

Supplementary Data

for

Convenient and efficient synthesis of novel 11*H*-benzo[5,6][1,4]thiazino[3,4-*a*]isoindol-11-ones derived from 2-bromo-(2/3-substitutedphenyl)-1*H*-indene-1,3(2*H*)-diones

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**Corresponding author*

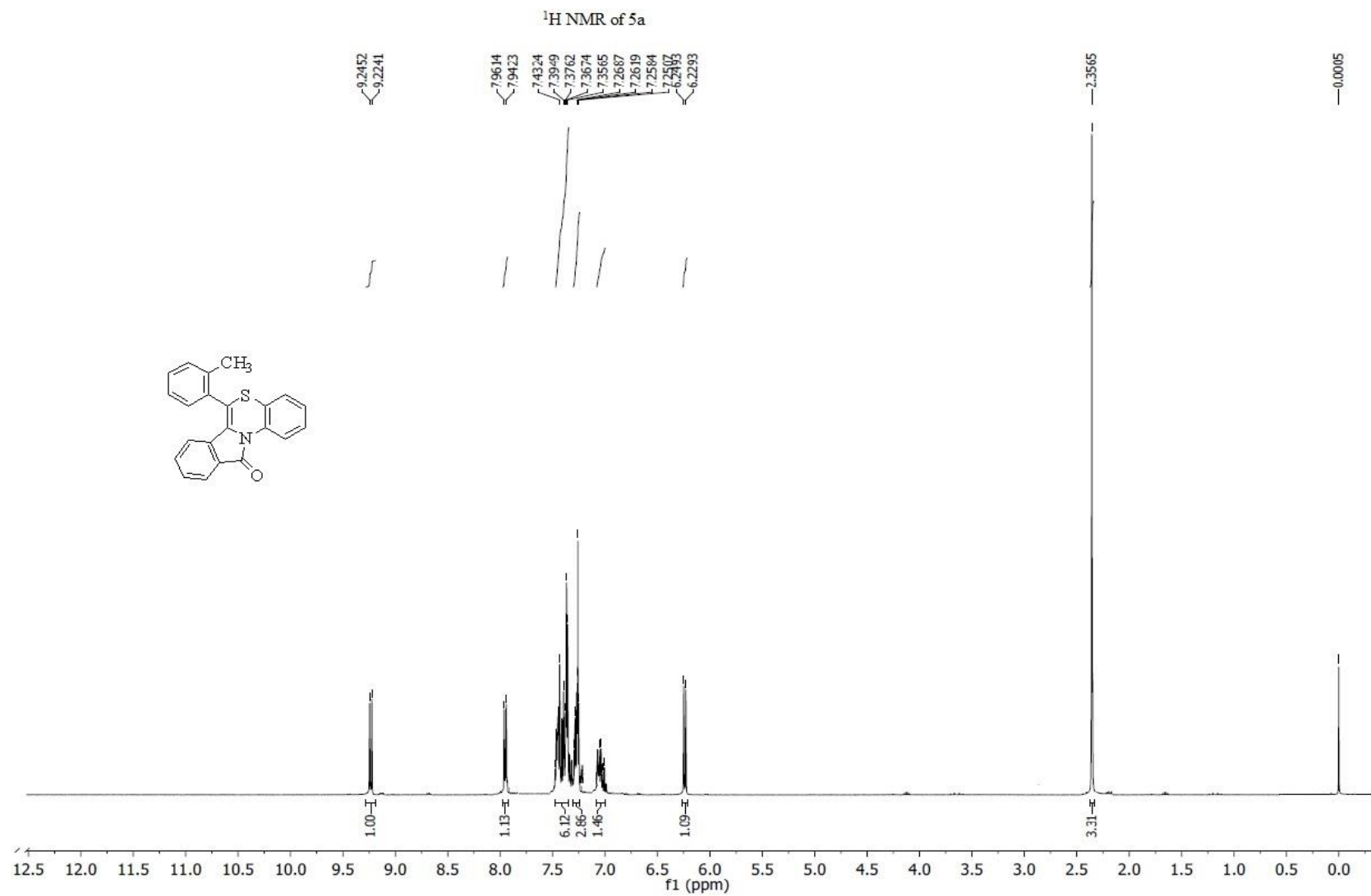
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NMR (¹H and ¹³C) spectra of **5a-r** and 2D-NMR of **5b**

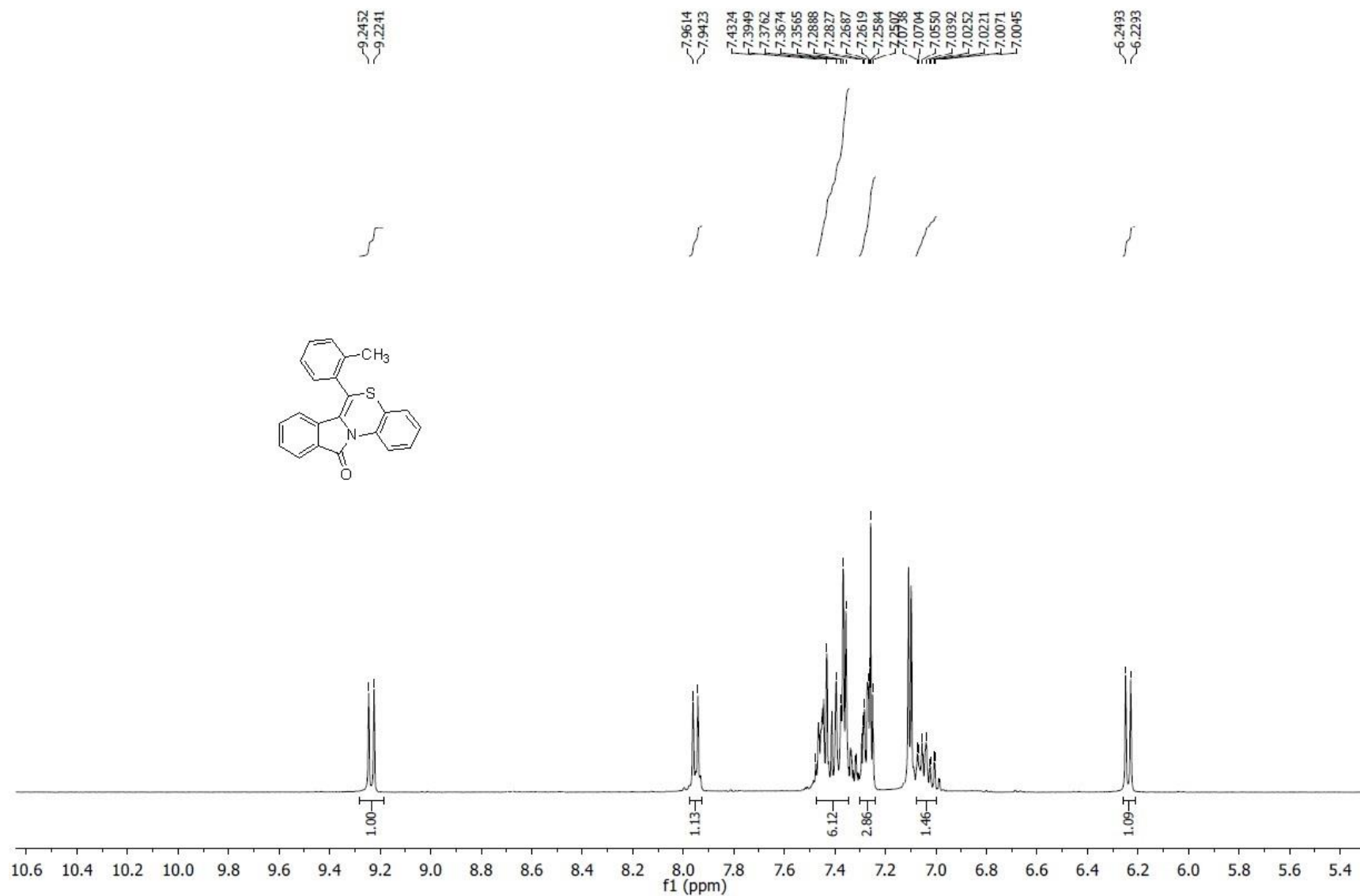
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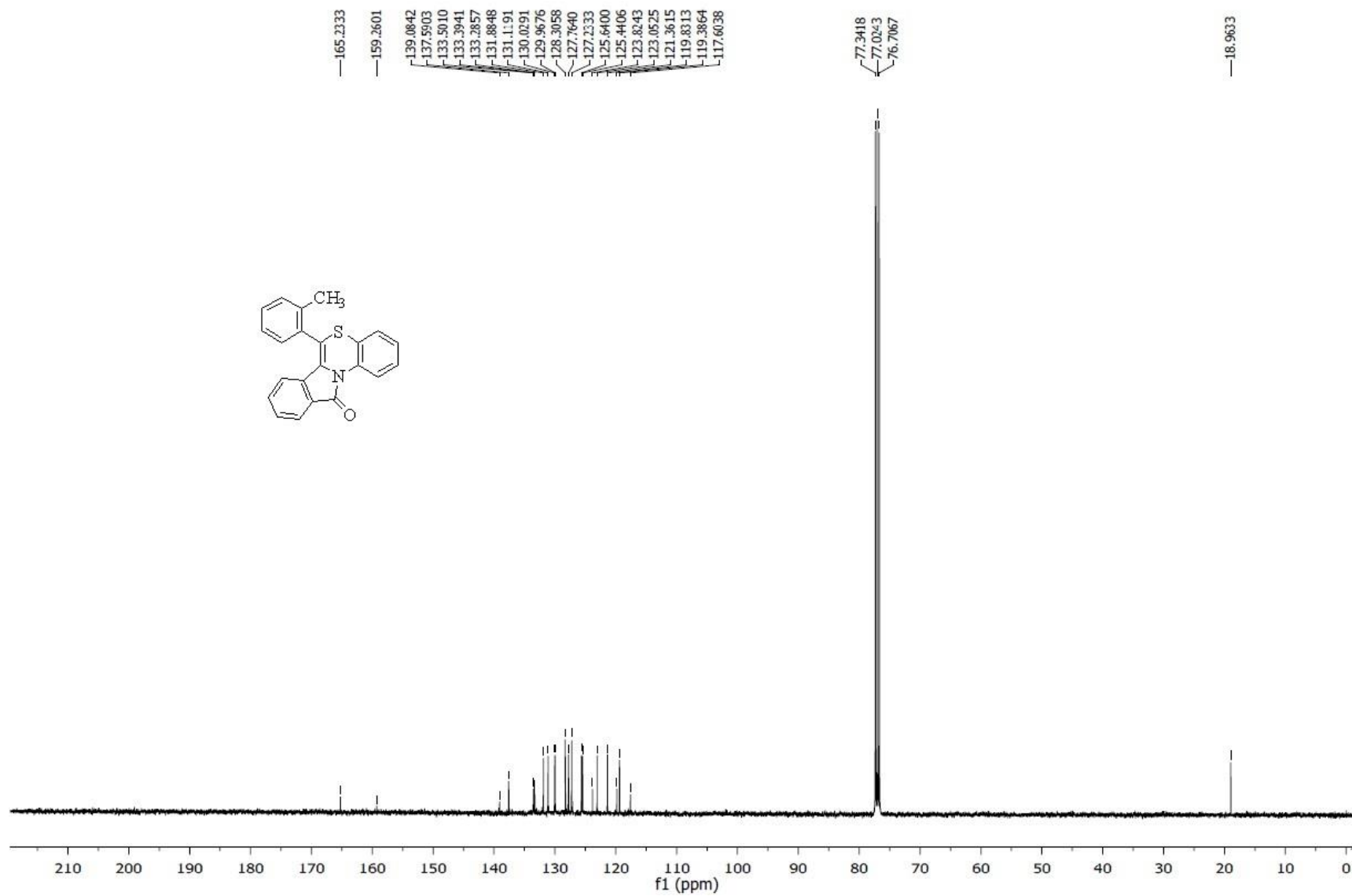
^1H and ^{13}C NMR of **5a-r**



¹H NMR of 5a



¹³C NMR of 5a



¹³C NMR of 5a

—165.2333

—159.2601

—139.0842

—137.5903

—133.5010

—133.3941

—133.2857

—131.8848

—131.1151

—130.0261

—129.9676

—128.3058

—127.7640

—127.2333

—125.6400

—125.4406

—123.8243

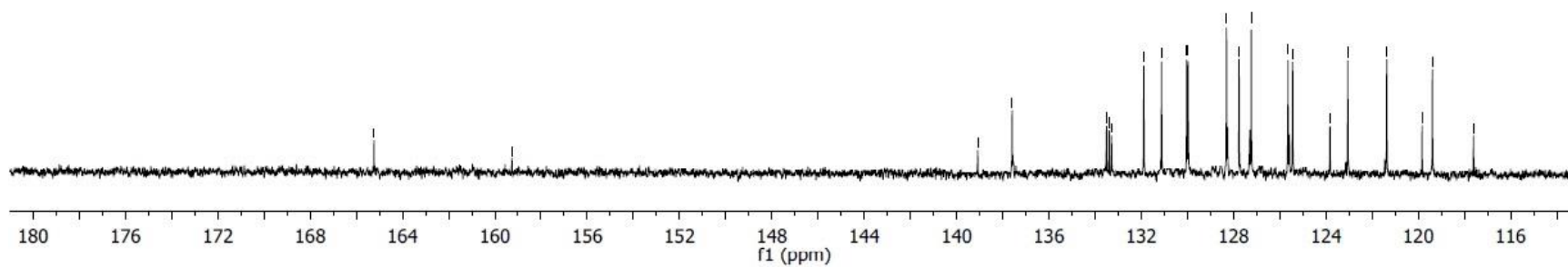
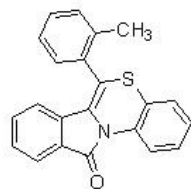
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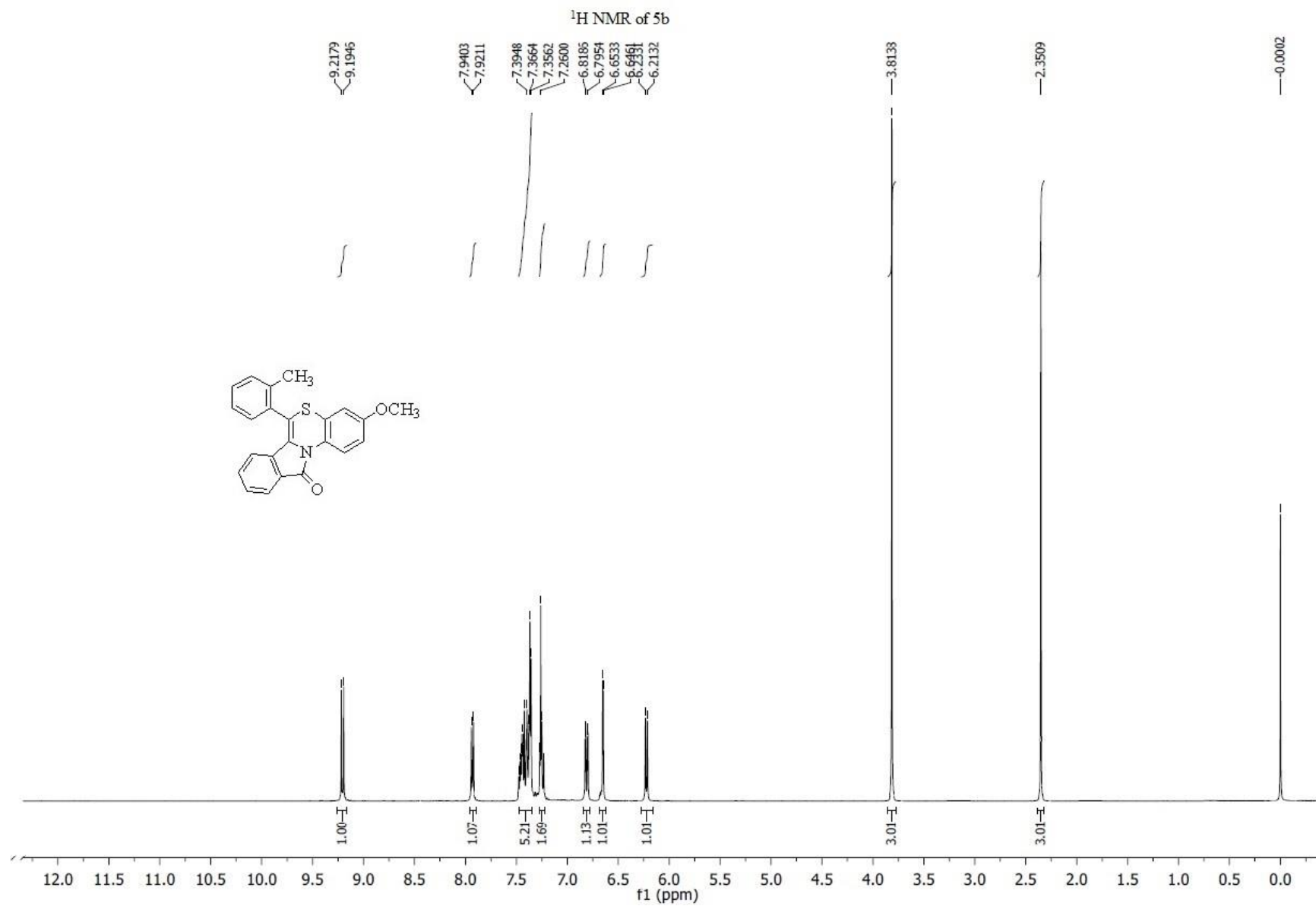
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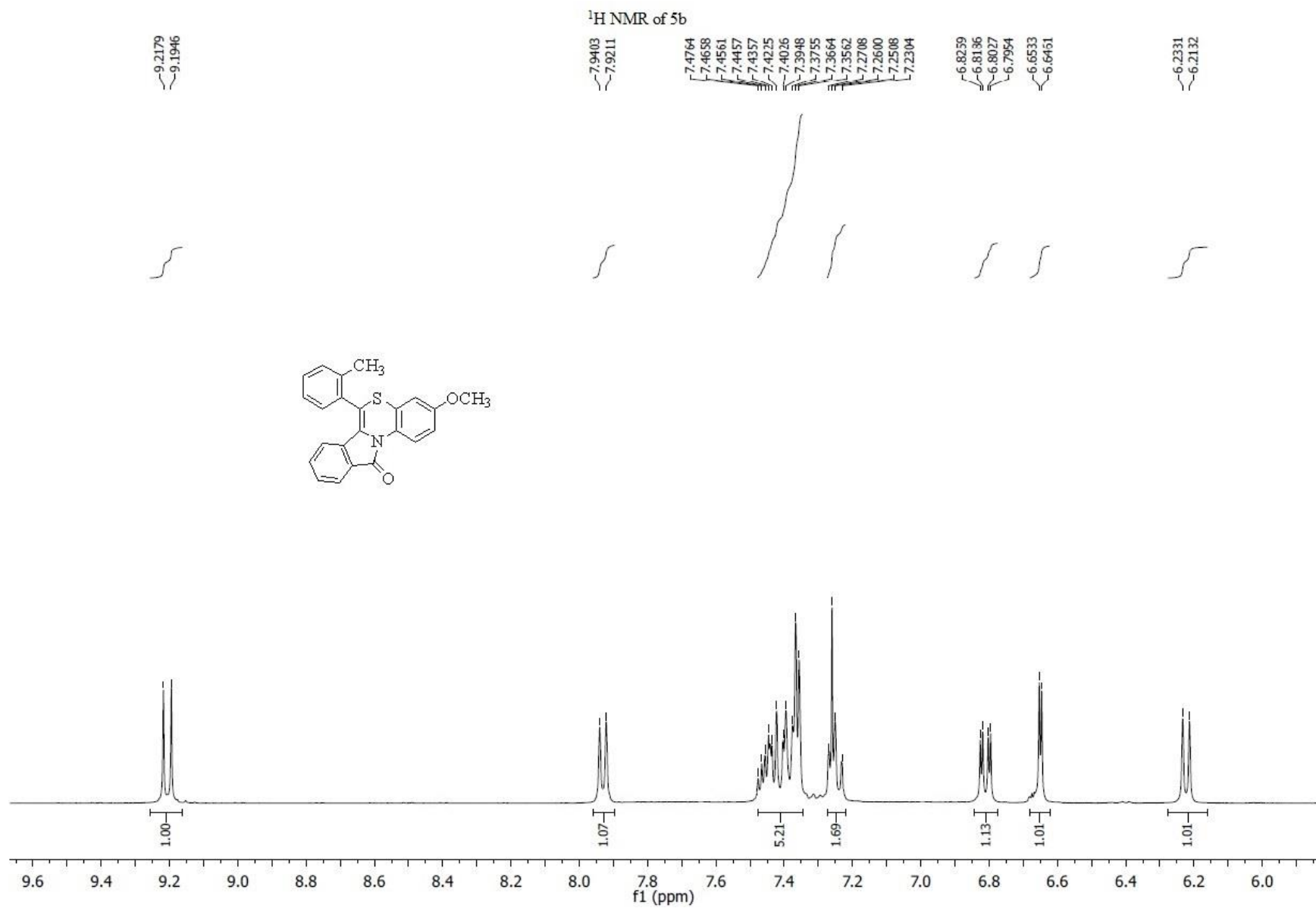
—119.8313

