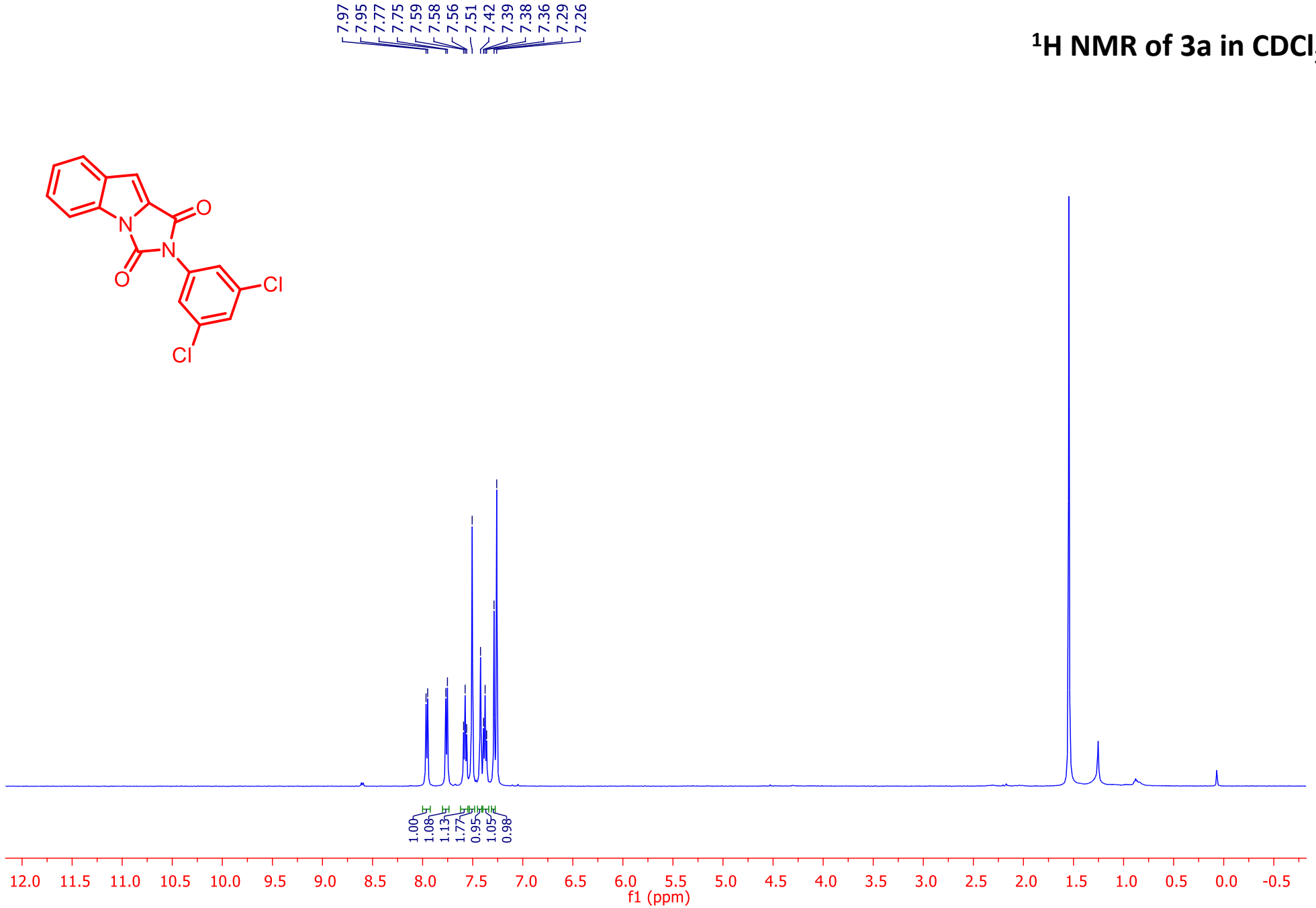
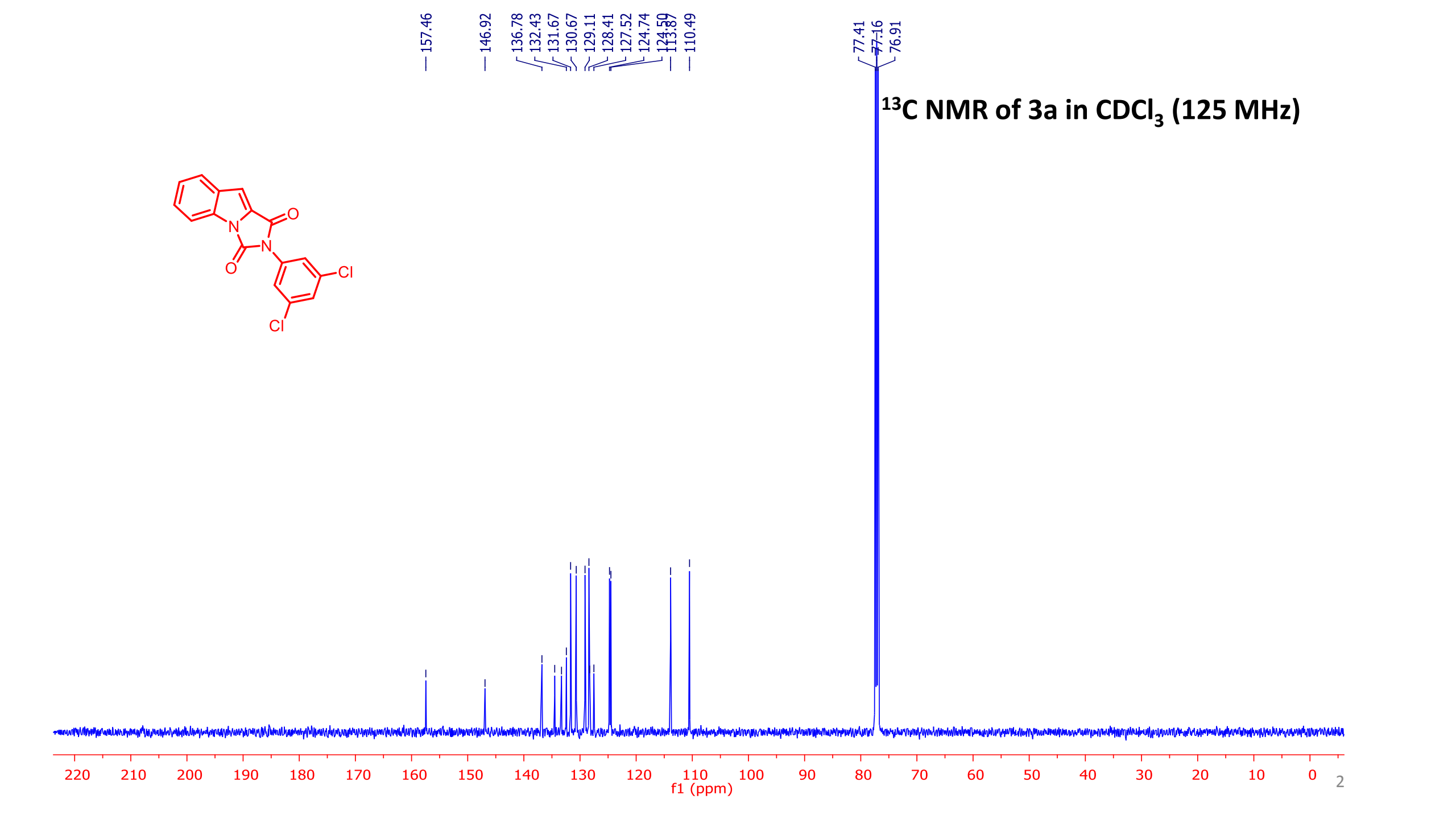
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

^{1}H NMR of 3a in $CDCl_3$ (500 MHz)

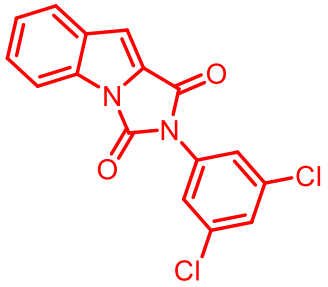




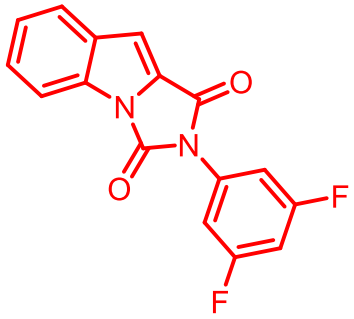
^{13}C NMR of 3a in $CDCl_3$ (125 MHz)

RS-1 #294 RT: 1.31 AV: 1 NL: 2.03E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

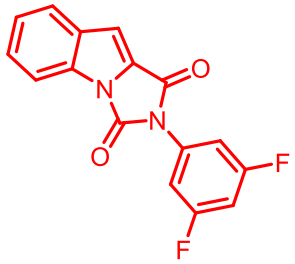
HRMS of 3a



^{1}H NMR of 3b in $CDCl_3$ (400 MHz)

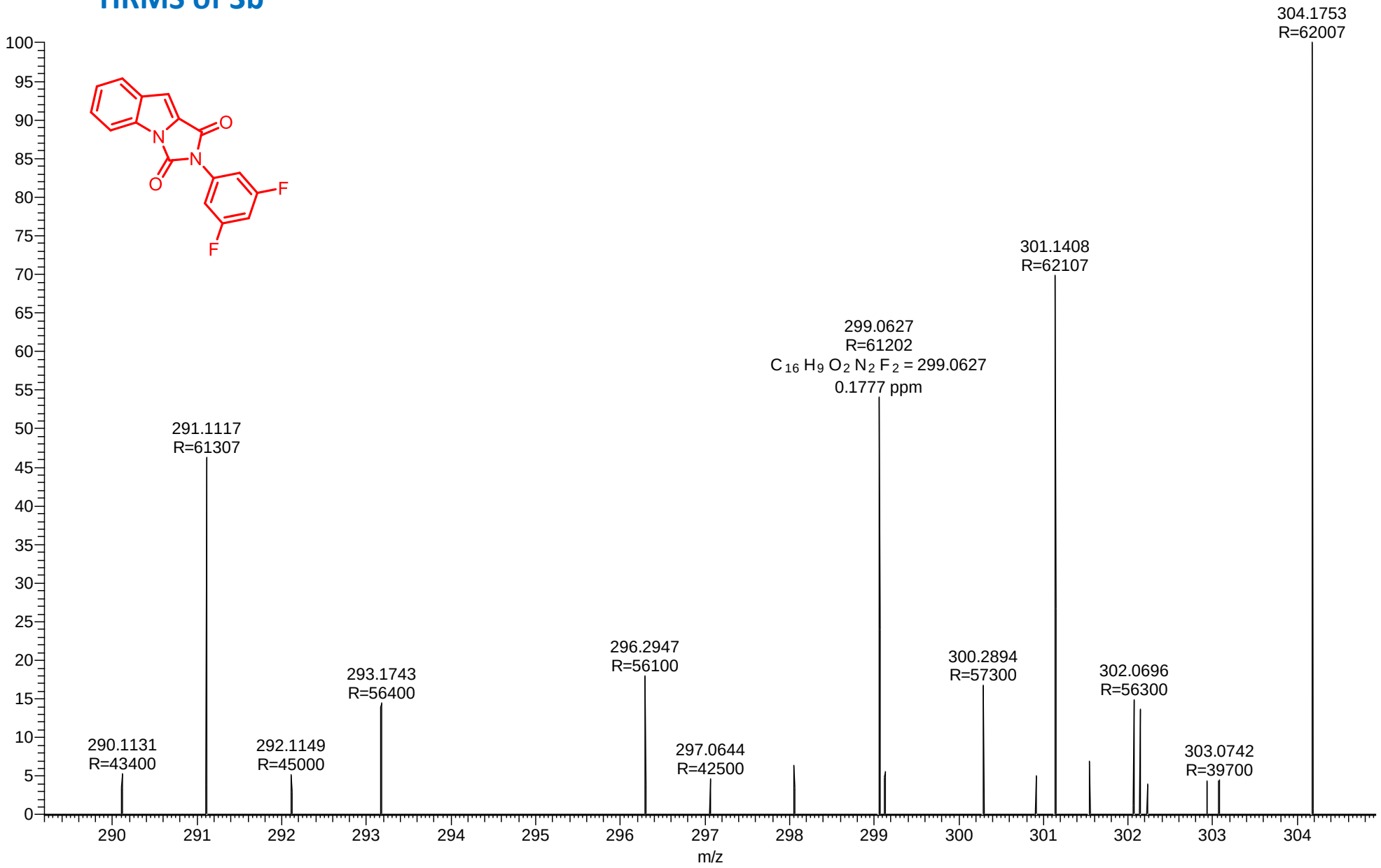


^{13}C NMR of 3b in $CDCl_3$ (100 MHz)

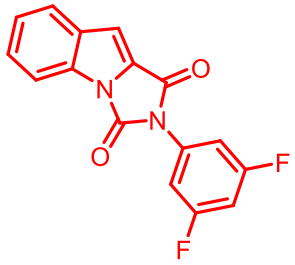


RS-2 #273 RT: 1.21 AV: 1 NL: 5.49E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

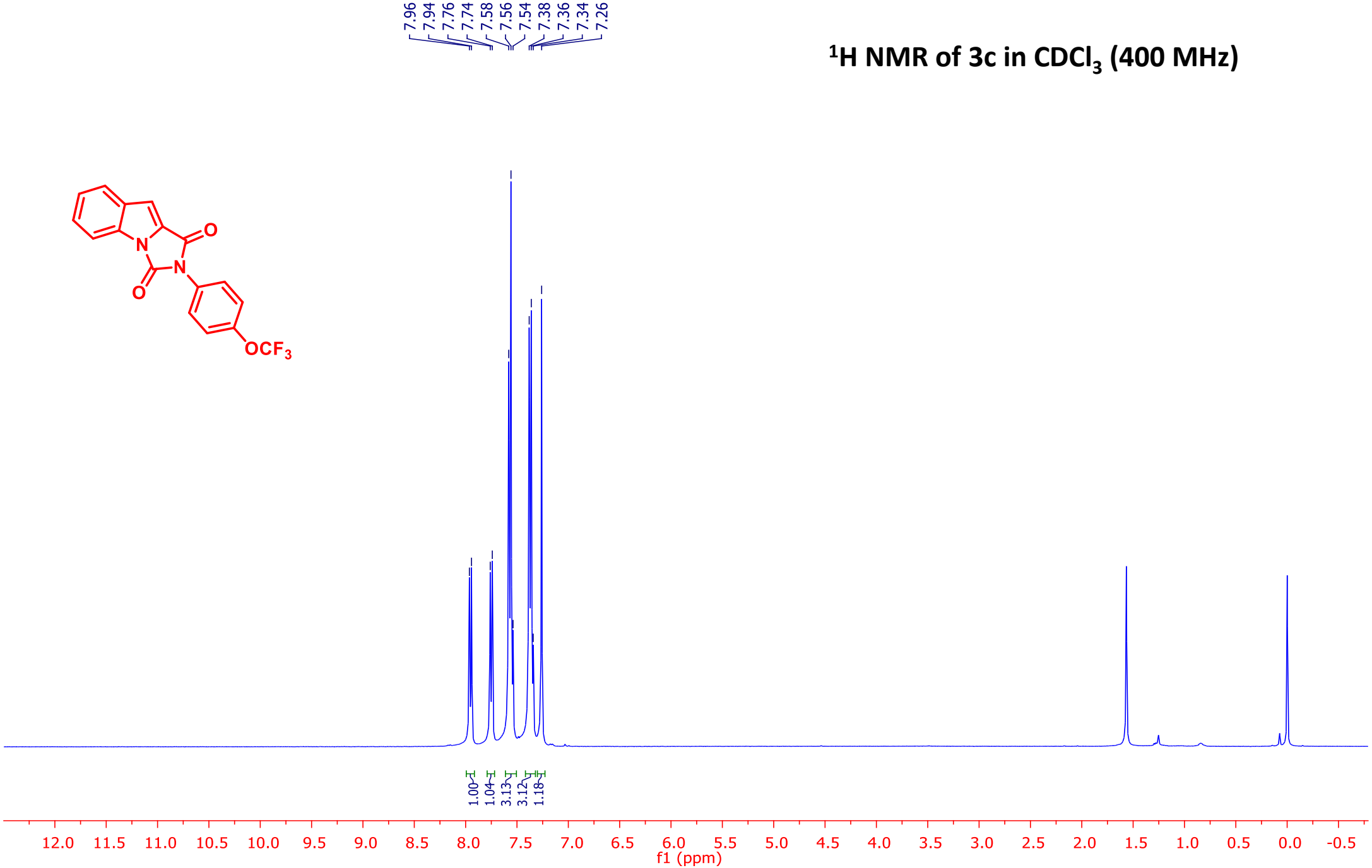
HRMS of 3b

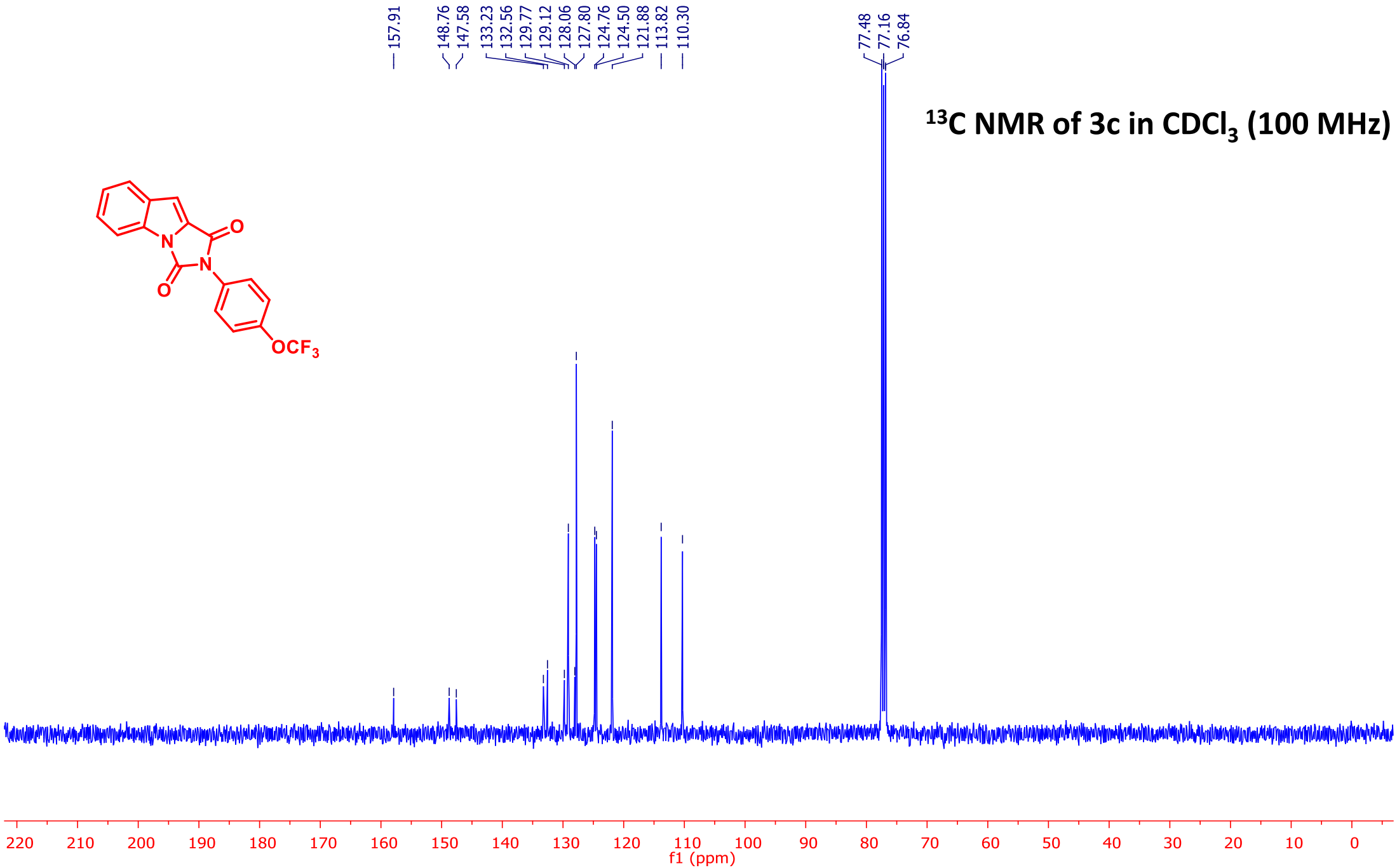


F^{19}-NMR of 3b in $CDCl_3$



^{1}H NMR of 3c in $CDCl_3$ (400 MHz)

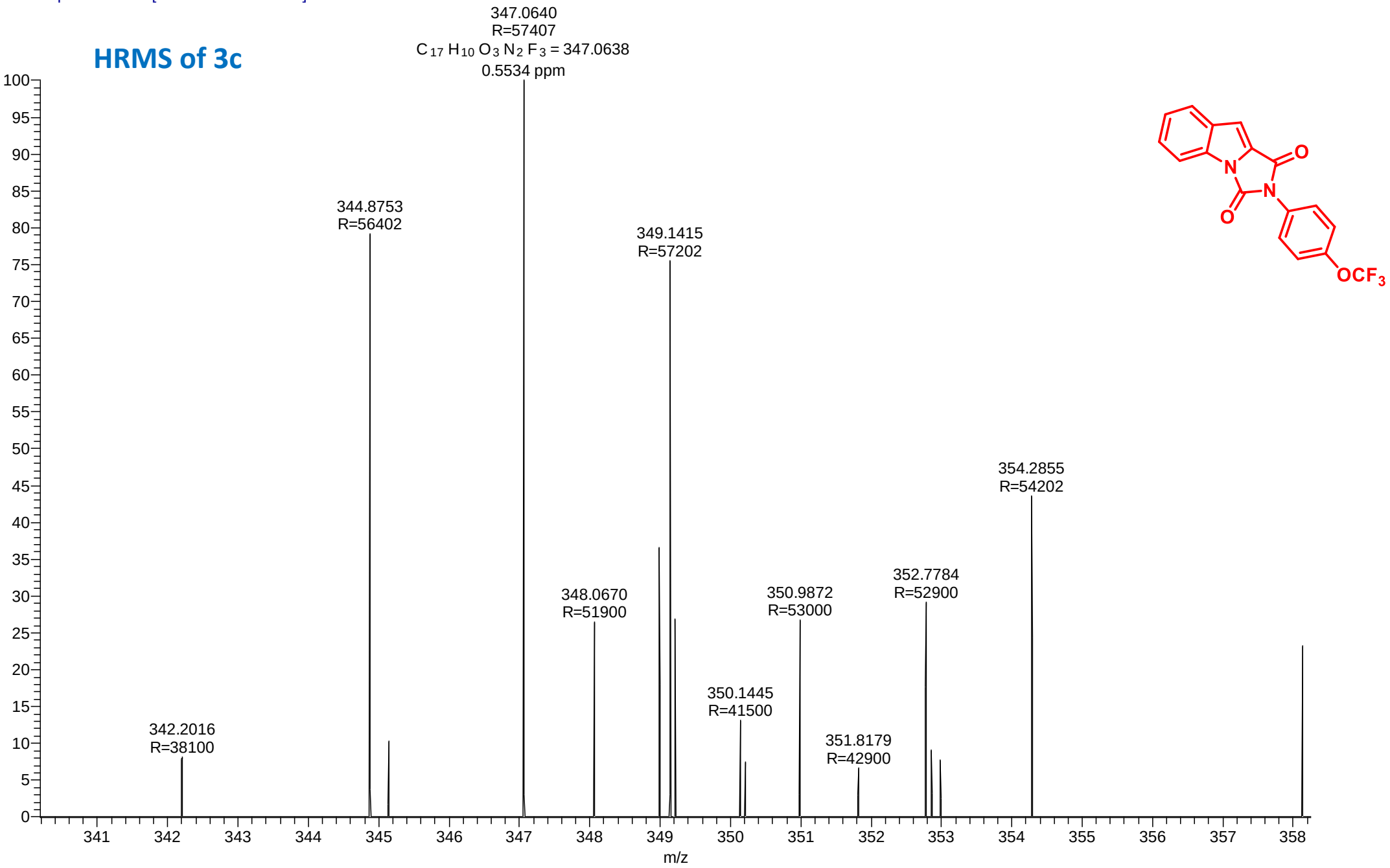




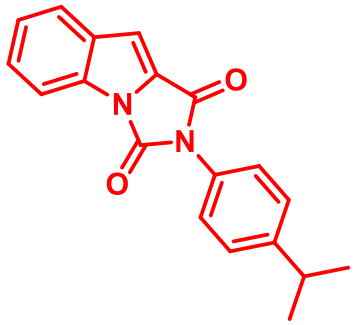
^{13}C NMR of 3c in $CDCl_3$ (100 MHz)

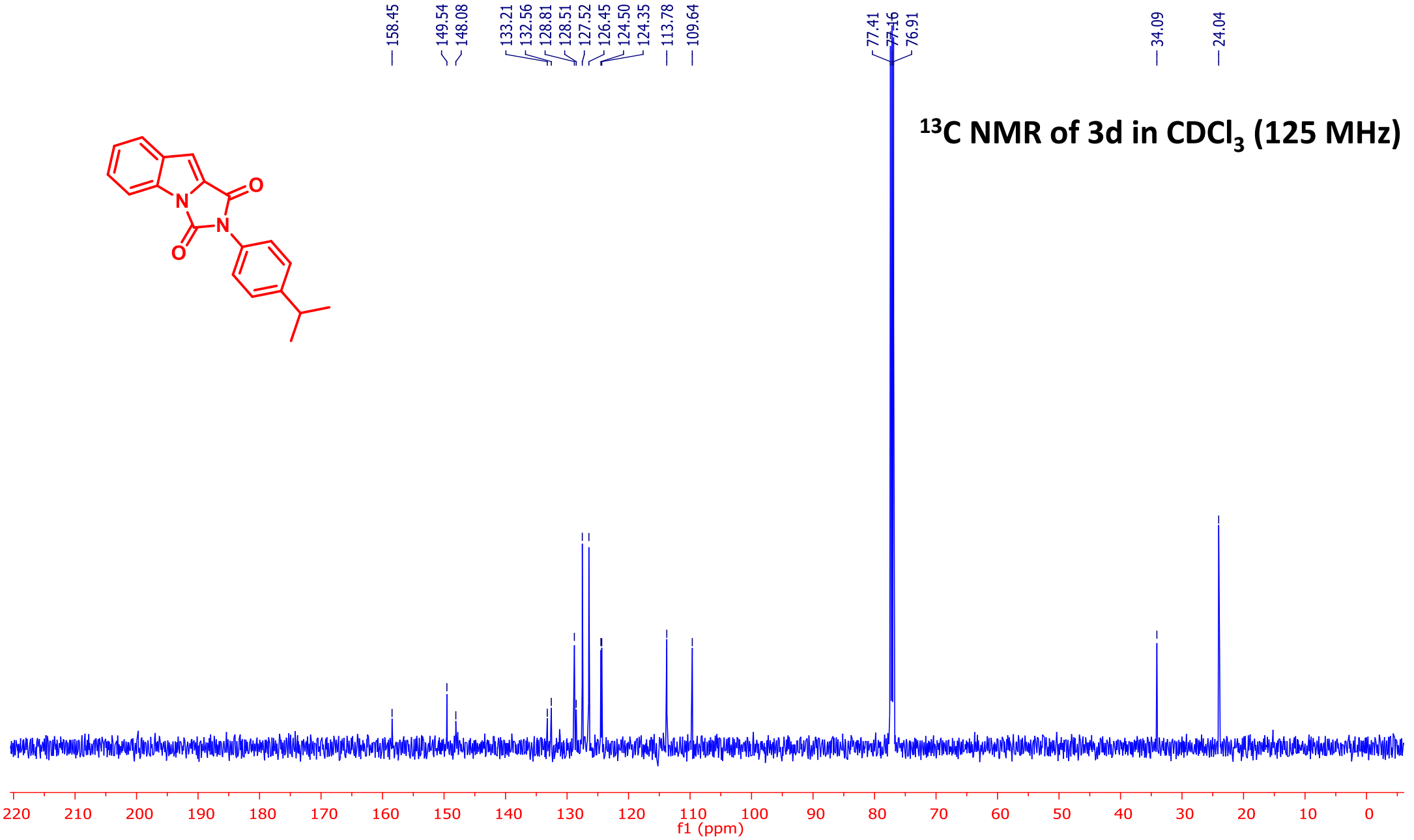
RS-3 #282 RT: 1.25 AV: 1 NL: 3.29E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

