Synthesis of biologically active isoindolones via N-acyliminium ion cyclisations

MAXIMILIAN TOBIAS FREEBAIRN

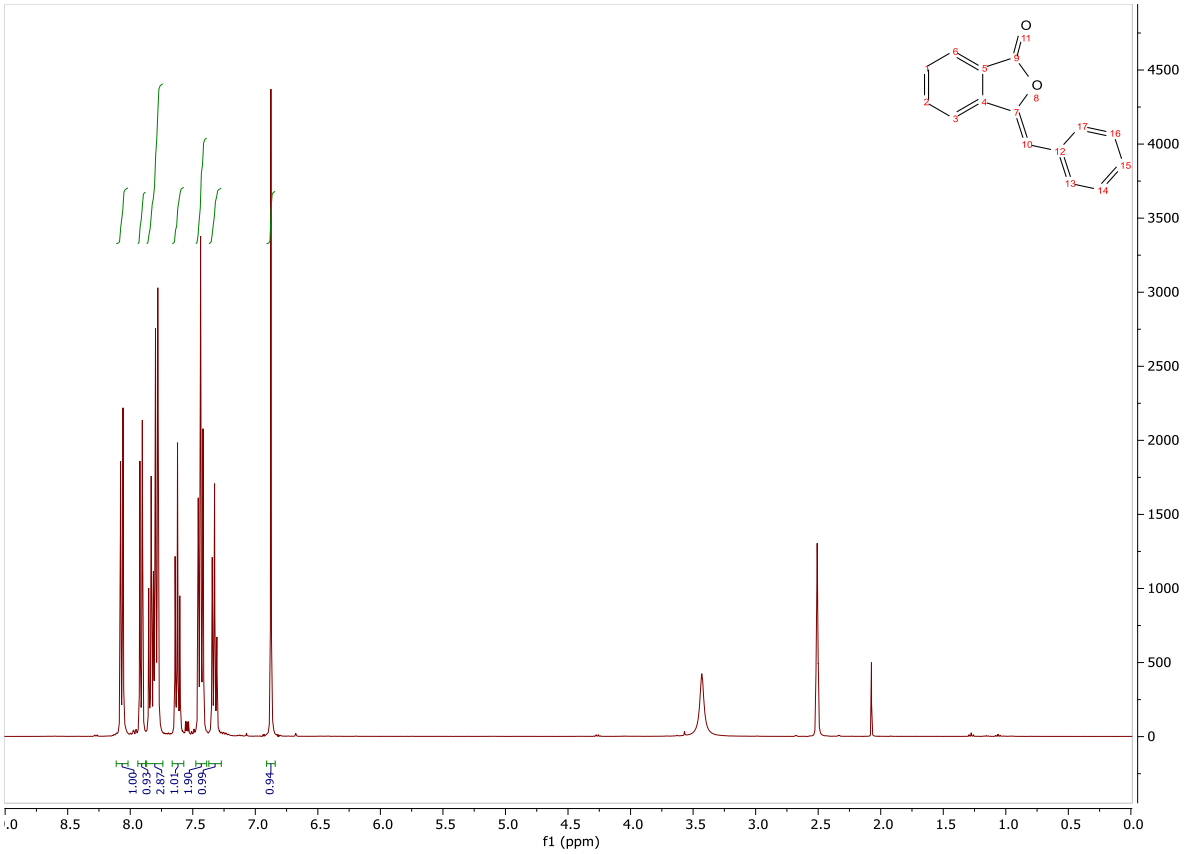
Supplementary information

Contents

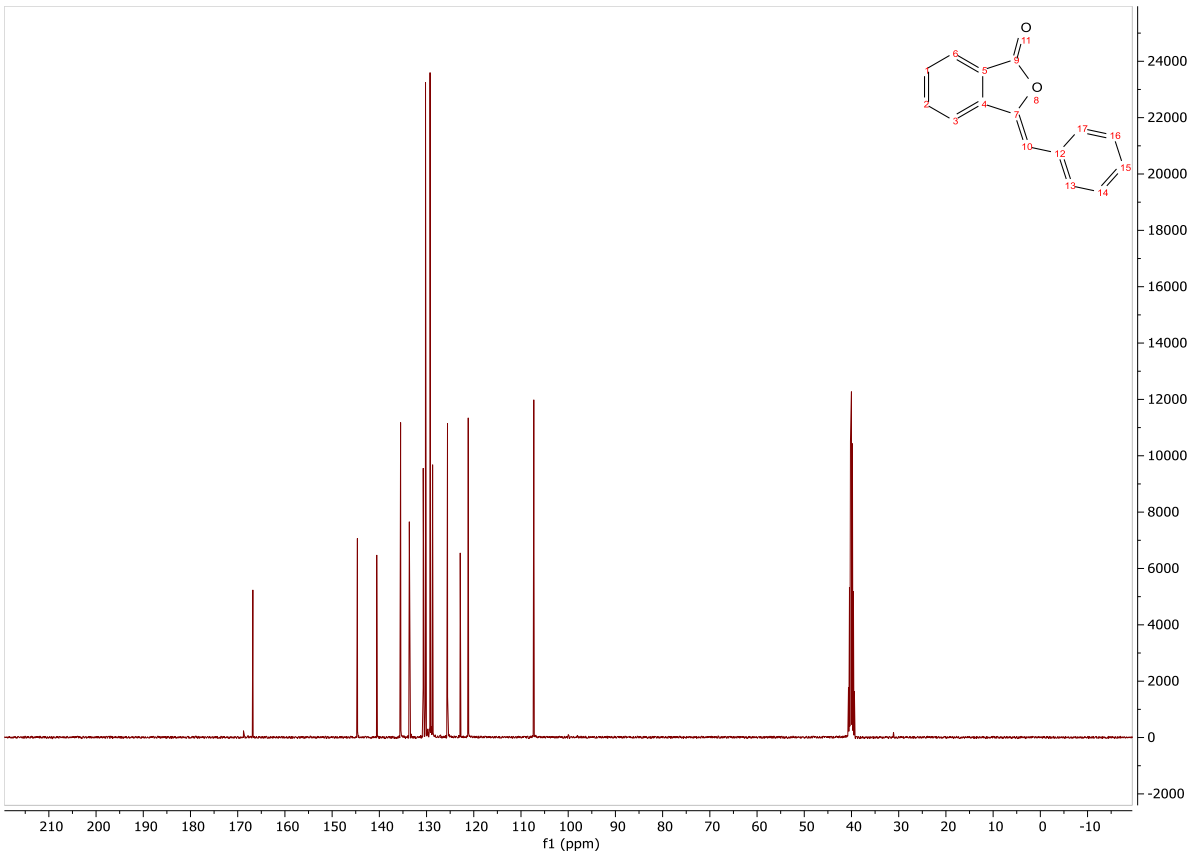
Synthesis of benzalphthalide derivatives **35-35k**

(*Z*)-3-(benzylidene)isobenzofuran-1(*H*)-one **35**

^{1}H:



^{13}C:



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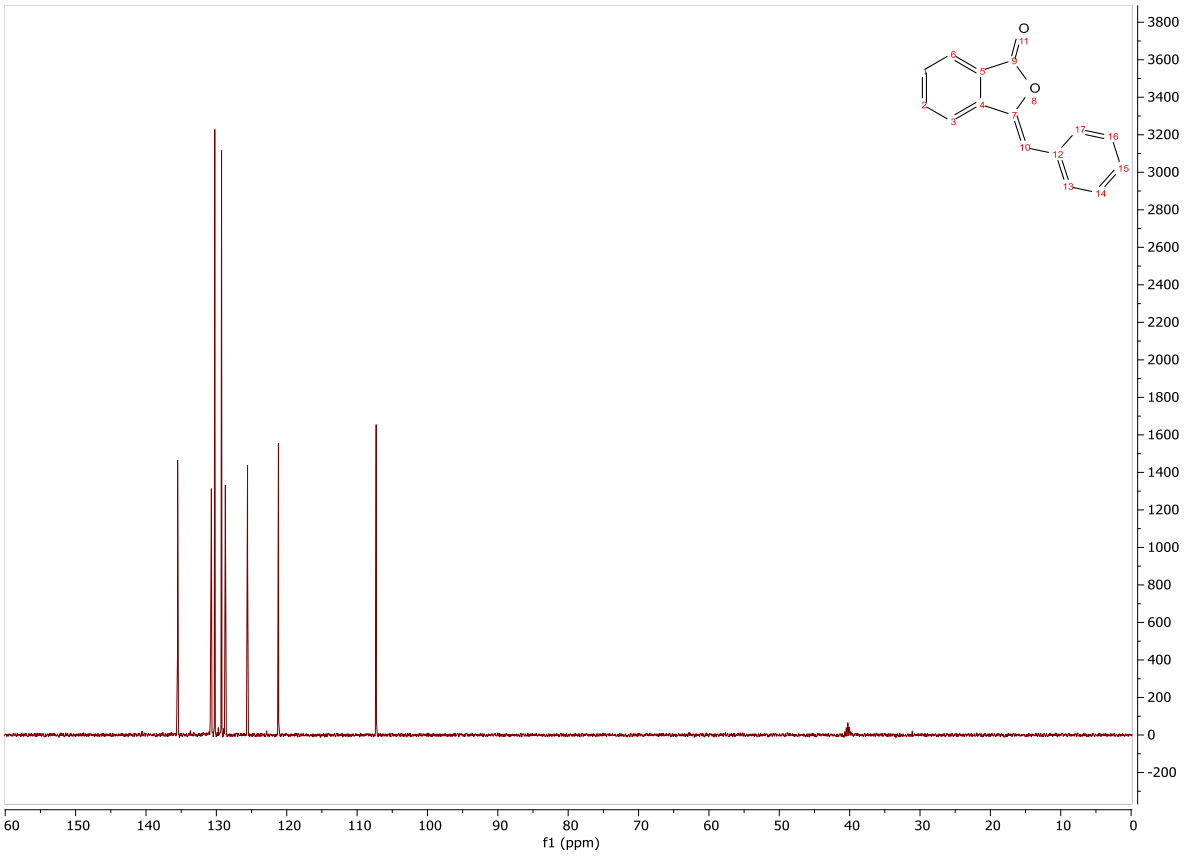
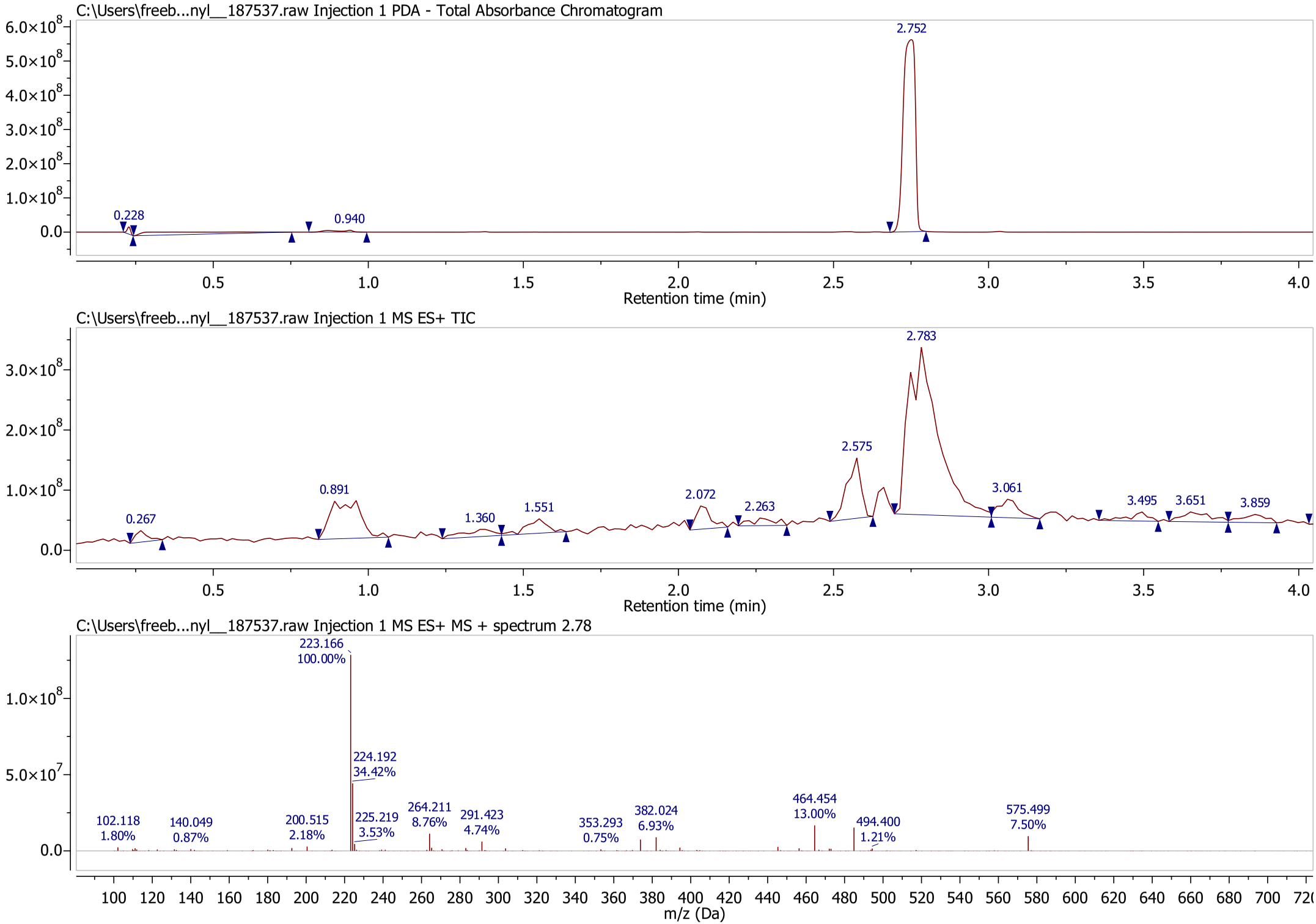

O
11
6
5
9
O
8
1
2
4
7
3
10
17
16
12
15
13
14
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


C:\Users\freeb...nyl__187537.raw Injection 1 PDA - Total Absorbance Chromatogram
6.0×10^8
5.0×10^8
4.0×10^8
3.0×10^8
2.0×10^8
1.0×10^8
0.0
2.752
0.228
0.940
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Retention time (min)
C:\Users\freeb...nyl__187537.raw Injection 1 MS ES+ TIC
3.0×10^8
2.0×10^8
1.0×10^8
0.0
2.783
2.575
0.891
3.061
2.072
2.263
1.551
1.360
3.495
3.651
3.859
0.267
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Retention time (min)
C:\Users\freeb...nyl__187537.raw Injection 1 MS ES+ MS + spectrum 2.78
1.0×10^8
5.0×10^7
0.0
223.166
100.00%
224.192
34.42%
102.118
1.80%
140.049
0.87%
200.515
2.18%
225.219
3.53%
264.211
8.76%
291.423
4.74%
353.293
0.75%
382.024
6.93%
464.454
13.00%
494.400
1.21%
575.499
7.50%
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700 72(
m/z (Da)

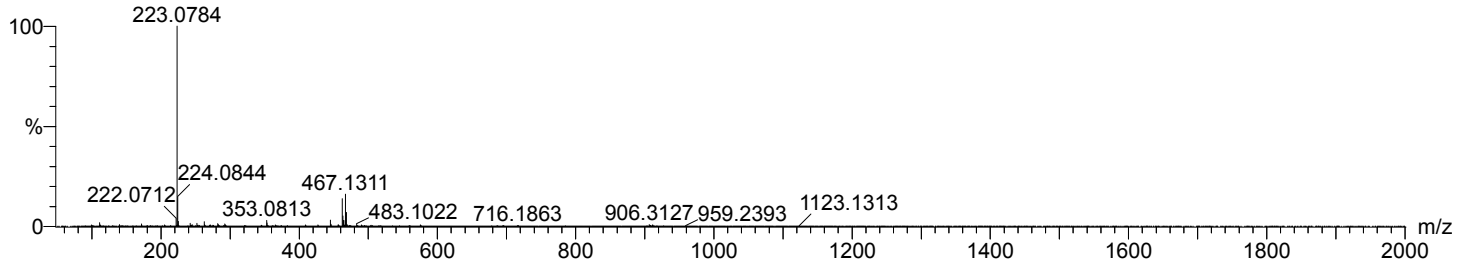
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
252 formula(e) evaluated with 5 results within limits (up to 500 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-4 O: 0-4 Cl: 0-2 I: 0-2

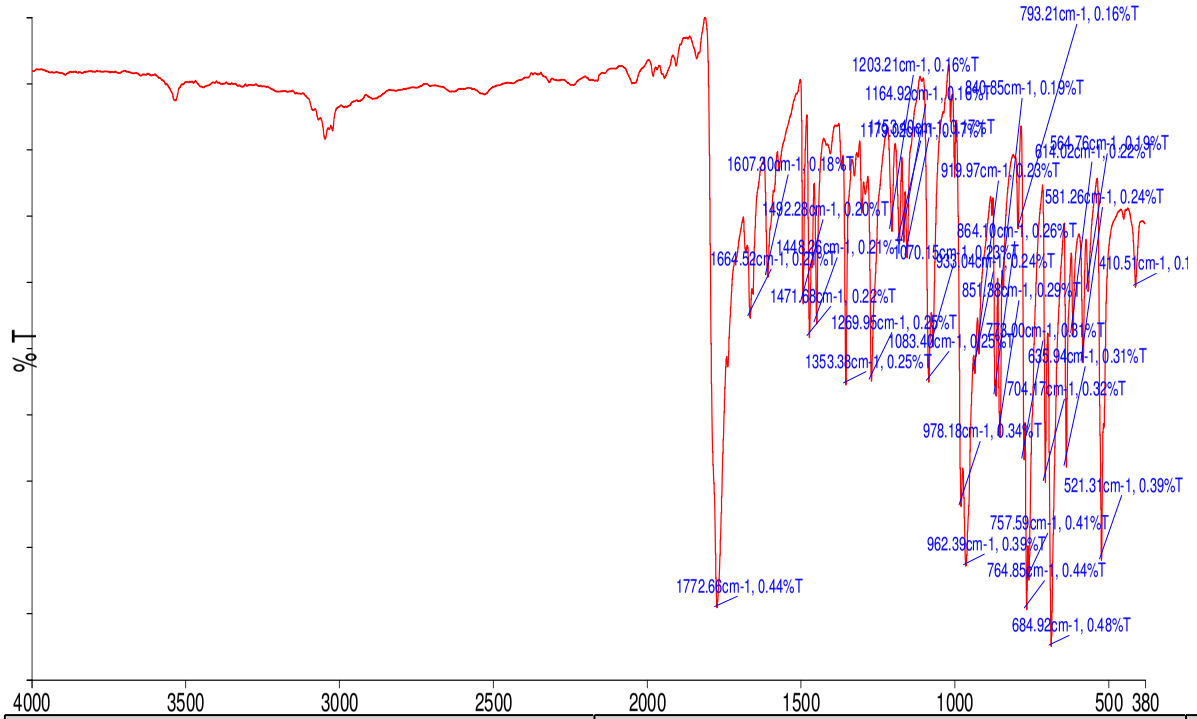
28-Aug-2018
IRB-Het-H 513 (4.313) Cm (512:513)

1: TOF MS ES+
2.83e+004



Minimum:				-1.5			
Maximum:		5.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
223.0784	223.0759	2.5	11.2	10.5	315.5	0.0	C15 H11 O2
	223.0831	-4.7	-21.1	6.5	318.7	3.2	C9 H11 N4 O3
	223.0750	3.4	15.2	6.5	335.2	19.8	C10 H12 N4 Cl
	223.0737	4.7	21.1	1.5	335.2	19.8	C9 H16 O4 Cl
	223.0769	1.5	6.7	1.5	337.6	22.2	C9 H17 N2 Cl2

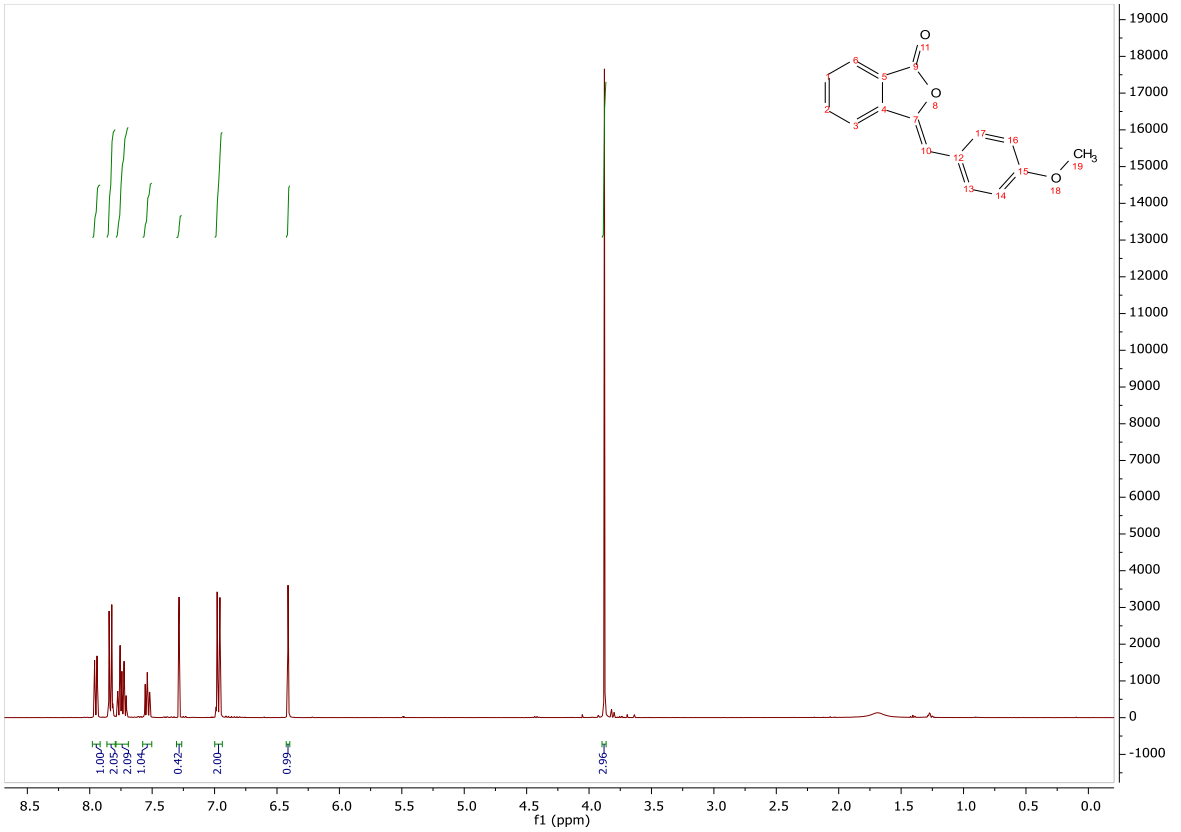
Analyst Professor Ian Baxendale
Date 24 August 2018 13:32



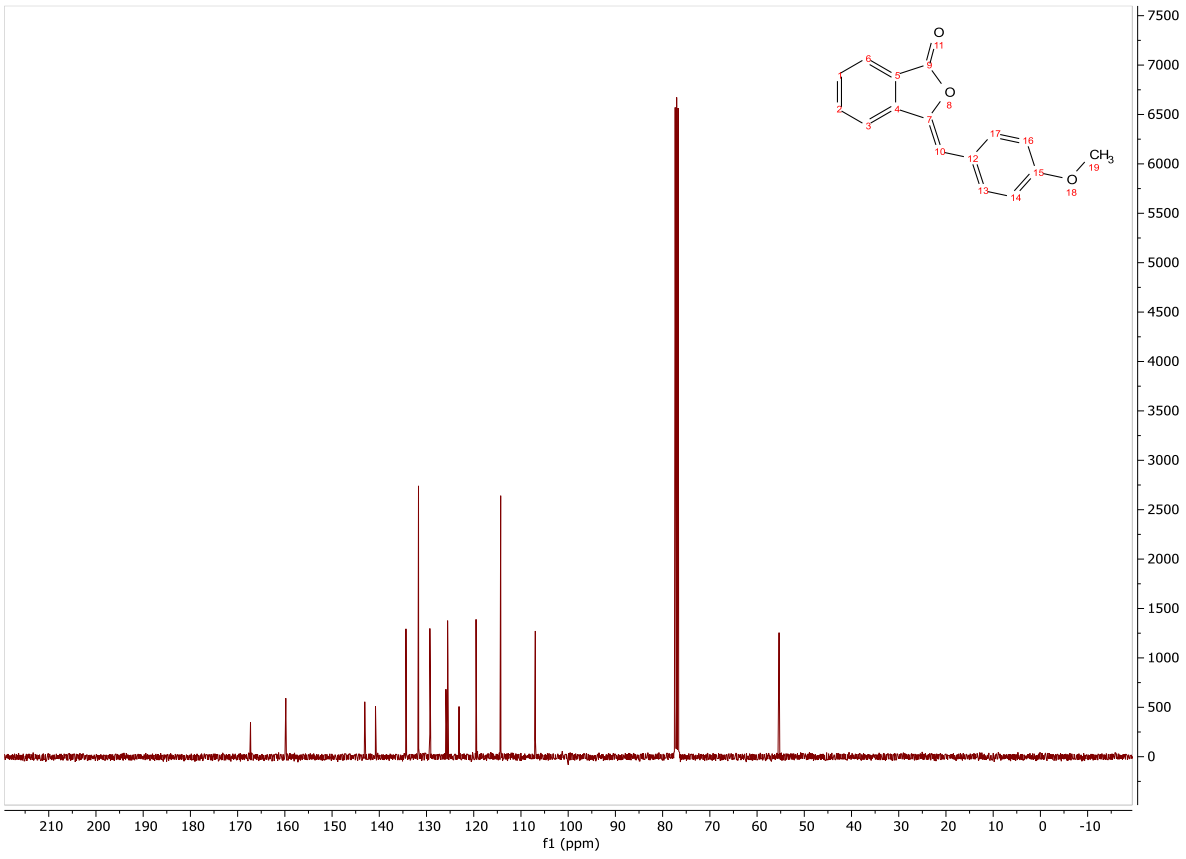
Sample Name	Description	Quality Checks
IRB 133	Sample 133 By IRB Date Friday, August 24 2018	The Quality Checks do not report any warnings for the sample.

(*Z*) -3-(4-methoxybenzylidene)isobenzofuran-1(*H*)-one **35b**

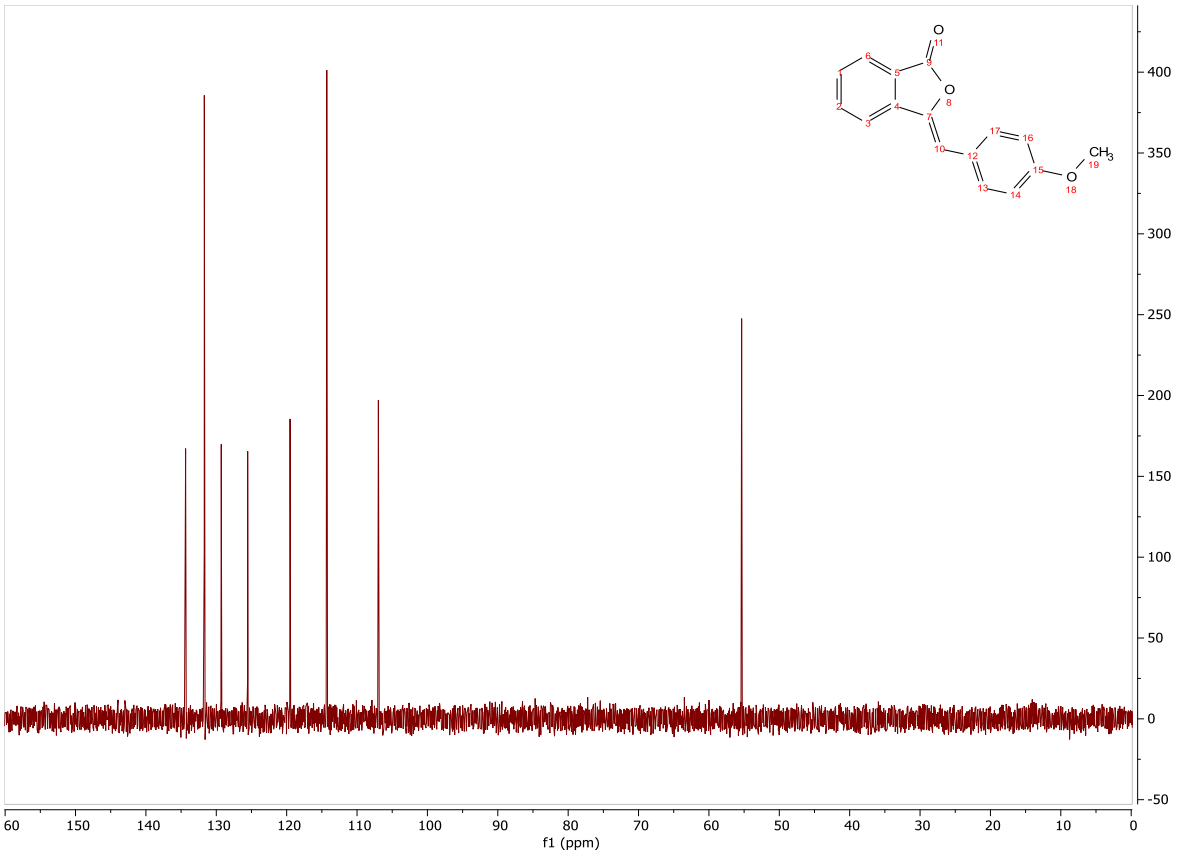
^{1}H:

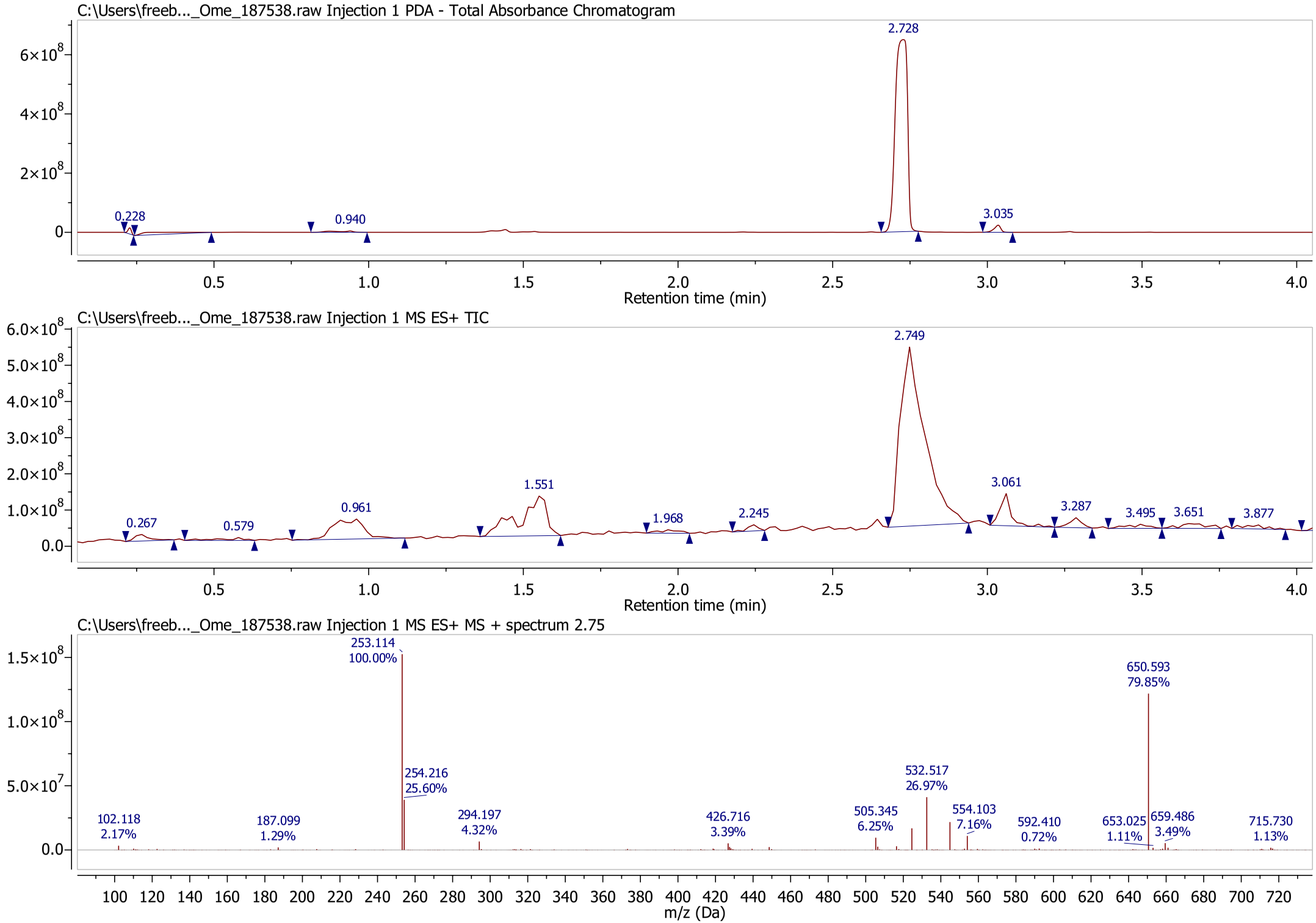


^{13}C:



DEPT-135:


O
11
6
5
9
O
8
1
4
7
2
3
10
17
16
12
15
CH3
19
O
18
13
14
400
350
300
250
200
150
100
50
0
-50
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


C:\Users\freeb..._Ome_187538.raw Injection 1 PDA - Total Absorbance Chromatogram
2.728
0.228
0.940
3.035
Retention time (min)
C:\Users\freeb..._Ome_187538.raw Injection 1 MS ES+ TIC
2.749
1.551
0.961
0.267
0.579
1.968
2.245
3.061
3.287
3.495
3.651
3.877
Retention time (min)
C:\Users\freeb..._Ome_187538.raw Injection 1 MS ES+ MS + spectrum 2.75
253.114
100.00%
650.593
79.85%
254.216
25.60%
532.517
26.97%
102.118
2.17%
187.099
1.29%
294.197
4.32%
426.716
3.39%
505.345
6.25%
554.103
7.16%
592.410
0.72%
653.025
1.11%
659.486
3.49%
715.730
1.13%
m/z (Da)

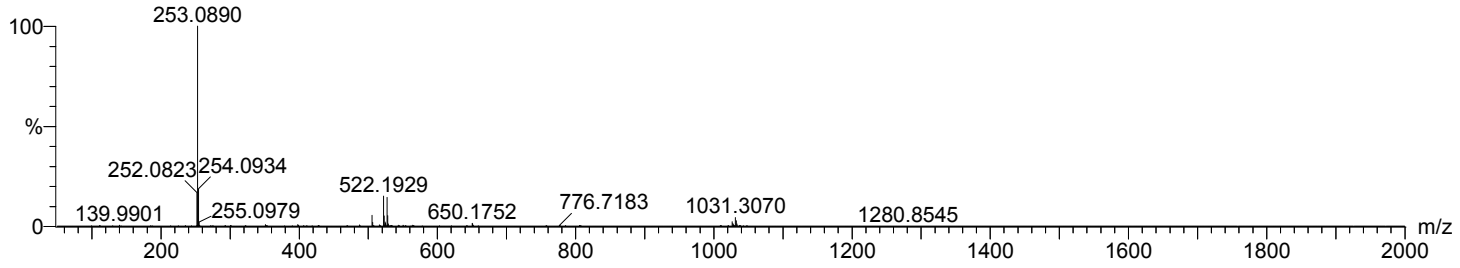
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
309 formula(e) evaluated with 4 results within limits (up to 500 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-4 O: 0-4 Cl: 0-2 I: 0-2

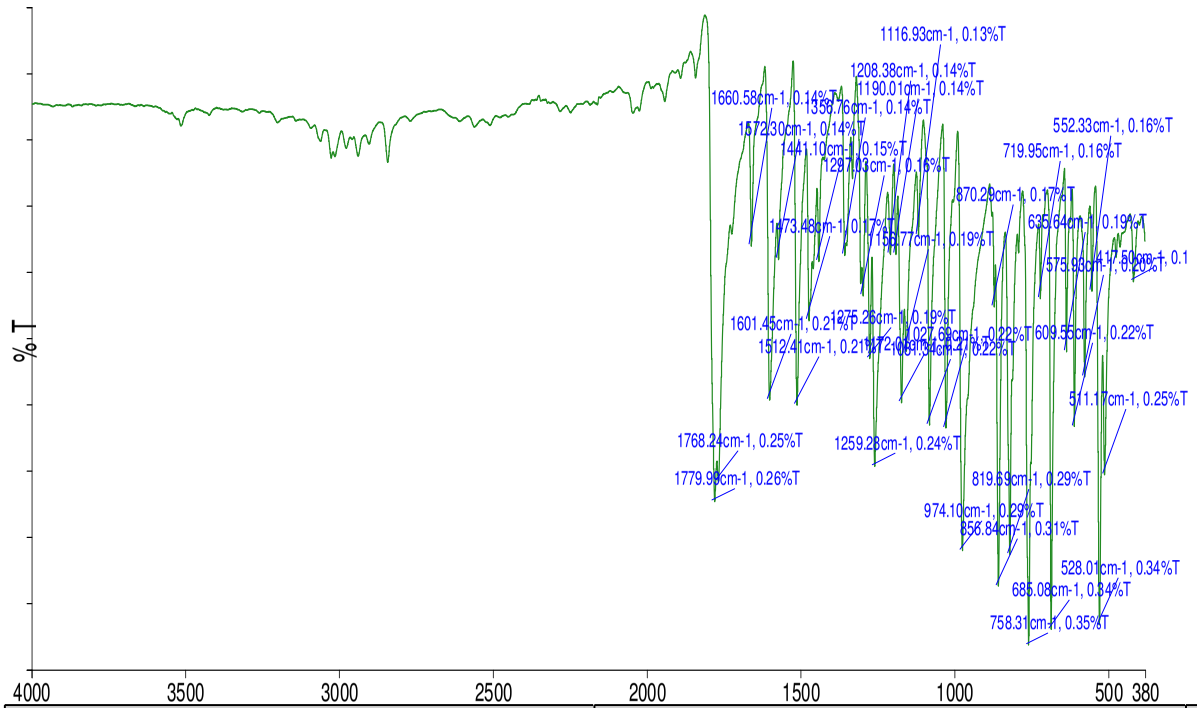
28-Aug-2018
IRB-Het-4-OMe 505 (4.246) Cm (500:517)

1: TOF MS ES+
5.18e+005



Minimum:				-1.5							
Maximum:		5.0	10.0	100.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula				
253.0890	253.0865	2.5	9.9	10.5	996.0	0.0	C16	H13	O3		
	253.0937	-4.7	-18.6	6.5	1005.6	9.6	C10	H13	N4	O4	
	253.0856	3.4	13.4	6.5	1024.8	28.7	C11	H14	N4	O	Cl
	253.0874	1.6	6.3	1.5	1026.6	30.5	C10	H19	N2	O	Cl2

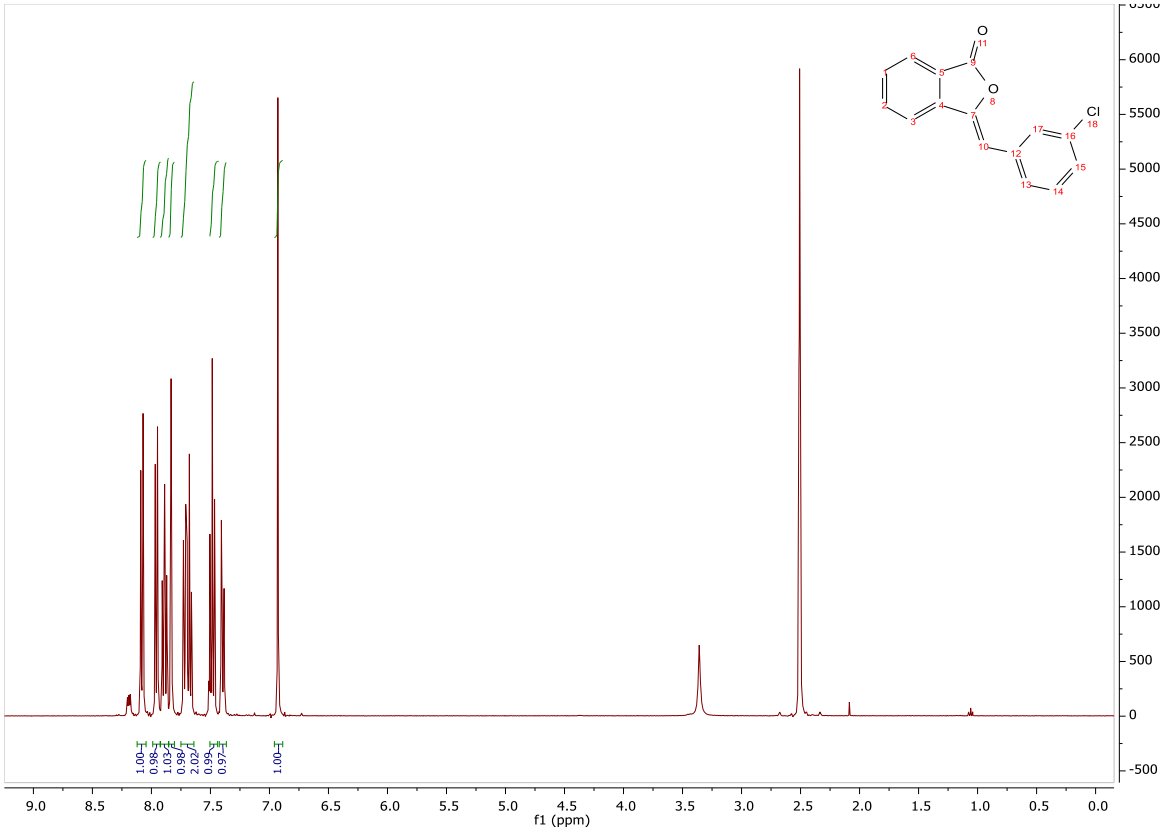
Analyst	Professor Ian Baxendale
Date	24 August 2018 13:45



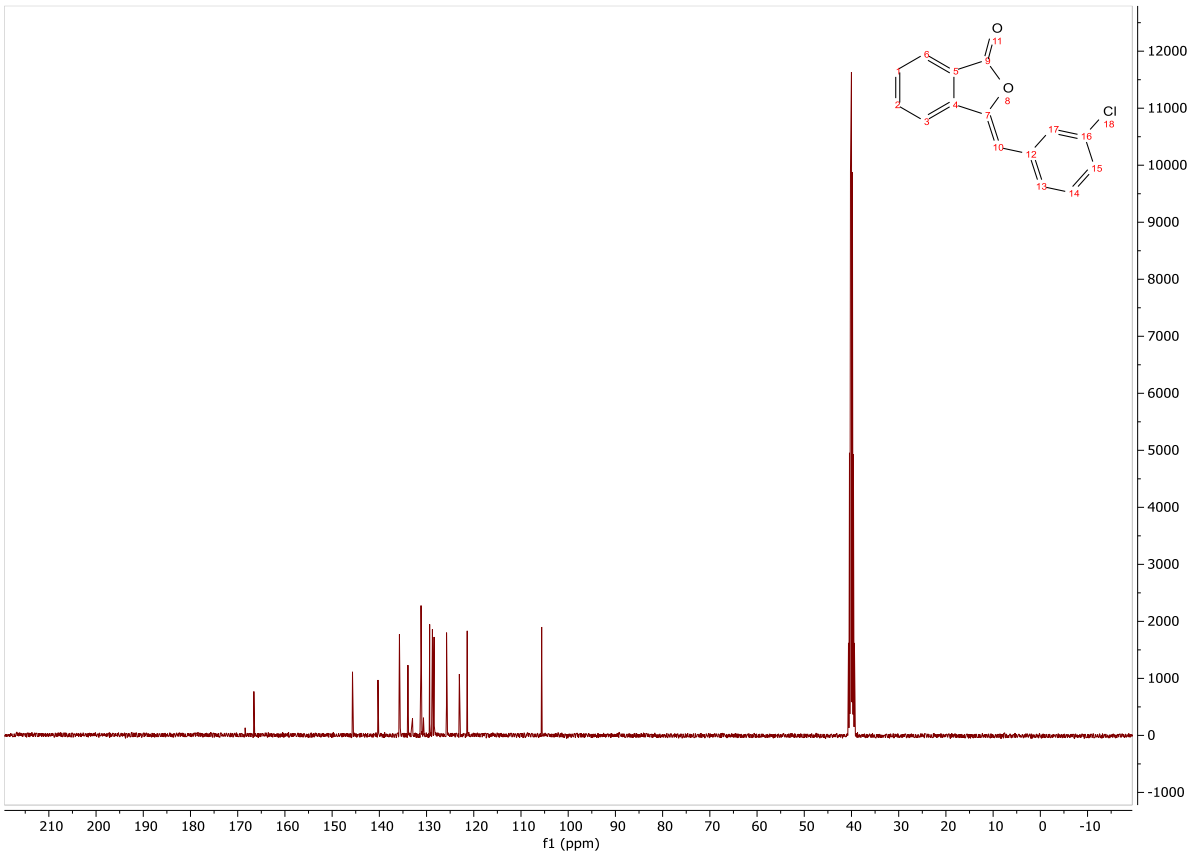
Sample Name	Description	Quality Checks
IRB 136	Sample 136 By IRB Date Friday, August 24 2018	The Quality Checks do not report any warnings for the sample.

(*Z*)-3-(3-chlorobenzylidene)isobenzofuran-1(*H*)-one **35c**

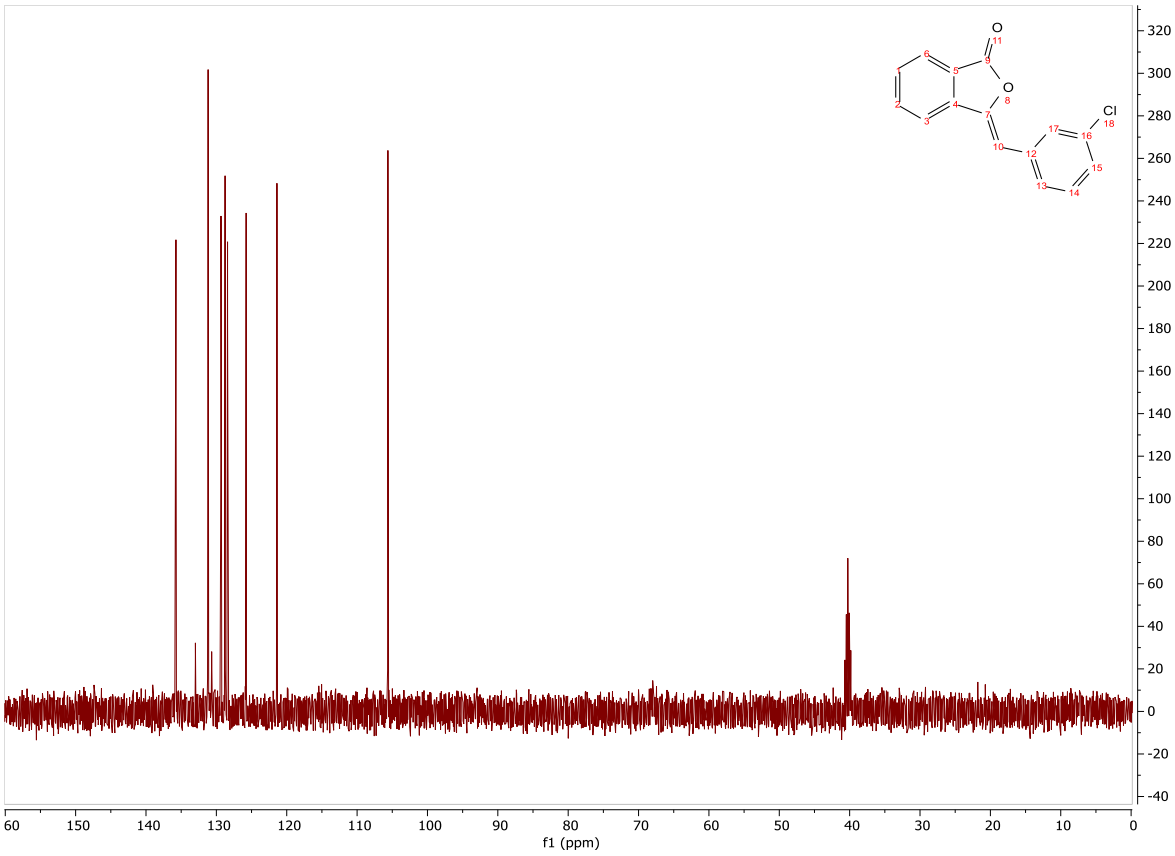
^{1}H:

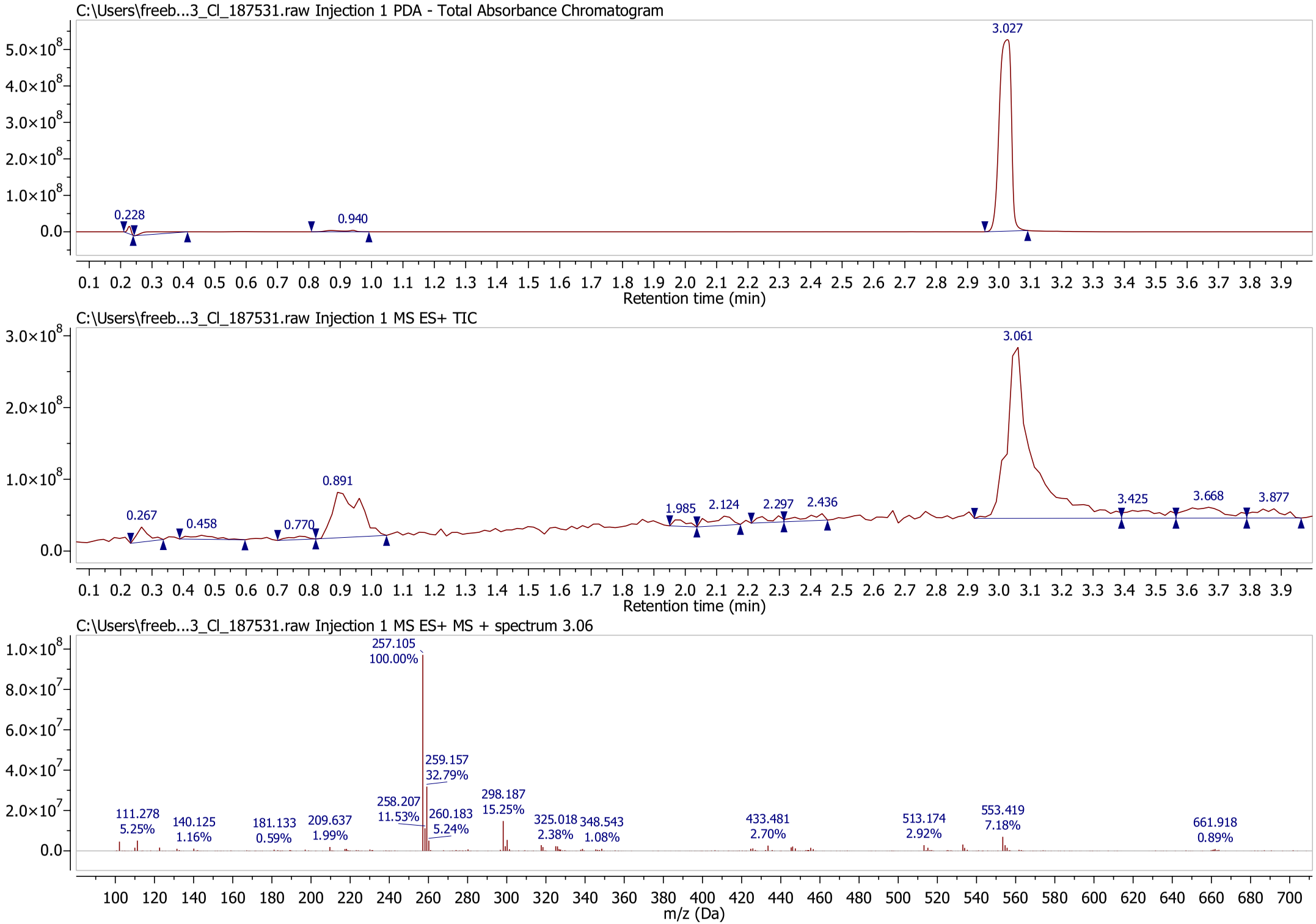


^{13}C:



DEPT-135:


O
11
6
5
1
O
8
2
4
7
3
10
Cl
18
17
16
12
15
13
14
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
-40
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


C:\Users\freeb...3_Cl_187531.raw Injection 1 PDA - Total Absorbance Chromatogram
3.027
0.228
0.940
Retention time (min)
C:\Users\freeb...3_Cl_187531.raw Injection 1 MS ES+ TIC
3.061
0.891
0.267
0.458
0.770
1.985
2.124
2.297
2.436
3.425
3.668
3.877
Retention time (min)
C:\Users\freeb...3_Cl_187531.raw Injection 1 MS ES+ MS + spectrum 3.06
257.105
100.00%
259.157
32.79%
298.187
15.25%
258.207
11.53%
260.183
5.24%
111.278
5.25%
140.125
1.16%
181.133
0.59%
209.637
1.99%
325.018
2.38%
348.543
1.08%
433.481
2.70%
513.174
2.92%
553.419
7.18%
661.918
0.89%
m/z (Da)

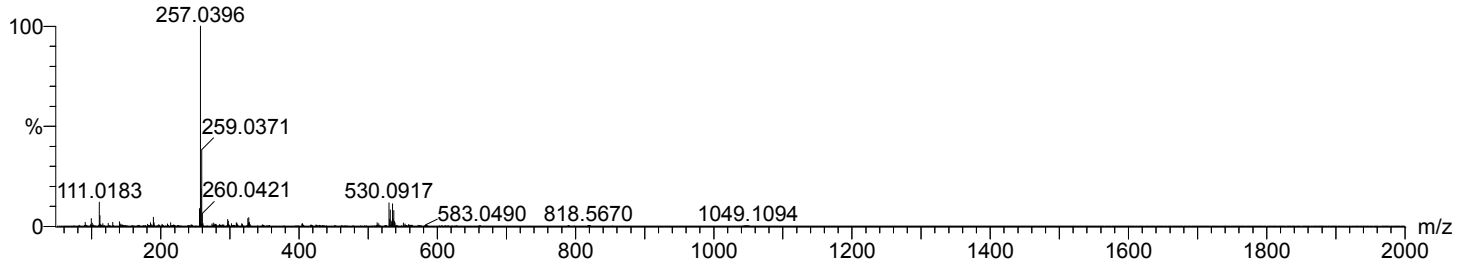
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
321 formula(e) evaluated with 7 results within limits (up to 500 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-4 O: 0-4 Cl: 0-2 I: 0-2

28-Aug-2018
IRB-Het-3-Cl 554 (4.661) Cm (546:560)

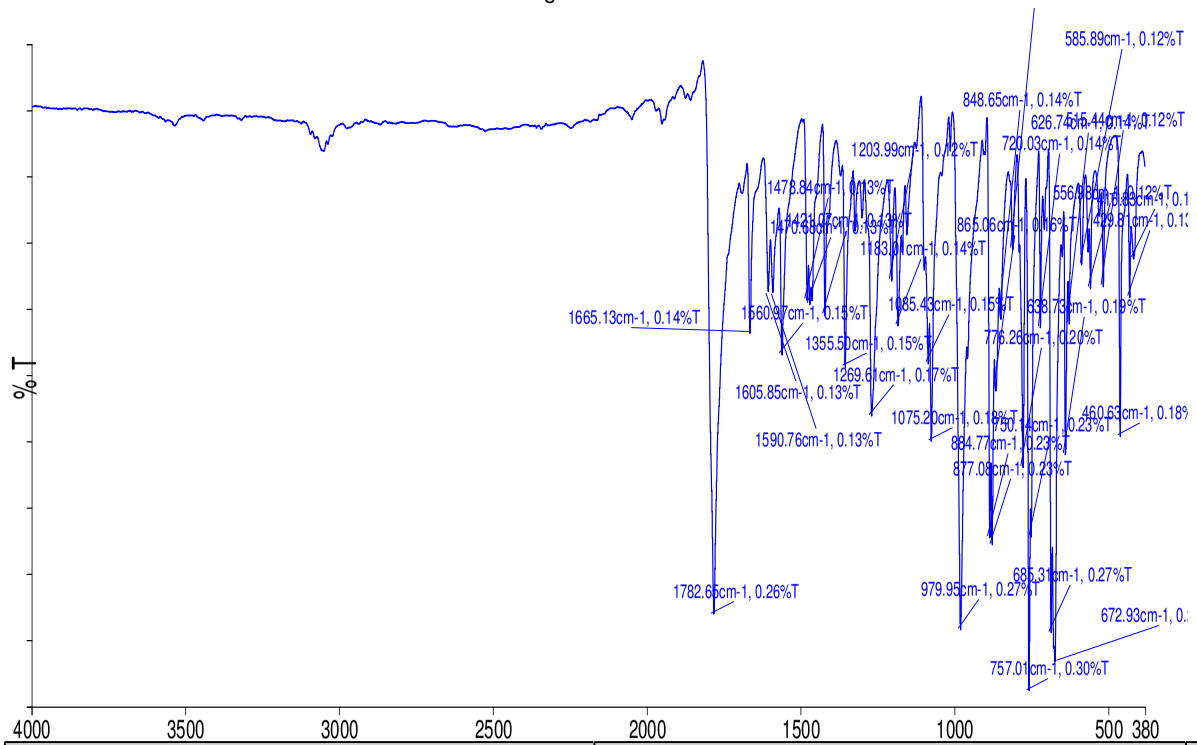
1: TOF MS ES+
4.38e+004



Minimum:				-1.5			
Maximum:		5.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
257.0396	257.0369	2.7	10.5	10.5	557.9	0.0	C15 H10 O2 Cl
	257.0441	-4.5	-17.5	6.5	562.9	5.0	C9 H10 N4 O3 Cl
	257.0351	4.5	17.5	15.5	572.6	14.7	C16 H5 N2 O2
	257.0361	3.5	13.6	6.5	573.0	15.2	C10 H11 N4 Cl2
	257.0402	-0.6	-2.3	-0.5	573.1	15.3	C8 H18 O I
	257.0391	0.5	1.9	19.5	573.3	15.4	C21 H5
	257.0347	4.9	19.1	1.5	573.4	15.6	C9 H15 O4 Cl2

Analyst Professor Ian Baxendale

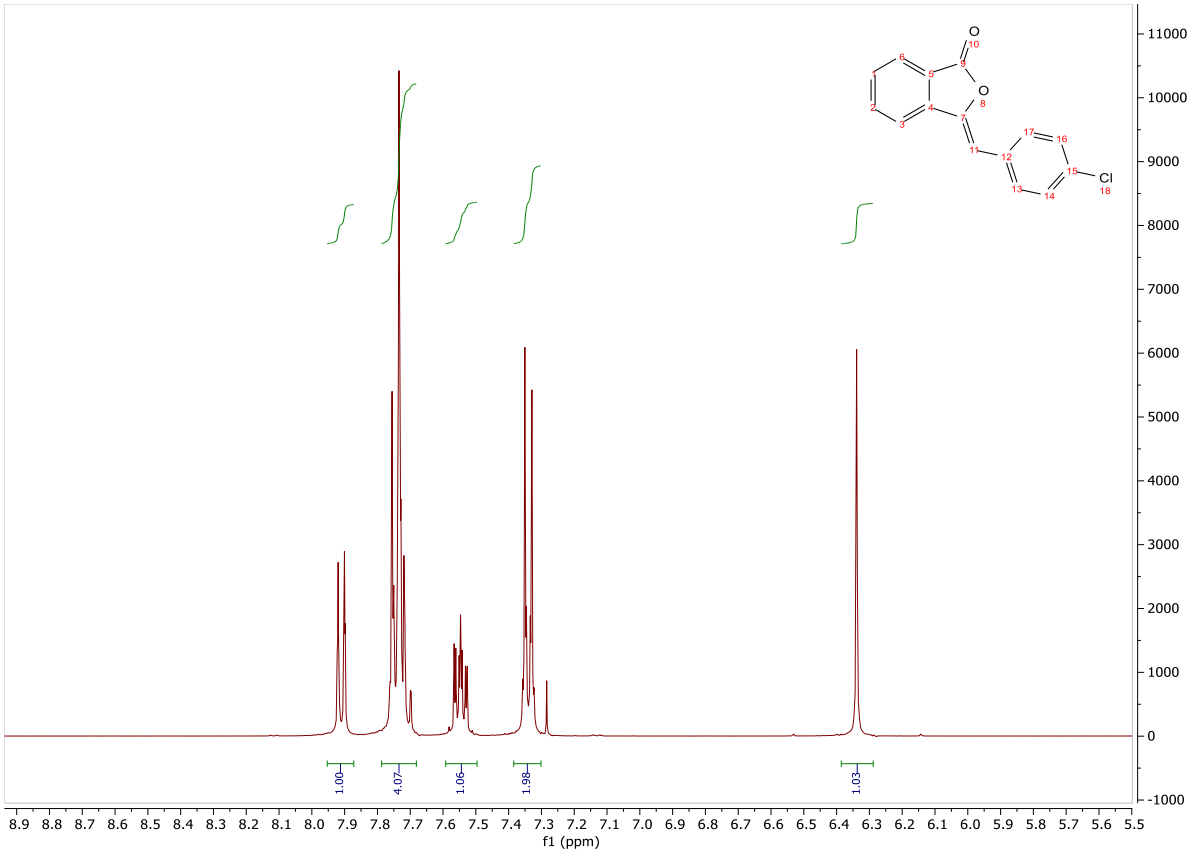
Date 24 August 2018 13:36



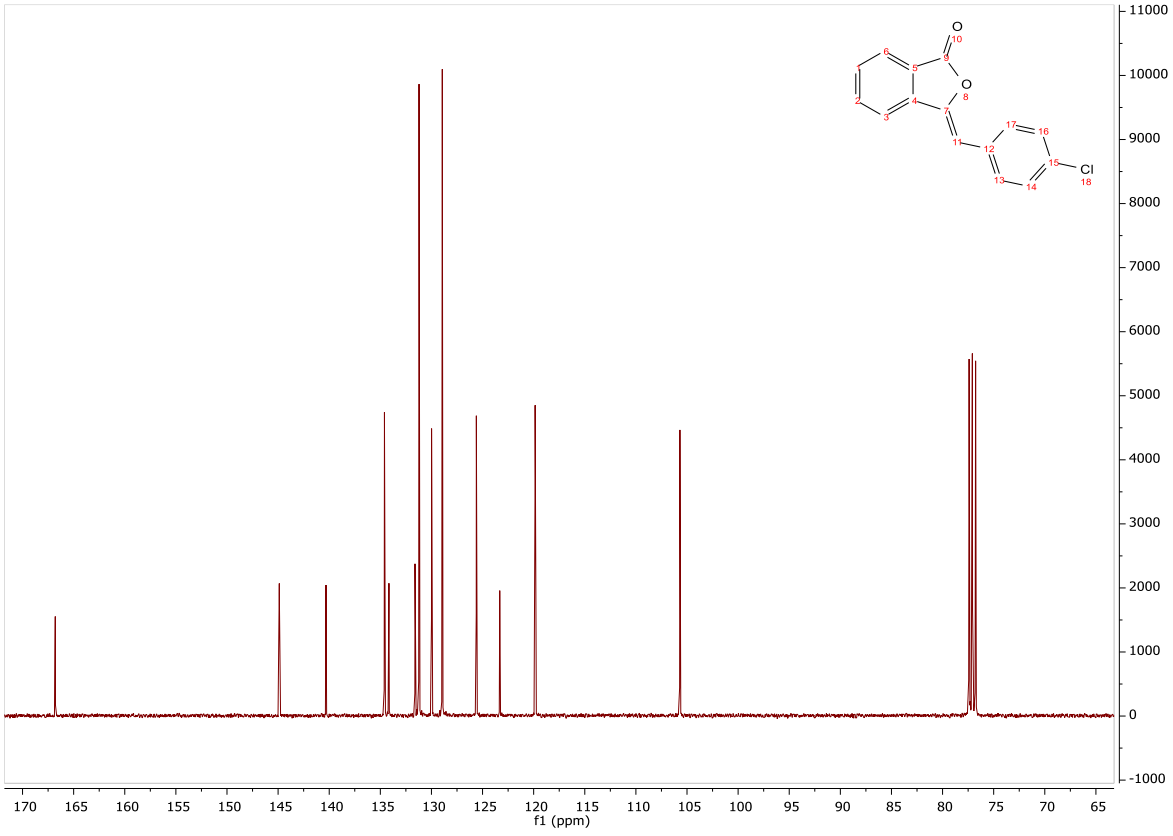
Sample Name	Description	Quality Checks
IRB 134	Sample 134 By IRB Date Friday, August 24 2018	The Quality Checks do not report any warnings for the sample.

(*Z*)-3-(4-chlorobenzylidene)isobenzofuran-1(*H*)-one **35d**

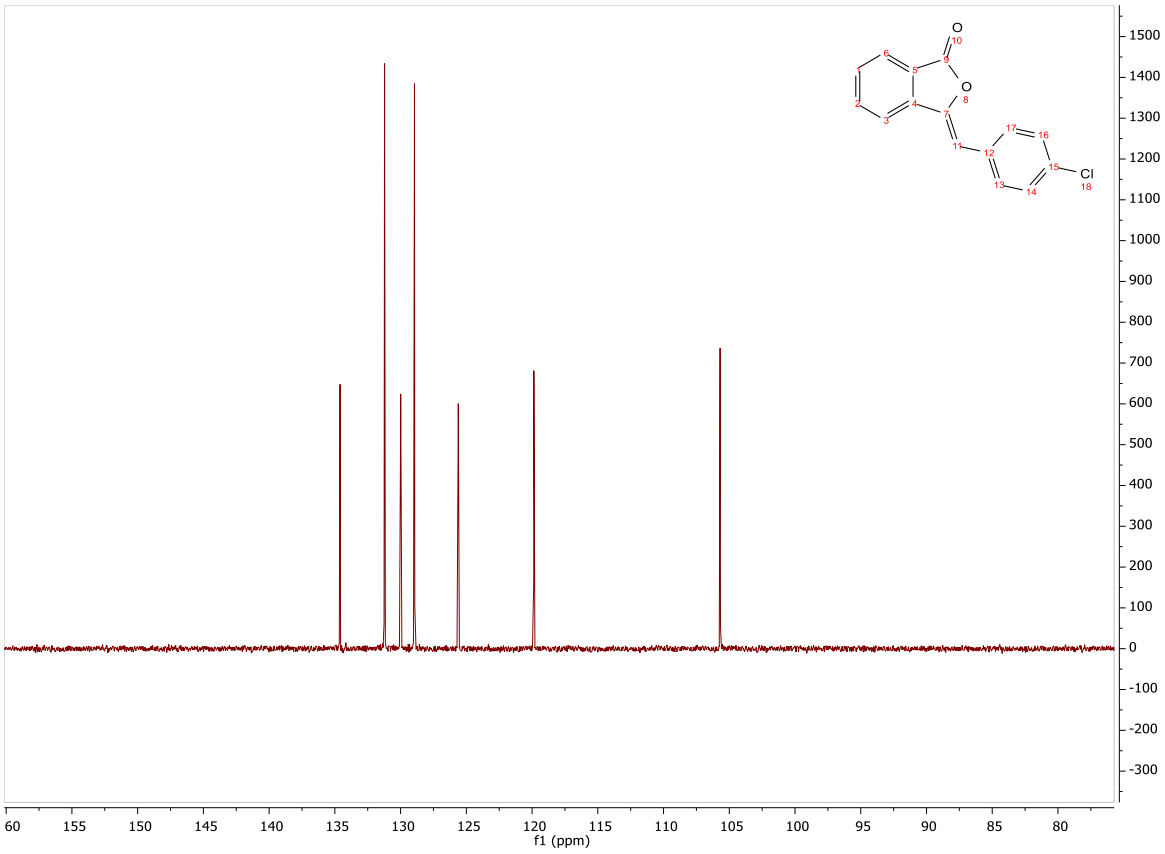
^{1}H:

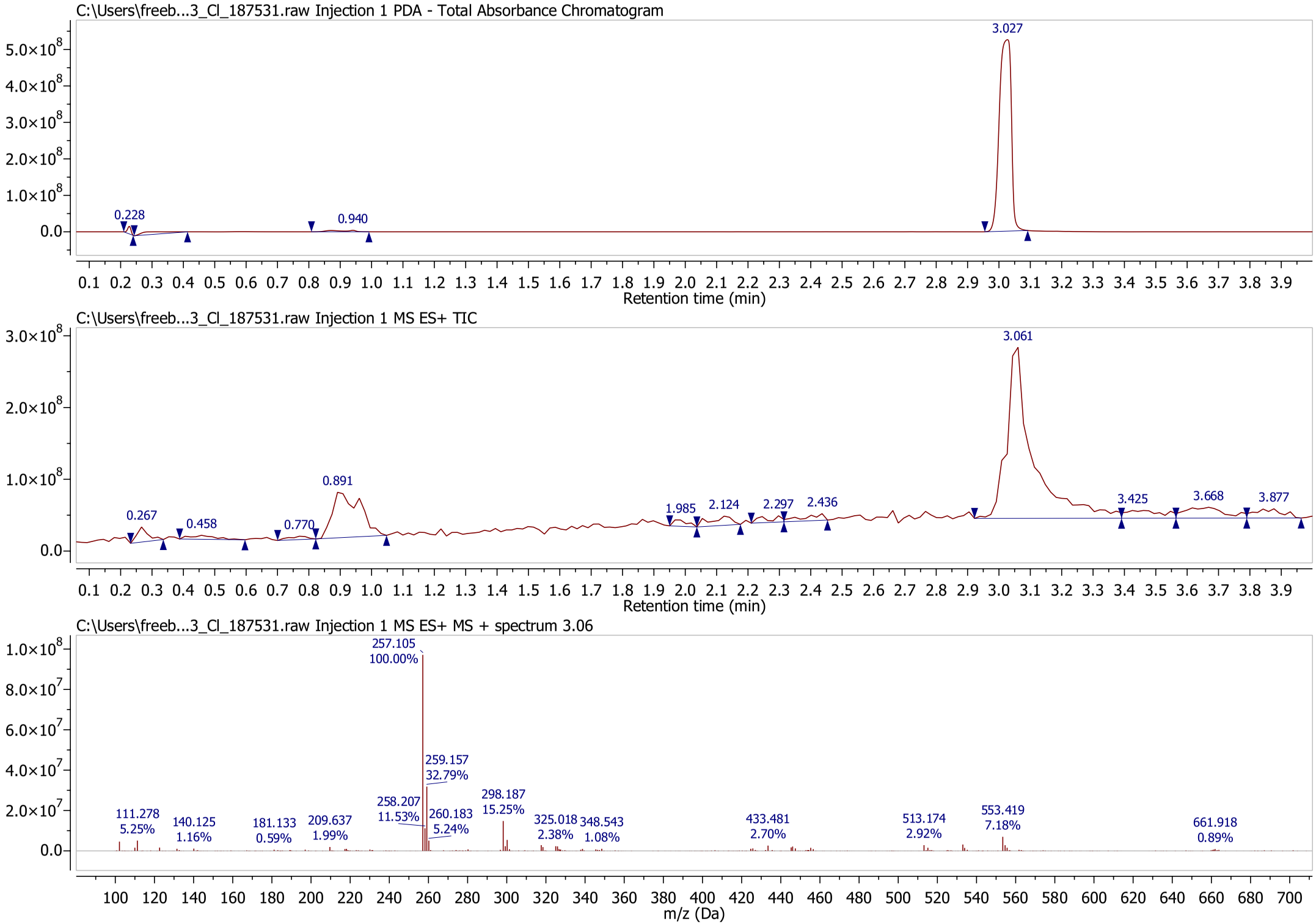


13C:



DEPT-135:


O
10
6
5
9
1
O
8
2
4
7
3
11
17
16
12
15
Cl
18
13
14
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
-300
60
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
f1 (ppm)


C:\Users\freeb...3_Cl_187531.raw Injection 1 PDA - Total Absorbance Chromatogram
3.027
0.228
0.940
Retention time (min)
C:\Users\freeb...3_Cl_187531.raw Injection 1 MS ES+ TIC
3.061
0.891
0.267
0.458
0.770
1.985
2.124
2.297
2.436
3.425
3.668
3.877
Retention time (min)
C:\Users\freeb...3_Cl_187531.raw Injection 1 MS ES+ MS + spectrum 3.06
257.105
100.00%
259.157
32.79%
298.187
15.25%
258.207
11.53%
260.183
5.24%
111.278
5.25%
140.125
1.16%
181.133
0.59%
209.637
1.99%
325.018
2.38%
348.543
1.08%
433.481
2.70%
513.174
2.92%
553.419
7.18%
661.918
0.89%
m/z (Da)

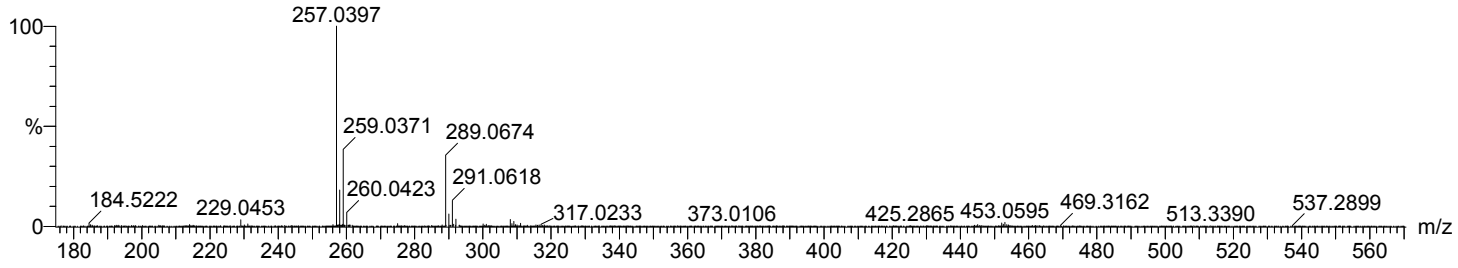
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
321 formula(e) evaluated with 7 results within limits (up to 500 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-4 O: 0-4 Cl: 0-2 I: 0-2

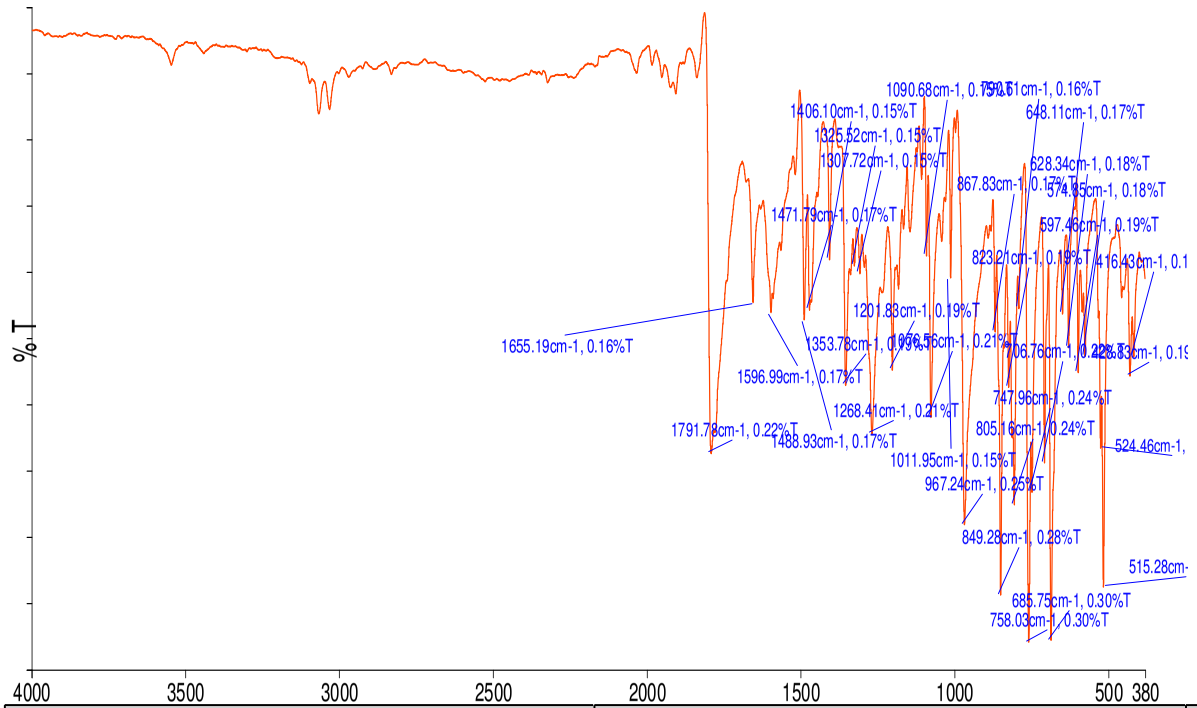
28-Aug-2018
IRB-Het-4-Cl 500 (4.205)

1: TOF MS ES+
1.13e+004



Minimum:				-1.5			
Maximum:		5.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
257.0397	257.0369	2.8	10.9	10.5	247.7	0.0	C15 H10 O2 Cl
	257.0441	-4.4	-17.1	6.5	254.7	7.1	C9 H10 N4 O3 Cl
	257.0347	5.0	19.5	1.5	265.9	18.2	C9 H15 O4 Cl2
	257.0361	3.6	14.0	6.5	265.9	18.2	C10 H11 N4 Cl2
	257.0351	4.6	17.9	15.5	271.0	23.3	C16 H5 N2 O2
	257.0402	-0.5	-1.9	-0.5	271.5	23.9	C8 H18 O I
	257.0391	0.6	2.3	19.5	271.7	24.0	C21 H5

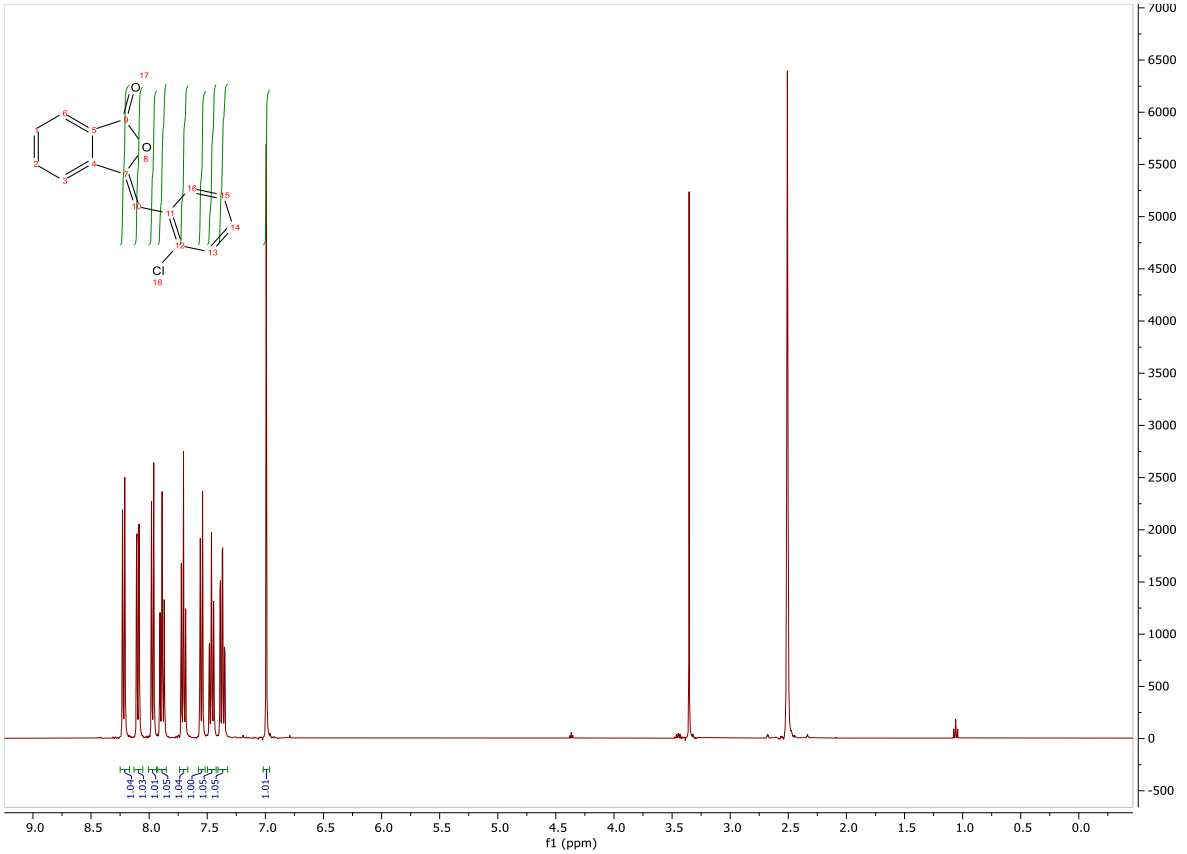
Analyst Professor Ian Baxendale
Date 24 August 2018 14:02



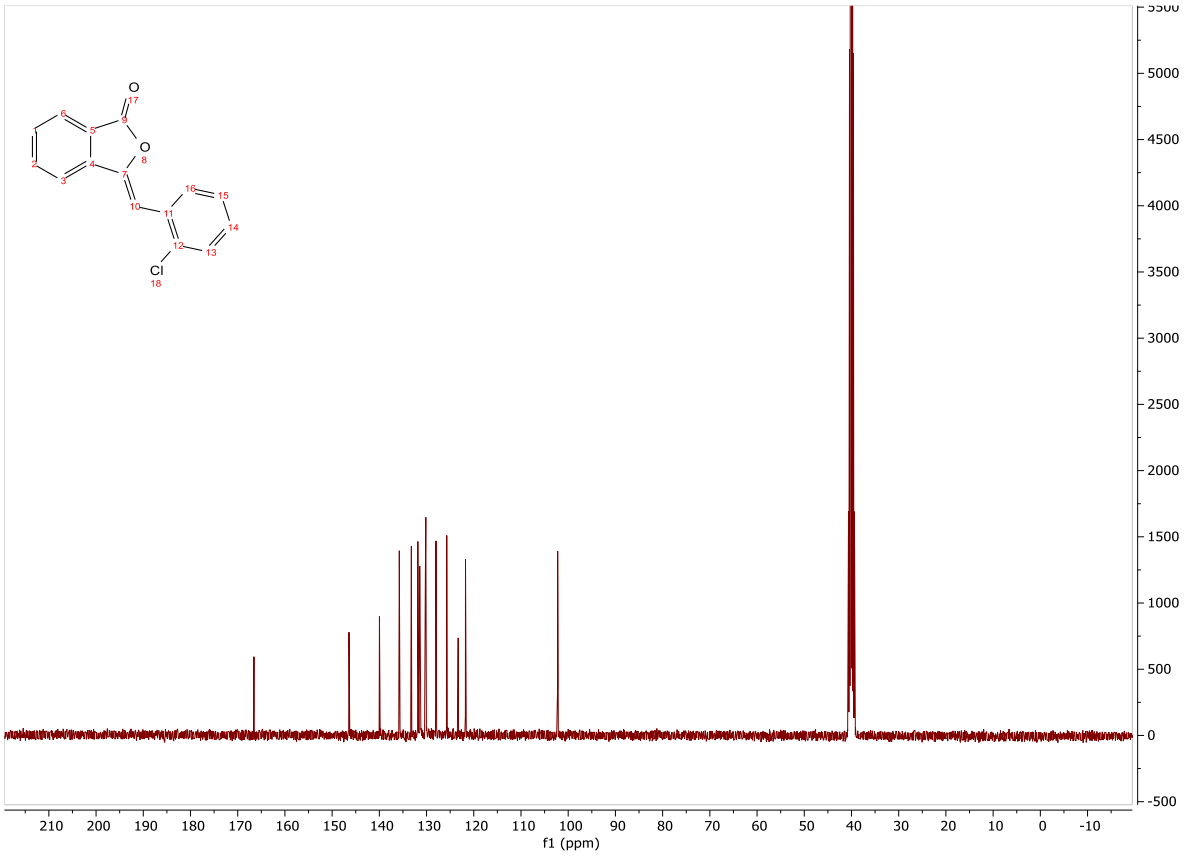
Sample Name	Description	Quality Checks
IRB 140	Sample 140 By IRB Date Friday, August 24 2018	The Quality Checks do not report any warnings for the sample.

(*Z*)-3-(2-chlorobenzylidene)isobenzofuran-1(*H*)-one **35e**

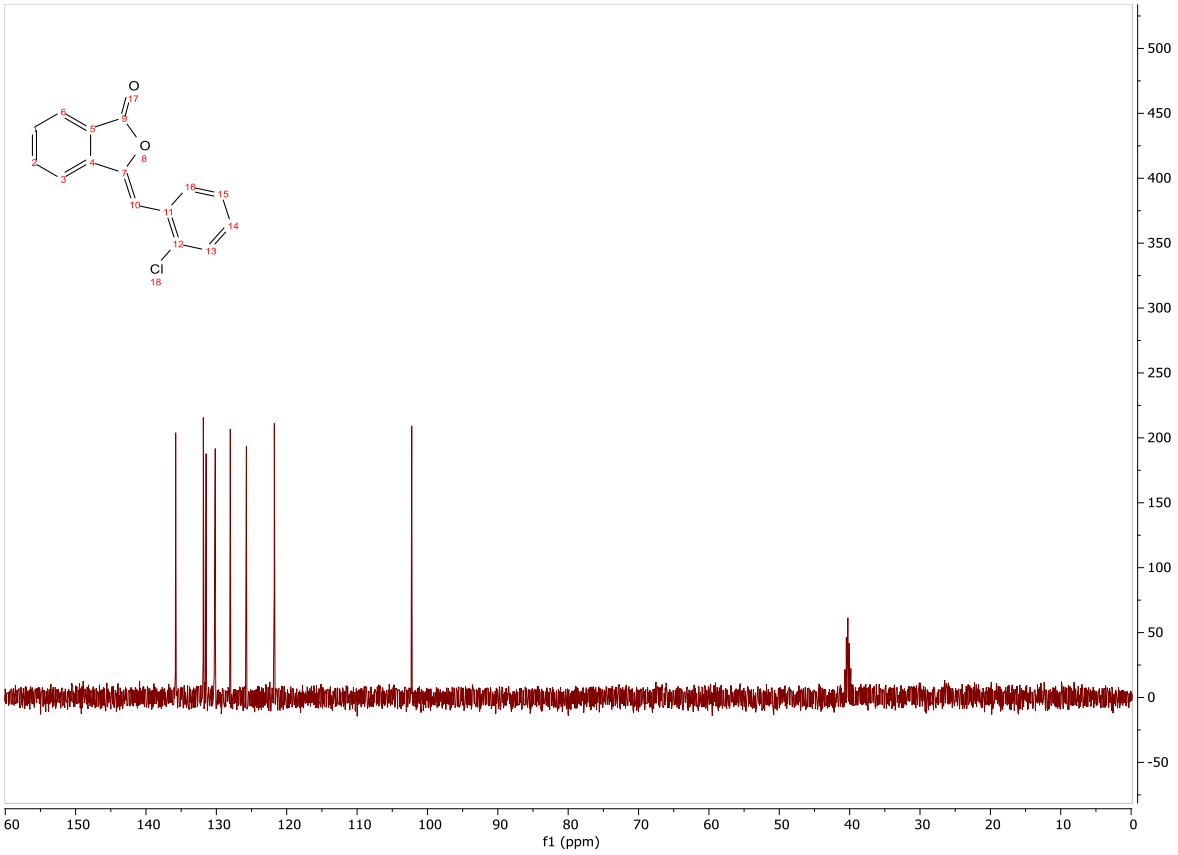
^{1}H:

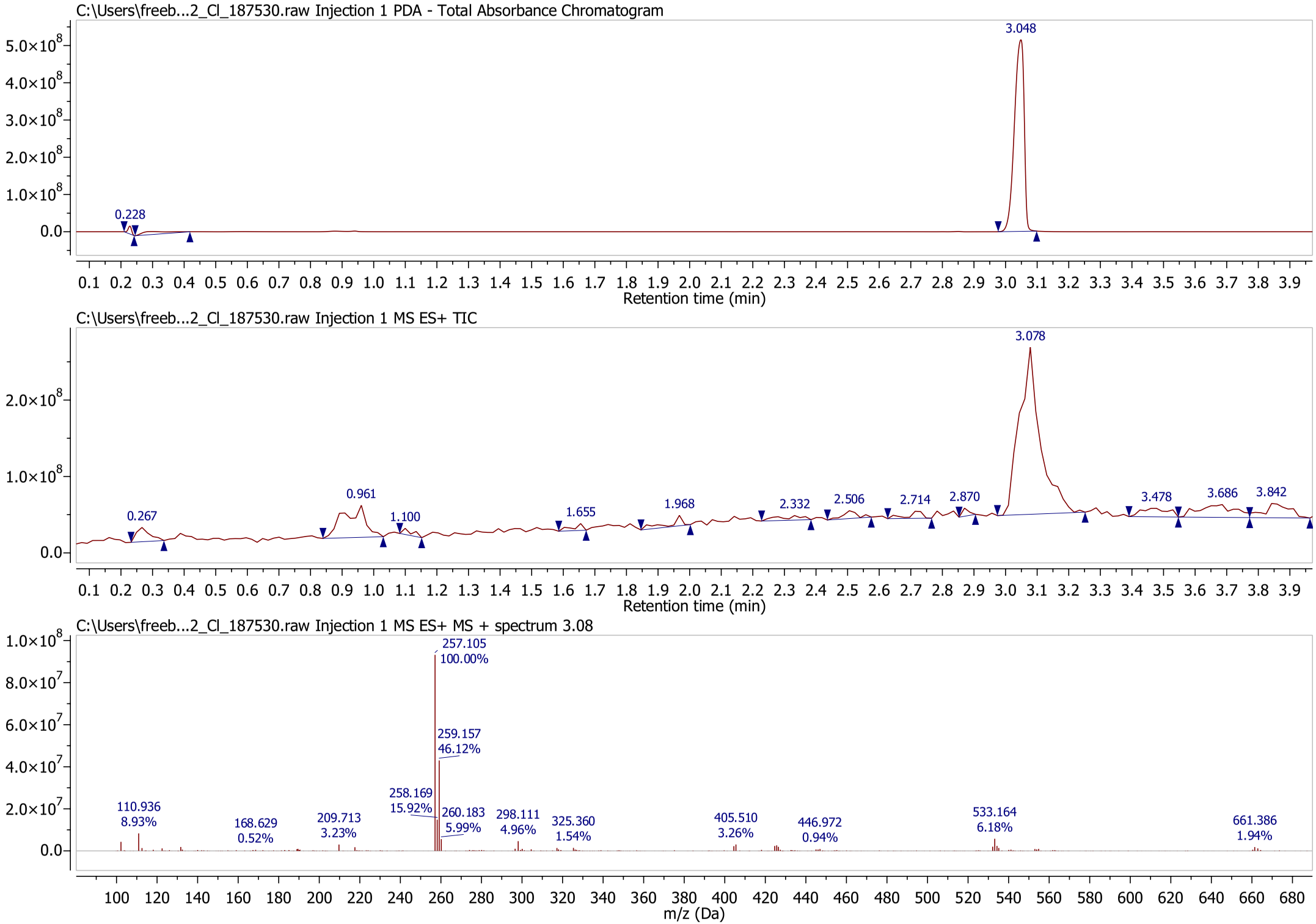


13C:



DEPT-135:


O
17
6
5
9
O
8
1
2
4
7
3
16
15
10
11
14
12
13
Cl
18
500
450
400
350
300
250
200
150
100
50
0
-50
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


C:\Users\freeb...2_Cl_187530.raw Injection 1 PDA - Total Absorbance Chromatogram
3.048
0.228
Retention time (min)
C:\Users\freeb...2_Cl_187530.raw Injection 1 MS ES+ TIC
3.078
0.961
0.267
1.100
1.655
1.968
2.332
2.506
2.714
2.870
3.478
3.686
3.842
Retention time (min)
C:\Users\freeb...2_Cl_187530.raw Injection 1 MS ES+ MS + spectrum 3.08
257.105
100.00%
259.157
46.12%
258.169
15.92%
260.183
5.99%
110.936
8.93%
168.629
0.52%
209.713
3.23%
298.111
4.96%
325.360
1.54%
405.510
3.26%
446.972
0.94%
533.164
6.18%
661.386
1.94%
m/z (Da)

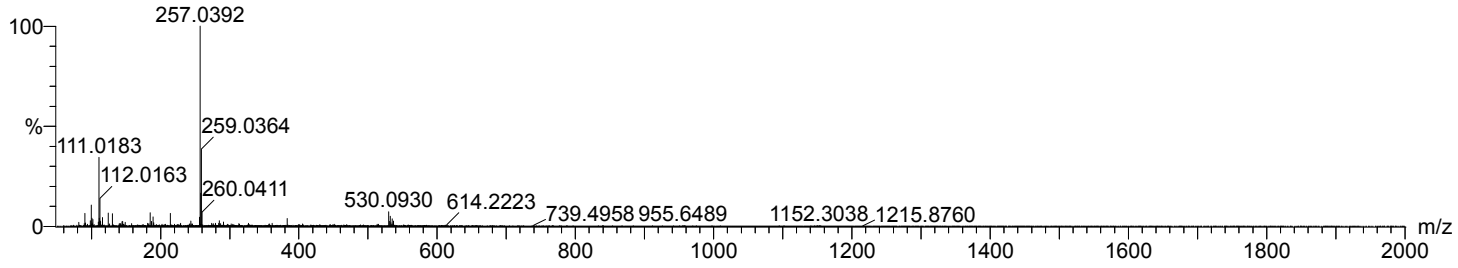
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
321 formula(e) evaluated with 7 results within limits (up to 500 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-4 O: 0-4 Cl: 0-2 I: 0-2

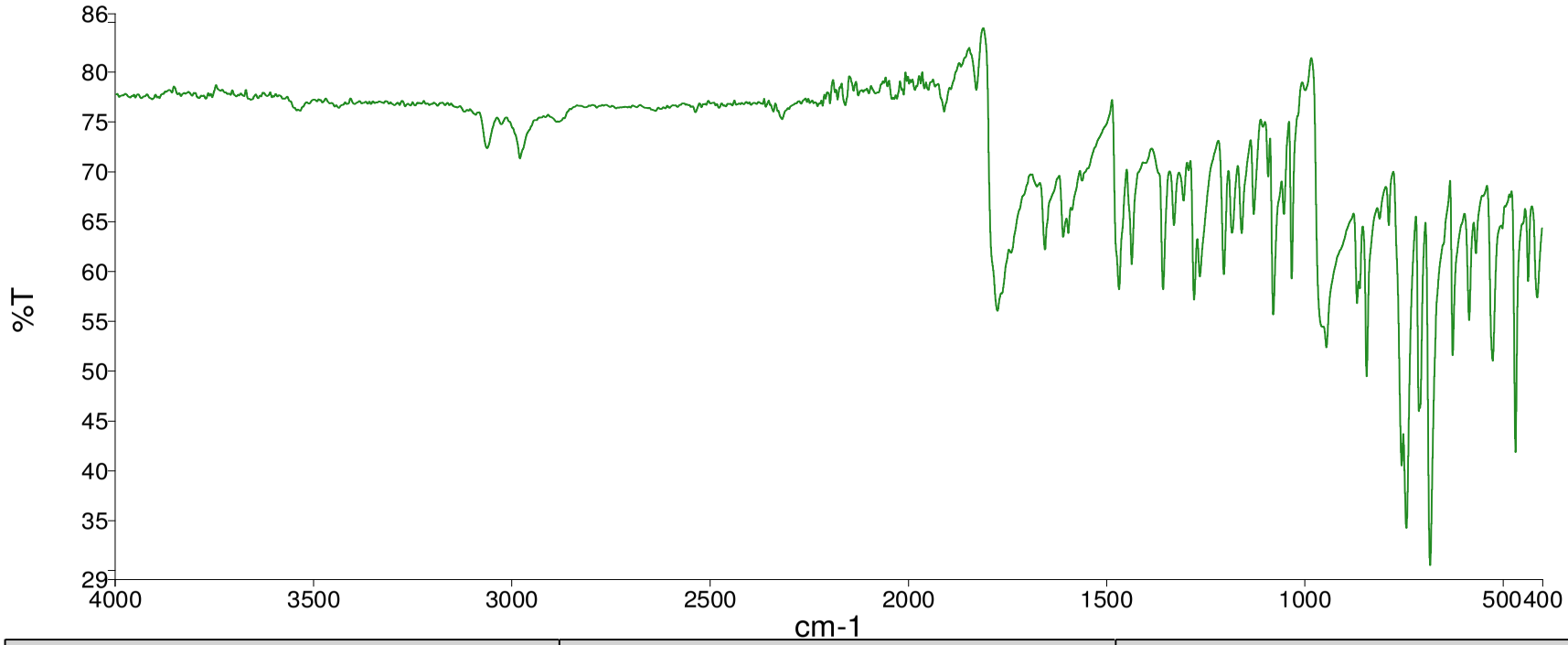
28-Aug-2018
IRB-Het-2-Cl 564 (4.743) Cm (564:571)

1: TOF MS ES+
7.66e+003



Minimum:				-1.5			
Maximum:		5.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
257.0392	257.0369	2.3	8.9	10.5	314.0	0.0	C15 H10 O2 Cl
	257.0441	-4.9	-19.1	6.5	320.6	6.5	C9 H10 N4 O3 Cl
	257.0361	3.1	12.1	6.5	332.5	18.5	C10 H11 N4 Cl2
	257.0347	4.5	17.5	1.5	332.7	18.7	C9 H15 O4 Cl2
	257.0351	4.1	16.0	15.5	338.3	24.3	C16 H5 N2 O2
	257.0402	-1.0	-3.9	-0.5	338.8	24.8	C8 H18 O I
	257.0391	0.1	0.4	19.5	339.1	25.1	C21 H5

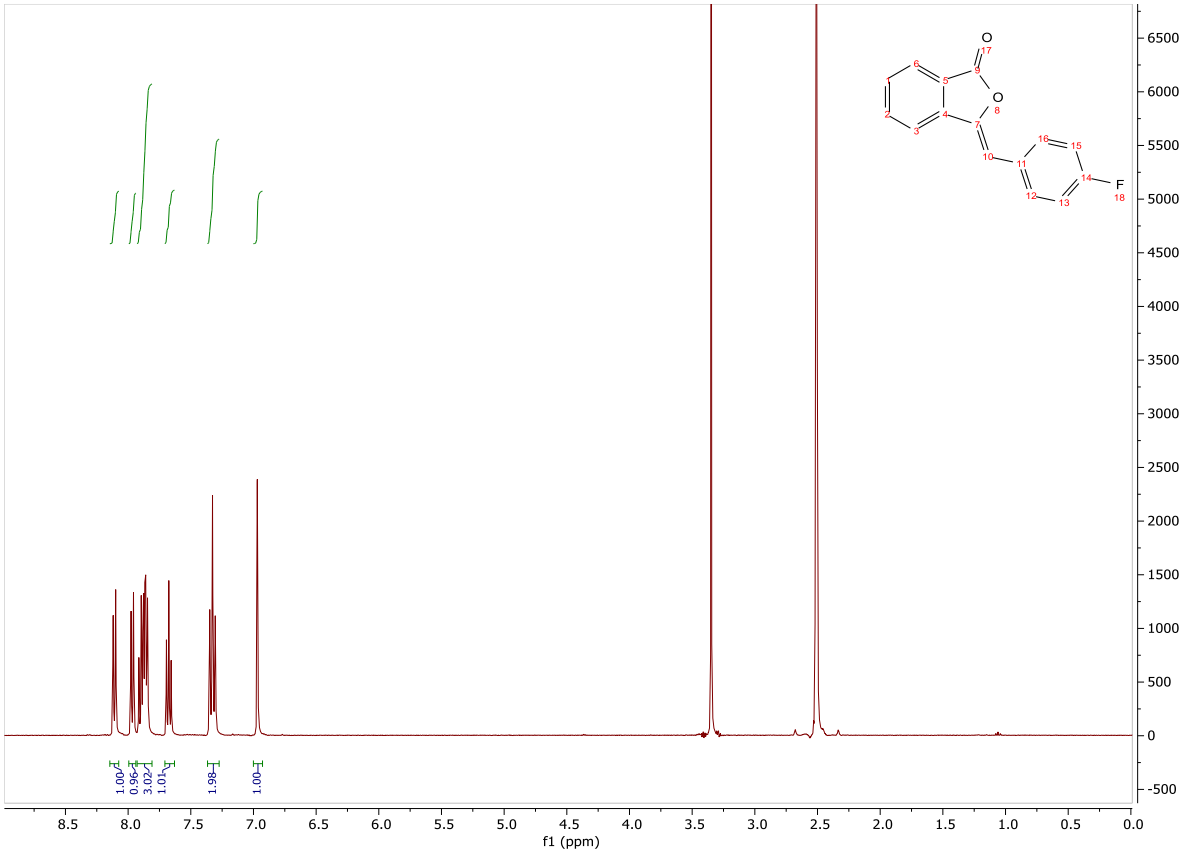
Analyst Lenny Lauchlan
Date 21 October 2022 08:18



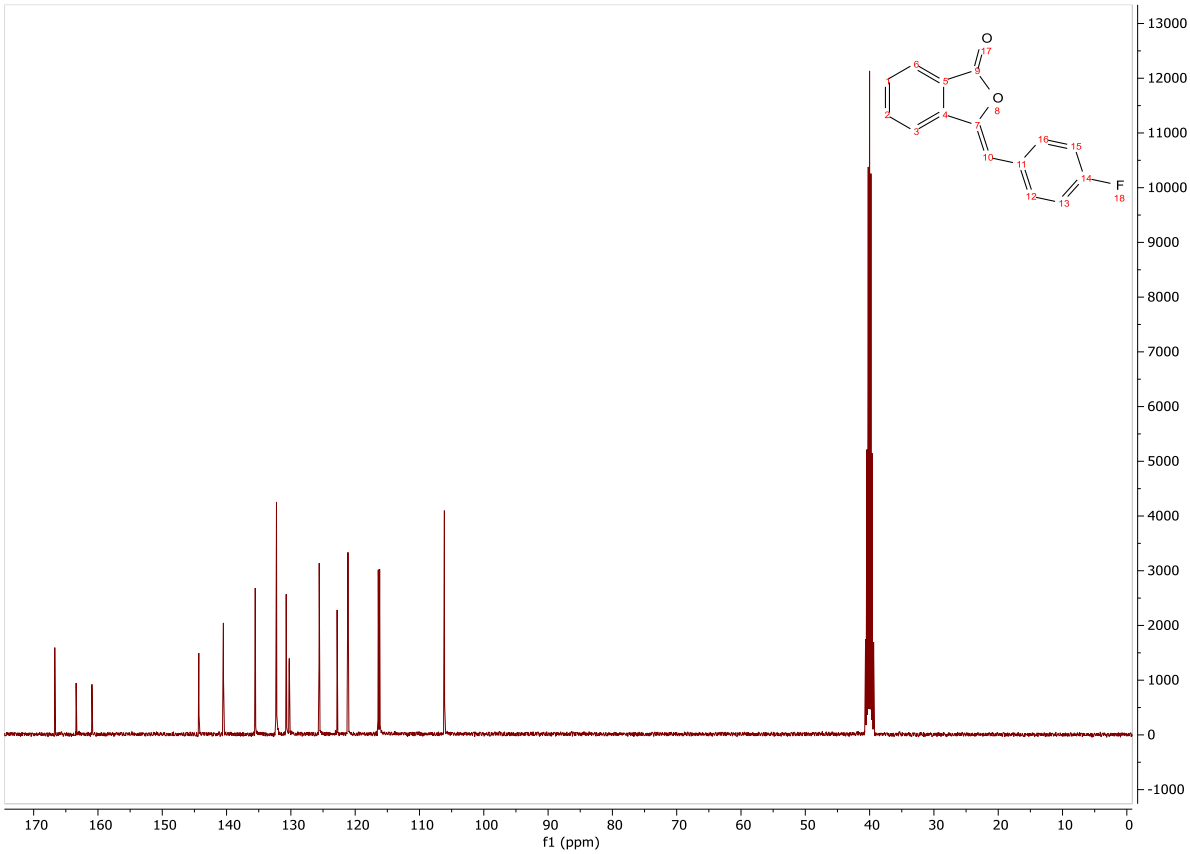
Sample Name	Description	Quality Checks
2-Chloro MAX	Sample 021 By Lenny Date Friday, October 21 2022	The Quality Checks do not report any warnings for the sample.

(*Z*)-3-(4-fluorobenzylidene)isobenzofuran-1(*H*)-one **35f**

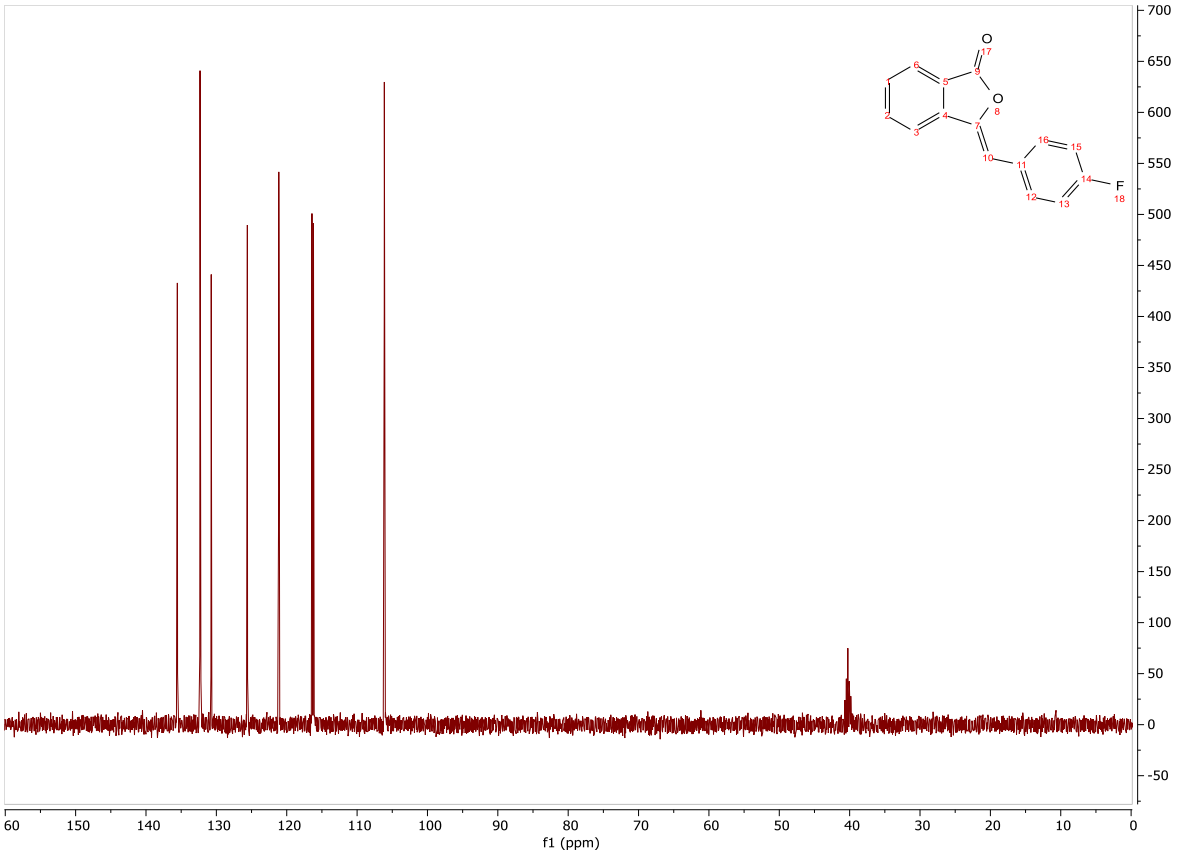
^{1}H:



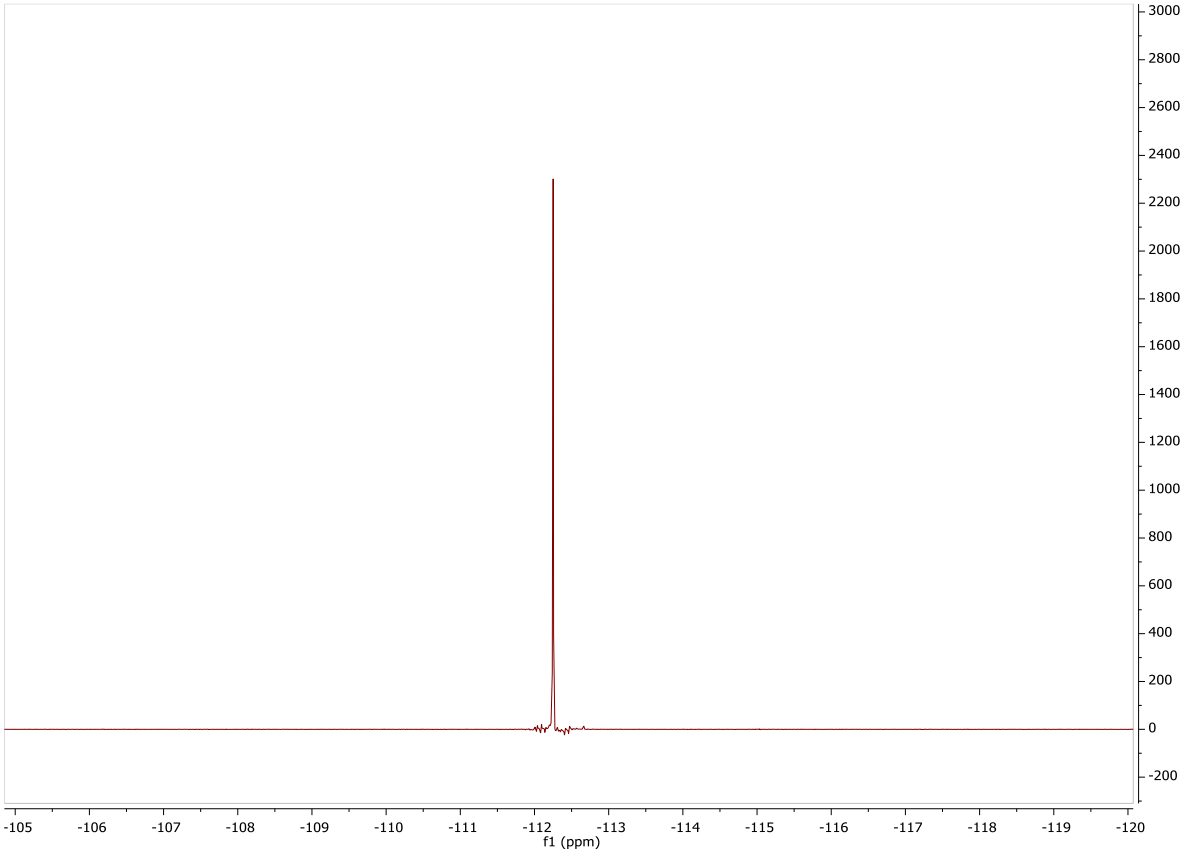
^{13}C:

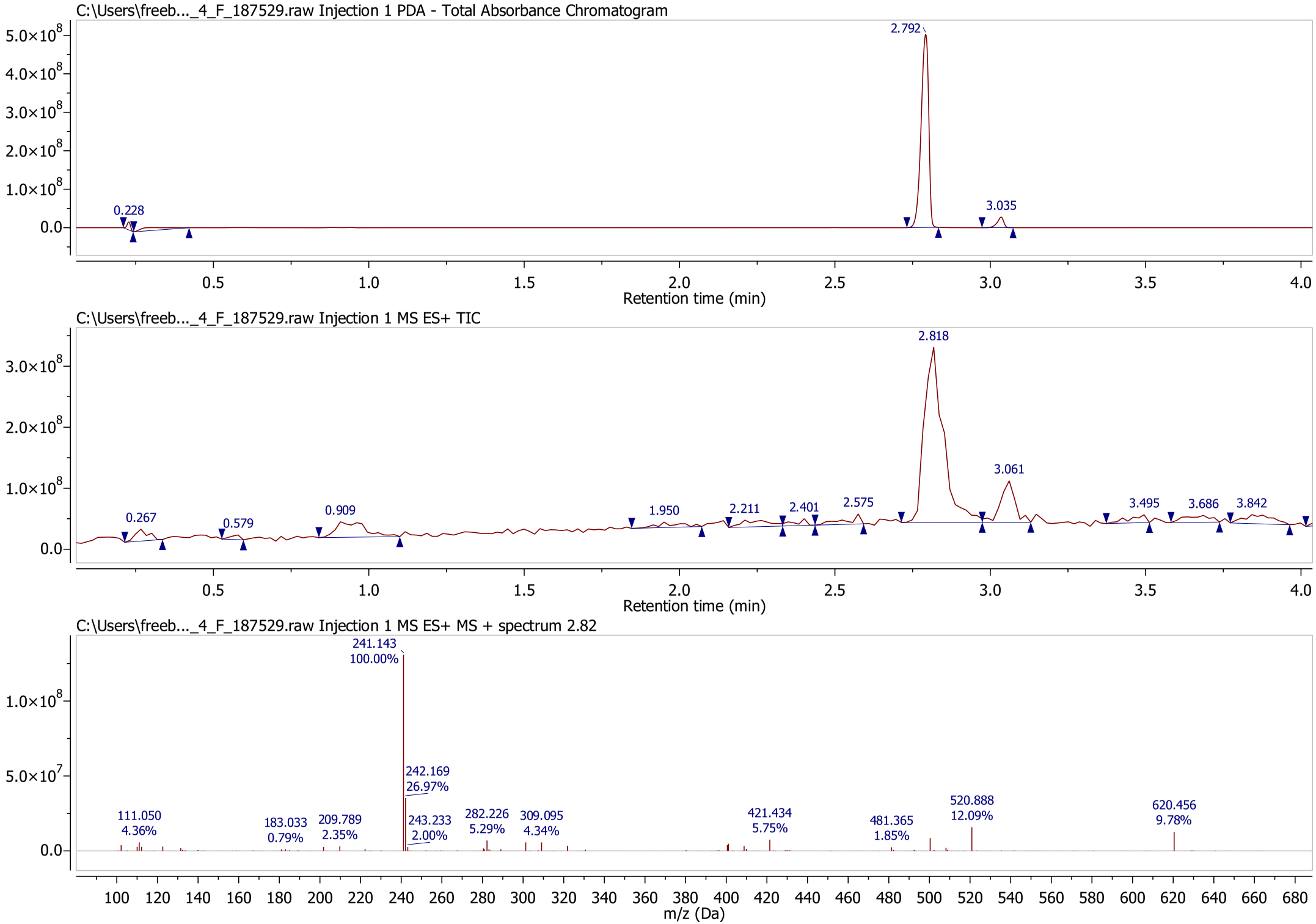


DEPT-135:


O
17
9
O
8
7
10
11
12
13
14
15
16
F
18
1
2
3
4
5
6
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{19}F:


3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
-105
-106
-107
-108
-109
-110
-111
-112
-113
-114
-115
-116
-117
-118
-119
-120
f1 (ppm)


C:\Users\freeb..._4_F_187529.raw Injection 1 PDA - Total Absorbance Chromatogram
5.0×10^8
4.0×10^8
3.0×10^8
2.0×10^8
1.0×10^8
0.0
2.792
0.228
3.035
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Retention time (min)
C:\Users\freeb..._4_F_187529.raw Injection 1 MS ES+ TIC
3.0×10^8
2.0×10^8
1.0×10^8
0.0
2.818
3.061
0.267
0.579
0.909
1.950
2.211
2.401
2.575
3.495
3.686
3.842
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Retention time (min)
C:\Users\freeb..._4_F_187529.raw Injection 1 MS ES+ MS + spectrum 2.82
1.0×10^8
5.0×10^7
0.0
241.143
100.00%
242.169
26.97%
111.050
4.36%
183.033
0.79%
209.789
2.35%
243.233
2.00%
282.226
5.29%
309.095
4.34%
421.434
5.75%
481.365
1.85%
520.888
12.09%
620.456
9.78%
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640
660
680
m/z (Da)

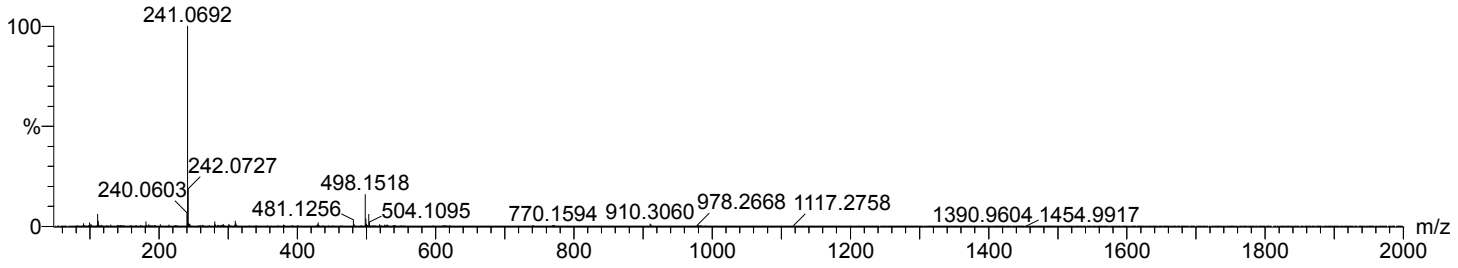
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
511 formula(e) evaluated with 10 results within limits (up to 500 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-6 O: 0-4 F: 0-3 I: 0-2

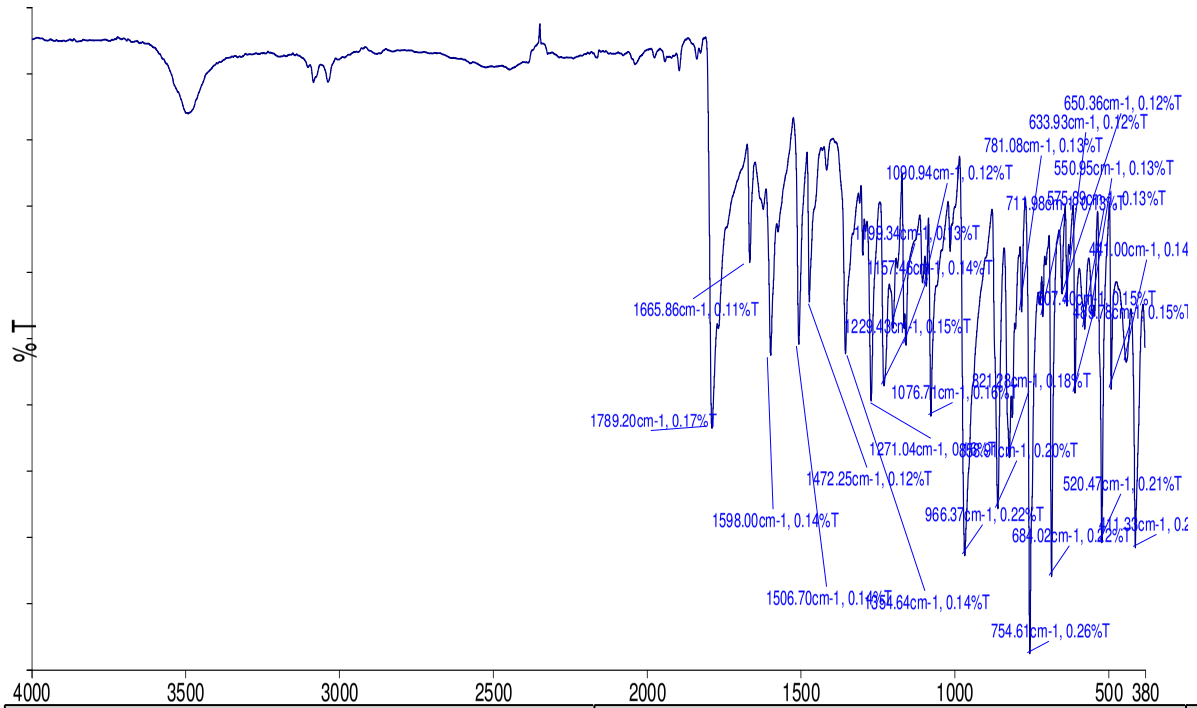
28-Aug-2018
IRB-Het-4-F 519 (4.370) Cm (515:519)

1: TOF MS ES+
4.74e+004



Minimum:				-1.5			
Maximum:		5.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
241.0692	241.0665	2.7	11.2	10.5	464.2	0.5	C15 H10 O2 F
	241.0726	-3.4	-14.1	10.5	465.5	1.7	C12 H9 N4 O2
	241.0676	1.6	6.6	6.5	465.9	2.2	C12 H11 O3 F2
	241.0653	3.9	16.2	14.5	466.2	2.5	C18 H9 O
	241.0688	0.4	1.7	2.5	467.8	4.1	C9 H12 O4 F3
	241.0701	-0.9	-3.7	7.5	467.9	4.2	C10 H8 N4 F3
	241.0737	-4.5	-18.7	6.5	468.9	5.2	C9 H10 N4 O3 F
	241.0649	4.3	17.8	7.5	470.7	7.0	C8 H7 N6 O F2
	241.0685	0.7	2.9	6.5	470.7	7.0	C7 H9 N6 O4
	241.0661	3.1	12.9	3.5	473.6	9.9	C5 H8 N6 O2 F3

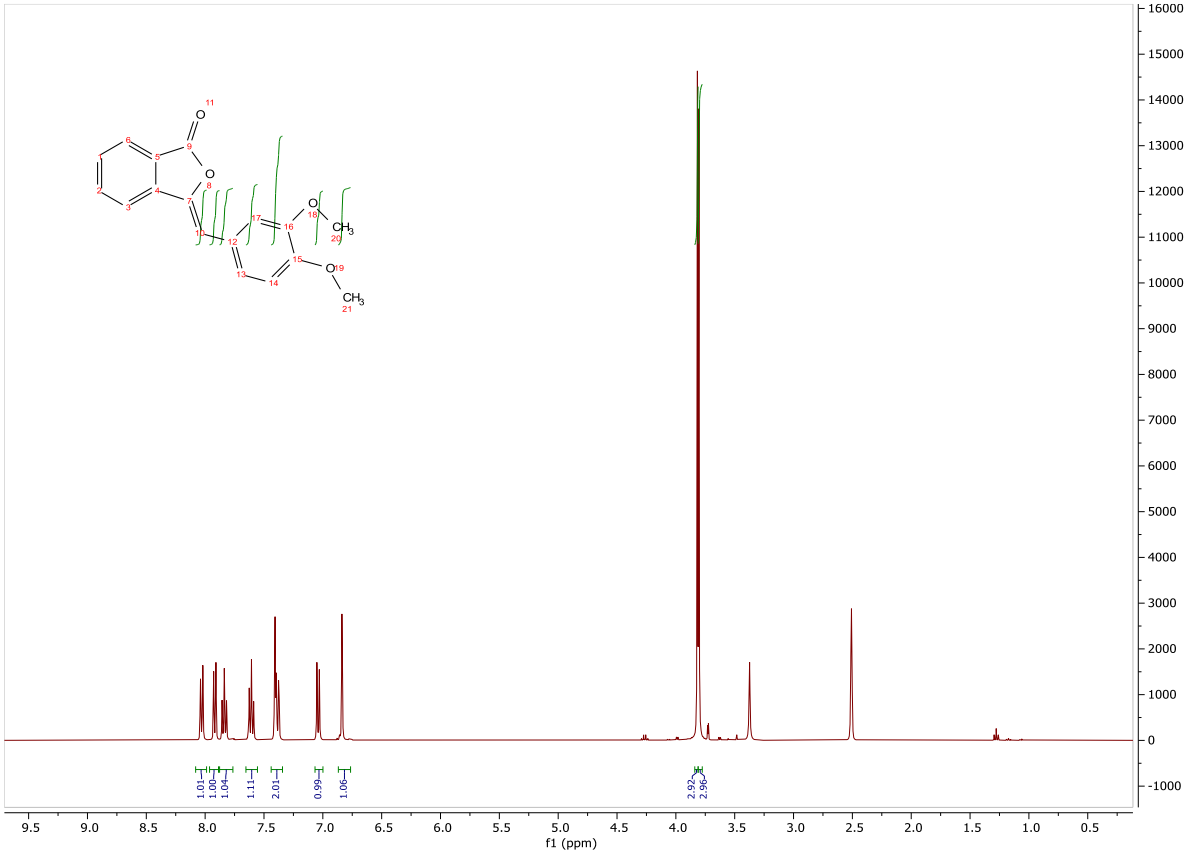
Analyst Professor Ian Baxendale
Date 24 August 2018 14:07



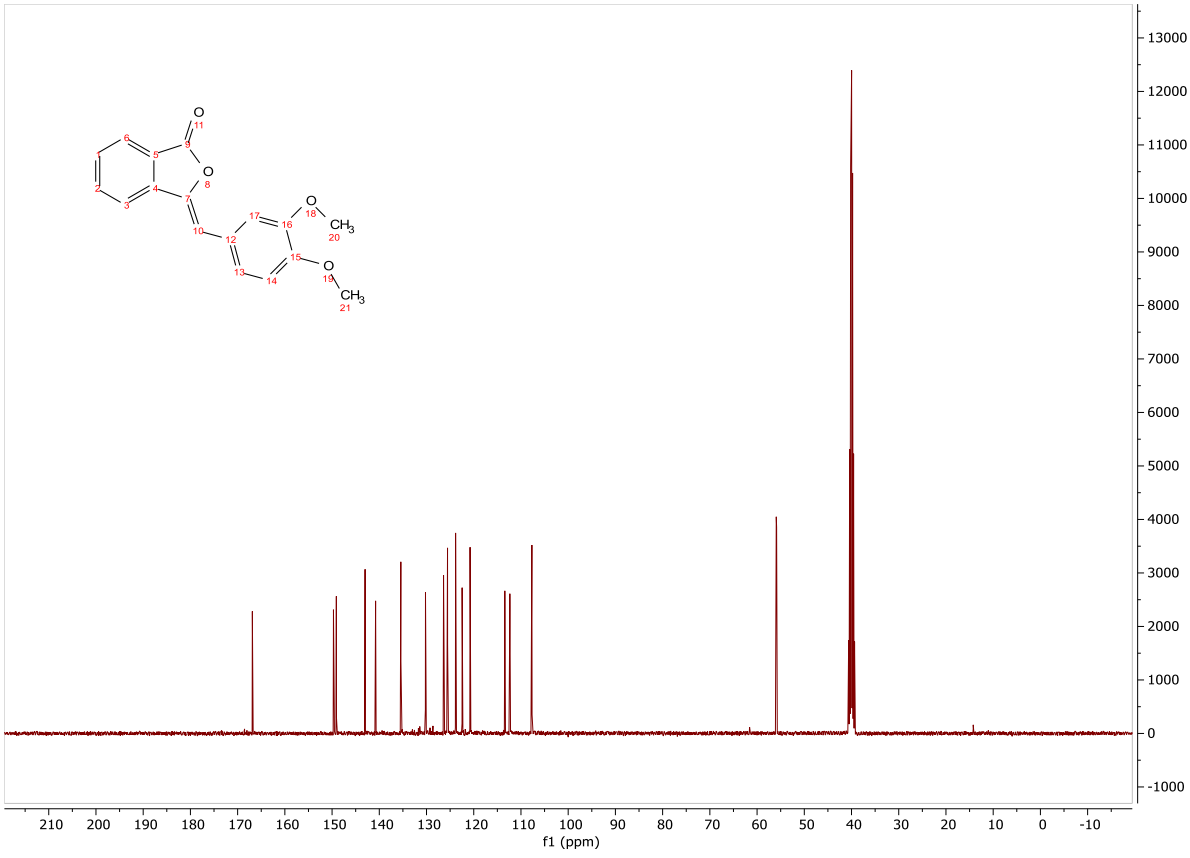
Sample Name	Description	Quality Checks
IRB 141	Sample 141 By IRB Date Friday, August 24 2018	The Quality Checks give rise to a Weak Bands warning for the sample.

(*Z*)-3-(3,4-dimethoxybenzylidene)isobenzofuran-1(*H*)-one **35g**

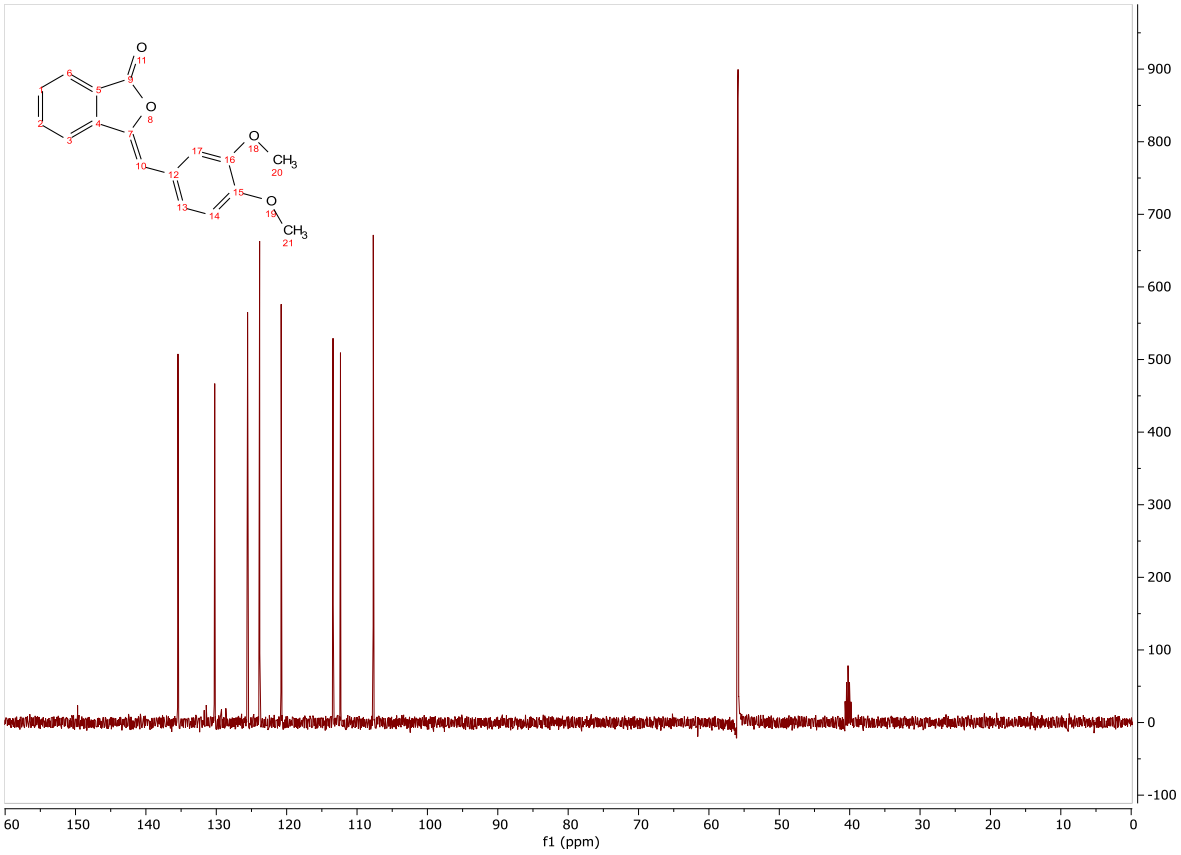
^{1}H:

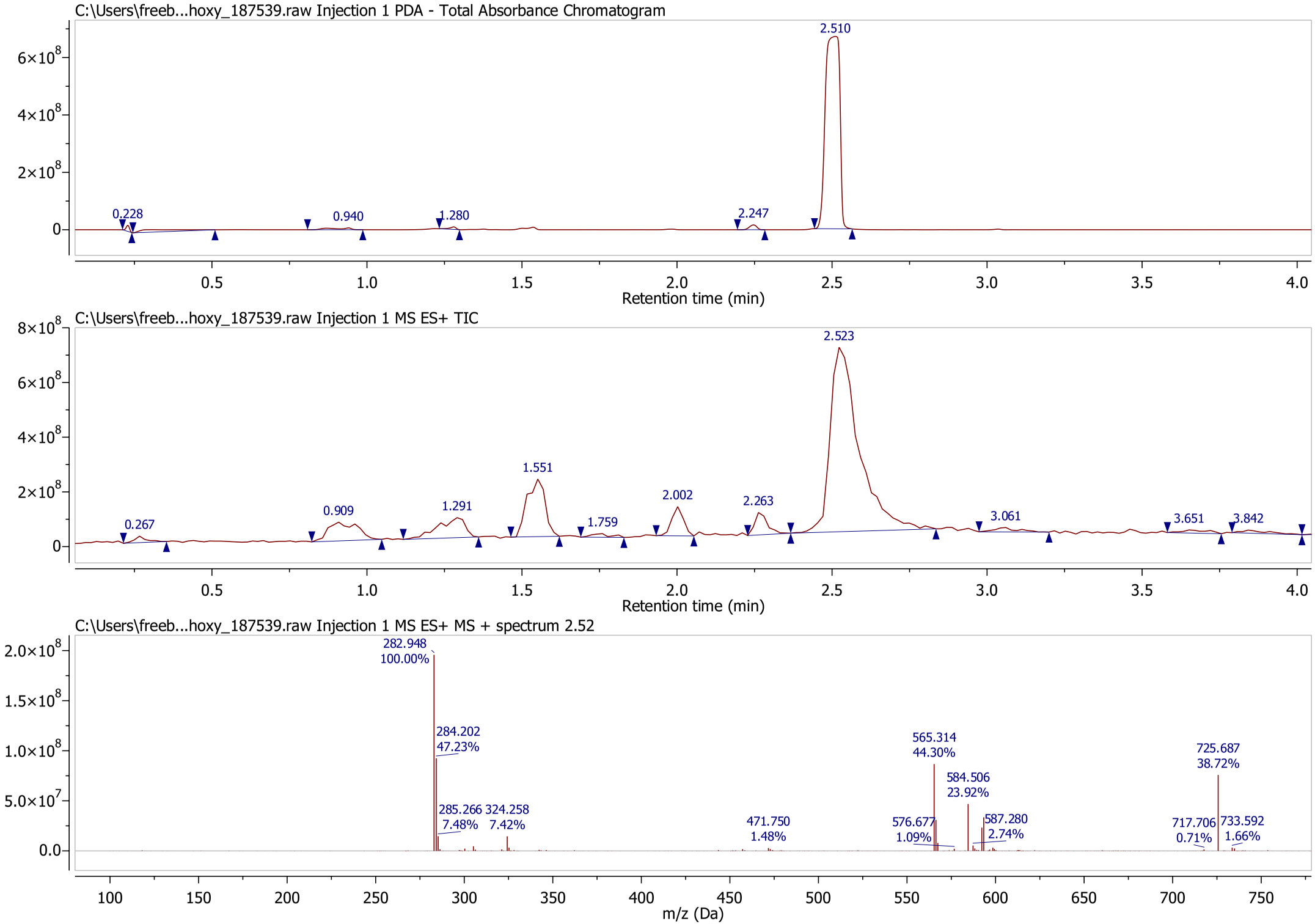


^{13}C:



DEPT-135:


O
11
6
5
9
O
8
2
3
4
7
10
12
17
16
O
18
CH3
20
13
14
15
O
19
CH3
21
900
800
700
600
500
400
300
200
100
0
-100
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


C:\Users\freeb...hoxy_187539.raw Injection 1 PDA - Total Absorbance Chromatogram
6×10^8
4×10^8
2×10^8
0
2.510
0.228
0.940
1.280
2.247
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Retention time (min)
C:\Users\freeb...hoxy_187539.raw Injection 1 MS ES+ TIC
8×10^8
6×10^8
4×10^8
2×10^8
0
2.523
1.551
0.909
1.291
2.002
2.263
0.267
1.759
3.061
3.651
3.842
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Retention time (min)
C:\Users\freeb...hoxy_187539.raw Injection 1 MS ES+ MS + spectrum 2.52
2.0×10^8
1.5×10^8
1.0×10^8
5.0×10^7
0.0
282.948
100.00%
284.202
47.23%
285.266
7.48%
324.258
7.42%
471.750
1.48%
565.314
44.30%
584.506
23.92%
576.677
1.09%
587.280
2.74%
725.687
38.72%
717.706
0.71%
733.592
1.66%
100
150
200
250
300
350
400
450
500
550
600
650
700
750
m/z (Da)

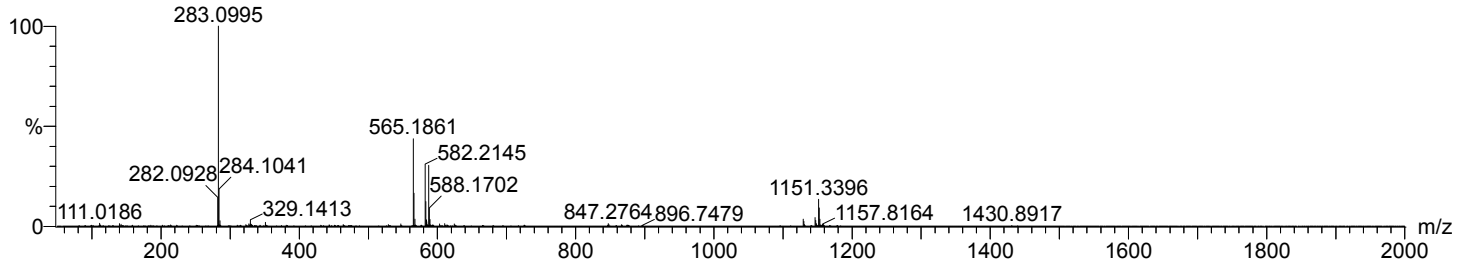
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
373 formula(e) evaluated with 6 results within limits (up to 500 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-4 O: 0-4 Cl: 0-2 I: 0-2

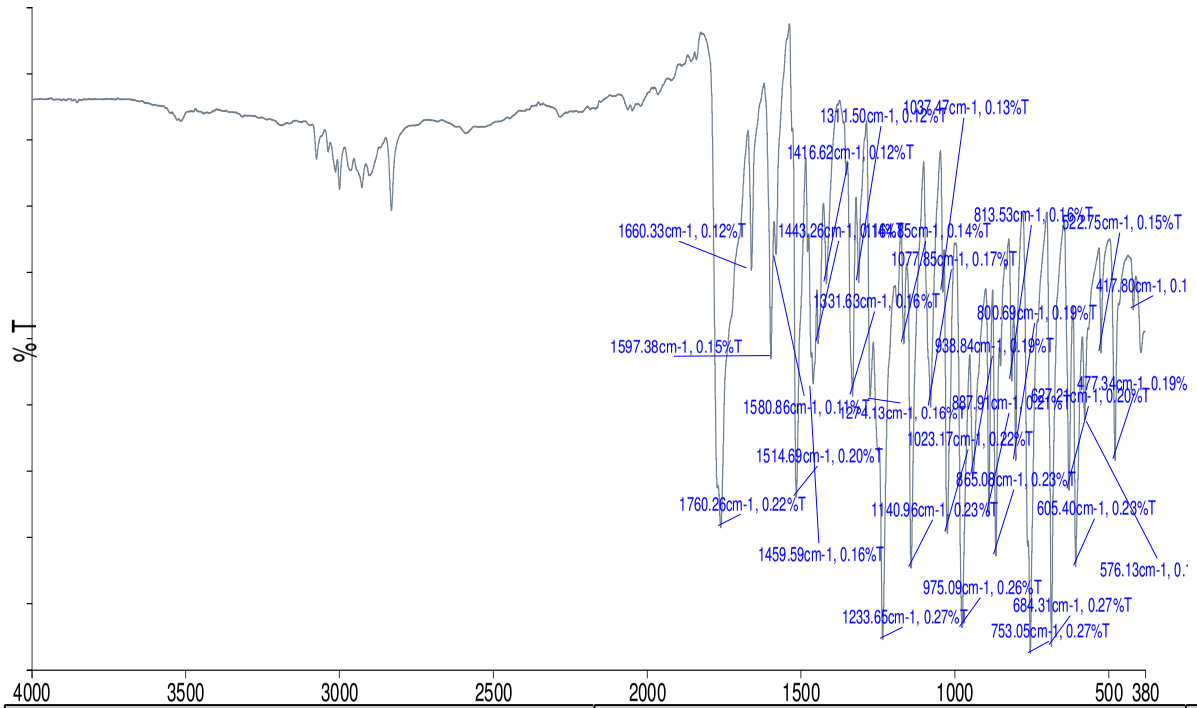
28-Aug-2018
IRB-Het-34-OMe 458 (3.851) Cm (453:458)

1: TOF MS ES+
5.99e+004



Minimum:				-1.5						
Maximum:		5.0	10.0	100.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
283.0995	283.0970	2.5	8.8	10.5	475.1	0.0	C17	H15	O4	
	283.0984	1.1	3.9	15.5	481.3	6.3	C18	H11	N4	
	283.1002	-0.7	-2.5	10.5	500.0	24.9	C17	H16	N2	Cl
	283.0962	3.3	11.7	6.5	500.0	24.9	C12	H16	N4	O2 Cl
	283.1020	-2.5	-8.8	5.5	502.2	27.1	C16	H21	Cl2	
	283.0980	1.5	5.3	1.5	502.2	27.1	C11	H21	N2	O2 Cl2

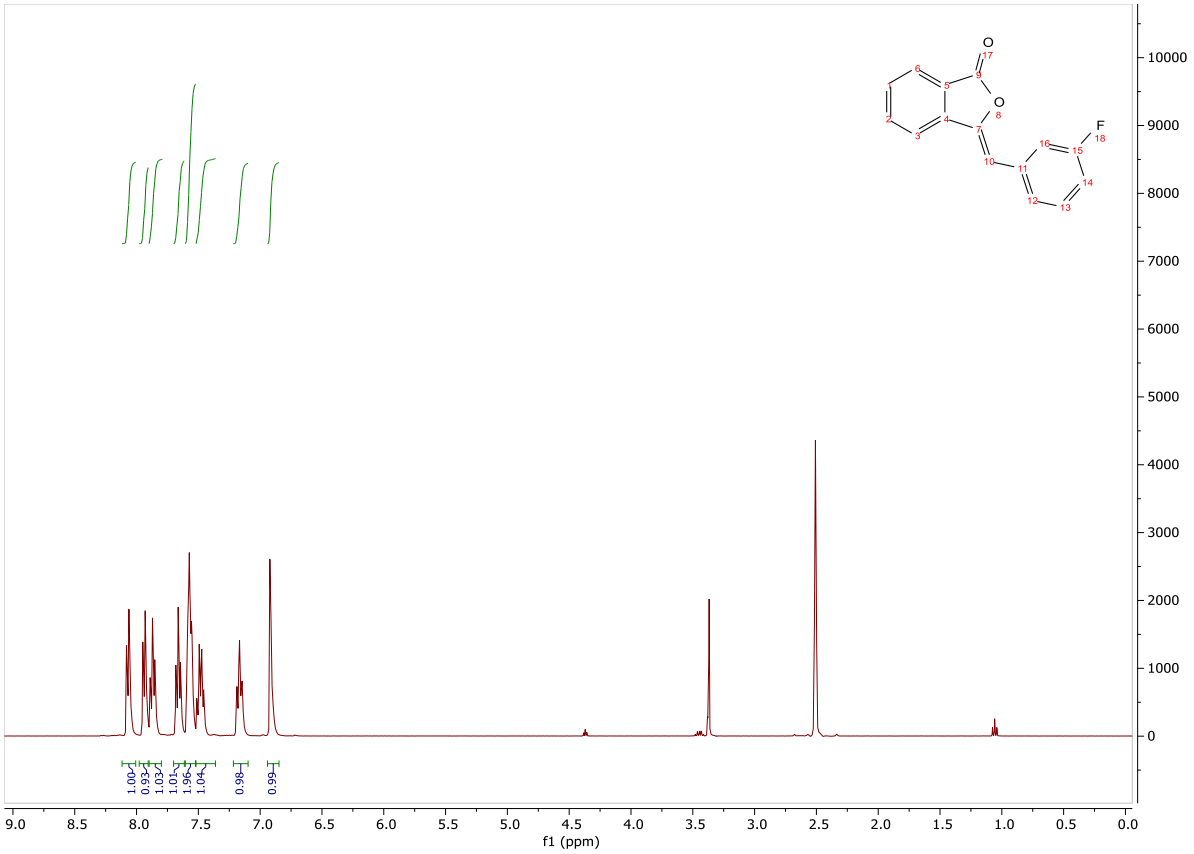
Analyst Professor Ian Baxendale
Date 24 August 2018 13:57



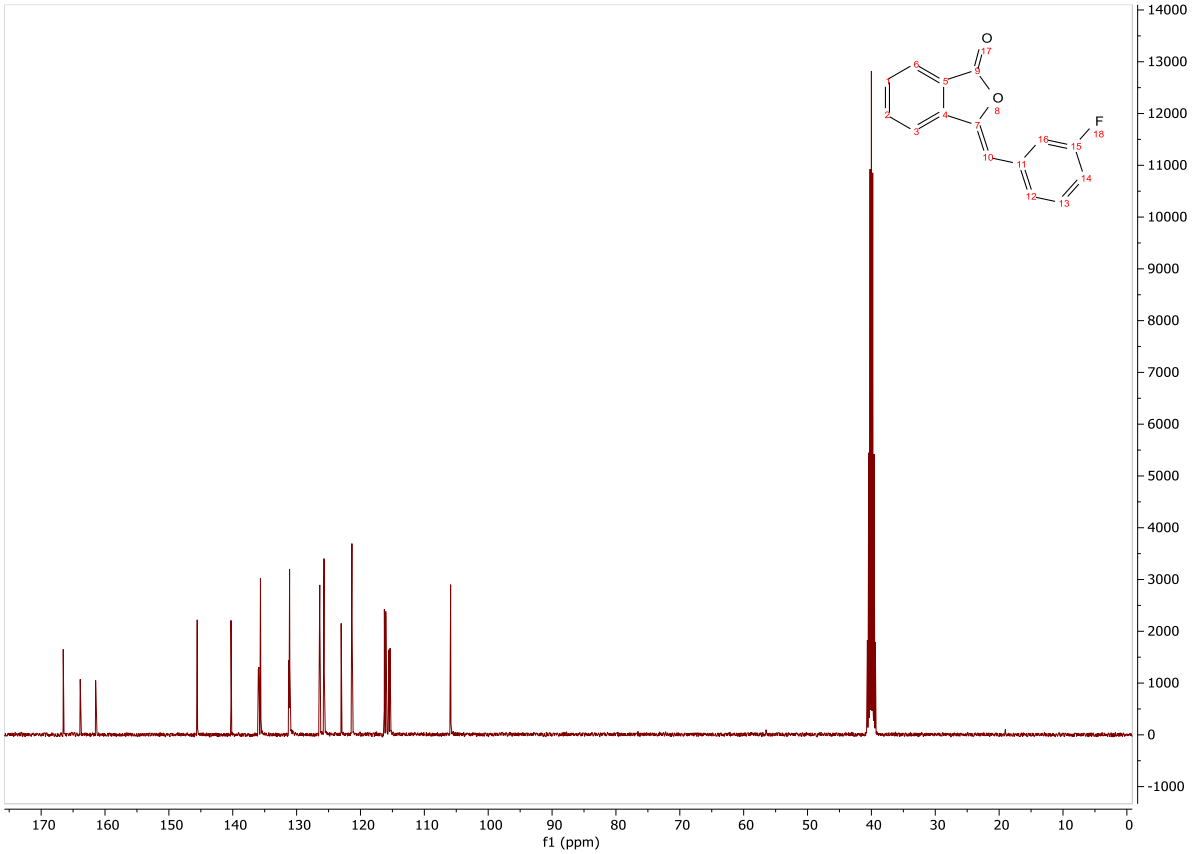
Sample Name	Description	Quality Checks
IRB 139	Sample 139 By IRB Date Friday, August 24 2018	The Quality Checks do not report any warnings for the sample.

