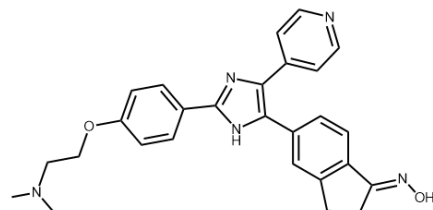


12.765  
12.687  
10.984  
10.860  
8.575  
8.561  
8.460  
8.456  
8.449  
8.445  
8.022  
8.009  
8.004  
8.000  
7.644  
7.624  
7.569  
7.551  
7.533  
7.521  
7.517  
7.509  
7.505  
7.483  
7.468  
7.401  
7.381  
7.082  
7.071  
7.060  
7.048  
4.125  
4.111  
4.096  
3.320  
3.066  
3.051  
3.034  
3.013  
2.999  
2.981  
2.870  
2.859  
2.853  
2.836  
2.827  
2.810  
2.660  
2.645  
2.631  
2.509  
2.504  
2.500  
2.495  
2.490  
2.230



Mixt. syn-anti isomers



SB-590885

Chemical Formula:  $C_{27}H_{27}N_5O_2$   
Molecular Weight: 453.55

Current Data Parameters  
NAME NSC-754362-R3  
EXPNO 1  
PROCNO 1

#### F2 - Acquisition Parameters

Date\_ 20221026  
Time 16.02 h  
INSTRUM spect  
PROBHD Z104450\_0348 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 80.6  
DW 60.800 usec  
DE 6.50 usec  
TE 298.5 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324710 MHz  
NUC1 1H  
P0 4.99 usec  
P1 14.96 usec  
PLW1 9.92000008 W

#### F2 - Processing parameters

SI 32768  
SF 400.1300032 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.0099

