

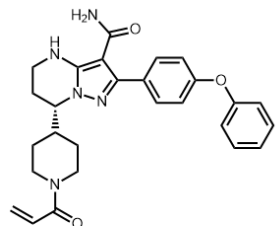


Current Data Parameters  
 NAME NSC-823807-Z2\_DMSO  
 EXPNO 1  
 PROCNO 1

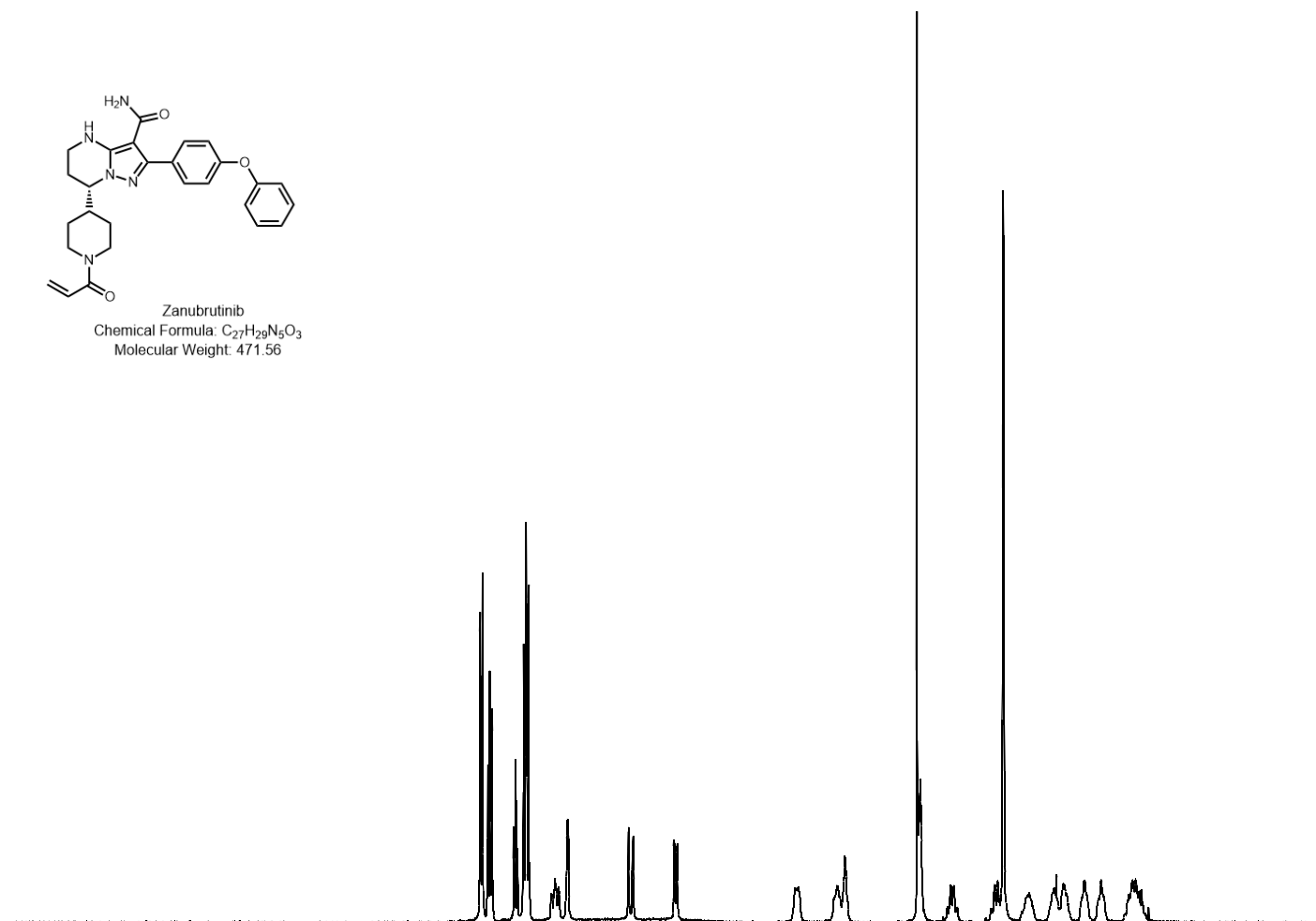
F2 - Acquisition Parameters  
 Date\_ 20200922  
 Time 11.45 h  
 INSTRUM spect  
 PROBHD Z104450\_0348 (zg30)  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 64  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 3.9845889 sec  
 RG 144  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.5 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324710 MHz  
 NUC1 1H  
 P0 4.87 usec  
 P1 14.60 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