(*Z*)-3-(3-fluoroybenzylidene)isobenzofuran-1(*H*)-one **35h**

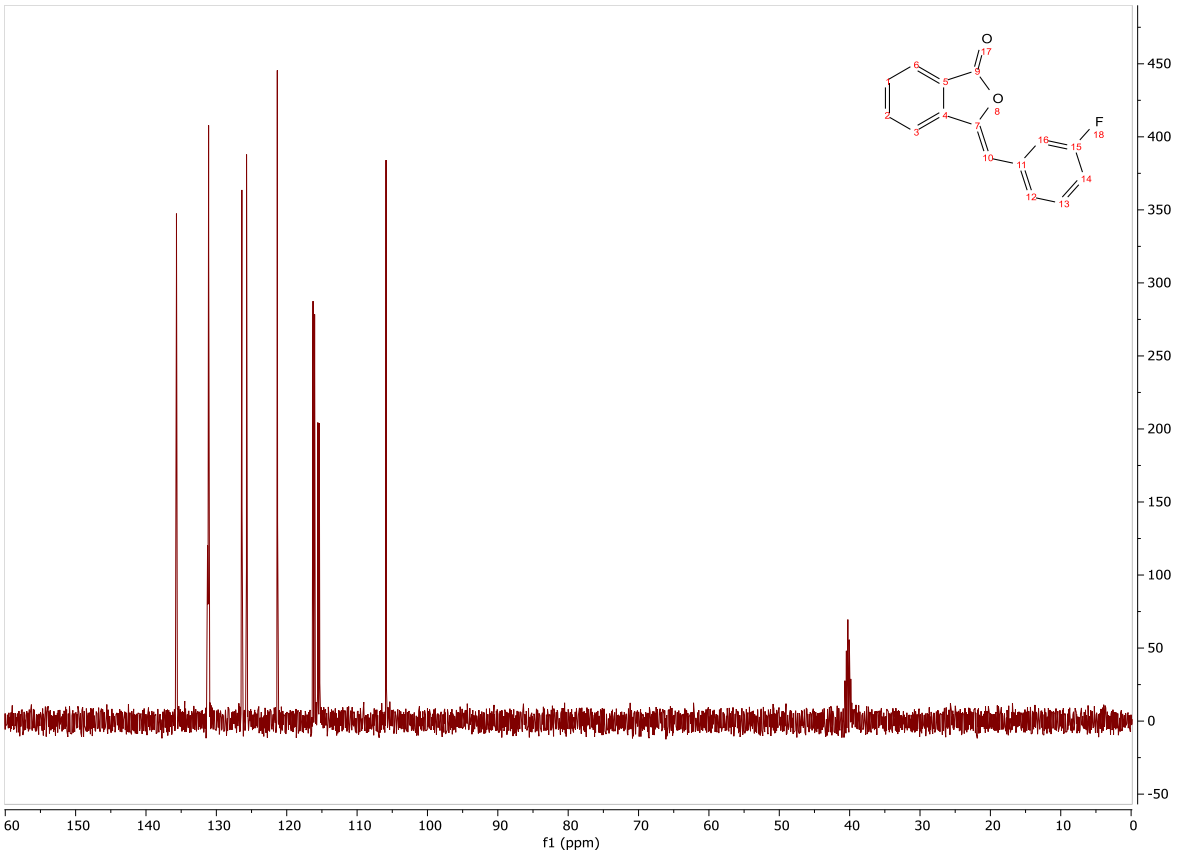
^{1}H:



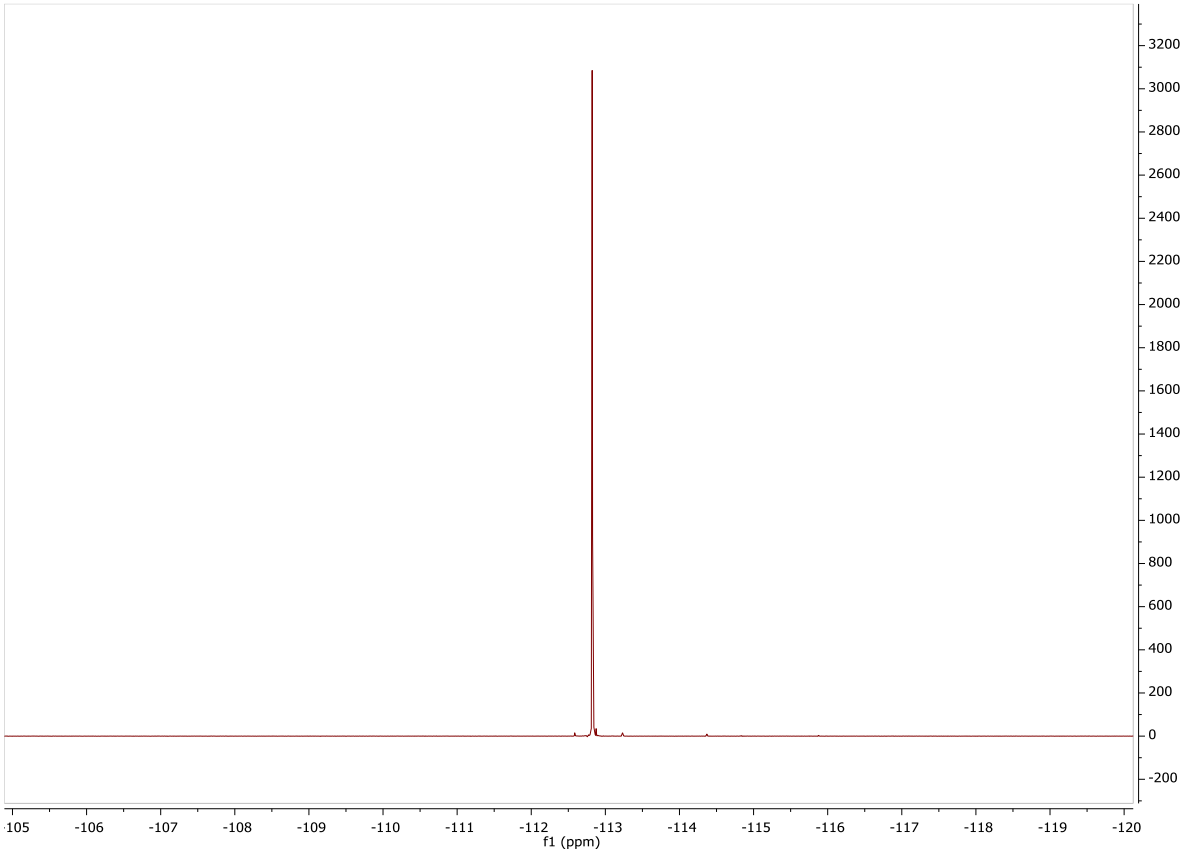
^{13}C:

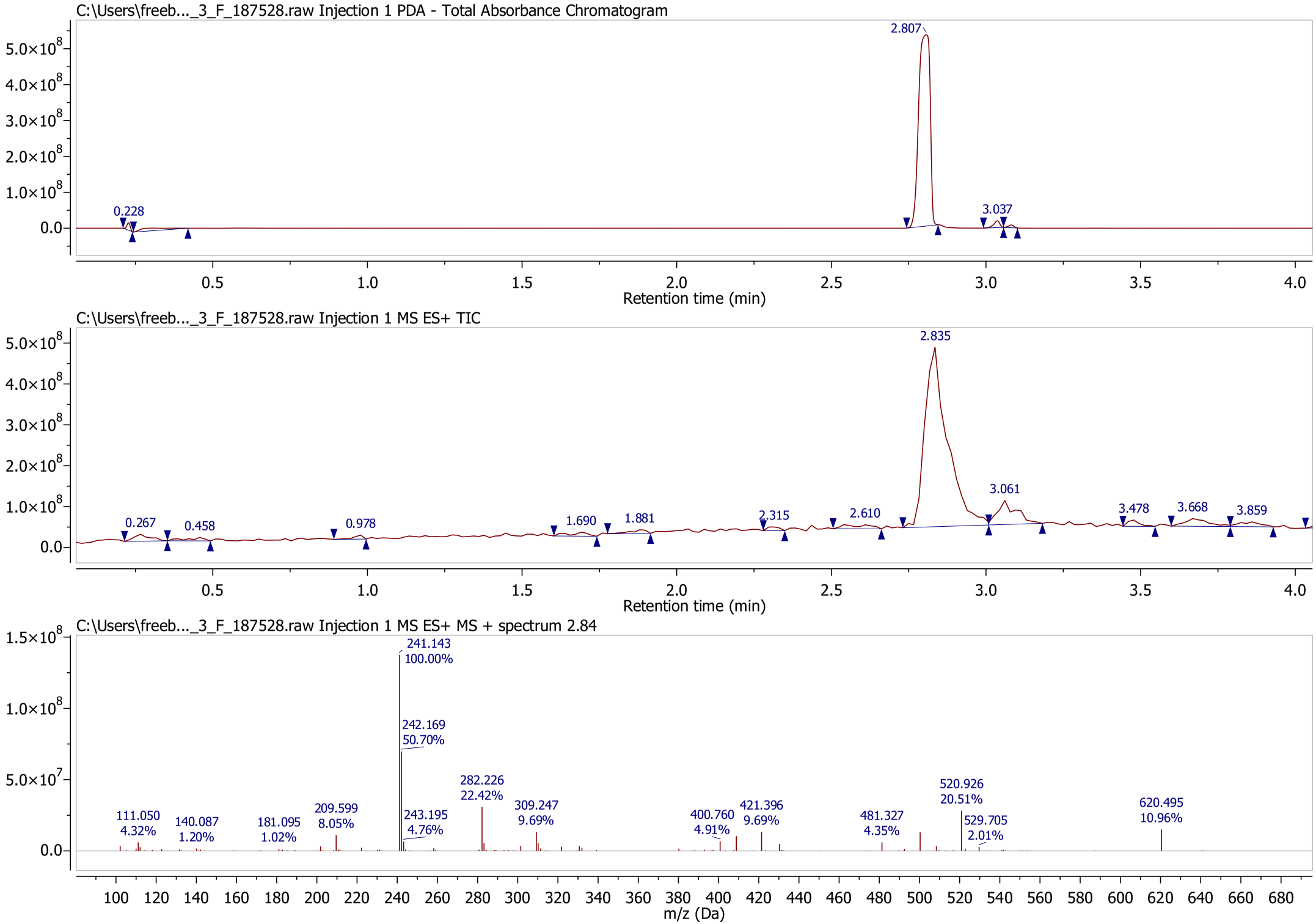


DEPT-135:


O
17
6
5
9
1
O
8
2
4
7
3
F
18
16
15
10
11
14
12
13
450
400
350
300
250
200
150
100
50
0
-50
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{19}F:


3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
105
-106
-107
-108
-109
-110
-111
-112
-113
-114
-115
-116
-117
-118
-119
-120
f1 (ppm)


C:\Users\freeb..._3_F_187528.raw Injection 1 PDA - Total Absorbance Chromatogram
2.807
0.228
3.037
Retention time (min)
C:\Users\freeb..._3_F_187528.raw Injection 1 MS ES+ TIC
2.835
3.061
0.267
0.458
0.978
1.690
1.881
2.315
2.610
3.478
3.668
3.859
Retention time (min)
C:\Users\freeb..._3_F_187528.raw Injection 1 MS ES+ MS + spectrum 2.84
241.143
100.00%
242.169
50.70%
282.226
22.42%
309.247
9.69%
111.050
4.32%
140.087
1.20%
181.095
1.02%
209.599
8.05%
243.195
4.76%
400.760
4.91%
421.396
9.69%
481.327
4.35%
520.926
20.51%
529.705
2.01%
620.495
10.96%
m/z (Da)

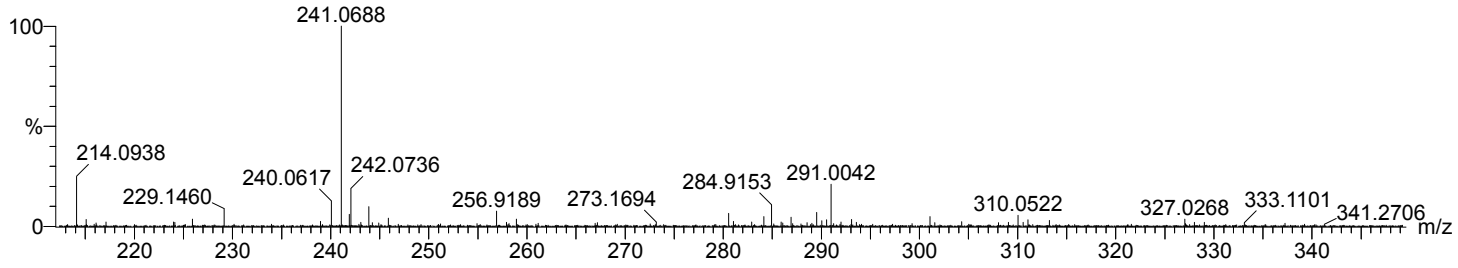
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
511 formula(e) evaluated with 10 results within limits (up to 500 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-6 O: 0-4 F: 0-3 I: 0-2

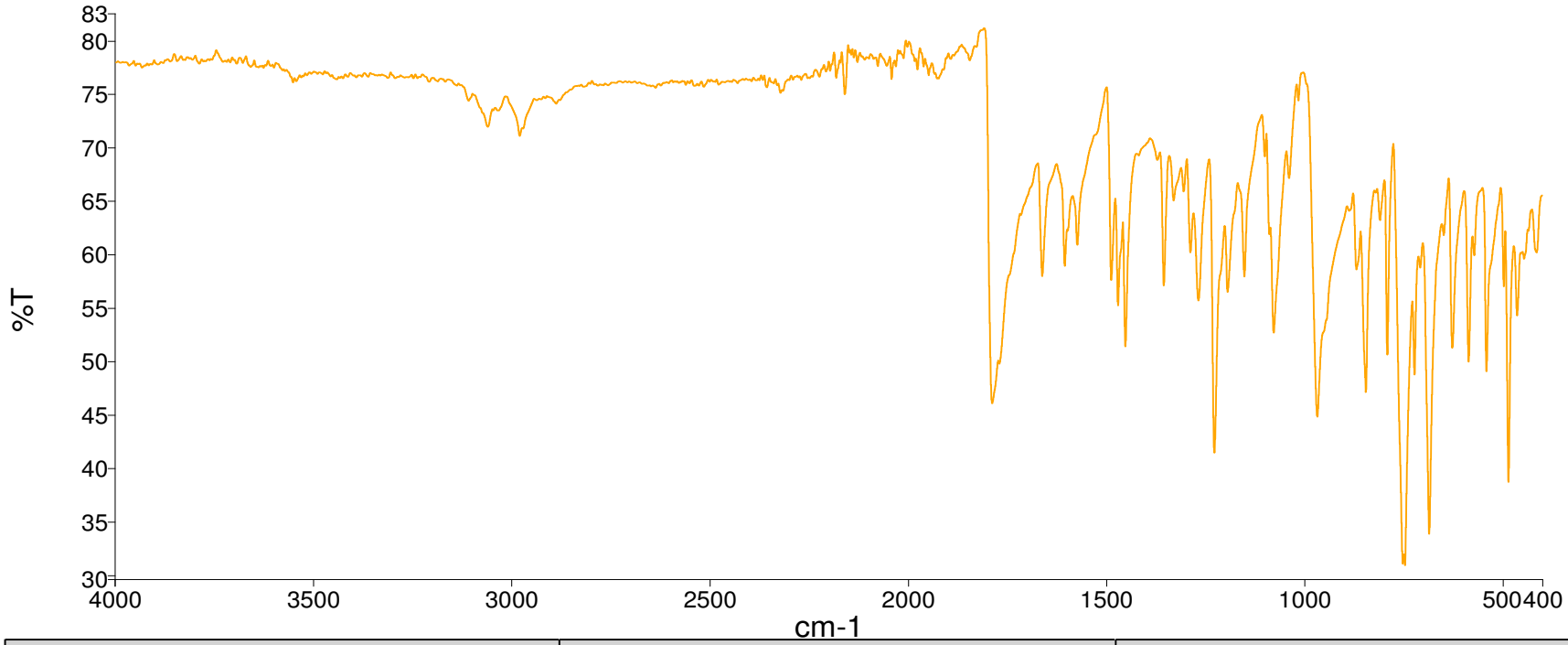
28-Aug-2018
IRB-Het-3-F 534 (4.490) Cm (534:547)

1: TOF MS ES+
5.18e+003



Minimum:				-1.5			
Maximum:		5.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
241.0688	241.0653	3.5	14.5	14.5	371.2	0.7	C18 H9 O
	241.0665	2.3	9.5	10.5	371.4	0.8	C15 H10 O2 F
	241.0726	-3.8	-15.8	10.5	374.4	3.9	C12 H9 N4 O2
	241.0676	1.2	5.0	6.5	375.0	4.4	C12 H11 O3 F2
	241.0701	-1.3	-5.4	7.5	377.4	6.8	C10 H8 N4 F3
	241.0688	0.0	0.0	2.5	377.5	6.9	C9 H12 O4 F3
	241.0737	-4.9	-20.3	6.5	377.9	7.3	C9 H10 N4 O3 F
	241.0685	0.3	1.2	6.5	379.0	8.5	C7 H9 N6 O4
	241.0649	3.9	16.2	7.5	379.1	8.6	C8 H7 N6 O F2
	241.0661	2.7	11.2	3.5	381.4	10.8	C5 H8 N6 O2 F3

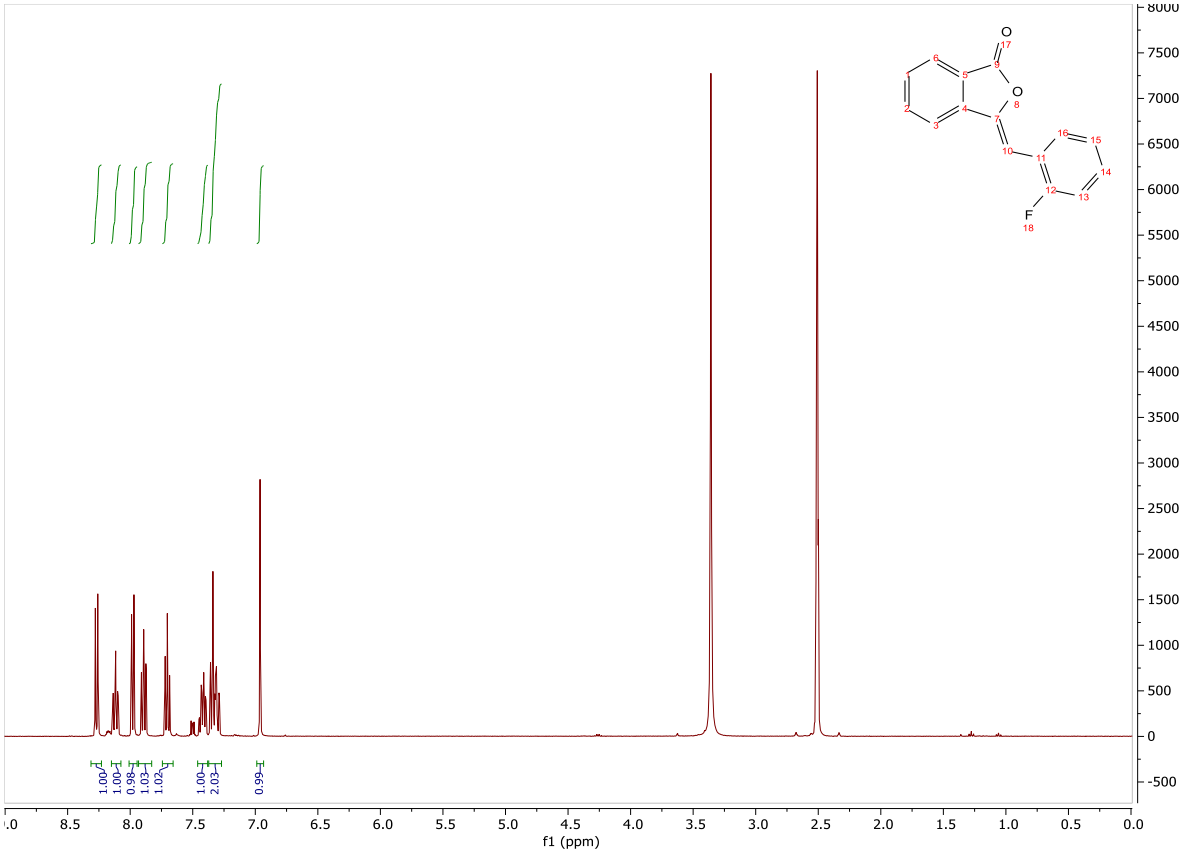
Analyst Lenny Lauchlan
Date 21 October 2022 08:19



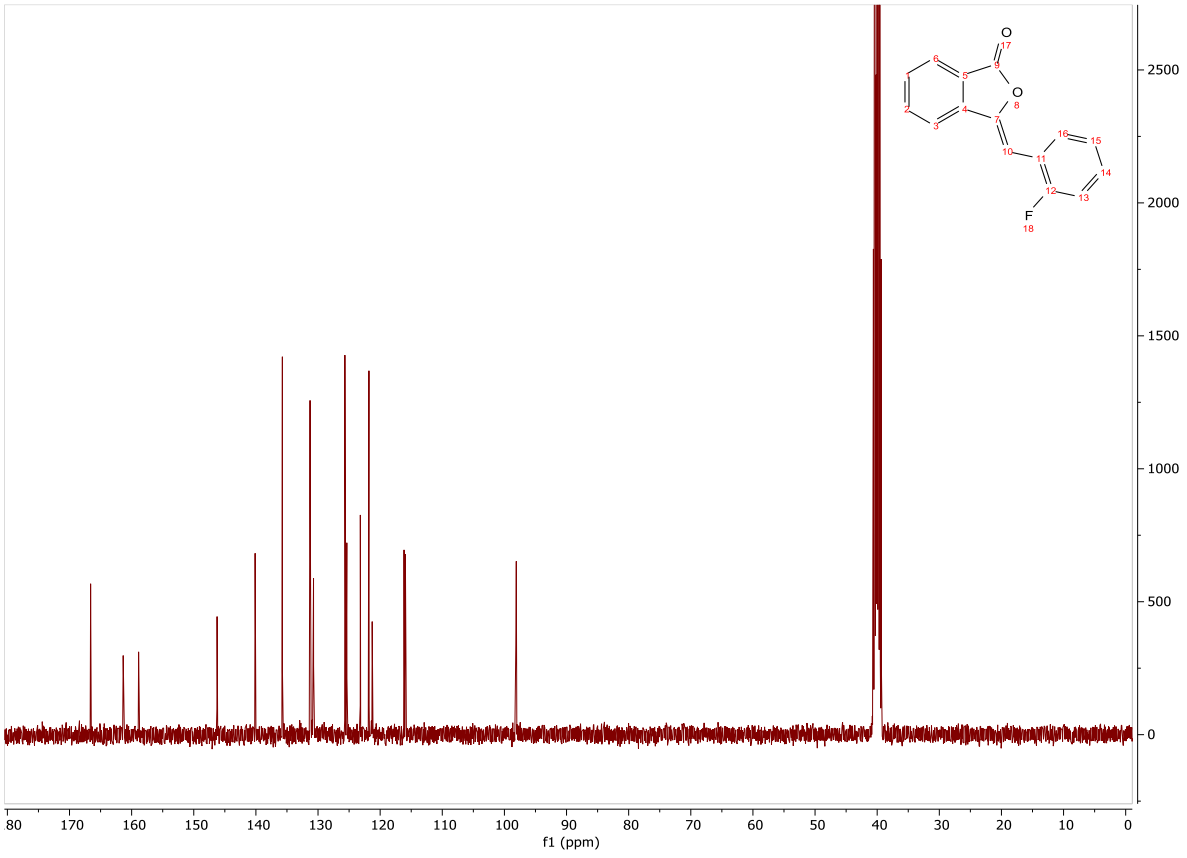
Sample Name	Description	Quality Checks
3-Fluoro MAX	Sample 022 By Lenny Date Friday, October 21 2022	The Quality Checks do not report any warnings for the sample.

(*Z*)-3-(2-fluoroybenzylidene)isobenzofuran-1(*H*)-one **35i**

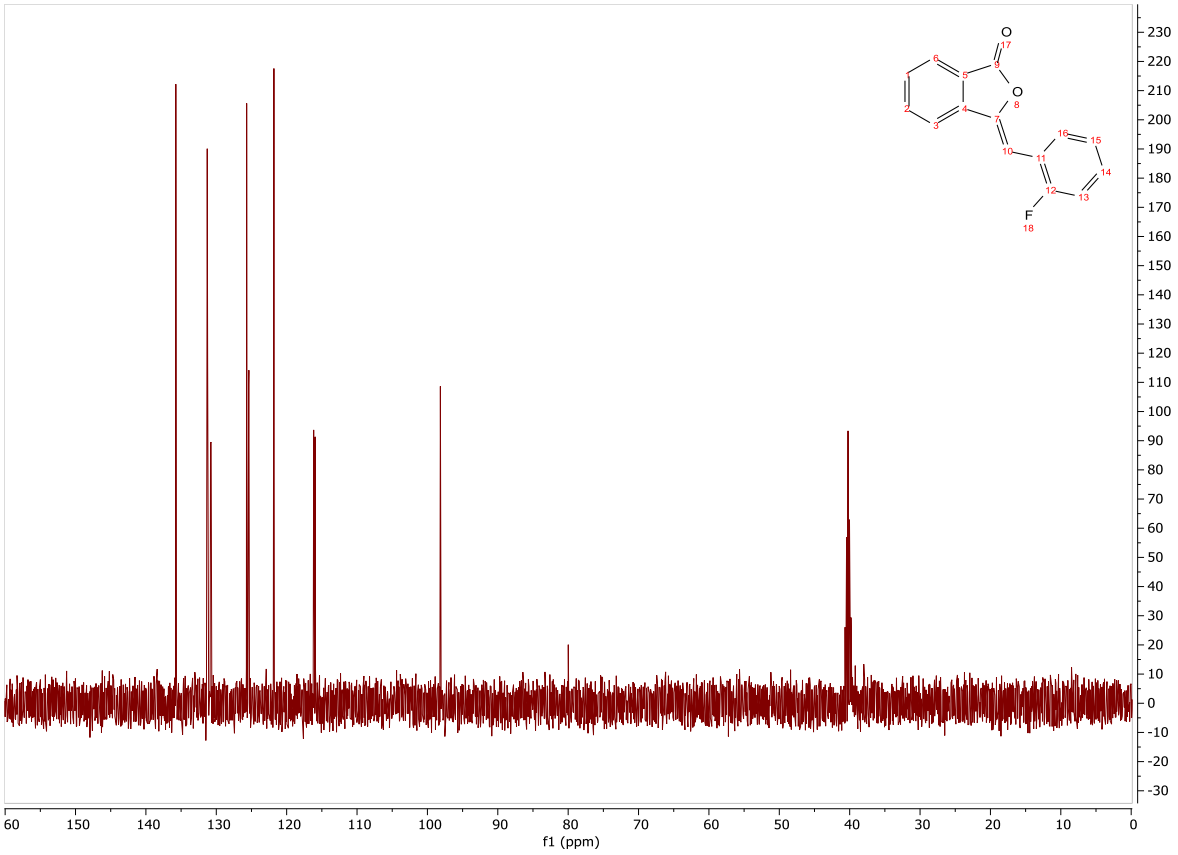
^{1}H:



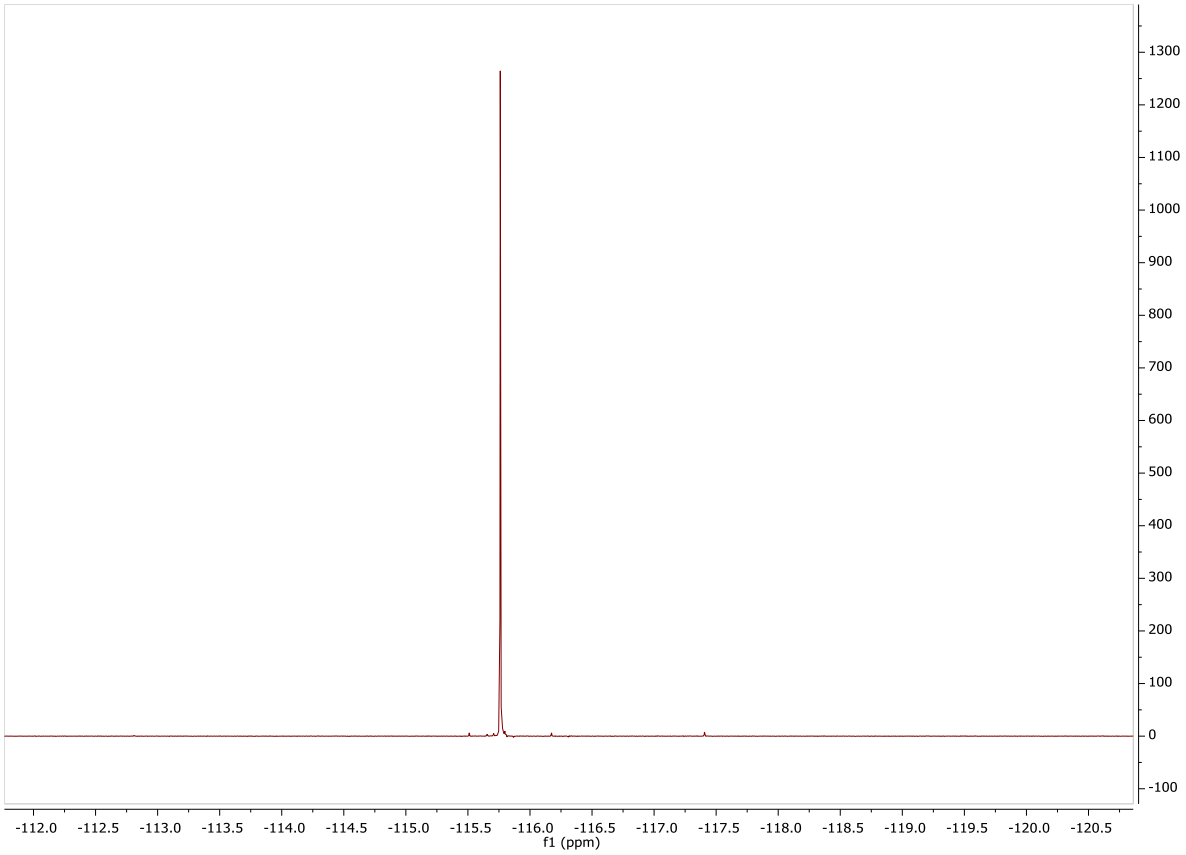
^{13}C:

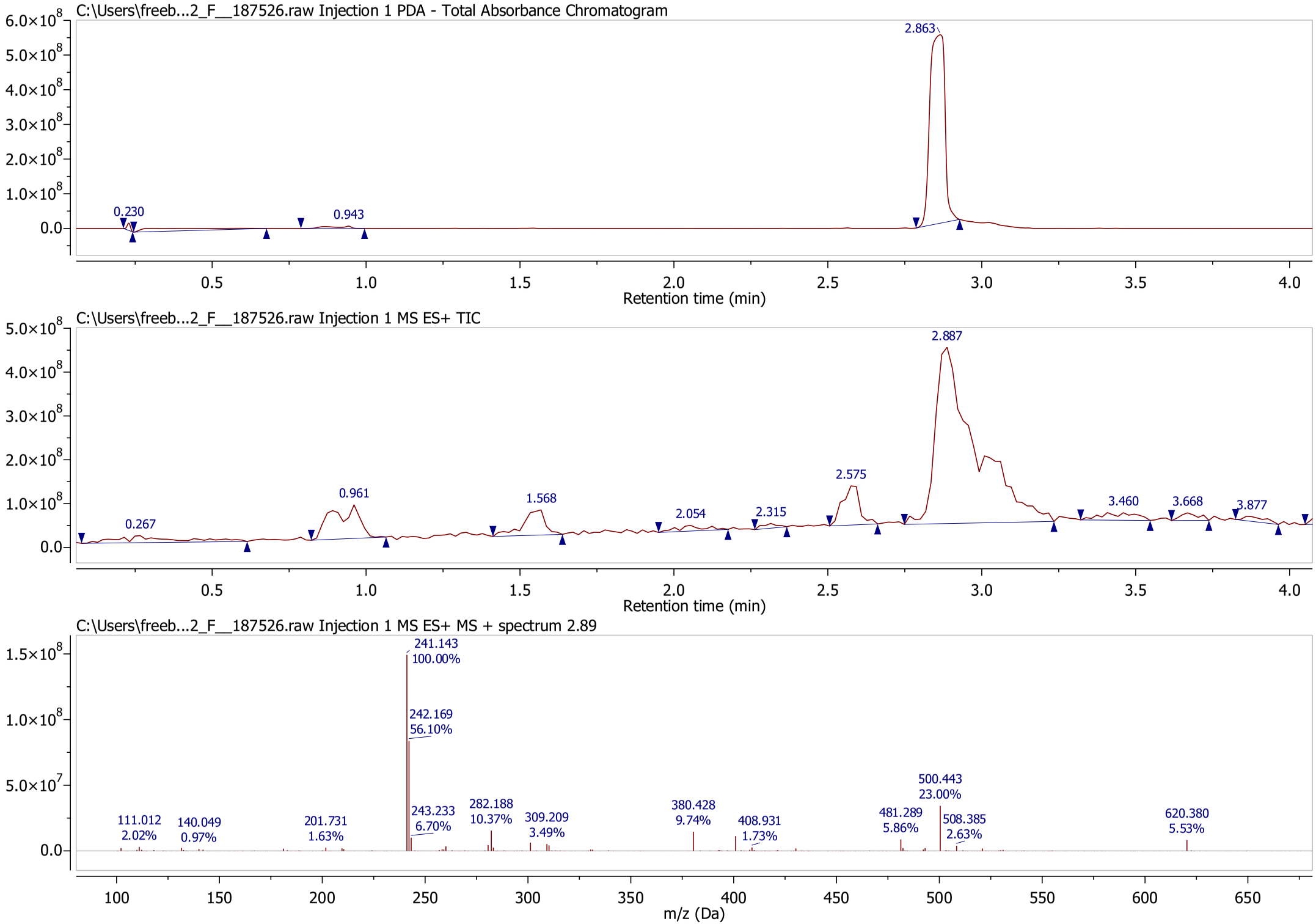


DEPT-135:


O
17
6
5
9
O
8
2
4
7
3
16
15
10
11
14
12
13
F
18
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{19}F:


1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-112.0
-112.5
-113.0
-113.5
-114.0
-114.5
-115.0
-115.5
-116.0
-116.5
-117.0
-117.5
-118.0
-118.5
-119.0
-119.5
-120.0
-120.5
f1 (ppm)


C:\Users\freeb...2_F__187526.raw Injection 1 PDA - Total Absorbance Chromatogram
6.0×10^8
5.0×10^8
4.0×10^8
3.0×10^8
2.0×10^8
1.0×10^8
0.0
2.863
0.230
0.943
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Retention time (min)
C:\Users\freeb...2_F__187526.raw Injection 1 MS ES+ TIC
5.0×10^8
4.0×10^8
3.0×10^8
2.0×10^8
1.0×10^8
0.0
2.887
0.267
0.961
1.568
2.054
2.315
2.575
3.460
3.668
3.877
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Retention time (min)
C:\Users\freeb...2_F__187526.raw Injection 1 MS ES+ MS + spectrum 2.89
1.5×10^8
1.0×10^8
5.0×10^7
0.0
241.143
100.00%
242.169
56.10%
111.012
2.02%
140.049
0.97%
201.731
1.63%
243.233
6.70%
282.188
10.37%
309.209
3.49%
380.428
9.74%
408.931
1.73%
481.289
5.86%
500.443
23.00%
508.385
2.63%
620.380
5.53%
100
150
200
250
300
350
400
450
500
550
600
650
m/z (Da)

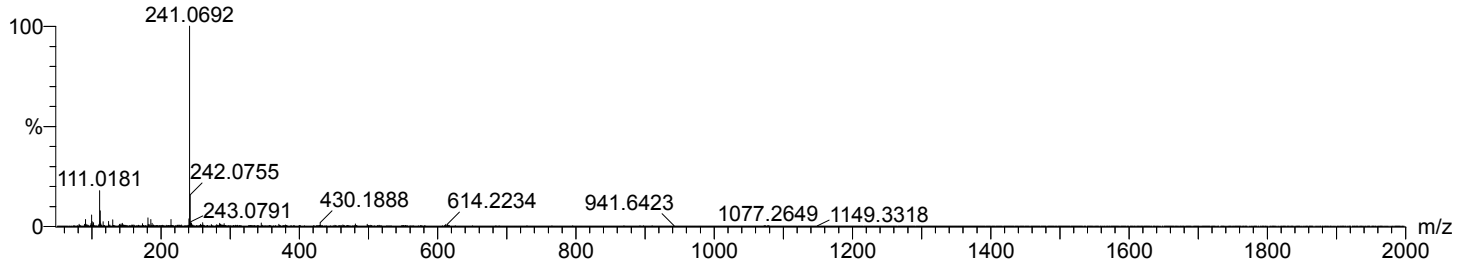
Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
511 formula(e) evaluated with 10 results within limits (up to 500 best isotopic matches for each mass)
Elements Used:
C: 0-60 H: 0-100 N: 0-6 O: 0-4 F: 0-3 I: 0-2

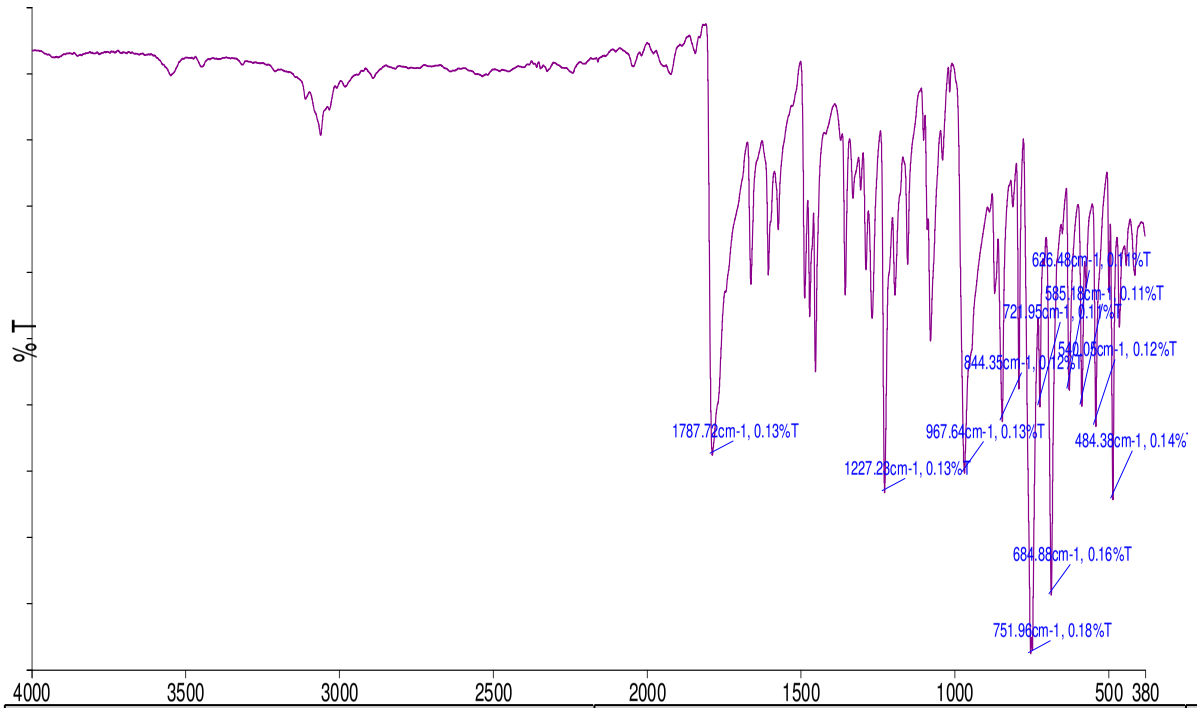
28-Aug-2018
IRB-Het-2-F 534 (4.489) Cm (534:544)

1: TOF MS ES+
2.78e+004



Minimum:				-1.5			
Maximum:		5.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
241.0692	241.0665	2.7	11.2	10.5	431.9	0.2	C15 H10 O2 F
	241.0726	-3.4	-14.1	10.5	433.5	1.9	C12 H9 N4 O2
	241.0676	1.6	6.6	6.5	434.5	2.9	C12 H11 O3 F2
	241.0653	3.9	16.2	14.5	437.4	5.7	C18 H9 O
	241.0737	-4.5	-18.7	6.5	439.1	7.5	C9 H10 N4 O3 F
	241.0701	-0.9	-3.7	7.5	439.2	7.6	C10 H8 N4 F3
	241.0688	0.4	1.7	2.5	439.4	7.8	C9 H12 O4 F3
	241.0649	4.3	17.8	7.5	441.3	9.7	C8 H7 N6 O F2
	241.0685	0.7	2.9	6.5	441.3	9.7	C7 H9 N6 O4
	241.0661	3.1	12.9	3.5	444.2	12.6	C5 H8 N6 O2 F3

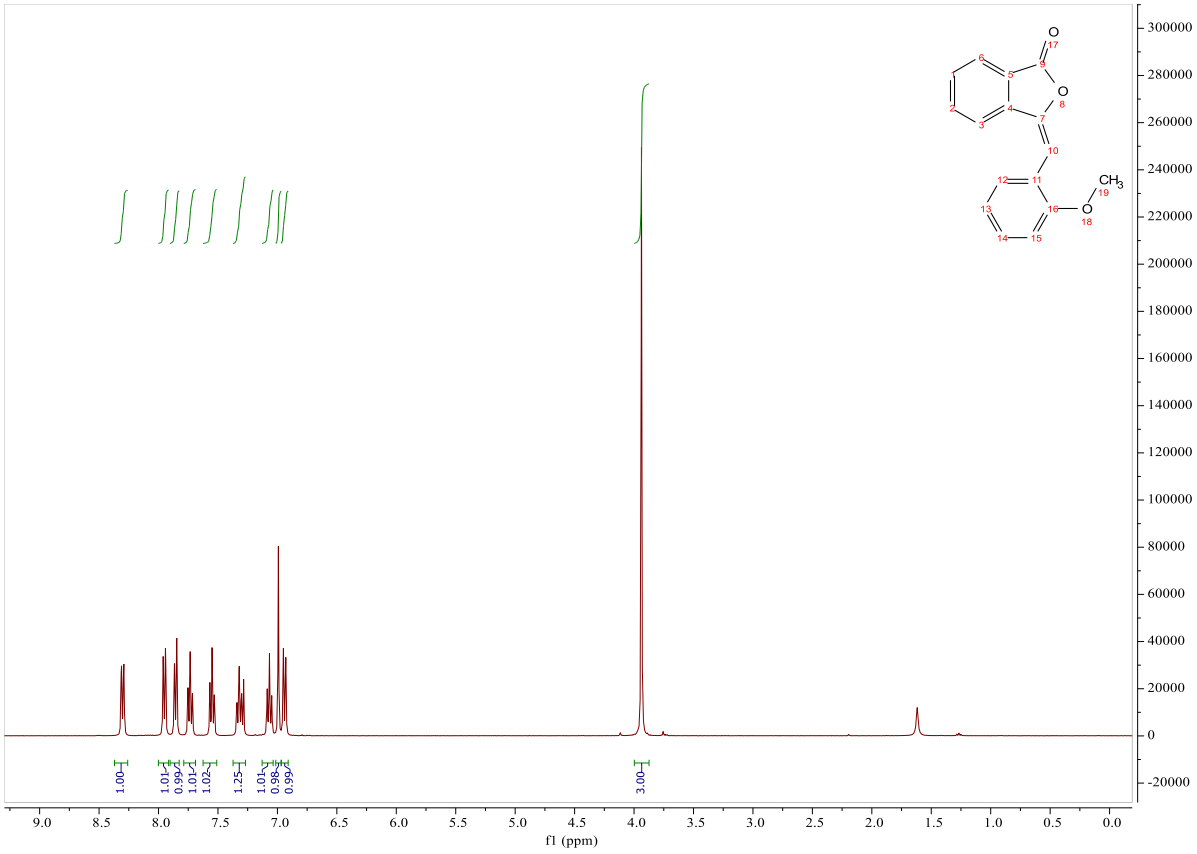
Analyst Professor Ian Baxendale
Date 24 August 2018 13:53



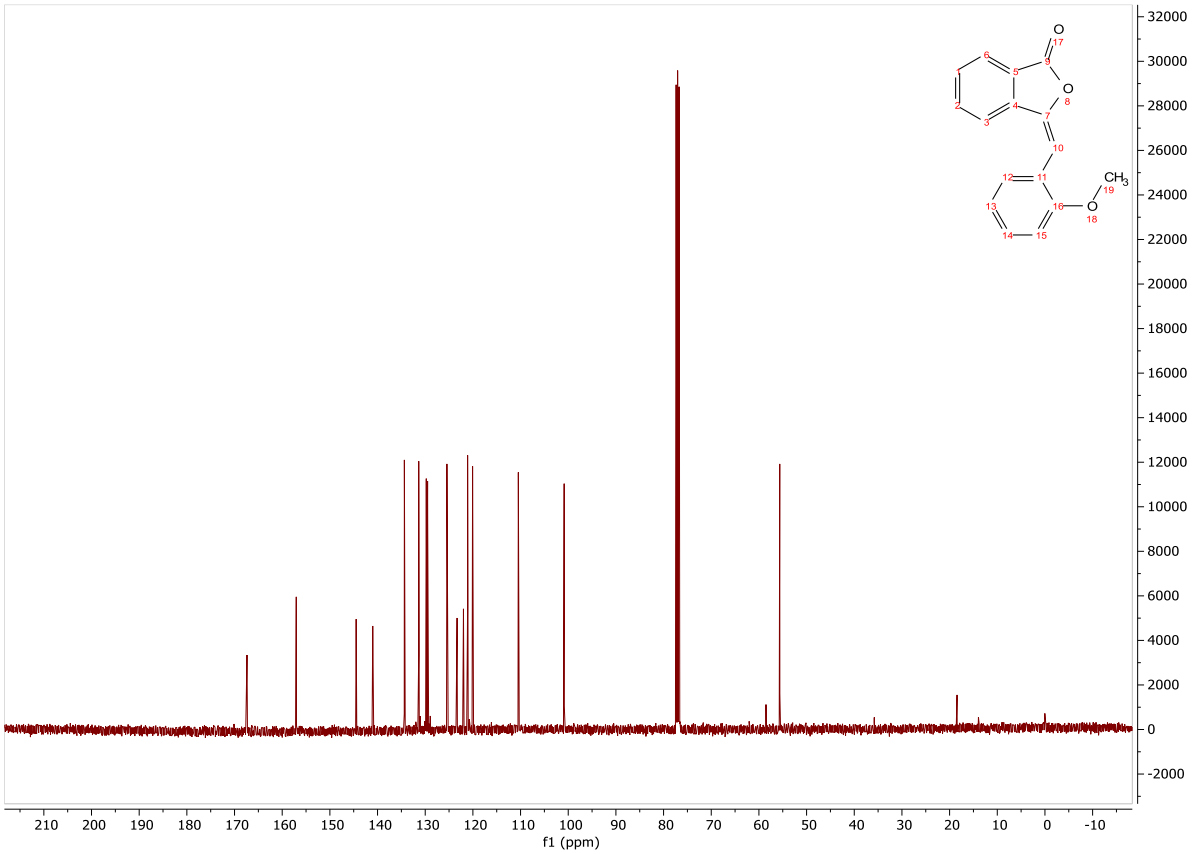
Sample Name	Description	Quality Checks
IRB 138	Sample 138 By IRB Date Friday, August 24 2018	The Quality Checks give rise to a Weak Bands warning for the sample.

(*Z*)-3-(2-methoxybenzylidene)isobenzofuran-1(3*H*)-one **35j**

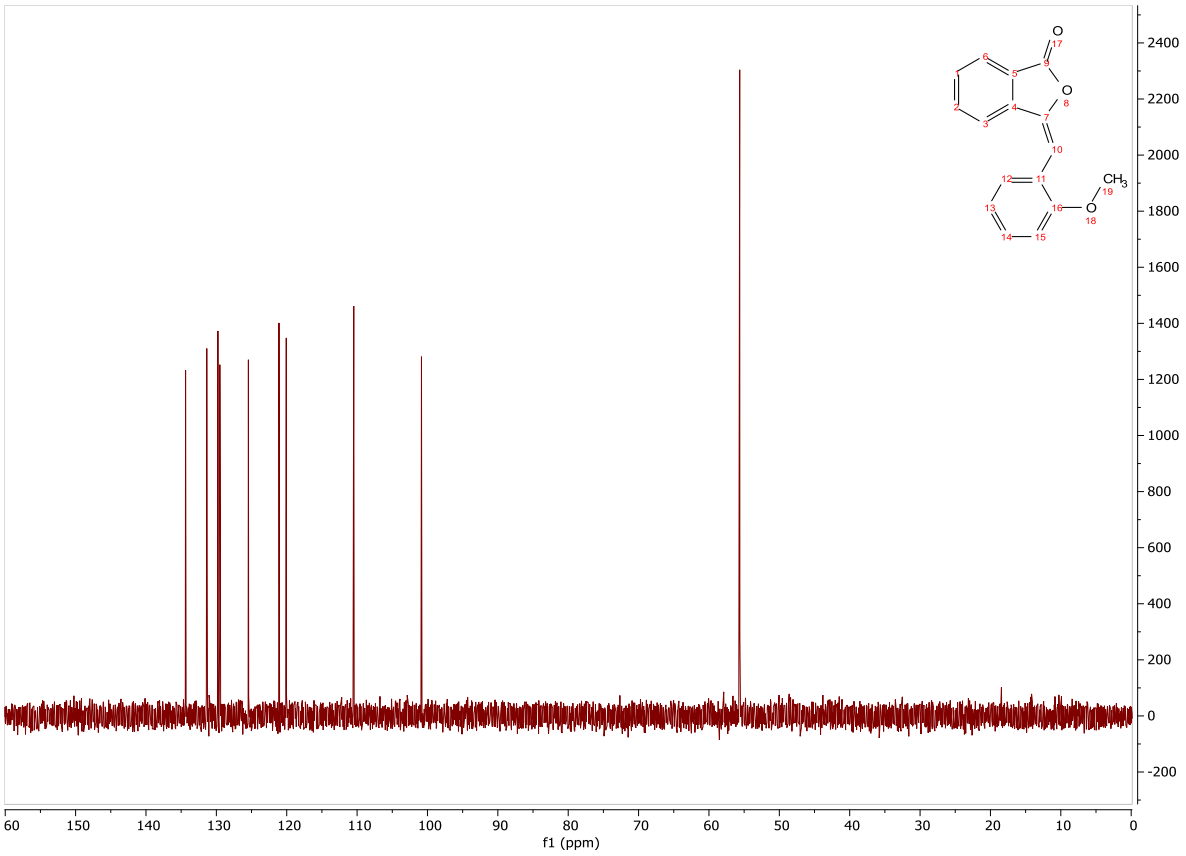
^{1}H:

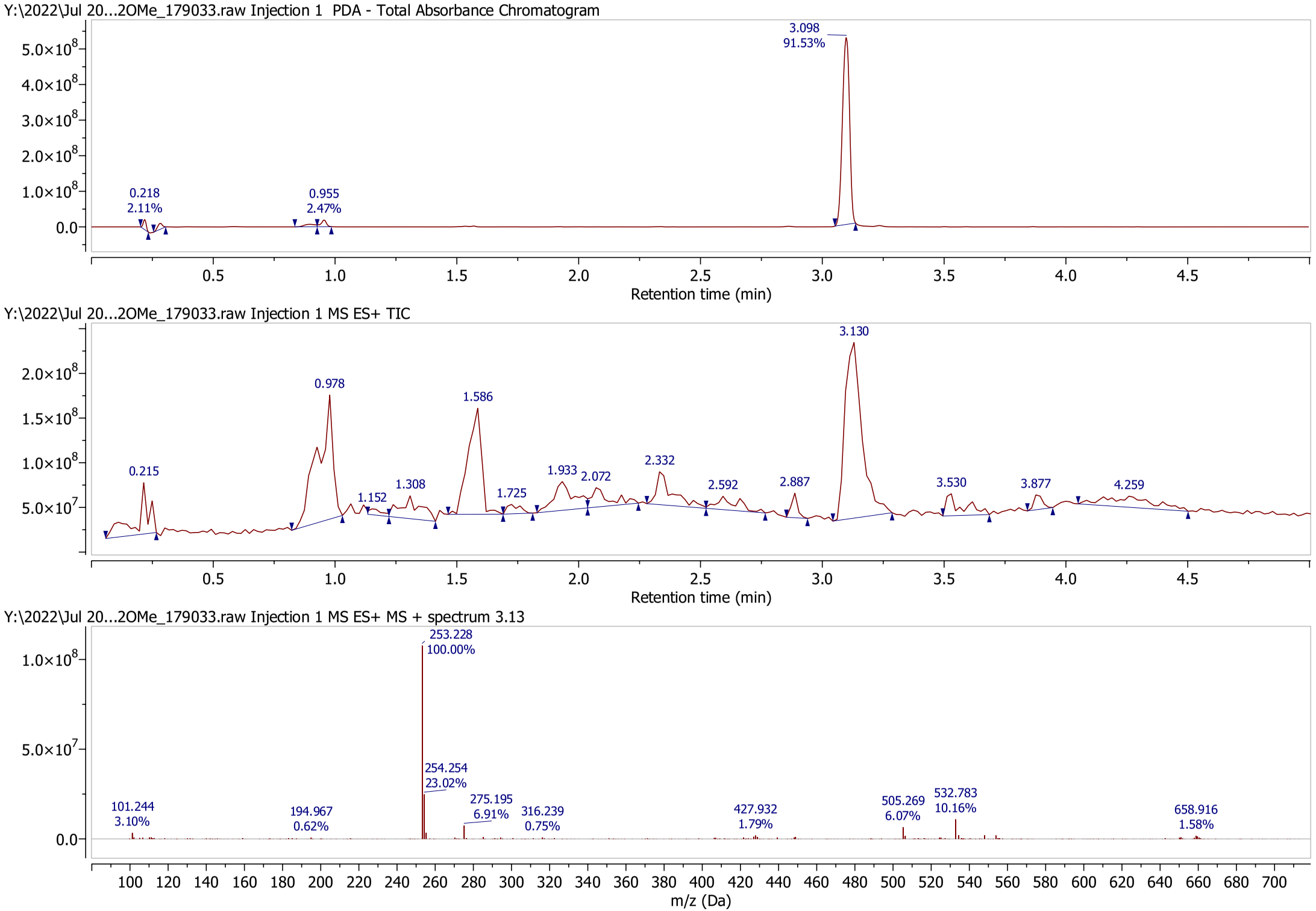


^{13}C:



DEPT-135:


O
17
6
5
9
O
8
1
2
4
7
3
10
12
11
CH3
19
13
16
O
18
14
15
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Y:\2022\Jul 20...2OMe_179033.raw Injection 1 PDA - Total Absorbance Chromatogram
3.098
91.53%
0.218
2.11%
0.955
2.47%
Retention time (min)
Y:\2022\Jul 20...2OMe_179033.raw Injection 1 MS ES+ TIC
3.130
0.978
1.586
0.215
1.152
1.308
1.725
1.933
2.072
2.332
2.592
2.887
3.530
3.877
4.259
Retention time (min)
Y:\2022\Jul 20...2OMe_179033.raw Injection 1 MS ES+ MS + spectrum 3.13
253.228
100.00%
254.254
23.02%
101.244
3.10%
194.967
0.62%
275.195
6.91%
316.239
0.75%
427.932
1.79%
505.269
6.07%
532.783
10.16%
658.916
1.58%
m/z (Da)

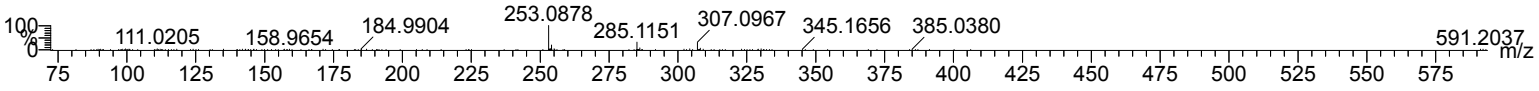
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
509 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-5 O: 0-6 P: 0-2

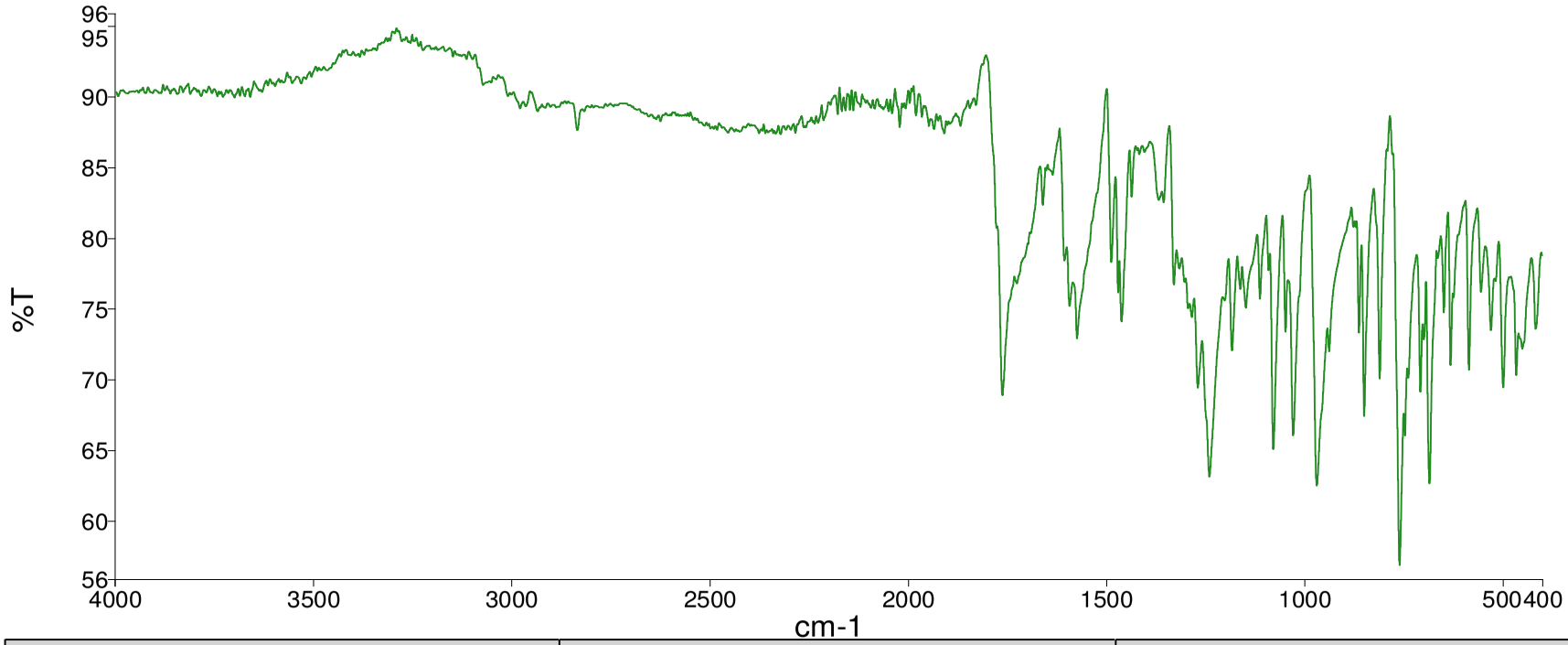
21-Jul-2022
MTF_MTF2OMe_179358 517 (4.341) Cm (513:519)

21-Jul-2022
1: TOF MS ES+
7.55e+003



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
253.0878	253.0871	0.7	2.8	1.5	179.6	15.215	0.00	C8 H19 N2 O3 P2
	253.0865	1.3	5.1	10.5	164.4	0.001	99.92	C16 H13 O3
	253.0895	-1.7	-6.7	10.5	171.5	7.119	0.08	C15 H14 N2 P
	253.0854	2.4	9.5	6.5	177.2	12.816	0.00	C10 H14 N4 O2 P

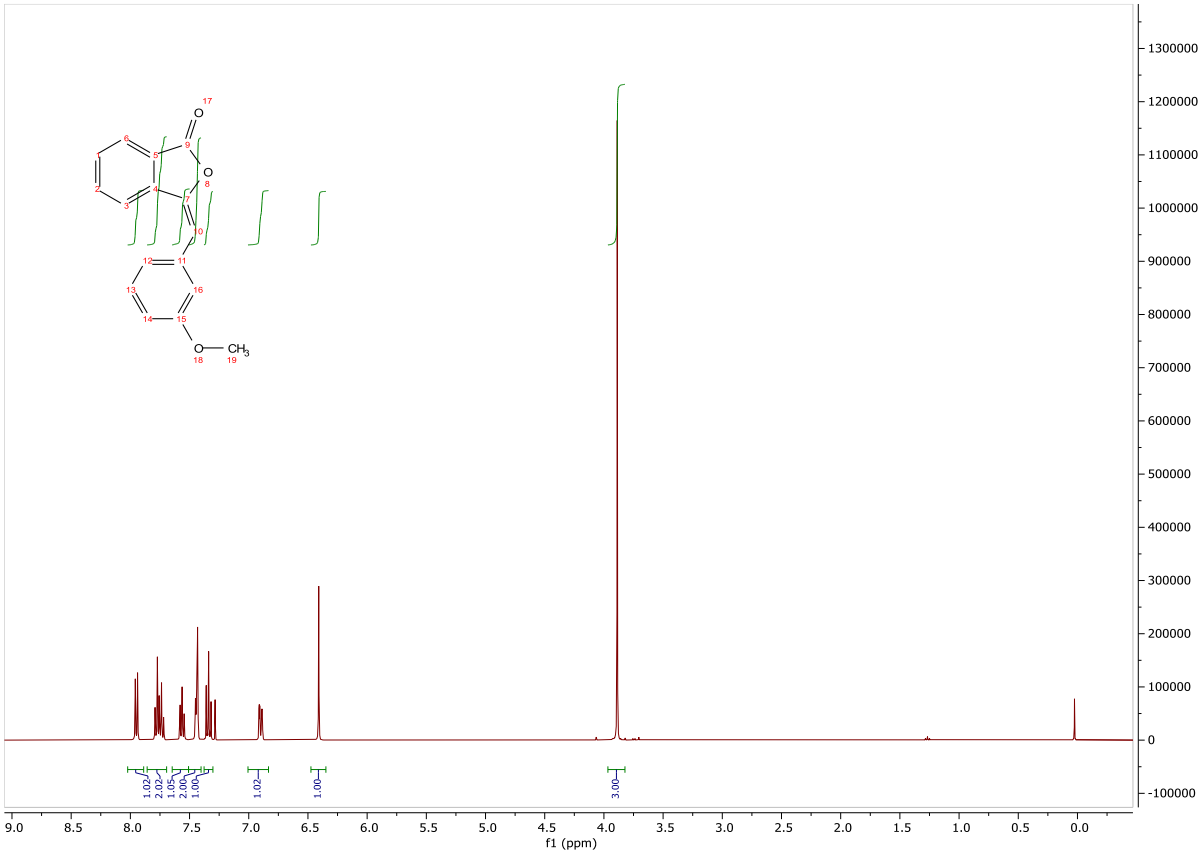
Analyst Lenny Lauchlan
Date 22 July 2022 14:30



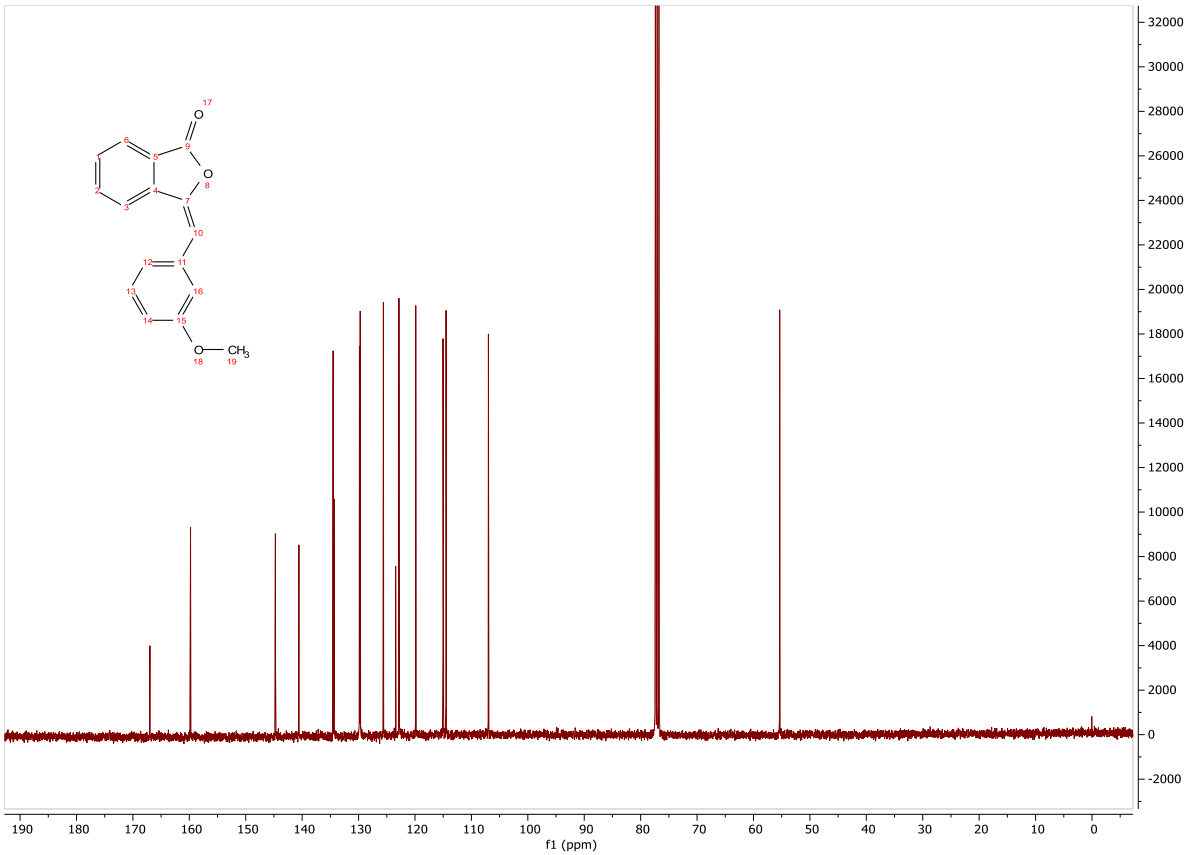
Sample Name	Description	Quality Checks
MTF 001J	Sample 020 By Lenny Date Friday, July 22 2022	The Quality Checks do not report any warnings for the sample.

(*Z*)-3-(3-methoxybenzylidene)isobenzofuran-1(3*H*)-one **35k**

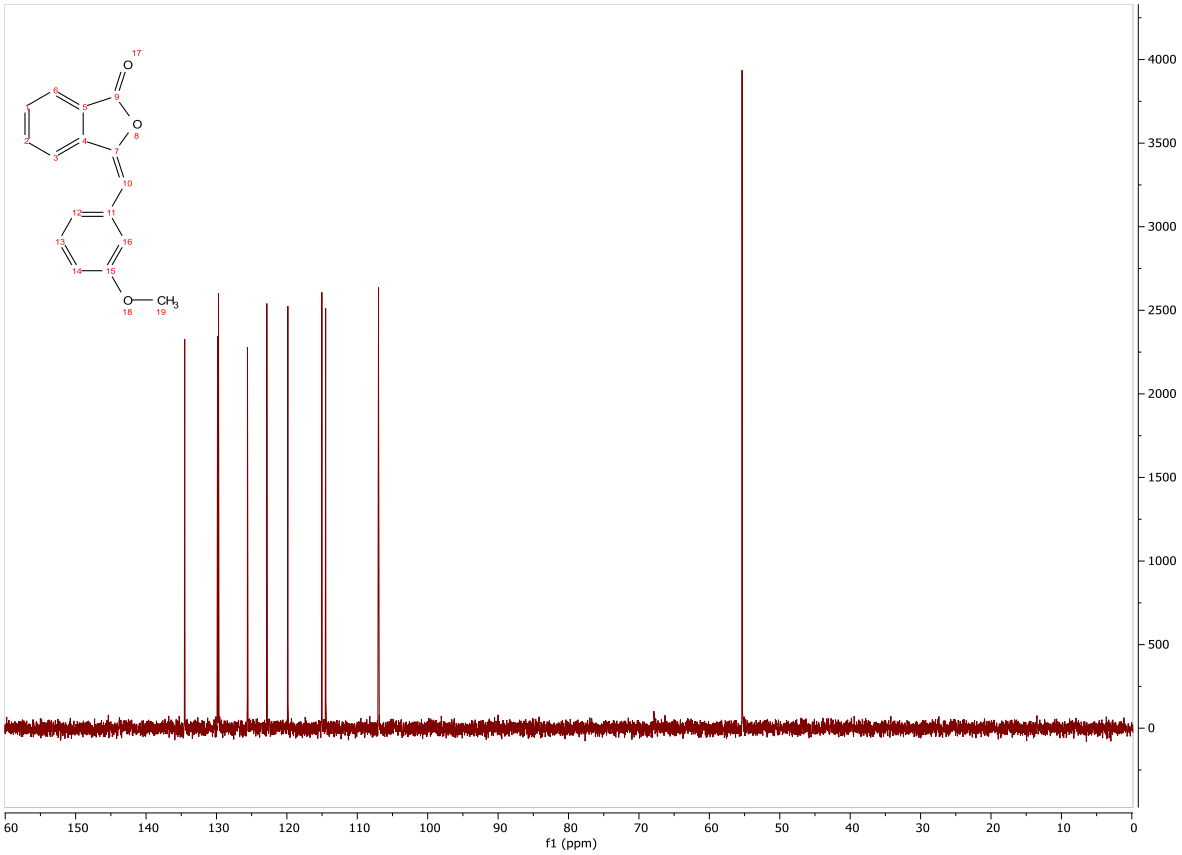
^{1}H:

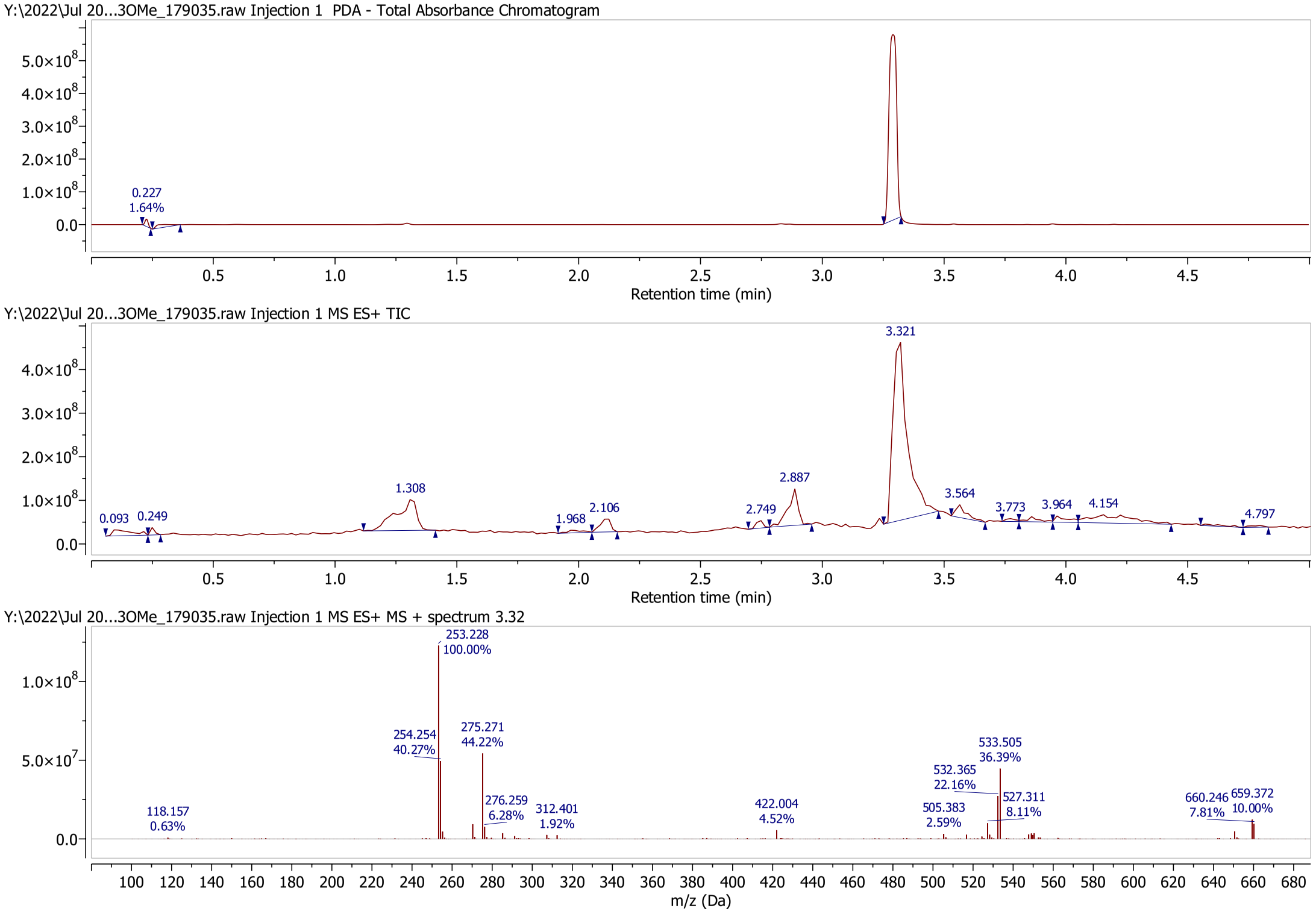


^{13}C:



DEPT-135:


4000
3500
3000
2500
2000
1500
1000
500
0
60
150
140
130
120
110
100
90
80
f1 (ppm)
70
60
50
40
30
20
10
0


Y:\2022\Jul 20...3OMe_179035.raw Injection 1 PDA - Total Absorbance Chromatogram
0.227
1.64%
Retention time (min)
Y:\2022\Jul 20...3OMe_179035.raw Injection 1 MS ES+ TIC
3.321
1.308
2.887
0.093
0.249
1.968
2.106
2.749
3.564
3.773
3.964
4.154
4.797
Retention time (min)
Y:\2022\Jul 20...3OMe_179035.raw Injection 1 MS ES+ MS + spectrum 3.32
253.228
100.00%
254.254
40.27%
275.271
44.22%
276.259
6.28%
312.401
1.92%
118.157
0.63%
422.004
4.52%
533.505
36.39%
532.365
22.16%
527.311
8.11%
505.383
2.59%
660.246
7.81%
659.372
10.00%
m/z (Da)

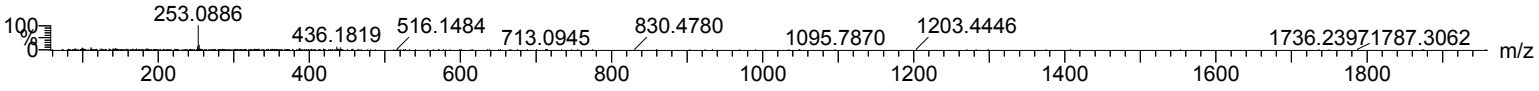
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
509 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-5 O: 0-6 P: 0-2

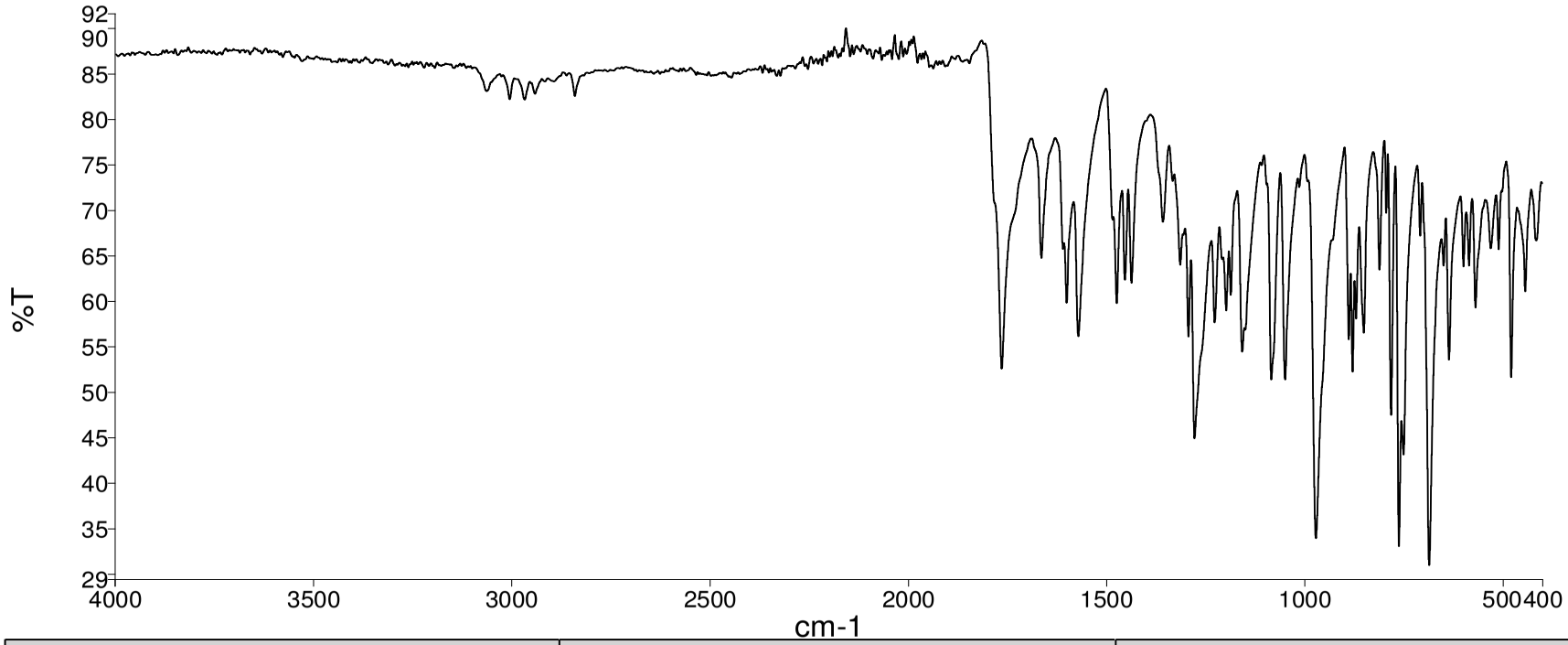
21-Jul-2022
MTF_MTF3OMe_179359 557 (4.679) Cm (557:561)

21-Jul-2022
1: TOF MS ES+
2.18e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
253.0886	253.0895	-0.9	-3.6	10.5	167.0	2.766	6.29	C15 H14 N2 P
	253.0871	1.5	5.9	1.5	174.5	10.304	0.00	C8 H19 N2 O3 P2
	253.0865	2.1	8.3	10.5	164.3	0.068	93.39	C16 H13 O3
	253.0911	-2.5	-9.9	5.5	169.9	5.761	0.31	C13 H19 O P2

Analyst Lenny Lauchlan
Date 22 July 2022 14:23

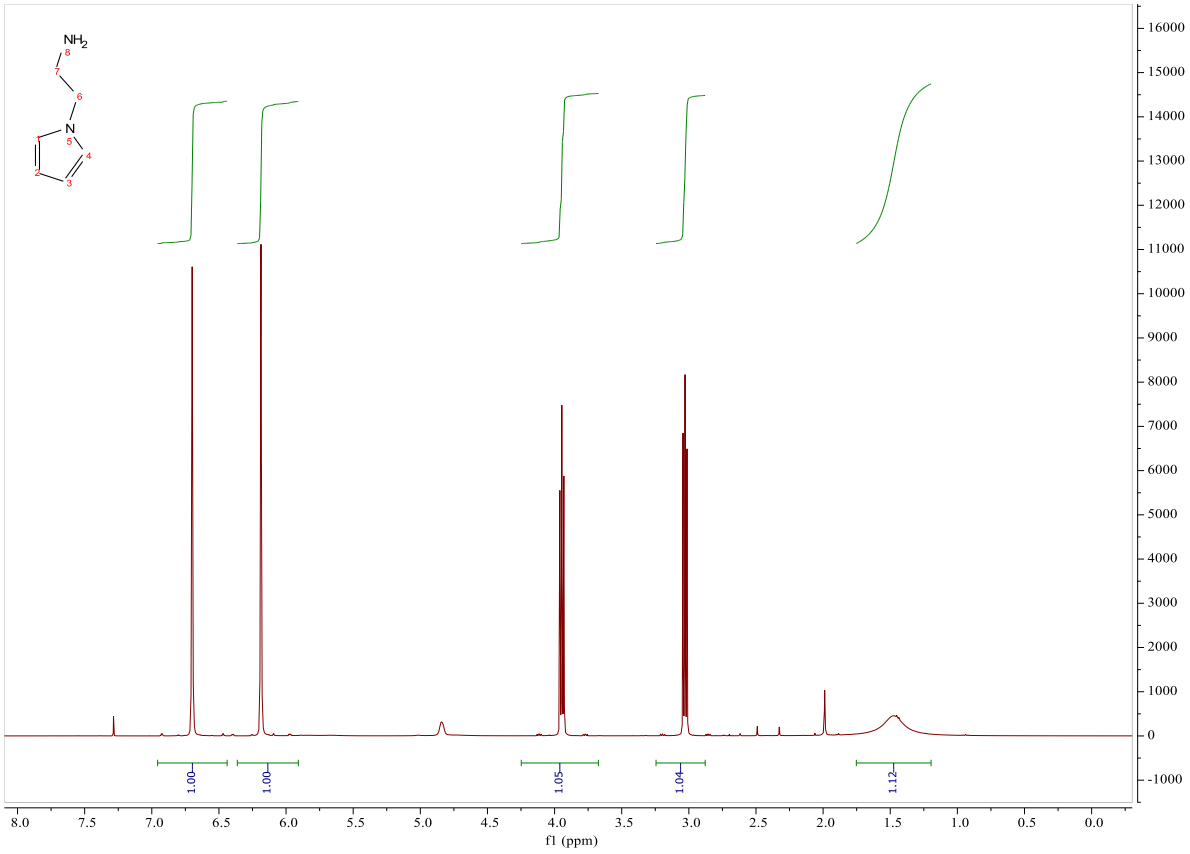


Sample Name	Description	Quality Checks
MTF 001k	Sample 016 By Lenny Date Friday, July 22 2022	The Quality Checks do not report any warnings for the sample.

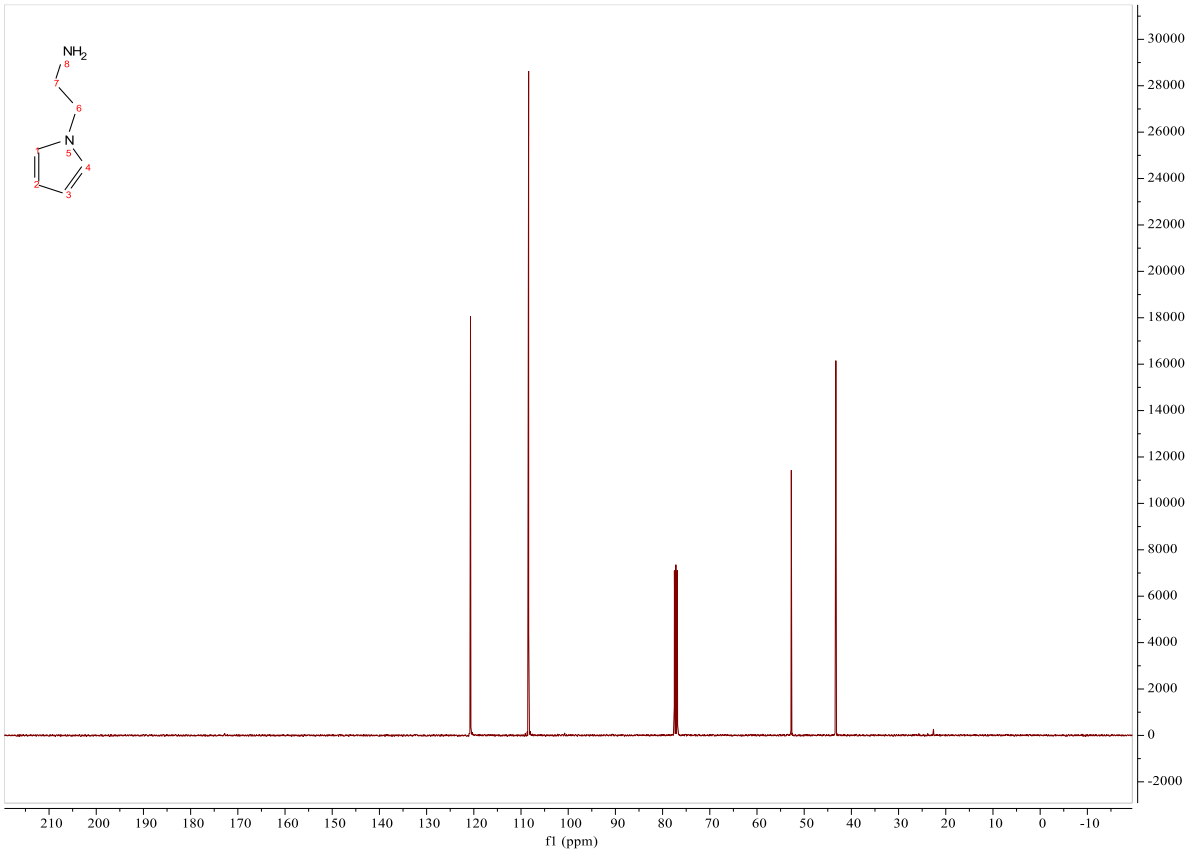
Synthesis of amine components **38** and **42**

2-(1*H*-pyrrol-1-yl)ethan-1-amine **38**

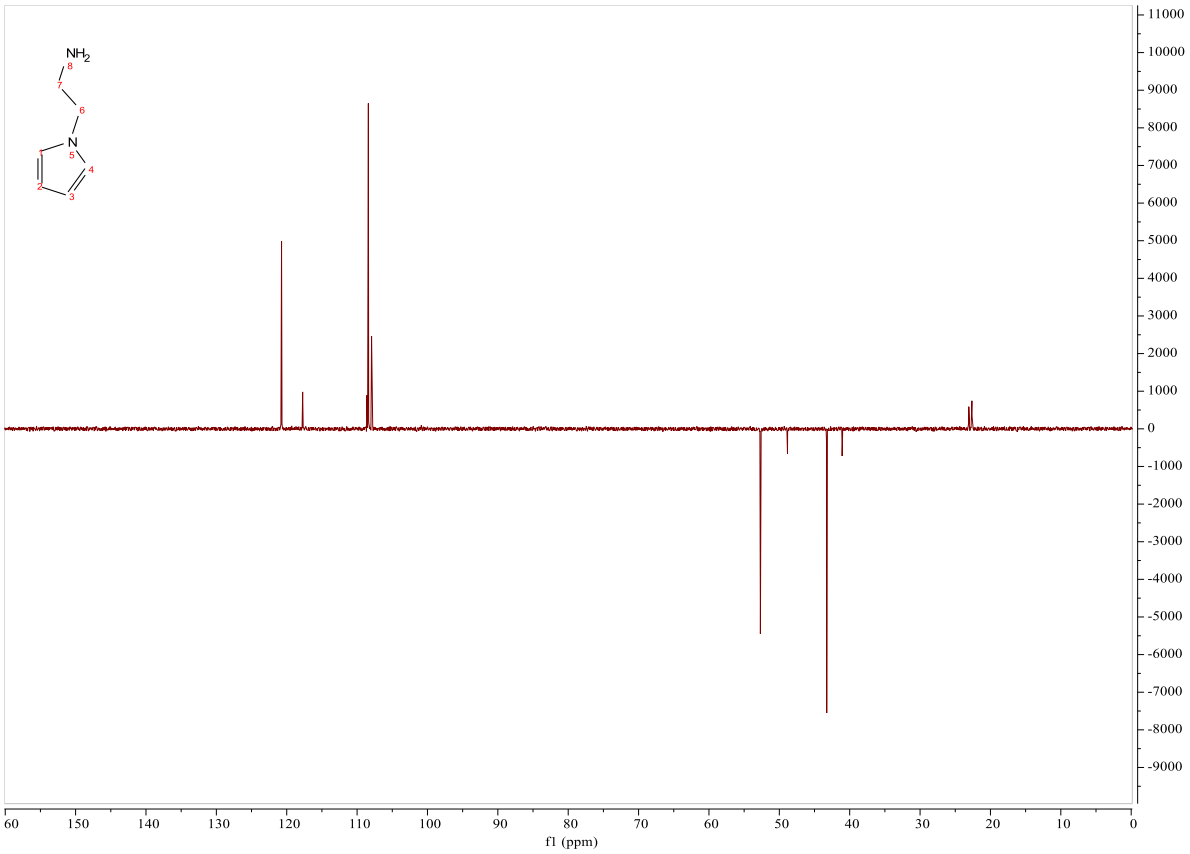
^{1}H:

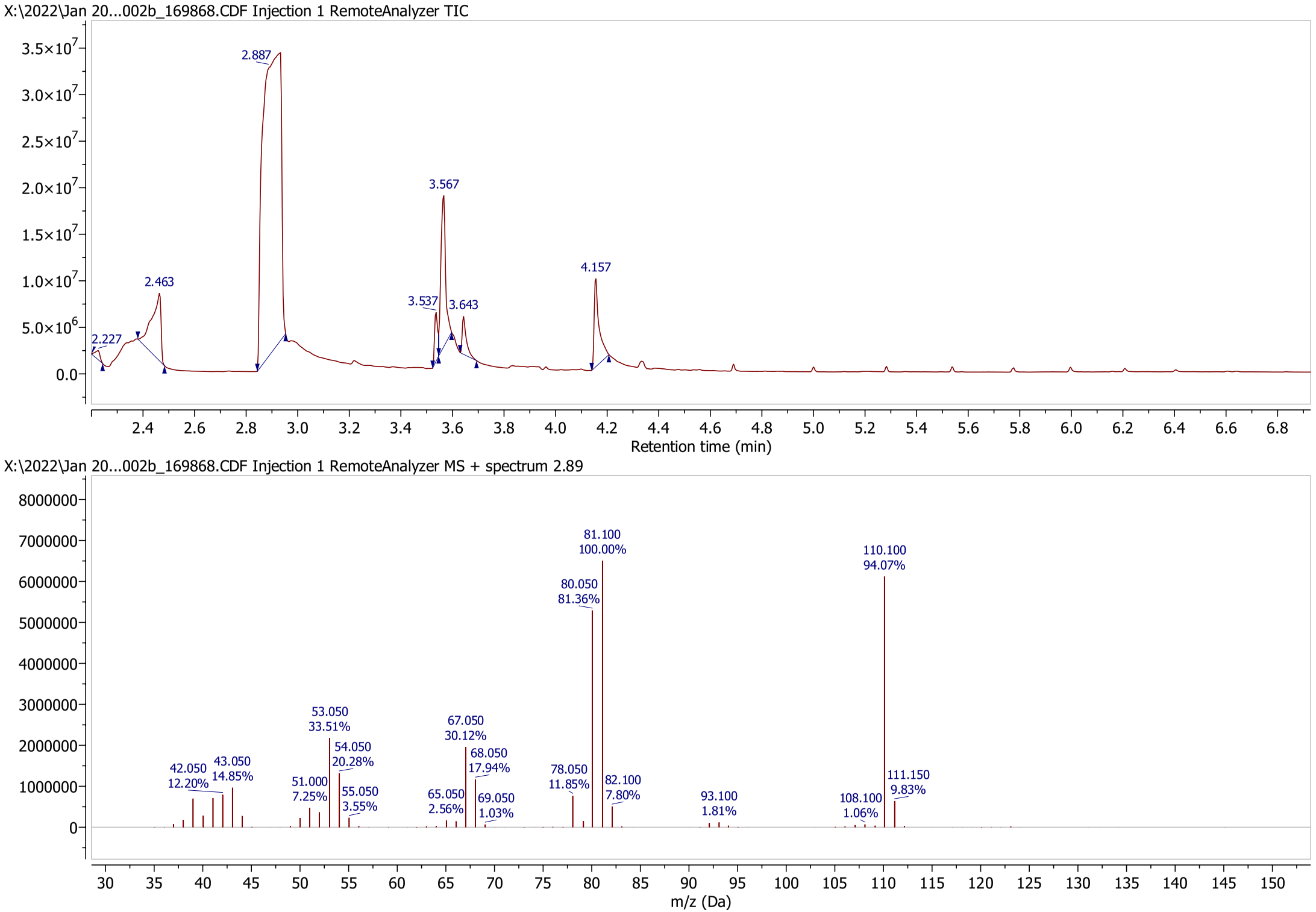


^{13}C:

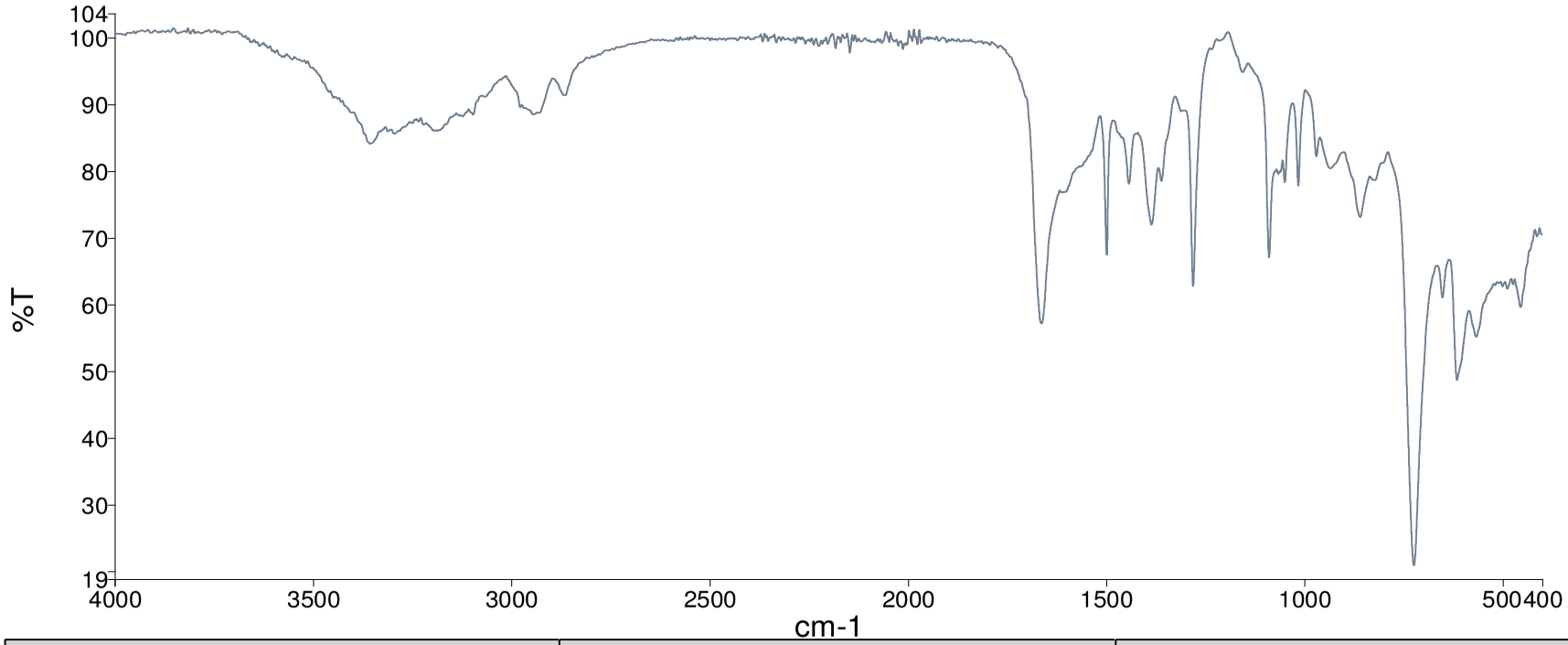


DEPT-135:


NH2
8
7
6
N
5
1
2
3
4
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
-5000
-6000
-7000
-8000
-9000
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


X:\2022\Jan 20...002b_169868.CDF Injection 1 RemoteAnalyzer TIC
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
2.887
3.567
4.157
2.463
3.537
3.643
2.227
2.4 2.6 2.8 3.0 3.2 3.4 3.6 3.8 4.0 4.2 4.4 4.6 4.8 5.0 5.2 5.4 5.6 5.8 6.0 6.2 6.4 6.6 6.8
Retention time (min)
X:\2022\Jan 20...002b_169868.CDF Injection 1 RemoteAnalyzer MS + spectrum 2.89
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
81.100
100.00%
110.100
94.07%
80.050
81.36%
53.050
33.51%
67.050
30.12%
54.050
20.28%
68.050
17.94%
42.050
12.20%
43.050
14.85%
51.000
7.25%
55.050
3.55%
65.050
2.56%
69.050
1.03%
78.050
11.85%
82.100
7.80%
93.100
1.81%
108.100
1.06%
111.150
9.83%
30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150
m/z (Da)

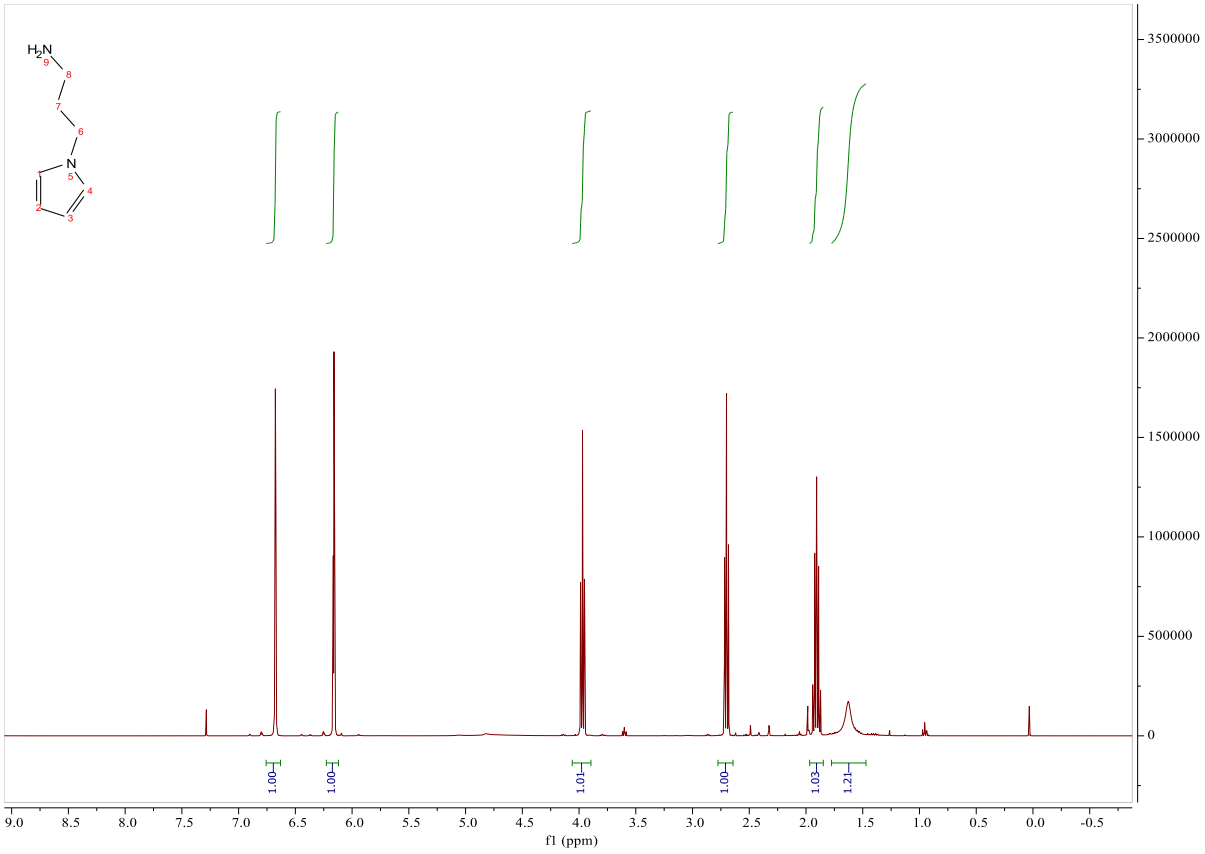
Analyst Lenny Lauchlan
Date 22 July 2022 14:34



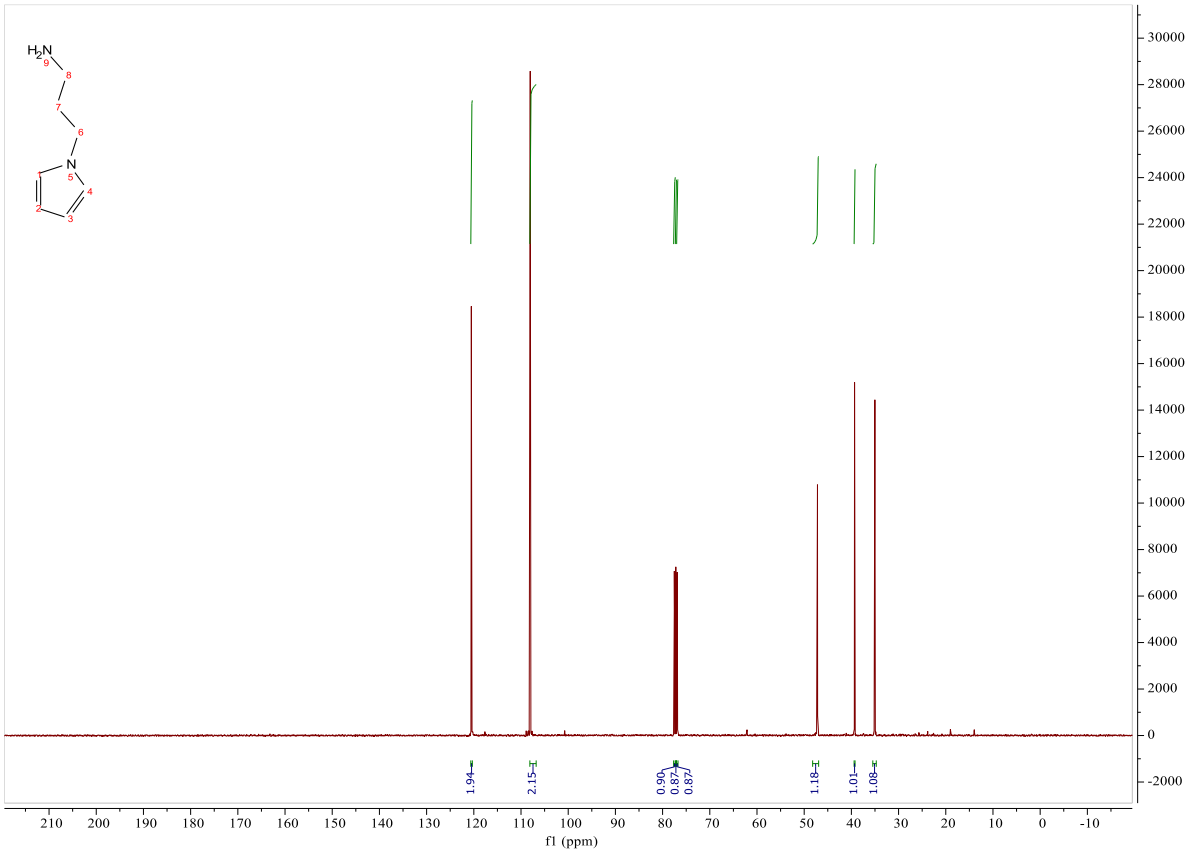
Sample Name	Description	Quality Checks
MTF 002B	Sample 023 By Lenny Date Friday, July 22 2022	The Quality Checks do not report any warnings for the sample.

3-(1*H*-pyrrol-1-yl)propan-1-amine **42**

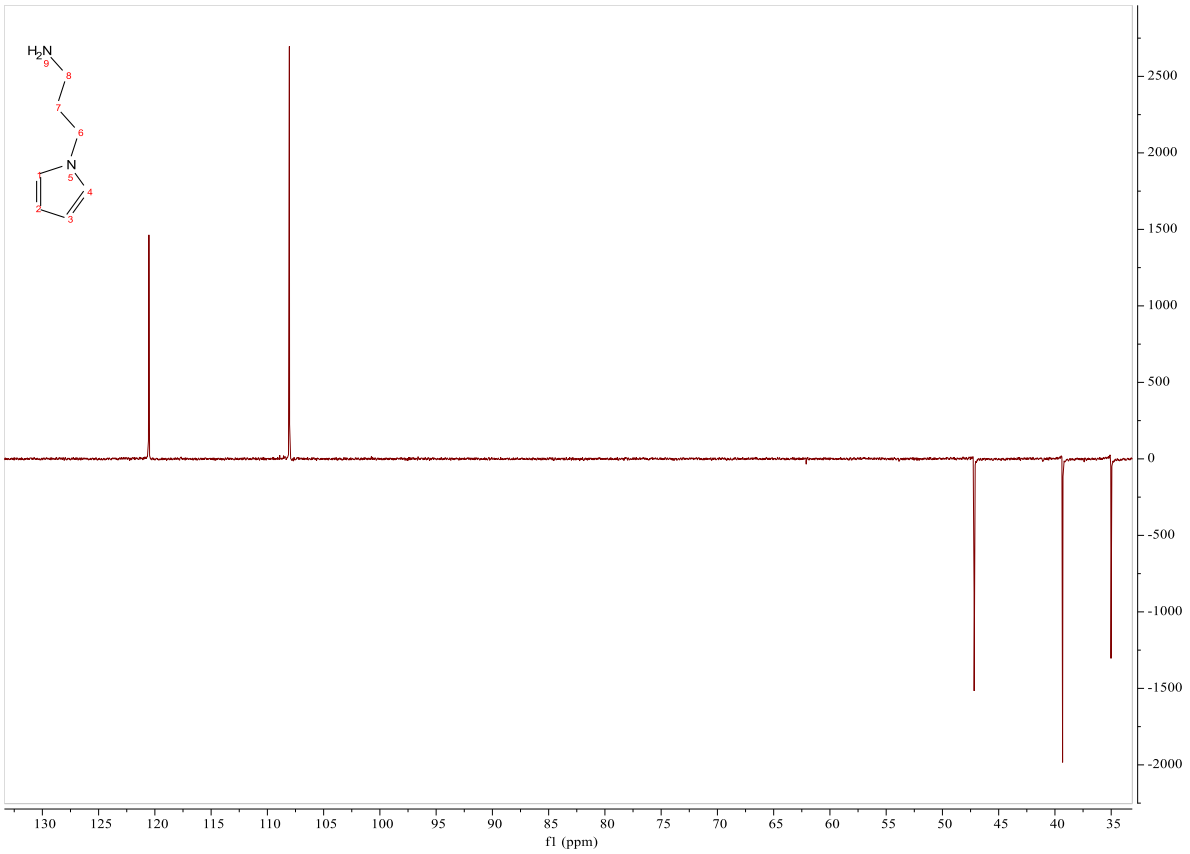
^{1}H:

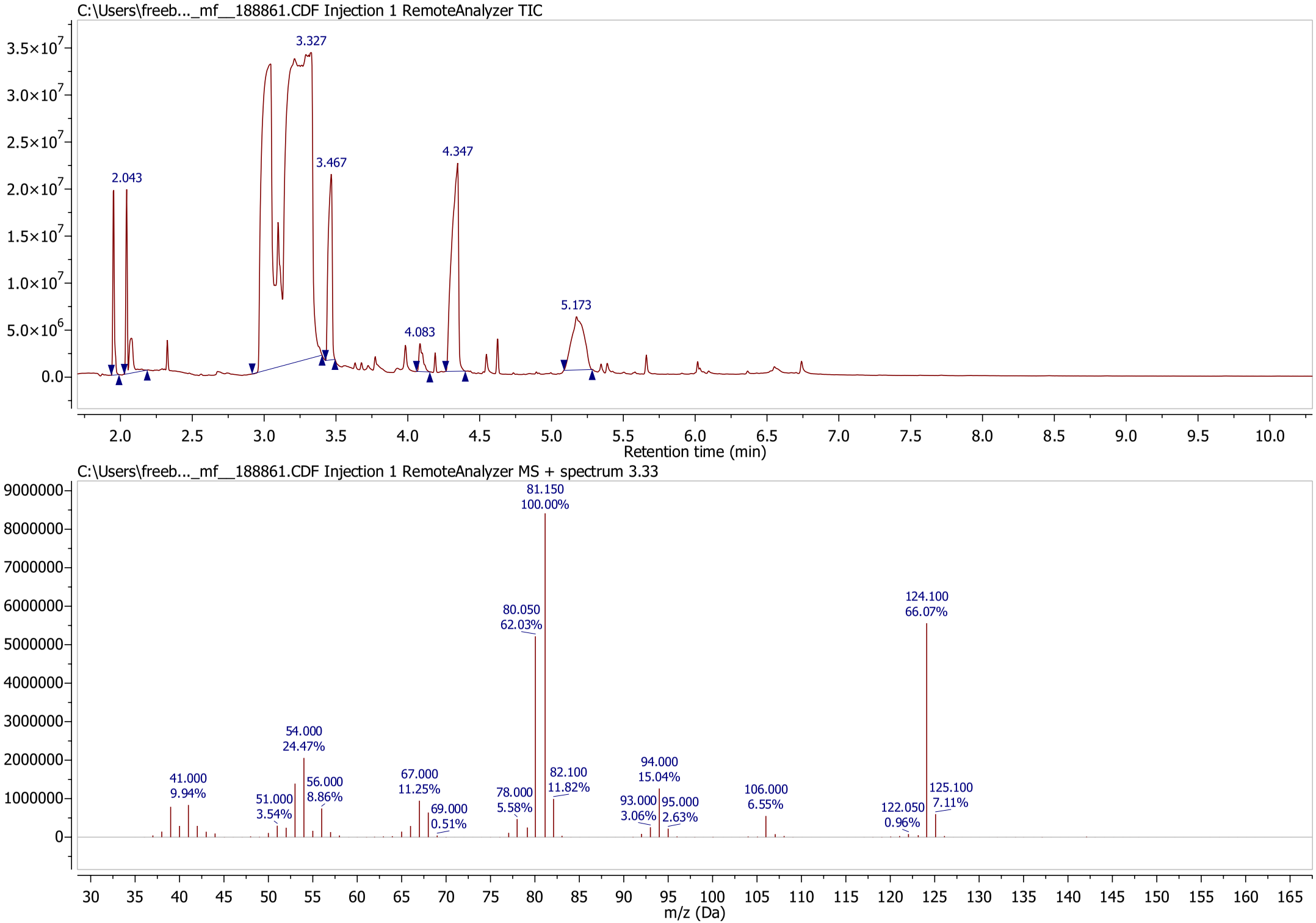


^{13}C:

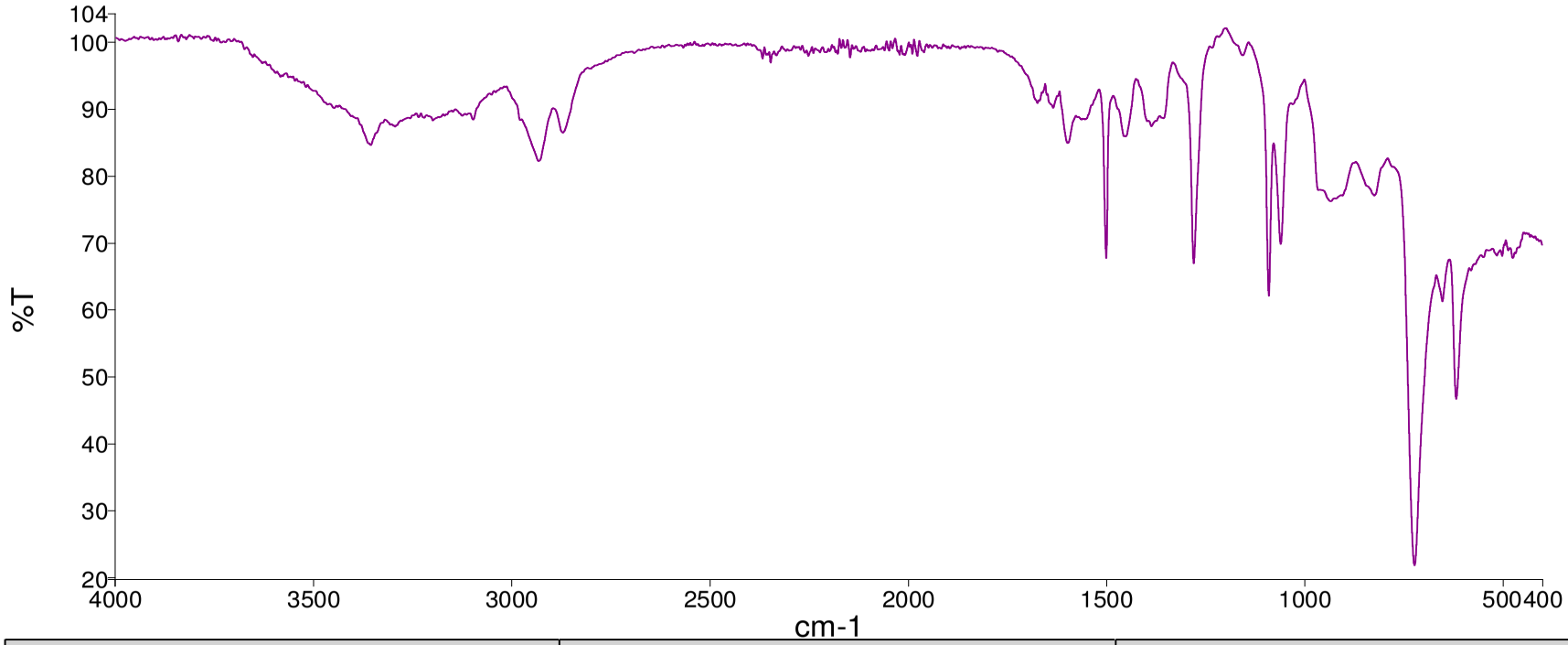


DEPT-135:


H2N
9
8
7
6
N
5
4
1
2
3
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
f1 (ppm)


C:\Users\freeb..._mf__188861.CDF Injection 1 RemoteAnalyzer TIC
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
2.043
3.327
3.467
4.083
4.347
5.173
2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0 8.5 9.0 9.5 10.0
Retention time (min)
C:\Users\freeb..._mf__188861.CDF Injection 1 RemoteAnalyzer MS + spectrum 3.33
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
81.150
100.00%
80.050
62.03%
124.100
66.07%
54.000
24.47%
41.000
9.94%
56.000
8.86%
51.000
3.54%
67.000
11.25%
69.000
0.51%
78.000
5.58%
82.100
11.82%
94.000
15.04%
93.000
3.06%
95.000
2.63%
106.000
6.55%
122.050
0.96%
125.100
7.11%
30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160 165
m/z (Da)

Analyst Lenny Lauchlan
Date 22 July 2022 14:33

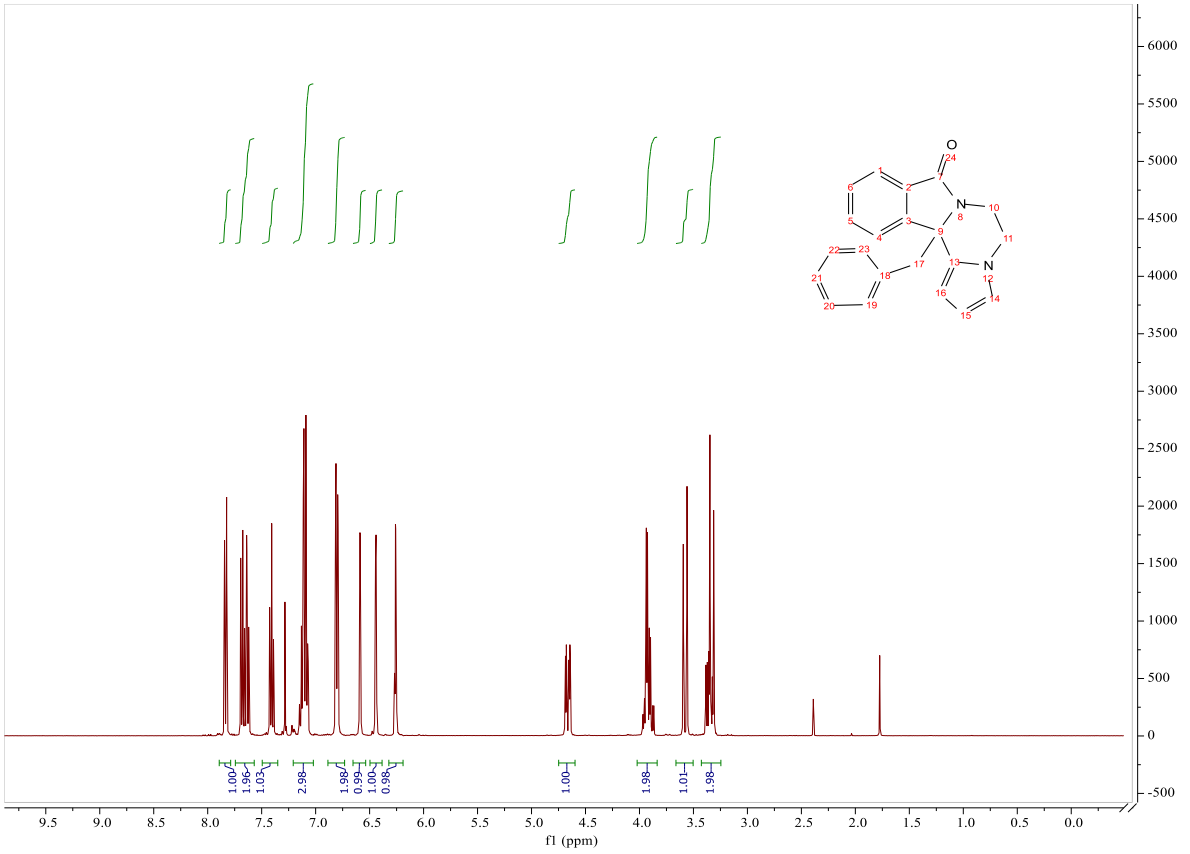


Sample Name	Description	Quality Checks
MTF 002C	Sample 022 By Lenny Date Friday, July 22 2022	The Quality Checks do not report any warnings for the sample.

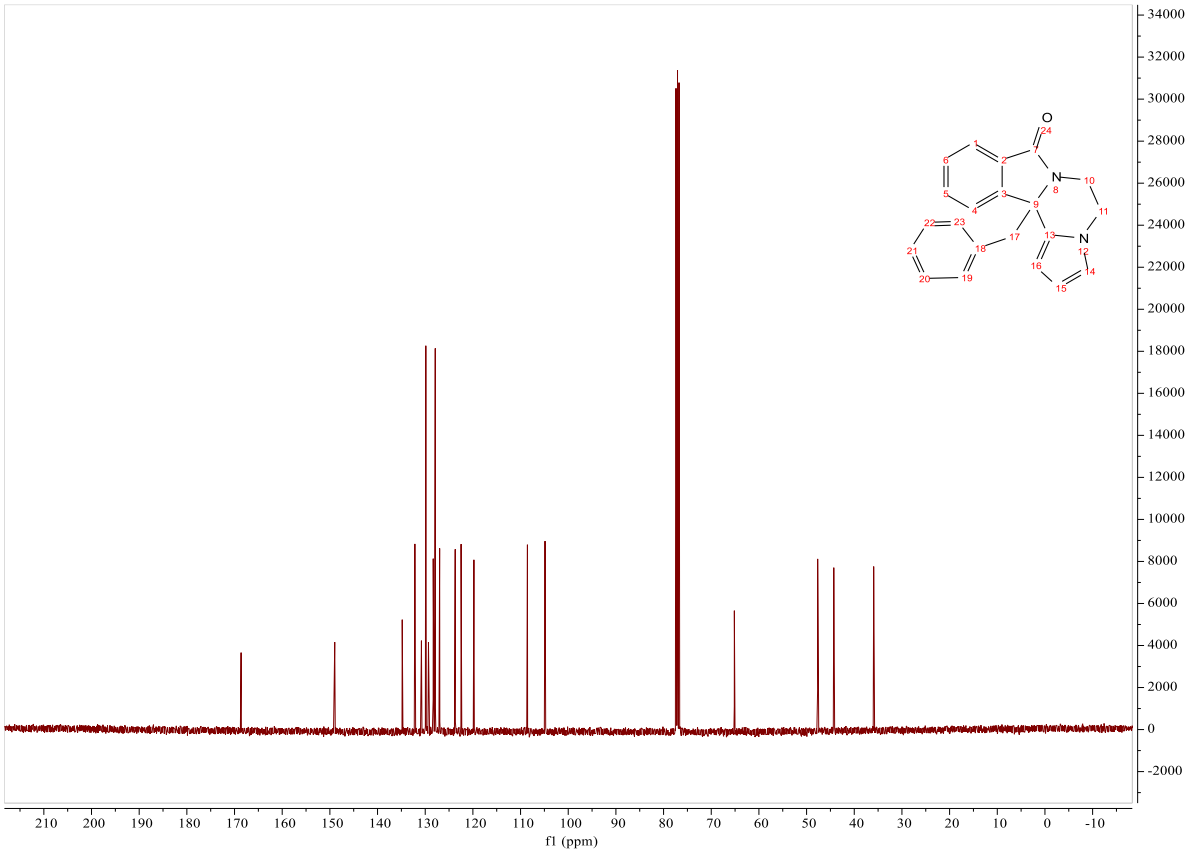
Synthesis of isoindolone product and substituted derivatives **1-1k**

12*b*-benzyl-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1**

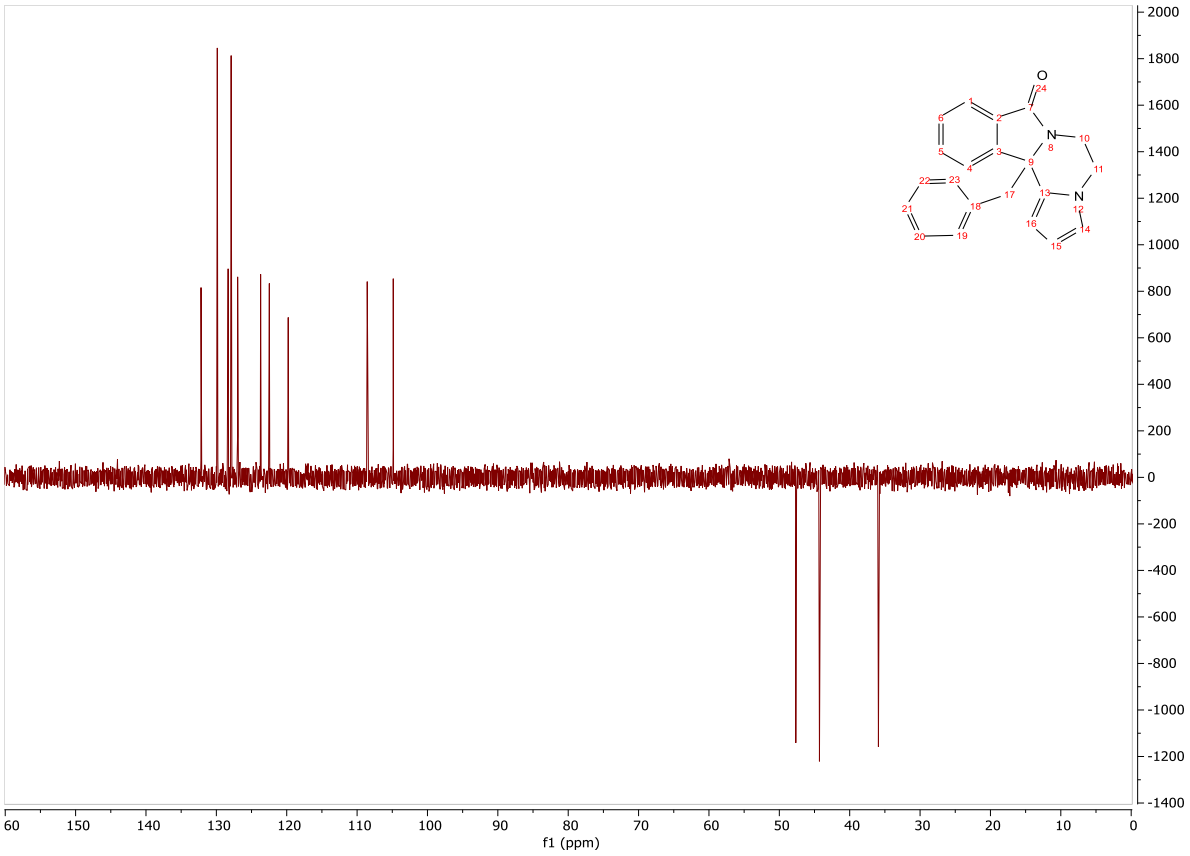
^{1}H:

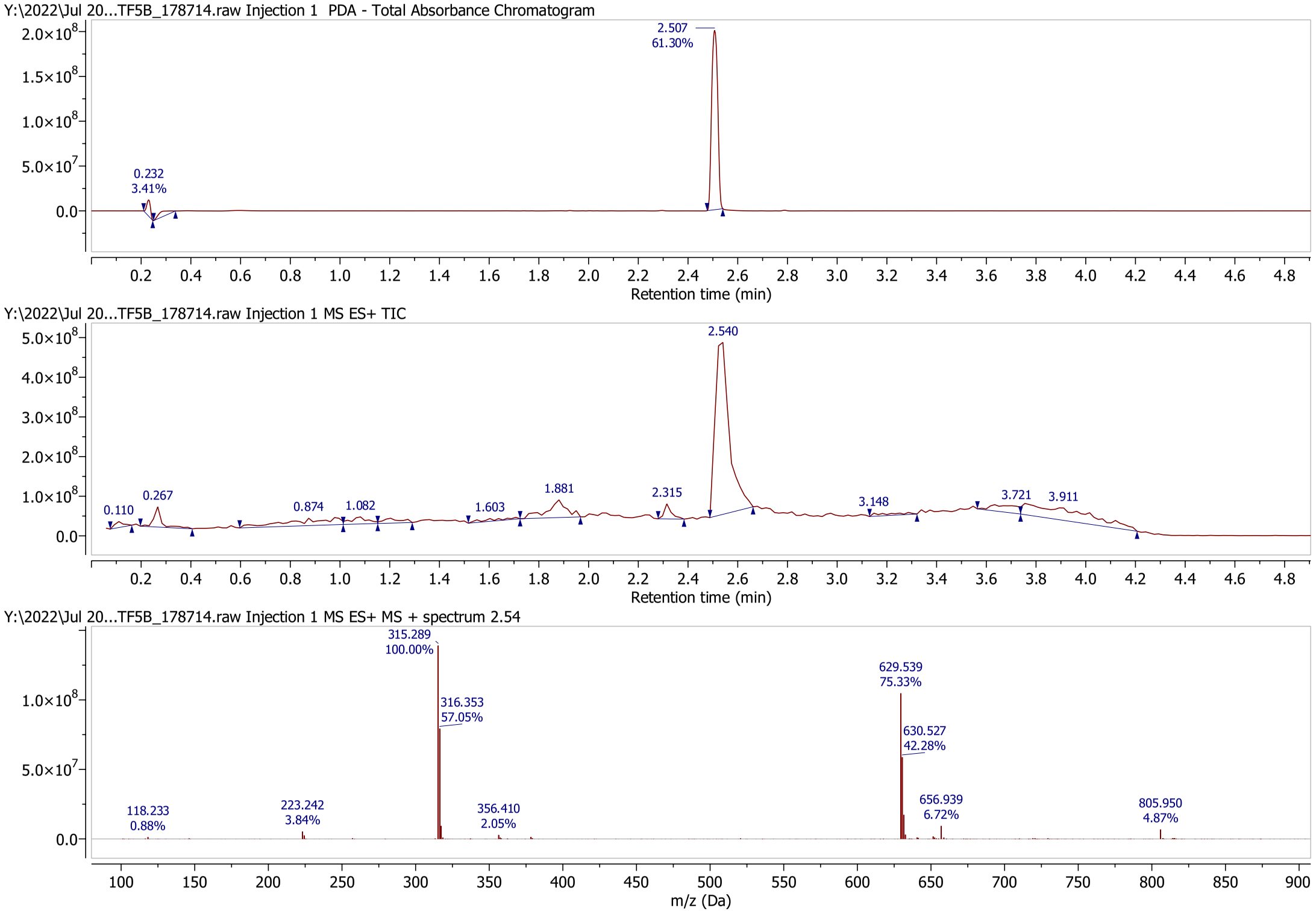


^{13}C:



DEPT-135:


2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
-400
-600
-800
-1000
-1200
-1400
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
N
N


Y:\2022\Jul 20...TF5B_178714.raw Injection 1 PDA - Total Absorbance Chromatogram
2.507
61.30%
0.232
3.41%
Retention time (min)
Y:\2022\Jul 20...TF5B_178714.raw Injection 1 MS ES+ TIC
2.540
0.110
0.267
0.874
1.082
1.603
1.881
2.315
3.148
3.721
3.911
Retention time (min)
Y:\2022\Jul 20...TF5B_178714.raw Injection 1 MS ES+ MS + spectrum 2.54
315.289
100.00%
316.353
57.05%
629.539
75.33%
630.527
42.28%
118.233
0.88%
223.242
3.84%
356.410
2.05%
656.939
6.72%
805.950
4.87%
m/z (Da)

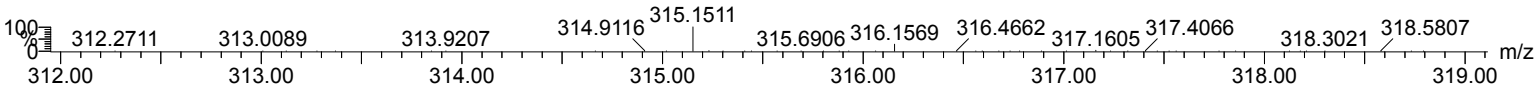
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
1356 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 Cl: 0-2

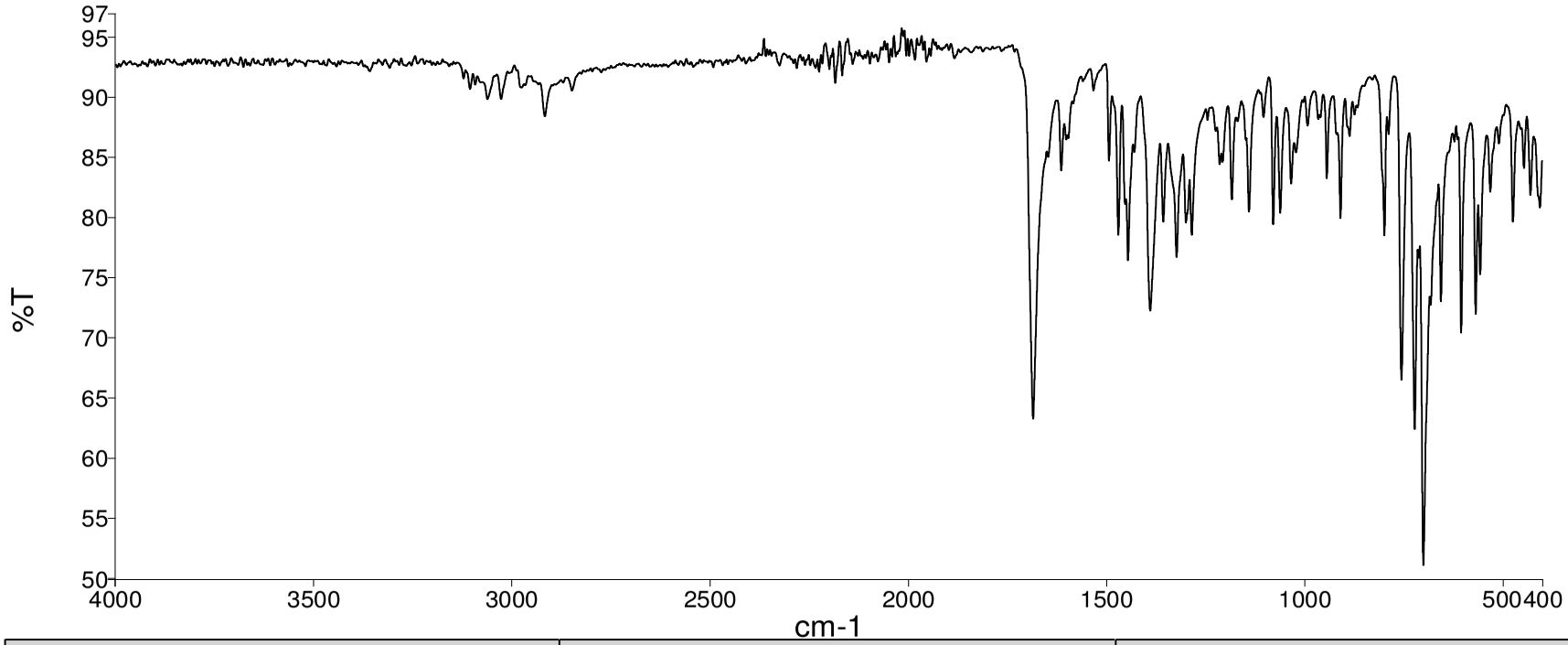
21-Jul-2022
MTF_MTF5B_179340 498 (4.185) Cm (498)

21-Jul-2022
1: TOF MS ES+
5.61e+002



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
315.1511	315.1507	0.4	1.3	-3.5	92.8	22.626	0.00	C4 H24 N8 O6 Cl
	315.1516	-0.5	-1.6	8.5	92.1	21.925	0.00	C20 H24 O Cl
	315.1516	-0.5	-1.6	0.5	78.6	8.493	0.02	C9 H23 N4 O8
	315.1497	1.4	4.4	13.5	70.1	0.001	99.94	C21 H19 N2 O
	315.1526	-1.5	-4.8	-8.5	94.3	24.139	0.00	C3 H29 N6 O6 Cl2
	315.1494	1.7	5.4	-8.5	92.9	22.801	0.00	C3 H28 N4 O10 Cl
	315.1494	1.7	5.4	-0.5	94.2	24.054	0.00	C14 H29 O3 Cl2
	315.1529	-1.8	-5.7	5.5	78.1	7.963	0.03	C10 H19 N8 O4
	315.1489	2.2	7.0	1.5	82.8	12.677	0.00	C5 H19 N10 O6
	315.1534	-2.3	-7.3	-4.5	92.0	21.848	0.00	C8 H28 N2 O8 Cl
	315.1539	-2.8	-8.9	-3.5	94.6	24.498	0.00	C4 H25 N10 O2 Cl2

Analyst Lenny Lauchlan
Date 28 June 2022 12:47



Sample Name	Description	Quality Checks
MTF 005B	Sample 016 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

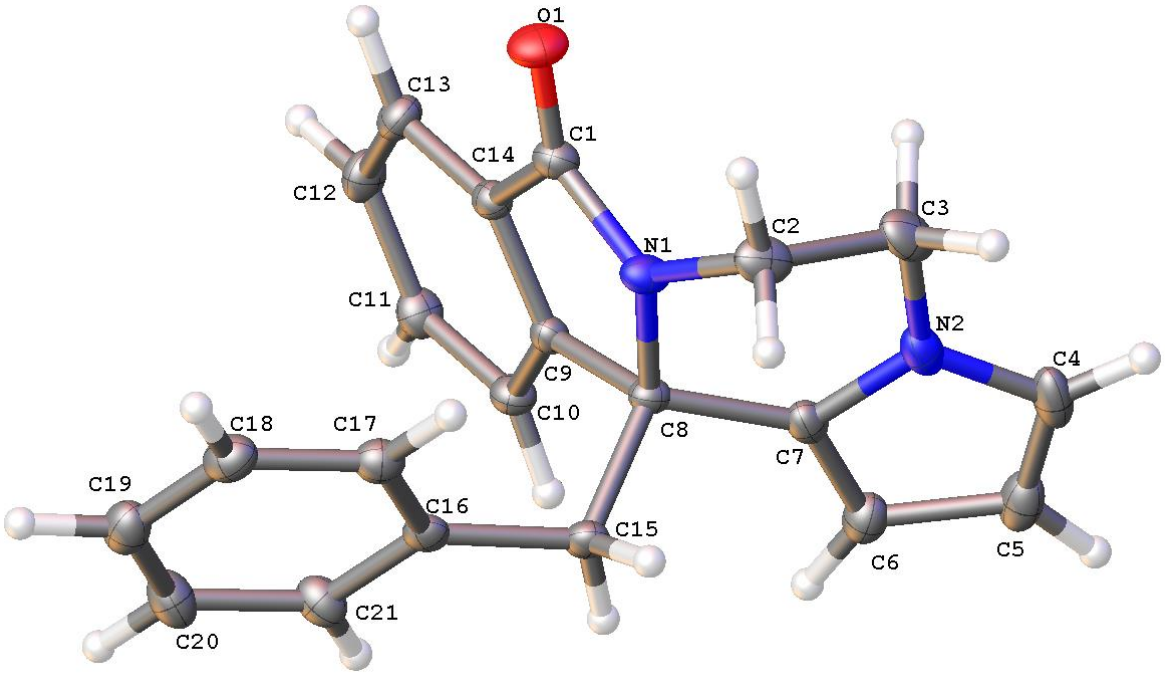


Table 1 Crystal data and structure refinement for 22srv006.	
Identification code	22srv006
Empirical formula	$C_{21}H_{18}N_2O$
Formula weight	314.37
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.0288(5)
b/Å	7.4406(2)
c/Å	15.8296(5)
α/°	90
β/°	100.0890(10)
γ/°	90
Volume/Å^3	1626.79(9)
Z	4
ρ_{calc}g/cm^3	1.284
μ/mm^{-1}	0.080

F(000)	664.0
Crystal size/mm^3	0.17 × 0.11 × 0.09
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.228 to 60
Index ranges	-19 ≤ h ≤ 19, -10 ≤ k ≤ 10, -22 ≤ l ≤ 22
Reflections collected	28536
Independent reflections	4725 [R_{int} = 0.0401, R_{sigma} = 0.0287]
Data/restraints/parameters	4725/0/289
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0473, wR_2 = 0.1132
Final R indexes [all data]	R_1 = 0.0550, wR_2 = 0.1178
Largest diff. peak/hole / e $Å^{-3}$	0.37/-0.23

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 22srv006. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	7693.5(7)	1105.8(11)	3711.3(6)	25.1(2)
N1	8340.1(7)	3736.0(12)	3290.9(6)	17.61(19)
N2	10093.3(7)	5304.1(15)	3837.2(6)	21.2(2)
C1	7757.0(8)	2748.1(15)	3719.7(7)	17.4(2)
C2	9170.7(9)	2986.5(17)	2984.0(8)	23.2(2)
C3	10068.4(9)	3385.2(18)	3642.1(9)	26.3(3)
C4	10905.6(9)	6284(2)	4150.0(8)	26.2(3)
C5	10631.0(9)	8006(2)	4286.8(8)	26.3(3)
C6	9605.4(9)	8089.1(17)	4049.1(8)	22.0(2)
C7	9292.6(8)	6392.2(15)	3784.0(7)	17.3(2)
C8	8293.8(8)	5686.6(14)	3433.8(7)	15.0(2)
C9	7588.6(7)	5772.7(14)	4059.8(7)	14.4(2)
C10	7271.3(8)	7244.8(15)	4470.3(7)	17.7(2)
C11	6628.1(8)	6929.0(16)	5033.8(8)	20.2(2)
C12	6310.1(8)	5197.8(17)	5179.3(8)	21.3(2)
C13	6620.5(8)	3732.0(16)	4757.1(8)	19.8(2)
C14	7259.1(8)	4059.5(14)	4195.9(7)	15.3(2)
C15	7893.0(8)	6660.2(16)	2575.4(7)	17.8(2)
C16	6866.6(8)	6188.7(15)	2183.9(7)	17.0(2)
C17	6640.2(9)	4580.8(16)	1737.1(7)	20.4(2)
C18	5685.5(9)	4189.5(17)	1372.5(8)	23.6(2)
C19	4951.6(9)	5398.5(19)	1443.8(8)	25.1(3)

C20	5169.8(9)	6997.0(19)	1883.7(8)	25.7(3)
C21	6124.1(9)	7385.7(17)	2253.3(8)	21.8(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv006. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	33.3(5)	13.3(4)	29.6(5)	-0.2(3)	7.9(4)	-0.2(3)
N1	22.1(4)	13.9(4)	18.1(4)	0.9(3)	6.8(3)	3.4(3)
N2	16.7(4)	29.0(5)	18.3(5)	4.2(4)	4.3(3)	5.5(4)
C1	20.0(5)	15.8(5)	15.9(5)	1.2(4)	2.0(4)	1.1(4)
C2	29.3(6)	21.3(5)	21.8(6)	-0.2(4)	12.3(5)	6.6(5)
C3	24.6(6)	28.1(6)	28.2(6)	4.4(5)	10.2(5)	12.3(5)
C4	15.2(5)	45.7(8)	17.0(5)	4.5(5)	0.9(4)	2.3(5)
C5	20.1(5)	41.0(7)	17.1(5)	-0.3(5)	1.2(4)	-7.5(5)
C6	19.7(5)	25.8(6)	20.4(5)	0.1(4)	3.0(4)	-3.1(4)
C7	15.6(5)	21.6(5)	15.1(5)	3.2(4)	3.9(4)	2.3(4)
C8	16.5(5)	13.0(4)	15.9(5)	1.6(4)	4.0(4)	1.3(4)
C9	13.9(4)	15.6(5)	13.6(4)	2.1(4)	2.0(3)	1.1(4)
C10	19.7(5)	14.4(5)	18.9(5)	0.6(4)	3.1(4)	1.3(4)
C11	19.6(5)	21.4(5)	19.9(5)	-2.9(4)	4.6(4)	2.7(4)
C12	17.5(5)	27.2(6)	20.4(5)	-1.0(4)	7.1(4)	-1.9(4)
C13	18.5(5)	20.3(5)	20.8(5)	0.9(4)	4.1(4)	-4.6(4)
C14	15.5(5)	14.5(5)	15.2(5)	0.6(4)	0.8(4)	-0.1(4)
C15	19.4(5)	17.8(5)	15.9(5)	4.4(4)	2.7(4)	-1.3(4)
C16	20.0(5)	17.8(5)	13.2(4)	3.8(4)	3.1(4)	0.1(4)
C17	23.5(5)	19.5(5)	18.7(5)	1.0(4)	4.8(4)	0.5(4)
C18	27.5(6)	21.7(6)	21.0(5)	-0.1(4)	2.4(4)	-5.2(5)
C19	21.4(5)	32.8(7)	20.2(5)	2.7(5)	1.2(4)	-3.6(5)
C20	21.6(5)	33.0(7)	21.8(6)	-0.5(5)	1.7(4)	6.8(5)
C21	23.6(5)	22.9(6)	17.7(5)	-1.9(4)	0.7(4)	3.8(4)

Table 4 Bond Lengths for 22srv006.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
O1	C1	1.2251(14)		C8	C15	1.5555(15)
N1	C1	1.3655(14)		C9	C10	1.3862(15)
N1	C2	1.4503(14)		C9	C14	1.3856(14)
N1	C8	1.4721(14)		C10	C11	1.3955(16)
N2	C3	1.4600(17)		C11	C12	1.3954(17)
N2	C4	1.3704(16)		C12	C13	1.3885(17)
N2	C7	1.3752(14)		C13	C14	1.3892(15)
C1	C14	1.4807(15)		C15	C16	1.5059(15)
C2	C3	1.5164(19)		C16	C17	1.3978(16)

C4	C5	1.366(2)		C16	C21	1.3894(16)
C5	C6	1.4233(17)		C17	C18	1.3932(17)
C6	C7	1.3777(17)		C18	C19	1.3867(19)
C7	C8	1.5081(15)		C19	C20	1.3851(19)
C8	C9	1.5193(14)		C20	C21	1.3942(17)

Table 5 Bond Angles for 22srv006.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C2	123.09(10)		C7	C8	C15	109.23(9)
C1	N1	C8	114.08(9)		C9	C8	C15	111.91(9)
C2	N1	C8	119.36(9)		C10	C9	C8	129.66(10)
C4	N2	C3	125.76(10)		C14	C9	C8	109.61(9)
C4	N2	C7	109.12(11)		C14	C9	C10	120.72(10)
C7	N2	C3	125.02(10)		C9	C10	C11	117.60(10)
O1	C1	N1	125.47(11)		C10	C11	C12	121.47(11)
O1	C1	C14	128.53(11)		C13	C12	C11	120.63(11)
N1	C1	C14	105.99(9)		C12	C13	C14	117.50(11)
N1	C2	C3	108.30(10)		C9	C14	C1	109.10(9)
N2	C3	C2	108.84(10)		C9	C14	C13	122.06(10)
C5	C4	N2	108.46(11)		C13	C14	C1	128.65(10)
C4	C5	C6	107.39(11)		C16	C15	C8	115.10(9)
C7	C6	C5	107.10(11)		C17	C16	C15	121.58(10)
N2	C7	C6	107.92(10)		C21	C16	C15	119.62(10)
N2	C7	C8	120.93(10)		C21	C16	C17	118.80(11)
C6	C7	C8	131.06(10)		C18	C17	C16	120.34(11)
N1	C8	C7	109.67(9)		C19	C18	C17	120.29(12)
N1	C8	C9	101.13(8)		C20	C19	C18	119.74(11)
N1	C8	C15	110.11(9)		C19	C20	C21	120.04(12)
C7	C8	C9	114.50(9)		C16	C21	C20	120.79(11)

Table 6 Torsion Angles for 22srv006.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
O1	C1	C14	C9	176.36(11)		C7	N2	C3	C2	28.17(15)
O1	C1	C14	C13	1.5(2)		C7	N2	C4	C5	-0.84(13)
N1	C1	C14	C9	-2.18(12)		C7	C8	C9	C10	59.25(15)
N1	C1	C14	C13	-177.05(11)		C7	C8	C9	C14	-120.71(10)
N1	C2	C3	N2	-51.65(13)		C7	C8	C15	C16	-175.61(9)
N1	C8	C9	C10	177.07(11)		C8	N1	C1	O1	-178.36(11)
N1	C8	C9	C14	-2.89(11)		C8	N1	C1	C14	0.23(12)
N1	C8	C15	C16	63.90(12)		C8	N1	C2	C3	61.20(13)
N2	C4	C5	C6	0.08(14)		C8	C9	C10	C11	-178.69(10)
N2	C7	C8	N1	7.12(14)		C8	C9	C14	C1	3.22(12)

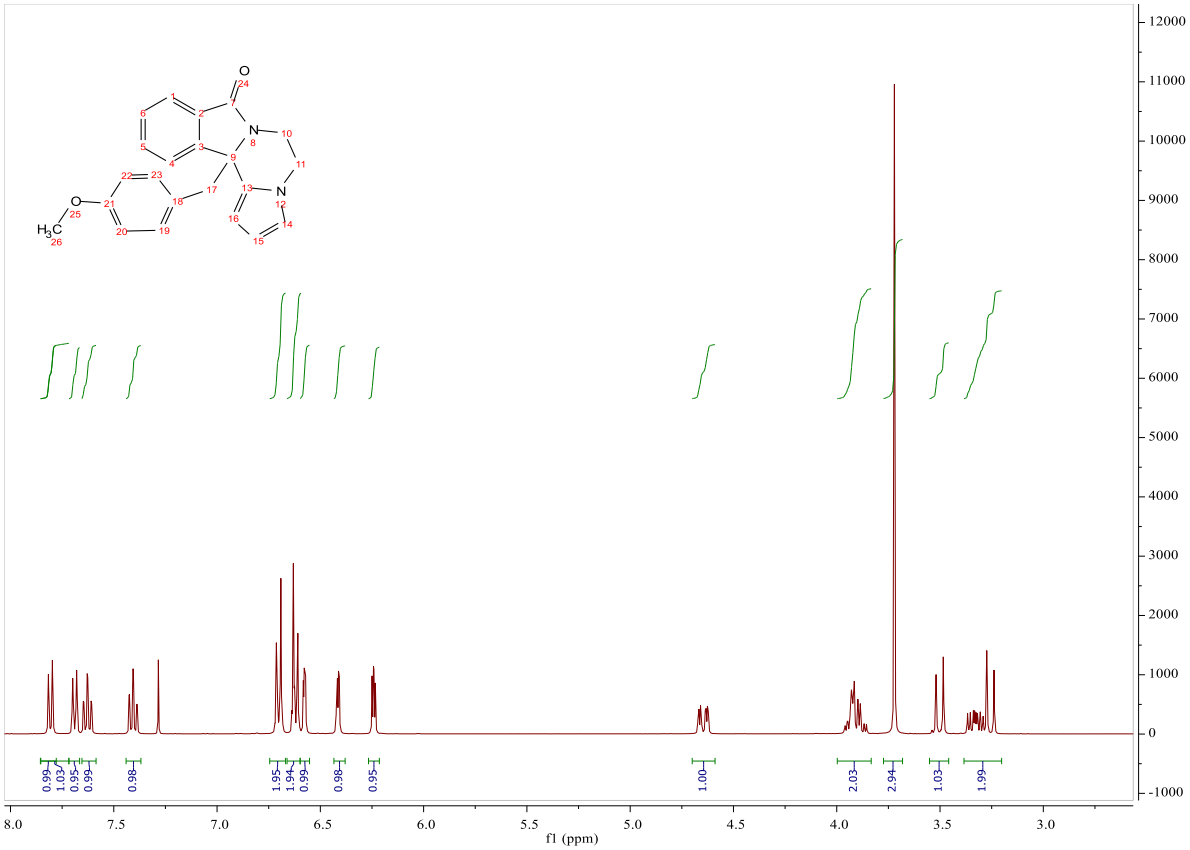
N2	C7	C8	C9	119.97(11)		C8	C9	C14	C13	178.50(10)
N2	C7	C8	C15	-113.64(11)		C8	C15	C16	C17	-77.77(13)
C1	N1	C2	C3	-96.51(13)		C8	C15	C16	C21	103.29(12)
C1	N1	C8	C7	122.84(10)		C9	C8	C15	C16	-47.74(13)
C1	N1	C8	C9	1.57(12)		C9	C10	C11	C12	-0.24(17)
C1	N1	C8	C15	-116.93(10)		C10	C9	C14	C1	-176.74(10)
C2	N1	C1	O1	-19.59(18)		C10	C9	C14	C13	-1.47(16)
C2	N1	C1	C14	159.00(10)		C10	C11	C12	C13	-0.64(18)
C2	N1	C8	C7	-36.78(13)		C11	C12	C13	C14	0.48(17)
C2	N1	C8	C9	-158.06(9)		C12	C13	C14	C1	174.84(11)
C2	N1	C8	C15	83.44(12)		C12	C13	C14	C9	0.56(17)
C3	N2	C4	C5	-177.23(11)		C14	C9	C10	C11	1.26(16)
C3	N2	C7	C6	177.71(11)		C15	C8	C9	C10	-65.75(14)
C3	N2	C7	C8	-5.45(16)		C15	C8	C9	C14	114.29(10)
C4	N2	C3	C2	-156.00(11)		C15	C16	C17	C18	-179.21(10)
C4	N2	C7	C6	1.29(13)		C15	C16	C21	C20	178.84(11)
C4	N2	C7	C8	178.13(10)		C16	C17	C18	C19	0.50(18)
C4	C5	C6	C7	0.70(14)		C17	C16	C21	C20	-0.13(17)
C5	C6	C7	N2	-1.21(13)		C17	C18	C19	C20	-0.34(19)
C5	C6	C7	C8	-177.62(11)		C18	C19	C20	C21	-0.04(19)
C6	C7	C8	N1	-176.86(11)		C19	C20	C21	C16	0.28(19)
C6	C7	C8	C9	-64.02(15)		C21	C16	C17	C18	-0.26(17)
C6	C7	C8	C15	62.38(15)						

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv006.