HRMS of 3c



^{1}H NMR of 3d in $CDCl_3$ (500 MHz)

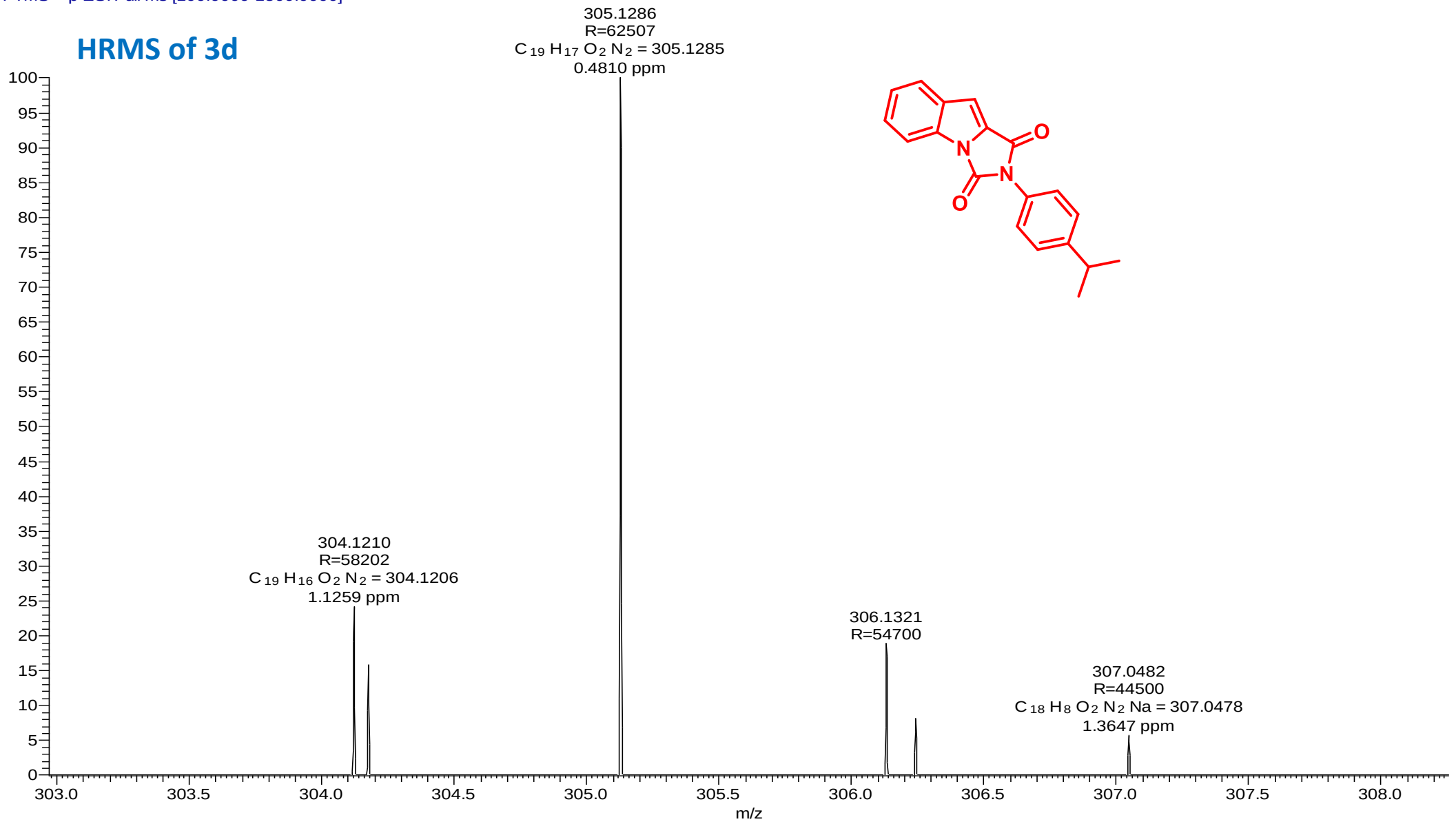


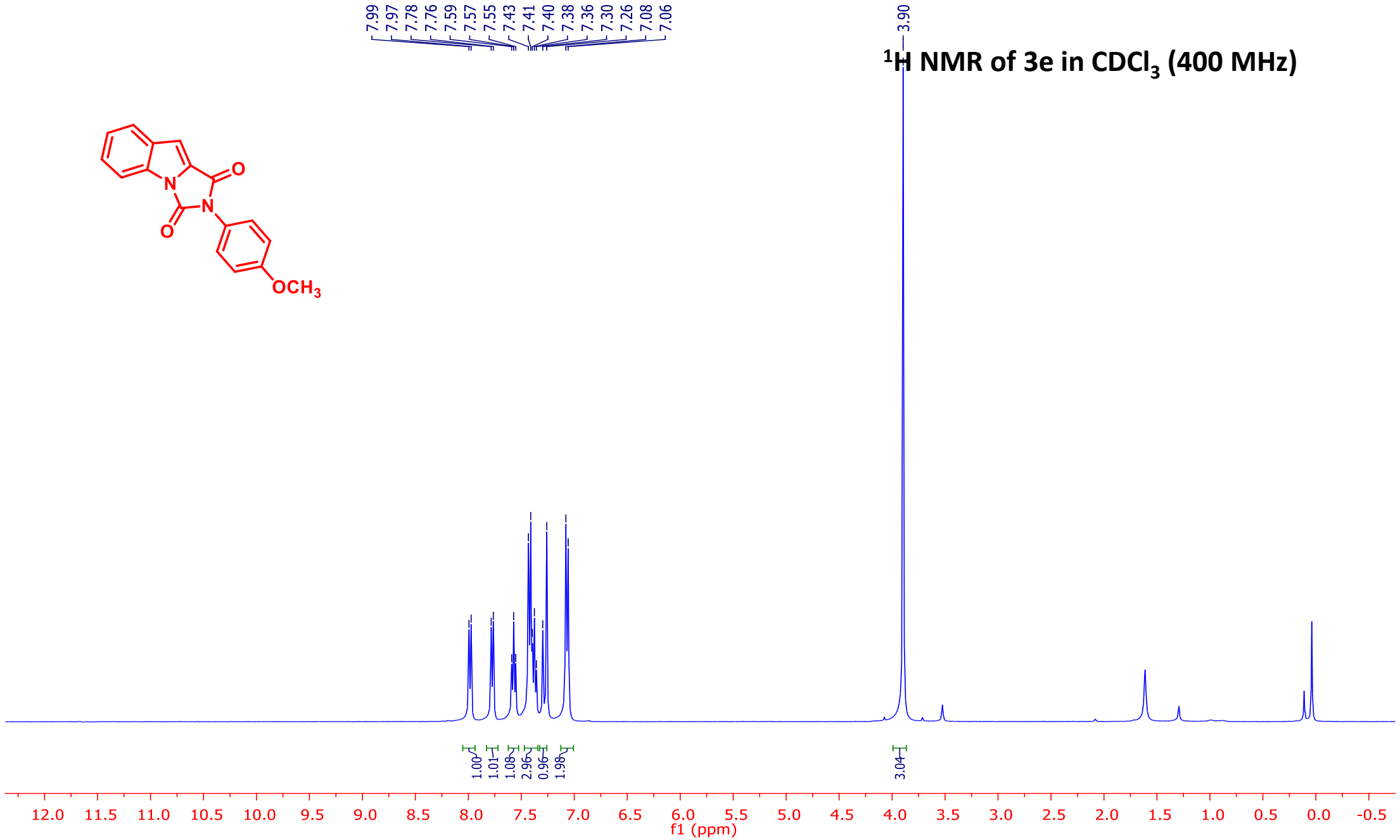


^{13}C NMR of 3d in $CDCl_3$ (125 MHz)

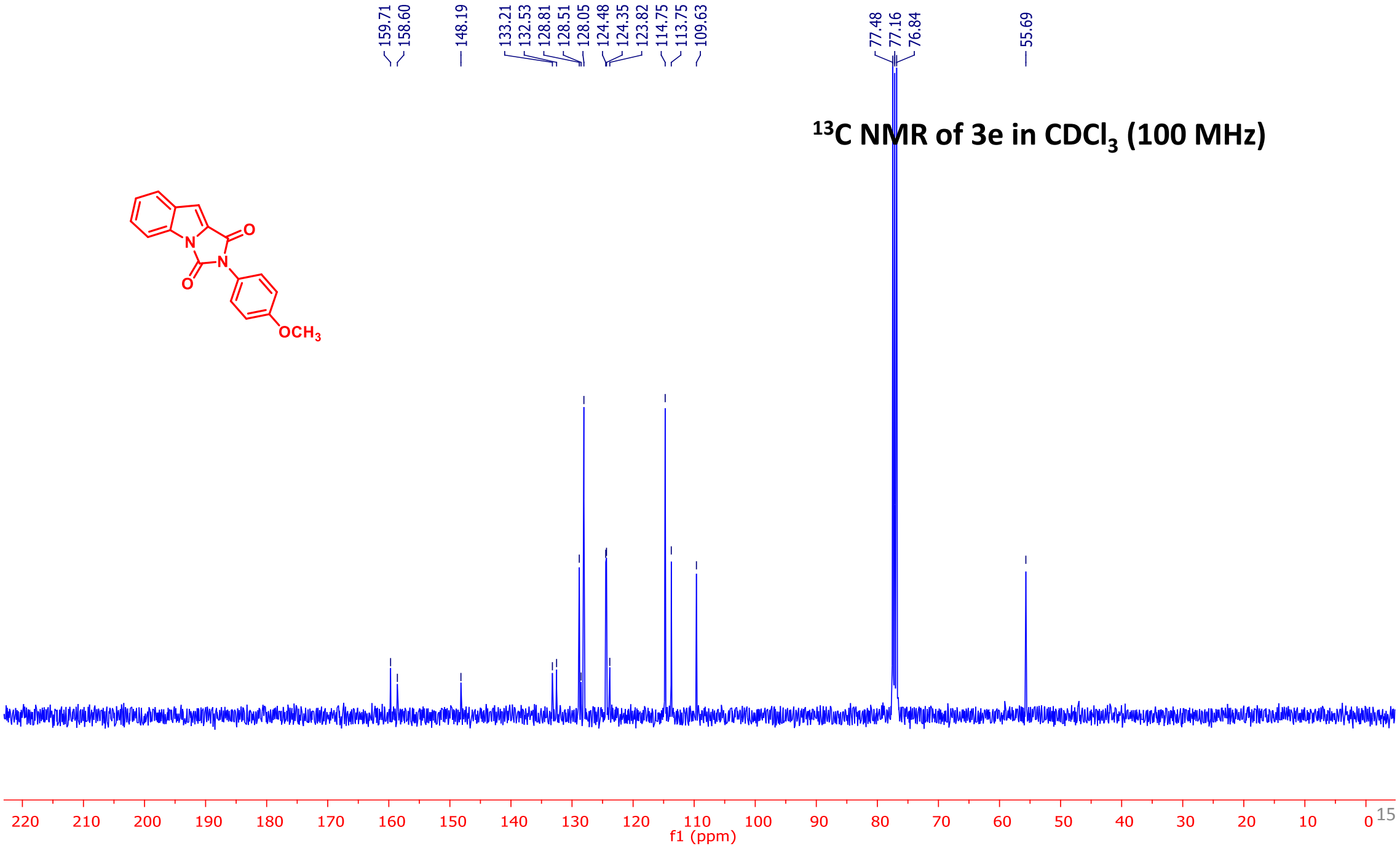
RS-4 #292 RT: 1.30 AV: 1 NL: 5.66E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

HRMS of 3d





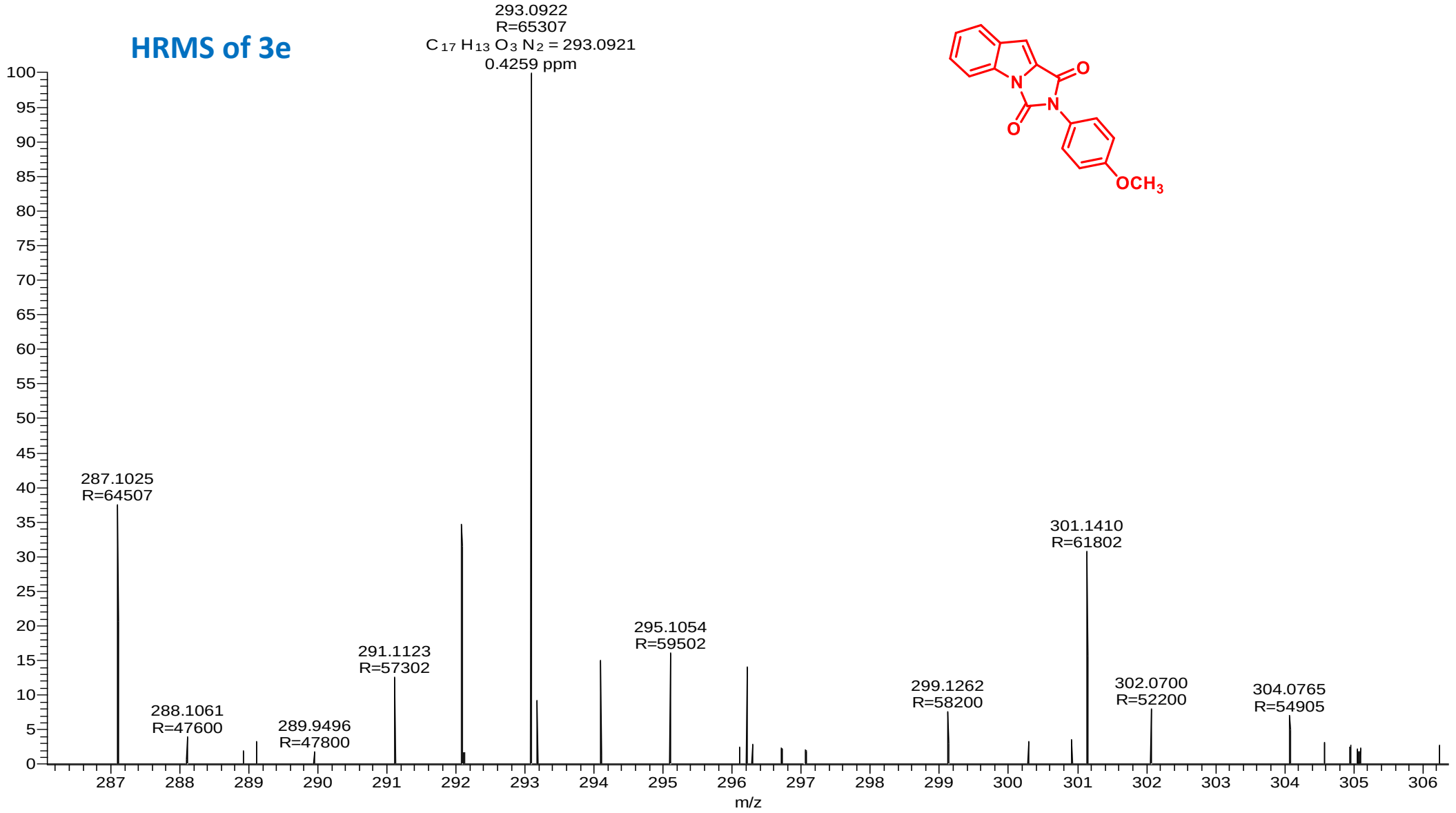
^{1}H NMR of 3e in $CDCl_3$ (400 MHz)

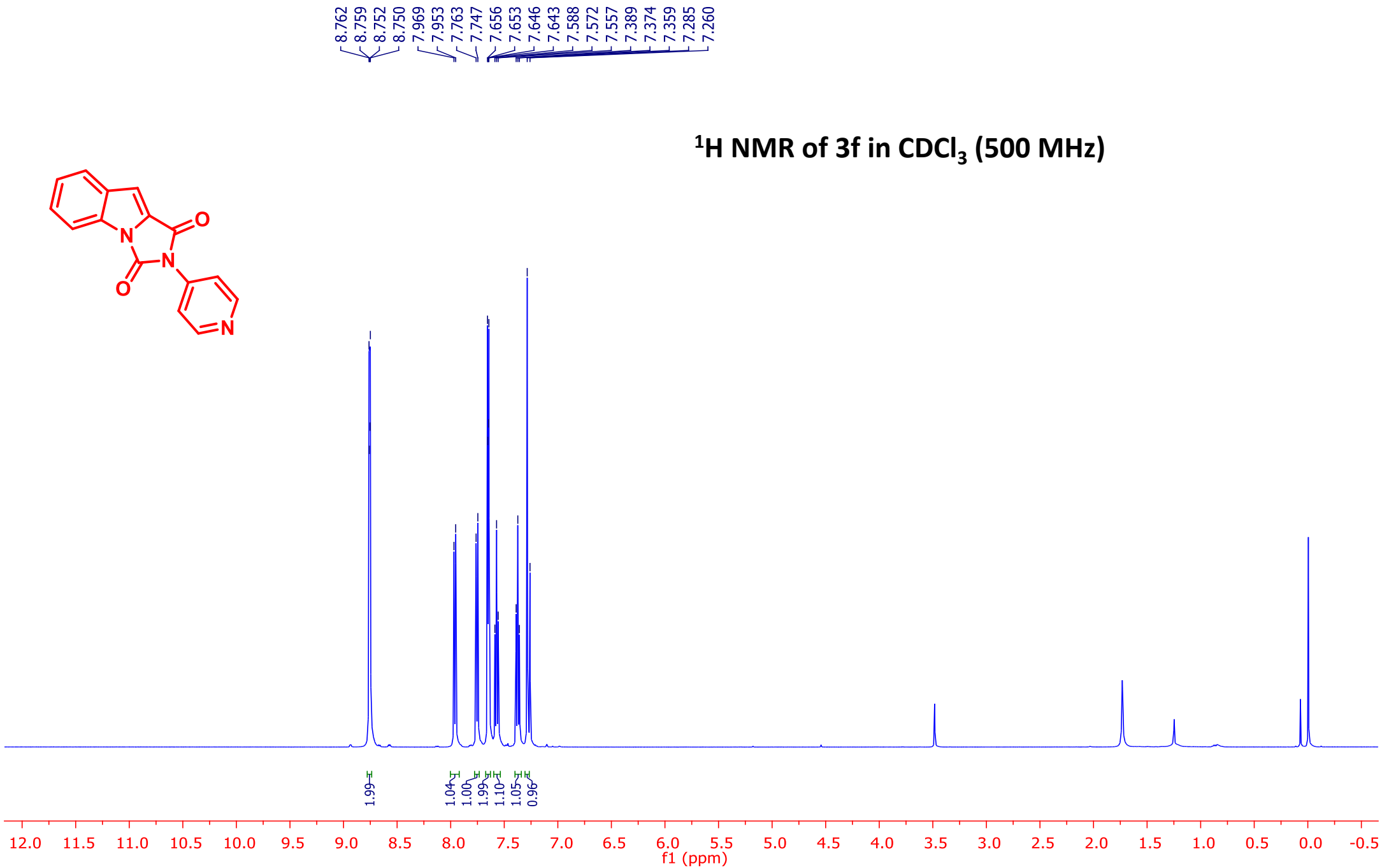


^{13}C NMR of 3e in $CDCl_3$ (100 MHz)

RS-5 #264 RT: 1.18 AV: 1 NL: 1.14E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]

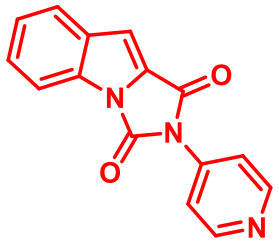
HRMS of 3e





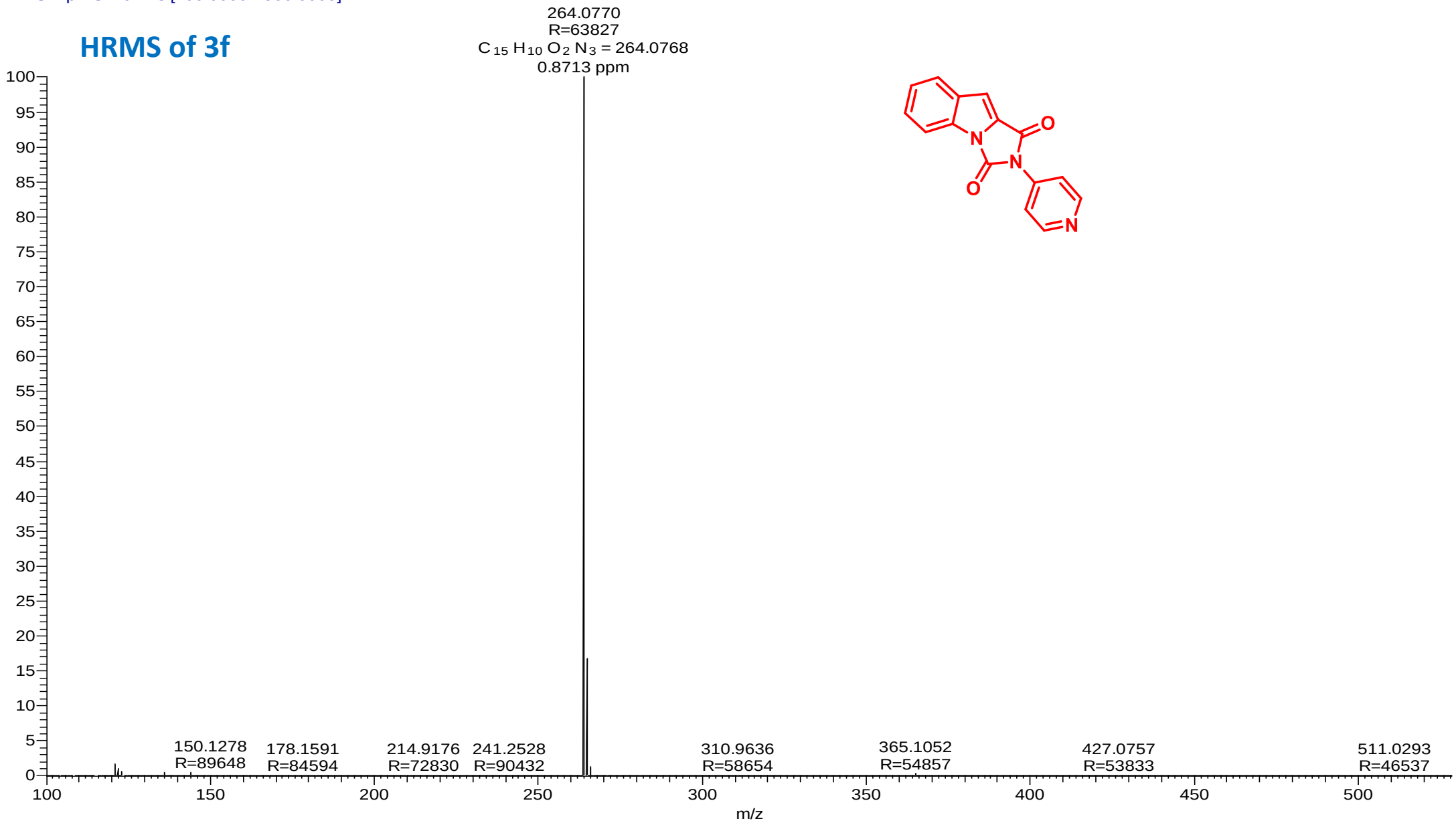
^{1}H NMR of 3f in $CDCl_3$ (500 MHz)

^{13}C NMR of 3f in $CDCl_3$ (125 MHz)