7.506  
7.494  
7.489  
7.437  
7.432  
7.419  
7.416  
7.402  
7.398  
7.392  
7.389  
7.171  
7.152  
7.152  
7.095  
7.093  
7.088  
7.074  
7.067  
7.062  
7.050  
7.045  
6.789  
6.762  
6.673  
6.092  
6.086  
6.050  
6.045  
5.653  
5.648  
5.627  
5.622  
4.463  
4.090  
4.017  
4.002  
3.325  
3.320  
3.297  
3.003  
2.974  
2.582  
2.551  
2.508  
2.504  
2.500  
2.495  
2.491  
1.987  
1.925  
1.909  
1.722  
1.559  
1.264  
1.233



Zanubrutinib  
 Chemical Formula: C<sub>27</sub>H<sub>29</sub>N<sub>5</sub>O<sub>3</sub>  
 Molecular Weight: 471.56



2.0000  
1.9185  
1.0463  
3.8356  
1.1151  
1.0646  
1.1456  
1.1208  
0.9355  
1.9347  
1.7701  
0.9193  
0.8303  
1.0549  
2.0156  
0.9812  
1.0110  
2.1245

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

7.511  
7.506  
7.494  
7.489  
7.443  
7.437  
7.432  
7.419  
7.416  
7.402  
7.398  
7.392  
7.189  
7.171  
7.152  
7.095  
7.093  
7.088  
7.074  
7.067  
7.062  
7.050  
7.045  
6.830  
6.820  
6.804  
6.789  
6.780  
6.762  
6.754  
6.673