0.9598

2.0133

2.0014

4.9374

2.0000

2.0148

1.9971

1.9622

2.0912

6.0417

—12.765  
—12.687

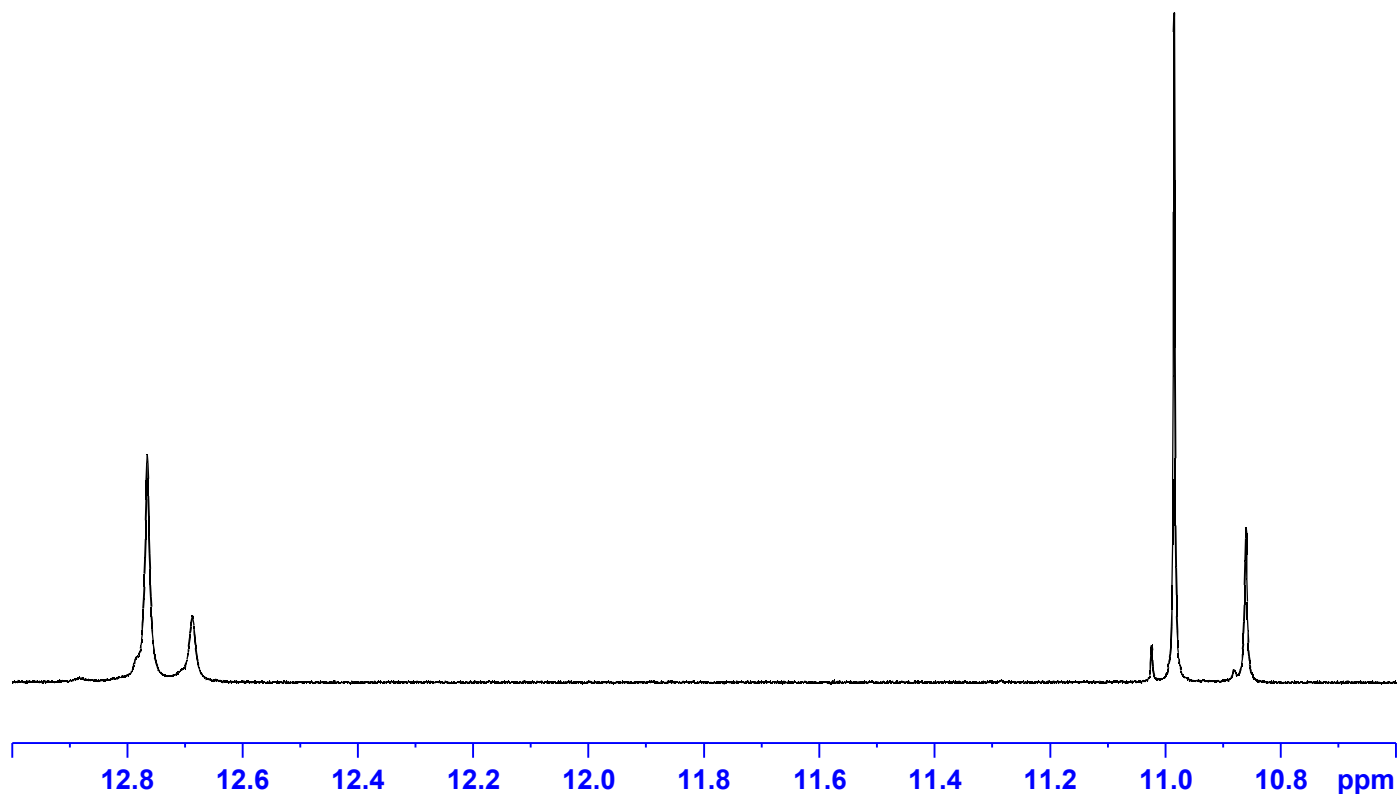
—11.023  
—10.984  
—10.860



Current Data Parameters  
NAME NSC-754362-R3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221026  
Time 16.02 h  
INSTRUM spect  
PROBHD Z104450\_0348 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
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DW 60.800 usec  
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D1 1.00000000 sec  
TD0 1  
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NUC1 1H  
P0 4.99 usec  
P1 14.96 usec  
PLW1 9.92000008 W

F2 - Processing parameters  
SI 32768  
SF 400.1300032 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



1.0099

0.9598

8.575  
8.561  
8.460  
8.456  
8.449  
8.445

8.022  
8.009  
8.004  
8.000

7.644  
7.624  
7.569  
7.551  
7.533  
7.521  
7.517  
7.509  
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7.483  
7.468  
7.401  
7.381

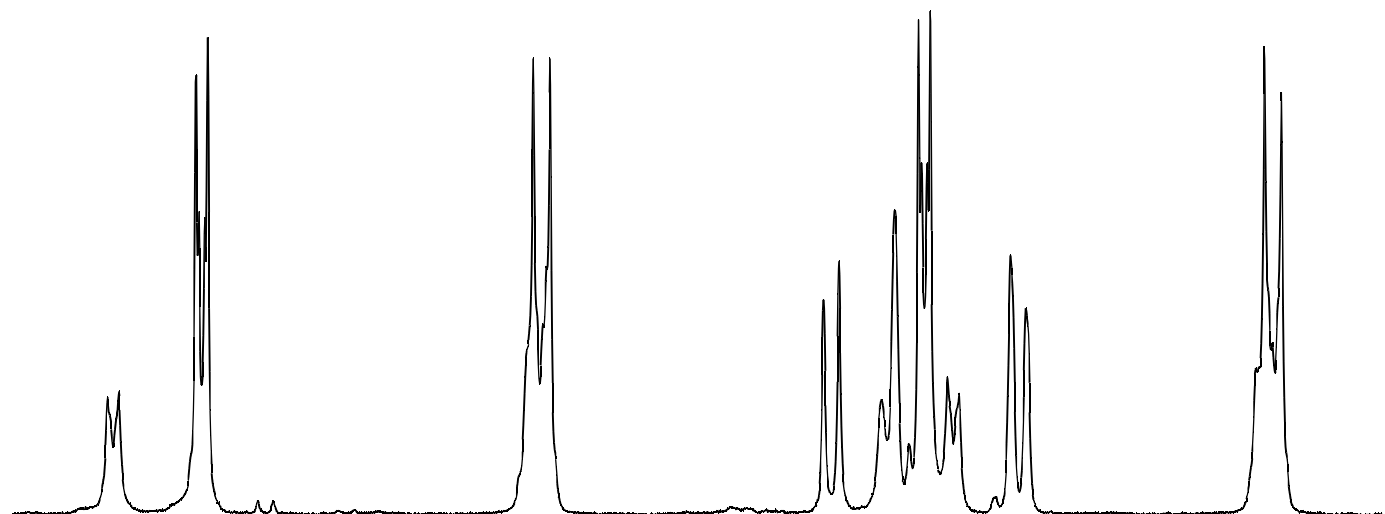
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7.071  
7.060  
7.048