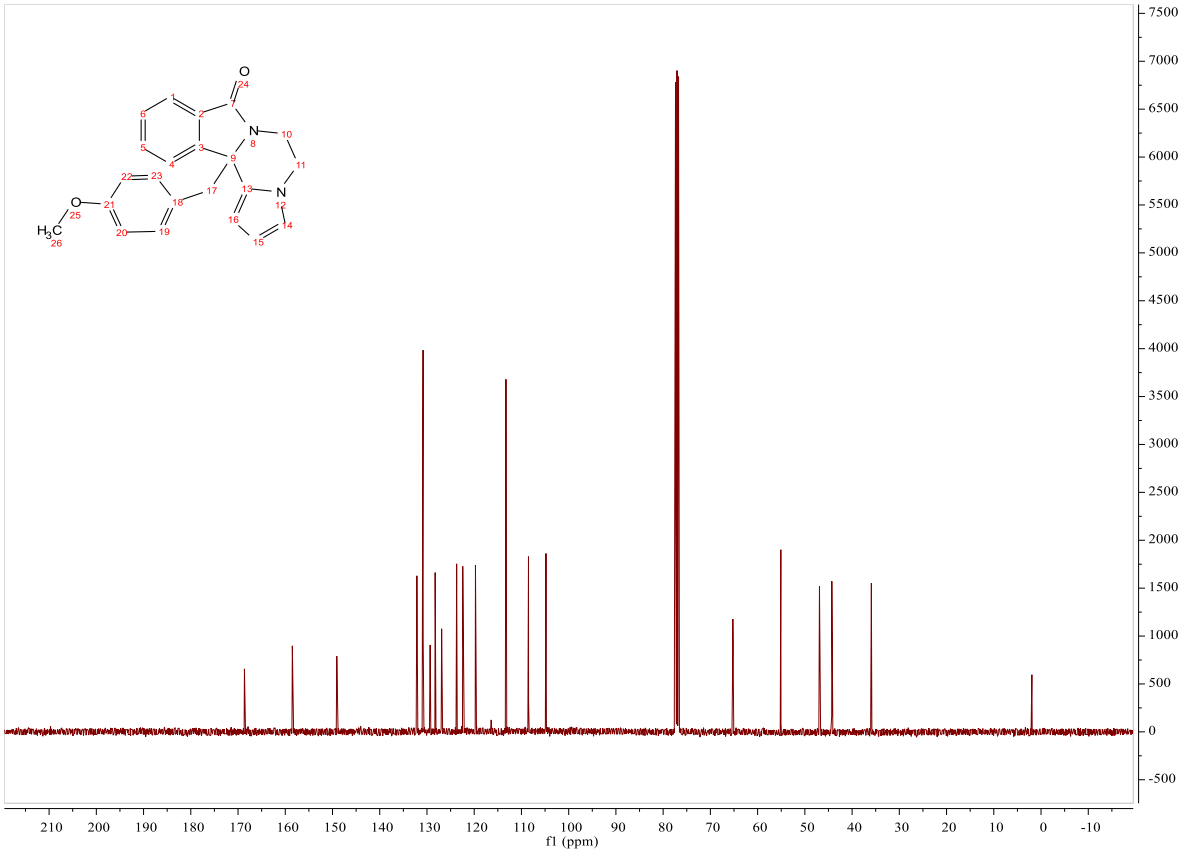
Atom	***x***	***y***	***z***	**U(eq)**
H2A	9219(11)	3550(20)	2425(10)	25(4)
H2B	9079(12)	1670(20)	2928(11)	34(4)
H3A	10068(11)	2660(20)	4170(11)	29(4)
H3B	10663(12)	3120(20)	3406(11)	32(4)
H4	11529(12)	5730(20)	4226(11)	33(4)
H5	11071(13)	8980(30)	4509(12)	40(5)
H6	9183(12)	9140(20)	4071(11)	36(4)
H10	7468(12)	8480(20)	4358(11)	28(4)
H11	6402(11)	7930(20)	5343(10)	24(4)
H12	5874(11)	5010(20)	5579(10)	26(4)
H13	6416(11)	2510(20)	4855(10)	26(4)
H15A	7952(10)	7950(20)	2690(10)	21(4)
H15B	8343(11)	6360(20)	2178(10)	24(4)
H17	7147(12)	3730(20)	1660(11)	30(4)
H18	5517(12)	3080(20)	1070(11)	34(4)
H19	4269(12)	5110(20)	1201(11)	33(4)
H20	4649(13)	7840(20)	1942(11)	35(4)
H21	6297(11)	8520(20)	2550(10)	23(4)

12*b*-(4-methoxybenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1b**

^{1}H:



^{13}C:



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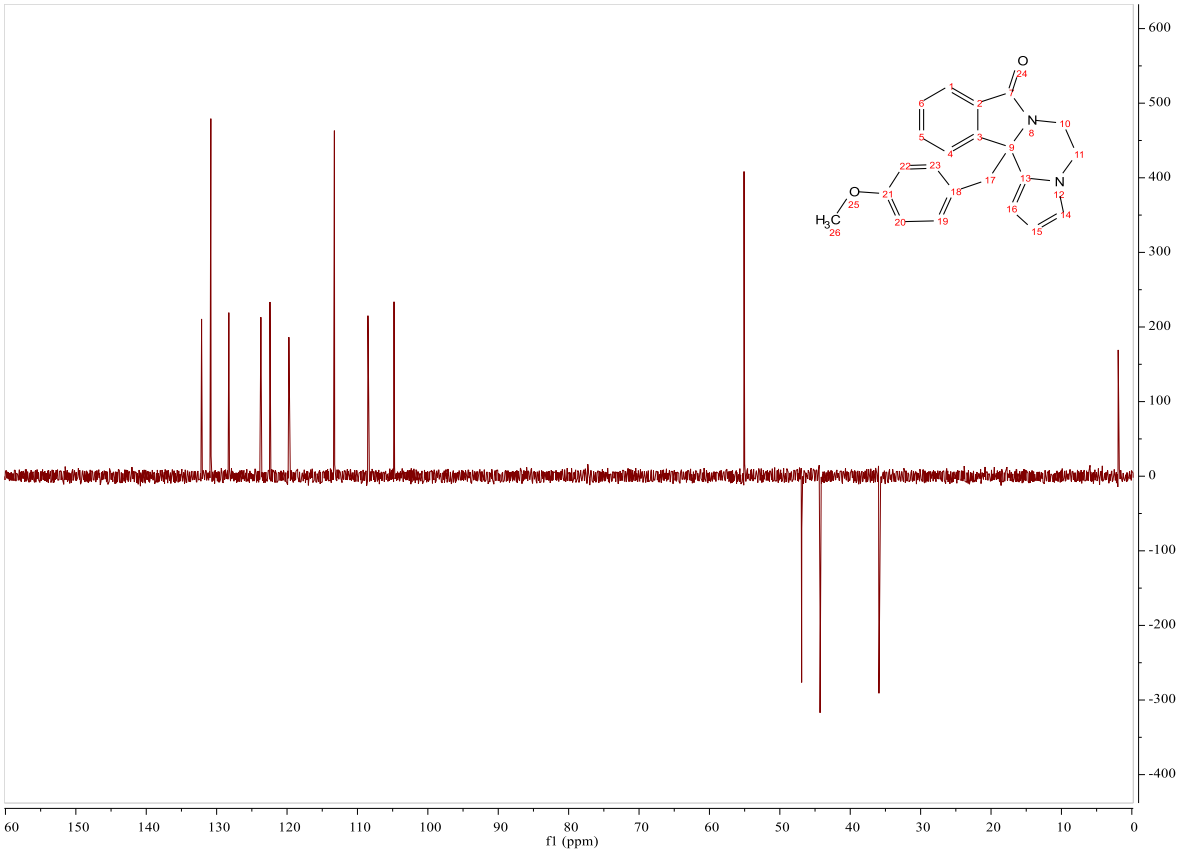
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500
400
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200
100
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-100
-200
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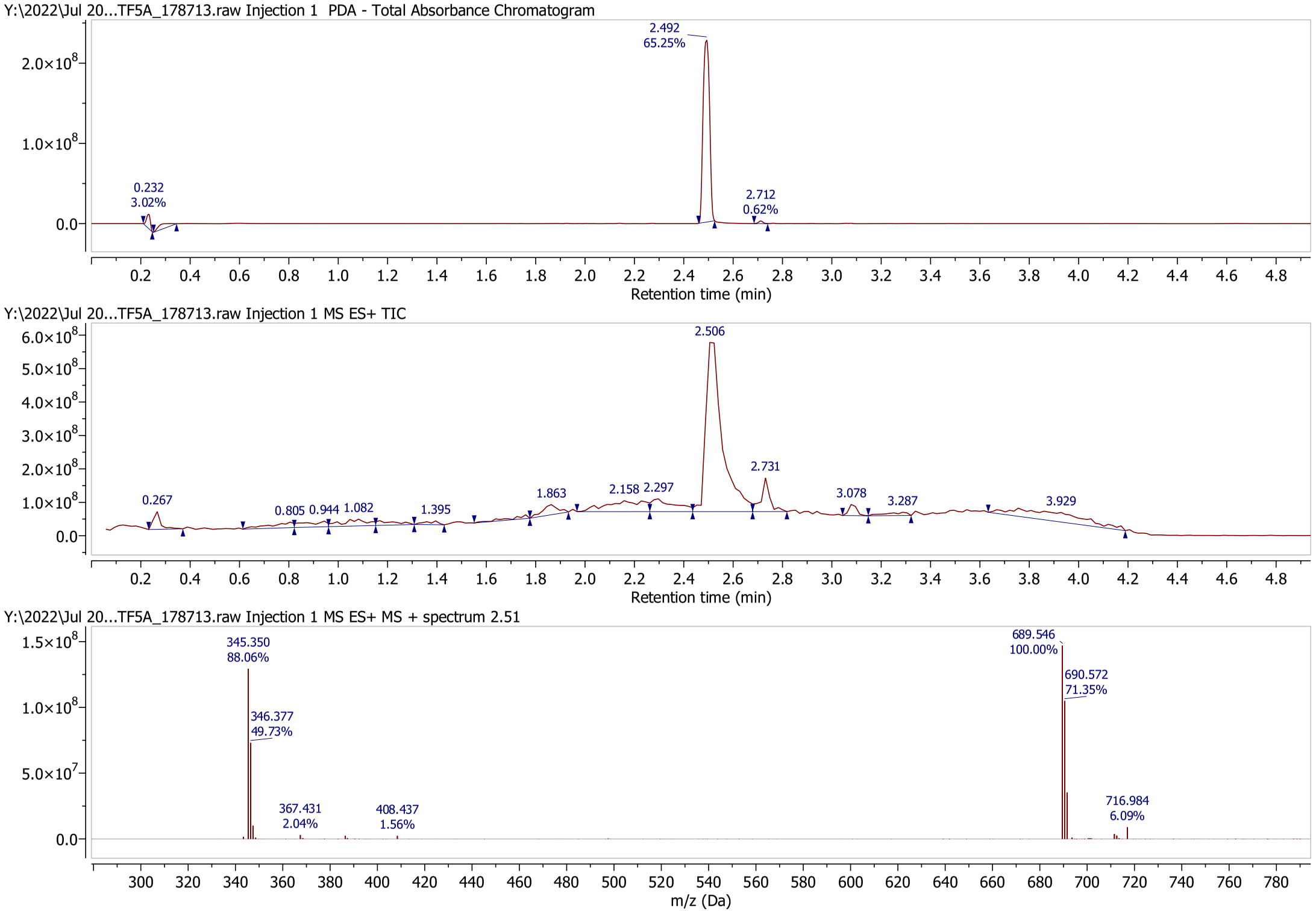
70
60
50
40
30
20
10
0
f1 (ppm)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65.25%
0.232
3.02%
2.712
0.62%
Retention time (min)
Y:\2022\Jul 20...TF5A_178713.raw Injection 1 MS ES+ TIC
2.506
2.731
0.267
0.805 0.944 1.082
1.395
1.863
2.158 2.297
3.078
3.287
3.929
Retention time (min)
Y:\2022\Jul 20...TF5A_178713.raw Injection 1 MS ES+ MS + spectrum 2.51
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88.06%
346.377
49.73%
367.431
2.04%
408.437
1.56%
689.546
100.00%
690.572
71.35%
716.984
6.09%
m/z (Da)

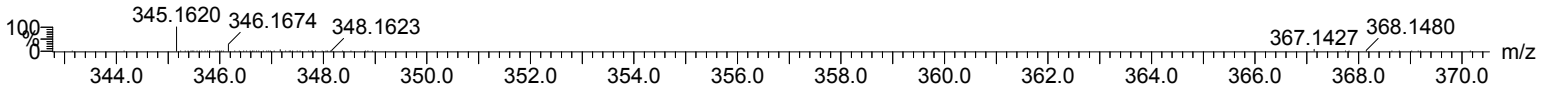
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
520 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10

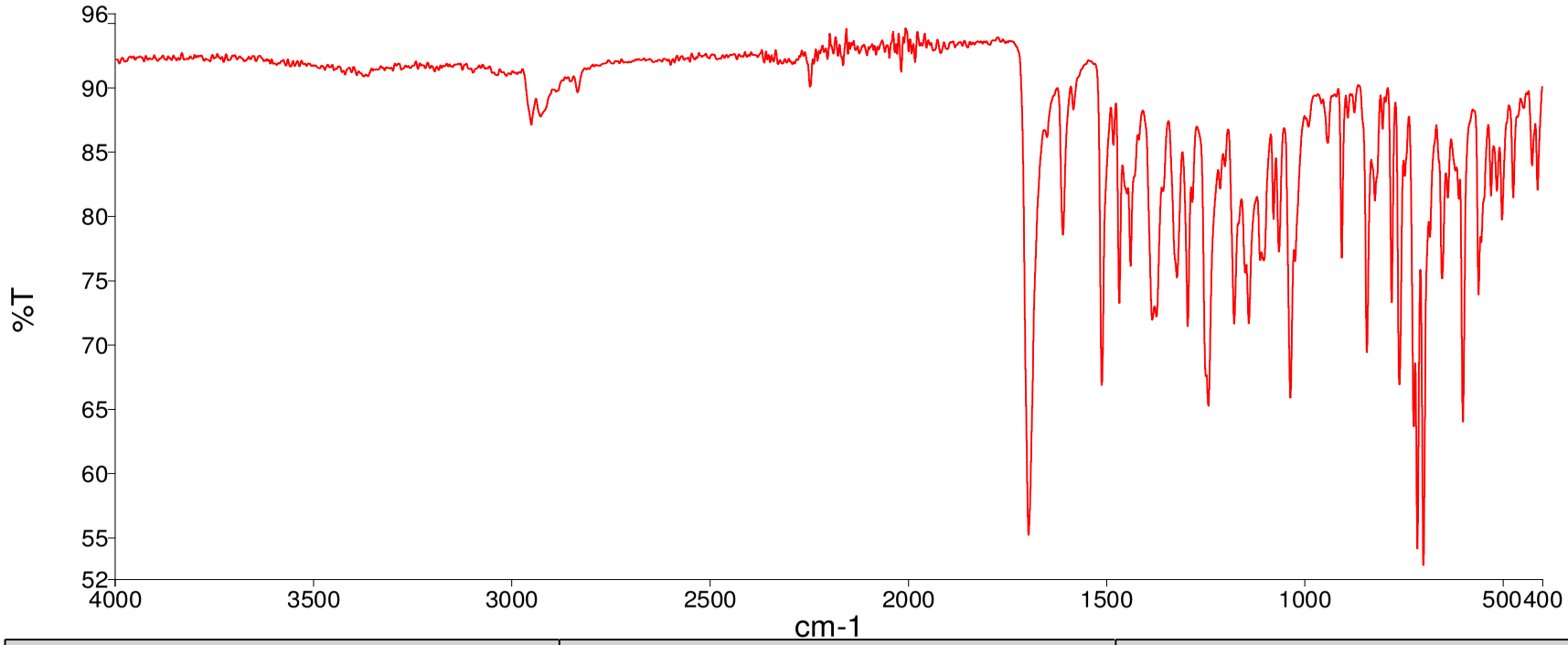
21-Jul-2022
MTF_MTF5A_179339 496 (4.170) Cm (496:497)

21-Jul-2022
1: TOF MS ES+
7.95e+004



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
345.1620	345.1622	-0.2	-0.6	0.5	556.0	10.556	0.00	C10 H25 N4 O9
	345.1635	-1.5	-4.3	5.5	554.7	9.247	0.01	C11 H21 N8 O5
	345.1603	1.7	4.9	13.5	546.7	1.264	28.24	C22 H21 N2 O2
	345.1643	-2.3	-6.7	17.5	545.8	0.332	71.74	C27 H21
	345.1595	2.5	7.2	1.5	558.0	12.600	0.00	C6 H21 N10 O7

Analyst Lenny Lauchlan
Date 22 June 2022 08:08



Sample Name	Description	Quality Checks
MTF 005A	Sample 017 By Lenny Date Wednesday, June 22 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

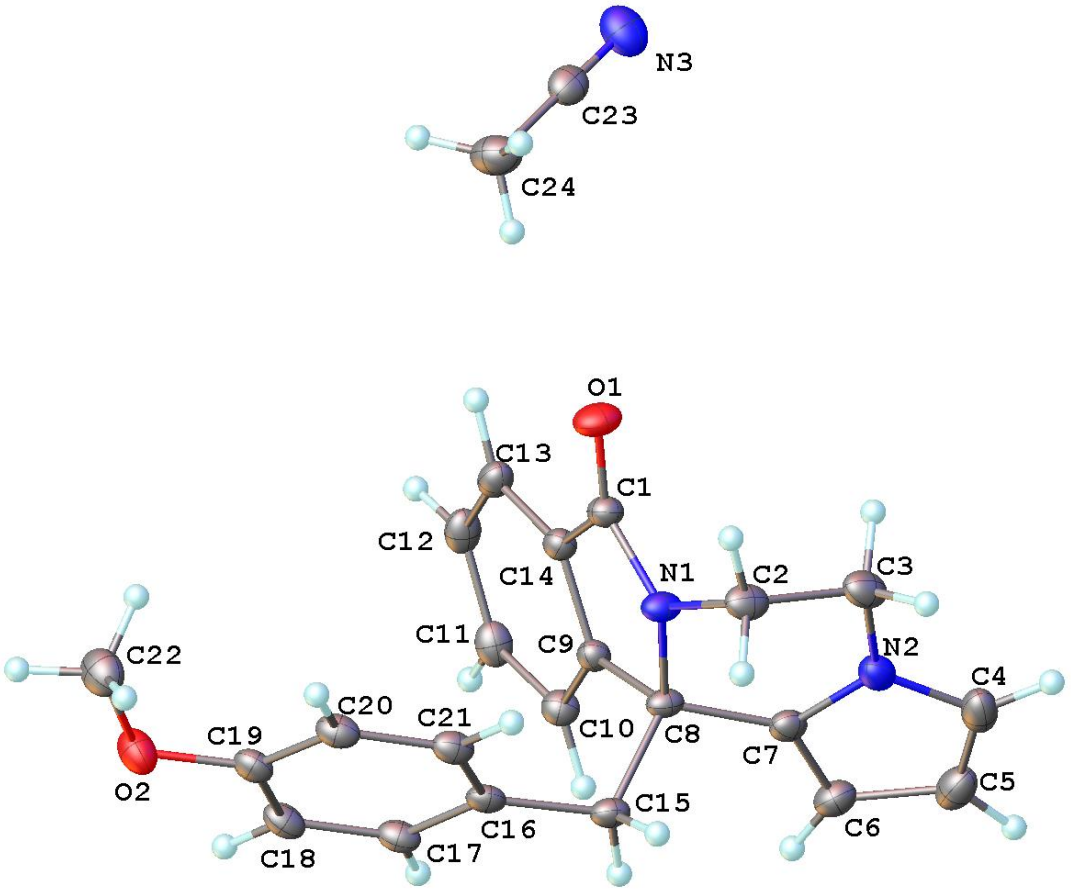


Table 1 Crystal data and structure refinement for 22srv059.	
Identification code	22srv059
Empirical formula	$C_{24}H_{23}N_3O_2$
Formula weight	385.45
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.8742(4)
b/Å	19.0273(8)
c/Å	10.9252(5)
α/°	90
β/°	107.0305(15)
γ/°	90
Volume/Å^3	1962.61(15)

Z	4
ρ_{calc}g/cm^3	1.305
μ/mm^{-1}	0.084
F(000)	816.0
Crystal size/mm^3	0.26 × 0.17 × 0.15
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.314 to 59.988
Index ranges	-13 ≤ h ≤ 13, -26 ≤ k ≤ 26, -15 ≤ l ≤ 15
Reflections collected	41640
Independent reflections	5706 [R_{int} = 0.0381, R_{sigma} = 0.0252]
Data/restraints/parameters	5706/0/354
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0429, wR_2 = 0.1021
Final R indexes [all data]	R_1 = 0.0528, wR_2 = 0.1075
Largest diff. peak/hole / e Å^{-3}	0.36/-0.23

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 22srv059. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	3649.9(9)	4372.3(4)	6017.9(8)	26.81(19)
O2	324.8(9)	6661.9(5)	1545.9(8)	26.79(19)
N1	4286.5(9)	5476.3(5)	6864.6(9)	18.36(18)
N2	5787.4(10)	5751.2(5)	9322.9(9)	21.76(19)
C1	3370.1(11)	4925.4(5)	6462.1(10)	18.3(2)
C2	5812.0(11)	5404.3(6)	7182.0(12)	22.7(2)
C3	6398.5(12)	5256.4(6)	8607.5(12)	25.7(2)
C4	6356.4(13)	5920.3(7)	10592.3(12)	28.3(3)
C5	5489.0(14)	6401.3(7)	10916.7(12)	29.2(3)
C6	4347.8(13)	6534.8(6)	9803.1(11)	24.4(2)
C7	4549.5(11)	6122.9(5)	8833.4(11)	19.0(2)
C8	3705.7(10)	6056.4(5)	7444.1(10)	16.69(19)
C9	2203.6(10)	5801.5(5)	7259.9(10)	16.20(19)
C10	1084.0(11)	6132.8(6)	7554.8(10)	19.7(2)
C11	-205.5(11)	5777.2(6)	7278.9(11)	22.9(2)
C12	-367.7(12)	5108.3(6)	6738.0(11)	23.6(2)
C13	750.0(12)	4780.5(6)	6434.7(10)	21.4(2)

C14	2022.4(11)	5144.1(5)	6689.9(10)	16.84(19)
C15	3748.1(11)	6759.0(5)	6725.9(11)	19.0(2)
C16	2895.4(11)	6746.7(5)	5336.7(10)	17.9(2)
C17	1519.9(11)	7021.4(5)	4945.9(11)	20.0(2)
C18	702.3(12)	6992.7(6)	3678.9(11)	21.2(2)
C19	1240.9(12)	6682.5(5)	2763.5(10)	20.0(2)
C20	2621.9(12)	6425.9(6)	3119.2(11)	20.8(2)
C21	3432.2(11)	6459.2(5)	4398.9(11)	19.9(2)
C22	677.2(15)	6205.4(7)	655.4(12)	30.8(3)
N3	2464.0(12)	1979.7(6)	6648.1(11)	32.9(2)
C23	2511.2(12)	2345.1(6)	5831.1(11)	23.7(2)
C24	2535.7(17)	2818.4(7)	4796.6(14)	33.3(3)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 22srv059. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	29.1(4)	18.0(4)	34.7(5)	-7.6(3)	11.6(4)	0.0(3)
O2	28.6(4)	30.2(4)	21.7(4)	4.4(3)	7.6(3)	8.4(3)
N1	16.2(4)	13.9(4)	26.2(5)	-2.9(3)	8.2(3)	0.5(3)
N2	19.1(4)	18.8(4)	25.6(5)	2.9(4)	3.8(4)	-0.9(3)
C1	19.9(5)	14.8(4)	20.1(5)	-0.4(4)	5.8(4)	-0.1(4)
C2	16.0(5)	19.8(5)	33.9(6)	-1.6(4)	9.7(4)	1.8(4)
C3	18.2(5)	20.6(5)	37.3(6)	1.9(5)	6.8(5)	2.6(4)
C4	26.4(6)	28.6(6)	25.3(6)	6.5(5)	0.6(5)	-5.9(5)
C5	33.8(6)	29.6(6)	22.7(6)	-1.3(5)	5.7(5)	-10.0(5)
C6	26.0(5)	21.1(5)	26.0(6)	-4.1(4)	7.8(4)	-4.0(4)
C7	16.9(5)	15.6(4)	24.3(5)	-0.6(4)	5.5(4)	-2.6(4)
C8	15.4(4)	12.9(4)	22.9(5)	-2.8(4)	7.2(4)	-0.5(3)
C9	16.0(4)	15.0(4)	17.7(5)	1.4(4)	5.1(4)	-1.0(3)
C10	19.6(5)	19.9(5)	20.9(5)	-0.2(4)	8.0(4)	0.9(4)
C11	17.8(5)	30.9(6)	21.4(5)	3.9(4)	8.2(4)	1.1(4)
C12	17.8(5)	30.2(6)	22.0(5)	4.0(4)	4.6(4)	-6.1(4)
C13	22.5(5)	20.4(5)	19.6(5)	1.2(4)	3.7(4)	-5.4(4)
C14	18.1(5)	15.3(4)	16.9(4)	1.3(4)	4.9(4)	-0.4(4)
C15	19.0(5)	13.6(4)	25.3(5)	-1.8(4)	8.0(4)	-1.6(4)
C16	19.3(5)	11.7(4)	24.4(5)	1.5(4)	9.0(4)	-1.1(3)
C17	22.4(5)	15.5(4)	25.6(5)	2.0(4)	12.5(4)	3.1(4)
C18	19.7(5)	18.8(5)	27.6(6)	5.8(4)	10.9(4)	4.9(4)
C19	23.0(5)	16.3(5)	22.2(5)	5.1(4)	9.3(4)	1.6(4)
C20	23.4(5)	17.3(5)	25.6(5)	1.5(4)	13.5(4)	2.7(4)
C21	17.1(5)	16.4(5)	28.2(5)	1.6(4)	10.1(4)	1.0(4)
C22	36.3(7)	33.8(7)	23.0(6)	1.3(5)	9.6(5)	5.7(5)
N3	31.1(6)	36.6(6)	33.6(6)	4.9(5)	13.4(5)	9.9(5)
C23	19.0(5)	24.2(5)	28.1(6)	-3.9(4)	7.0(4)	3.2(4)
C24	44.2(8)	23.7(6)	33.8(7)	-0.1(5)	14.3(6)	-2.9(5)

Table 4 Bond Lengths for 22srv059.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
O1	C1	1.2239(13)		C8	C15	1.5568(15)
O2	C19	1.3728(14)		C9	C10	1.3900(14)
O2	C22	1.4213(15)		C9	C14	1.3853(14)
N1	C1	1.3703(13)		C10	C11	1.3948(15)
N1	C2	1.4499(13)		C11	C12	1.3925(17)
N1	C8	1.4700(13)		C12	C13	1.3896(17)
N2	C3	1.4619(15)		C13	C14	1.3891(14)
N2	C4	1.3734(15)		C15	C16	1.5049(15)
N2	C7	1.3775(14)		C16	C17	1.4001(14)
C1	C14	1.4833(14)		C16	C21	1.3958(15)
C2	C3	1.5204(17)		C17	C18	1.3843(16)
C4	C5	1.3691(19)		C18	C19	1.3939(15)
C5	C6	1.4183(17)		C19	C20	1.3922(15)
C6	C7	1.3783(16)		C20	C21	1.3941(16)
C7	C8	1.5078(15)		N3	C23	1.1432(16)
C8	C9	1.5169(14)		C23	C24	1.4508(18)

Table 5 Bond Angles for 22srv059.								
Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C19	O2	C22	117.18(9)		C9	C8	C15	112.17(8)
C1	N1	C2	123.14(9)		C10	C9	C8	129.59(9)
C1	N1	C8	114.10(8)		C14	C9	C8	109.93(9)
C2	N1	C8	118.49(8)		C14	C9	C10	120.47(9)
C4	N2	C3	125.45(10)		C9	C10	C11	117.87(10)
C4	N2	C7	109.01(10)		C12	C11	C10	121.29(10)
C7	N2	C3	125.54(10)		C13	C12	C11	120.72(10)
O1	C1	N1	125.49(10)		C14	C13	C12	117.60(10)
O1	C1	C14	128.72(10)		C9	C14	C1	108.94(9)
N1	C1	C14	105.79(8)		C9	C14	C13	122.01(10)
N1	C2	C3	108.65(9)		C13	C14	C1	129.03(10)
N2	C3	C2	109.60(9)		C16	C15	C8	113.91(8)
C5	C4	N2	108.43(11)		C17	C16	C15	120.53(9)
C4	C5	C6	107.32(11)		C21	C16	C15	121.73(9)
C7	C6	C5	107.47(11)		C21	C16	C17	117.74(10)
N2	C7	C6	107.76(10)		C18	C17	C16	121.32(10)
N2	C7	C8	120.91(9)		C17	C18	C19	120.05(10)
C6	C7	C8	131.29(10)		O2	C19	C18	115.20(10)
N1	C8	C7	109.04(8)		O2	C19	C20	125.03(10)
N1	C8	C9	101.09(8)		C20	C19	C18	119.78(10)
N1	C8	C15	110.88(8)		C19	C20	C21	119.44(10)

C7	C8	C9	113.01(8)		C20	C21	C16	121.61(10)
C7	C8	C15	110.29(8)		N3	C23	C24	178.42(13)

Table 6 Torsion Angles for 22srv059.

A	B	C	D	Angle/˚		A	B	C	D	Angle/˚
N1	C2	C3	N2	-47.52(12)		C8	C15	C16	C17	97.40(11)
N1	C8	C7	N2	9.57(13)		C8	C15	C16	C21	-82.04(12)
C1	C14	C9	C8	-0.07(11)		C9	C8	N1	C1	-3.72(11)
C1	C14	C9	C10	178.87(9)		C9	C8	N1	C2	-161.27(9)
C2	N1	C1	O1	-19.42(17)		C9	C8	C7	N2	121.15(10)
C2	C3	N2	C4	-159.09(10)		C9	C8	C15	C16	-51.40(12)
C2	C3	N2	C7	20.89(15)		C9	C14	C1	O1	177.36(11)
C3	C2	N1	C1	-92.16(12)		C9	C14	C1	N1	-2.22(11)
C3	C2	N1	C8	63.23(12)		C10	C9	C8	N1	-176.69(10)
C6	C7	N2	C3	-179.39(10)		C10	C9	C8	C15	-58.52(14)
C6	C7	N2	C4	0.60(12)		C10	C9	C14	C13	-2.42(16)
C6	C7	C8	N1	-173.07(11)		C13	C14	C1	O1	-1.23(19)
C6	C7	C8	C9	-61.50(15)		C13	C14	C1	N1	179.20(11)
C6	C7	C8	C15	64.96(14)		C14	C1	N1	C2	160.17(10)
C7	C8	N1	C1	115.56(10)		C14	C1	N1	C8	3.81(12)
C7	C8	N1	C2	-41.98(12)		C14	C9	C8	N1	2.13(11)
C7	C8	C9	C10	66.92(14)		C14	C9	C8	C15	120.29(9)
C7	C8	C9	C14	-114.26(10)		C15	C8	N1	C1	-122.82(10)
C7	C8	C15	C16	-178.32(9)		C15	C8	N1	C2	79.63(11)
C8	N1	C1	O1	-175.78(10)		C15	C8	C7	N2	-112.40(10)
C8	C7	N2	C3	-1.47(16)		C16	C15	C8	N1	60.79(11)
C8	C7	N2	C4	178.51(9)		C18	C19	O2	C22	-164.78(10)
C8	C9	C14	C13	178.64(10)		C20	C19	O2	C22	15.62(16)

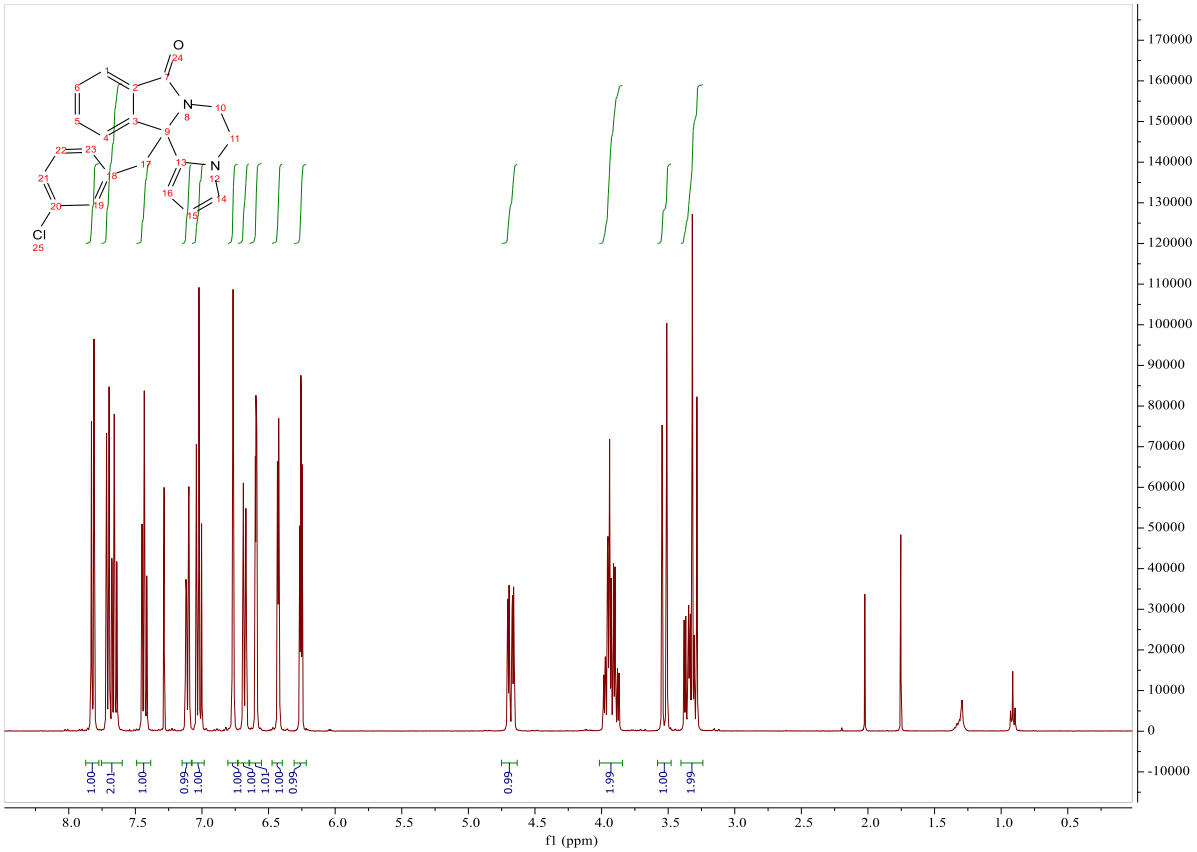
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv059.

Atom	*x*	*y*	*z*	U(eq)
H2A	6211(15)	5847(8)	6946(13)	25(3)
H2B	6035(15)	5027(8)	6693(13)	24(3)
H3A	6145(16)	4778(8)	8793(14)	32(4)
H3B	7434(17)	5313(8)	8904(15)	35(4)
H4	7242(17)	5710(8)	11091(15)	37(4)
H5	5651(17)	6607(9)	11764(16)	41(4)
H6	3576(17)	6859(8)	9717(15)	34(4)
H10	1198(15)	6603(8)	7951(14)	26(4)
H11	-1011(16)	6003(8)	7487(14)	32(4)
H12	-1281(16)	4874(8)	6549(14)	29(4)

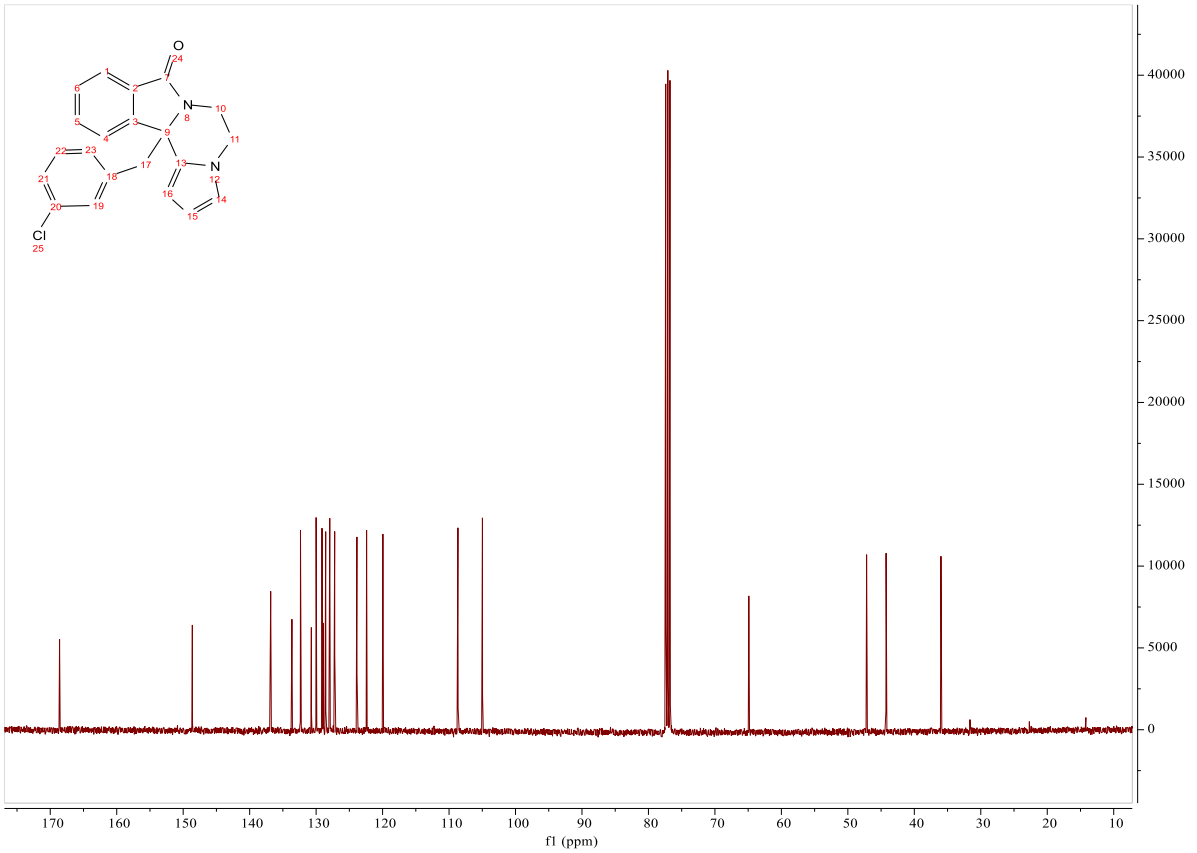
H13	660(15)	4308(8)	6074(14)	27(4)
H15A	3392(15)	7123(7)	7188(13)	23(3)
H15B	4743(16)	6865(8)	6829(13)	27(4)
H17	1127(15)	7231(7)	5556(13)	23(3)
H18	-240(16)	7181(7)	3410(13)	26(4)
H20	3029(15)	6221(8)	2469(14)	29(4)
H21	4396(16)	6277(8)	4631(14)	29(4)
H22A	791(17)	5722(9)	999(15)	36(4)
H22B	1534(18)	6352(9)	471(15)	37(4)
H22C	-117(18)	6235(8)	-150(16)	39(4)
H24A	2640(20)	3273(11)	5085(19)	57(5)
H24B	3420(30)	2735(13)	4570(20)	88(8)
H24C	1710(30)	2752(14)	4100(30)	101(9)

12*b*-(3-chlorobenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1c**

^{1}H:



^{13}C:



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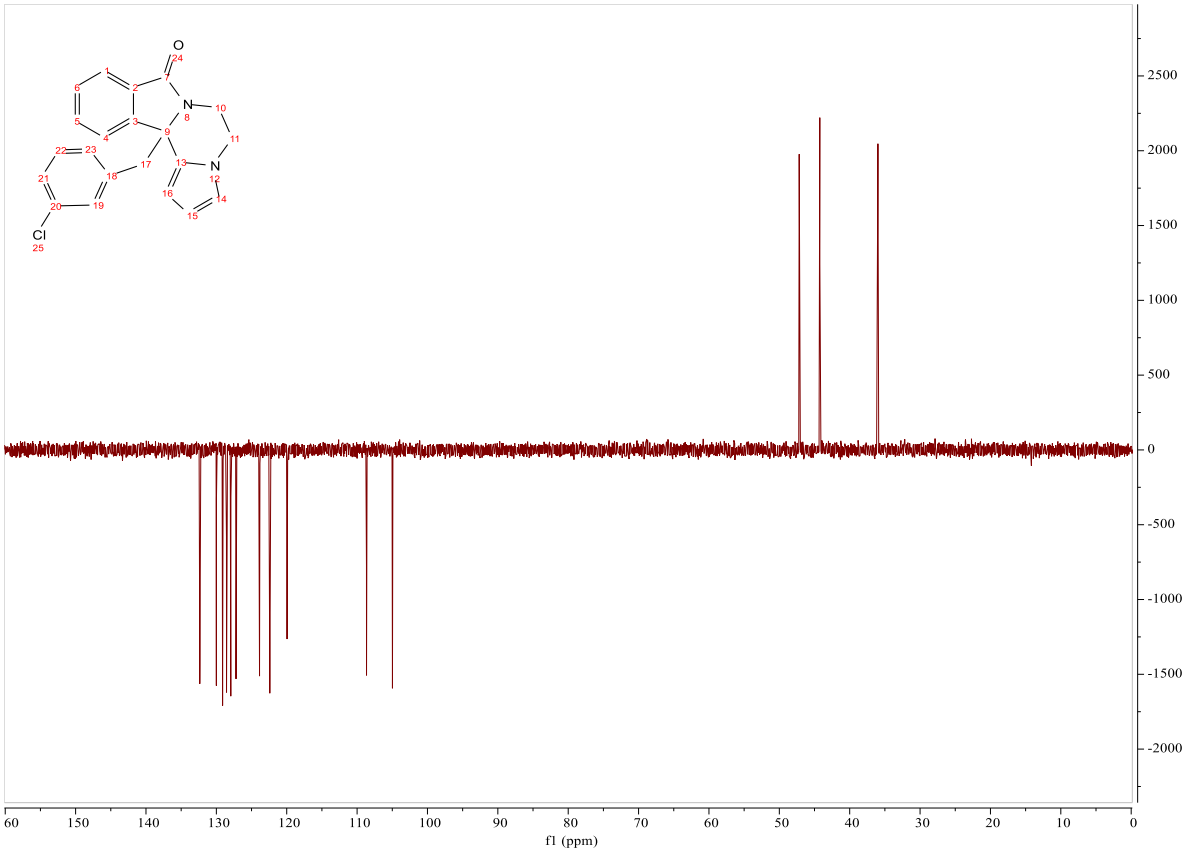
O
24
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2
6
7
N
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3
9
11
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22
23
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21
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17
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15
Cl
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2500
2000
1500
1000
500
0
-500
-1000
-1500
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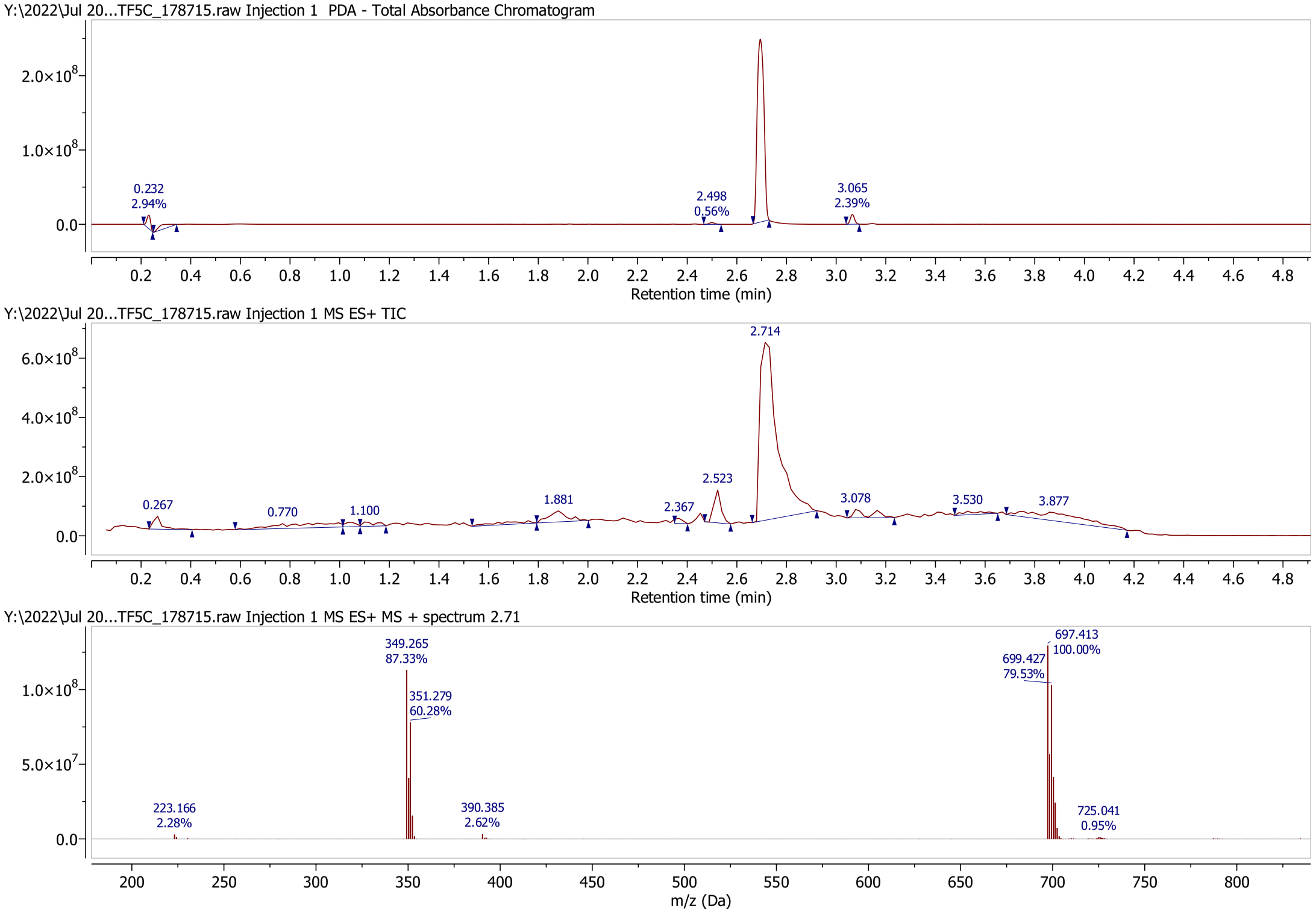
f1 (ppm)


Y:\2022\Jul 20...TF5C_178715.raw Injection 1 PDA - Total Absorbance Chromatogram
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2.498
0.56%
3.065
2.39%
Retention time (min)
Y:\2022\Jul 20...TF5C_178715.raw Injection 1 MS ES+ TIC
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2.523
0.267
0.770
1.100
1.881
2.367
3.078
3.530
3.877
Retention time (min)
Y:\2022\Jul 20...TF5C_178715.raw Injection 1 MS ES+ MS + spectrum 2.71
349.265
87.33%
351.279
60.28%
697.413
100.00%
699.427
79.53%
223.166
2.28%
390.385
2.62%
725.041
0.95%
m/z (Da)

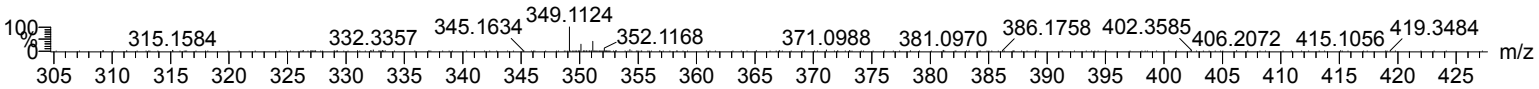
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
1468 formula(e) evaluated with 12 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 Cl: 0-2

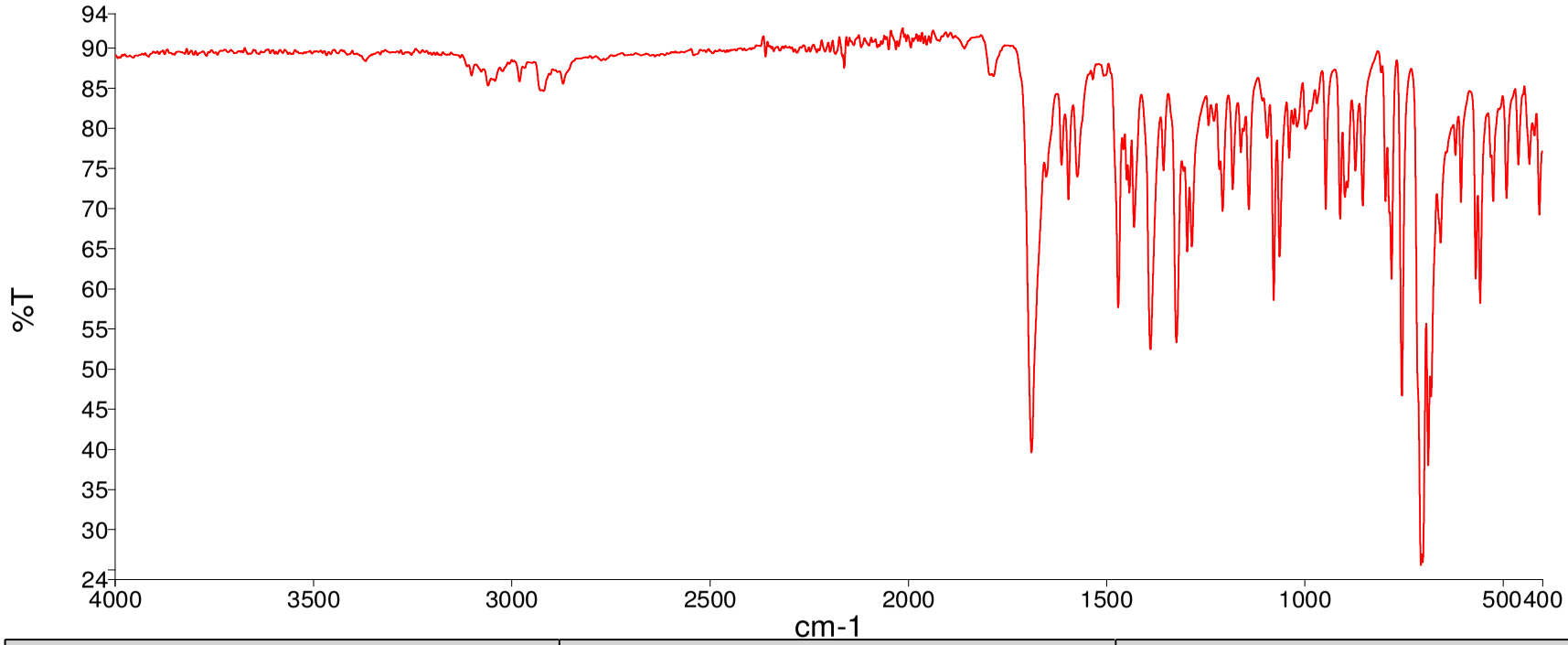
21-Jul-2022
MTF_MTF5C_179341 550 (4.621) Cm (550:552)

21-Jul-2022
1: TOF MS ES+
1.24e+003



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
349.1124	349.1108	1.6	4.6	5.5	186.7	19.248	0.00	C10 H17 N6 O8
	349.1140	-1.6	-4.6	5.5	175.7	8.319	0.02	C10 H18 N8 O4 Cl
	349.1121	0.3	0.9	10.5	186.4	18.963	0.00	C11 H13 N10 O4
	349.1135	-1.1	-3.2	4.5	187.2	19.748	0.00	C14 H21 O10
	349.1148	-2.4	-6.9	9.5	187.5	20.081	0.00	C15 H17 N4 O6
	349.1126	-0.2	-0.6	8.5	184.5	17.070	0.00	C20 H23 O Cl2
	349.1108	1.6	4.6	13.5	167.4	0.000	99.97	C21 H18 N2 O Cl
	349.1104	2.0	5.7	-8.5	187.0	19.577	0.00	C3 H27 N4 O10 Cl2
	349.1118	0.6	1.7	-3.5	186.6	19.206	0.00	C4 H23 N8 O6 Cl2
	349.1099	2.5	7.2	1.5	180.3	12.914	0.00	C5 H18 N10 O6 Cl
	349.1144	-2.0	-5.7	-4.5	185.2	17.784	0.00	C8 H27 N2 O8 Cl2
	349.1126	-0.2	-0.6	0.5	176.6	9.246	0.01	C9 H22 N4 O8 Cl

Analyst Lenny Lauchlan
Date 28 June 2022 12:48



Sample Name	Description	Quality Checks
MTF 005C	Sample 017 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

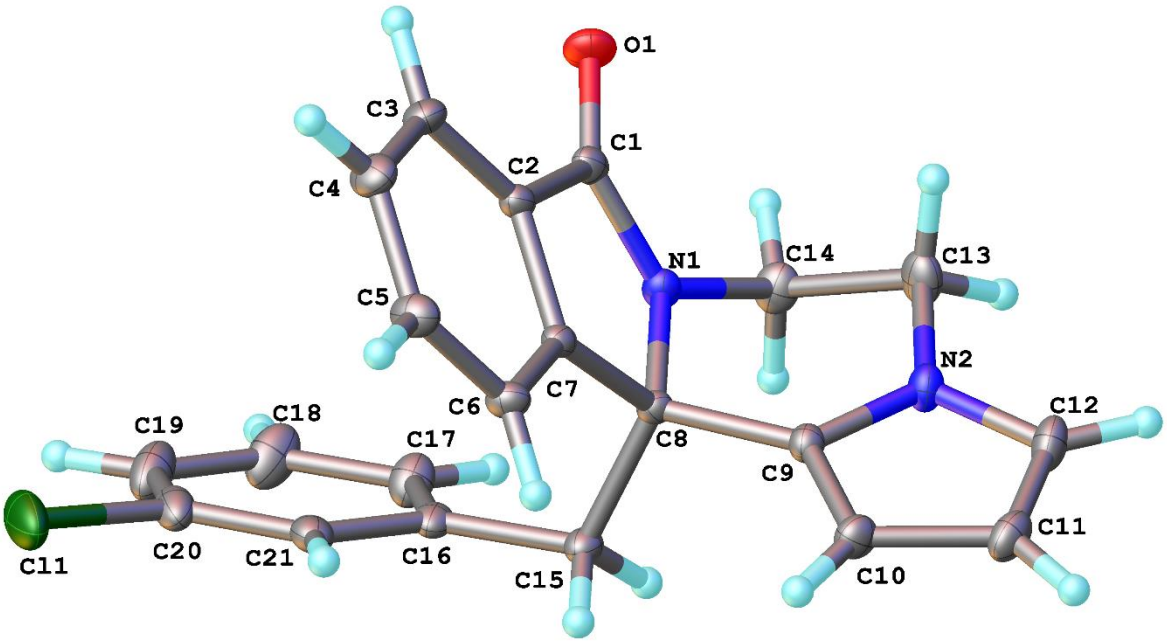


Table 1 Crystal data and structure refinement for 21srv468.	
Identification code	21srv468
Empirical formula	$C_{21}H_{17}ClN_2O$
Formula weight	348.82
Temperature/K	120.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.2495(4)
b/Å	9.5835(3)
c/Å	14.0702(4)
α/°	90
β/°	117.1379(9)
γ/°	90
Volume/Å^3	1709.90(9)
Z	4
ρ_{calc}g/cm^3	1.355
μ/mm^{-1}	0.234

F(000)	728.0
Crystal size/mm^3	0.25 × 0.18 × 0.15
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.426 to 59.982
Index ranges	-20 ≤ h ≤ 20, -13 ≤ k ≤ 13, -19 ≤ l ≤ 19
Reflections collected	28335
Independent reflections	4958 [R_{int} = 0.0303, R_{sigma} = 0.0222]
Data/restraints/parameters	4958/0/226
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0416, wR_2 = 0.1047
Final R indexes [all data]	R_1 = 0.0477, wR_2 = 0.1084
Largest diff. peak/hole / e $Å^{-3}$	0.93/-0.36

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 21srv468. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	3953.4(3)	8074.9(5)	2667.7(3)	36.26(11)
O1	7934.9(8)	8692.4(10)	7832.6(7)	22.0(2)
N1	8503.0(8)	8974.8(10)	6546.5(8)	14.14(19)
N2	10453.2(8)	8418.7(11)	6746.3(8)	16.9(2)
C1	7969.5(9)	8319.0(12)	7015.9(9)	14.5(2)
C2	7472.8(9)	7074.4(12)	6352.9(9)	13.4(2)
C3	6801.6(10)	6099.5(14)	6453.8(10)	18.3(2)
C4	6463.6(10)	4994.0(14)	5736.3(10)	20.8(2)
C5	6797.0(10)	4879.7(13)	4945.1(10)	19.8(2)
C6	7469.6(9)	5860.8(12)	4848.5(9)	16.0(2)
C7	7806.3(9)	6962.7(12)	5569.0(9)	12.4(2)
C8	8492.1(9)	8206.4(11)	5635.2(9)	12.0(2)
C9	9610.8(9)	7834.6(12)	5883.0(9)	13.7(2)
C10	10001.8(10)	7036.3(13)	5329.1(10)	17.9(2)
C11	11119.3(10)	7129.0(13)	5887.5(11)	20.9(2)
C12	11372.7(10)	7979.2(13)	6751.3(11)	21.2(2)
C13	10383.5(10)	9275.3(14)	7571.9(11)	21.9(3)
C14	9319.6(10)	10008.2(13)	7095.1(10)	19.5(2)
C15	7987.1(9)	9094.8(12)	4594.4(9)	15.1(2)
C16	6880.9(9)	9575.4(13)	4300.6(9)	16.1(2)
C17	6692.2(10)	10849.8(13)	4661.9(11)	22.2(3)
C18	5665.9(12)	11281.0(15)	4387.9(14)	30.1(3)

C19	4815.1(11)	10449.1(16)	3756.7(13)	29.6(3)
C20	5006.7(10)	9176.8(15)	3415.5(10)	23.3(3)
C21	6019.2(10)	8728.9(14)	3666.9(9)	18.7(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 21srv468. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	19.58(16)	51.1(2)	27.98(18)	6.85(16)	2.07(13)	-13.09(15)
O1	26.2(5)	27.2(5)	16.7(4)	-4.6(4)	13.3(4)	0.4(4)
N1	14.3(4)	14.6(4)	14.0(4)	-3.1(3)	6.9(4)	-0.3(3)
N2	12.4(4)	17.0(5)	20.1(5)	-2.3(4)	6.3(4)	-0.8(4)
C1	12.7(5)	17.7(5)	12.5(5)	0.5(4)	5.4(4)	3.6(4)
C2	12.6(5)	16.6(5)	11.3(5)	0.9(4)	5.7(4)	1.9(4)
C3	17.7(5)	24.0(6)	16.5(5)	2.1(4)	10.7(4)	-1.1(4)
C4	20.9(6)	21.7(6)	21.3(6)	1.0(5)	10.9(5)	-6.2(5)
C5	23.6(6)	17.7(5)	18.0(5)	-2.1(4)	9.2(5)	-4.9(5)
C6	19.2(5)	16.4(5)	14.0(5)	-1.3(4)	8.9(4)	-1.3(4)
C7	11.8(5)	14.3(5)	10.9(5)	2.1(4)	5.1(4)	1.7(4)
C8	12.4(5)	12.7(5)	11.7(5)	-0.2(4)	6.3(4)	0.4(4)
C9	12.1(5)	14.0(5)	14.7(5)	1.2(4)	6.0(4)	0.6(4)
C10	17.1(5)	19.3(5)	19.6(5)	-0.3(4)	10.4(5)	2.8(4)
C11	17.2(5)	20.1(6)	30.0(7)	3.5(5)	14.6(5)	3.6(4)
C12	12.4(5)	20.1(6)	30.7(7)	1.8(5)	9.3(5)	0.3(4)
C13	16.4(5)	23.9(6)	21.6(6)	-8.8(5)	5.4(5)	-3.5(5)
C14	19.7(5)	15.9(5)	23.0(6)	-6.3(4)	9.8(5)	-2.6(4)
C15	14.3(5)	17.0(5)	15.4(5)	3.7(4)	7.9(4)	1.4(4)
C16	15.2(5)	18.3(5)	15.3(5)	6.7(4)	7.5(4)	2.1(4)
C17	19.7(6)	17.0(6)	30.9(7)	3.3(5)	12.4(5)	1.1(4)
C18	27.4(7)	19.7(6)	48.7(9)	5.7(6)	22.3(7)	5.6(5)
C19	19.2(6)	29.8(7)	42.2(8)	13.9(6)	15.9(6)	6.4(5)
C20	16.0(5)	30.2(7)	20.7(6)	8.6(5)	5.8(5)	-3.9(5)
C21	18.0(5)	22.7(6)	14.3(5)	4.3(4)	6.5(4)	-0.3(4)

Table 4 Bond Lengths for 21srv468.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Cl1	C20	1.7419(14)		C7	C8	1.5170(15)
O1	C1	1.2258(14)		C8	C9	1.5108(15)
N1	C1	1.3666(15)		C8	C15	1.5575(16)
N1	C8	1.4725(14)		C9	C10	1.3782(16)
N1	C14	1.4530(15)		C10	C11	1.4212(17)
N2	C9	1.3782(15)		C11	C12	1.3678(19)
N2	C12	1.3733(15)		C13	C14	1.5211(18)

N2	C13	1.4624(16)		C15	C16	1.5078(16)
C1	C2	1.4804(16)		C16	C17	1.3953(18)
C2	C3	1.3898(16)		C16	C21	1.4007(17)
C2	C7	1.3900(15)		C17	C18	1.3942(19)
C3	C4	1.3891(18)		C18	C19	1.383(2)
C4	C5	1.3998(18)		C19	C20	1.382(2)
C5	C6	1.3928(17)		C20	C21	1.3876(18)
C6	C7	1.3890(16)				

Table 5 Bond Angles for 21srv468.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C8	113.80(9)		C7	C8	C15	111.31(9)
C1	N1	C14	122.96(10)		C9	C8	C7	114.28(9)
C14	N1	C8	119.42(9)		C9	C8	C15	109.41(9)
C9	N2	C13	125.50(10)		N2	C9	C8	120.72(10)
C12	N2	C9	108.99(10)		C10	C9	N2	108.03(10)
C12	N2	C13	125.34(11)		C10	C9	C8	131.04(11)
O1	C1	N1	126.01(11)		C9	C10	C11	107.02(11)
O1	C1	C2	127.87(11)		C12	C11	C10	107.67(11)
N1	C1	C2	106.11(9)		C11	C12	N2	108.28(11)
C3	C2	C1	129.11(10)		N2	C13	C14	108.90(10)
C3	C2	C7	121.98(11)		N1	C14	C13	108.37(10)
C7	C2	C1	108.89(10)		C16	C15	C8	113.68(9)
C4	C3	C2	117.72(11)		C17	C16	C15	121.24(11)
C3	C4	C5	120.44(11)		C17	C16	C21	118.70(11)
C6	C5	C4	121.54(11)		C21	C16	C15	120.05(11)
C7	C6	C5	117.77(11)		C18	C17	C16	120.72(13)
C2	C7	C8	109.55(10)		C19	C18	C17	120.56(14)
C6	C7	C2	120.55(11)		C20	C19	C18	118.52(13)
C6	C7	C8	129.83(10)		C19	C20	Cl1	119.49(10)
N1	C8	C7	101.36(9)		C19	C20	C21	122.09(13)
N1	C8	C9	109.02(9)		C21	C20	Cl1	118.40(11)
N1	C8	C15	111.24(9)		C20	C21	C16	119.39(12)

Table 6 Selected Torsion Angles for 21srv468.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C8	C9	N2	-11.64(14)		C9	C8	C15	C16	-177.50(10)
N1	C14	C13	N2	49.88(14)		C10	C9	N2	C12	-0.91(14)
C7	C8	N1	C1	2.60(12)		C10	C9	N2	C13	-176.33(12)
C7	C8	N1	C14	161.27(10)		C10	C9	C8	N1	174.33(12)
C7	C8	C9	N2	-124.24(11)		C10	C9	C8	C15	-63.82(16)
C7	C8	C9	C10	61.74(16)		C13	C14	N1	C1	94.70(13)

C7	C8	C15	C16	55.25(13)		C13	C14	N1	C8	-61.92(14)
C8	C9	N2	C12	-176.18(10)		C14	C13	N2	C9	-27.78(17)
C8	C9	N2	C13	8.40(18)		C14	C13	N2	C12	157.53(12)
C8	C15	C16	C17	90.79(14)		C15	C8	N1	C1	121.01(10)
C8	C15	C16	C21	-88.25(13)		C15	C8	N1	C14	-80.33(12)
C9	C8	N1	C1	-118.26(10)		C15	C8	C9	N2	110.20(12)
C9	C8	N1	C14	40.41(13)		C16	C15	C8	N1	-56.99(13)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 21srv468.

Atom	*x*	*y*	*z*	U(eq)
H3	6581.5	6186.09	6994.78	22
H4	6003.12	4311.07	5782.98	25
H5	6558.97	4115.15	4462.81	24
H6	7690.71	5779.04	4307.97	19
H10	9600.28	6521.49	4694.14	22
H11	11603.21	6681.13	5695.52	25
H12	12065.85	8223.66	7266.24	25
H13A	10958.28	9974.37	7841.78	26
H13B	10458.57	8679.96	8177.59	26
H14A	9206.64	10460.23	7667.28	23
H14B	9296.6	10737.05	6586.23	23
H15A	8435.36	9923.15	4685.26	18
H15B	7976	8535.05	3997.96	18
H17	7269.37	11429.88	5099.41	27
H18	5550.15	12153.9	4636.9	36
H19	4114.6	10745.28	3561.76	36
H21	6127.01	7856.18	3411.6	22

Refinement model description

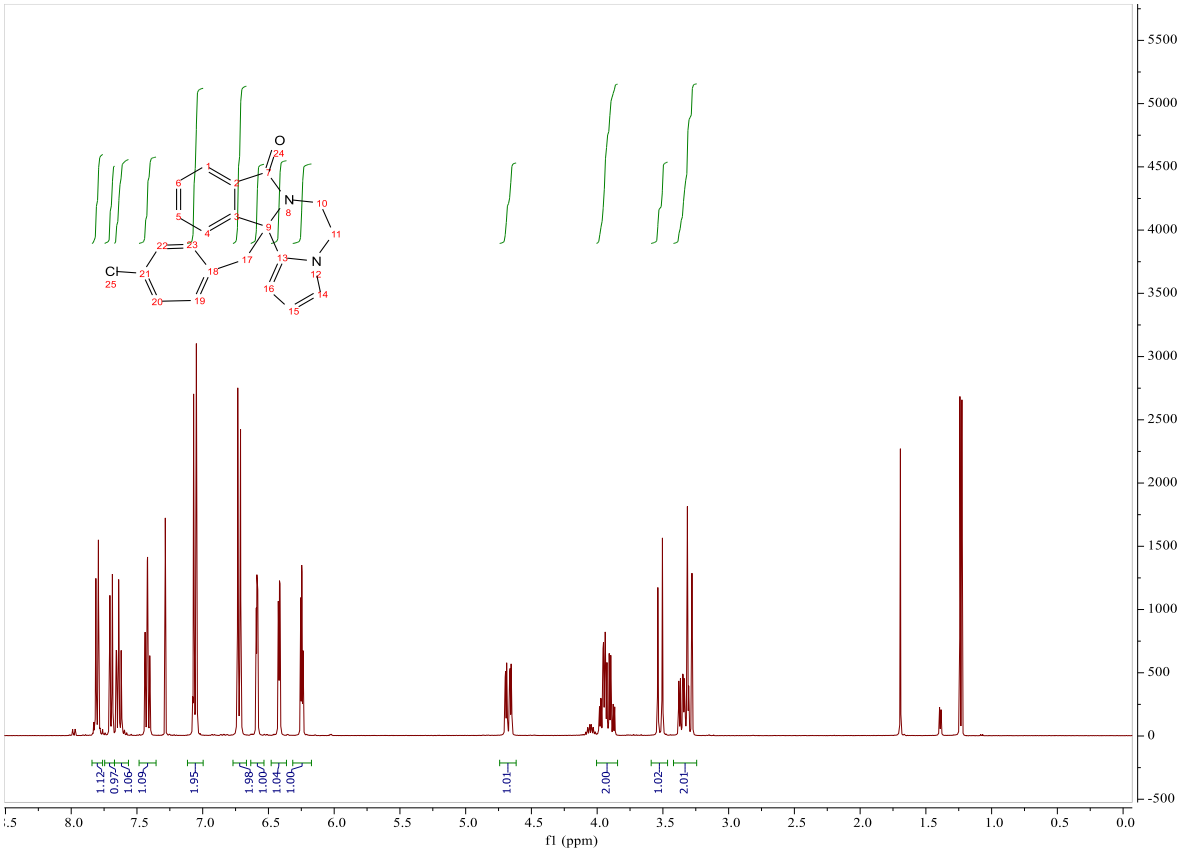
Number of restraints - 0, number of constraints - unknown.

Details:

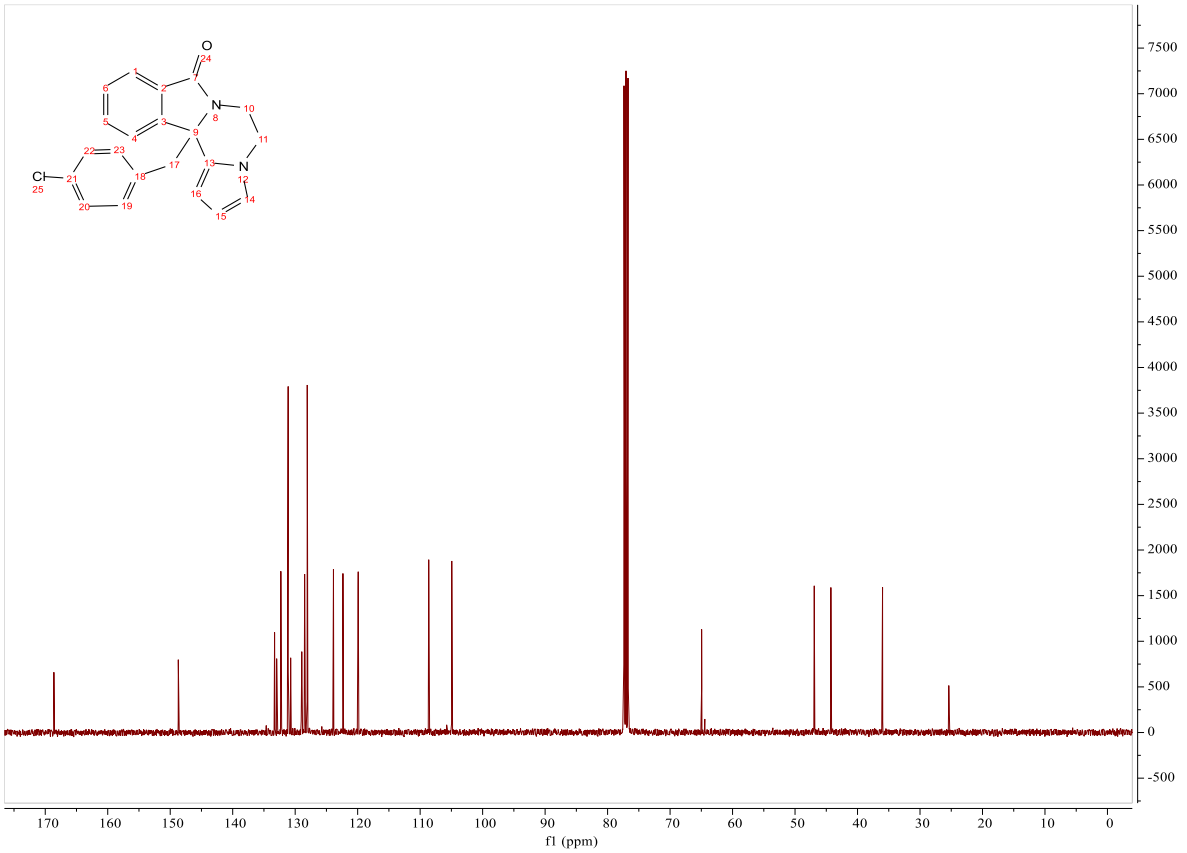
1. Fixed Uiso
 At 1.2 times of:
  All C(H) groups, All C(H,H) groups
2.a Secondary CH2 refined with riding coordinates:
 C13(H13A,H13B), C14(H14A,H14B), C15(H15A,H15B)
2.b Aromatic/amide H refined with riding coordinates:
 C3(H3), C4(H4), C5(H5), C6(H6), C10(H10), C11(H11), C12(H12), C17(H17),
 C18(H18), C19(H19), C21(H21)

12*b*-(4-chlorobenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1d**

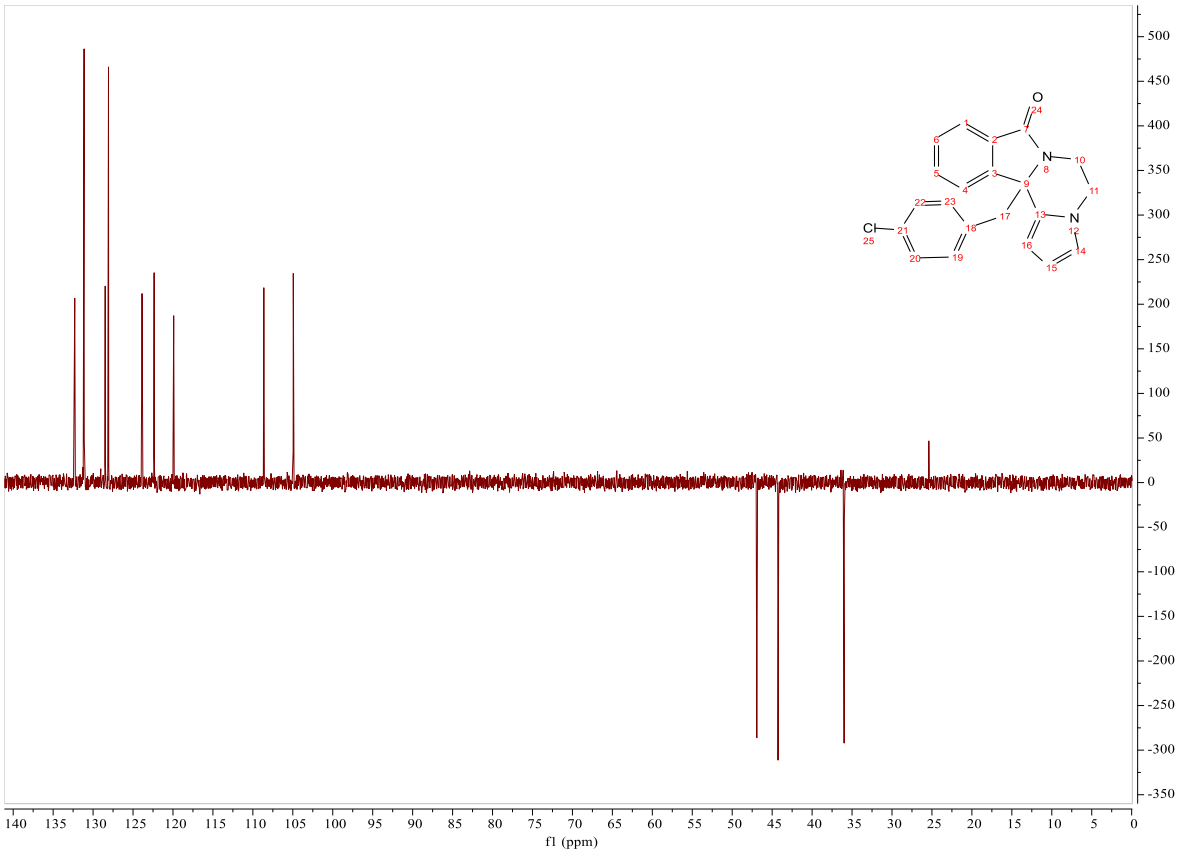
^{1}H:

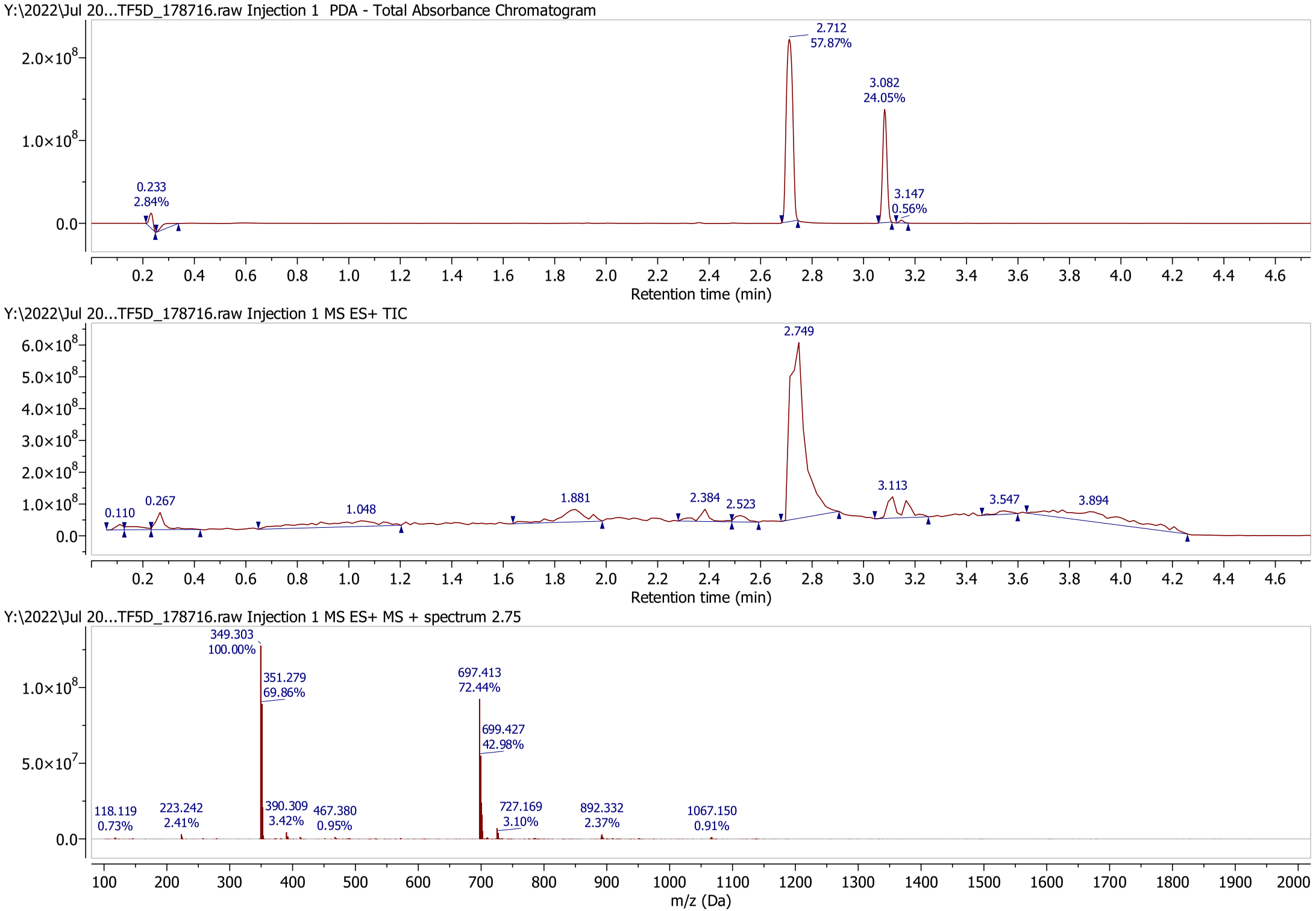


^{13}C:



DEPT-135:


O
24
1
2
7
6
N
8
10
11
5
4
3
9
22
23
17
13
N
12
Cl
25
21
18
16
14
20
19
15
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)


Y:\2022\Jul 20...TF5D_178716.raw Injection 1 PDA - Total Absorbance Chromatogram
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57.87%
3.082
24.05%
0.233
2.84%
3.147
0.56%
Retention time (min)
Y:\2022\Jul 20...TF5D_178716.raw Injection 1 MS ES+ TIC
2.749
0.110
0.267
1.048
1.881
2.384
2.523
3.113
3.547
3.894
Retention time (min)
Y:\2022\Jul 20...TF5D_178716.raw Injection 1 MS ES+ MS + spectrum 2.75
349.303
100.00%
351.279
69.86%
697.413
72.44%
699.427
42.98%
118.119
0.73%
223.242
2.41%
390.309
3.42%
467.380
0.95%
727.169
3.10%
892.332
2.37%
1067.150
0.91%
m/z (Da)

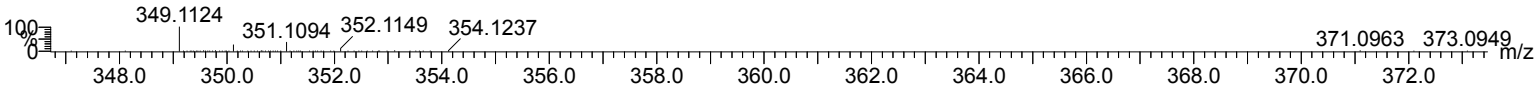
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
1468 formula(e) evaluated with 12 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 Cl: 0-2

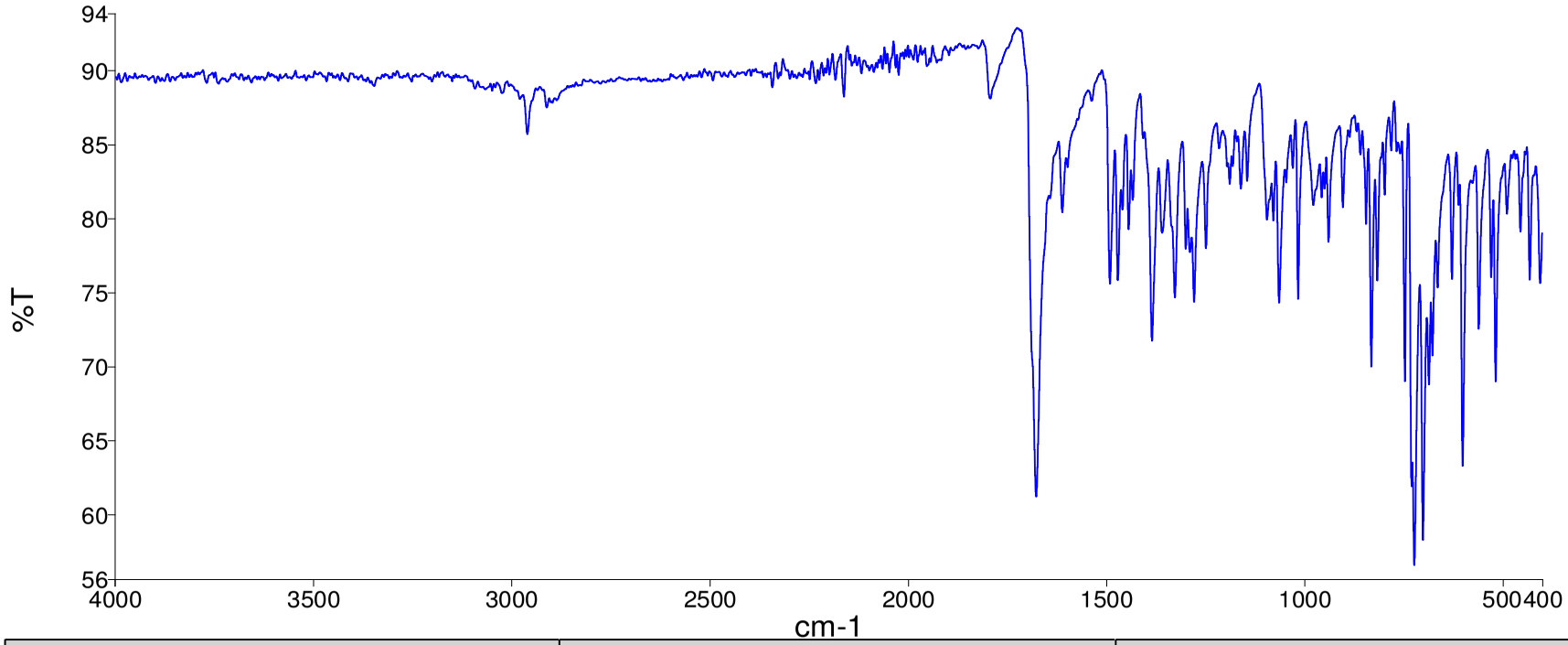
21-Jul-2022
MTF_MTF5D_179342 533 (4.475) Cm (531:533)

21-Jul-2022
1: TOF MS ES+
6.83e+004



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
349.1124	349.1126	-0.2	-0.6	0.5	704.1	15.783	0.00	C9 H22 N4 O8 Cl
	349.1126	-0.2	-0.6	8.5	717.2	28.884	0.00	C20 H23 O Cl2
	349.1121	0.3	0.9	10.5	715.1	26.722	0.00	C11 H13 N10 O4
	349.1118	0.6	1.7	-3.5	718.0	29.682	0.00	C4 H23 N8 O6 Cl2
	349.1135	-1.1	-3.2	4.5	715.1	26.768	0.00	C14 H21 O10
	349.1140	-1.6	-4.6	5.5	703.0	14.647	0.00	C10 H18 N8 O4 Cl
	349.1108	1.6	4.6	5.5	715.2	26.881	0.00	C10 H17 N6 O8
	349.1108	1.6	4.6	13.5	688.4	0.000	100.00	C21 H18 N2 O Cl
	349.1144	-2.0	-5.7	-4.5	717.8	29.425	0.00	C8 H27 N2 O8 Cl2
	349.1104	2.0	5.7	-8.5	718.5	30.173	0.00	C3 H27 N4 O10 Cl2
	349.1148	-2.4	-6.9	9.5	715.2	26.822	0.00	C15 H17 N4 O6
	349.1099	2.5	7.2	1.5	707.4	19.088	0.00	C5 H18 N10 O6 Cl

Analyst Lenny Lauchlan
Date 28 June 2022 12:50



Sample Name	Description	Quality Checks
MTF 005D	Sample 018 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

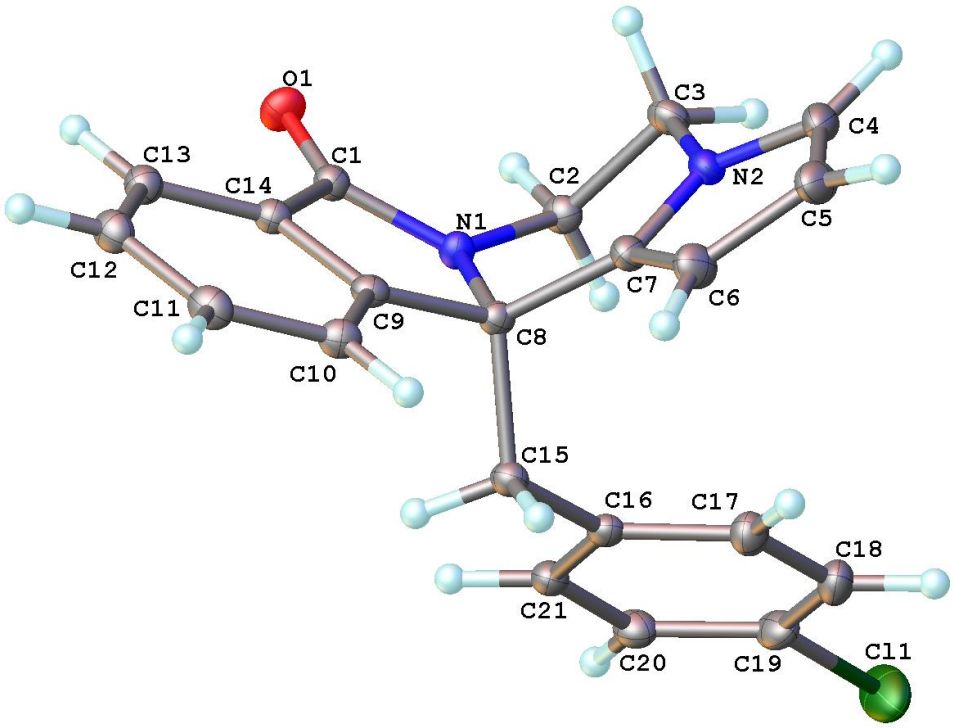


Table 1 Crystal data and structure refinement for 22srv040.	
Identification code	22srv040
Empirical formula	$C_{21}H_{17}ClN_2O$
Formula weight	348.82
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.4849(2)
b/Å	27.8691(6)
c/Å	7.8403(2)
α/°	90
β/°	93.0887(9)
γ/°	90
Volume/Å^3	1633.09(7)
Z	4
ρ_{calc}g/cm^3	1.419
μ/mm^{-1}	0.245

F(000)	728.0
Crystal size/mm^3	0.25 × 0.2 × 0.03
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.404 to 60
Index ranges	-10 ≤ h ≤ 10, -39 ≤ k ≤ 39, -11 ≤ l ≤ 11
Reflections collected	28852
Independent reflections	4751 [R_{int} = 0.0395, R_{sigma} = 0.0276]
Data/restraints/parameters	4751/0/294
Goodness-of-fit on F^2	1.085
Final R indexes [I>=2σ (I)]	R_1 = 0.0440, wR_2 = 0.0982
Final R indexes [all data]	R_1 = 0.0517, wR_2 = 0.1017
Largest diff. peak/hole / e $Å^{-3}$	0.38/-0.43

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 22srv040. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	2760.1(6)	4908.2(2)	2213.5(5)	34.30(12)
O1	7459.1(13)	2322.5(3)	5868.3(13)	18.9(2)
N1	8134.8(14)	3106.8(4)	5210.2(14)	13.6(2)
N2	9100.5(15)	3816.8(4)	7458.6(14)	15.7(2)
C1	8485.6(17)	2624.6(5)	5342.2(16)	14.0(2)
C2	6708.3(17)	3336.6(5)	6091.5(17)	15.5(2)
C3	7447.9(18)	3559.5(5)	7750.4(17)	17.3(3)
C4	9901(2)	4143.5(5)	8569.5(18)	20.4(3)
C5	11496(2)	4277.0(5)	7945.8(19)	23.5(3)
C6	11693(2)	4021.9(5)	6403.6(18)	20.8(3)
C7	10205.7(17)	3736.1(5)	6140.9(16)	14.7(2)
C8	9676.9(16)	3392.1(4)	4717.2(16)	12.9(2)
C9	11043.6(16)	3001.6(5)	4435.7(16)	13.3(2)
C10	12740.4(17)	3039.4(5)	3819.9(17)	16.5(2)
C11	13692.3(18)	2619.9(5)	3545.2(17)	18.4(3)
C12	12956.8(18)	2172.9(5)	3869.9(17)	18.3(3)
C13	11245.0(18)	2134.7(5)	4473.4(17)	16.1(2)
C14	10309.9(16)	2555.5(5)	4739.4(16)	13.9(2)
C15	9310.2(17)	3651.5(5)	2972.6(16)	14.9(2)
C16	7689.4(17)	3970.8(5)	2819.0(16)	14.6(2)
C17	7686.2(19)	4431.9(5)	3514.1(18)	19.1(3)
C18	6168(2)	4718.9(5)	3345.2(19)	21.7(3)

C19	4656(2)	4545.7(5)	2454.8(18)	21.1(3)
C20	4623.5(19)	4091.2(5)	1739.5(17)	19.2(3)
C21	6139.3(18)	3804.7(5)	1932.9(17)	16.1(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv040. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	35.3(2)	35.3(2)	31.7(2)	-3.16(16)	-4.05(16)	21.11(17)
O1	16.4(4)	17.6(4)	23.1(5)	2.7(4)	4.3(4)	-2.8(4)
N1	12.3(5)	14.0(5)	14.7(5)	-0.1(4)	2.9(4)	-0.9(4)
N2	19.5(5)	15.3(5)	12.3(5)	-0.9(4)	0.7(4)	1.0(4)
C1	14.0(5)	15.4(6)	12.5(5)	-0.3(4)	0.3(4)	-0.4(4)
C2	13.7(6)	16.9(6)	16.1(6)	0.9(5)	3.1(4)	1.3(5)
C3	18.8(6)	20.3(6)	13.3(6)	0.4(5)	3.8(5)	2.0(5)
C4	31.1(7)	15.0(6)	14.7(6)	-1.9(5)	-2.3(5)	1.2(5)
C5	32.4(8)	18.4(6)	19.0(6)	-1.4(5)	-4.6(6)	-5.0(6)
C6	22.8(7)	19.9(6)	19.3(6)	-1.2(5)	-1.0(5)	-5.8(5)
C7	17.4(6)	14.1(5)	12.4(5)	0.0(4)	-0.7(4)	-0.1(4)
C8	11.9(5)	13.8(5)	13.1(5)	0.6(4)	1.4(4)	-1.6(4)
C9	13.0(5)	16.0(6)	10.7(5)	-0.1(4)	-1.0(4)	-0.6(4)
C10	13.5(6)	19.4(6)	16.8(6)	1.1(5)	1.0(4)	-2.5(5)
C11	12.7(6)	25.2(7)	17.4(6)	-1.0(5)	1.3(4)	1.1(5)
C12	16.5(6)	20.8(6)	17.7(6)	-1.7(5)	1.4(5)	4.4(5)
C13	16.5(6)	16.3(6)	15.3(6)	-0.6(5)	-0.2(5)	0.0(5)
C14	13.2(5)	16.5(6)	12.0(5)	0.2(4)	0.4(4)	-0.4(4)
C15	15.9(6)	15.7(6)	13.2(5)	0.7(5)	1.5(4)	0.8(4)
C16	16.9(6)	14.8(6)	12.2(5)	2.2(4)	2.8(4)	0.5(4)
C17	21.3(7)	16.6(6)	19.4(6)	-1.4(5)	1.4(5)	-1.9(5)
C18	29.7(7)	14.3(6)	21.6(7)	-1.2(5)	4.5(5)	2.1(5)
C19	24.1(7)	21.1(6)	18.2(6)	3.2(5)	2.3(5)	8.7(5)
C20	20.0(6)	21.8(6)	15.6(6)	1.4(5)	-0.8(5)	2.3(5)
C21	20.1(6)	15.5(6)	12.8(5)	0.3(5)	1.4(4)	0.2(5)

Table 4 Bond Lengths for 22srv040.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Cl1	C19	1.7437(14)		C8	C15	1.5583(17)
O1	C1	1.2262(15)		C9	C10	1.3869(18)
N1	C1	1.3719(16)		C9	C14	1.3850(17)
N1	C2	1.4516(16)		C10	C11	1.3919(19)
N1	C8	1.4705(16)		C11	C12	1.391(2)
N2	C3	1.4584(17)		C12	C13	1.3937(19)
N2	C4	1.3749(17)		C13	C14	1.3871(18)

N2	C7	1.3763(17)		C15	C16	1.5042(18)
C1	C14	1.4814(17)		C16	C17	1.3959(18)
C2	C3	1.5187(19)		C16	C21	1.3986(18)
C4	C5	1.366(2)		C17	C18	1.390(2)
C5	C6	1.417(2)		C18	C19	1.385(2)
C6	C7	1.3753(18)		C19	C20	1.385(2)
C7	C8	1.5079(17)		C20	C21	1.3889(19)
C8	C9	1.5179(17)				

Table 5 Bond Angles for 22srv040.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C2	122.61(10)		C9	C8	C15	107.04(10)
C1	N1	C8	113.57(10)		C10	C9	C8	129.28(12)
C2	N1	C8	119.63(10)		C14	C9	C8	110.01(11)
C4	N2	C3	124.79(11)		C14	C9	C10	120.47(12)
C4	N2	C7	108.95(11)		C9	C10	C11	118.42(12)
C7	N2	C3	125.91(11)		C12	C11	C10	120.86(12)
O1	C1	N1	125.24(12)		C11	C12	C13	120.71(12)
O1	C1	C14	128.54(12)		C14	C13	C12	117.84(12)
N1	C1	C14	106.22(10)		C9	C14	C1	108.60(11)
N1	C2	C3	110.16(11)		C9	C14	C13	121.67(12)
N2	C3	C2	109.87(10)		C13	C14	C1	129.73(12)
C5	C4	N2	108.24(12)		C16	C15	C8	116.60(10)
C4	C5	C6	107.58(13)		C17	C16	C15	122.12(12)
C7	C6	C5	107.32(13)		C17	C16	C21	118.67(12)
N2	C7	C8	121.01(11)		C21	C16	C15	119.20(12)
C6	C7	N2	107.89(12)		C18	C17	C16	120.75(13)
C6	C7	C8	131.08(12)		C19	C18	C17	119.30(13)
N1	C8	C7	109.13(10)		C18	C19	Cl1	119.43(11)
N1	C8	C9	101.25(10)		C18	C19	C20	121.26(13)
N1	C8	C15	112.21(10)		C20	C19	Cl1	119.31(12)
C7	C8	C9	114.29(10)		C19	C20	C21	119.03(13)
C7	C8	C15	112.44(10)		C20	C21	C16	120.99(12)

Table 6 Selected Torsion Angles for 22srv040.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C2	C3	N2	44.78(14)		C9	C8	N1	C2	161.37(11)
N1	C8	C7	N2	-12.77(16)		C9	C8	C7	N2	-125.30(12)
C1	C14	C9	C10	-178.54(11)		C9	C8	C7	C6	56.47(19)
C2	N1	C1	O1	16.8(2)		C9	C8	C15	C16	165.68(11)
C2	C3	N2	C4	164.92(12)		C9	C14	C1	O1	-173.79(13)
C2	C3	N2	C7	-22.65(17)		C9	C14	C1	N1	5.93(14)

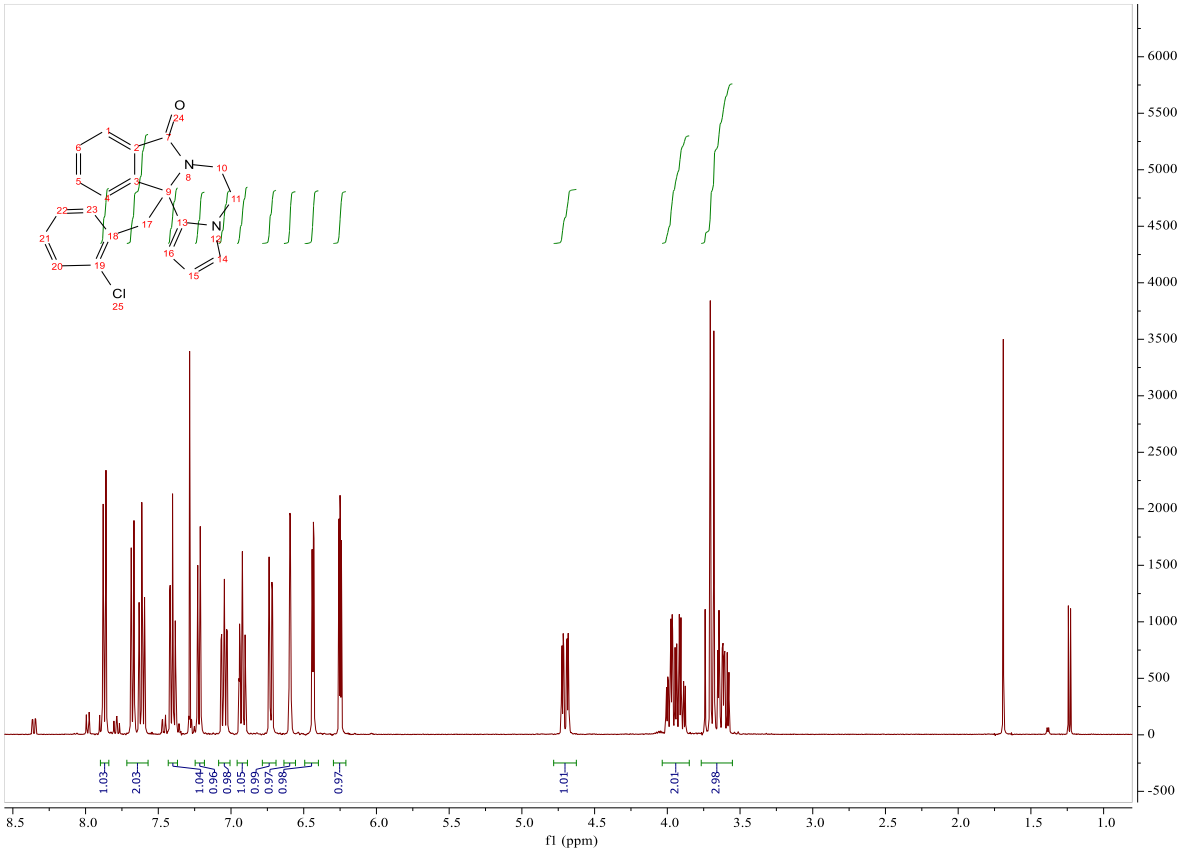
C3	C2	N1	C1	96.60(14)		C10	C9	C8	N1	174.46(13)
C3	C2	N1	C8	-58.89(15)		C10	C9	C14	C13	1.22(19)
C6	C7	N2	C3	-174.78(12)		C13	C14	C1	O1	6.5(2)
C6	C7	N2	C4	-1.35(15)		C13	C14	C1	N1	-173.81(13)
C6	C7	C8	N1	168.99(14)		C14	C1	N1	C2	-162.88(11)
C6	C7	C8	C15	-65.83(18)		C14	C1	N1	C8	-6.05(14)
C7	C8	N1	C1	-117.08(11)		C14	C9	C8	N1	0.19(13)
C7	C8	N1	C2	40.51(15)		C14	C9	C8	C7	117.34(12)
C7	C8	C9	C10	-68.39(17)		C14	C9	C8	C15	-117.46(11)
C8	N1	C1	O1	173.68(12)		C15	C8	N1	C1	117.61(12)
C8	C7	N2	C3	6.62(19)		C15	C8	N1	C2	-84.80(13)
C8	C7	N2	C4	-179.95(11)		C15	C8	C7	N2	112.40(13)
C8	C9	C14	C1	-3.69(14)		C15	C8	C9	C10	56.81(17)
C8	C9	C14	C13	176.07(11)		C16	C15	C8	N1	55.46(15)
C8	C15	C16	C17	78.58(16)		C16	C15	C8	C7	-68.01(14)
C9	C8	N1	C1	3.78(13)		C21	C16	C15	C8	-102.30(14)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv040.

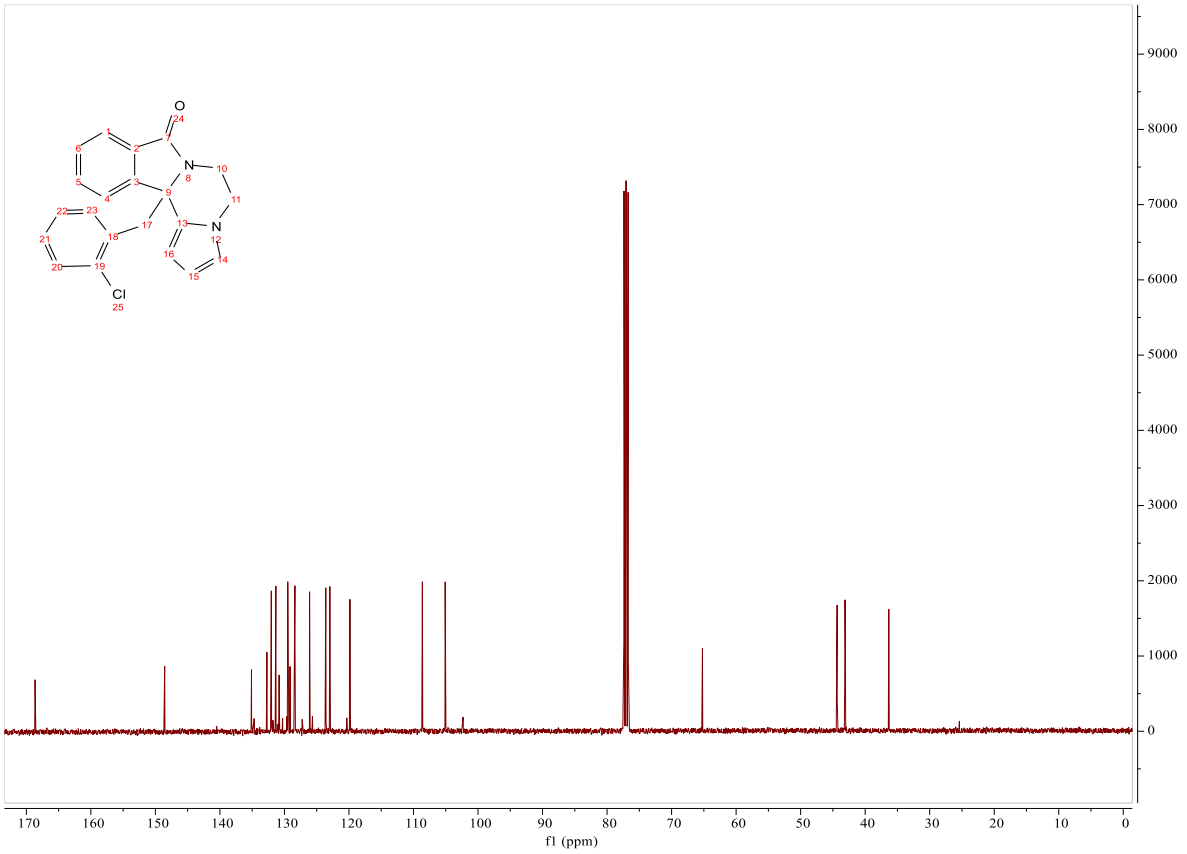
Atom	***x***	***y***	***z***	**U(eq)**
H2A	5830(20)	3084(6)	6330(20)	17(4)
H3A	6570(20)	3790(6)	8170(20)	18(4)
H2B	6140(20)	3575(6)	5360(20)	14(4)
H3B	7690(20)	3299(6)	8620(20)	19(4)
H4	9300(20)	4237(7)	9620(20)	26(5)
H5	12330(30)	4508(7)	8470(30)	32(5)
H6	12710(30)	4046(7)	5640(30)	33(5)
H15A	9180(20)	3398(7)	2110(20)	24(5)
H10	13250(20)	3352(7)	3590(20)	23(4)
H12	13630(20)	1878(7)	3660(20)	25(5)
H11	14880(20)	2642(6)	3110(20)	23(4)
H13	10760(20)	1827(7)	4700(20)	23(4)
H15B	10400(20)	3842(6)	2760(20)	23(4)
H17	8770(30)	4554(7)	4100(20)	29(5)
H18	6180(20)	5034(7)	3850(20)	25(5)
H21	6140(20)	3485(7)	1440(20)	21(4)
H20	3560(20)	3973(6)	1120(20)	24(4)

12*b*-(2-chlorobenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1e**

^{1}H:



^{13}C:



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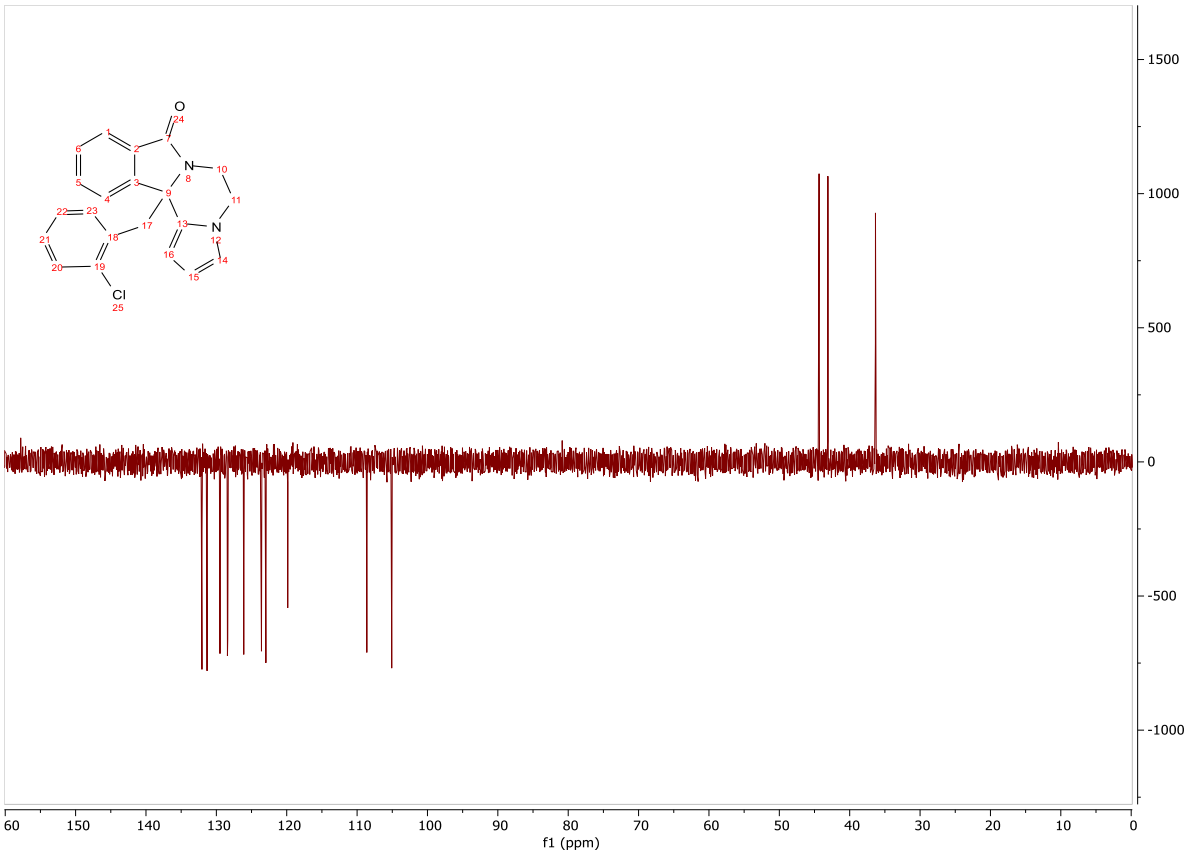
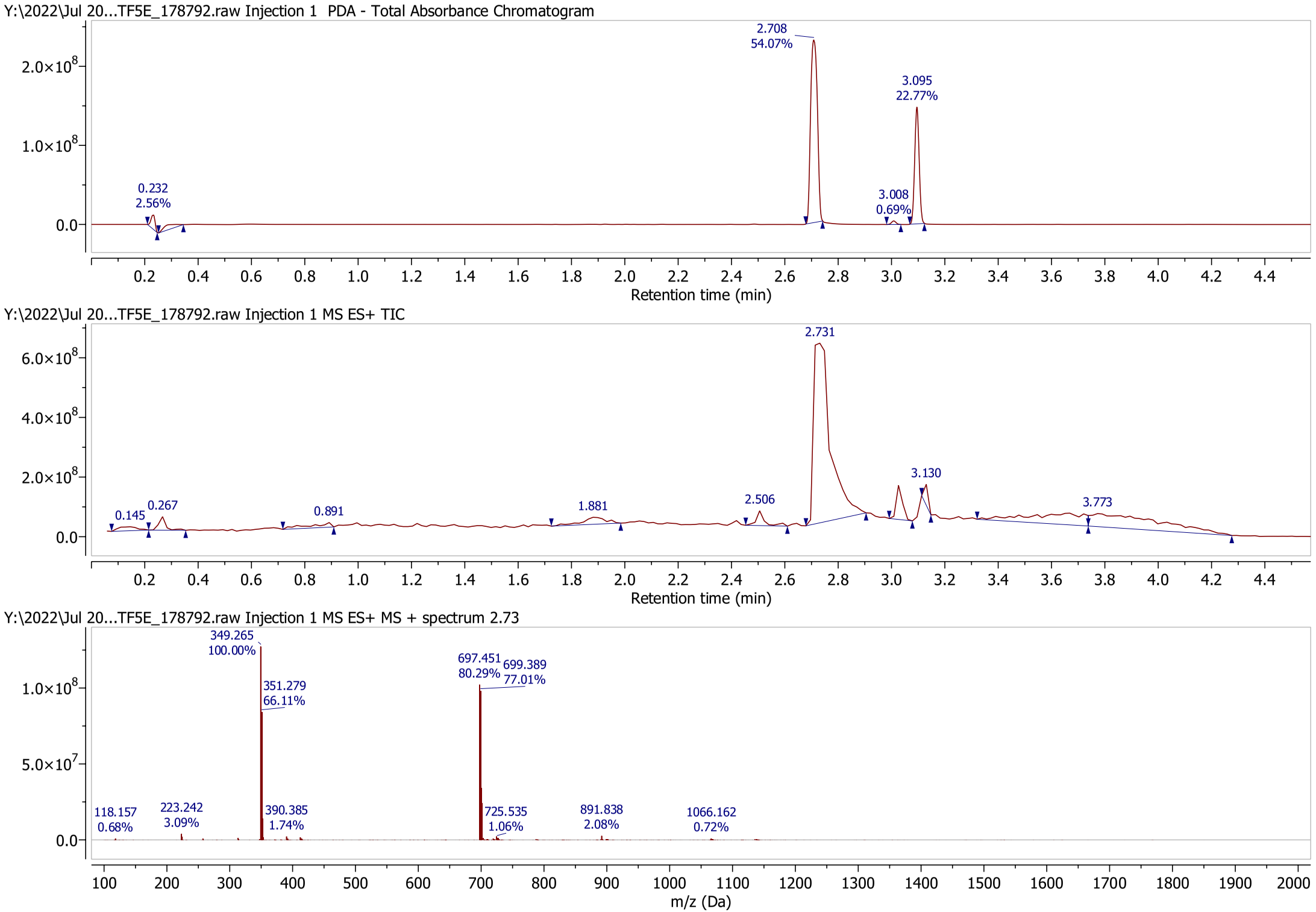

O
24
1
2
7
6
N
8
10
11
5
3
9
4
22
23
17
13
N
12
21
18
16
14
20
19
15
Cl
25
1500
1000
500
0
-500
-1000
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Y:\2022\Jul 20...TF5E_178792.raw Injection 1 PDA - Total Absorbance Chromatogram
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54.07%
3.095
22.77%
0.232
2.56%
3.008
0.69%
Retention time (min)
Y:\2022\Jul 20...TF5E_178792.raw Injection 1 MS ES+ TIC
2.731
3.130
0.145
0.267
0.891
1.881
2.506
3.773
Retention time (min)
Y:\2022\Jul 20...TF5E_178792.raw Injection 1 MS ES+ MS + spectrum 2.73
349.265
100.00%
351.279
66.11%
697.451
80.29%
699.389
77.01%
118.157
0.68%
223.242
3.09%
390.385
1.74%
725.535
1.06%
891.838
2.08%
1066.162
0.72%
m/z (Da)

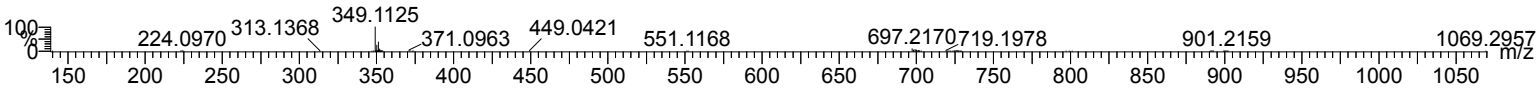
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
1468 formula(e) evaluated with 12 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 Cl: 0-2

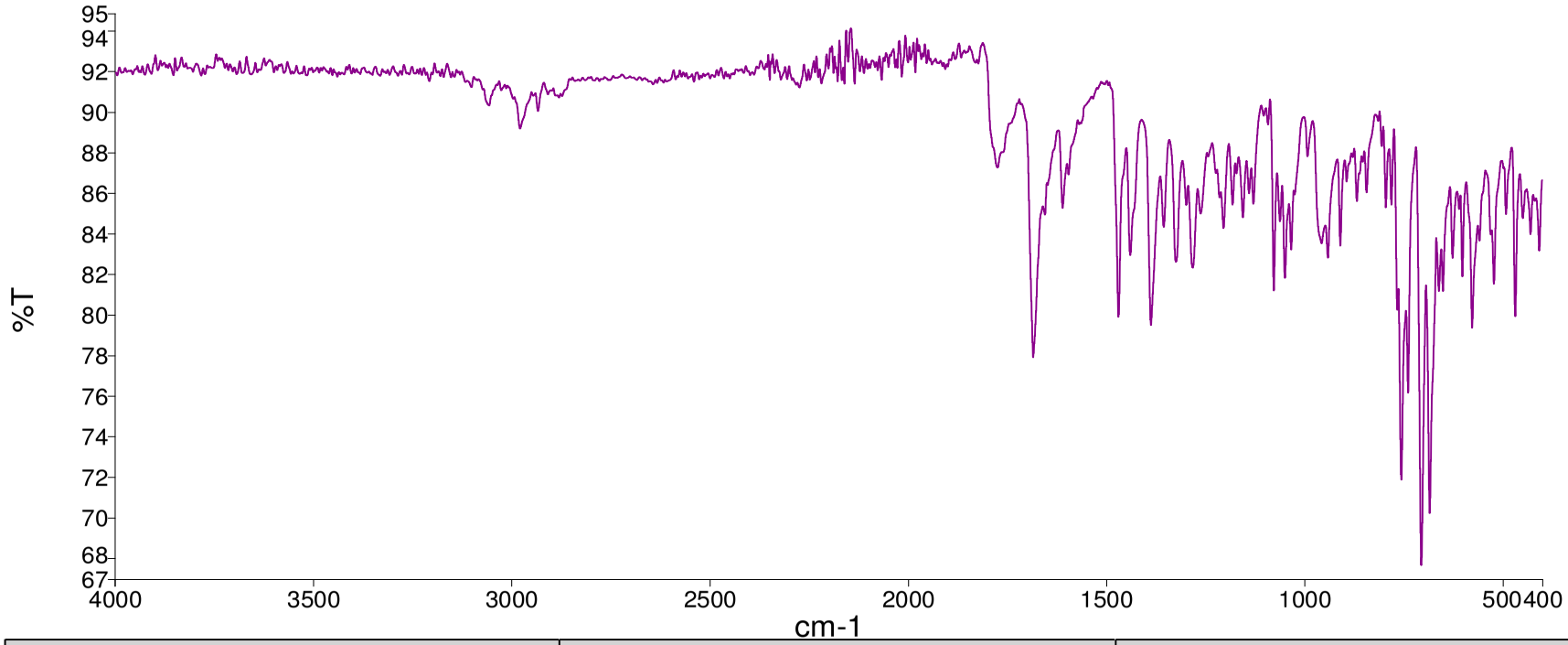
21-Jul-2022
MTF_MTF5E_179343 538 (4.521) Cm (538:540)

21-Jul-2022
1: TOF MS ES+
7.03e+004



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
349.1125	349.1126	-0.1	-0.3	0.5	614.0	16.763	0.00	C9 H22 N4 O8 Cl
	349.1126	-0.1	-0.3	8.5	628.6	31.349	0.00	C20 H23 O Cl2
	349.1121	0.4	1.1	10.5	625.9	28.655	0.00	C11 H13 N10 O4
	349.1118	0.7	2.0	-3.5	629.2	31.984	0.00	C4 H23 N8 O6 Cl2
	349.1135	-1.0	-2.9	4.5	626.0	28.785	0.00	C14 H21 O10
	349.1140	-1.5	-4.3	5.5	612.5	15.283	0.00	C10 H18 N8 O4 Cl
	349.1108	1.7	4.9	5.5	626.0	28.824	0.00	C10 H17 N6 O8
	349.1108	1.7	4.9	13.5	597.2	0.000	100.00	C21 H18 N2 O Cl
	349.1144	-1.9	-5.4	-4.5	629.0	31.799	0.00	C8 H27 N2 O8 Cl2
	349.1104	2.1	6.0	-8.5	629.7	32.433	0.00	C3 H27 N4 O10 Cl2
	349.1148	-2.3	-6.6	9.5	626.0	28.822	0.00	C15 H17 N4 O6
	349.1099	2.6	7.4	1.5	617.3	20.060	0.00	C5 H18 N10 O6 Cl

Analyst Lenny Lauchlan
Date 07 July 2022 08:10



Sample Name	Description	Quality Checks
5E	Sample 022 By Lenny Date Thursday, July 07 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

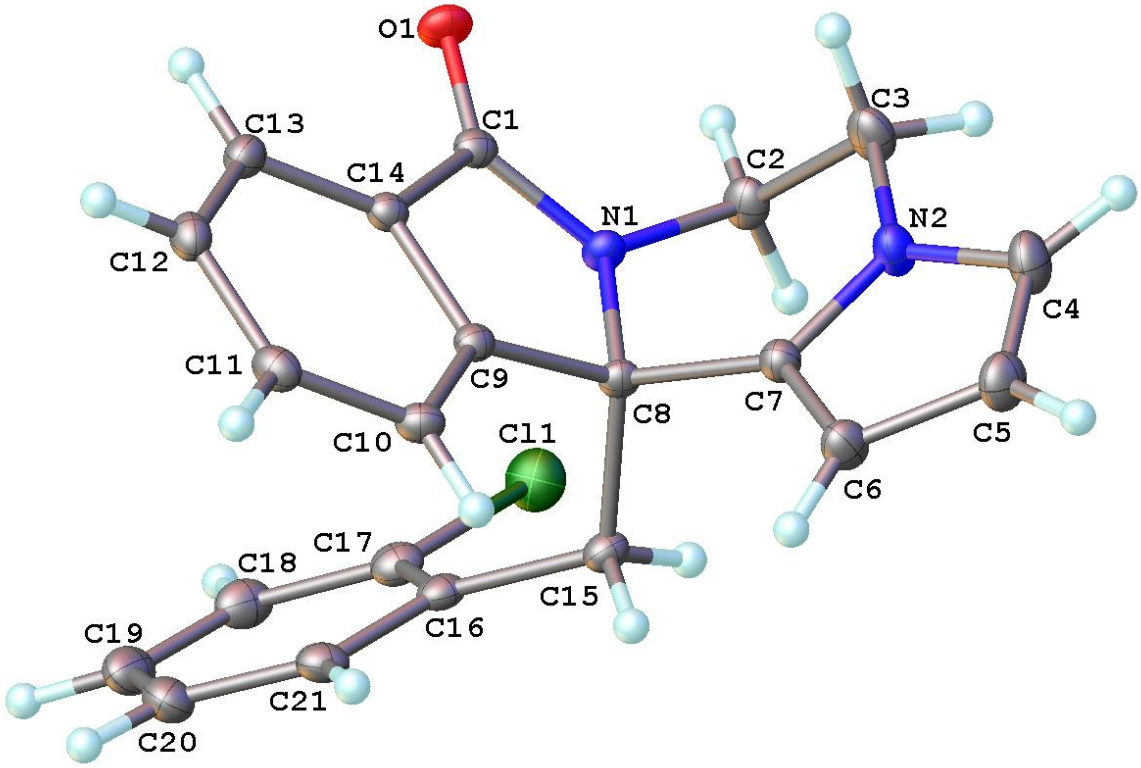


Table 1 Crystal data and structure refinement for 22srv041.	
Identification code	22srv041
Empirical formula	$C_{21}H_{17}ClN_2O$
Formula weight	348.82
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.6679(4)
b/Å	10.0995(3)
c/Å	13.8218(4)
α/°	90
β/°	118.0822(10)
γ/°	90
Volume/Å^3	1683.33(9)
Z	4

ρ_{calc}g/cm^3	1.376
μ/mm^{-1}	0.238
F(000)	728.0
Crystal size/mm^3	0.21 × 0.12 × 0.05
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.262 to 59.988
Index ranges	-19 ≤ h ≤ 19, -14 ≤ k ≤ 14, -19 ≤ l ≤ 19
Reflections collected	39362
Independent reflections	4877 [R_{int} = 0.0388, R_{sigma} = 0.0227]
Data/restraints/parameters	4877/0/294
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0384, wR_2 = 0.0942
Final R indexes [all data]	R_1 = 0.0434, wR_2 = 0.0972
Largest diff. peak/hole / e Å^{-3}	0.43/-0.36

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 22srv041. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	8177.5(3)	-1382.9(3)	5109.5(3)	23.23(9)
O1	9911.9(7)	1504.0(9)	7735.4(7)	17.75(17)
N1	8070.4(8)	1213.7(9)	6481.9(8)	13.06(17)
N2	6304.8(8)	1711.4(10)	6829.6(8)	17.36(19)
C1	9060.3(9)	1866.5(11)	6930.2(9)	13.0(2)
C2	7798.3(10)	227.5(12)	7081.5(10)	17.5(2)
C3	7211.0(10)	918.9(13)	7641.0(10)	20.5(2)
C4	5372.1(11)	2101.1(13)	6891.4(11)	22.0(2)
C5	4736.7(10)	2859.0(13)	5990.9(11)	21.6(2)
C6	5295.5(10)	2942.5(12)	5351.3(10)	18.4(2)
C7	6263.4(9)	2232.5(11)	5890.1(9)	13.9(2)
C8	7165.1(9)	1941.3(10)	5582.1(8)	11.90(19)
C9	7765.5(9)	3169.7(10)	5514.8(8)	11.81(19)
C10	7364.5(9)	4242.0(11)	4806.5(9)	14.7(2)
C11	8116.7(10)	5217.1(11)	4883.3(9)	16.3(2)
C12	9237.7(10)	5136.2(12)	5654.4(9)	16.6(2)
C13	9637.2(9)	4062.0(11)	6361.9(9)	15.4(2)
C14	8882.4(9)	3086.2(11)	6274.0(9)	12.49(19)
C15	6675.9(9)	1146.6(11)	4488.2(9)	14.3(2)

C16	7464.5(9)	960.8(11)	4017.8(9)	14.6(2)
C17	8173.1(10)	-124.1(11)	4247.3(9)	17.1(2)
C18	8883.4(10)	-263.8(13)	3790.2(10)	21.0(2)
C19	8916.2(10)	704.0(14)	3100.3(10)	22.7(3)
C20	8225.9(11)	1799.8(13)	2856.2(10)	20.4(2)
C21	7505.0(10)	1912.2(12)	3299.5(9)	17.1(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv041. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Cl1	27.00(16)	13.50(13)	29.60(16)	1.43(10)	13.65(13)	2.89(10)
O1	13.1(4)	20.4(4)	14.4(4)	2.3(3)	2.0(3)	3.6(3)
N1	11.5(4)	12.8(4)	12.7(4)	2.6(3)	4.0(3)	1.5(3)
N2	16.4(4)	19.9(5)	18.5(5)	4.5(4)	10.4(4)	3.4(4)
C1	13.0(5)	14.5(5)	11.7(4)	-1.0(4)	6.0(4)	1.9(4)
C2	17.3(5)	16.2(5)	19.1(5)	6.5(4)	8.6(4)	2.5(4)
C3	20.7(6)	23.8(6)	18.9(5)	8.7(4)	11.0(5)	5.4(5)
C4	21.3(6)	24.8(6)	27.0(6)	3.4(5)	17.2(5)	2.9(5)
C5	16.9(5)	24.4(6)	26.6(6)	1.1(5)	12.9(5)	3.7(4)
C6	14.7(5)	22.5(6)	18.2(5)	2.7(4)	7.9(4)	4.1(4)
C7	13.2(5)	15.0(5)	14.1(5)	0.3(4)	6.8(4)	0.3(4)
C8	10.7(4)	12.2(4)	11.2(4)	1.3(3)	3.9(4)	1.7(3)
C9	12.1(4)	12.4(4)	11.1(4)	-1.4(3)	5.6(4)	0.7(4)
C10	14.9(5)	14.2(5)	12.4(5)	0.1(4)	4.3(4)	1.4(4)
C11	21.1(5)	13.8(5)	14.7(5)	0.7(4)	9.1(4)	0.4(4)
C12	18.1(5)	16.4(5)	18.0(5)	-1.6(4)	10.7(4)	-2.9(4)
C13	12.7(5)	18.4(5)	15.2(5)	-1.6(4)	6.6(4)	-1.0(4)
C14	12.6(5)	13.7(5)	11.3(4)	-0.5(4)	5.7(4)	1.4(4)
C15	11.8(5)	14.9(5)	14.2(5)	-1.8(4)	4.5(4)	0.0(4)
C16	12.5(5)	16.2(5)	12.4(5)	-4.5(4)	3.6(4)	-0.9(4)
C17	16.7(5)	14.9(5)	16.8(5)	-3.5(4)	5.5(4)	-0.9(4)
C18	17.7(5)	22.9(6)	20.8(5)	-5.2(4)	7.8(4)	3.9(4)
C19	18.7(6)	31.9(7)	19.0(5)	-6.1(5)	10.1(5)	0.5(5)
C20	21.7(6)	24.8(6)	15.3(5)	-1.6(4)	9.2(4)	-1.0(5)
C21	17.2(5)	18.7(5)	12.8(5)	-2.7(4)	4.9(4)	0.9(4)

Table 4 Bond Lengths for 22srv041.

Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
Cl1	C17	1.7405(12)		C8	C15	1.5574(15)
O1	C1	1.2279(13)		C9	C10	1.3880(15)
N1	C1	1.3638(14)		C9	C14	1.3894(14)
N1	C2	1.4517(14)		C10	C11	1.3912(16)

N1	C8	1.4728(13)		C11	C12	1.3974(16)
N2	C3	1.4576(15)		C12	C13	1.3888(16)
N2	C4	1.3746(15)		C13	C14	1.3901(15)
N2	C7	1.3776(14)		C15	C16	1.5098(15)
C1	C14	1.4804(15)		C16	C17	1.3965(16)
C2	C3	1.5213(17)		C16	C21	1.4014(16)
C4	C5	1.3681(18)		C17	C18	1.3925(17)
C5	C6	1.4170(17)		C18	C19	1.3809(19)
C6	C7	1.3753(16)		C19	C20	1.3889(18)
C7	C8	1.5100(15)		C20	C21	1.3884(17)
C8	C9	1.5142(15)				

Table 5 Bond Angles for 22srv041.

Atom	Atom	Atom	Angle/˚		Atom	Atom	Atom	Angle/˚
C1	N1	C2	122.56(9)		C9	C8	C15	111.10(9)
C1	N1	C8	113.70(9)		C10	C9	C8	129.57(10)
C2	N1	C8	119.03(9)		C10	C9	C14	120.58(10)
C4	N2	C3	125.91(10)		C14	C9	C8	109.78(9)
C4	N2	C7	108.75(10)		C9	C10	C11	117.79(10)
C7	N2	C3	125.30(10)		C10	C11	C12	121.50(10)
O1	C1	N1	125.59(10)		C13	C12	C11	120.61(11)
O1	C1	C14	128.00(10)		C12	C13	C14	117.56(10)
N1	C1	C14	106.39(9)		C9	C14	C1	108.57(9)
N1	C2	C3	108.27(10)		C9	C14	C13	121.96(10)
N2	C3	C2	108.76(10)		C13	C14	C1	129.44(10)
C5	C4	N2	108.29(11)		C16	C15	C8	114.51(9)
C4	C5	C6	107.65(11)		C17	C16	C15	124.00(10)
C7	C6	C5	107.14(11)		C17	C16	C21	116.39(10)
N2	C7	C8	120.97(10)		C21	C16	C15	119.62(10)
C6	C7	N2	108.17(10)		C16	C17	Cl1	120.47(9)
C6	C7	C8	130.81(10)		C18	C17	Cl1	117.27(9)
N1	C8	C7	109.38(9)		C18	C17	C16	122.25(11)
N1	C8	C9	101.33(8)		C19	C18	C17	119.85(11)
N1	C8	C15	111.64(9)		C18	C19	C20	119.52(11)
C7	C8	C9	113.30(9)		C21	C20	C19	120.00(12)
C7	C8	C15	109.85(9)		C20	C21	C16	121.98(11)

Table 6 Torsion Angles for 22srv041.

A	B	C	D	Angle/˚		A	B	C	D	Angle/˚
N1	C2	C3	N2	51.19(13)		C8	C9	C14	C13	177.66(10)
N1	C8	C7	N2	-6.99(14)		C8	C15	C16	C17	91.29(13)
C1	C14	C9	C8	-4.20(12)		C8	C15	C16	C21	-89.08(12)

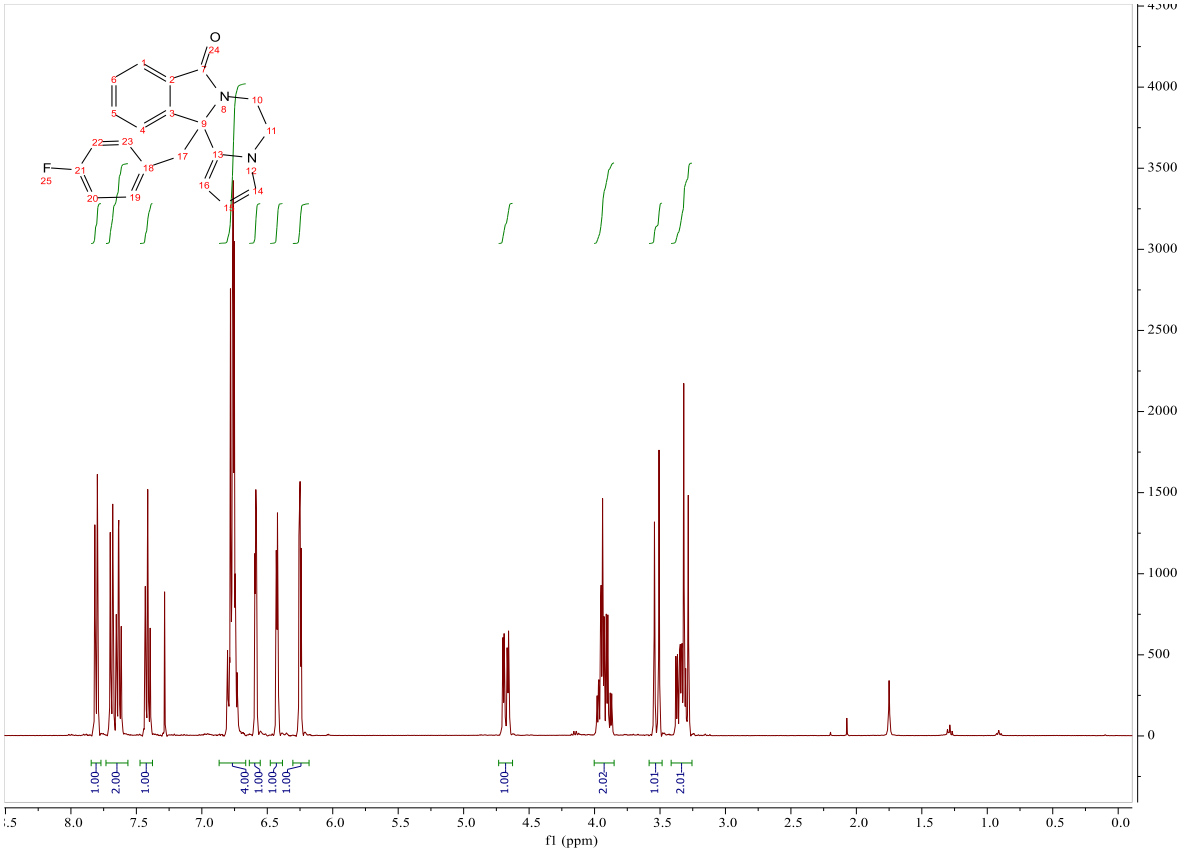
C1	C14	C9	C10	178.51(9)		C9	C8	N1	C1	1.46(11)
C2	N1	C1	O1	19.25(17)		C9	C8	N1	C2	157.79(9)
C2	C3	N2	C4	156.06(12)		C9	C8	C7	N2	-119.22(11)
C2	C3	N2	C7	-26.35(16)		C9	C8	C15	C16	45.84(12)
C3	C2	N1	C1	91.89(12)		C9	C14	C1	O1	-173.53(11)
C3	C2	N1	C8	-62.25(13)		C9	C14	C1	N1	5.01(12)
C6	C7	N2	C3	-178.54(12)		C10	C9	C8	N1	178.80(11)
C6	C7	N2	C4	-0.60(14)		C10	C9	C8	C15	60.09(14)
C6	C7	C8	N1	175.93(12)		C10	C9	C14	C13	0.37(16)
C6	C7	C8	C9	63.71(16)		C13	C14	C1	O1	4.43(19)
C6	C7	C8	C15	-61.20(16)		C13	C14	C1	N1	-177.04(11)
C7	C8	N1	C1	-118.42(10)		C14	C1	N1	C2	-159.33(10)
C7	C8	N1	C2	37.91(13)		C14	C1	N1	C8	-3.95(12)
C7	C8	C9	C10	-64.14(14)		C14	C9	C8	N1	1.83(11)
C7	C8	C9	C14	118.88(10)		C14	C9	C8	C15	-116.88(10)
C7	C8	C15	C16	172.01(9)		C15	C8	N1	C1	119.79(10)
C8	N1	C1	O1	174.63(10)		C15	C8	N1	C2	-83.89(12)
C8	C7	N2	C3	3.79(18)		C15	C8	C7	N2	115.87(11)
C8	C7	N2	C4	-178.28(10)		C16	C15	C8	N1	-66.47(12)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv041.