—119.3864

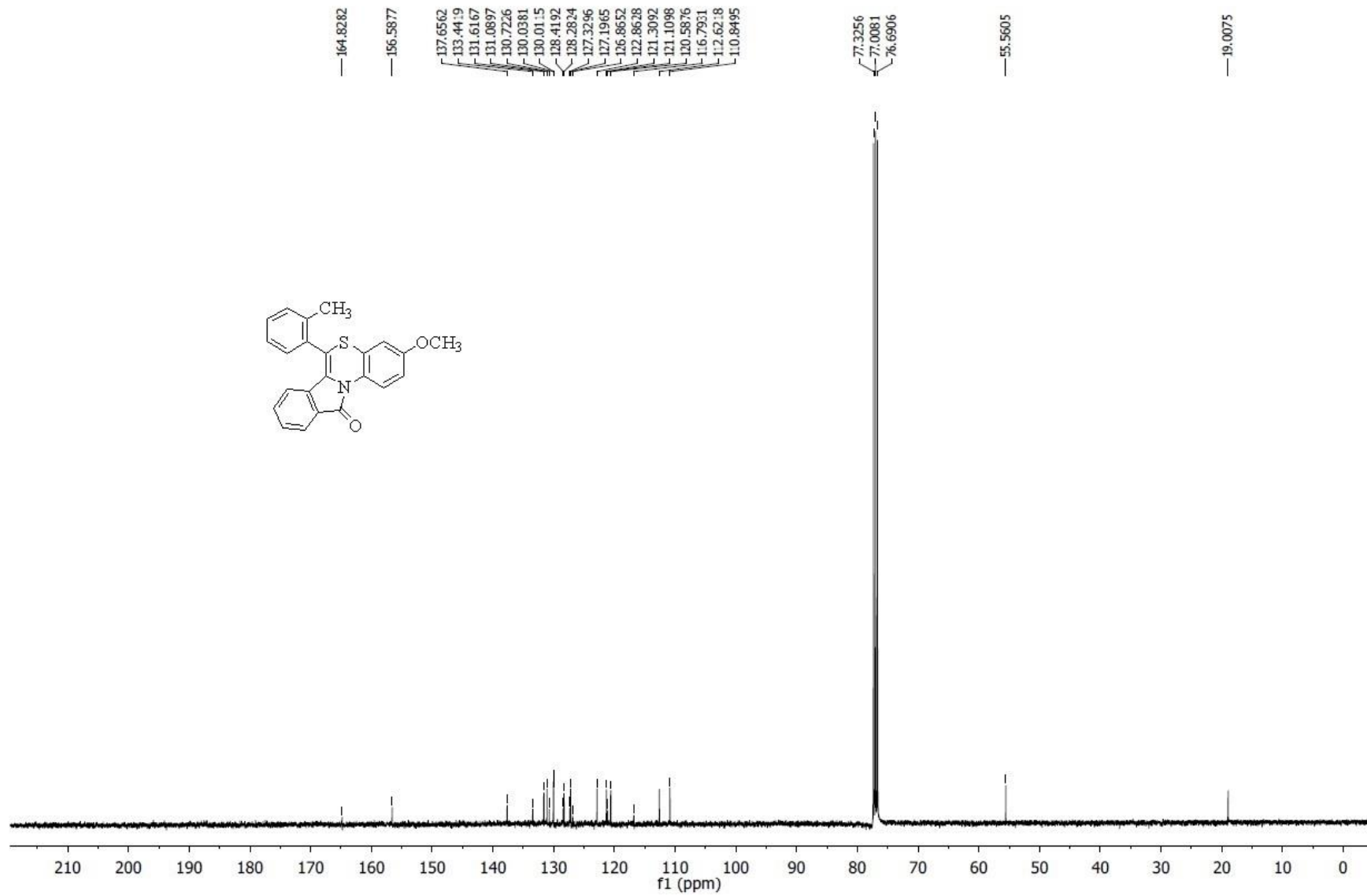
—117.6038







¹³C NMR of 5b



¹³C NMR of 5b

—164.8282

—156.5877

—137.6562

—133.4419

—131.6167

—131.0897

—130.7225

—130.0381

—130.0115

—128.4192

—128.2824

—127.3295

—127.1965

—126.8652

—122.8628

—121.3092

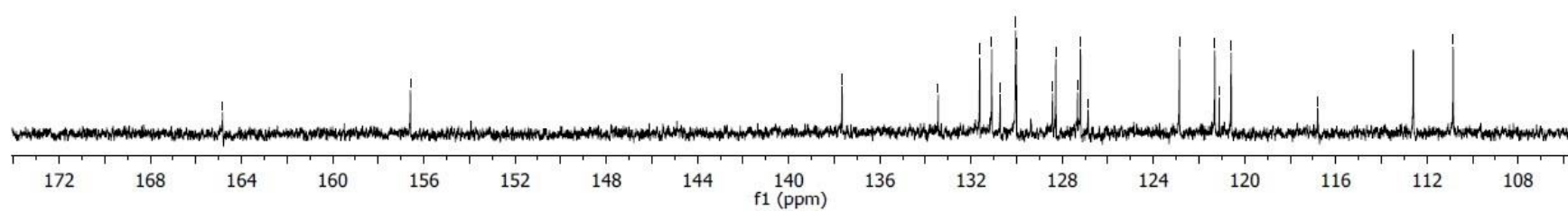
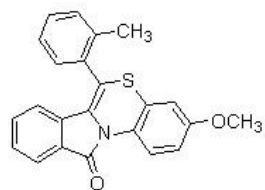
—121.1098

—120.5876

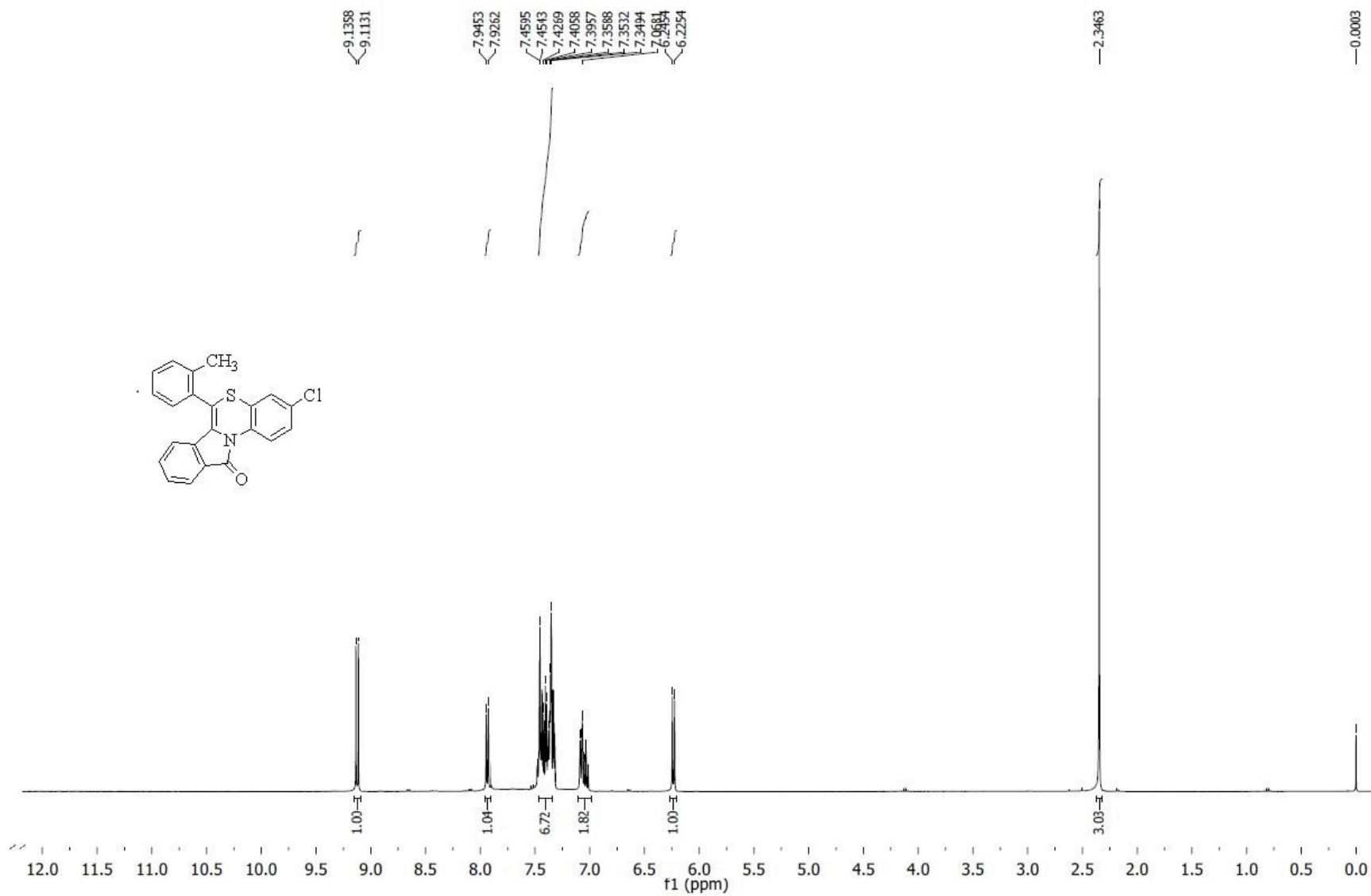
—116.7931

—112.6218

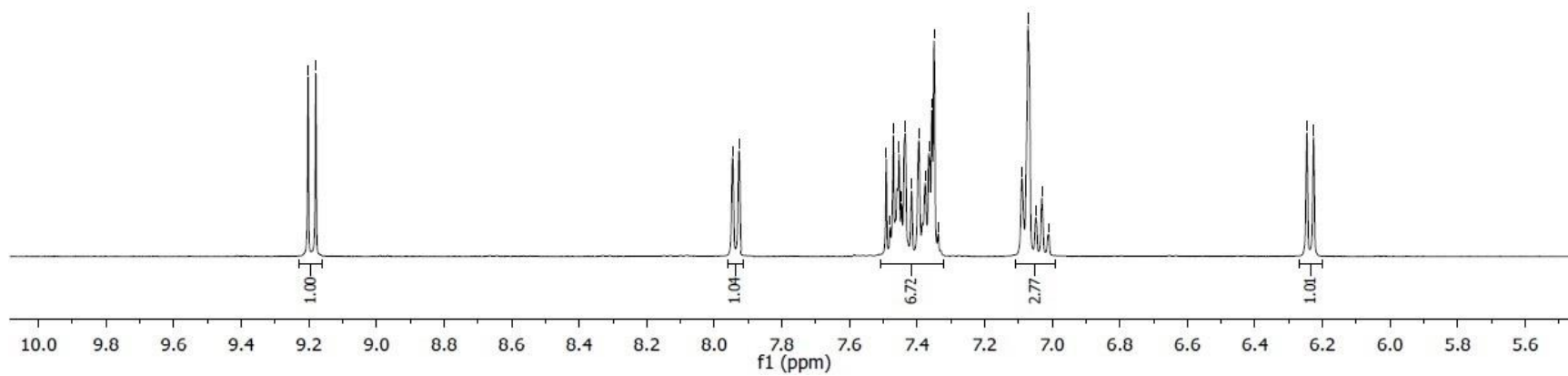
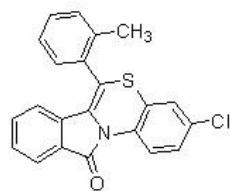
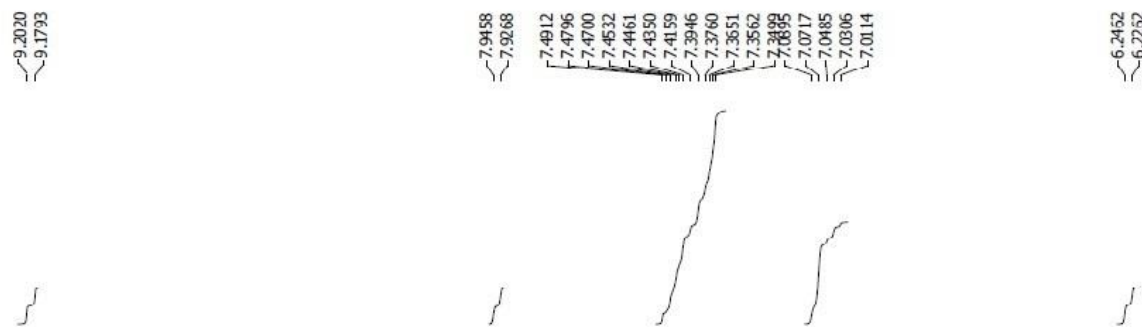
—110.8495