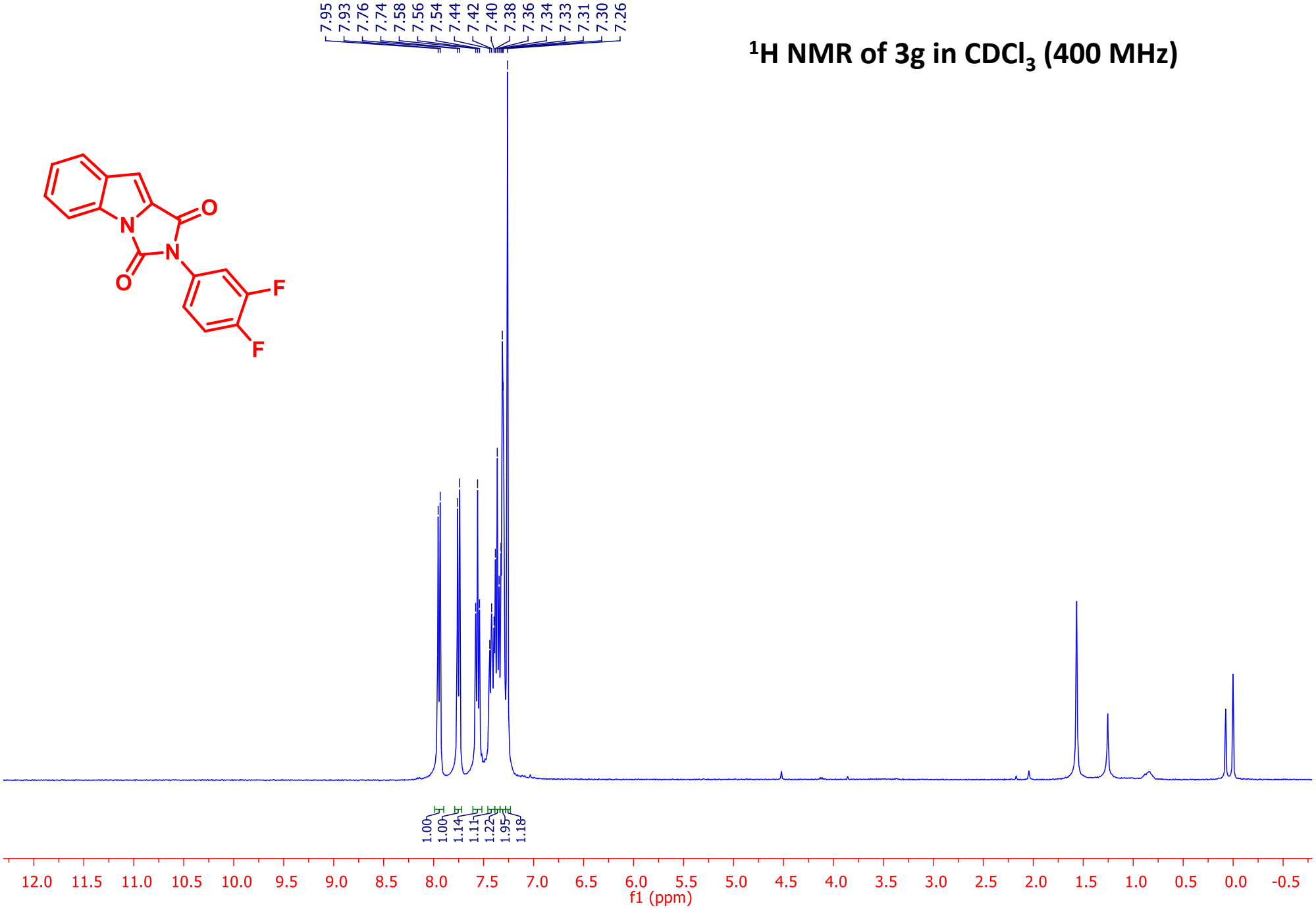


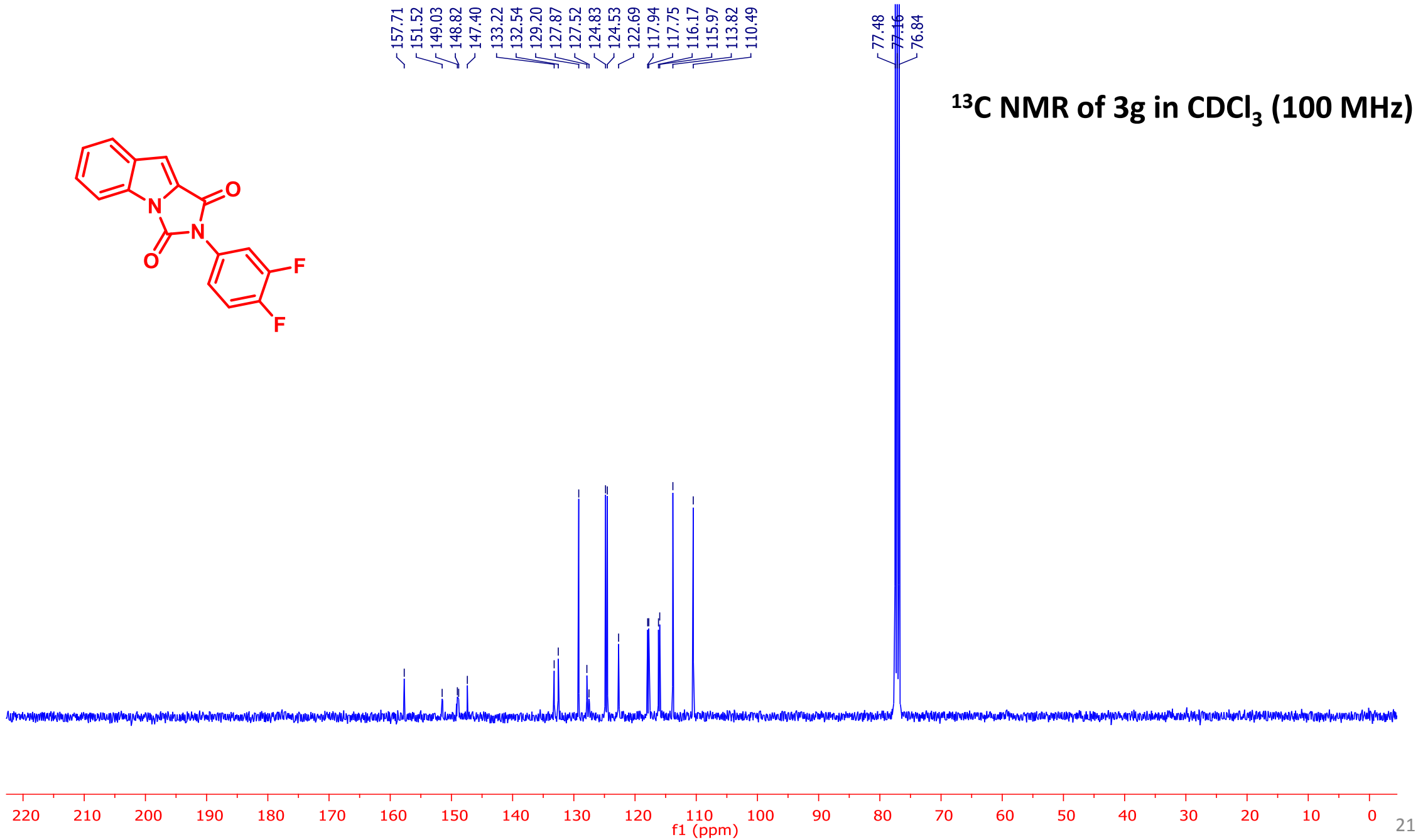
RS-6 #367-370 RT: 1.63-1.65 AV: 4 NL: 6.18E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]

HRMS of 3f



^{1}H NMR of 3g in $CDCl_3$ (400 MHz)

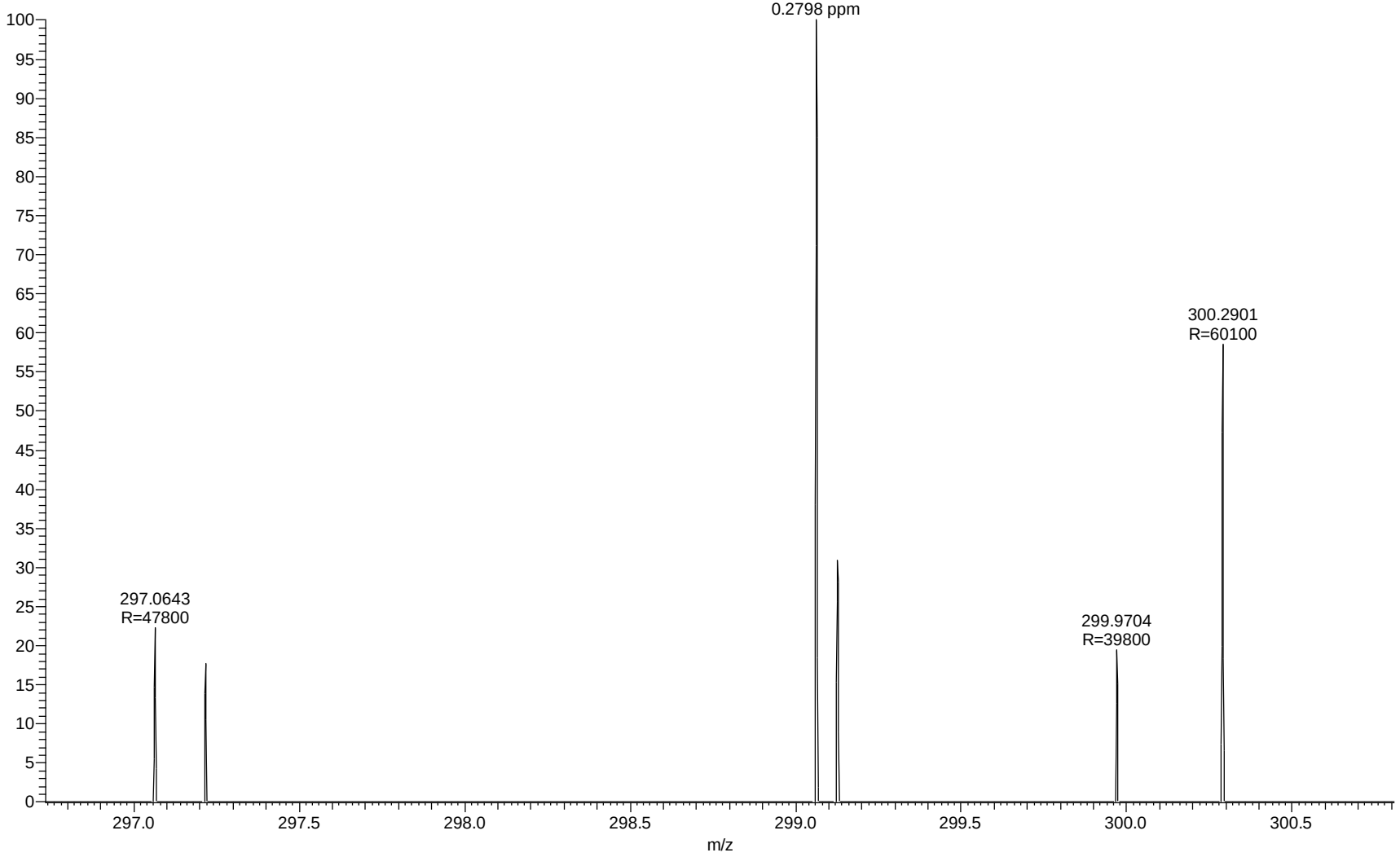


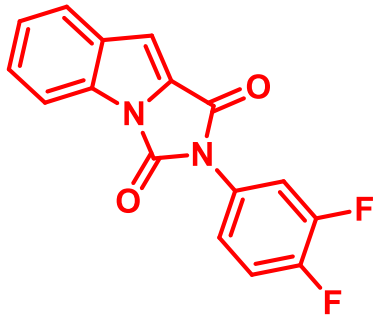


^{13}C NMR of 3g in $CDCl_3$ (100 MHz)

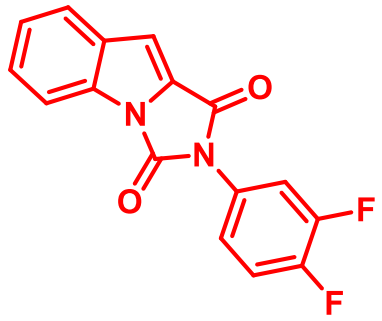
RS-7 #281 RT: 1.25 AV: 1 NL: 1.10E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

HRMS of 3g



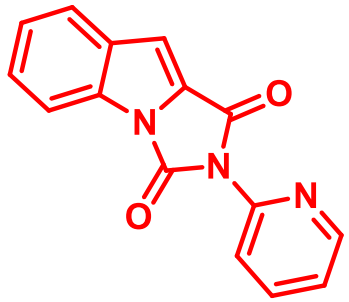


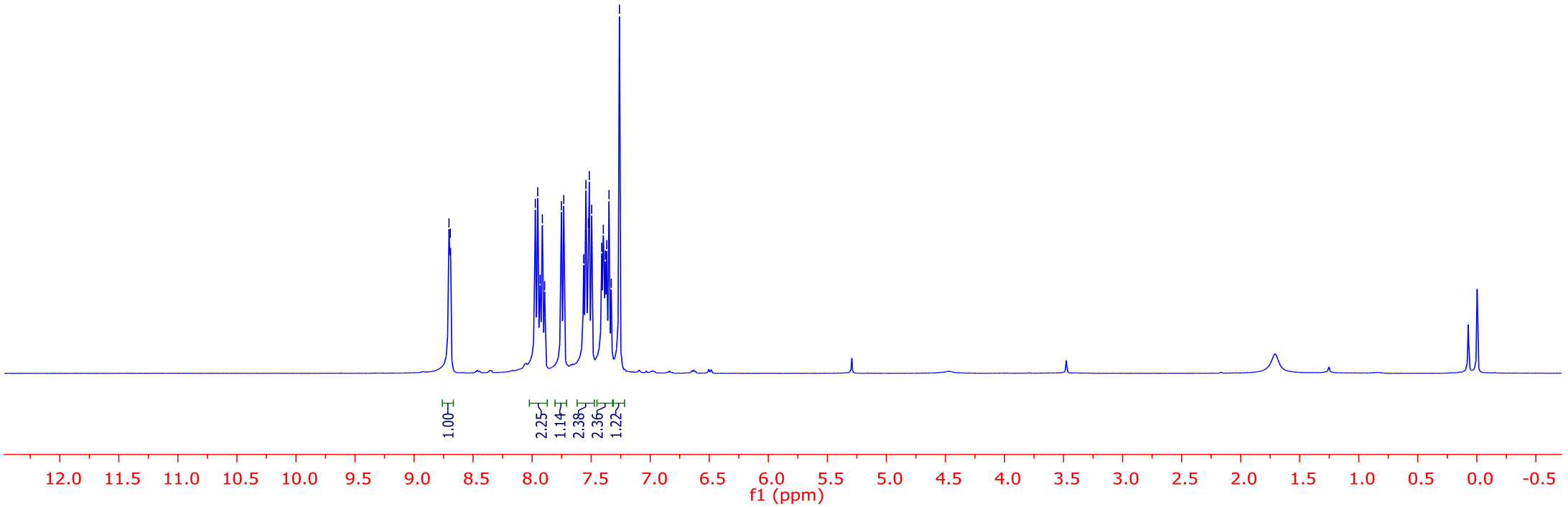
F^{19}-NMR of 3g in $CDCl_3$

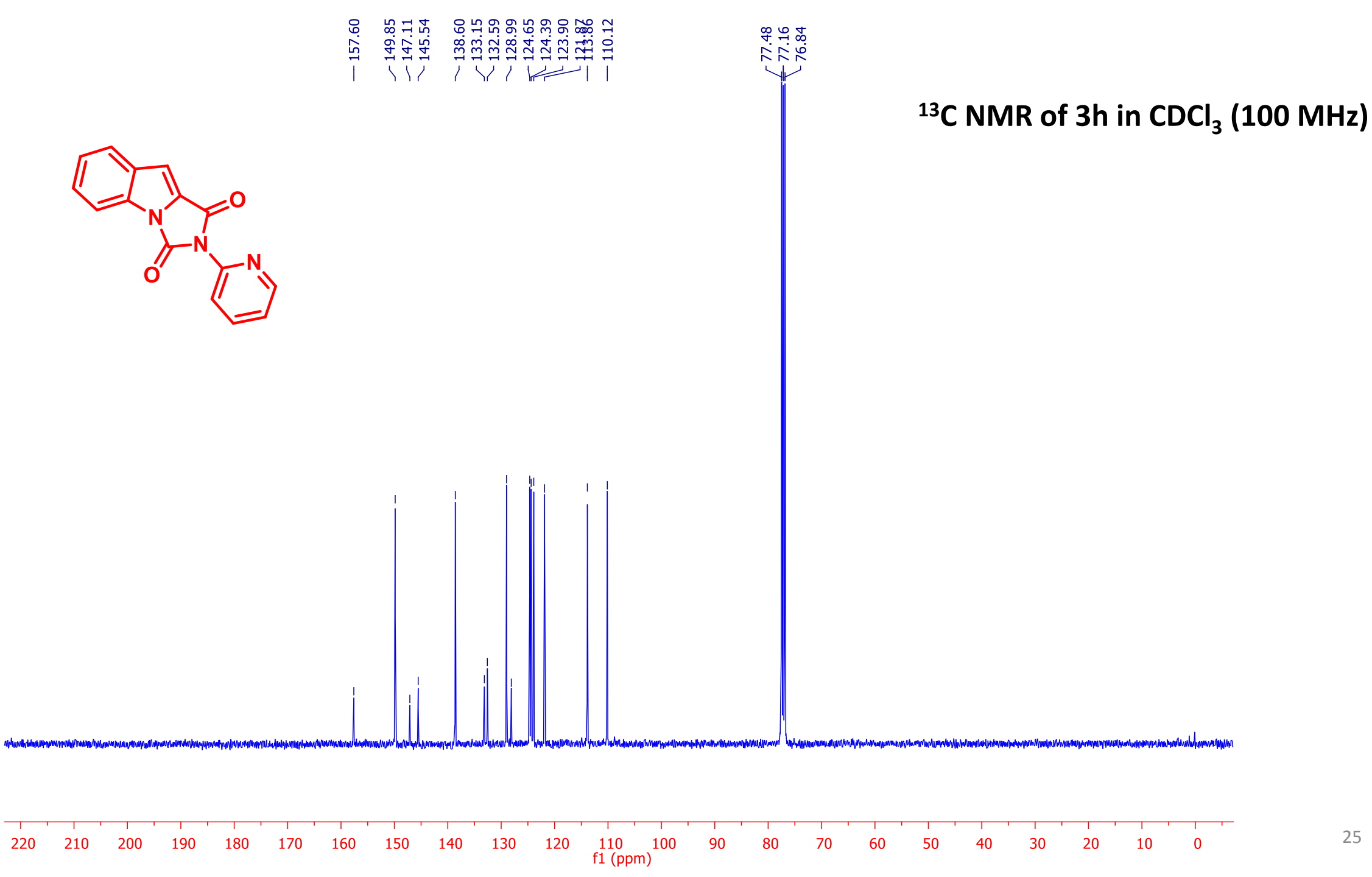


8.70
8.69
7.97
7.95
7.93
7.91
7.89
7.75
7.73
7.56
7.54
7.52
7.52
7.50
7.41
7.40
7.38
7.37
7.35
7.33
7.26

^{1}H NMR of 3h in $CDCl_3$ (400 MHz)



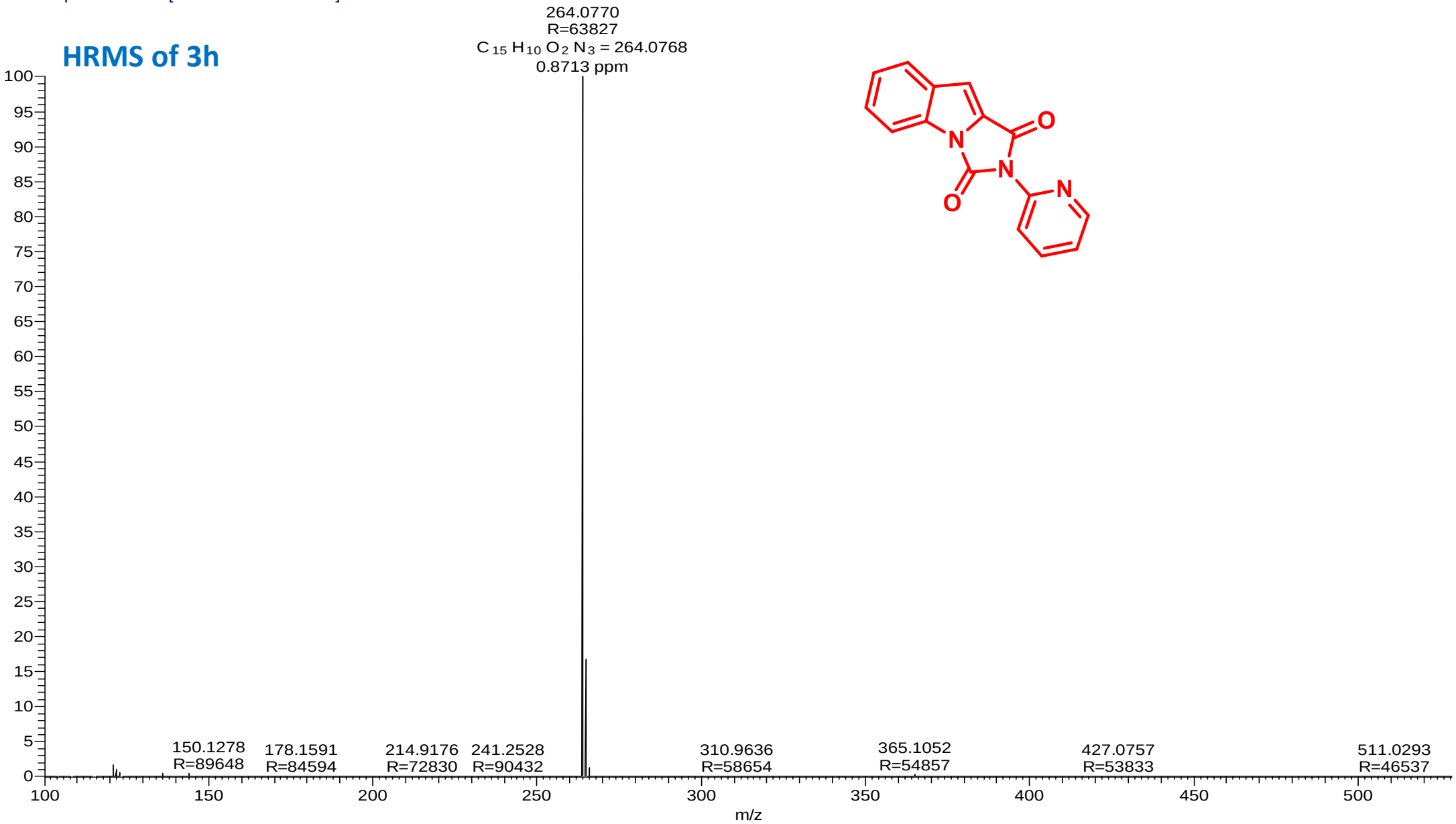




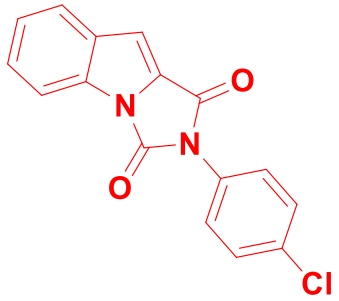
^{13}C NMR of 3h in $CDCl_3$ (100 MHz)

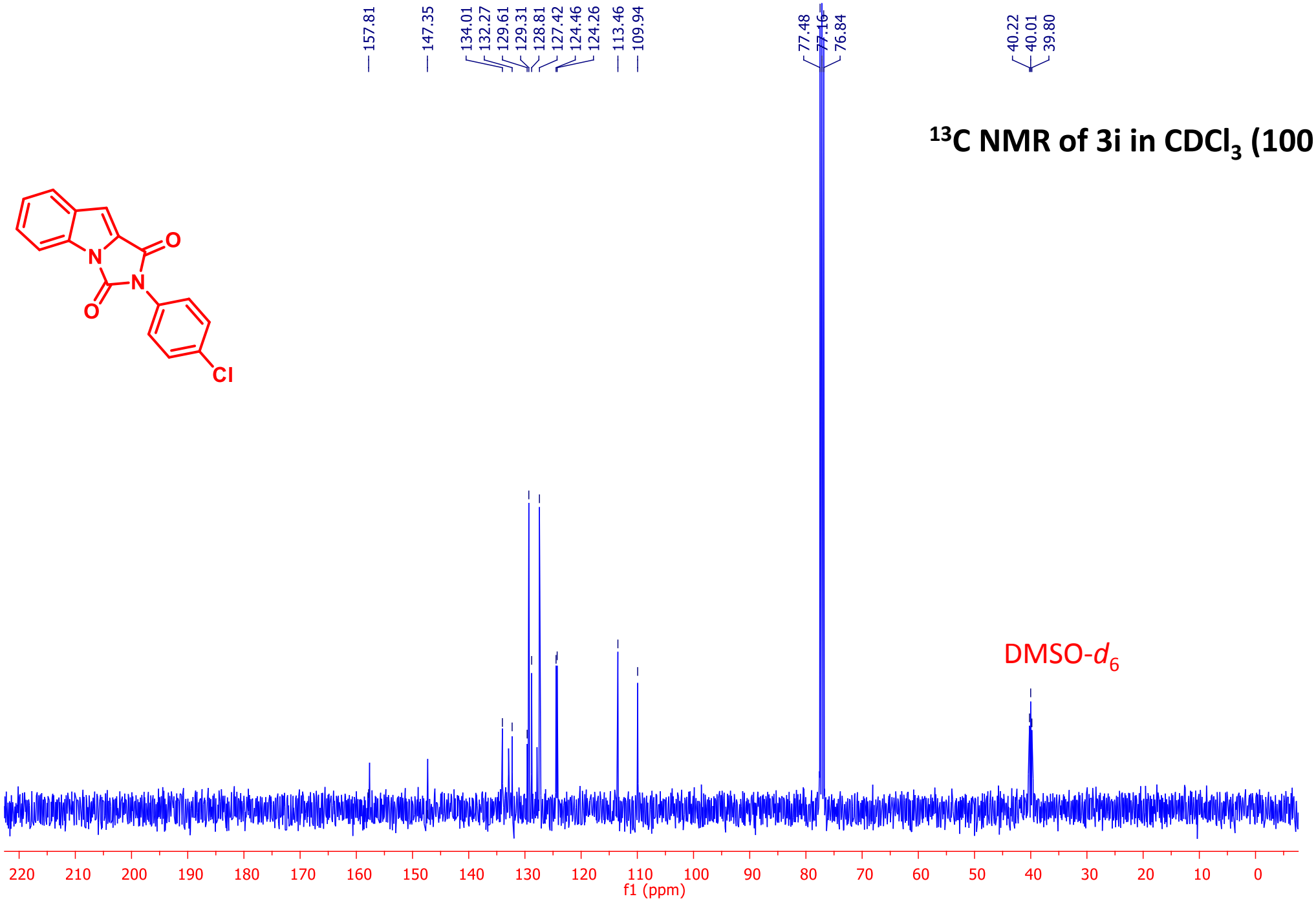
RS-6 #367-370 RT: 1.63-1.65 AV: 4 NL: 6.18E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]

HRMS of 3h

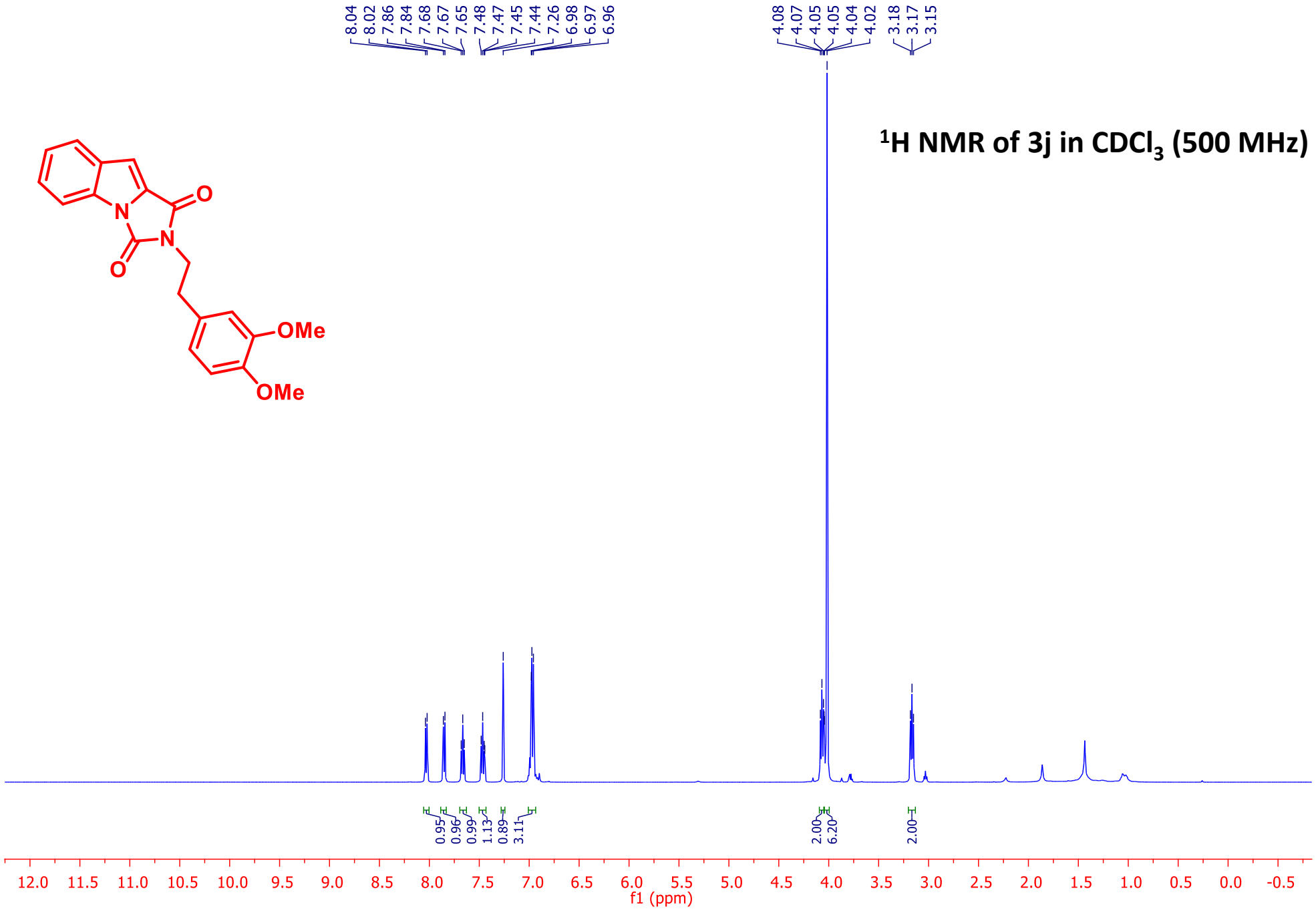


^{1}H NMR of 3i in $CDCl_3$ &DMSO-d_6 (400 MHz)