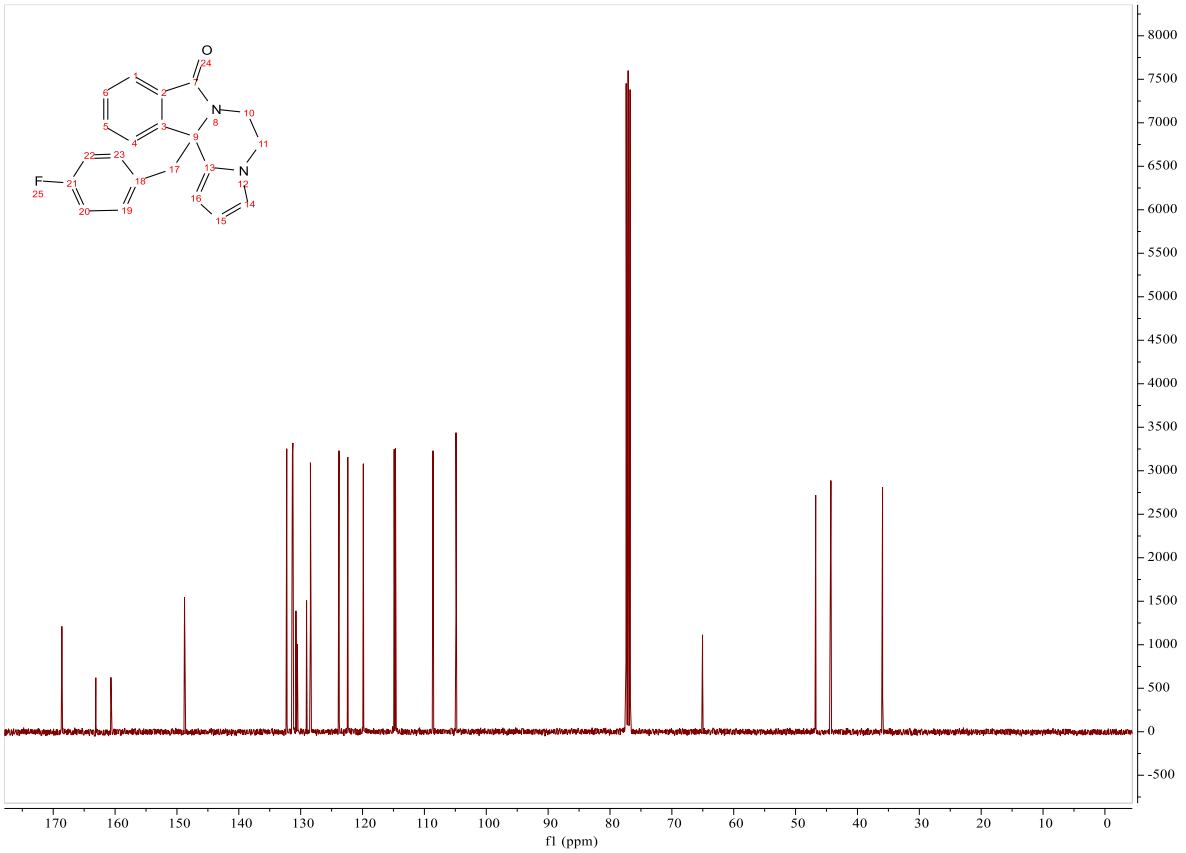
Atom	***x***	***y***	***z***	**U(eq)**
H2A	8463(14)	-188(17)	7617(14)	25(4)
H2B	7334(13)	-469(17)	6582(13)	21(4)
H3A	7731(14)	1500(16)	8225(13)	22(4)
H3B	6906(14)	275(17)	7943(14)	26(4)
H4	5280(15)	1839(18)	7496(15)	30(4)
H5	4032(14)	3246(17)	5819(13)	23(4)
H6	5069(14)	3368(17)	4677(14)	24(4)
H15A	6429(13)	321(17)	4621(13)	20(4)
H10	6628(14)	4311(16)	4296(13)	21(4)
H11	7856(13)	5970(16)	4392(13)	17(4)
H13	10414(14)	3983(16)	6896(14)	23(4)
H12	9714(14)	5812(17)	5707(13)	24(4)
H15B	6036(13)	1649(16)	3981(13)	17(4)
H21	7001(13)	2655(16)	3111(12)	16(3)
H18	9349(14)	-1018(18)	3976(14)	27(4)
H20	8281(12)	2459(16)	2381(12)	16(3)
H19	9397(14)	596(17)	2769(14)	27(4)

12*b*-(4-fluorobenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1f**

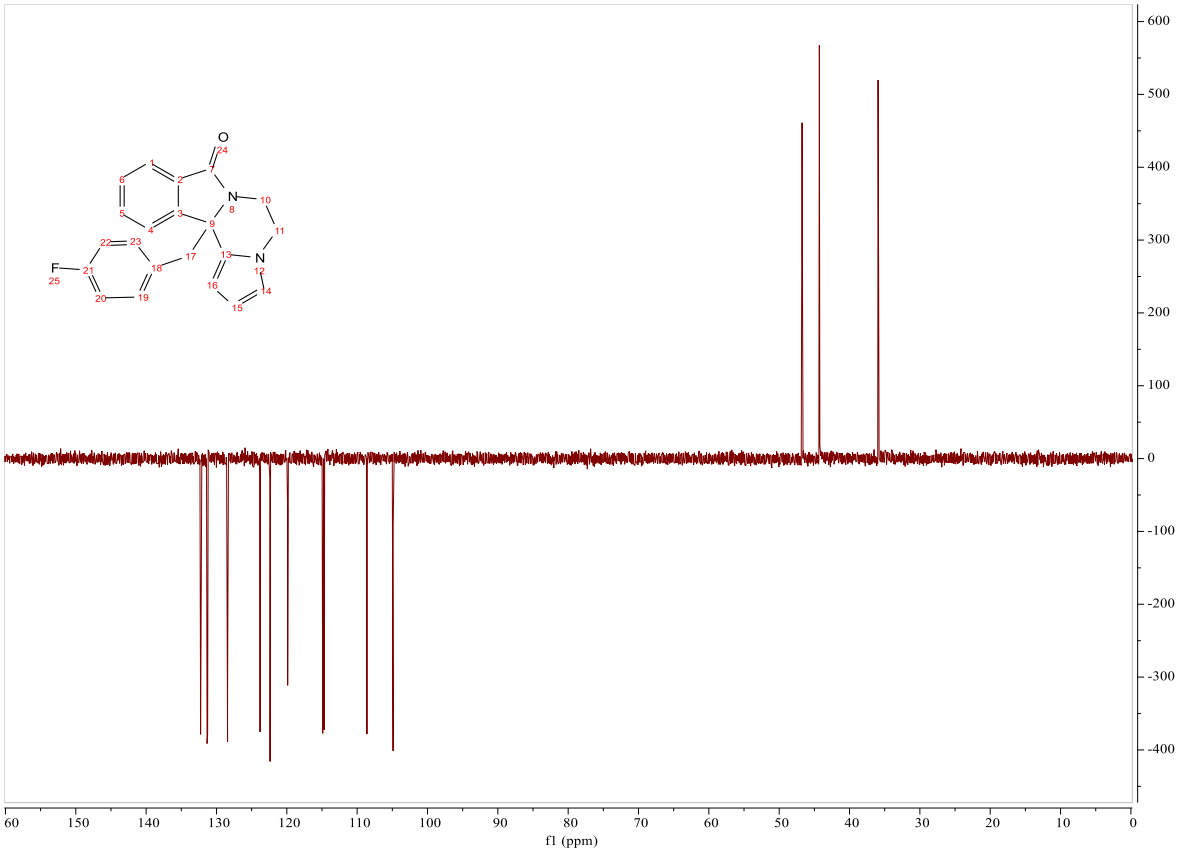
^{1}H:



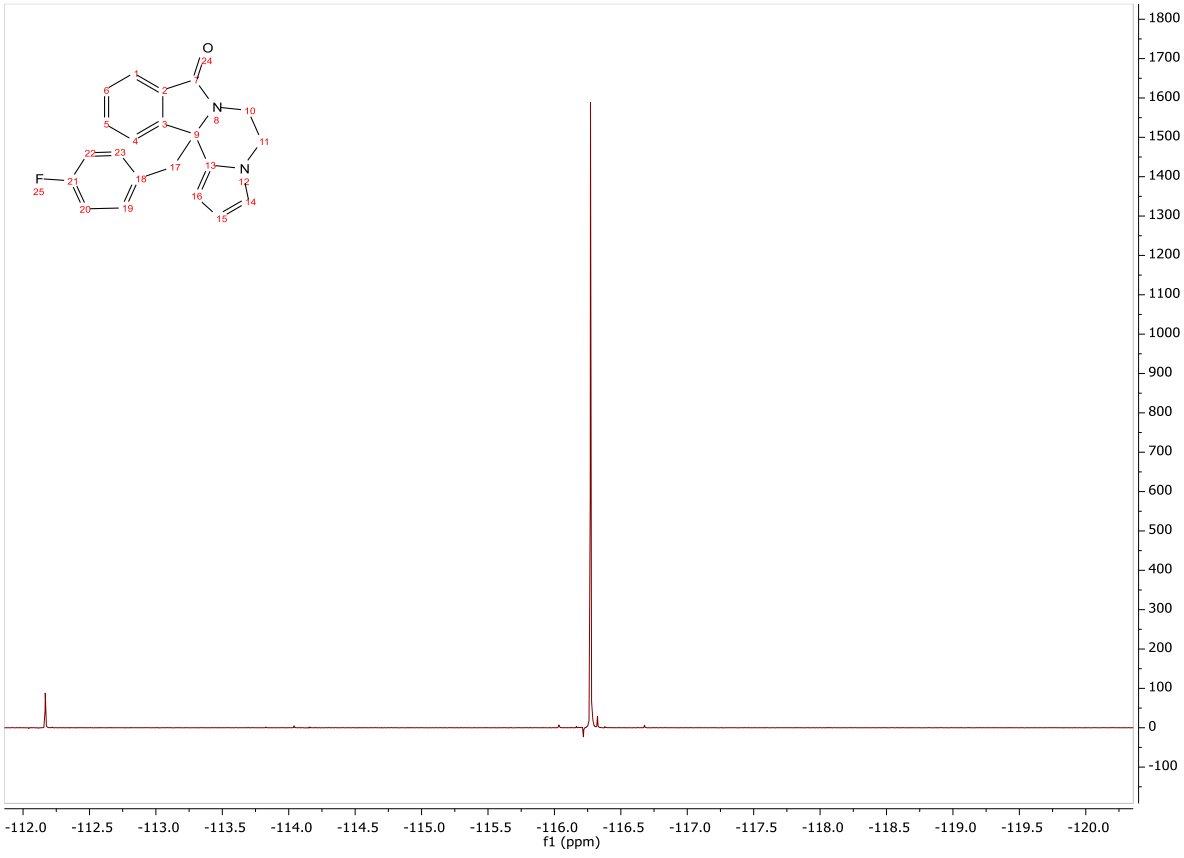
^{13}C:



DEPT-135:


O
24
1
2
6
N
8
10
11
5
4
3
9
22
23
17
13
N
12
F
25
21
18
16
14
20
19
15
600
500
400
300
200
100
0
-100
-200
-300
-400
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{19}F:


O
24
1
2
6
N
8
10
11
5
4
3
9
22
23
17
13
N
12
F
25
21
18
16
14
20
19
15
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-112.0
-112.5
-113.0
-113.5
-114.0
-114.5
-115.0
-115.5
-116.0
-116.5
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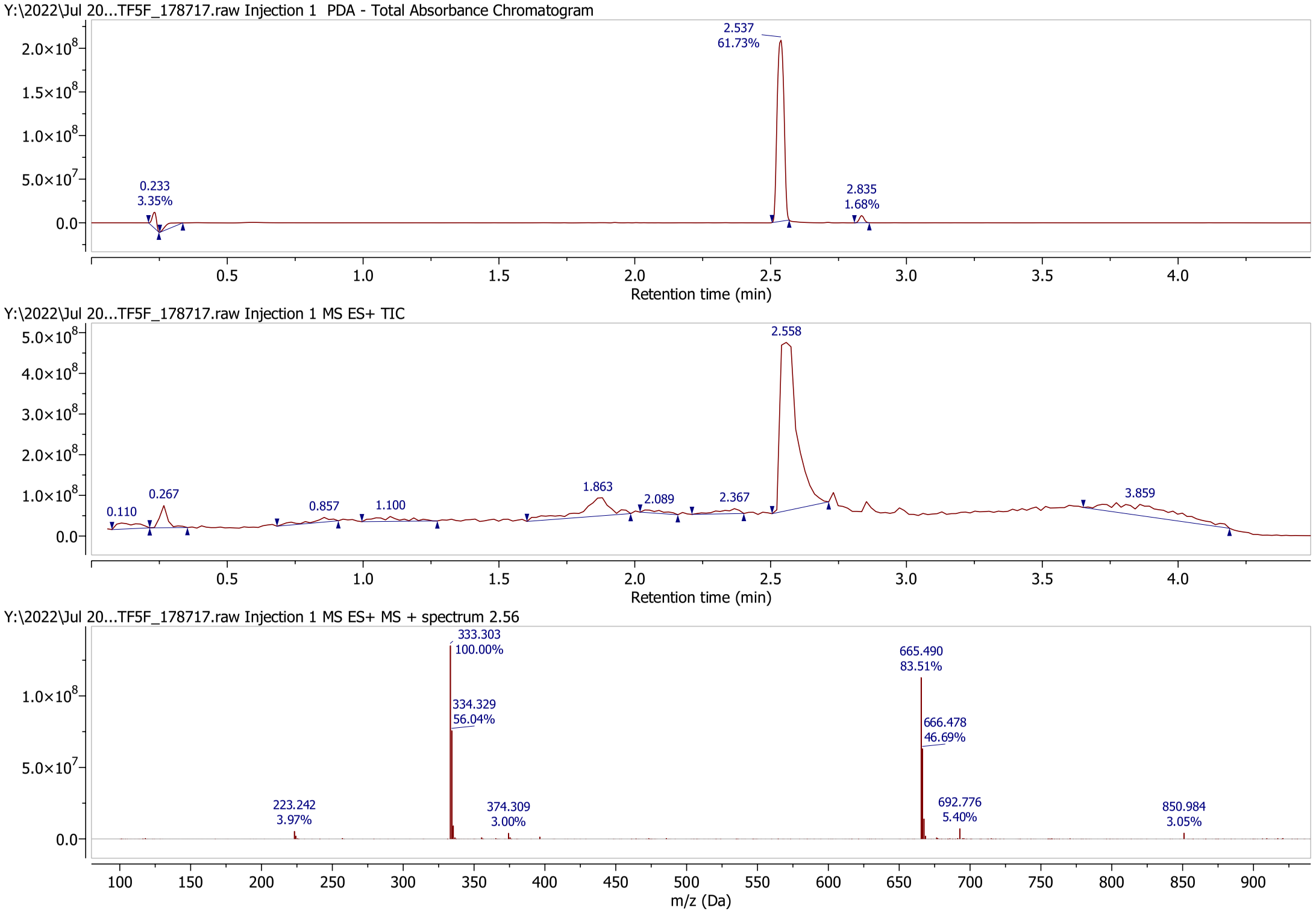
-119.0
-119.5
-120.0
f1 (ppm)


Y:\2022\Jul 20...TF5F_178717.raw Injection 1 PDA - Total Absorbance Chromatogram
2.537
61.73%
0.233
3.35%
2.835
1.68%
Retention time (min)
Y:\2022\Jul 20...TF5F_178717.raw Injection 1 MS ES+ TIC
2.558
0.110
0.267
0.857
1.100
1.863
2.089
2.367
3.859
Retention time (min)
Y:\2022\Jul 20...TF5F_178717.raw Injection 1 MS ES+ MS + spectrum 2.56
333.303
100.00%
334.329
56.04%
665.490
83.51%
666.478
46.69%
223.242
3.97%
374.309
3.00%
692.776
5.40%
850.984
3.05%
m/z (Da)

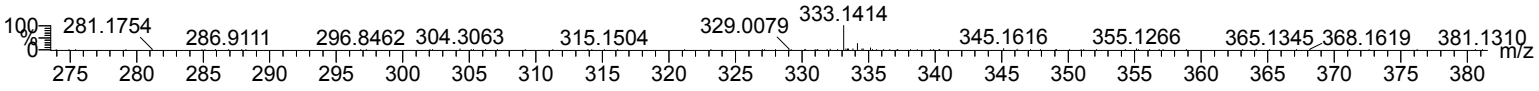
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
3006 formula(e) evaluated with 23 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 F: 0-6

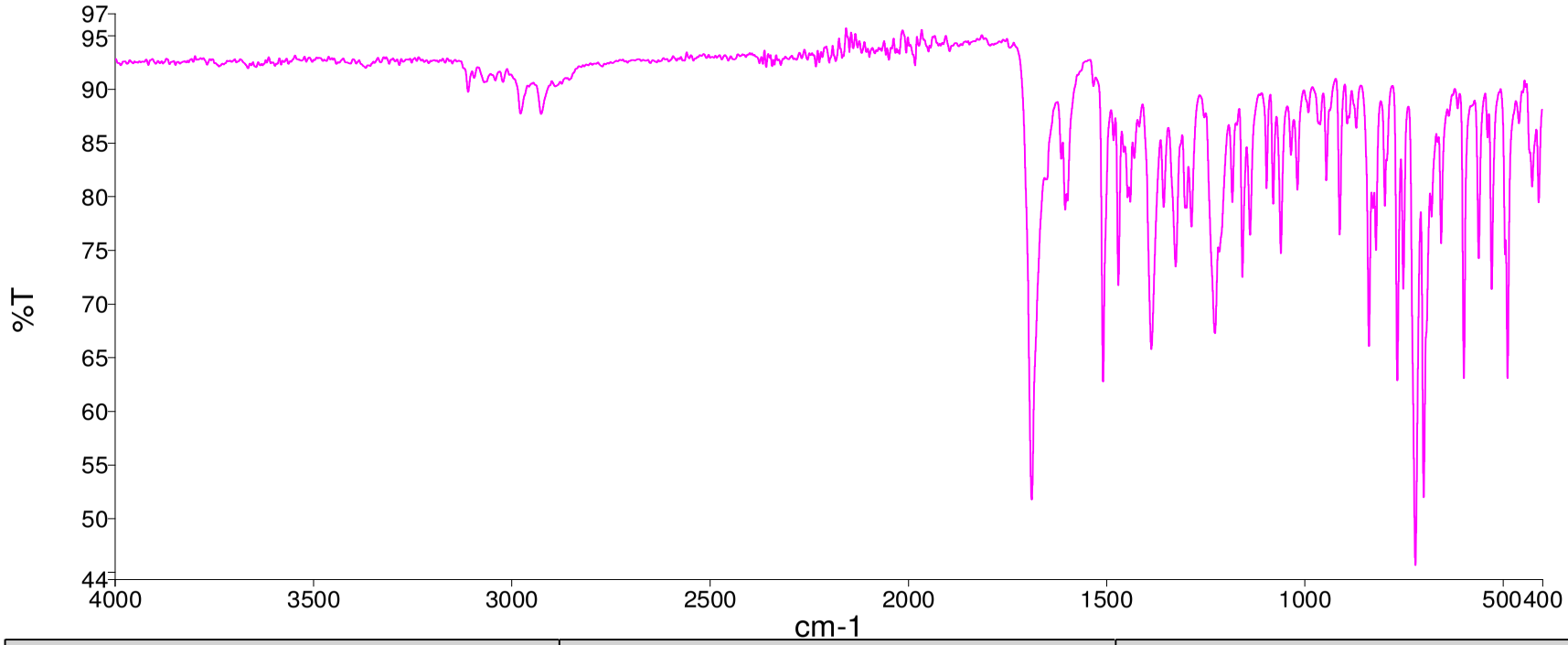
21-Jul-2022
MTF_MTF5F_179344 517 (4.344) Cm (517)

21-Jul-2022
1: TOF MS ES+
1.58e+003



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
333.1414	333.1442	-2.8	-8.4	-3.5	104.0	13.567	0.00	C H21 N10 O10
	333.1435	-2.1	-6.3	5.5	98.6	8.082	0.03	C10 H18 N8 O4 F
	333.1386	2.8	8.4	1.5	99.7	9.202	0.01	C10 H20 N4 O5 F3
	333.1399	1.5	4.5	6.5	99.0	8.541	0.02	C11 H16 N8 O F3
	333.1437	-2.3	-6.9	1.5	97.8	7.359	0.06	C12 H21 N2 O4 F4
	333.1410	0.4	1.2	4.5	97.1	6.660	0.13	C12 H21 N4 O7
	333.1424	-1.0	-3.0	9.5	96.5	5.999	0.25	C13 H17 N8 O3
	333.1402	1.2	3.6	2.5	98.2	7.730	0.04	C13 H19 N2 O F6
	333.1388	2.6	7.8	10.5	97.3	6.861	0.10	C14 H15 N8 F2
	333.1426	-1.2	-3.6	5.5	95.8	5.323	0.49	C15 H20 N2 O3 F3
	333.1390	2.4	7.2	6.5	96.6	6.180	0.21	C16 H18 N2 F5
	333.1415	-0.1	-0.3	9.5	93.7	3.237	3.93	C18 H19 N2 O2 F2
	333.1406	0.8	2.4	-2.5	103.9	13.447	0.00	C2 H19 N10 O7 F2
	333.1433	-1.9	-5.7	-5.5	104.1	13.667	0.00	C2 H19 N8 O4 F6
	333.1403	1.1	3.3	13.5	91.9	1.390	24.90	C21 H18 N2 O F
	333.1392	2.2	6.6	17.5	90.8	0.360	69.80	C24 H17 N2
	333.1409	0.5	1.5	-6.5	102.7	12.211	0.00	C4 H22 N4 O7 F5
	333.1395	1.9	5.7	1.5	102.1	11.626	0.00	C5 H18 N10 O6 F
	333.1422	-0.8	-2.4	-1.5	102.3	11.862	0.00	C5 H18 N8 O3 F5
	333.1433	-1.9	-5.7	-3.5	100.9	10.417	0.00	C6 H23 N4 O9 F2
	333.1397	1.7	5.1	-2.5	101.2	10.717	0.00	C7 H21 N4 O6 F4
	333.1411	0.3	0.9	2.5	100.7	10.192	0.00	C8 H17 N8 O2 F4
	333.1422	-0.8	-2.4	0.5	99.1	8.605	0.02	C9 H22 N4 O8 F

Analyst Lenny Lauchlan
Date 28 June 2022 12:52



Sample Name	Description	Quality Checks
MTF 005F	Sample 019 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

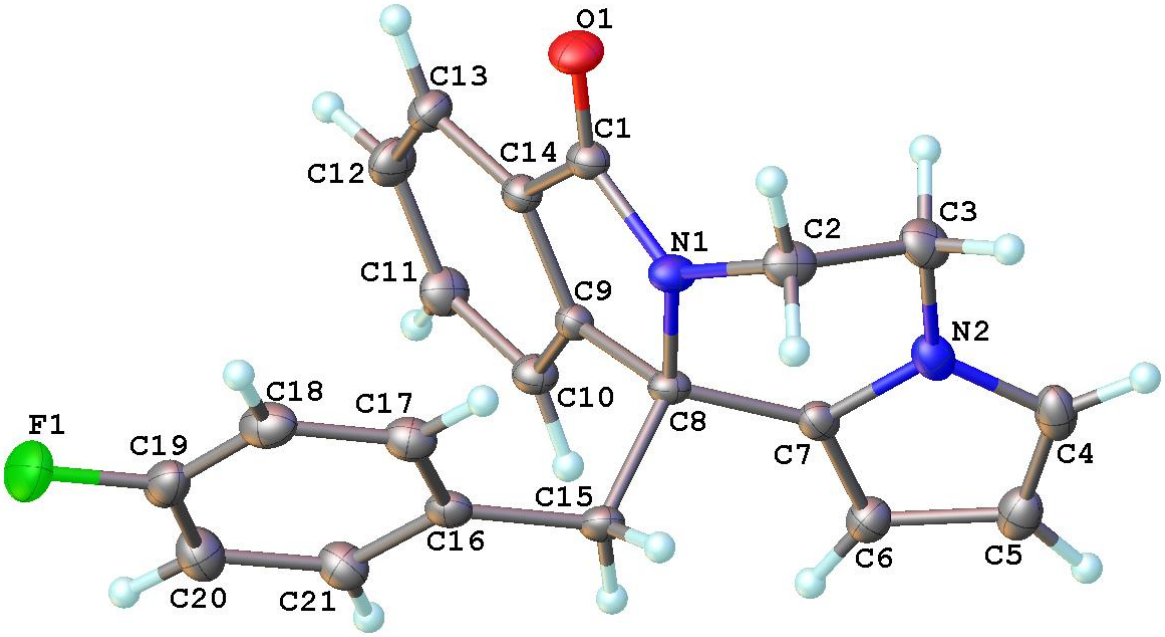


Table 1 Crystal data and structure refinement for 22srv128.	
Identification code	22srv128
Empirical formula	$C_{21}H_{17}FN_2O$
Formula weight	332.36
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.4336(4)
b/Å	7.3808(2)
c/Å	15.9267(5)
α/°	90
β/°	98.7023(12)
γ/°	90
Volume/Å^3	1677.16(8)
Z	4
ρ_{calc}g/cm^3	1.316
μ/mm^{-1}	0.090

F(000)	696.0
Crystal size/mm^3	0.34 × 0.21 × 0.08
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.174 to 59.988
Index ranges	-20 ≤ h ≤ 20, -10 ≤ k ≤ 10, -22 ≤ l ≤ 22
Reflections collected	38607
Independent reflections	4863 [R_{int} = 0.0372, R_{sigma} = 0.0217]
Data/restraints/parameters	4863/0/294
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	R_1 = 0.0454, wR_2 = 0.1124
Final R indexes [all data]	R_1 = 0.0512, wR_2 = 0.1161
Largest diff. peak/hole / e $Å^{-3}$	0.35/-0.23

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 22srv128. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	-617.7(6)	-18.9(12)	1156.8(6)	38.1(2)
O1	2841.1(6)	-3858.0(11)	3647.9(6)	24.57(19)
N1	3488.9(6)	-1160.3(12)	3300.7(6)	17.36(18)
N2	5158.0(6)	465.4(14)	3894.2(6)	19.94(19)
C1	2891.0(7)	-2204.2(14)	3684.4(7)	17.3(2)
C2	4330.5(8)	-1883.9(16)	3029.5(7)	22.0(2)
C3	5151.3(8)	-1472.4(17)	3720.1(8)	23.5(2)
C4	5933.1(8)	1492.0(18)	4180.3(7)	23.8(2)
C5	5646.4(8)	3232.5(18)	4291.7(7)	23.8(2)
C6	4654.8(8)	3271.1(16)	4060.5(7)	20.7(2)
C7	4373.0(7)	1537.3(14)	3824.4(6)	16.7(2)
C8	3419.9(7)	790.7(13)	3468.8(6)	15.31(19)
C9	2700.5(7)	810.1(14)	4070.8(6)	14.73(19)
C10	2359.9(8)	2252.6(15)	4491.3(7)	18.4(2)
C11	1686.7(8)	1877.1(16)	5009.3(7)	21.9(2)
C12	1353.1(8)	124.1(17)	5091.4(8)	23.1(2)
C13	1684.6(8)	-1315.7(15)	4658.2(7)	20.5(2)
C14	2363.4(7)	-930.7(14)	4150.9(6)	15.85(19)
C15	3049.1(8)	1815.7(15)	2629.4(7)	18.7(2)
C16	2070.6(8)	1311.1(14)	2232.7(6)	17.7(2)
C17	1891.3(8)	-302.6(16)	1782.6(7)	21.7(2)
C18	982.0(9)	-764.2(17)	1423.5(7)	25.5(2)

C19	268.1(8)	422.5(17)	1514.5(8)	25.1(2)
C20	413.4(9)	2032.8(18)	1948.8(8)	26.3(2)
C21	1325.7(8)	2464.9(16)	2312.3(7)	22.6(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv128. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	26.2(4)	41.4(5)	43.2(5)	5.6(4)	-6.4(3)	-11.0(3)
O1	28.9(4)	13.1(4)	32.4(4)	-0.7(3)	6.9(3)	0.1(3)
N1	21.1(4)	13.0(4)	19.2(4)	0.7(3)	6.8(3)	2.2(3)
N2	18.2(4)	24.0(5)	18.0(4)	1.7(3)	4.0(3)	4.5(3)
C1	18.9(5)	14.8(4)	17.9(4)	1.1(4)	2.0(4)	0.4(4)
C2	26.8(5)	19.8(5)	21.6(5)	-1.2(4)	10.9(4)	4.1(4)
C3	22.8(5)	23.2(5)	25.8(5)	0.3(4)	8.0(4)	8.4(4)
C4	17.7(5)	35.7(6)	17.6(5)	1.5(4)	1.7(4)	1.4(4)
C5	21.5(5)	31.6(6)	18.0(5)	-0.8(4)	2.0(4)	-4.7(5)
C6	20.1(5)	21.1(5)	21.1(5)	0.2(4)	3.9(4)	-1.4(4)
C7	16.6(4)	18.3(5)	15.7(4)	2.6(4)	4.3(3)	2.2(4)
C8	18.0(4)	12.4(4)	16.1(4)	1.5(3)	4.5(3)	1.0(3)
C9	14.8(4)	14.7(4)	14.6(4)	1.9(3)	2.0(3)	1.0(3)
C10	20.8(5)	15.2(5)	19.6(5)	0.7(4)	4.1(4)	1.2(4)
C11	22.9(5)	21.3(5)	22.6(5)	-2.1(4)	7.5(4)	3.5(4)
C12	20.7(5)	25.4(6)	25.1(5)	1.0(4)	9.6(4)	-0.6(4)
C13	18.9(5)	18.9(5)	24.2(5)	1.8(4)	5.1(4)	-2.9(4)
C14	16.3(4)	14.3(4)	16.7(4)	0.9(3)	1.6(3)	0.5(3)
C15	21.1(5)	17.3(5)	17.7(5)	5.1(4)	2.9(4)	-1.4(4)
C16	22.2(5)	16.7(5)	14.3(4)	3.0(4)	2.7(4)	-0.1(4)
C17	27.5(5)	18.6(5)	19.1(5)	-0.2(4)	3.8(4)	1.5(4)
C18	33.9(6)	20.1(5)	21.3(5)	-0.8(4)	0.6(4)	-4.9(5)
C19	22.4(5)	29.3(6)	22.3(5)	5.1(4)	-0.5(4)	-5.9(4)
C20	23.5(5)	29.1(6)	26.0(6)	0.1(5)	2.7(4)	4.2(5)
C21	26.0(5)	20.6(5)	20.5(5)	-1.9(4)	1.5(4)	2.5(4)

Table 4 Bond Lengths for 22srv128.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
F1	C19	1.3583(14)		C8	C15	1.5588(14)
O1	C1	1.2236(13)		C9	C10	1.3868(14)
N1	C1	1.3679(13)		C9	C14	1.3866(14)
N1	C2	1.4513(14)		C10	C11	1.3944(15)
N1	C8	1.4708(13)		C11	C12	1.3935(16)
N2	C3	1.4566(15)		C12	C13	1.3908(16)
N2	C4	1.3708(15)		C13	C14	1.3903(14)

N2	C7	1.3726(13)		C15	C16	1.5042(15)
C1	C14	1.4788(14)		C16	C17	1.3941(15)
C2	C3	1.5203(17)		C16	C21	1.3922(15)
C4	C5	1.3693(18)		C17	C18	1.3923(17)
C5	C6	1.4231(16)		C18	C19	1.3767(18)
C6	C7	1.3777(15)		C19	C20	1.3752(18)
C7	C8	1.5103(14)		C20	C21	1.3929(17)
C8	C9	1.5163(14)				

Table 5 Bond Angles for 22srv128.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C2	122.60(9)		C9	C8	C15	111.02(8)
C1	N1	C8	113.92(8)		C10	C9	C8	129.74(9)
C2	N1	C8	119.82(9)		C14	C9	C8	109.44(9)
C4	N2	C3	125.99(10)		C14	C9	C10	120.80(9)
C4	N2	C7	109.29(10)		C9	C10	C11	117.57(10)
C7	N2	C3	124.68(10)		C12	C11	C10	121.44(10)
O1	C1	N1	125.26(10)		C13	C12	C11	120.88(10)
O1	C1	C14	128.81(10)		C14	C13	C12	117.24(10)
N1	C1	C14	105.91(9)		C9	C14	C1	109.16(9)
N1	C2	C3	107.87(9)		C9	C14	C13	122.06(10)
N2	C3	C2	108.41(9)		C13	C14	C1	128.60(10)
C5	C4	N2	108.32(10)		C16	C15	C8	114.76(9)
C4	C5	C6	107.28(11)		C17	C16	C15	121.13(10)
C7	C6	C5	107.21(10)		C21	C16	C15	119.95(10)
N2	C7	C6	107.89(9)		C21	C16	C17	118.92(10)
N2	C7	C8	120.92(9)		C18	C17	C16	120.69(11)
C6	C7	C8	130.98(9)		C19	C18	C17	118.37(11)
N1	C8	C7	110.04(8)		F1	C19	C18	118.38(11)
N1	C8	C9	101.31(8)		F1	C19	C20	118.72(11)
N1	C8	C15	110.06(8)		C20	C19	C18	122.90(11)
C7	C8	C9	115.56(8)		C19	C20	C21	118.01(11)
C7	C8	C15	108.64(8)		C16	C21	C20	121.10(11)

Table 6 Selected Torsion Angles for 22srv128.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C2	C3	N2	-53.82(12)		C8	C7	N2	C3	-6.10(15)
N1	C8	C7	N2	4.49(13)		C8	C7	N2	C4	176.07(9)
C2	N1	C1	O1	-20.05(17)		C8	C15	C16	C17	-76.82(13)
C2	C3	N2	C4	-151.20(10)		C8	C15	C16	C21	103.18(12)
C2	C3	N2	C7	31.33(14)		C9	C8	N1	C1	2.79(11)
C3	C2	N1	C1	-97.11(12)		C9	C8	N1	C2	-156.19(9)

C3	C2	N1	C8	59.99(12)		C9	C8	C7	N2	118.43(10)
C6	C7	N2	C3	178.49(10)		C9	C8	C15	C16	-47.60(12)
C6	C7	N2	C4	0.66(12)		C10	C9	C8	N1	176.86(10)
C6	C7	C8	N1	178.70(10)		C10	C9	C8	C15	-66.30(14)
C6	C7	C8	C9	-67.36(14)		C14	C1	N1	C2	158.47(10)
C6	C7	C8	C15	58.15(14)		C14	C1	N1	C8	0.15(12)
C7	C8	N1	C1	125.56(9)		C14	C9	C8	N1	-4.86(11)
C7	C8	N1	C2	-33.42(12)		C14	C9	C8	C15	111.98(10)
C7	C8	C9	C10	57.98(14)		C15	C8	N1	C1	-114.75(10)
C7	C8	C9	C14	-123.73(10)		C15	C8	N1	C2	86.27(11)
C7	C8	C15	C16	-175.72(9)		C15	C8	C7	N2	-116.06(10)
C8	N1	C1	O1	-178.37(10)		C16	C15	C8	N1	63.74(12)

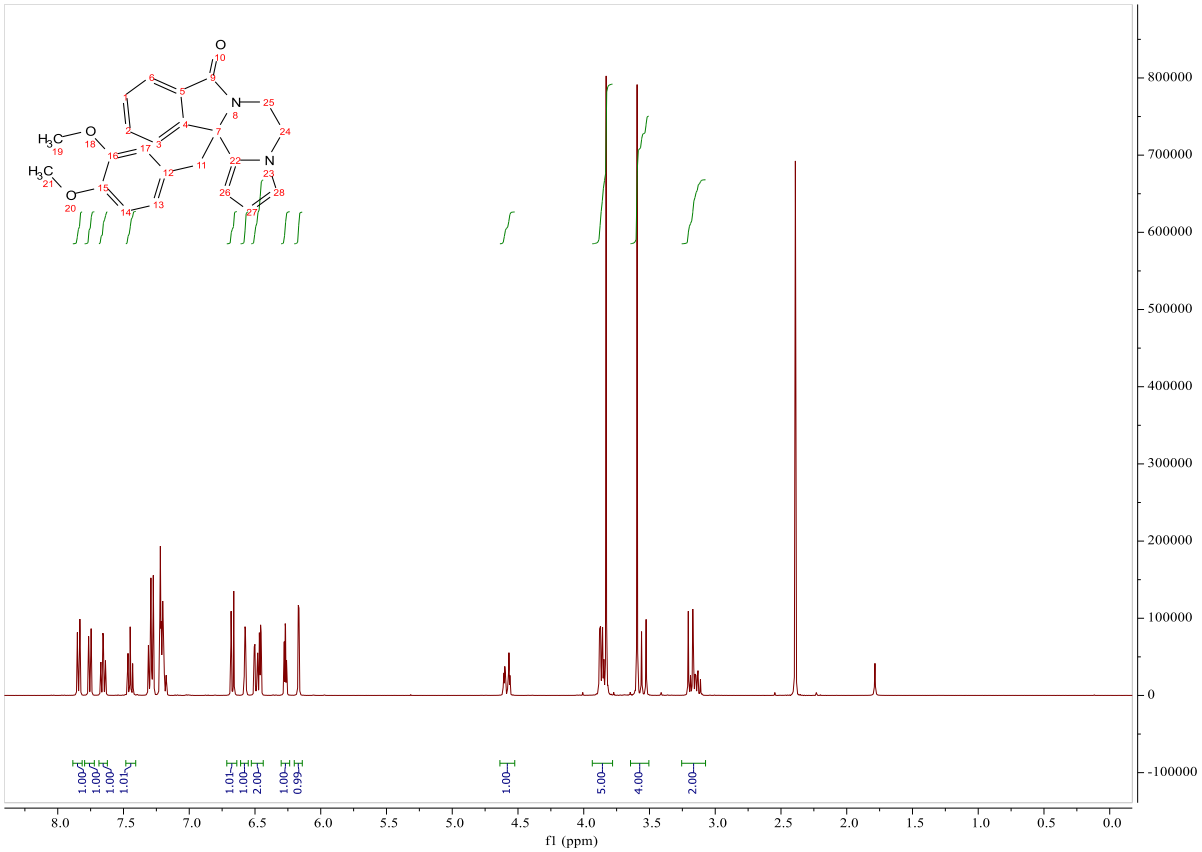
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv128.

Atom	***x***	***y***	***z***	**U(eq)**
H2A	4421(11)	-1350(20)	2472(10)	26(4)
H2B	4239(10)	-3220(20)	2947(10)	23(4)
H3A	5102(11)	-2170(20)	4234(10)	26(4)
H3B	5749(12)	-1790(20)	3535(10)	31(4)
H4	6538(11)	920(20)	4256(10)	30(4)
H5	6060(12)	4230(20)	4497(11)	38(4)
H6	4242(11)	4320(20)	4056(10)	30(4)
H10	2572(11)	3480(20)	4420(10)	29(4)
H11	1446(11)	2850(20)	5307(10)	32(4)
H12	880(11)	-100(20)	5446(11)	31(4)
H13	1464(11)	-2540(20)	4725(10)	27(4)
H15A	3494(10)	1510(20)	2229(10)	25(4)
H15B	3080(11)	3100(20)	2757(10)	25(4)
H17	2404(12)	-1100(20)	1716(10)	33(4)
H18	838(12)	-1890(20)	1124(11)	36(4)
H20	-120(13)	2800(20)	1993(11)	39(5)
H21	1446(11)	3600(20)	2609(10)	27(4)

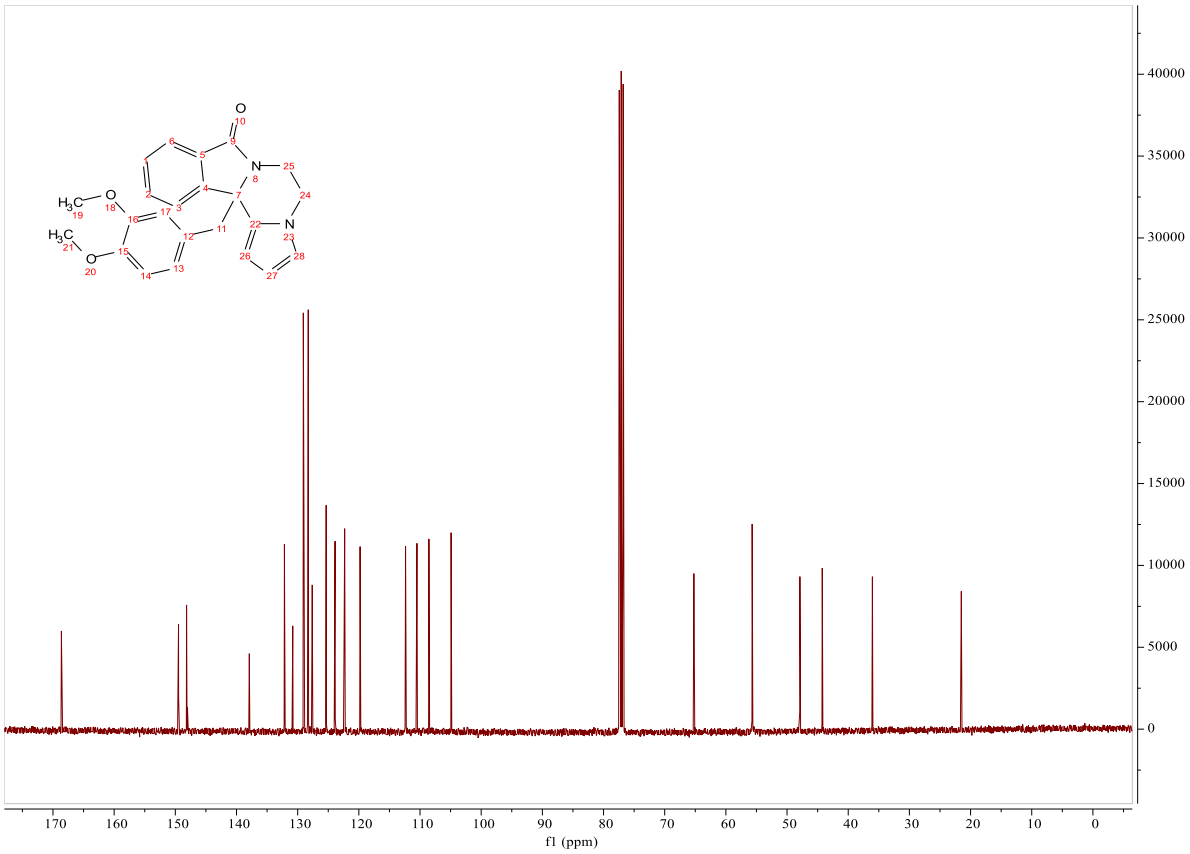
12*b*-(3,4-dimethoxybenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one

1g

^{1}H:



^{13}C: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30000
25000
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10000
5000
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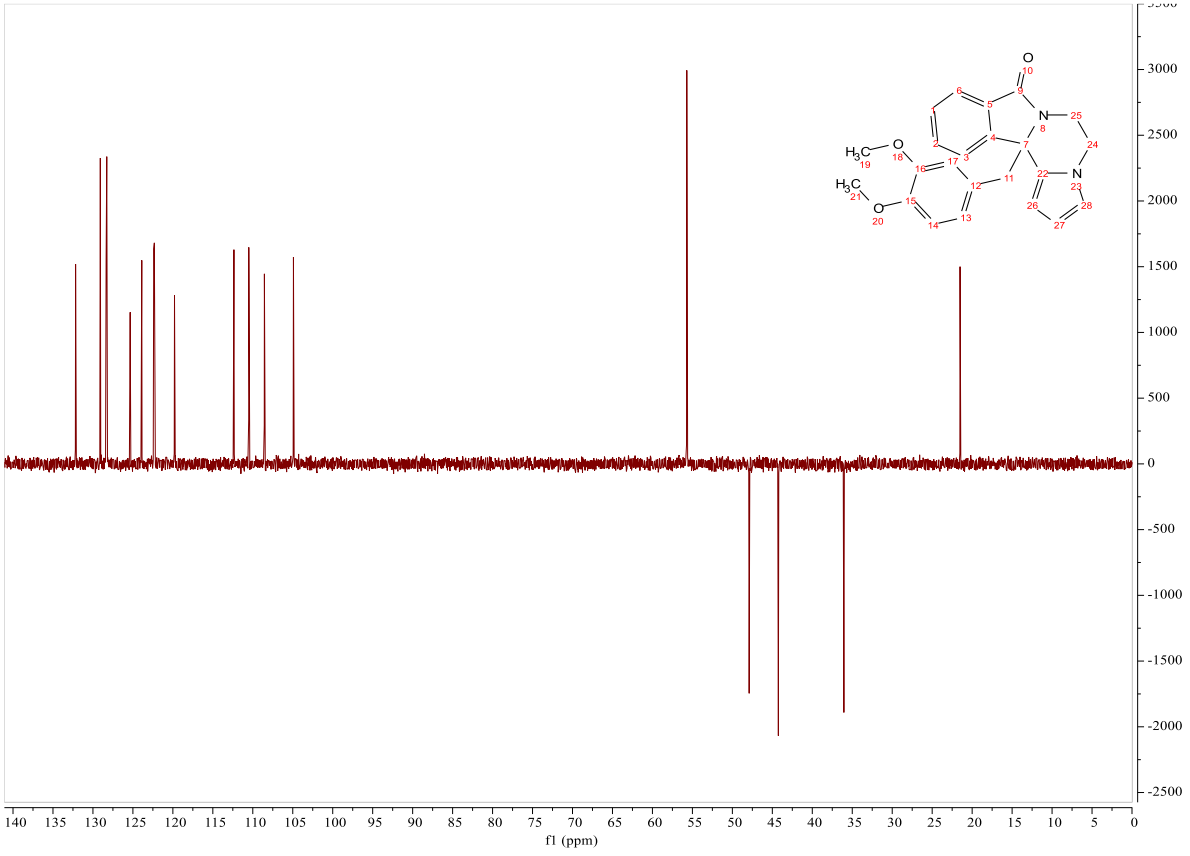
f1 (ppm)

DEPT-135: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0
-500
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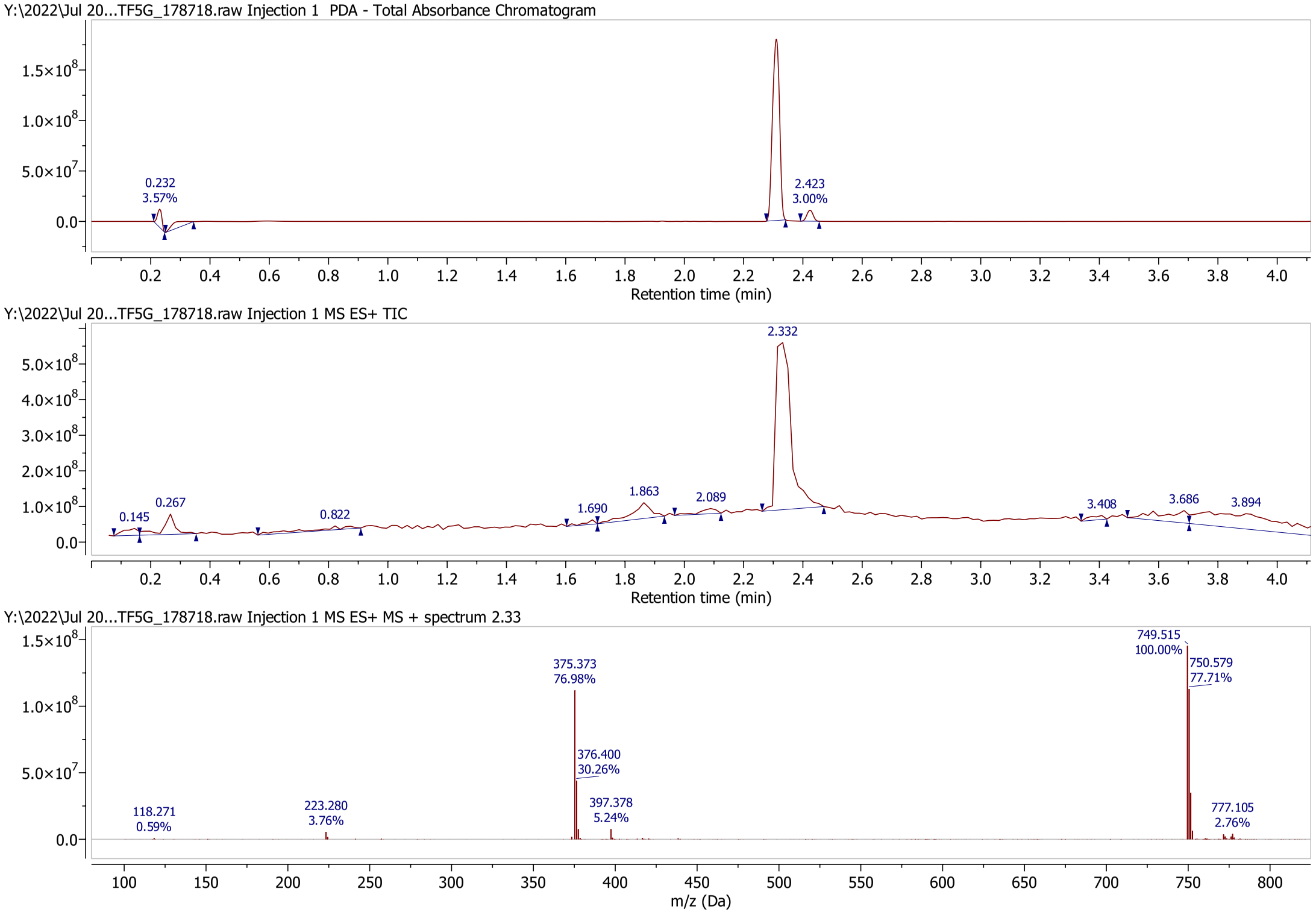
-2000
-2500
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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3.57%
2.423
3.00%
Retention time (min)
Y:\2022\Jul 20...TF5G_178718.raw Injection 1 MS ES+ TIC
2.332
0.145
0.267
0.822
1.690
1.863
2.089
3.408
3.686
3.894
Retention time (min)
Y:\2022\Jul 20...TF5G_178718.raw Injection 1 MS ES+ MS + spectrum 2.33
749.515
100.00%
375.373
76.98%
750.579
77.71%
376.400
30.26%
397.378
5.24%
223.280
3.76%
118.271
0.59%
777.105
2.76%
m/z (Da)

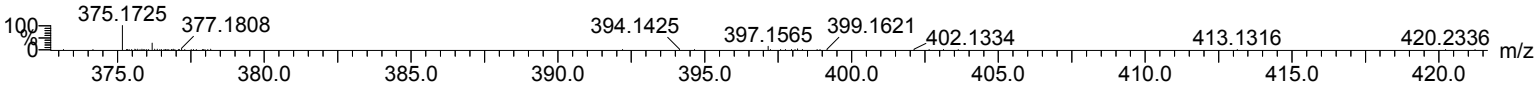
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
3344 formula(e) evaluated with 27 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 F: 0-6

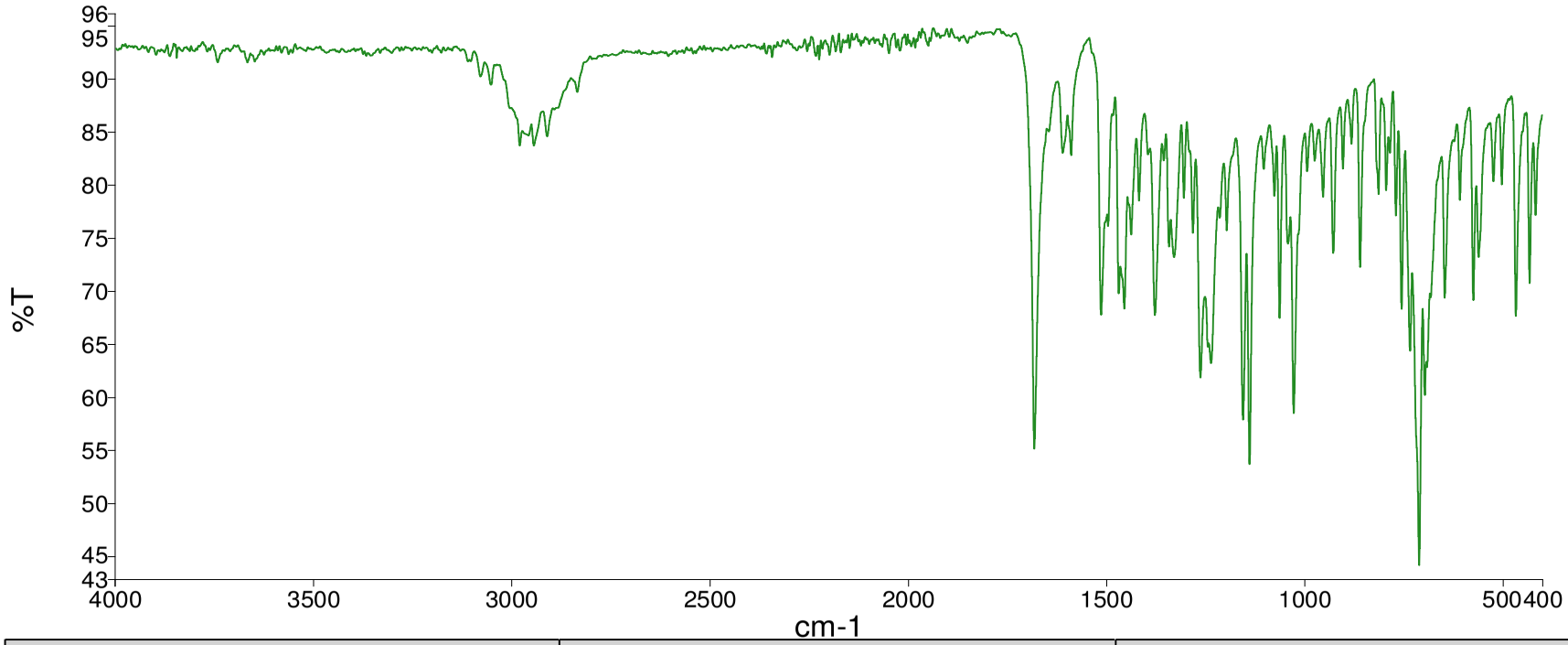
21-Jul-2022
MTF_MTF5G_179345 470 (3.951) Cm (468:470)

21-Jul-2022
1: TOF MS ES+
2.58e+004



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
375.1725	375.1723	0.2	0.5	-6.5	389.1	22.661	0.00	C H25 N10 O10 F2
	375.1750	-2.5	-6.7	-9.5	389.3	22.861	0.00	C H25 N8 O7 F6
	375.1716	0.9	2.4	2.5	381.8	15.405	0.00	C10 H22 N8 O4 F3
	375.1754	-2.9	-7.7	-2.5	381.1	14.683	0.00	C11 H27 N2 O7 F4
	375.1727	-0.2	-0.5	0.5	380.5	14.062	0.00	C11 H27 N4 O10
	375.1741	-1.6	-4.3	5.5	379.1	12.653	0.00	C12 H23 N8 O6
	375.1719	0.6	1.6	-1.5	380.4	13.933	0.00	C12 H25 N2 O4 F6
	375.1732	-0.7	-1.9	3.5	379.8	13.365	0.00	C13 H21 N6 F6
	375.1705	2.0	5.3	6.5	379.2	12.755	0.00	C13 H21 N8 O3 F2
	375.1743	-1.8	-4.8	1.5	378.0	11.526	0.00	C14 H26 N2 O6 F3
	375.1707	1.8	4.8	2.5	377.9	11.473	0.00	C15 H24 N2 O3 F5
	375.1732	-0.7	-1.9	5.5	374.4	7.922	0.04	C17 H25 N2 O5 F2
	375.1745	-2.0	-5.3	10.5	372.8	6.331	0.18	C18 H21 N6 O F2
	375.1696	2.9	7.7	6.5	374.9	8.431	0.02	C18 H23 N2 O2 F4
	375.1720	0.5	1.3	9.5	370.2	3.807	2.22	C20 H24 N2 O4 F
	375.1747	-2.2	-5.9	6.5	372.2	5.768	0.31	C20 H24 O F5
	375.1733	-0.8	-2.1	14.5	367.8	1.404	24.56	C21 H20 N6 F
	375.1736	-1.1	-2.9	10.5	367.3	0.852	42.67	C23 H23 F4
	375.1709	1.6	4.3	13.5	367.7	1.231	29.21	C23 H23 N2 O3
	375.1749	-2.4	-6.4	17.5	371.3	4.848	0.78	C28 H23 O
	375.1712	1.3	3.5	-2.5	386.4	19.998	0.00	C4 H24 N10 O9 F
	375.1739	-1.4	-3.7	-5.5	386.5	20.084	0.00	C4 H24 N8 O6 F5
	375.1714	1.1	2.9	-6.5	384.8	18.409	0.00	C6 H27 N4 O9 F4
	375.1700	2.5	6.7	1.5	384.2	17.769	0.00	C7 H23 N10 O8
	375.1728	-0.3	-0.8	-1.5	384.2	17.808	0.00	C7 H23 N8 O5 F4
	375.1752	-2.7	-7.2	1.5	382.1	15.675	0.00	C9 H24 N8 O7 F
	375.1703	2.2	5.9	-2.5	383.0	16.524	0.00	C9 H26 N4 O8 F3

Analyst Lenny Lauchlan
Date 28 June 2022 12:53



Sample Name	Description	Quality Checks
MTF 005G	Sample 020 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

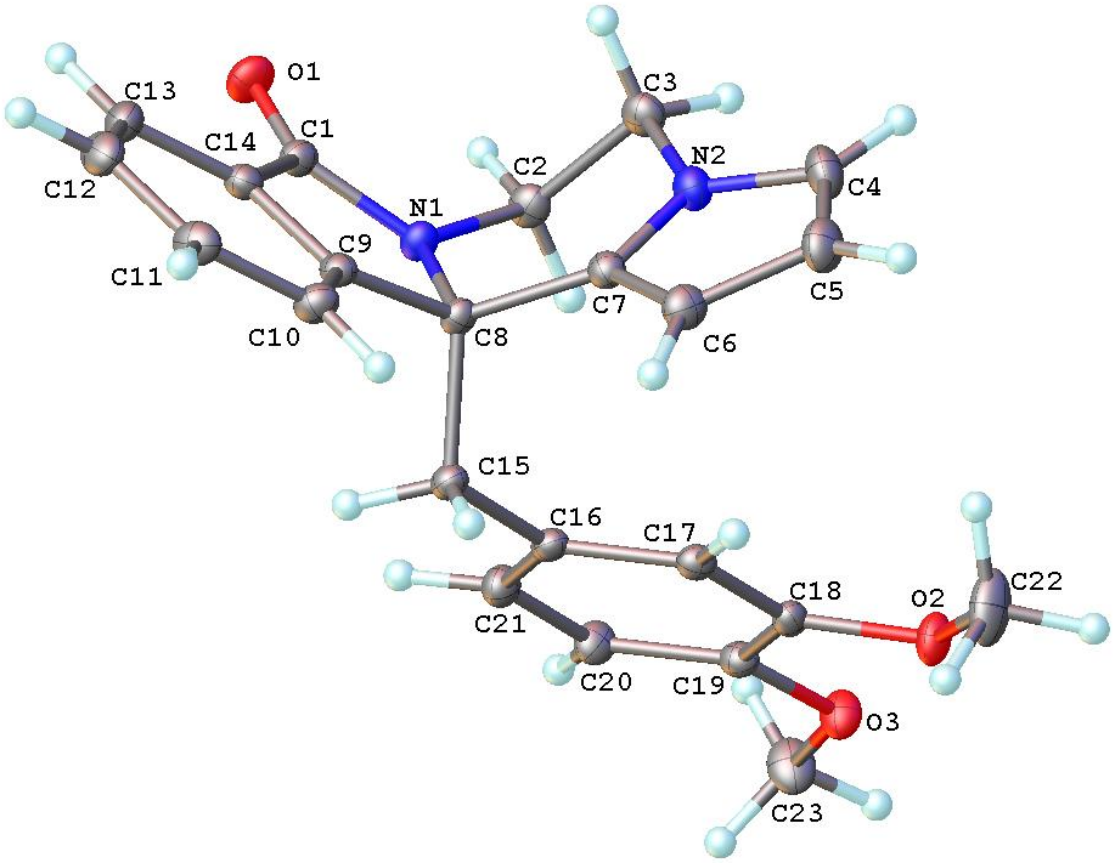


Table 1 Crystal data and structure refinement for 22srv182.	
Identification code	22srv182
Empirical formula	$C_{30}H_{30}N_2O_3$
Formula weight	466.56
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.2621(5)
b/Å	7.3267(4)
c/Å	36.416(2)
α/°	90
β/°	94.354(2)
γ/°	90
Volume/Å^3	2464.1(2)

Z	4
ρ_{calc}g/cm^3	1.258
μ/mm^{-1}	0.081
F(000)	992.0
Crystal size/mm^3	0.21 × 0.03 × 0.02
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.41 to 60
Index ranges	-13 ≤ h ≤ 13, -10 ≤ k ≤ 10, -51 ≤ l ≤ 51
Reflections collected	86517
Independent reflections	7189 [R_{int} = 0.0837, R_{sigma} = 0.0445]
Data/restraints/parameters	7189/0/436
Goodness-of-fit on F^2	1.080
Final R indexes [I>=2σ (I)]	R_1 = 0.0529, wR_2 = 0.1212
Final R indexes [all data]	R_1 = 0.0739, wR_2 = 0.1294
Largest diff. peak/hole / e Å^{-3}	0.53/-0.31

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 22srv182. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	2095.3(11)	14469.7(13)	3930.5(3)	20.1(2)
O2	3576.9(10)	6709.6(13)	2363.9(3)	18.1(2)
O3	1764.0(10)	8635.0(13)	1963.7(2)	18.3(2)
N1	2494.0(12)	11735.6(14)	3641.7(3)	13.6(2)
N2	5081.4(12)	10209.9(16)	3487.9(3)	17.0(2)
C1	2184.4(13)	12800.8(18)	3935.1(3)	14.5(2)
C2	3250.9(15)	12495.0(18)	3339.6(4)	16.4(3)
C3	4862.7(15)	12154.5(19)	3414.4(4)	18.0(3)
C4	6315.1(15)	9241(2)	3434.3(4)	22.2(3)
C5	6164.0(15)	7529(2)	3577.6(4)	22.9(3)
C6	4795.9(15)	7449.3(19)	3727.7(4)	18.8(3)
C7	4153.4(13)	9128.2(18)	3668.4(3)	13.7(2)
C8	2642.4(13)	9776.5(17)	3735.4(3)	12.5(2)
C9	2327.5(13)	9785.5(17)	4138.5(3)	13.0(2)
C10	2321.7(15)	8347.9(18)	4385.2(4)	17.0(3)
C11	2011.2(15)	8746(2)	4745.1(4)	19.4(3)
C12	1708.5(15)	10522(2)	4854.4(4)	20.3(3)
C13	1697.8(14)	11953.1(19)	4605.4(4)	17.9(3)

C14	2010.3(13)	11549.6(17)	4246.1(3)	14.2(2)
C15	1457.9(14)	8619.6(17)	3516.7(3)	13.8(2)
C16	1501.6(13)	8651.0(17)	3103.4(3)	13.3(2)
C17	2543.0(13)	7623.2(17)	2932.5(3)	13.5(2)
C18	2601.9(13)	7654.0(17)	2554.2(3)	13.2(2)
C19	1610.8(13)	8722.3(17)	2333.8(3)	13.9(2)
C20	581.8(14)	9733.7(19)	2500.2(4)	16.8(3)
C21	528.5(14)	9687.6(18)	2883.7(4)	16.5(3)
C22	4551.3(19)	5521(3)	2569.8(5)	31.0(4)
C23	718.4(16)	9599(2)	1731.2(4)	23.6(3)
C1S	7775.4(16)	4543(2)	4368.4(4)	23.9(3)
C2S	7945.3(17)	2756(2)	4250.6(4)	25.2(3)
C3S	6891.5(18)	1435(2)	4294.4(4)	28.1(3)
C4S	5638.1(18)	1899(2)	4458.6(5)	30.9(4)
C5S	5438.4(17)	3685(3)	4570.7(5)	31.9(4)
C6S	6488.2(17)	4991(2)	4526.9(5)	28.1(3)
C7S	8933.3(19)	5955(3)	4334.2(5)	31.7(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv182. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	26.6(5)	11.3(4)	22.6(5)	-0.5(4)	3.1(4)	1.7(4)
O2	19.3(5)	19.4(5)	16.1(4)	1.4(4)	4.2(3)	8.3(4)
O3	18.9(5)	23.4(5)	12.5(4)	1.6(4)	0.6(3)	4.0(4)
N1	16.9(5)	10.6(5)	13.6(5)	1.3(4)	2.8(4)	0.3(4)
N2	15.9(5)	18.7(5)	16.9(5)	1.1(4)	3.4(4)	0.3(4)
C1	13.5(6)	13.3(6)	16.7(6)	-1.2(5)	0.6(4)	0.3(4)
C2	20.7(6)	13.5(6)	15.5(6)	3.1(5)	3.9(5)	-1.1(5)
C3	18.6(6)	16.8(6)	18.9(6)	2.4(5)	3.9(5)	-2.2(5)
C4	15.7(6)	30.0(8)	21.3(7)	1.1(6)	5.4(5)	3.3(6)
C5	18.9(7)	26.0(7)	23.8(7)	0.1(6)	2.3(5)	8.4(6)
C6	18.4(6)	17.5(6)	20.1(6)	0.8(5)	-0.5(5)	2.8(5)
C7	14.1(6)	14.7(6)	12.3(5)	-0.2(5)	0.8(4)	0.1(5)
C8	15.0(6)	10.1(5)	12.7(5)	0.1(4)	1.8(4)	0.5(4)
C9	12.7(5)	13.7(6)	12.6(5)	-0.7(4)	0.2(4)	-1.5(4)
C10	20.5(6)	14.2(6)	16.1(6)	0.0(5)	0.9(5)	-1.5(5)
C11	22.0(7)	21.2(7)	15.0(6)	2.9(5)	1.3(5)	-3.7(5)
C12	21.4(6)	25.7(7)	13.9(6)	-2.4(5)	2.9(5)	-2.2(6)
C13	17.7(6)	18.6(6)	17.5(6)	-4.3(5)	2.8(5)	0.0(5)
C14	13.0(5)	14.3(6)	15.4(6)	-0.5(5)	0.7(4)	-1.4(5)
C15	15.5(6)	12.7(6)	13.5(6)	-1.3(5)	1.8(4)	-1.1(5)
C16	14.8(6)	12.2(5)	12.9(5)	-1.9(4)	1.4(4)	-2.0(4)
C17	13.9(6)	11.5(5)	14.9(6)	0.5(5)	-0.2(4)	-0.3(5)
C18	13.1(5)	11.0(5)	15.8(6)	-1.3(5)	2.5(4)	-0.2(4)

C19	14.4(6)	15.0(6)	12.2(5)	0.3(5)	0.2(4)	-1.8(5)
C20	15.7(6)	17.6(6)	16.6(6)	0.4(5)	-1.3(5)	4.3(5)
C21	15.9(6)	16.3(6)	17.2(6)	-1.3(5)	1.5(5)	2.2(5)
C22	34.1(9)	35.8(9)	23.9(8)	7.1(7)	8.3(6)	22.3(7)
C23	21.0(7)	33.2(8)	16.2(6)	4.8(6)	-1.9(5)	5.7(6)
C1S	22.5(7)	29.2(8)	19.5(7)	1.1(6)	-1.7(5)	1.4(6)
C2S	25.7(7)	30.7(8)	18.7(7)	-1.5(6)	-1.8(5)	4.6(6)
C3S	32.8(8)	27.5(8)	22.1(7)	-1.7(6)	-9.8(6)	0.9(6)
C4S	24.0(8)	36.0(9)	31.1(8)	3.0(7)	-9.0(6)	-6.7(7)
C5S	18.9(7)	42.3(10)	34.1(9)	-2.3(7)	0.0(6)	-0.4(7)
C6S	22.5(7)	30.8(9)	30.8(8)	-2.0(7)	0.9(6)	2.4(6)
C7S	26.5(8)	33.3(9)	35.8(9)	-1.0(7)	5.1(7)	-3.5(7)

Table 4 Bond Lengths for 22srv182.

Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
O1	C1	1.2256(16)		C9	C14	1.3885(17)
O2	C18	1.3673(15)		C10	C11	1.3937(19)
O2	C22	1.4253(18)		C11	C12	1.396(2)
O3	C19	1.3676(15)		C12	C13	1.386(2)
O3	C23	1.4244(16)		C13	C14	1.3931(18)
N1	C1	1.3710(16)		C15	C16	1.5089(17)
N1	C2	1.4588(16)		C16	C17	1.4055(17)
N1	C8	1.4794(16)		C16	C21	1.3854(18)
N2	C3	1.4610(18)		C17	C18	1.3833(17)
N2	C4	1.3718(17)		C18	C19	1.4097(17)
N2	C7	1.3727(16)		C19	C20	1.3829(18)
C1	C14	1.4753(18)		C20	C21	1.4016(18)
C2	C3	1.5177(19)		C1S	C2S	1.391(2)
C4	C5	1.369(2)		C1S	C6S	1.402(2)
C5	C6	1.419(2)		C1S	C7S	1.502(2)
C6	C7	1.3763(18)		C2S	C3S	1.392(2)
C7	C8	1.5151(17)		C3S	C4S	1.388(2)
C8	C9	1.5184(17)		C4S	C5S	1.387(3)
C8	C15	1.5568(17)		C5S	C6S	1.382(2)
C9	C10	1.3847(18)				

Table 5 Bond Angles for 22srv182.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C18	O2	C22	117.31(11)		C9	C10	C11	117.53(12)
C19	O3	C23	116.48(10)		C10	C11	C12	121.56(13)
C1	N1	C2	120.76(11)		C13	C12	C11	120.71(12)
C1	N1	C8	113.19(10)		C12	C13	C14	117.53(13)

C2	N1	C8	120.16(10)		C9	C14	C1	108.90(11)
C4	N2	C3	125.73(12)		C9	C14	C13	121.74(12)
C4	N2	C7	109.15(11)		C13	C14	C1	129.18(12)
C7	N2	C3	124.59(11)		C16	C15	C8	115.51(10)
O1	C1	N1	125.10(12)		C17	C16	C15	120.30(11)
O1	C1	C14	128.27(12)		C21	C16	C15	121.24(11)
N1	C1	C14	106.63(11)		C21	C16	C17	118.45(11)
N1	C2	C3	108.93(11)		C18	C17	C16	120.83(12)
N2	C3	C2	108.30(11)		O2	C18	C17	125.03(11)
C5	C4	N2	108.02(12)		O2	C18	C19	114.78(11)
C4	C5	C6	107.75(13)		C17	C18	C19	120.18(11)
C7	C6	C5	106.89(13)		O3	C19	C18	115.04(11)
N2	C7	C6	108.19(11)		O3	C19	C20	125.69(11)
N2	C7	C8	121.04(11)		C20	C19	C18	119.26(11)
C6	C7	C8	130.43(12)		C19	C20	C21	120.09(12)
N1	C8	C7	109.74(10)		C16	C21	C20	121.19(12)
N1	C8	C9	101.39(9)		C2S	C1S	C6S	117.84(15)
N1	C8	C15	111.15(10)		C2S	C1S	C7S	121.65(14)
C7	C8	C9	113.87(10)		C6S	C1S	C7S	120.50(15)
C7	C8	C15	111.76(10)		C1S	C2S	C3S	121.49(15)
C9	C8	C15	108.50(10)		C4S	C3S	C2S	119.73(16)
C10	C9	C8	129.38(11)		C5S	C4S	C3S	119.49(16)
C10	C9	C14	120.91(12)		C6S	C5S	C4S	120.55(16)
C14	C9	C8	109.71(11)		C5S	C6S	C1S	120.87(16)

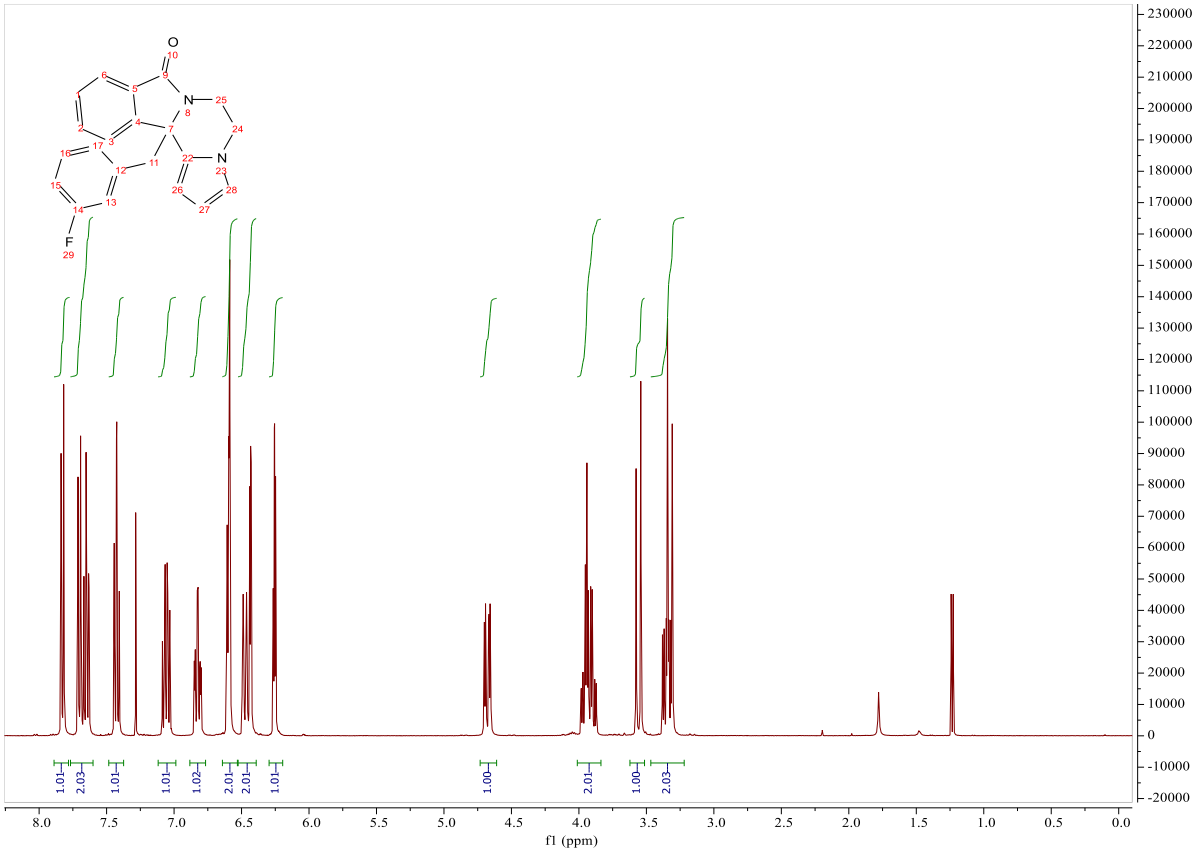
Table 6 Selected Torsion Angles for 22srv182.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C2	C3	N2	52.70(14)		C8	C15	C16	C17	76.66(15)
N1	C8	C7	N2	-9.99(16)		C8	C15	C16	C21	-103.17(14)
C2	C3	N2	C4	154.36(13)		C9	C8	N1	C1	1.57(13)
C2	C3	N2	C7	-34.97(17)		C9	C8	N1	C2	154.78(11)
C3	C2	N1	C1	93.45(14)		C9	C8	C7	N2	-122.84(12)
C3	C2	N1	C8	-57.72(15)		C9	C8	C15	C16	172.96(10)
C6	C7	N2	C3	-172.48(12)		C10	C9	C8	N1	-178.87(13)
C6	C7	N2	C4	-0.48(15)		C10	C9	C8	C15	64.03(16)
C6	C7	C8	N1	177.51(13)		C14	C9	C8	N1	1.33(13)
C6	C7	C8	C9	64.67(18)		C14	C9	C8	C15	-115.77(11)
C6	C7	C8	C15	-58.72(18)		C15	C8	N1	C1	116.73(11)
C7	C8	N1	C1	-119.14(11)		C15	C8	N1	C2	-90.07(13)
C7	C8	N1	C2	34.06(15)		C15	C8	C7	N2	113.78(13)
C7	C8	C9	C10	-61.10(17)		C16	C15	C8	N1	62.30(14)
C7	C8	C9	C14	119.10(12)		C17	C18	O2	C22	3.8(2)
C7	C8	C15	C16	-60.68(14)		C18	C19	O3	C23	175.86(12)
C8	C7	N2	C3	13.53(19)		C19	C18	O2	C22	-176.38(13)
C8	C7	N2	C4	-174.48(11)		C20	C19	O3	C23	-3.52(19)

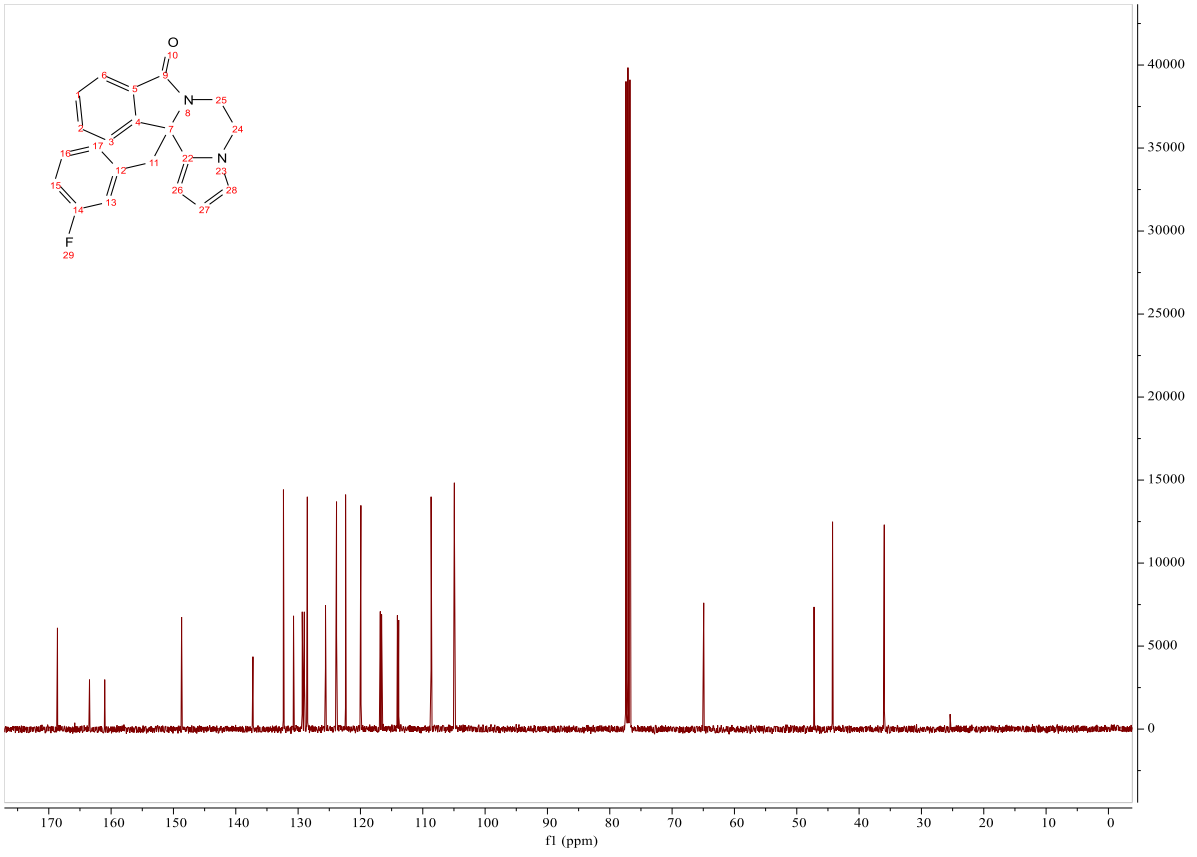
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv182.				
Atom	***x***	***y***	***z***	**U(eq)**
H2A	3050(17)	13810(20)	3331(4)	17(4)
H2B	2860(17)	11900(20)	3108(4)	15(4)
H3A	5239(18)	12860(20)	3633(4)	18(4)
H3B	5415(19)	12510(20)	3200(5)	24(4)
H4	7081(19)	9770(20)	3304(5)	23(4)
H5	6820(20)	6540(30)	3565(5)	34(5)
H6	4341(19)	6320(20)	3836(5)	27(5)
H10	2500(17)	7130(20)	4309(4)	16(4)
H11	2028(19)	7750(20)	4921(5)	26(4)
H12	1498(19)	10770(20)	5106(5)	27(4)
H13	1497(18)	13230(20)	4670(5)	22(4)
H15A	1579(17)	7360(20)	3610(4)	18(4)
H15B	499(17)	9080(20)	3588(4)	14(4)
H17	3239(18)	6890(20)	3079(4)	20(4)
H20	-101(19)	10480(30)	2354(5)	27(5)
H21	-216(19)	10430(20)	2993(5)	27(5)
H22A	5150(20)	4990(30)	2382(5)	39(5)
H22B	3960(20)	4450(30)	2682(5)	38(5)
H22C	5170(20)	6190(30)	2753(6)	37(5)
H23A	754(19)	10900(30)	1789(5)	26(4)
H23B	-250(20)	9120(30)	1771(5)	29(5)
H23C	970(20)	9330(30)	1482(5)	32(5)
H2S	8850(20)	2410(30)	4138(5)	37(5)
H3S	7010(20)	170(30)	4215(5)	32(5)
H4S	4890(20)	980(30)	4501(6)	45(6)
H5S	4510(20)	4050(30)	4684(6)	52(6)
H6S	6386(19)	6220(30)	4603(5)	25(4)
H7SA	8560(30)	7080(30)	4214(6)	59(7)
H7SB	9740(20)	5480(30)	4185(6)	42(6)
H7SC	9350(20)	6310(30)	4593(6)	48(6)

12*b*-(3-fluorobenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1h**

^{1}H:



^{13}C:



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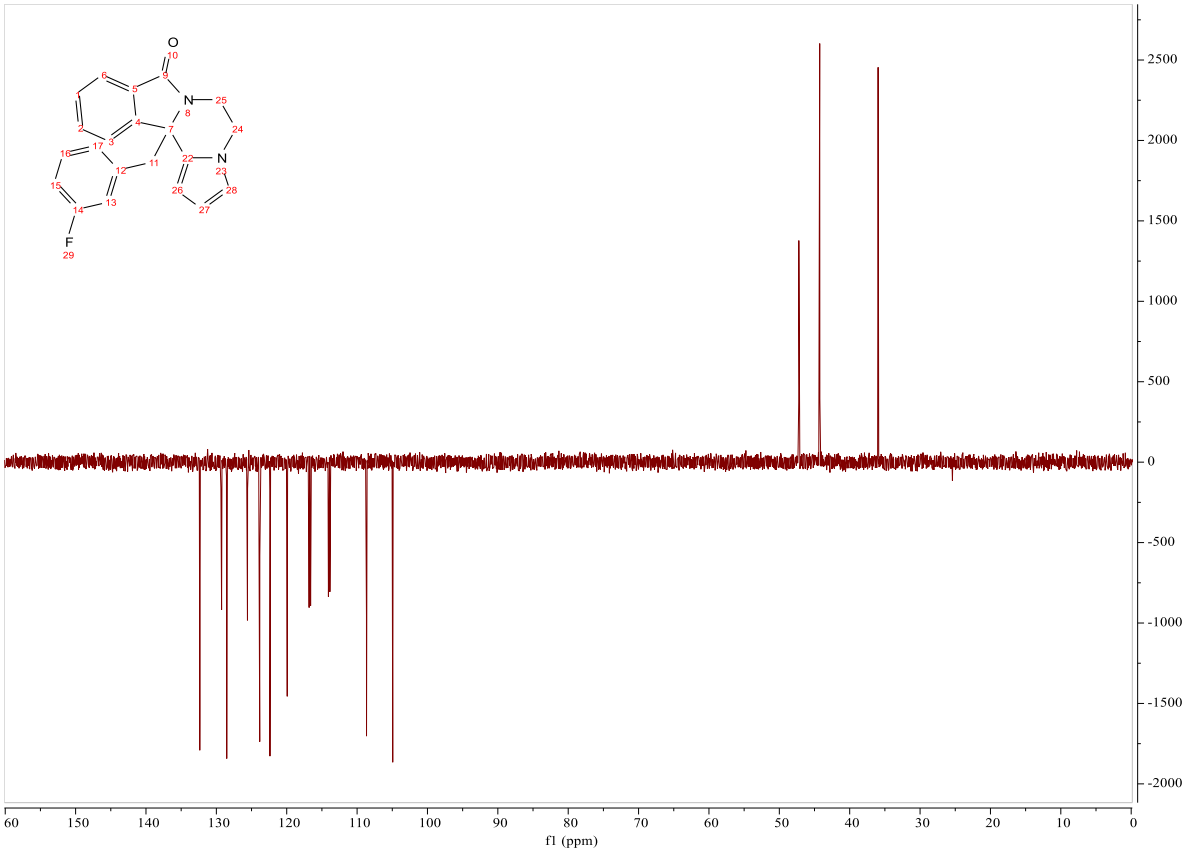
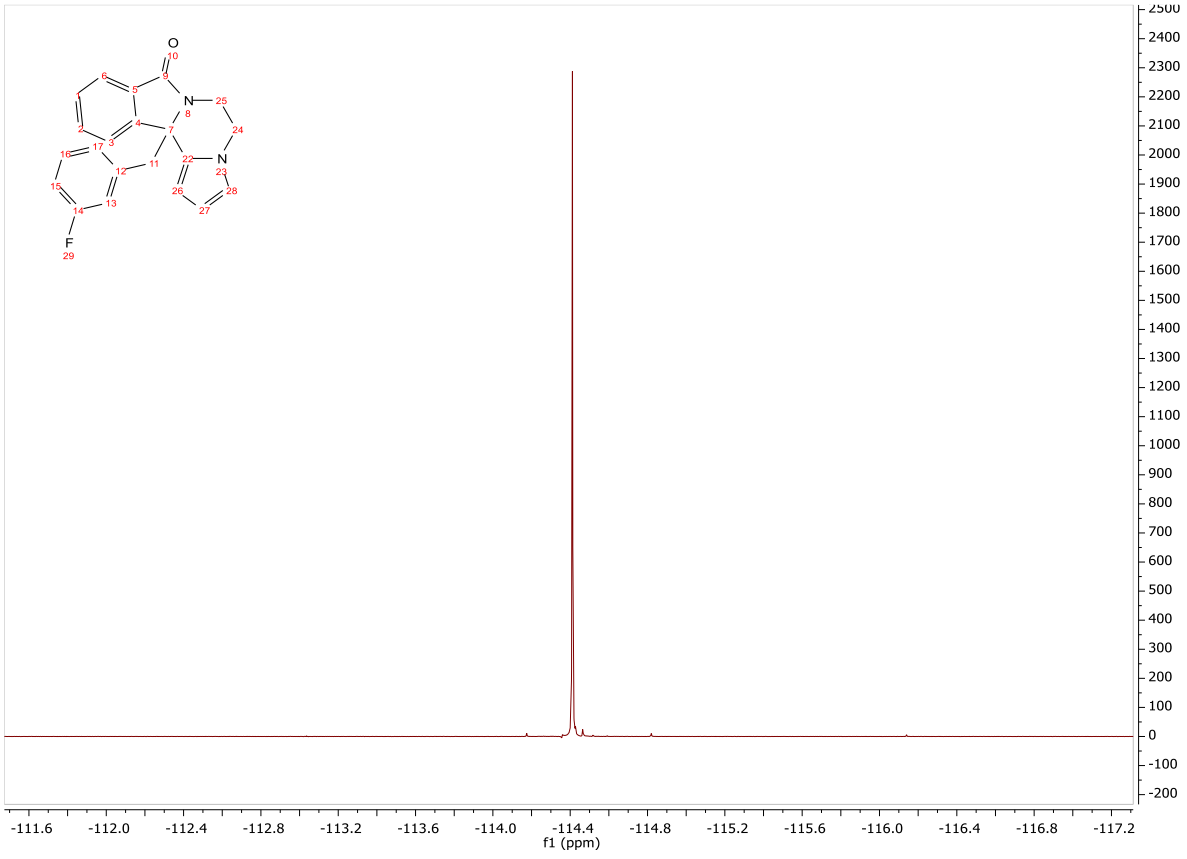

O
10
9
N
8
25
24
7
22
N
23
26
28
27
6
5
4
3
2
1
17
16
15
14
13
12
11
F
29
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{19}F:


O
10
9
N
8
25
24
7
22
N
23
26
28
27
6
5
4
3
2
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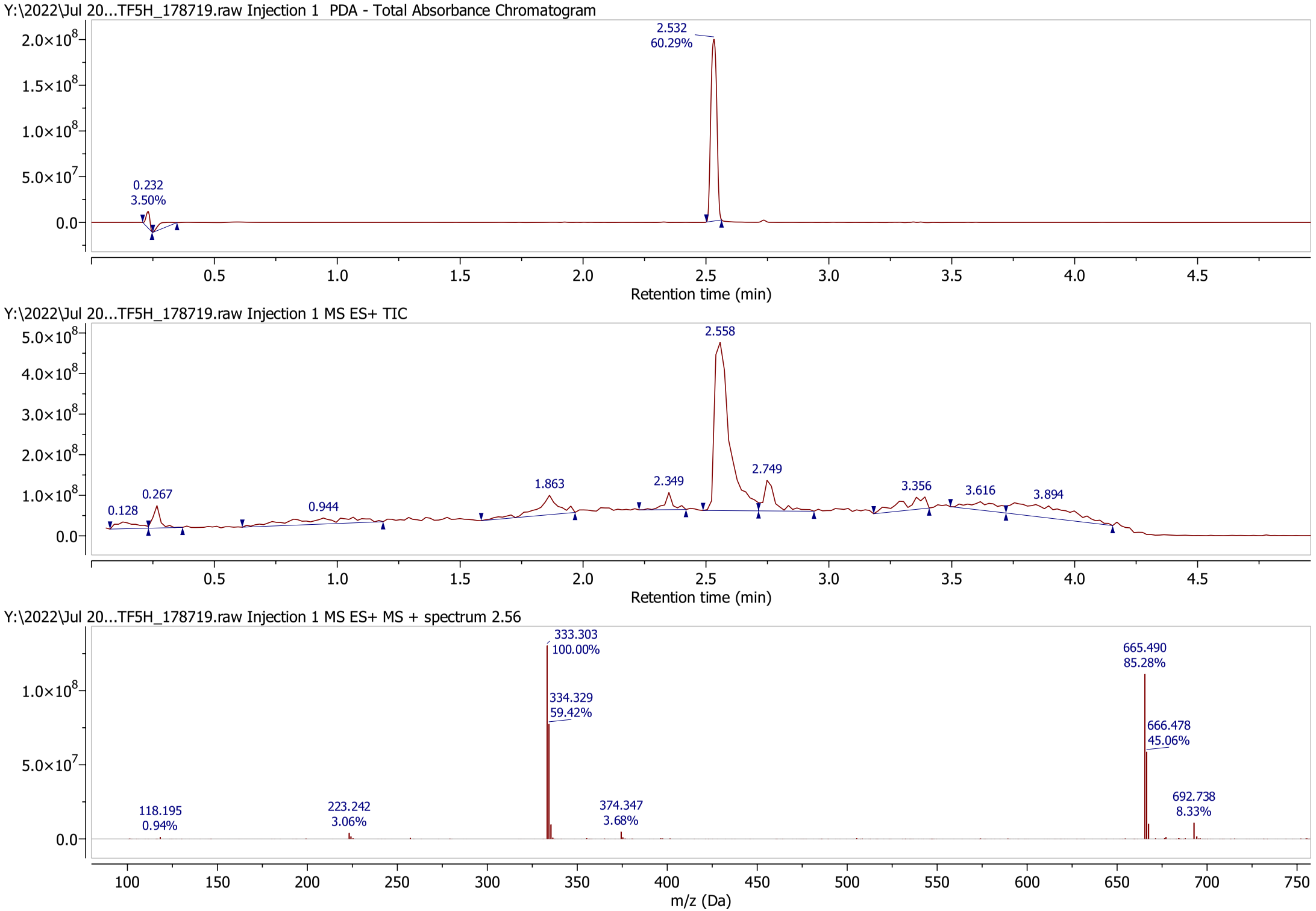
17
16
15
14
13
12
11
F
29
2500
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
-111.6
-112.0
-112.4
-112.8
-113.2
-113.6
-114.0
-114.4
-114.8
-115.2
-115.6
-116.0
-116.4
-116.8
-117.2
f1 (ppm)


Y:\2022\Jul 20...TF5H_178719.raw Injection 1 PDA - Total Absorbance Chromatogram
2.532
60.29%
0.232
3.50%
Retention time (min)
Y:\2022\Jul 20...TF5H_178719.raw Injection 1 MS ES+ TIC
2.558
0.128
0.267
0.944
1.863
2.349
2.749
3.356
3.616
3.894
Retention time (min)
Y:\2022\Jul 20...TF5H_178719.raw Injection 1 MS ES+ MS + spectrum 2.56
333.303
100.00%
334.329
59.42%
665.490
85.28%
666.478
45.06%
692.738
8.33%
118.195
0.94%
223.242
3.06%
374.347
3.68%
m/z (Da)

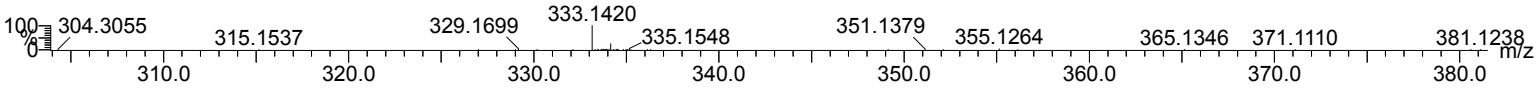
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
3006 formula(e) evaluated with 24 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 F: 0-6

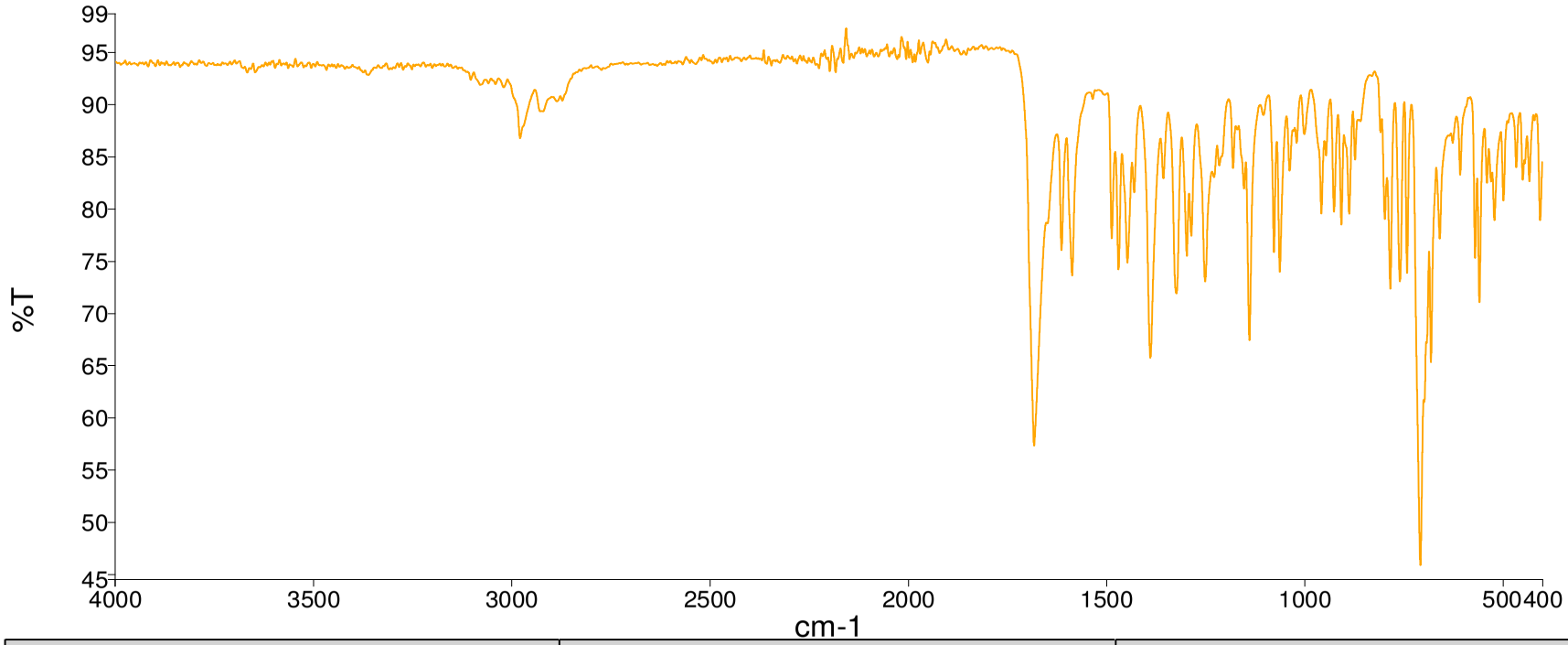
21-Jul-2022
MTF_MTF5H_179346 511 (4.295) Cm (511:513)

21-Jul-2022
1: TOF MS ES+
1.81e+004



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
333.1420	333.1422	-0.2	-0.6	-1.5	277.2	19.433	0.00	C5 H18 N8 O3 F5
	333.1422	-0.2	-0.6	0.5	273.7	15.953	0.00	C9 H22 N4 O8 F
	333.1424	-0.4	-1.2	9.5	268.5	10.736	0.00	C13 H17 N8 O3
	333.1415	0.5	1.5	9.5	262.9	5.142	0.58	C18 H19 N2 O2 F2
	333.1426	-0.6	-1.8	5.5	268.0	10.249	0.00	C15 H20 N2 O3 F3
	333.1411	0.9	2.7	2.5	275.0	17.233	0.00	C8 H17 N8 O2 F4
	333.1410	1.0	3.0	4.5	270.5	12.753	0.00	C12 H21 N4 O7
	333.1409	1.1	3.3	-6.5	277.9	20.169	0.00	C4 H22 N4 O7 F5
	333.1433	-1.3	-3.9	-5.5	279.1	21.305	0.00	C2 H19 N8 O4 F6
	333.1433	-1.3	-3.9	-3.5	276.2	18.460	0.00	C6 H23 N4 O9 F2
	333.1406	1.4	4.2	-2.5	278.6	20.786	0.00	C2 H19 N10 O7 F2
	333.1435	-1.5	-4.5	5.5	272.2	14.454	0.00	C10 H18 N8 O4 F
	333.1403	1.7	5.1	13.5	257.8	0.033	96.79	C21 H18 N2 O F
	333.1437	-1.7	-5.1	1.5	271.8	14.064	0.00	C12 H21 N2 O4 F4
	333.1402	1.8	5.4	2.5	271.6	13.832	0.00	C13 H19 N2 O F6
	333.1399	2.1	6.3	6.5	272.3	14.561	0.00	C11 H16 N8 O F3
	333.1442	-2.2	-6.6	-3.5	278.9	21.093	0.00	C H21 N10 O10
	333.1397	2.3	6.9	-2.5	276.0	18.228	0.00	C7 H21 N4 O6 F4
	333.1395	2.5	7.5	1.5	276.5	18.676	0.00	C5 H18 N10 O6 F
	333.1445	-2.5	-7.5	-7.5	278.2	20.468	0.00	C3 H24 N4 O10 F3
	333.1446	-2.6	-7.8	1.5	275.1	17.334	0.00	C7 H19 N8 O5 F2
	333.1392	2.8	8.4	17.5	261.4	3.643	2.62	C24 H17 N2
	333.1449	-2.9	-8.7	-2.5	274.8	17.049	0.00	C9 H22 N2 O5 F5
	333.1390	3.0	9.0	6.5	268.4	10.615	0.00	C16 H18 N2 F5

Analyst Lenny Lauchlan
Date 28 June 2022 12:55



Sample Name	Description	Quality Checks
MTF 005H	Sample 021 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

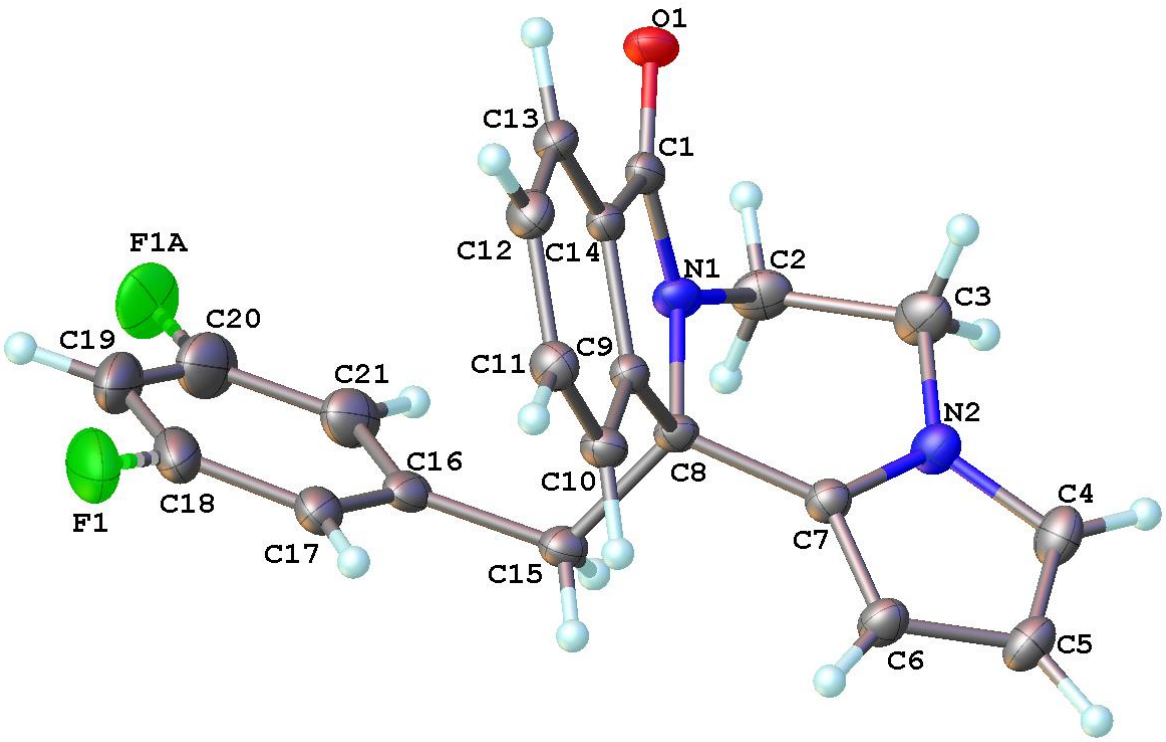


Table 1 Crystal data and structure refinement for 22srv124.	
Identification code	22srv124
Empirical formula	$C_{21}H_{17}FN_2O$
Formula weight	332.36
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.0341(3)
b/Å	9.5589(2)
c/Å	14.0998(4)
α/°	90
β/°	119.3469(9)
γ/°	90
Volume/Å^3	1648.76(7)
Z	4

ρ_{calc}g/cm^3	1.339
μ/mm^{-1}	0.091
F(000)	696.0
Crystal size/mm^3	0.23 × 0.11 × 0.07
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.398 to 59.996
Index ranges	-19 ≤ h ≤ 19, -13 ≤ k ≤ 13, -19 ≤ l ≤ 19
Reflections collected	38671
Independent reflections	4778 [R_{int} = 0.0428, R_{sigma} = 0.0254]
Data/restraints/parameters	4778/1/287
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0485, wR_2 = 0.1166
Final R indexes [all data]	R_1 = 0.0569, wR_2 = 0.1215
Largest diff. peak/hole / e Å^{-3}	0.35/-0.38

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 22srv124. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	10983.1(11)	7788.2(18)	7496.9(12)	50.7(4)
F1A	10022(2)	11845(3)	5706(2)	49.9(7)
O1	7133.9(7)	8563.2(10)	2280.8(7)	24.97(19)
N1	6573.4(8)	8855.9(10)	3554.4(8)	19.11(19)
N2	4534.7(8)	8355.3(11)	3247.8(8)	21.8(2)
C1	7098.1(9)	8175.1(12)	3091.1(9)	18.7(2)
C2	5743.2(11)	9913.1(13)	2979.4(11)	25.3(2)
C3	4633.3(11)	9203.5(14)	2438.7(11)	27.5(3)
C4	3574.6(10)	7972.6(13)	3209.8(11)	25.9(3)
C5	3819.0(10)	7145.9(13)	4089.2(11)	25.7(3)
C6	4972.4(10)	7008.3(13)	4691.6(10)	23.0(2)
C7	5394.6(9)	7759.8(12)	4151.0(9)	18.5(2)
C8	6562.2(9)	8074.3(11)	4448.6(8)	16.8(2)
C9	7230.9(8)	6794.6(11)	4514.7(8)	16.4(2)
C10	7545.9(9)	5669.6(12)	5224.8(9)	19.7(2)
C11	8211.1(10)	4655.7(13)	5138.6(10)	22.8(2)
C12	8558.0(9)	4762.6(14)	4365.6(10)	23.7(2)
C13	8242.8(9)	5891.4(13)	3658.8(9)	21.9(2)
C14	7578.5(9)	6899.1(12)	3747.6(8)	17.6(2)

C15	7118.7(10)	8920.2(13)	5529.5(9)	20.9(2)
C16	8300.1(10)	9257.8(13)	5915.0(9)	24.0(2)
C17	9120.6(10)	8328.1(15)	6586.0(10)	27.9(3)
C18	10190.8(11)	8649.1(17)	6899.9(11)	38.8(4)
C19	10503.0(13)	9849(2)	6602.9(14)	48.3(5)
C20	9686.8(15)	10757(2)	5950.8(14)	48.4(4)
C21	8589.5(13)	10487.6(16)	5593.0(12)	35.0(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv124. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	24.5(6)	78.2(11)	39.5(8)	-9.8(8)	8.1(6)	-0.3(7)
F1A	53.7(17)	37.8(14)	58.0(17)	2.2(12)	27.1(14)	-30.7(12)
O1	30.0(4)	30.8(5)	18.4(4)	0.9(3)	15.1(3)	-5.9(4)
N1	23.2(5)	19.3(4)	17.6(4)	2.1(3)	12.1(4)	-3.0(3)
N2	20.5(5)	21.5(5)	24.1(5)	5.1(4)	11.4(4)	2.4(4)
C1	17.9(5)	22.8(5)	15.1(5)	-2.6(4)	7.9(4)	-7.5(4)
C2	32.4(6)	20.5(5)	27.6(6)	6.3(5)	18.2(5)	1.9(5)
C3	26.2(6)	29.7(6)	26.7(6)	11.7(5)	13.1(5)	6.3(5)
C4	18.9(5)	24.6(6)	34.2(6)	1.7(5)	12.9(5)	2.0(4)
C5	22.8(6)	24.2(6)	35.2(7)	0.4(5)	18.3(5)	-1.8(4)
C6	22.6(5)	24.9(6)	24.5(6)	3.2(4)	13.8(5)	-1.3(4)
C7	19.0(5)	18.6(5)	18.8(5)	0.9(4)	10.0(4)	-0.2(4)
C8	19.5(5)	17.8(5)	15.3(5)	0.5(4)	10.4(4)	-2.5(4)
C9	15.7(4)	19.4(5)	14.2(4)	-2.6(4)	7.4(4)	-3.6(4)
C10	21.7(5)	22.3(5)	16.5(5)	-0.2(4)	10.2(4)	-1.8(4)
C11	21.7(5)	24.5(6)	20.8(5)	1.1(4)	9.3(4)	0.5(4)
C12	19.3(5)	28.5(6)	23.6(6)	-2.5(4)	10.7(4)	1.2(4)
C13	18.1(5)	30.7(6)	19.3(5)	-3.5(4)	10.9(4)	-3.2(4)
C14	16.1(5)	23.1(5)	13.5(4)	-2.1(4)	7.0(4)	-5.2(4)
C15	24.3(5)	22.6(5)	18.6(5)	-4.4(4)	12.7(4)	-4.6(4)
C16	27.5(6)	29.2(6)	18.7(5)	-10.5(4)	13.8(5)	-10.8(5)
C17	25.4(6)	37.5(7)	21.1(5)	-9.1(5)	11.7(5)	-9.2(5)
C18	25.0(6)	62.1(10)	27.6(7)	-18.2(7)	11.7(5)	-11.5(6)
C19	32.6(8)	75.7(12)	40.2(8)	-24.1(8)	20.6(7)	-29.1(8)
C20	50.9(10)	54.6(10)	45.3(9)	-16.7(8)	27.9(8)	-34.1(8)
C21	40.9(8)	33.3(7)	32.3(7)	-9.3(6)	19.1(6)	-17.0(6)

Table 4 Bond Lengths for 22srv124.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
F1	C18	1.3057(15)		C8	C15	1.5556(15)
O1	C1	1.2254(13)		C9	C10	1.3858(15)

N1	C1	1.3653(14)		C9	C14	1.3910(14)
N1	C2	1.4526(15)		C10	C11	1.3916(16)
N1	C8	1.4723(13)		C11	C12	1.3985(17)
N2	C3	1.4604(15)		C12	C13	1.3860(18)
N2	C4	1.3716(15)		C13	C14	1.3882(16)
N2	C7	1.3769(15)		C15	C16	1.5051(16)
C1	C14	1.4789(16)		C16	C17	1.3939(19)
C2	C3	1.5178(19)		C16	C21	1.3906(18)
C4	C5	1.3648(18)		C17	C18	1.3764(18)
C5	C6	1.4183(17)		C18	C19	1.365(3)
C6	C7	1.3751(15)		C19	C20	1.371(3)
C7	C8	1.5091(15)		C20	C21	1.390(2)
C8	C9	1.5166(15)				

Table 5 Bond Angles for 22srv124.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C2	122.53(10)		C9	C8	C15	111.14(9)
C1	N1	C8	113.73(9)		C10	C9	C8	129.72(10)
C2	N1	C8	119.25(9)		C10	C9	C14	120.55(10)
C4	N2	C3	125.79(10)		C14	C9	C8	109.66(9)
C4	N2	C7	108.96(10)		C9	C10	C11	117.87(10)
C7	N2	C3	125.19(10)		C10	C11	C12	121.46(11)
O1	C1	N1	125.44(11)		C13	C12	C11	120.46(11)
O1	C1	C14	128.24(11)		C12	C13	C14	117.85(10)
N1	C1	C14	106.31(9)		C9	C14	C1	108.66(10)
N1	C2	C3	108.33(10)		C13	C14	C1	129.50(10)
N2	C3	C2	108.82(10)		C13	C14	C9	121.82(10)
C5	C4	N2	108.32(11)		C16	C15	C8	113.61(9)
C4	C5	C6	107.62(11)		C17	C16	C15	120.38(11)
C7	C6	C5	107.16(11)		C21	C16	C15	120.64(13)
N2	C7	C8	120.99(10)		C21	C16	C17	118.97(12)
C6	C7	N2	107.95(10)		C18	C17	C16	118.97(13)
C6	C7	C8	130.85(10)		F1	C18	C17	121.14(15)
N1	C8	C7	109.20(9)		F1	C18	C19	115.31(15)
N1	C8	C9	101.30(8)		C19	C18	C17	123.54(15)
N1	C8	C15	111.36(9)		C18	C19	C20	116.73(14)
C7	C8	C9	114.29(9)		C19	C20	C21	122.62(16)
C7	C8	C15	109.35(9)		C20	C21	C16	119.16(16)

Table 6 Selected Torsion Angles for 22srv124.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C2	C3	N2	50.92(13)		C8	C9	C14	C13	177.51(10)

N1	C8	C7	N2	-9.37(14)		C8	C15	C16	C17	-88.70(13)
C1	C14	C9	C8	-4.15(12)		C8	C15	C16	C21	90.16(14)
C1	C14	C9	C10	178.62(10)		C9	C8	N1	C1	2.87(11)
C2	N1	C1	O1	17.62(17)		C9	C8	N1	C2	159.74(10)
C2	C3	N2	C4	155.18(12)		C9	C8	C7	N2	-122.00(11)
C2	C3	N2	C7	-27.79(16)		C9	C8	C15	C16	51.44(13)
C3	C2	N1	C1	92.79(12)		C9	C14	C1	O1	-173.14(11)
C3	C2	N1	C8	-61.96(13)		C9	C14	C1	N1	5.83(12)
C6	C7	N2	C3	-178.07(12)		C10	C9	C8	N1	177.90(11)
C6	C7	N2	C4	-0.62(14)		C10	C9	C8	C15	59.50(14)
C6	C7	C8	N1	176.58(12)		C10	C9	C14	C13	0.28(16)
C6	C7	C8	C9	63.95(16)		C13	C14	C1	O1	5.03(19)
C6	C7	C8	C15	-61.34(16)		C13	C14	C1	N1	-176.00(11)
C7	C8	N1	C1	-118.04(10)		C14	C1	N1	C2	-161.39(10)
C7	C8	N1	C2	38.82(13)		C14	C1	N1	C8	-5.39(12)
C7	C8	C9	C10	-64.84(15)		C14	C9	C8	N1	1.00(11)
C7	C8	C9	C14	118.26(10)		C14	C9	C8	C15	-117.40(10)
C7	C8	C15	C16	178.53(10)		C15	C8	N1	C1	121.10(10)
C8	N1	C1	O1	173.62(10)		C15	C8	N1	C2	-82.03(12)
C8	C7	N2	C3	6.65(17)		C15	C8	C7	N2	112.71(12)
C8	C7	N2	C4	-175.89(10)		C16	C15	C8	N1	-60.69(13)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv124.

Atom	***x***	***y***	***z***	**U(eq)**
H17	8943.8	7485.89	6822.99	33
H19	11249.33	10045.09	6836.66	58
H20	9878.94	11604.9	5734.78	58
H21	8043.88	11135.27	5134.24	42
H2A	5793(13)	10610(18)	3535(14)	32(4)
H2B	5901(13)	10338(17)	2442(13)	28(4)
H3A	4559(12)	8609(17)	1815(13)	28(4)
H3B	4032(14)	9901(19)	2139(14)	39(5)
H4	2870(15)	8296(19)	2593(15)	40(5)
H5	3287(14)	6734(18)	4273(13)	32(4)
H6	5402(13)	6512(18)	5349(14)	31(4)
H10	7335(12)	5583(16)	5776(13)	24(4)
H11	8445(13)	3854(18)	5648(13)	30(4)
H12	9012(14)	4046(19)	4322(14)	36(4)
H13	8502(13)	5997(16)	3117(13)	27(4)
H15A	7045(11)	8349(16)	6075(12)	20(3)
H15B	6685(13)	9784(18)	5405(13)	30(4)

Table 8 Atomic Occupancy for 22srv124.							
Atom	***Occupancy***		**Atom**	***Occupancy***		**Atom**	***Occupancy***
F1	0.65		F1A	0.35			

Refinement model description

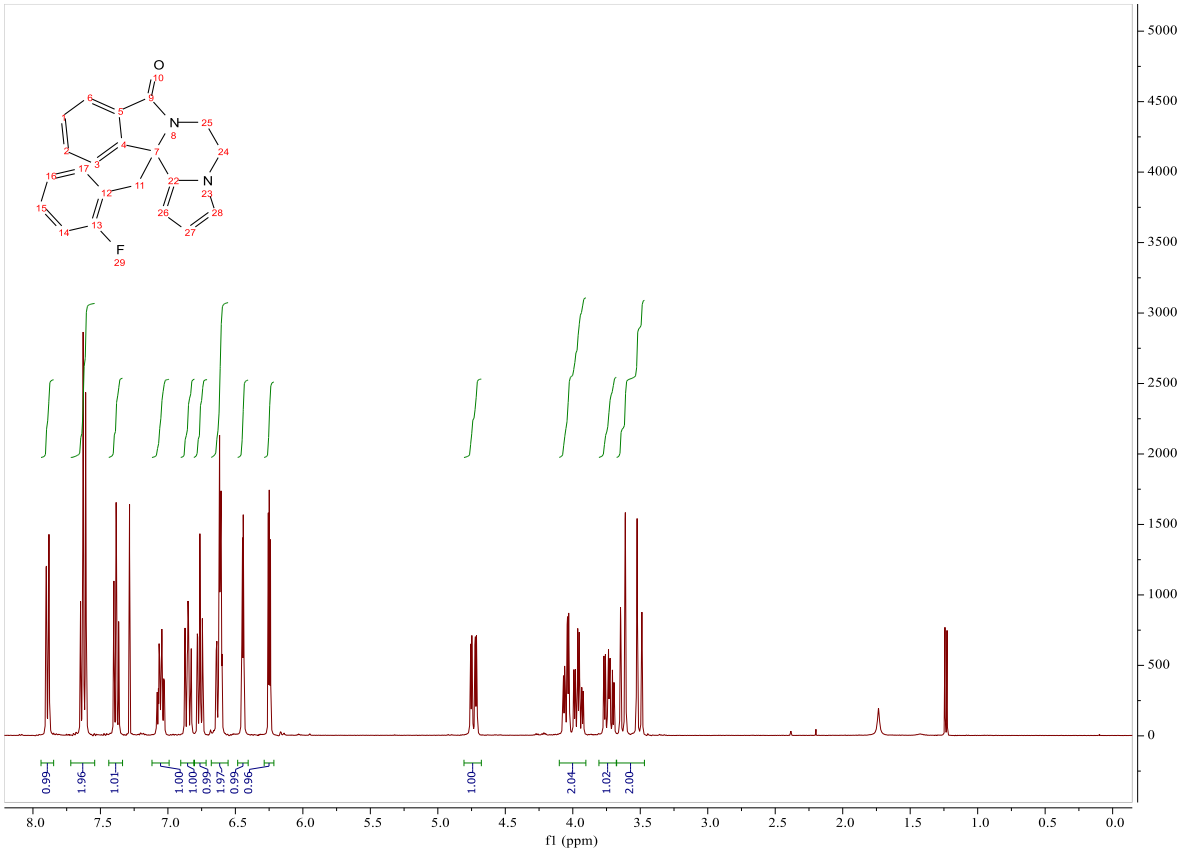
Number of restraints - 1, number of constraints - unknown.

Details:

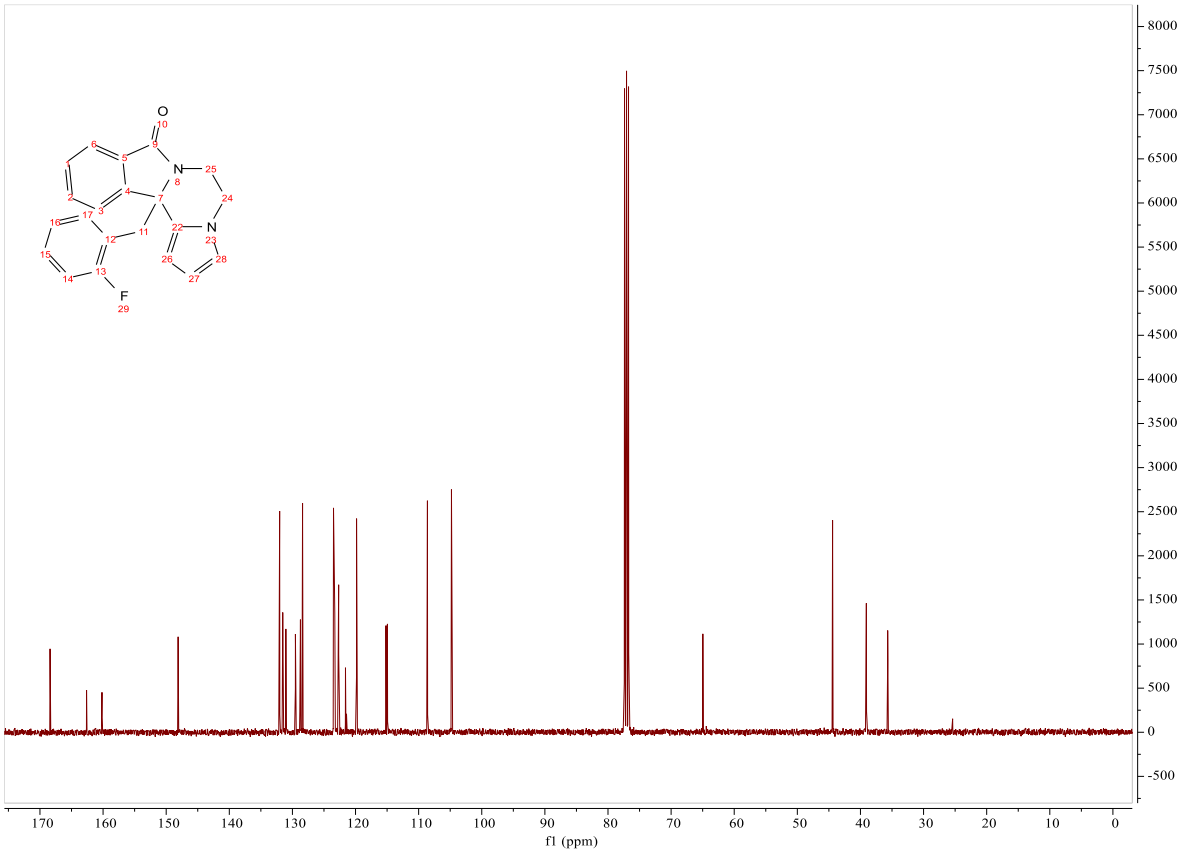
1. Fixed Uiso
 At 1.2 times of: All C(H) groups
2. Restrained distances
 F1-C18 1.33 with sigma of 0.002
3. Others
 Fixed Sof: F1(0.65) F1A(0.35)
4.a Aromatic/amide H refined with riding coordinates:
 C17(H17), C19(H19), C20(H20), C21(H21)

12*b*-(2-fluorobenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1i**

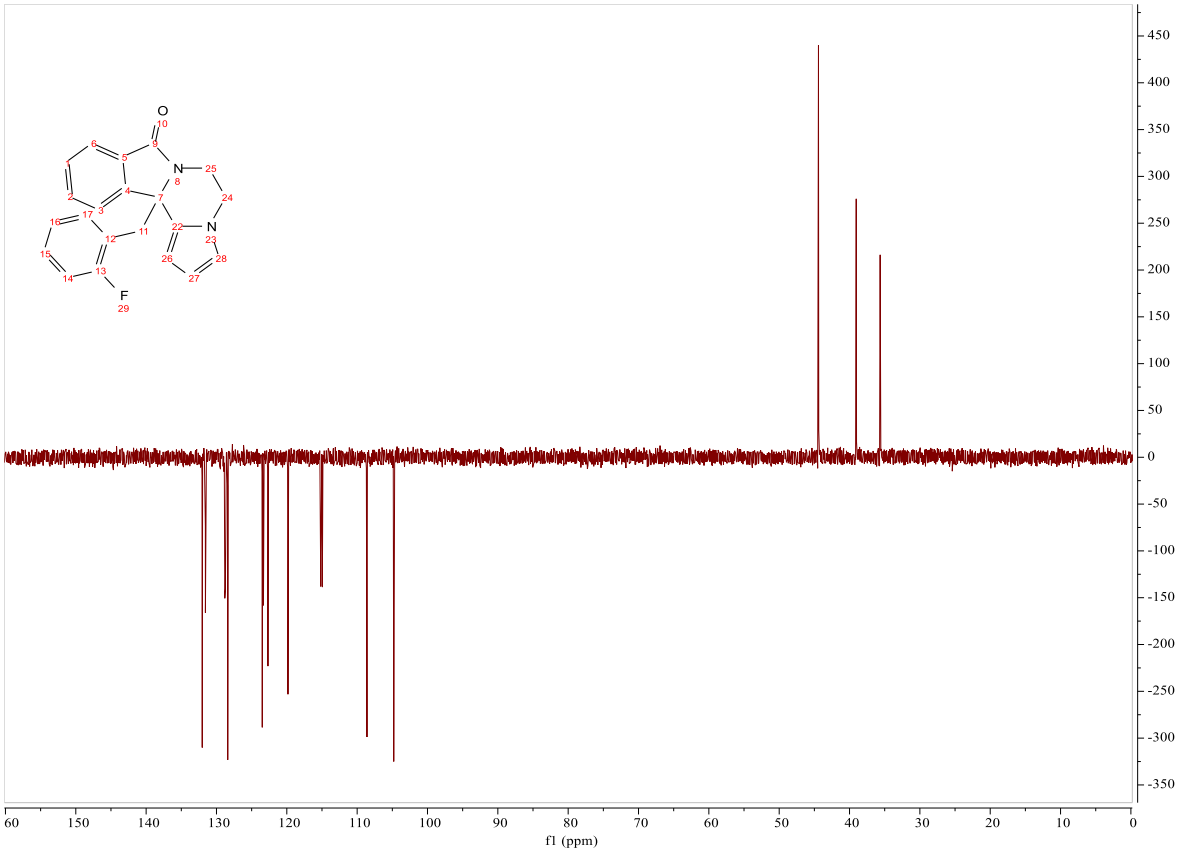
^{1}H:



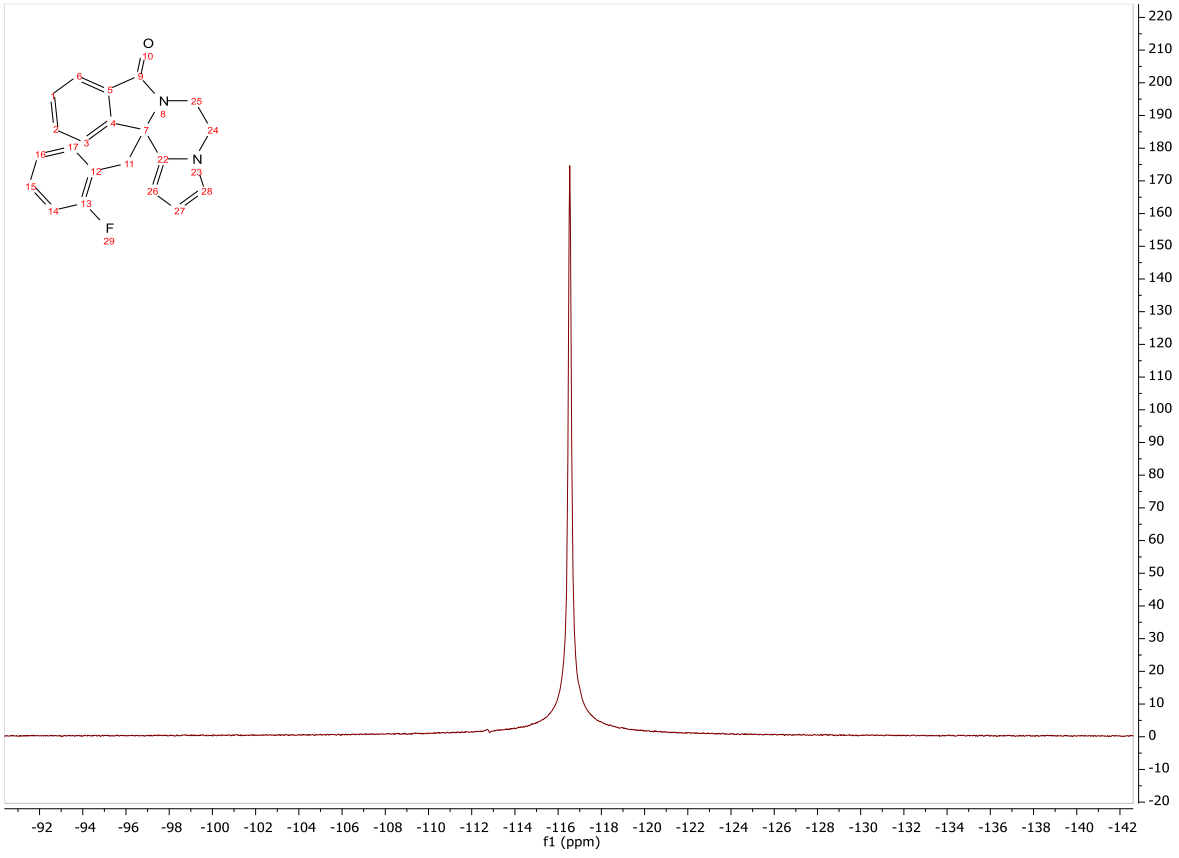
^{13}C:



DEPT-135:


O
10
6
5
9
N
8
25
1
2
4
7
24
3
17
16
11
22
N
12
23
15
26
28
14
13
27
F
29
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{19}F:


O
10
6
5
9
N
8
25
1
2
4
7
24
3
17
16
11
22
N
12
23
15
26
28
14
13
27
F
29
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-92
-94
-96
-98
-100
-102
-104
-106
-108
-110
-112
-114
-116
-118
-120
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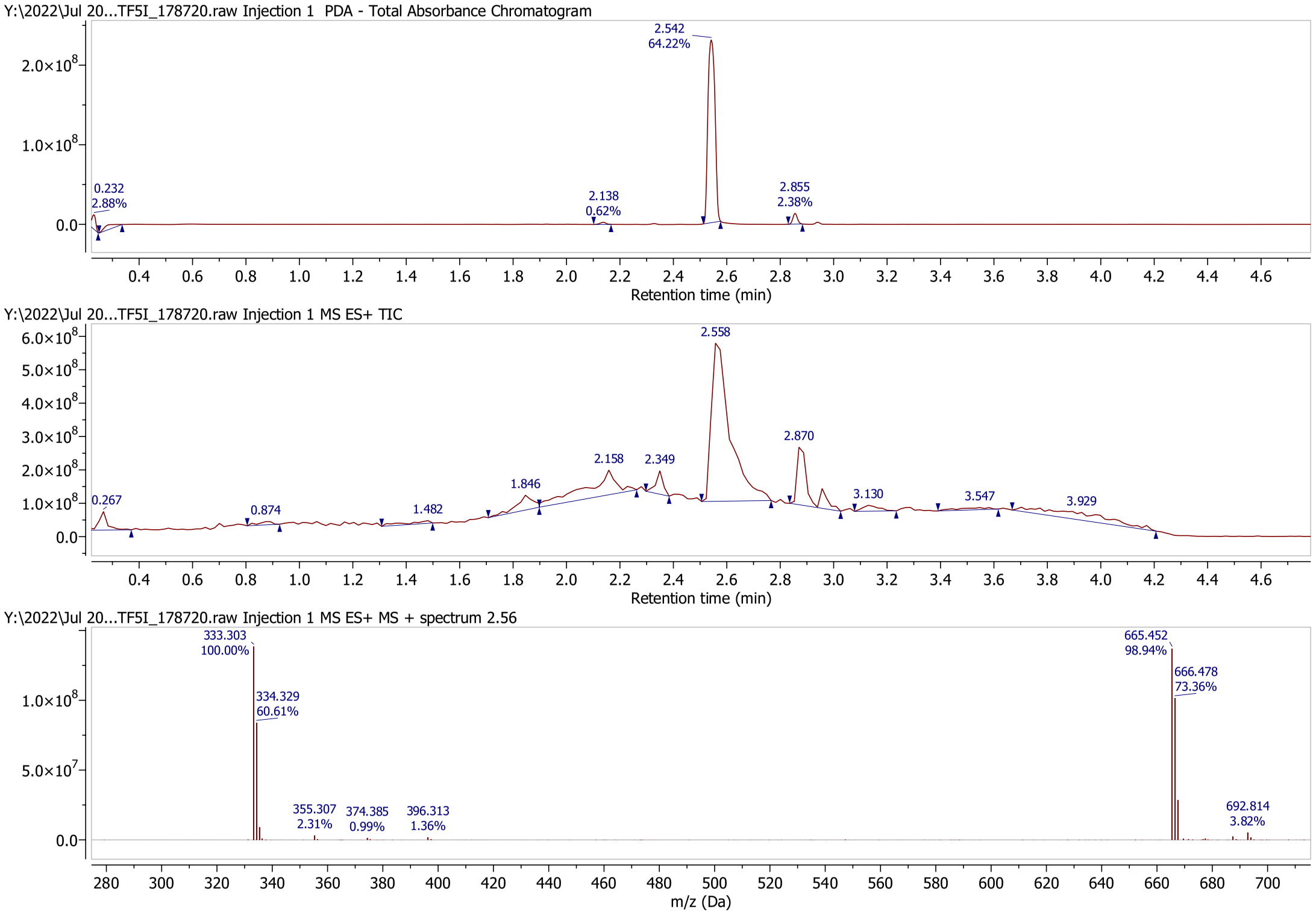
-124
-126
-128
-130
-132
-134
-136
-138
-140
-142
f1 (ppm)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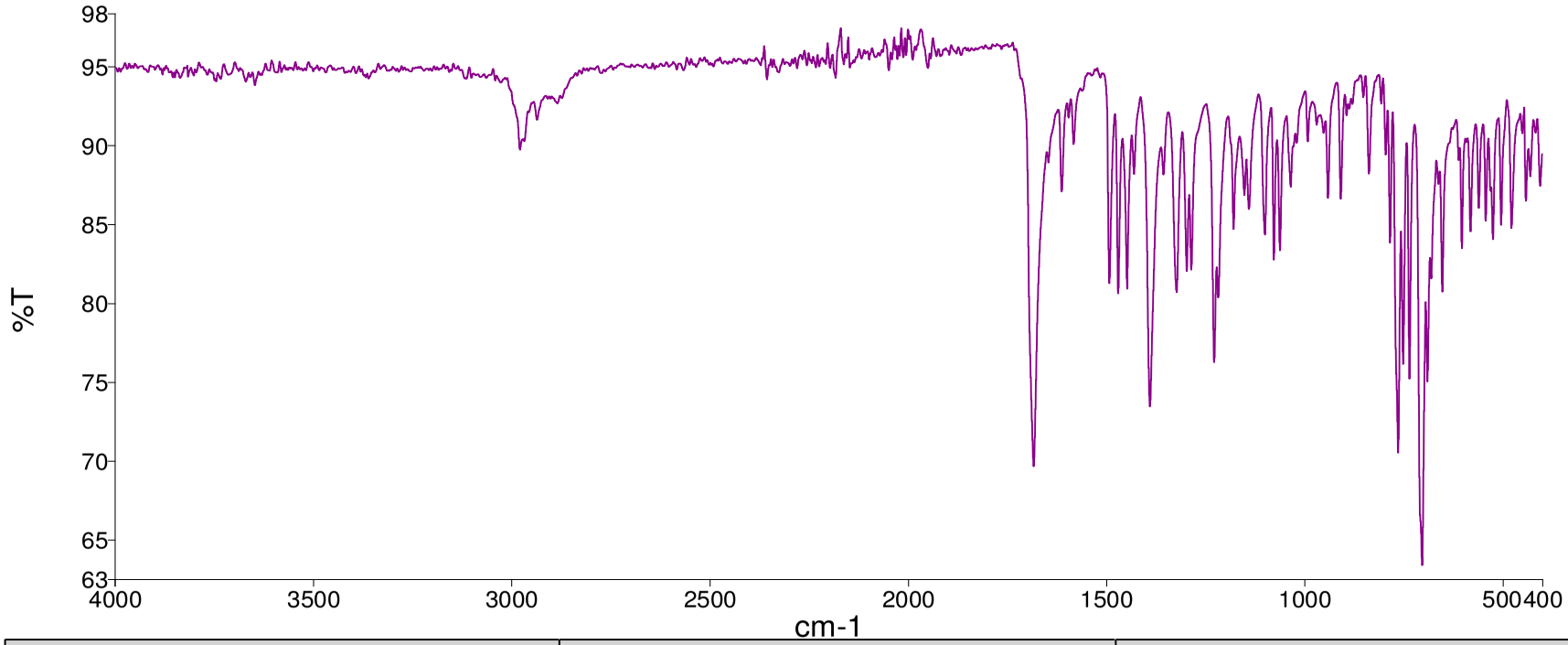
64.22%
0.232
2.88%
2.138
0.62%
2.855
2.38%
Retention time (min)
Y:\2022\Jul 20...TF5I_178720.raw Injection 1 MS ES+ TIC
2.558
2.870
2.158
2.349
1.846
0.267
0.874
1.482
3.130
3.547
3.929
Retention time (min)
Y:\2022\Jul 20...TF5I_178720.raw Injection 1 MS ES+ MS + spectrum 2.56
333.303
100.00%
334.329
60.61%
355.307
2.31%
374.385
0.99%
396.313
1.36%
665.452
98.94%
666.478
73.36%
692.814
3.82%
m/z (Da)

Analyst Lenny Lauchlan
Date 28 June 2022 12:56



Sample Name	Description	Quality Checks
MTF 005I	Sample 022 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

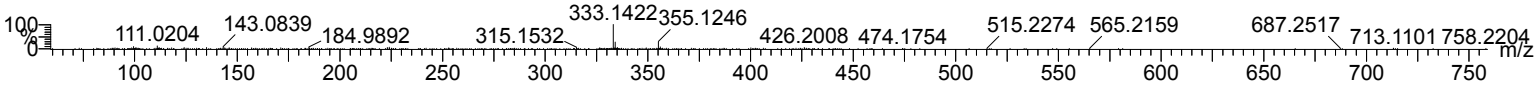
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
3006 formula(e) evaluated with 24 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 F: 0-6

21-Jul-2022
MTF_MTF5I_179347 571 (4.794) Cm (549:573)

21-Jul-2022
1: TOF MS ES+
1.20e+004



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
333.1422	333.1442	-2.0	-6.0	-3.5	332.6	10.219	0.00	C H21 N10 O10
	333.1435	-1.3	-3.9	5.5	327.3	4.901	0.74	C10 H18 N8 O4 F
	333.1399	2.3	6.9	6.5	327.2	4.829	0.80	C11 H16 N8 O F3
	333.1437	-1.5	-4.5	1.5	327.7	5.360	0.47	C12 H21 N2 O4 F4
	333.1410	1.2	3.6	4.5	326.6	4.189	1.52	C12 H21 N4 O7
	333.1451	-2.9	-8.7	6.5	327.1	4.700	0.91	C13 H17 N6 F4
	333.1424	-0.2	-0.6	9.5	325.4	3.067	4.66	C13 H17 N8 O3
	333.1402	2.0	6.0	2.5	328.1	5.722	0.33	C13 H19 N2 O F6
	333.1426	-0.4	-1.2	5.5	326.0	3.644	2.62	C15 H20 N2 O3 F3
	333.1450	-2.8	-8.4	8.5	324.2	1.854	15.66	C17 H21 N2 O5
	333.1415	0.7	2.1	9.5	324.3	1.916	14.72	C18 H19 N2 O2 F2
	333.1406	1.6	4.8	-2.5	332.0	9.590	0.01	C2 H19 N10 O7 F2
	333.1433	-1.1	-3.3	-5.5	332.2	9.864	0.01	C2 H19 N8 O4 F6
	333.1403	1.9	5.7	13.5	322.9	0.568	56.65	C21 H18 N2 O F
	333.1445	-2.3	-6.9	-7.5	331.5	9.167	0.01	C3 H24 N4 O10 F3
	333.1409	1.3	3.9	-6.5	331.2	8.811	0.01	C4 H22 N4 O7 F5
	333.1395	2.7	8.1	1.5	329.9	7.516	0.05	C5 H18 N10 O6 F
	333.1422	0.0	0.0	-1.5	330.3	7.892	0.04	C5 H18 N8 O3 F5
	333.1433	-1.1	-3.3	-3.5	329.9	7.522	0.05	C6 H23 N4 O9 F2
	333.1446	-2.4	-7.2	1.5	329.0	6.650	0.13	C7 H19 N8 O5 F2
	333.1397	2.5	7.5	-2.5	329.7	7.363	0.06	C7 H21 N4 O6 F4
	333.1411	1.1	3.3	2.5	328.7	6.326	0.18	C8 H17 N8 O2 F4
	333.1449	-2.7	-8.1	-2.5	329.3	6.921	0.10	C9 H22 N2 O5 F5
	333.1422	0.0	0.0	0.5	328.3	5.908	0.27	C9 H22 N4 O8 F

X-ray crystallography data

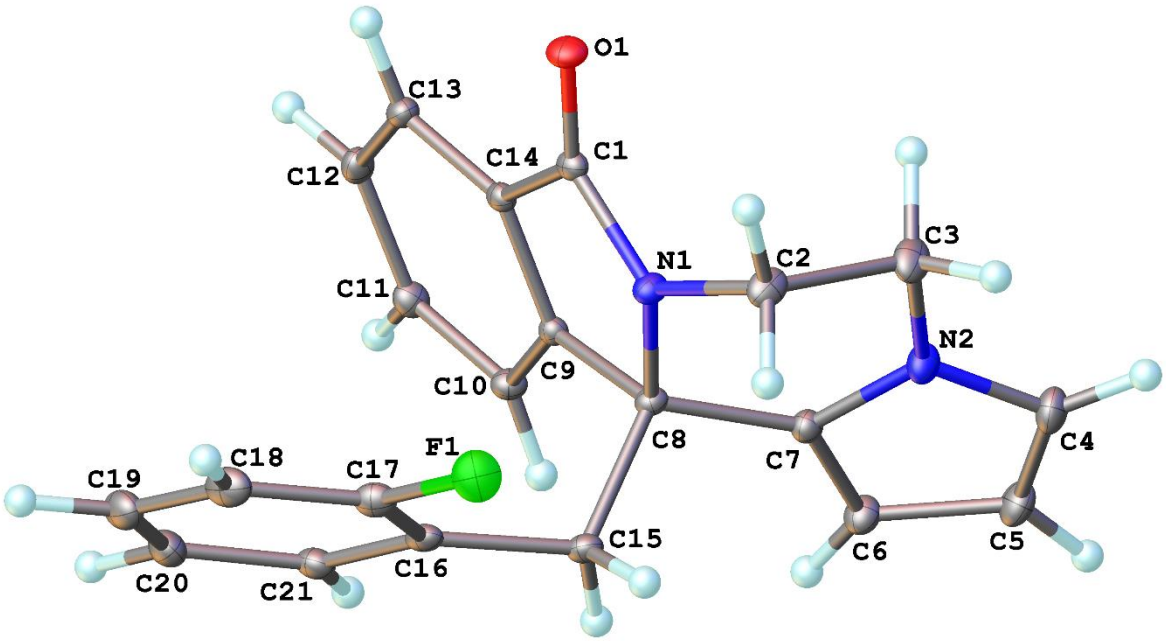


Table 1 Crystal data and structure refinement for 22srv130.	
Identification code	22srv130
Empirical formula	$C_{21}H_{17}FN_2O$
Formula weight	332.36
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.8025(3)
b/Å	9.6560(2)
c/Å	13.9900(3)
α/°	90
β/°	118.9275(8)
γ/°	90
Volume/Å^3	1631.91(6)
Z	4
ρ_{calc}g/cm^3	1.353
μ/mm^{-1}	0.092
F(000)	696.0

Crystal size/mm^3	0.23 × 0.14 × 0.09
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.4 to 59.994
Index ranges	-19 ≤ h ≤ 19, -13 ≤ k ≤ 13, -19 ≤ l ≤ 19
Reflections collected	38242
Independent reflections	4736 [R_{int} = 0.0411, R_{sigma} = 0.0239]
Data/restraints/parameters	4736/0/294
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0457, wR_2 = 0.1116
Final R indexes [all data]	R_1 = 0.0530, wR_2 = 0.1164
Largest diff. peak/hole / e $Å^{-3}$	0.40/-0.22

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 22srv130. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	8080.0(7)	6149.0(8)	4831.6(7)	31.1(2)
O1	9889.5(7)	3559.2(9)	7650.9(7)	20.81(18)
N1	8055.2(8)	3850.1(10)	6363.5(8)	15.71(18)
N2	6298.3(8)	3436.3(11)	6705.8(8)	20.7(2)
C1	9043.9(9)	3164.6(11)	6845.0(9)	15.1(2)
C2	7791.5(10)	4948.1(12)	6911.1(10)	21.8(2)
C3	7206.4(11)	4300.2(15)	7486.0(11)	26.2(3)
C4	5364.2(11)	3090.9(14)	6765.6(11)	24.9(3)
C5	4725.7(11)	2253.2(14)	5903.6(11)	24.8(3)
C6	5284.6(10)	2068.8(13)	5288.0(10)	21.5(2)
C7	6257.7(9)	2807.6(11)	5806.2(9)	16.4(2)
C8	7147.7(9)	3055.0(11)	5494.6(9)	14.1(2)
C9	7747.9(9)	1755.8(11)	5466.3(8)	13.50(19)
C10	7345.2(9)	601.4(12)	4797.9(9)	17.0(2)
C11	8098.1(10)	-429.8(12)	4906.1(9)	19.6(2)
C12	9225.6(10)	-306.1(12)	5652.9(9)	19.8(2)
C13	9624.4(9)	850.0(12)	6322.0(9)	17.6(2)
C14	8865.9(9)	1866.7(11)	6216.2(8)	14.3(2)
C15	6644.8(9)	3833.1(12)	4382.4(9)	17.3(2)
C16	7444.0(9)	3998.6(12)	3943.4(9)	17.5(2)
C17	8144.2(10)	5131.0(12)	4194.3(10)	21.5(2)
C18	8896.6(11)	5289.1(14)	3815.1(11)	27.1(3)
C19	8978.7(11)	4257.9(15)	3169.9(11)	27.9(3)
C20	8293.5(11)	3110.5(14)	2896.2(10)	24.5(3)

C21	7529.6(10)	2993.9(13)	3270.1(9)	20.2(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv130. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	39.1(5)	17.0(4)	38.9(5)	-2.9(3)	20.1(4)	-5.5(3)
O1	15.5(4)	23.3(4)	17.5(4)	-2.0(3)	3.0(3)	-4.4(3)
N1	13.5(4)	14.5(4)	16.7(4)	-3.2(3)	5.3(3)	-2.1(3)
N2	19.8(5)	21.5(5)	23.5(5)	-6.6(4)	12.5(4)	-2.6(4)
C1	14.3(5)	16.4(5)	14.2(4)	1.8(4)	6.6(4)	-2.4(4)
C2	19.9(5)	17.2(5)	25.9(6)	-8.0(4)	9.3(5)	-2.9(4)
C3	24.6(6)	29.9(6)	25.8(6)	-13.8(5)	13.7(5)	-5.9(5)
C4	24.5(6)	25.6(6)	32.1(6)	-4.0(5)	19.7(5)	-0.9(5)
C5	20.0(6)	24.3(6)	34.4(7)	-1.6(5)	16.7(5)	-2.8(4)
C6	18.0(5)	22.6(6)	24.1(6)	-4.1(4)	10.3(4)	-4.0(4)
C7	15.9(5)	16.5(5)	17.3(5)	-1.0(4)	8.4(4)	-0.1(4)
C8	12.1(4)	13.3(4)	14.8(4)	-0.4(4)	4.8(4)	-1.1(3)
C9	14.1(5)	13.5(4)	13.0(4)	1.4(3)	6.6(4)	0.0(3)
C10	16.3(5)	15.8(5)	15.8(5)	-0.8(4)	5.5(4)	-1.3(4)
C11	23.3(5)	16.4(5)	18.8(5)	-1.4(4)	10.1(4)	0.3(4)
C12	21.1(5)	19.9(5)	21.2(5)	2.3(4)	12.3(4)	4.5(4)
C13	14.5(5)	21.0(5)	16.8(5)	2.6(4)	7.2(4)	1.5(4)
C14	14.4(5)	16.2(5)	12.6(4)	1.5(4)	6.8(4)	-1.4(4)
C15	14.3(5)	17.5(5)	16.9(5)	3.0(4)	5.0(4)	1.1(4)
C16	14.4(5)	18.4(5)	15.6(5)	5.3(4)	4.0(4)	0.0(4)
C17	22.0(5)	17.3(5)	21.2(5)	3.9(4)	7.3(4)	-1.1(4)
C18	24.7(6)	26.2(6)	27.6(6)	7.7(5)	10.6(5)	-6.0(5)
C19	24.8(6)	36.5(7)	24.1(6)	8.2(5)	13.2(5)	-1.9(5)
C20	25.3(6)	29.7(6)	18.9(5)	3.0(5)	11.0(5)	0.3(5)
C21	19.2(5)	22.4(5)	15.6(5)	3.3(4)	5.6(4)	-1.2(4)

Table 4 Bond Lengths for 22srv130.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
F1	C17	1.3586(15)		C8	C15	1.5564(15)
O1	C1	1.2270(13)		C9	C10	1.3868(15)
N1	C1	1.3656(14)		C9	C14	1.3882(14)
N1	C2	1.4537(15)		C10	C11	1.3936(16)
N1	C8	1.4707(13)		C11	C12	1.3981(17)
N2	C3	1.4610(16)		C12	C13	1.3881(17)
N2	C4	1.3730(16)		C13	C14	1.3899(15)
N2	C7	1.3738(14)		C15	C16	1.5083(16)
C1	C14	1.4818(15)		C16	C17	1.3873(16)

C2	C3	1.5229(18)		C16	C21	1.3965(17)
C4	C5	1.3628(19)		C17	C18	1.3842(18)
C5	C6	1.4182(17)		C18	C19	1.385(2)
C6	C7	1.3771(16)		C19	C20	1.3850(19)
C7	C8	1.5080(15)		C20	C21	1.3898(17)
C8	C9	1.5144(15)				

Table 5 Bond Angles for 22srv130.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C2	122.59(9)		C9	C8	C15	111.03(9)
C1	N1	C8	113.77(9)		C10	C9	C8	129.61(10)
C2	N1	C8	119.08(9)		C10	C9	C14	120.53(10)
C4	N2	C3	125.78(10)		C14	C9	C8	109.79(9)
C4	N2	C7	108.97(10)		C9	C10	C11	117.81(10)
C7	N2	C3	125.23(10)		C10	C11	C12	121.47(11)
O1	C1	N1	125.60(10)		C13	C12	C11	120.50(11)
O1	C1	C14	128.24(10)		C12	C13	C14	117.62(10)
N1	C1	C14	106.14(9)		C9	C14	C1	108.57(9)
N1	C2	C3	108.10(10)		C9	C14	C13	122.05(10)
N2	C3	C2	108.81(10)		C13	C14	C1	129.35(10)
C5	C4	N2	108.34(11)		C16	C15	C8	113.45(9)
C4	C5	C6	107.64(11)		C17	C16	C15	122.53(11)
C7	C6	C5	107.09(11)		C17	C16	C21	116.25(11)
N2	C7	C6	107.96(10)		C21	C16	C15	121.21(10)
N2	C7	C8	121.12(10)		F1	C17	C16	118.53(11)
C6	C7	C8	130.79(10)		F1	C17	C18	118.10(11)
N1	C8	C7	109.33(9)		C18	C17	C16	123.36(12)
N1	C8	C9	101.31(8)		C17	C18	C19	118.92(12)
N1	C8	C15	111.34(9)		C18	C19	C20	119.68(12)
C7	C8	C9	114.12(9)		C19	C20	C21	120.10(12)
C7	C8	C15	109.49(9)		C20	C21	C16	121.65(11)

Table 6 Selected Torsion Angles for 22srv130.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C2	C3	N2	-50.91(13)		C8	C9	C14	C13	-176.55(10)
N1	C8	C7	N2	8.02(14)		C8	C15	C16	C17	-89.58(13)
C1	C14	C9	C8	5.30(11)		C8	C15	C16	C21	89.30(12)
C1	C14	C9	C10	-177.40(9)		C9	C8	N1	C1	-2.71(11)
C2	N1	C1	O1	-17.02(17)		C9	C8	N1	C2	-159.41(9)
C2	C3	N2	C4	-155.19(12)		C9	C8	C7	N2	120.65(11)
C2	C3	N2	C7	26.62(17)		C9	C8	C15	C16	-47.12(12)
C3	C2	N1	C1	-92.26(12)		C9	C14	C1	O1	171.78(11)

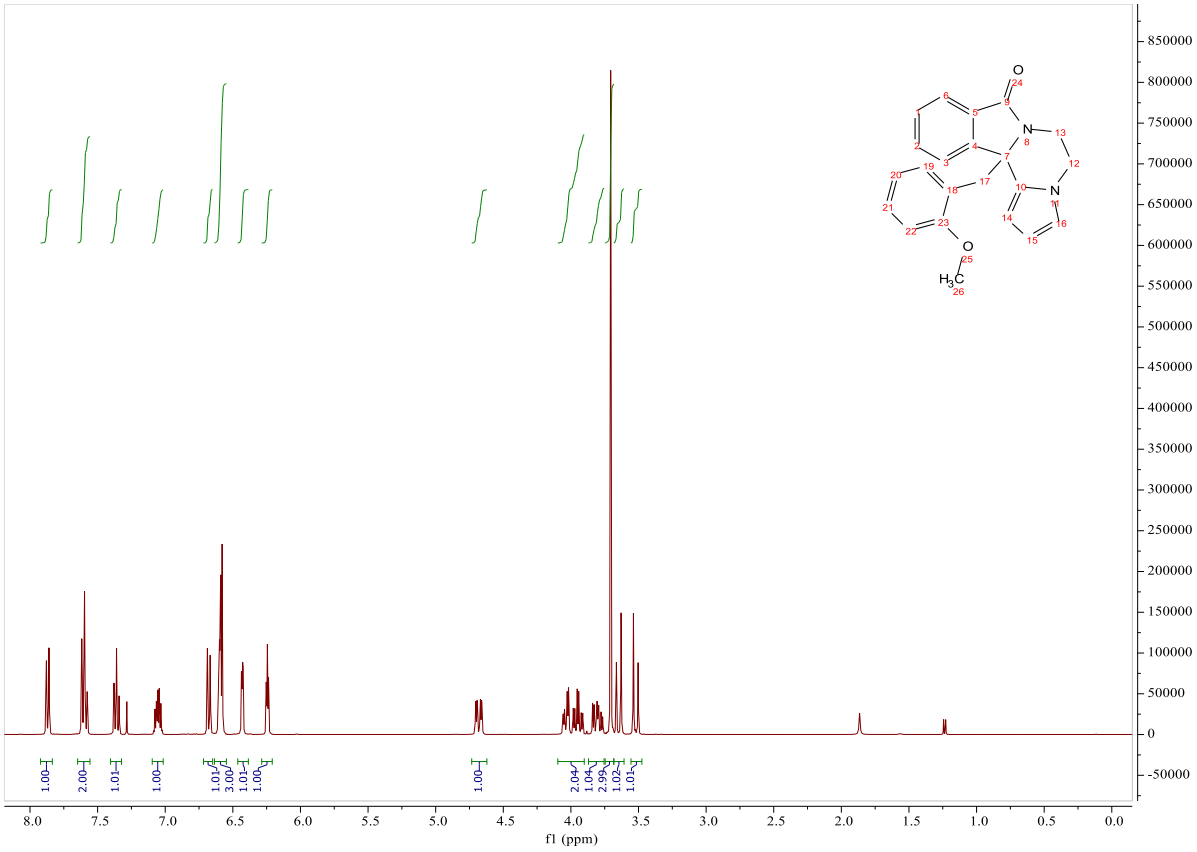
C3	C2	N1	C8	62.29(13)		C9	C14	C1	N1	-6.83(11)
C6	C7	N2	C3	178.98(12)		C10	C9	C8	N1	-178.80(11)
C6	C7	N2	C4	0.53(14)		C10	C9	C8	C15	-60.48(14)
C6	C7	C8	N1	-176.58(12)		C10	C9	C14	C13	0.75(16)
C6	C7	C8	C9	-63.96(16)		C13	C14	C1	O1	-6.19(19)
C6	C7	C8	C15	61.19(15)		C13	C14	C1	N1	175.19(11)
C7	C8	N1	C1	118.08(10)		C14	C1	N1	C2	161.64(10)
C7	C8	N1	C2	-38.62(13)		C14	C1	N1	C8	5.86(12)
C7	C8	C9	C10	63.85(15)		C14	C9	C8	N1	-1.82(11)
C7	C8	C9	C14	-119.17(10)		C14	C9	C8	C15	116.50(10)
C7	C8	C15	C16	-174.04(9)		C15	C8	N1	C1	-120.80(10)
C8	N1	C1	O1	-172.80(10)		C15	C8	N1	C2	82.49(12)
C8	C7	N2	C3	-4.68(18)		C15	C8	C7	N2	-114.21(11)
C8	C7	N2	C4	176.87(10)		C16	C15	C8	N1	64.95(12)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv130.

