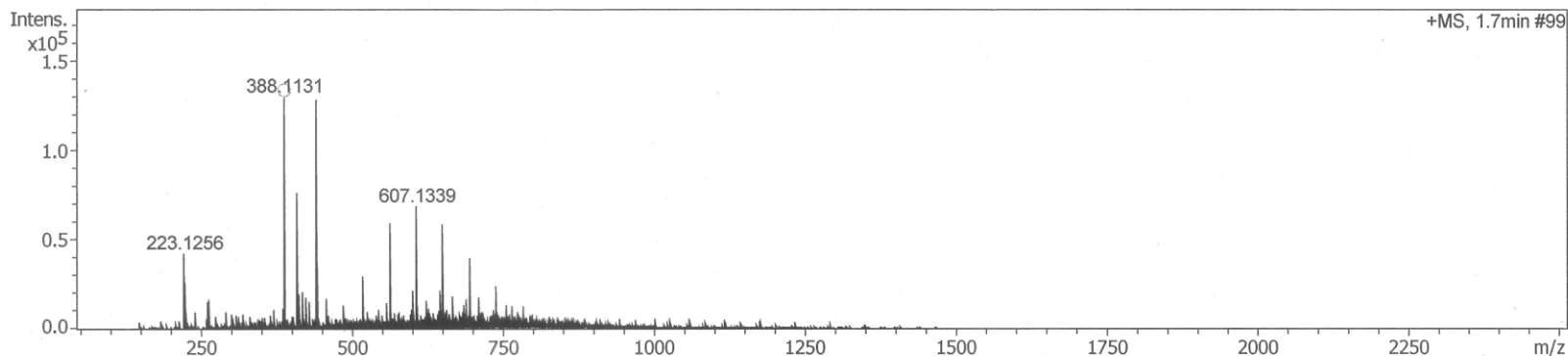
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02180 P rere000001.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02180 P rere  
 Comment

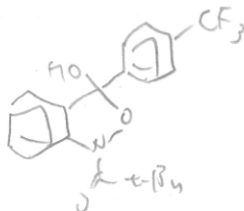
Acquisition Date 8/8/2022 2:58:39 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

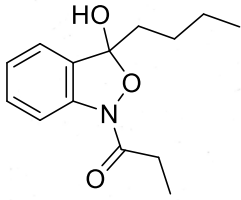
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
388.1131	1	C <sub>19</sub> H <sub>18</sub> F <sub>3</sub> NNaO <sub>3</sub>	388.1131	0.0	2.2	1	100.00	10.0	even	ok





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# Mass Spectrum SmartFormula Report

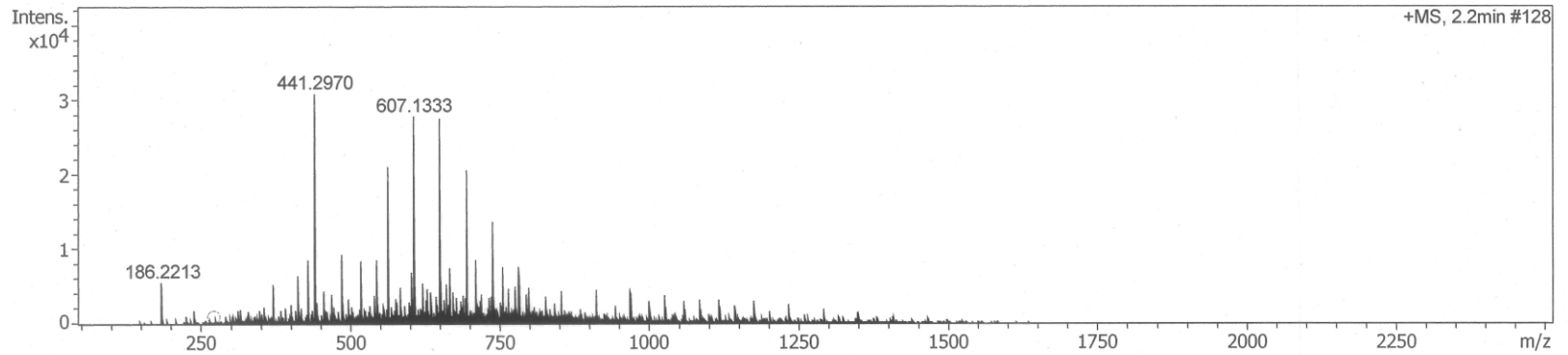
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02059 P.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02059 P  
 Comment