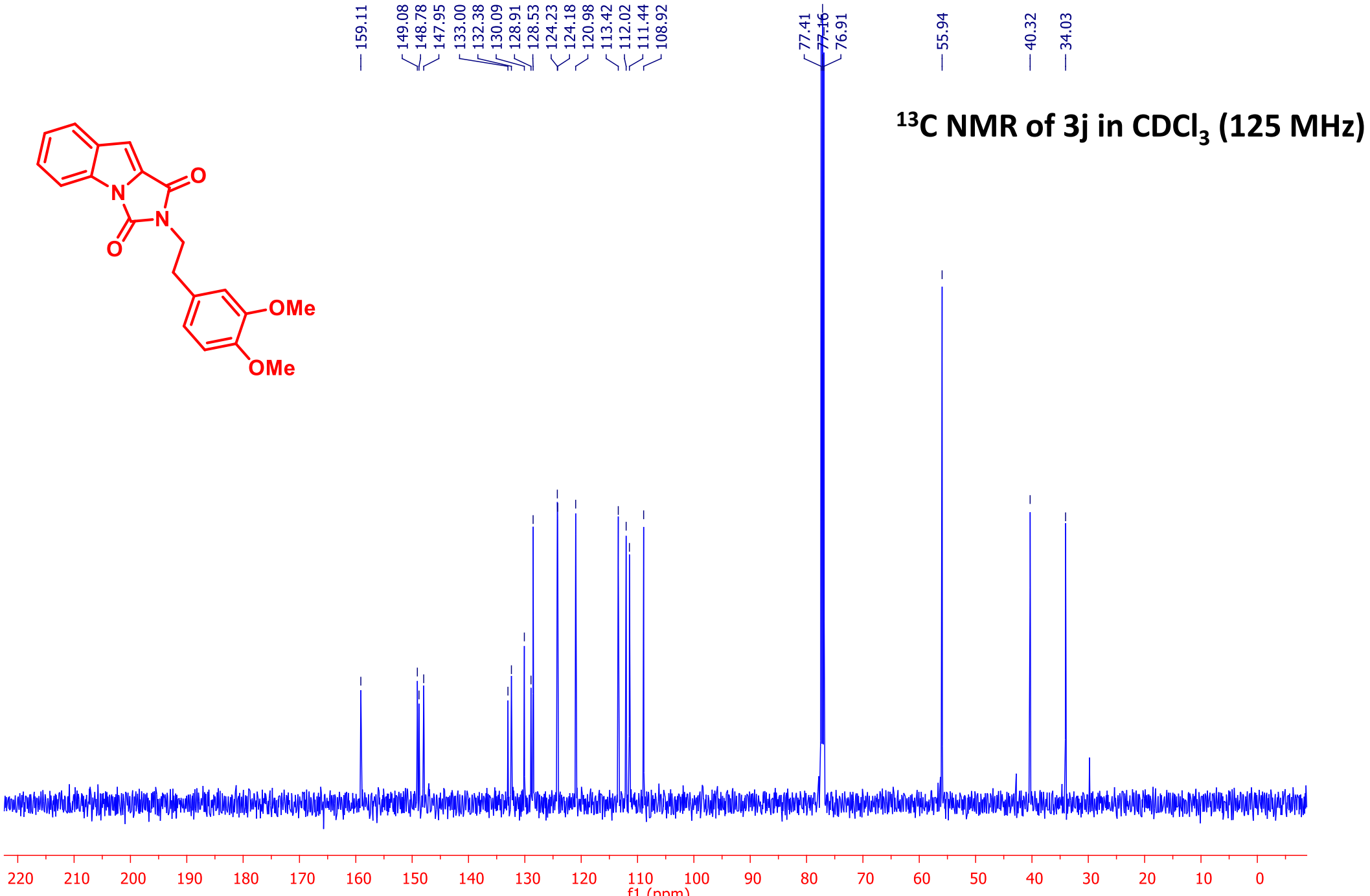




^{13}C NMR of 3i in $CDCl_3$ (100 MHz)

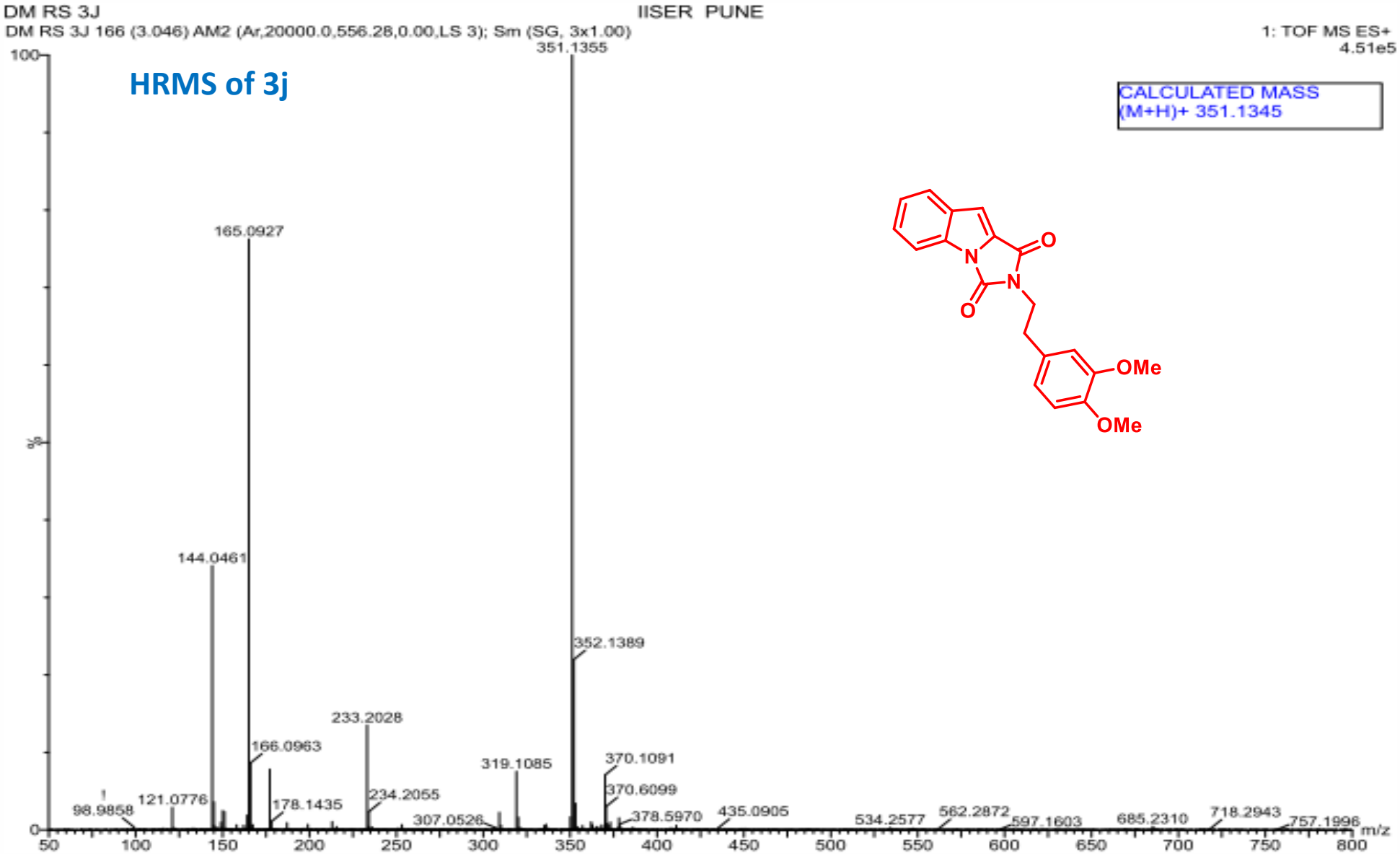


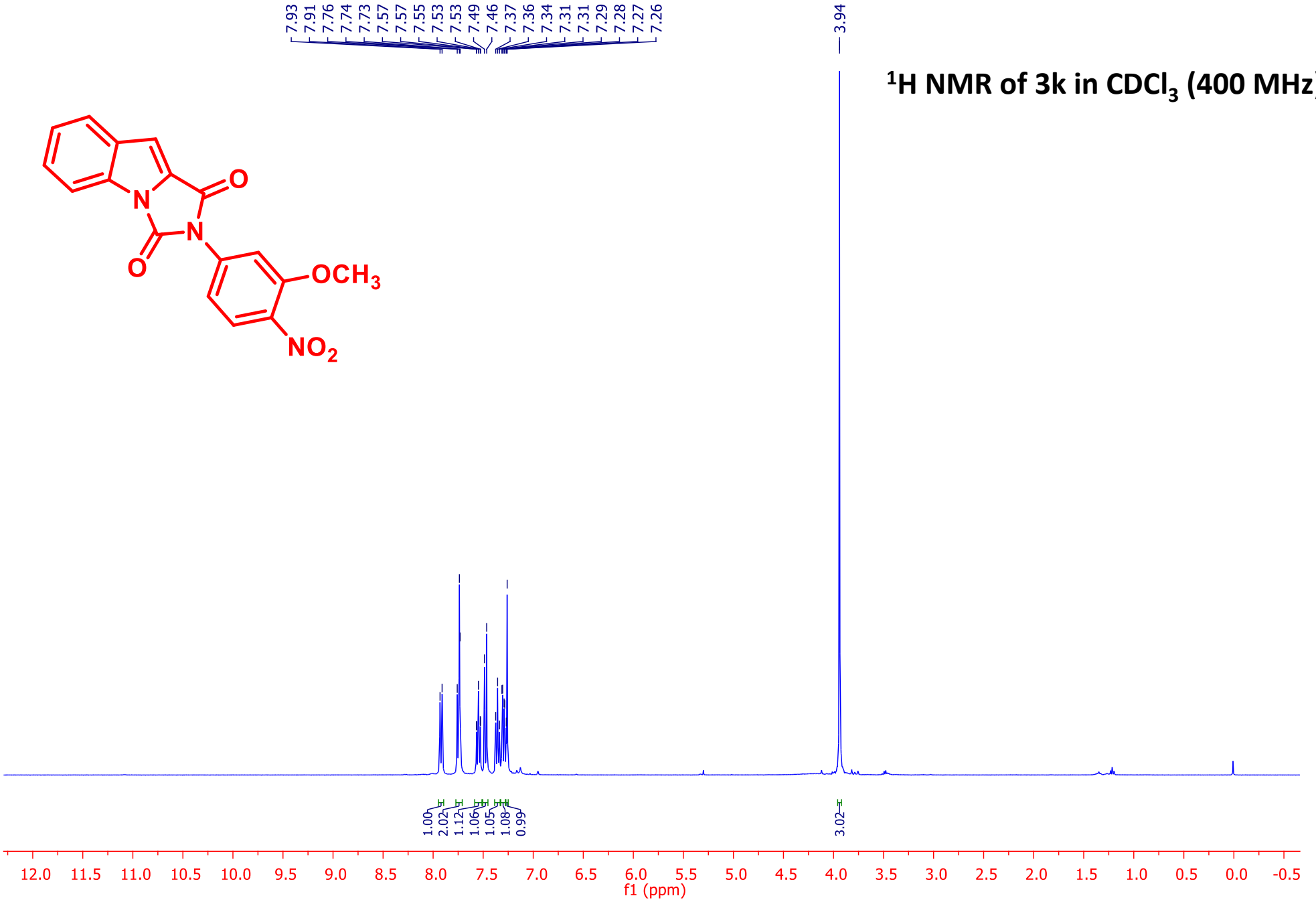
^{1}H NMR of 3j in $CDCl_3$ (500 MHz)



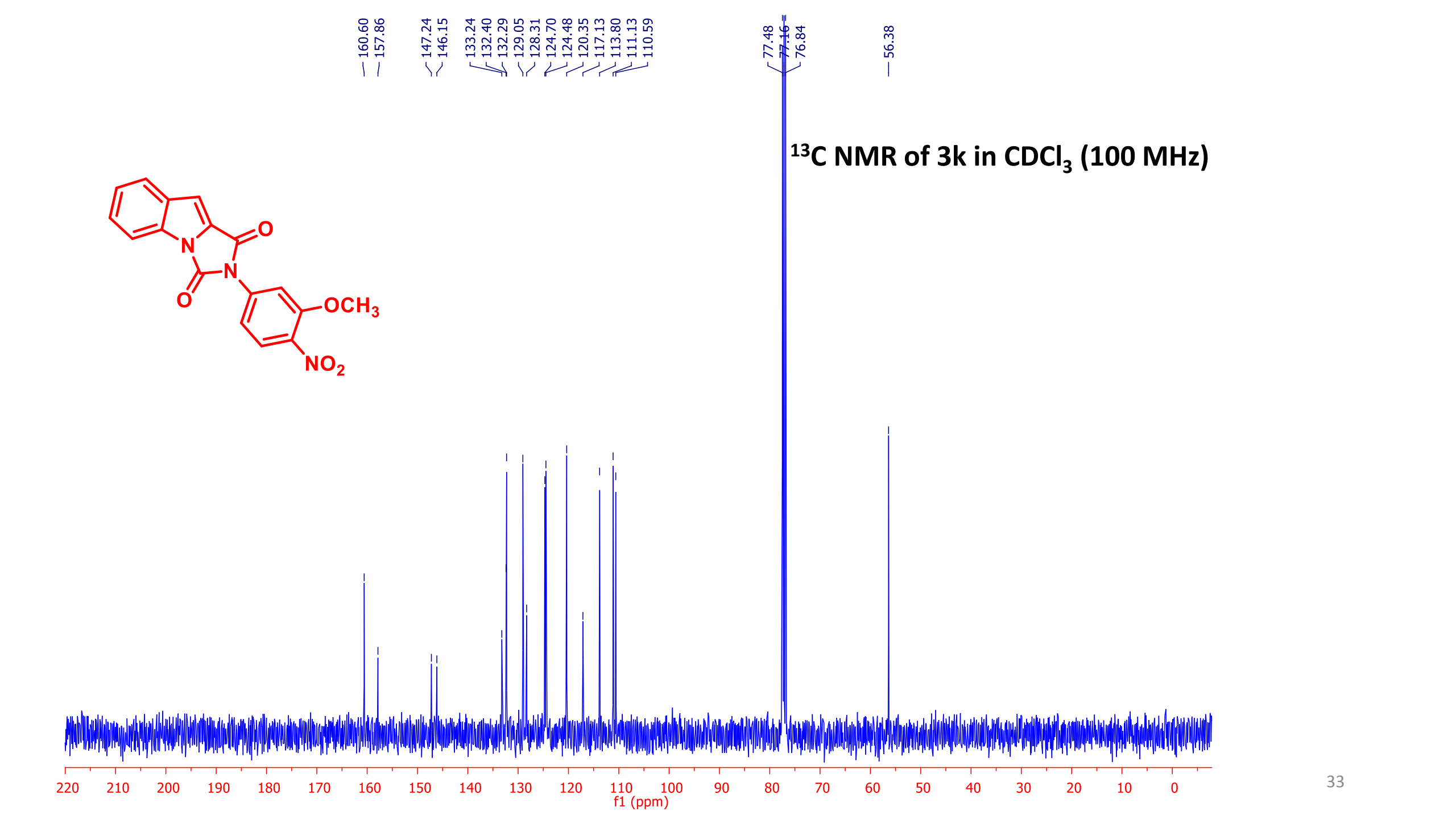
^{13}C NMR of 3j in $CDCl_3$ (125 MHz)

HRMS of 3j


DM RS 3J
IISER PUNE
DM RS 3J 166 (3.046) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES+
4.51e5
CALCULATED MASS
(M+H)+ 351.1345
351.1355
165.0927
144.0461
352.1389
233.2028
166.0963
319.1085
370.1091
370.6099
234.2055
178.1435
121.0776
98.9858
307.0526
378.5970
435.0905
534.2577
562.2872
597.1603
685.2310
718.2943
757.1996
%
m/z
OMe
OMe

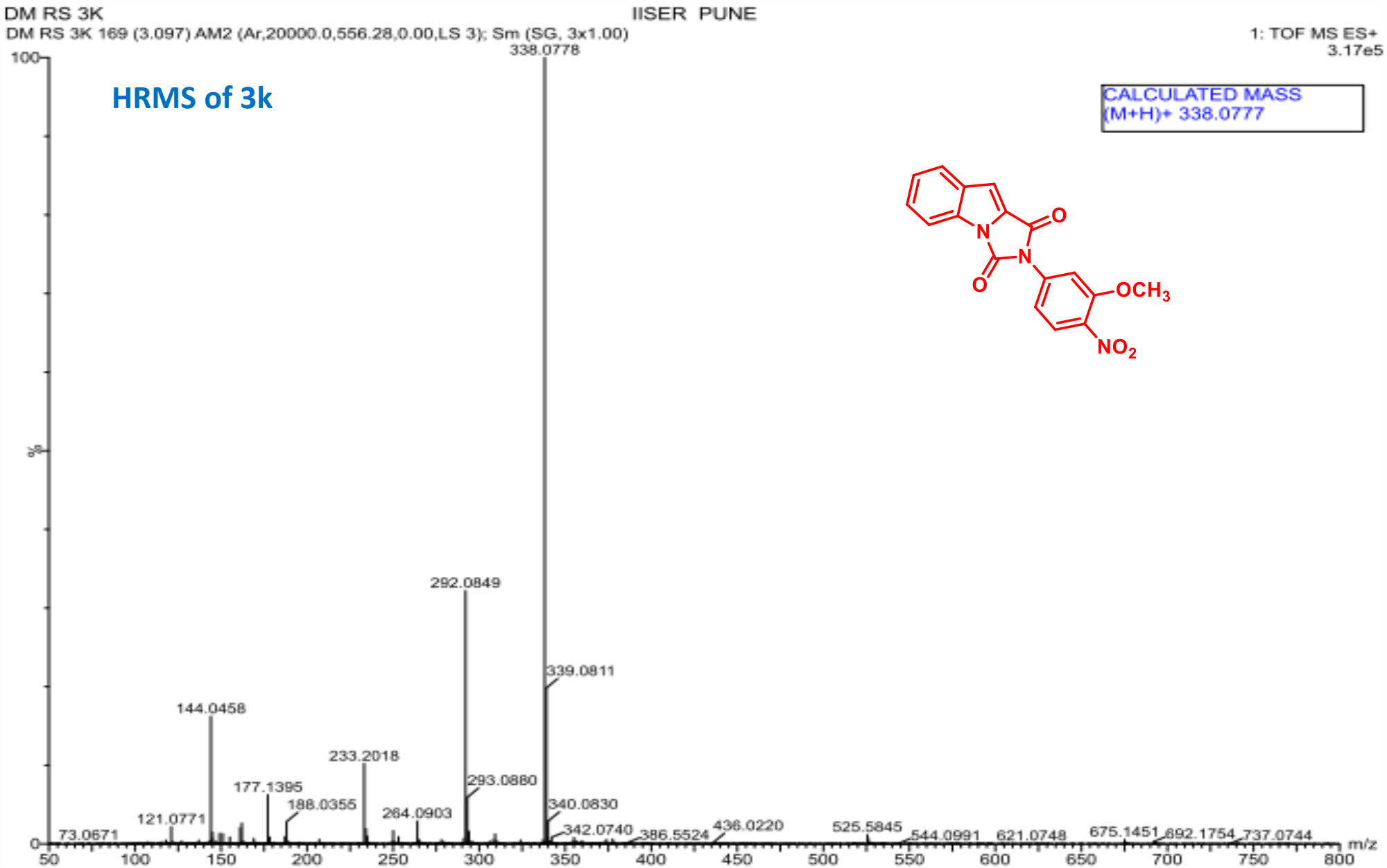


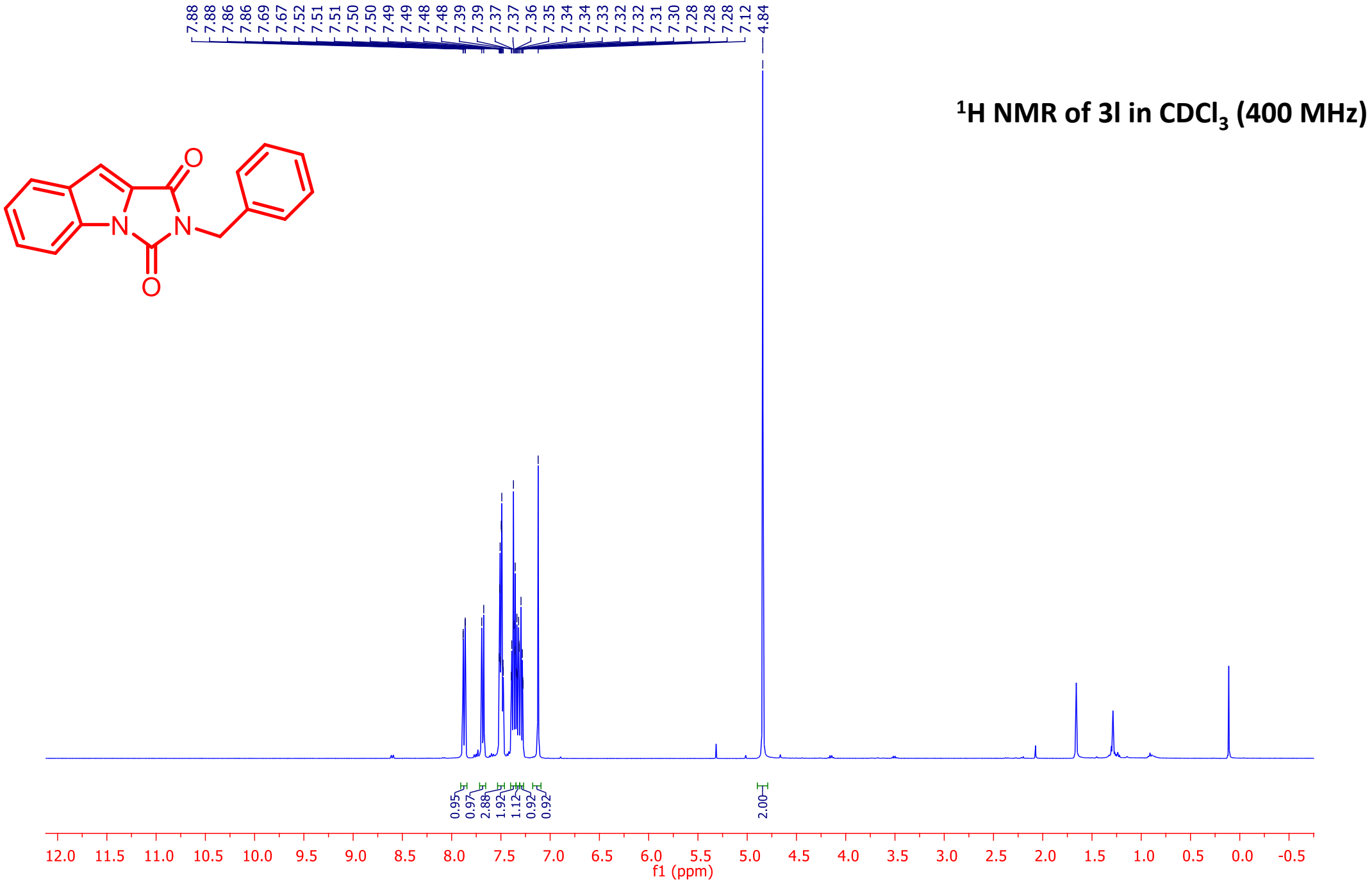
^{1}H NMR of 3k in $CDCl_3$ (400 MHz)



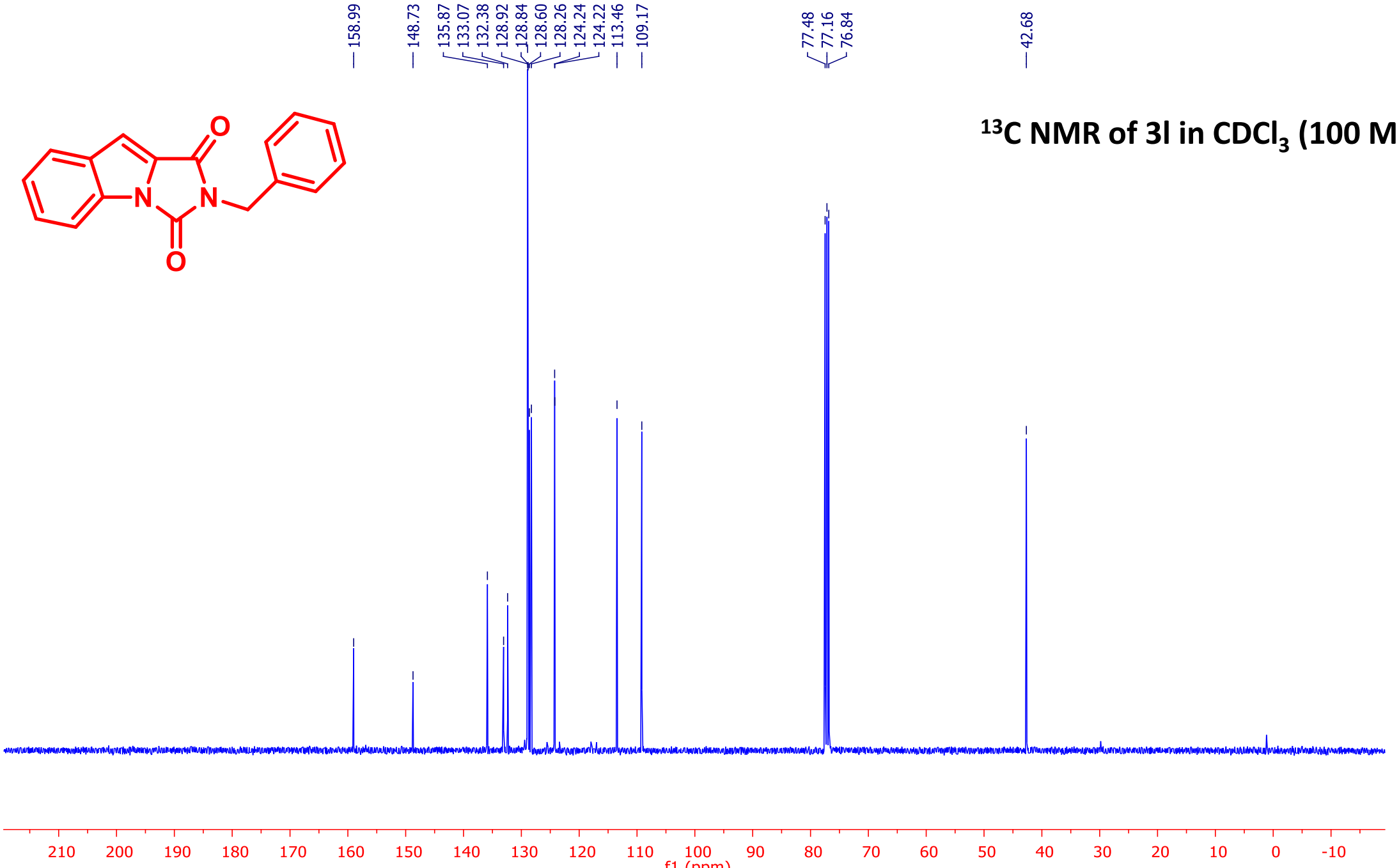
^{13}C NMR of 3k in $CDCl_3$ (100 MHz)