Current Data Parameters  
NAME NSC-754362-R3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221026  
Time 16.02 h  
INSTRUM spect  
PROBHD Z104450\_0348 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 80.6  
DW 60.800 usec  
DE 6.50 usec  
TE 298.5 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324710 MHz  
NUC1 1H  
P0 4.99 usec  
P1 14.96 usec  
PLW1 9.92000008 W

F2 - Processing parameters  
SI 32768  
SF 400.1300032 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 ppm

2.0133

2.0014

4.9374

2.0000

4.125  
4.111  
4.096

3.320

3.066  
3.051  
3.034  
3.013  
2.999  
2.981  
2.870  
2.859  
2.853  
2.836  
2.827  
2.810  
2.794  
2.660  
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2.504  
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2.495  
2.490  
2.394

2.230



Current Data Parameters  
NAME NSC-754362-R3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221026  
Time 16.02 h  
INSTRUM spect  
PROBHD zg30  
PULPROG 104450\_0348  
TD 65536  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 80.6  
DW 60.800 usec  
DE 6.50 usec  
TE 298.5 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324710 MHz  
NUC1 1H  
P0 4.99 usec  
P1 14.96 usec  
PLW1 9.92000008 W

F2 - Processing parameters  
SI 32768  
SF 400.1300032 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 ppm

2.0148

1.9971

1.9622

2.0912

6.0417

# Qualitative Analysis Report

**Data Filename** 754362-R3\_11.d **Sample Name** 754362-R3  
**Sample Type** Sample **Position** P1-B1  
**Instrument Name** Instrument 1 **User Name**  
**Acq Method** 5-95\_10min\_pos.m **Acquired Time** 10/24/2022 4:10:56 PM (UTC-07:00)  
**IRM Calibration Status** Not Applicable **DA Method** Default.m

## Comment

## Sample Group

**Stream Name** LC 1

## Info.

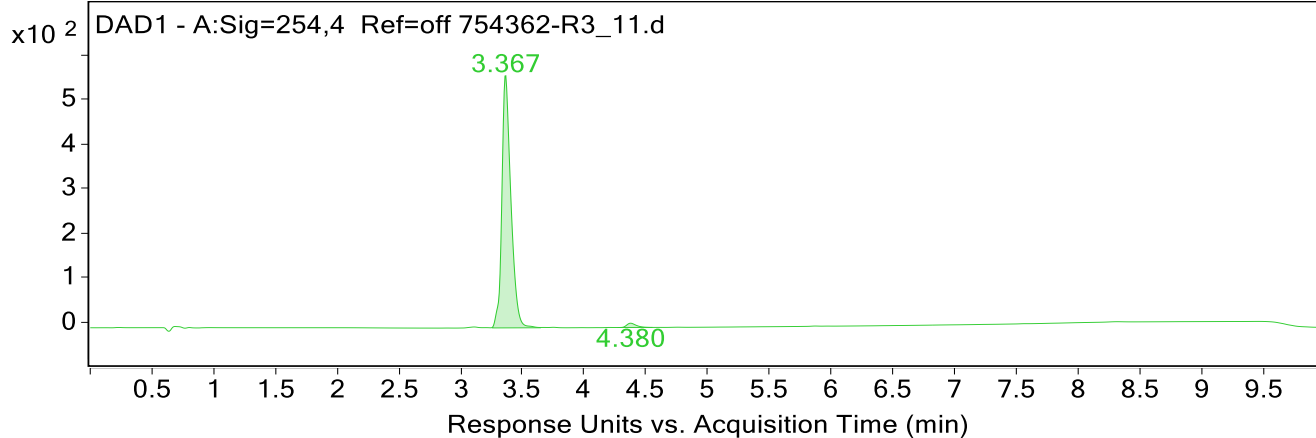
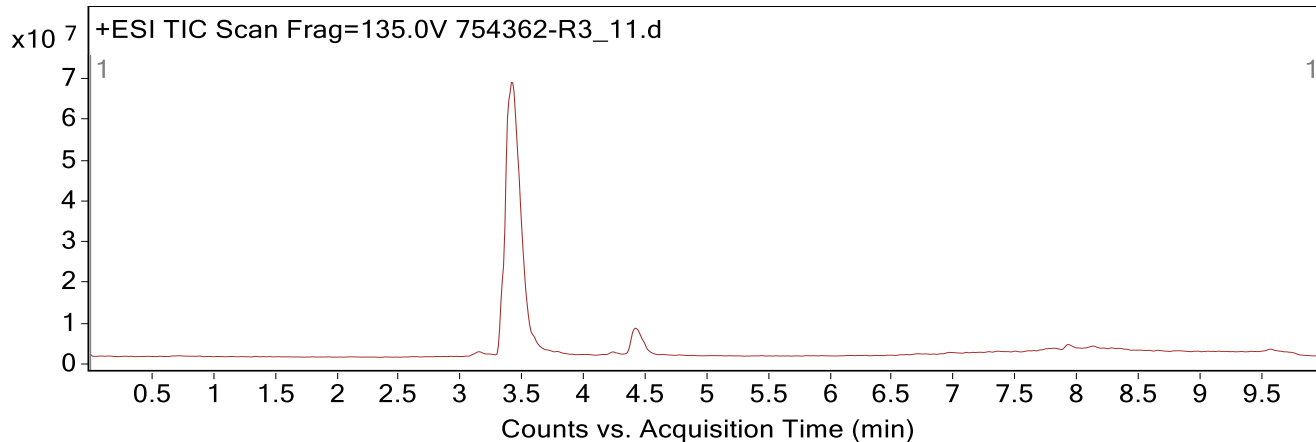
**Acquisition Time (Local)** 10/24/2022 4:10:56 PM (UTC-07:00)