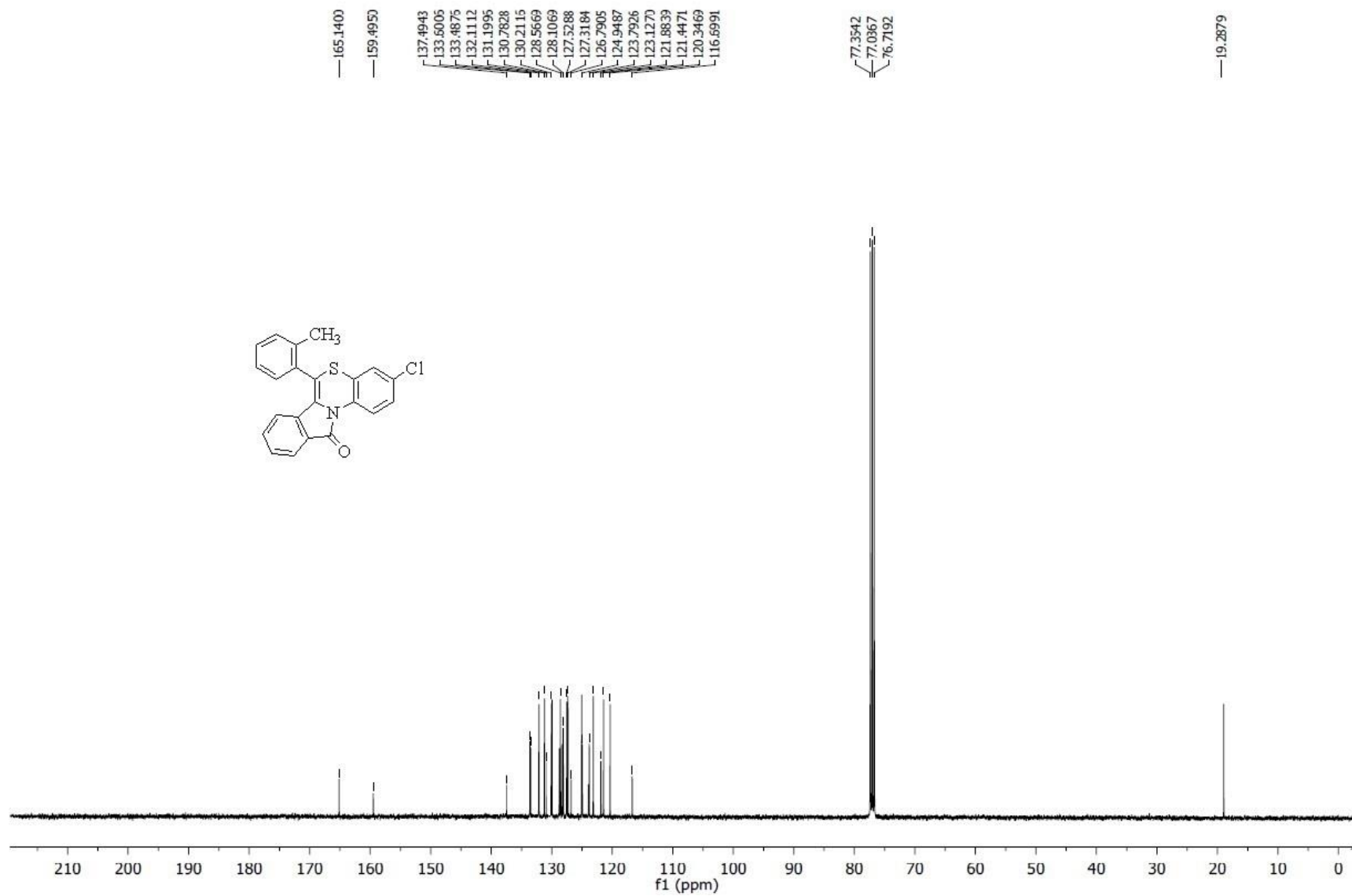
¹H NMR of 5c



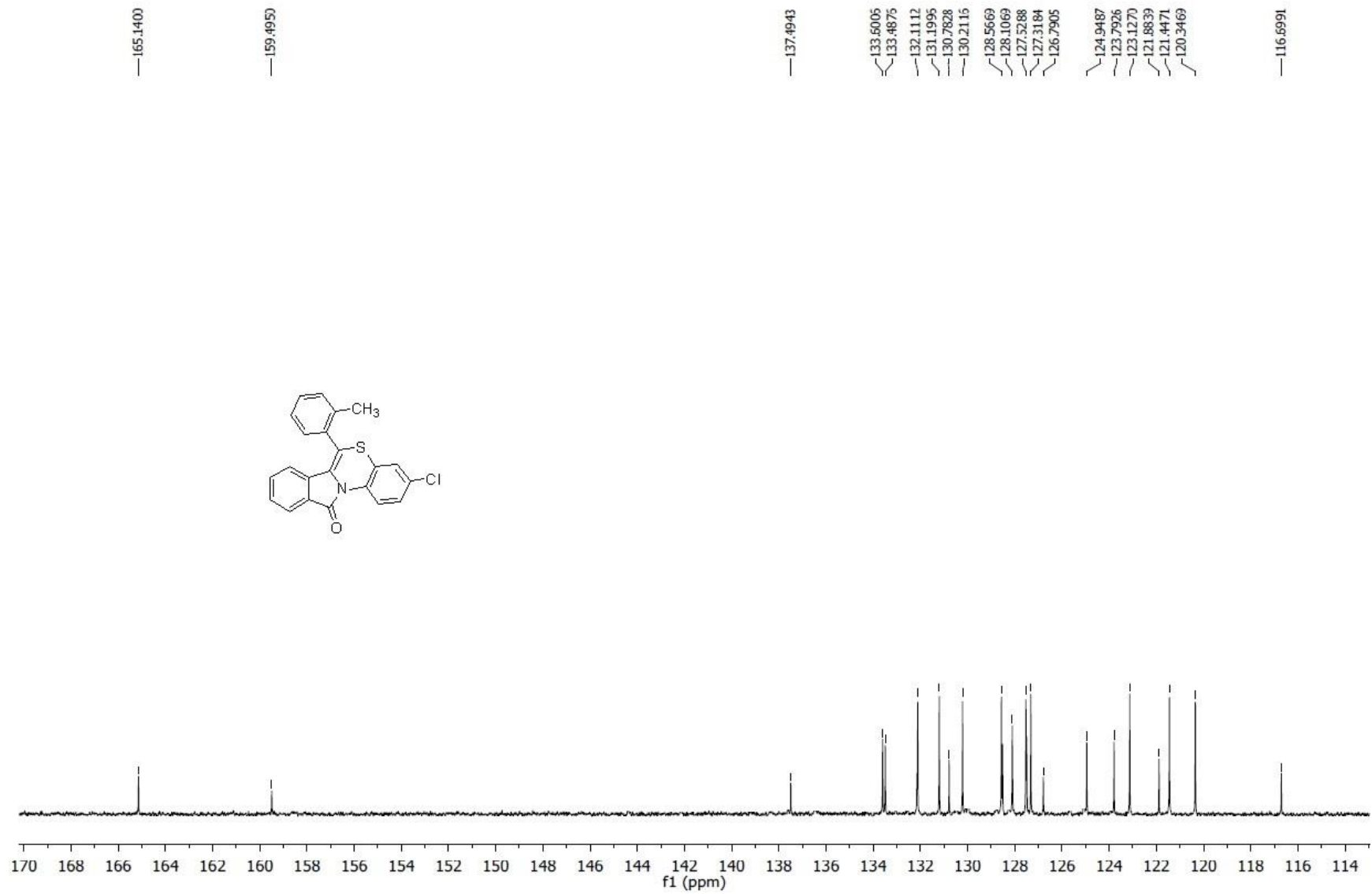
¹H NMR of 5c

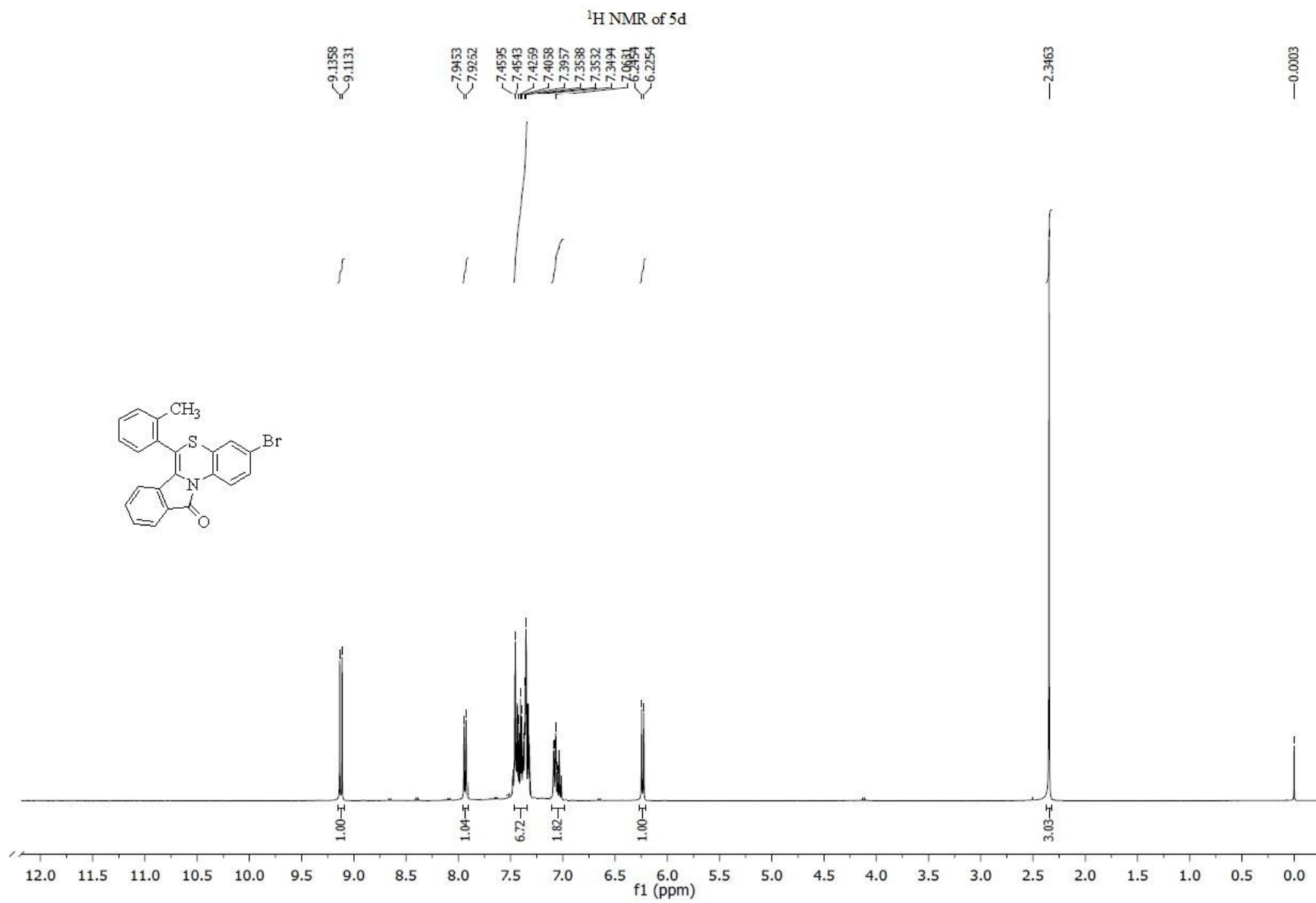


¹³C NMR of 5c

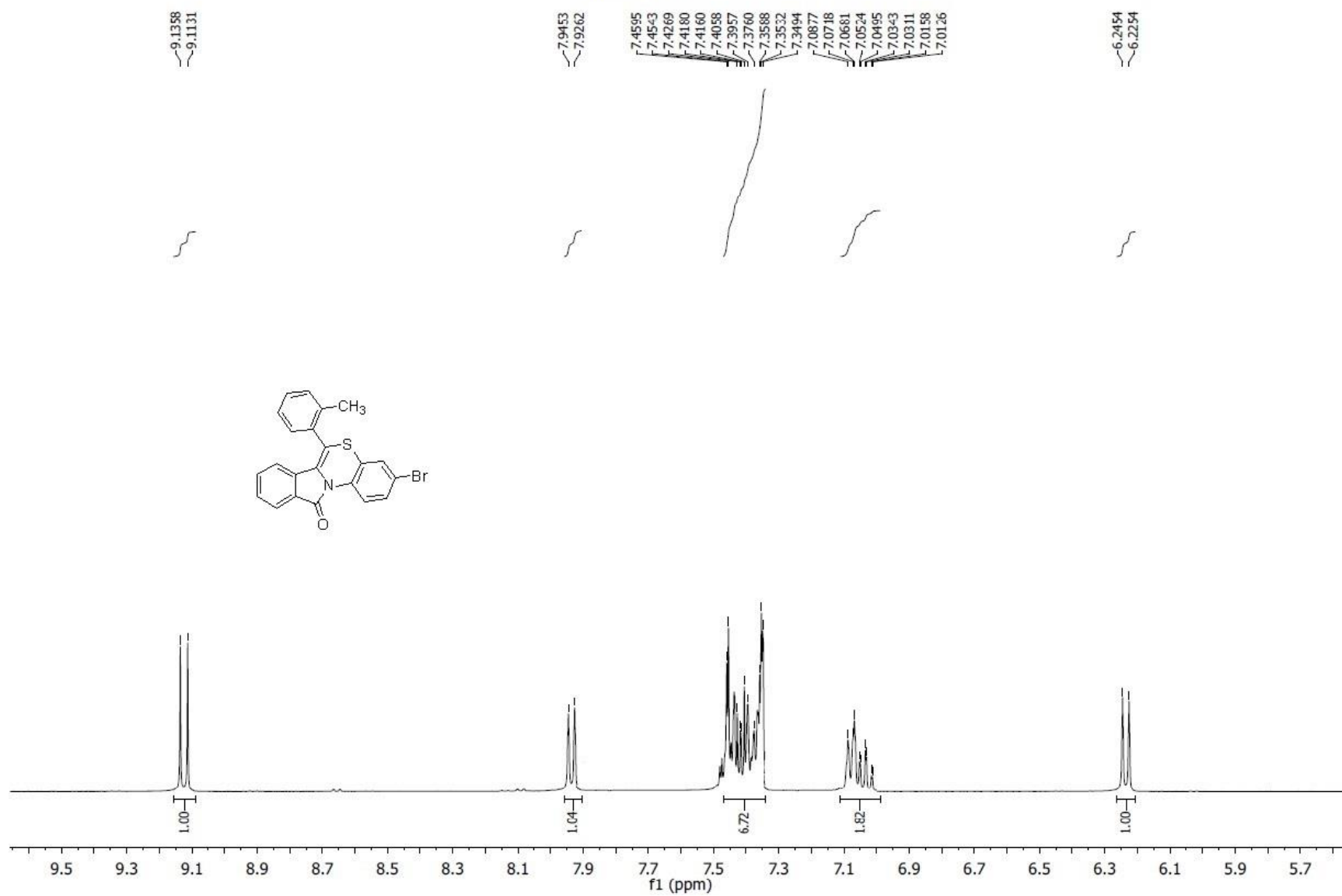


¹³C NMR of 5c

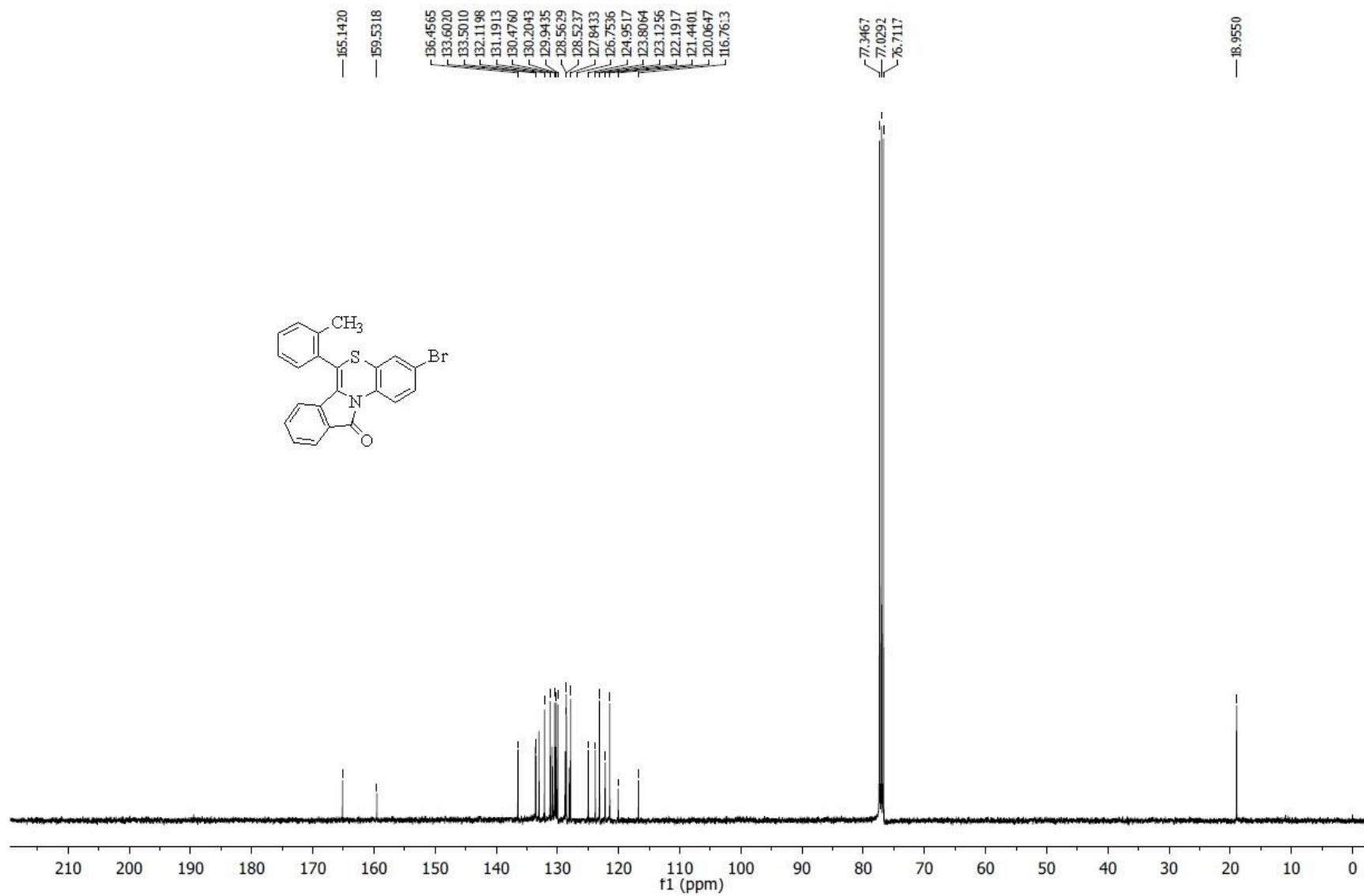




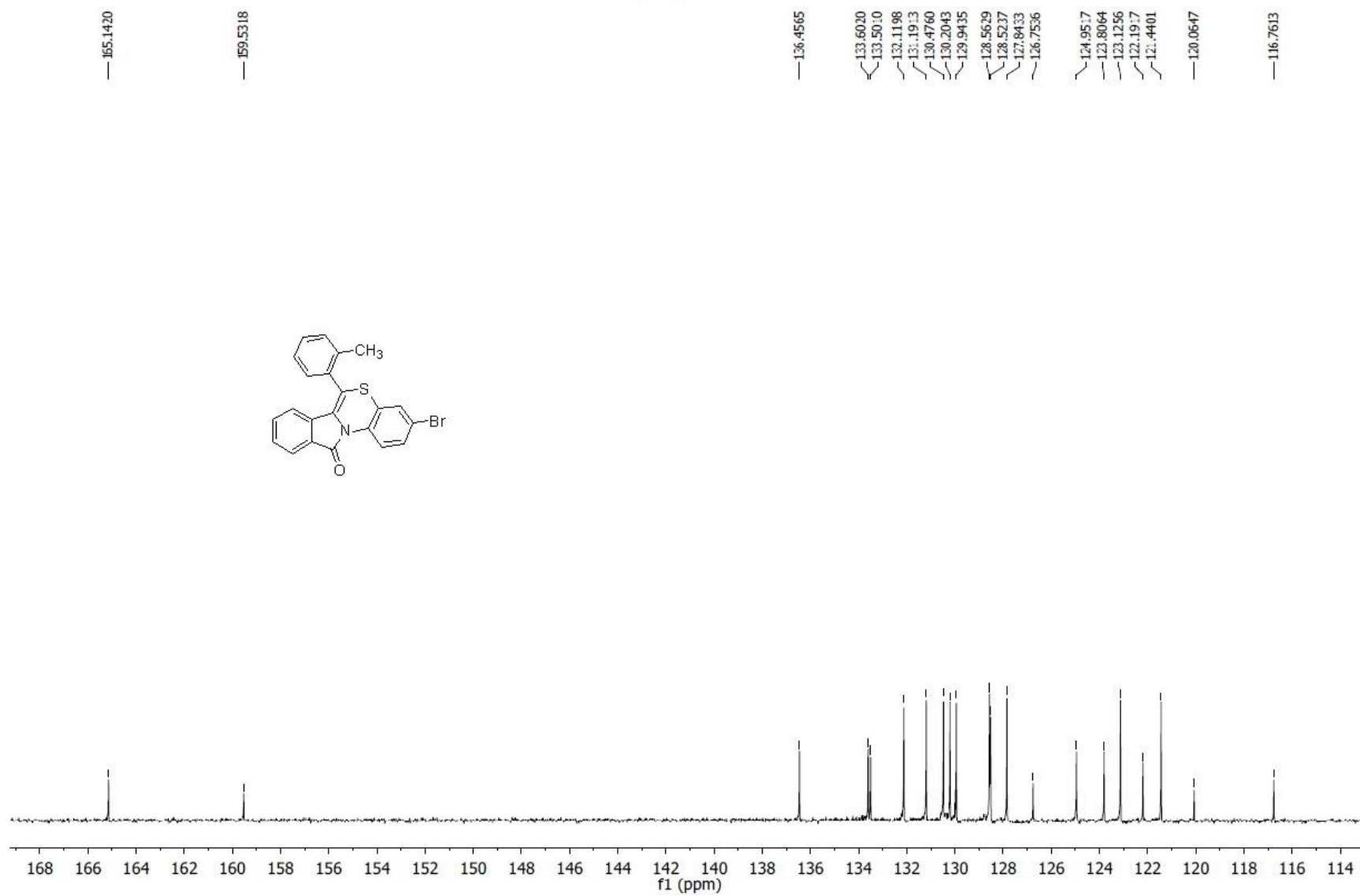
¹H NMR of 5d

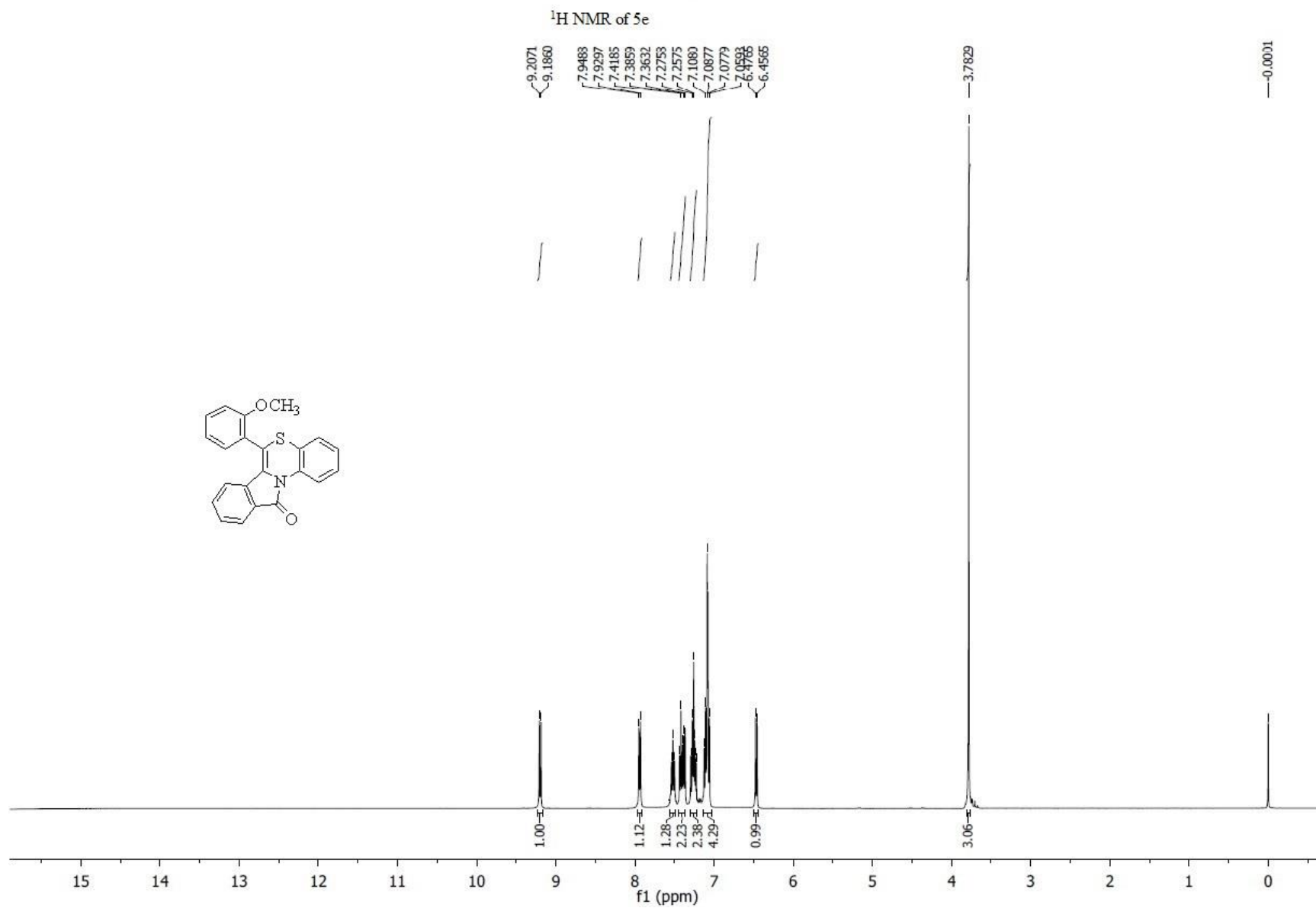


¹³C NMR of 5d

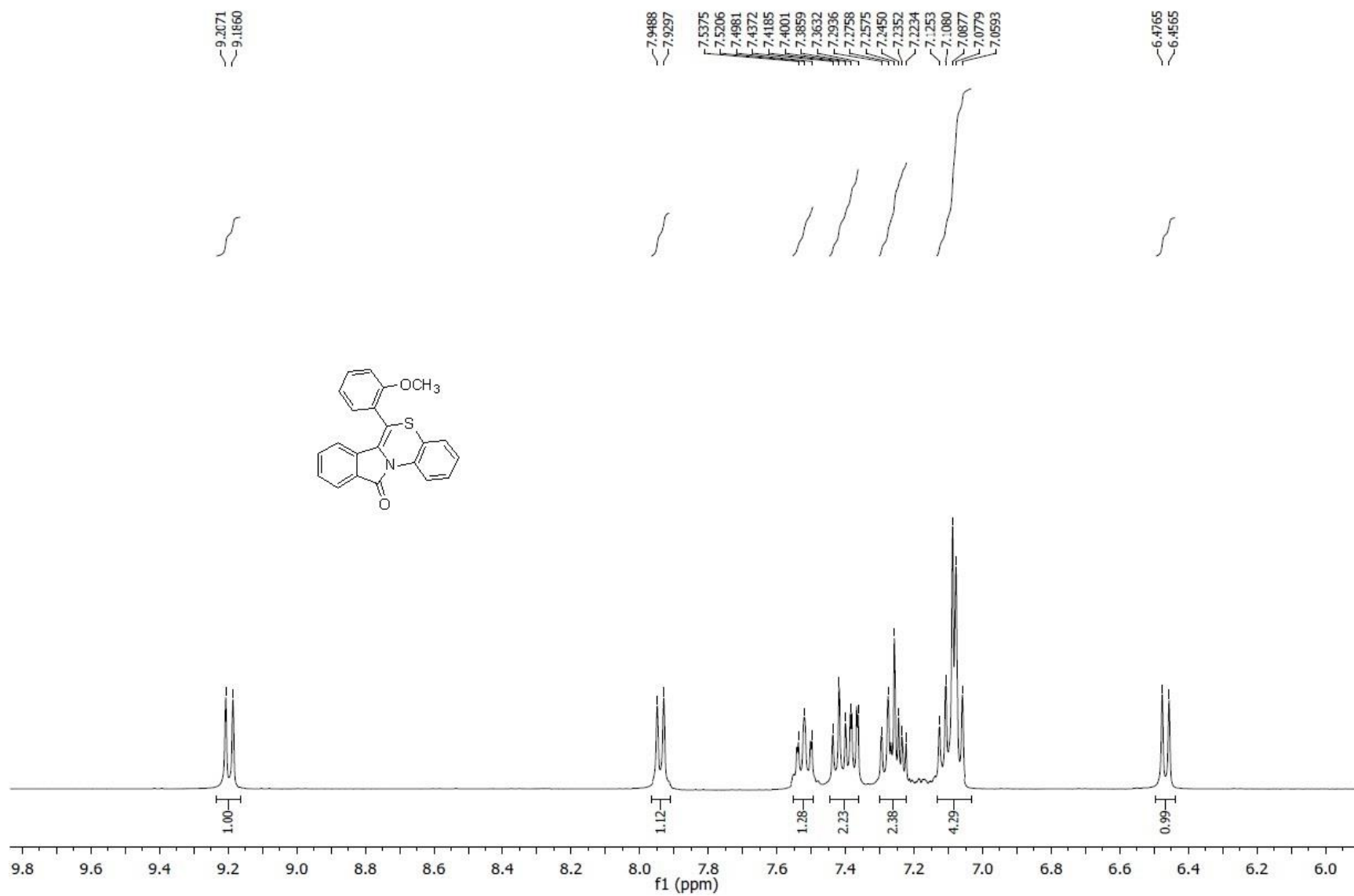


¹³C NMR of 5d



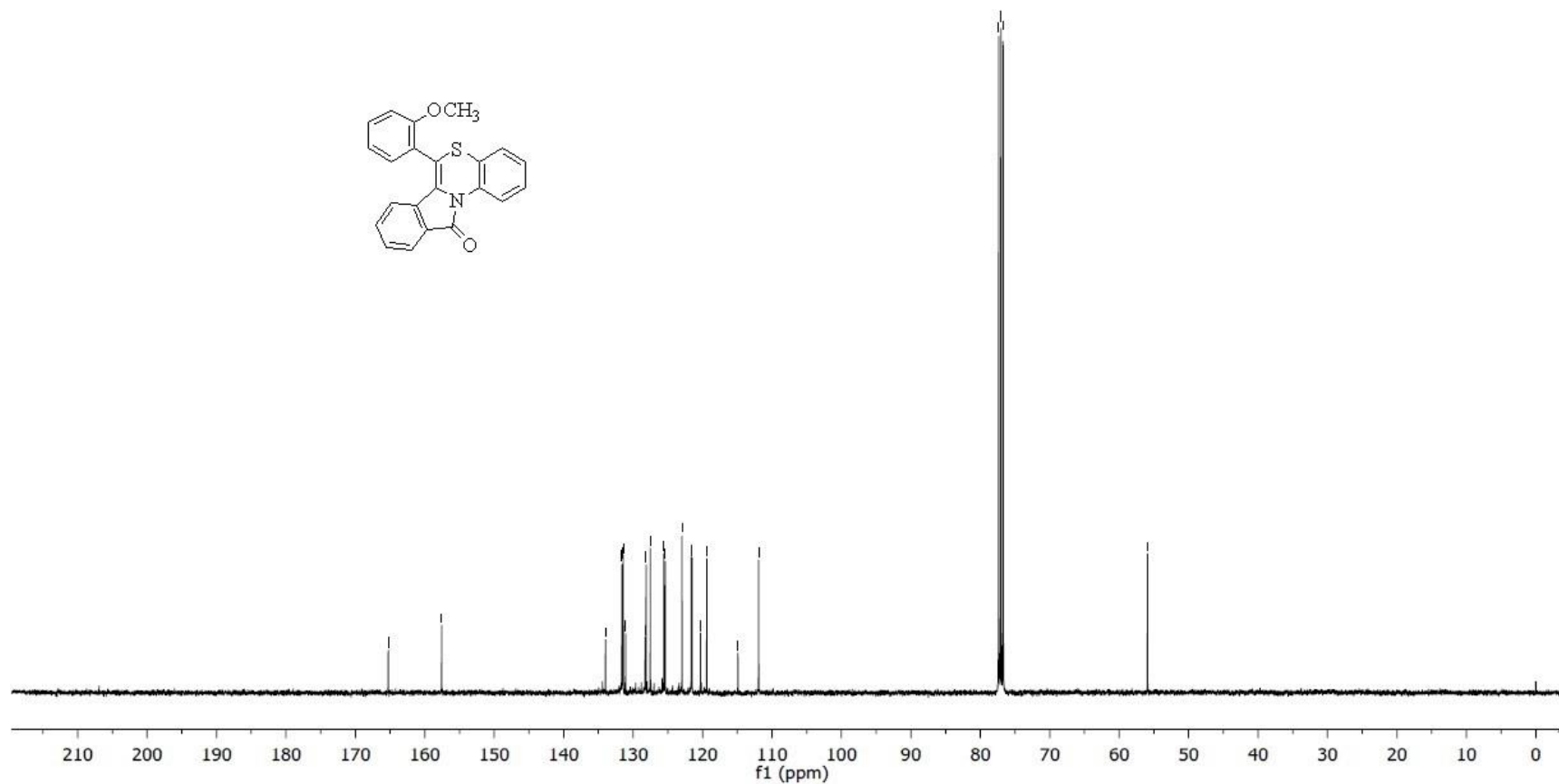
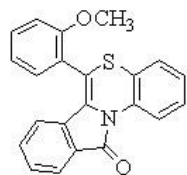