HRMS of 3k


DM RS 3K
IISER PUNE
DM RS 3K 169 (3.097) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES+
3.17e5
CALCULATED MASS
(M+H)+ 338.0777
338.0778
292.0849
339.0811
144.0458
233.2018
293.0880
177.1395
188.0355
340.0830
121.0771
264.0903
342.0740
386.5524
436.0220
525.5845
73.0671
544.0991
621.0748
675.1451
692.1754
737.0744
%
m/z

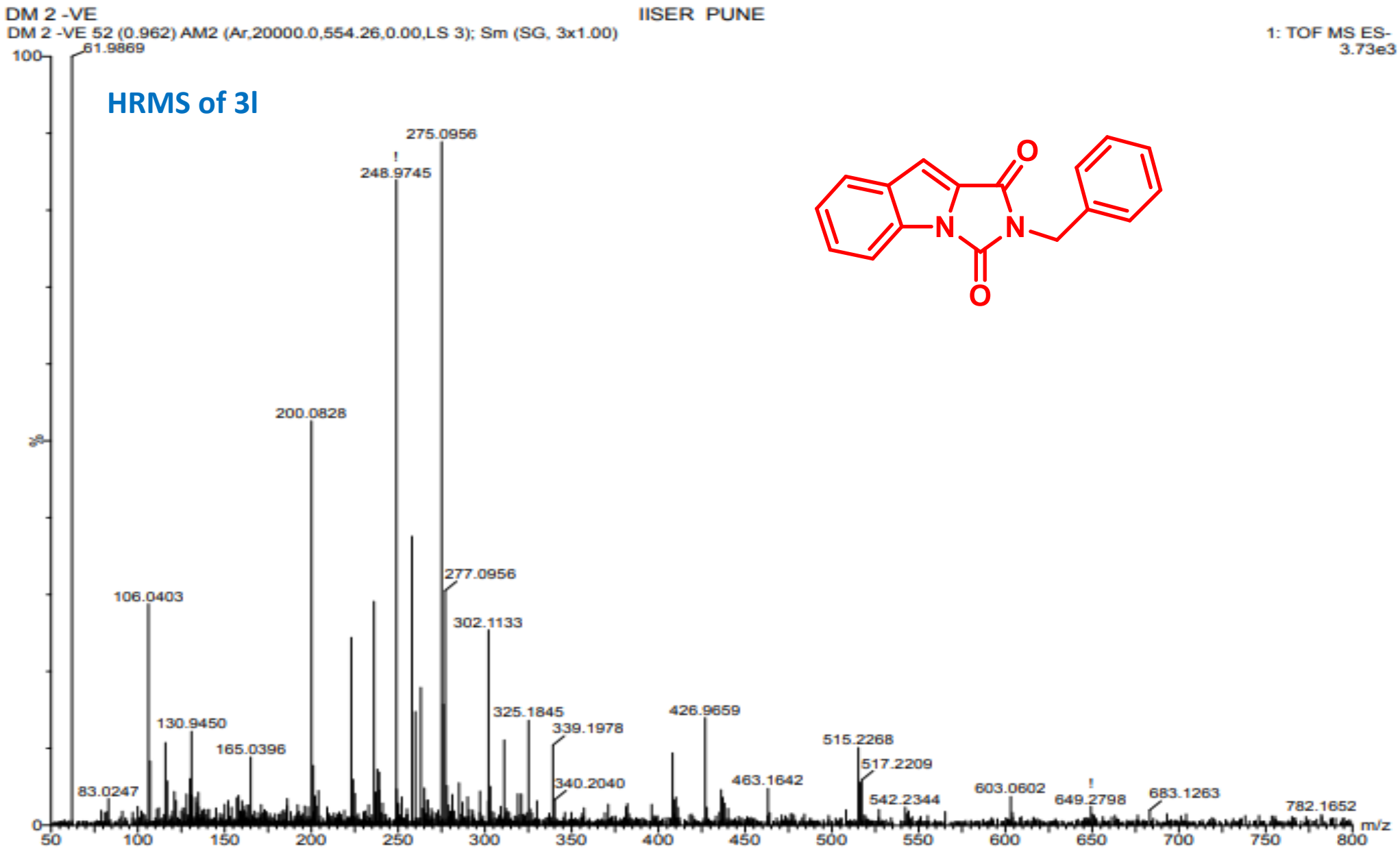


^{1}H NMR of 3l in $CDCl_3$ (400 MHz)

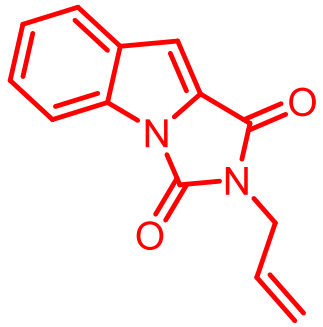


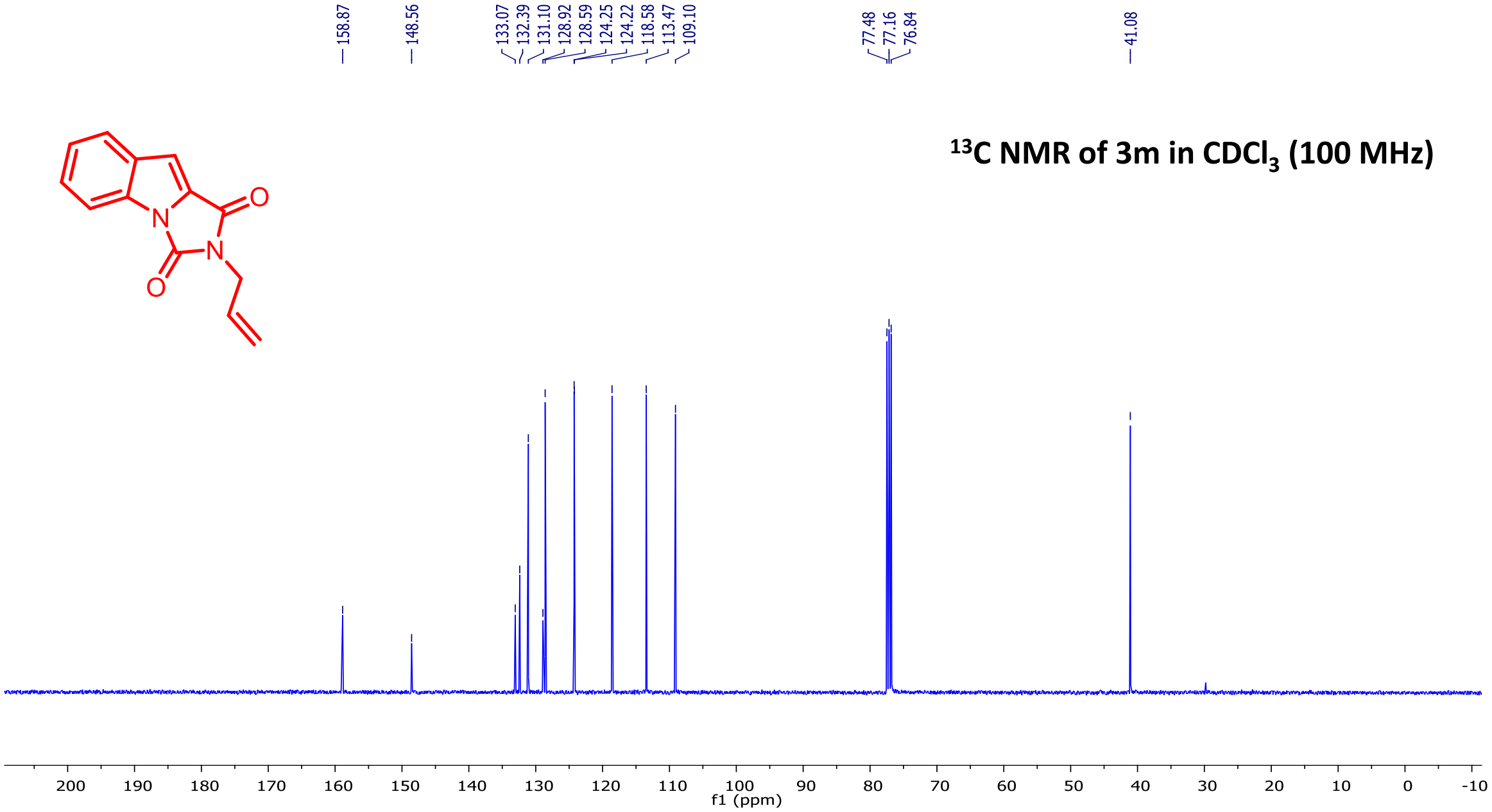
^{13}C NMR of 3l in $CDCl_3$ (100 MHz)

HRMS of 3l

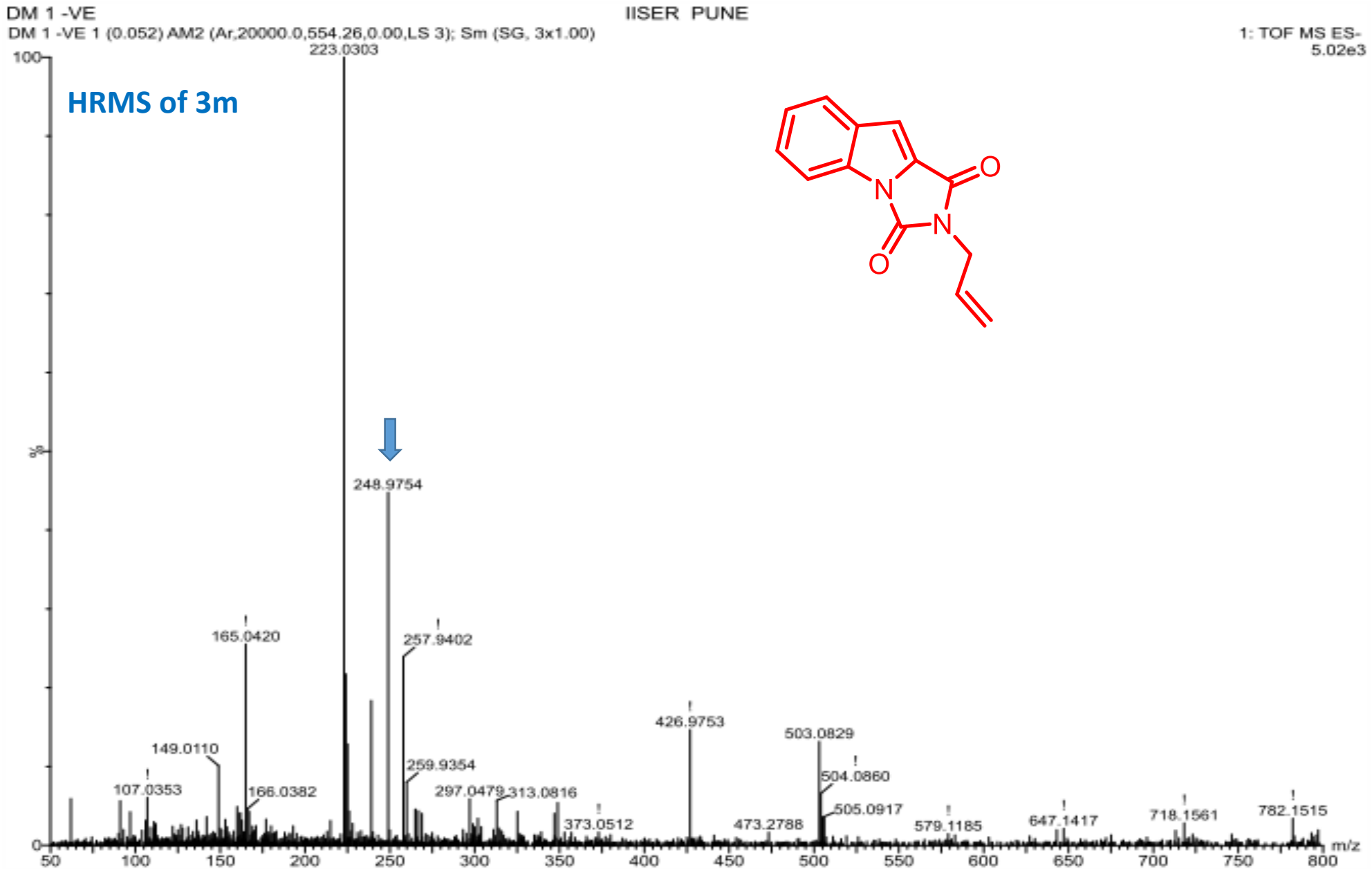

DM 2 -VE
IISER PUNE
DM 2 -VE 52 (0.962) AM2 (Ar,20000.0,554.26,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES-
3.73e3
61.9869
275.0956
248.9745
200.0828
277.0956
106.0403
302.1133
325.1845
339.1978
426.9659
130.9450
165.0396
515.2268
517.2209
340.2040
463.1642
603.0602
649.2798
683.1263
542.2344
782.1652
83.0247
%
m/z

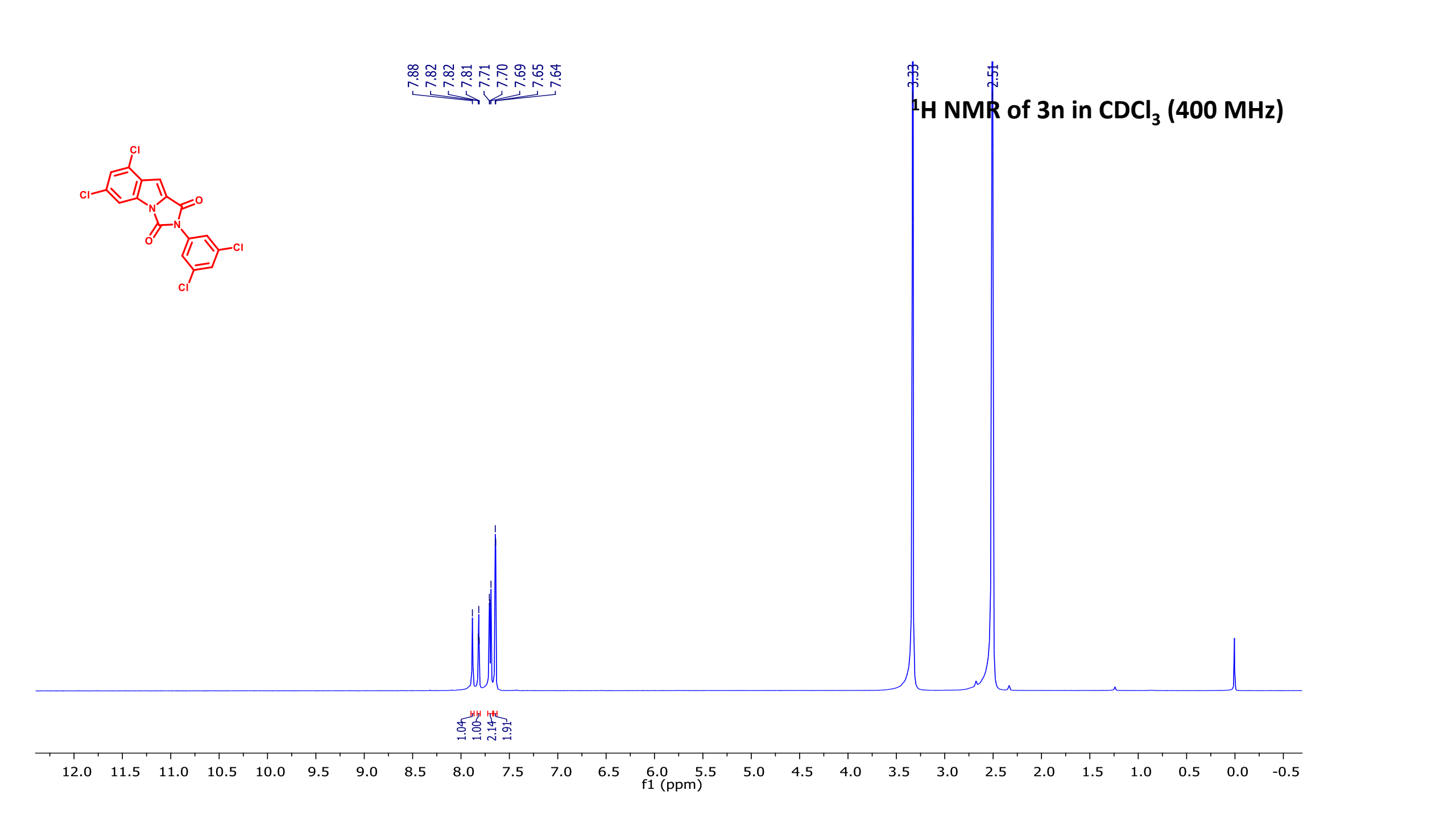
^{1}H NMR of 3m in $CDCl_3$ (400 MHz)



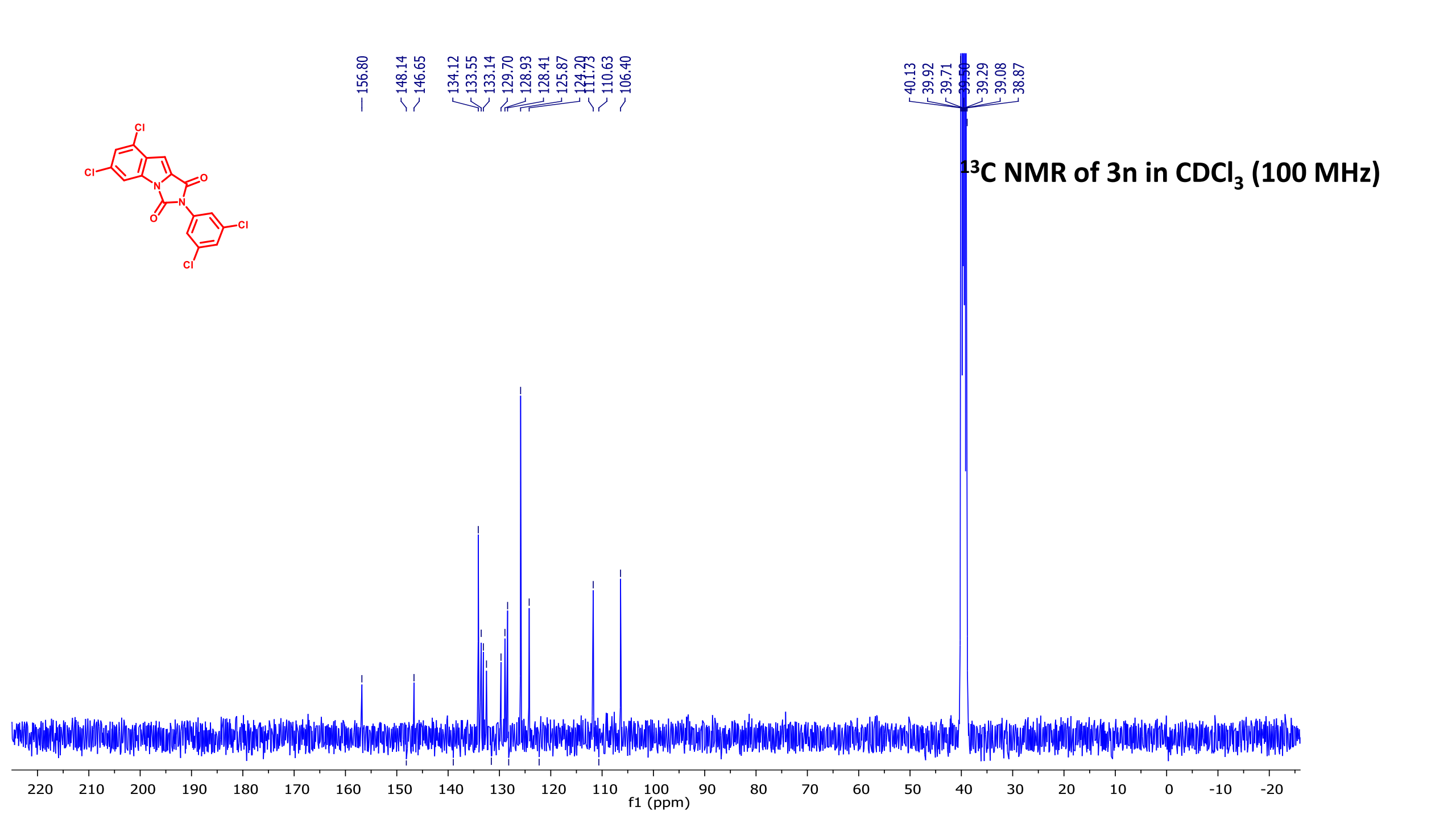


^{13}C NMR of 3m in $CDCl_3$ (100 MHz)

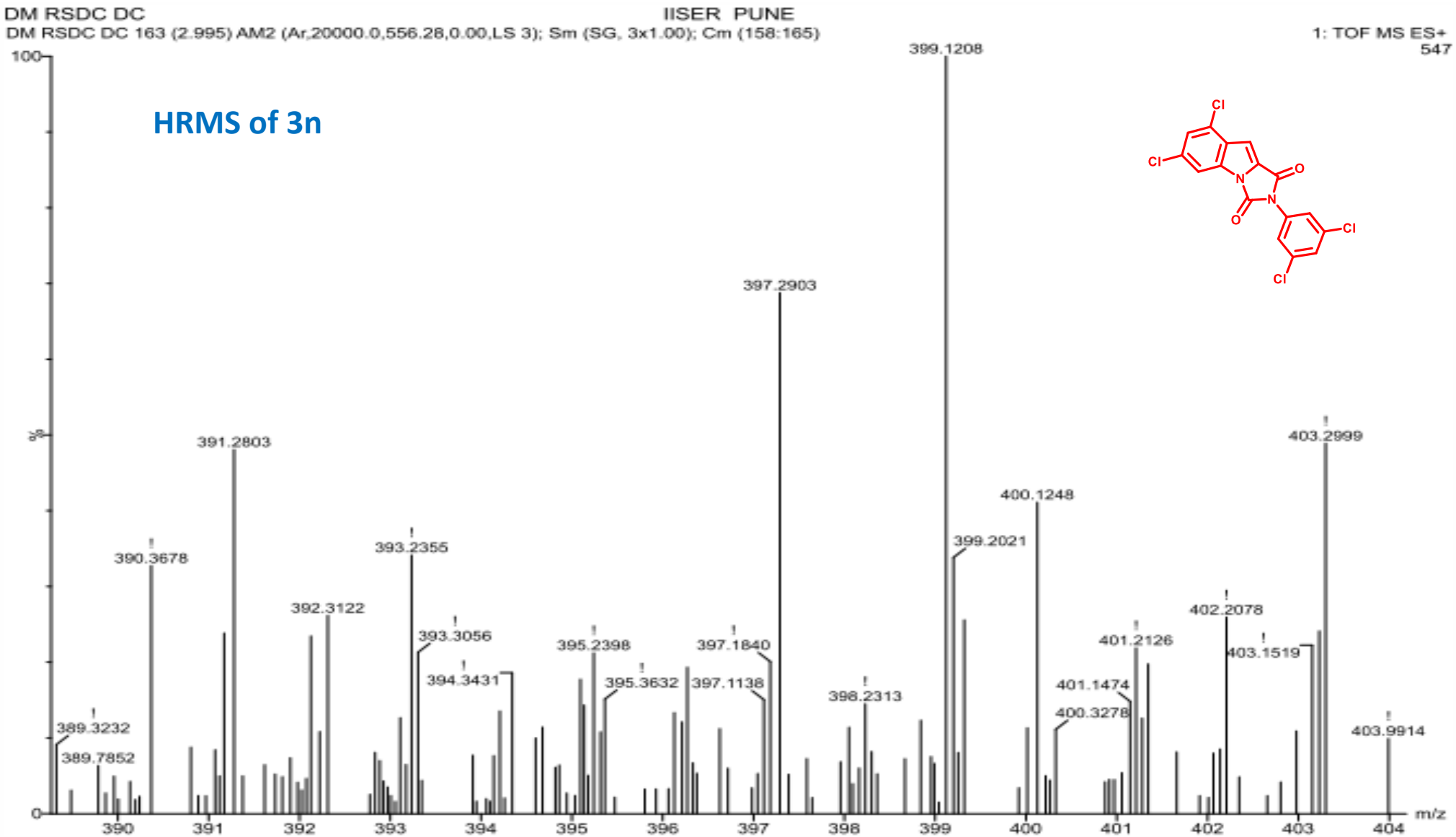

DM 1 -VE
IISER PUNE
DM 1 -VE 1 (0.052) AM2 (Ar,20000.0,554.26,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES-
5.02e3
HRMS of 3m
223.0303
248.9754
165.0420
257.9402
426.9753
503.0829
149.0110
504.0860
107.0353
166.0382
259.9354
297.0479
313.0816
505.0917
373.0512
473.2788
579.1185
647.1417
718.1561
782.1515
%
m/z
100
0
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
O
N
N
O