6.092  
6.086  
6.050  
6.045

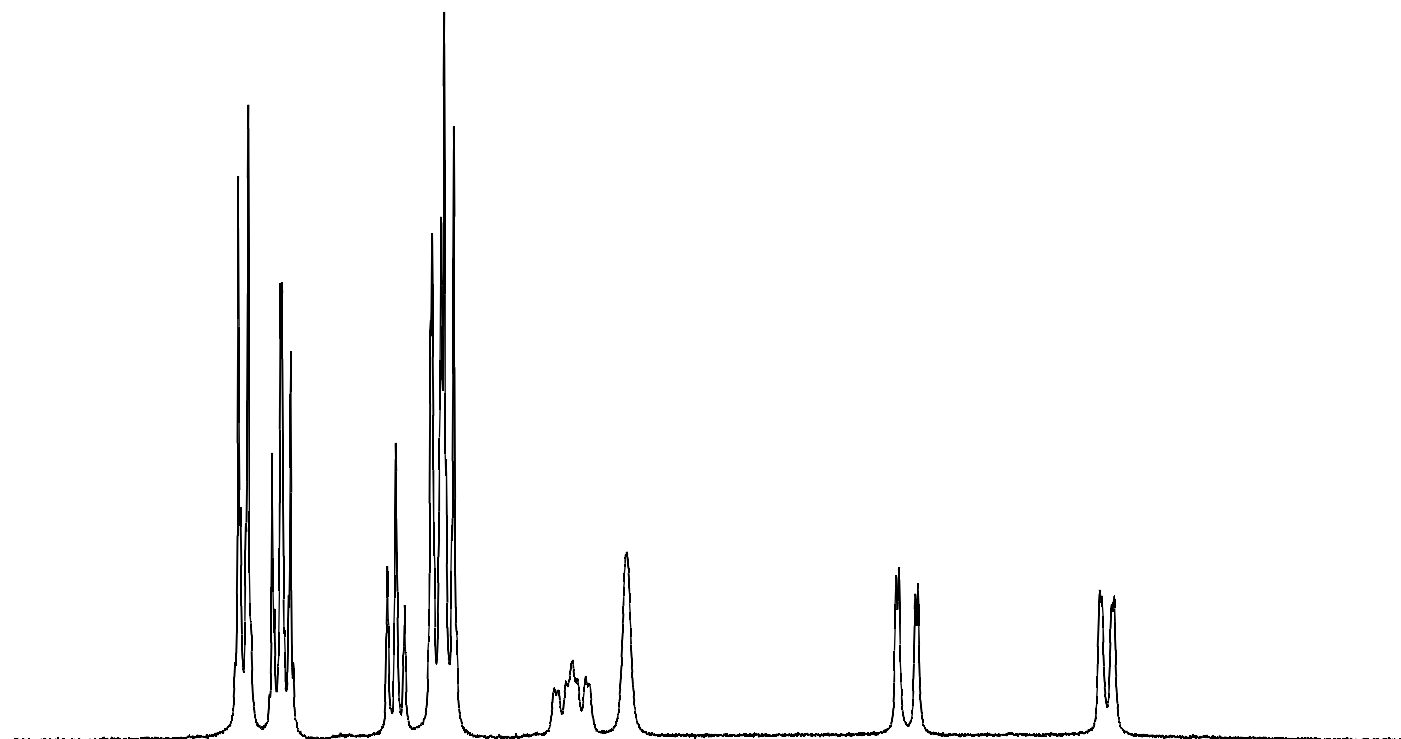
5.653  
5.648  
5.627  
5.622



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TD0 1  
SFO1 400.1324710 MHz  
NUC1 1H  
P0 4.87 usec  
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SF 400.1300032 MHz  
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SSB 0  
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GB 0  
PC 1.00