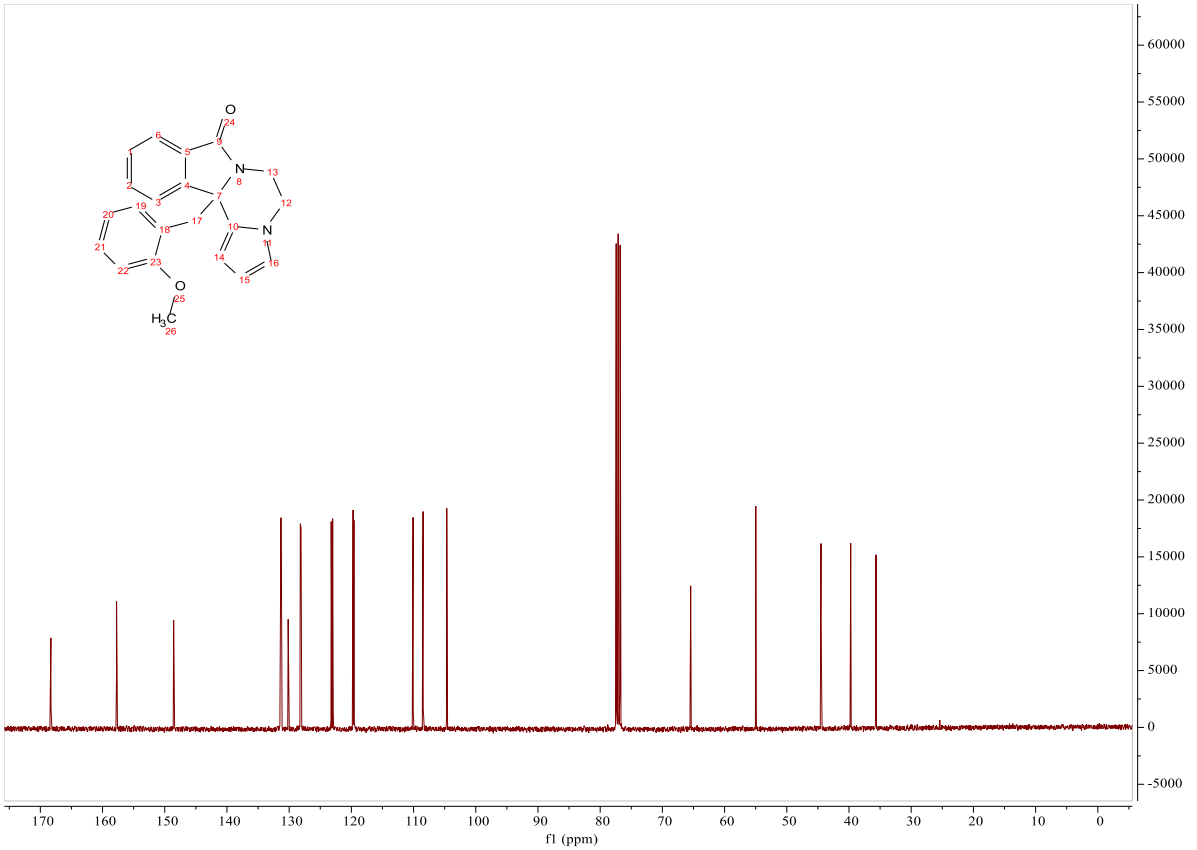
Atom	***x***	***y***	***z***	**U(eq)**
H2A	7314(13)	5625(17)	6355(13)	24(4)
H2B	8468(14)	5372(18)	7433(14)	28(4)
H3A	7778(14)	3699(18)	8133(14)	32(4)
H3B	6894(16)	5030(20)	7754(15)	42(5)
H4	5265(15)	3450(19)	7367(15)	35(5)
H5	3999(15)	1856(19)	5727(14)	34(5)
H6	5045(14)	1559(18)	4648(14)	29(4)
H10	6597(13)	512(17)	4278(13)	23(4)
H11	7833(13)	-1256(18)	4440(13)	27(4)
H12	9742(14)	-1058(18)	5713(13)	28(4)
H13	10392(14)	960(16)	6827(13)	23(4)
H15A	6006(13)	3283(16)	3855(12)	19(4)
H15B	6360(13)	4732(17)	4476(12)	22(4)
H18	9341(15)	6079(19)	4029(15)	36(5)
H19	9505(15)	4355(19)	2902(15)	36(5)
H20	8347(14)	2374(19)	2416(14)	32(4)
H21	7032(14)	2201(17)	3072(13)	25(4)

12*b*-(2-methoxybenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1j**

^{1}H:



^{13}C:



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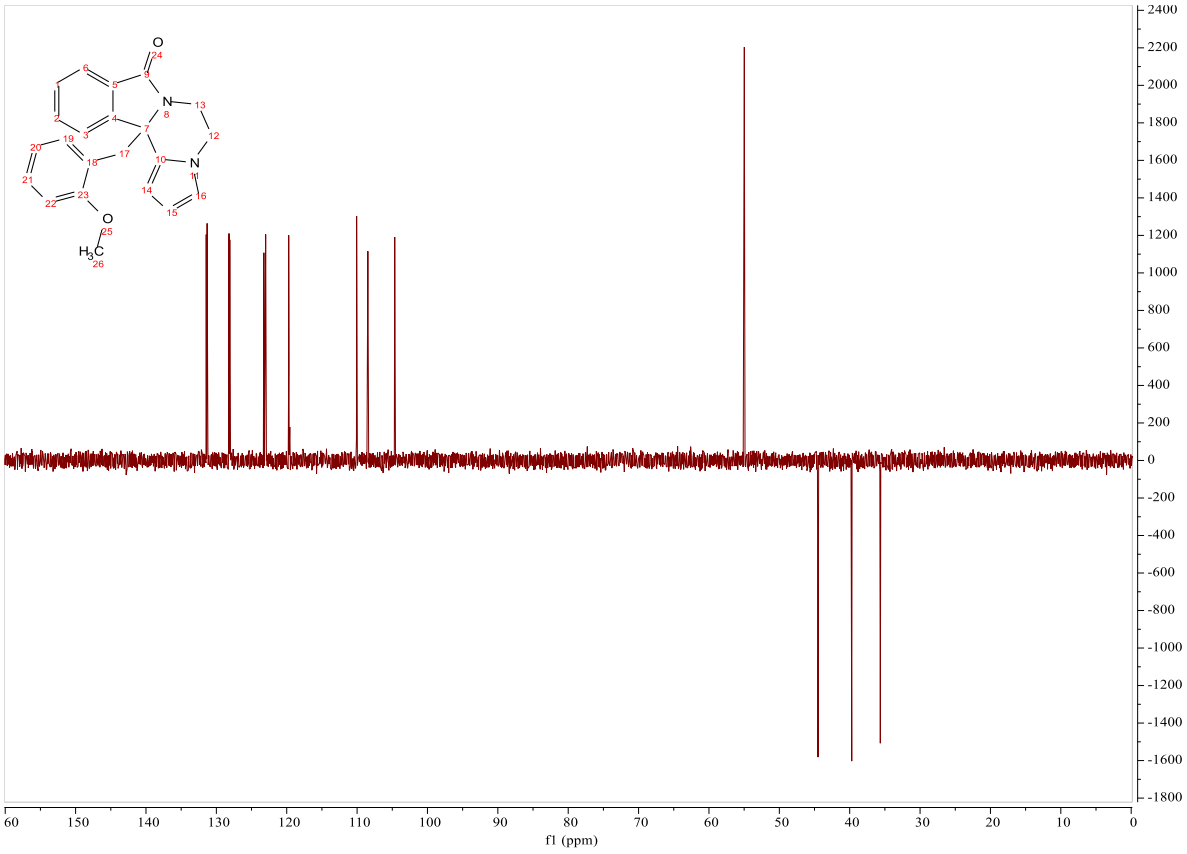
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21
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14
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15
O
25
H3C
26
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
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-400
-600
-800
-1000
-1200
-1400
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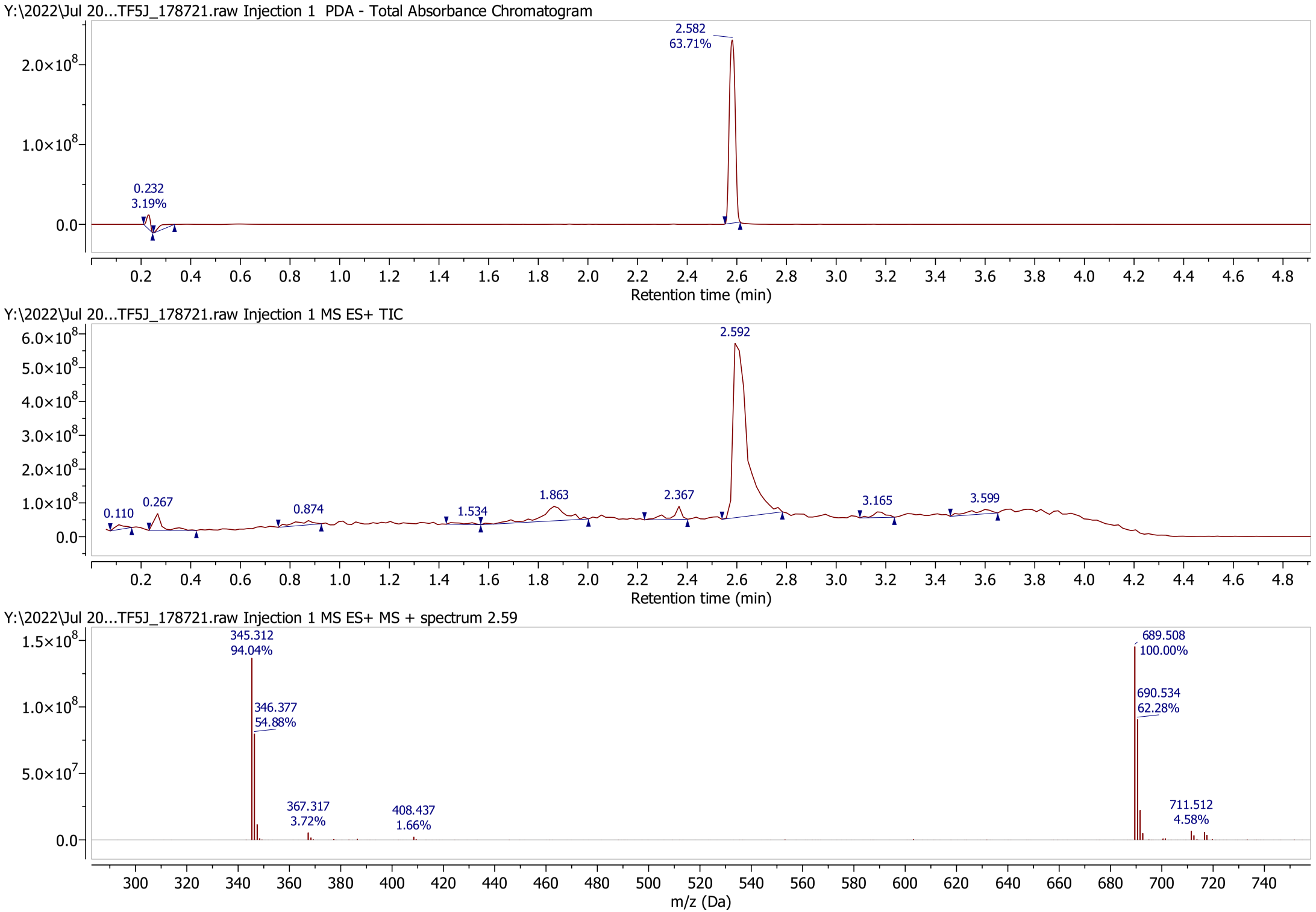
f1 (ppm)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63.71%
0.232
3.19%
Retention time (min)
Y:\2022\Jul 20...TF5J_178721.raw Injection 1 MS ES+ TIC
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0.110
0.267
0.874
1.534
1.863
2.367
3.165
3.599
Retention time (min)
Y:\2022\Jul 20...TF5J_178721.raw Injection 1 MS ES+ MS + spectrum 2.59
345.312
94.04%
346.377
54.88%
367.317
3.72%
408.437
1.66%
689.508
100.00%
690.534
62.28%
711.512
4.58%
m/z (Da)

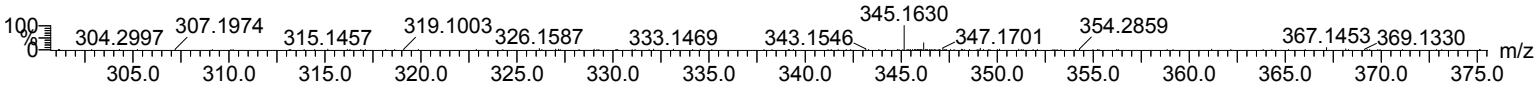
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
3124 formula(e) evaluated with 25 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 F: 0-6

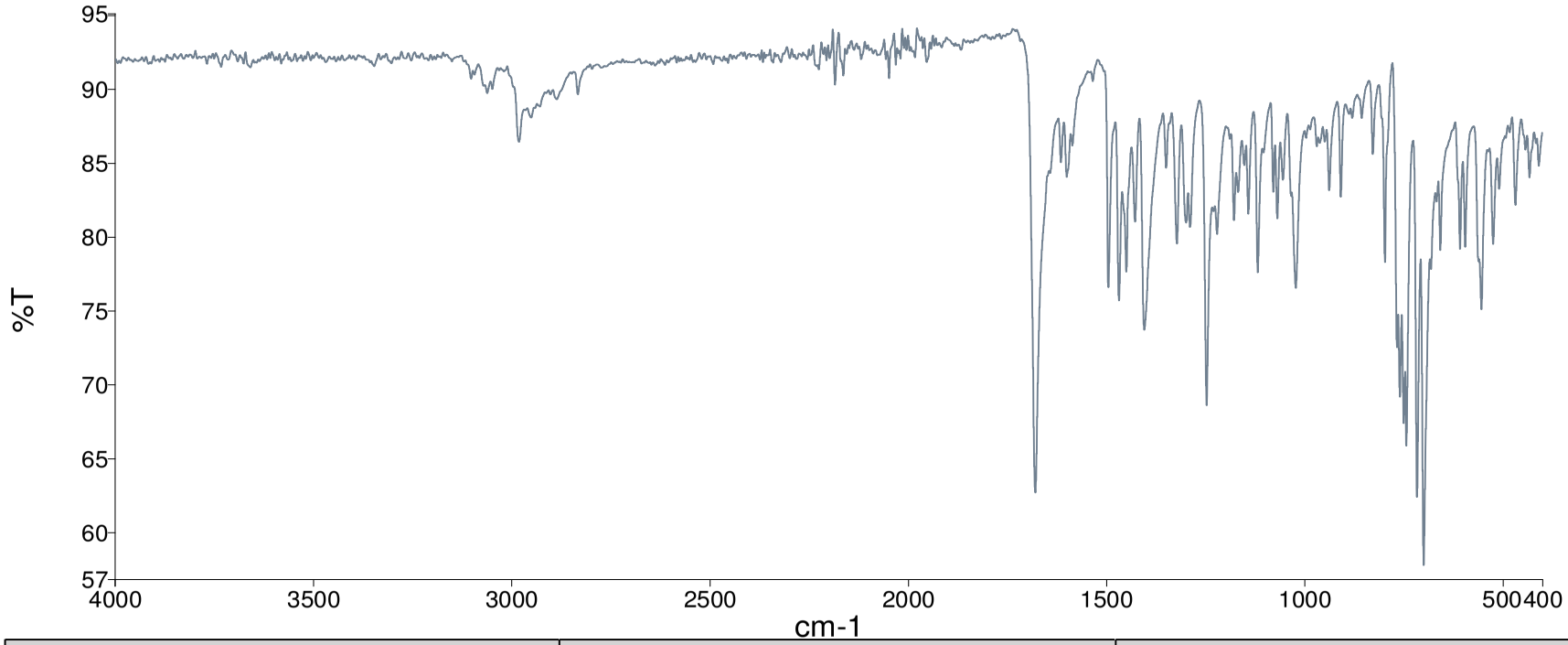
21-Jul-2022
MTF_MTF5J_179348 531 (4.464) Cm (529:531)

21-Jul-2022
1: TOF MS ES+
1.81e+003



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
345.1630	345.1649	-1.9	-5.5	-2.5	182.8	5.036	0.65	C10 H25 N2 O6 F4
	345.1622	0.8	2.3	0.5	182.1	4.317	1.33	C10 H25 N4 O9
	345.1635	-0.5	-1.4	5.5	181.5	3.717	2.43	C11 H21 N8 O5
	345.1613	1.7	4.9	-1.5	182.7	4.993	0.68	C11 H23 N2 O3 F6
	345.1637	-0.7	-2.0	1.5	181.7	3.997	1.84	C13 H24 N2 O5 F3
	345.1651	-2.1	-6.1	6.5	181.4	3.605	2.72	C14 H20 N6 O F3
	345.1601	2.9	8.4	2.5	181.8	4.066	1.71	C14 H22 N2 O2 F5
	345.1626	0.4	1.2	5.5	180.7	3.001	4.98	C16 H23 N2 O4 F2
	345.1653	-2.3	-6.7	2.5	181.8	4.097	1.66	C16 H23 O F6
	345.1639	-0.9	-2.6	10.5	180.5	2.796	6.10	C17 H19 N6 F2
	345.1642	-1.2	-3.5	6.5	181.1	3.373	3.43	C19 H22 F5
	345.1614	1.6	4.6	9.5	179.9	2.142	11.74	C19 H22 N2 O3 F
	345.1603	2.7	7.8	13.5	179.3	1.541	21.43	C22 H21 N2 O2
	345.1655	-2.5	-7.2	13.5	179.5	1.750	17.38	C24 H22 O F
	345.1643	-1.3	-3.8	17.5	179.4	1.697	18.32	C27 H21
	345.1606	2.4	7.0	-2.5	183.9	6.104	0.22	C3 H22 N10 O8 F
	345.1633	-0.3	-0.9	-5.5	184.4	6.605	0.14	C3 H22 N8 O5 F5
	345.1658	-2.8	-8.1	-2.5	183.6	5.846	0.29	C5 H23 N8 O7 F2
	345.1609	2.1	6.1	-6.5	184.0	6.254	0.19	C5 H25 N4 O8 F4
	345.1622	0.8	2.3	-1.5	183.4	5.602	0.37	C6 H21 N8 O4 F4
	345.1633	-0.3	-0.9	-3.5	183.2	5.410	0.45	C7 H26 N4 O10 F
	345.1646	-1.6	-4.6	1.5	182.5	4.775	0.84	C8 H22 N8 O6 F
	345.1610	2.0	5.8	2.5	182.4	4.627	0.98	C9 H20 N8 O3 F3
	345.1618	1.2	3.5	-6.5	185.0	7.234	0.07	H23 N10 O9 F2
	345.1645	-1.5	-4.3	-9.5	185.4	7.694	0.05	H23 N8 O6 F6

Analyst Lenny Lauchlan
Date 28 June 2022 12:58



Sample Name	Description	Quality Checks
MTF 005J	Sample 023 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

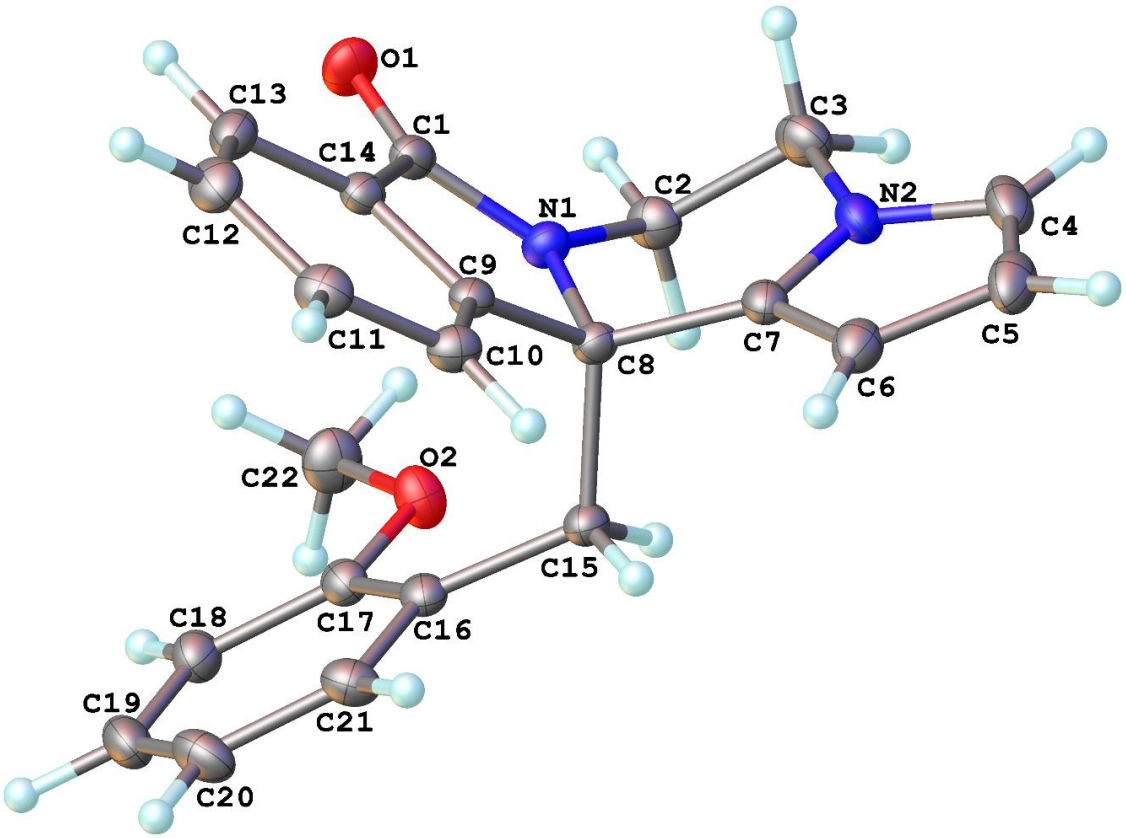


Table 1 Crystal data and structure refinement for 22srv149.	
Identification code	22srv149
Empirical formula	$C_{22}H_{20}N_2O_2$
Formula weight	344.40
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.0740(2)
b/Å	7.5318(2)
c/Å	20.9844(5)
α/°	90
β/°	92.9918(9)
γ/°	90
Volume/Å^3	1747.86(7)
Z	4

ρ_{calc}g/cm^3	1.309
μ/mm^{-1}	0.085
F(000)	728.0
Crystal size/mm^3	0.22 × 0.12 × 0.05
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.546 to 59.996
Index ranges	-15 ≤ h ≤ 15, -10 ≤ k ≤ 10, -29 ≤ l ≤ 29
Reflections collected	51064
Independent reflections	5082 [R_{int} = 0.0467, R_{sigma} = 0.0239]
Data/restraints/parameters	5082/0/315
Goodness-of-fit on F^2	1.086
Final R indexes [I>=2σ (I)]	R_1 = 0.0456, wR_2 = 0.1080
Final R indexes [all data]	R_1 = 0.0534, wR_2 = 0.1121
Largest diff. peak/hole / e Å^{-3}	0.35/-0.20

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 22srv149. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	7317.1(8)	1103.6(11)	6178.5(4)	25.52(19)
O2	10262.3(8)	3395.0(12)	5796.6(4)	23.29(18)
N1	7662.4(8)	3671.1(12)	5621.5(4)	17.63(19)
N2	6543.7(9)	5298.2(14)	4604.1(5)	21.9(2)
C1	7313.4(10)	2726.5(15)	6131.5(5)	17.7(2)
C2	7870.3(11)	2923.8(16)	5001.8(6)	21.5(2)
C3	6815.0(12)	3408.3(18)	4541.8(6)	25.3(2)
C4	5884.7(11)	6291(2)	4161.9(6)	27.7(3)
C5	5726.7(11)	7950.6(19)	4407.2(6)	28.2(3)
C6	6309.7(10)	7983.8(17)	5027.6(6)	23.3(2)
C7	6789.7(9)	6320.0(15)	5139.2(5)	18.4(2)
C8	7569.8(9)	5598.9(14)	5691.3(5)	15.7(2)
C9	7030.5(9)	5743.7(14)	6338.8(5)	15.8(2)
C10	6707.0(10)	7236.3(15)	6674.8(6)	19.9(2)
C11	6272.3(10)	6982.9(17)	7280.7(6)	22.6(2)
C12	6157.7(11)	5287.8(18)	7538.7(6)	24.0(2)
C13	6482.9(10)	3799.4(16)	7199.3(6)	21.4(2)
C14	6928.5(9)	4059.0(15)	6598.9(5)	16.5(2)
C15	8835.5(9)	6507.8(15)	5690.1(5)	17.3(2)

C16	9715.9(9)	6123.6(15)	6246.9(5)	17.6(2)
C17	10431.6(10)	4586.0(15)	6284.2(5)	18.4(2)
C18	11277.2(10)	4330.6(17)	6793.9(6)	22.6(2)
C19	11405.9(11)	5605.0(18)	7269.5(6)	25.8(3)
C20	10711.3(11)	7128.8(19)	7243.1(6)	27.3(3)
C21	9875.4(10)	7374.4(16)	6732.2(6)	22.4(2)
C22	10829.2(13)	1700.0(17)	5871.2(7)	27.9(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv149. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	34.3(5)	14.9(4)	27.0(4)	2.2(3)	-1.3(4)	-0.5(3)
O2	24.5(4)	24.3(4)	20.8(4)	-3.1(3)	-1.9(3)	6.3(3)
N1	19.4(4)	15.6(4)	17.9(4)	-0.1(3)	1.7(3)	-1.0(3)
N2	18.1(4)	28.2(5)	19.0(4)	1.7(4)	-2.7(3)	-2.2(4)
C1	16.7(5)	16.5(5)	19.6(5)	1.5(4)	-2.3(4)	-1.2(4)
C2	23.2(5)	21.7(5)	19.7(5)	-3.7(4)	2.2(4)	-0.8(4)
C3	25.4(6)	28.2(6)	21.9(6)	-4.3(5)	-1.6(4)	-4.6(5)
C4	17.7(5)	43.9(8)	21.0(6)	5.8(5)	-3.9(4)	-0.6(5)
C5	18.9(5)	38.5(7)	27.1(6)	11.9(5)	-0.5(4)	4.7(5)
C6	18.2(5)	26.7(6)	24.9(6)	6.2(5)	1.1(4)	1.8(4)
C7	14.6(5)	22.6(5)	18.0(5)	3.0(4)	0.3(4)	-2.0(4)
C8	15.3(4)	14.4(5)	17.3(5)	1.3(4)	1.0(4)	-0.9(4)
C9	12.3(4)	17.5(5)	17.4(5)	1.3(4)	0.1(3)	-1.5(4)
C10	17.7(5)	18.1(5)	24.0(5)	-0.3(4)	2.0(4)	-0.4(4)
C11	19.0(5)	25.1(6)	24.2(6)	-3.8(4)	4.2(4)	1.4(4)
C12	21.4(5)	31.3(6)	19.8(5)	0.7(5)	4.9(4)	-1.0(5)
C13	18.8(5)	23.7(6)	21.6(5)	6.3(4)	1.1(4)	-0.6(4)
C14	13.3(4)	17.4(5)	18.6(5)	1.7(4)	-1.2(4)	-0.7(4)
C15	15.2(5)	18.4(5)	18.3(5)	2.8(4)	0.5(4)	-1.8(4)
C16	14.1(4)	20.9(5)	17.8(5)	1.9(4)	1.6(4)	-2.3(4)
C17	16.9(5)	21.9(5)	16.3(5)	0.8(4)	2.0(4)	-1.6(4)
C18	18.8(5)	26.3(6)	22.4(5)	4.2(4)	-1.4(4)	-0.2(4)
C19	20.9(5)	35.6(7)	20.5(5)	2.1(5)	-4.0(4)	-4.5(5)
C20	22.5(6)	33.8(7)	25.1(6)	-7.9(5)	-1.9(4)	-4.9(5)
C21	17.9(5)	23.2(5)	26.1(6)	-3.3(4)	0.7(4)	-2.2(4)
C22	32.4(7)	21.1(6)	30.1(6)	0.2(5)	0.7(5)	5.5(5)

Table 4 Bond Lengths for 22srv149.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
O1	C1	1.2263(14)		C8	C9	1.5164(15)
O2	C17	1.3663(14)		C8	C15	1.5600(15)

O2	C22	1.4276(15)		C9	C10	1.3841(15)
N1	C1	1.3580(14)		C9	C14	1.3882(15)
N1	C2	1.4465(14)		C10	C11	1.3959(16)
N1	C8	1.4634(14)		C11	C12	1.3951(18)
N2	C3	1.4620(17)		C12	C13	1.3858(18)
N2	C4	1.3719(15)		C13	C14	1.3906(15)
N2	C7	1.3768(15)		C15	C16	1.5101(15)
C1	C14	1.4814(15)		C16	C17	1.4032(16)
C2	C3	1.5208(17)		C16	C21	1.3918(16)
C4	C5	1.367(2)		C17	C18	1.3976(15)
C5	C6	1.4229(17)		C18	C19	1.3866(18)
C6	C7	1.3766(16)		C19	C20	1.3811(19)
C7	C8	1.5097(15)		C20	C21	1.3916(17)

Table 5 Bond Angles for 22srv149.

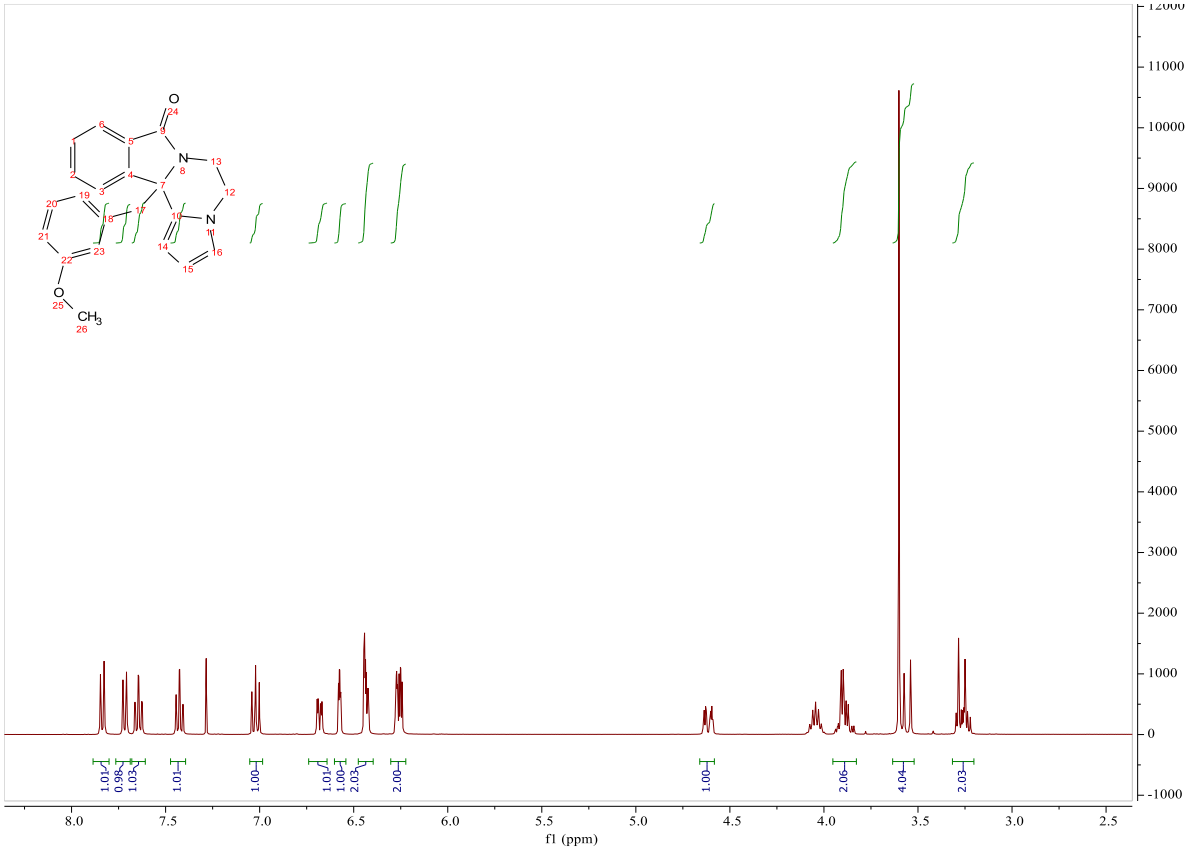
Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C17	O2	C22	117.56(9)		C9	C8	C15	111.45(8)
C1	N1	C2	124.74(10)		C10	C9	C8	129.75(10)
C1	N1	C8	114.62(9)		C10	C9	C14	120.90(10)
C2	N1	C8	119.43(9)		C14	C9	C8	109.30(9)
C4	N2	C3	125.08(11)		C9	C10	C11	117.63(11)
C4	N2	C7	108.82(11)		C12	C11	C10	121.41(11)
C7	N2	C3	125.75(10)		C13	C12	C11	120.63(11)
O1	C1	N1	125.85(11)		C12	C13	C14	117.76(11)
O1	C1	C14	128.46(11)		C9	C14	C1	109.08(9)
N1	C1	C14	105.69(9)		C9	C14	C13	121.65(10)
N1	C2	C3	108.92(10)		C13	C14	C1	129.23(10)
N2	C3	C2	109.36(10)		C16	C15	C8	117.29(9)
C5	C4	N2	108.54(11)		C17	C16	C15	122.77(10)
C4	C5	C6	107.45(11)		C21	C16	C15	119.25(10)
C7	C6	C5	107.00(12)		C21	C16	C17	117.91(10)
N2	C7	C8	120.38(10)		O2	C17	C16	116.43(9)
C6	C7	N2	108.17(10)		O2	C17	C18	122.89(10)
C6	C7	C8	131.19(11)		C18	C17	C16	120.68(10)
N1	C8	C7	108.69(9)		C19	C18	C17	119.67(11)
N1	C8	C9	101.19(8)		C20	C19	C18	120.68(11)
N1	C8	C15	111.56(9)		C19	C20	C21	119.21(12)
C7	C8	C9	115.18(9)		C20	C21	C16	121.84(12)
C7	C8	C15	108.61(8)					

Table 6 Selected Torsion Angles for 22srv149.										
A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C2	C3	N2	46.90(13)		C8	C7	N2	C3	10.13(16)
N1	C8	C7	N2	-15.79(13)		C8	C7	N2	C4	-176.37(10)
C2	C3	N2	C4	161.83(11)		C8	C15	C16	C17	81.89(13)
C2	C3	N2	C7	-25.68(16)		C8	C15	C16	C21	-101.27(12)
C3	C2	N1	C1	104.93(12)		C9	C8	N1	C1	-2.61(11)
C3	C2	N1	C8	-61.80(13)		C9	C8	N1	C2	165.41(9)
C6	C7	N2	C3	-175.07(11)		C9	C8	C7	N2	-128.46(10)
C6	C7	N2	C4	-1.56(13)		C9	C8	C15	C16	45.60(13)
C6	C7	C8	N1	170.77(11)		C15	C8	N1	C1	116.01(10)
C6	C7	C8	C9	58.11(16)		C15	C8	N1	C2	-75.96(12)
C6	C7	C8	C15	-67.67(15)		C15	C8	C7	N2	105.76(11)
C7	C8	N1	C1	-124.26(10)		C16	C15	C8	N1	-66.70(12)
C7	C8	N1	C2	43.76(12)		C16	C17	O2	C22	-170.10(10)
C7	C8	C15	C16	173.53(9)		C18	C17	O2	C22	10.74(16)

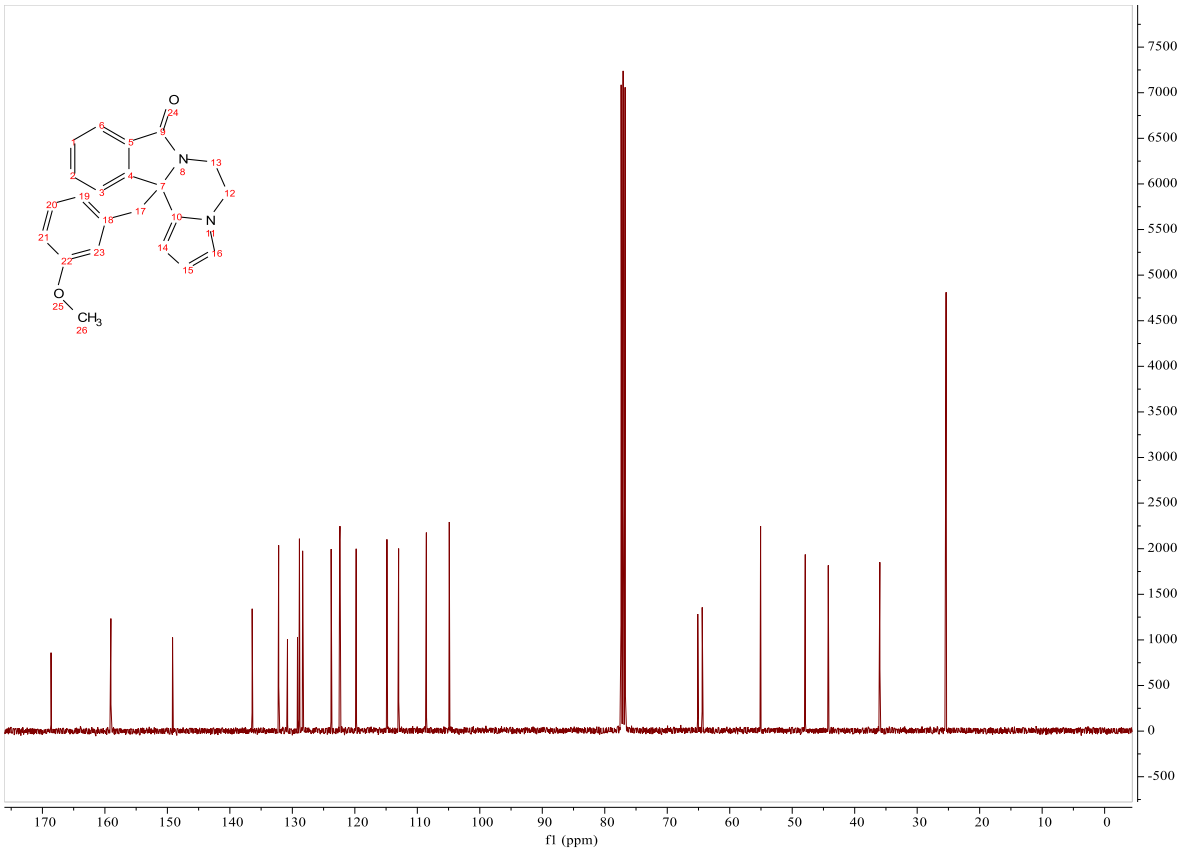
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv149.				
Atom	***x***	***y***	***z***	**U(eq)**
H2A	7929(14)	1600(20)	5044(7)	26(4)
H2B	8673(14)	3400(20)	4836(7)	25(4)
H3A	6079(14)	2680(20)	4647(7)	27(4)
H3B	7029(15)	3150(20)	4079(8)	31(4)
H4	5610(15)	5740(20)	3761(8)	33(4)
H5	5267(16)	8910(20)	4200(9)	43(5)
H6	6391(14)	8990(20)	5329(8)	31(4)
H10	6792(14)	8460(20)	6507(7)	24(4)
H11	6034(14)	8010(20)	7527(8)	30(4)
H12	5835(15)	5150(20)	7961(8)	35(4)
H13	6393(13)	2600(20)	7366(7)	21(4)
H15A	9179(13)	6172(19)	5287(7)	21(3)
H15B	8664(13)	7790(20)	5677(7)	21(3)
H18	11762(14)	3270(20)	6819(7)	25(4)
H19	12019(15)	5400(20)	7633(8)	31(4)
H20	10805(15)	8030(20)	7572(8)	37(4)
H21	9366(13)	8460(20)	6704(7)	23(4)
H22A	11723(16)	1810(20)	5862(8)	35(4)
H22B	10631(15)	1170(20)	6281(8)	33(4)
H22C	10496(15)	970(20)	5507(8)	36(4)

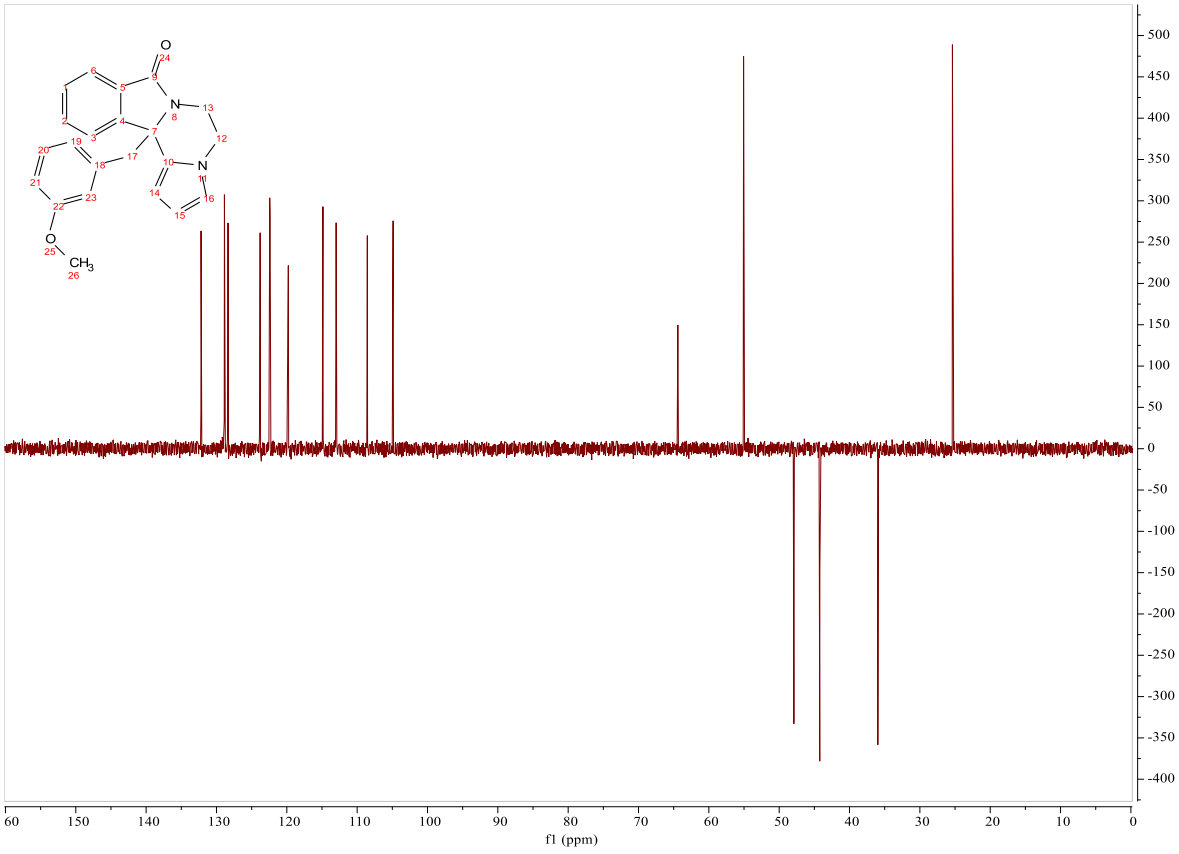
12*b*-(3-methoxybenzyl)-5,6-dihydropyrrolo[2',1':3,4]pyrazino[2,1-*a*]isoindol-8(12*bH*)-one **1k**

^{1}H:



^{13}C:

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24
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9
N
8
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12
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2
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7
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20
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17
10
N
11
14
16
15
21
22
23
O
25
CH3
26
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
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30
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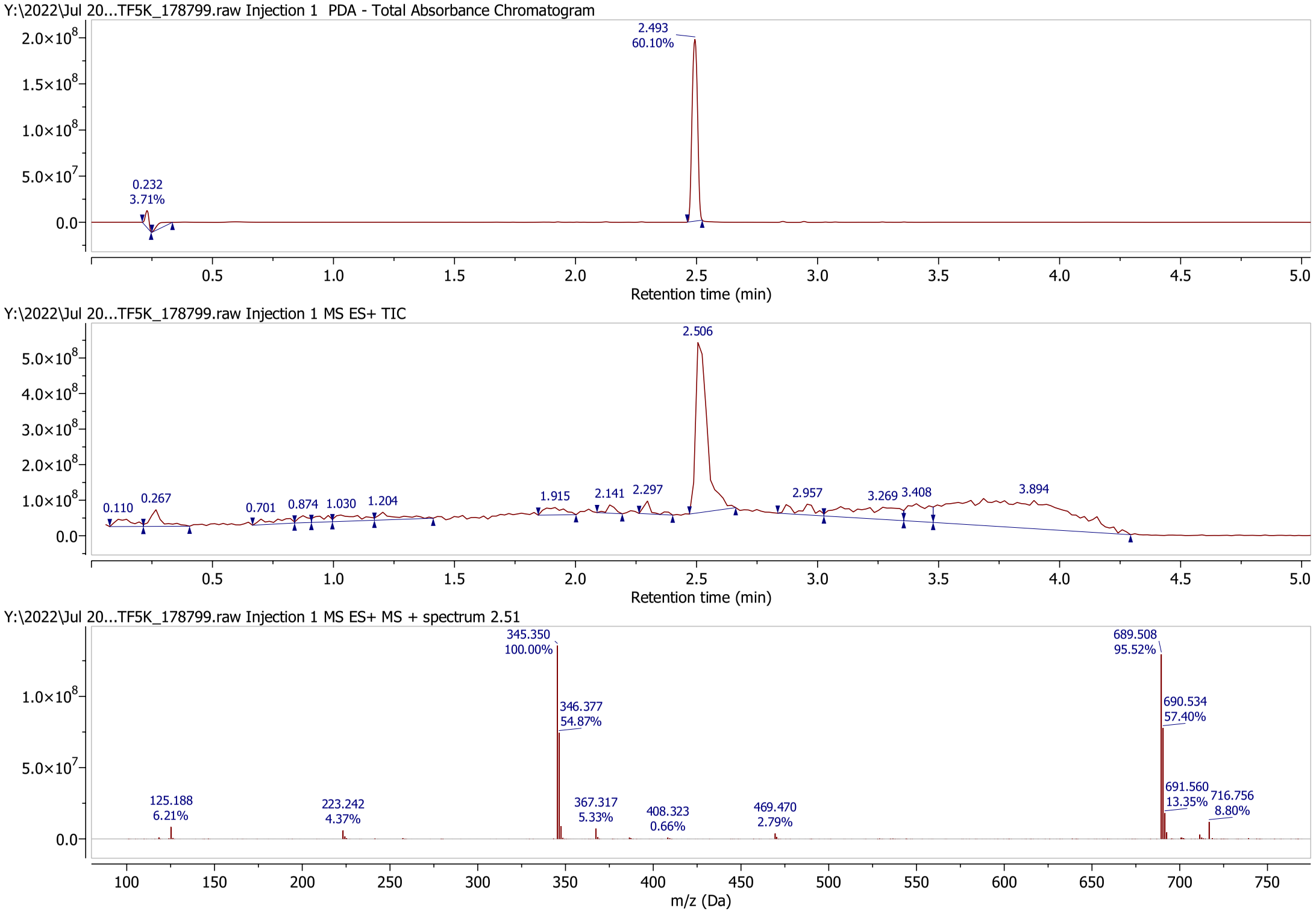
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60.10%
0.232
3.71%
Retention time (min)
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0.267
0.701
0.874
1.030
1.204
1.915
2.141
2.297
2.957
3.269
3.408
3.894
Retention time (min)
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345.350
100.00%
346.377
54.87%
689.508
95.52%
690.534
57.40%
691.560
13.35%
716.756
8.80%
125.188
6.21%
223.242
4.37%
367.317
5.33%
408.323
0.66%
469.470
2.79%
m/z (Da)

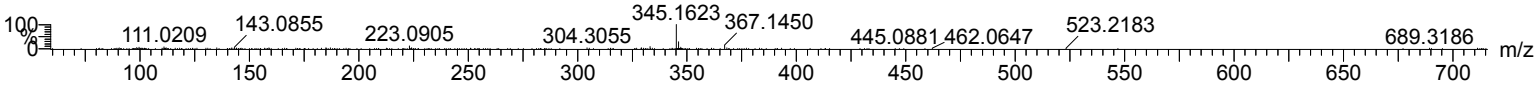
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
3124 formula(e) evaluated with 25 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 F: 0-6

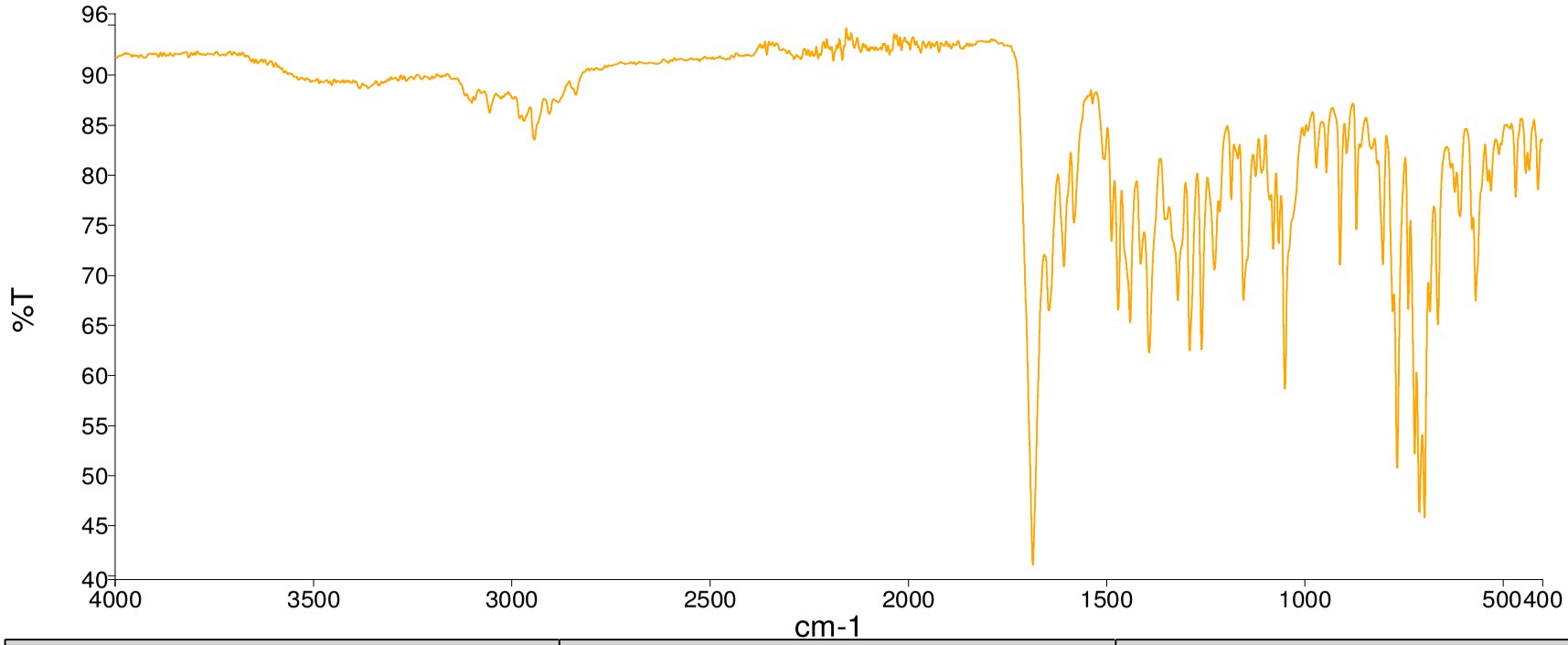
21-Jul-2022
MTF_MTF5K_179349 511 (4.296) Cm (510:517)

21-Jul-2022
1: TOF MS ES+
5.10e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
345.1623	345.1622	0.1	0.3	-1.5	199.6	12.611	0.00	C6 H21 N8 O4 F4
	345.1622	0.1	0.3	0.5	196.9	9.848	0.01	C10 H25 N4 O9
	345.1626	-0.3	-0.9	5.5	193.7	6.658	0.13	C16 H23 N2 O4 F2
	345.1618	0.5	1.4	-6.5	204.1	17.135	0.00	H23 N10 O9 F2
	345.1614	0.9	2.6	9.5	191.1	4.058	1.73	C19 H22 N2 O3 F
	345.1613	1.0	2.9	-1.5	197.9	10.881	0.00	C11 H23 N2 O3 F6
	345.1633	-1.0	-2.9	-3.5	198.7	11.727	0.00	C7 H26 N4 O10 F
	345.1633	-1.0	-2.9	-5.5	201.5	14.483	0.00	C3 H22 N8 O5 F5
	345.1635	-1.2	-3.5	5.5	195.9	8.898	0.01	C11 H21 N8 O5
	345.1610	1.3	3.8	2.5	198.0	10.947	0.00	C9 H20 N8 O3 F3
	345.1609	1.4	4.1	-6.5	200.4	13.352	0.00	C5 H25 N4 O8 F4
	345.1637	-1.4	-4.1	1.5	195.9	8.943	0.01	C13 H24 N2 O5 F3
	345.1639	-1.6	-4.6	10.5	193.2	6.178	0.21	C17 H19 N6 F2
	345.1606	1.7	4.9	-2.5	201.3	14.333	0.00	C3 H22 N10 O8 F
	345.1642	-1.9	-5.5	6.5	194.0	7.045	0.09	C19 H22 F5
	345.1643	-2.0	-5.8	17.5	187.3	0.345	70.80	C27 H21
	345.1603	2.0	5.8	13.5	188.3	1.311	26.97	C22 H21 N2 O2
	345.1601	2.2	6.4	2.5	196.3	9.335	0.01	C14 H22 N2 O2 F5
	345.1645	-2.2	-6.4	-9.5	204.5	17.508	0.00	H23 N8 O6 F6
	345.1646	-2.3	-6.7	1.5	198.1	11.049	0.00	C8 H22 N8 O6 F
	345.1599	2.4	7.0	6.5	196.2	9.208	0.01	C12 H19 N8 O2 F2
	345.1649	-2.6	-7.5	-2.5	198.0	10.977	0.00	C10 H25 N2 O6 F4
	345.1597	2.6	7.5	-2.5	198.9	11.910	0.00	C8 H24 N4 O7 F3
	345.1651	-2.8	-8.1	6.5	195.4	8.397	0.02	C14 H20 N6 O F3
	345.1595	2.8	8.1	1.5	199.5	12.459	0.00	C6 H21 N10 O7

Analyst Lenny Lauchlan
Date 07 July 2022 08:09



Sample Name	Description	Quality Checks
MTF 005K	Sample 021 By Lenny Date Thursday, July 07 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

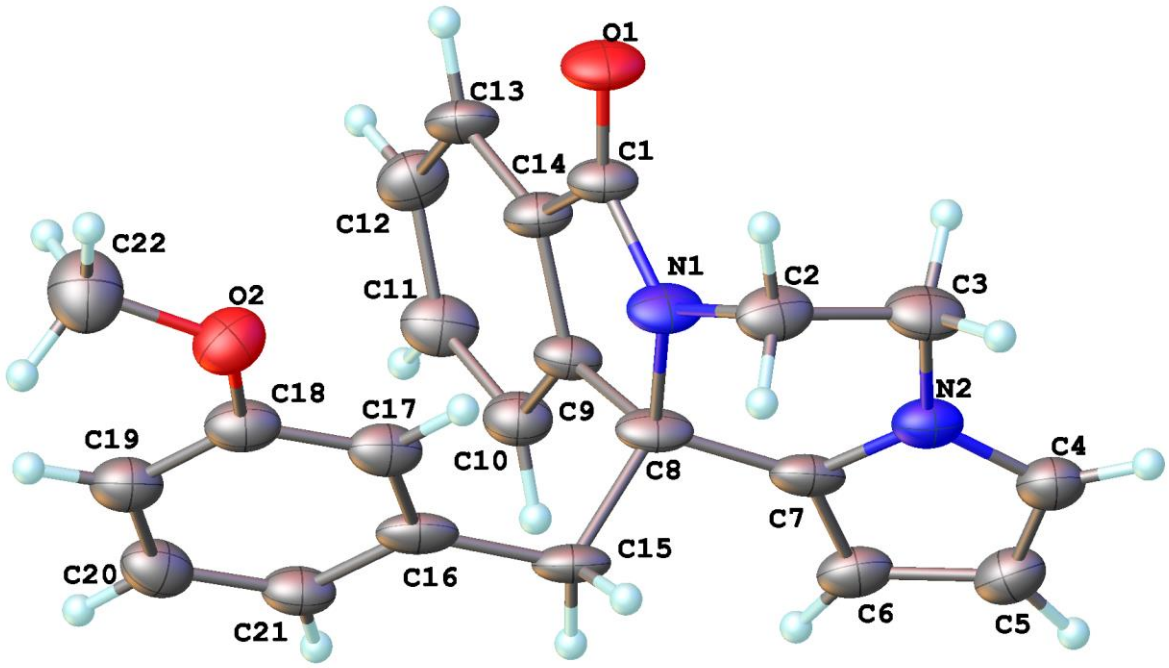


Table 1 Crystal data and structure refinement for 22srv180.	
Identification code	22srv180
Empirical formula	$C_{22}H_{20}N_2O_2$
Formula weight	344.40
Temperature/K	100.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	32.325(3)
b/Å	7.2919(6)
c/Å	15.5017(14)
α/°	90
β/°	103.775(2)
γ/°	90
Volume/Å^3	3548.8(5)
Z	8
ρ_{calc}g/cm^3	1.289
μ/mm^{-1}	0.078

F(000)	1456.0
Crystal size/mm^3	0.06 × 0.02 × 0.001
Radiation	Synchrotron (λ = 0.6889)
2Θ range for data collection/°	1.258 to 49
Index ranges	-38 ≤ h ≤ 38, -8 ≤ k ≤ 8, -18 ≤ l ≤ 18
Reflections collected	33898
Independent reflections	6488 [R_{int} = 0.0851, R_{sigma} = 0.1109]
Data/restraints/parameters	6488/0/472
Goodness-of-fit on F^2	1.081
Final R indexes [I>=2σ (I)]	R_1 = 0.0989, wR_2 = 0.2600
Final R indexes [all data]	R_1 = 0.1096, wR_2 = 0.2739
Largest diff. peak/hole / e $Å^{-3}$	0.88/-0.36

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 22srv180. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	3905.8(10)	9016(4)	5093(2)	41.0(8)
O2	2782.7(10)	7299(4)	6642(2)	39.9(8)
N1	4119.7(11)	6287(4)	5807(2)	32.3(8)
N2	4914.9(11)	4855(4)	6242(2)	33.2(8)
C1	3936.0(13)	7358(5)	5098(3)	28.8(9)
C2	4409.6(13)	7023(5)	6590(3)	35.5(10)
C3	4862.9(15)	6761(5)	6506(3)	39.3(10)
C4	5295.2(14)	3964(5)	6340(3)	35.4(9)
C5	5215.3(14)	2267(6)	5993(3)	36.8(10)
C6	4768.1(14)	2090(5)	5653(3)	35.0(10)
C7	4591.8(14)	3714(5)	5800(2)	32.0(9)
C8	4132.1(13)	4315(5)	5615(3)	31.0(9)
C9	3904.3(12)	4293(5)	4632(2)	28.1(8)
C10	3799.4(13)	2796(6)	4071(3)	32.7(9)
C11	3585.4(14)	3184(5)	3191(3)	37.6(10)
C12	3480.7(14)	4949(6)	2891(3)	36.9(10)
C13	3582.1(13)	6426(6)	3468(3)	35.4(10)
C14	3790.1(13)	6051(5)	4352(3)	29.3(9)
C15	3890.2(13)	3163(5)	6186(3)	31.8(9)
C16	3428.1(14)	3609(5)	6050(2)	33.2(9)
C17	3292.0(13)	5243(5)	6383(2)	33.0(9)
C18	2865.1(14)	5626(5)	6276(3)	34.2(9)

C19	2555.0(13)	4405(6)	5853(3)	36.8(10)
C20	2685.7(14)	2777(6)	5528(3)	37.2(10)
C21	3111.4(14)	2395(5)	5615(3)	32.8(10)
C22	2351.8(15)	7900(8)	6409(4)	51.7(13)
O1A	1090.7(10)	-4039(3)	1175(2)	40.0(8)
O2A	2239.1(9)	-2215(4)	3824(2)	41.1(8)
N1A	884.2(11)	-1303(4)	1683(2)	29.2(8)
N2A	86.7(12)	130(4)	1329(2)	33.5(8)
C1A	1065.2(13)	-2366(5)	1147(3)	28.4(9)
C2A	592.5(13)	-2034(5)	2186(3)	34.7(10)
C3A	138.8(15)	-1772(5)	1650(3)	38.8(10)
C4A	-294.7(14)	1016(6)	1050(3)	36.4(10)
C5A	-218.1(14)	2703(6)	766(3)	32.2(9)
C6A	226.5(14)	2890(5)	873(3)	35.1(10)
C7A	411.0(14)	1257(5)	1205(3)	33.1(9)
C8A	865.9(13)	665(5)	1472(2)	28.7(9)
C9A	1099.8(12)	680(5)	714(2)	29.1(9)
C10A	1200.2(13)	2174(5)	240(3)	31.0(9)
C11A	1411.8(14)	1786(5)	-423(3)	34.5(9)
C12A	1515.1(14)	-23(6)	-612(3)	36.8(10)
C13A	1418.4(14)	-1456(5)	-128(3)	35.3(10)
C14A	1214.6(13)	-1076(5)	550(2)	29.1(9)
C15A	1108.3(13)	1836(5)	2276(3)	30.4(9)
C16A	1576.1(13)	1423(5)	2601(2)	31.3(9)
C17A	1712.2(13)	-189(5)	3065(2)	30.1(9)
C18A	2142.3(14)	-559(5)	3381(3)	35.5(9)
C19A	2450.5(13)	687(6)	3242(3)	36.9(10)
C20A	2308.4(15)	2330(6)	2782(3)	38.3(10)
C21A	1882.4(14)	2639(5)	2463(3)	31.7(10)
C22A	2666.6(14)	-2767(7)	4008(3)	42.5(11)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 22srv180. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	64(2)	15.8(14)	43.2(18)	-0.8(12)	12.5(14)	2.8(12)
O2	47(2)	32.8(16)	38.2(16)	-7.2(13)	7.5(15)	6.4(13)
N1	53(2)	14.1(16)	29.0(17)	-6.4(13)	7.8(15)	0.4(14)
N2	47(2)	22.8(17)	28.6(17)	1.9(13)	7.0(15)	0.1(14)
C1	46(3)	16.4(18)	26(2)	0.7(14)	10.9(18)	1.1(15)
C2	55(3)	22(2)	26(2)	-6.1(16)	3.8(18)	0.1(18)
C3	60(3)	21(2)	37(2)	-3.5(17)	11(2)	-3.4(19)
C4	43(2)	30(2)	33(2)	6.2(17)	8.5(17)	1.6(17)
C5	45(3)	33(2)	33(2)	5.3(18)	10(2)	8.4(19)
C6	52(3)	27(2)	26(2)	3.8(17)	8.3(18)	4.7(19)

C7	53(3)	19.1(18)	23.4(18)	4.0(15)	8.6(16)	-3.2(17)
C8	56(3)	12.4(18)	25.6(19)	-2.8(15)	10.6(17)	-0.7(16)
C9	43(2)	18.2(18)	24.6(19)	0.6(14)	10.7(16)	-2.3(16)
C10	44(3)	25(2)	31(2)	-1.2(16)	11.1(19)	0.4(17)
C11	56(3)	30(2)	29(2)	-6.9(18)	13.2(18)	-1.8(19)
C12	46(3)	37(2)	27(2)	1.5(17)	7.6(17)	4.8(19)
C13	49(3)	27(2)	32(2)	12.4(16)	12.3(18)	3.4(17)
C14	43(2)	18.5(18)	27.6(19)	2.5(15)	10.3(16)	3.9(16)
C15	56(3)	15.8(18)	25.2(19)	5.3(15)	12.2(17)	2.8(17)
C16	62(3)	19.5(18)	19.6(18)	4.4(14)	12.6(17)	1.1(17)
C17	52(3)	23.7(19)	22.9(18)	-2.4(15)	7.3(17)	-3.2(17)
C18	53(3)	23.5(19)	26.8(19)	-0.8(16)	10.9(17)	1.9(18)
C19	49(3)	29(2)	33(2)	2.8(17)	10.0(18)	-0.5(18)
C20	50(3)	31(2)	30(2)	-2.0(17)	8(2)	-7.6(19)
C21	50(3)	19.6(18)	29(2)	-0.4(15)	11(2)	-0.9(17)
C22	52(3)	49(3)	55(3)	-15(2)	13(2)	0(2)
O1A	62(2)	11.9(13)	46.7(18)	-0.6(12)	14.5(15)	1.3(12)
O2A	41.4(19)	38.0(18)	45.0(17)	19.4(14)	12.7(15)	4.3(14)
N1A	49(2)	13.1(15)	28.9(16)	3.3(12)	16.3(14)	0.0(13)
N2A	54(2)	20.4(16)	27.3(17)	-3.1(13)	12.6(15)	-5.0(14)
C1A	40(3)	18.5(18)	26(2)	-1.2(14)	5.2(18)	2.3(15)
C2A	54(3)	24(2)	29(2)	7.1(17)	15.5(19)	-2.3(19)
C3A	61(3)	22(2)	37(2)	1.3(17)	18(2)	-4.0(18)
C4A	45(3)	32(2)	32(2)	-7.2(17)	9.9(18)	5.4(18)
C5A	39(3)	30(2)	28(2)	-1.3(16)	7.7(18)	6.2(17)
C6A	50(3)	21(2)	34(2)	-0.7(17)	10.0(19)	3.1(18)
C7A	59(3)	18.3(18)	24.6(19)	-1.7(15)	15.0(17)	-3.6(18)
C8A	49(3)	10.8(17)	27.1(19)	1.6(14)	10.7(17)	1.0(15)
C9A	43(2)	20.0(19)	24.8(19)	-3.3(15)	9.0(16)	-1.0(16)
C10A	45(3)	22.2(19)	25(2)	1.2(16)	8.3(18)	2.7(17)
C11A	50(3)	27(2)	28(2)	4.1(16)	11.9(18)	-0.8(18)
C12A	46(2)	39(2)	27(2)	-4.3(17)	12.5(18)	3.1(19)
C13A	51(3)	27(2)	27(2)	-5.0(16)	8.1(18)	11.2(18)
C14A	45(2)	16.2(17)	23.9(18)	-2.9(14)	4.8(16)	0.7(16)
C15A	48(2)	15.9(18)	27.0(19)	-1.0(15)	9.1(16)	0.3(16)
C16A	54(3)	18.7(18)	23.6(19)	-2.3(14)	13.3(17)	1.6(17)
C17A	47(2)	19.5(18)	25.7(19)	-1.3(15)	12.8(16)	-1.4(16)
C18A	57(3)	19.5(18)	32(2)	1.8(15)	15.2(18)	3.0(18)
C19A	49(3)	28(2)	33(2)	3.1(17)	7.6(18)	-0.1(18)
C20A	52(3)	30(2)	33(2)	1.0(17)	11(2)	-5.0(19)
C21A	49(3)	17.9(18)	27(2)	0.6(15)	6.9(19)	-2.7(16)
C22A	44(3)	42(3)	43(3)	11(2)	13(2)	9(2)

Table 4 Bond Lengths for 22srv180.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
O1	C1	1.213(5)		O1A	C1A	1.223(5)
O2	C18	1.398(5)		O2A	C18A	1.388(5)
O2	C22	1.422(6)		O2A	C22A	1.402(5)
N1	C1	1.363(5)		N1A	C1A	1.365(5)
N1	C2	1.449(5)		N1A	C2A	1.460(5)
N1	C8	1.471(4)		N1A	C8A	1.470(4)
N2	C3	1.469(5)		N2A	C3A	1.469(5)
N2	C4	1.366(5)		N2A	C4A	1.368(6)
N2	C7	1.383(5)		N2A	C7A	1.381(5)
C1	C14	1.486(5)		C1A	C14A	1.480(6)
C2	C3	1.514(6)		C2A	C3A	1.516(6)
C4	C5	1.350(6)		C4A	C5A	1.349(6)
C5	C6	1.422(6)		C5A	C6A	1.413(6)
C6	C7	1.357(5)		C6A	C7A	1.376(5)
C7	C8	1.510(6)		C7A	C8A	1.493(6)
C8	C9	1.527(5)		C8A	C9A	1.541(5)
C8	C15	1.558(5)		C8A	C15A	1.559(5)
C9	C10	1.386(5)		C9A	C10A	1.395(5)
C9	C14	1.375(5)		C9A	C14A	1.373(5)
C10	C11	1.403(6)		C10A	C11A	1.392(6)
C11	C12	1.383(5)		C11A	C12A	1.408(6)
C12	C13	1.389(6)		C12A	C13A	1.365(6)
C13	C14	1.401(5)		C13A	C14A	1.395(6)
C15	C16	1.494(6)		C15A	C16A	1.506(6)
C16	C17	1.410(5)		C16A	C17A	1.393(5)
C16	C21	1.399(6)		C16A	C21A	1.383(6)
C17	C18	1.379(6)		C17A	C18A	1.386(6)
C18	C19	1.383(6)		C18A	C19A	1.402(6)
C19	C20	1.395(6)		C19A	C20A	1.413(6)
C20	C21	1.378(6)		C20A	C21A	1.366(5)

Table 5 Bond Angles for 22srv180.								
Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C18	O2	C22	115.8(3)		C18A	O2A	C22A	116.5(3)
C1	N1	C2	122.3(3)		C1A	N1A	C2A	122.9(3)
C1	N1	C8	115.2(3)		C1A	N1A	C8A	114.8(3)
C2	N1	C8	119.2(3)		C2A	N1A	C8A	118.5(3)
C4	N2	C3	125.3(4)		C4A	N2A	C3A	125.1(4)
C4	N2	C7	108.8(3)		C4A	N2A	C7A	109.4(3)
C7	N2	C3	125.7(4)		C7A	N2A	C3A	125.4(4)
O1	C1	N1	126.5(4)		O1A	C1A	N1A	125.5(4)
O1	C1	C14	128.6(4)		O1A	C1A	C14A	128.8(4)

N1	C1	C14	104.9(3)		N1A	C1A	C14A	105.7(3)
N1	C2	C3	109.0(3)		N1A	C2A	C3A	109.0(3)
N2	C3	C2	108.7(3)		N2A	C3A	C2A	108.8(3)
C5	C4	N2	108.0(4)		C5A	C4A	N2A	108.2(4)
C4	C5	C6	108.2(4)		C4A	C5A	C6A	108.1(4)
C7	C6	C5	106.8(4)		C7A	C6A	C5A	107.4(4)
N2	C7	C8	120.8(3)		N2A	C7A	C8A	121.3(3)
C6	C7	N2	108.1(4)		C6A	C7A	N2A	106.9(4)
C6	C7	C8	131.0(4)		C6A	C7A	C8A	131.6(4)
N1	C8	C7	108.6(3)		N1A	C8A	C7A	109.2(3)
N1	C8	C9	100.5(3)		N1A	C8A	C9A	100.1(3)
N1	C8	C15	111.8(3)		N1A	C8A	C15A	111.8(3)
C7	C8	C9	113.9(3)		C7A	C8A	C9A	114.6(3)
C7	C8	C15	109.9(3)		C7A	C8A	C15A	109.7(3)
C9	C8	C15	111.9(3)		C9A	C8A	C15A	111.1(3)
C10	C9	C8	128.5(3)		C10A	C9A	C8A	128.7(3)
C14	C9	C8	109.6(3)		C14A	C9A	C8A	109.8(3)
C14	C9	C10	121.9(4)		C14A	C9A	C10A	121.5(4)
C9	C10	C11	116.2(4)		C11A	C10A	C9A	116.6(4)
C12	C11	C10	122.6(4)		C10A	C11A	C12A	121.7(4)
C11	C12	C13	120.2(4)		C13A	C12A	C11A	120.4(4)
C12	C13	C14	117.6(4)		C12A	C13A	C14A	118.2(4)
C9	C14	C1	109.9(3)		C9A	C14A	C1A	109.5(3)
C9	C14	C13	121.4(4)		C9A	C14A	C13A	121.5(4)
C13	C14	C1	128.7(3)		C13A	C14A	C1A	128.9(3)
C16	C15	C8	115.0(3)		C16A	C15A	C8A	115.6(3)
C17	C16	C15	121.4(4)		C17A	C16A	C15A	120.7(4)
C21	C16	C15	121.5(4)		C21A	C16A	C15A	121.2(4)
C21	C16	C17	117.0(4)		C21A	C16A	C17A	118.1(4)
C18	C17	C16	121.2(4)		C18A	C17A	C16A	120.9(4)
C17	C18	O2	114.2(4)		O2A	C18A	C19A	123.7(4)
C17	C18	C19	121.2(4)		C17A	C18A	O2A	115.7(4)
C19	C18	O2	124.6(4)		C17A	C18A	C19A	120.6(4)
C18	C19	C20	118.1(4)		C18A	C19A	C20A	118.0(4)
C21	C20	C19	121.2(4)		C21A	C20A	C19A	120.1(4)
C20	C21	C16	121.2(4)		C20A	C21A	C16A	122.3(4)

Table 6 Torsion Angles for 22srv180.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C2	C3	N2	-48.4(4)		C15	C8	N1	C2	79.6(4)
N1	C8	C7	N2	11.4(5)		C15	C8	C7	N2	-111.2(4)
C2	N1	C1	O1	-17.8(7)		C16	C15	C8	N1	60.4(4)
C2	C3	N2	C4	-160.4(4)		N1A	C2A	C3A	N2A	-48.5(4)
C2	C3	N2	C7	24.2(5)		N1A	C8A	C7A	N2A	11.5(5)

C3	C2	N1	C1	-95.2(4)		C2A	N1A	C1A	O1A	-17.9(6)
C3	C2	N1	C8	63.1(4)		C2A	C3A	N2A	C4A	-160.3(4)
C6	C7	N2	C3	178.2(4)		C2A	C3A	N2A	C7A	24.3(5)
C6	C7	N2	C4	2.3(4)		C3A	C2A	N1A	C1A	-94.4(4)
C6	C7	C8	N1	-173.4(4)		C3A	C2A	N1A	C8A	62.6(4)
C6	C7	C8	C9	-62.4(5)		C6A	C7A	N2A	C3A	178.1(3)
C6	C7	C8	C15	64.1(5)		C6A	C7A	N2A	C4A	2.1(4)
C7	C8	N1	C1	118.1(4)		C6A	C7A	C8A	N1A	-173.2(4)
C7	C8	N1	C2	-41.7(5)		C6A	C7A	C8A	C9A	-61.9(5)
C7	C8	C9	C10	67.0(5)		C6A	C7A	C8A	C15A	64.0(5)
C7	C8	C9	C14	-115.7(4)		C7A	C8A	N1A	C1A	117.4(4)
C7	C8	C15	C16	-179.0(3)		C7A	C8A	N1A	C2A	-41.4(4)
C8	N1	C1	O1	-177.0(4)		C7A	C8A	C15A	C16A	-178.3(3)
C8	C7	N2	C3	-5.6(6)		C8A	N1A	C1A	O1A	-175.7(4)
C8	C7	N2	C4	178.5(3)		C8A	C7A	N2A	C3A	-5.5(6)
C8	C15	C16	C17	-73.0(4)		C8A	C7A	N2A	C4A	178.5(3)
C8	C15	C16	C21	109.3(4)		C8A	C15A	C16A	C17A	-72.5(5)
C9	C8	N1	C1	-1.7(4)		C8A	C15A	C16A	C21A	108.6(4)
C9	C8	N1	C2	-161.5(3)		C9A	C8A	N1A	C1A	-3.2(4)
C9	C8	C7	N2	122.4(4)		C9A	C8A	N1A	C2A	-162.0(3)
C9	C8	C15	C16	-51.4(4)		C9A	C8A	C7A	N2A	122.8(4)
C10	C9	C8	N1	-177.1(4)		C9A	C8A	C15A	C16A	-50.6(4)
C10	C9	C8	C15	-58.4(5)		C14A	C1A	N1A	C2A	161.8(3)
C14	C1	N1	C2	161.5(4)		C14A	C1A	N1A	C8A	4.0(5)
C14	C1	N1	C8	2.4(5)		C15A	C8A	N1A	C1A	-121.0(4)
C14	C9	C8	N1	0.2(4)		C15A	C8A	N1A	C2A	80.2(4)
C14	C9	C8	C15	119.0(4)		C15A	C8A	C7A	N2A	-111.4(4)
C15	C8	N1	C1	-120.5(4)		C16A	C15A	C8A	N1A	60.3(4)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv180.

Atom	***x***	***y***	***z***	**U(eq)**
H2A	4368.34	6382.34	7126.76	43
H2B	4351.55	8344.06	6650.4	43
H3A	4923.66	7612.55	6053.93	47
H3B	5064.74	7026.54	7080.39	47
H4	5568.06	4453.3	6607.23	42
H5	5422.16	1350.29	5977.65	44
H6	4621.07	1036.34	5376.89	42
H10	3868.61	1577.48	4270.53	39
H11	3509.27	2194.9	2785.74	45
H12	3339	5152.23	2287.65	44
H13	3512.97	7646.15	3271.67	42
H15A	3917.5	1848.94	6048.66	38

H15B	4030.8	3346.68	6820.66	38
H17	3498.16	6094.95	6686.19	40
H19	2261.26	4668.88	5787.05	44
H20	2477.73	1914.62	5240.85	45
H21	3191.12	1288.06	5374.81	39
H22A	2254.73	7976.17	5760.68	78
H22B	2330.6	9111.92	6668.25	78
H22C	2173.13	7026.89	6636.16	78
H2AA	634.29	-1384.85	2761.43	42
H2AB	650.09	-3353.82	2307.69	42
H3AA	77.84	-2629.55	1140.36	47
H3AB	-62.98	-2031.26	2025.22	47
H4A	-566.61	527.15	1054.79	44
H5A	-426.55	3607.5	535.53	39
H6A	371.14	3947.8	739.79	42
H10A	1127.91	3392.98	362.67	37
H11A	1488.55	2767.69	-756.56	41
H12A	1653	-246.47	-1078.54	44
H13A	1487.89	-2679.23	-250.76	42
H15C	1076.3	3146.6	2105.7	36
H15D	970.02	1653.1	2774.36	36
H17A	1507.53	-1044.86	3167.23	36
H19A	2745.79	434.29	3449.74	44
H20A	2509.19	3219.95	2695.78	46
H21A	1793.5	3727.2	2133.88	38
H22D	2766.15	-2759.8	3458.3	64
H22E	2692.54	-4008.62	4257.49	64
H22F	2839.91	-1919.84	4436.91	64

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

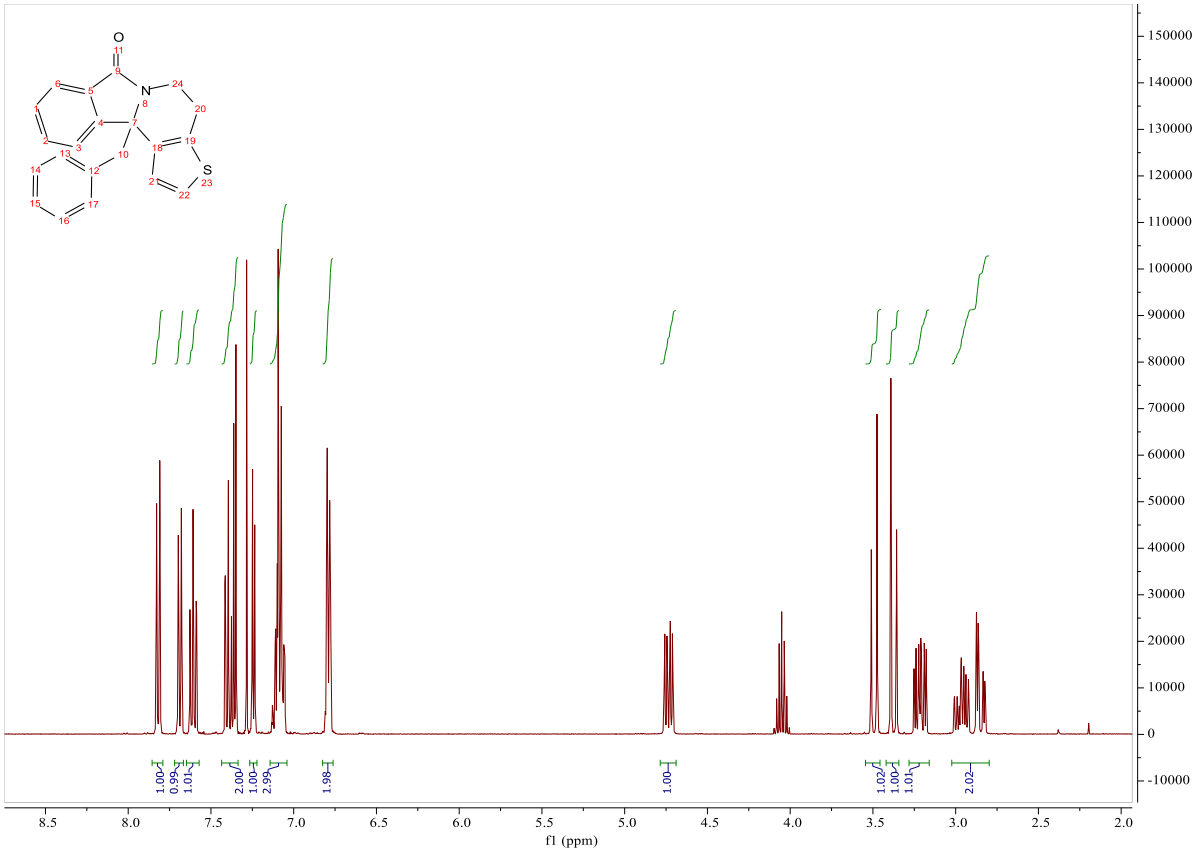
1. Twinned data refinement
Scales: 0.723(3) 0.277(3)
2. Fixed Uiso
At 1.2 times of: All C(H) groups, All C(H,H) groups
At 1.5 times of: All C(H,H,H) groups
3.a Secondary CH2 refined with riding coordinates:
C2(H2A,H2B), C3(H3A,H3B), C15(H15A,H15B), C2A(H2AA,H2AB), C3A(H3AA,H3AB), C15A(H15C,H15D)
3.b Aromatic/amide H refined with riding coordinates:
C4(H4), C5(H5), C6(H6), C10(H10), C11(H11), C12(H12), C13(H13), C17(H17), C19(H19), C20(H20), C21(H21), C4A(H4A), C5A(H5A), C6A(H6A), C10A(H10A), C11A(H11A), C12A(H12A), C13A(H13A), C17A(H17A), C19A(H19A), C20A(H20A), C21A(H21A)

3.c Idealised Me refined as rotating group:
C22(H22A,H22B,H22C), C22A(H22D,H22E,H22F)

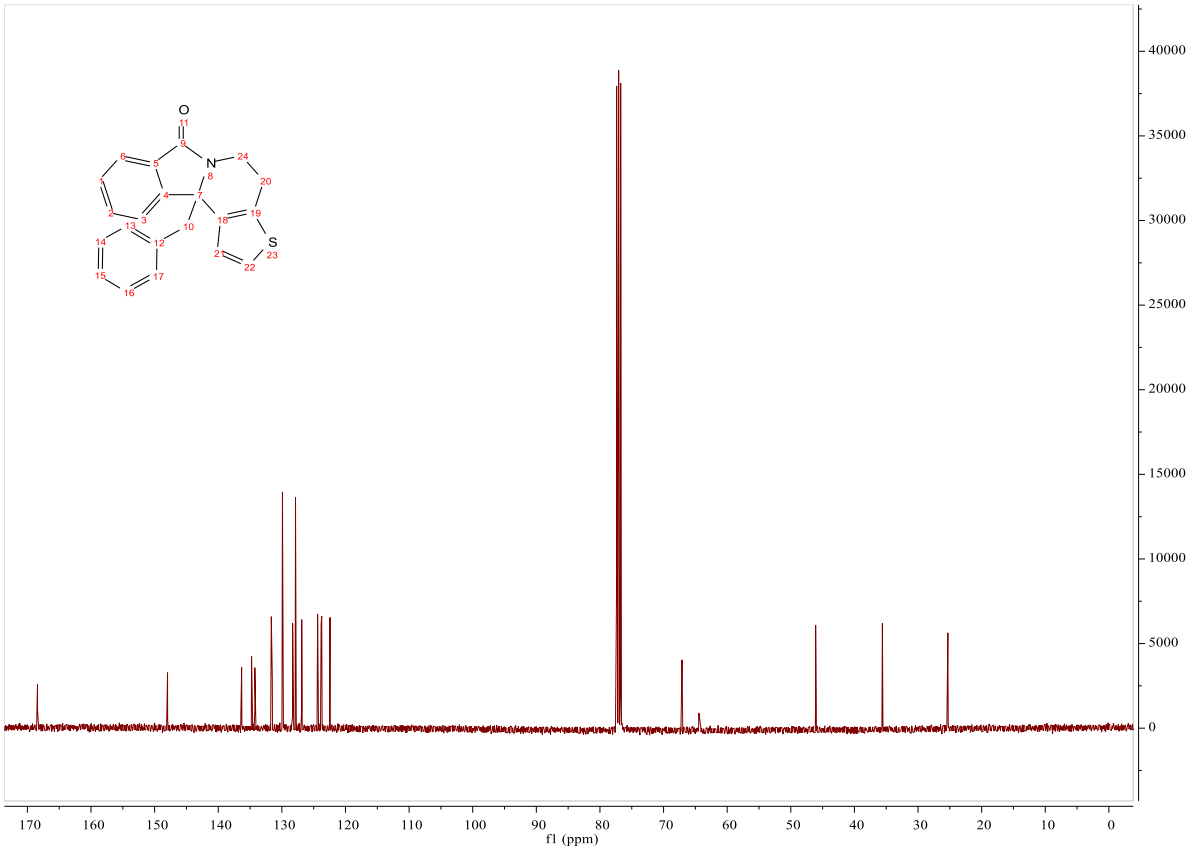
Synthesis of **80-96** through implementation of alternative amine components

11*b*-benzyl-4,11*b*-dihydrothieno[3',2':3,4]pyrido[2,1-*a*]isoindol-7(5*H*)-one **80**

^{1}H:



^{13}C:



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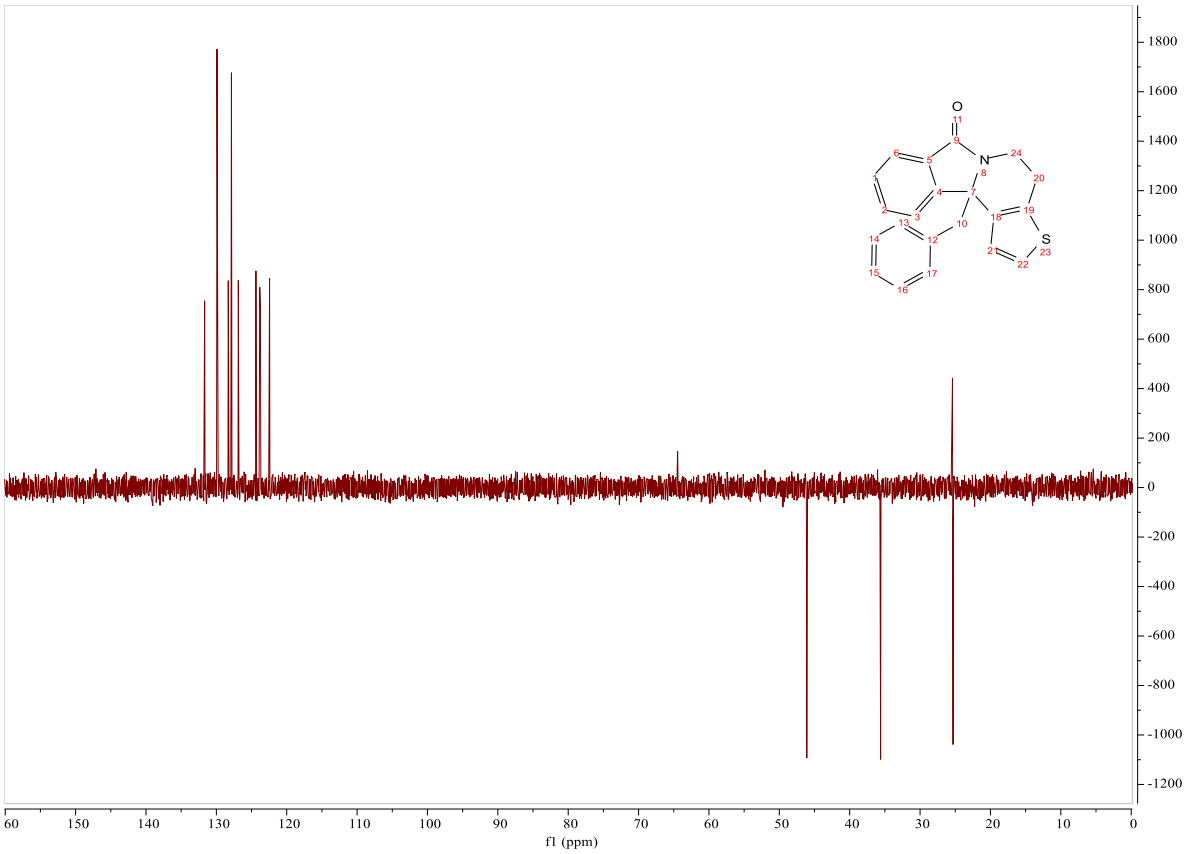
O
N
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200
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-600
-800
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110
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90
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70
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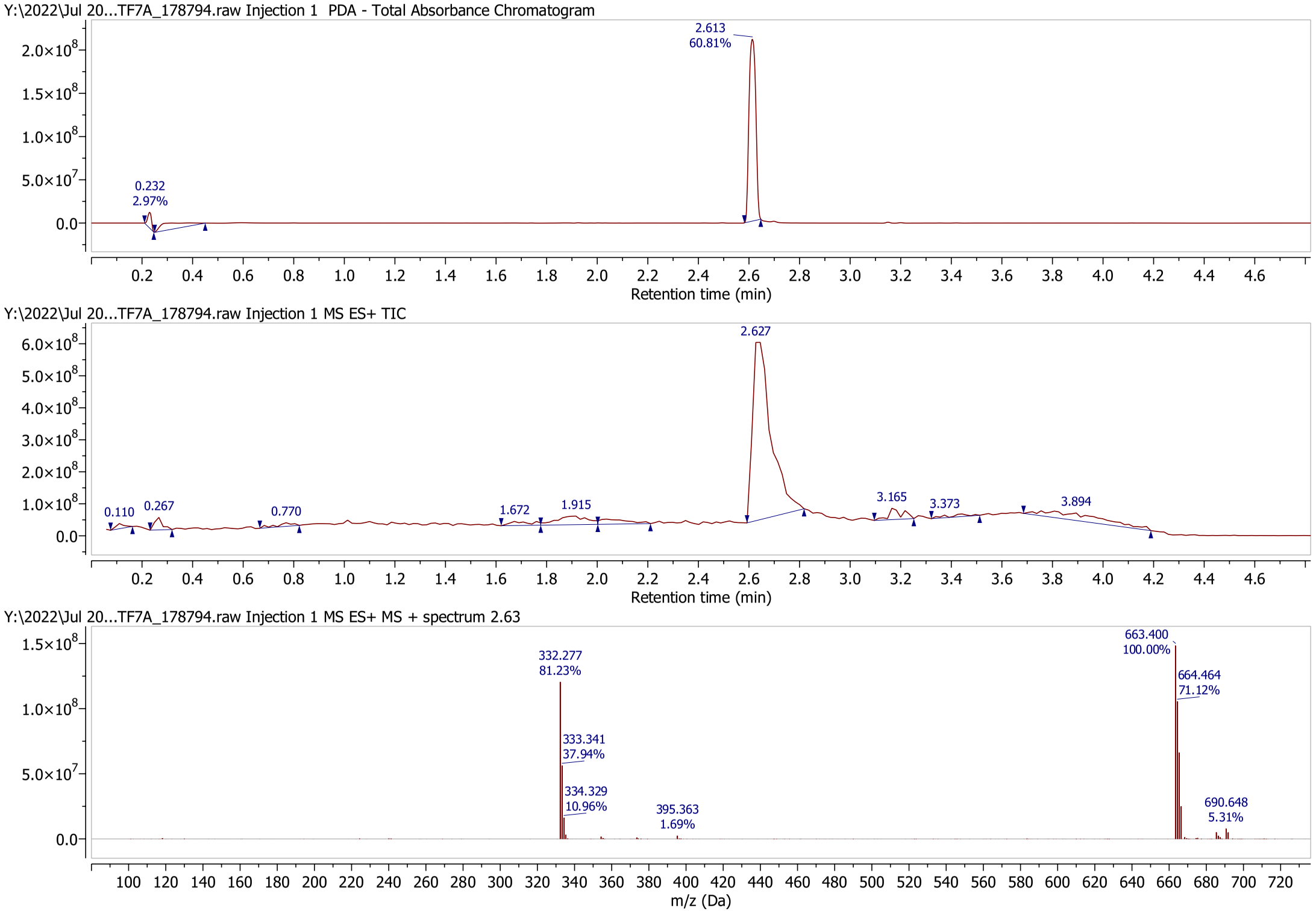
50
40
30
20
10
0
f1 (ppm)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0.232
2.97%
Retention time (min)
Y:\2022\Jul 20...TF7A_178794.raw Injection 1 MS ES+ TIC
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0.110
0.267
0.770
1.672
1.915
3.165
3.373
3.894
Retention time (min)
Y:\2022\Jul 20...TF7A_178794.raw Injection 1 MS ES+ MS + spectrum 2.63
663.400
100.00%
332.277
81.23%
664.464
71.12%
333.341
37.94%
334.329
10.96%
395.363
1.69%
690.648
5.31%
m/z (Da)

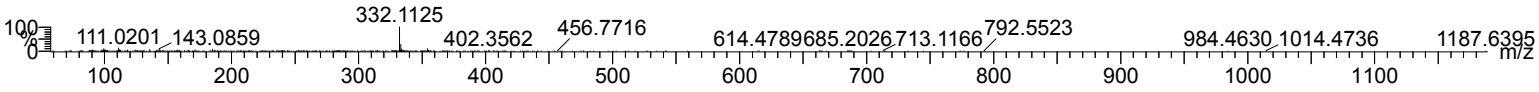
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
2127 formula(e) evaluated with 16 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 S: 0-4

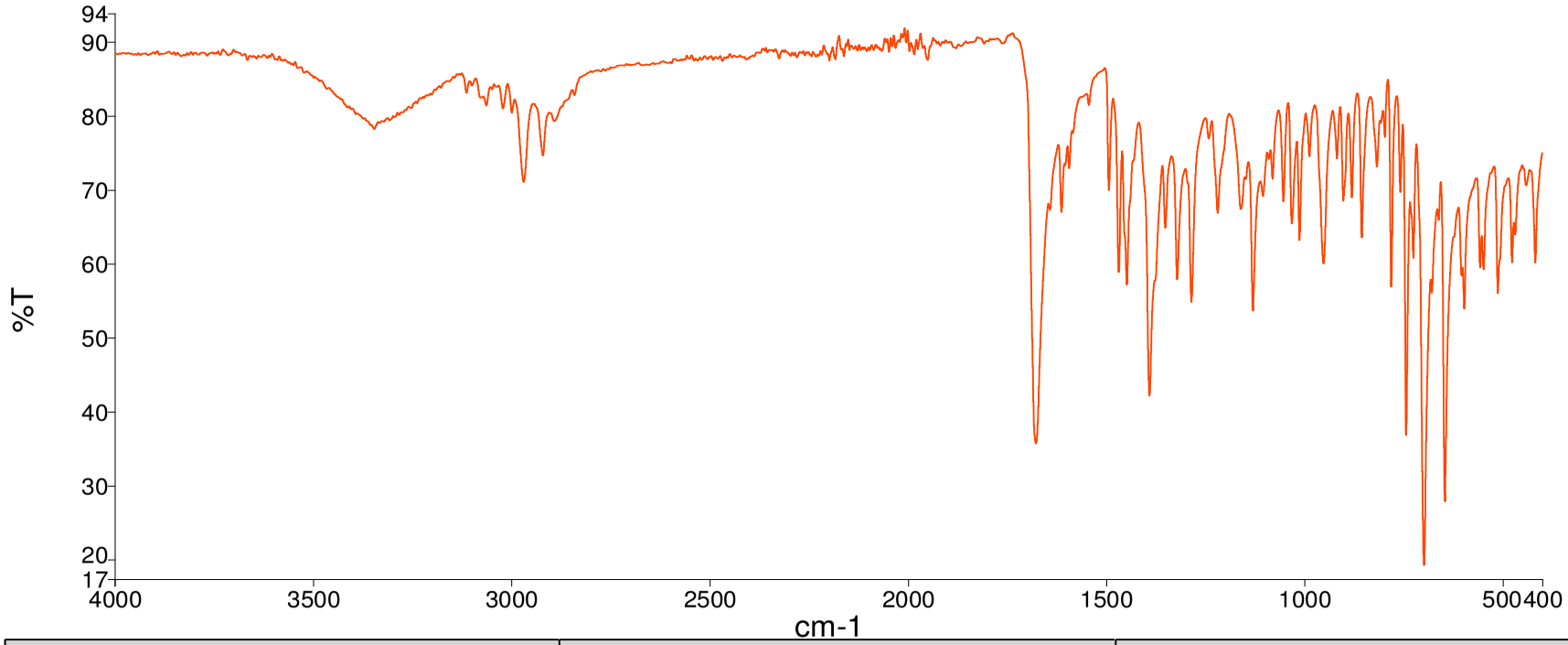
21-Jul-2022
MTF_MTF7A_179350 548 (4.604) Cm (547:558)

21-Jul-2022
1: TOF MS ES+
4.17e+003



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
332.1125	332.1121	0.4	1.2	-8.5	255.6	18.088	0.00	C H26 N5 O10 S2
	332.1141	-1.6	-4.8	5.5	249.2	11.653	0.00	C10 H18 N7 O4 S
	332.1136	-1.1	-3.3	-0.5	252.9	15.381	0.00	C10 H26 N3 O3 S3
	332.1107	1.8	5.4	10.5	252.6	15.067	0.00	C13 H14 N7 O4
	332.1103	2.2	6.6	4.5	248.1	10.566	0.00	C13 H22 N3 O3 S2
	332.1134	-0.9	-2.7	9.5	250.9	13.370	0.00	C17 H18 N O6
	332.1147	-2.2	-6.6	14.5	250.8	13.285	0.00	C18 H14 N5 O2
	332.1143	-1.8	-5.4	8.5	246.0	8.471	0.02	C18 H22 N O S2
	332.1134	-0.9	-2.7	-3.5	254.2	16.678	0.00	C2 H22 N9 O6 S2
	332.1130	-0.5	-1.5	-9.5	257.9	20.344	0.00	C2 H30 N5 O5 S4
	332.1109	1.6	4.8	13.5	237.5	0.000	99.98	C21 H18 N O S
	332.1143	-1.8	-5.4	-4.5	257.0	19.489	0.00	C3 H26 N9 O S4
	332.1101	2.4	7.2	1.5	252.9	15.345	0.00	C5 H18 N9 O6 S
	332.1096	2.9	8.7	-4.5	254.8	17.302	0.00	C5 H26 N5 O5 S3
	332.1109	1.6	4.8	0.5	253.4	15.903	0.00	C6 H22 N9 O S3
	332.1128	-0.3	-0.9	0.5	250.8	13.271	0.00	C9 H22 N3 O8 S

Analyst Lenny Lauchlan
Date 28 June 2022 12:59



Sample Name	Description	Quality Checks
MTF 007A	Sample 024 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

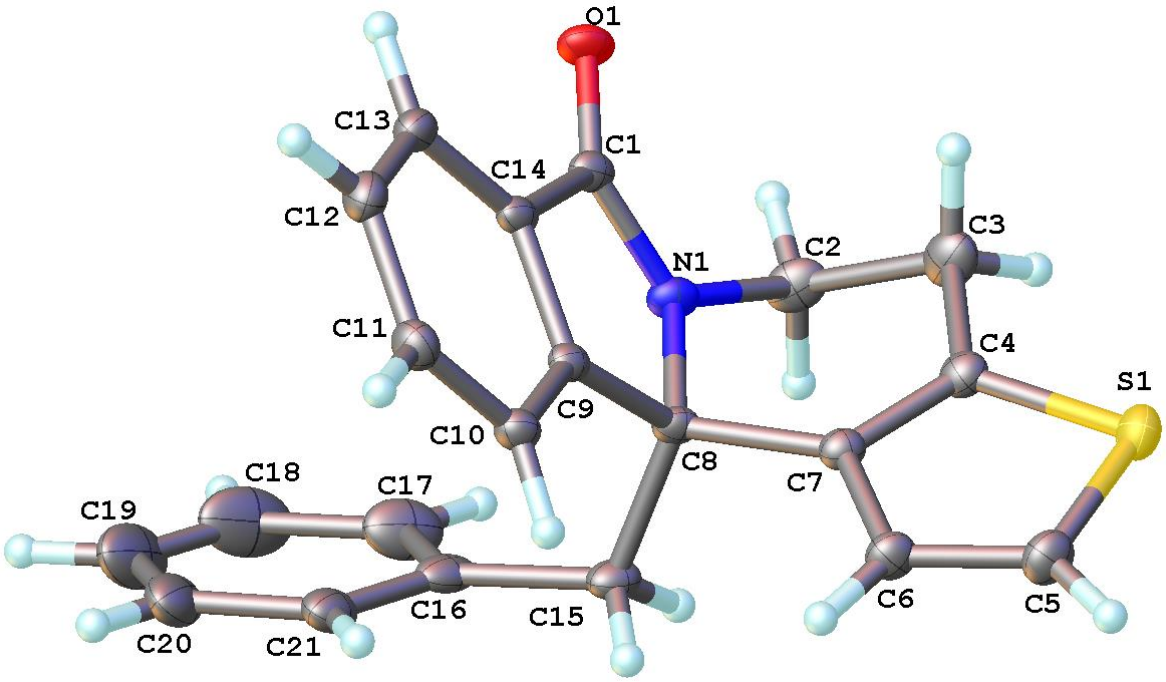


Table 1 Crystal data and structure refinement for 22srv070.	
Identification code	22srv070
Empirical formula	$C_{21}H_{17}NOS$
Formula weight	331.42
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.9177(3)
b/Å	9.5917(2)
c/Å	14.2503(3)
α/°	90
β/°	119.0699(8)
γ/°	90
Volume/Å^3	1662.69(6)
Z	4
ρ_{calc}g/cm^3	1.324
μ/mm^{-1}	0.201

F(000)	696.0
Crystal size/mm^3	0.19 × 0.18 × 0.06
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.36 to 59.994
Index ranges	-19 ≤ h ≤ 19, -13 ≤ k ≤ 13, -20 ≤ l ≤ 20
Reflections collected	38796
Independent reflections	4818 [R_{int} = 0.0385, R_{sigma} = 0.0219]
Data/restraints/parameters	4818/0/285
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0404, wR_2 = 0.0956
Final R indexes [all data]	R_1 = 0.0451, wR_2 = 0.0981
Largest diff. peak/hole / e Å^{-3}	0.38/-0.34

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 22srv070. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	9833.3(2)	2116.8(3)	3122.8(2)	21.61(9)
O1	5139.9(7)	1538.0(10)	2242.0(7)	22.29(18)
N1	6939.1(8)	1142.3(10)	3531.0(8)	17.37(19)
C1	5976.7(9)	1868.1(12)	3068.2(9)	16.7(2)
C2	7178.6(10)	88.8(13)	2940.8(11)	23.6(2)
C3	7778.4(11)	768.8(14)	2401.8(11)	24.8(3)
C4	8685.6(9)	1659.6(12)	3216.7(9)	18.1(2)
C5	10373.7(10)	3022.4(13)	4310.3(10)	22.7(2)
C6	9710.1(9)	2977.0(13)	4762.5(10)	19.7(2)
C7	8730.7(9)	2192.6(11)	4126.8(9)	15.8(2)
C8	7848.2(9)	1885.4(11)	4432.1(9)	15.2(2)
C9	7260.1(9)	3164.7(11)	4520.3(8)	14.7(2)
C10	7650.7(9)	4257.5(12)	5252.0(9)	17.9(2)
C11	6913.8(10)	5301.1(13)	5157.8(10)	21.2(2)
C12	5810.7(10)	5261.9(14)	4360.1(10)	22.5(2)
C13	5418.9(9)	4157.4(13)	3640.2(9)	20.0(2)
C14	6158.5(9)	3121.2(12)	3737.8(8)	16.0(2)
C15	8356.6(9)	1000.4(13)	5478.5(9)	20.2(2)
C16	7576.1(10)	697.8(14)	5902.6(10)	24.9(3)
C17	6919.8(13)	-492.7(18)	5590.4(14)	39.0(4)
C18	6185.9(16)	-729(2)	5983.0(17)	57.6(6)
C19	6095.3(14)	208(3)	6665.6(15)	56.5(6)

C20	6741.3(13)	1389(2)	6979.5(13)	42.3(4)
C21	7485.9(11)	1623.3(17)	6610.4(10)	28.8(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv070. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	20.94(15)	22.09(15)	25.91(16)	-0.05(11)	14.62(12)	1.80(11)
O1	15.3(4)	28.6(5)	16.2(4)	-0.6(3)	2.4(3)	-5.8(3)
N1	14.5(4)	16.4(4)	16.7(4)	-0.9(3)	4.0(3)	-3.7(3)
C1	14.0(5)	20.2(5)	14.5(5)	2.4(4)	6.0(4)	-4.2(4)
C2	20.8(5)	17.0(5)	27.7(6)	-5.5(5)	7.5(5)	-3.7(4)
C3	23.0(6)	25.8(6)	24.6(6)	-10.0(5)	10.7(5)	-3.0(5)
C4	16.7(5)	16.9(5)	19.8(5)	-0.5(4)	8.2(4)	0.8(4)
C5	17.9(5)	23.4(6)	26.8(6)	-1.3(5)	10.9(5)	-4.3(4)
C6	16.5(5)	21.0(5)	19.9(5)	-1.7(4)	7.4(4)	-4.1(4)
C7	14.2(5)	15.0(5)	16.6(5)	1.4(4)	6.2(4)	-0.7(4)
C8	11.8(4)	16.4(5)	13.8(5)	0.8(4)	3.4(4)	-2.6(4)
C9	13.6(5)	17.5(5)	12.7(4)	2.9(4)	6.1(4)	-1.6(4)
C10	15.4(5)	21.6(5)	14.9(5)	0.5(4)	6.0(4)	-1.9(4)
C11	22.4(5)	23.7(6)	18.1(5)	-2.3(4)	10.4(4)	-0.8(4)
C12	20.2(5)	27.4(6)	22.7(6)	2.2(5)	12.6(5)	3.8(5)
C13	14.0(5)	28.5(6)	17.4(5)	3.2(4)	7.5(4)	0.6(4)
C14	13.1(5)	21.6(5)	12.6(4)	2.8(4)	5.7(4)	-2.5(4)
C15	15.5(5)	21.7(5)	18.8(5)	6.7(4)	4.7(4)	0.0(4)
C16	16.5(5)	31.2(6)	20.3(6)	14.3(5)	3.7(4)	-1.6(5)
C17	35.0(8)	37.0(8)	36.8(8)	13.3(7)	10.9(7)	-12.6(6)
C18	39.9(9)	69.7(13)	50.7(11)	25.0(10)	12.3(8)	-27.3(9)
C19	33.1(8)	98.0(17)	39.2(9)	27.5(10)	18.3(7)	-12.9(9)
C20	28.0(7)	74.5(13)	25.8(7)	19.9(8)	14.3(6)	3.2(7)
C21	20.2(6)	43.8(8)	19.9(6)	12.5(5)	7.8(5)	-0.1(5)

Table 4 Bond Lengths for 22srv070.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
S1	C4	1.7232(12)		C8	C15	1.5555(15)
S1	C5	1.7167(13)		C9	C10	1.3894(16)
O1	C1	1.2289(13)		C9	C14	1.3909(14)
N1	C1	1.3620(14)		C10	C11	1.3922(17)
N1	C2	1.4533(16)		C11	C12	1.3982(17)
N1	C8	1.4761(14)		C12	C13	1.3886(18)
C1	C14	1.4780(16)		C13	C14	1.3884(16)
C2	C3	1.5282(19)		C15	C16	1.5057(17)
C3	C4	1.4994(17)		C16	C17	1.393(2)

C4	C7	1.3668(16)		C16	C21	1.394(2)
C5	C6	1.3596(17)		C17	C18	1.401(3)
C6	C7	1.4300(15)		C18	C19	1.374(4)
C7	C8	1.5177(15)		C19	C20	1.379(3)
C8	C9	1.5138(16)		C20	C21	1.3894(19)

Table 5 Bond Angles for 22srv070.								
Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C5	S1	C4	91.77(6)		C9	C8	C7	114.33(9)
C1	N1	C2	121.55(10)		C9	C8	C15	112.03(9)
C1	N1	C8	113.59(9)		C10	C9	C8	130.06(10)
C2	N1	C8	119.89(9)		C10	C9	C14	120.08(10)
O1	C1	N1	125.69(11)		C14	C9	C8	109.81(9)
O1	C1	C14	127.83(11)		C9	C10	C11	117.96(10)
N1	C1	C14	106.46(9)		C10	C11	C12	121.70(11)
N1	C2	C3	109.21(10)		C13	C12	C11	120.20(11)
C4	C3	C2	108.30(10)		C14	C13	C12	117.79(11)
C3	C4	S1	123.26(9)		C9	C14	C1	108.56(10)
C7	C4	S1	111.20(8)		C13	C14	C1	129.16(10)
C7	C4	C3	125.53(11)		C13	C14	C9	122.25(11)
C6	C5	S1	112.20(9)		C16	C15	C8	114.15(9)
C5	C6	C7	112.00(11)		C17	C16	C15	121.25(14)
C4	C7	C6	112.83(10)		C17	C16	C21	118.50(14)
C4	C7	C8	121.93(10)		C21	C16	C15	120.24(12)
C6	C7	C8	125.14(10)		C16	C17	C18	119.81(19)
N1	C8	C7	108.39(9)		C19	C18	C17	120.80(18)
N1	C8	C9	101.19(8)		C18	C19	C20	119.83(16)
N1	C8	C15	111.64(9)		C19	C20	C21	119.89(19)
C7	C8	C15	109.04(9)		C20	C21	C16	121.13(15)

Table 6 Torsion Angles for 22srv070.										
A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
C1	C14	C9	C8	-2.77(12)		C8	N1	C1	O1	172.01(10)
C1	C14	C9	C10	179.26(10)		C8	C7	C4	S1	-176.93(8)
C2	N1	C1	O1	17.03(17)		C8	C9	C14	C13	179.19(10)
C2	C3	C4	S1	156.63(9)		C8	C15	C16	C17	90.48(15)
C2	C3	C4	C7	-22.20(17)		C8	C15	C16	C21	-88.63(14)
C3	C2	N1	C1	91.07(13)		C9	C8	N1	C1	4.79(12)
C3	C2	N1	C8	-62.38(14)		C9	C8	N1	C2	160.23(10)
C3	C4	C7	C6	178.63(11)		C9	C8	C15	C16	48.97(14)
C3	C4	C7	C8	2.03(18)		C9	C14	C1	O1	-172.87(11)
C4	C3	C2	N1	47.64(13)		C9	C14	C1	N1	5.68(12)

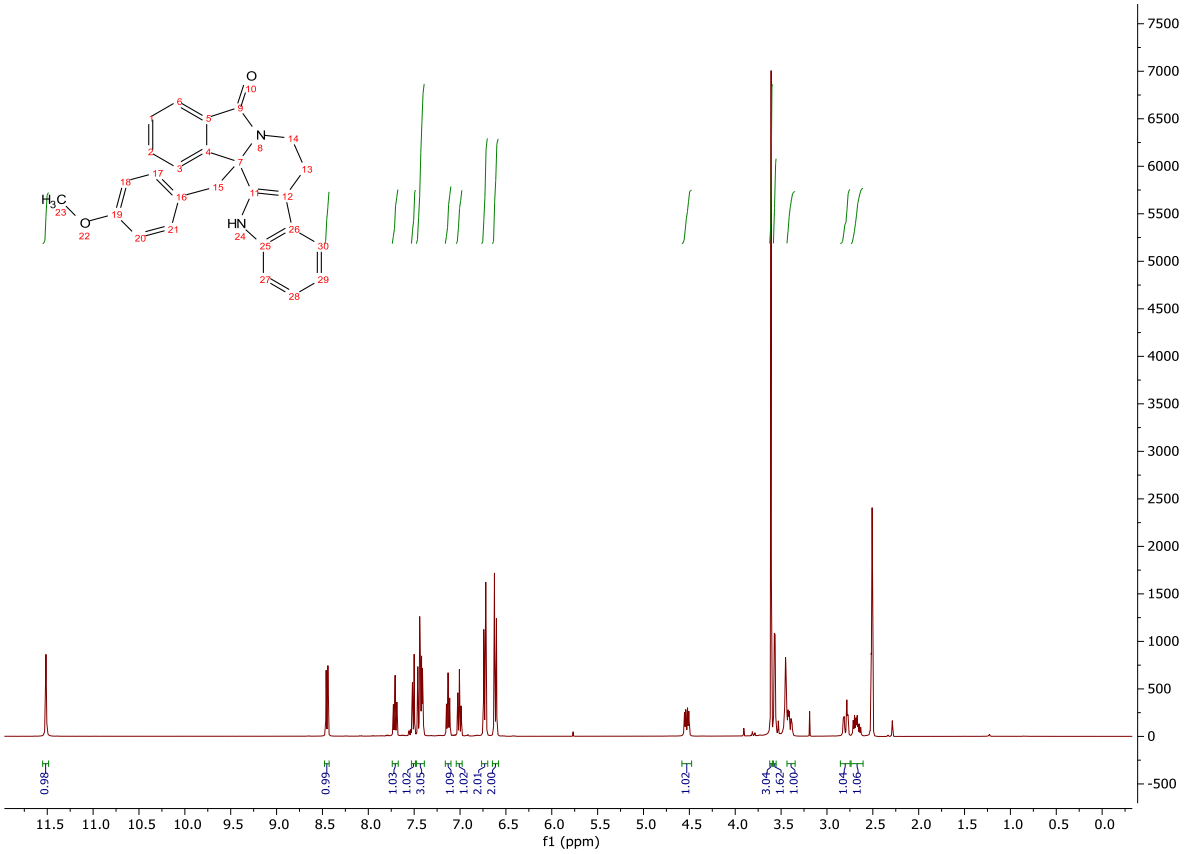
C4	C7	C8	N1	-8.00(14)		C10	C9	C8	N1	176.76(11)
C4	C7	C8	C9	-120.01(12)		C10	C9	C8	C15	57.71(15)
C4	C7	C8	C15	113.73(12)		C10	C9	C14	C13	1.22(16)
C6	C7	C4	S1	-0.32(13)		C13	C14	C1	O1	4.99(19)
C6	C7	C8	N1	175.82(10)		C13	C14	C1	N1	-176.45(11)
C6	C7	C8	C9	63.82(14)		C14	C1	N1	C2	-161.57(10)
C6	C7	C8	C15	-62.45(14)		C14	C1	N1	C8	-6.58(12)
C7	C8	N1	C1	-115.77(10)		C14	C9	C8	N1	-0.94(11)
C7	C8	N1	C2	39.68(13)		C14	C9	C8	C15	-119.99(10)
C7	C8	C9	C10	-66.98(15)		C15	C8	N1	C1	124.11(10)
C7	C8	C9	C14	115.32(10)		C15	C8	N1	C2	-80.44(13)
C7	C8	C15	C16	176.55(10)		C16	C15	C8	N1	-63.72(14)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv070.

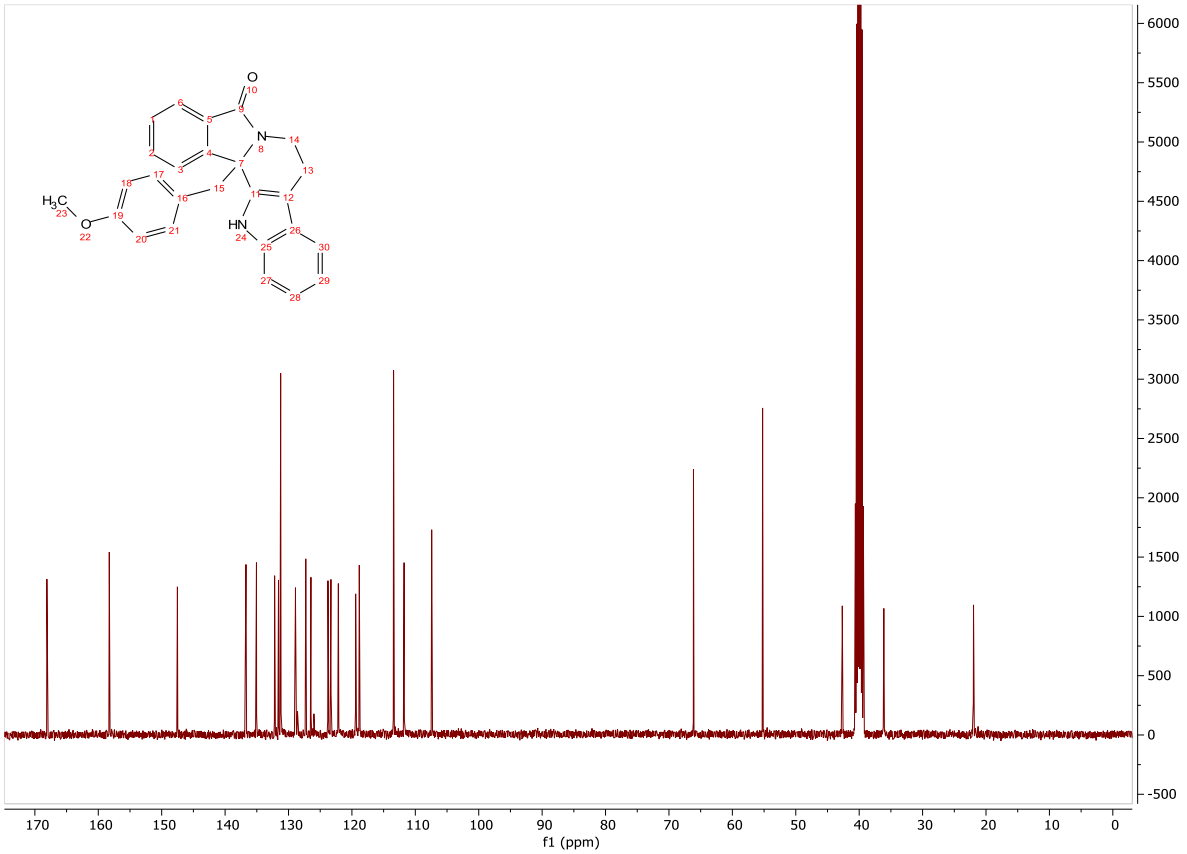
Atom	***x***	***y***	***z***	**U(eq)**
H2A	7642(14)	-633(19)	3456(14)	32(4)
H2B	6484(15)	-324(19)	2403(14)	33(4)
H3A	7244(13)	1354(18)	1780(14)	28(4)
H3B	8063(14)	60(20)	2121(14)	34(4)
H5	11061(14)	3461(18)	4556(14)	29(4)
H6	9878(14)	3425(18)	5431(14)	29(4)
H10	8392(13)	4281(16)	5813(13)	21(4)
H11	7171(13)	6043(18)	5655(13)	27(4)
H12	5316(14)	6005(19)	4314(14)	32(4)
H13	4656(14)	4107(18)	3090(13)	30(4)
H15A	8989(13)	1527(17)	6020(12)	22(4)
H15B	8626(13)	164(19)	5338(13)	27(4)
H17	6973(15)	-1110(20)	5116(15)	35(5)
H18	5776(19)	-1500(30)	5759(18)	60(6)
H19	5585(19)	70(30)	6945(18)	63(7)
H20	6683(18)	2060(20)	7471(19)	57(6)
H21	7940(14)	2469(19)	6836(14)	30(4)

13*b*-(4-methoxybenzyl)-7,8,13,13*b*-tetrahydro-5*H*-benzo[1,2]indolizino[8,7-*b*]indol-5-one **83**

^{1}H:



^{13}C:



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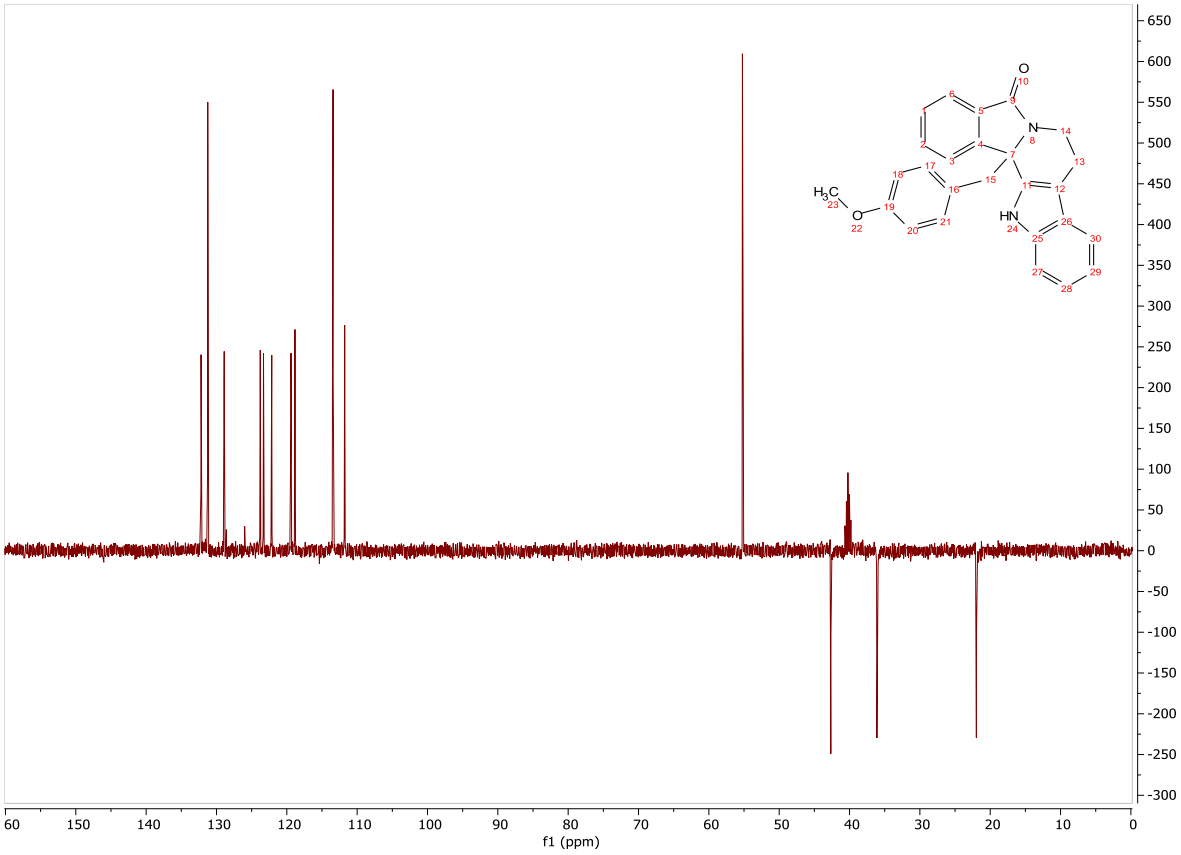
650
600
550
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300
250
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50
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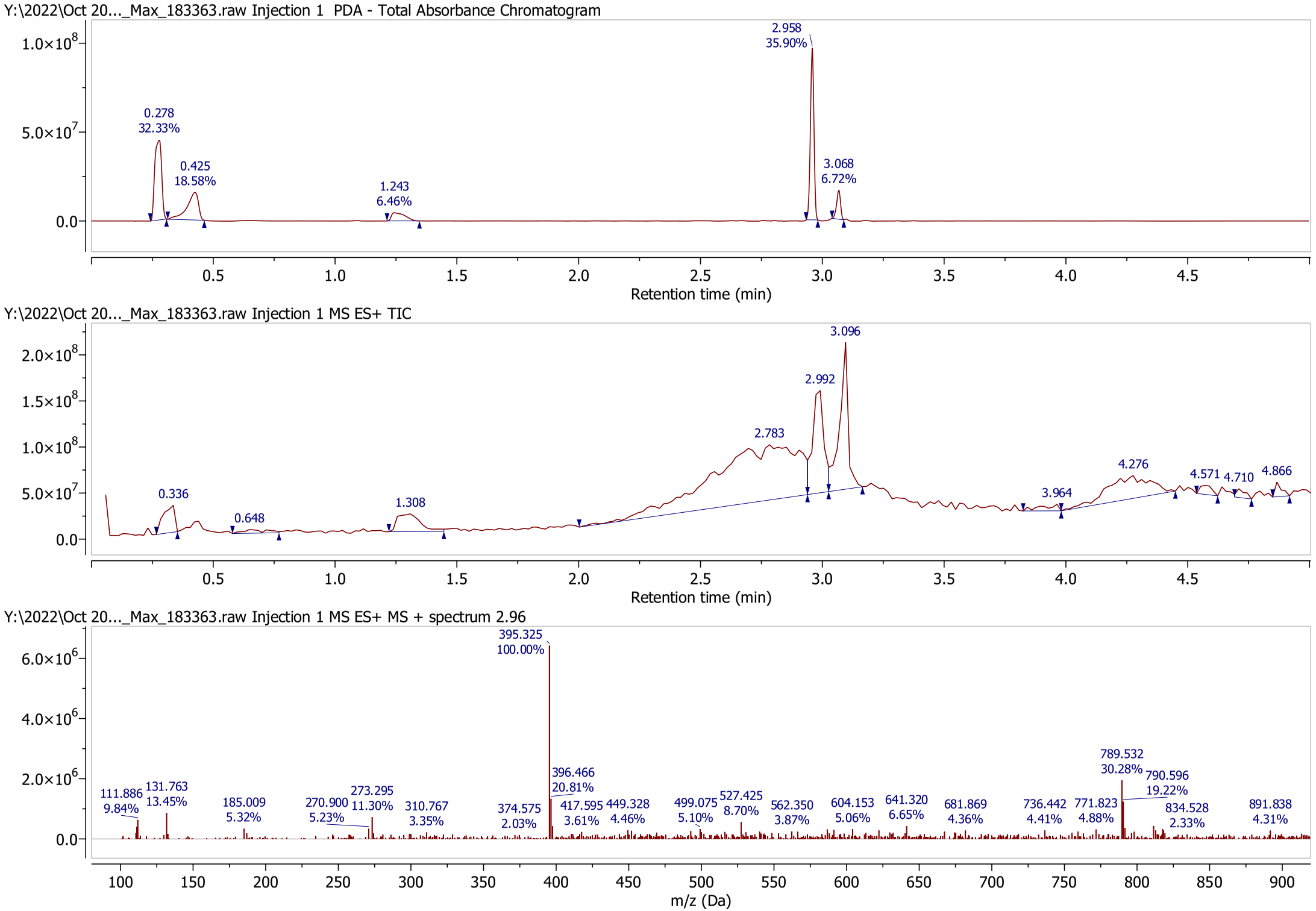
-300
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
10
6
5
9
N
8
14
1
2
4
3
7
13
17
18
15
16
11
12
H3C
23
O
22
19
21
20
HN
24
26
25
30
27
29
28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5.0×10^7
0.0
0.278
32.33%
0.425
18.58%
1.243
6.46%
2.958
35.90%
3.068
6.72%
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Oct 20..._Max_183363.raw Injection 1 MS ES+ TIC
2.0×10^8
1.5×10^8
1.0×10^8
5.0×10^7
0.0
0.336
0.648
1.308
2.783
2.992
3.096
3.964
4.276
4.571
4.710
4.866
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Oct 20..._Max_183363.raw Injection 1 MS ES+ MS + spectrum 2.96
6.0×10^6
4.0×10^6
2.0×10^6
0.0
111.886
9.84%
131.763
13.45%
185.009
5.32%
270.900
5.23%
273.295
11.30%
310.767
3.35%
374.575
2.03%
395.325
100.00%
396.466
20.81%
417.595
3.61%
449.328
4.46%
499.075
5.10%
527.425
8.70%
562.350
3.87%
604.153
5.06%
641.320
6.65%
681.869
4.36%
736.442
4.41%
771.823
4.88%
789.532
30.28%
790.596
19.22%
834.528
2.33%
891.838
4.31%
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
m/z (Da)

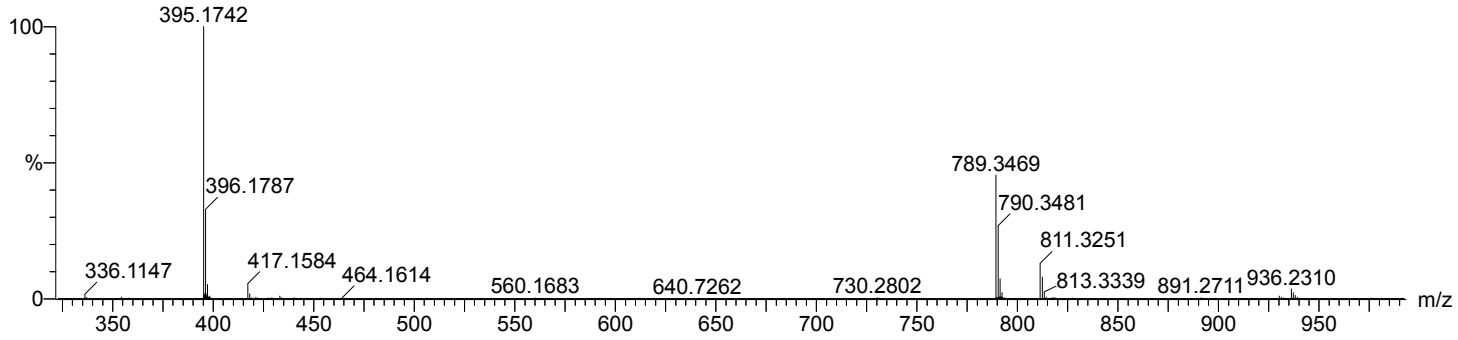
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
131 formula(e) evaluated with 2 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-4 O: 0-4

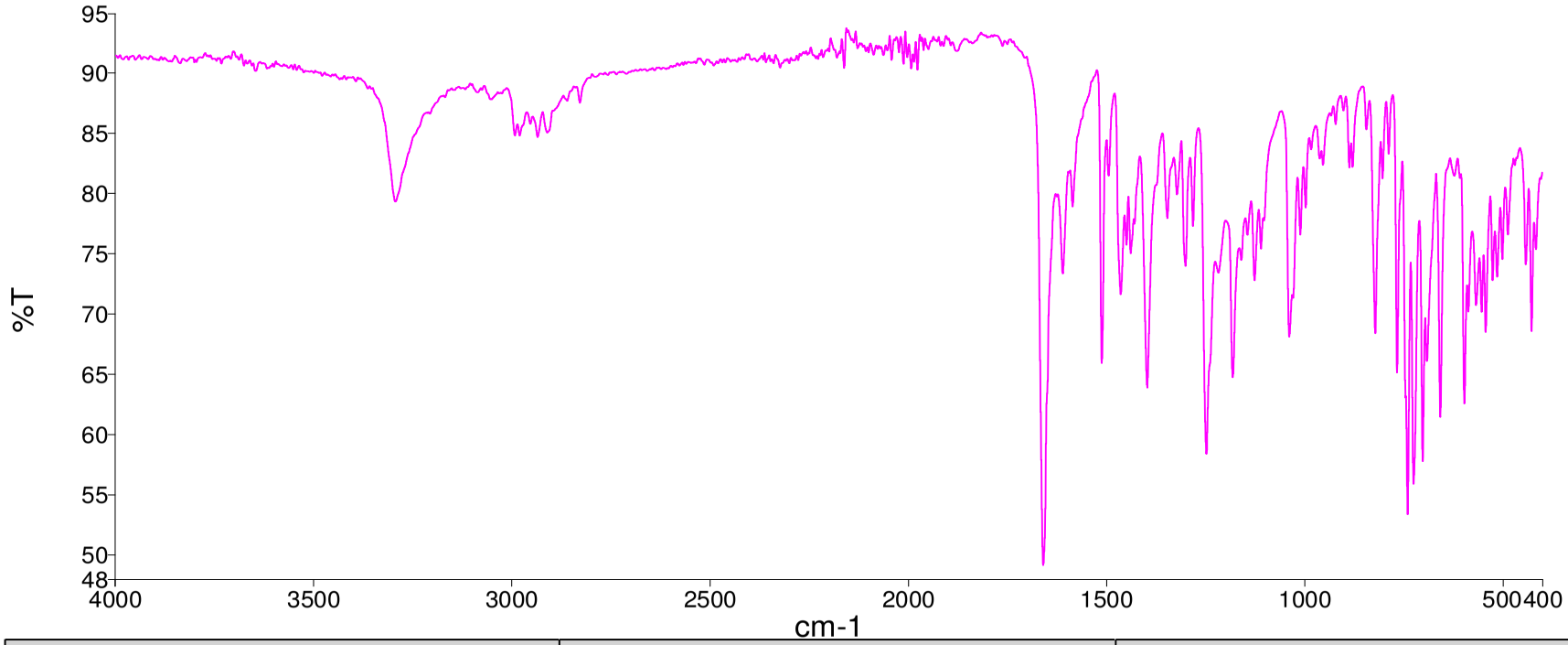
IRB_Cycloadduct_Max 468 (4.020) Cm (463:481)

1: TOF MS ES+
4.69e+004



Minimum:				-1.5						
Maximum:		3.0	5.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
395.1742	395.1760	-1.8	-4.6	16.5	815.3	0.0	C26	H23	N2	O2
	395.1719	2.3	5.8	12.5	821.2	5.9	C21	H23	N4	O4

Analyst Lenny Lauchlan
Date 21 October 2022 08:16



Sample Name	Description	Quality Checks
Cyclo adduct	Sample 020 By Lenny Date Friday, October 21 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

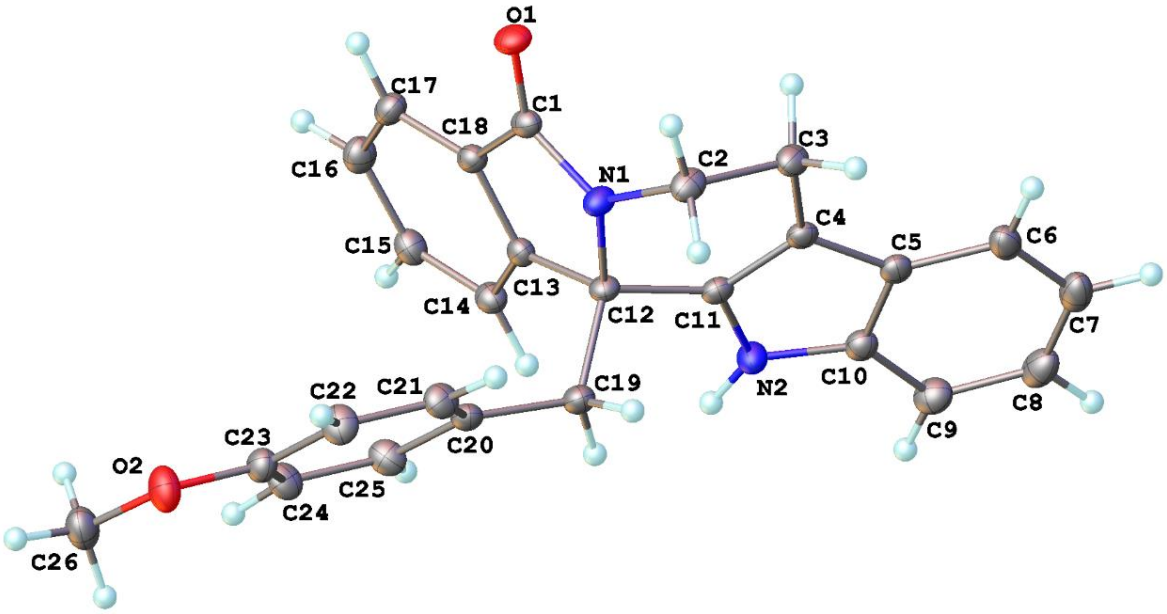


Table 1 Crystal data and structure refinement for 22srv271.	
Identification code	22srv271
Empirical formula	$C_{26}H_{22}N_2O_2$
Formula weight	394.45
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.4584(4)
b/Å	13.8652(5)
c/Å	12.6042(4)
α/°	90
β/°	103.3267(11)
γ/°	90
Volume/Å^3	1948.54(12)
Z	4
ρ_{calc}g/cm^3	1.345
μ/mm^{-1}	0.086
F(000)	832.0

Crystal size/mm^3	0.18 × 0.11 × 0.01
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.334 to 59.992
Index ranges	-16 ≤ h ≤ 16, -19 ≤ k ≤ 19, -17 ≤ l ≤ 17
Reflections collected	41416
Independent reflections	5689 [R_{int} = 0.0632, R_{sigma} = 0.0482]
Data/restraints/parameters	5689/0/359
Goodness-of-fit on F^2	1.060
Final R indexes [I>=2σ (I)]	R_1 = 0.0524, wR_2 = 0.1023
Final R indexes [all data]	R_1 = 0.0788, wR_2 = 0.1127
Largest diff. peak/hole / e $Å^{-3}$	0.29/-0.26