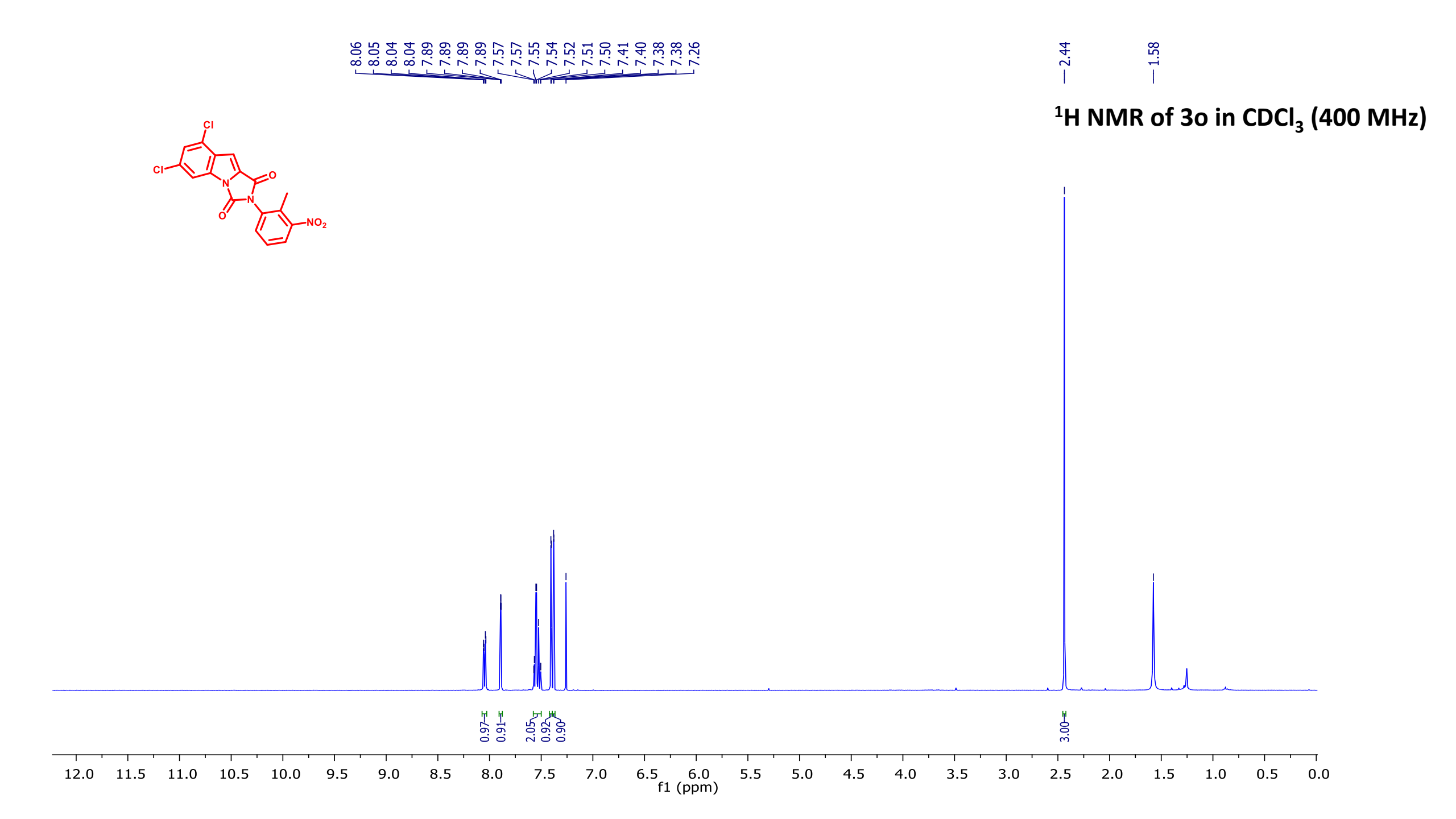


^{1}H NMR of 3n in $CDCl_3$ (400 MHz)

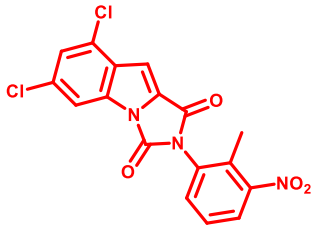

156.80
148.14
146.65
134.12
133.55
133.14
129.70
128.93
128.41
125.87
124.20
111.73
110.63
106.40
40.13
39.92
39.71
39.50
39.29
39.08
38.87
Cl
Cl
Cl
Cl
O
O
N
N
13C NMR of 3n in CDCl3 (100 MHz)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

HRMS of 3n


DM RSDC DC
IISER PUNE
DM RSDC DC 163 (2.995) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00); Cm (158:165)
1: TOF MS ES+
547
100
%
0
m/z
390
391
392
393
394
395
396
397
398
399
400
401
402
403
404
399.1208
397.2903
391.2803
403.2999
400.1248
399.2021
390.3678
393.2355
392.3122
402.2078
393.3056
401.2126
395.2398
397.1840
403.1519
394.3431
395.3632
397.1138
401.1474
398.2313
400.3278
389.3232
403.9914
389.7852
Cl
Cl
Cl
Cl
N
N
O
O



^{1}H NMR of 3o in $CDCl_3$ (400 MHz)

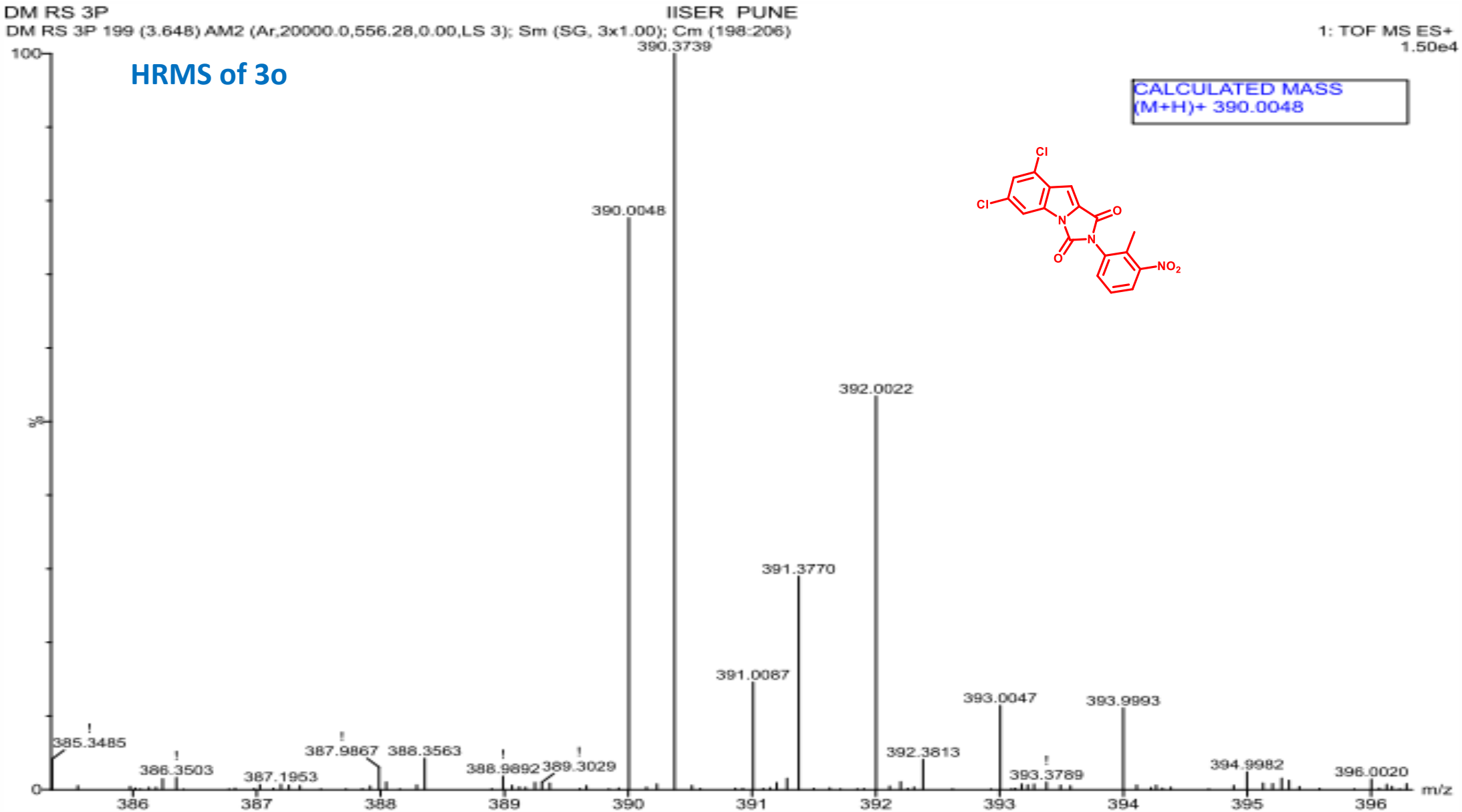


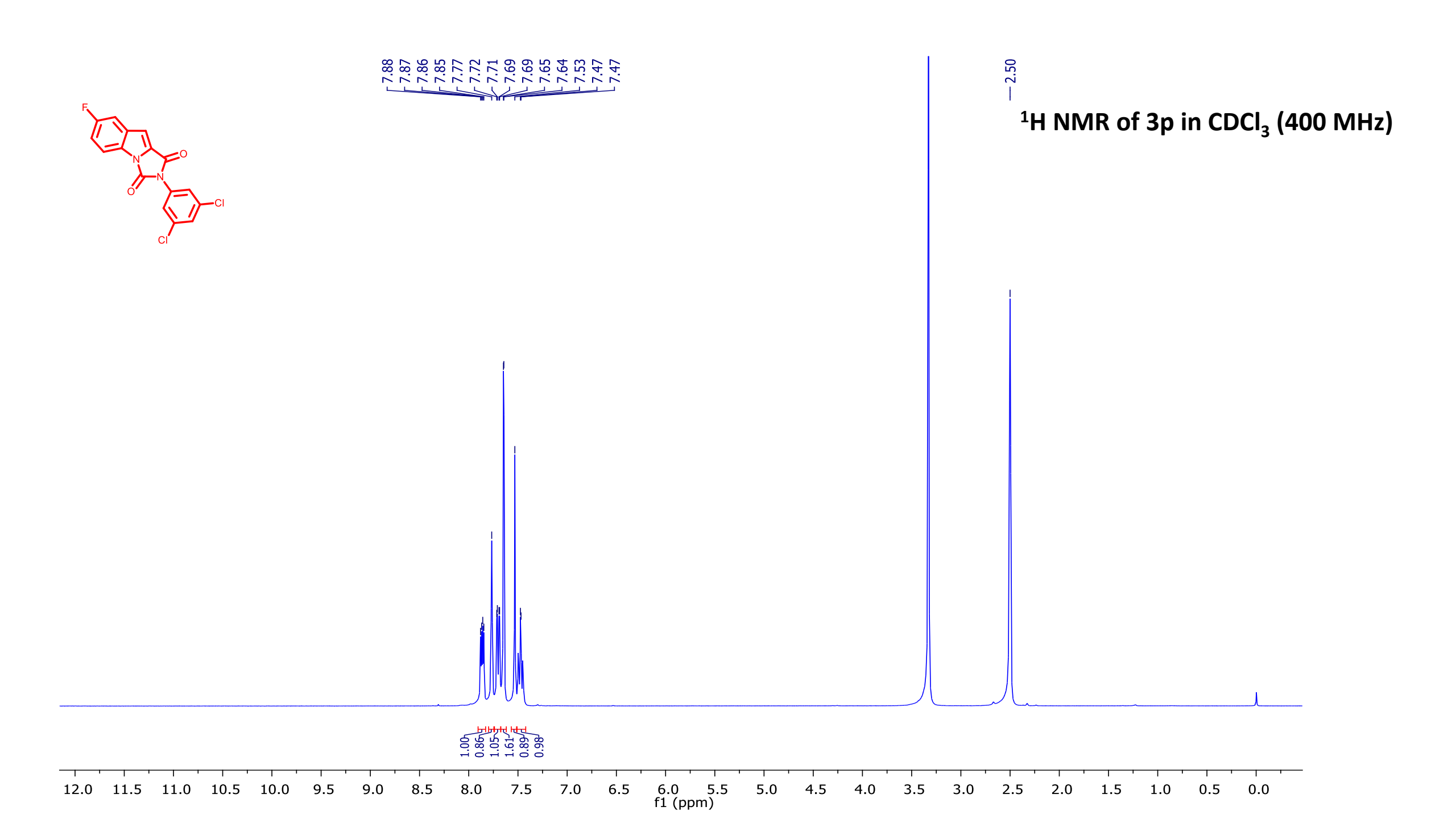
156.91
151.33
146.77
135.78
133.56
133.49
132.62
131.63
130.20
130.14
128.46
127.52
126.15
125.39
112.71
108.58
77.48
77.16
76.84
14.97

^{13}C NMR of 3o in $CDCl_3$ (100 MHz)

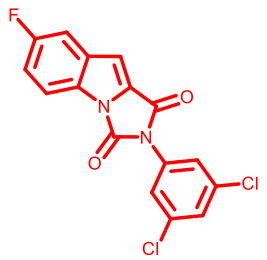
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

HRMS of 3o


DM RS 3P
IISER PUNE
DM RS 3P 199 (3.648) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00); Cm (198:206)
1: TOF MS ES+
1.50e4
CALCULATED MASS
(M+H)+ 390.0048
Cl
Cl
O
N
N
O
NO2
390.3739
390.0048
392.0022
391.3770
391.0087
393.0047
393.9993
385.3485
386.3503
387.1953
387.9867
388.3563
388.9892
389.3029
392.3813
393.3789
394.9982
396.0020
%
m/z
100
0
386
387
388
389
390
391
392
393
394
395
396



^{1}H NMR of 3p in $CDCl_3$ (400 MHz)

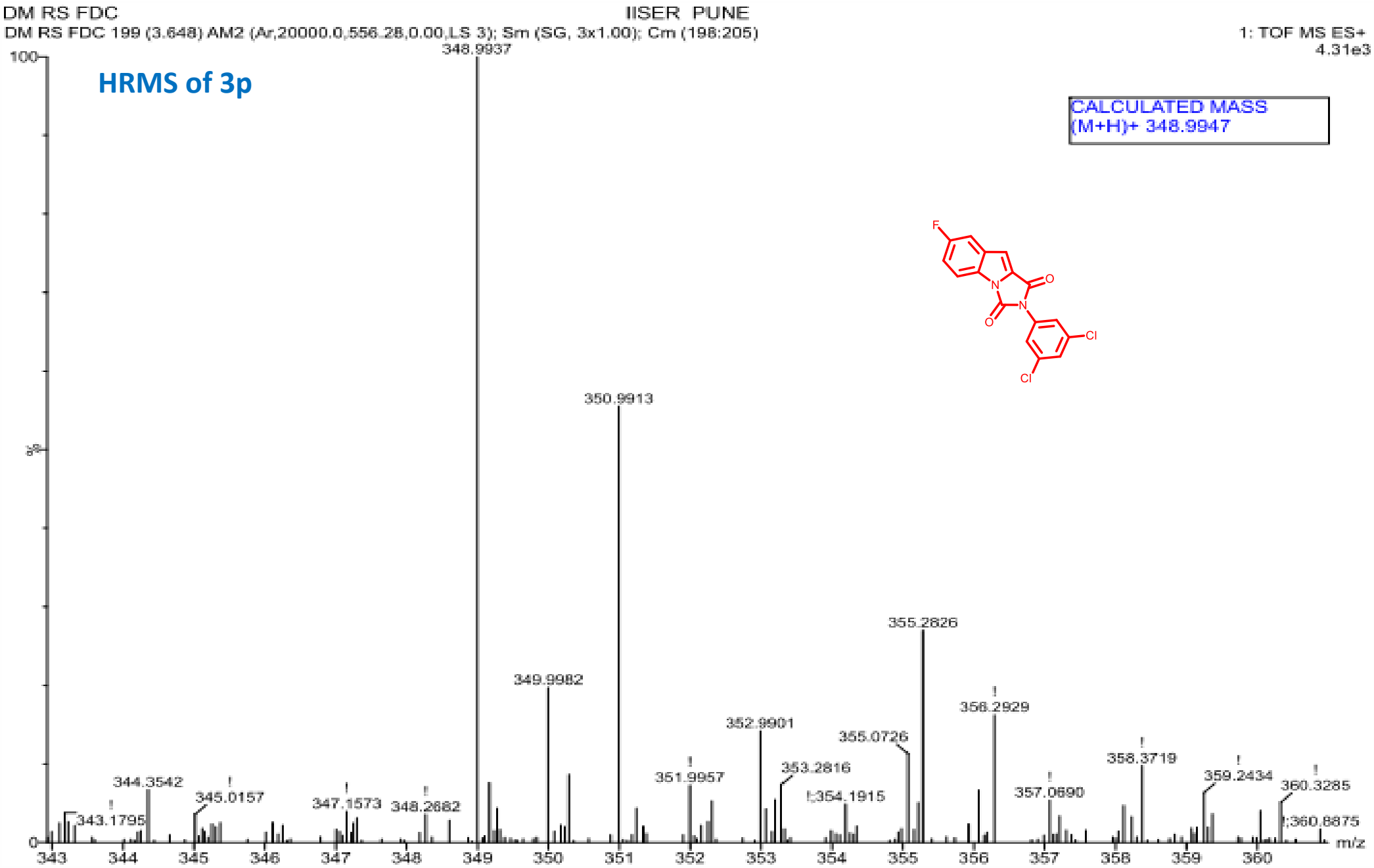


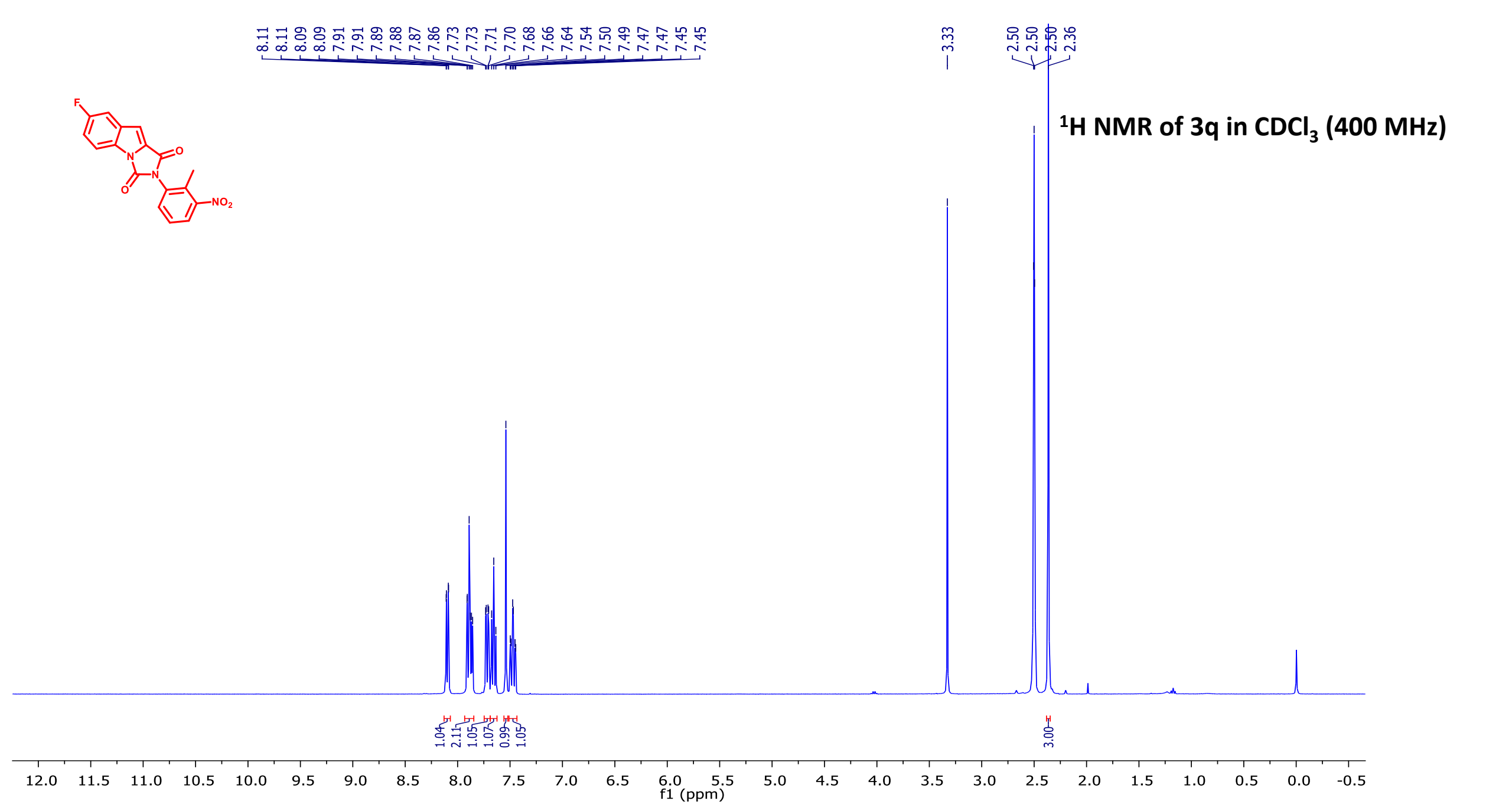
160.13
157.75
157.17
146.86
134.04
133.39
133.16
130.05
128.89
128.13
125.85
116.72
114.13
114.04
110.07
109.82
108.87
40.13
39.92
39.71
39.50
39.29
39.08
38.87

^{13}C NMR of 3p in $CDCl_3$ (100 MHz)

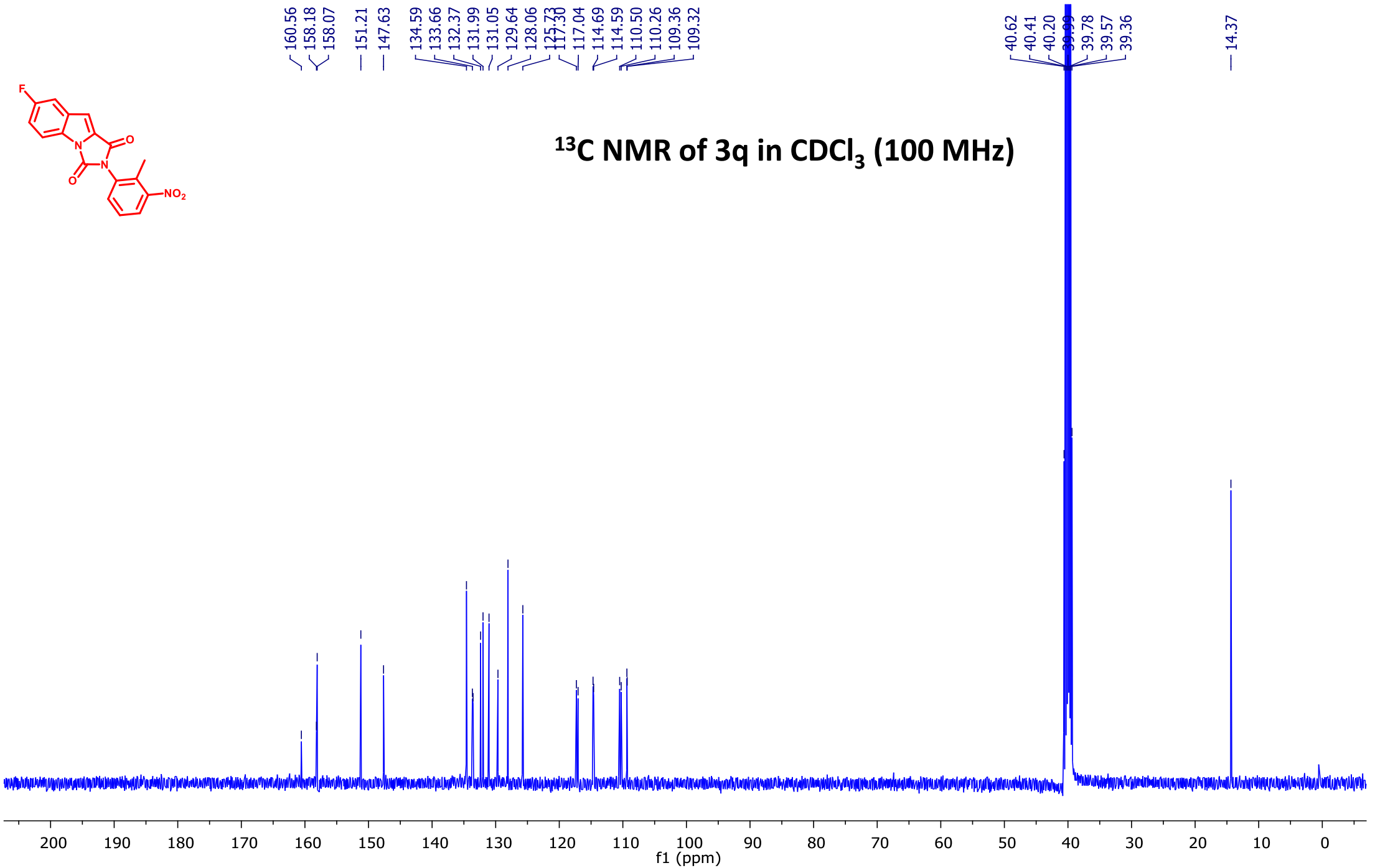
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)


DM RS FDC
IISER PUNE
DM RS FDC 199 (3.648) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00); Cm (198:205)
1: TOF MS ES+
4.31e3
HRMS of 3p
CALCULATED MASS
(M+H)+ 348.9947
348.9937
350.9913
349.9982
352.9901
355.0726
355.2826
358.2929
351.9957
353.2816
354.1915
358.3719
359.2434
360.3285
360.8875
344.3542
345.0157
347.1573
348.2682
343.1795
357.0690
m/z

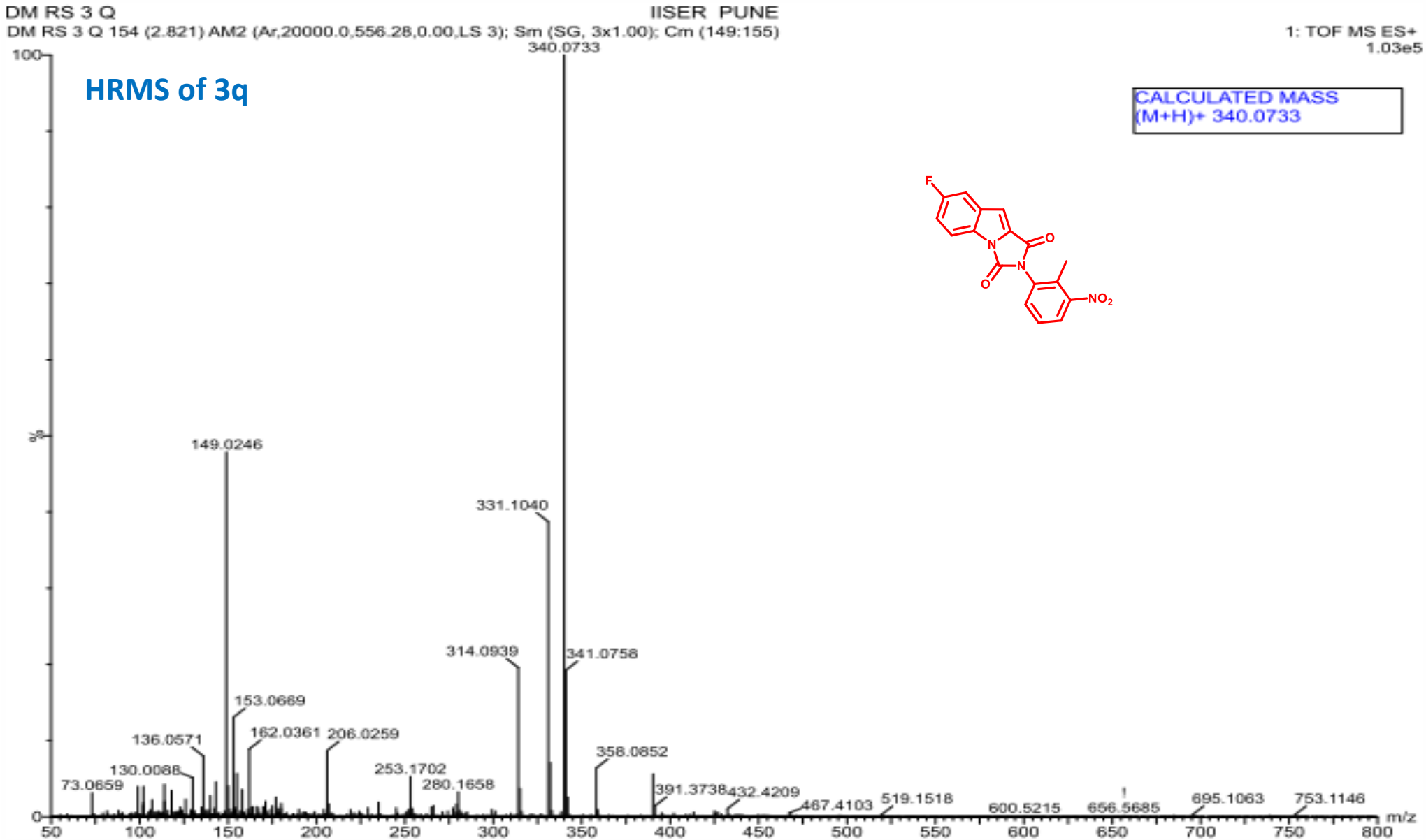


^{1}H NMR of 3q in $CDCl_3$ (400 MHz)