## Acquisition SW Version

6400 Series Triple  
Quadrupole  
B.08.02 (B8260.0)

## Chromatograms

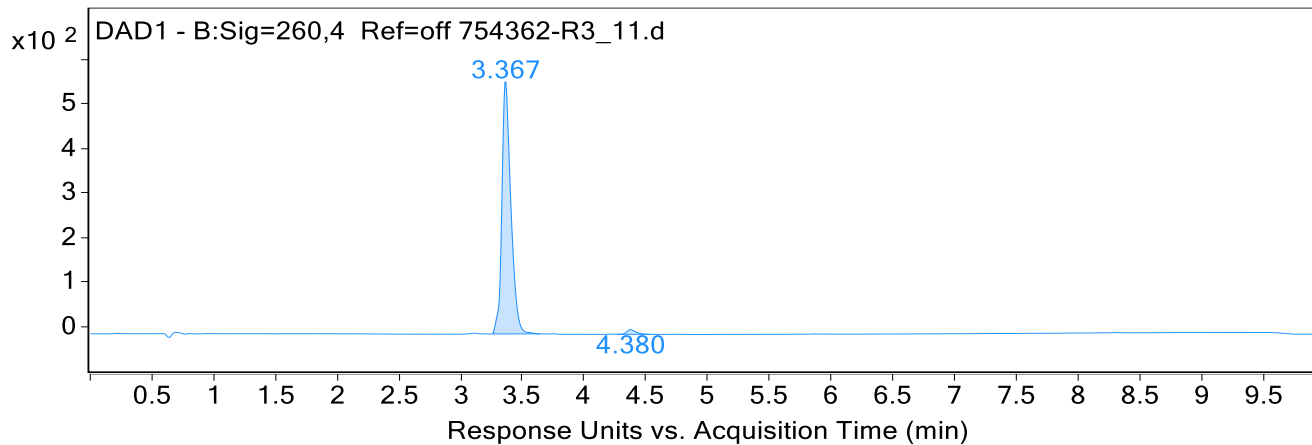
**Fragmentor Voltage** 135 **Collision Energy** 0 **Ionization Mode** ESI



## Integration Peak List

Peak	Start	RT	End	Height	Area	Area Sum %
1	3.260	3.367	3.647	564.9	2885.7	98.3
2	4.273	4.380	4.555	9.6	51.2	1.7