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 22srv271. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	5608.1(9)	3186.6(8)	5477.1(8)	20.6(2)
O2	7400.4(10)	4719.7(8)	604.4(10)	26.4(3)
N1	3988.8(10)	3684.7(9)	4136.7(10)	16.5(2)
N2	999.9(11)	2877.1(9)	2527.0(10)	18.2(3)
C1	4897.2(12)	3073.1(10)	4584.4(11)	16.0(3)
C2	3544.7(14)	4441.4(11)	4753.1(13)	19.7(3)
C3	2412.9(13)	4101.9(12)	5101.3(12)	19.5(3)
C4	1592.4(12)	3604.4(10)	4165.9(11)	15.8(3)
C5	318.6(13)	3453.7(10)	3951.2(12)	16.7(3)
C6	-568.1(14)	3658.6(11)	4521.7(13)	22.0(3)
C7	-1746.8(15)	3406.1(12)	4059.5(14)	25.9(4)
C8	-2060.9(15)	2960.3(12)	3038.3(14)	26.5(4)
C9	-1208.0(14)	2752.5(12)	2453.7(14)	23.6(3)
C10	-16.2(13)	2999.0(10)	2923.4(12)	18.1(3)
C11	1966.7(12)	3243.3(10)	3289.4(11)	15.4(3)
C12	3213.4(12)	3320.8(10)	3107.2(11)	14.8(3)
C13	3805.5(12)	2364.1(10)	2982.2(11)	14.9(3)
C14	3470.1(13)	1652.0(11)	2194.8(12)	18.1(3)
C15	4189.1(14)	834.0(11)	2275.2(13)	19.9(3)
C16	5229.7(14)	732.7(11)	3099.8(13)	21.5(3)
C17	5558.3(13)	1444.3(11)	3890.6(12)	19.4(3)
C18	4823.4(12)	2252.2(10)	3820.7(11)	15.6(3)
C19	3188.4(13)	4024.3(11)	2140.4(12)	18.5(3)
C20	4344.0(13)	4169.5(10)	1780.3(11)	16.5(3)

C21	5121.1(14)	4936.0(11)	2165.2(12)	20.4(3)
C22	6135.9(14)	5097.5(12)	1768.0(13)	22.7(3)
C23	6392.5(13)	4491.5(11)	970.4(12)	19.2(3)
C24	5644.1(14)	3722.4(11)	582.1(13)	20.7(3)
C25	4627.7(14)	3576.2(11)	987.1(12)	20.9(3)
C26	7701.5(16)	4098.9(13)	-189.8(15)	27.4(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv271. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	17.4(5)	25.3(6)	16.4(5)	0.4(4)	-1.8(4)	-1.3(4)
O2	20.2(6)	29.5(6)	32.4(6)	-5.9(5)	11.7(5)	-4.9(5)
N1	14.9(6)	17.5(6)	15.2(6)	-2.8(5)	-0.6(5)	0.8(5)
N2	14.3(6)	23.4(7)	16.2(6)	-2.9(5)	2.3(5)	-1.0(5)
C1	13.9(6)	18.8(7)	15.2(7)	2.5(5)	2.9(5)	-1.9(5)
C2	19.4(7)	18.3(7)	19.1(7)	-5.3(6)	-0.1(6)	0.8(6)
C3	20.1(7)	21.3(8)	16.1(7)	-3.1(6)	2.6(6)	3.1(6)
C4	16.7(7)	14.6(7)	15.4(7)	3.3(5)	2.1(5)	2.3(5)
C5	18.2(7)	14.1(7)	17.6(7)	3.4(5)	3.7(5)	2.6(5)
C6	23.9(8)	21.6(8)	22.8(8)	4.7(6)	9.8(6)	5.0(6)
C7	22.2(8)	24.9(8)	33.5(9)	8.6(7)	12.2(7)	3.5(6)
C8	17.1(8)	27.0(9)	34.4(9)	8.2(7)	4.3(7)	-1.4(6)
C9	20.3(8)	24.3(8)	24.7(8)	0.7(7)	1.8(6)	-3.5(6)
C10	17.5(7)	17.2(7)	19.5(7)	2.9(6)	3.7(6)	0.7(5)
C11	15.7(6)	14.2(6)	15.0(6)	1.6(5)	0.8(5)	1.3(5)
C12	13.8(6)	17.0(7)	12.2(6)	-0.7(5)	0.3(5)	-0.4(5)
C13	14.6(6)	16.1(7)	14.9(7)	1.4(5)	5.2(5)	-0.7(5)
C14	16.3(7)	21.7(7)	15.9(7)	-0.9(6)	3.2(6)	-1.7(6)
C15	21.6(7)	19.5(7)	20.1(7)	-2.5(6)	8.0(6)	-2.3(6)
C16	21.6(7)	18.6(7)	25.5(8)	0.8(6)	7.6(6)	2.3(6)
C17	15.6(7)	20.6(7)	21.5(7)	3.3(6)	3.2(6)	2.0(6)
C18	14.6(6)	17.4(7)	14.9(7)	2.2(5)	3.5(5)	-0.7(5)
C19	17.1(7)	21.0(8)	16.8(7)	3.3(6)	2.7(6)	2.2(6)
C20	16.9(7)	17.3(7)	14.9(7)	3.0(5)	2.7(5)	1.5(5)
C21	23.1(8)	19.0(7)	18.9(7)	-4.4(6)	4.7(6)	0.4(6)
C22	20.5(8)	22.2(8)	24.8(8)	-6.0(6)	3.8(6)	-6.4(6)
C23	15.6(7)	21.1(7)	21.3(7)	0.9(6)	5.1(6)	-0.4(6)
C24	24.6(8)	19.0(7)	19.4(7)	-5.2(6)	7.0(6)	-1.9(6)
C25	23.2(8)	19.0(7)	20.5(7)	-2.3(6)	5.1(6)	-5.8(6)
C26	27.8(9)	27.5(9)	30.8(9)	0.7(7)	14.5(7)	3.7(7)

Table 4 Bond Lengths for 22srv271.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
O1	C1	1.2376(16)		C9	C10	1.400(2)
O2	C23	1.3756(17)		C11	C12	1.5020(19)
O2	C26	1.422(2)		C12	C13	1.5145(19)
N1	C1	1.3603(18)		C12	C19	1.556(2)
N1	C2	1.4647(19)		C13	C14	1.390(2)
N1	C12	1.4821(17)		C13	C18	1.3905(19)
N2	C10	1.3791(19)		C14	C15	1.392(2)
N2	C11	1.3848(18)		C15	C16	1.397(2)
C1	C18	1.480(2)		C16	C17	1.391(2)
C2	C3	1.536(2)		C17	C18	1.392(2)
C3	C4	1.496(2)		C19	C20	1.509(2)
C4	C5	1.4371(19)		C20	C21	1.399(2)
C4	C11	1.369(2)		C20	C25	1.390(2)
C5	C6	1.402(2)		C21	C22	1.386(2)
C5	C10	1.412(2)		C22	C23	1.393(2)
C6	C7	1.387(2)		C23	C24	1.385(2)
C7	C8	1.398(2)		C24	C25	1.390(2)
C8	C9	1.383(2)				

Table 5 Bond Angles for 22srv271.								
Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C23	O2	C26	117.11(12)		N1	C12	C13	101.35(11)
C1	N1	C2	123.56(12)		N1	C12	C19	111.80(12)
C1	N1	C12	113.45(12)		C11	C12	C13	114.70(11)
C2	N1	C12	119.79(11)		C11	C12	C19	108.55(11)
C10	N2	C11	108.11(12)		C13	C12	C19	113.29(11)
O1	C1	N1	125.32(14)		C14	C13	C12	129.77(13)
O1	C1	C18	128.02(13)		C14	C13	C18	120.60(13)
N1	C1	C18	106.63(12)		C18	C13	C12	109.64(12)
N1	C2	C3	110.59(12)		C13	C14	C15	117.73(14)
C4	C3	C2	109.56(12)		C14	C15	C16	121.71(14)
C5	C4	C3	129.94(13)		C17	C16	C15	120.37(14)
C11	C4	C3	123.21(13)		C16	C17	C18	117.74(14)
C11	C4	C5	106.76(12)		C13	C18	C1	108.70(12)
C6	C5	C4	134.30(14)		C13	C18	C17	121.82(13)
C6	C5	C10	119.02(14)		C17	C18	C1	129.39(13)
C10	C5	C4	106.68(12)		C20	C19	C12	117.40(12)
C7	C6	C5	118.94(15)		C21	C20	C19	121.96(13)
C6	C7	C8	121.17(15)		C25	C20	C19	120.28(13)
C9	C8	C7	121.26(15)		C25	C20	C21	117.60(13)
C8	C9	C10	117.65(15)		C22	C21	C20	121.14(14)
N2	C10	C5	108.28(13)		C21	C22	C23	119.84(14)

N2	C10	C9	129.76(14)		O2	C23	C22	115.89(13)
C9	C10	C5	121.96(14)		O2	C23	C24	123.90(14)
N2	C11	C12	123.85(12)		C24	C23	C22	120.20(14)
C4	C11	N2	110.17(13)		C23	C24	C25	119.04(14)
C4	C11	C12	125.68(13)		C20	C25	C24	122.18(14)
N1	C12	C11	106.85(11)					

Table 6 Hydrogen Bonds for 22srv271.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N2	H2	O1[1]	0.913(19)	2.03(2)	2.9186(16)	164.0(17)

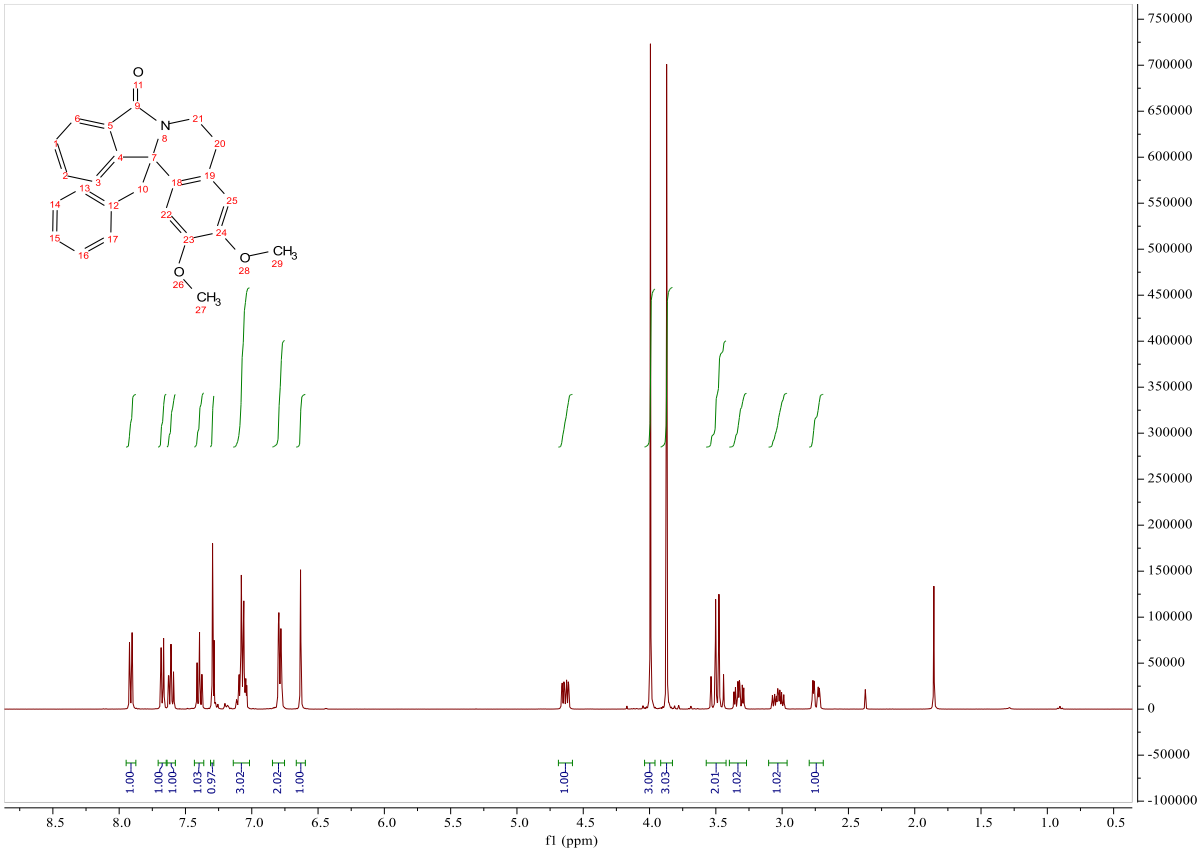
[1]-1/2+X,1/2-Y,-1/2+Z

Table 7 Selected Torsion Angles for 22srv271.										
A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C12	C11	N2	-176.34(12)		C12	C19	C20	C21	-95.00(17)
C1	C18	C13	C12	4.85(15)		C12	C19	C20	C25	89.63(17)
C1	C18	C13	C14	-174.99(12)		C13	C12	N1	C1	-0.30(15)
C2	N1	C1	O1	-15.1(2)		C13	C12	N1	C2	-160.78(12)
C2	C3	C4	C5	-156.74(14)		C13	C12	C11	N2	-64.89(18)
C2	C3	C4	C11	19.26(19)		C13	C12	C19	C20	-48.39(17)
C3	C2	N1	C1	-98.24(16)		C13	C18	C1	O1	172.82(14)
C3	C2	N1	C12	60.17(17)		C13	C18	C1	N1	-4.94(15)
C3	C4	C11	N2	-176.42(13)		C14	C13	C12	N1	176.94(14)
C3	C4	C11	C12	-2.6(2)		C14	C13	C12	C19	-63.15(19)
C4	C3	C2	N1	-44.07(16)		C14	C13	C18	C17	1.7(2)
C4	C11	C12	N1	10.62(19)		C17	C18	C1	O1	-3.5(2)
C4	C11	C12	C13	122.07(15)		C17	C18	C1	N1	178.69(14)
C4	C11	C12	C19	-110.10(15)		C18	C1	N1	C2	162.76(13)
C5	C4	C11	N2	0.38(16)		C18	C1	N1	C12	3.13(16)
C5	C4	C11	C12	174.22(13)		C18	C13	C12	N1	-2.88(14)
C11	C12	N1	C1	120.11(13)		C18	C13	C12	C19	117.03(13)
C11	C12	N1	C2	-40.37(16)		C19	C12	N1	C1	-121.27(13)
C11	C12	C13	C14	62.25(19)		C19	C12	N1	C2	78.25(16)
C11	C12	C13	C18	-117.57(13)		C19	C12	C11	N2	62.94(17)
C11	C12	C19	C20	-177.02(12)		C20	C19	C12	N1	65.37(16)
C12	N1	C1	O1	-174.71(13)		C22	C23	O2	C26	178.42(14)
C12	C13	C18	C17	-178.46(13)		C24	C23	O2	C26	-2.5(2)

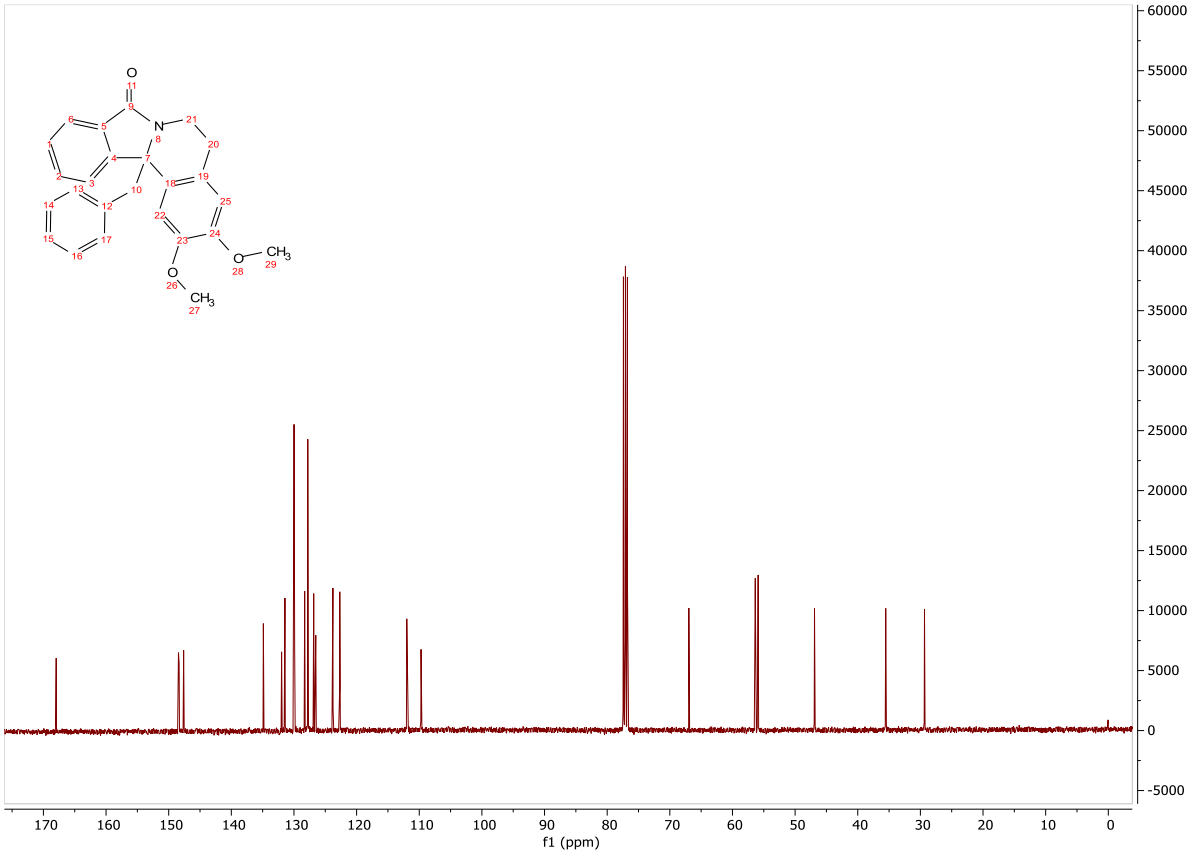
Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv271.				
Atom	***x***	***y***	***z***	**U(eq)**
H2	1014(17)	2596(14)	1875(16)	35(5)
H2A	3346(15)	5035(13)	4276(14)	23(4)
H2B	4164(15)	4590(12)	5387(14)	19(4)
H3A	2008(16)	4684(14)	5352(15)	32(5)
H3B	2645(16)	3670(13)	5739(14)	25(5)
H6	-346(16)	3991(13)	5261(15)	28(5)
H7	-2364(17)	3536(13)	4444(16)	34(5)
H8	-2899(17)	2794(13)	2729(14)	31(5)
H9	-1396(15)	2452(12)	1733(14)	22(4)
H14	2727(15)	1723(12)	1592(14)	21(4)
H15	3988(15)	303(12)	1734(14)	23(4)
H16	5735(16)	165(13)	3135(14)	29(5)
H17	6274(17)	1397(13)	4492(15)	32(5)
H19A	2559(16)	3773(12)	1516(14)	25(5)
H19B	2885(14)	4648(13)	2350(13)	21(4)
H21	4926(16)	5384(13)	2678(15)	30(5)
H22	6673(15)	5644(13)	2013(14)	24(4)
H24	5789(15)	3331(12)	1(14)	22(4)
H25	4072(15)	3045(13)	694(14)	26(5)
H26A	7040(17)	4077(13)	-870(15)	30(5)
H26B	8494(18)	4377(15)	-339(16)	42(6)
H26C	7863(16)	3425(14)	108(14)	28(5)

12*b*-benzyl-2,3-dimethoxy-5,12*b*-dihydroisoindolo[1,2-*a*]isoquinolin-8(6*H*)-one **86a**

^{1}H:



^{13}C:



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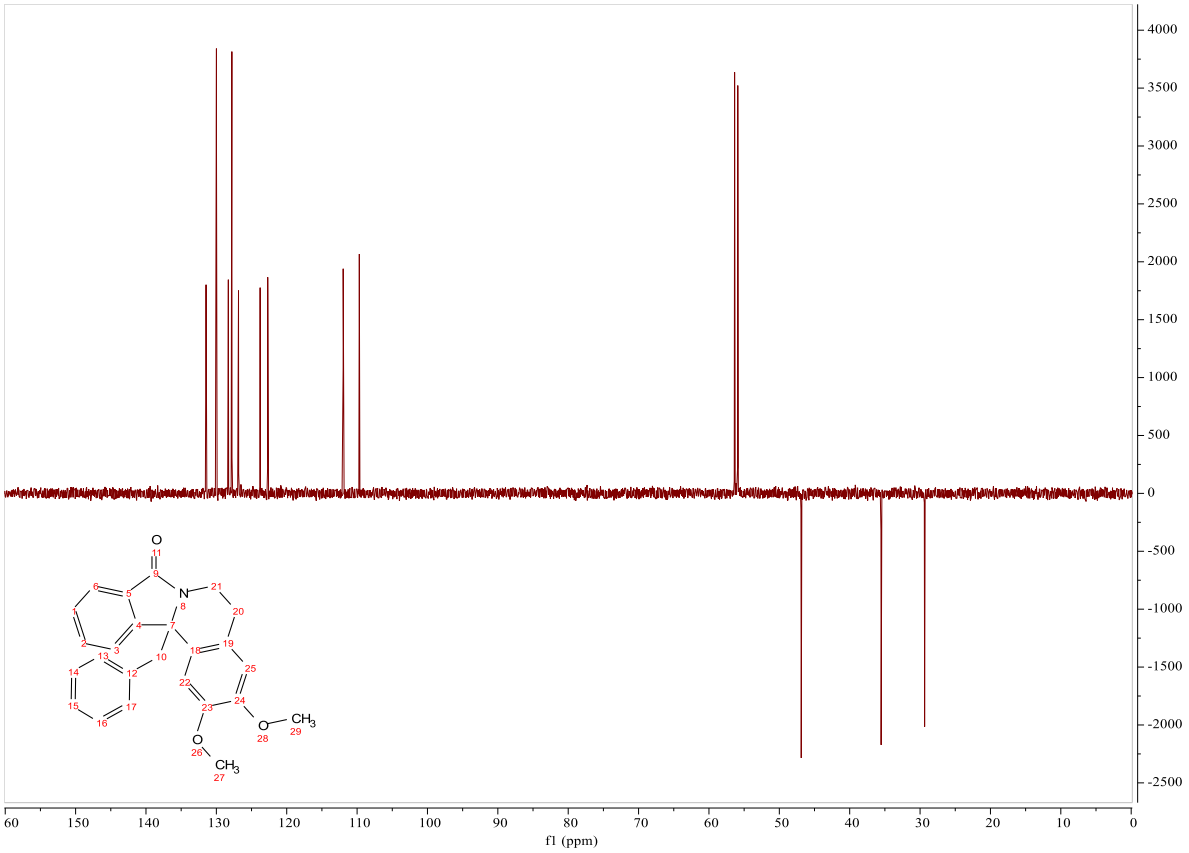
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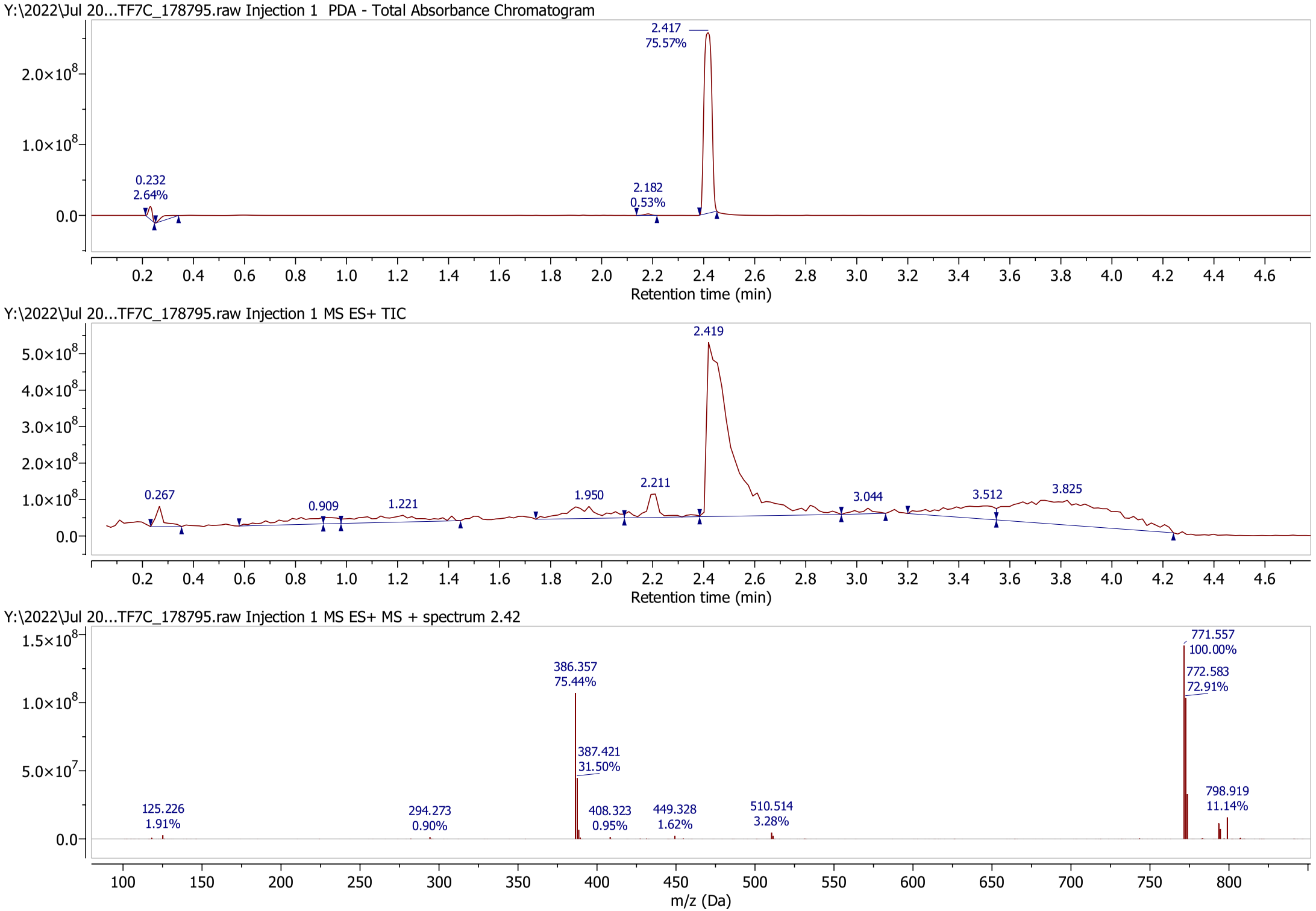
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
11
8
N
21
6
5
20
1
4
7
2
3
19
13
10
18
25
14
12
22
24
15
17
23
O
CH3
29
16
28
O
26
CH3
27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75.57%
0.232
2.64%
2.182
0.53%
Retention time (min)
Y:\2022\Jul 20...TF7C_178795.raw Injection 1 MS ES+ TIC
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0.267
0.909
1.221
1.950
2.211
3.044
3.512
3.825
Retention time (min)
Y:\2022\Jul 20...TF7C_178795.raw Injection 1 MS ES+ MS + spectrum 2.42
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100.00%
772.583
72.91%
386.357
75.44%
387.421
31.50%
798.919
11.14%
125.226
1.91%
294.273
0.90%
408.323
0.95%
449.328
1.62%
510.514
3.28%
m/z (Da)

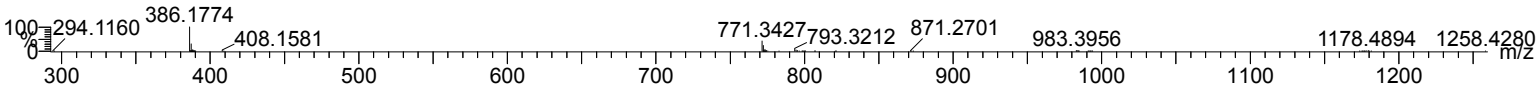
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
2425 formula(e) evaluated with 16 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 S: 0-4

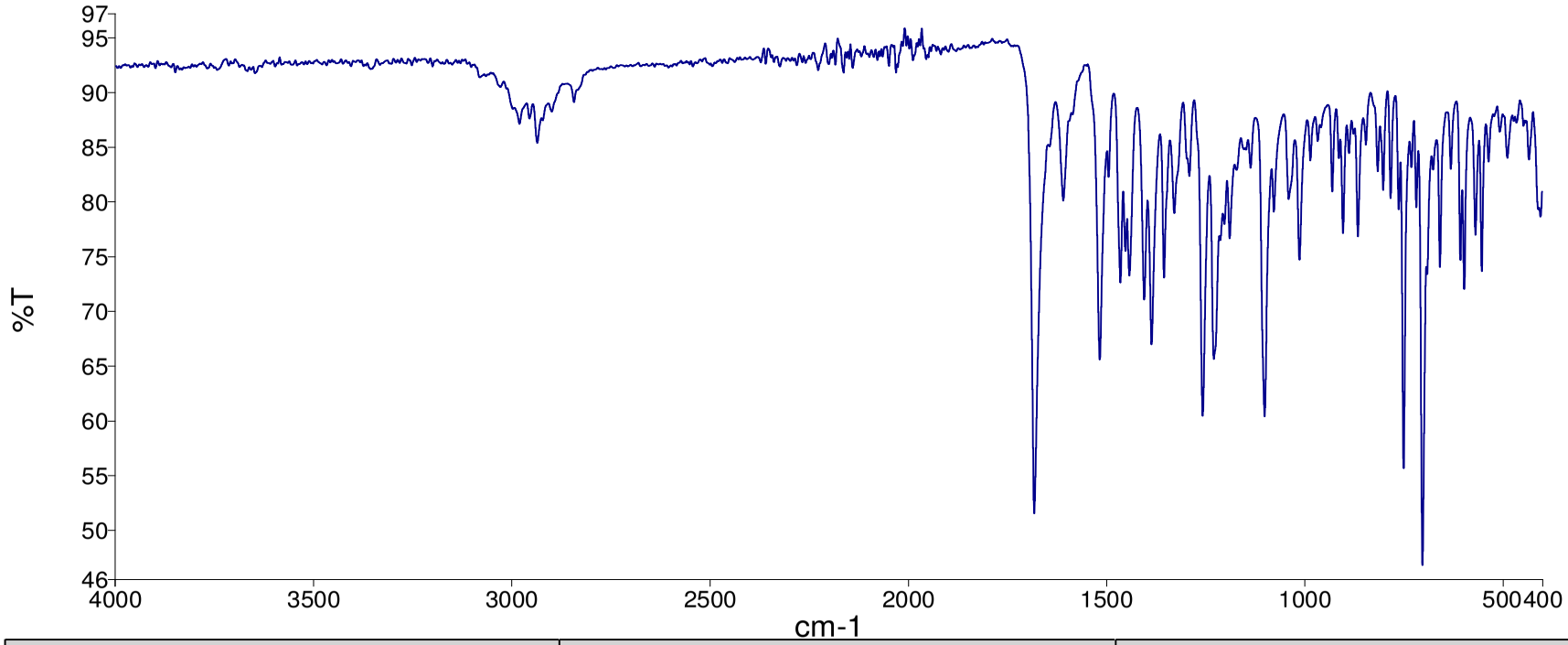
21-Jul-2022
MTF_MTF7C_179352 487 (4.096) Cm (485:491)

21-Jul-2022
1: TOF MS ES+
2.58e+005



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
386.1774	386.1757	1.7	4.4	1.5	609.4	28.052	0.00	C10 H28 N9 O3 S2
	386.1752	2.2	5.7	-4.5	616.8	35.459	0.00	C10 H36 N5 O2 S4
	386.1775	-0.1	-0.3	1.5	599.5	18.157	0.00	C13 H28 N3 O10
	386.1788	-1.4	-3.6	6.5	598.2	16.845	0.00	C14 H24 N7 O6
	386.1783	-0.9	-2.3	0.5	609.9	28.608	0.00	C14 H32 N3 O5 S2
	386.1797	-2.3	-6.0	5.5	609.3	28.011	0.00	C15 H28 N7 O S2
	386.1792	-1.8	-4.7	-0.5	617.2	35.891	0.00	C15 H36 N3 S4
	386.1750	2.4	6.2	5.5	602.1	20.801	0.00	C17 H28 N3 O5 S
	386.1763	1.1	2.8	10.5	599.8	18.489	0.00	C18 H24 N7 O S
	386.1758	1.6	4.1	4.5	614.9	33.547	0.00	C18 H32 N3 S3
	386.1790	-1.6	-4.1	9.5	601.4	20.113	0.00	C22 H28 N O3 S
	386.1756	1.8	4.7	14.5	581.3	0.000	100.00	C25 H24 N O3
	386.1782	-0.8	-2.1	-2.5	605.8	24.519	0.00	C6 H28 N9 O8 S
	386.1777	-0.3	-0.8	-8.5	613.6	32.329	0.00	C6 H36 N5 O7 S3
	386.1790	-1.6	-4.1	-3.5	613.5	32.216	0.00	C7 H32 N9 O3 S3
	386.1748	2.6	6.7	2.5	601.9	20.613	0.00	C9 H24 N9 O8

Analyst Lenny Lauchlan
Date 28 June 2022 13:01



Sample Name	Description	Quality Checks
MTF 007C	Sample 025 By Lenny Date Tuesday, June 28 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

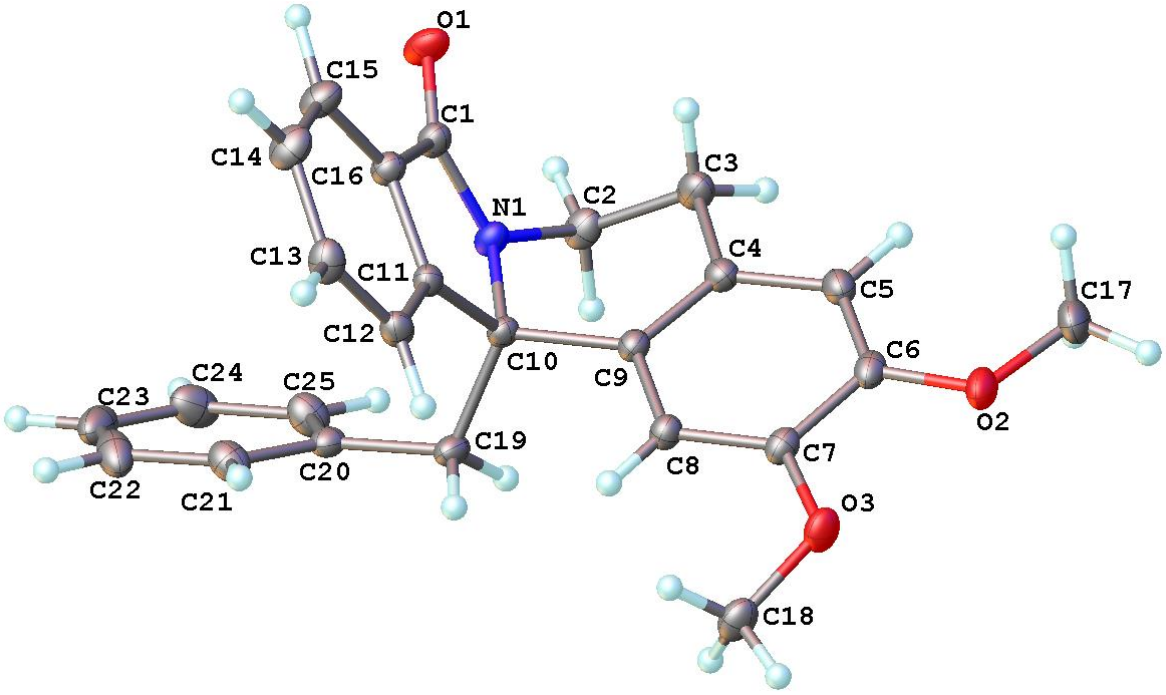


Table 1 Crystal data and structure refinement for 22srv120.	
Identification code	22srv120
Empirical formula	$C_{25}H_{23}NO_3$
Formula weight	385.44
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.5911(2)
b/Å	16.9315(4)
c/Å	13.5723(4)
α/°	90
β/°	97.5953(11)
γ/°	90
Volume/Å^3	1956.91(9)
Z	4
ρ_{calc}g/cm^3	1.308
μ/mm^{-1}	0.086
F(000)	816.0

Crystal size/mm^3	0.24 × 0.18 × 0.16
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.354 to 60
Index ranges	-12 ≤ h ≤ 12, -23 ≤ k ≤ 23, -19 ≤ l ≤ 19
Reflections collected	46441
Independent reflections	5662 [R_{int} = 0.0434, R_{sigma} = 0.0248]
Data/restraints/parameters	5662/0/354
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0458, wR_2 = 0.1126
Final R indexes [all data]	R_1 = 0.0529, wR_2 = 0.1172
Largest diff. peak/hole / e Å^{-3}	0.40/-0.20

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 22srv120. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	5603.0(11)	2044.8(5)	2419.5(6)	25.80(19)
O2	6849.4(10)	6068.5(5)	5381.6(7)	24.23(18)
O3	8667.0(10)	5212.2(5)	6620.9(6)	23.17(18)
N1	7645.2(11)	2749.4(5)	3266.3(6)	16.65(18)
C1	6449.6(13)	2215.5(6)	3189.8(8)	18.0(2)
C2	7663.0(14)	3360.3(7)	2517.5(8)	21.2(2)
C3	6568.9(15)	4012.9(7)	2773.3(9)	22.7(2)
C4	7041.7(12)	4269.5(6)	3840.7(8)	18.0(2)
C5	6644.6(13)	5036.0(7)	4120.4(9)	20.5(2)
C6	7159.5(13)	5332.7(6)	5052.7(9)	19.2(2)
C7	8132.9(13)	4860.3(6)	5734.0(8)	17.8(2)
C8	8484.3(12)	4095.6(6)	5477.1(8)	17.0(2)
C9	7924.8(12)	3787.6(6)	4536.8(8)	15.75(19)
C10	8313.6(12)	2931.4(6)	4297.1(7)	14.83(19)
C11	7461.1(12)	2332.3(6)	4865.0(7)	14.98(19)
C12	7637.5(13)	2162.3(6)	5876.4(8)	18.2(2)
C13	6683.4(14)	1578.6(7)	6203.2(8)	22.0(2)
C14	5564.7(15)	1182.7(7)	5540.1(9)	25.0(2)
C15	5398.8(14)	1348.2(7)	4532.9(9)	22.7(2)
C16	6382.8(12)	1916.0(6)	4209.4(8)	16.9(2)
C17	6004.3(16)	6588.5(8)	4674.3(12)	31.1(3)
C18	9872.0(15)	4792.8(7)	7226.3(9)	23.6(2)
C19	10114.9(13)	2793.4(6)	4449.4(9)	18.9(2)
C20	10610.3(12)	1990.7(6)	4124.8(8)	17.0(2)

C21	10809.1(14)	1354.2(7)	4777.4(9)	23.5(2)
C22	11275.8(15)	618.3(7)	4468.1(11)	29.6(3)
C23	11534.7(14)	506.7(8)	3490.8(11)	30.4(3)
C24	11342.6(15)	1131.5(8)	2836.0(10)	29.7(3)
C25	10891.1(14)	1867.2(7)	3147.4(9)	24.1(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv120. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	31.5(5)	25.4(4)	17.9(4)	0.3(3)	-6.6(3)	-8.5(3)
O2	22.5(4)	14.8(4)	35.7(5)	-3.8(3)	4.9(3)	2.7(3)
O3	32.2(4)	16.8(4)	20.3(4)	-5.4(3)	2.6(3)	0.2(3)
N1	20.9(4)	15.3(4)	13.3(4)	-0.1(3)	0.4(3)	-2.8(3)
C1	21.1(5)	15.5(5)	16.6(5)	-0.5(4)	-0.3(4)	-1.2(4)
C2	28.6(6)	19.0(5)	15.9(5)	2.2(4)	2.1(4)	-3.6(4)
C3	26.6(6)	19.6(5)	20.2(5)	2.4(4)	-3.5(4)	-0.5(4)
C4	17.1(5)	16.3(5)	20.1(5)	0.6(4)	0.8(4)	-1.2(4)
C5	17.7(5)	16.5(5)	26.7(5)	2.4(4)	1.2(4)	1.1(4)
C6	16.7(5)	14.1(5)	28.1(5)	-1.5(4)	7.4(4)	-0.5(4)
C7	19.8(5)	15.5(5)	18.9(5)	-2.5(4)	5.2(4)	-2.2(4)
C8	19.1(5)	14.4(4)	17.3(5)	-1.0(4)	2.2(4)	-0.6(4)
C9	15.4(4)	13.8(4)	18.0(5)	-0.6(3)	2.0(4)	-0.9(3)
C10	16.1(4)	13.9(4)	14.0(4)	-1.8(3)	0.0(3)	-1.2(3)
C11	15.6(4)	13.3(4)	15.7(4)	-0.6(3)	0.7(3)	1.1(3)
C12	20.9(5)	17.2(5)	15.7(5)	-1.2(4)	-0.5(4)	2.3(4)
C13	29.9(6)	19.9(5)	16.7(5)	1.8(4)	4.8(4)	2.1(4)
C14	30.4(6)	22.6(5)	23.1(5)	1.8(4)	7.2(4)	-7.0(4)
C15	24.9(5)	21.8(5)	21.0(5)	-0.9(4)	2.3(4)	-7.7(4)
C16	18.3(5)	16.2(5)	15.8(4)	-0.3(3)	0.8(4)	-1.5(4)
C17	26.7(6)	18.6(6)	46.9(8)	-1.2(5)	0.7(5)	6.7(4)
C18	32.1(6)	20.0(5)	18.1(5)	-4.0(4)	1.3(4)	-3.6(4)
C19	16.0(5)	17.5(5)	22.6(5)	-4.5(4)	0.6(4)	-1.8(4)
C20	13.5(4)	17.5(5)	19.9(5)	-2.6(4)	1.6(4)	-1.5(3)
C21	20.9(5)	26.6(6)	23.5(5)	3.7(4)	5.4(4)	2.9(4)
C22	21.9(5)	21.2(6)	47.3(8)	8.1(5)	9.9(5)	2.5(4)
C23	19.3(5)	22.3(6)	49.4(8)	-11.7(5)	4.0(5)	0.6(4)
C24	25.4(6)	37.8(7)	25.4(6)	-11.3(5)	1.4(5)	7.4(5)
C25	24.3(5)	27.7(6)	20.9(5)	1.1(4)	5.4(4)	5.2(4)

Table 4 Bond Lengths for 22srv120.

Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
O1	C1	1.2267(13)		C9	C10	1.5322(14)

O2	C6	1.3616(13)		C10	C11	1.5194(14)
O2	C17	1.4281(16)		C10	C19	1.5516(15)
O3	C7	1.3670(13)		C11	C12	1.3912(14)
O3	C18	1.4234(15)		C11	C16	1.3887(14)
N1	C1	1.3619(14)		C12	C13	1.3932(16)
N1	C2	1.4516(14)		C13	C14	1.3980(17)
N1	C10	1.4730(13)		C14	C15	1.3842(16)
C1	C16	1.4820(15)		C15	C16	1.3892(15)
C2	C3	1.5203(17)		C19	C20	1.5074(15)
C3	C4	1.5156(15)		C20	C21	1.3912(16)
C4	C5	1.4068(15)		C20	C25	1.3950(15)
C4	C9	1.3945(14)		C21	C22	1.3906(17)
C5	C6	1.3789(16)		C22	C23	1.387(2)
C6	C7	1.4106(15)		C23	C24	1.377(2)
C7	C8	1.3844(14)		C24	C25	1.3871(17)
C8	C9	1.4034(14)				

Table 5 Bond Angles for 22srv120.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C6	O2	C17	116.61(10)		N1	C10	C11	100.87(8)
C7	O3	C18	115.14(8)		N1	C10	C19	110.60(8)
C1	N1	C2	119.82(9)		C9	C10	C19	110.84(8)
C1	N1	C10	113.99(8)		C11	C10	C9	113.00(8)
C2	N1	C10	118.49(8)		C11	C10	C19	111.78(8)
O1	C1	N1	125.28(10)		C12	C11	C10	129.92(9)
O1	C1	C16	128.57(10)		C16	C11	C10	109.83(9)
N1	C1	C16	106.13(9)		C16	C11	C12	120.24(10)
N1	C2	C3	107.10(9)		C11	C12	C13	117.96(10)
C4	C3	C2	109.33(9)		C12	C13	C14	121.24(10)
C5	C4	C3	118.58(10)		C15	C14	C13	120.73(11)
C9	C4	C3	122.21(10)		C14	C15	C16	117.69(10)
C9	C4	C5	119.12(10)		C11	C16	C1	108.65(9)
C6	C5	C4	121.59(10)		C11	C16	C15	122.07(10)
O2	C6	C5	125.54(10)		C15	C16	C1	129.21(10)
O2	C6	C7	115.39(10)		C20	C19	C10	114.33(8)
C5	C6	C7	119.04(10)		C21	C20	C19	121.87(10)
O3	C7	C6	115.53(9)		C21	C20	C25	117.85(10)
O3	C7	C8	124.78(10)		C25	C20	C19	120.27(10)
C8	C7	C6	119.69(10)		C22	C21	C20	121.19(11)
C7	C8	C9	121.11(10)		C23	C22	C21	120.00(12)
C4	C9	C8	119.27(9)		C24	C23	C22	119.46(12)
C4	C9	C10	121.61(9)		C23	C24	C25	120.50(12)
C8	C9	C10	119.12(9)		C24	C25	C20	120.99(11)
N1	C10	C9	109.34(8)					

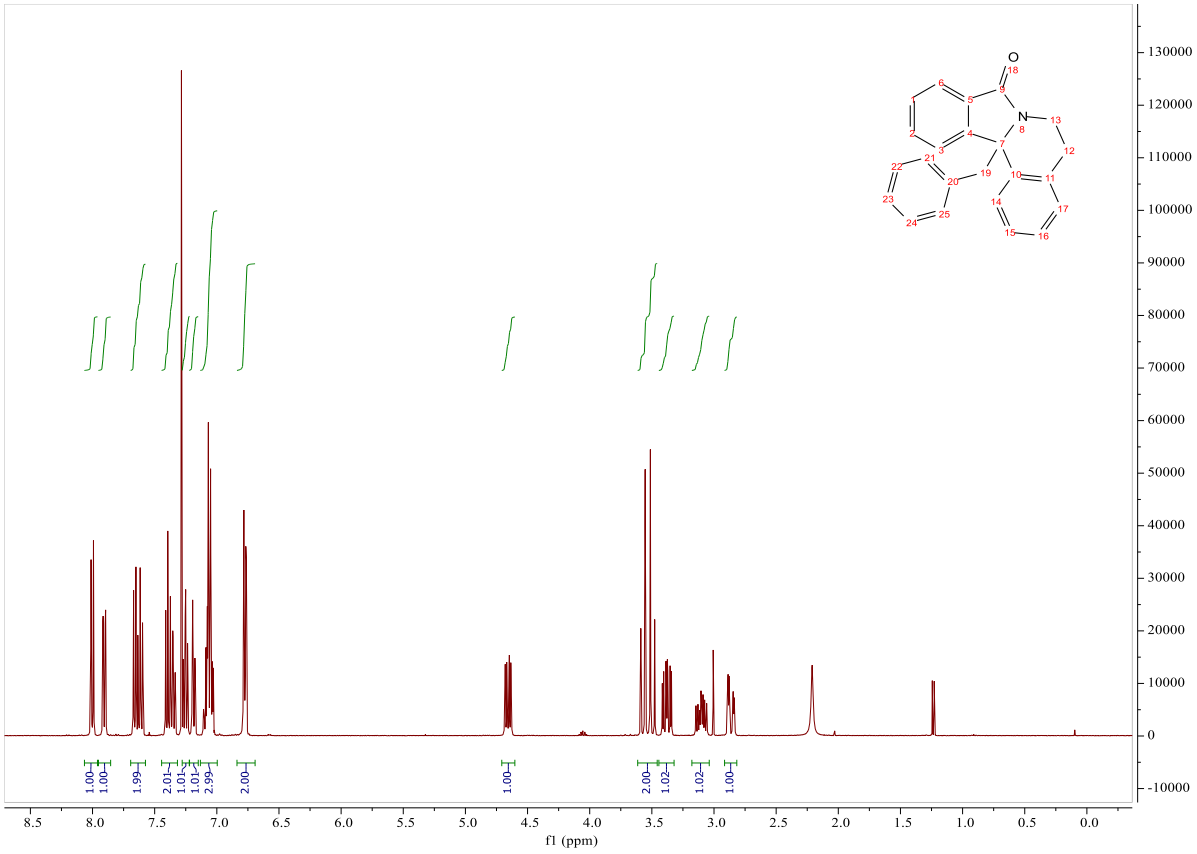
Table 6 Selected Torsion Angles for 22srv120.										
A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
C1	C16	C11	C10	-0.47(12)		C9	C10	C11	C12	-67.85(14)
C1	C16	C11	C12	-179.74(9)		C9	C10	C11	C16	112.97(10)
C2	N1	C1	O1	22.11(17)		C9	C10	C19	C20	-173.74(9)
C2	C3	C4	C5	155.35(10)		C10	N1	C1	O1	171.09(11)
C2	C3	C4	C9	-21.20(15)		C10	C11	C16	C15	-177.69(10)
C3	C2	N1	C1	81.04(12)		C10	C19	C20	C21	-91.50(13)
C3	C2	N1	C10	-66.57(12)		C10	C19	C20	C25	88.76(13)
C3	C4	C9	C8	172.32(10)		C11	C10	N1	C1	7.04(11)
C3	C4	C9	C10	-7.07(16)		C11	C10	N1	C2	156.46(9)
C4	C3	C2	N1	53.54(12)		C11	C10	C19	C20	59.23(12)
C4	C9	C10	N1	1.01(13)		C11	C16	C1	O1	-173.81(11)
C4	C9	C10	C11	-110.46(11)		C11	C16	C1	N1	4.80(12)
C4	C9	C10	C19	123.18(10)		C12	C11	C10	N1	175.55(10)
C5	C4	C9	C8	-4.21(15)		C12	C11	C10	C19	58.00(14)
C5	C4	C9	C10	176.39(9)		C12	C11	C16	C15	3.04(16)
C5	C6	O2	C17	-4.26(16)		C15	C16	C1	O1	3.1(2)
C6	C7	O3	C18	-168.72(10)		C15	C16	C1	N1	-178.24(11)
C7	C6	O2	C17	173.69(10)		C16	C1	N1	C2	-156.56(9)
C8	C7	O3	C18	11.15(15)		C16	C1	N1	C10	-7.58(12)
C8	C9	C10	N1	-178.39(9)		C16	C11	C10	N1	-3.63(11)
C8	C9	C10	C11	70.14(12)		C16	C11	C10	C19	-121.18(9)
C8	C9	C10	C19	-56.21(12)		C19	C10	N1	C1	125.45(10)
C9	C10	N1	C1	-112.23(10)		C19	C10	N1	C2	-85.13(11)
C9	C10	N1	C2	37.19(12)		C20	C19	C10	N1	-52.31(12)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv120.				
Atom	***x***	***y***	***z***	**U(eq)**
H17A	5990(20)	7101(11)	5045(13)	37(4)
H2A	8780(18)	3548(9)	2546(11)	25(4)
H2B	7300(18)	3113(9)	1861(11)	22(4)
H3A	5490(20)	3821(9)	2680(12)	29(4)
H3B	6610(20)	4485(10)	2319(12)	34(4)
H5	6000(19)	5364(9)	3622(12)	29(4)
H8	9119(18)	3789(9)	5955(11)	23(4)
H12	8389(18)	2440(9)	6334(11)	21(3)
H13	6779(18)	1447(9)	6917(12)	27(4)
H14	4910(20)	776(10)	5782(12)	34(4)
H15	4580(19)	1082(9)	4053(12)	29(4)
H17B	6598(19)	6643(10)	4058(12)	31(4)

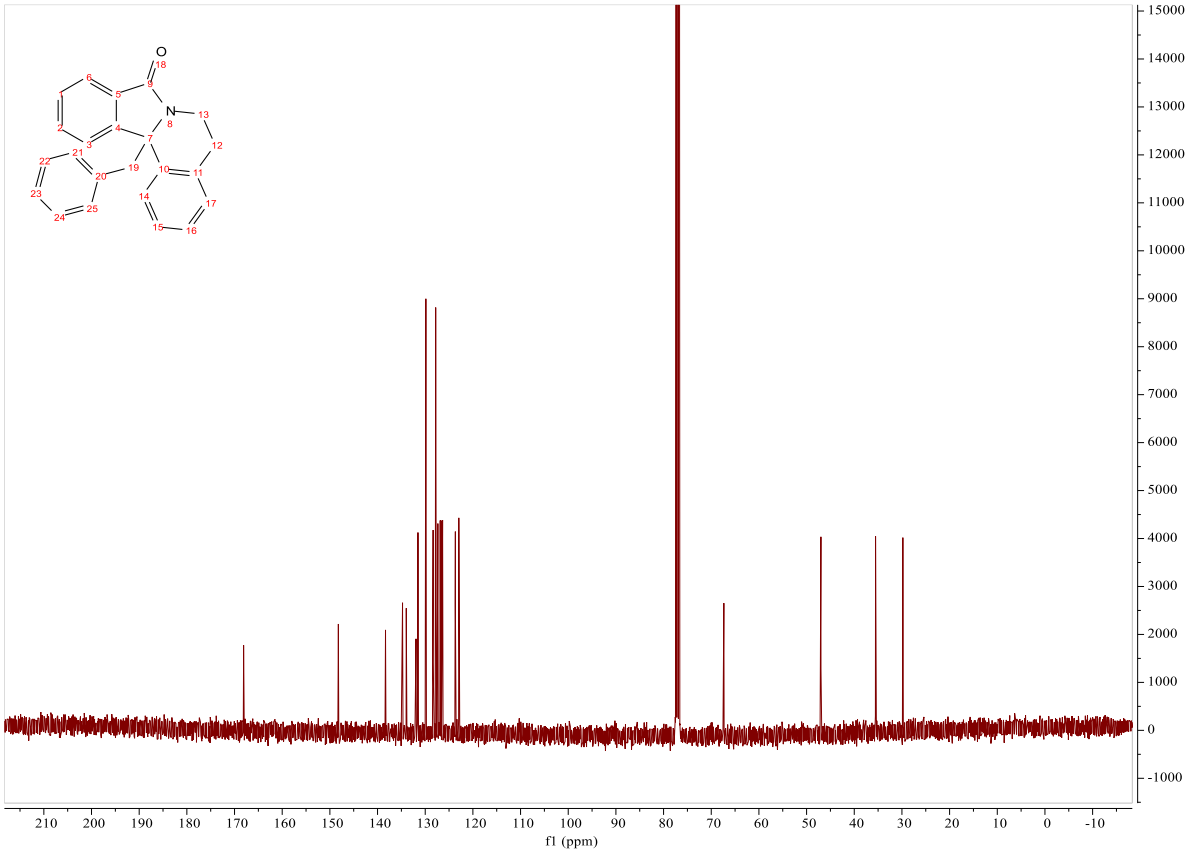
H17C	4920(20)	6385(11)	4504(13)	42(5)
H18A	9505(18)	4288(9)	7436(11)	24(4)
H18B	10779(19)	4700(9)	6864(12)	30(4)
H18C	10195(19)	5121(10)	7806(12)	31(4)
H19A	10572(19)	3208(9)	4075(12)	28(4)
H19B	10490(18)	2869(9)	5149(11)	23(4)
H21	10580(20)	1414(10)	5475(13)	35(4)
H22	11450(20)	177(11)	4946(13)	37(4)
H23	11860(20)	-12(11)	3250(13)	41(5)
H24	11590(20)	1048(11)	2154(14)	46(5)
H25	10750(20)	2309(11)	2662(14)	43(5)

12*b*-benzyl-5,12*b*-dihydroisoindolo[1,2-*a*]isoquinolin-8(6*H*)-one **86b**

^{1}H:



^{13}C:



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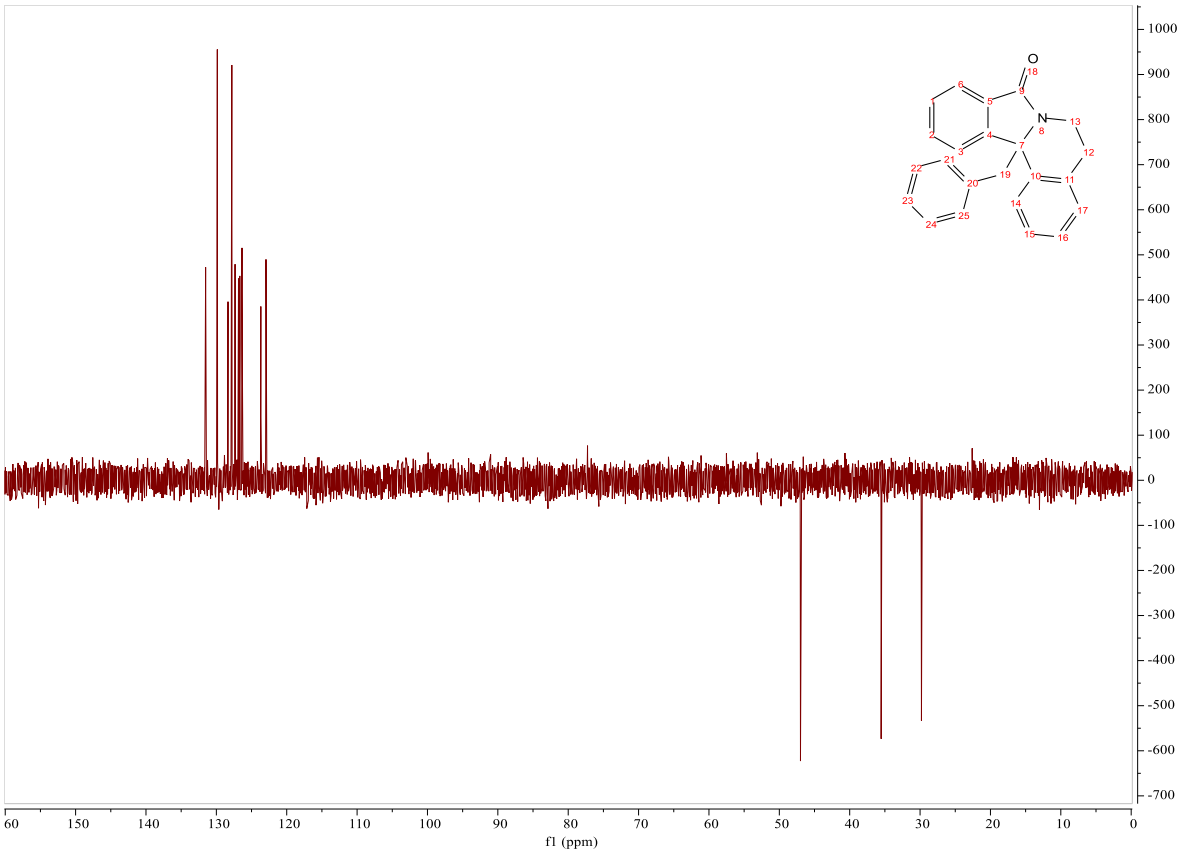
O
18
6
5
9
N
13
8
2
4
7
12
3
21
22
19
10
11
20
23
14
17
25
24
15
16
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
-300
-400
-500
-600
-700
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140
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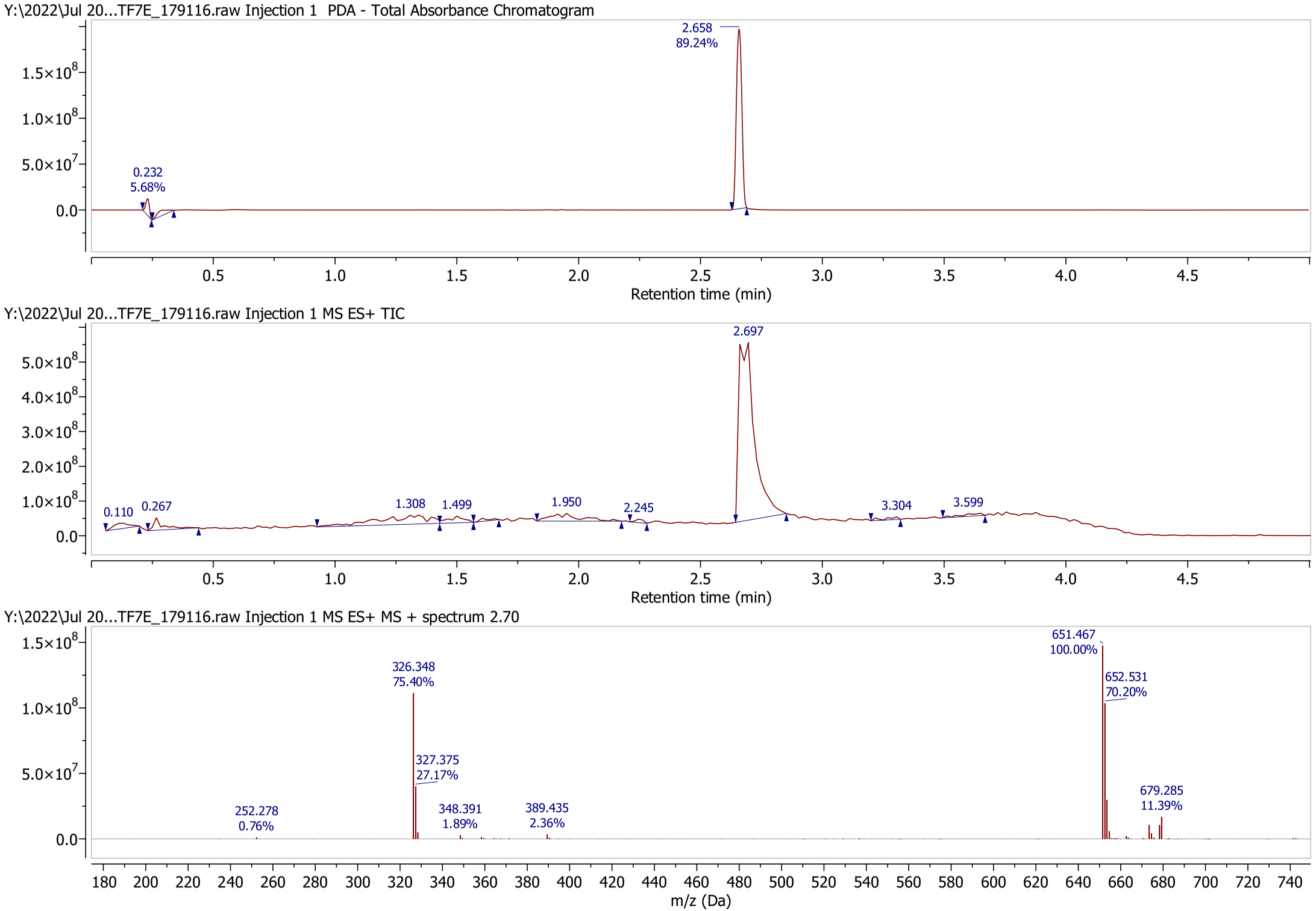
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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89.24%
0.232
5.68%
1.5×10^8
1.0×10^8
5.0×10^7
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Jul 20...TF7E_179116.raw Injection 1 MS ES+ TIC
2.697
0.110
0.267
1.308
1.499
1.950
2.245
3.304
3.599
5.0×10^8
4.0×10^8
3.0×10^8
2.0×10^8
1.0×10^8
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Jul 20...TF7E_179116.raw Injection 1 MS ES+ MS + spectrum 2.70
651.467
100.00%
326.348
75.40%
652.531
70.20%
327.375
27.17%
679.285
11.39%
252.278
0.76%
348.391
1.89%
389.435
2.36%
1.5×10^8
1.0×10^8
5.0×10^7
0.0
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640
660
680
700
720
740
m/z (Da)

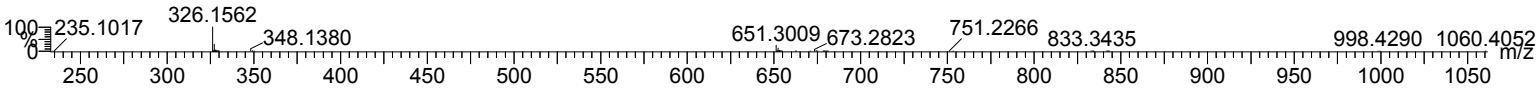
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
2060 formula(e) evaluated with 13 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 S: 0-4

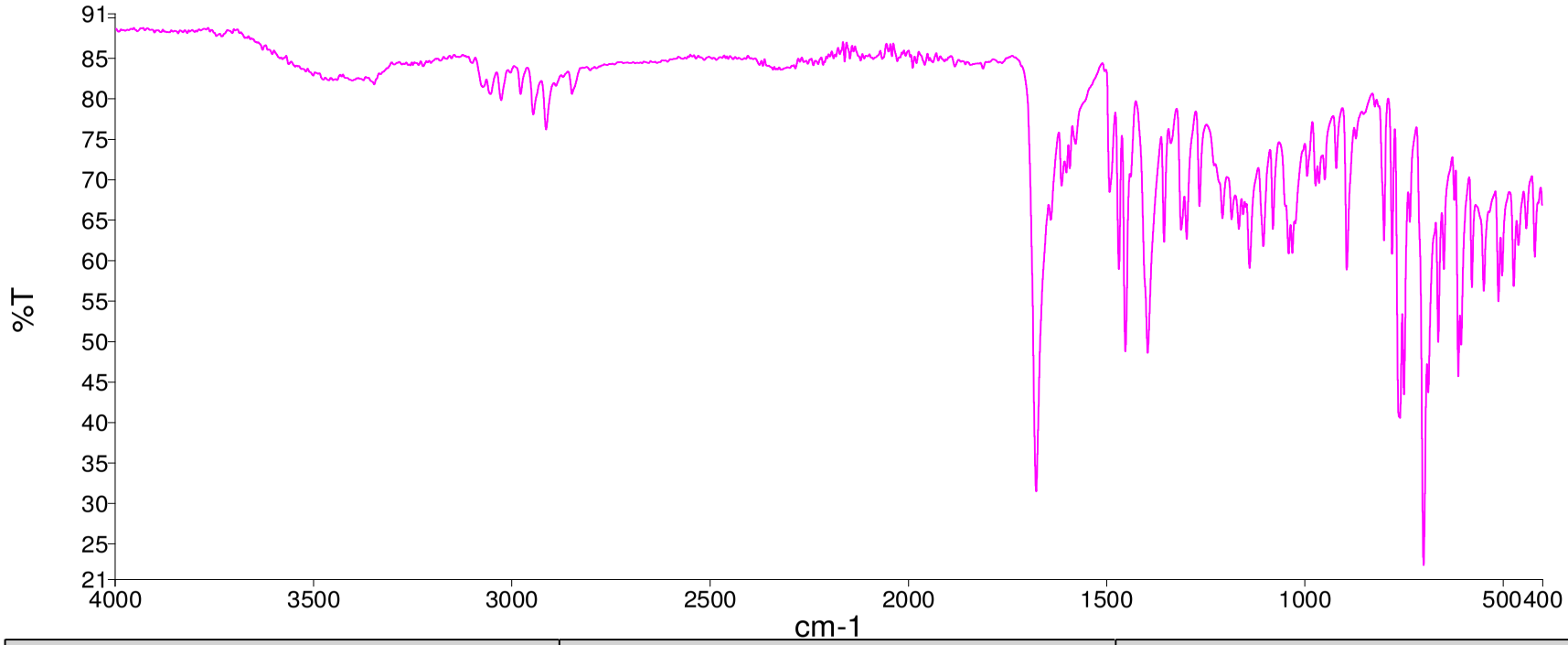
21-Jul-2022
MTF_MTF7E_179354 528 (4.434) Cm (526:529)

21-Jul-2022
1: TOF MS ES+
1.70e+005



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
326.1562	326.1563	-0.1	-0.3	1.5	565.0	12.248	0.00	C11 H24 N3 O8
	326.1566	-0.4	-1.2	-8.5	583.8	31.034	0.00	C4 H32 N5 O5 S3
	326.1557	0.5	1.5	-7.5	576.7	23.938	0.00	C3 H28 N5 O10 S
	326.1570	-0.8	-2.5	-2.5	574.7	21.961	0.00	C4 H24 N9 O6 S
	326.1572	-1.0	-3.1	0.5	581.6	28.803	0.00	C12 H28 N3 O3 S2
	326.1577	-1.5	-4.6	6.5	563.3	10.543	0.00	C12 H20 N7 O4
	326.1579	-1.7	-5.2	9.5	574.6	21.837	0.00	C20 H24 N O S
	326.1579	-1.7	-5.2	-3.5	583.7	30.923	0.00	C5 H28 N9 O S3
	326.1545	1.7	5.2	1.5	581.2	28.379	0.00	C8 H24 N9 O S2
	326.1545	1.7	5.2	14.5	552.8	0.000	100.00	C23 H20 N O
	326.1541	2.1	6.4	-4.5	584.7	31.963	0.00	C8 H32 N5 S4
	326.1538	2.4	7.4	5.5	574.3	21.539	0.00	C15 H24 N3 O3 S
	326.1537	2.5	7.7	2.5	567.1	14.297	0.00	C7 H20 N9 O6

Analyst Lenny Lauchlan
Date 22 July 2022 14:28



Sample Name	Description	Quality Checks
MTF 007Ei	Sample 019 By Lenny Date Friday, July 22 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

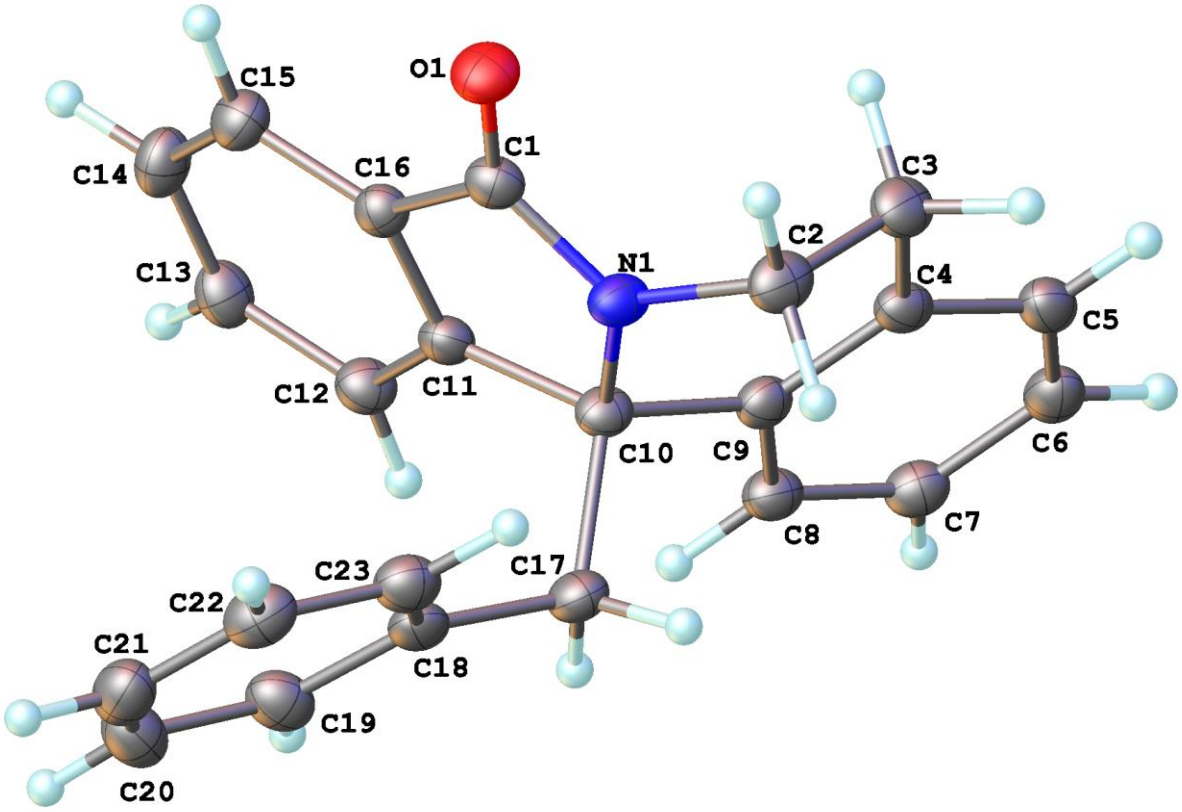


Table 1 Crystal data and structure refinement for 22srv206.	
Identification code	22srv206
Empirical formula	$C_{23}H_{19}NO$
Formula weight	325.39
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.0084(5)
b/Å	7.6983(3)
c/Å	16.0076(6)
α/°	90
β/°	99.0852(13)
γ/°	90
Volume/Å^3	1704.62(11)
Z	4

ρ_{calc}g/cm^3	1.268
μ/mm^{-1}	0.077
F(000)	688.0
Crystal size/mm^3	0.16 × 0.11 × 0.01
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.154 to 55.992
Index ranges	-18 ≤ h ≤ 18, -10 ≤ k ≤ 10, -21 ≤ l ≤ 21
Reflections collected	34352
Independent reflections	4112 [R_{int} = 0.0759, R_{sigma} = 0.0424]
Data/restraints/parameters	4112/0/303
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0479, wR_2 = 0.1050
Final R indexes [all data]	R_1 = 0.0832, wR_2 = 0.1219
Largest diff. peak/hole / e Å^{-3}	0.32/-0.20

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 22srv206. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	2565.1(9)	1366.3(15)	3764.5(8)	28.0(3)
N1	3254.3(10)	3819.7(18)	3291.9(9)	22.4(3)
C1	2654.9(12)	2949(2)	3737.4(10)	21.7(4)
C2	4068.2(14)	2991(2)	2991.5(12)	26.6(4)
C3	4958.3(14)	3339(2)	3637.2(12)	27.8(4)
C4	5075.6(13)	5248(2)	3826.7(10)	22.7(4)
C5	5998.3(13)	5915(2)	4110.8(11)	26.2(4)
C6	6139.9(13)	7650(3)	4296.5(11)	26.5(4)
C7	5357.2(13)	8763(2)	4194.1(11)	25.2(4)
C8	4433.2(13)	8136(2)	3906.0(11)	23.6(4)
C9	4282.0(12)	6376(2)	3728.6(10)	21.7(4)
C10	3257.1(12)	5719(2)	3404.4(10)	20.6(3)
C11	2547.6(12)	5909(2)	4028.1(10)	20.9(4)
C12	2241.9(13)	7380(2)	4413.2(11)	24.0(4)
C13	1597.1(13)	7160(2)	4985.5(12)	26.4(4)
C14	1250.0(13)	5520(3)	5154.4(12)	28.1(4)
C15	1533.2(13)	4064(2)	4751.5(12)	26.5(4)
C16	2181.8(12)	4291(2)	4193.0(10)	19.9(3)
C17	2878.3(13)	6599(2)	2542.4(11)	24.7(4)

C18	1847.3(13)	6152(2)	2171.5(10)	24.3(4)
C19	1108.2(14)	7327(3)	2237.1(11)	28.3(4)
C20	162.0(14)	6963(3)	1878.1(12)	32.5(4)
C21	-62.8(14)	5421(3)	1456.6(12)	32.5(5)
C22	661.9(15)	4228(3)	1395.9(12)	31.3(4)
C23	1612.9(14)	4591(2)	1746.5(11)	27.7(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv206. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	33.4(7)	17.9(6)	33.3(7)	0.0(5)	7.0(6)	-1.5(5)
N1	28.8(8)	17.6(7)	22.3(7)	0.6(6)	8.4(6)	2.2(6)
C1	23.6(8)	21.2(9)	19.5(8)	0.3(7)	1.0(7)	0.9(7)
C2	33.5(10)	21.8(9)	26.7(9)	-2.4(7)	11.8(8)	3.2(8)
C3	30.8(10)	22.6(9)	31.9(10)	1.4(8)	10.7(8)	7.0(8)
C4	26.9(9)	22.9(9)	19.6(8)	3.2(7)	7.9(7)	4.4(7)
C5	25.6(9)	30.6(10)	23.2(9)	5.1(7)	6.5(7)	6.0(8)
C6	25.4(9)	34.2(10)	19.8(8)	3.8(7)	3.3(7)	-0.7(8)
C7	30.4(9)	23.5(9)	22.1(9)	0.6(7)	5.7(7)	-1.2(7)
C8	27.8(9)	21.4(9)	22.6(8)	2.8(7)	7.5(7)	2.4(7)
C9	24.4(9)	22.5(8)	19.6(8)	1.8(7)	7.7(7)	1.3(7)
C10	25.0(8)	15.9(8)	22.0(8)	0.7(6)	6.5(7)	1.9(7)
C11	21.8(8)	21.6(8)	19.0(8)	3.5(6)	2.3(7)	2.8(7)
C12	27.0(9)	21.3(9)	24.0(9)	0.3(7)	4.6(7)	3.0(7)
C13	24.3(9)	27.6(10)	27.4(9)	-4.4(7)	4.2(7)	4.2(8)
C14	24.4(9)	35.6(11)	26.0(9)	-3.1(8)	9.2(8)	-0.3(8)
C15	24.4(9)	27.6(10)	27.9(9)	2.1(8)	5.7(7)	-2.3(7)
C16	20.1(8)	21.2(8)	18.0(8)	-0.2(6)	2.0(6)	0.7(7)
C17	26.7(9)	23.8(9)	24.2(9)	5.1(7)	6.0(7)	-2.1(8)
C18	27.0(9)	28.7(9)	17.9(8)	6.4(7)	5.4(7)	2.3(7)
C19	32.4(10)	30.1(10)	21.8(9)	0.1(8)	2.1(8)	5.0(8)
C20	30.8(10)	39.0(11)	27.4(10)	1.6(8)	3.5(8)	9.1(9)
C21	27.0(10)	42.3(12)	28.0(10)	4.4(9)	3.8(8)	-3.2(9)
C22	36.8(11)	30.2(10)	27.2(9)	0.3(8)	5.8(8)	-6.3(9)
C23	32.5(10)	28.1(10)	23.0(9)	2.5(7)	6.1(8)	1.6(8)

Table 4 Bond Lengths for 22srv206.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
O1	C1	1.226(2)		C10	C17	1.554(2)
N1	C1	1.361(2)		C11	C12	1.389(2)
N1	C2	1.453(2)		C11	C16	1.388(2)
N1	C10	1.473(2)		C12	C13	1.395(2)

C1	C16	1.480(2)		C13	C14	1.394(3)
C2	C3	1.512(3)		C14	C15	1.382(3)
C3	C4	1.504(2)		C15	C16	1.383(2)
C4	C5	1.398(3)		C17	C18	1.512(2)
C4	C9	1.400(2)		C18	C19	1.391(2)
C5	C6	1.376(3)		C18	C23	1.394(3)
C6	C7	1.381(3)		C19	C20	1.387(3)
C7	C8	1.390(3)		C20	C21	1.377(3)
C8	C9	1.394(2)		C21	C22	1.384(3)
C9	C10	1.533(2)		C22	C23	1.390(3)
C10	C11	1.523(2)				

Table 5 Bond Angles for 22srv206.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C2	122.58(14)		C11	C10	C9	114.80(14)
C1	N1	C10	114.51(13)		C11	C10	C17	111.94(14)
C2	N1	C10	119.27(14)		C12	C11	C10	130.40(16)
O1	C1	N1	125.68(16)		C16	C11	C10	109.70(14)
O1	C1	C16	128.29(16)		C16	C11	C12	119.90(15)
N1	C1	C16	105.99(14)		C11	C12	C13	117.99(17)
N1	C2	C3	107.55(14)		C14	C13	C12	121.28(17)
C4	C3	C2	111.27(15)		C15	C14	C13	120.60(17)
C5	C4	C3	119.36(16)		C14	C15	C16	117.73(17)
C5	C4	C9	119.06(16)		C11	C16	C1	108.99(14)
C9	C4	C3	121.58(16)		C15	C16	C1	128.41(16)
C6	C5	C4	121.39(17)		C15	C16	C11	122.44(16)
C5	C6	C7	119.48(17)		C18	C17	C10	114.85(14)
C6	C7	C8	120.28(17)		C19	C18	C17	119.88(17)
C7	C8	C9	120.58(17)		C19	C18	C23	118.45(17)
C4	C9	C10	121.21(15)		C23	C18	C17	121.66(16)
C8	C9	C4	119.19(16)		C20	C19	C18	120.73(18)
C8	C9	C10	119.58(15)		C21	C20	C19	120.45(19)
N1	C10	C9	110.67(14)		C20	C21	C22	119.53(19)
N1	C10	C11	100.73(13)		C21	C22	C23	120.34(19)
N1	C10	C17	109.30(14)		C22	C23	C18	120.48(18)
C9	C10	C17	109.08(13)					

Table 6 Selected Torsion Angles for 22srv206.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
C2	C3	C4	C5	-153.88(16)		C8	C9	C10	C11	-64.5(2)
C2	C3	C4	C9	26.4(2)		C8	C9	C10	C17	62.06(19)
C3	C2	N1	C1	-95.50(19)		C9	C10	N1	C1	122.78(15)

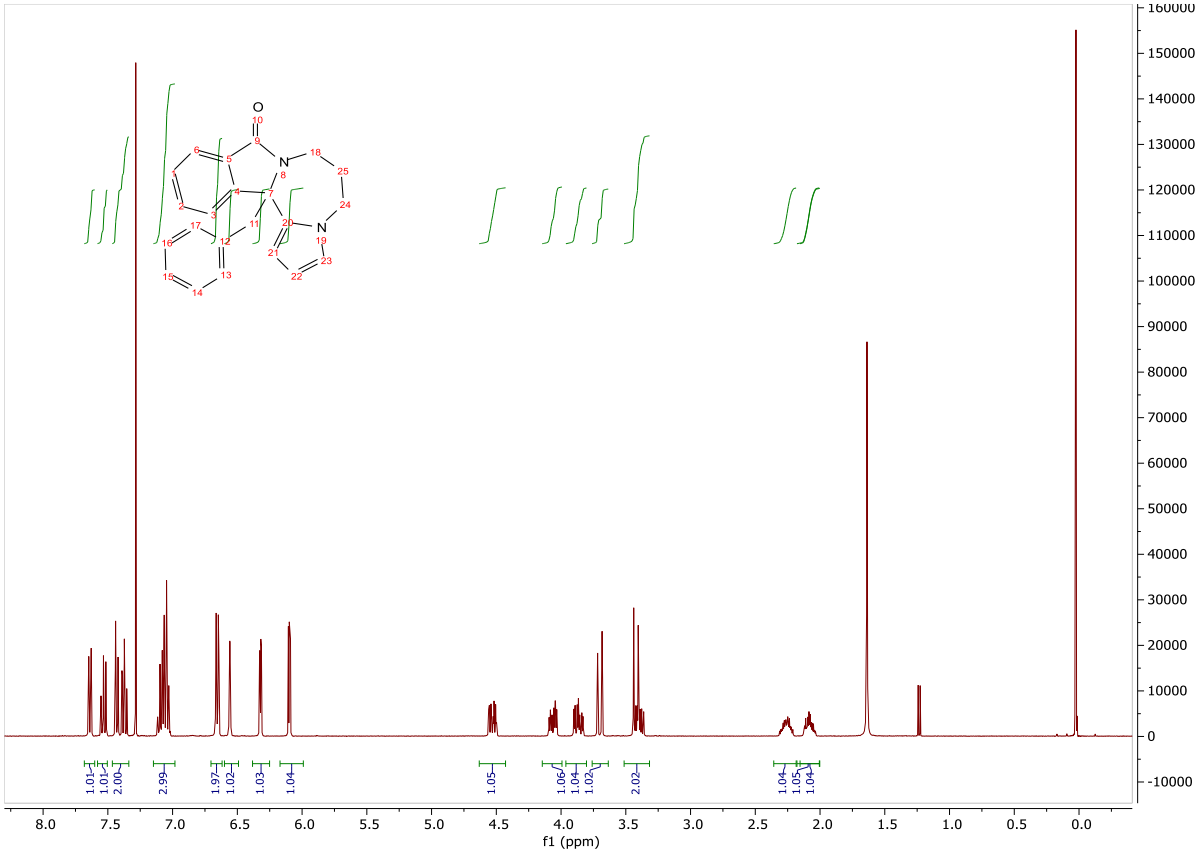
C3	C2	N1	C10	61.83(19)		C9	C10	N1	C2	-36.3(2)
C3	C4	C9	C8	-179.42(16)		C9	C10	C17	C18	-176.50(14)
C3	C4	C9	C10	-1.3(2)		C10	C17	C18	C19	101.82(19)
C4	C3	C2	N1	-52.70(19)		C10	C17	C18	C23	-79.4(2)
C4	C9	C10	N1	4.3(2)		C11	C10	N1	C1	0.92(18)
C4	C9	C10	C11	117.44(17)		C11	C10	N1	C2	-158.17(14)
C4	C9	C10	C17	-116.03(17)		C11	C10	C17	C18	-48.3(2)
C5	C4	C9	C8	0.8(2)		C17	C10	N1	C1	-117.07(15)
C5	C4	C9	C10	178.91(15)		C17	C10	N1	C2	83.84(18)
C8	C9	C10	N1	-177.65(14)		C18	C17	C10	N1	62.37(19)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv206.

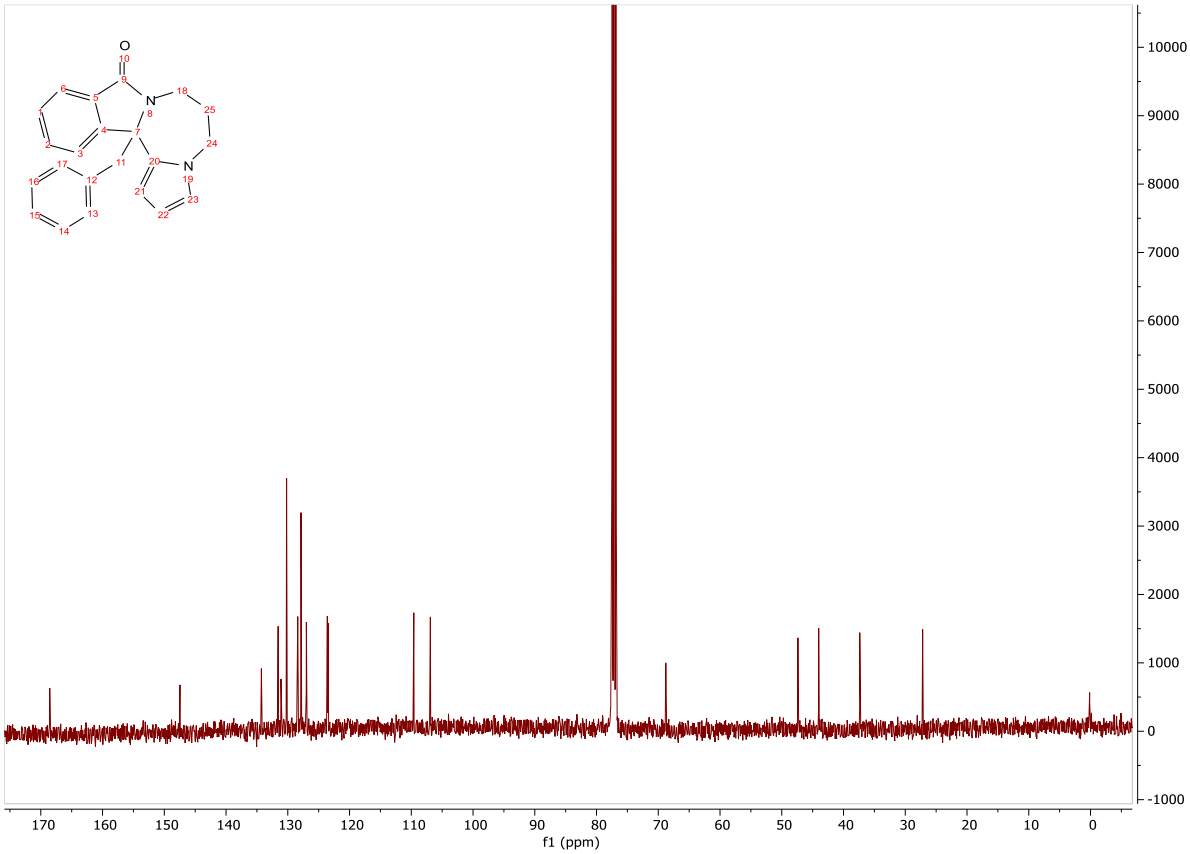
Atom	***x***	***y***	***z***	**U(eq)**
H2A	3912(14)	1680(30)	2955(13)	36(6)
H2B	4121(14)	3550(30)	2407(13)	34(5)
H3A	4895(14)	2690(30)	4172(14)	36(6)
H3B	5589(17)	2910(30)	3418(15)	52(7)
H5	6537(15)	5090(30)	4152(13)	37(6)
H6	6809(14)	8110(30)	4496(12)	31(5)
H7	5446(13)	10000(20)	4335(11)	20(5)
H8	3873(14)	8970(30)	3843(12)	29(5)
H12	2451(14)	8540(30)	4288(13)	32(5)
H13	1371(14)	8190(30)	5287(12)	32(5)
H14	802(15)	5390(30)	5557(13)	38(6)
H15	1314(16)	2860(30)	4872(14)	45(6)
H17A	3351(13)	6240(20)	2141(12)	25(5)
H17B	2924(14)	7890(30)	2637(13)	36(6)
H19	1262(14)	8430(30)	2512(12)	28(5)
H20	-306(16)	7830(30)	1930(14)	43(6)
H21	-721(16)	5200(30)	1204(14)	43(6)
H22	497(15)	3140(30)	1109(13)	39(6)
H23	2165(15)	3730(30)	1709(12)	33(5)

13*b*-benzyl-6,7-dihydro-5*H*-pyrrolo[2',1':3,4][1,4]diazepino[2,1-*a*]isoindol-9(13*bH*)-one **90**

^{1}H:



^{13}C:



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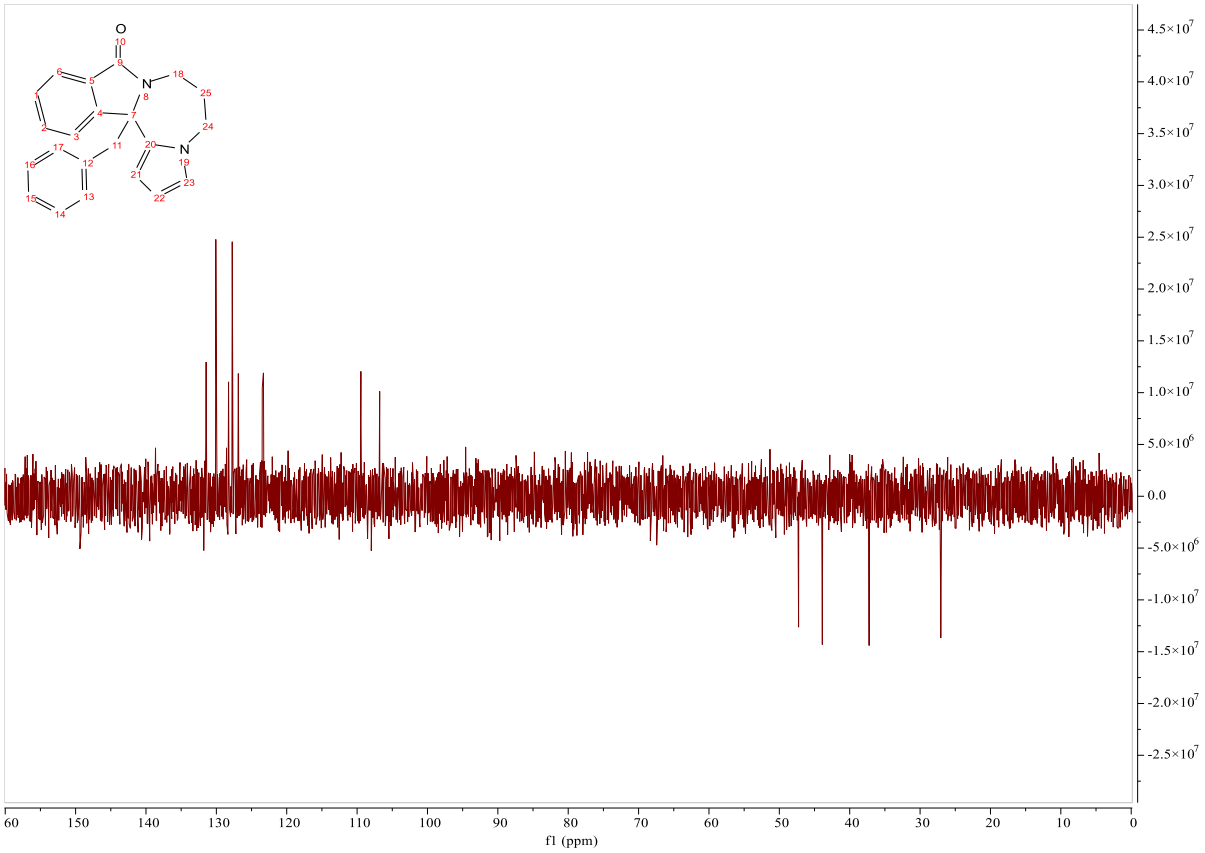
O
N
N
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4.0×10^7
3.5×10^7
3.0×10^7
2.5×10^7
2.0×10^7
1.5×10^7
1.0×10^7
5.0×10^6
0.0
-5.0×10^6
-1.0×10^7
-1.5×10^7
-2.0×10^7
-2.5×10^7
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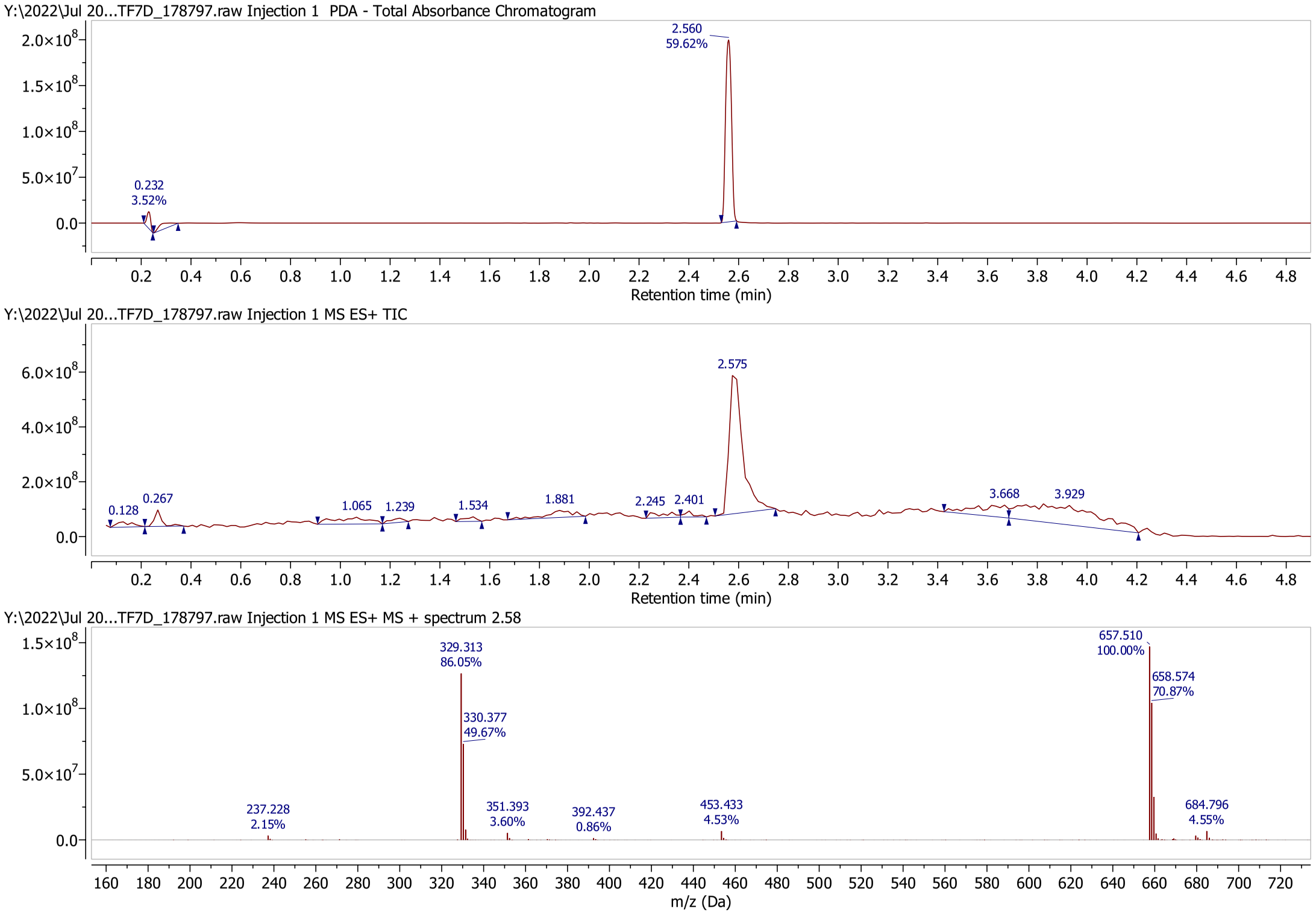
f1 (ppm)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59.62%
0.232
3.52%
Retention time (min)
Y:\2022\Jul 20...TF7D_178797.raw Injection 1 MS ES+ TIC
2.575
0.128
0.267
1.065
1.239
1.534
1.881
2.245
2.401
3.668
3.929
Retention time (min)
Y:\2022\Jul 20...TF7D_178797.raw Injection 1 MS ES+ MS + spectrum 2.58
329.313
86.05%
330.377
49.67%
657.510
100.00%
658.574
70.87%
237.228
2.15%
351.393
3.60%
392.437
0.86%
453.433
4.53%
684.796
4.55%
m/z (Da)

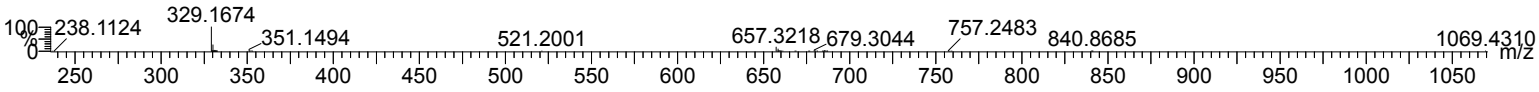
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
2134 formula(e) evaluated with 15 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 S: 0-4

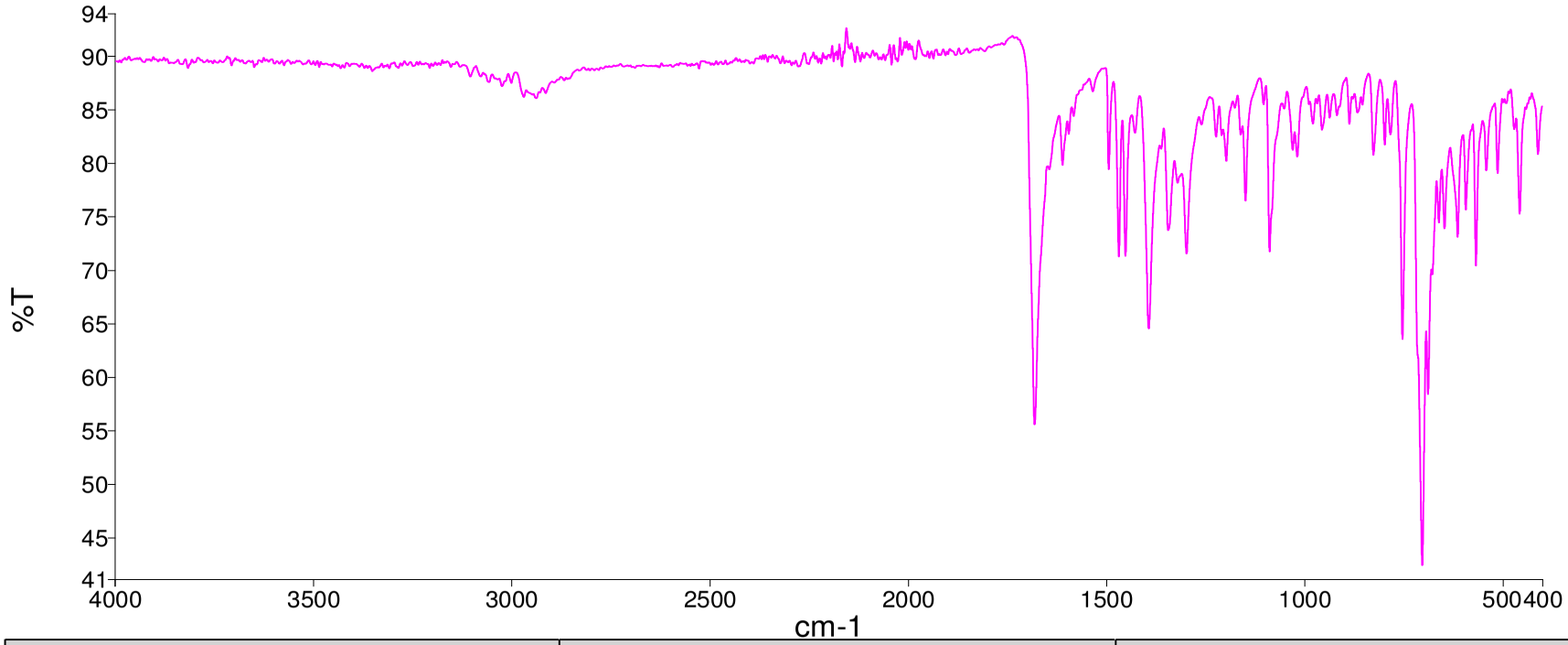
21-Jul-2022
MTF_MTF7D_179353 513 (4.311) Cm (509:517)

21-Jul-2022
1: TOF MS ES+
2.52e+005



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
329.1674	329.1672	0.2	0.6	0.5	653.5	11.413	0.00	C10 H25 N4 O8
	329.1668	0.6	1.8	-5.5	674.8	32.716	0.00	C10 H33 O7 S2
	329.1686	-1.2	-3.6	5.5	652.1	10.014	0.00	C11 H21 N8 O4
	329.1681	-0.7	-2.1	-0.5	674.5	32.463	0.00	C11 H29 N4 O3 S2
	329.1676	-0.2	-0.6	-6.5	677.4	35.280	0.00	C11 H37 O2 S4
	329.1647	2.7	8.2	4.5	667.5	25.454	0.00	C14 H25 N4 O3 S
	329.1688	-1.4	-4.3	8.5	667.7	25.645	0.00	C19 H25 N2 O S
	329.1666	0.8	2.4	-8.5	669.8	27.770	0.00	C2 H29 N6 O10 S
	329.1654	2.0	6.1	13.5	642.1	0.000	99.99	C22 H21 N2 O
	329.1679	-0.5	-1.5	-3.5	668.0	25.907	0.00	C3 H25 N10 O6 S
	329.1675	-0.1	-0.3	-9.5	676.6	34.563	0.00	C3 H33 N6 O5 S3
	329.1688	-1.4	-4.3	-4.5	676.6	34.571	0.00	C4 H29 N10 O S3
	329.1646	2.8	8.5	1.5	657.7	15.602	0.00	C6 H21 N10 O6
	329.1654	2.0	6.1	0.5	674.4	32.320	0.00	C7 H25 N10 O S2
	329.1650	2.4	7.3	-5.5	677.5	35.467	0.00	C7 H33 N6 S4

Analyst Lenny Lauchlan
Date 07 July 2022 08:06



Sample Name	Description	Quality Checks
MTF 007D	Sample 019 By Lenny Date Thursday, July 07 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

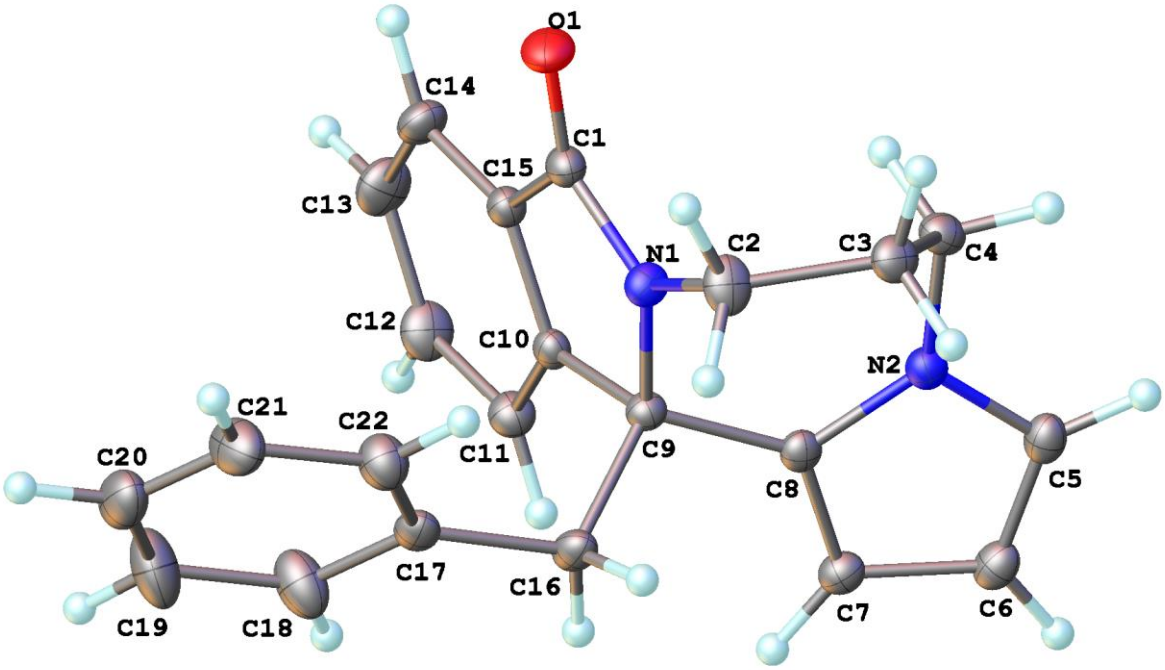


Table 1 Crystal data and structure refinement for 22srv188.	
Identification code	22srv188
Empirical formula	$C_{22}H_{20}N_2O$
Formula weight	328.40
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.6844(4)
b/Å	7.3610(2)
c/Å	16.2628(4)
α/°	90
β/°	105.5710(9)
γ/°	90
Volume/Å^3	1693.36(8)
Z	4
ρ_{calc}g/cm^3	1.288
μ/mm^{-1}	0.080

F(000)	696.0
Crystal size/mm^3	0.22 × 0.09 × 0.02
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.224 to 57.992
Index ranges	-20 ≤ h ≤ 20, -10 ≤ k ≤ 10, -22 ≤ l ≤ 22
Reflections collected	45810
Independent reflections	4485 [R_{int} = 0.0756, R_{sigma} = 0.0372]
Data/restraints/parameters	4485/0/306
Goodness-of-fit on F^2	1.086
Final R indexes [I>=2σ (I)]	R_1 = 0.0519, wR_2 = 0.1136
Final R indexes [all data]	R_1 = 0.0624, wR_2 = 0.1188
Largest diff. peak/hole / e $Å^{-3}$	0.34/-0.27

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 22srv188. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	7585.1(8)	9104.3(14)	2698.3(7)	25.0(2)
N1	8195.1(8)	6466.5(16)	3388.3(7)	16.0(2)
N2	10017.2(8)	4866.1(16)	3517.6(7)	16.1(2)
C1	7711.5(9)	7458.4(19)	2705.8(9)	16.6(3)
C2	8658.0(10)	7285(2)	4208.8(9)	22.3(3)
C3	9731.7(10)	7492(2)	4369.1(9)	19.2(3)
C4	10096.0(10)	6843.2(19)	3631.5(9)	18.2(3)
C5	10788.5(10)	3749(2)	3614.0(9)	19.0(3)
C6	10489.4(10)	1980(2)	3526.7(9)	19.1(3)
C7	9494.2(10)	2010.0(19)	3368.3(8)	17.3(3)
C8	9217.5(9)	3796.9(19)	3370.1(8)	15.1(3)
C9	8218.8(9)	4506.4(18)	3224.7(8)	14.1(2)
C10	7671.4(9)	4430.9(18)	2286.7(8)	14.3(3)
C11	7459.9(10)	2946(2)	1744.2(9)	18.8(3)
C12	6964.7(11)	3260(2)	898.8(9)	24.3(3)
C13	6690.6(11)	5003(2)	600.9(9)	26.3(3)
C14	6894.1(10)	6481(2)	1147.3(9)	21.8(3)
C15	7385.8(9)	6154.0(18)	1994.4(8)	15.5(3)
C16	7722.2(10)	3411(2)	3798.8(9)	18.6(3)
C17	6700.3(9)	3905.2(19)	3700.0(8)	18.1(3)
C18	5989.9(12)	2810(3)	3214.5(11)	31.1(4)
C19	5043.5(12)	3226(3)	3120.6(12)	37.4(4)

C20	4798.4(11)	4734(3)	3516.3(11)	31.0(4)
C21	5497.5(12)	5826(2)	4008.5(12)	30.3(4)
C22	6442.9(11)	5416(2)	4098.9(10)	25.0(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv188. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	25.8(5)	13.4(5)	34.3(6)	0.5(4)	5.5(4)	1.3(4)
N1	17.4(5)	15.4(5)	14.2(5)	-2.7(4)	2.4(4)	0.1(4)
N2	16.1(5)	17.4(6)	14.8(5)	0.5(4)	4.1(4)	-0.4(4)
C1	14.5(6)	15.6(6)	20.0(6)	0.8(5)	5.0(5)	0.0(5)
C2	21.0(7)	27.7(8)	17.7(7)	-9.2(6)	4.3(5)	-1.7(6)
C3	20.5(7)	19.3(7)	16.2(6)	-2.7(5)	2.2(5)	-2.1(5)
C4	19.6(6)	17.0(6)	17.7(6)	0.2(5)	4.4(5)	-2.8(5)
C5	16.3(6)	25.1(7)	16.0(6)	0.8(5)	4.9(5)	2.0(5)
C6	19.1(6)	22.3(7)	16.8(6)	0.7(5)	6.3(5)	4.7(5)
C7	19.2(6)	17.2(6)	15.7(6)	0.6(5)	5.4(5)	2.0(5)
C8	15.6(6)	17.8(6)	11.3(5)	0.6(5)	2.9(4)	0.2(5)
C9	15.1(6)	13.1(6)	14.1(6)	-0.5(5)	3.9(5)	0.4(5)
C10	12.7(6)	16.6(6)	14.2(6)	1.0(5)	4.5(4)	-0.7(5)
C11	19.9(6)	17.6(7)	19.2(6)	-1.6(5)	5.5(5)	0.1(5)
C12	25.5(7)	27.6(8)	18.8(7)	-8.0(6)	4.1(6)	-2.0(6)
C13	27.5(8)	33.9(9)	14.8(6)	0.5(6)	0.8(5)	2.8(6)
C14	22.3(7)	22.9(7)	19.0(7)	6.3(6)	3.3(5)	3.5(6)
C15	13.9(6)	16.5(6)	16.0(6)	1.2(5)	3.9(5)	-0.4(5)
C16	18.1(6)	21.2(7)	18.3(6)	6.1(5)	8.0(5)	3.0(5)
C17	18.8(6)	20.9(7)	16.0(6)	4.9(5)	7.2(5)	0.5(5)
C18	25.8(8)	35.3(9)	36.1(9)	-11.0(7)	14.9(7)	-6.5(7)
C19	22.3(8)	51.5(12)	39.3(10)	-13.1(9)	9.7(7)	-10.5(8)
C20	21.0(7)	38.9(9)	35.7(9)	8.0(7)	12.0(6)	4.0(7)
C21	26.6(8)	26.3(8)	42.6(10)	-0.2(7)	17.4(7)	4.3(6)
C22	22.7(7)	26.5(8)	27.2(7)	-3.1(6)	8.8(6)	-0.9(6)

Table 4 Bond Lengths for 22srv188.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
O1	C1	1.2253(17)		C9	C16	1.5556(18)
N1	C1	1.3588(17)		C10	C11	1.3868(19)
N1	C2	1.4555(17)		C10	C15	1.3797(18)
N1	C9	1.4693(17)		C11	C12	1.391(2)
N2	C4	1.4677(18)		C12	C13	1.392(2)
N2	C5	1.3743(18)		C13	C14	1.386(2)
N2	C8	1.3801(17)		C14	C15	1.3939(18)

C1	C15	1.4805(19)		C16	C17	1.5102(19)
C2	C3	1.535(2)		C17	C18	1.385(2)
C3	C4	1.516(2)		C17	C22	1.390(2)
C5	C6	1.369(2)		C18	C19	1.391(2)
C6	C7	1.4144(19)		C19	C20	1.378(3)
C7	C8	1.3769(19)		C20	C21	1.379(2)
C8	C9	1.5142(18)		C21	C22	1.390(2)
C9	C10	1.5225(17)				

Table 5 Bond Angles for 22srv188.

Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C2	122.65(12)		C8	C9	C16	108.53(10)
C1	N1	C9	114.35(11)		C10	C9	C16	112.08(11)
C2	N1	C9	123.00(11)		C11	C10	C9	129.36(12)
C5	N2	C4	122.98(12)		C15	C10	C9	109.97(11)
C5	N2	C8	108.38(12)		C15	C10	C11	120.67(12)
C8	N2	C4	128.46(11)		C10	C11	C12	117.78(13)
O1	C1	N1	125.73(13)		C11	C12	C13	121.51(14)
O1	C1	C15	128.11(13)		C14	C13	C12	120.54(13)
N1	C1	C15	106.16(11)		C13	C14	C15	117.59(14)
N1	C2	C3	113.73(11)		C10	C15	C1	108.81(11)
C4	C3	C2	113.52(11)		C10	C15	C14	121.89(13)
N2	C4	C3	112.30(11)		C14	C15	C1	129.28(13)
C6	C5	N2	109.01(12)		C17	C16	C9	115.06(11)
C5	C6	C7	106.91(12)		C18	C17	C16	119.68(13)
C8	C7	C6	107.80(12)		C18	C17	C22	118.29(14)
N2	C8	C9	125.00(12)		C22	C17	C16	122.02(13)
C7	C8	N2	107.90(12)		C17	C18	C19	120.80(16)
C7	C8	C9	127.10(12)		C20	C19	C18	120.28(16)
N1	C9	C8	112.30(11)		C19	C20	C21	119.60(15)
N1	C9	C10	100.69(10)		C20	C21	C22	120.10(16)
N1	C9	C16	111.27(11)		C21	C22	C17	120.92(15)
C8	C9	C10	111.88(10)					

Table 6 Torsion Angles for 22srv188.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
O1	C1	C15	C10	-179.04(14)		C7	C8	C9	C16	48.66(17)
O1	C1	C15	C14	2.6(2)		C8	N2	C4	C3	58.03(18)
N1	C1	C15	C10	1.26(14)		C8	N2	C5	C6	0.21(15)
N1	C1	C15	C14	-177.07(13)		C8	C9	C10	C11	59.27(18)
N1	C2	C3	C4	1.39(19)		C8	C9	C10	C15	-119.97(12)
N1	C9	C10	C11	178.74(13)		C8	C9	C16	C17	-177.55(12)

N1	C9	C10	C15	-0.50(13)		C9	N1	C1	O1	178.62(13)
N1	C9	C16	C17	58.39(15)		C9	N1	C1	C15	-1.67(15)
N2	C5	C6	C7	0.14(15)		C9	N1	C2	C3	77.64(17)
N2	C8	C9	N1	-8.92(17)		C9	C10	C11	C12	-178.30(13)
N2	C8	C9	C10	103.46(14)		C9	C10	C15	C1	-0.42(14)
N2	C8	C9	C16	-132.36(13)		C9	C10	C15	C14	178.05(12)
C1	N1	C2	C3	-101.68(16)		C9	C16	C17	C18	101.17(16)
C1	N1	C9	C8	120.53(12)		C9	C16	C17	C22	-80.32(17)
C1	N1	C9	C10	1.37(14)		C10	C9	C16	C17	-53.49(16)
C1	N1	C9	C16	-117.58(12)		C10	C11	C12	C13	0.2(2)
C2	N1	C1	O1	-2.0(2)		C11	C10	C15	C1	-179.73(12)
C2	N1	C1	C15	177.71(11)		C11	C10	C15	C14	-1.3(2)
C2	N1	C9	C8	-58.84(16)		C11	C12	C13	C14	-0.9(2)
C2	N1	C9	C10	-178.00(11)		C12	C13	C14	C15	0.6(2)
C2	N1	C9	C16	63.05(16)		C13	C14	C15	C1	178.66(14)
C2	C3	C4	N2	-68.29(16)		C13	C14	C15	C10	0.5(2)
C4	N2	C5	C6	175.73(12)		C15	C10	C11	C12	0.9(2)
C4	N2	C8	C7	-175.69(12)		C16	C9	C10	C11	-62.91(17)
C4	N2	C8	C9	5.2(2)		C16	C9	C10	C15	117.86(12)
C5	N2	C4	C3	-116.54(14)		C16	C17	C18	C19	179.34(15)
C5	N2	C8	C7	-0.49(15)		C16	C17	C22	C21	-179.01(14)
C5	N2	C8	C9	-179.64(12)		C17	C18	C19	C20	-0.4(3)
C5	C6	C7	C8	-0.43(15)		C18	C17	C22	C21	-0.5(2)
C6	C7	C8	N2	0.57(15)		C18	C19	C20	C21	-0.2(3)
C6	C7	C8	C9	179.69(12)		C19	C20	C21	C22	0.5(3)
C7	C8	C9	N1	172.09(12)		C20	C21	C22	C17	-0.2(3)
C7	C8	C9	C10	-75.52(16)		C22	C17	C18	C19	0.8(2)

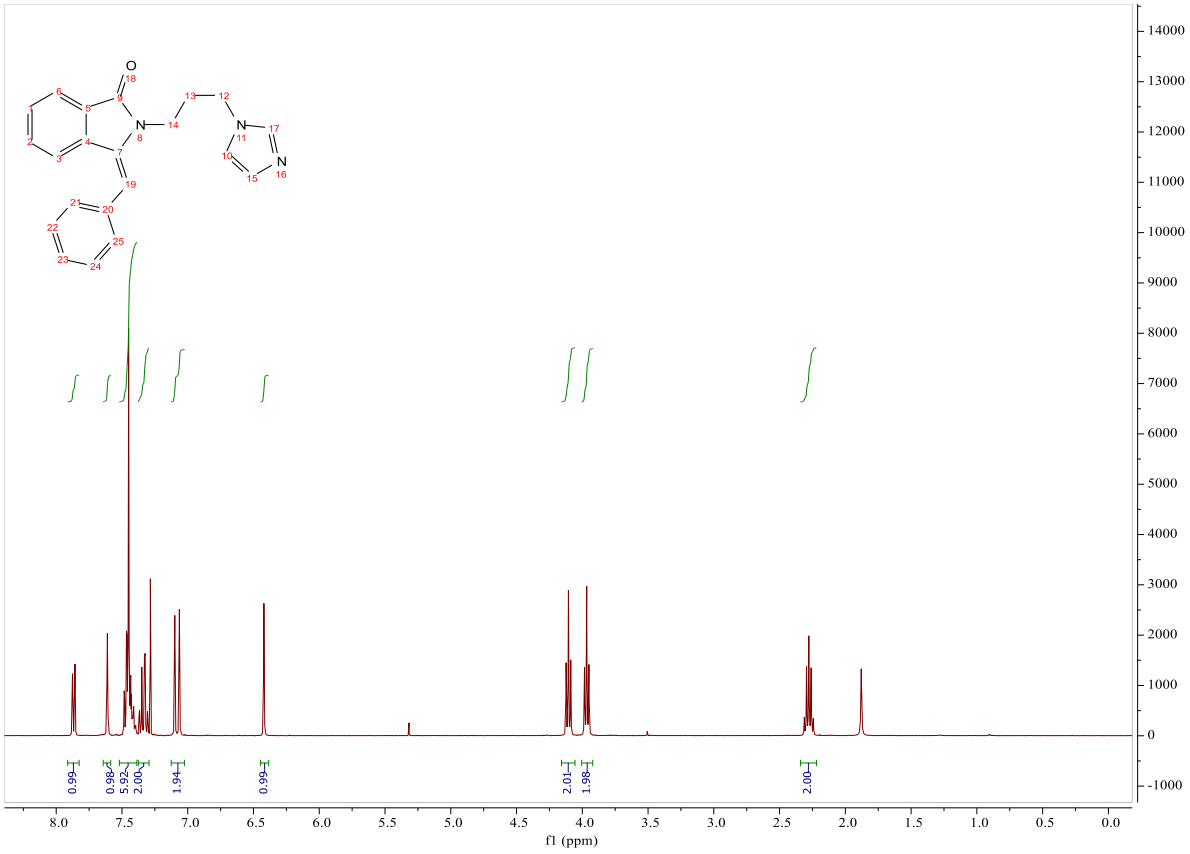
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv188.

Atom	***x***	***y***	***z***	**U(eq)**
H2A	8506(13)	6530(30)	4659(12)	29(5)
H2B	8371(14)	8470(30)	4234(13)	38(5)
H3A	10068(13)	6820(30)	4904(12)	29(5)
H3B	9883(14)	8780(30)	4474(13)	39(5)
H4A	9754(11)	7460(20)	3099(11)	15(4)
H4B	10774(13)	7110(20)	3741(11)	23(4)
H5	11425(13)	4280(20)	3723(11)	25(4)
H6	10893(13)	930(30)	3551(12)	28(5)
H7	9060(12)	960(20)	3263(11)	21(4)
H11	7644(13)	1750(30)	1947(11)	25(5)
H12	6811(13)	2210(30)	514(12)	28(5)
H13	6351(14)	5160(30)	-1(14)	41(6)
H14	6709(12)	7720(30)	948(11)	23(4)

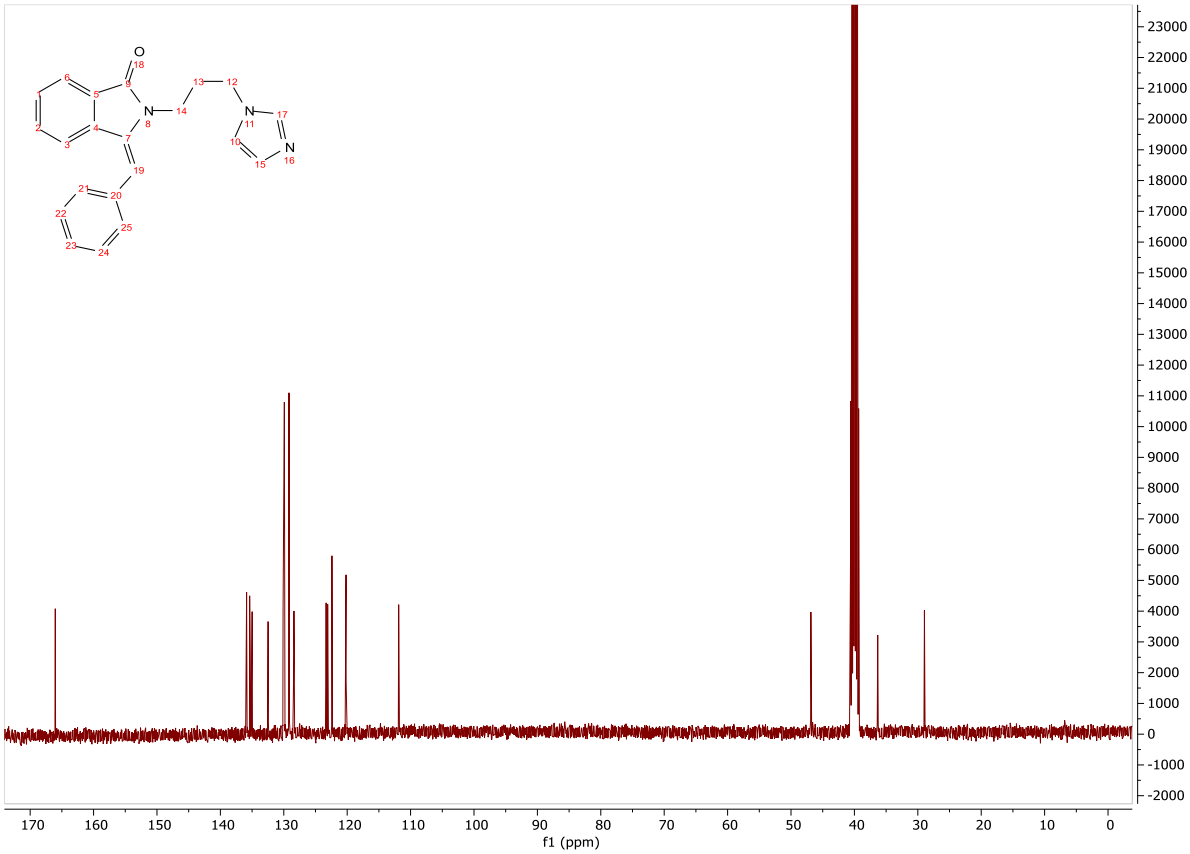
H16A	7764(12)	2090(20)	3645(11)	20(4)
H16B	8115(12)	3600(20)	4408(11)	22(4)
H18	6180(14)	1730(30)	2958(13)	40(6)
H19	4582(16)	2420(30)	2780(15)	50(6)
H20	4131(14)	5030(30)	3449(13)	37(5)
H21	5314(15)	6880(30)	4289(14)	41(6)
H22	6933(14)	6230(30)	4442(12)	33(5)

13*b*-benzyl-6,7-dihydro-5*H*-imidazo[2',1':3,4][1,4]diazepino[2,1-a]isoindol-9(13*bH*)-one **96**

^{1}H:



^{13}C:



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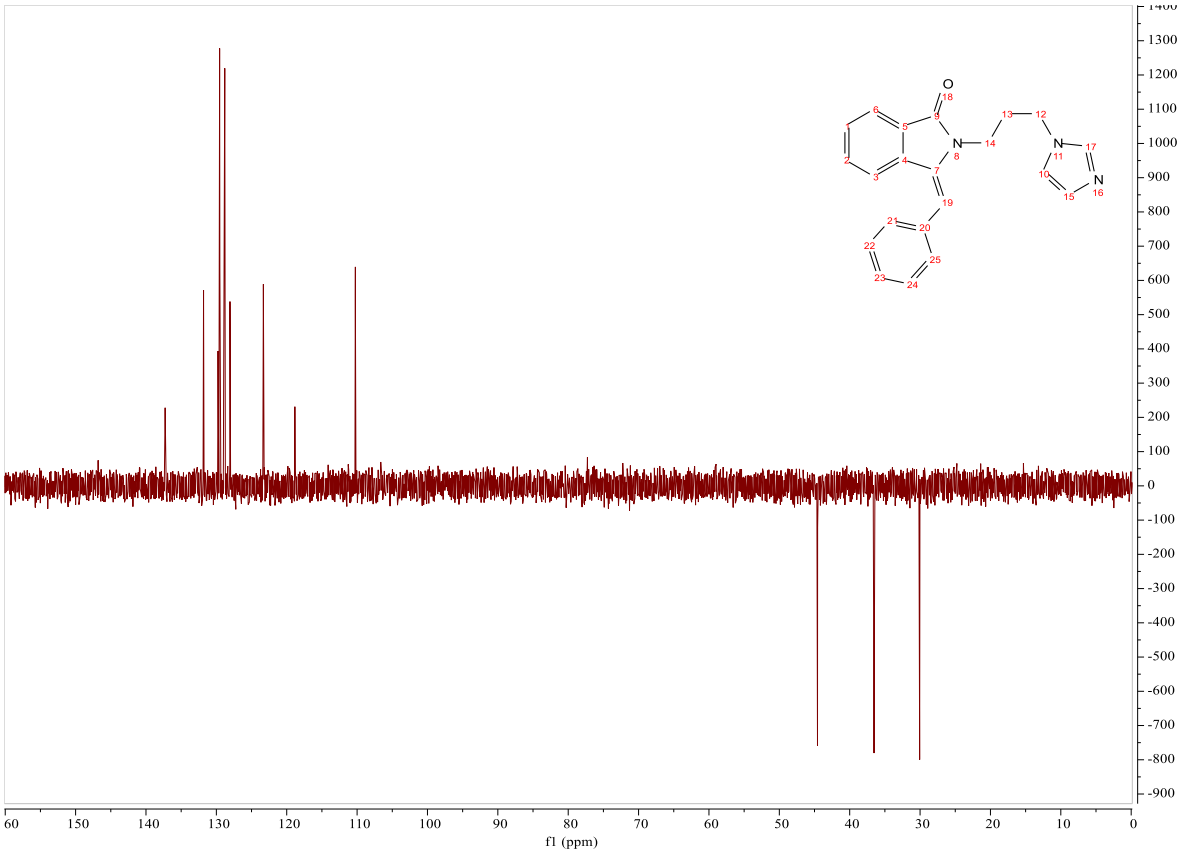
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-400
-500
-600
-700
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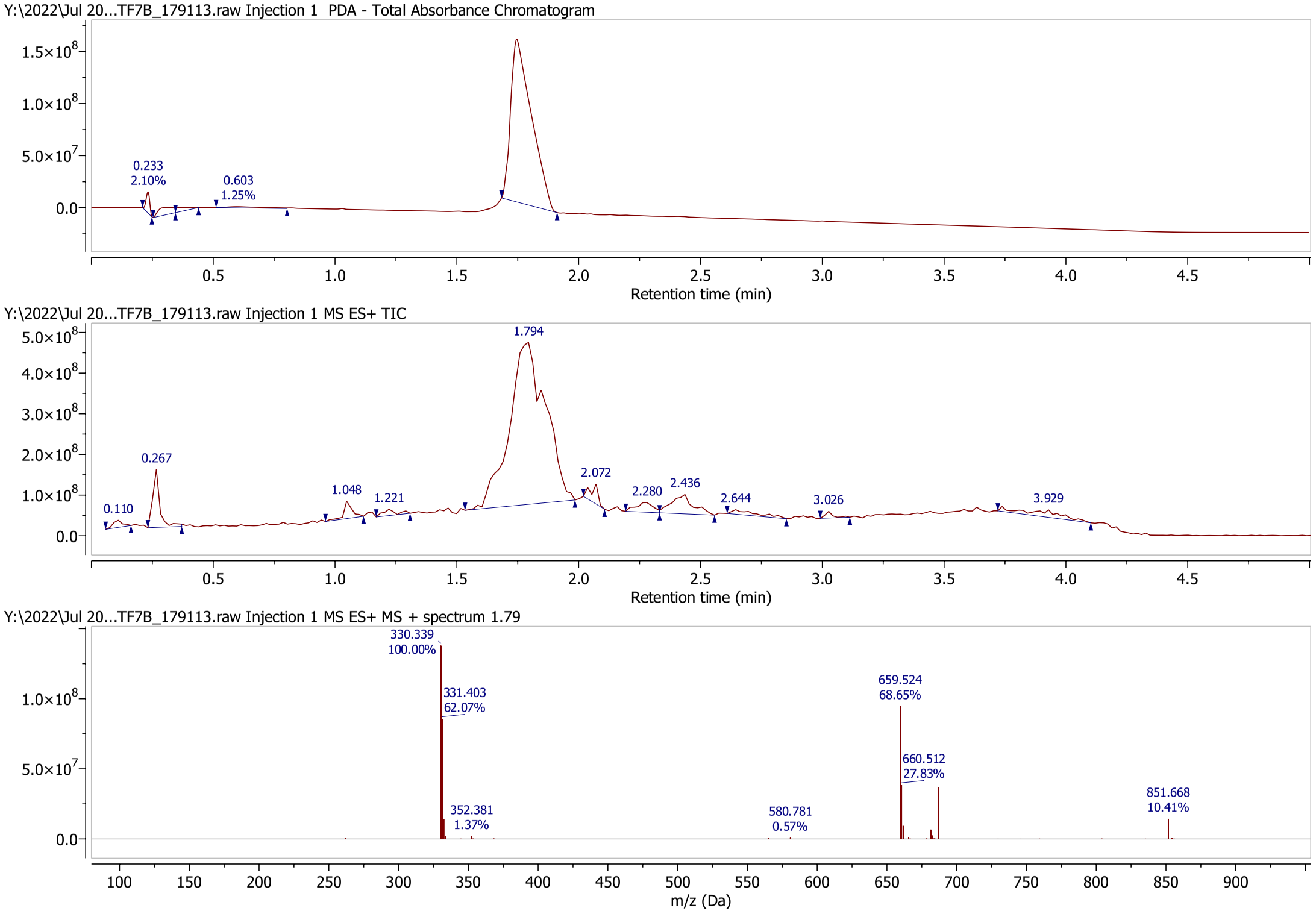
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0.603
1.25%
Retention time (min)
Y:\2022\Jul 20...TF7B_179113.raw Injection 1 MS ES+ TIC
1.794
0.267
0.110
1.048
1.221
2.072
2.280
2.436
2.644
3.026
3.929
Retention time (min)
Y:\2022\Jul 20...TF7B_179113.raw Injection 1 MS ES+ MS + spectrum 1.79
330.339
100.00%
331.403
62.07%
352.381
1.37%
580.781
0.57%
659.524
68.65%
660.512
27.83%
851.668
10.41%
m/z (Da)

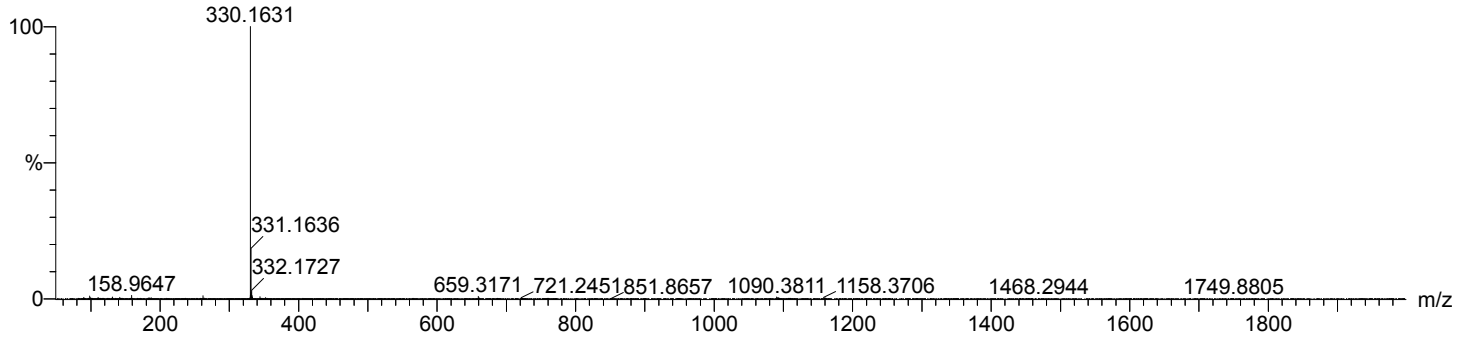
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
302 formula(e) evaluated with 2 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-8 O: 0-8

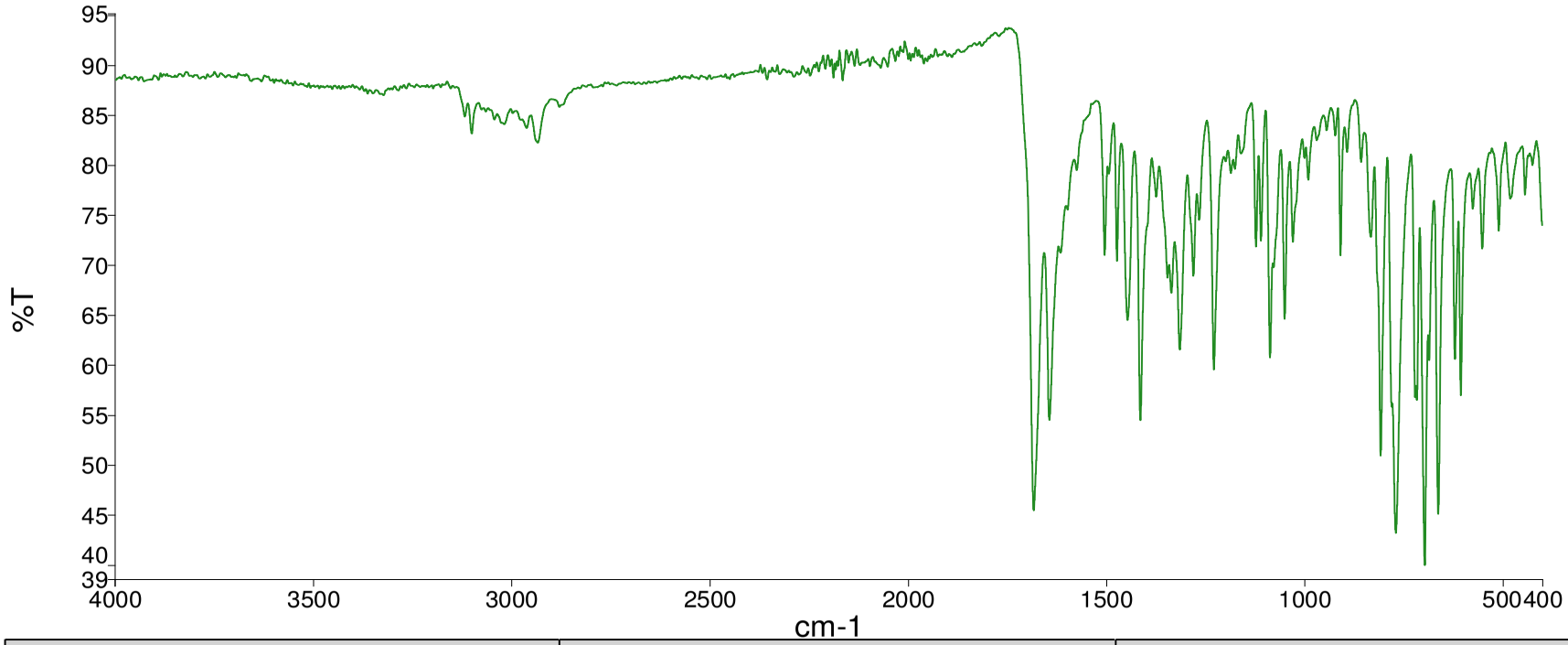
MTF_MTF7B_179351 380 (3.197) Cm (380:382)

1: TOF MS ES+
1.67e+004



Minimum:				-1.5			
Maximum:		3.0	100.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
330.1631	330.1625	0.6	1.8	0.5	280.2	0.8	C9 H24 N5 O8
	330.1606	2.5	7.6	13.5	279.9	0.6	C21 H20 N3 O

Analyst Lenny Lauchlan
Date 07 July 2022 08:07



Sample Name	Description	Quality Checks
MTF 007B	Sample 020 By Lenny Date Thursday, July 07 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

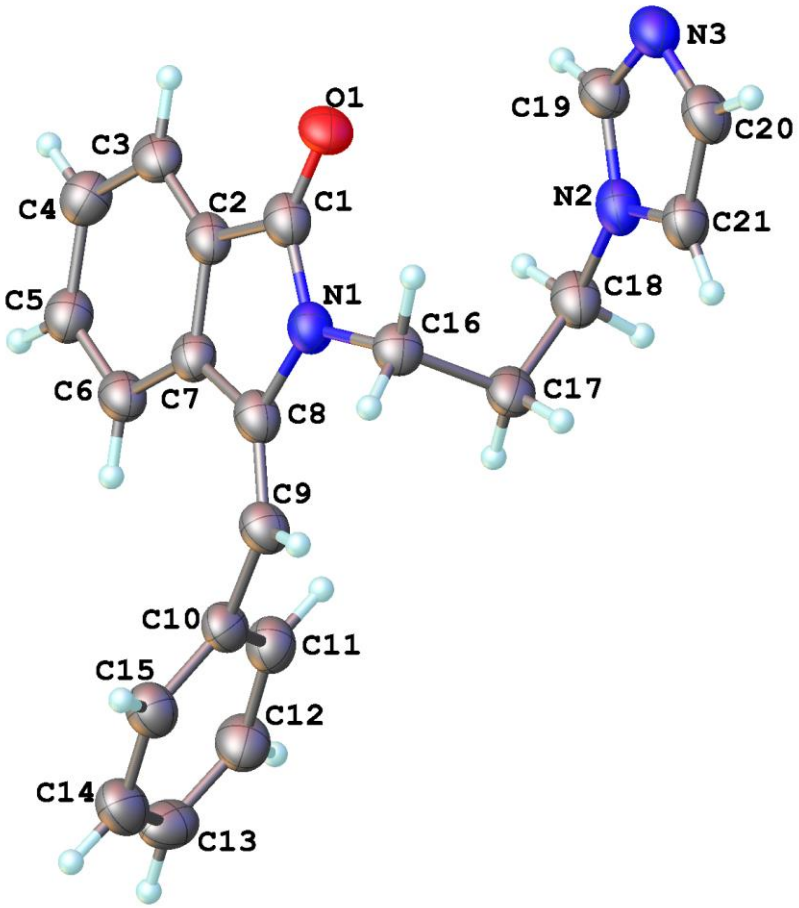


Table 1 Crystal data and structure refinement for 22srv091.	
Identification code	22srv091
Empirical formula	$C_{21}H_{19}N_3O$
Formula weight	329.39
Temperature/K	120.00
Crystal system	triclinic
Space group	P-1
a/Å	10.3572(4)
b/Å	12.0296(5)
c/Å	15.5730(6)
α/°	76.184(3)
β/°	89.161(3)
γ/°	65.778(3)
Volume/Å^3	1710.65(12)

Z	4
ρ_{calc}g/cm^3	1.279
μ/mm^{-1}	0.637
F(000)	696.0
Crystal size/mm^3	0.16 × 0.09 × 0.01
Radiation	Mo Kα (λ = 1.54178)
2Θ range for data collection/°	5.87 to 139.996
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 14, -18 ≤ l ≤ 18
Reflections collected	24922
Independent reflections	6422 [R_{int} = 0.1790, R_{sigma} = 0.1761]
Data/restraints/parameters	6422/0/452
Goodness-of-fit on F^2	0.987
Final R indexes [I>=2σ (I)]	R_1 = 0.0841, wR_2 = 0.2038
Final R indexes [all data]	R_1 = 0.1408, wR_2 = 0.2528
Largest diff. peak/hole / e Å^{-3}	0.33/-0.34

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 22srv091. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	625(3)	662(2)	1101.5(17)	40.3(7)
N2	522(4)	3680(3)	995(2)	38.5(8)
N3	-1834(4)	4516(3)	865(2)	41.5(8)
N1	2869(3)	86(3)	1740.7(19)	35.3(7)
C8	4286(4)	-746(3)	1683(2)	36.2(9)
C1	1901(4)	13(3)	1189(2)	37.5(9)
C2	2740(4)	-983(3)	744(2)	34.9(8)
C6	5191(4)	-2360(3)	689(2)	37.6(9)
C7	4176(4)	-1409(3)	1020(2)	34.1(8)
C10	6909(4)	-1578(3)	2096(2)	37.9(9)
C4	3289(4)	-2397(3)	-169(2)	40.2(9)
C21	100(4)	4482(3)	1548(2)	39.4(9)
C20	-1339(4)	4978(3)	1459(3)	43.0(10)
C5	4723(4)	-2847(3)	101(2)	38.9(9)
C11	7469(5)	-1262(3)	1299(3)	42.9(10)
C16	2500(4)	1084(3)	2207(2)	36.5(9)
C14	9273(5)	-3072(4)	2732(3)	49.4(11)
C15	7834(4)	-2482(3)	2815(3)	42.9(10)

C9	5389(4)	-866(3)	2194(2)	38.3(9)
C3	2270(4)	-1449(3)	152(2)	37.3(9)
C18	2002(4)	2940(3)	848(2)	41.4(10)
C19	-659(4)	3749(3)	601(2)	39.2(9)
C17	2917(4)	2133(3)	1719(3)	39.7(9)
C13	9828(4)	-2753(4)	1933(3)	48.2(10)
C12	8912(5)	-1841(4)	1223(3)	47.0(10)
O1A	4168(3)	-549(2)	6170.9(17)	43.4(7)
N1A	1901(3)	-51(3)	6617.5(19)	37.2(8)
N2A	4441(4)	-3684(3)	7334(2)	38.4(8)
C1A	2895(4)	96(3)	6050(2)	37.8(9)
N3A	6799(4)	-4493(3)	7529(2)	45.4(9)
C9A	-625(4)	880(3)	6748(2)	39.2(9)
C10A	-2137(4)	1719(3)	6395(2)	37.7(9)
C15A	-2810(5)	1406(4)	5802(3)	47.5(11)
C18A	3015(4)	-3000(3)	6876(2)	41.2(9)
C7A	628(4)	1623(3)	5453(2)	37.0(9)
C16A	2292(4)	-1030(3)	7452(2)	40.3(9)
C8A	500(5)	825(3)	6303(2)	40.7(10)
C20A	6271(4)	-4967(3)	8283(3)	43.9(10)
C21A	4829(4)	-4482(3)	8169(3)	41.7(9)
C2A	2048(4)	1187(3)	5299(2)	39.3(9)
C19A	5662(4)	-3736(4)	6986(3)	42.0(9)
C6A	-384(5)	2691(4)	4860(3)	45.2(10)
C17A	1959(4)	-2138(3)	7384(2)	41.2(9)
C4A	1521(5)	2823(4)	3977(3)	47.1(10)
C3A	2519(4)	1764(4)	4561(2)	41.3(9)
C14A	-4220(5)	2144(4)	5488(3)	52.1(11)
C13A	-4982(5)	3216(4)	5765(3)	56.1(12)
C5A	95(5)	3285(4)	4129(3)	48.8(10)
C11A	-2904(5)	2778(5)	6702(4)	64.3(14)
C12A	-4329(5)	3512(5)	6372(4)	72.2(17)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 22srv091. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	25.6(14)	40.3(13)	50.8(14)	-12.0(11)	8.8(11)	-9.5(10)
N2	39.0(19)	29.1(13)	43.3(16)	-7.0(12)	12.2(14)	-11.7(12)
N3	31.6(17)	35.3(15)	52.2(18)	-7.3(13)	6.8(14)	-11.0(13)
N1	34.2(17)	29.4(13)	40.7(15)	-9.5(11)	8.4(13)	-11.7(12)
C8	34(2)	30.6(16)	39.5(17)	-7.2(13)	10.8(15)	-10.1(14)
C1	35(2)	32.5(16)	41.6(18)	-8.1(14)	11.4(16)	-12.3(14)
C2	30.5(19)	29.2(15)	42.0(17)	-8.0(13)	12.6(15)	-10.4(13)
C6	31.4(19)	33.5(16)	44.1(18)	-7.5(14)	8.3(15)	-11.4(14)

C7	31.7(19)	30.1(15)	40.2(17)	-7.8(13)	9.2(15)	-13.5(14)
C10	32(2)	30.1(16)	48.9(19)	-13.9(14)	5.4(16)	-8.6(14)
C4	42(2)	40.7(18)	42.1(18)	-14.8(15)	10.7(16)	-19.6(16)
C21	40(2)	30.7(16)	44.4(18)	-10.3(14)	8.0(16)	-12.1(15)
C20	39(2)	32.3(16)	49.2(19)	-9.9(14)	11.2(17)	-6.8(15)
C5	38(2)	35.3(17)	45.7(19)	-13.5(14)	13.2(16)	-15.8(15)
C11	42(2)	36.4(18)	50(2)	-12.0(15)	10.3(17)	-15.5(16)
C16	33(2)	35.8(17)	39.6(17)	-13.0(14)	12.1(15)	-12.0(14)
C14	42(2)	38.2(19)	61(2)	-15.9(17)	1.9(19)	-8.7(17)
C15	41(2)	38.3(18)	45.4(19)	-11.6(15)	5.4(16)	-12.4(16)
C9	34(2)	34.6(17)	41.9(18)	-10.6(14)	7.2(15)	-9.2(14)
C3	30.0(19)	36.7(17)	44.3(18)	-7.4(14)	9.2(15)	-14.8(14)
C18	37(2)	35.8(17)	48.2(19)	-9.6(15)	14.9(17)	-12.8(15)
C19	33(2)	36.1(17)	43.4(19)	-8.0(14)	4.7(16)	-11.1(15)
C17	28.7(19)	33.3(17)	54(2)	-12.4(15)	10.1(16)	-9.7(14)
C13	30(2)	51(2)	69(3)	-32(2)	9.8(18)	-13.1(16)
C12	38(2)	42.9(19)	60(2)	-16.8(17)	15.4(19)	-15.2(16)
O1A	34.3(15)	42.3(14)	49.3(14)	-11.1(11)	10.0(12)	-12.3(11)
N1A	35.9(18)	33.1(14)	41.2(15)	-11.1(12)	11.1(13)	-12.3(12)
N2A	35.4(18)	33.8(14)	46.7(16)	-12.9(12)	8.6(14)	-13.9(12)
C1A	36(2)	34.8(17)	45.6(19)	-13.8(14)	13.8(16)	-16.7(15)
N3A	37.5(19)	39.4(16)	53.7(18)	-11.7(14)	10.5(15)	-11.0(13)
C9A	38(2)	35.9(17)	40.6(17)	-9.9(14)	9.9(16)	-12.7(15)
C10A	37(2)	32.7(17)	45.2(18)	-10.9(14)	13.0(16)	-16.2(15)
C15A	52(3)	46(2)	47(2)	-18.7(17)	11.6(19)	-19.8(18)
C18A	34(2)	38.7(18)	49(2)	-13.7(15)	7.9(16)	-11.4(15)
C7A	36(2)	35.7(17)	42.6(18)	-12.3(14)	9.6(15)	-16.9(14)
C16A	35(2)	36.6(18)	46.1(19)	-10.7(15)	10.9(16)	-11.8(15)
C8A	45(2)	32.7(17)	42.8(18)	-12.3(14)	13.8(17)	-12.9(15)
C20A	40(2)	37.6(18)	44.5(19)	-5.6(15)	7.9(16)	-10.3(16)
C21A	41(2)	33.0(17)	48.6(19)	-9.4(15)	11.5(17)	-13.4(15)
C2A	38(2)	39.6(18)	45.4(19)	-18.3(15)	9.1(16)	-16.8(15)
C19A	35(2)	41.5(19)	53(2)	-14.9(16)	12.6(17)	-18.3(15)
C6A	38(2)	46(2)	50(2)	-10.1(17)	10.5(18)	-17.4(17)
C17A	35(2)	35.7(17)	45.1(19)	-5.8(15)	7.0(16)	-10.2(15)
C4A	47(3)	52(2)	43.2(19)	-6.6(16)	12.7(18)	-25.1(18)
C3A	35(2)	49(2)	46.2(19)	-17.6(16)	12.2(16)	-21.3(16)
C14A	51(3)	61(3)	49(2)	-16.0(19)	6(2)	-27(2)
C13A	39(2)	54(2)	69(3)	-12(2)	5(2)	-14.5(19)
C5A	46(2)	50(2)	50(2)	-6.2(17)	6.8(19)	-24.2(18)
C11A	43(3)	61(3)	97(4)	-47(3)	10(3)	-15(2)
C12A	45(3)	55(3)	114(4)	-45(3)	7(3)	-6(2)

Table 4 Bond Lengths for 22srv091.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
O1	C1	1.218(5)		O1A	C1A	1.214(5)
N2	C21	1.380(4)		N1A	C1A	1.386(5)
N2	C18	1.471(4)		N1A	C16A	1.461(5)
N2	C19	1.340(6)		N1A	C8A	1.406(5)
N3	C20	1.387(6)		N2A	C18A	1.456(5)
N3	C19	1.321(4)		N2A	C21A	1.370(5)
N1	C8	1.414(4)		N2A	C19A	1.352(5)
N1	C1	1.372(6)		C1A	C2A	1.487(5)
N1	C16	1.466(4)		N3A	C20A	1.386(5)
C8	C7	1.477(5)		N3A	C19A	1.309(6)
C8	C9	1.340(6)		C9A	C10A	1.495(5)
C1	C2	1.482(4)		C9A	C8A	1.333(5)
C2	C7	1.396(5)		C10A	C15A	1.372(6)
C2	C3	1.373(6)		C10A	C11A	1.389(5)
C6	C7	1.400(4)		C15A	C14A	1.382(6)
C6	C5	1.384(6)		C18A	C17A	1.526(4)
C10	C11	1.399(5)		C7A	C8A	1.478(5)
C10	C15	1.396(6)		C7A	C2A	1.383(5)
C10	C9	1.478(5)		C7A	C6A	1.400(6)
C4	C5	1.388(6)		C16A	C17A	1.534(6)
C4	C3	1.390(4)		C20A	C21A	1.358(6)
C21	C20	1.354(6)		C2A	C3A	1.386(5)
C11	C12	1.383(6)		C6A	C5A	1.392(5)
C16	C17	1.530(5)		C4A	C3A	1.383(6)
C14	C15	1.382(6)		C4A	C5A	1.388(6)
C14	C13	1.399(6)		C14A	C13A	1.375(6)
C18	C17	1.528(5)		C13A	C12A	1.361(8)
C13	C12	1.387(6)		C11A	C12A	1.399(7)

Table 5 Bond Angles for 22srv091.								
Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C21	N2	C18	125.4(4)		C1A	N1A	C16A	122.6(3)
C19	N2	C21	107.3(3)		C1A	N1A	C8A	113.2(3)
C19	N2	C18	127.3(3)		C8A	N1A	C16A	124.2(3)
C19	N3	C20	103.6(4)		C21A	N2A	C18A	127.2(3)
C8	N1	C16	123.1(3)		C19A	N2A	C18A	126.3(3)
C1	N1	C8	113.0(3)		C19A	N2A	C21A	106.3(4)
C1	N1	C16	122.9(3)		O1A	C1A	N1A	125.6(4)
N1	C8	C7	104.8(3)		O1A	C1A	C2A	129.8(3)
C9	C8	N1	122.6(3)		N1A	C1A	C2A	104.6(3)
C9	C8	C7	132.5(3)		C19A	N3A	C20A	104.0(3)
O1	C1	N1	125.1(3)		C8A	C9A	C10A	124.8(3)

O1	C1	C2	129.2(4)		C15A	C10A	C9A	120.0(3)
N1	C1	C2	105.7(3)		C15A	C10A	C11A	119.1(4)
C7	C2	C1	108.2(4)		C11A	C10A	C9A	120.8(4)
C3	C2	C1	128.9(4)		C10A	C15A	C14A	121.1(4)
C3	C2	C7	122.9(3)		N2A	C18A	C17A	113.3(3)
C5	C6	C7	118.4(4)		C2A	C7A	C8A	108.3(3)
C2	C7	C8	108.3(3)		C2A	C7A	C6A	120.0(3)
C2	C7	C6	119.0(4)		C6A	C7A	C8A	131.7(4)
C6	C7	C8	132.6(4)		N1A	C16A	C17A	112.2(3)
C11	C10	C9	119.8(3)		N1A	C8A	C7A	104.9(3)
C15	C10	C11	118.8(4)		C9A	C8A	N1A	123.7(3)
C15	C10	C9	121.1(3)		C9A	C8A	C7A	131.3(4)
C5	C4	C3	120.9(4)		C21A	C20A	N3A	110.5(4)
C20	C21	N2	105.0(4)		C20A	C21A	N2A	106.1(3)
C21	C20	N3	111.3(3)		C7A	C2A	C1A	109.0(3)
C6	C5	C4	121.4(3)		C7A	C2A	C3A	122.2(4)
C12	C11	C10	120.6(4)		C3A	C2A	C1A	128.8(4)
N1	C16	C17	111.5(3)		N3A	C19A	N2A	113.2(4)
C15	C14	C13	120.5(4)		C5A	C6A	C7A	117.7(4)
C14	C15	C10	120.5(4)		C18A	C17A	C16A	113.1(3)
C8	C9	C10	126.0(3)		C3A	C4A	C5A	120.6(4)
C2	C3	C4	117.4(4)		C4A	C3A	C2A	117.9(4)
N2	C18	C17	112.0(3)		C13A	C14A	C15A	120.5(5)
N3	C19	N2	112.7(4)		C12A	C13A	C14A	118.6(5)
C18	C17	C16	113.9(4)		C4A	C5A	C6A	121.6(4)
C12	C13	C14	119.0(4)		C10A	C11A	C12A	118.7(5)
C11	C12	C13	120.6(4)		C13A	C12A	C11A	122.0(4)

Table 6 Selected Torsion Angles for 22srv091.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
C8	C9	C10	C11	58.6(6)		C10A	C9A	C8A	N1A	-174.1(4)
C8	C9	C10	C15	-127.7(4)		C10A	C9A	C8A	C7A	9.3(7)
C7	C8	C9	C10	13.0(7)		C15A	C10A	C9A	C8A	77.4(5)
C10	C9	C8	N1	-171.3(3)		C18A	C17A	C16A	N1A	75.4(4)
C16	C17	C18	N2	66.4(4)		C16A	C17A	C18A	N2A	67.0(4)
C18	C17	C16	N1	70.6(4)		C8A	C9A	C10A	C11A	-106.6(5)
C17	C16	N1	C8	69.3(4)		C17A	C18A	N2A	C21A	57.6(5)
C17	C16	N1	C1	-98.5(4)		C17A	C18A	N2A	C19A	-128.4(4)
C17	C18	N2	C21	53.8(5)		C17A	C16A	N1A	C1A	-103.0(4)
C17	C18	N2	C19	-129.1(4)		C17A	C16A	N1A	C8A	76.5(4)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv091.				
Atom	***x***	***y***	***z***	**U(eq)**
H6	6176.14	-2663.6	862.11	45
H4	2999.5	-2741.29	-578.34	48
H21	690.85	4649.63	1912.05	47
H20	-1932.64	5567.1	1765.19	52
H5	5397.92	-3502.8	-121.52	47
H11	6852.68	-645.19	805.71	51
H16A	2993.65	718.32	2814.61	44
H16B	1463.08	1443.59	2260.28	44
H14	9889.19	-3699.4	3221.74	59
H15	7472.24	-2693.74	3364.36	51
H9	5173.24	-455.18	2662.49	46
H3	1287.48	-1135.78	-31.52	45
H18A	2411.98	3519.05	532.17	50
H18B	2017.7	2385.56	465.29	50
H19	-652.64	3293.99	177.73	47
H17A	2845.08	2686.08	2113.97	48
H17B	3923.06	1749.81	1591.89	48
H13	10817.73	-3153.87	1878.28	58
H12	9278.59	-1612.04	679.74	56
H9A	-453.58	347.76	7331.85	47
H15A	-2297.6	669.45	5603.19	57
H18C	2661.97	-3614.8	6779.19	49
H18D	3061.23	-2485.96	6286.67	49
H16C	1769.17	-661.05	7924.75	48
H16D	3321.91	-1345.25	7622.58	48
H20A	6836.91	-5548.43	8806.63	53
H21A	4214.26	-4660.43	8584.06	50
H19A	5691.9	-3271.37	6405.6	50
H6A	-1365.16	2999.86	4952.41	54
H17C	1966.44	-2640.02	7990.16	49
H17D	991.27	-1803.75	7082.7	49
H4A	1815.01	3239.1	3466.55	56
H3A	3496.95	1442.49	4459.97	50
H14A	-4665.67	1910.2	5077.99	62
H13A	-5943.72	3737.66	5538.73	67
H5A	-569.15	4023.49	3725.85	59
H11A	-2470.45	2998.6	7127.41	77
H12A	-4856.06	4239.28	6576.82	87

Refinement model description

Number of restraints - 0, number of constraints - unknown.