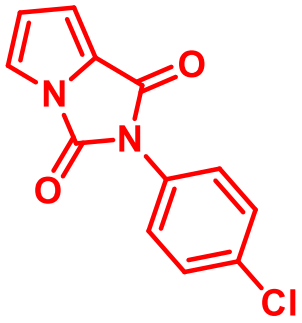


^{13}C NMR of 3q in $CDCl_3$ (100 MHz)

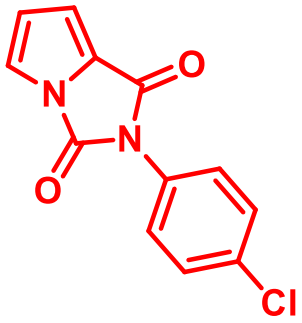
HRMS of 3q


DM RS 3 Q
IISER PUNE
DM RS 3 Q 154 (2.821) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00); Cm (149:155)
1: TOF MS ES+
1.03e5
340.0733
CALCULATED MASS
(M+H)+ 340.0733
F
O
N
N
O
NO2
%
149.0246
331.1040
314.0939
341.0758
153.0669
136.0571
162.0361
206.0259
358.0852
130.0088
253.1702
73.0659
280.1658
391.3738
432.4209
467.4103
519.1518
600.5215
656.5685
695.1063
753.1146
m/z
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800

^{1}H NMR of 4a in $CDCl_3$ (400 MHz)

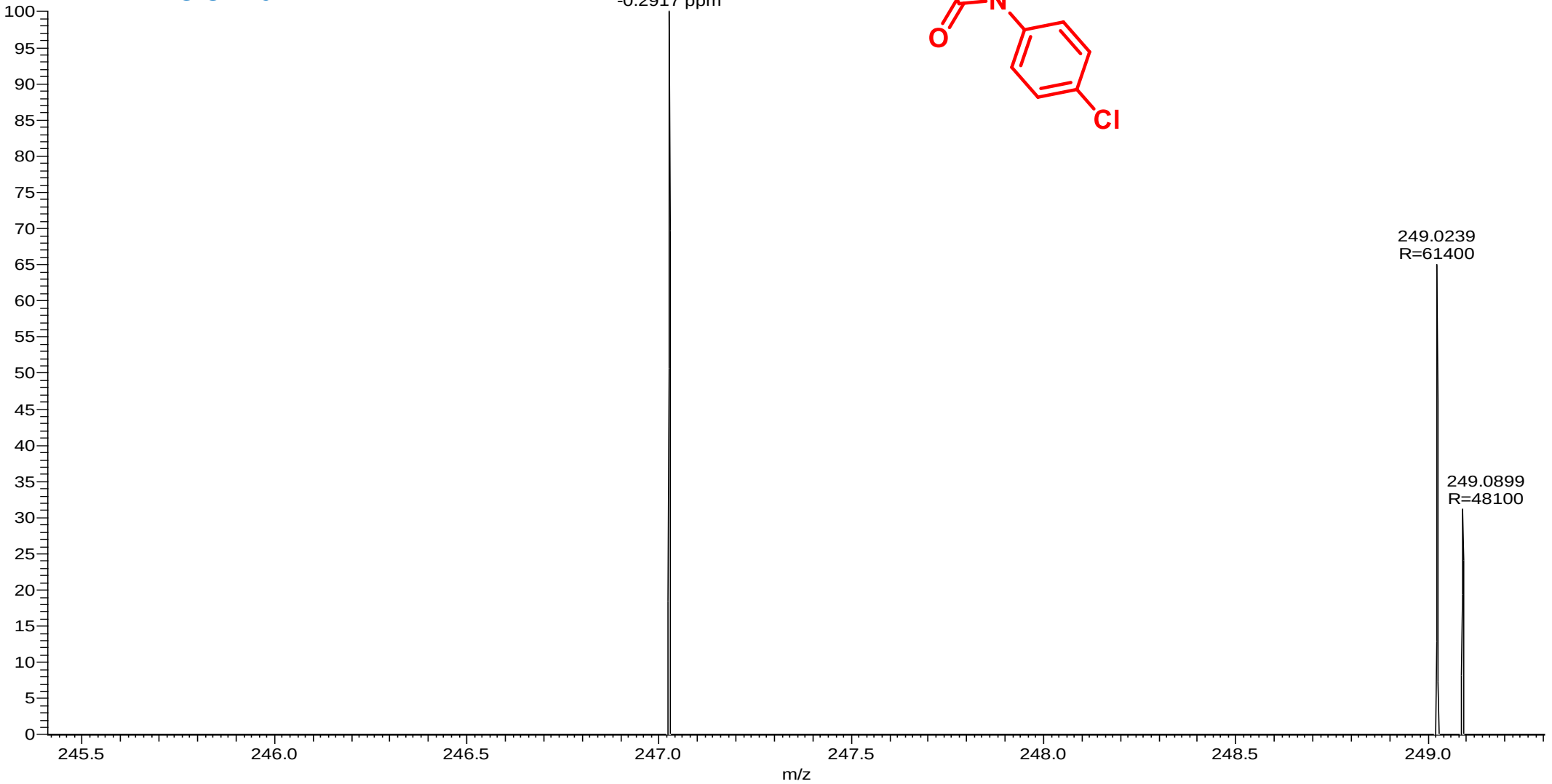


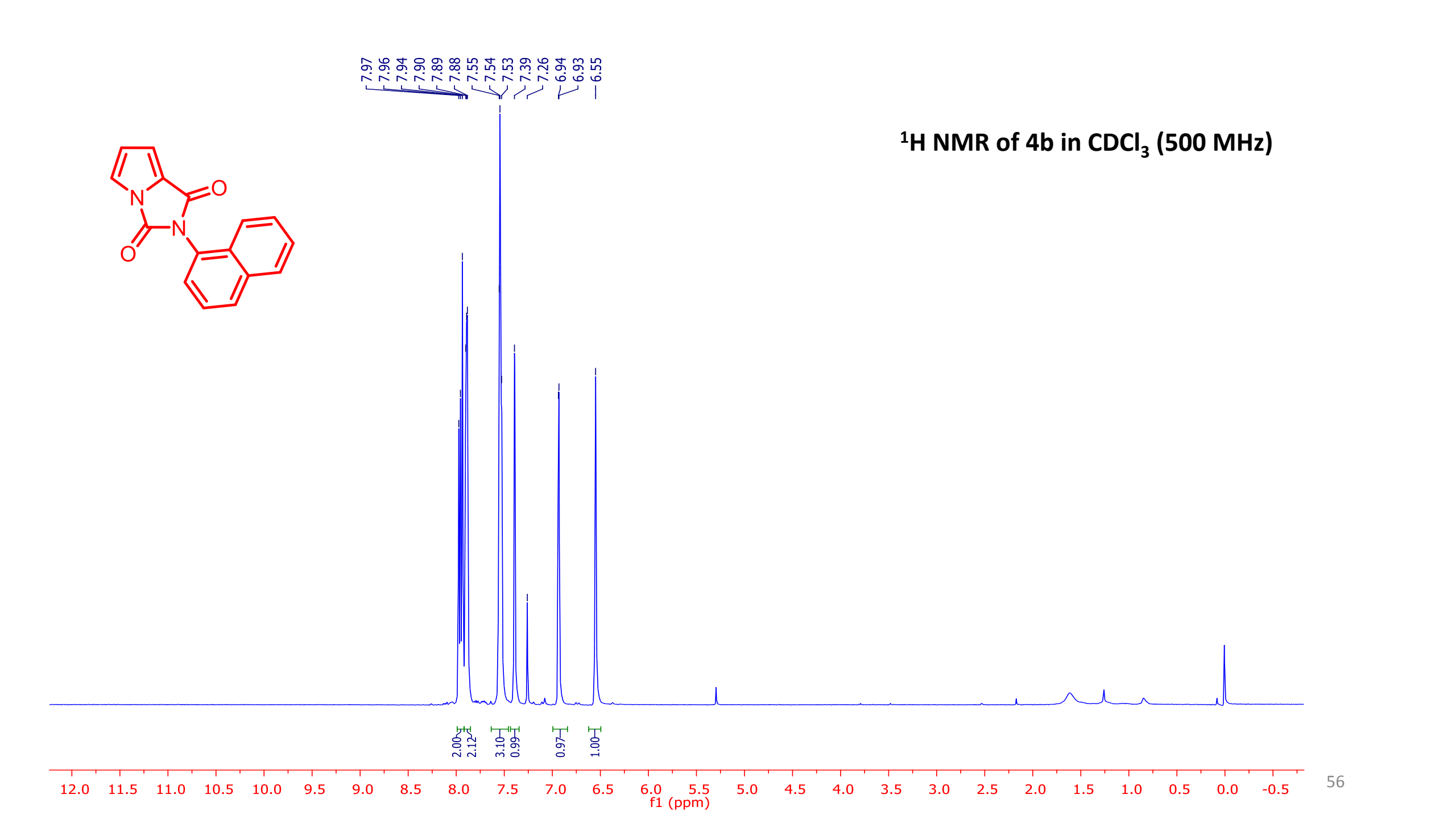
^{13}C NMR of 4a in $CDCl_3$ (100 MHz)



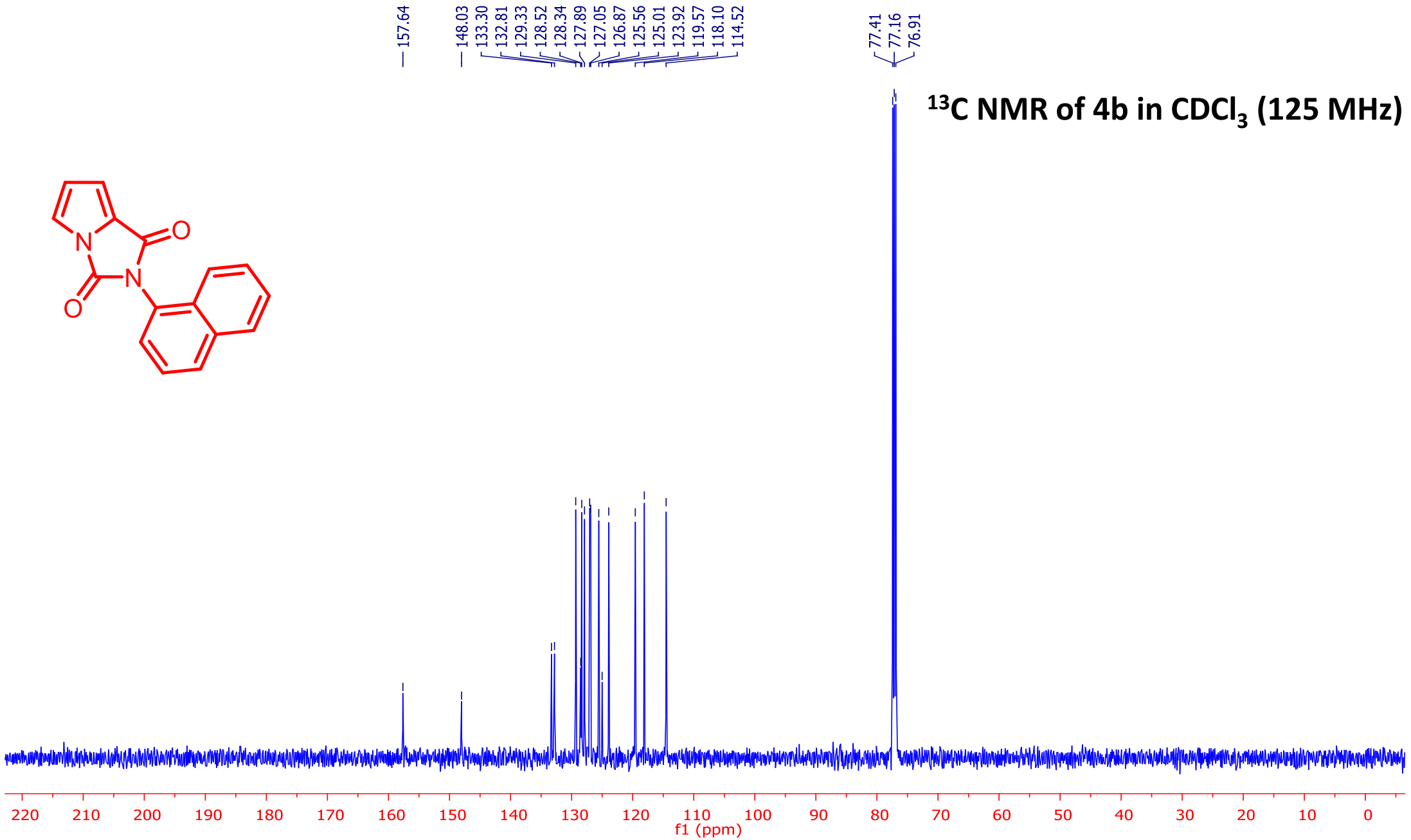
SR-18 #262 RT: 1.17 AV: 1 NL: 1.09E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

HRMS of 4a





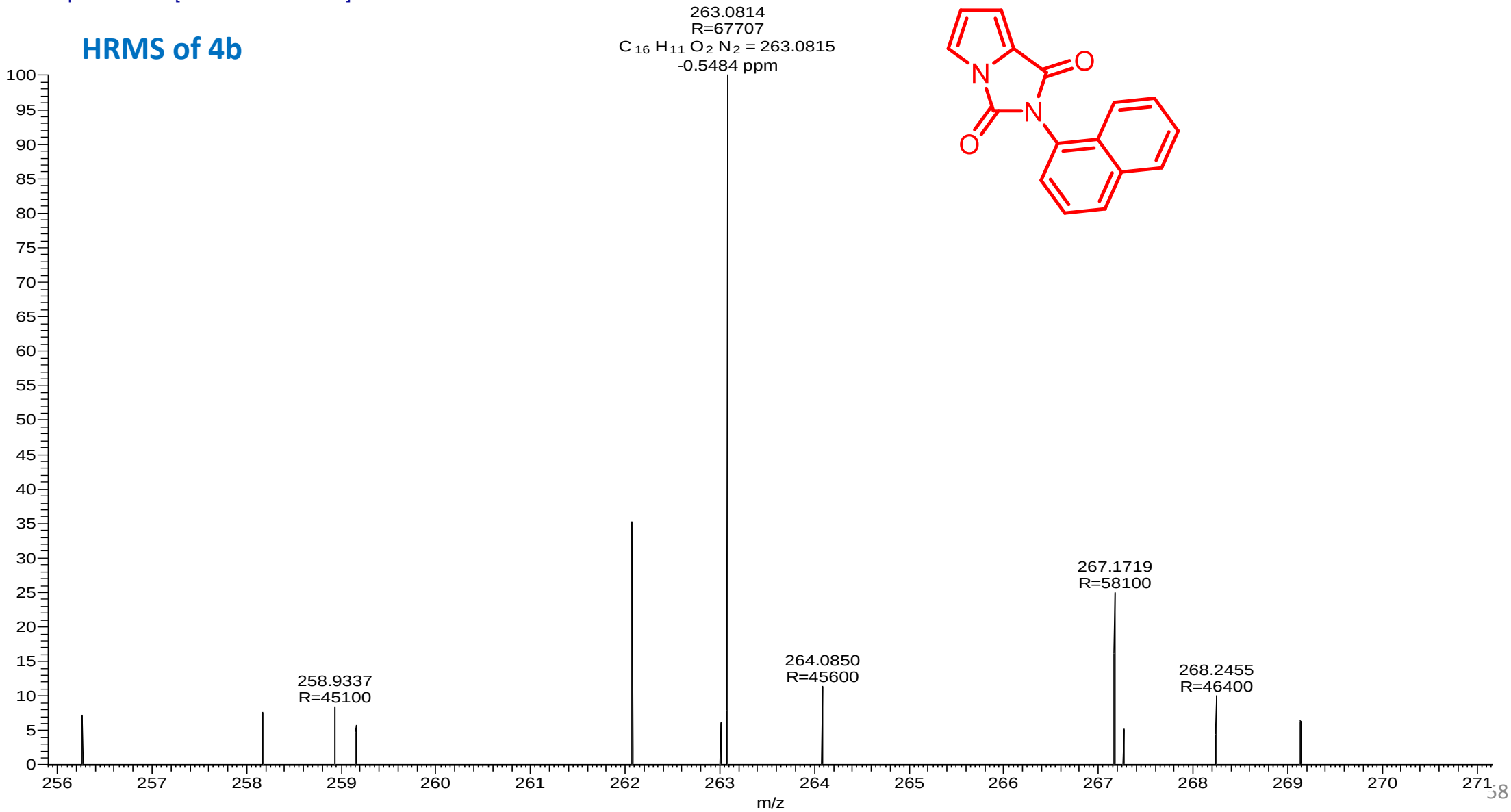
^{1}H NMR of 4b in $CDCl_3$ (500 MHz)

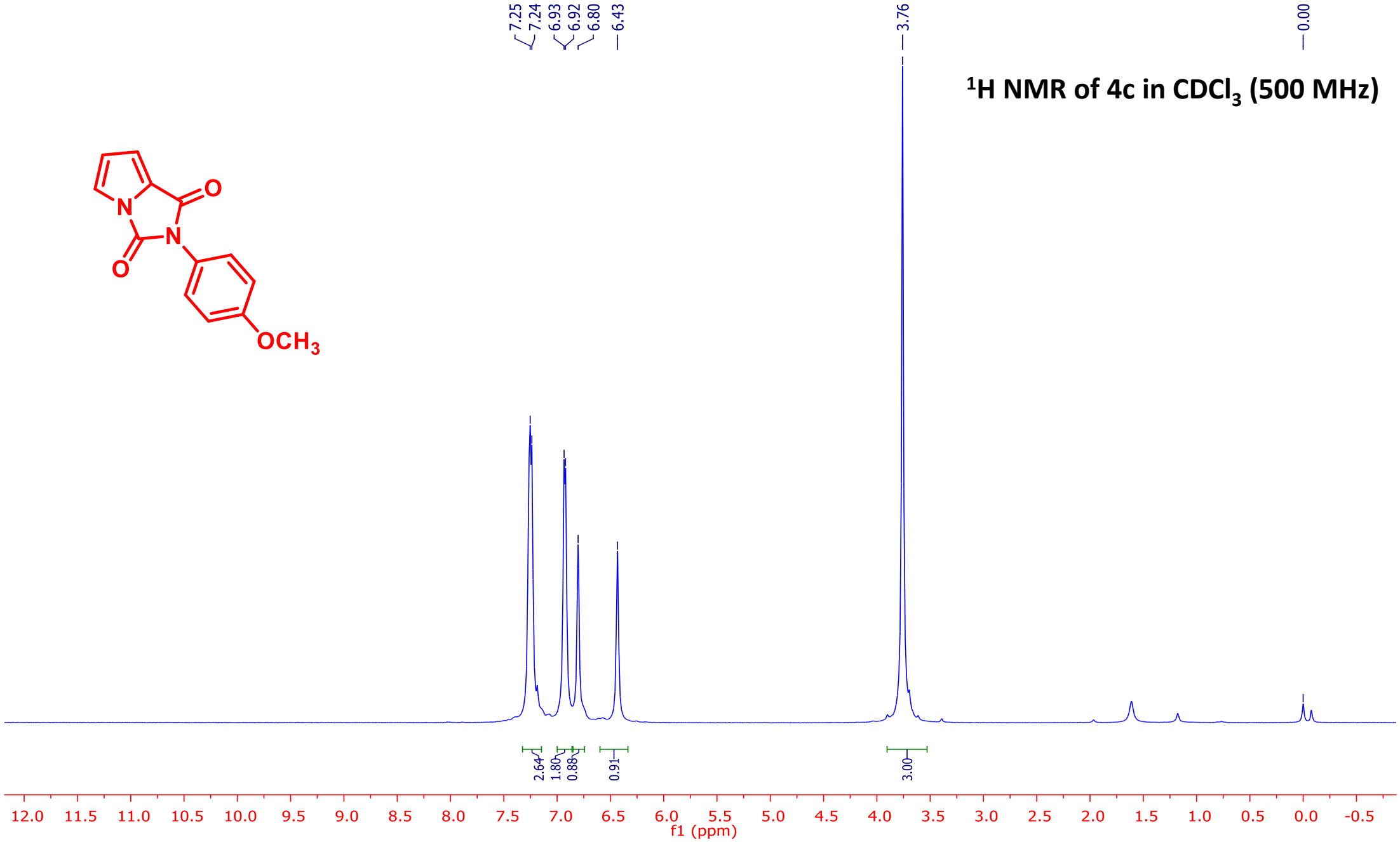


^{13}C NMR of 4b in $CDCl_3$ (125 MHz)

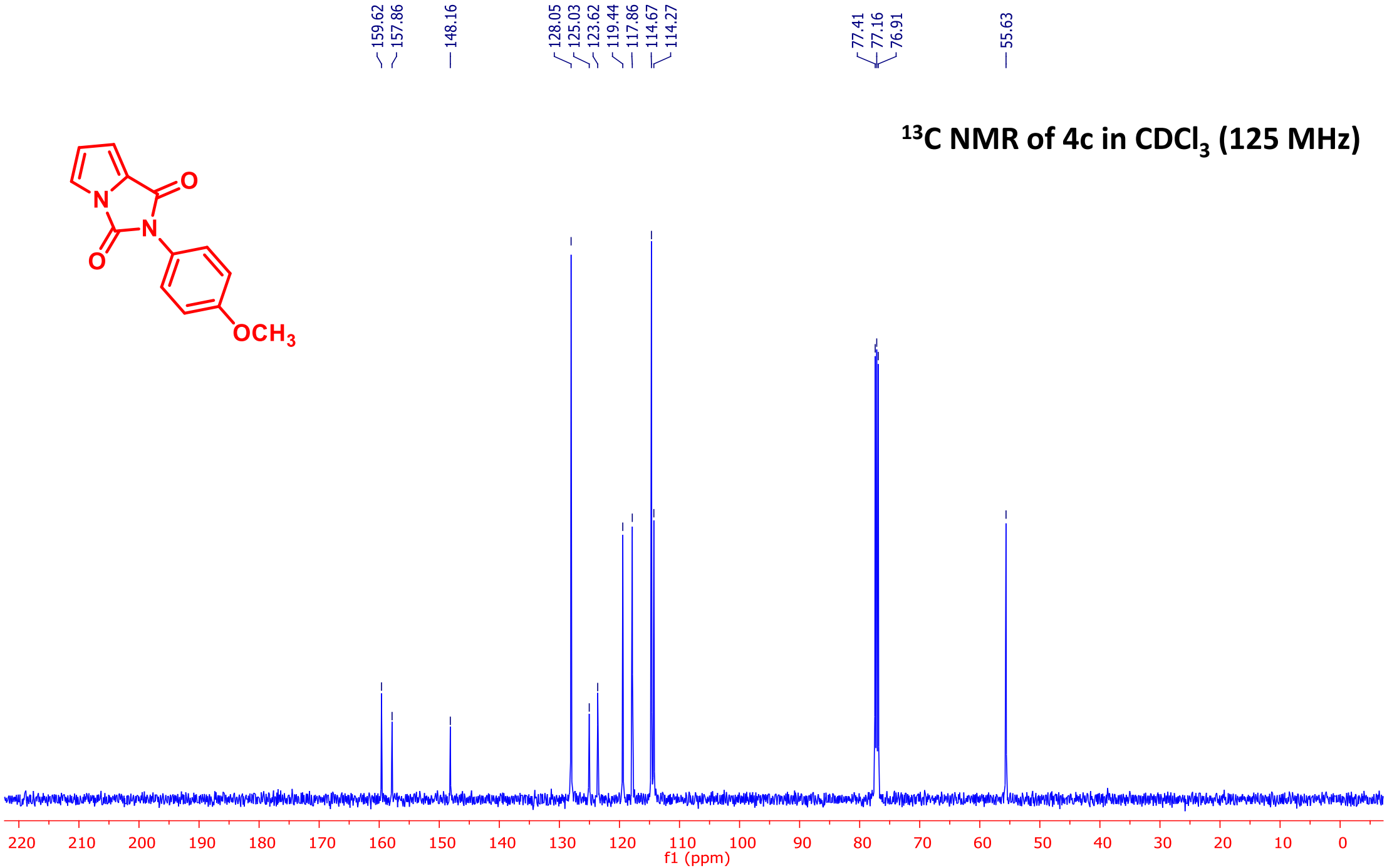
SR-20 #265 RT: 1.18 AV: 1 NL: 3.27E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]