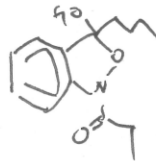
Acquisition Date 5/25/2022 4:15:17 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

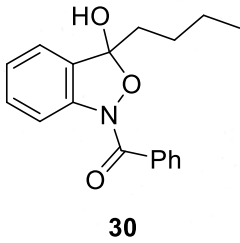
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
272.1257	1	C <sub>14</sub> H <sub>19</sub> NNaO <sub>3</sub>	272.1257	-0.0	n.a.	1	100.00	6.0	even	ok





# Mass Spectrum SmartFormula Report

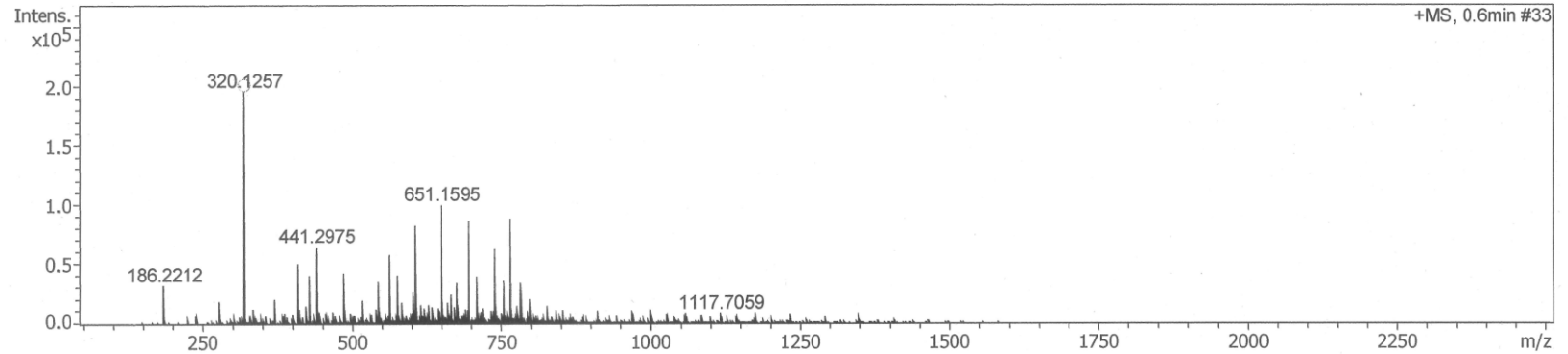
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02062 P.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK02062 P  
 Comment

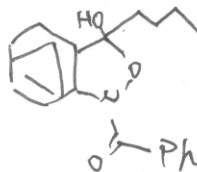
Acquisition Date 5/25/2022 3:54:29 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

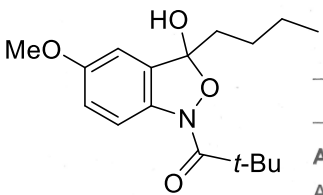
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
320.1257	1	C <sub>18</sub> H <sub>19</sub> NNaO <sub>3</sub>	320.1257	0.2	3.0	1	100.00	10.0	even	ok





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# Mass Spectrum SmartFormula Report