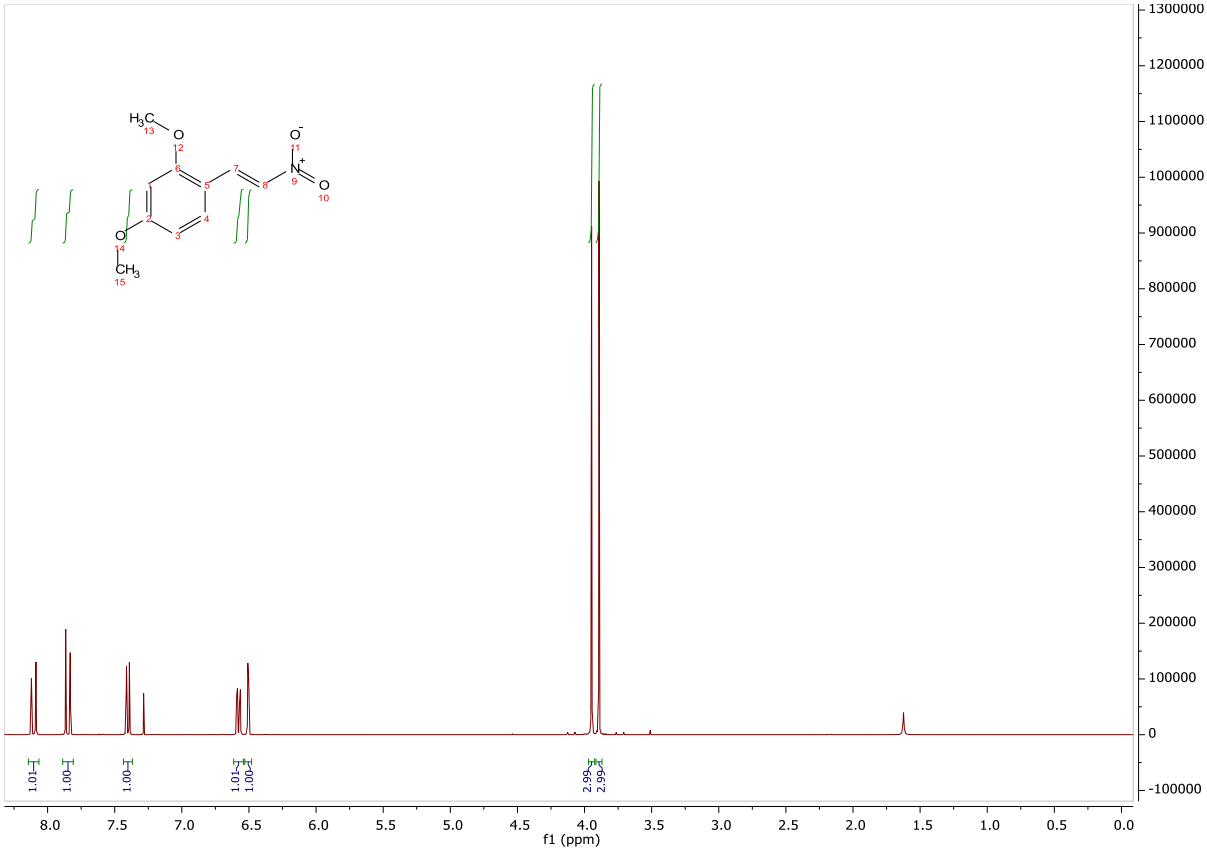
Details:

1. Fixed Uiso
At 1.2 times of: All C(H) groups, All C(H,H) groups
2.a Secondary CH2 refined with riding coordinates:
C16(H16A,H16B), C18(H18A,H18B), C17(H17A,H17B), C18A(H18C,H18D), C16A(H16C, H16D), C17A(H17C,H17D)
2.b Aromatic/amide H refined with riding coordinates:
C6(H6), C4(H4), C21(H21), C20(H20), C5(H5), C11(H11), C14(H14), C15(H15), C9(H9), C3(H3), C19(H19), C13(H13), C12(H12), C9A(H9A), C15A(H15A), C20A(H20A), C21A(H21A), C19A(H19A), C6A(H6A), C4A(H4A), C3A(H3A), C14A(H14A), C13A(H13A), C5A(H5A), C11A(H11A), C12A(H12A)

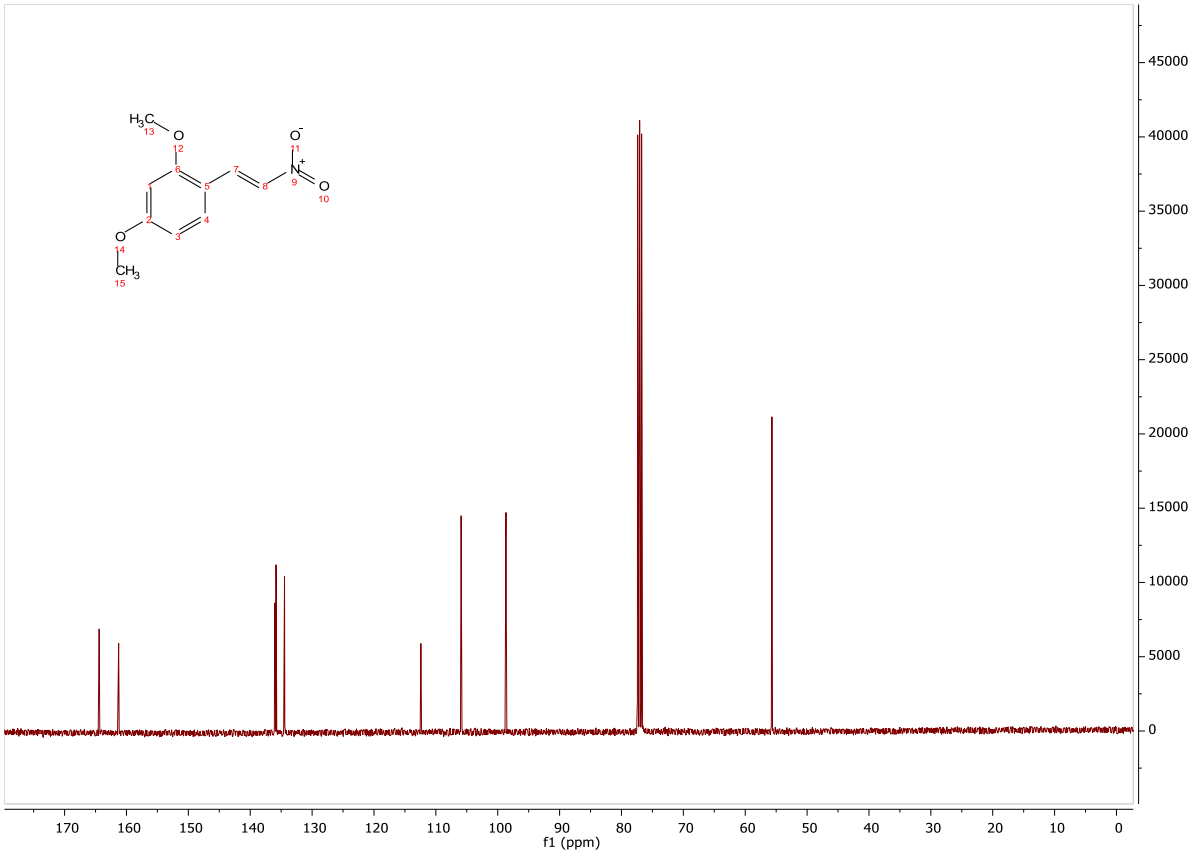
Synthesis of β-nitrostyrenes 88c-88k via the Henry reaction

(*E*)-2,4-dimethoxy-1-(2-nitrovinyl)benzene **88c**

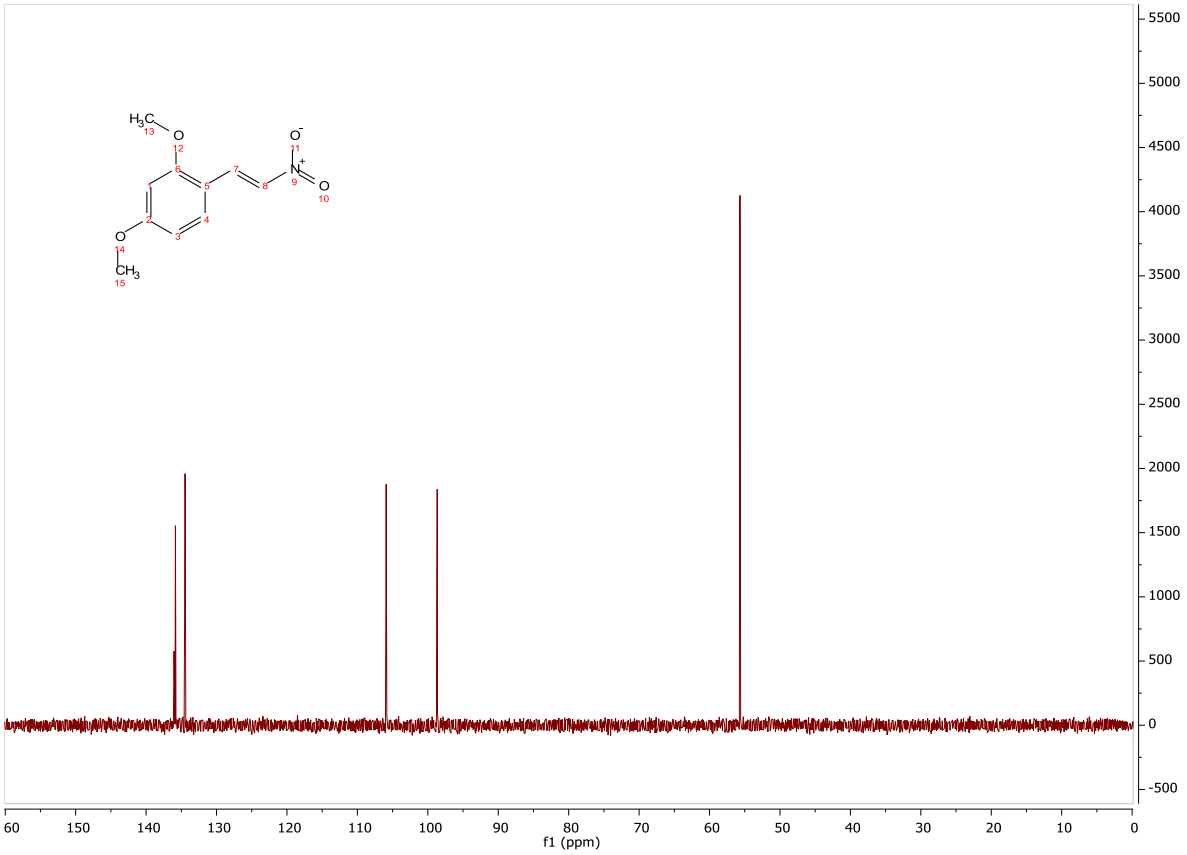
^{1}H:



^{13}C:



DEPT-135: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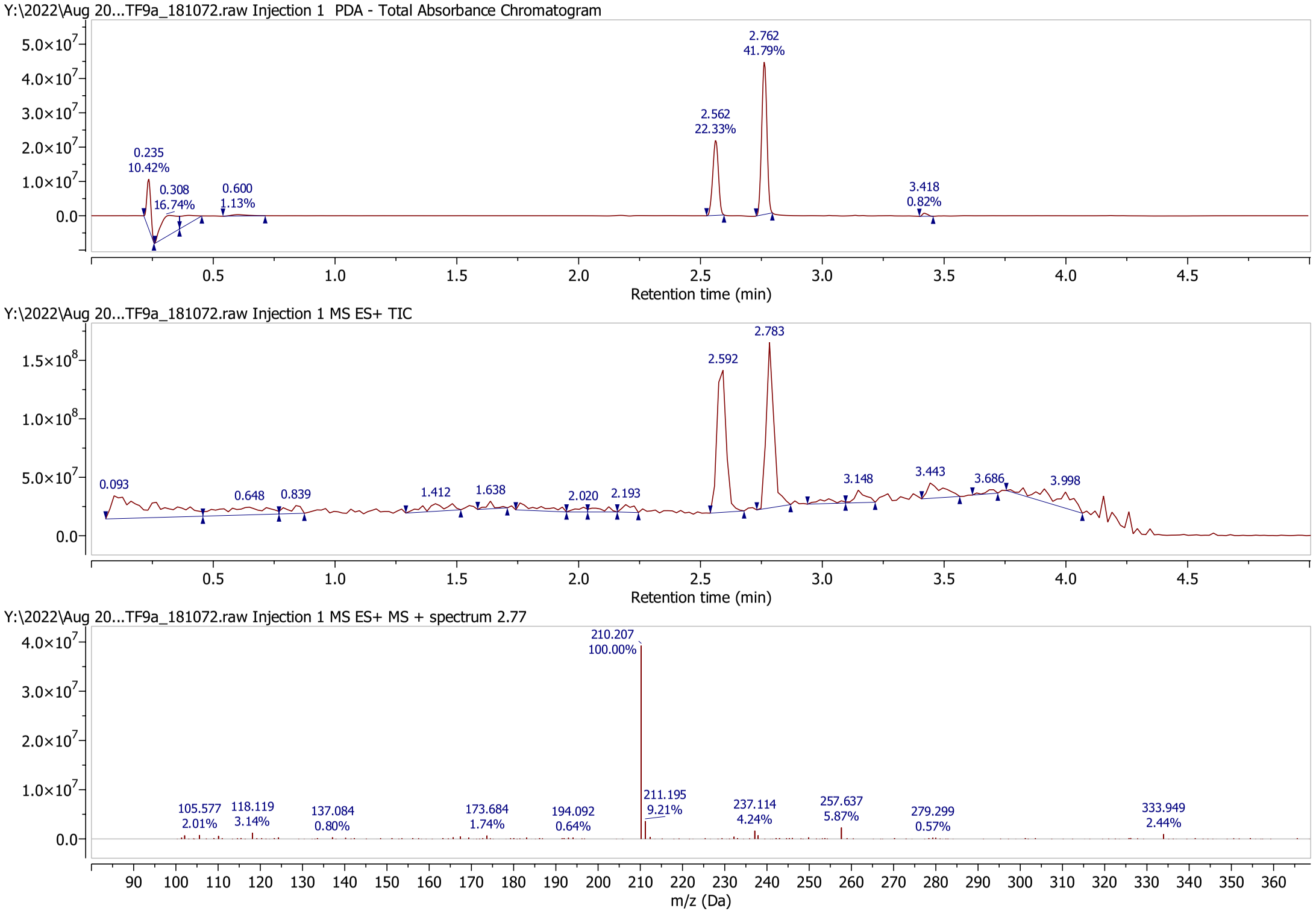
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16.74%
0.600
1.13%
2.562
22.33%
2.762
41.79%
3.418
0.82%
Retention time (min)
Y:\2022\Aug 20...TF9a_181072.raw Injection 1 MS ES+ TIC
0.093
0.648
0.839
1.412
1.638
2.020
2.193
2.592
2.783
3.148
3.443
3.686
3.998
Retention time (min)
Y:\2022\Aug 20...TF9a_181072.raw Injection 1 MS ES+ MS + spectrum 2.77
210.207
100.00%
105.577
2.01%
118.119
3.14%
137.084
0.80%
173.684
1.74%
194.092
0.64%
211.195
9.21%
237.114
4.24%
257.637
5.87%
279.299
0.57%
333.949
2.44%
m/z (Da)

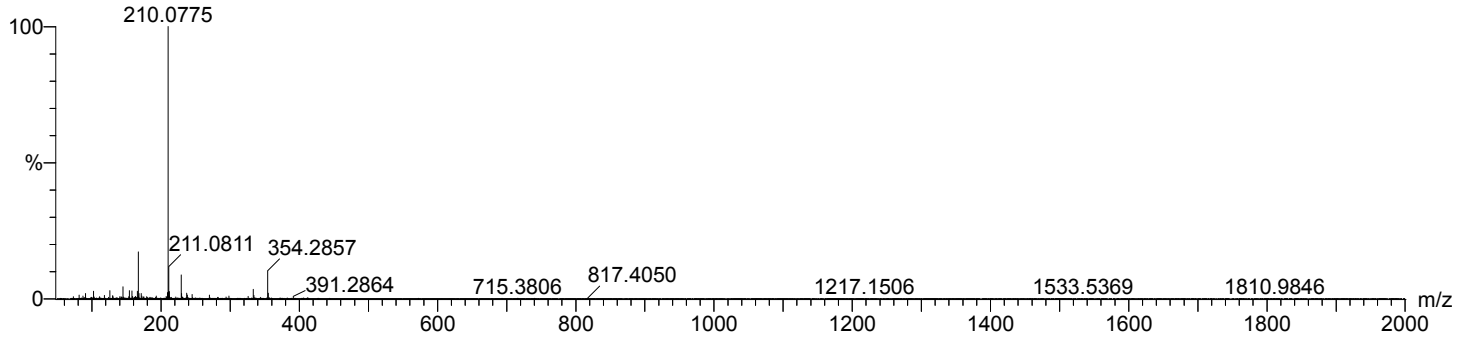
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
657 formula(e) evaluated with 7 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3

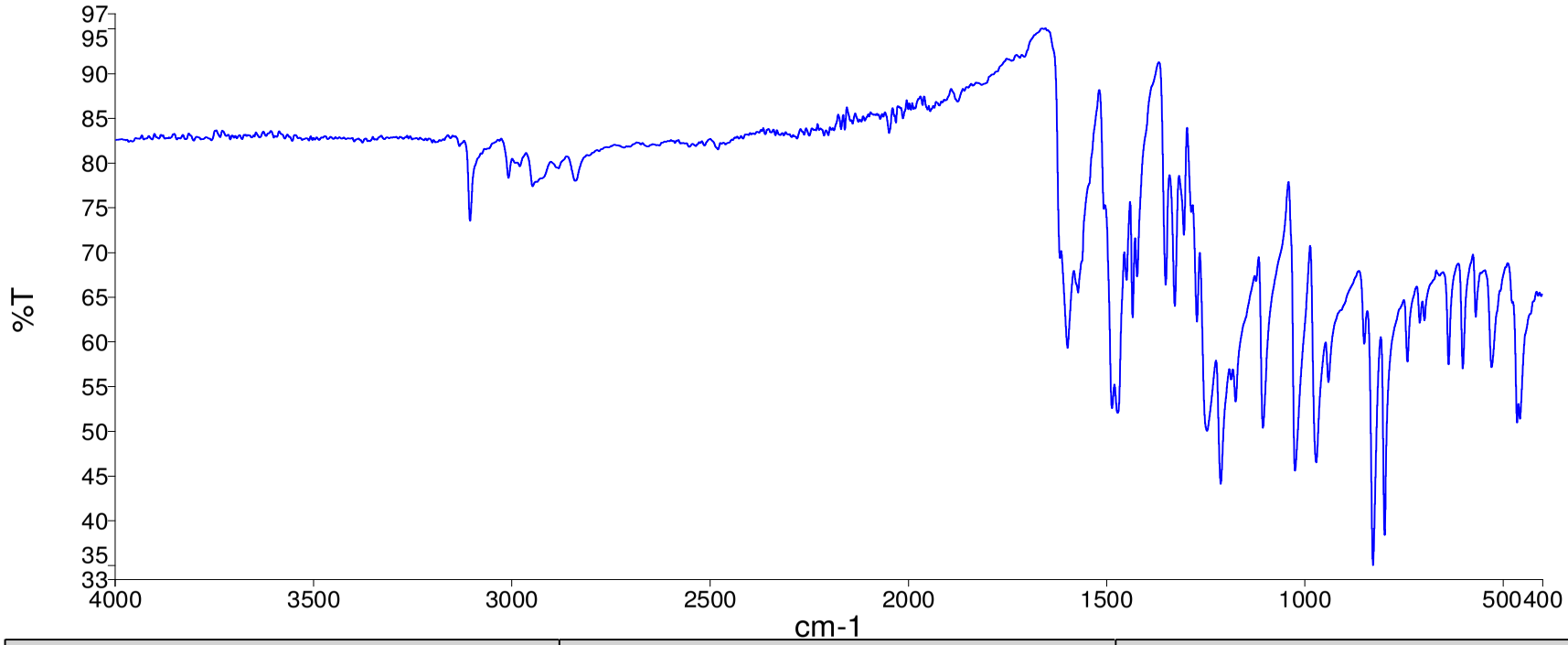
MTF9a 429 (3.638) Cm (429:432)

1: TOF MS ES+
1.19e+004



Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
210.0775	210.0778	-0.3	-1.4	1.5	225.4	1.5	C7 H13 N O5 F
	210.0780	-0.5	-2.4	10.5	228.0	4.2	C11 H8 N5
	210.0766	0.9	4.3	5.5	224.2	0.3	C10 H12 N O4
	210.0762	1.3	6.2	-1.5	237.8	13.9	H10 N7 O4 F2
	210.0791	-1.6	-7.6	6.5	228.6	4.7	C8 H9 N5 O F
	210.0751	2.4	11.4	2.5	233.8	9.9	C3 H9 N7 O3 F
	210.0803	-2.8	-13.3	2.5	231.4	7.5	C5 H10 N5 O2 F2

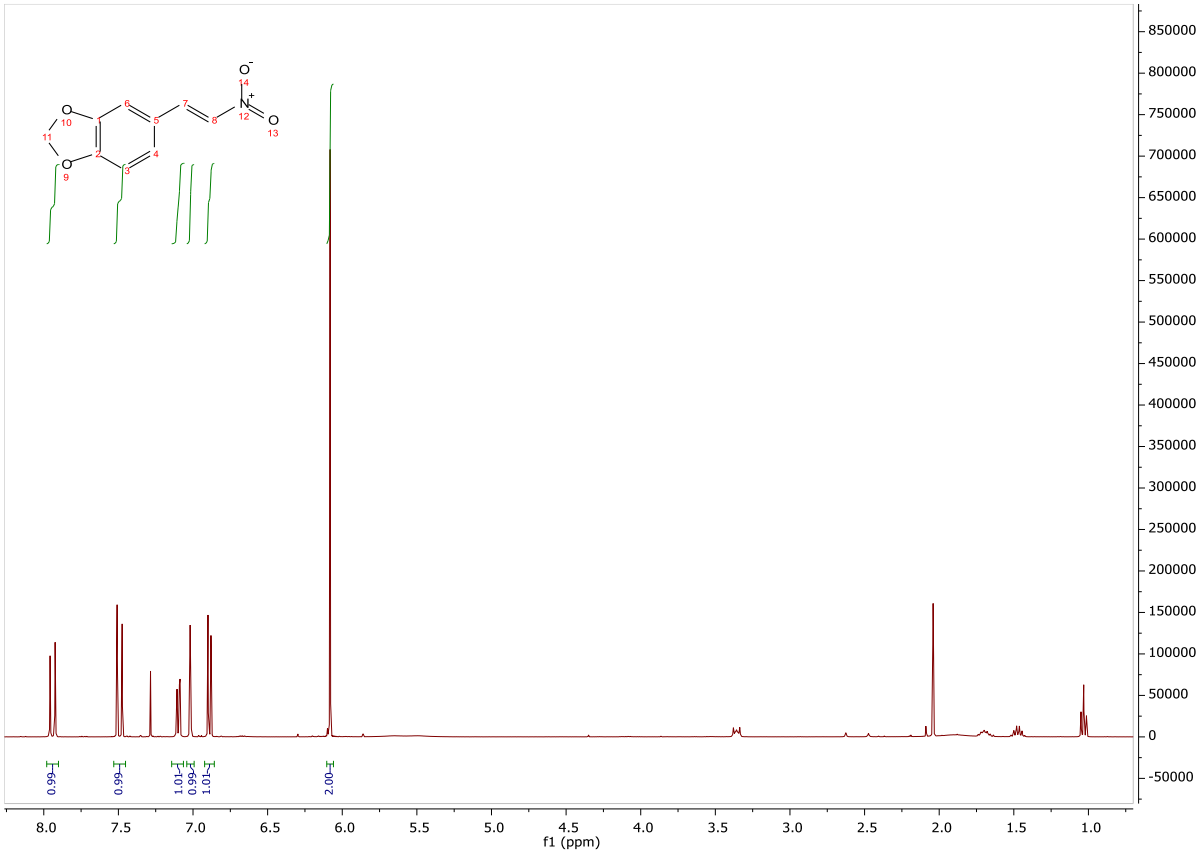
Analyst Lenny Lauchlan
Date 31 August 2022 08:00



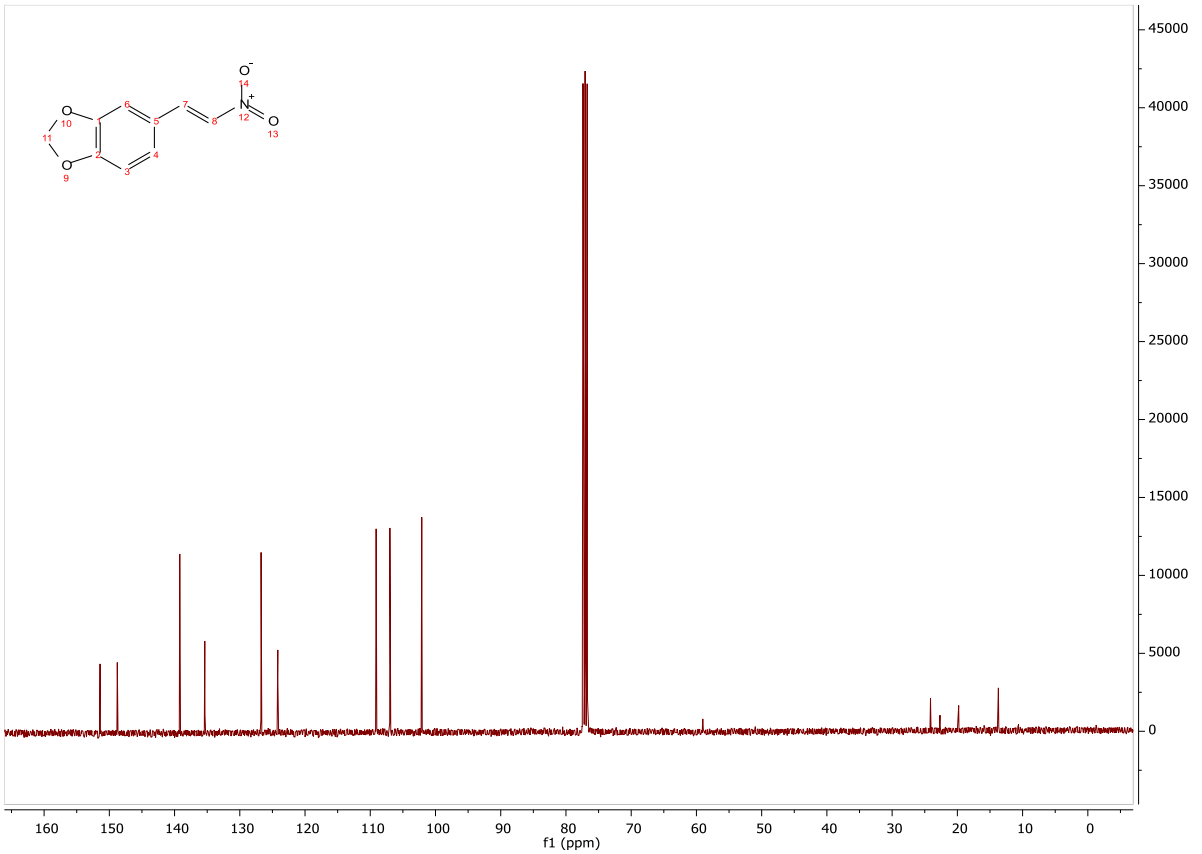
Sample Name	Description	Quality Checks
MTF 9a	Sample 018 By Lenny Date Wednesday, August 31 2022	The Quality Checks do not report any warnings for the sample.

(*E*)-5-(2-nitrovinyl)benzo[*d*][1,3]dioxole **88d**

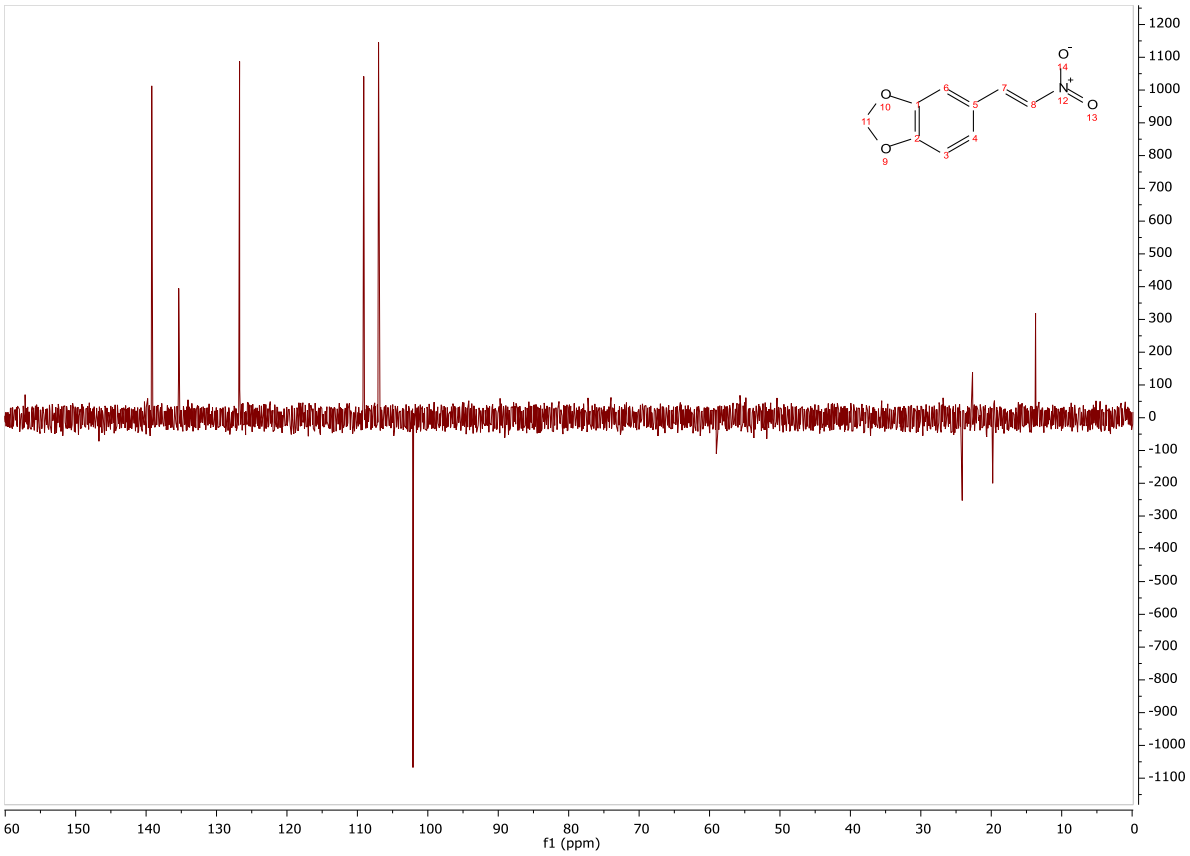
^{1}H:

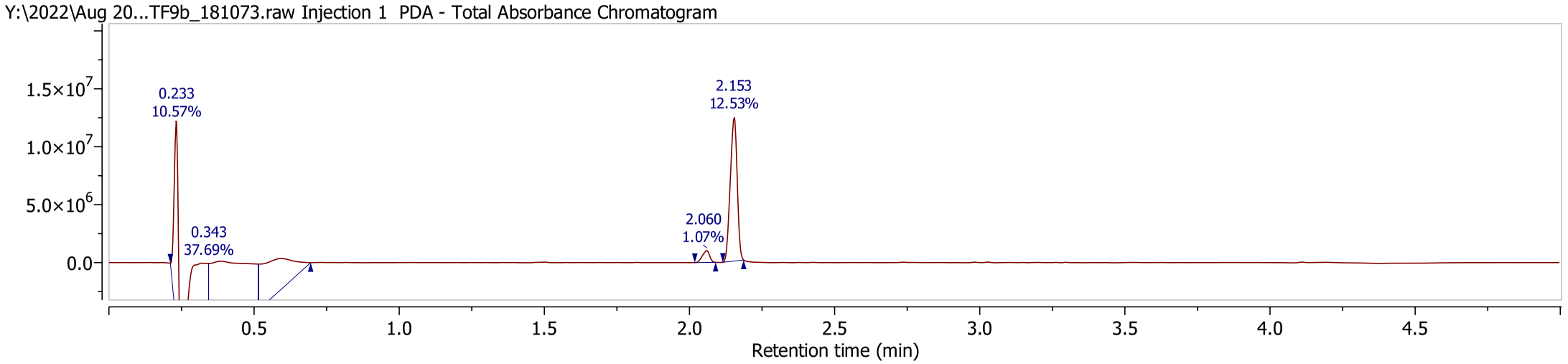


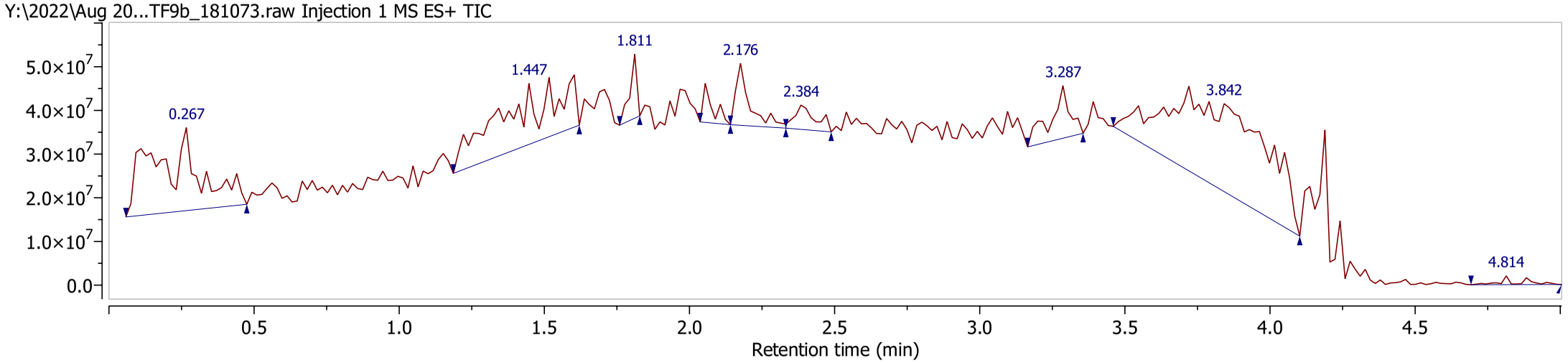
^{13}C:

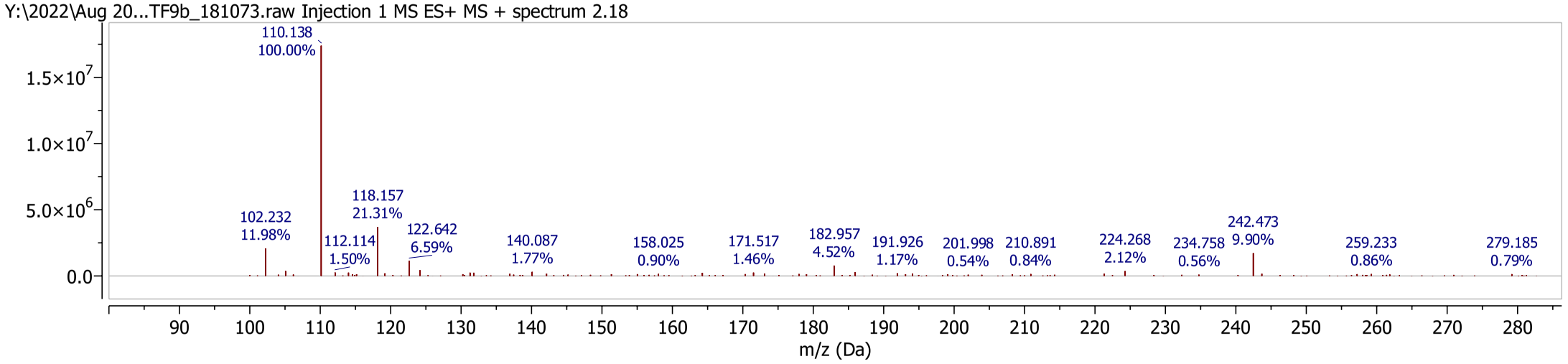


DEPT-135:


1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
-300
-400
-500
-600
-700
-800
-900
-1000
-1100
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Y:\2022\Aug 20...TF9b_181073.raw Injection 1 PDA - Total Absorbance Chromatogram
0.233
10.57%
0.343
37.69%
2.060
1.07%
2.153
12.53%
Retention time (min)


Y:\2022\Aug 20...TF9b_181073.raw Injection 1 MS ES+ TIC
0.267
1.447
1.811
2.176
2.384
3.287
3.842
4.814
Retention time (min)


Y:\2022\Aug 20...TF9b_181073.raw Injection 1 MS ES+ MS + spectrum 2.18
110.138
100.00%
102.232
11.98%
112.114
1.50%
118.157
21.31%
122.642
6.59%
140.087
1.77%
158.025
0.90%
171.517
1.46%
182.957
4.52%
191.926
1.17%
201.998
0.54%
210.891
0.84%
224.268
2.12%
234.758
0.56%
242.473
9.90%
259.233
0.86%
279.185
0.79%
m/z (Da)

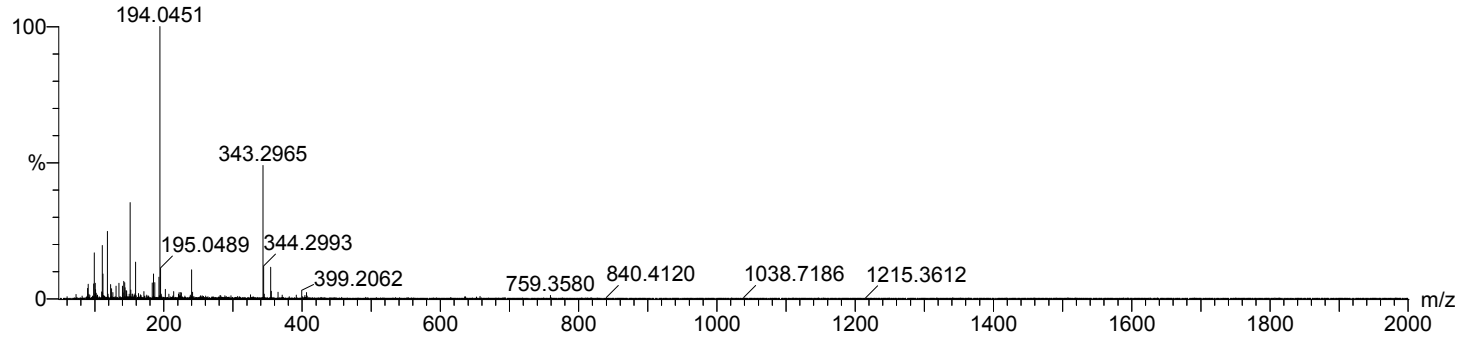
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
548 formula(e) evaluated with 9 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3

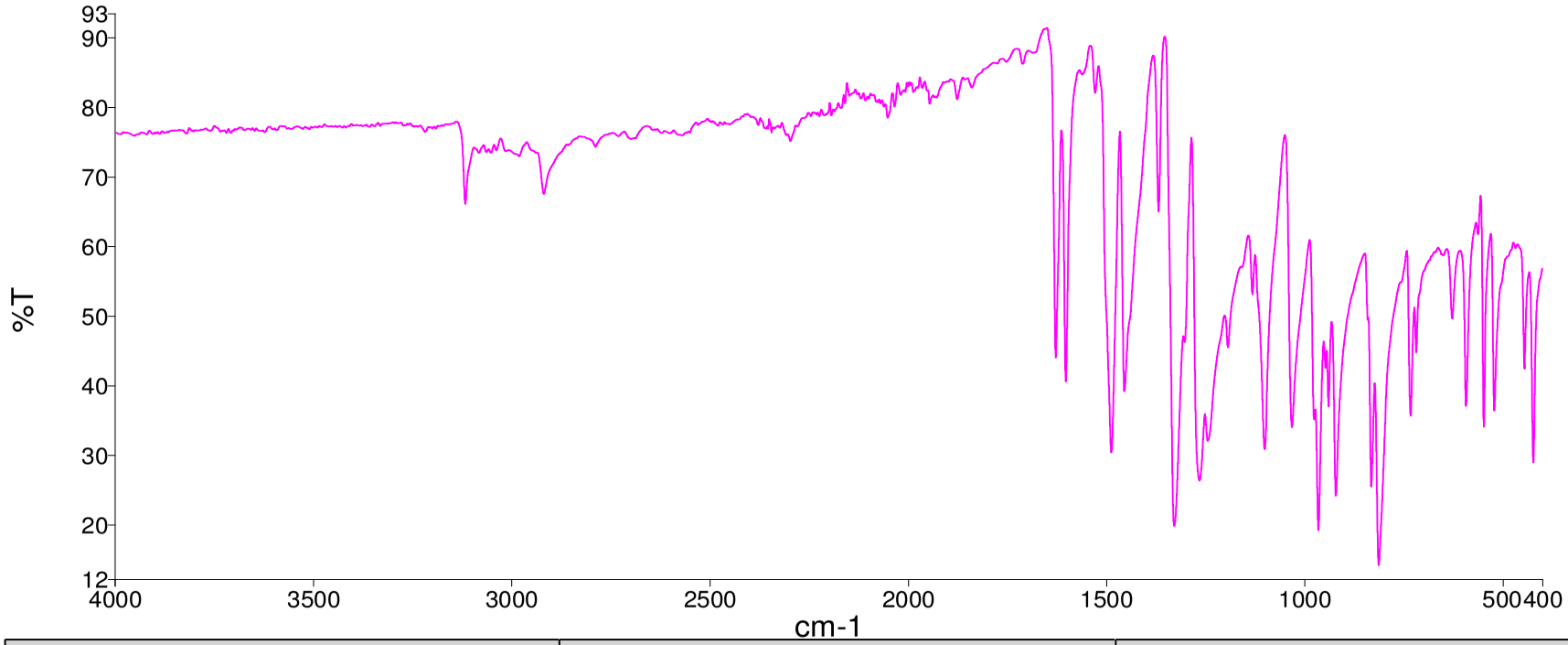
MTF9b 418 (3.541) Cm (416:420)

1: TOF MS ES+
1.20e+003



Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
194.0451	194.0453	-0.2	-1.0	6.5	118.1	0.1	C9 H8 N O4
	194.0438	1.3	6.7	3.5	127.6	9.6	C2 H5 N7 O3 F
	194.0465	-1.4	-7.2	2.5	122.2	4.1	C6 H9 N O5 F
	194.0467	-1.6	-8.2	11.5	121.5	3.5	C10 H4 N5
	194.0429	2.2	11.3	3.5	123.0	5.0	C7 H7 N O2 F3
	194.0476	-2.5	-12.9	-1.5	126.0	8.0	C3 H10 N O6 F2
	194.0426	2.5	12.9	7.5	124.9	6.8	C5 H4 N7 O2
	194.0425	2.6	13.4	-1.5	128.6	10.6	C H9 N3 O7 F
	194.0478	-2.7	-13.9	7.5	123.1	5.1	C7 H5 N5 O F

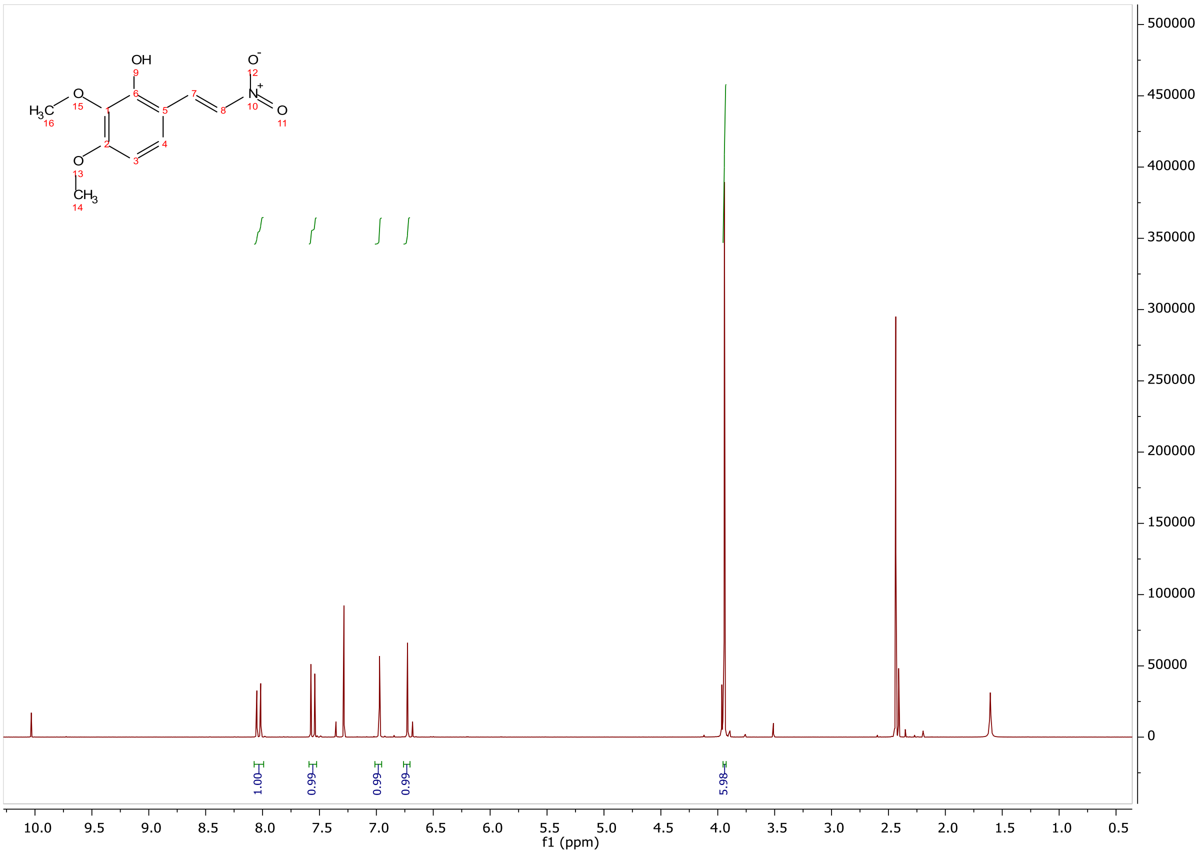
Analyst Lenny Lauchlan
Date 31 August 2022 08:02



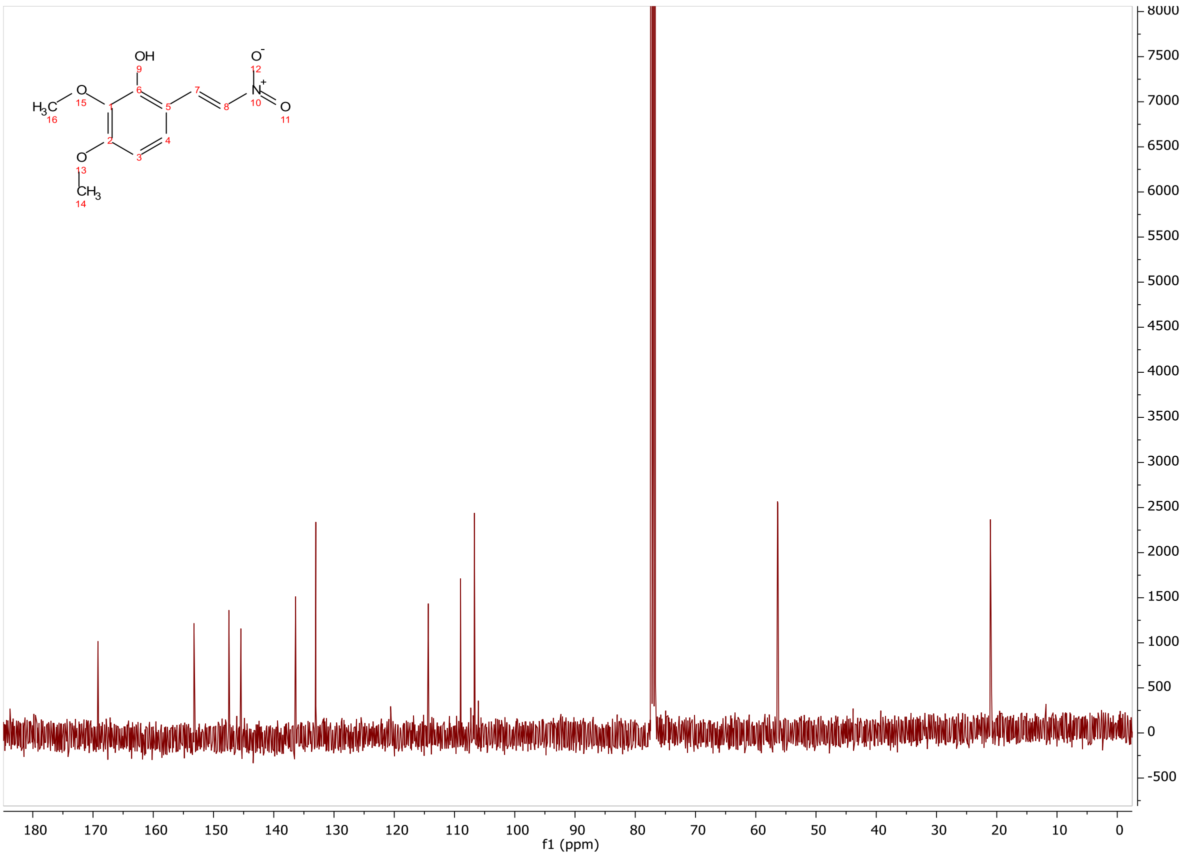
Sample Name	Description	Quality Checks
MTF 9b	Sample 019 By Lenny Date Wednesday, August 31 2022	The Quality Checks do not report any warnings for the sample.

(*E*)-2,3-dimethoxy-6-(2-nitrovinyl)phenol **88e**

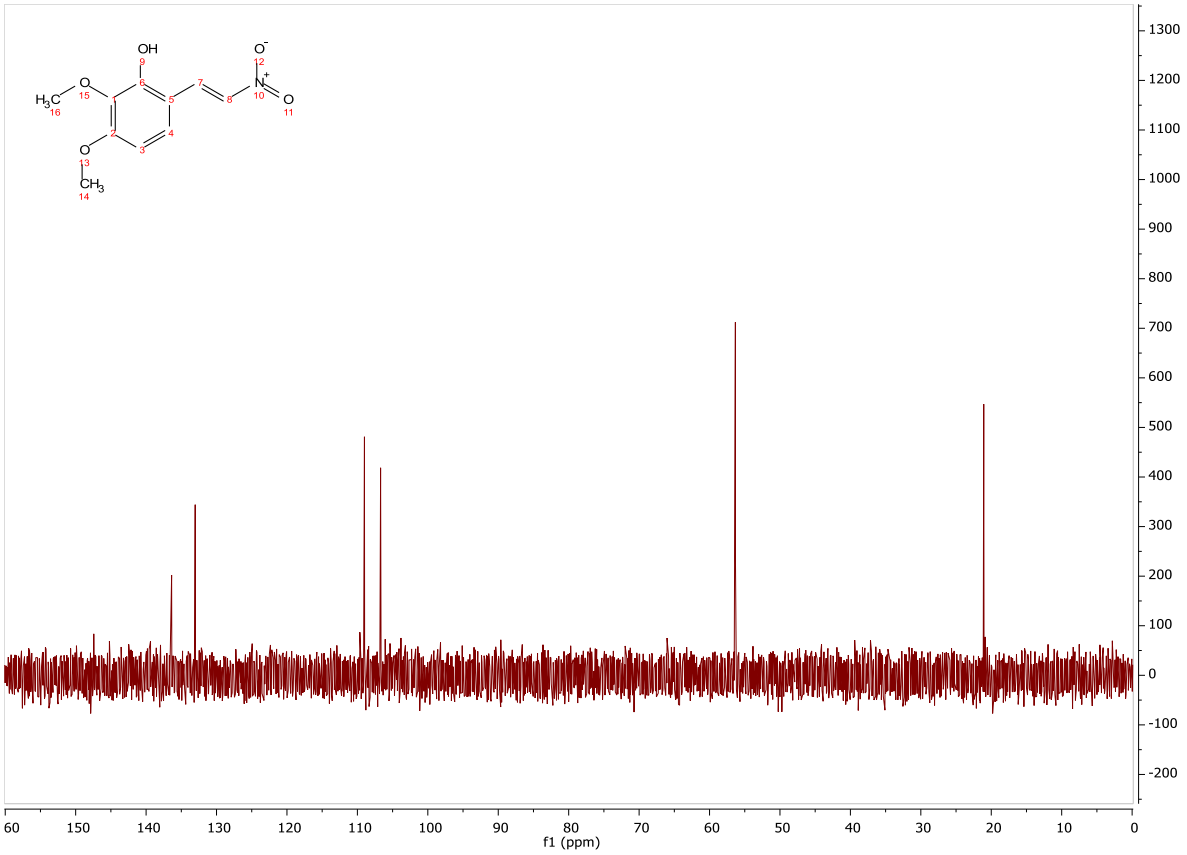
^{1}H:

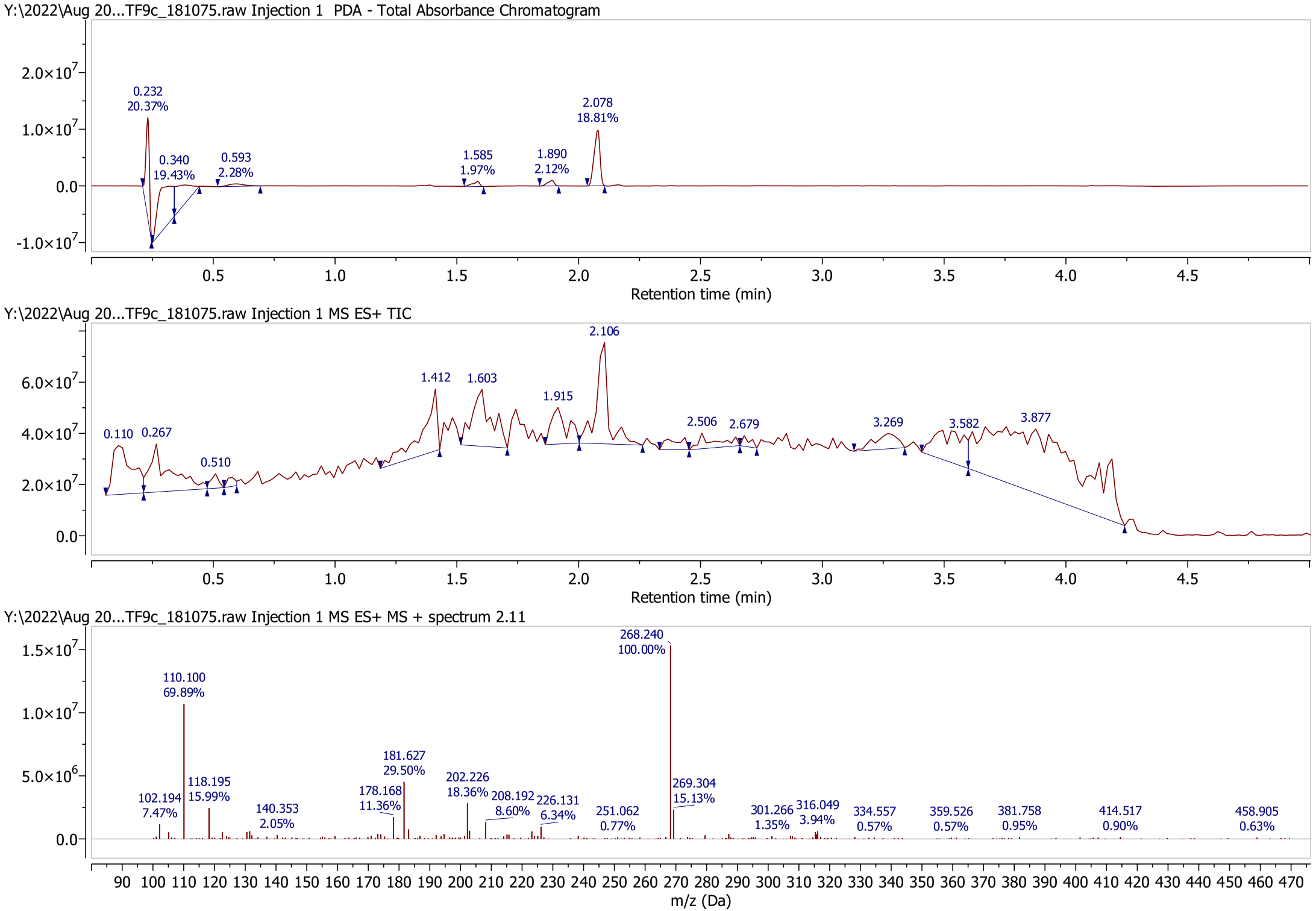


^{13}C:



DEPT-135:


OH
O
12
O
15
16
1
6
7
N
10
O
11
2
5
8
4
3
O
13
CH3
14
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Y:\2022\Aug 20...TF9c_181075.raw Injection 1 PDA - Total Absorbance Chromatogram
0.232
20.37%
0.340
19.43%
0.593
2.28%
1.585
1.97%
1.890
2.12%
2.078
18.81%
Retention time (min)
Y:\2022\Aug 20...TF9c_181075.raw Injection 1 MS ES+ TIC
0.110
0.267
0.510
1.412
1.603
1.915
2.106
2.506
2.679
3.269
3.582
3.877
Retention time (min)
Y:\2022\Aug 20...TF9c_181075.raw Injection 1 MS ES+ MS + spectrum 2.11
268.240
100.00%
110.100
69.89%
181.627
29.50%
118.195
15.99%
202.226
18.36%
269.304
15.13%
102.194
7.47%
178.168
11.36%
208.192
8.60%
226.131
6.34%
140.353
2.05%
251.062
0.77%
301.266
1.35%
316.049
3.94%
334.557
0.57%
359.526
0.57%
381.758
0.95%
414.517
0.90%
458.905
0.63%
m/z (Da)

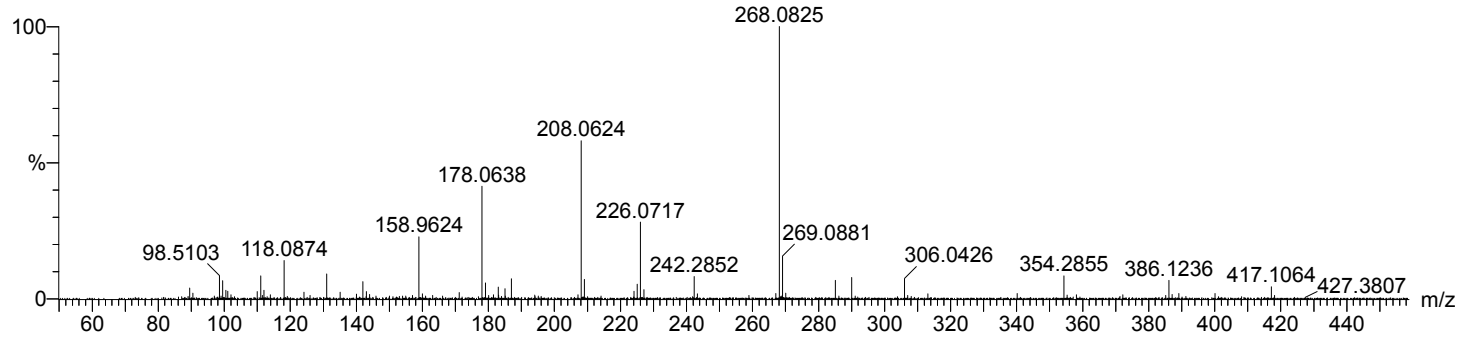
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
770 formula(e) evaluated with 8 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3

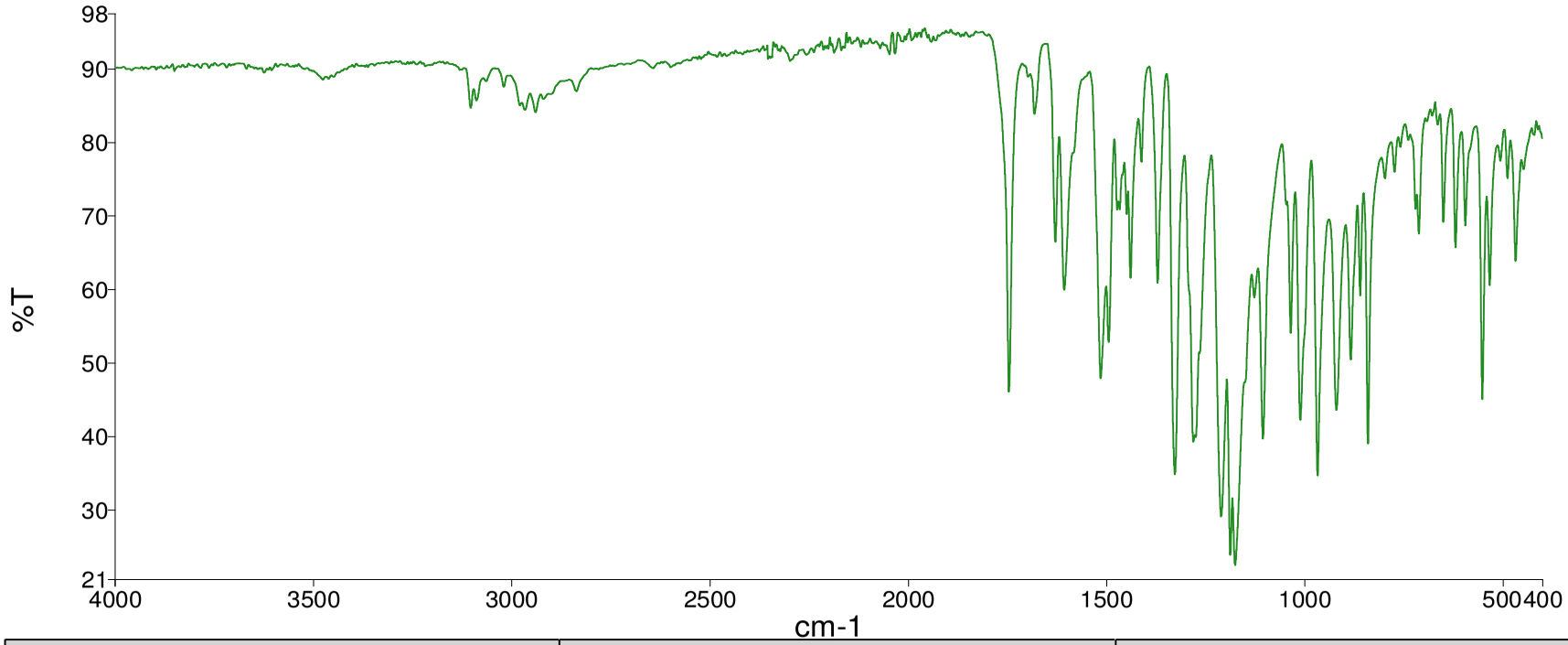
MTF9c 376 (3.191) Cm (375:378)

1: TOF MS ES+
1.34e+003



Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
226.0717	226.0715	0.2	0.9	5.5	66.3	0.5	C10 H12 N O5
	226.0711	0.6	2.7	-1.5	74.3	8.6	H10 N7 O5 F2
	226.0727	-1.0	-4.4	1.5	67.5	1.8	C7 H13 N O6 F
	226.0729	-1.2	-5.3	10.5	67.7	2.0	C11 H8 N5 O
	226.0700	1.7	7.5	2.5	71.6	5.9	C3 H9 N7 O4 F
	226.0740	-2.3	-10.2	6.5	68.4	2.7	C8 H9 N5 O2 F
	226.0691	2.6	11.5	2.5	69.3	3.6	C8 H11 N O3 F3
	226.0689	2.8	12.4	6.5	70.2	4.5	C6 H8 N7 O3

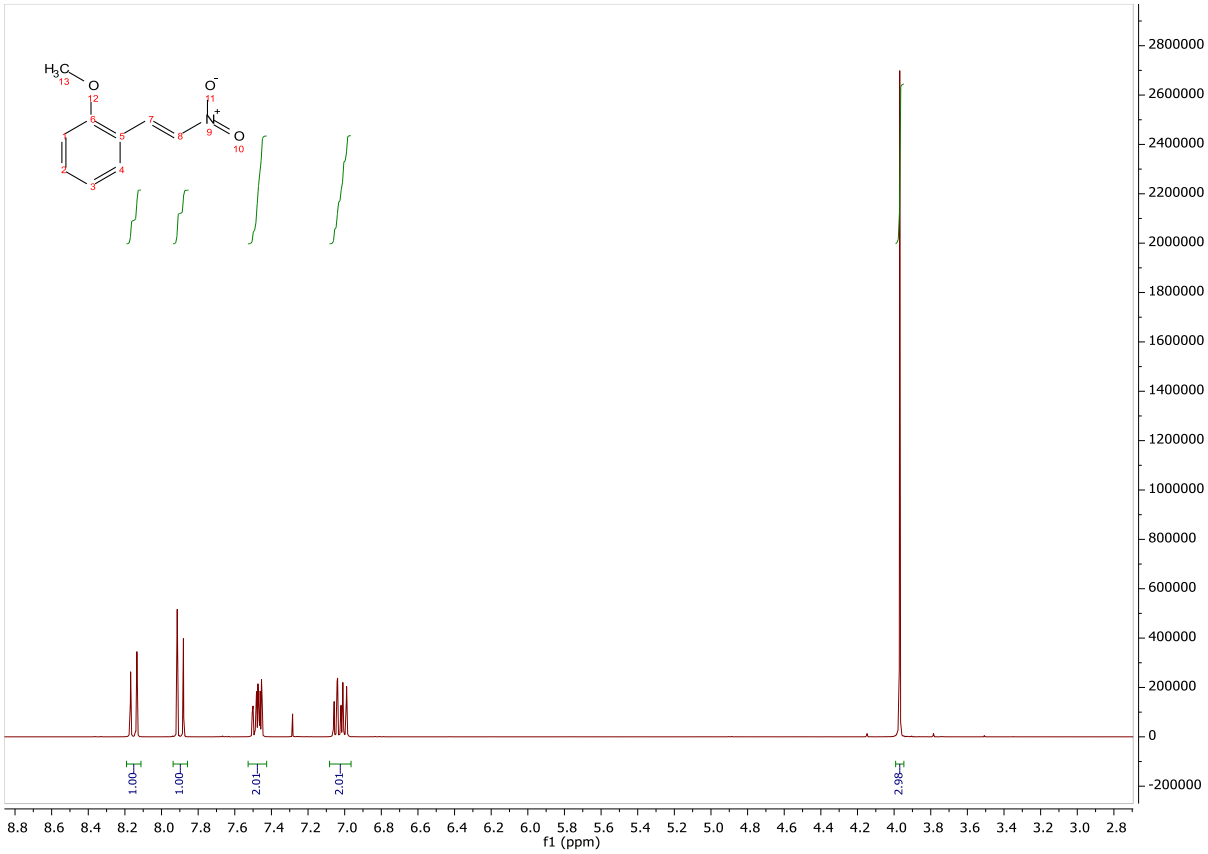
Analyst Lenny Lauchlan
Date 31 August 2022 08:04



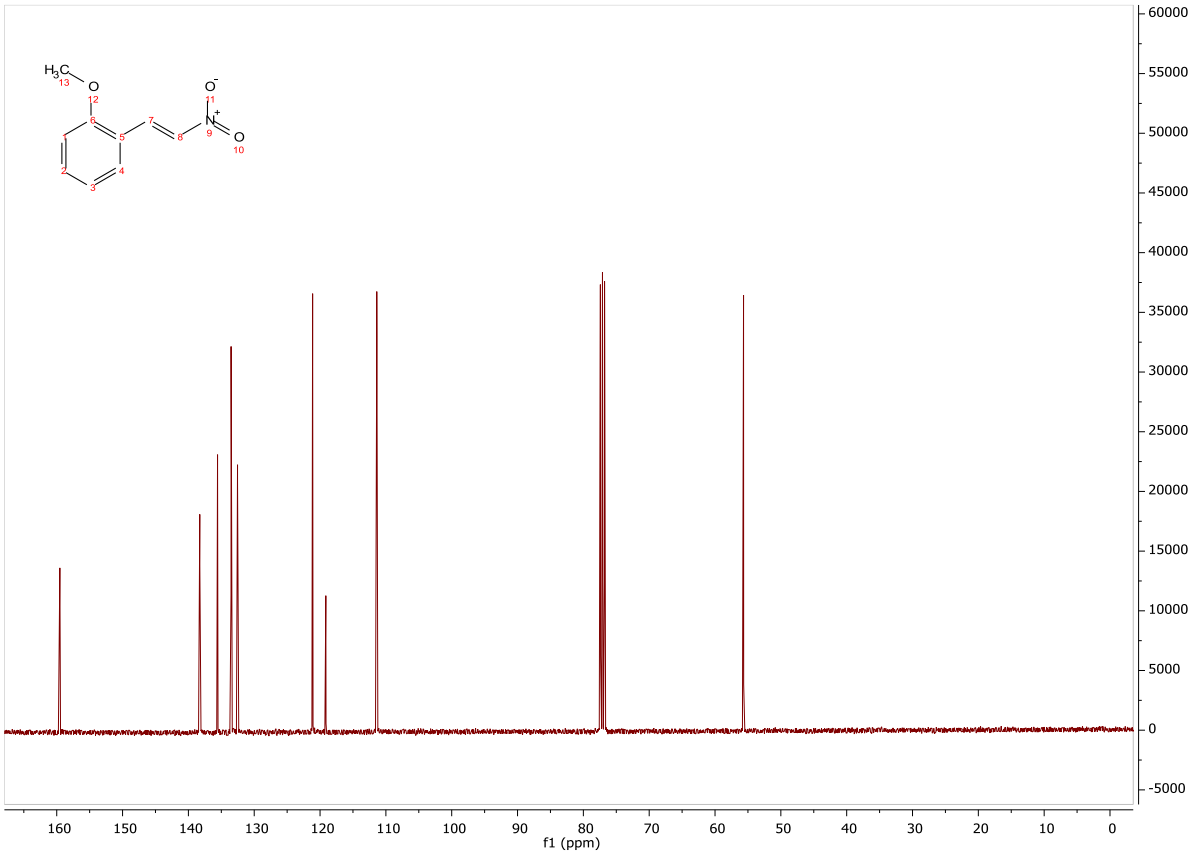
Sample Name	Description	Quality Checks
MTF 9c	Sample 020 By Lenny Date Wednesday, August 31 2022	The Quality Checks do not report any warnings for the sample.

(*E*)-1-methoxy-2-(2-nitrovinyl)benzene **88f**

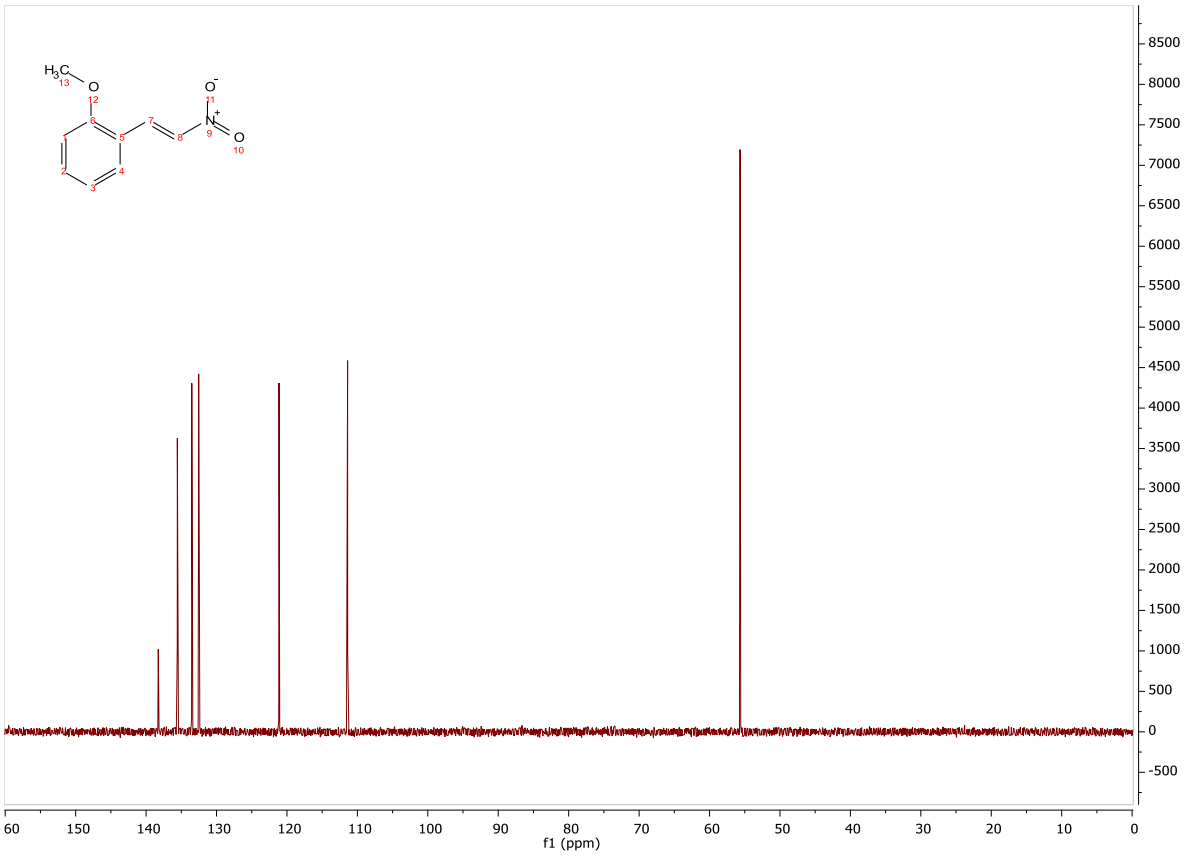
^{1}H:

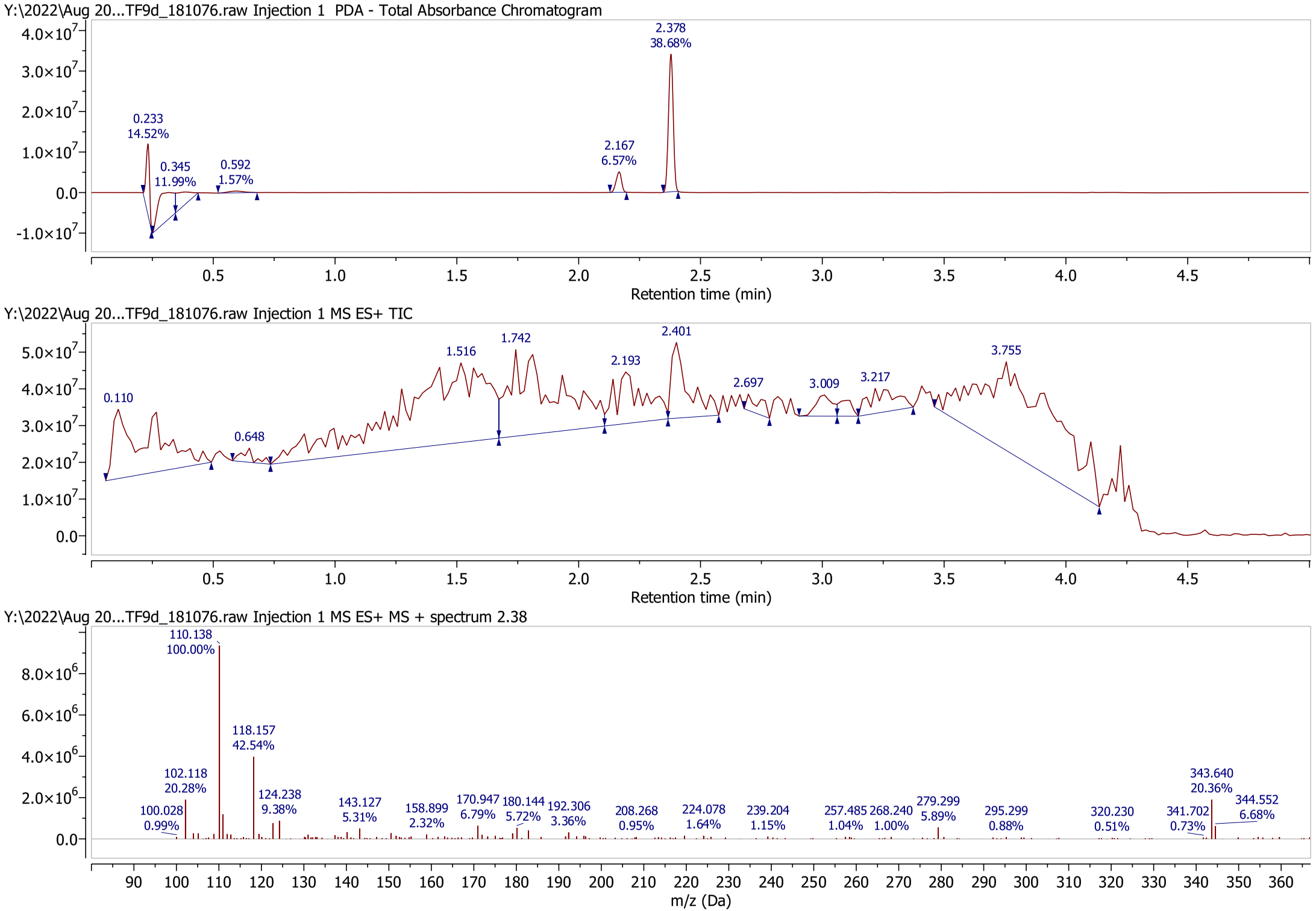


^{13}C:



DEPT-135:


H3C
13
O
12
1
6
5
7
8
N+
9
O-
11
O
10
2
3
4
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Y:\2022\Aug 20...TF9d_181076.raw Injection 1 PDA - Total Absorbance Chromatogram
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
-1.0×10^7
0.233
14.52%
0.345
11.99%
0.592
1.57%
2.167
6.57%
2.378
38.68%
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Aug 20...TF9d_181076.raw Injection 1 MS ES+ TIC
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
0.110
0.648
1.516
1.742
2.193
2.401
2.697
3.009
3.217
3.755
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Aug 20...TF9d_181076.raw Injection 1 MS ES+ MS + spectrum 2.38
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
110.138
100.00%
118.157
42.54%
102.118
20.28%
124.238
9.38%
100.028
0.99%
143.127
5.31%
158.899
2.32%
170.947
6.79%
180.144
5.72%
192.306
3.36%
208.268
0.95%
224.078
1.64%
239.204
1.15%
257.485
1.04%
268.240
1.00%
279.299
5.89%
295.299
0.88%
320.230
0.51%
341.702
0.73%
343.640
20.36%
344.552
6.68%
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320
330
340
350
360
m/z (Da)

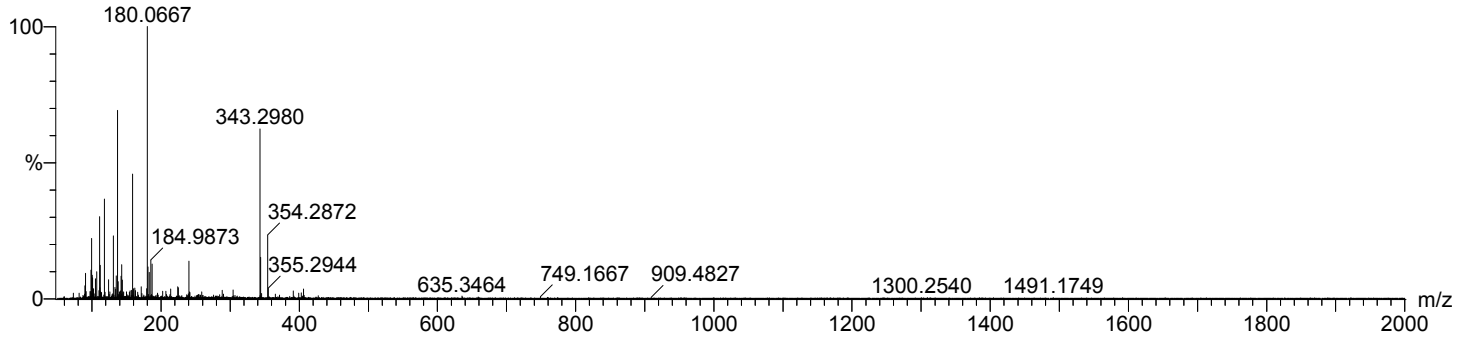
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
460 formula(e) evaluated with 5 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3

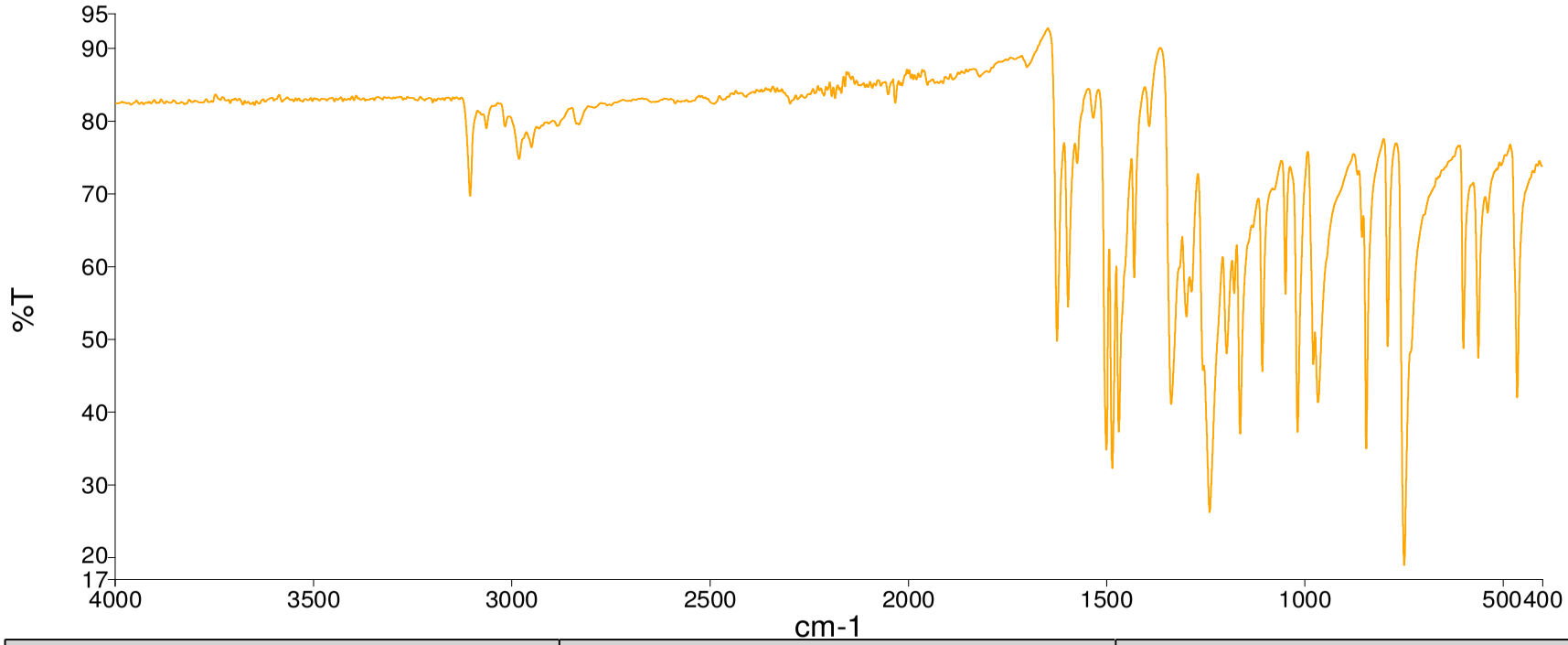
MTF9d 421 (3.566) Cm (418:428)

1: TOF MS ES+
1.66e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
180.0667	180.0672	-0.5	-2.8	1.5	141.7	3.6	C6 H11 N O4 F
	180.0661	0.6	3.3	5.5	138.1	0.0	C9 H10 N O3
	180.0685	-1.8	-10.0	6.5	143.2	5.1	C7 H7 N5 F
	180.0645	2.2	12.2	2.5	149.0	11.0	C2 H7 N7 O2 F
	180.0697	-3.0	-16.7	2.5	147.0	8.9	C4 H8 N5 O F2

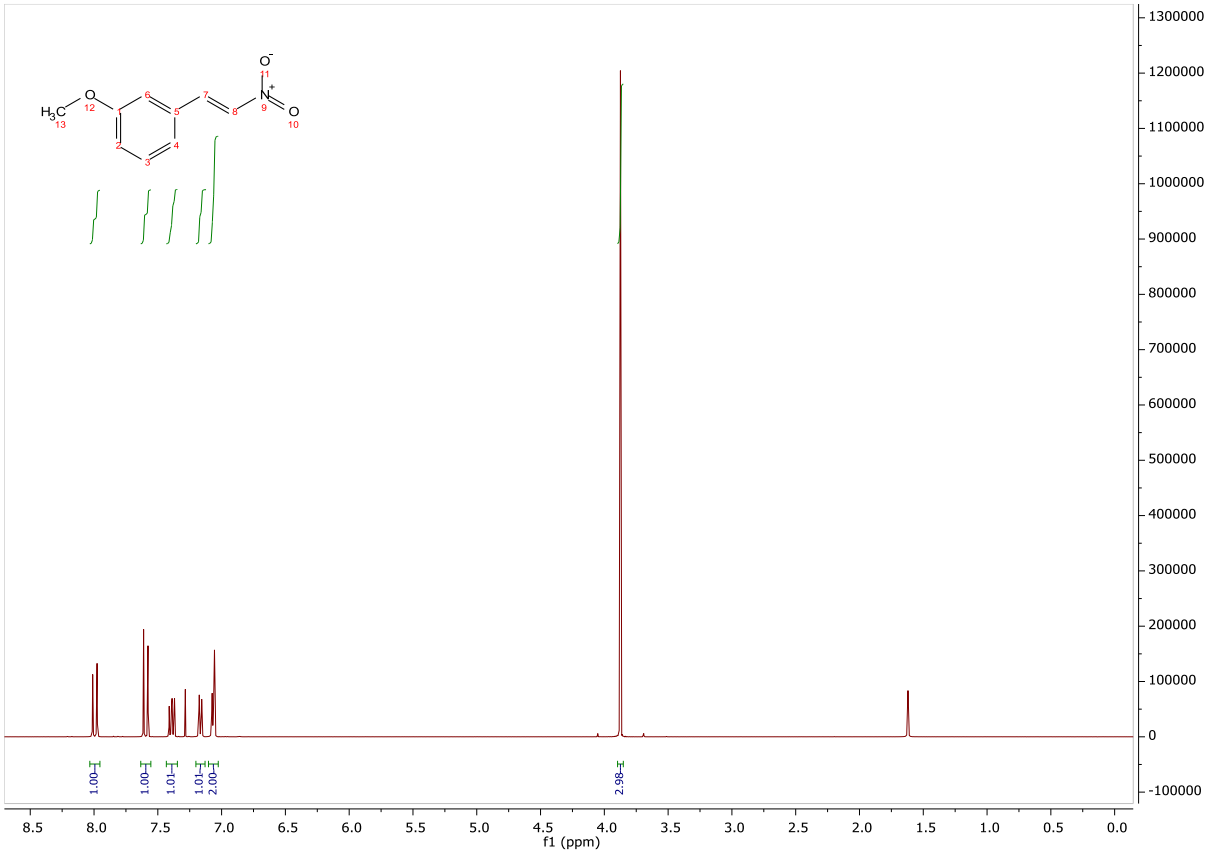
Analyst Lenny Lauchlan
Date 31 August 2022 08:05



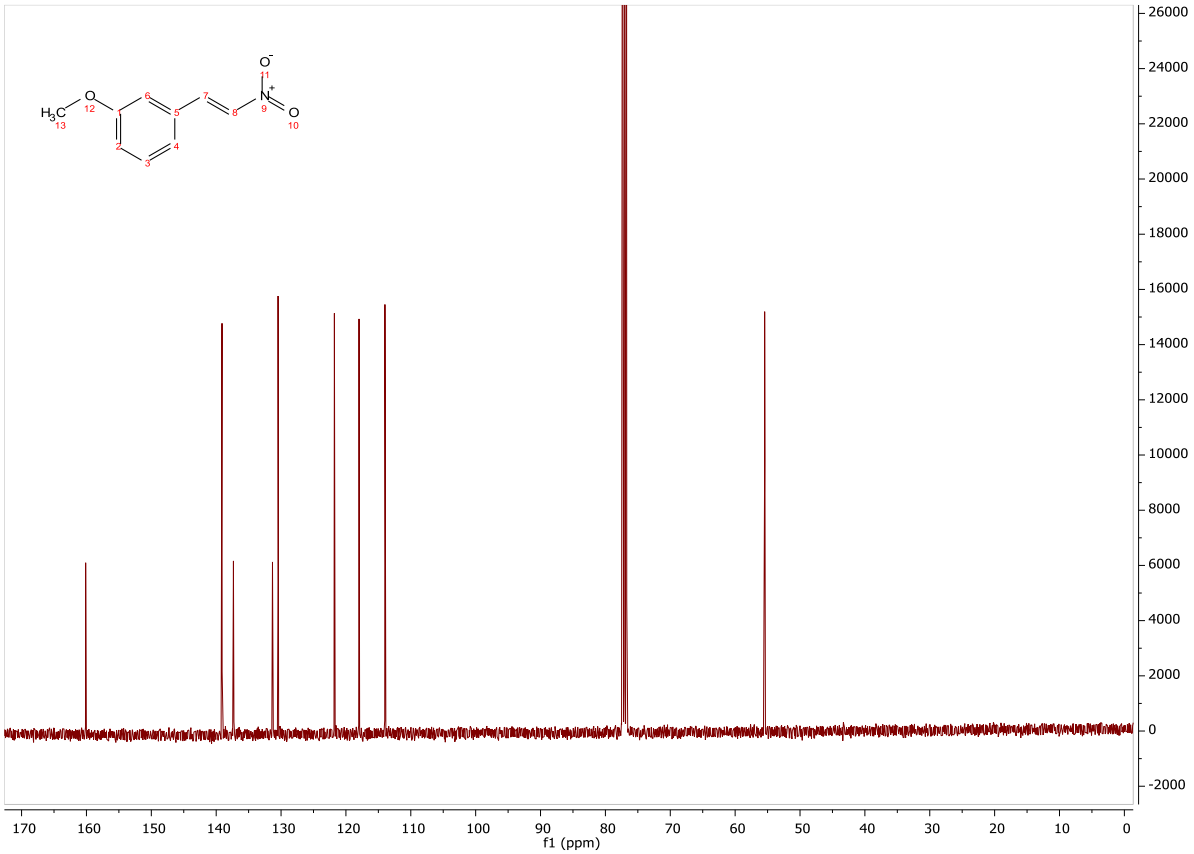
Sample Name	Description	Quality Checks
MTF 9d	Sample 021 By Lenny Date Wednesday, August 31 2022	The Quality Checks do not report any warnings for the sample.

(*E*)-1-methoxy-3-(2-nitrovinyl)benzene **88g**

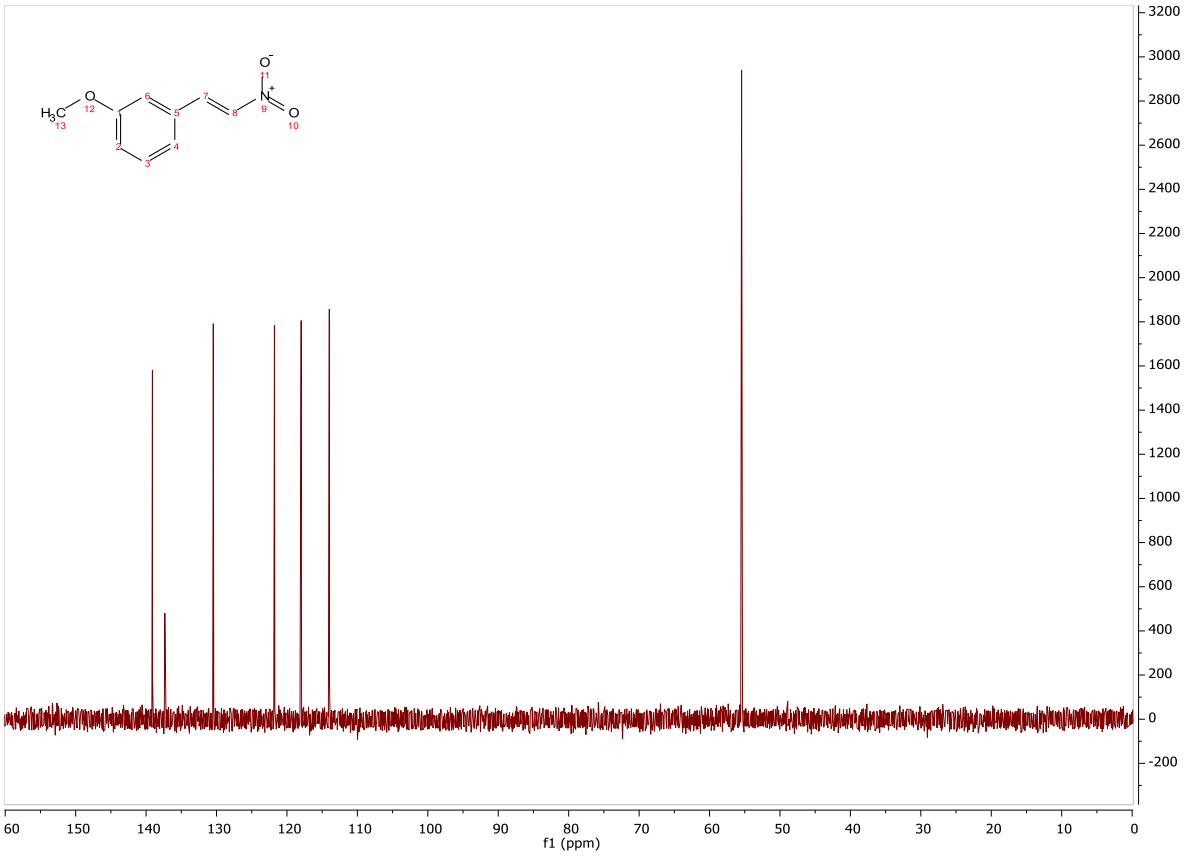
^{1}H:

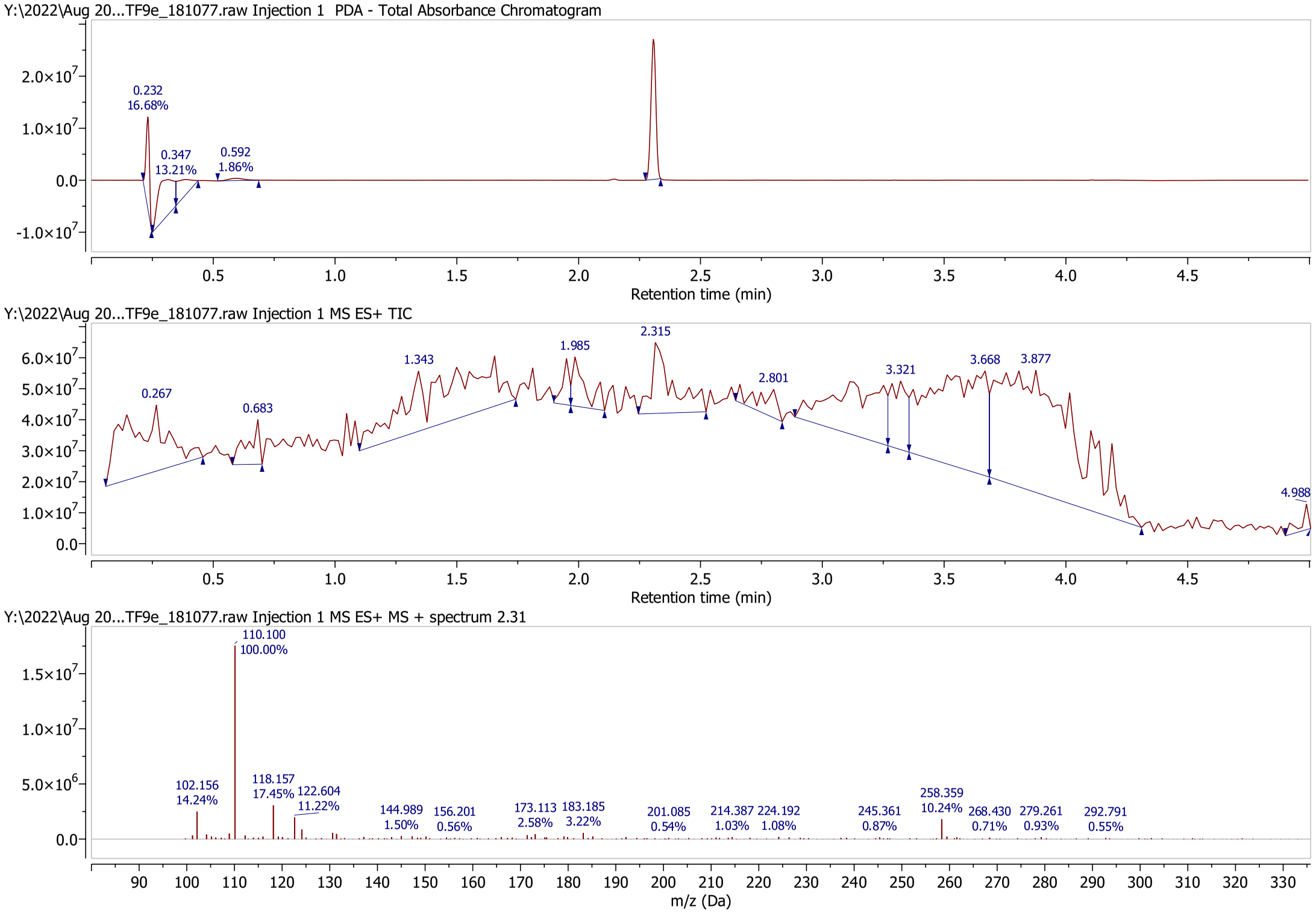


^{13}C:



DEPT-135:


3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Y:\2022\Aug 20...TF9e_181077.raw Injection 1 PDA - Total Absorbance Chromatogram
0.232
16.68%
0.347
13.21%
0.592
1.86%
Retention time (min)
Y:\2022\Aug 20...TF9e_181077.raw Injection 1 MS ES+ TIC
0.267
0.683
1.343
1.985
2.315
2.801
3.321
3.668
3.877
4.988
Retention time (min)
Y:\2022\Aug 20...TF9e_181077.raw Injection 1 MS ES+ MS + spectrum 2.31
110.100
100.00%
102.156
14.24%
118.157
17.45%
122.604
11.22%
144.989
1.50%
156.201
0.56%
173.113
2.58%
183.185
3.22%
201.085
0.54%
214.387
1.03%
224.192
1.08%
245.361
0.87%
258.359
10.24%
268.430
0.71%
279.261
0.93%
292.791
0.55%
m/z (Da)

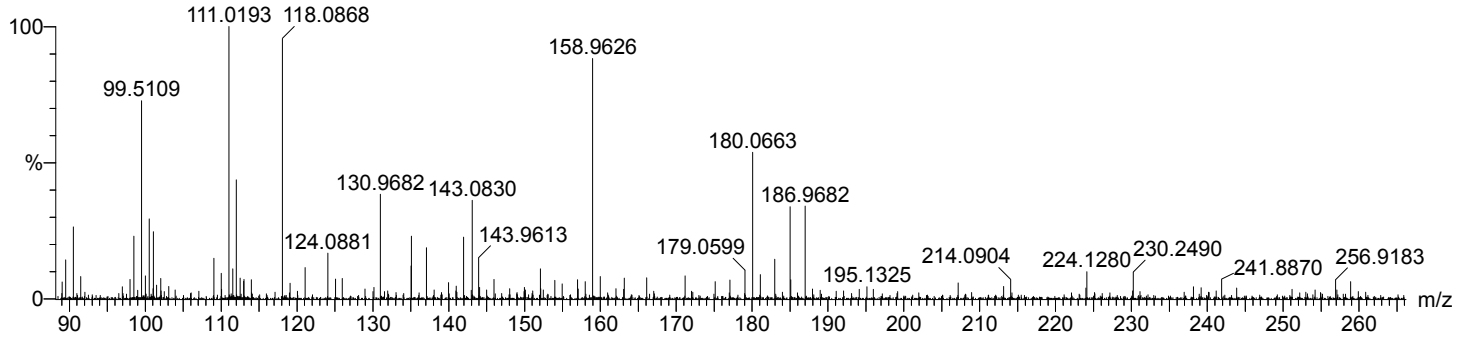
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
460 formula(e) evaluated with 6 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3

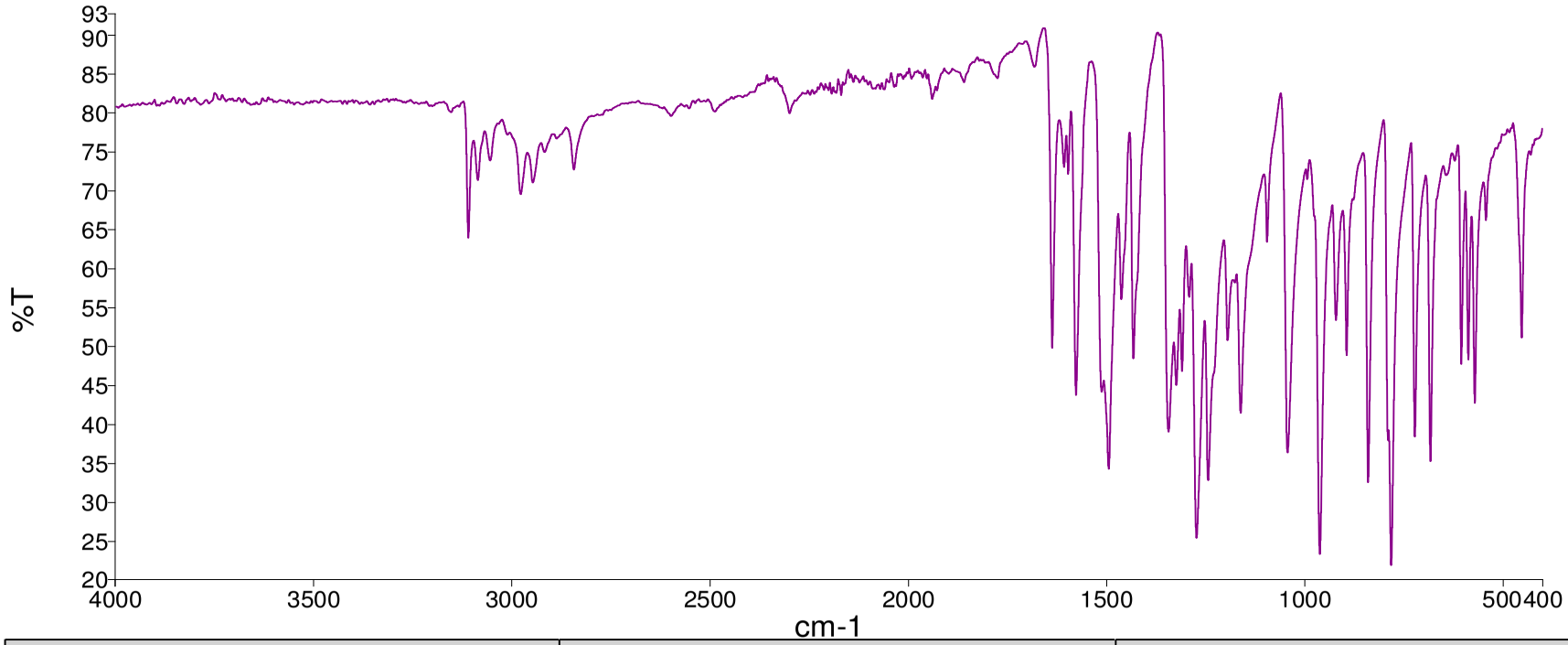
MTF9e 445 (3.767) Cm (438:448)

1: TOF MS ES+
6.33e+002



Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
180.0663	180.0661	0.2	1.1	5.5	73.3	0.2	C9 H10 N O3
	180.0672	-0.9	-5.0	1.5	75.1	2.0	C6 H11 N O4 F
	180.0645	1.8	10.0	2.5	79.5	6.4	C2 H7 N7 O2 F
	180.0685	-2.2	-12.2	6.5	76.0	3.0	C7 H7 N5 F
	180.0636	2.7	15.0	2.5	77.1	4.1	C7 H9 N O F3
	180.0634	2.9	16.1	6.5	78.2	5.2	C5 H6 N7 O

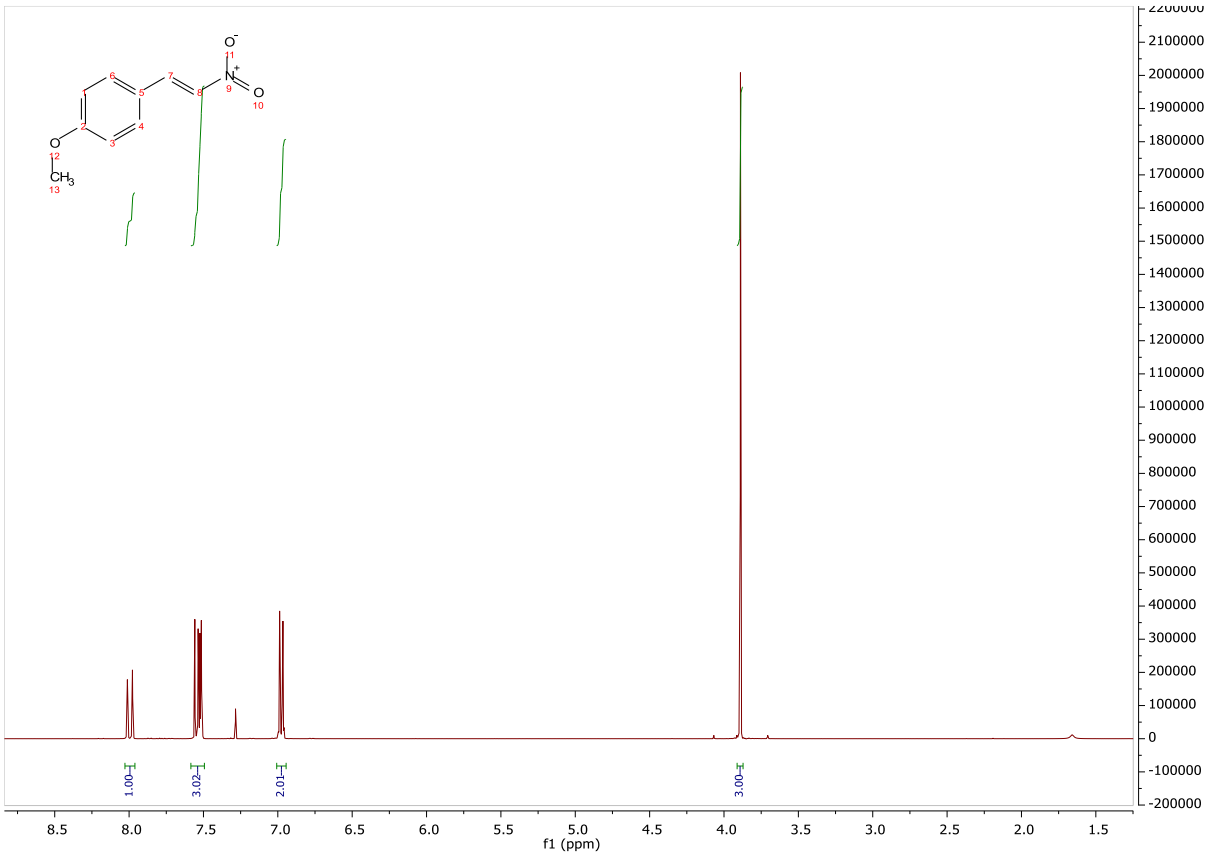
Analyst Lenny Lauchlan
Date 31 August 2022 08:07



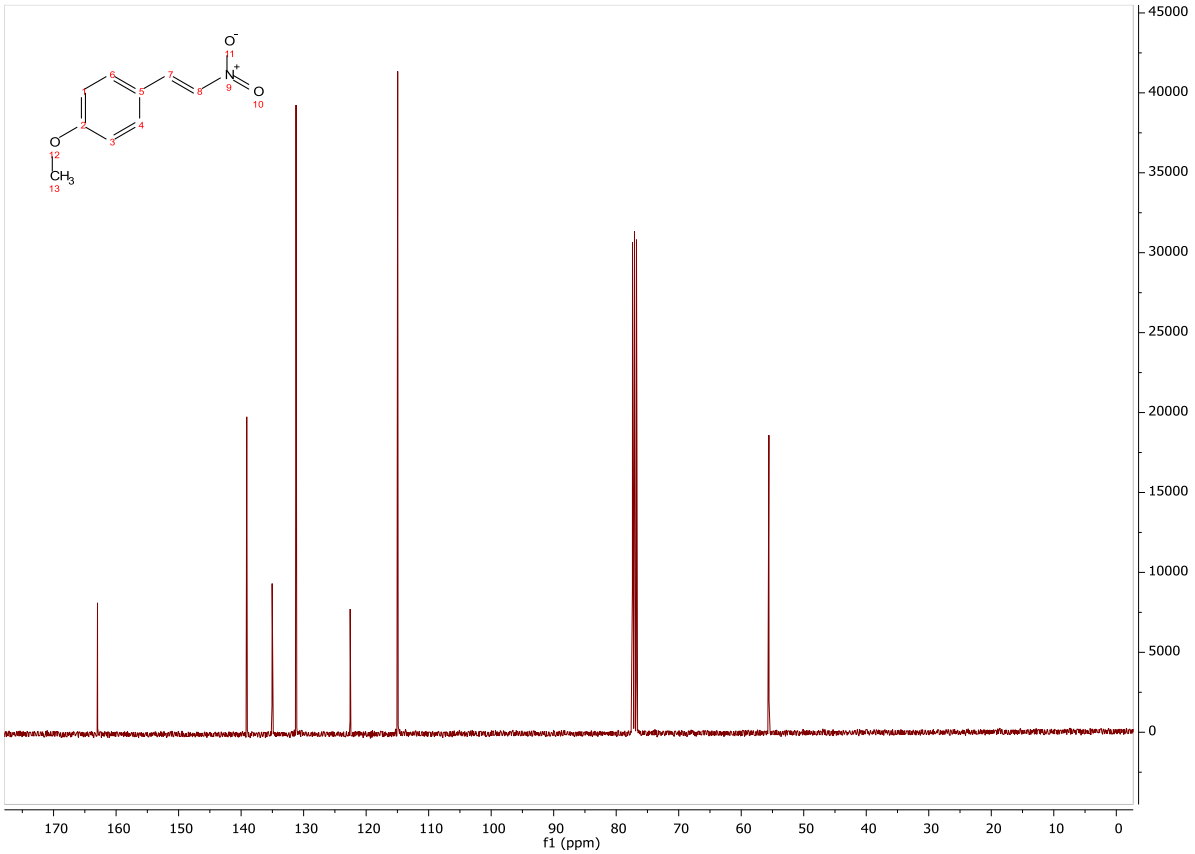
Sample Name	Description	Quality Checks
MTF 9e	Sample 022 By Lenny Date Wednesday, August 31 2022	The Quality Checks do not report any warnings for the sample.

(*E*)-1-methoxy-4-(2-nitrovinyl)benzene **88h**

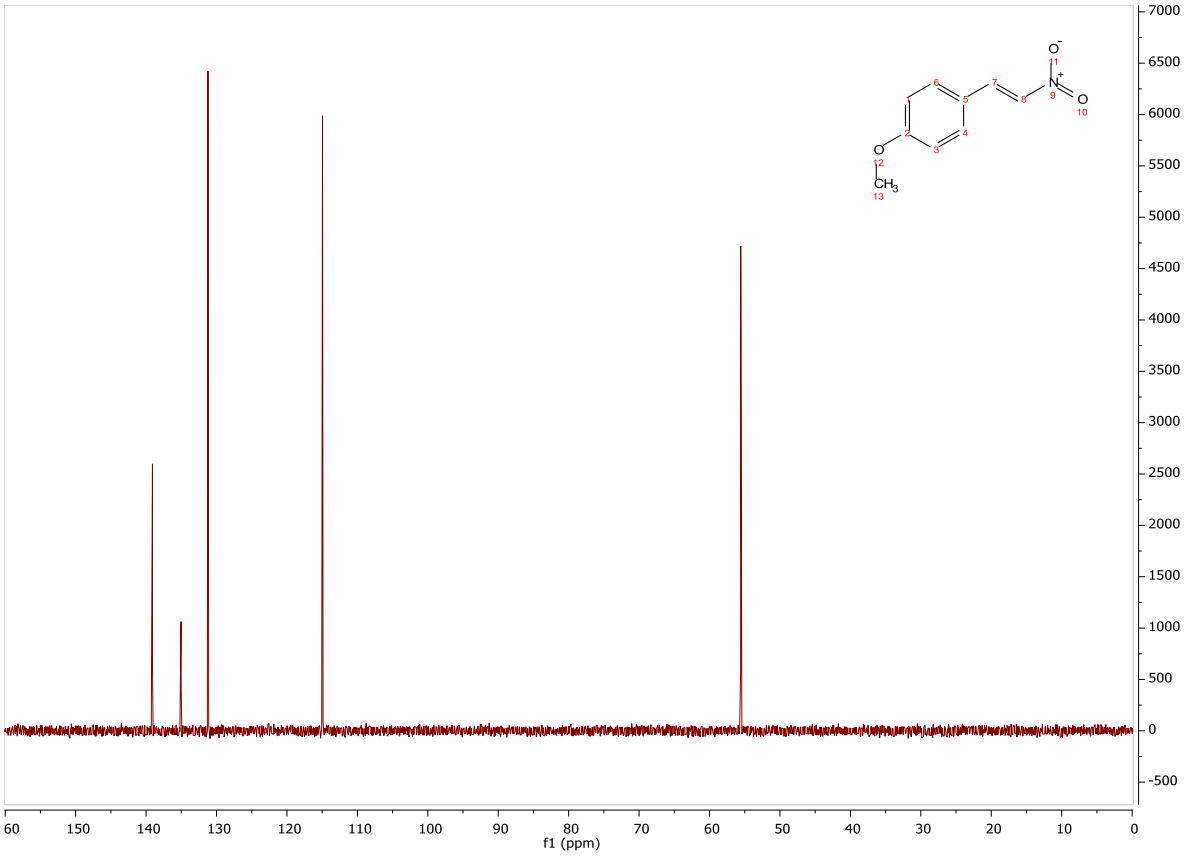
^{1}H:

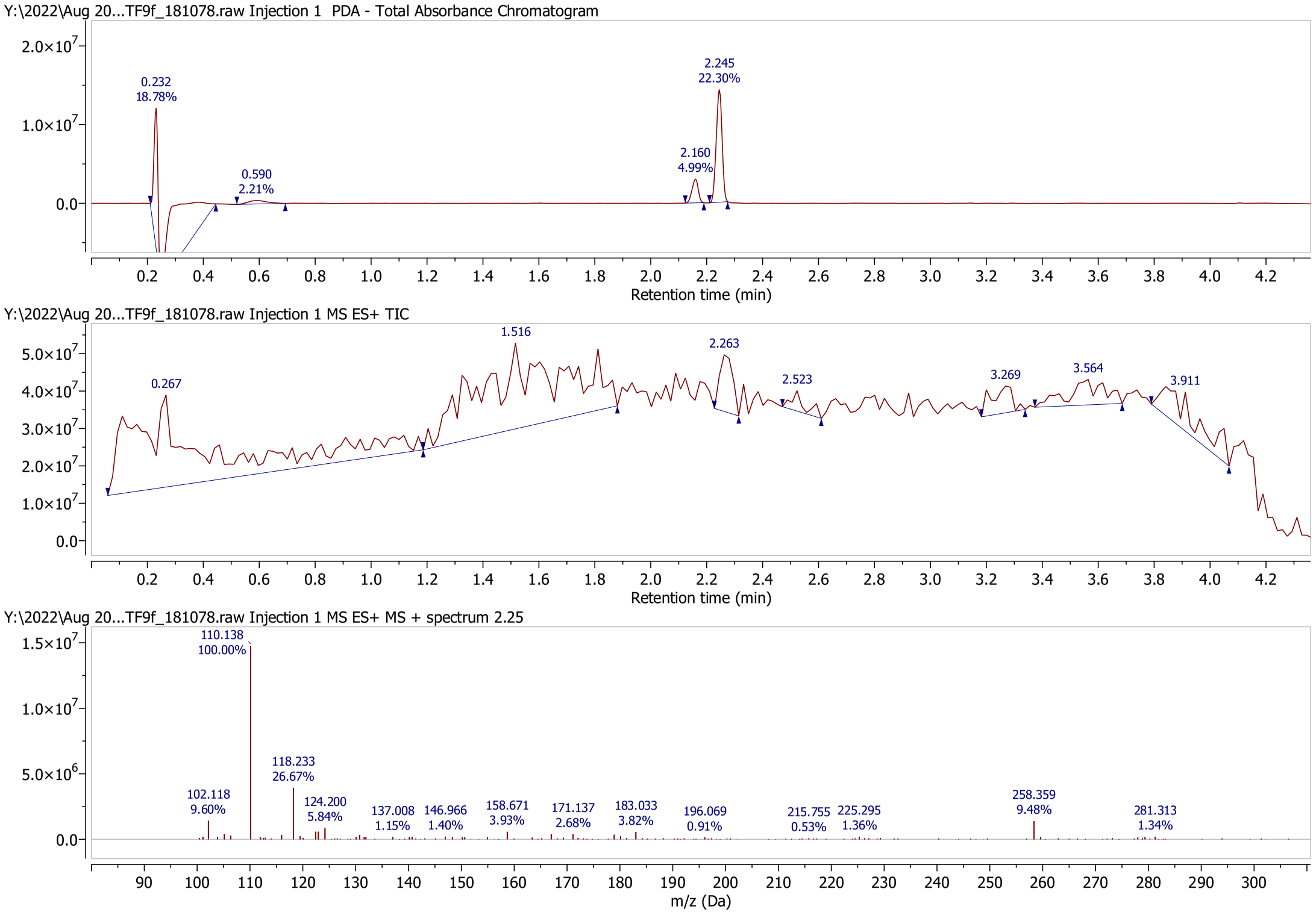


^{13}C:



DEPT-135:


7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
11
N
9
O
10
O
12
CH3
13


Y:\2022\Aug 20...TF9f_181078.raw Injection 1 PDA - Total Absorbance Chromatogram
0.232
18.78%
0.590
2.21%
2.160
4.99%
2.245
22.30%
Retention time (min)
Y:\2022\Aug 20...TF9f_181078.raw Injection 1 MS ES+ TIC
0.267
1.516
2.263
2.523
3.269
3.564
3.911
Retention time (min)
Y:\2022\Aug 20...TF9f_181078.raw Injection 1 MS ES+ MS + spectrum 2.25
110.138
100.00%
118.233
26.67%
102.118
9.60%
124.200
5.84%
137.008
1.15%
146.966
1.40%
158.671
3.93%
171.137
2.68%
183.033
3.82%
196.069
0.91%
215.755
0.53%
225.295
1.36%
258.359
9.48%
281.313
1.34%
m/z (Da)

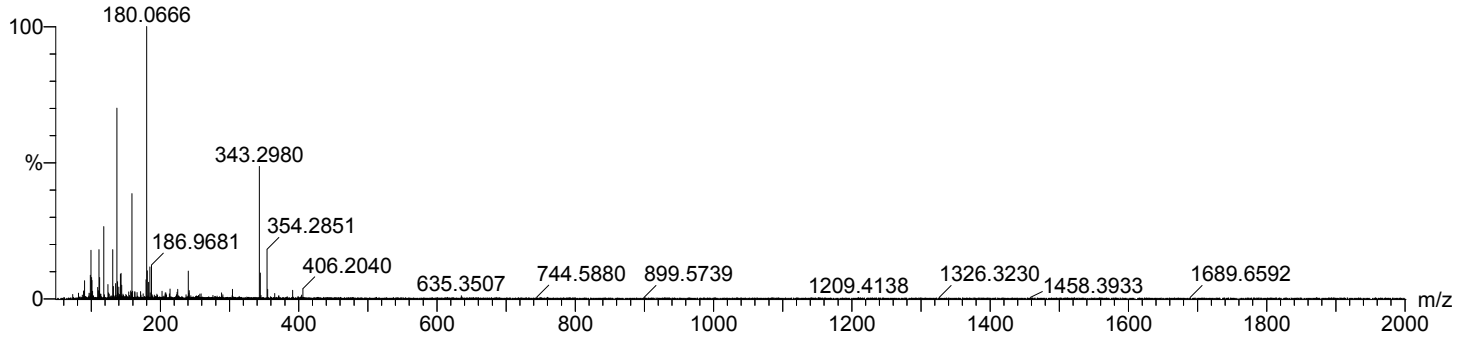
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
460 formula(e) evaluated with 5 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3

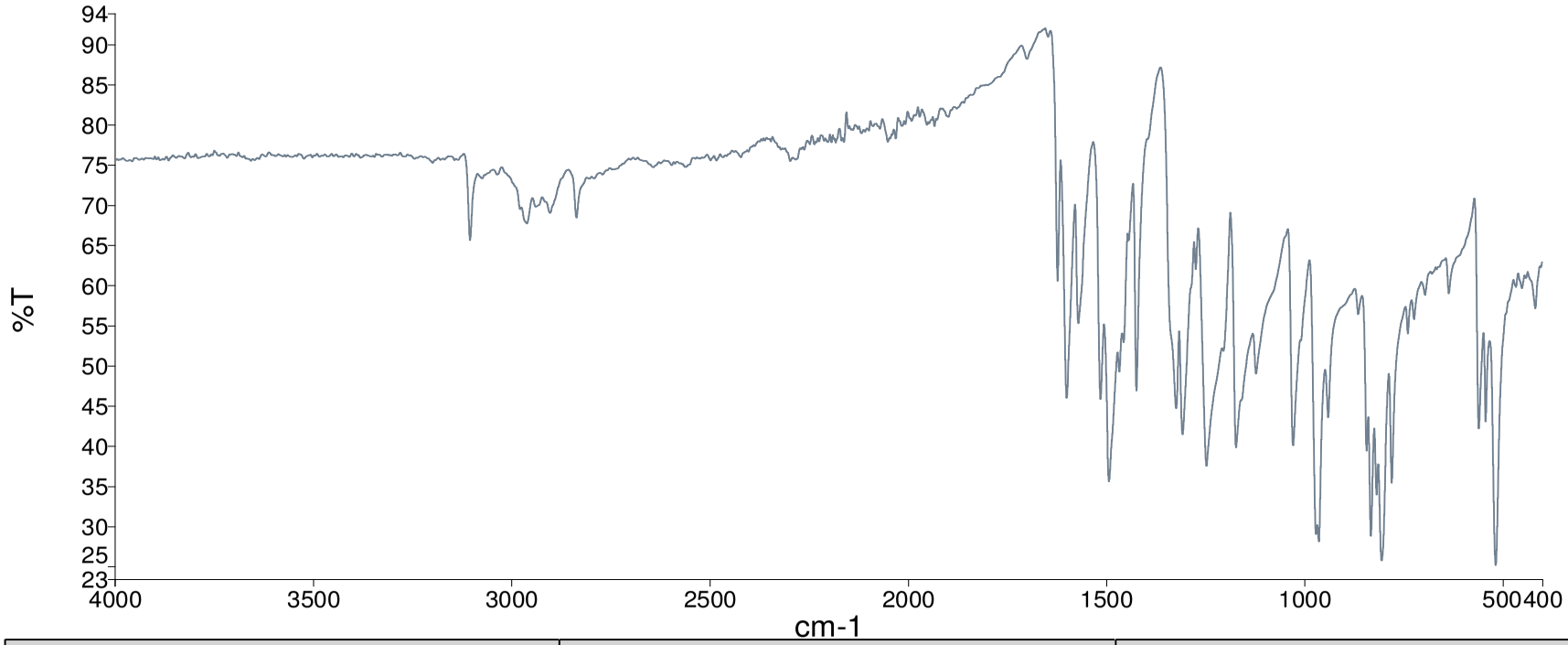
MTF9f 418 (3.540) Cm (415:419)

1: TOF MS ES+
9.61e+002



Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
180.0666	180.0661	0.5	2.8	5.5	96.7	0.2	C9 H10 N O3
	180.0672	-0.6	-3.3	1.5	98.7	2.2	C6 H11 N O4 F
	180.0685	-1.9	-10.6	6.5	99.8	3.4	C7 H7 N5 F
	180.0645	2.1	11.7	2.5	105.7	9.2	C2 H7 N7 O2 F
	180.0636	3.0	16.7	2.5	101.3	4.8	C7 H9 N O F3

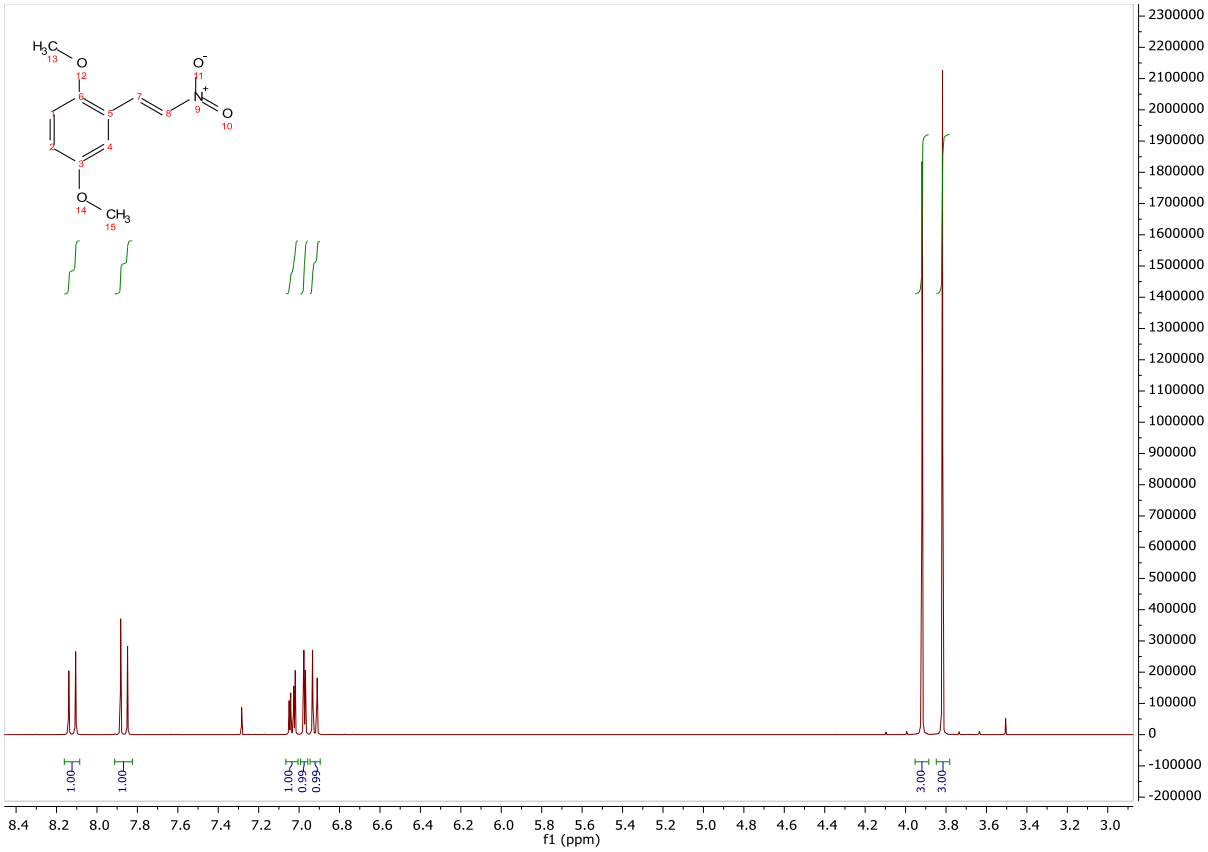
Analyst Lenny Lauchlan
Date 31 August 2022 08:08



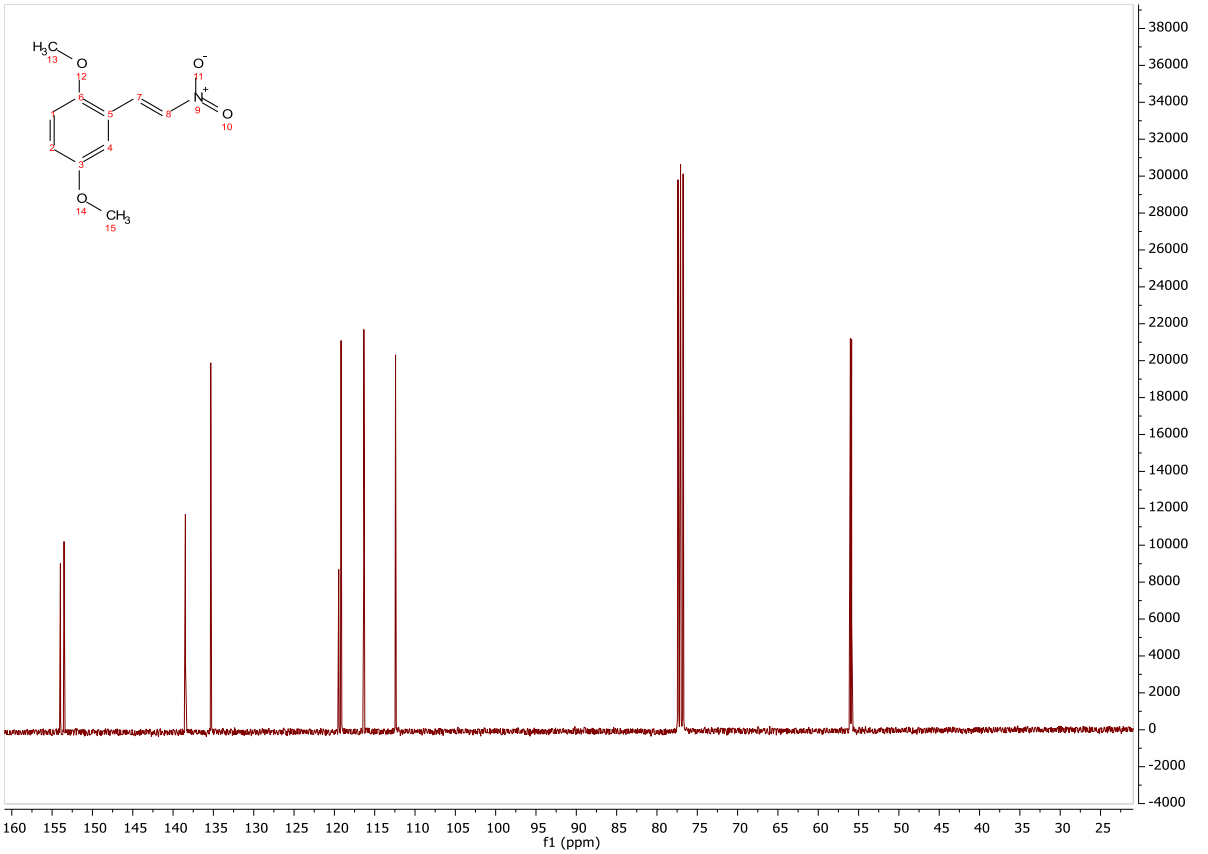
Sample Name	Description	Quality Checks
MTF 9f	Sample 023 By Lenny Date Wednesday, August 31 2022	The Quality Checks do not report any warnings for the sample.