¹H NMR of 5e

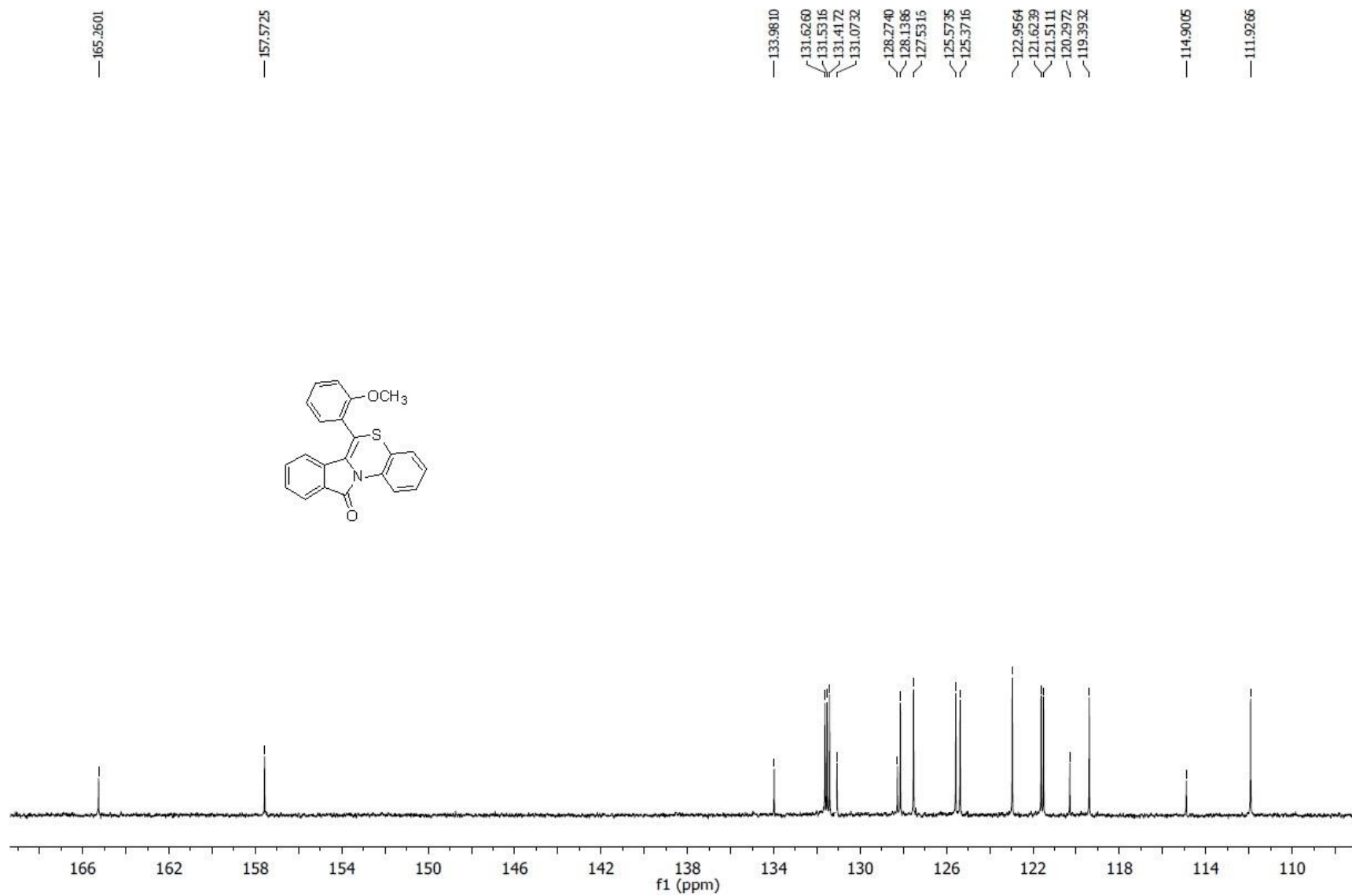


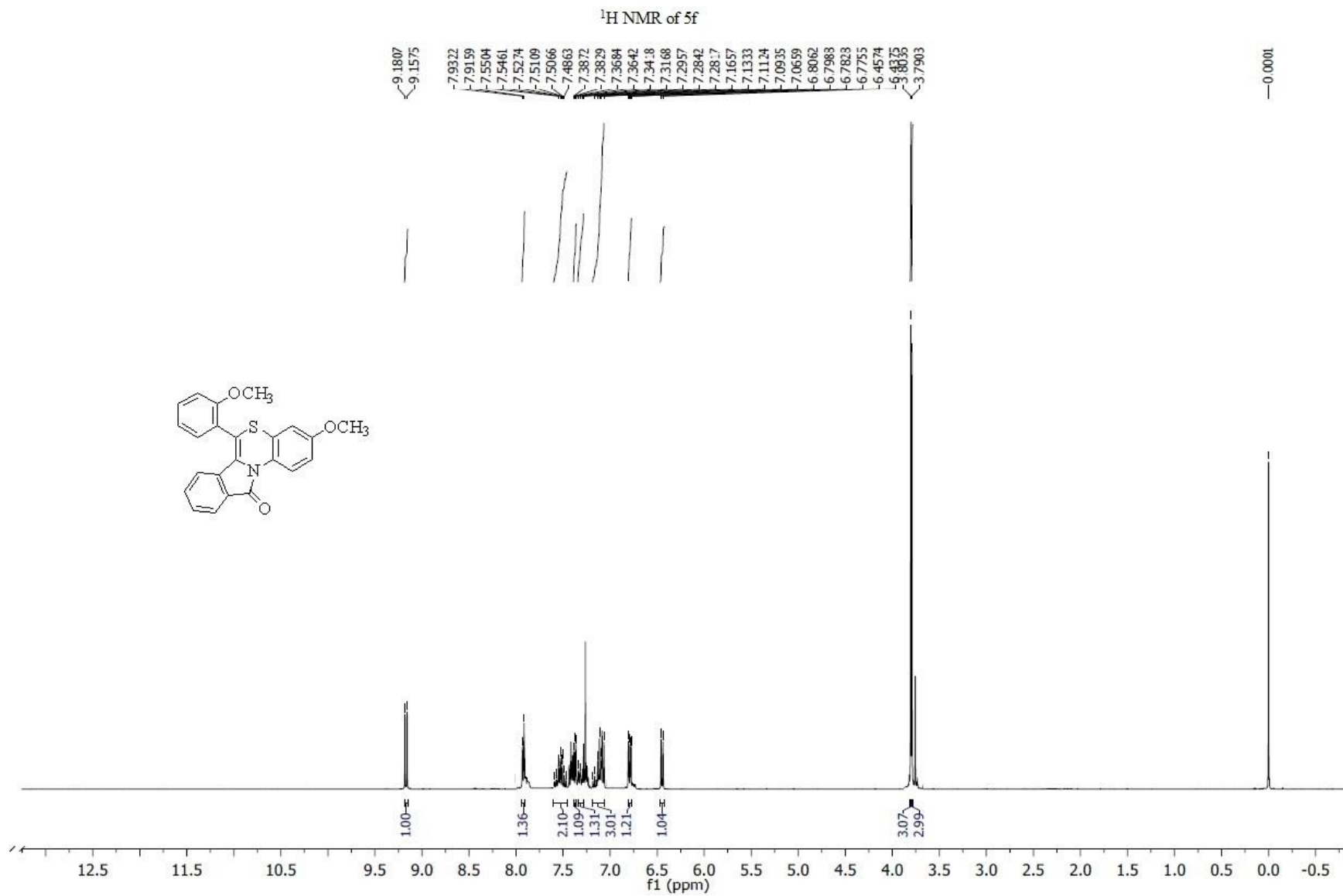
¹H NMR of 5e

165.2601
157.5725
133.9810
131.6260
131.5316
131.4172
131.0732
128.2740
128.1386
127.5316
125.5735
125.3716
122.9564
121.6239
121.5111
120.2972
119.3932
114.9005
111.9266
77.3557
77.0380
76.7204
55.9221

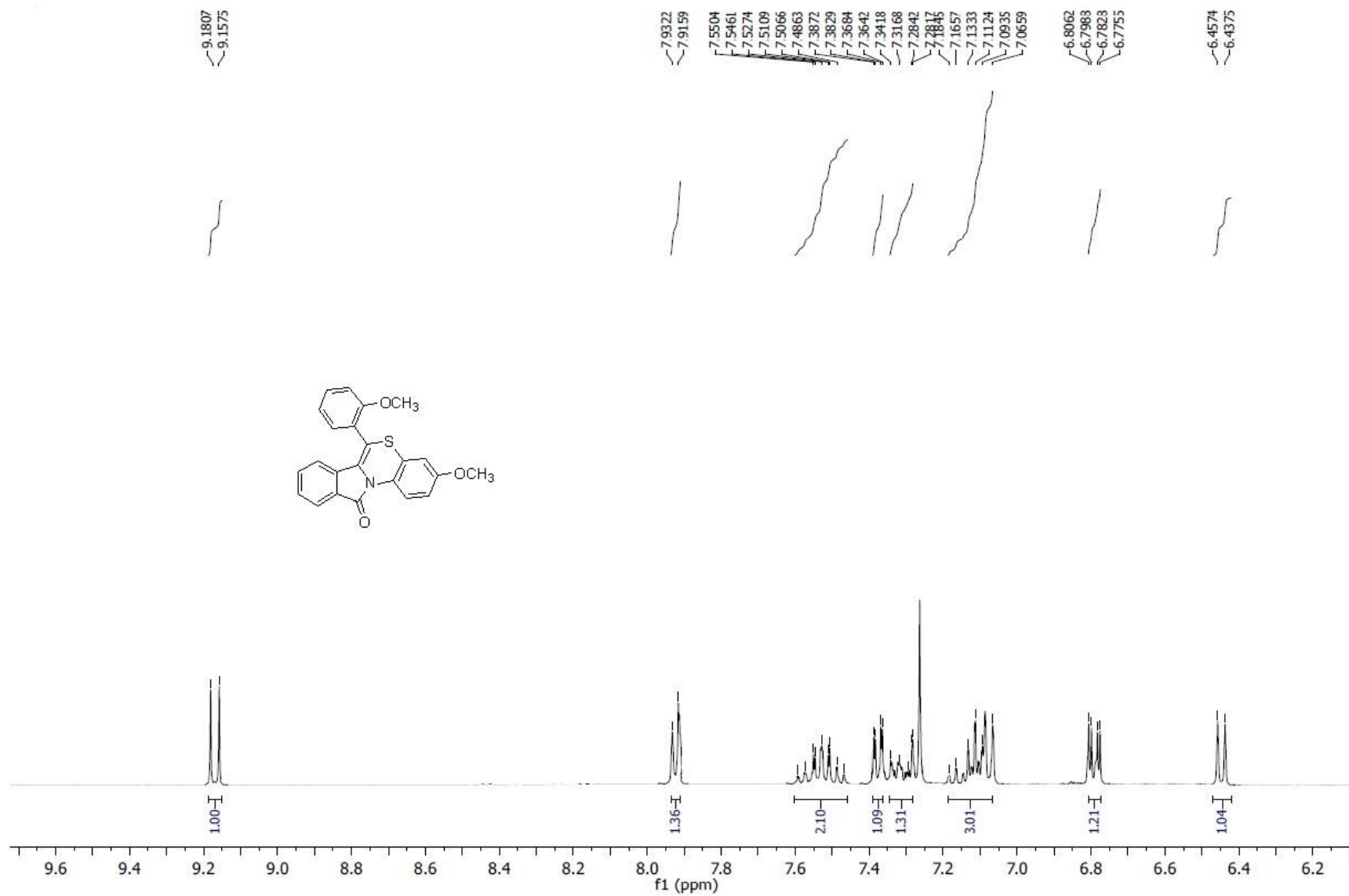


¹³C NMR of 5e

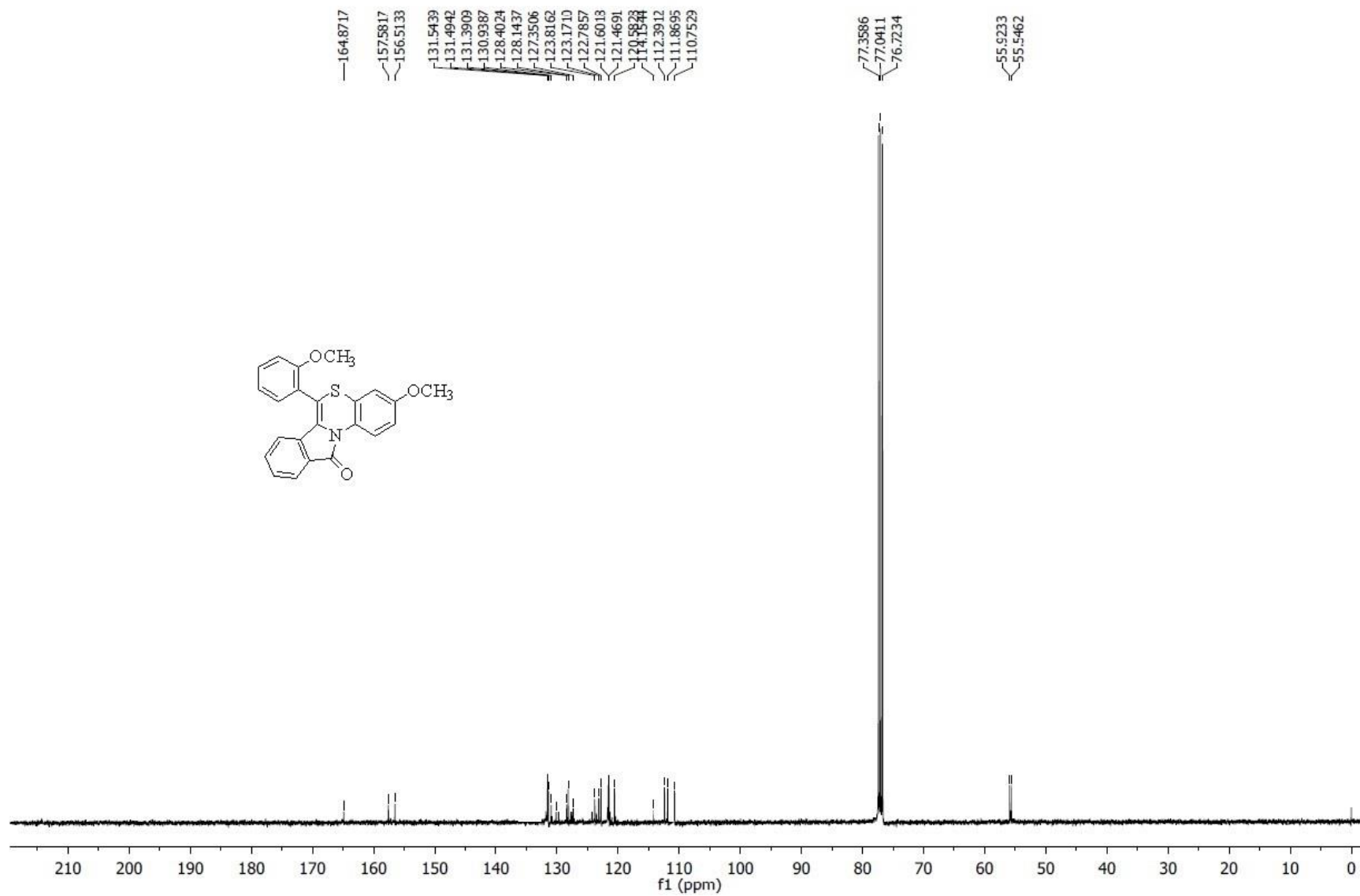




¹H NMR of 5f



¹³C NMR of 5f



¹³C NMR of 5f

—164.8717

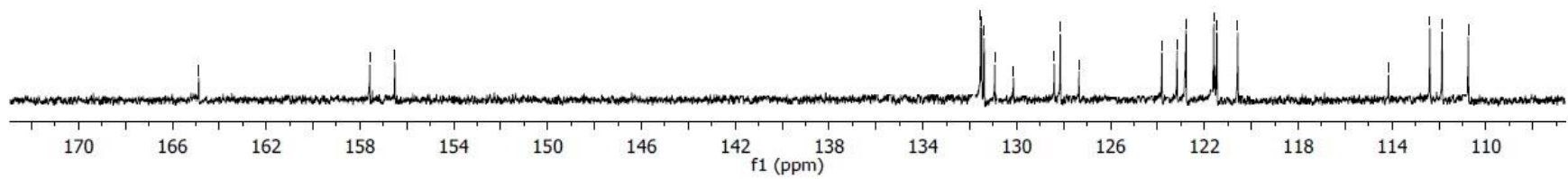
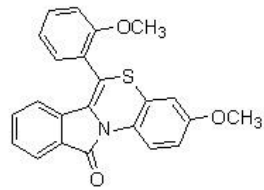
—157.5817

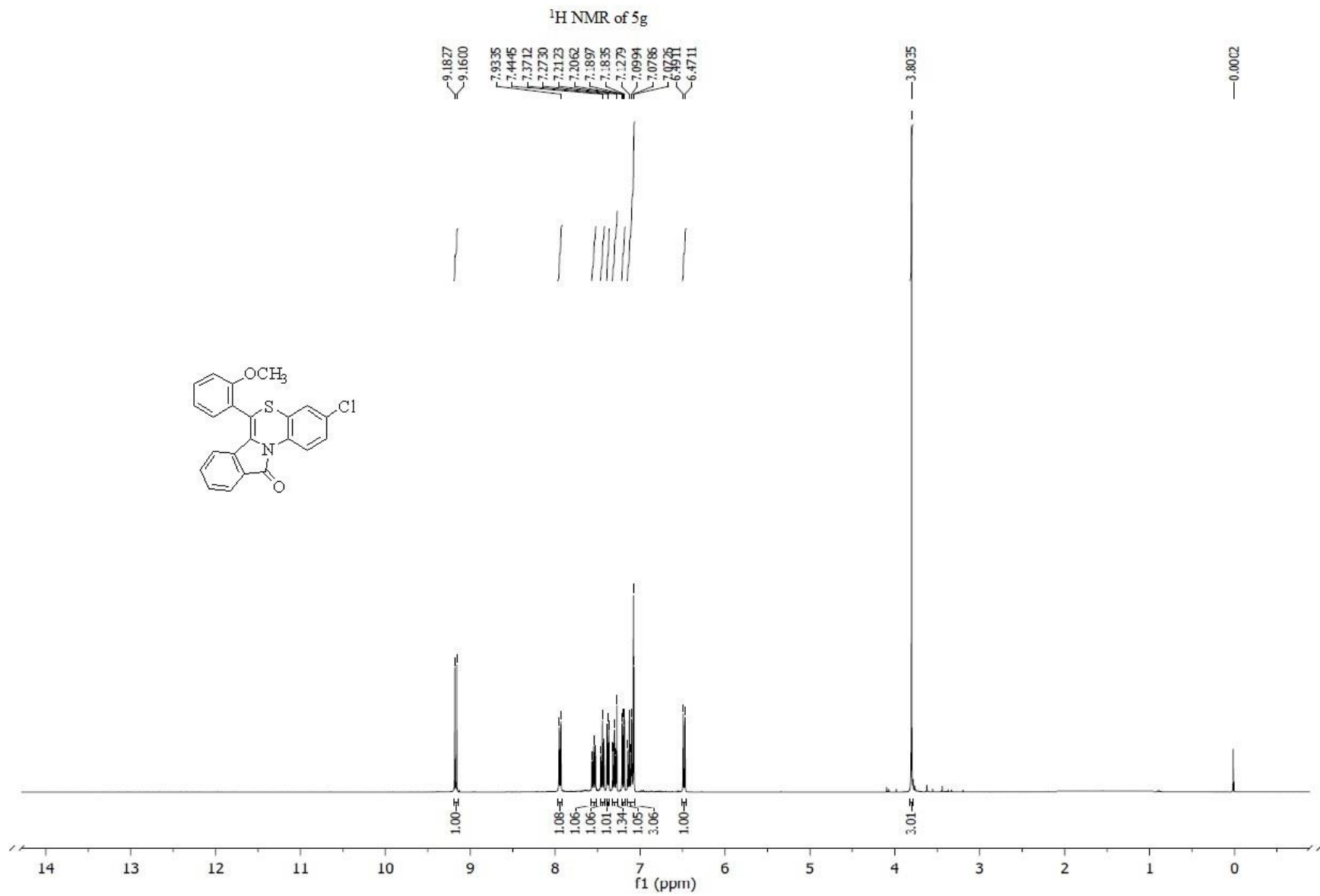
—156.5133

131.5439
131.4942
131.3909
130.9387
130.1399
128.4024
128.1437
127.3506

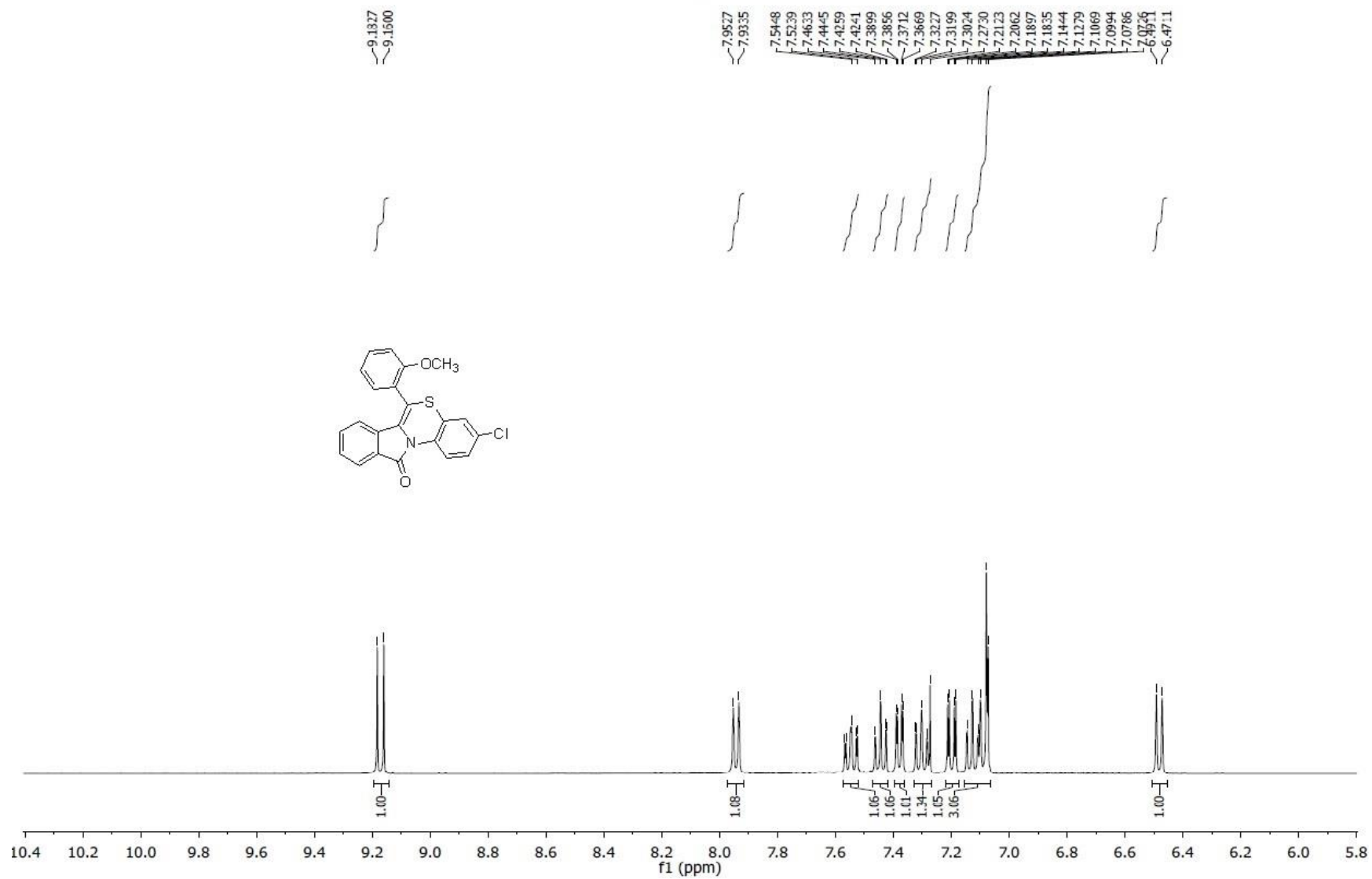
123.8162
123.1710
122.7857
121.6013
121.4691
120.5823