HRMS of 4b



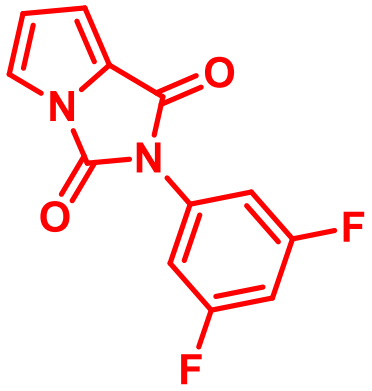


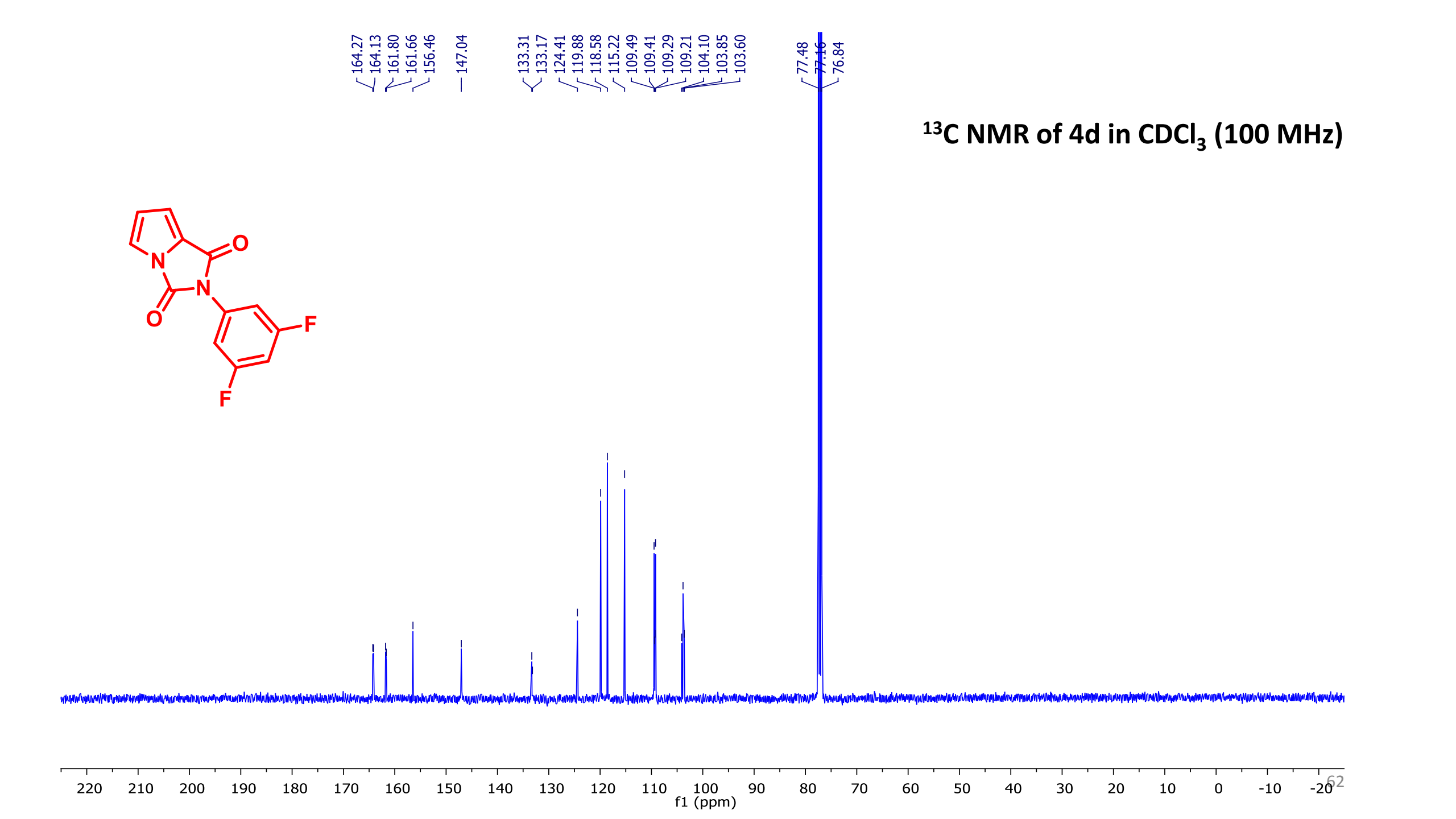
^{1}H NMR of 4c in $CDCl_3$ (500 MHz)



^{13}C NMR of 4c in $CDCl_3$ (125 MHz)

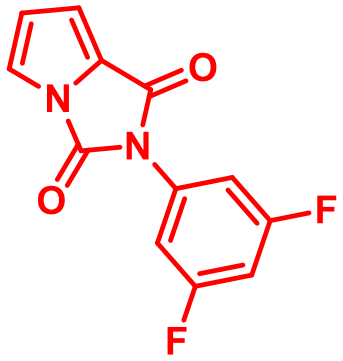
^{1}H NMR of 4d in $CDCl_3$ (400 MHz)





^{13}C NMR of 4d in $CDCl_3$ (100 MHz)

F^{19}-NMR of 4d in $CDCl_3$



DM RS 4D

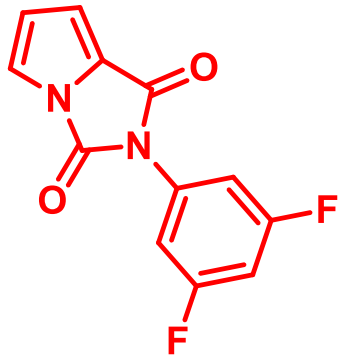
IISER PUNE

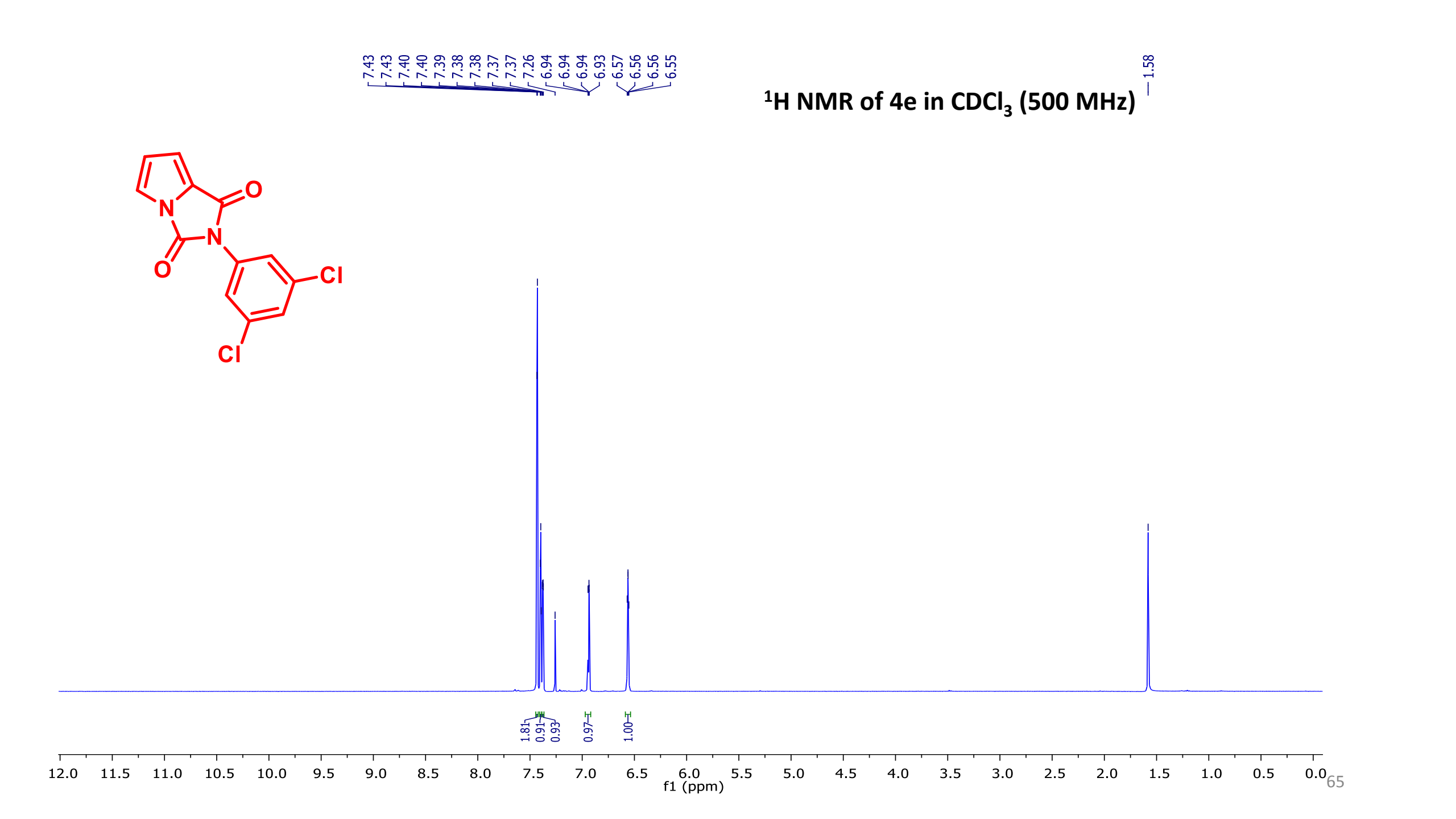
DM RS 4D 155 (2.838) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00); Cm (152:157-(1:151+158:273))

1: TOF MS ES+
1.97e4

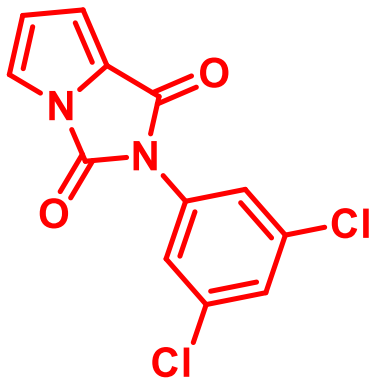
HRMS of 4d

CALCULATED MASS
(M+H)+ 249.0475




7.43
7.43
7.40
7.40
7.39
7.38
7.38
7.37
7.37
7.26
6.94
6.94
6.94
6.93
6.57
6.56
6.56
6.55
1.58
^{1}H NMR of 4e in CDCl$_3$ (500 MHz)
O
N
N
O
Cl
Cl
1.81
0.91
0.93
0.97
1.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

^{13}C NMR of 4e in $CDCl_3$ (125 MHz)



DM RS 4E

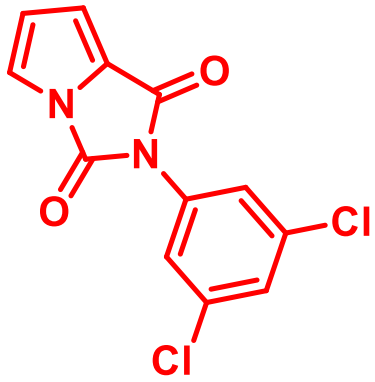
IISER PUNE

DM RS 4E 176 (3.216) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00); Cm (173:179-(2:172+180:273))

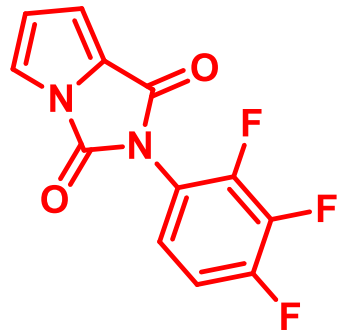
1: TOF MS ES+
2.28e4

HRMS of 4e

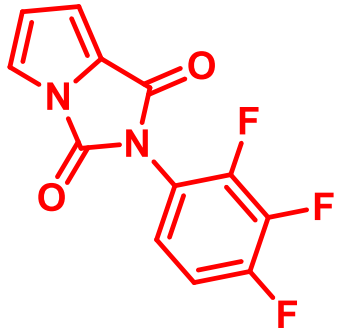
CALCULATED MASS
(M+H)+ 280.9884



^{1}H NMR of 4f in $CDCl_3$ (500 MHz)



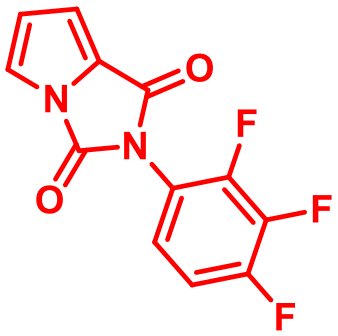
^{13}C NMR of 4f in $CDCl_3$ (125 MHz)

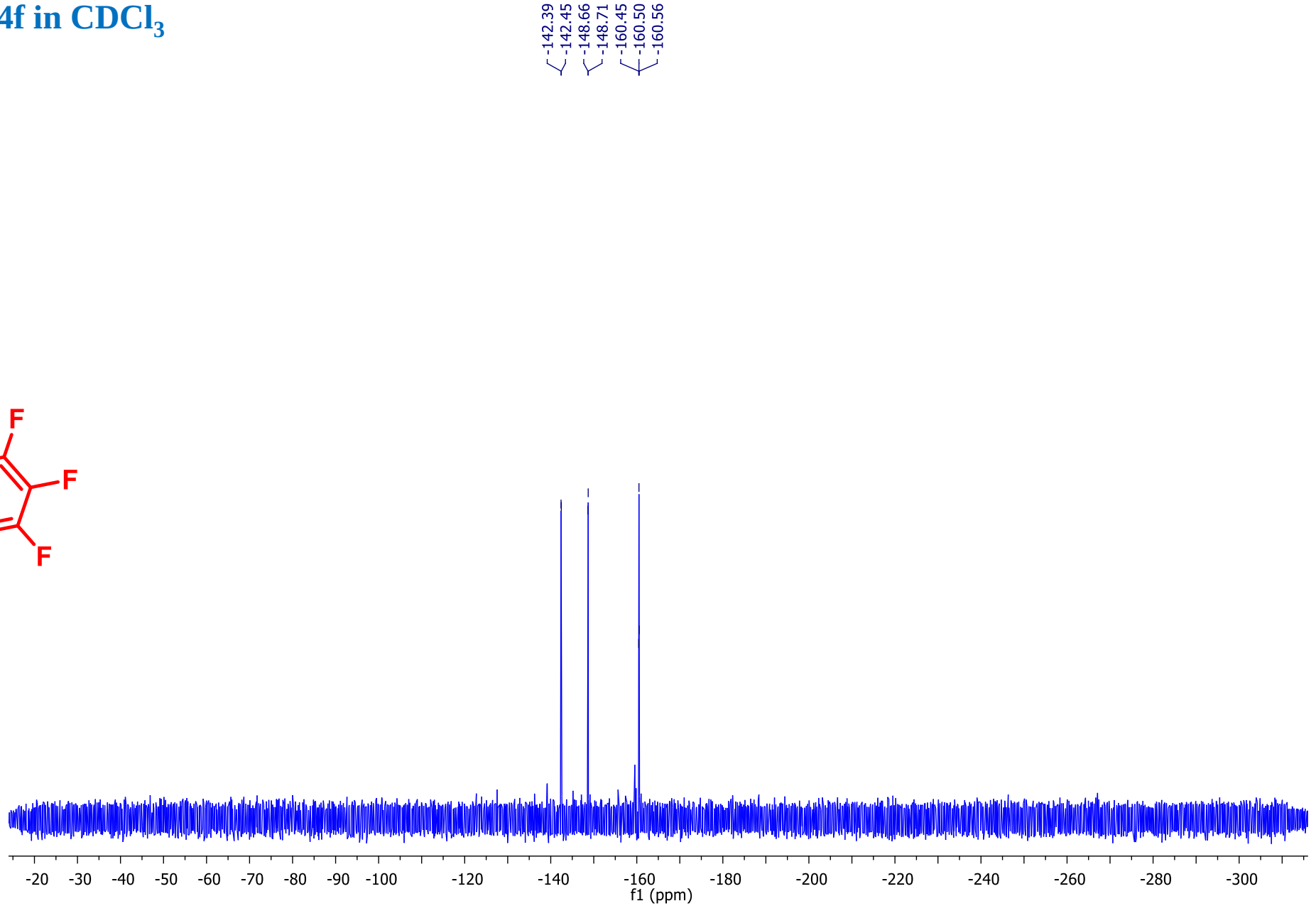


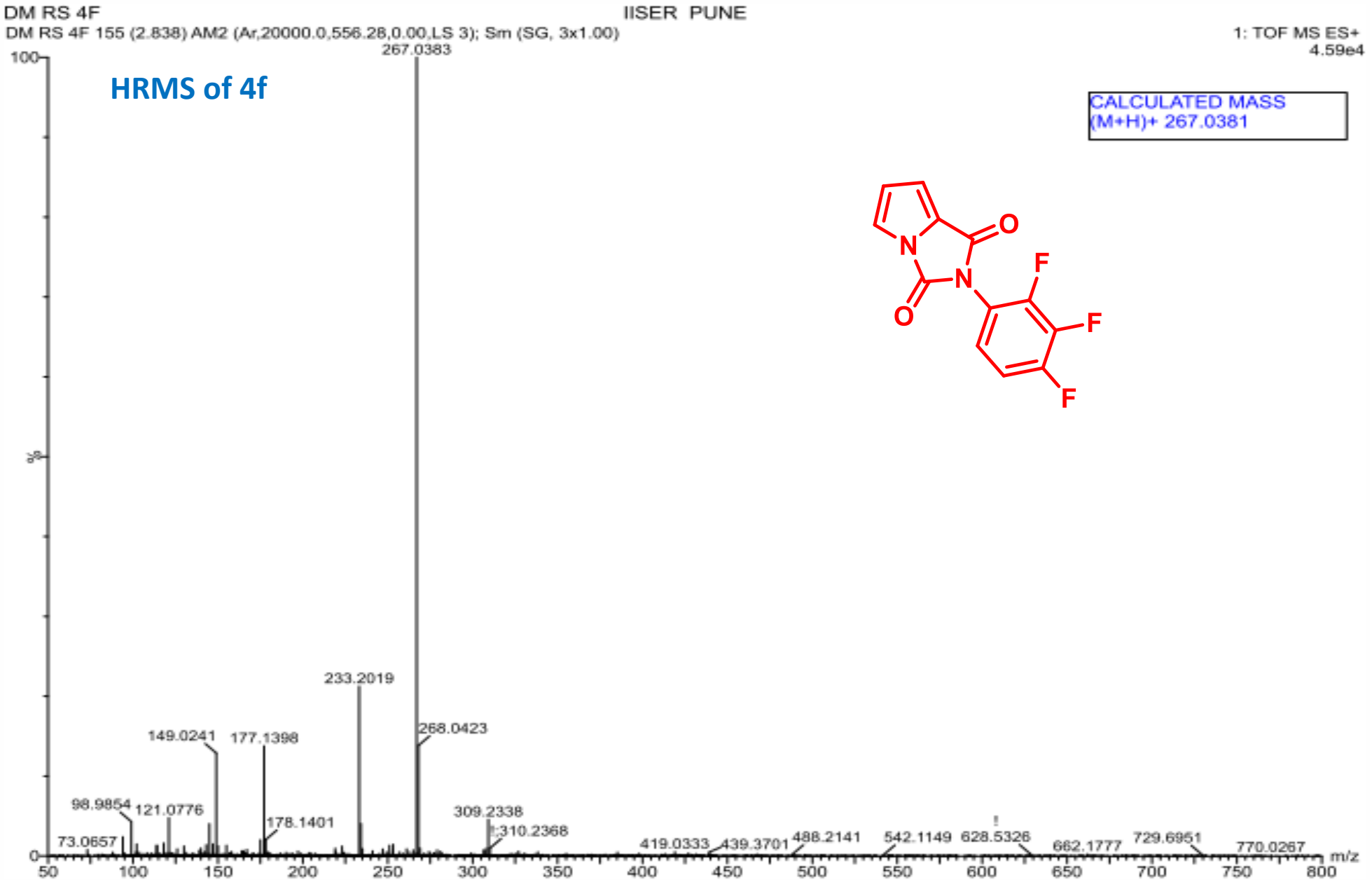
156.27
152.91
150.91
149.05
146.74
141.86
139.84
139.06
124.93
124.00
120.13
118.42
116.21
115.38
112.48
112.33
77.41
77.16
76.91

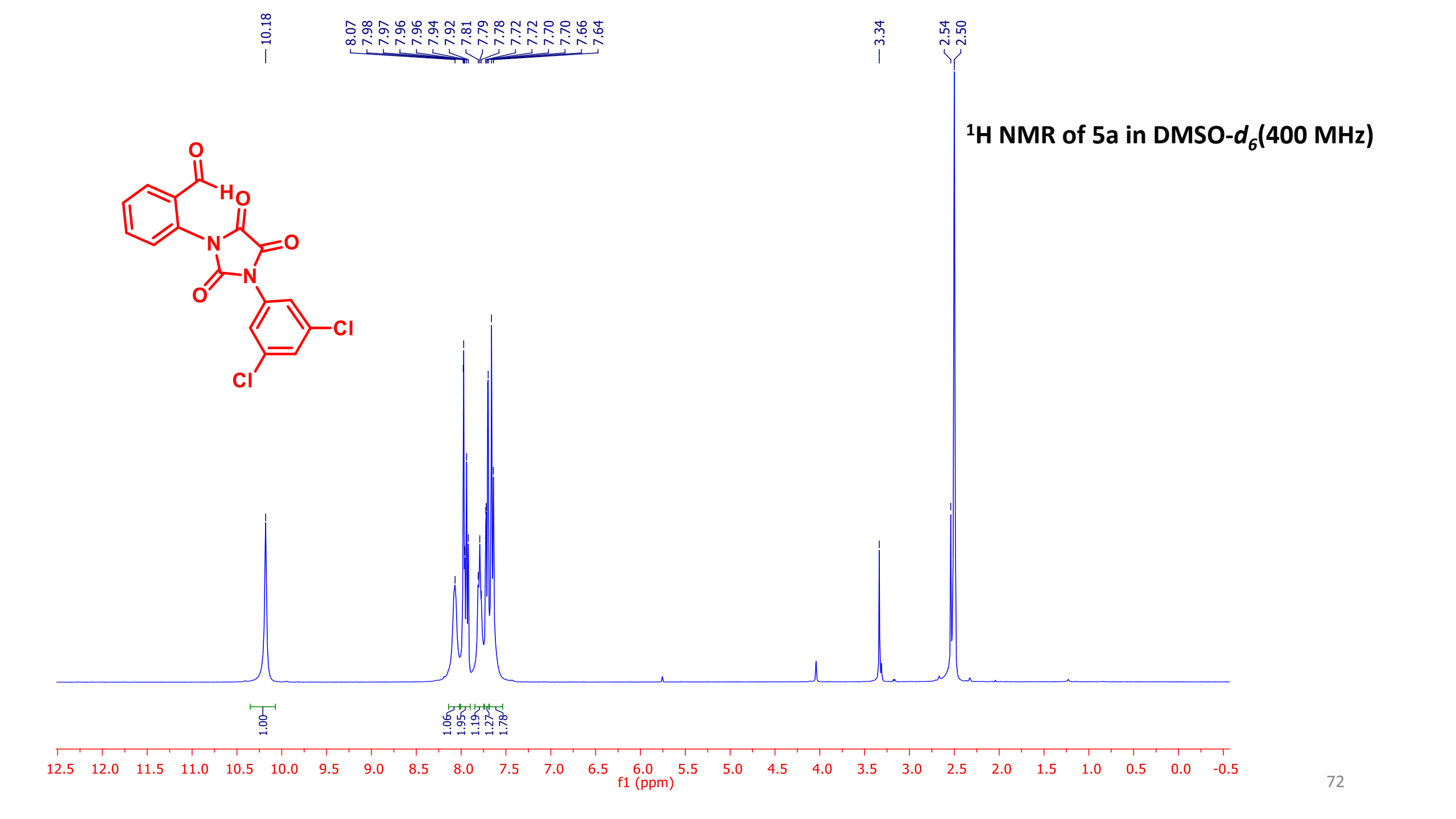
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

F^{19}-NMR of 4f in $CDCl_3$

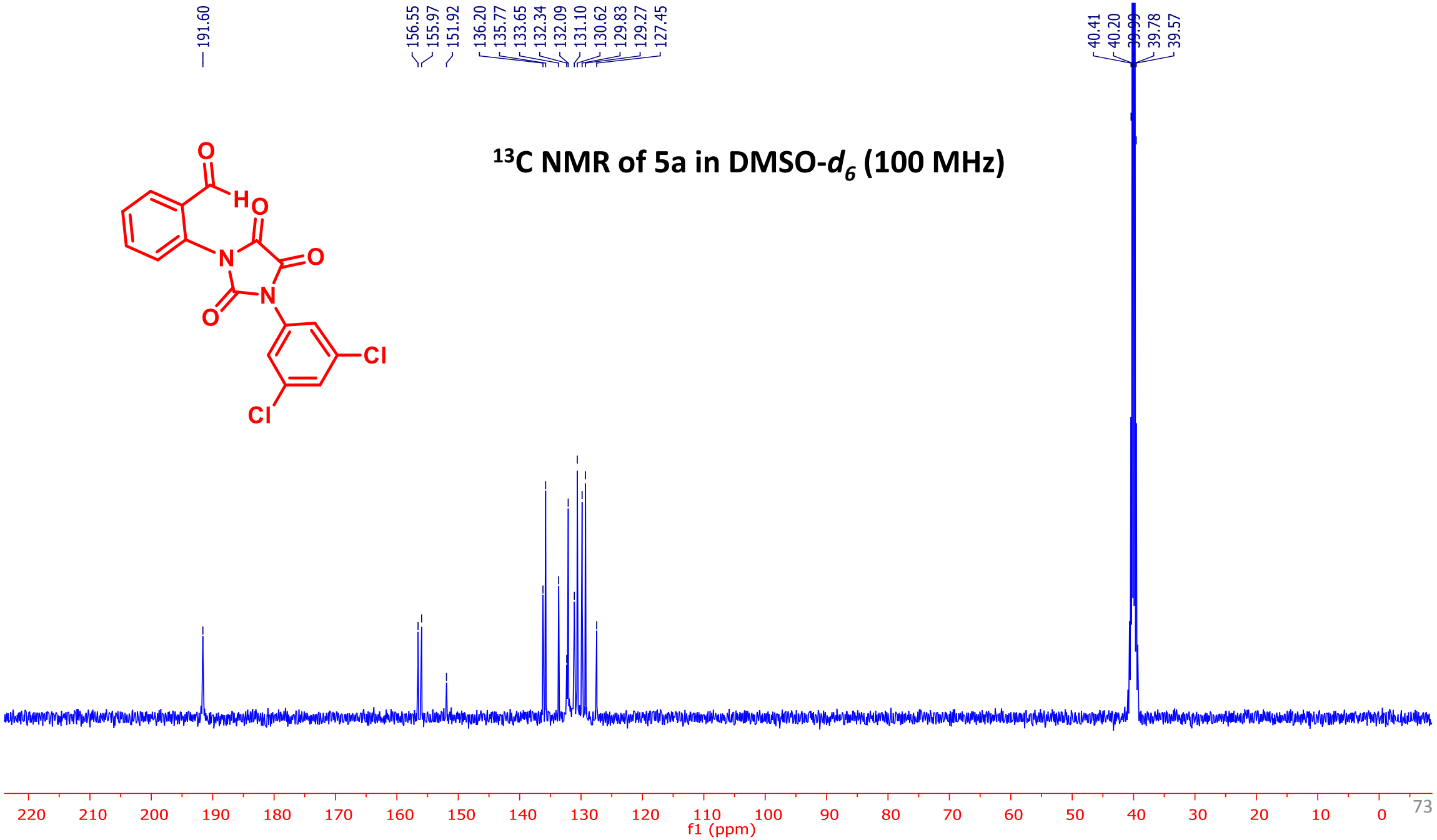





DM RS 4F
IISER PUNE
DM RS 4F 155 (2.838) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)
1: TOF MS ES+
4.59e4
HRMS of 4f
CALCULATED MASS
(M+H)+ 267.0381
267.0383
233.2019
268.0423
149.0241
177.1398
98.9854
121.0776
178.1401
309.2338
310.2368
73.0657
419.0333
439.3701
488.2141
542.1149
628.5326
662.1777
729.6951
770.0267
%
m/z
100
0
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
O
N
N
O
F
F
F



^{1}H NMR of 5a in DMSO-d_6(400 MHz)



^{13}C NMR of 5a in DMSO-d_6 (100 MHz)