(*E*)-1,4-dimethoxy-2-(2-nitrovinyl)benzene **88i**

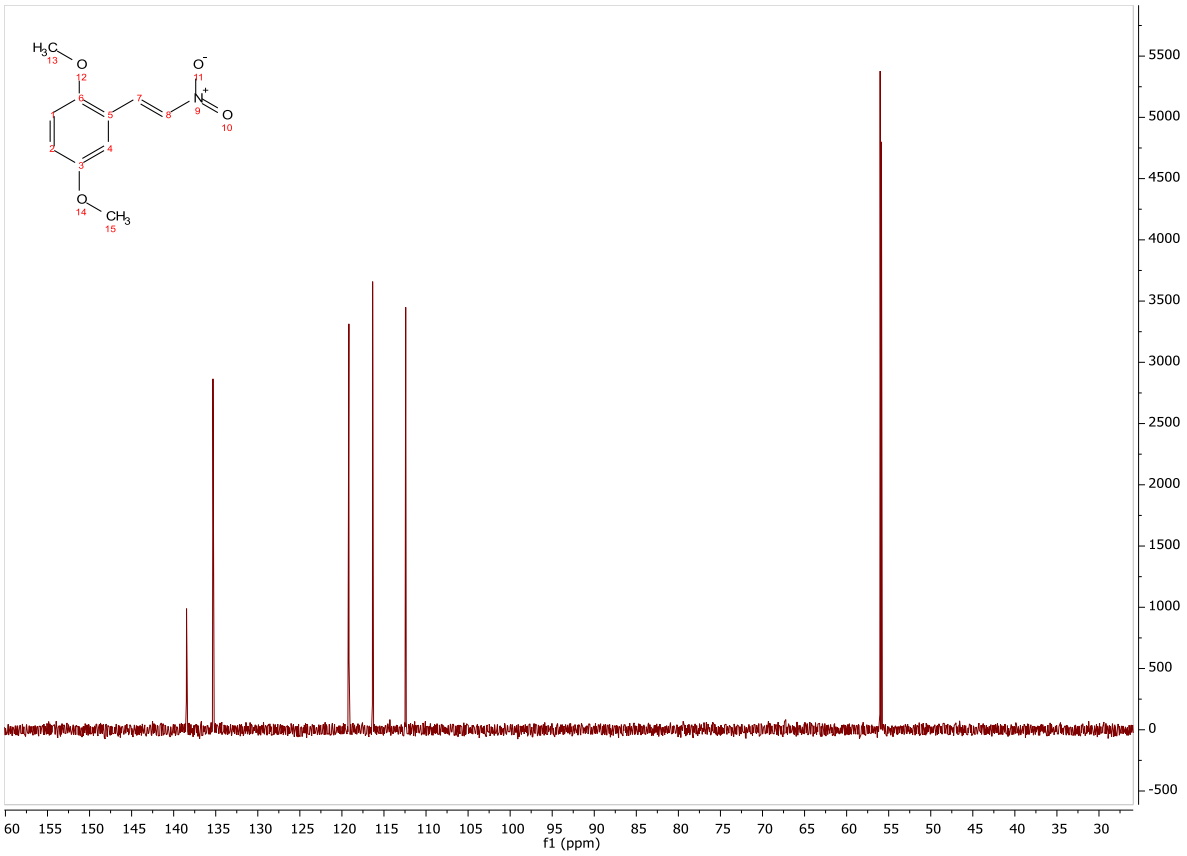
^{1}H:

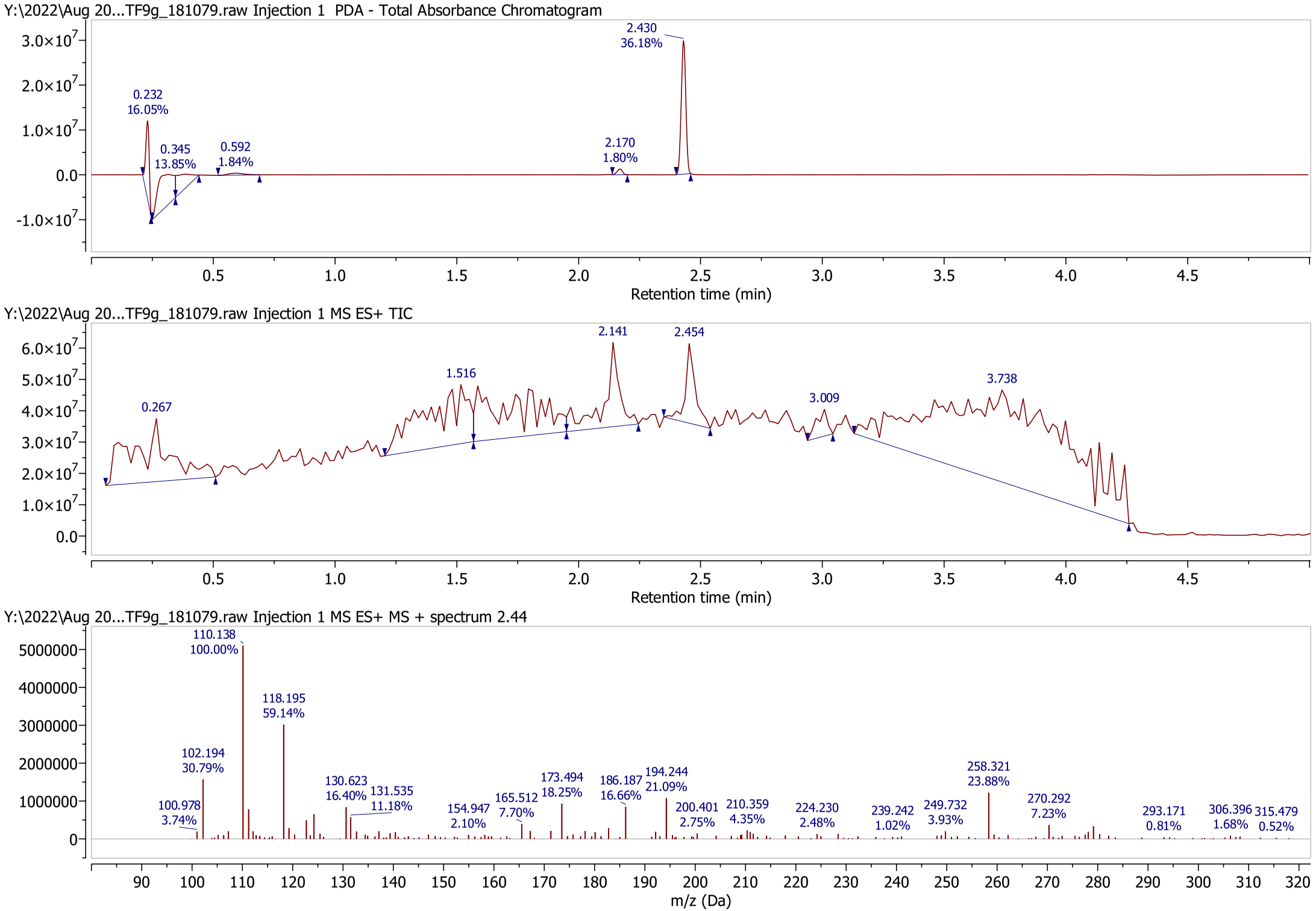


^{13}C:



DEPT-135:


H3C
13
O
12
O-
11
N+
9
O
10
O
14
CH3
15
1
2
3
4
5
6
7
8
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
60 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30
f1 (ppm)


Y:\2022\Aug 20...TF9g_181079.raw Injection 1 PDA - Total Absorbance Chromatogram
3.0×10^7
2.0×10^7
1.0×10^7
0.0
-1.0×10^7
0.232
16.05%
0.345
13.85%
0.592
1.84%
2.170
1.80%
2.430
36.18%
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Aug 20...TF9g_181079.raw Injection 1 MS ES+ TIC
6.0×10^7
5.0×10^7
4.0×10^7
3.0×10^7
2.0×10^7
1.0×10^7
0.0
0.267
1.516
2.141
2.454
3.009
3.738
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Aug 20...TF9g_181079.raw Injection 1 MS ES+ MS + spectrum 2.44
5000000
4000000
3000000
2000000
1000000
0
110.138
100.00%
118.195
59.14%
102.194
30.79%
100.978
3.74%
130.623
16.40%
131.535
11.18%
154.947
2.10%
165.512
7.70%
173.494
18.25%
186.187
16.66%
194.244
21.09%
200.401
2.75%
210.359
4.35%
224.230
2.48%
239.242
1.02%
249.732
3.93%
258.321
23.88%
270.292
7.23%
293.171
0.81%
306.396
1.68%
315.479
0.52%
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320
m/z (Da)

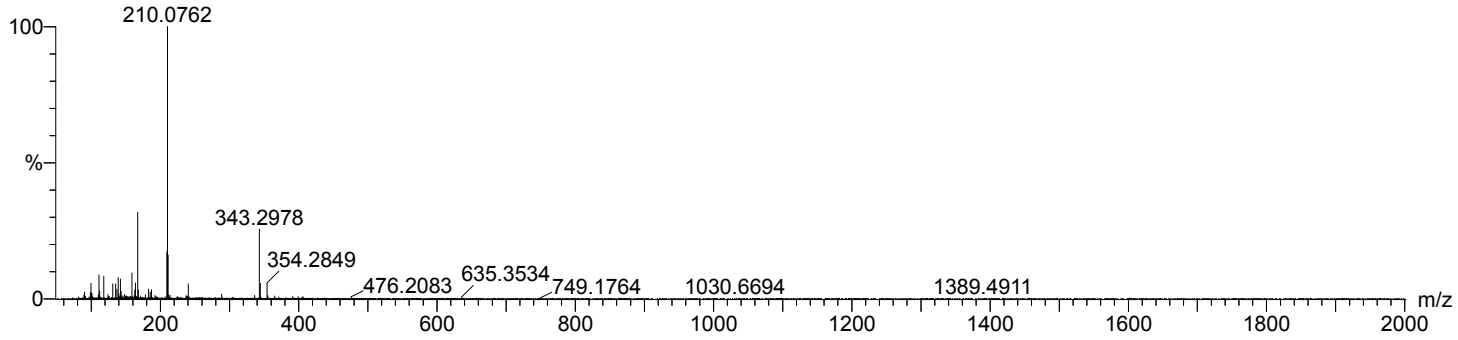
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
657 formula(e) evaluated with 8 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3

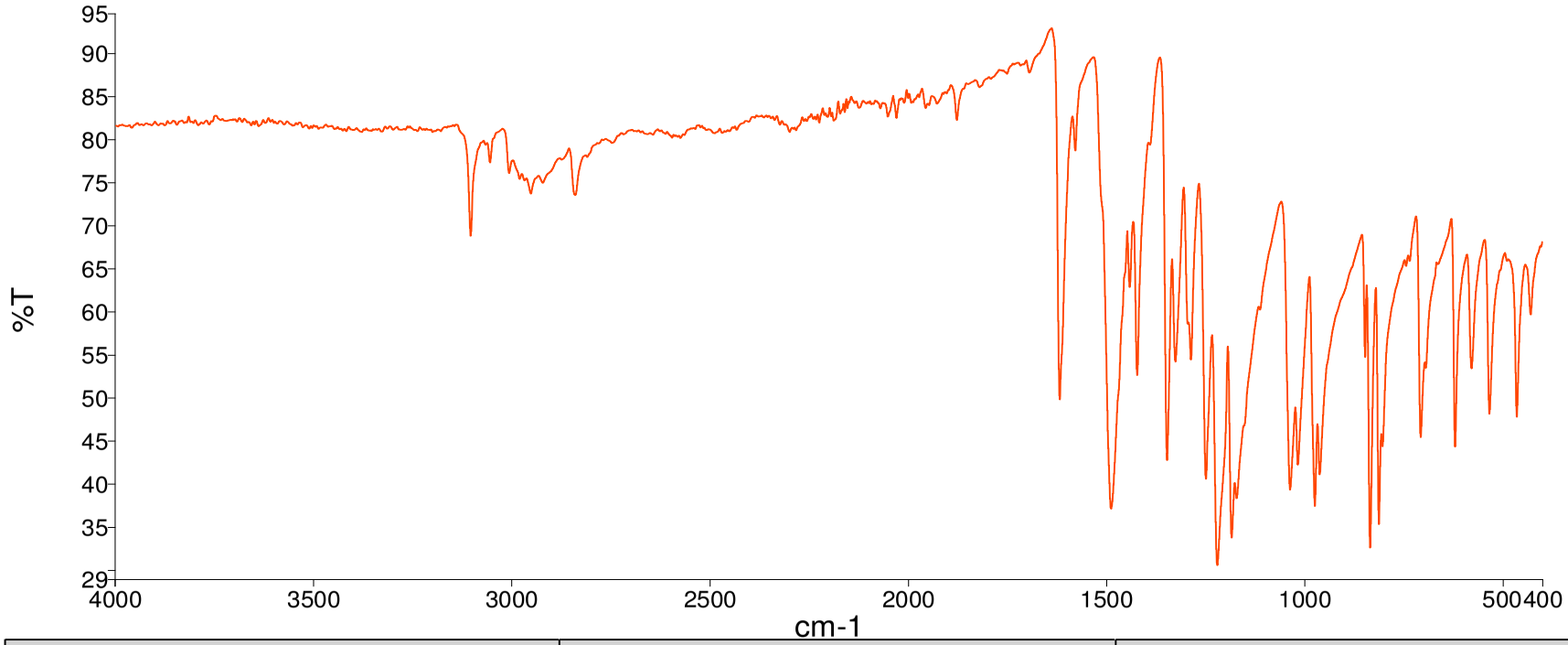
MTF9g 416 (3.529) Cm (416:418)

1: TOF MS ES+
1.74e+003



Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
210.0762	210.0762	0.0	0.0	-1.5	142.8	10.9	H10 N7 O4 F2
	210.0766	-0.4	-1.9	5.5	132.9	1.1	C10 H12 N O4
	210.0751	1.1	5.2	2.5	139.9	8.0	C3 H9 N7 O3 F
	210.0778	-1.6	-7.6	1.5	135.8	3.9	C7 H13 N O5 F
	210.0780	-1.8	-8.6	10.5	132.4	0.5	C11 H8 N5
	210.0742	2.0	9.5	2.5	136.1	4.2	C8 H11 N O2 F3
	210.0739	2.3	10.9	6.5	137.9	6.0	C6 H8 N7 O2
	210.0791	-2.9	-13.8	6.5	136.2	4.3	C8 H9 N5 O F

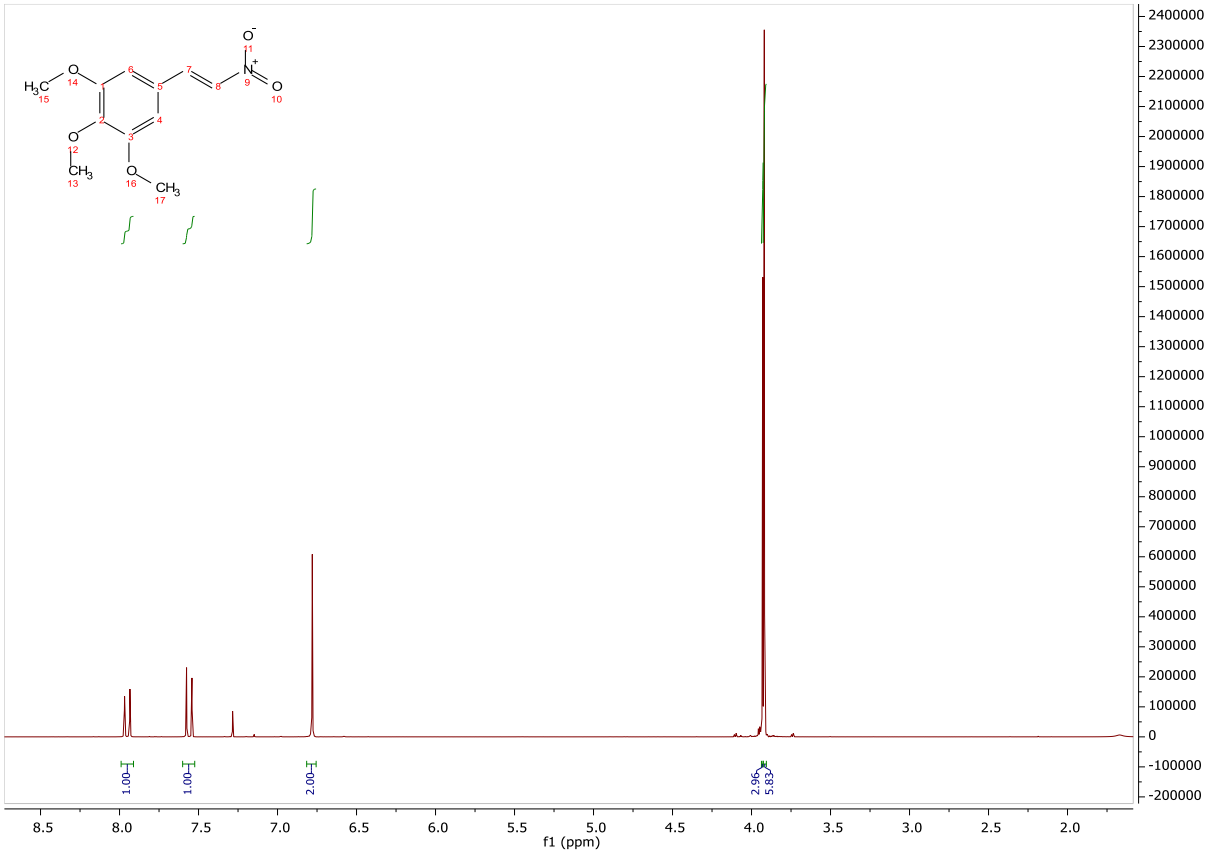
Analyst Lenny Lauchlan
Date 31 August 2022 08:10



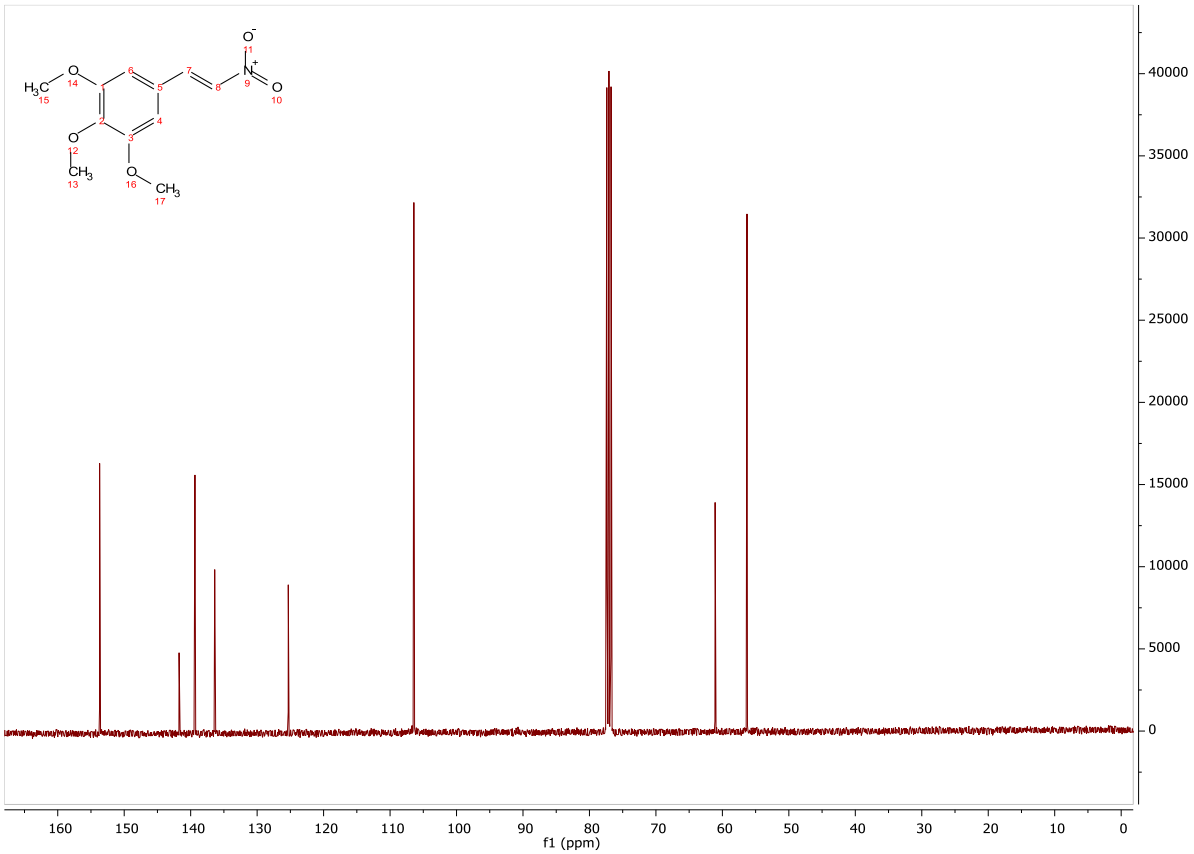
Sample Name	Description	Quality Checks
MTF 9g	Sample 024 By Lenny Date Wednesday, August 31 2022	The Quality Checks do not report any warnings for the sample.

(*E*)-1,2,3-trimethoxy-5-(2-nitrovinyl)benzene **88j**

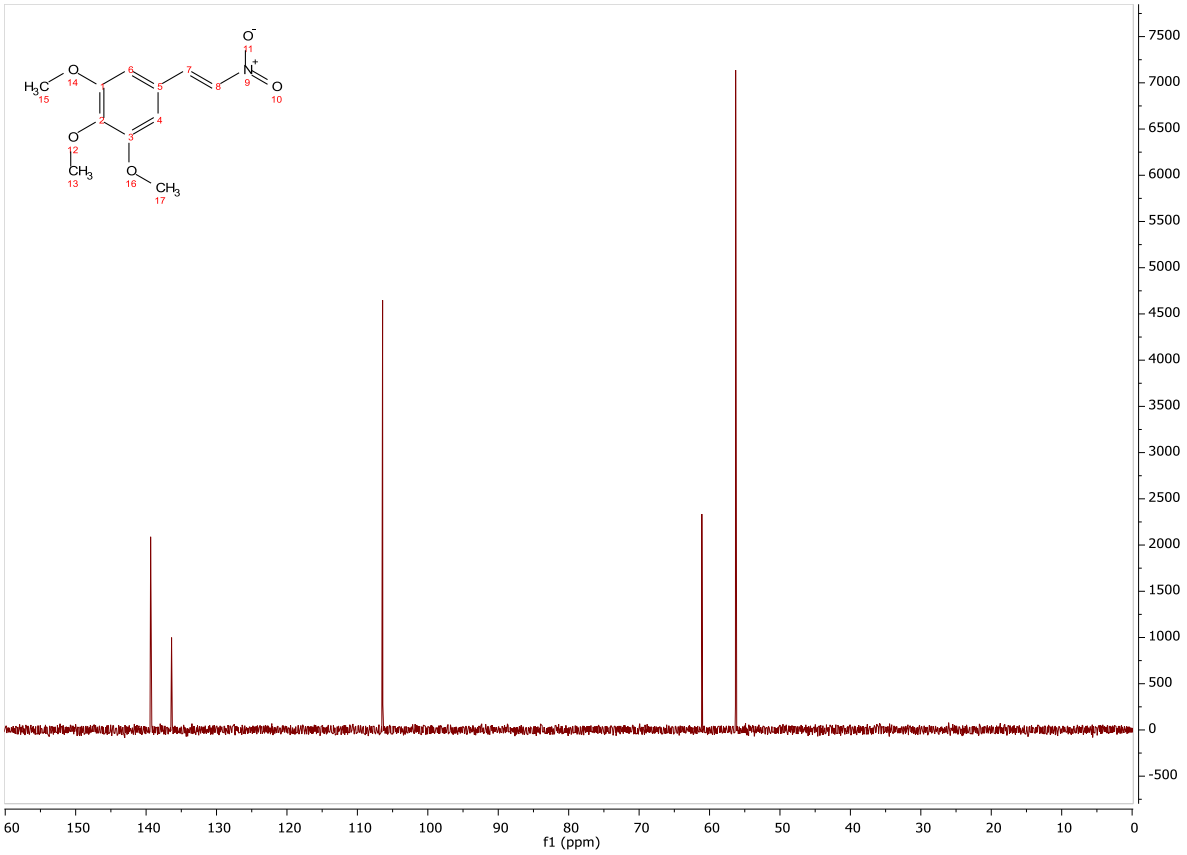
^{1}H:

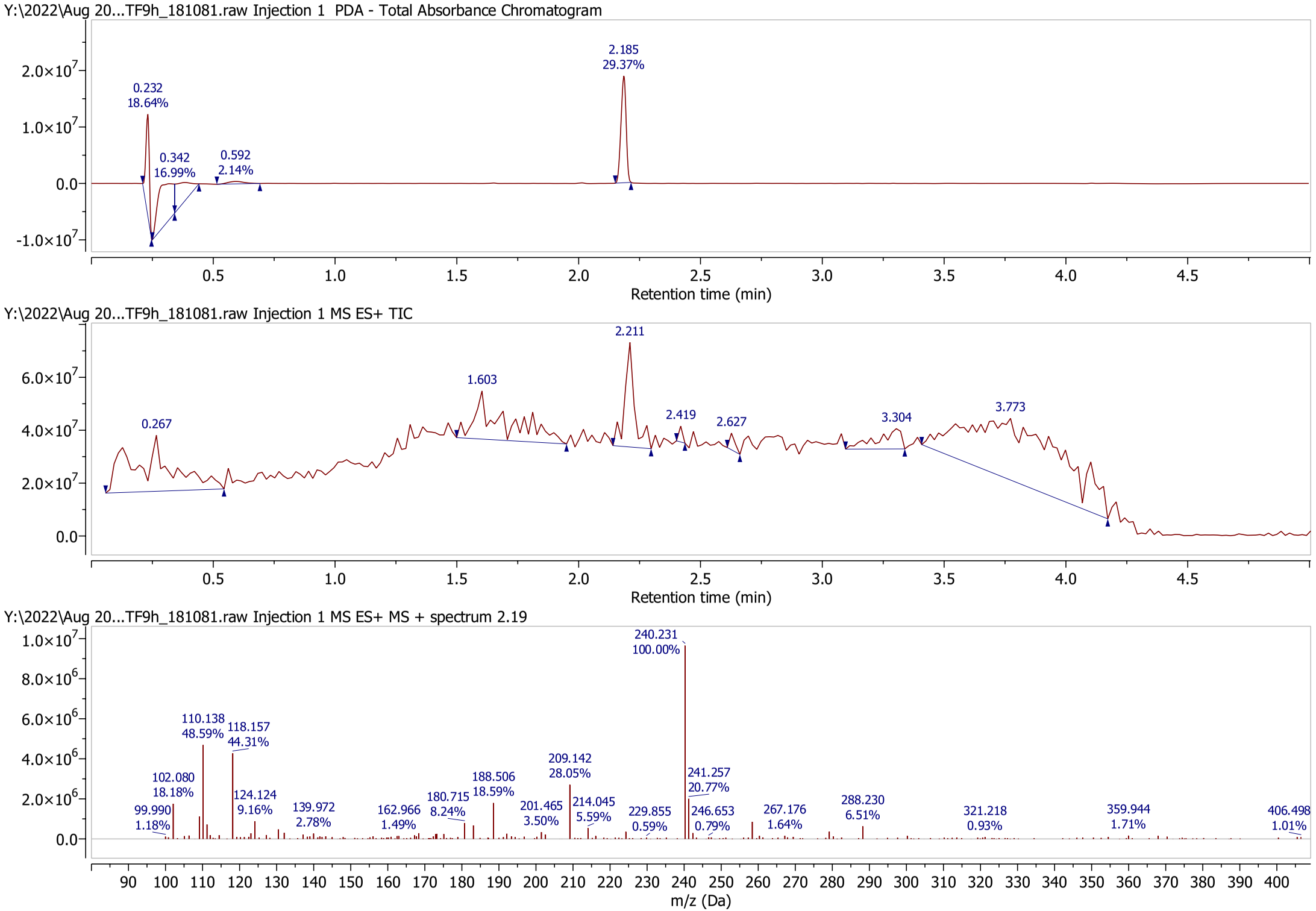


^{13}C:



DEPT-135:


7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Y:\2022\Aug 20...TF9h_181081.raw Injection 1 PDA - Total Absorbance Chromatogram
2.185
29.37%
0.232
18.64%
0.342
16.99%
0.592
2.14%
2.0×10^7
1.0×10^7
0.0
-1.0×10^7
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Aug 20...TF9h_181081.raw Injection 1 MS ES+ TIC
2.211
1.603
0.267
2.419
2.627
3.304
3.773
6.0×10^7
4.0×10^7
2.0×10^7
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
Retention time (min)
Y:\2022\Aug 20...TF9h_181081.raw Injection 1 MS ES+ MS + spectrum 2.19
240.231
100.00%
110.138
48.59%
118.157
44.31%
102.080
18.18%
124.124
9.16%
99.990
1.18%
139.972
2.78%
162.966
1.49%
180.715
8.24%
188.506
18.59%
209.142
28.05%
201.465
3.50%
214.045
5.59%
229.855
0.59%
241.257
20.77%
246.653
0.79%
267.176
1.64%
288.230
6.51%
321.218
0.93%
359.944
1.71%
406.498
1.01%
1.0×10^7
8.0×10^6
6.0×10^6
4.0×10^6
2.0×10^6
0.0
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320
330
340
350
360
370
380
390
400
m/z (Da)

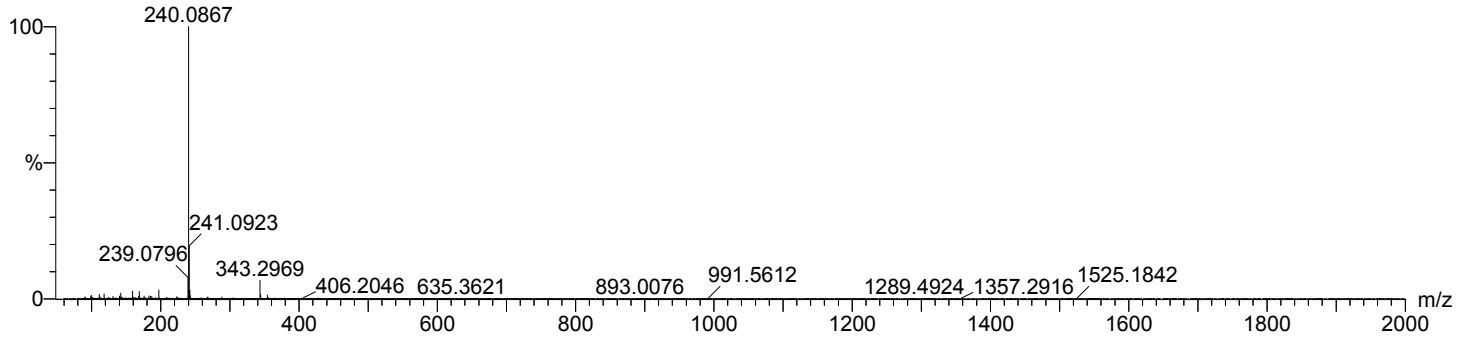
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
867 formula(e) evaluated with 8 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3

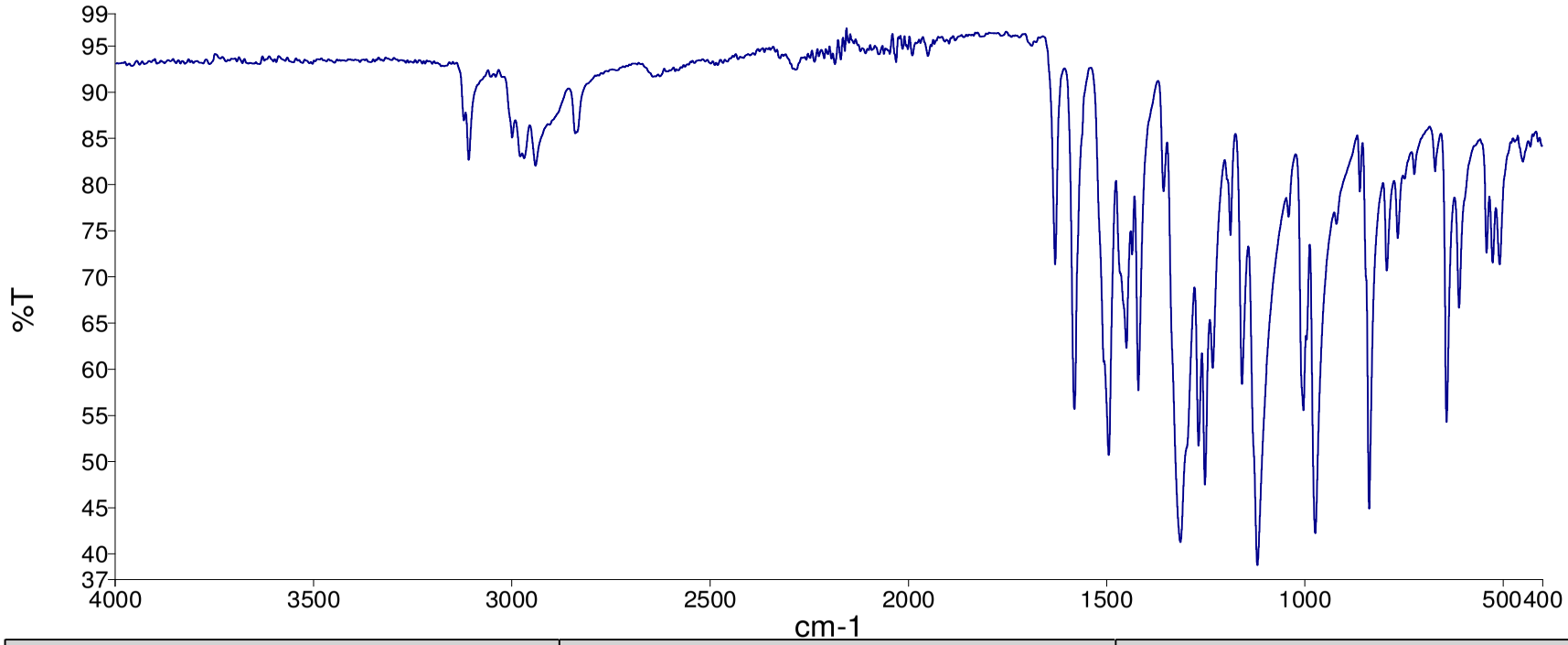
MTF9h 420 (3.559) Cm (417:421)

1: TOF MS ES+
9.89e+003



Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
240.0867	240.0868	-0.1	-0.4	-1.5	280.3	7.6	C H12 N7 O5 F2
	240.0872	-0.5	-2.1	5.5	273.6	1.0	C11 H14 N O5
	240.0857	1.0	4.2	2.5	278.1	5.5	C4 H11 N7 O4 F
	240.0883	-1.6	-6.7	1.5	275.1	2.4	C8 H15 N O6 F
	240.0885	-1.8	-7.5	10.5	273.7	1.0	C12 H10 N5 O
	240.0848	1.9	7.9	2.5	275.4	2.7	C9 H13 N O3 F3
	240.0845	2.2	9.2	6.5	276.5	3.9	C7 H10 N7 O3
	240.0897	-3.0	-12.5	6.5	275.5	2.8	C9 H11 N5 O2 F

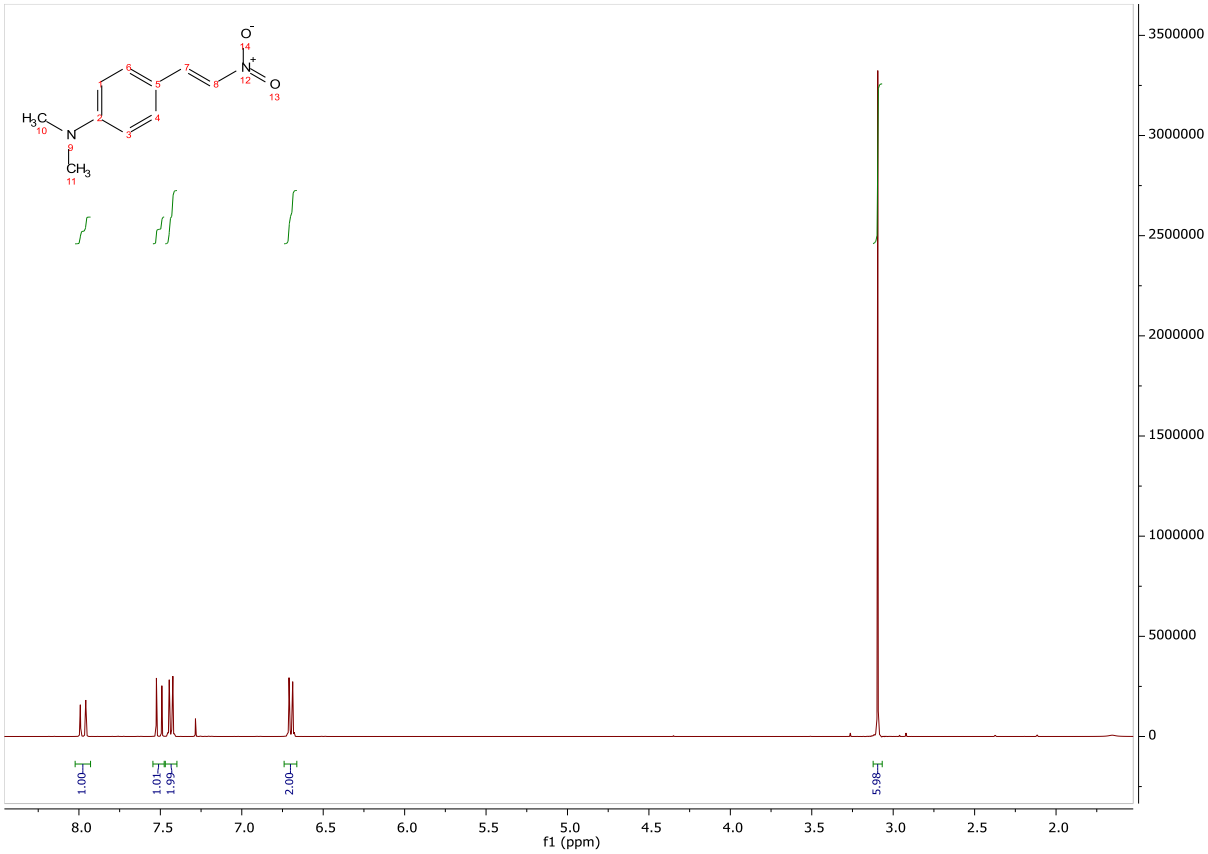
Analyst Lenny Lauchlan
Date 31 August 2022 08:11



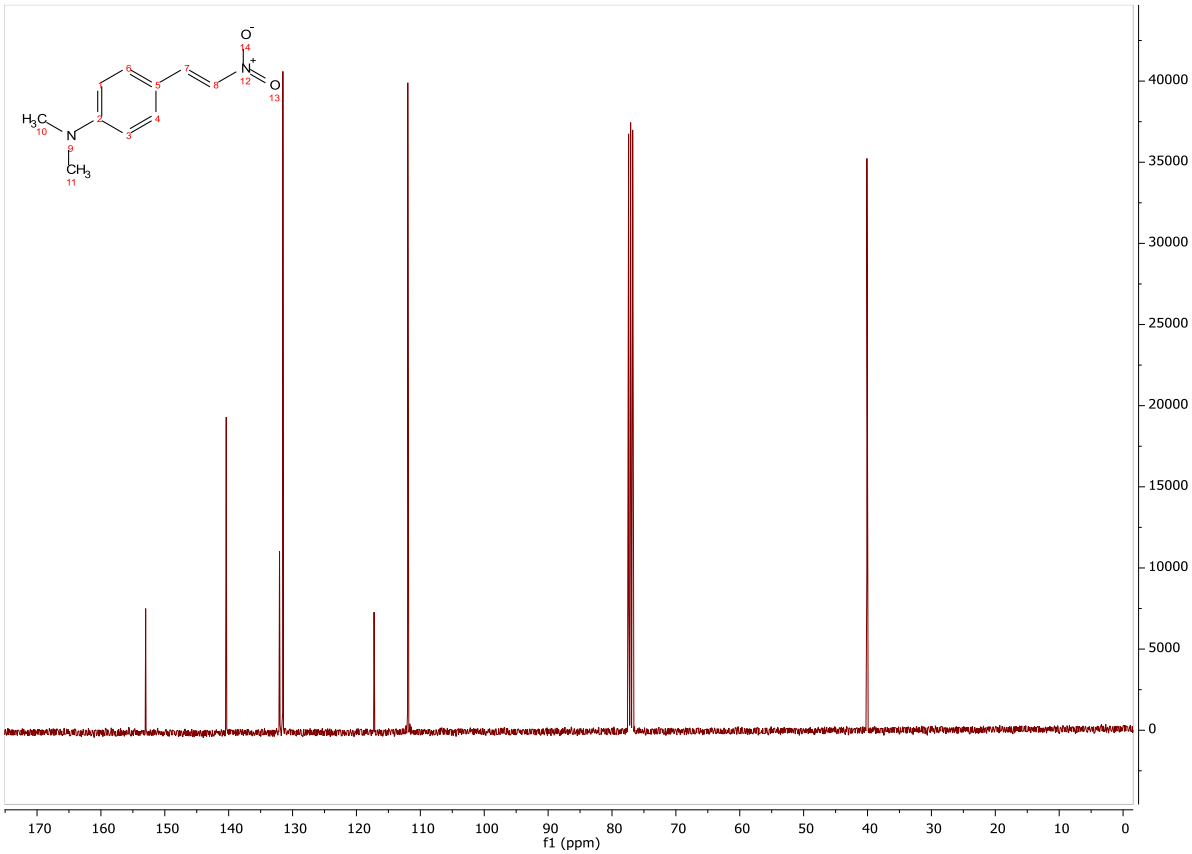
Sample Name	Description	Quality Checks
MTF 9h	Sample 025 By Lenny Date Wednesday, August 31 2022	The Quality Checks do not report any warnings for the sample.

(*E*)-*N*,*N*-dimethyl-4-(2-nitrovinyl)aniline **88k**

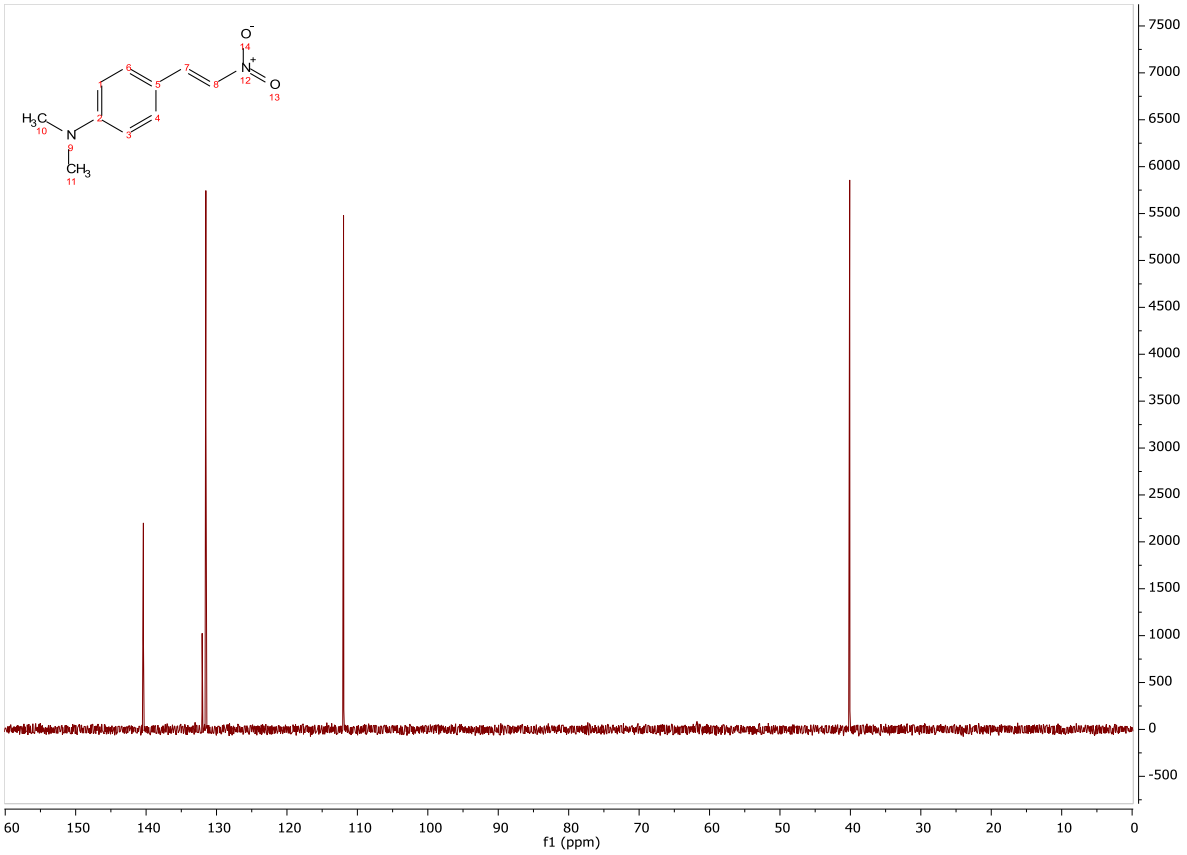
^{1}H:

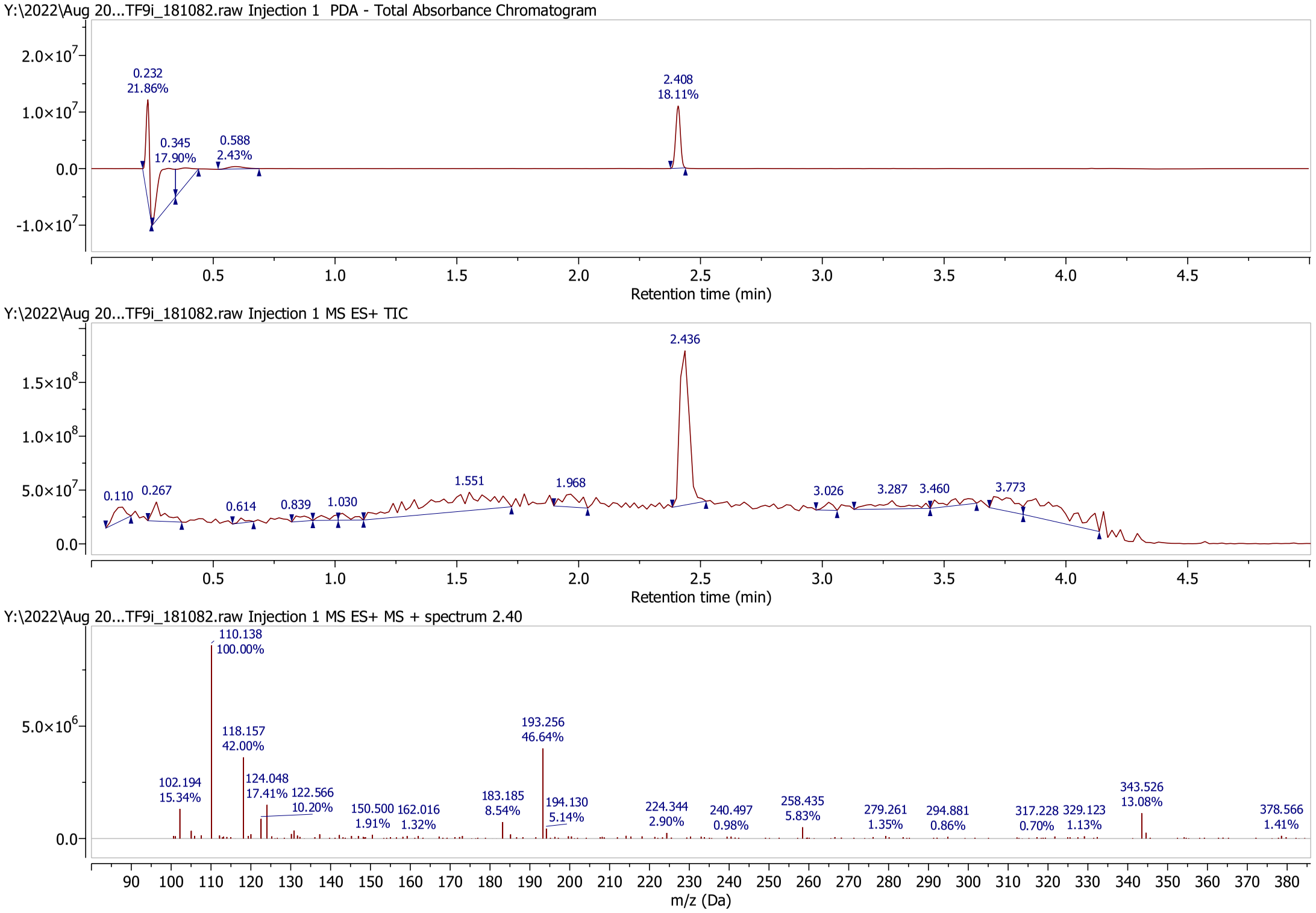


^{13}C:



DEPT-135:


7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Y:\2022\Aug 20...TF9i_181082.raw Injection 1 PDA - Total Absorbance Chromatogram
0.232
21.86%
0.345
17.90%
0.588
2.43%
2.408
18.11%
Retention time (min)
Y:\2022\Aug 20...TF9i_181082.raw Injection 1 MS ES+ TIC
0.110
0.267
0.614
0.839
1.030
1.551
1.968
2.436
3.026
3.287
3.460
3.773
Retention time (min)
Y:\2022\Aug 20...TF9i_181082.raw Injection 1 MS ES+ MS + spectrum 2.40
110.138
100.00%
118.157
42.00%
102.194
15.34%
124.048
17.41%
122.566
10.20%
150.500
1.91%
162.016
1.32%
183.185
8.54%
193.256
46.64%
194.130
5.14%
224.344
2.90%
240.497
0.98%
258.435
5.83%
279.261
1.35%
294.881
0.86%
317.228
0.70%
329.123
1.13%
343.526
13.08%
378.566
1.41%
m/z (Da)

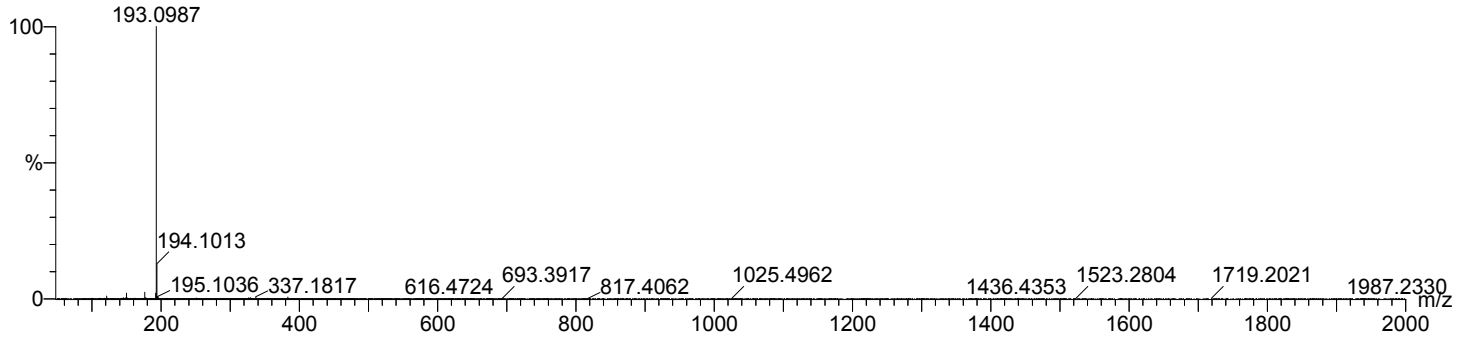
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
539 formula(e) evaluated with 5 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-3

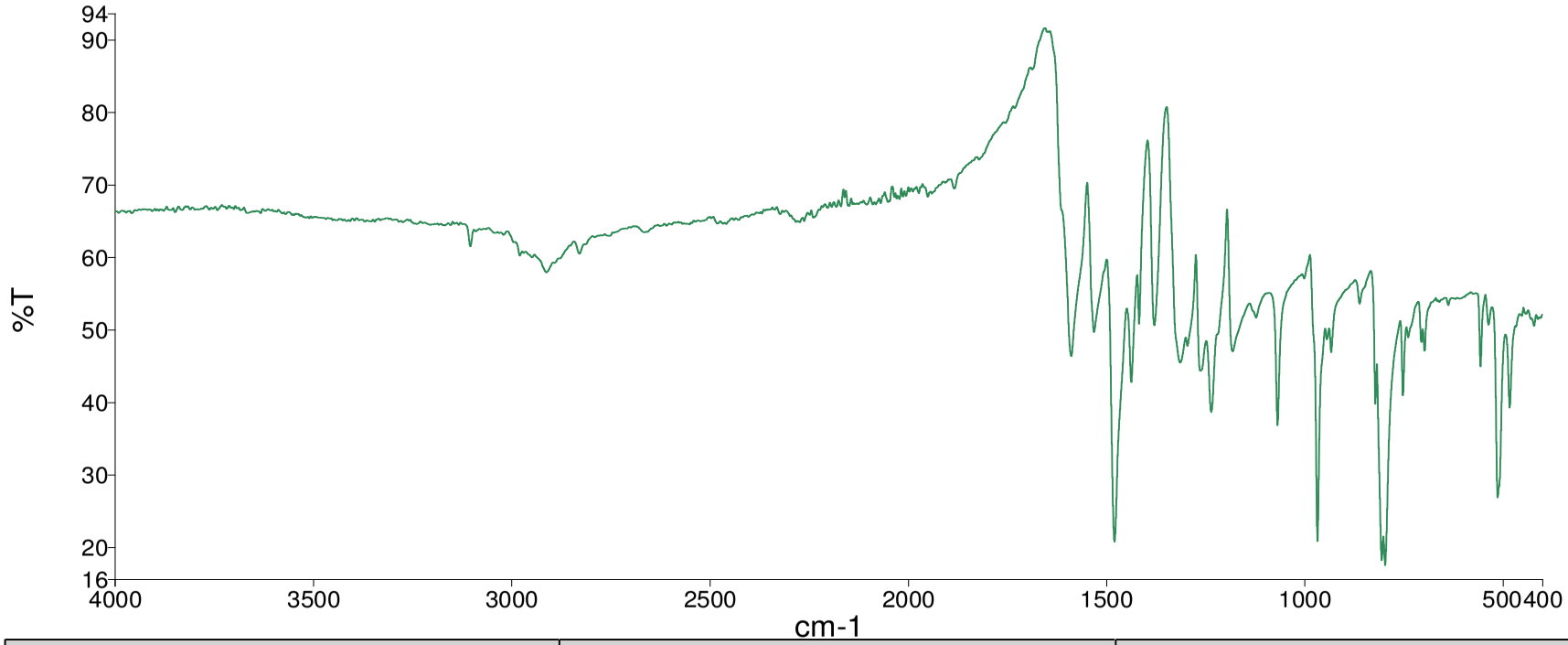
MTF9i 453 (3.842) Cm (452:454)

1: TOF MS ES+
6.05e+004



Minimum:				-1.5			
Maximum:		3.0	5.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
193.0987	193.0988	-0.1	-0.5	1.5	476.0	3.2	C7 H14 N2 O3 F
	193.0977	1.0	5.2	5.5	472.8	0.0	C10 H13 N2 O2
	193.0973	1.4	7.3	-1.5	489.6	16.8	H11 N8 O2 F2
	193.0962	2.5	12.9	2.5	484.9	12.1	C3 H10 N8 O F
	193.1013	-2.6	-13.5	2.5	481.7	8.9	C5 H11 N6 F2

Analyst Lenny Lauchlan
Date 31 August 2022 08:15

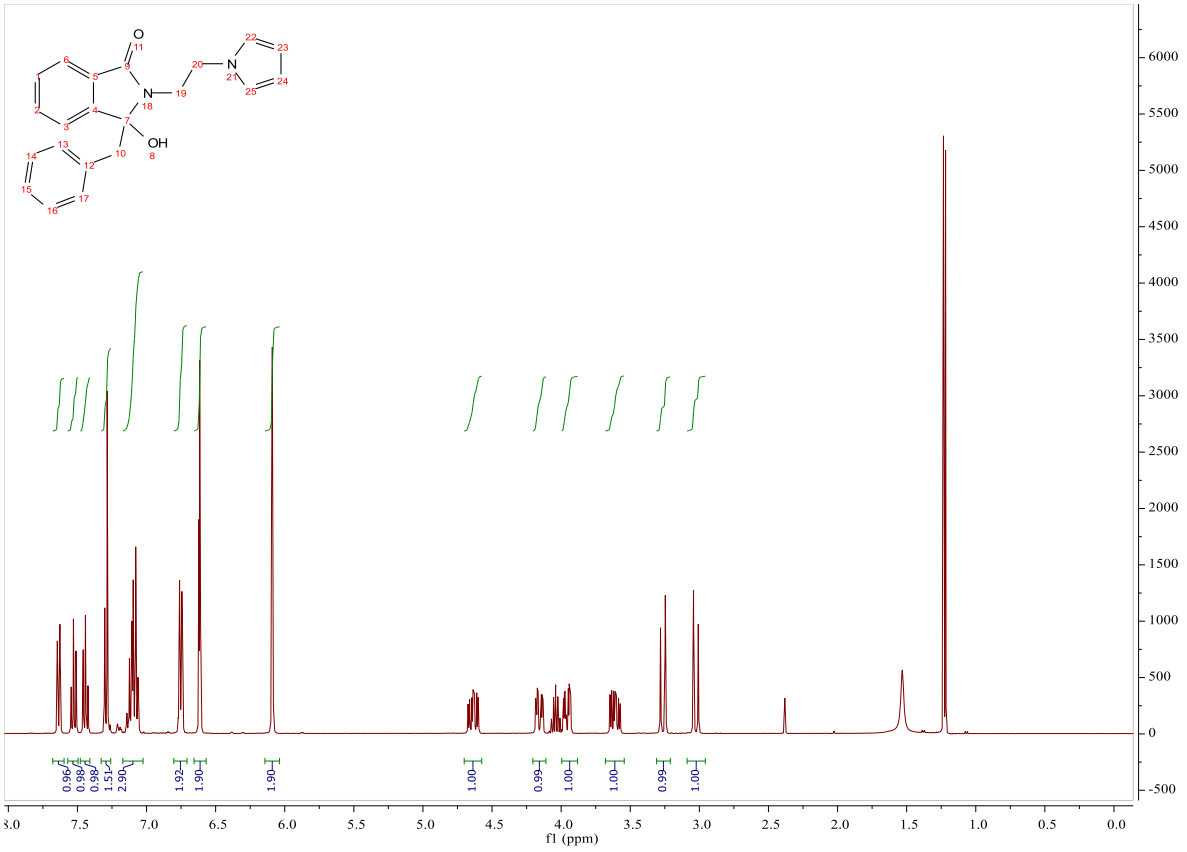


Sample Name	Description	Quality Checks
MTF 9i rpt	Sample 027 By Lenny Date Wednesday, August 31 2022	The Quality Checks do not report any warnings for the sample.

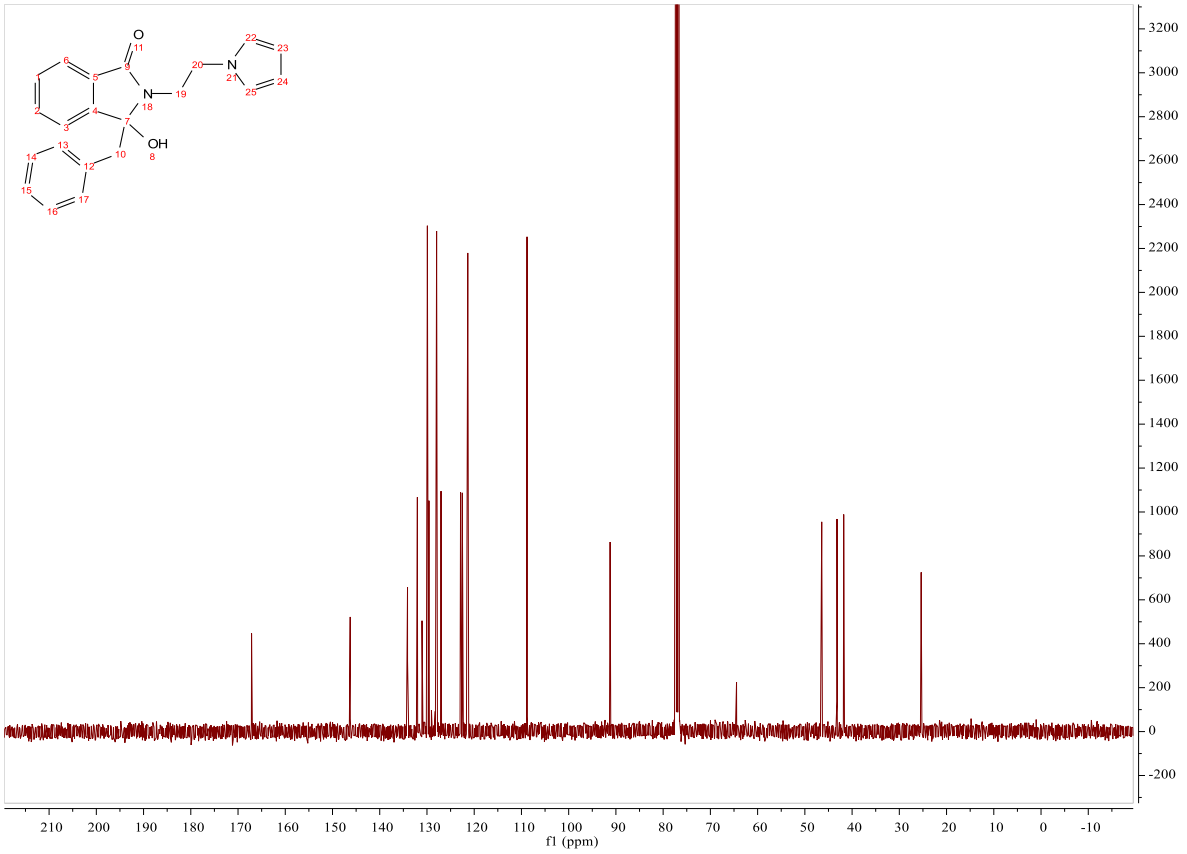
Miscellaneous

2-(2-(1*H*-pyrrol-1-yl)ethyl)-3-benzyl-3-hydroxyisoindolin-1-one **25**

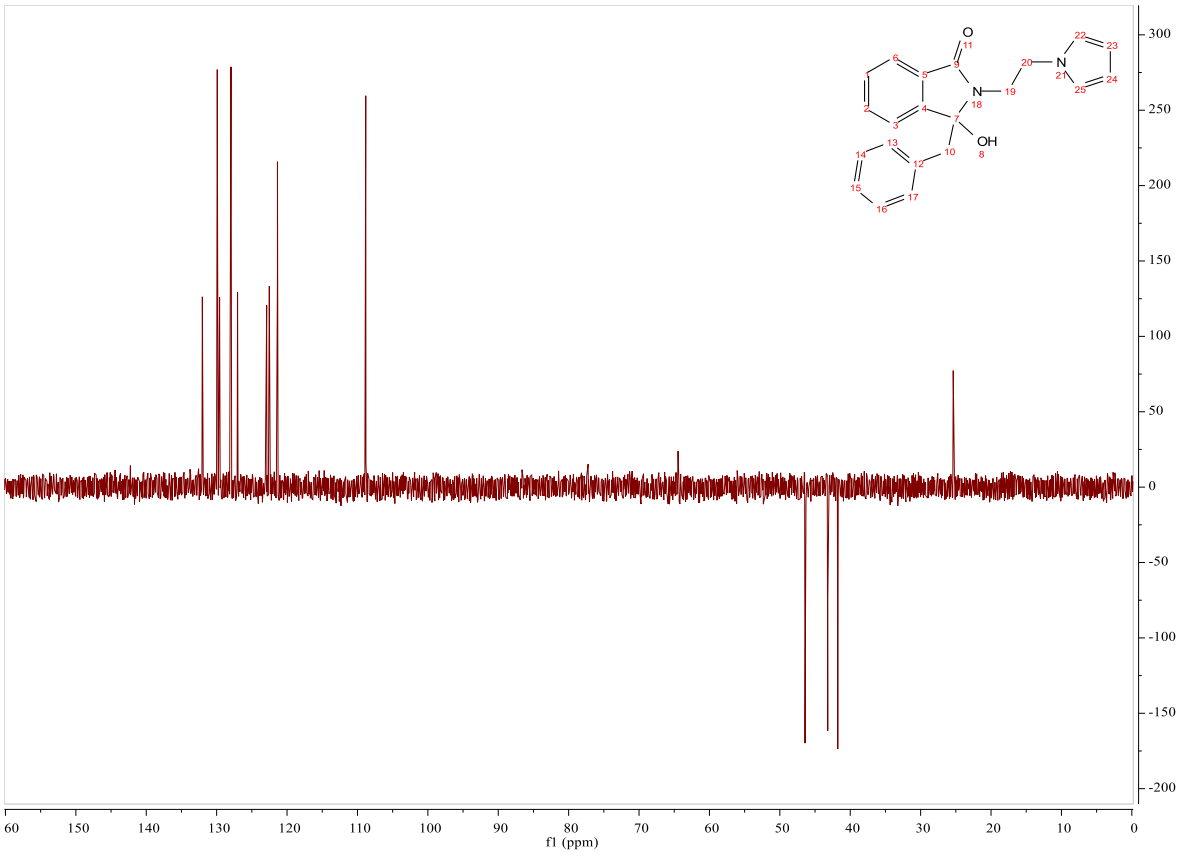
^{1}H:

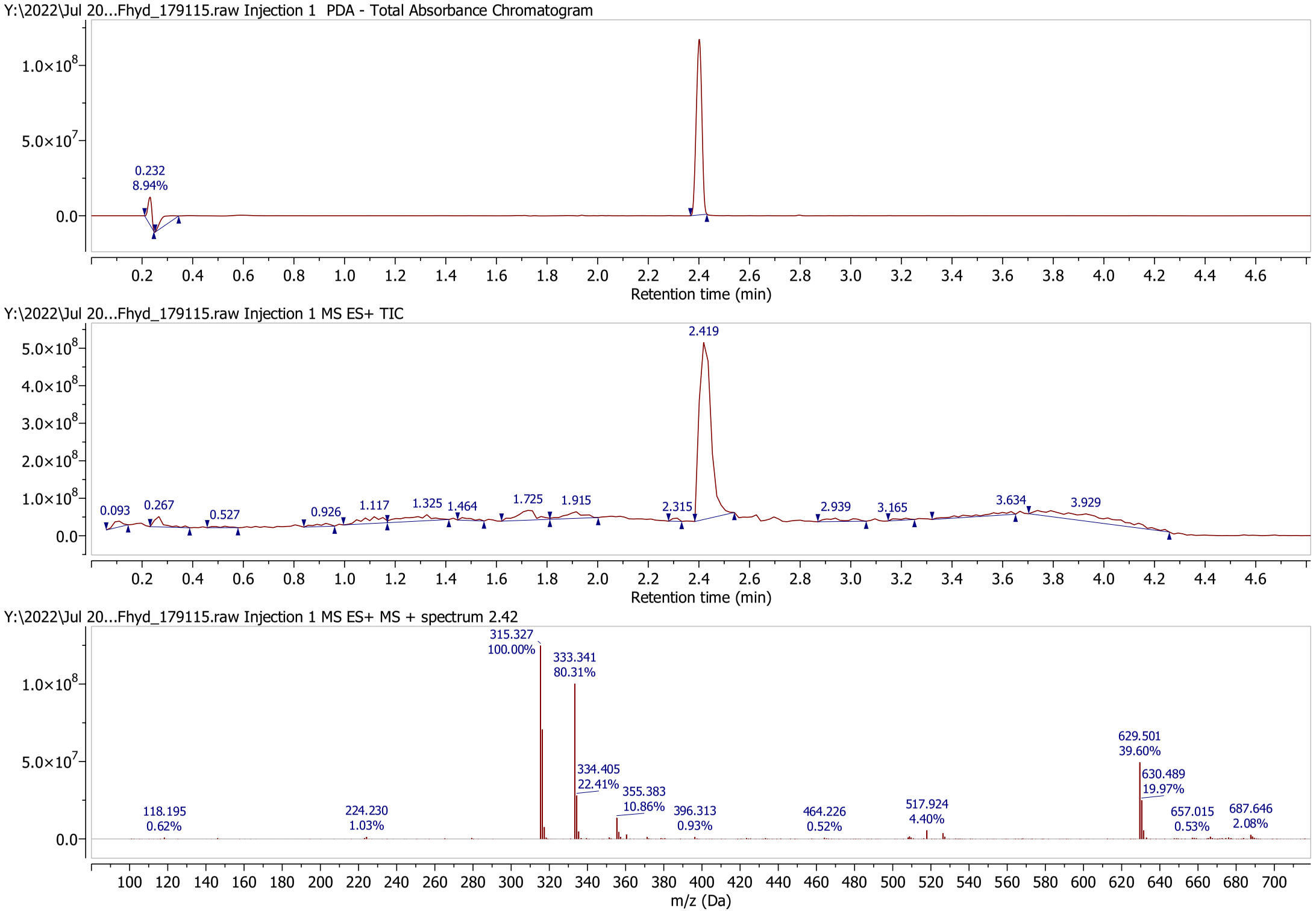


^{13}C:



DEPT-135:


O
11
6
5
9
N
18
19
20
N
21
22
23
24
25
2
4
3
7
OH
8
10
13
14
12
15
16
17
300
250
200
150
100
50
0
-50
-100
-150
-200
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Y:\2022\Jul 20...Fhyd_179115.raw Injection 1 PDA - Total Absorbance Chromatogram
1.0×10^8
5.0×10^7
0.0
0.232
8.94%
0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8 3.0 3.2 3.4 3.6 3.8 4.0 4.2 4.4 4.6
Retention time (min)
Y:\2022\Jul 20...Fhyd_179115.raw Injection 1 MS ES+ TIC
5.0×10^8
4.0×10^8
3.0×10^8
2.0×10^8
1.0×10^8
0.0
2.419
0.093 0.267 0.527 0.926 1.117 1.325 1.464 1.725 1.915 2.315 2.939 3.165 3.634 3.929
0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8 3.0 3.2 3.4 3.6 3.8 4.0 4.2 4.4 4.6
Retention time (min)
Y:\2022\Jul 20...Fhyd_179115.raw Injection 1 MS ES+ MS + spectrum 2.42
1.0×10^8
5.0×10^7
0.0
315.327
100.00%
333.341
80.31%
334.405
22.41%
355.383
10.86%
396.313
0.93%
464.226
0.52%
517.924
4.40%
629.501
39.60%
630.489
19.97%
657.015
0.53%
687.646
2.08%
118.195
0.62%
224.230
1.03%
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700
m/z (Da)

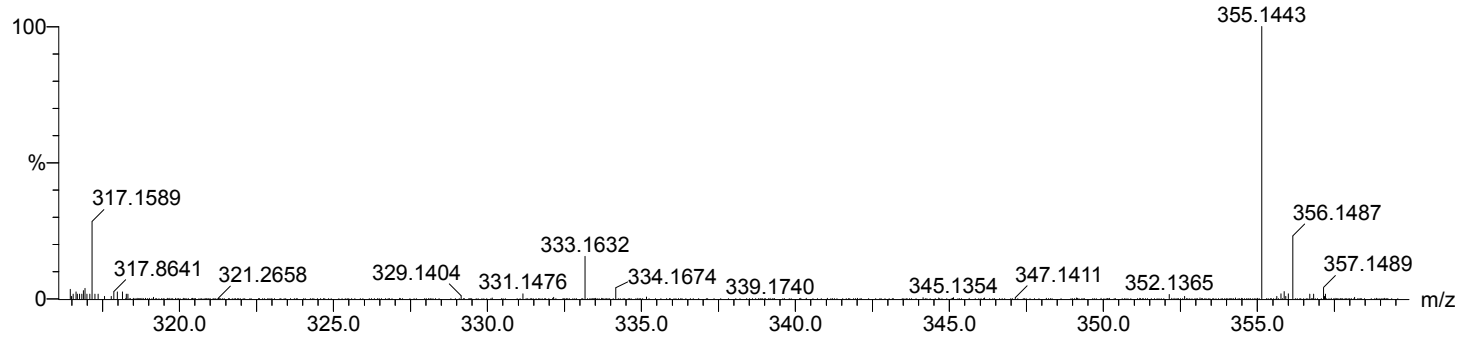
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
314 formula(e) evaluated with 4 results within limits (up to 200 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-8 O: 0-8

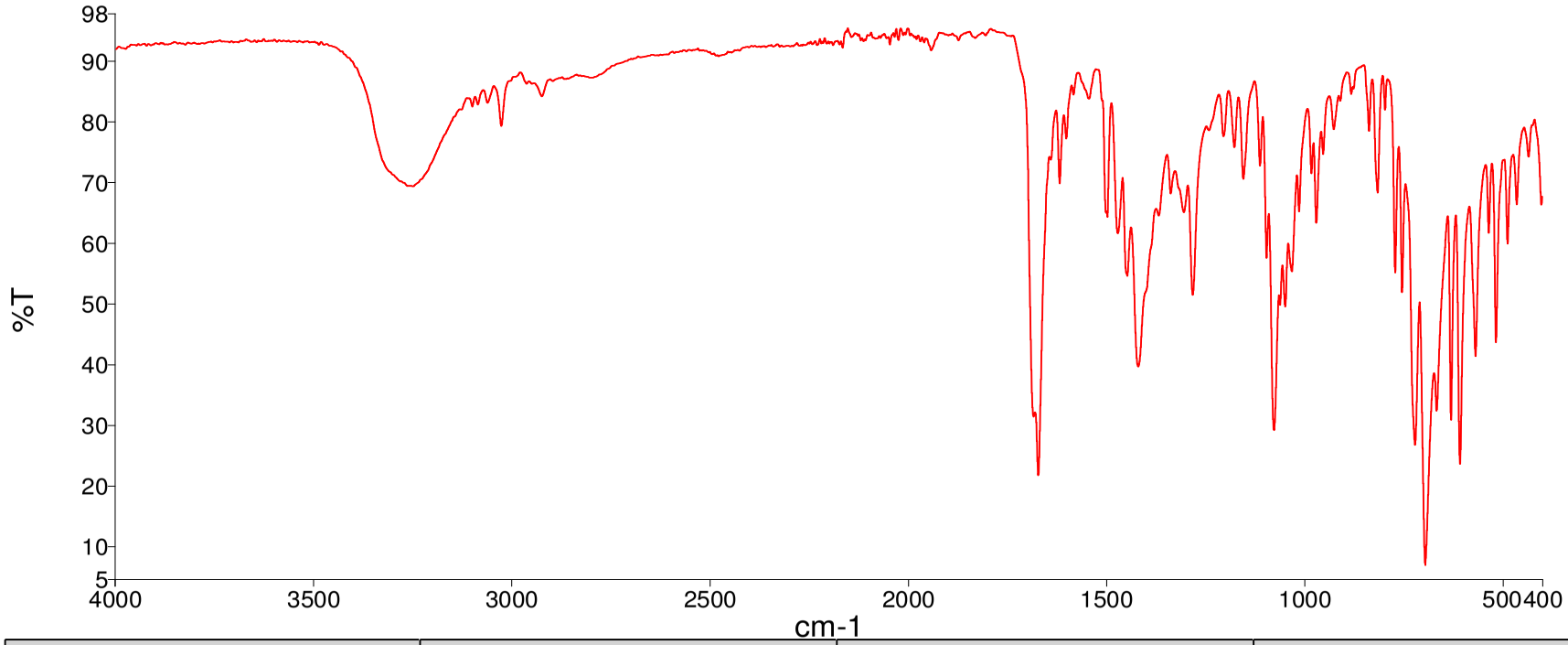
MTF_MTFhyd_179356 489 (4.111) Cm (489:491)

1: TOF MS ES+
6.01e+003



Minimum:				-1.5						
Maximum:		3.0	100.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula			
333.1632	333.1635	-0.3	-0.9	4.5	78.0	4.7	C10	H21	N8	O5
	333.1643	-1.1	-3.3	16.5	73.5	0.3	C26	H21		
	333.1603	2.9	8.7	12.5	74.8	1.6	C21	H21	N2	O2
	333.1662	-3.0	-9.0	3.5	78.4	5.1	C14	H25	N2	O7

Analyst Lenny Lauchlan
Date 19 November 2021 08:21



Sample Name	Description	Quality Checks	TimeStamp
21 srv 1159 MFr	Sample 012 By Lenny Date Friday, November 19 2021	The Quality Checks do not report any warnings for the sample.	3967693.346

X-ray crystallography data

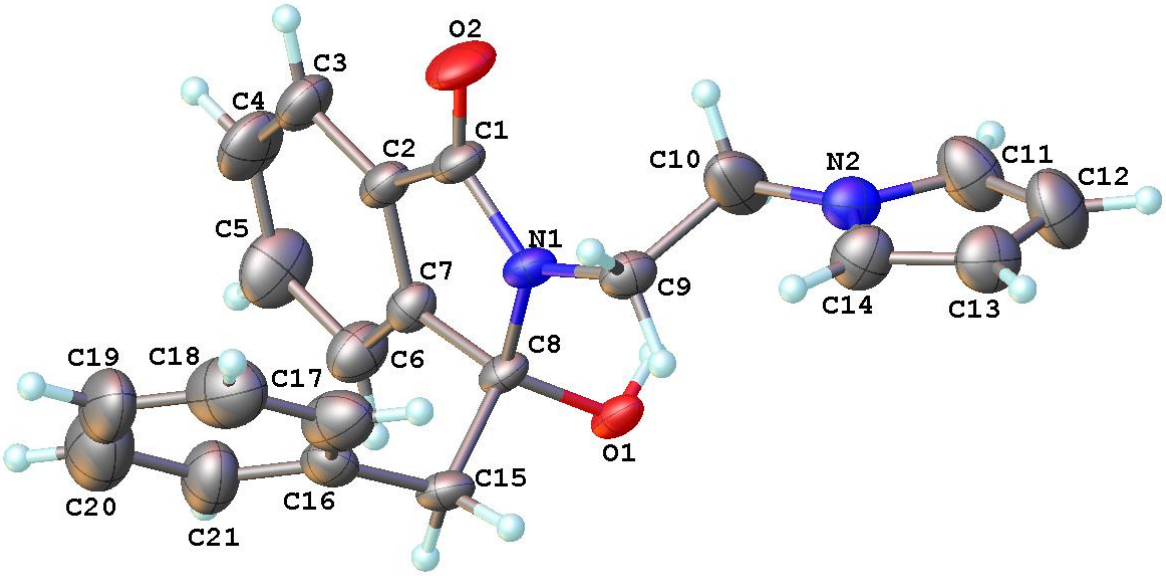


Table 1 Crystal data and structure refinement for 22srv021.	
Identification code	22srv021
Empirical formula	$C_{21}H_{20}N_2O_2$
Formula weight	332.39
Temperature/K	120.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.6547(11)
b/Å	9.1573(8)
c/Å	15.7046(13)
α/°	90
β/°	114.297(3)
γ/°	90
Volume/Å^3	1789.8(3)
Z	4
ρ_{calc}g/cm^3	1.234
μ/mm^{-1}	0.080
F(000)	704.0
Crystal size/mm^3	0.38 × 0.04 × 0.01

Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.146 to 52
Index ranges	-16 ≤ h ≤ 16, -11 ≤ k ≤ 11, -19 ≤ l ≤ 19
Reflections collected	22996
Independent reflections	3520 [R_{int} = 0.1172, R_{sigma} = 0.0867]
Data/restraints/parameters	3520/72/261
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0744, wR_2 = 0.1545
Final R indexes [all data]	R_1 = 0.1248, wR_2 = 0.1771
Largest diff. peak/hole / e $Å^{-3}$	0.31/-0.20

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 22srv021. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	8667.6(15)	4258(2)	4386.2(13)	29.8(5)
O2	7327.5(17)	7612(3)	2102.7(14)	50.4(7)
N1	8282.3(18)	6430(2)	3473.0(14)	27.3(6)
N2	10571(2)	5792(3)	2807.0(17)	36.8(6)
C1	7366(2)	6846(3)	2762.3(19)	31.3(7)
C2	6477(2)	6193(3)	2925.2(18)	30.9(7)
C3	5389(2)	6218(4)	2370(2)	43.1(8)
C4	4723(3)	5463(4)	2668(3)	55.8(10)
C5	5132(3)	4701(4)	3503(3)	58.9(10)
C6	6240(2)	4684(3)	4068(2)	43.0(8)
C7	6900(2)	5439(3)	3761.0(19)	28.7(7)
C8	8106(2)	5588(3)	4201.3(18)	25.4(6)
C9	9340(2)	6707(3)	3489.9(19)	32.0(7)
C10	9473(3)	5854(4)	2717(2)	56.7(10)
C11	10957(3)	4676(4)	2466(3)	55.2(10)
C12	12021(3)	4923(4)	2692(3)	60.0(11)
C13	12289(3)	6249(4)	3170(2)	47.3(9)
C14	11390(3)	6743(4)	3249(2)	45.0(9)
C15	8534(2)	6420(3)	5136.6(18)	30.7(7)
C16	8093(8)	7880(7)	5080(8)	36(3)
C17	8562(6)	9061(9)	4834(7)	56(3)
C18	8119(6)	10447(8)	4759(5)	70(3)
C19	7208(6)	10652(7)	4931(6)	66(3)
C20	6739(6)	9471(9)	5177(6)	79(3)
C21	7182(8)	8085(8)	5251(8)	56(3)

C16A	7927(7)	7879(6)	5123(7)	26(3)
C17A	8182(5)	9155(7)	4779(5)	29.0(17)
C18A	7614(4)	10431(5)	4740(4)	29.2(16)
C19A	6792(4)	10432(6)	5045(4)	36.6(18)
C20A	6536(5)	9155(7)	5388(5)	50(2)
C21A	7104(7)	7879(6)	5427(6)	41(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 22srv021. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	27.9(11)	24.8(11)	23.9(10)	-1.1(9)	-2.2(8)	4.9(9)
O2	47.5(14)	59.8(16)	35.7(12)	25.9(11)	8.9(11)	14.2(11)
N1	24.9(13)	28.9(13)	20.9(12)	2.8(10)	2.0(10)	-0.1(10)
N2	32.0(15)	43.5(16)	34.3(14)	1.3(12)	13.1(12)	-3.9(12)
C1	30.3(17)	31.2(17)	24.0(15)	5.6(13)	2.5(12)	7.3(13)
C2	26.6(16)	30.1(16)	27.2(15)	-0.1(12)	2.1(13)	5.6(13)
C3	27.3(18)	51(2)	39.5(18)	2.1(16)	1.9(15)	8.9(16)
C4	24.8(19)	69(3)	59(2)	-1(2)	2.6(17)	2.7(18)
C5	39(2)	59(3)	78(3)	6(2)	23(2)	-10.8(18)
C6	33.5(19)	45(2)	47.1(19)	8.1(16)	13.5(16)	0.1(15)
C7	24.8(16)	24.9(16)	31.3(15)	-1.1(12)	6.4(13)	-0.8(13)
C8	24.2(15)	21.5(15)	23.5(14)	5.1(11)	2.8(11)	2.9(12)
C9	26.0(16)	35.9(18)	28.6(15)	3.0(13)	5.7(12)	-2.8(13)
C10	33(2)	90(3)	43(2)	-21.9(19)	10.6(16)	-5.9(19)
C11	56(2)	57(2)	61(2)	-19.3(19)	33(2)	-14.7(19)
C12	54(3)	69(3)	70(3)	-15(2)	39(2)	-6(2)
C13	38(2)	52(2)	53(2)	0.0(18)	20.3(17)	-9.9(17)
C14	37(2)	41(2)	51(2)	-5.3(16)	11.6(16)	-5.4(16)
C15	31.9(17)	31.1(17)	20.2(14)	2.4(12)	1.7(12)	-0.4(13)
C16	42(5)	37(5)	24(4)	-6(4)	9(4)	0(3)
C17	67(5)	44(4)	44(4)	-6(3)	9(4)	4(4)
C18	87(6)	52(5)	61(4)	-5(4)	20(4)	3(4)
C19	70(5)	57(5)	65(5)	-8(4)	22(4)	25(4)
C20	74(5)	74(6)	83(5)	-16(5)	25(4)	14(4)
C21	52(5)	50(5)	63(5)	-8(4)	20(4)	10(4)
C16A	28(4)	23(4)	19(4)	-5(3)	1(3)	6(3)
C17A	35(4)	24(4)	28(3)	-2(3)	12(3)	-2(3)
C18A	31(4)	29(3)	28(3)	3(2)	14(3)	6(3)
C19A	37(4)	26(4)	43(3)	-1(3)	13(3)	3(3)
C20A	53(4)	56(4)	50(4)	-7(3)	30(3)	11(3)
C21A	48(4)	40(4)	39(4)	-3(3)	23(3)	3(3)

Table 4 Bond Lengths for 22srv021.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
O1	C8	1.404(3)		C11	C12	1.365(5)
O2	C1	1.233(3)		C12	C13	1.396(5)
N1	C1	1.344(3)		C13	C14	1.360(4)
N1	C8	1.479(3)		C15	C16	1.453(6)
N1	C9	1.455(3)		C15	C16A	1.567(5)
N2	C10	1.449(4)		C16	C17	1.3900
N2	C11	1.357(4)		C16	C21	1.3900
N2	C14	1.361(4)		C17	C18	1.3900
C1	C2	1.467(4)		C18	C19	1.3900
C2	C3	1.380(4)		C19	C20	1.3900
C2	C7	1.382(4)		C20	C21	1.3900
C3	C4	1.368(5)		C16A	C17A	1.3900
C4	C5	1.384(5)		C16A	C21A	1.3900
C5	C6	1.404(4)		C17A	C18A	1.3900
C6	C7	1.371(4)		C18A	C19A	1.3900
C7	C8	1.508(4)		C19A	C20A	1.3900
C8	C15	1.540(4)		C20A	C21A	1.3900
C9	C10	1.515(4)				

Table 5 Bond Angles for 22srv021.								
Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C8	113.5(2)		N1	C9	C10	109.9(2)
C1	N1	C9	122.9(2)		N2	C10	C9	113.7(3)
C9	N1	C8	123.5(2)		N2	C11	C12	108.5(3)
C11	N2	C10	123.1(3)		C11	C12	C13	107.4(3)
C11	N2	C14	108.2(3)		C14	C13	C12	107.0(3)
C14	N2	C10	128.7(3)		C13	C14	N2	108.9(3)
O2	C1	N1	124.2(3)		C8	C15	C16A	114.7(4)
O2	C1	C2	128.7(3)		C16	C15	C8	114.3(5)
N1	C1	C2	107.1(2)		C17	C16	C15	120.4(6)
C3	C2	C1	129.6(3)		C17	C16	C21	120.0
C3	C2	C7	121.9(3)		C21	C16	C15	119.6(6)
C7	C2	C1	108.5(2)		C16	C17	C18	120.0
C4	C3	C2	118.0(3)		C17	C18	C19	120.0
C3	C4	C5	120.9(3)		C20	C19	C18	120.0
C4	C5	C6	120.9(3)		C19	C20	C21	120.0
C7	C6	C5	117.7(3)		C20	C21	C16	120.0
C2	C7	C8	109.9(2)		C17A	C16A	C15	120.4(5)
C6	C7	C2	120.5(3)		C17A	C16A	C21A	120.0
C6	C7	C8	129.5(3)		C21A	C16A	C15	119.5(5)
O1	C8	N1	111.3(2)		C18A	C17A	C16A	120.0
O1	C8	C7	114.6(2)		C17A	C18A	C19A	120.0

O1	C8	C15	105.7(2)		C18A	C19A	C20A	120.0
N1	C8	C7	100.8(2)		C21A	C20A	C19A	120.0
N1	C8	C15	111.2(2)		C20A	C21A	C16A	120.0
C7	C8	C15	113.3(2)					

Table 6 Hydrogen Bonds for 22srv021.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1	H1	O2[1]	0.90(3)	1.75(3)	2.641(3)	169(3)

[1]3/2-X,-1/2+Y,1/2-Z

Table 7 Selected Torsion Angles for 22srv021.

A	B	C	D	Angle/°		A	B	C	D	Angle/°
N1	C9	C10	N2	-166.7(3)		C9	N1	C8	O1	-49.3(3)
C1	N1	C8	O1	127.1(2)		C9	C10	N2	C11	152.2(3)
C2	C7	C8	O1	-123.1(2)		C9	C10	N2	C14	-25.3(5)
C2	C7	C8	N1	-3.5(3)		C10	C9	N1	C1	-65.6(3)
C2	C7	C8	C15	115.4(3)		C10	C9	N1	C8	110.5(3)
C6	C7	C8	O1	55.9(4)		C15	C8	N1	C1	-115.3(3)
C6	C7	C8	N1	175.5(3)		C15	C8	N1	C9	68.3(3)
C6	C7	C8	C15	-65.6(4)		C16	C15	C8	O1	176.5(5)
C7	C8	N1	C1	5.1(3)		C16	C15	C8	N1	55.6(5)
C7	C8	N1	C9	-171.3(2)		C16A	C15	C8	O1	-173.6(4)
C7	C8	C15	C16	-57.1(5)		C16A	C15	C8	N1	65.4(4)
C7	C8	C15	C16A	-47.3(4)						

Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 22srv021.

Atom	*x*	*y*	*z*	U(eq)
H3	5109.35	6744.88	1798.45	52
H4	3971.04	5460.96	2296.28	67
H5	4656.23	4181.66	3696.26	71
H6	6522.18	4167.21	4643.42	52
H9A	9901.94	6411.06	4102.46	38
H9B	9423.73	7763.29	3404.66	38
H10A	9209.97	4845.35	2714.23	68
H10B	9018.55	6306.43	2109.71	68
H11	10554.77	3859.97	2126.99	66
H12	12492.74	4305.37	2549.27	72
H13	12969.87	6718.25	3398.16	57
H14	11342.25	7610.44	3561.04	54
H15C	9302.87	6645.22	5318.58	37

H15D	8485.03	5772.37	5622.27	37
H15A	8368.08	5846.14	5595.05	37
H15B	9325.26	6494.62	5374.52	37
H17	9184.24	8920.51	4716.2	68
H18	8439.4	11254.25	4591.01	84
H19	6905.51	11599.85	4880.08	79
H20	6116.45	9611.71	5294.35	95
H21	6861.27	7277.96	5419.55	67
H17A	8744.27	9154.64	4571.47	35
H18A	7788.65	11303.66	4505.98	35
H19A	6403.59	11304.14	5018.13	44
H20A	5974.14	9155.59	5595.77	60
H21A	6929.75	7006.55	5661.25	49
H1	8410(20)	3660(30)	3880(20)	48(10)

Table 9 Atomic Occupancy for 22srv021.

Atom	***Occupancy***		**Atom**	***Occupancy***		**Atom**	***Occupancy***
H15C	0.5		H15D	0.5		H15A	0.5
H15B	0.5		C16	0.5		C17	0.5
H17	0.5		C18	0.5		H18	0.5
C19	0.5		H19	0.5		C20	0.5
H20	0.5		C21	0.5		H21	0.5
C16A	0.5		C17A	0.5		H17A	0.5
C18A	0.5		H18A	0.5		C19A	0.5
H19A	0.5		C20A	0.5		H20A	0.5
C21A	0.5		H21A	0.5			

Refinement model description

Number of restraints - 72, number of constraints - unknown.

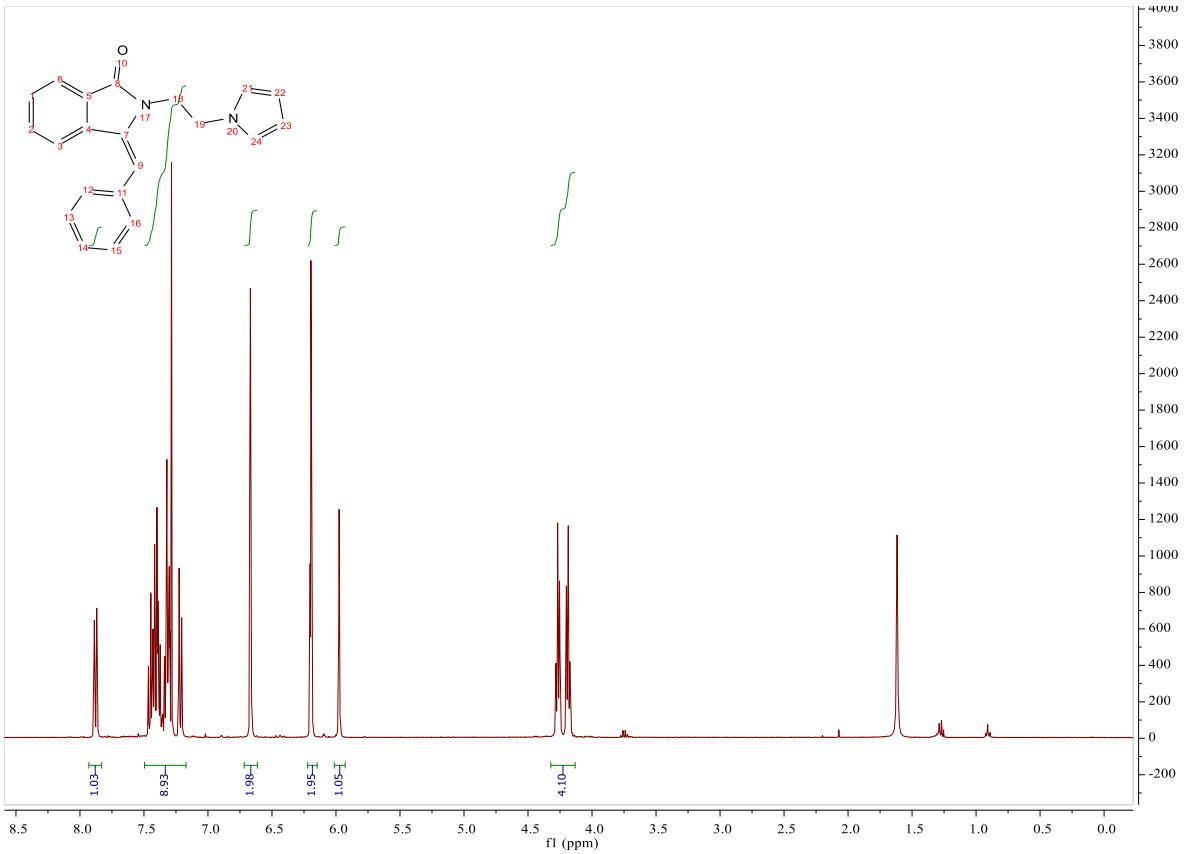
Details:

1. Fixed Uiso
At 1.2 times of: All C(H) groups, All C(H,H) groups, All C(H,H,H,H) groups
2. Uiso/Uaniso restraints and constraints
Uanis(C16A) ≈ Ueq, Uanis(C17A) ≈ Ueq, Uanis(C18A) ≈ Ueq,
Uanis(C20A) ≈ Ueq, Uanis(C21A) ≈ Ueq, Uanis(C16) ≈ Ueq, Uanis(C17)
≈ Ueq, Uanis(C18) ≈ Ueq, Uanis(C20) ≈ Ueq, Uanis(C21) ≈ Ueq,
Uanis(C19) ≈ Ueq, Uanis(C19A) ≈ Ueq: with sigma of 0.006 and sigma for
terminal atoms of 0.01
3. Others
Fixed Sof: H15C(0.5) H15D(0.5) H15A(0.5) H15B(0.5) C16(0.5) C17(0.5) H17(0.5) C18(0.5) H18(0.5) C19(0.5)
H19(0.5) C20(0.5) H20(0.5) C21(0.5) H21(0.5) C16A(0.5) C17A(0.5) H17A(0.5) C18A(0.5) H18A(0.5) C19A(0.5)
H19A(0.5) C20A(0.5) H20A(0.5) C21A(0.5) H21A(0.5)
4.a Secondary CH2 refined with riding coordinates:
C9(H9A,H9B), C10(H10A,H10B), C15(H15C,H15D), C15(H15A,H15B)

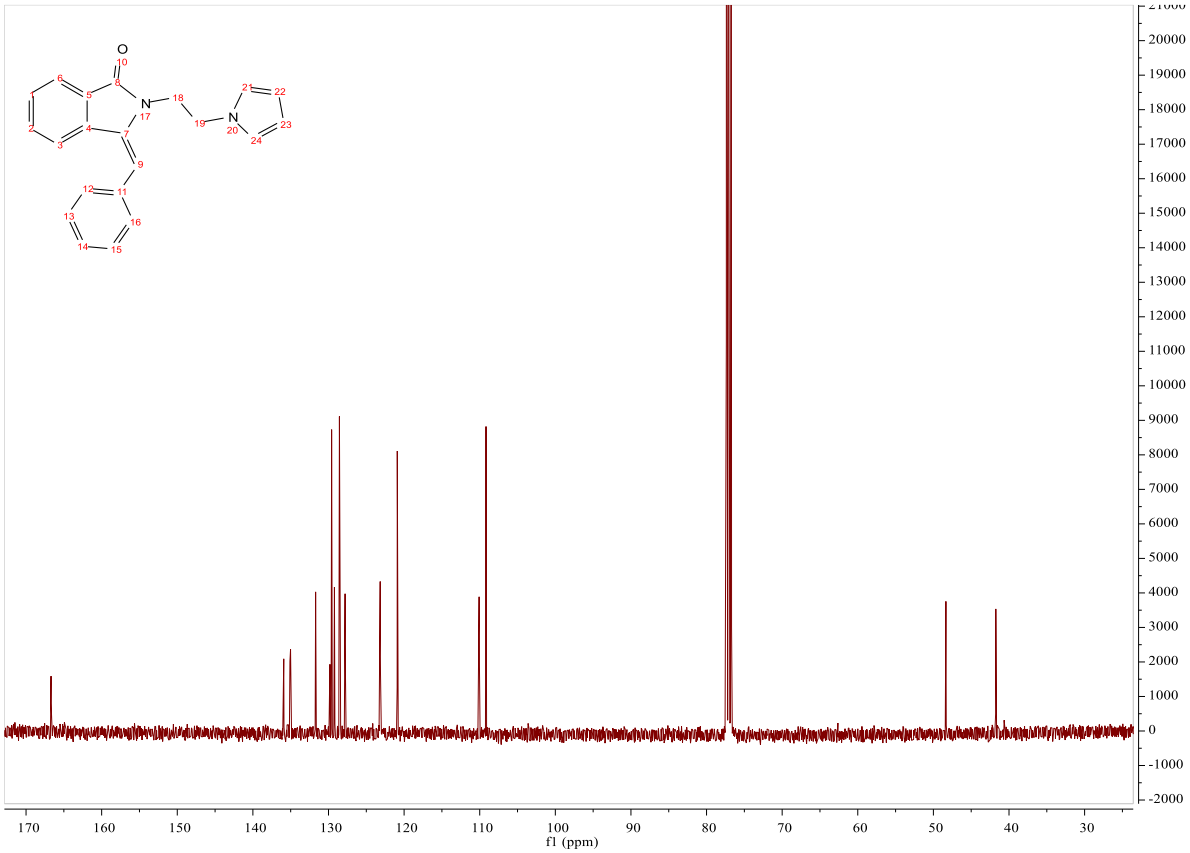
4.b Aromatic/amide H refined with riding coordinates:
C3(H3), C4(H4), C5(H5), C6(H6), C11(H11), C12(H12), C13(H13), C14(H14), C17(H17), C18(H18), C19(H19), C20(H20), C21(H21), C17A(H17A), C18A(H18A), C19A(H19A), C20A(H20A), C21A(H21A)
4.c Fitted hexagon refined as free rotating group:
C16(C17,C18,C19,C20,C21), C16A(C17A,C18A,C19A,C20A,C21A)

(*E*)-2-(2-(1*H*-pyrrol-1-yl)ethyl)-3-benzylideneisoindolin-1-one **43**

^{1}H:



^{13}C:



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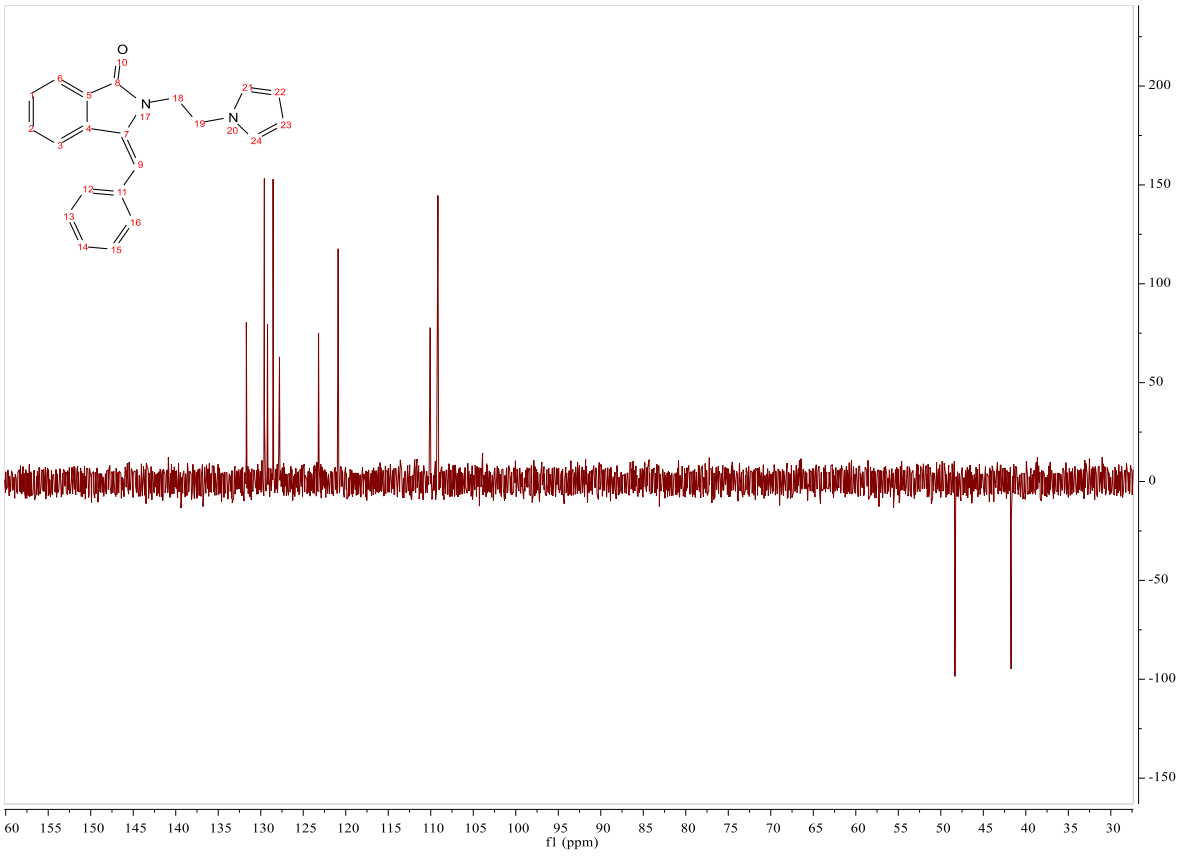
O
10
6
5
9
1
N
18
21
22
2
4
7
17
19
N
20
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9
12
11
13
16
14
15
200
150
100
50
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-100
-150
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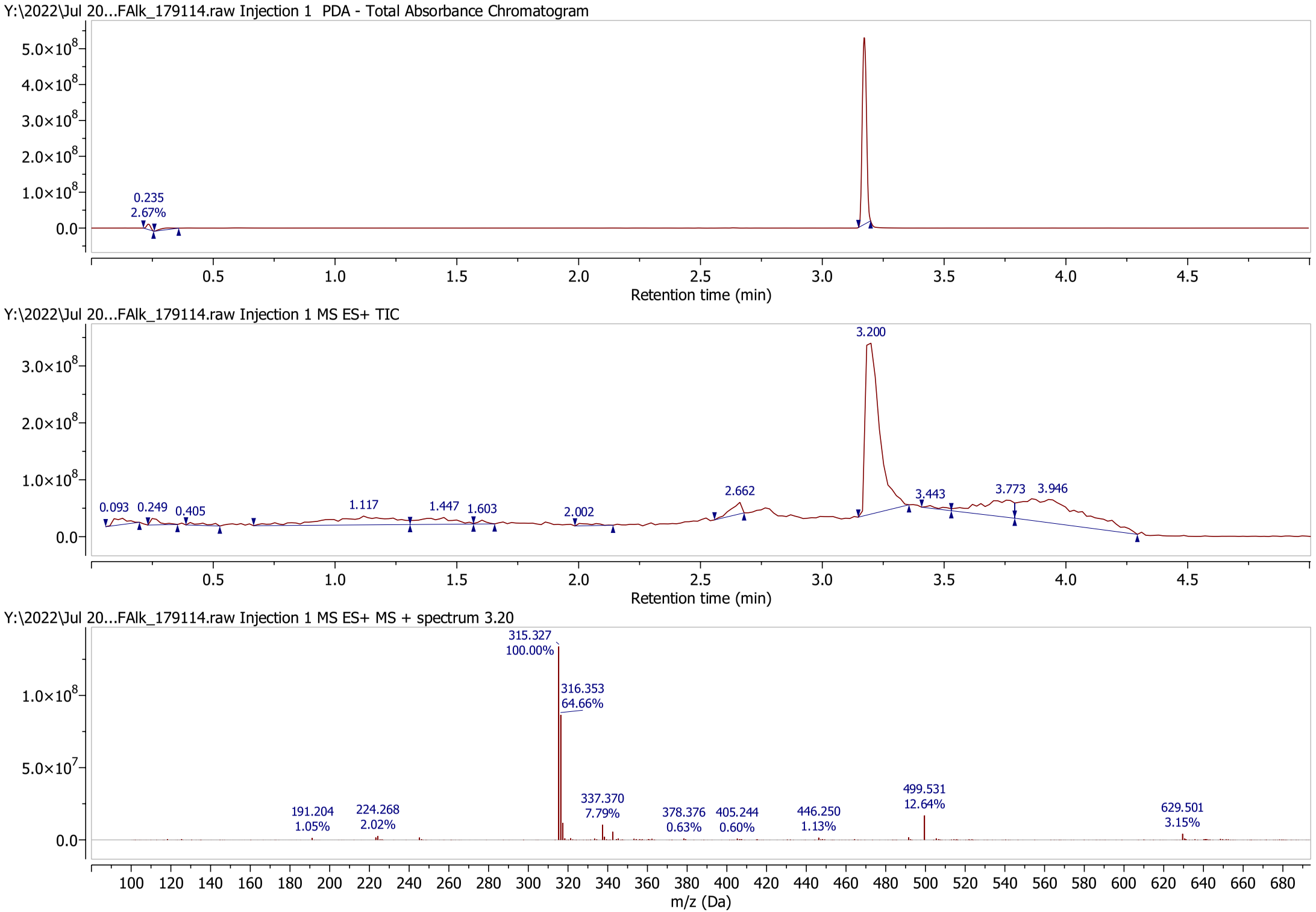
f1 (ppm)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2.67%
Retention time (min)
Y:\2022\Jul 20...FAlk_179114.raw Injection 1 MS ES+ TIC
3.200
0.093
0.249
0.405
1.117
1.447
1.603
2.002
2.662
3.443
3.773
3.946
Retention time (min)
Y:\2022\Jul 20...FAlk_179114.raw Injection 1 MS ES+ MS + spectrum 3.20
315.327
100.00%
316.353
64.66%
191.204
1.05%
224.268
2.02%
337.370
7.79%
378.376
0.63%
405.244
0.60%
446.250
1.13%
499.531
12.64%
629.501
3.15%
m/z (Da)

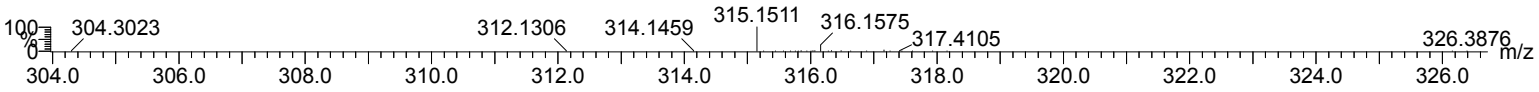
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
2017 formula(e) evaluated with 17 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-10 O: 0-10 S: 0-4

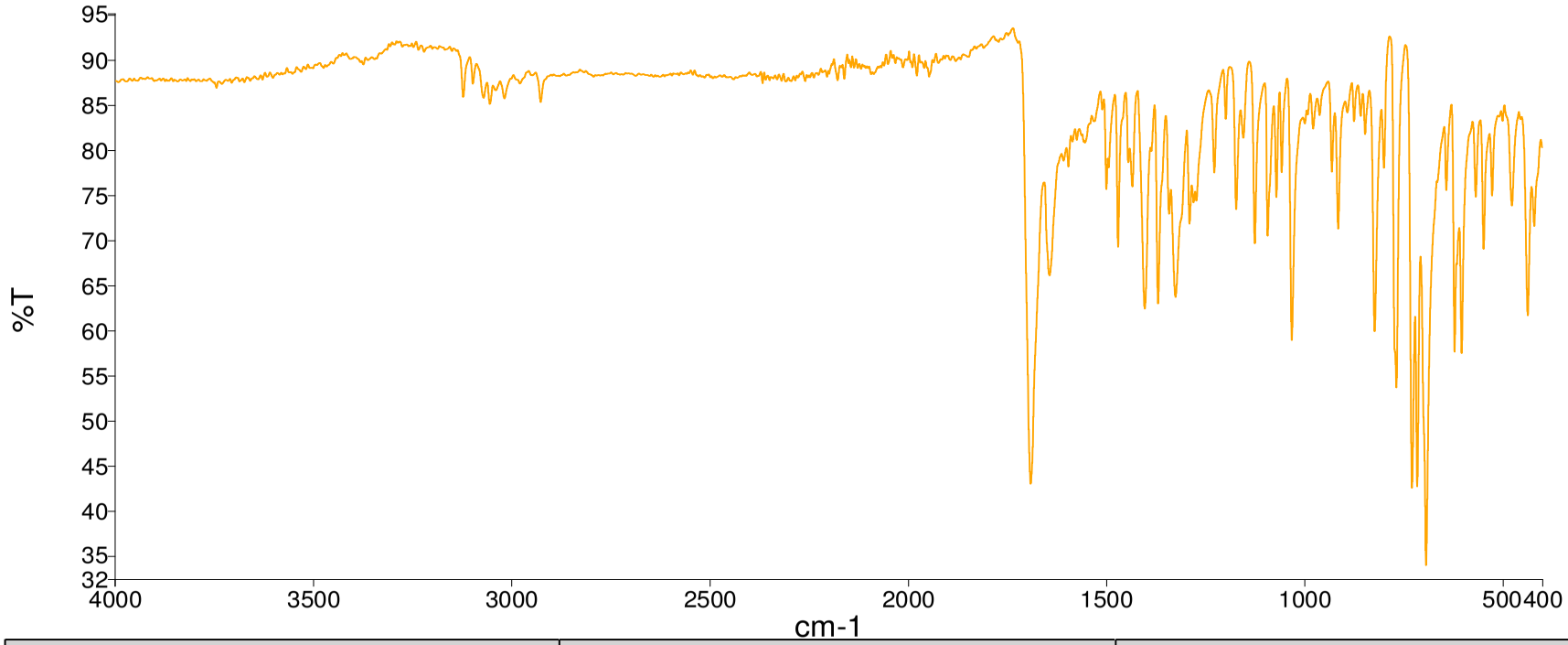
21-Jul-2022
MTF_MTFAlk_179355 566 (4.756) Cm (563:566)

21-Jul-2022
1: TOF MS ES+
1.79e+004



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
315.1511	315.1511	0.0	0.0	-5.5	248.7	29.890	0.00	C9 H31 O7 S2
	315.1509	0.2	0.6	-8.5	245.6	26.790	0.00	C H27 N6 O10 S
	315.1516	-0.5	-1.6	0.5	236.6	17.698	0.00	C9 H23 N4 O8
	315.1518	-0.7	-2.2	-9.5	252.8	33.990	0.00	C2 H31 N6 O5 S3
	315.1520	-0.9	-2.9	-6.5	254.2	35.342	0.00	C10 H35 O2 S4
	315.1523	-1.2	-3.8	-3.5	244.1	25.256	0.00	C2 H23 N10 O6 S
	315.1498	1.3	4.1	0.5	247.6	28.788	0.00	C6 H23 N10 O S2
	315.1497	1.4	4.4	13.5	218.9	0.000	100.00	C21 H19 N2 O
	315.1525	-1.4	-4.4	-0.5	247.9	29.078	0.00	C10 H27 N4 O3 S2
	315.1493	1.8	5.7	-5.5	254.4	35.563	0.00	C6 H31 N6 S4
	315.1529	-1.8	-5.7	5.5	235.5	16.597	0.00	C10 H19 N8 O4
	315.1531	-2.0	-6.3	8.5	238.9	20.083	0.00	C18 H23 N2 O S
	315.1531	-2.0	-6.3	-4.5	252.4	33.503	0.00	C3 H27 N10 O S3
	315.1491	2.0	6.3	4.5	239.5	20.657	0.00	C13 H23 N4 O3 S
	315.1489	2.2	7.0	1.5	240.1	21.238	0.00	C5 H19 N10 O6
	315.1486	2.5	7.9	-1.5	252.3	33.450	0.00	C13 H31 O2 S3
	315.1484	2.7	8.6	-4.5	248.7	29.857	0.00	C5 H27 N6 O5 S2

Analyst Lenny Lauchlan
Date 22 July 2022 14:31



Sample Name	Description	Quality Checks
MTF Alk	Sample 021 By Lenny Date Friday, July 22 2022	The Quality Checks do not report any warnings for the sample.

X-ray crystallography data

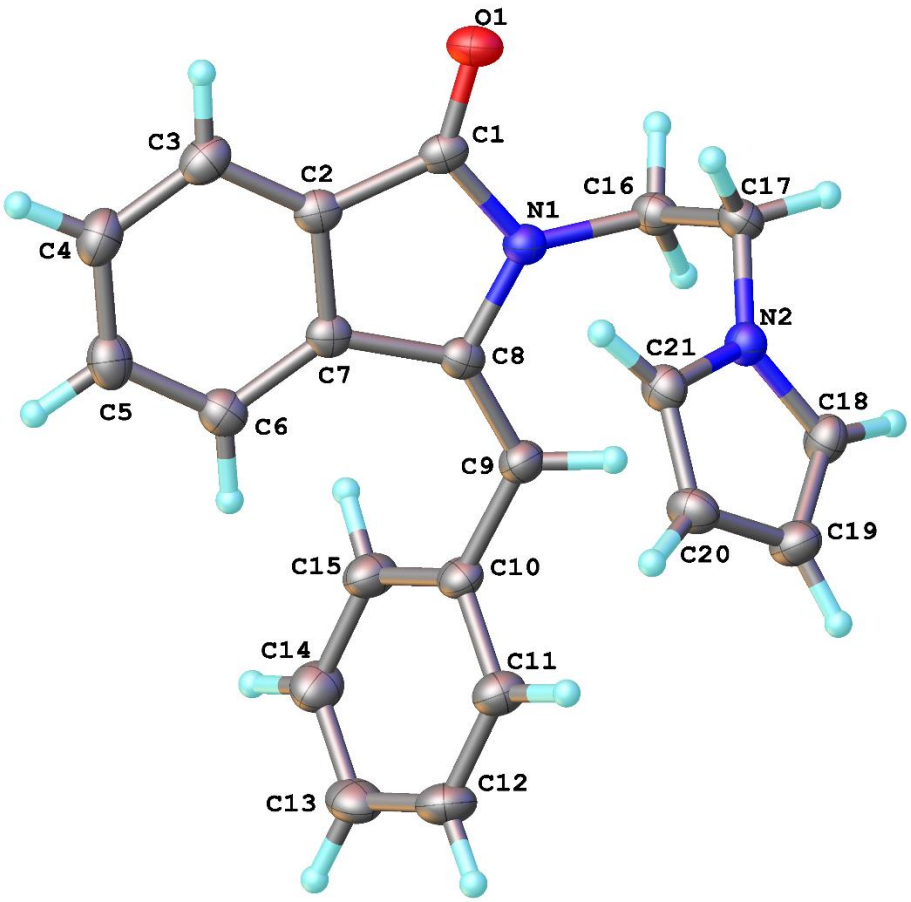


Table 1 Crystal data and structure refinement for 21srv467.	
Identification code	21srv467
Empirical formula	$C_{21}H_{18}N_2O$
Formula weight	314.37
Temperature/K	120.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.3276(4)
b/Å	12.1351(3)
c/Å	9.7437(3)
α/°	90
β/°	96.9734(11)
γ/°	90

Volume/Å^3	1681.57(8)
Z	4
ρ_{calc}g/cm^3	1.242
μ/mm^{-1}	0.077
F(000)	664.0
Crystal size/mm^3	0.26 × 0.19 × 0.14
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.386 to 59.99
Index ranges	-20 ≤ h ≤ 20, -17 ≤ k ≤ 17, -13 ≤ l ≤ 13
Reflections collected	28328
Independent reflections	4882 [R_{int} = 0.0451, R_{sigma} = 0.0370]
Data/restraints/parameters	4882/0/289
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0470, wR_2 = 0.1055
Final R indexes [all data]	R_1 = 0.0673, wR_2 = 0.1157
Largest diff. peak/hole / e Å^{-3}	0.28/-0.21

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 21srv467. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	100.4(6)	6294.1(8)	3839.9(9)	29.7(2)
N1	1300.3(7)	7403.3(8)	3275.0(10)	22.6(2)
N2	1044.6(7)	9701.5(8)	4256.1(10)	22.5(2)
C1	941.2(8)	6467.3(10)	3816.5(12)	22.6(2)
C2	1752.8(8)	5769.7(10)	4317.9(12)	22.9(2)
C3	1766.2(10)	4758.2(11)	4975.9(13)	28.8(3)
C4	2639.3(10)	4283.4(11)	5384.6(14)	32.6(3)
C5	3459.5(10)	4822.4(11)	5140.0(14)	30.7(3)
C6	3445.6(9)	5836.2(11)	4474.4(13)	27.0(3)
C7	2574.3(8)	6313.9(10)	4039.4(12)	22.3(2)
C8	2294.1(8)	7368.5(10)	3352.9(12)	22.3(2)
C9	2811.5(9)	8192.4(10)	2914.2(13)	25.9(3)
C10	3830.3(9)	8152.1(10)	2823.0(13)	24.7(3)
C11	4406.4(9)	9003.7(11)	3391.2(14)	29.9(3)
C12	5361.5(10)	9003.1(13)	3265.2(16)	36.1(3)
C13	5753.3(10)	8159.7(13)	2564.6(15)	35.2(3)

C14	5184.1(10)	7320.3(12)	1972.1(16)	34.9(3)
C15	4226.1(10)	7319.1(11)	2092.5(15)	31.5(3)
C16	681.3(9)	8215.1(11)	2533.5(13)	25.0(3)
C17	302.1(8)	9054.2(11)	3483.1(13)	25.2(3)
C18	1429.4(9)	10653.8(11)	3814.6(13)	27.2(3)
C19	2146.1(10)	10968.3(11)	4795.8(14)	31.4(3)
C20	2205.2(9)	10176.8(12)	5872.3(13)	29.3(3)
C21	1525.2(9)	9405.7(11)	5504.7(13)	25.6(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 21srv467. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	23.3(4)	36.6(5)	29.1(5)	-1.2(4)	2.8(3)	-7.1(4)
N1	21.3(5)	23.1(5)	23.6(5)	-0.7(4)	3.5(4)	-1.5(4)
N2	23.5(5)	23.2(5)	20.5(5)	1.0(4)	1.5(4)	0.6(4)
C1	26.3(6)	24.7(6)	17.1(5)	-4.1(4)	3.8(4)	-6.0(5)
C2	25.9(6)	25.8(6)	17.6(5)	-3.7(4)	5.2(4)	-2.4(5)
C3	36.0(7)	26.4(6)	25.5(6)	-1.2(5)	9.6(5)	-4.3(5)
C4	43.2(8)	25.6(6)	30.2(7)	2.0(5)	9.1(6)	3.1(6)
C5	35.4(7)	30.4(7)	26.6(6)	-0.7(5)	5.4(5)	7.9(6)
C6	26.7(6)	30.7(7)	24.0(6)	-2.4(5)	4.7(5)	1.0(5)
C7	24.5(6)	24.0(6)	18.6(5)	-4.7(4)	4.1(4)	-1.0(4)
C8	22.0(5)	24.2(6)	20.7(5)	-3.9(4)	2.8(4)	-0.7(4)
C9	25.2(6)	23.3(6)	29.5(6)	-0.2(5)	4.4(5)	-2.0(5)
C10	24.4(6)	24.0(6)	26.4(6)	3.5(5)	5.8(5)	-3.7(5)
C11	30.7(7)	28.8(7)	30.9(7)	-2.2(5)	6.3(5)	-6.2(5)
C12	29.4(7)	38.9(8)	39.8(8)	-2.5(6)	3.9(6)	-11.6(6)
C13	25.3(7)	41.9(8)	39.5(8)	5.2(6)	8.8(6)	-5.1(6)
C14	32.4(7)	33.5(7)	41.1(8)	-1.0(6)	14.1(6)	-0.5(6)
C15	30.1(7)	28.2(7)	37.4(7)	-4.1(6)	9.0(5)	-5.9(5)
C16	23.1(6)	29.4(6)	21.8(6)	1.3(5)	0.2(5)	-1.4(5)
C17	20.3(6)	28.2(6)	26.7(6)	-0.4(5)	0.7(5)	0.1(5)
C18	32.5(7)	24.3(6)	24.5(6)	3.5(5)	2.6(5)	0.5(5)
C19	31.9(7)	29.9(7)	31.9(7)	2.0(5)	2.2(5)	-6.4(5)
C20	25.8(6)	36.9(7)	24.2(6)	1.2(5)	-0.9(5)	-2.4(5)
C21	26.8(6)	29.0(6)	21.0(6)	3.6(5)	2.3(5)	0.8(5)

Table 4 Bond Lengths for 21srv467.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
O1	C1	1.2258(14)		C7	C8	1.4768(17)
N1	C1	1.3781(15)		C8	C9	1.3450(17)
N1	C8	1.4172(15)		C9	C10	1.4739(17)

N1	C16	1.4573(16)		C10	C11	1.3946(18)
N2	C17	1.4565(16)		C10	C15	1.3957(18)
N2	C18	1.3719(16)		C11	C12	1.3886(19)
N2	C21	1.3711(15)		C12	C13	1.386(2)
C1	C2	1.4729(17)		C13	C14	1.386(2)
C2	C3	1.3839(18)		C14	C15	1.3918(19)
C2	C7	1.4044(16)		C16	C17	1.5198(17)
C3	C4	1.391(2)		C18	C19	1.3696(19)
C4	C5	1.390(2)		C19	C20	1.4171(19)
C5	C6	1.3897(19)		C20	C21	1.3669(18)
C6	C7	1.3949(17)				

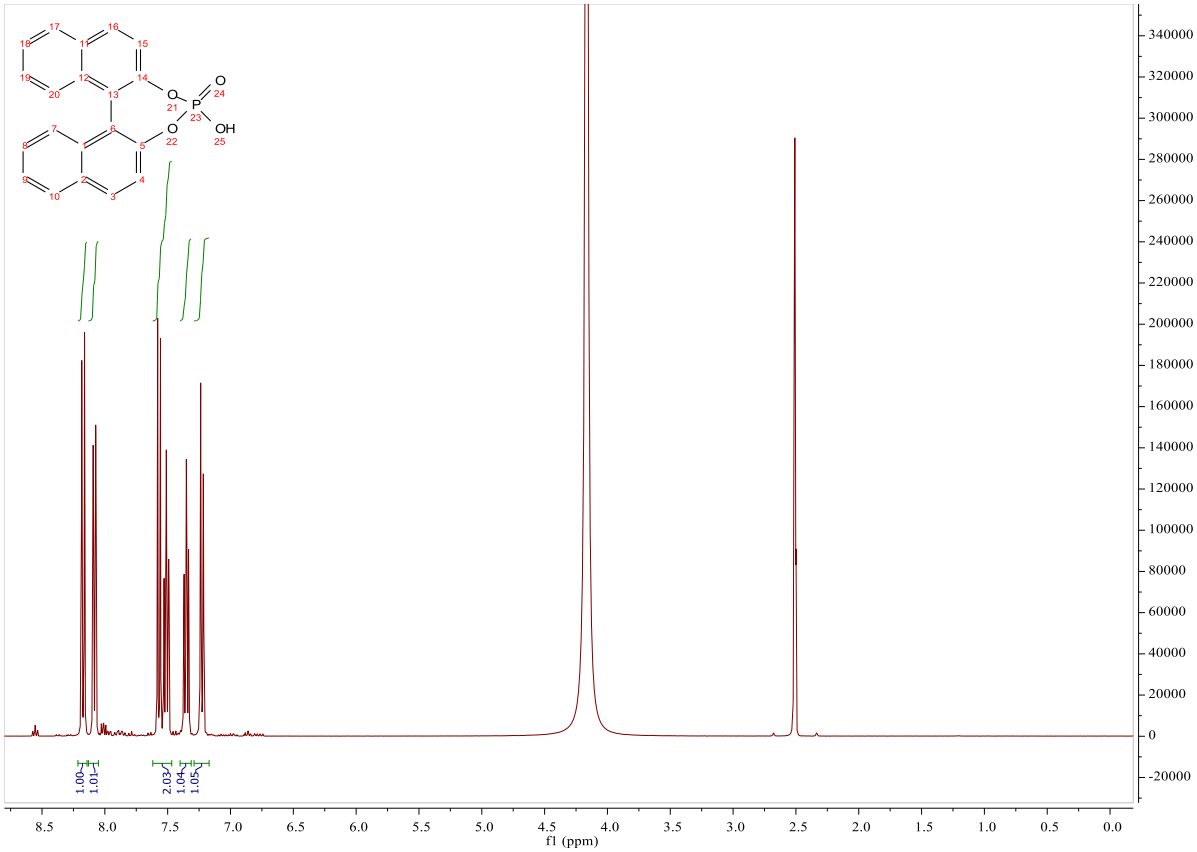
Table 5 Bond Angles for 21srv467.								
Atom	**Atom**	**Atom**	**Angle/˚**		**Atom**	**Atom**	**Atom**	**Angle/˚**
C1	N1	C8	111.98(10)		N1	C8	C7	105.44(10)
C1	N1	C16	120.93(10)		C9	C8	N1	123.35(11)
C8	N1	C16	126.42(10)		C9	C8	C7	131.16(11)
C18	N2	C17	126.03(10)		C8	C9	C10	125.63(12)
C21	N2	C17	125.05(11)		C11	C10	C9	119.62(11)
C21	N2	C18	108.73(10)		C11	C10	C15	118.79(12)
O1	C1	N1	124.19(12)		C15	C10	C9	121.42(11)
O1	C1	C2	129.30(11)		C12	C11	C10	120.44(13)
N1	C1	C2	106.51(10)		C13	C12	C11	120.42(13)
C3	C2	C1	129.00(11)		C12	C13	C14	119.64(13)
C3	C2	C7	122.81(12)		C13	C14	C15	120.14(13)
C7	C2	C1	108.18(11)		C14	C15	C10	120.54(13)
C2	C3	C4	117.47(12)		N1	C16	C17	113.08(10)
C5	C4	C3	120.36(13)		N2	C17	C16	112.56(10)
C6	C5	C4	122.14(13)		C19	C18	N2	108.16(11)
C5	C6	C7	118.12(12)		C18	C19	C20	107.47(12)
C2	C7	C8	107.87(10)		C21	C20	C19	107.07(12)
C6	C7	C2	119.07(11)		C20	C21	N2	108.57(11)
C6	C7	C8	132.98(11)					

Table 6 Selected Torsion Angles for 21srv467.										
A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
N1	C16	C17	N2	61.57(14)		C16	C17	N2	C18	86.99(15)
C7	C8	C9	C10	10.5(2)		C16	C17	N2	C21	-87.45(14)
C8	C9	C10	C11	-130.54(14)		C17	C16	N1	C1	85.63(13)
C8	C9	C10	C15	54.13(19)		C17	C16	N1	C8	-104.52(13)
C10	C9	C8	N1	-172.64(11)						

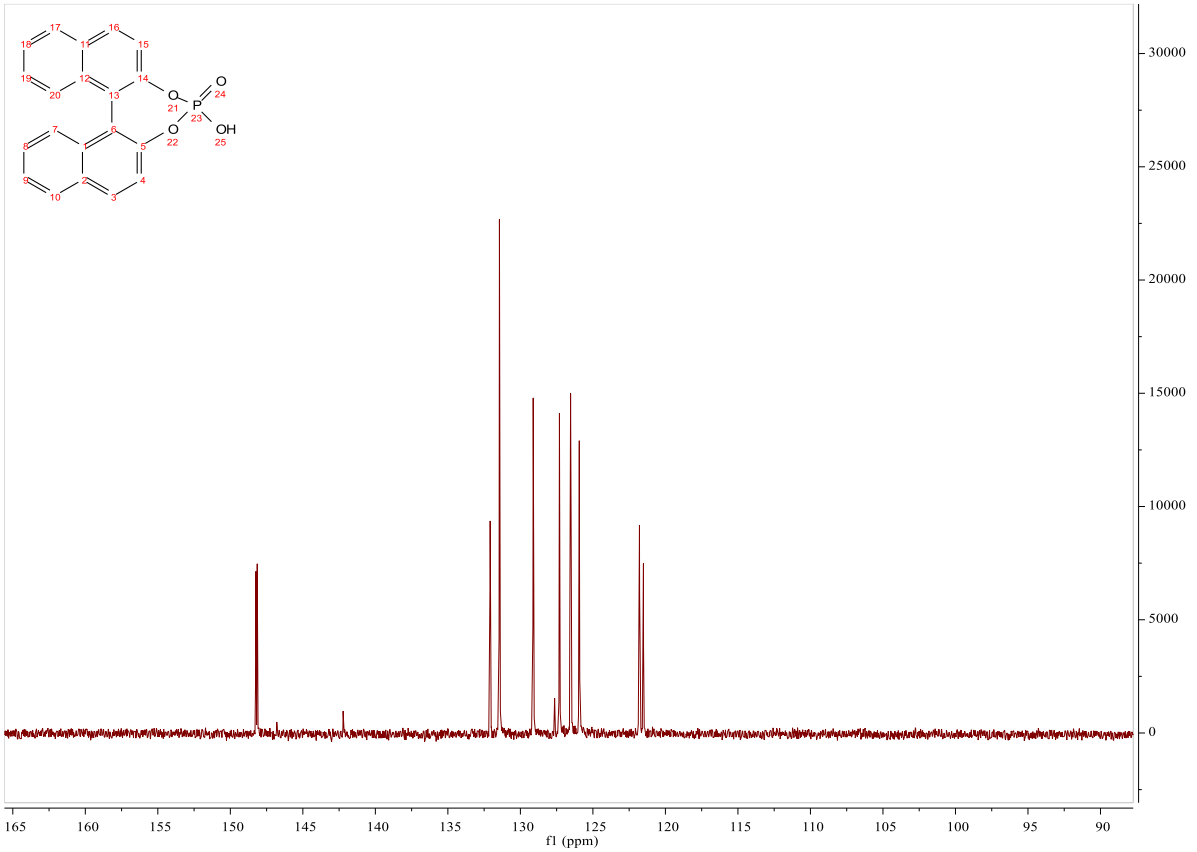
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 21srv467.				
Atom	***x***	***y***	***z***	**U(eq)**
H3	1183(10)	4402(12)	5092(15)	26(4)
H4	2685(10)	3571(13)	5855(15)	33(4)
H5	4066(11)	4474(12)	5461(15)	34(4)
H6	4028(11)	6212(12)	4292(15)	32(4)
H9	2480(10)	8877(13)	2634(15)	33(4)
H11	4104(11)	9610(13)	3873(16)	37(4)
H12	5753(13)	9603(15)	3705(18)	55(5)
H13	6440(13)	8143(14)	2466(17)	47(5)
H14	5465(12)	6717(15)	1414(18)	52(5)
H15	3793(12)	6727(15)	1639(17)	48(5)
H16A	1053(10)	8590(12)	1854(14)	28(4)
H16B	128(10)	7804(12)	2017(15)	30(4)
H17A	-59(10)	8690(13)	4178(16)	33(4)
H17B	-130(10)	9564(12)	2902(15)	28(4)
H18	1159(10)	11002(13)	2951(16)	35(4)
H19	2531(11)	11623(14)	4741(17)	43(4)
H20	2626(11)	10177(13)	6722(16)	38(4)
H21	1347(10)	8751(13)	5960(15)	32(4)

(*R*)-(−)-1,1′-Binaphthyl-2,2′-diyl hydrogen phosphate **150**

^{1}H:



^{13}C:



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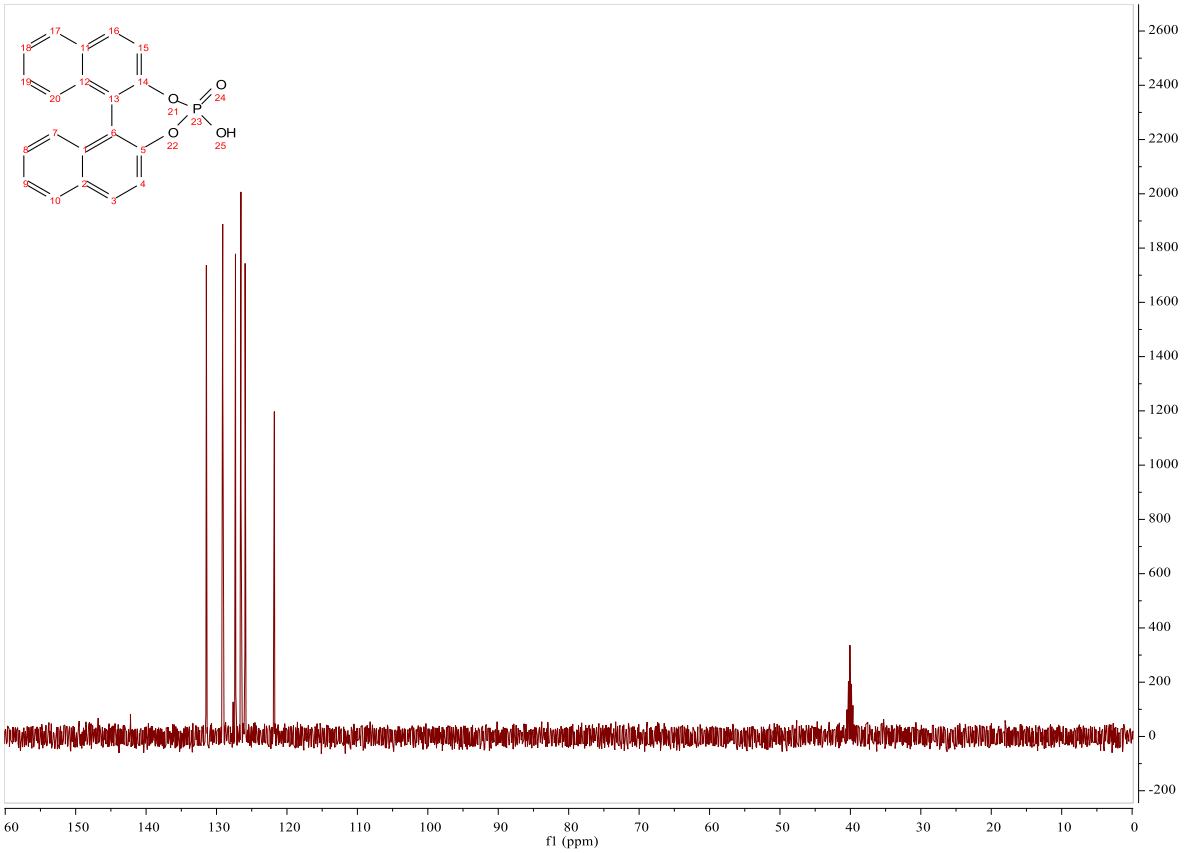
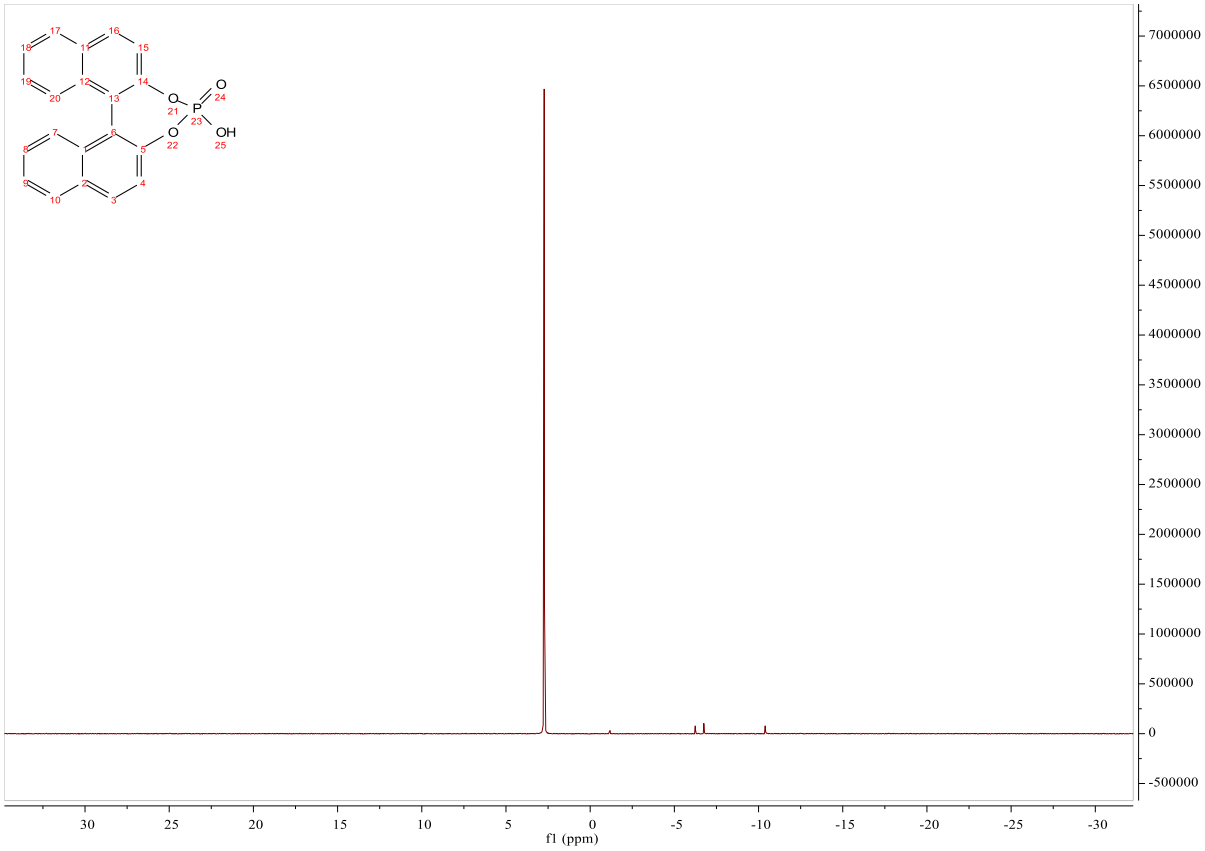
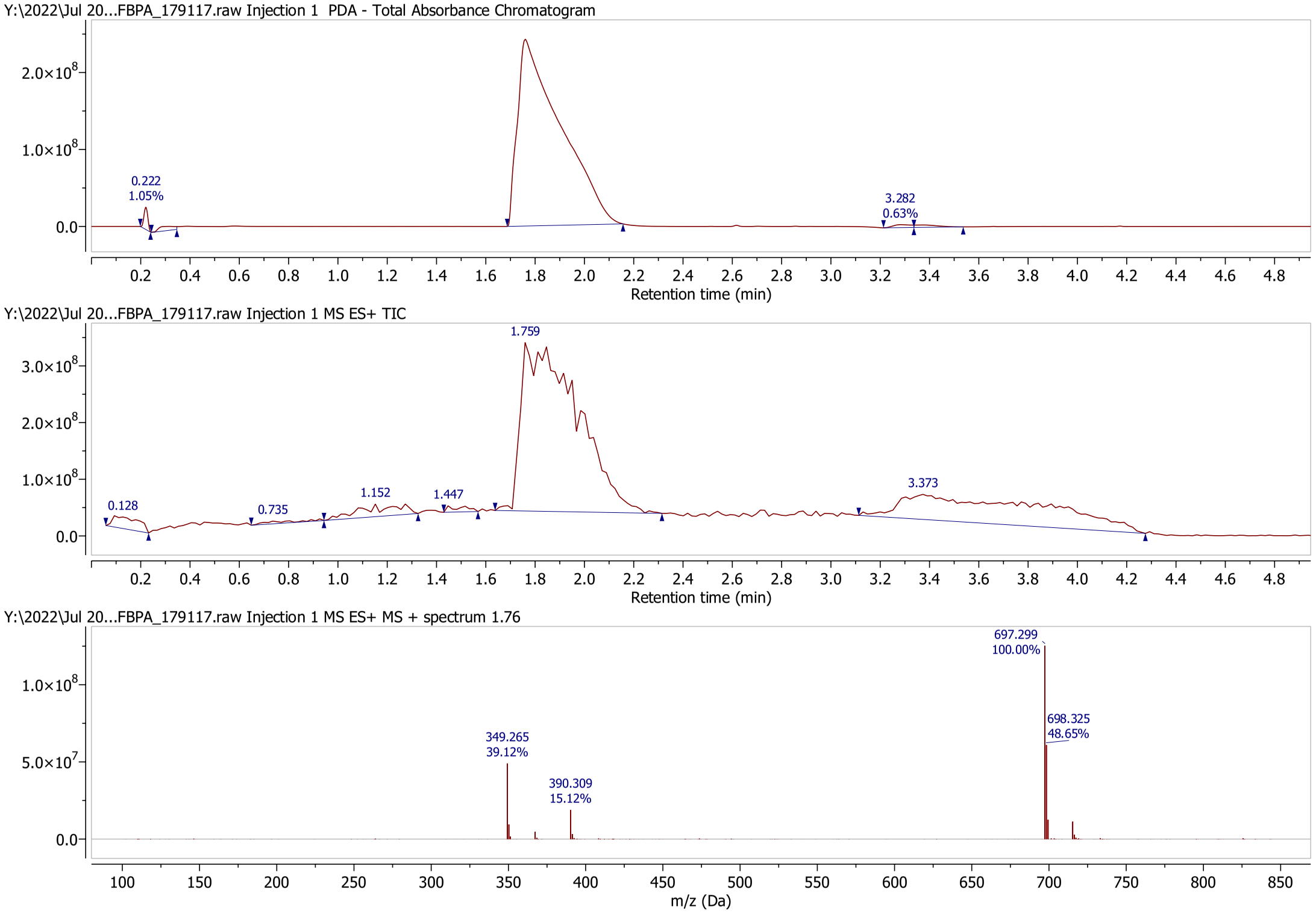


^{31}P:




Y:\2022\Jul 20...FBPA_179117.raw Injection 1 PDA - Total Absorbance Chromatogram
0.222
1.05%
3.282
0.63%
Retention time (min)
Y:\2022\Jul 20...FBPA_179117.raw Injection 1 MS ES+ TIC
1.759
0.128
0.735
1.152
1.447
3.373
Retention time (min)
Y:\2022\Jul 20...FBPA_179117.raw Injection 1 MS ES+ MS + spectrum 1.76
697.299
100.00%
698.325
48.65%
349.265
39.12%
390.309
15.12%
m/z (Da)

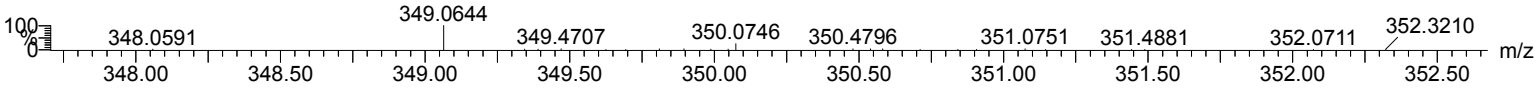
Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 9

Monoisotopic Mass, Even Electron Ions
545 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-50 H: 0-50 N: 0-5 O: 0-6 P: 0-2

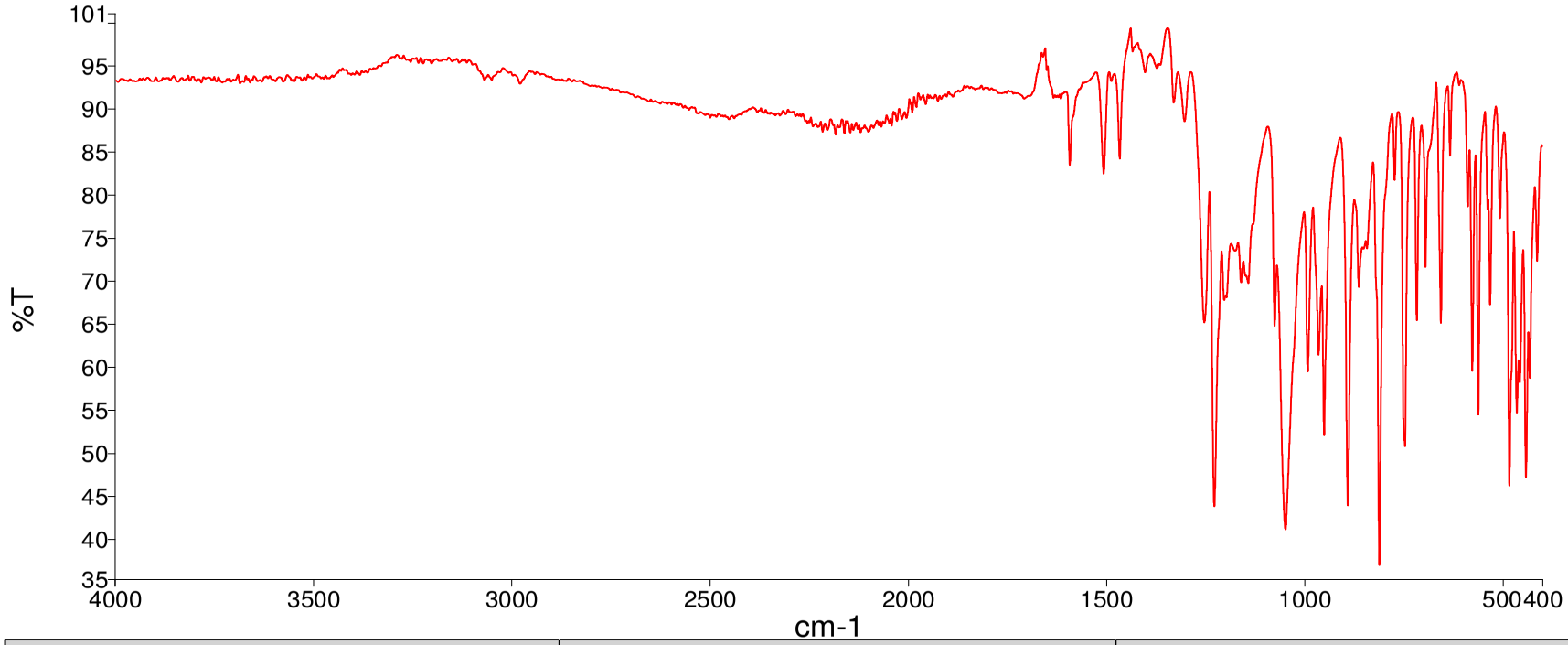
21-Jul-2022
MTF_MTFBPA_179357 457 (3.843) Cm (454:457)

21-Jul-2022
1: TOF MS ES+
4.56e+003



Minimum:				-10.0				
Maximum:		3.0	5.0	100.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
349.0644	349.0643	0.1	0.3	19.5	143.7	0.173	84.10	C21 H10 N4 P
	349.0653	-0.9	-2.6	23.5	152.5	8.984	0.01	C27 H9 O
	349.0630	1.4	4.0	14.5	145.4	1.897	15.01	C20 H14 O4 P
	349.0660	-1.6	-4.6	14.5	148.3	4.729	0.88	C19 H15 N2 O P2
	349.0619	2.5	7.2	10.5	156.6	13.058	0.00	C14 H15 N4 O3 P2

Analyst Lenny Lauchlan
Date 22 July 2022 14:25



Sample Name	Description	Quality Checks
MTF BPA	Sample 017 By Lenny Date Friday, July 22 2022	The Quality Checks do not report any warnings for the sample.