—114.1544
—112.3912
—111.8695
—110.7523

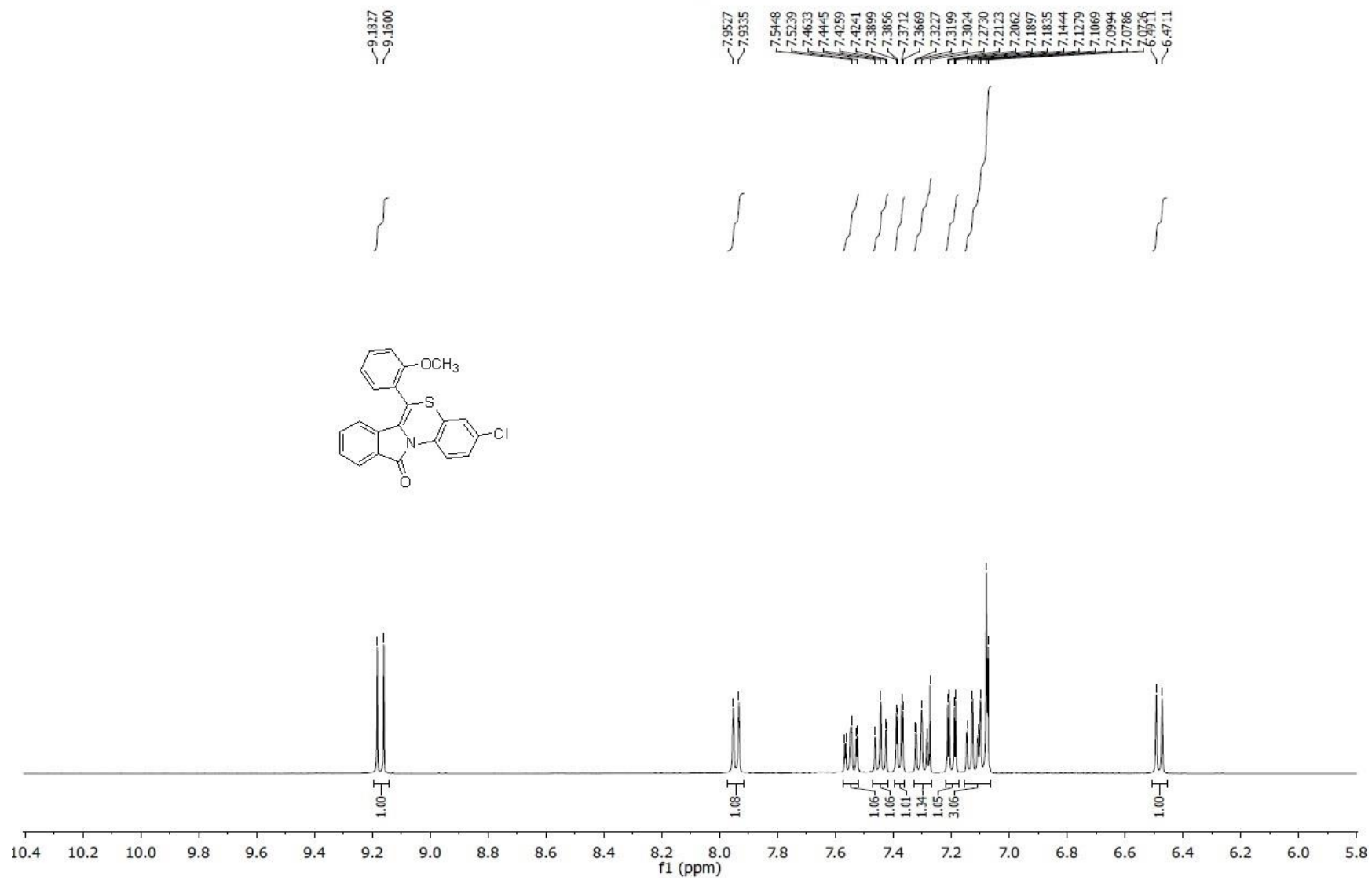




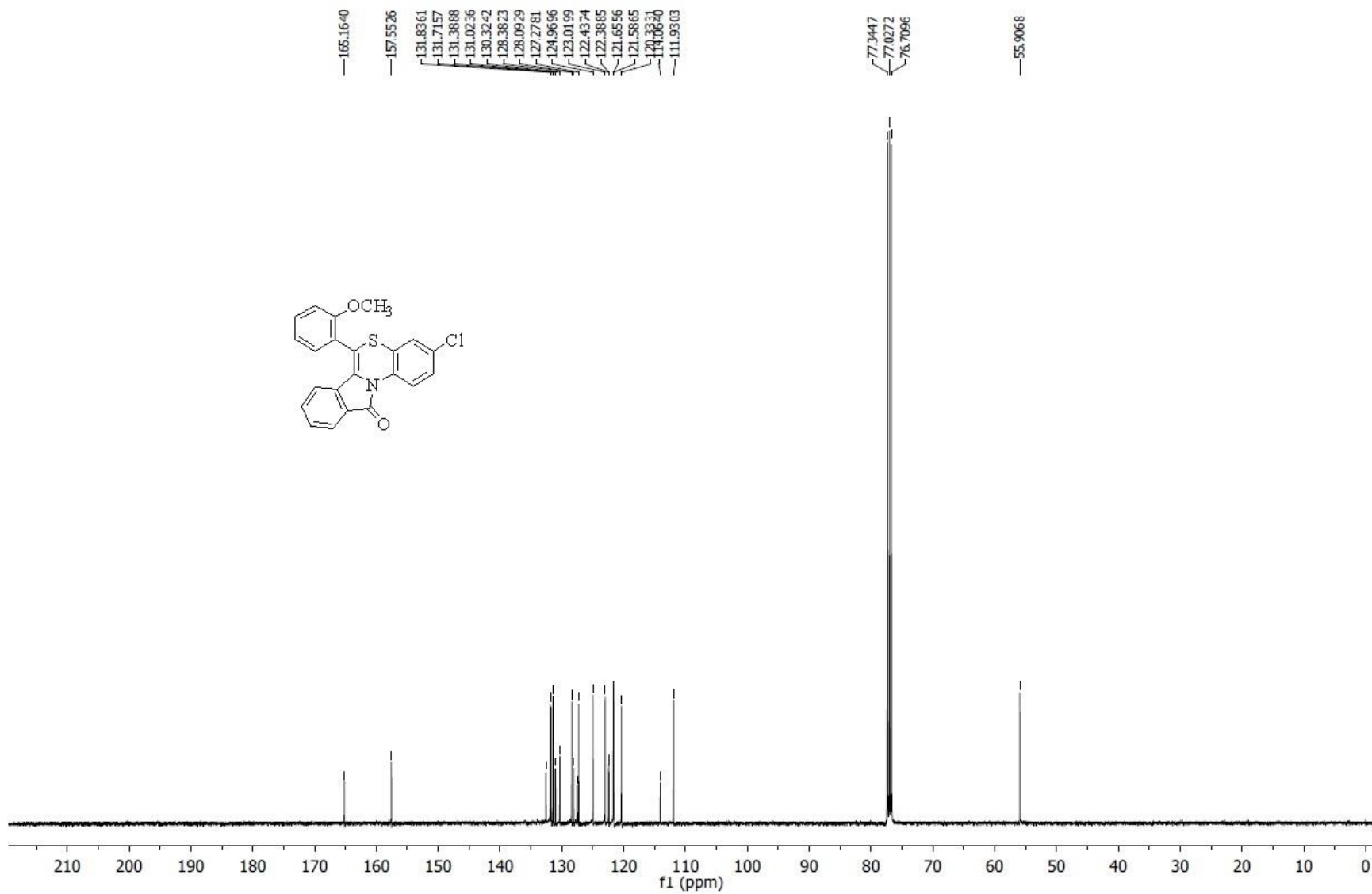
¹H NMR of 5g



¹H NMR of 5g



¹³C NMR of 5g



¹³C NMR of 5g

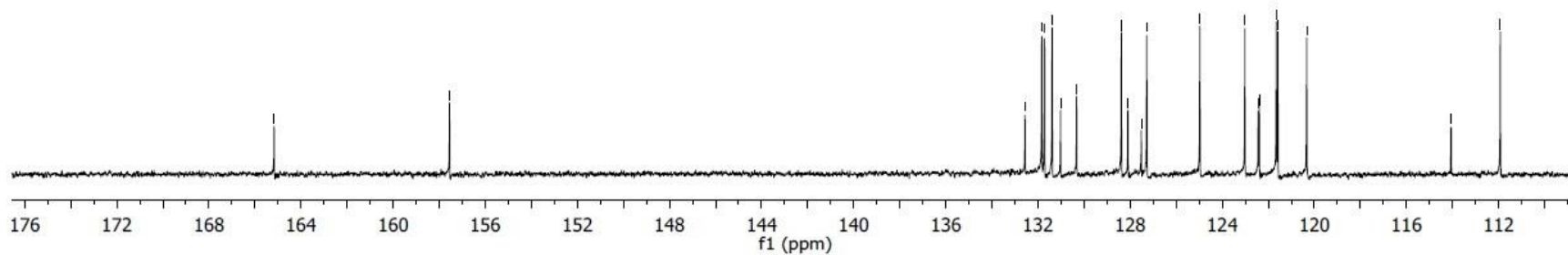
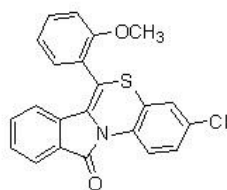
—165.1640

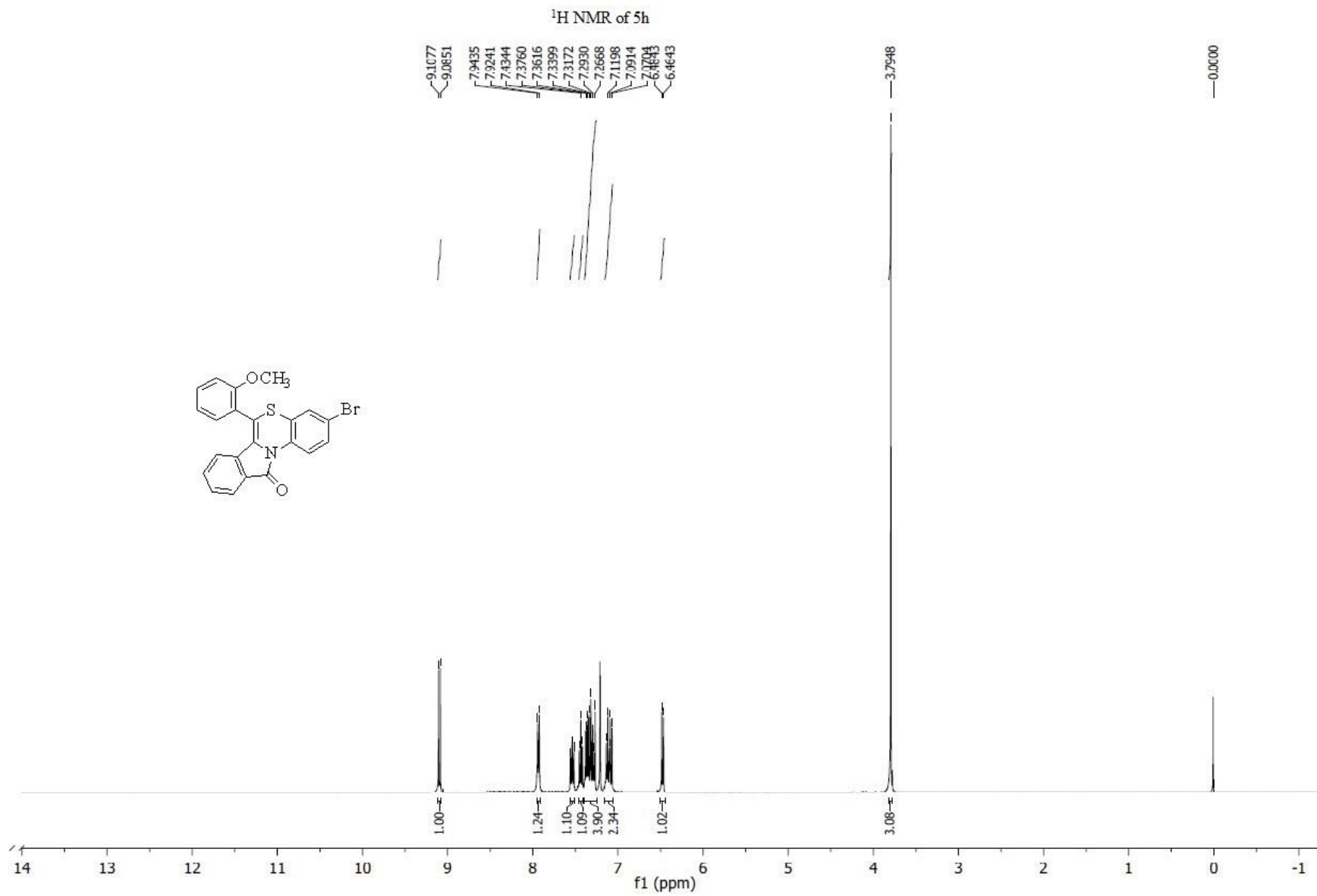
—157.5526

132.5647
131.8361
131.7157
131.3888
131.0236
130.3242
128.3823
128.0929
127.5139
127.2781
—124.9695
123.0199
122.4374
122.3885
121.6555
121.5865
120.3331