2.0000  
1.9185

1.0463  
3.8356

1.1151  
1.0646

1.1456

1.1208

7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 ppm

4.491  
4.463

4.090  
4.017  
4.002

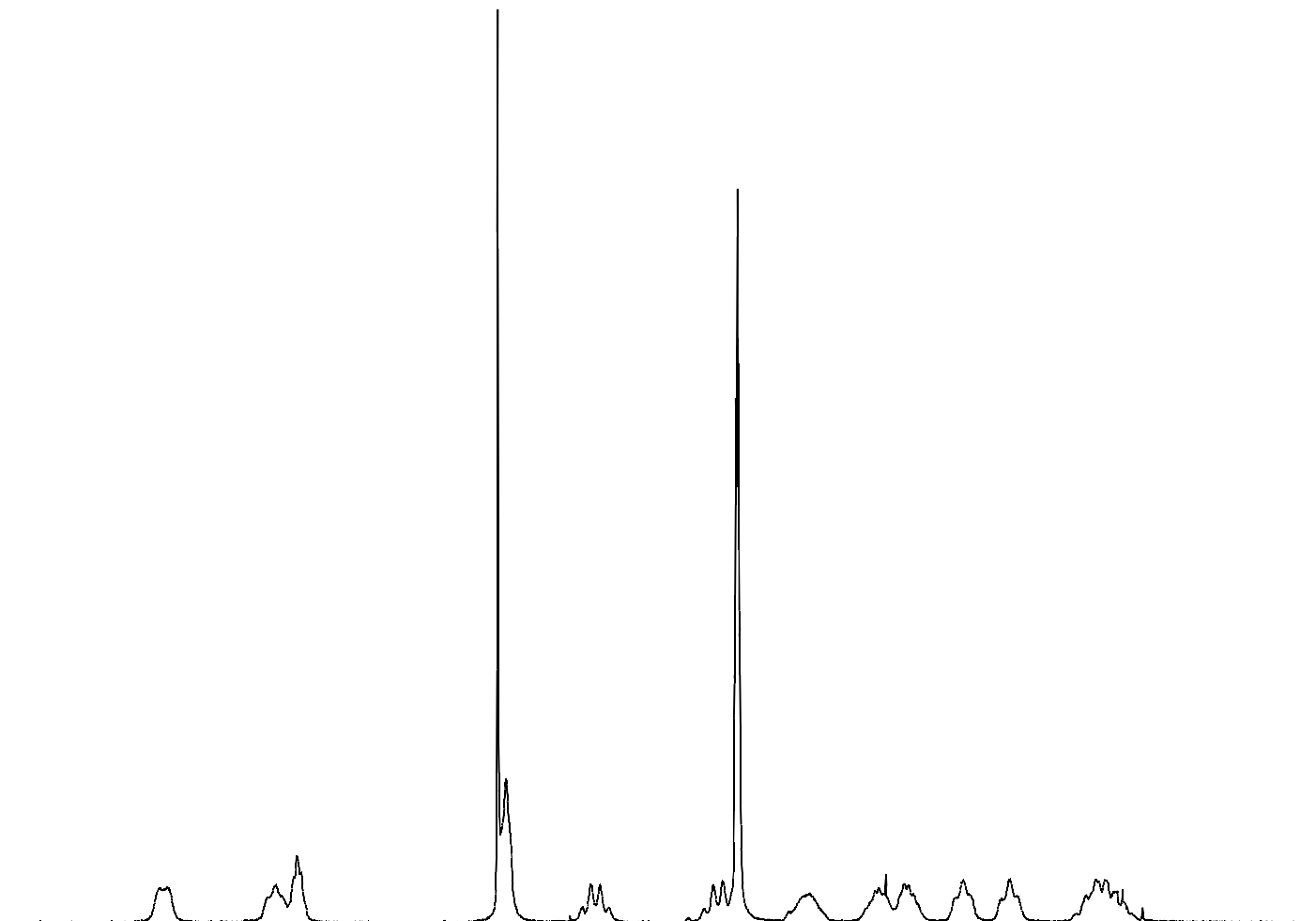
3.325  
3.320  
3.297  
3.032  
3.003  
2.974  
2.941  
2.614  
2.582  
2.551  
2.508  
2.504  
2.500  
2.495  
2.491  
2.321  
2.317  
2.268  
2.255  
2.251  
2.025  
2.010  
1.996  
1.987  
1.925  
1.909  
1.894  
1.746  
1.722  
1.702  
1.676  
1.588  
1.559  
1.536  
1.332  
1.297  
1.264  
1.233  
1.202  
1.190  
1.172