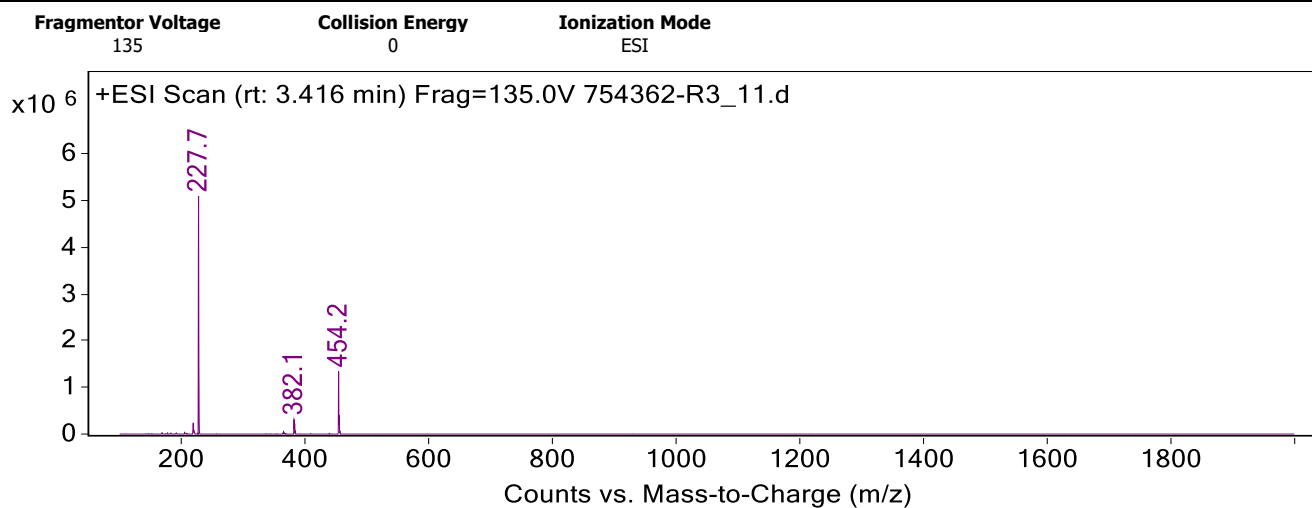
# Qualitative Analysis Report



## Integration Peak List

Peak	Start	RT	End	Height	Area	Area Sum %
1	3.267	3.367	3.644	565.3	2873.2	98.1
2	4.267	4.380	4.540	10.3	55.2	1.9

## Spectra

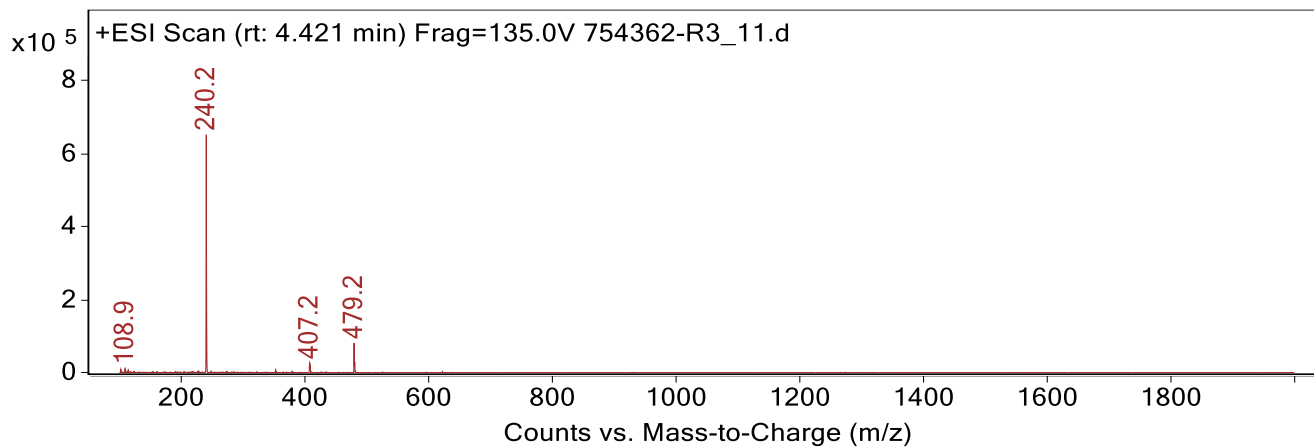


## Peak List

m/z	z	Abund
219.0		230085
219.9		70889
220.3		66859
227.7	2	5093236
365.1		55325
382.1		312101
383.1	1	220624
454.2	1	1342794
455.2	1	400260
456.2	1	65564

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI

# Qualitative Analysis Report



## Peak List

<i>m/z</i>	<i>z</i>	Abund
102.0		8720
108.9		11024
113.9		8017
240.2		650796
352.3		8503
407.2		25664
408.1		20587
479.2	1	80764
480.2	1	29158

--- End Of Report ---