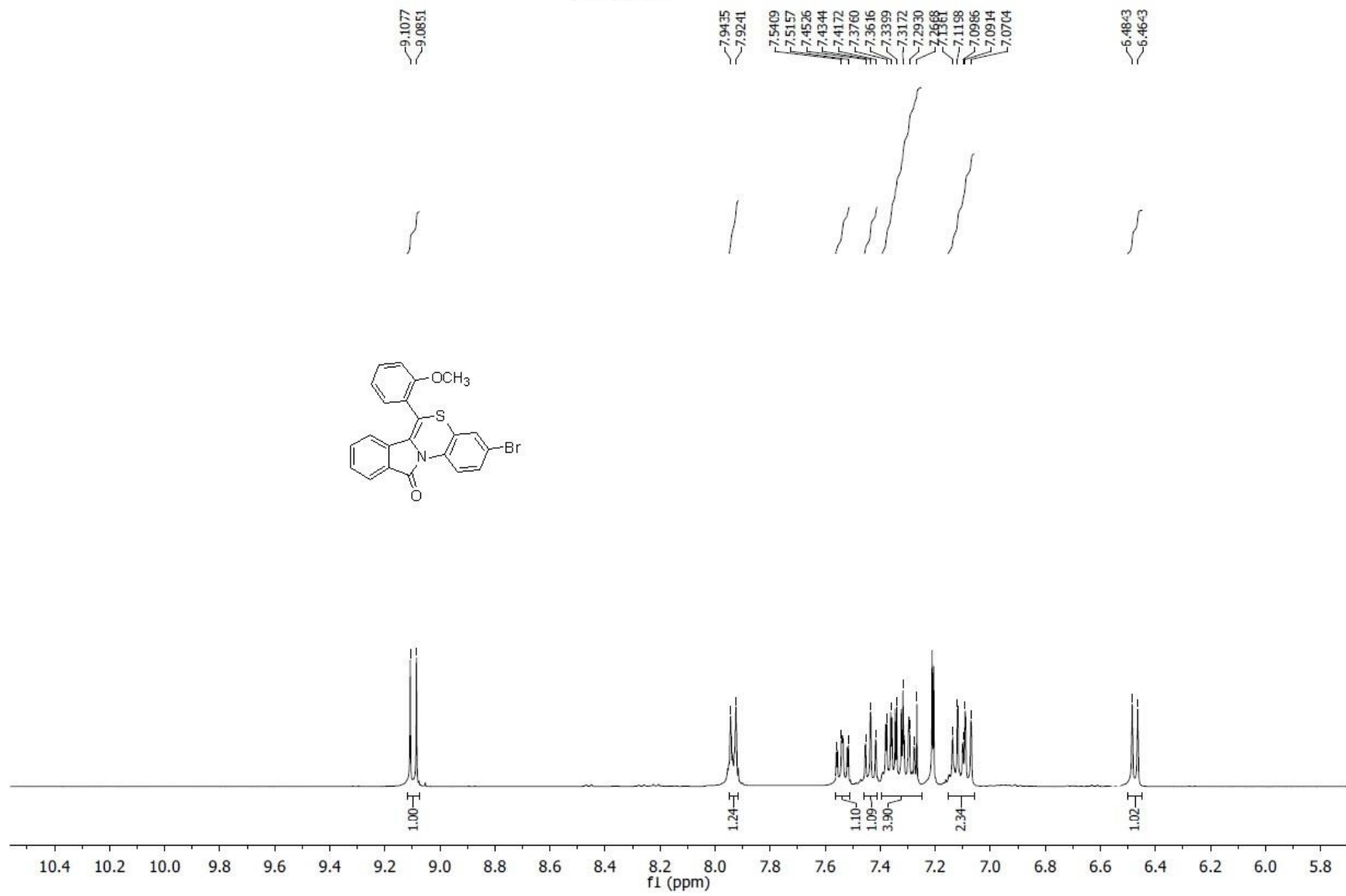
—114.0640

—111.9303

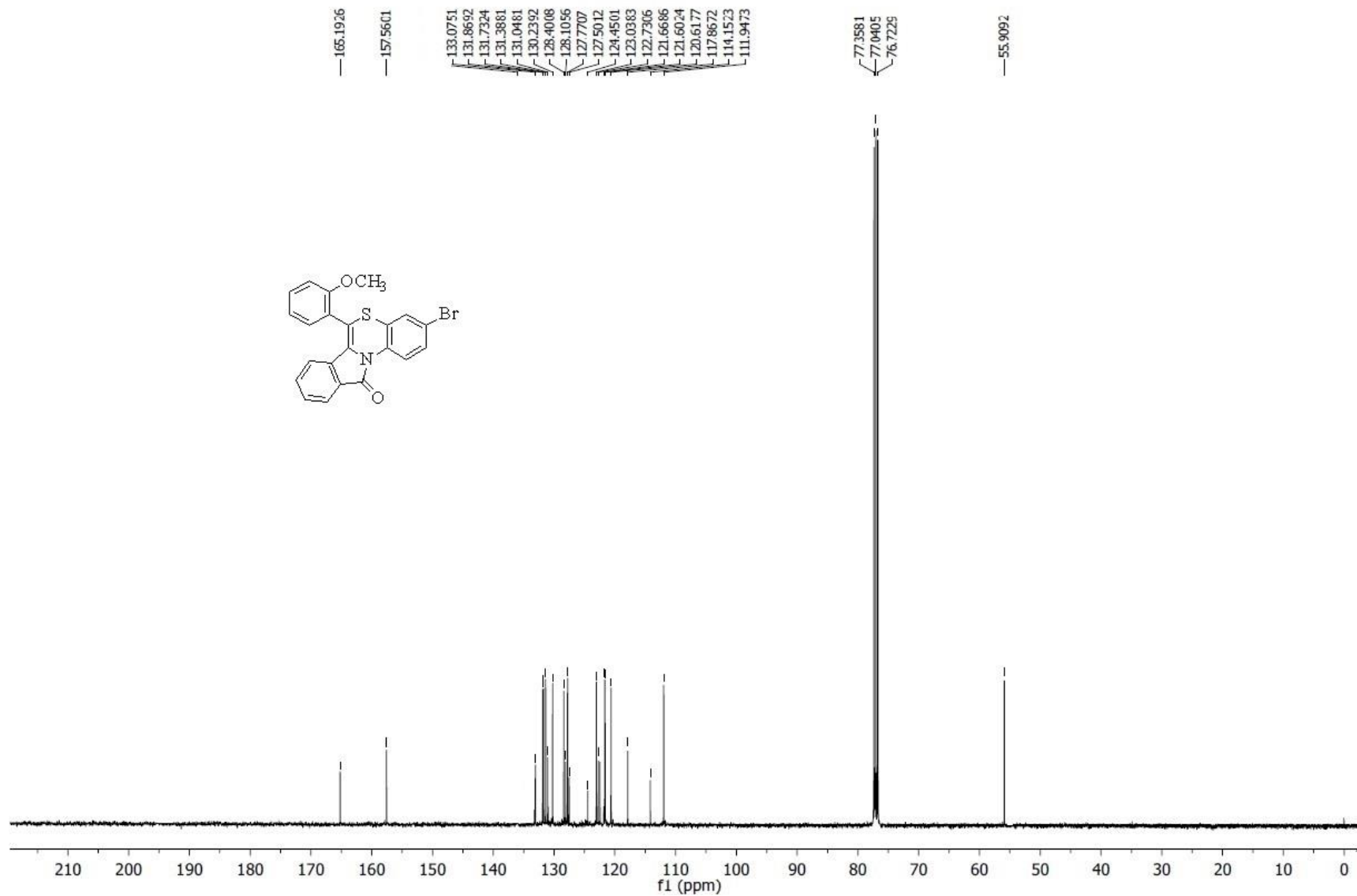




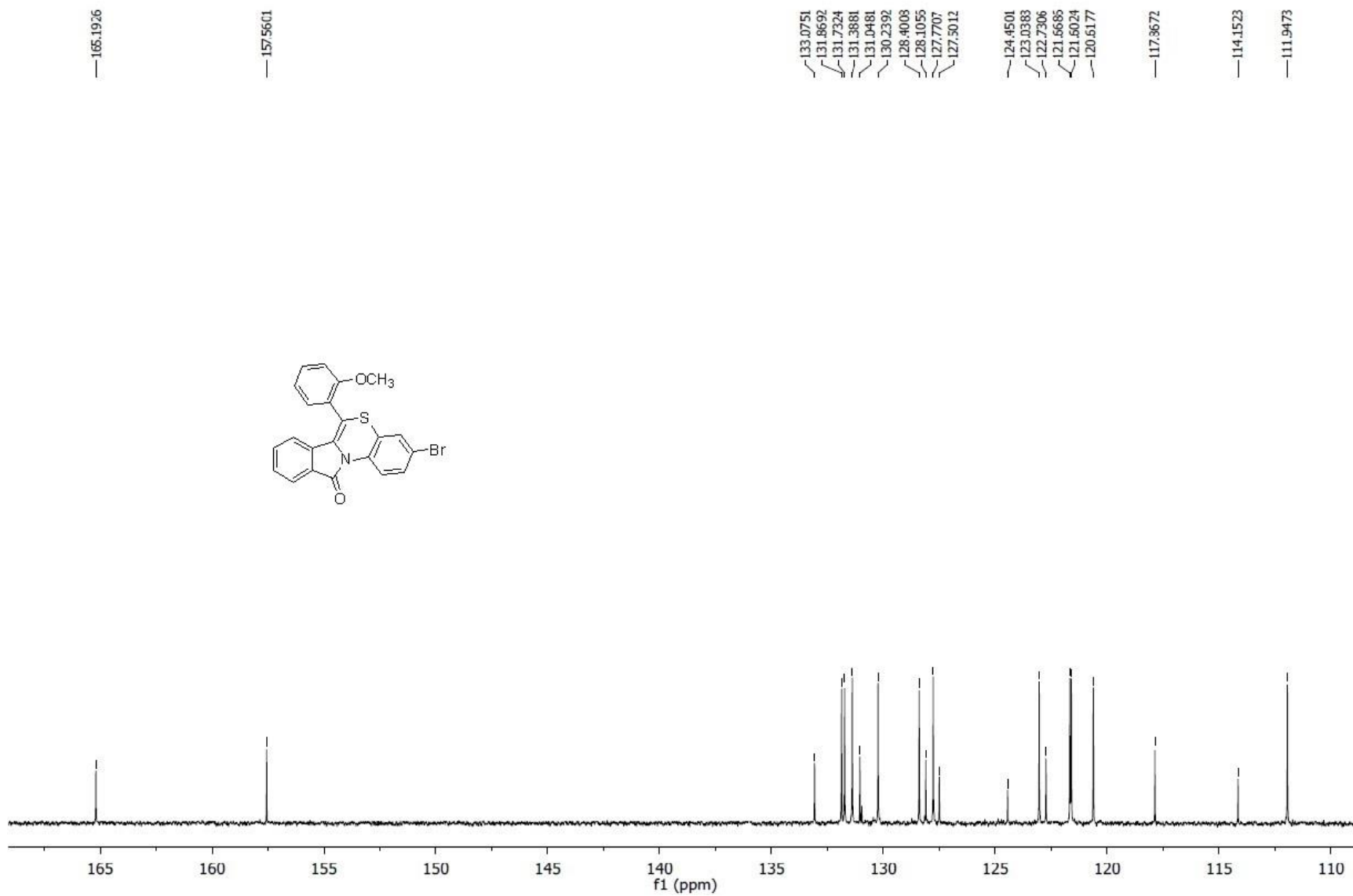
¹H NMR of 5h



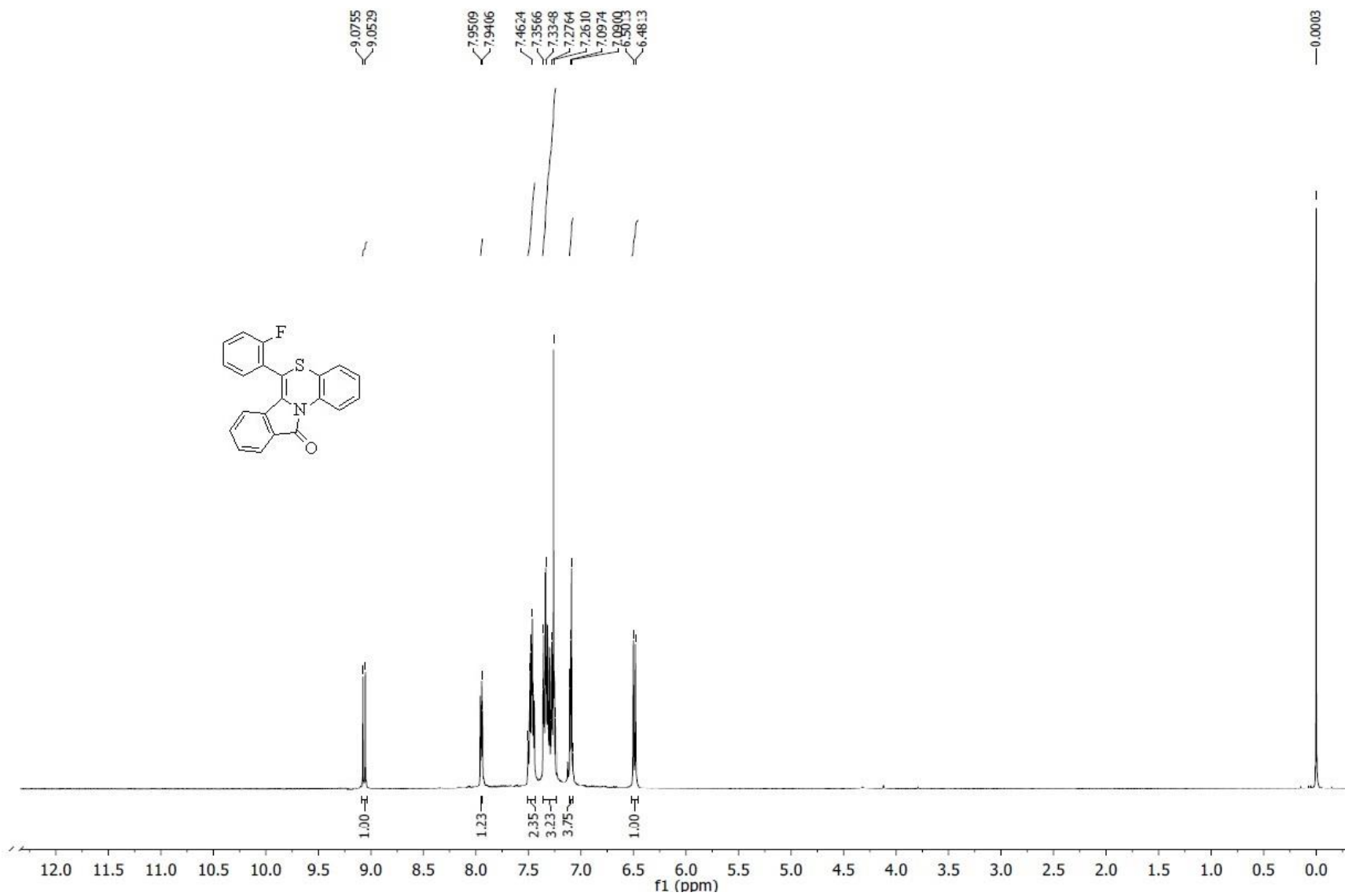
¹³C NMR of 5h



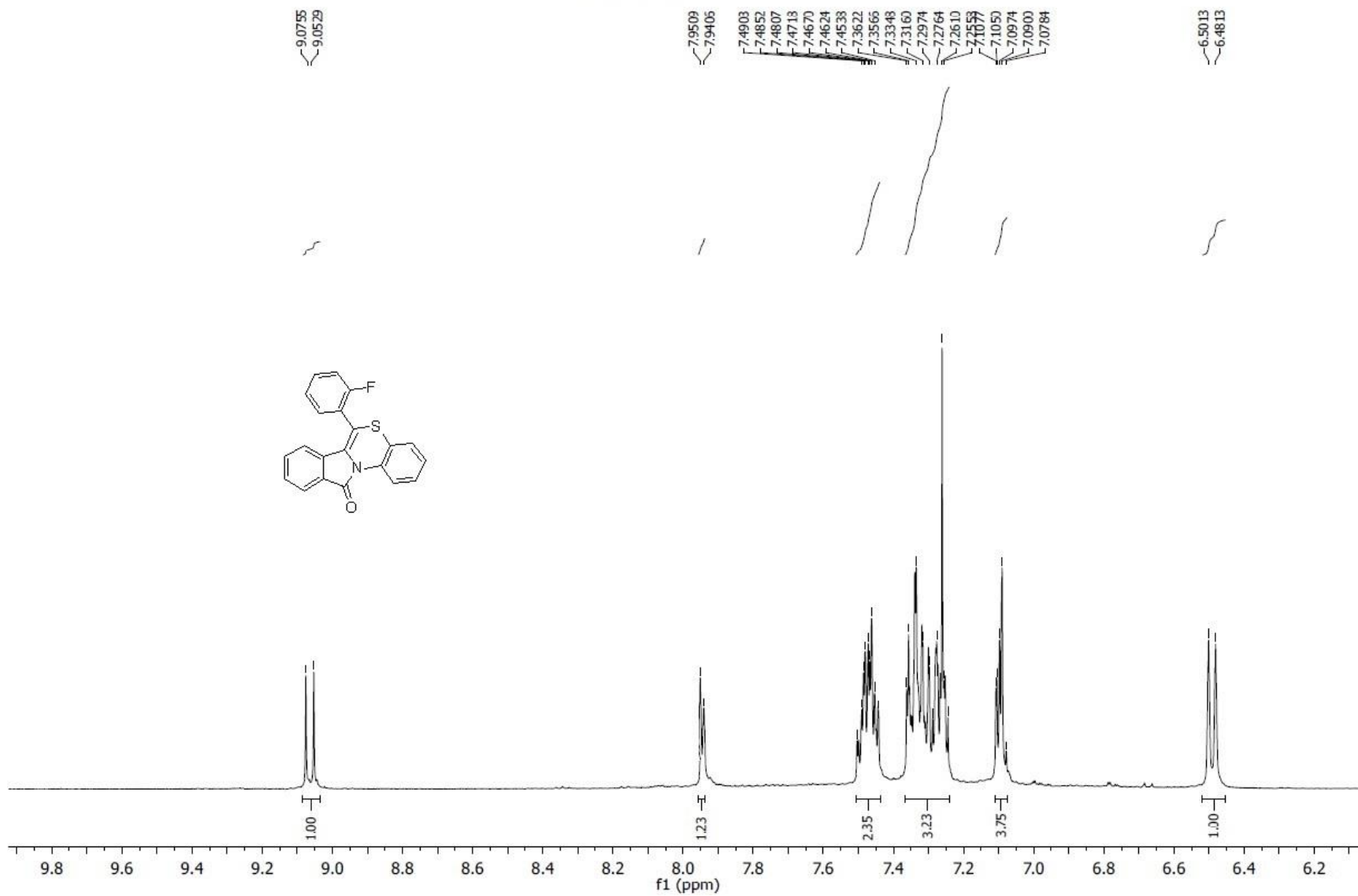
¹³C NMR of 5h



¹H NMR of 5i



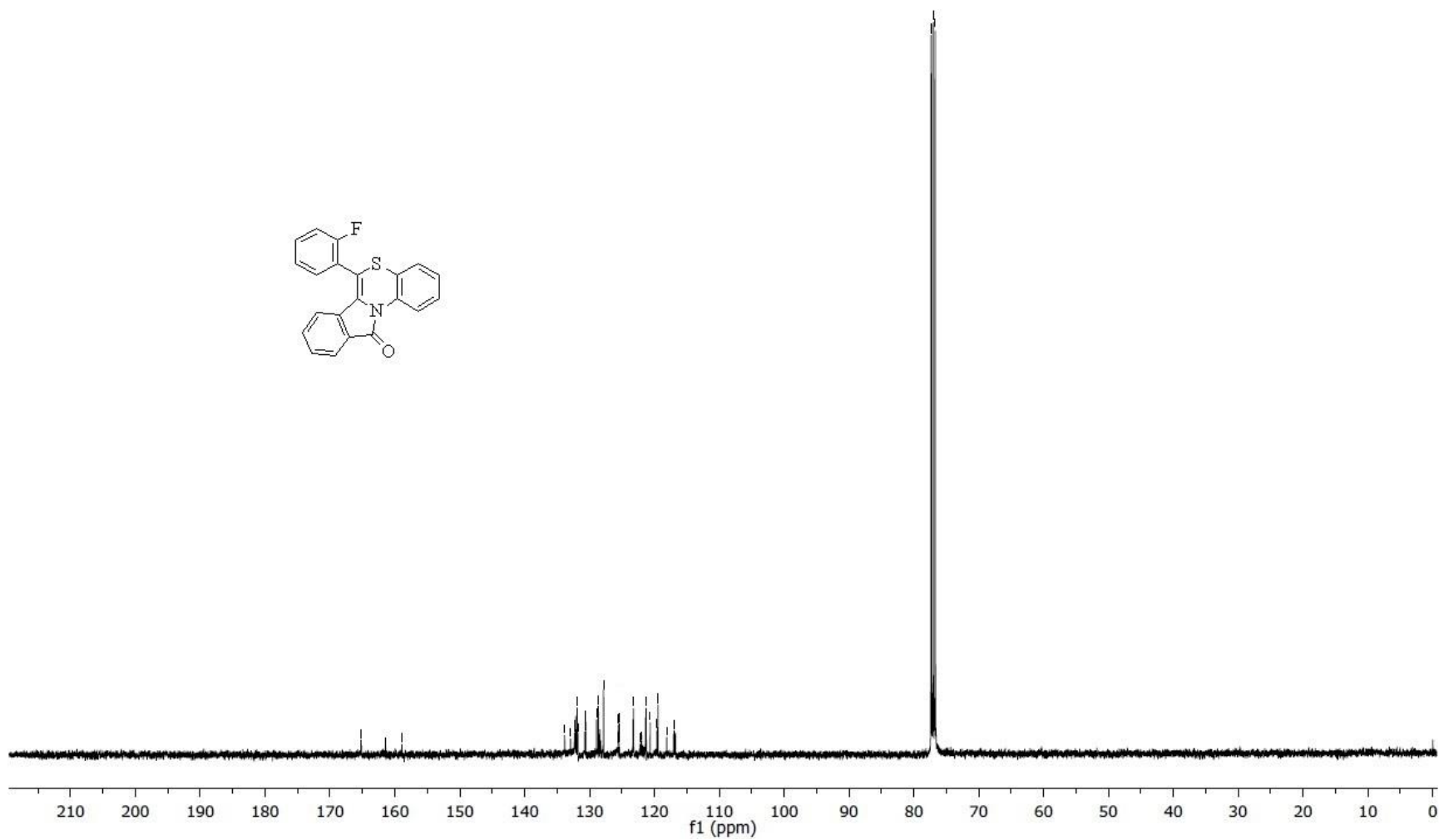
¹H NMR of 5i



¹³C NMR of 5i

165.2118
161.4177
158.9153
133.8157
132.9131
132.3015
132.2208
131.8917
131.8286
131.8003
131.7737
130.7146
130.5994
128.9039
128.6869
127.8273
125.4971
125.4881
123.2039
122.2665
122.0459
121.2630
120.6511
119.6991
119.4947
118.0956
116.9418

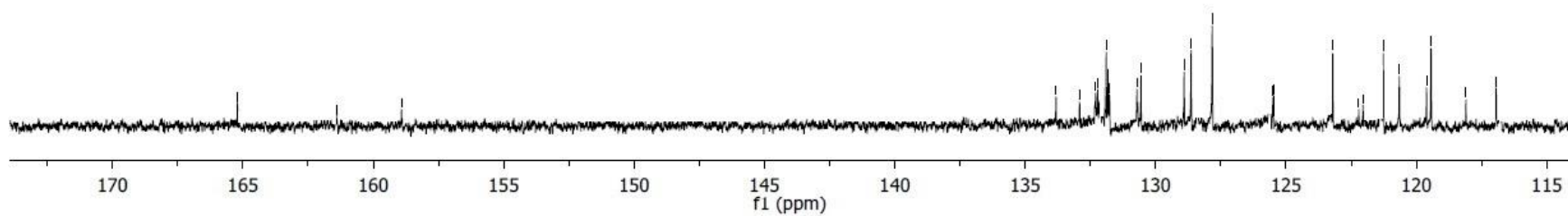
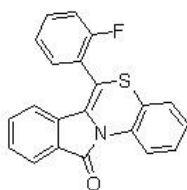
77.3413
77.0227
76.7053

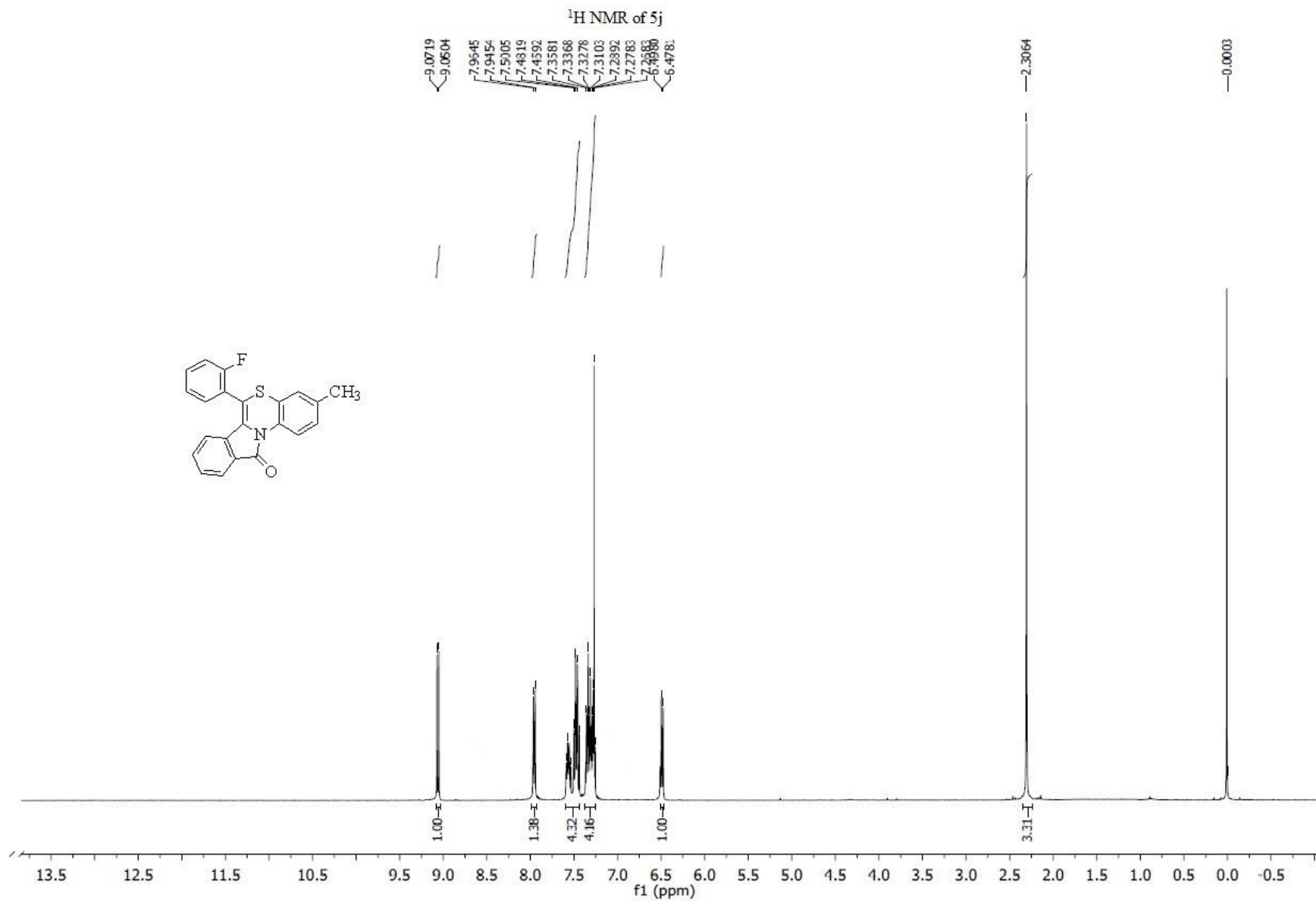


¹³C NMR of 5i

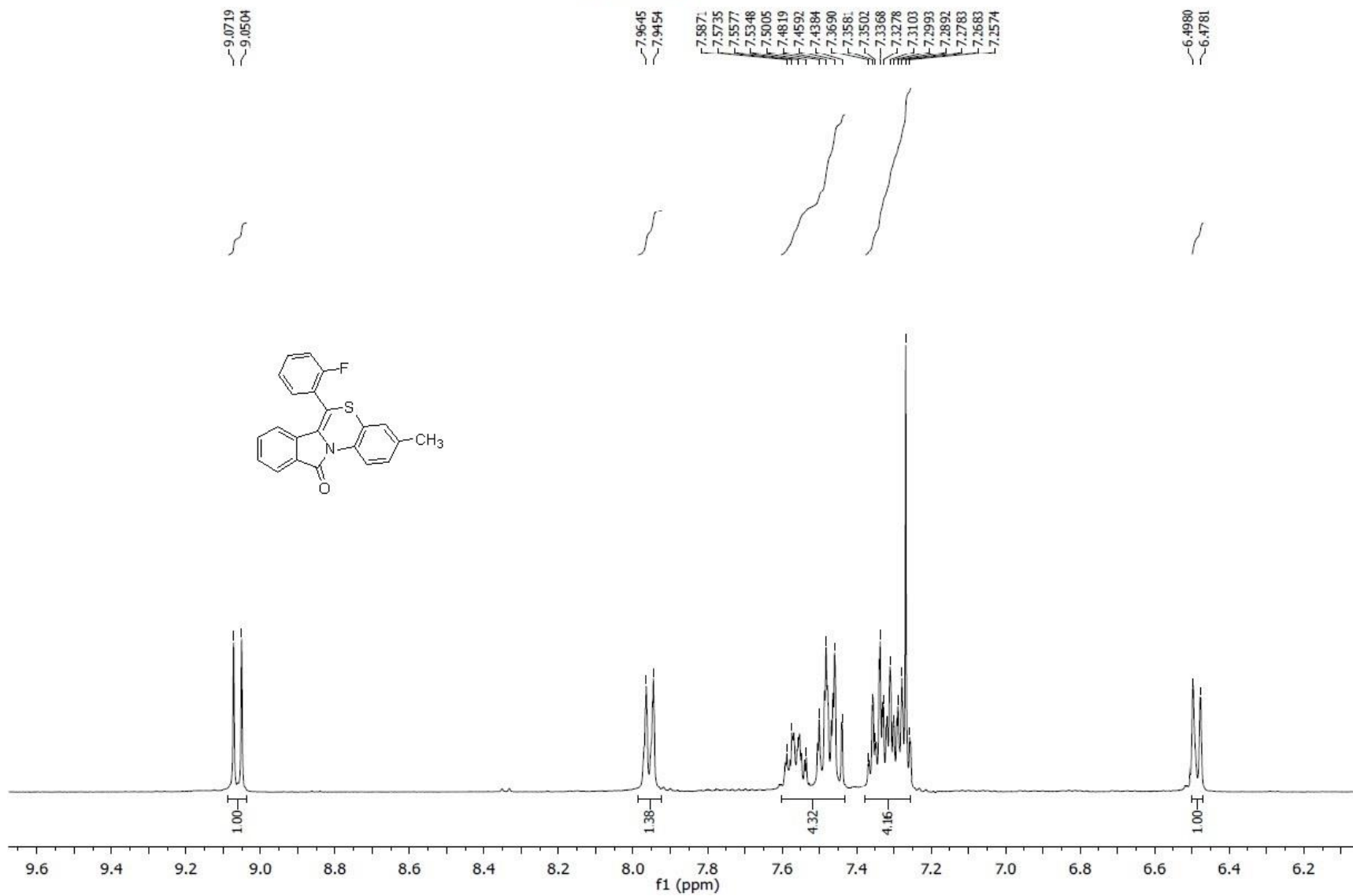
— 165.2118
— 161.4177
— 158.9153

133.8157
132.9131
132.3015
132.2208
131.8917
131.8286
131.8103
131.7737
130.7146
130.5594
128.9039
128.6369
127.8273
125.4971
125.4581
123.2039
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122.0459
121.2630
120.6511
119.6091
119.4347
118.0956
116.9418