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



4.5

4.0

3.5

3.0

2.5

2.0

1.5

1.0

ppm

0.9355

1.9347

1.7701

0.9193

0.8303

1.0549

2.0156

0.9812

1.0110

2.1245

# Qualitative Analysis Report

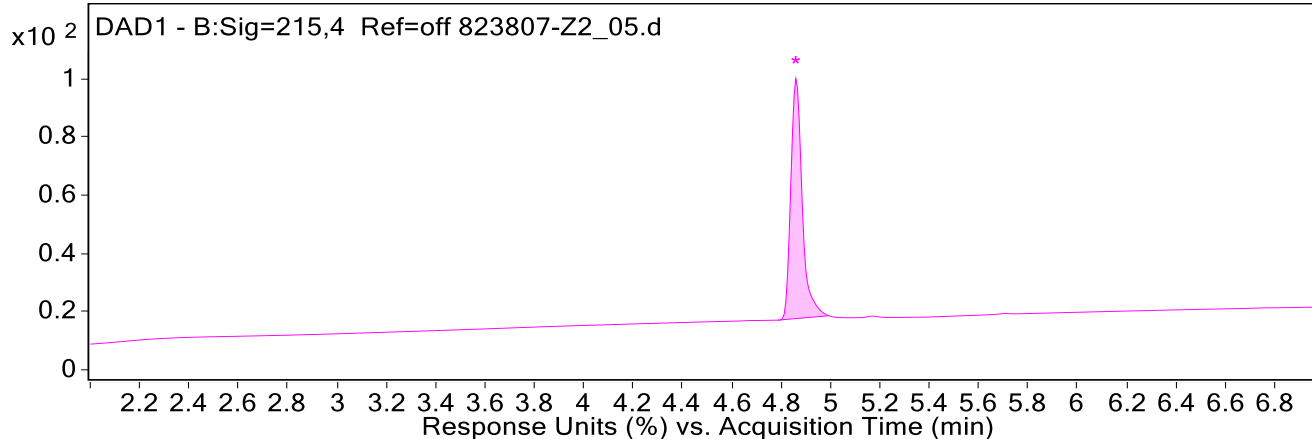
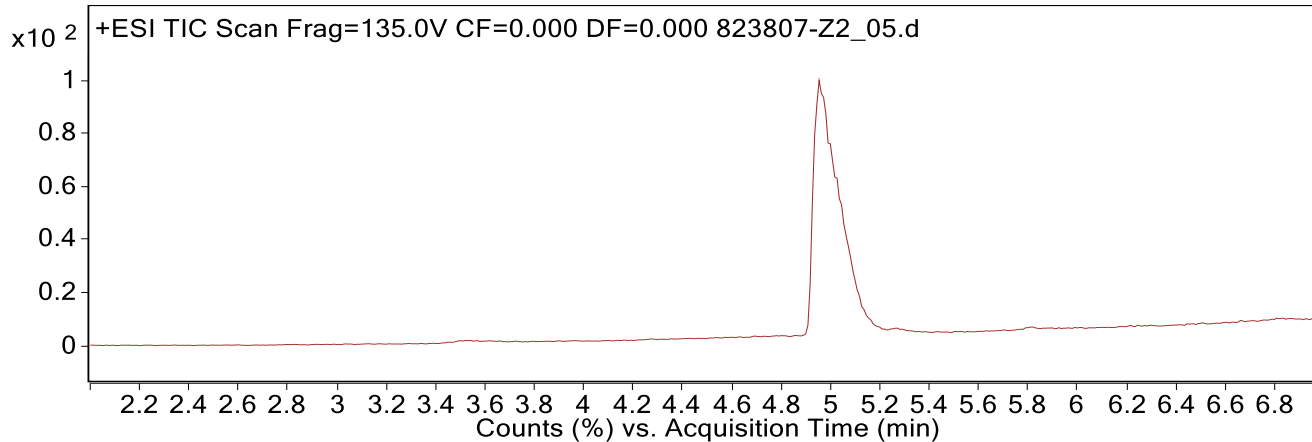
**Data Filename** 823807-Z2\_05.d **Sample Name** 823807-Z2  
**Sample Type** Sample **Position** P1-A6  
**Instrument Name** Instrument 1 **User Name**  
**Acq Method** Leidos\_10min\_pos.m **Acquired Time** 9/21/2020 1:08:07 PM  
**IRM Calibration Status** Not Applicable **DA Method** uv integration test.m  
**Comment**

**Sample Group**  
**Stream Name** LC 1

**Info.**  
**Acquisition SW** 6400 Series Triple  
**Version** Quadrupole  
B.08.00 (B8023.0)

## User Chromatograms

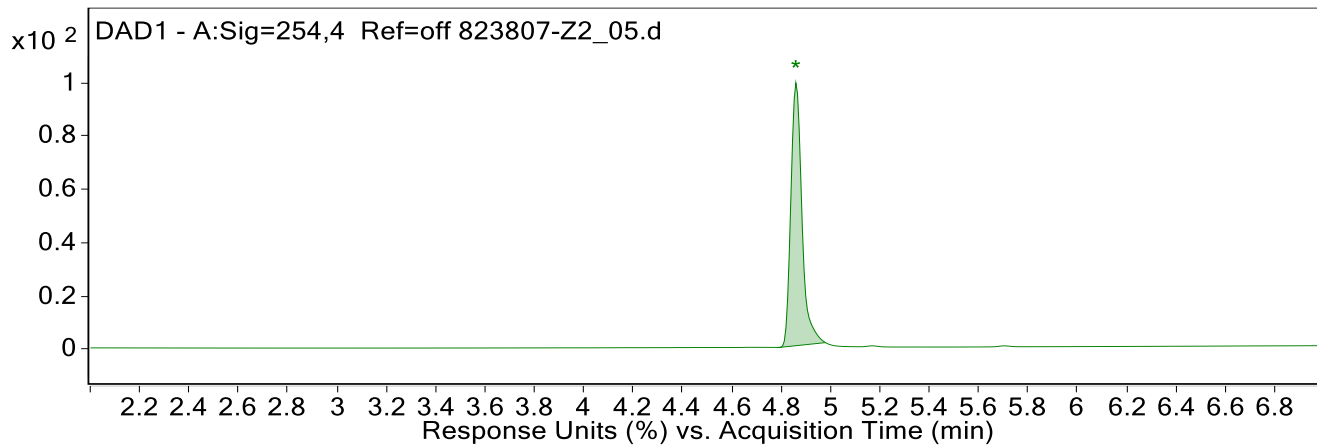
**Fragmentor Voltage** 135 **Collision Energy** 0 **Ionization Mode** ESI