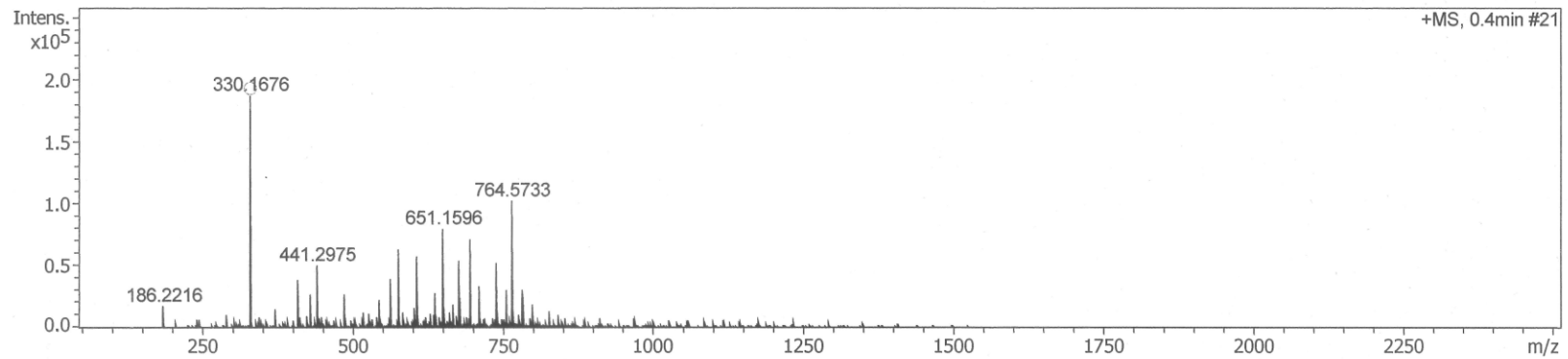
## Analysis Info

Analysis Name: D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02070 P.d  
 Method: esi\_pos\_low\_150to2500.m  
 Sample Name: SK02070 P  
 Comment:

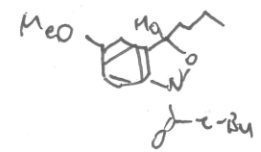
Acquisition Date: 5/25/2022 3:22:26 PM  
 Operator: Demo User  
 Instrument: compact  
 8255754.20198

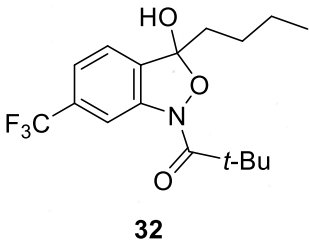
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
330.1676	1	C <sub>17</sub> H <sub>25</sub> NNaO <sub>4</sub>	330.1676	0.1	1.4	1	100.00	6.0	even	ok





# Mass Spectrum SmartFormula Report

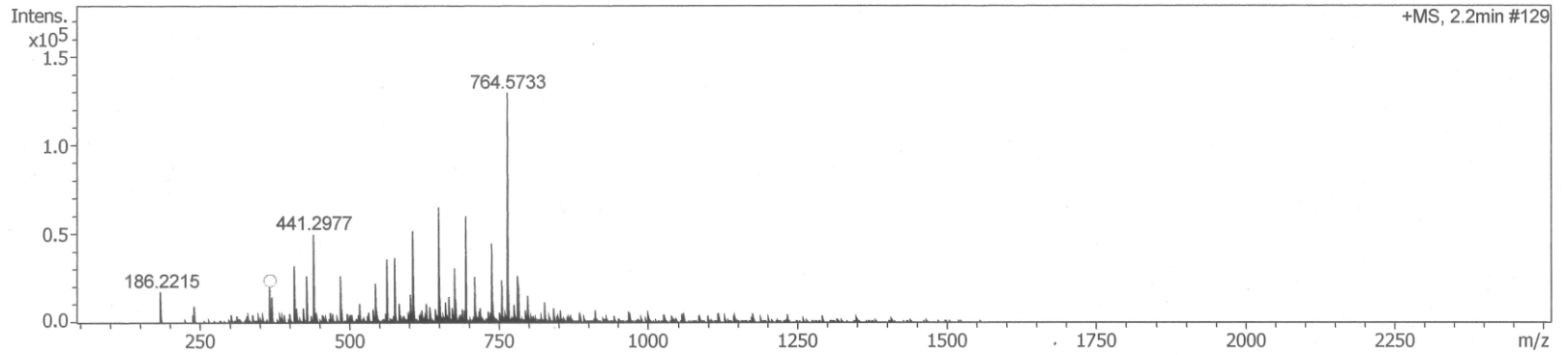
## Analysis Info

Analysis Name: D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK02071 Prere.d  
 Method: esi\_pos\_low\_150to2500.m  
 Sample Name: SK02071 Prere  
 Comment:

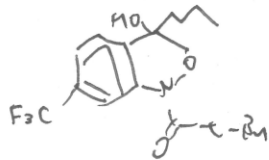
Acquisition Date: 5/25/2022 3:16:14 PM  
 Operator: Demo User  
 Instrument: compact  
 8255754.20198

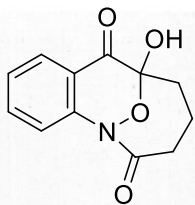
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
368.1444	1	C17H22F3NNaO3	368.1444	-0.1	19.7	1	100.00	6.0	even	ok





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# Mass Spectrum SmartFormula Report

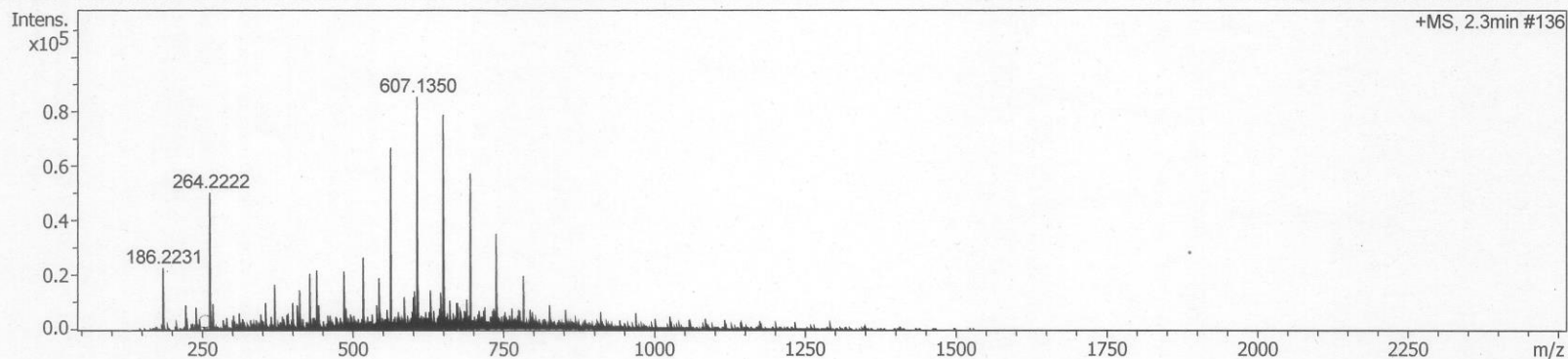
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01132 2.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK01132 2  
 Comment

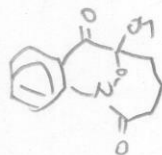
Acquisition Date 3/3/2022 3:05:52 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

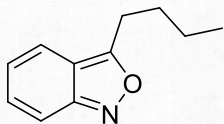
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
256.0580	1	C <sub>12</sub> H <sub>11</sub> NNaO <sub>4</sub>	256.0580	0.2	n.a.	1	100.00	8.0	even	ok





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# Mass Spectrum SmartFormula Report

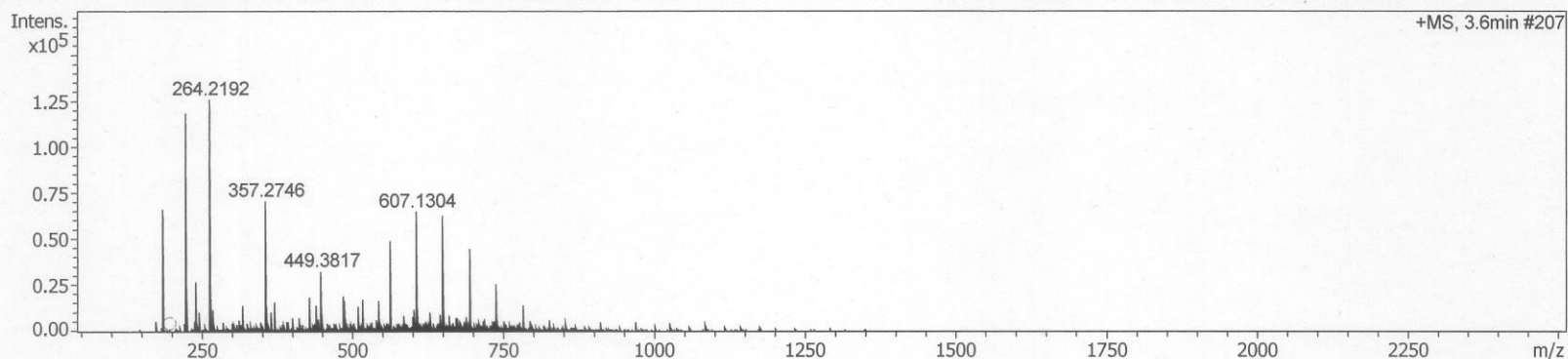
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01052 3.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK01052 3  
 Comment