¹H NMR of 5j

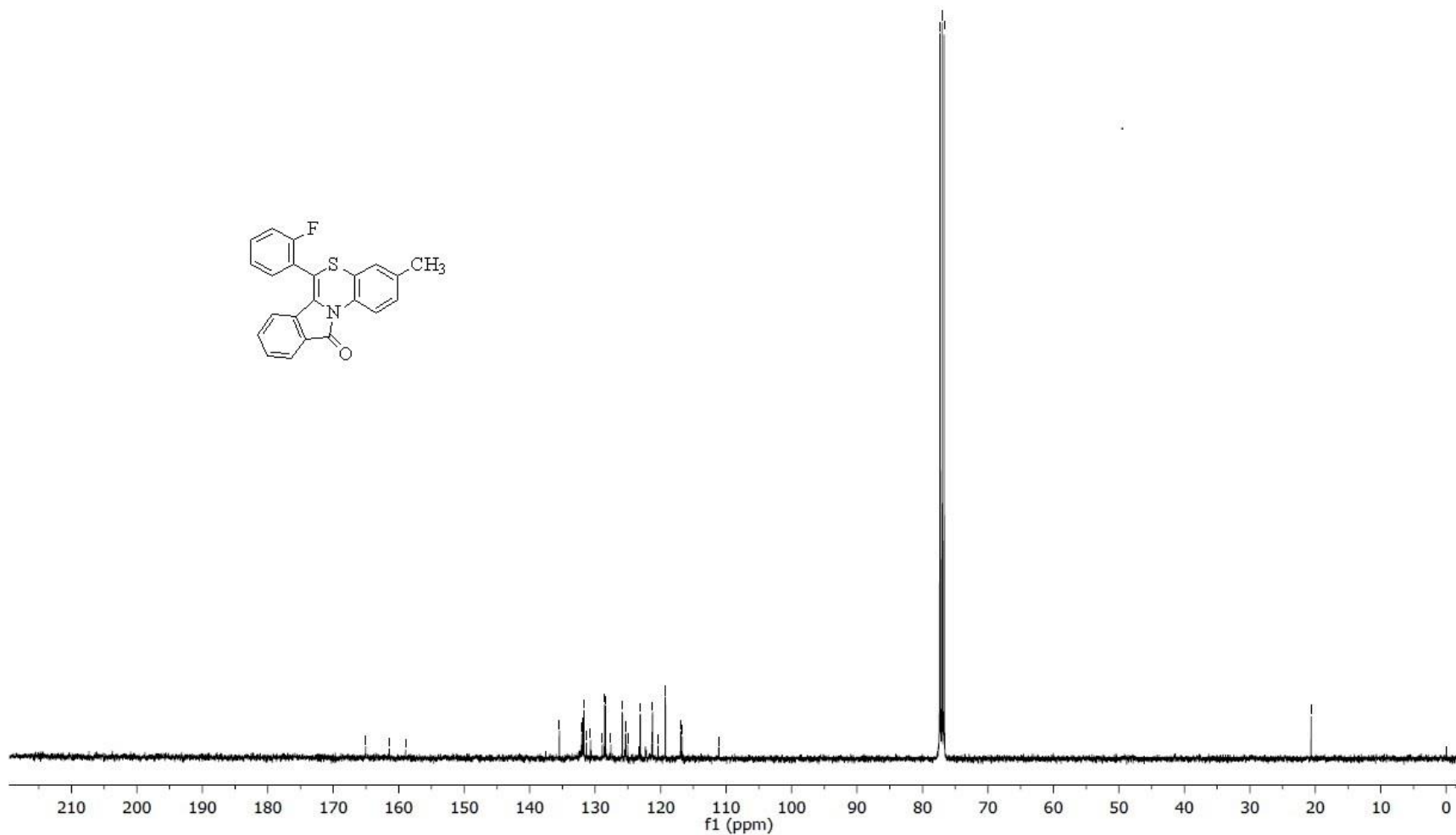
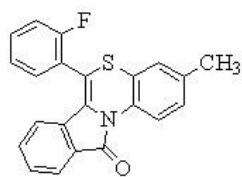


¹³C NMR of 5j

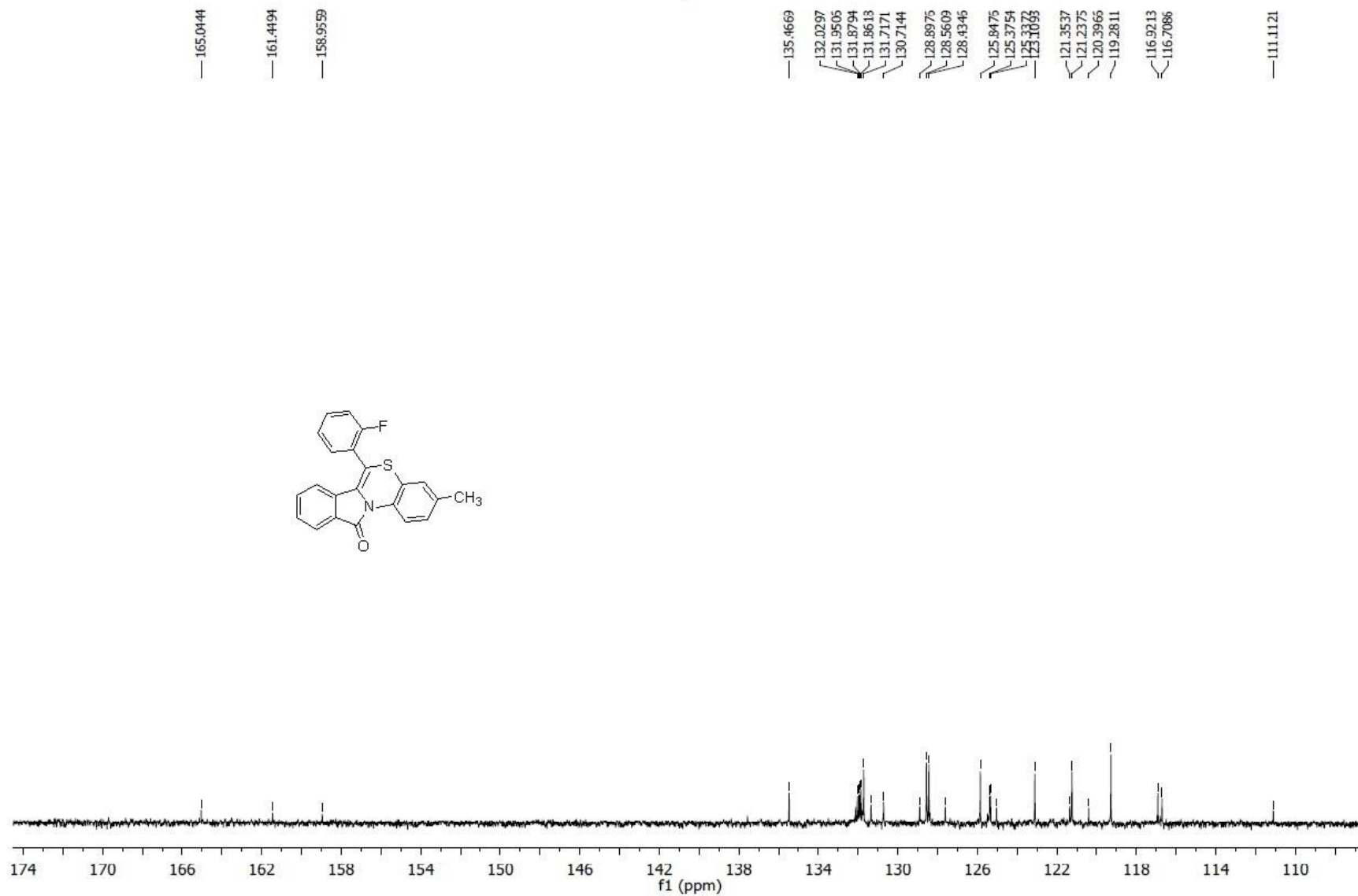
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161.4494
158.9559
135.4669
132.0297
131.9506
131.8794
131.8618
131.7171
130.7144
128.5509
128.4346
125.8476
125.3754
125.3372
123.1093
121.2375
119.2311
116.9213
116.7085
116.1121

77.3305
77.0131
76.6955

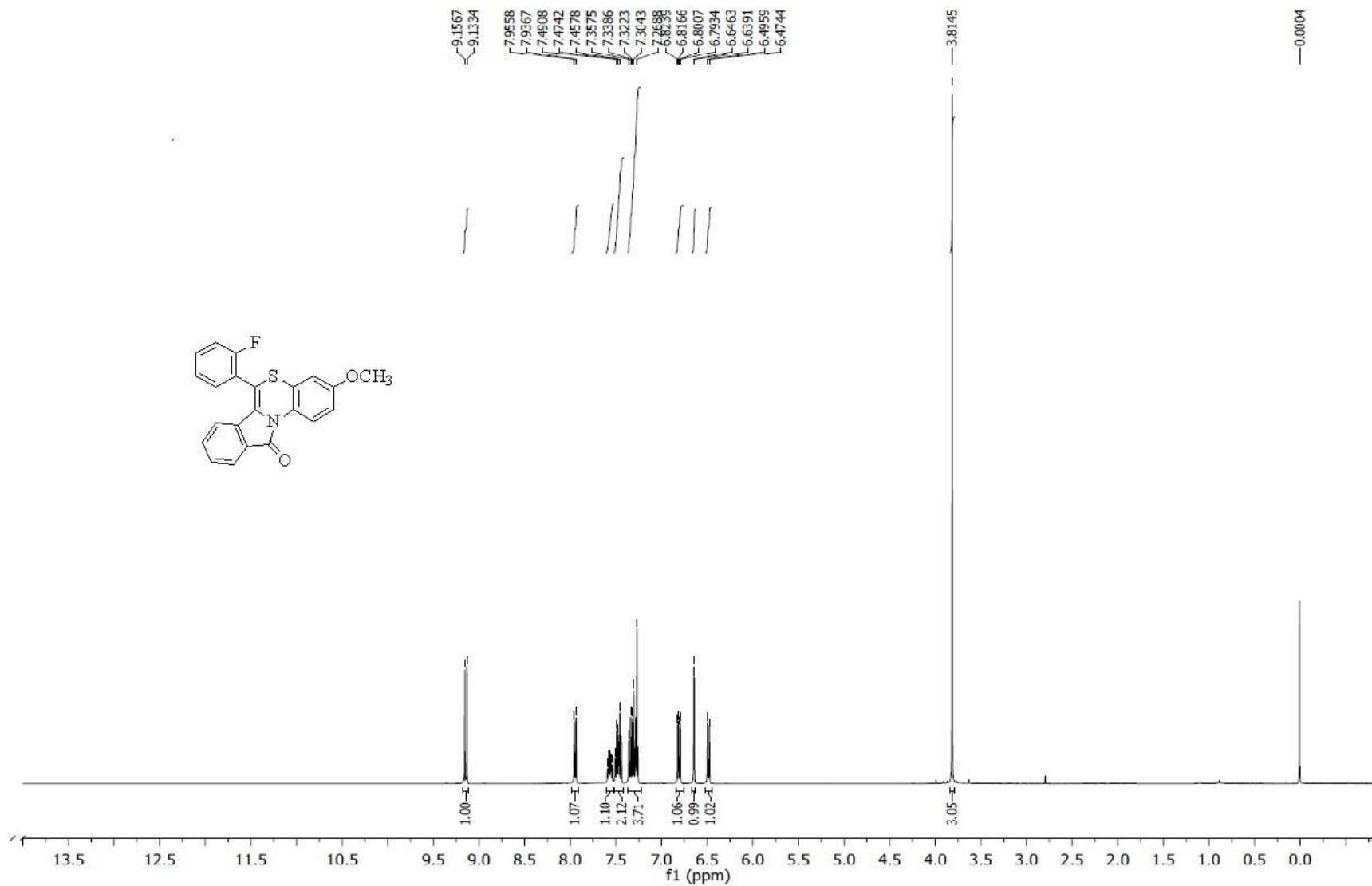
20.6495



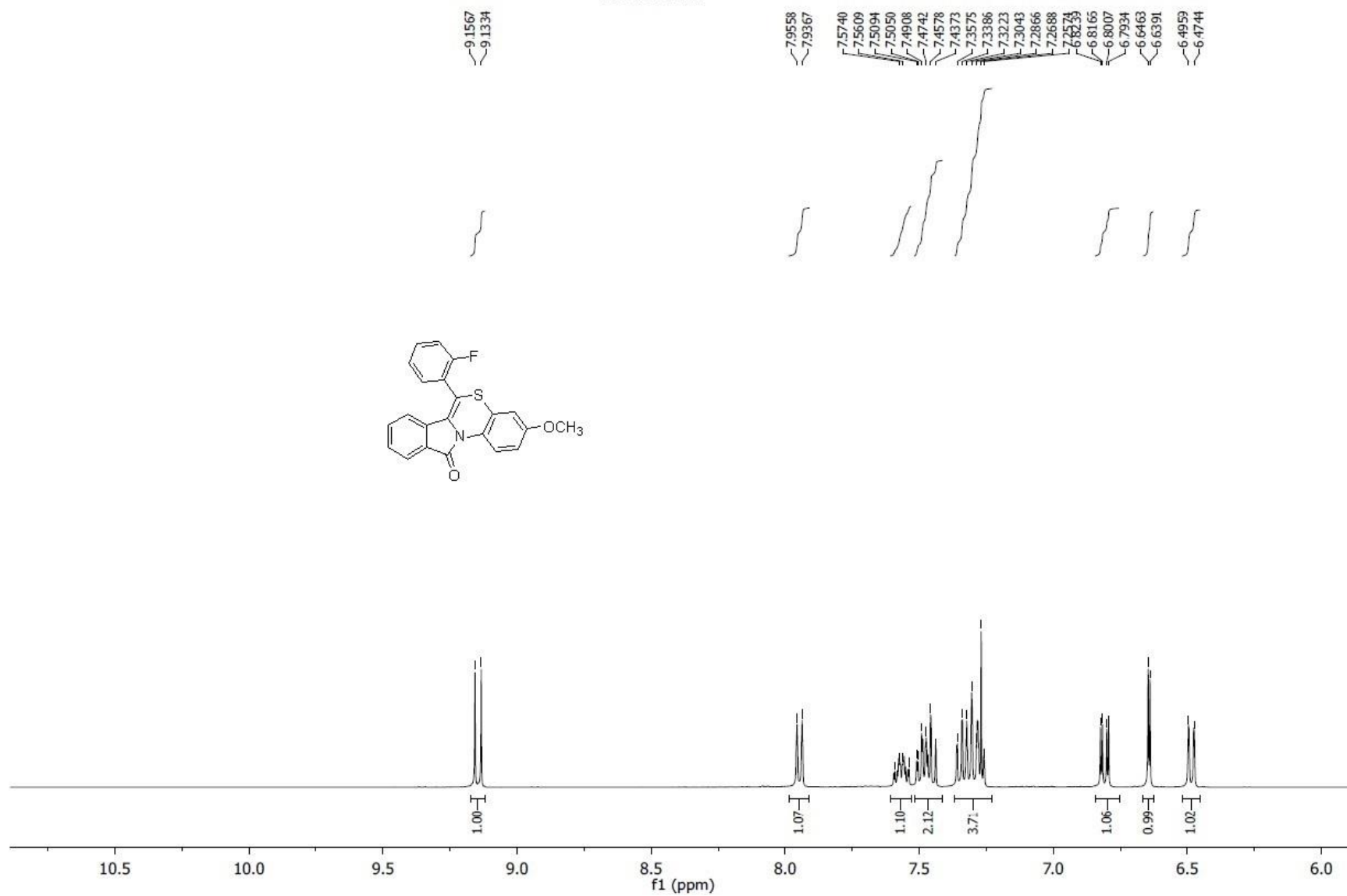
¹³C NMR of 5j



¹H NMR of 5k

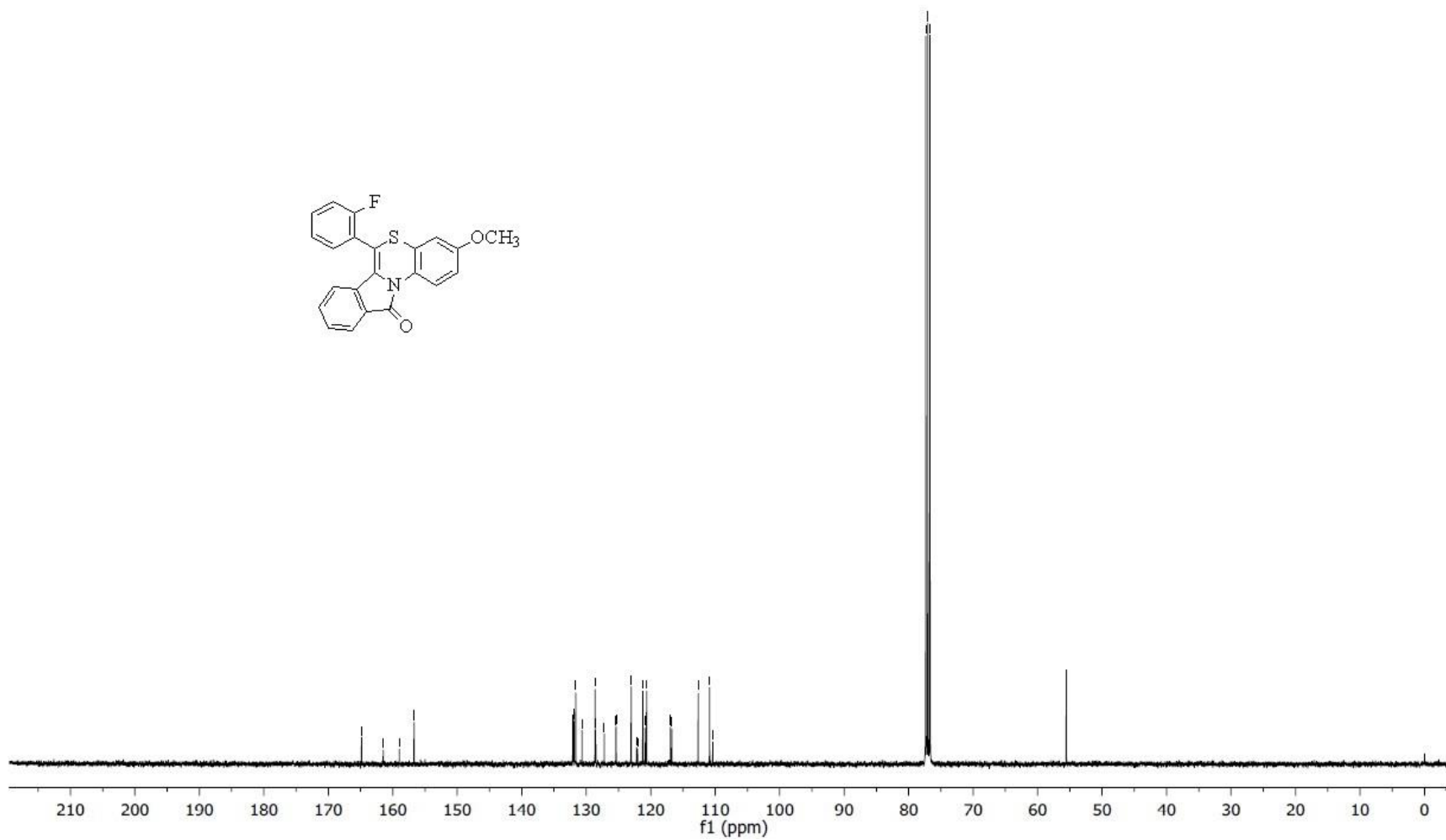
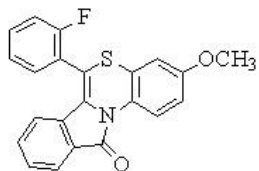


¹H NMR of 5k



¹³C NMR of 5k

- 164.8429
- 161.4620
- 158.9897
- 156.7016
- 132.0839
- 132.0041
- 131.9203
- 131.9024
- 131.6345
- 130.6540
- 128.6216
- 128.5819
- 128.4970
- 127.2032
- 125.3886
- 125.3510
- 123.0309
- 122.1927
- 122.0336
- 121.2311
- 120.8855
- 120.6409
- 116.9312
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- 112.6357
- 110.8661
- 110.3773
- 77.3350
- 77.0175
- 76.7000
- 55.5585



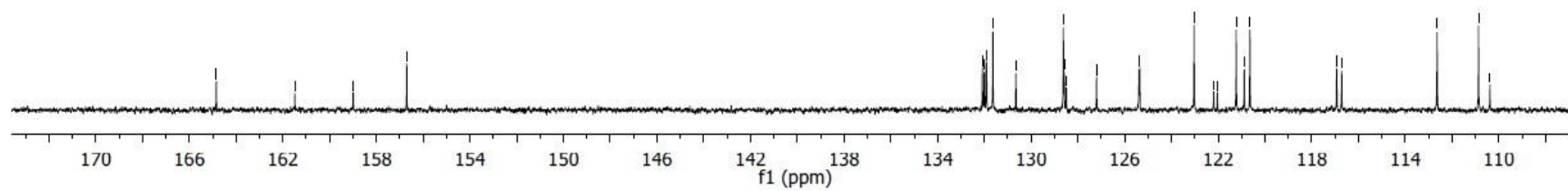
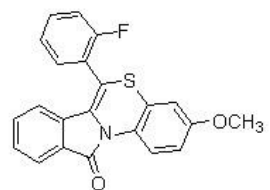
¹³C NMR of 5k