## Integration Peak List

| Peak | Start | RT    | End   | Height | Area   | Area Sum % |
|------|-------|-------|-------|--------|--------|------------|
| 1    | 4.787 | 4.860 | 4.993 | 1497.8 | 4830.1 | 100.0      |

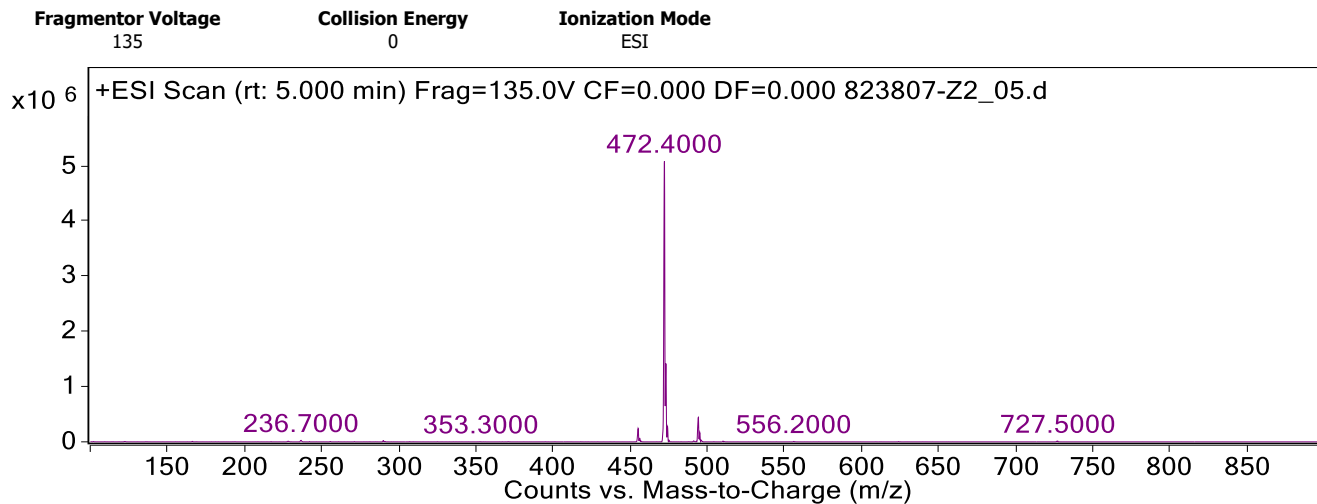
# Qualitative Analysis Report



## Integration Peak List

| Peak | Start | RT    | End   | Height | Area   | Area Sum % |
|------|-------|-------|-------|--------|--------|------------|
| 1    | 4.787 | 4.860 | 4.980 | 976.8  | 3057.6 | 100.0      |

## User Spectra



## Peak List

| m/z   | Abund   |
|-------|---------|
| 455.3 | 241566  |
| 456.4 | 61080   |
| 472.4 | 5082837 |
| 473.3 | 1417459 |
| 474.4 | 272130  |
| 494.4 | 442191  |
| 495.3 | 166143  |
| 496.2 | 32765   |
| 963.3 | 35348   |
| 965.6 | 47082   |

--- End Of Report ---