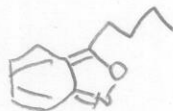
Acquisition Date 3/3/2022 2:35:46 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

## Acquisition Parameter

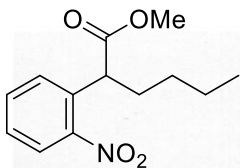
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	2500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
198.0889	1	C <sub>11</sub> H <sub>13</sub> NNaO	198.0889	0.1	185.8	1	100.00	6.0	even	ok







S14

# Mass Spectrum SmartFormula Report

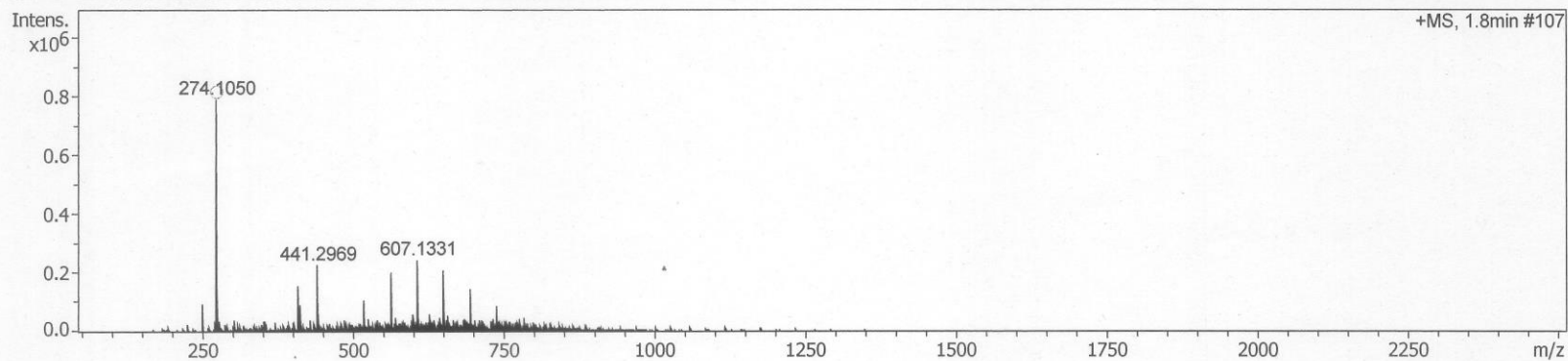
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01212.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK01212  
 Comment

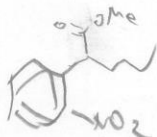
Acquisition Date 3/2/2022 3:34:42 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

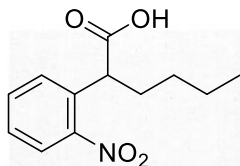
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
274.1050	1	C13H17NNaO4	274.1050	-0.2	1.3	1	100.00	6.0	even	ok





S15

# Mass Spectrum SmartFormula Report

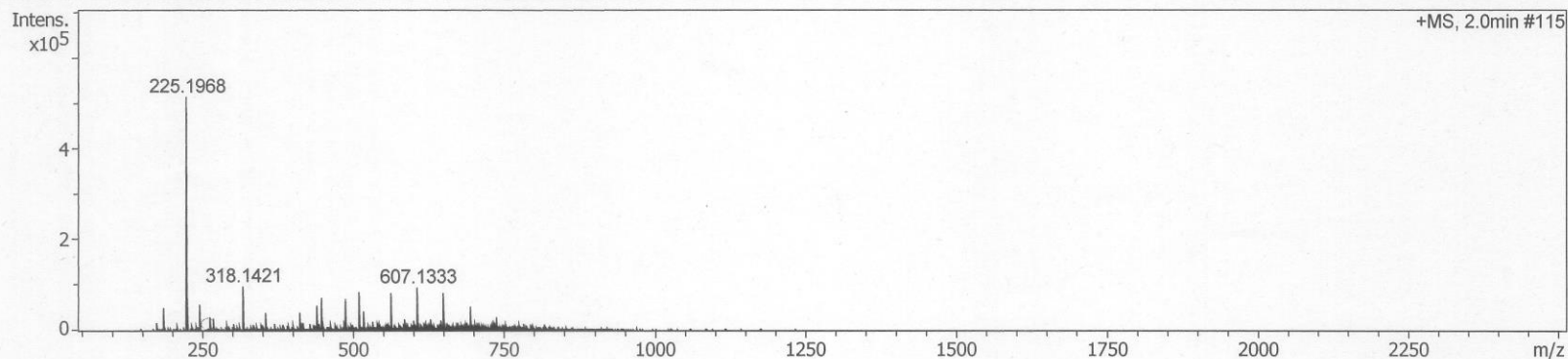
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01213.d  
Method esi\_pos\_low\_150to2500.m  
Sample Name SK01213  
Comment

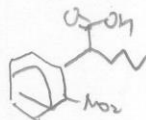
Acquisition Date 3/3/2022 2:42:57 PM  
Operator Demo User  
Instrument compact 8255754.20198

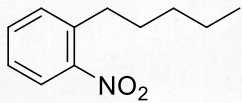
## Acquisition Parameter

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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
260.0893	1	C12H15NNaO4	260.0893	0.3	698.3	1	100.00	6.0	even	ok





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# Mass Spectrum SmartFormula Report

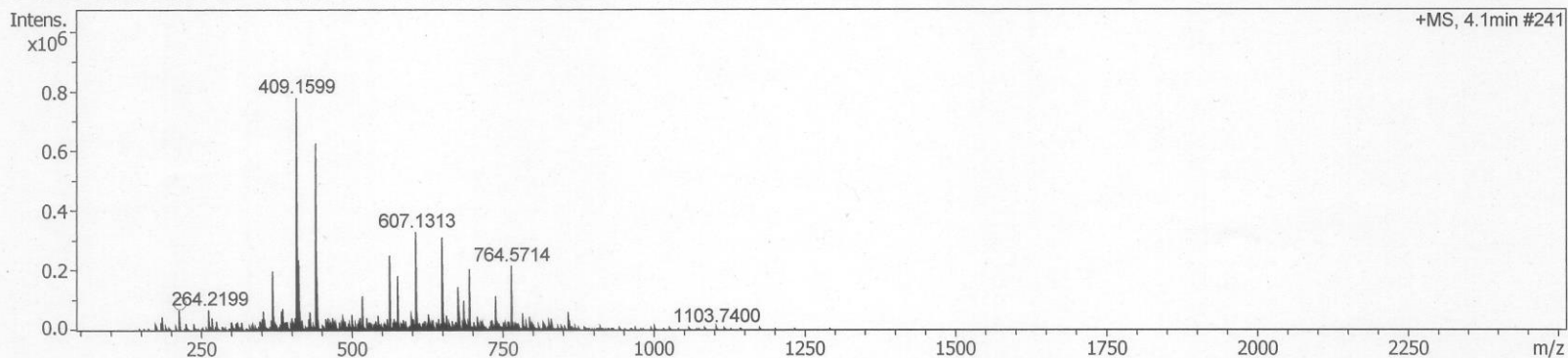
## Analysis Info

Analysis Name D:\Data\Data\_Lab\S. Yokoshima. Lab\Kitayama\SK01214 3.d  
 Method esi\_pos\_low\_150to2500.m  
 Sample Name SK01214 3  
 Comment

Acquisition Date 3/3/2022 3:21:14 PM  
 Operator Demo User  
 Instrument compact 8255754.20198

## 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	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



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
216.0995	1	C11H15NNO2	216.0995	-0.0	18.7	1	100.00	5.0	even	ok