— 164.8429
— 161.4820
— 158.9897
— 156.7016

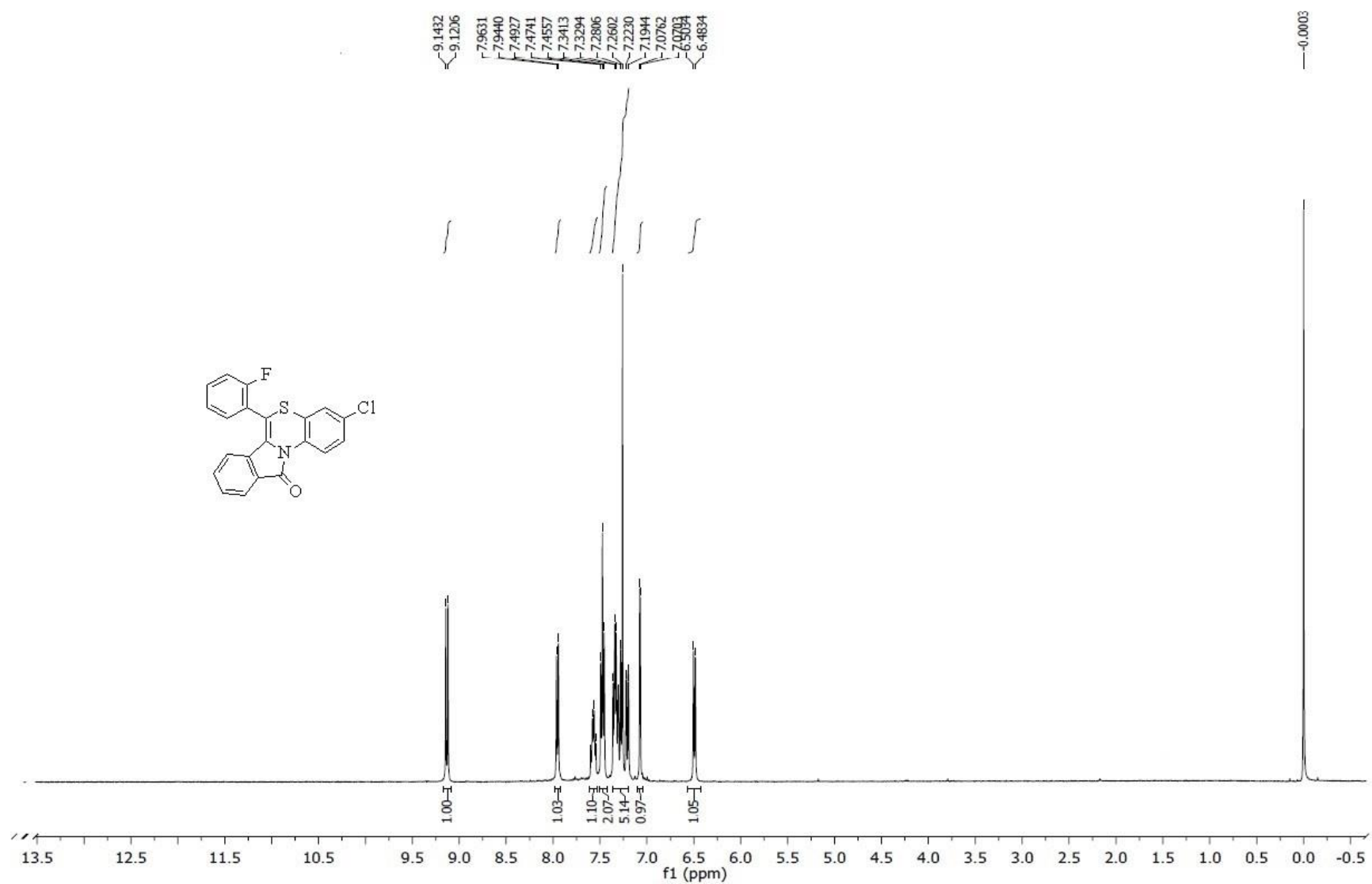
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132.0041
131.9203
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120.8855
120.6409

116.9312
116.7193

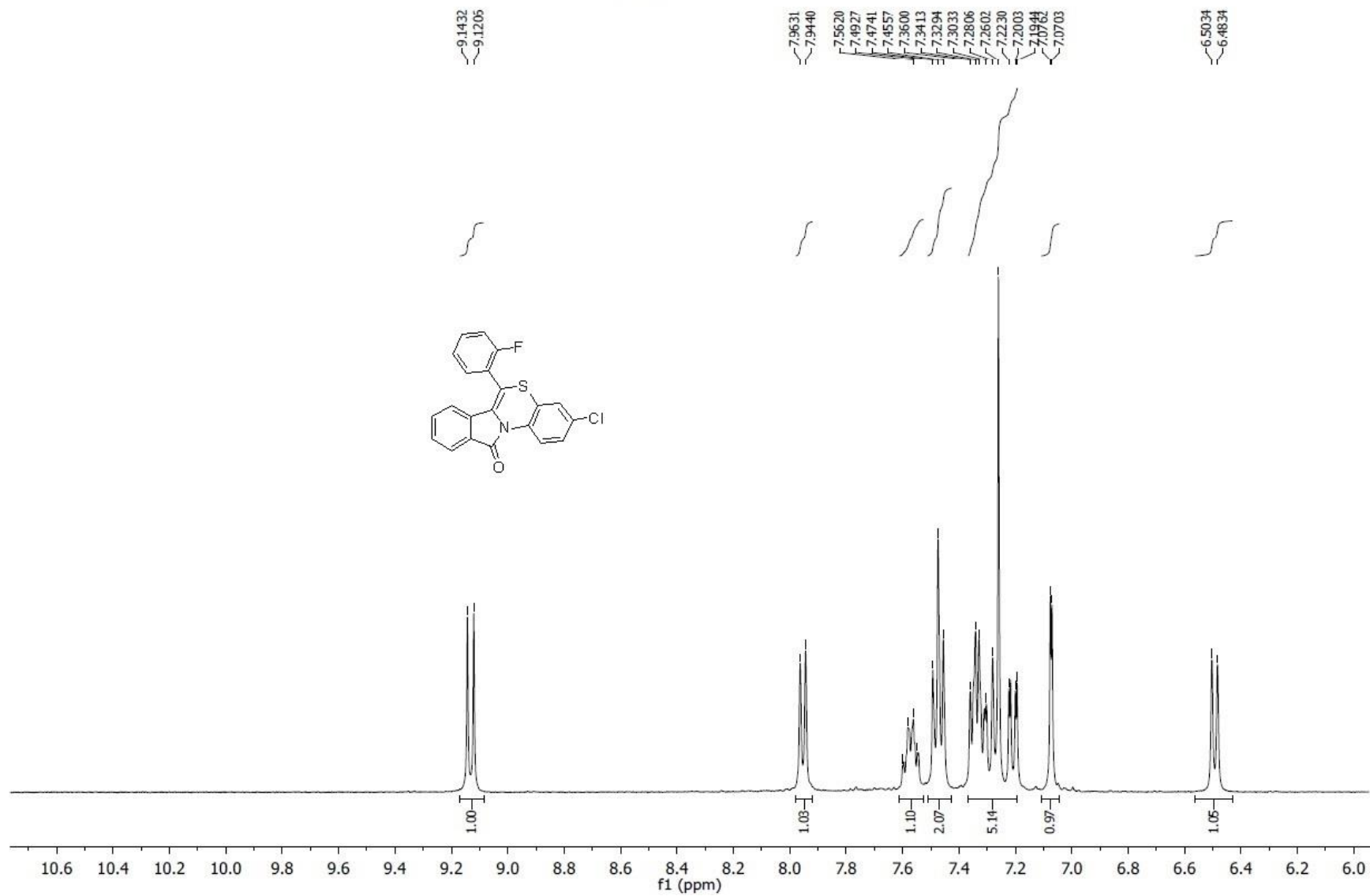
112.6357
110.8651
110.3773



¹H NMR of 51

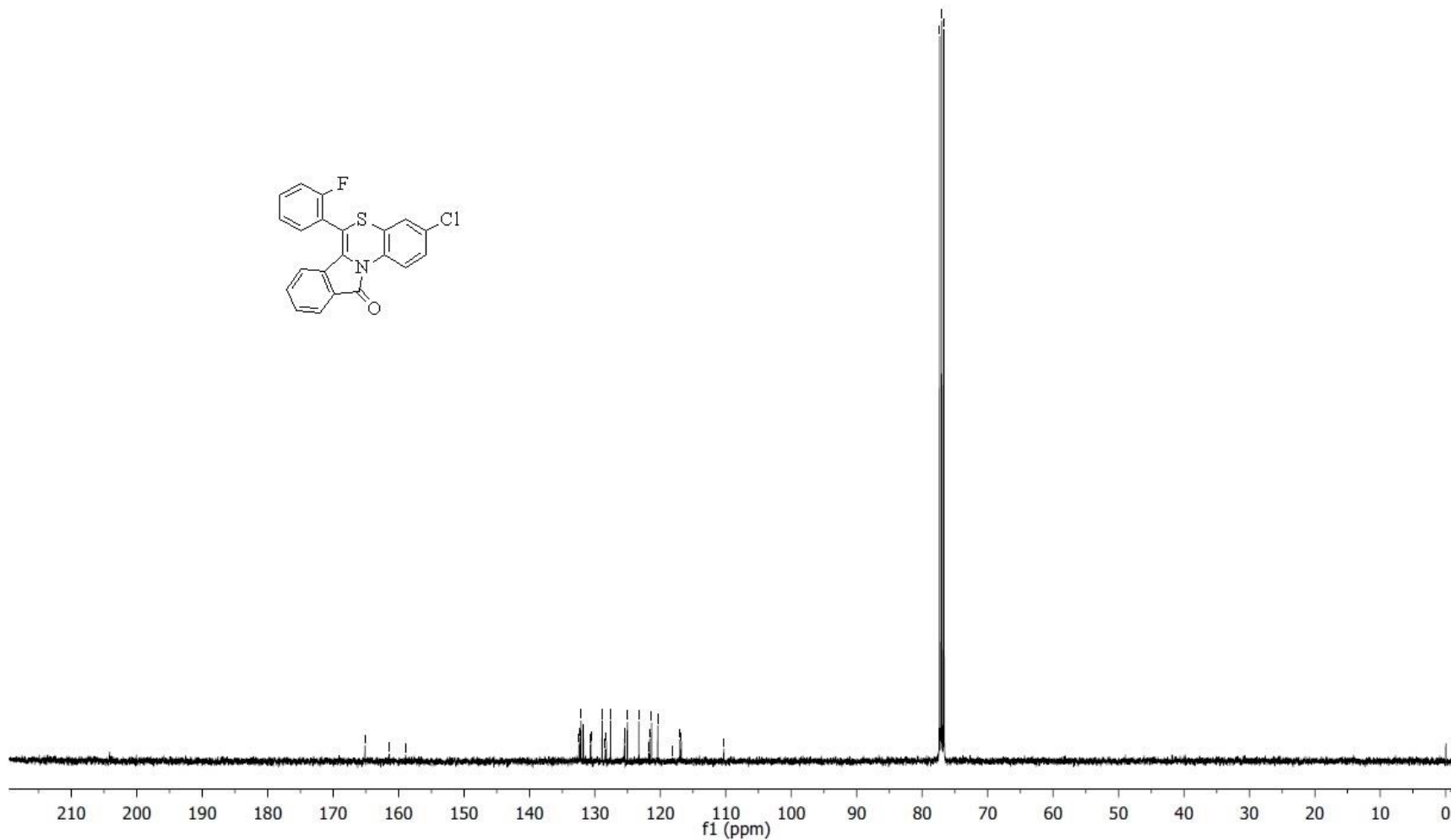


¹H NMR of 51



¹³C NMR of 51

165.1387
161.4187
158.9243
132.2517
132.2121
132.1144
131.7933
131.7760
130.6026
128.9009
128.2592
127.6137
125.4879
125.0381
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121.6604
121.3535
120.3865
117.0144
116.8032
77.3275
77.0100
76.6925

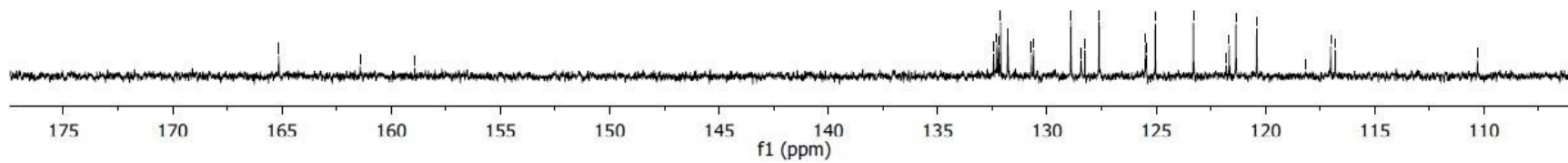
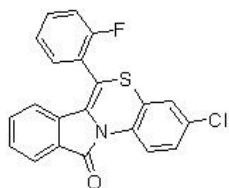


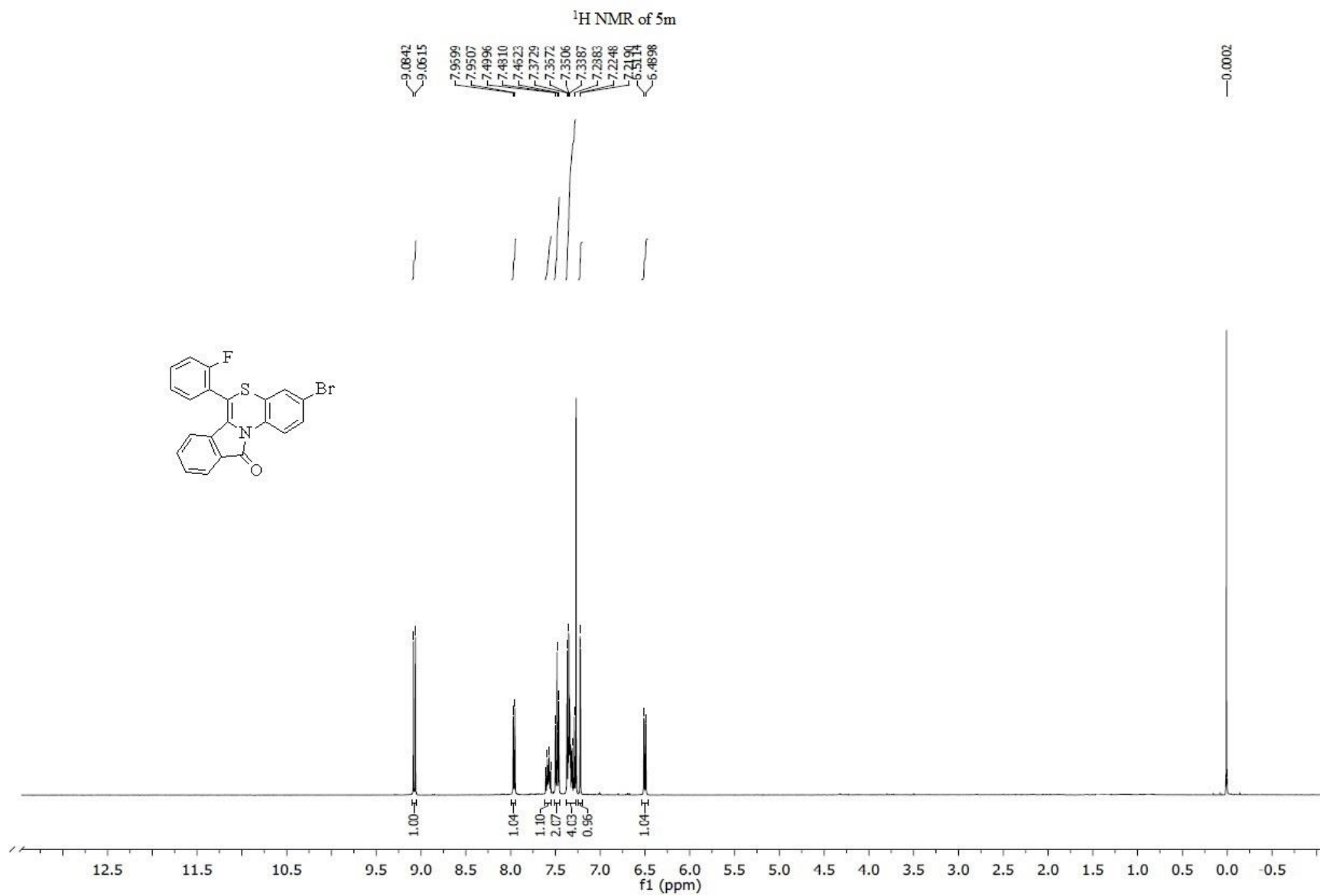
¹³C NMR of 51

— 165.1387
— 161.4187
— 158.9243

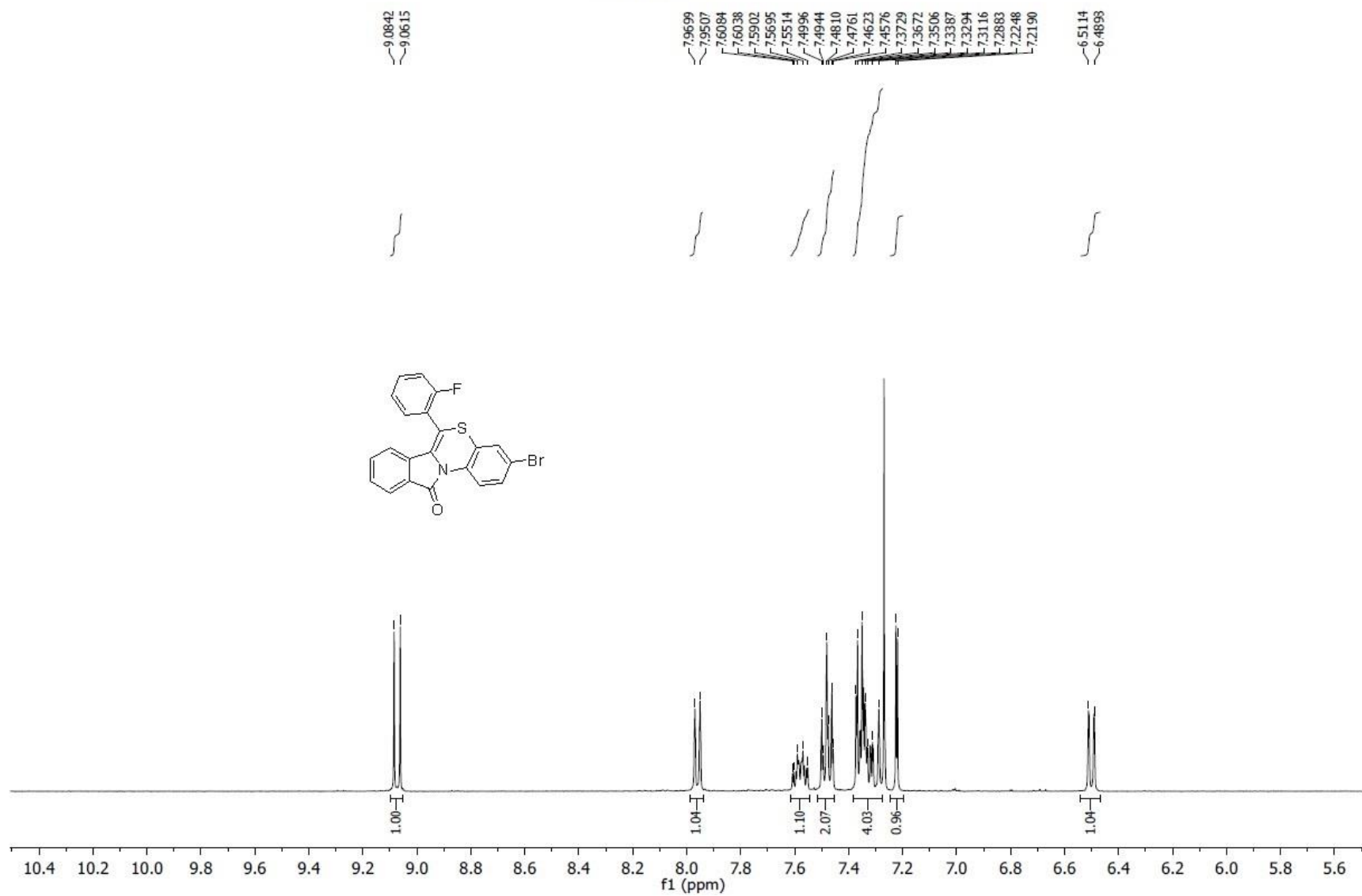
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127.6137
125.4879
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120.3965
118.1728
117.0144
116.8032

— 110.3015



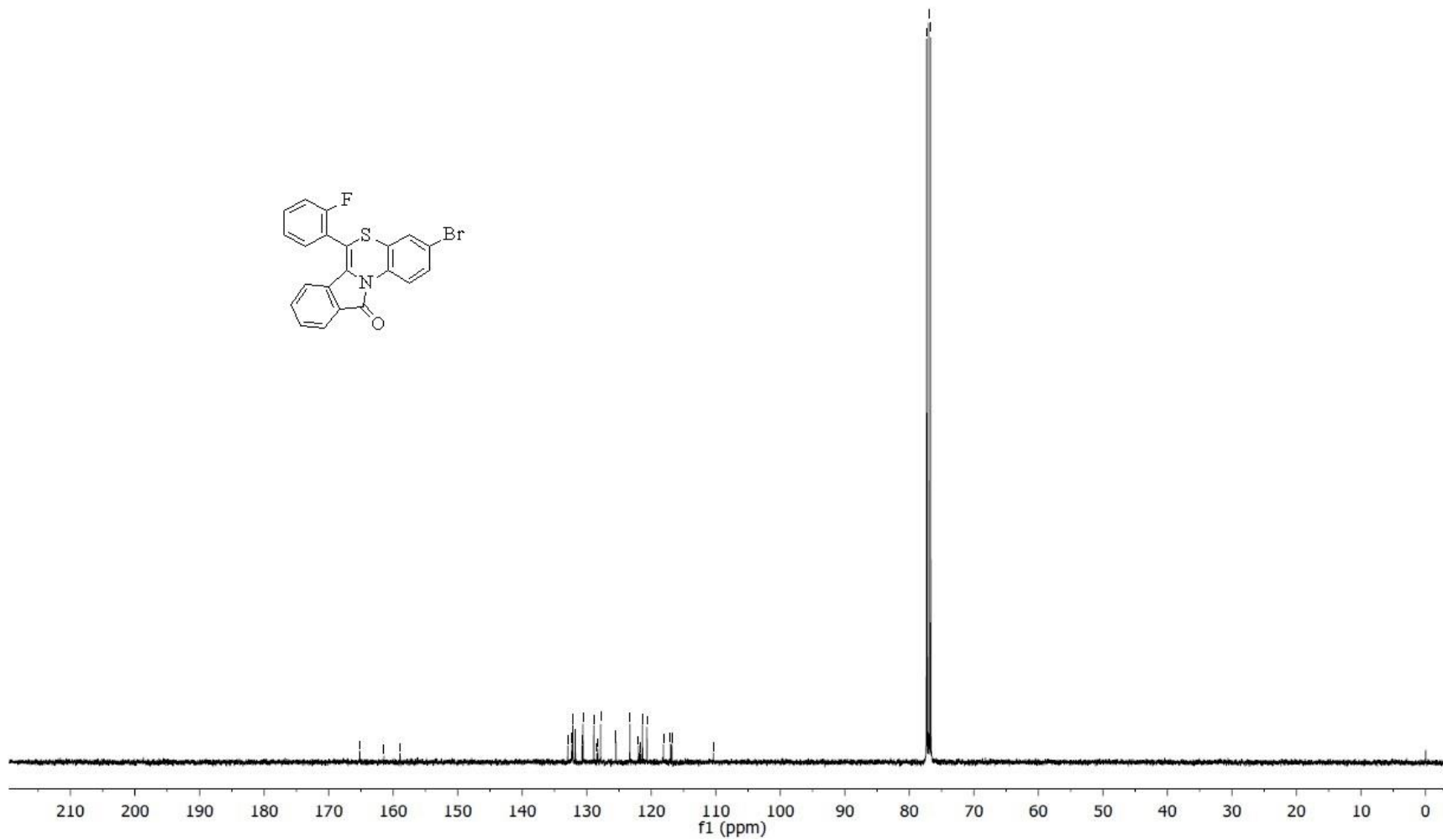
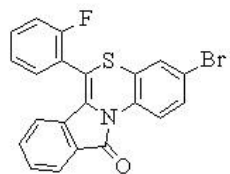


¹H NMR of 5m



¹³C NMR of 5m

165.1528
161.4092
158.9137
132.2979
132.2178
132.1365
131.7831
131.7648
130.7129
130.5715
128.9084
127.8274
125.4929
125.4588
123.3013
121.3570
120.6634
118.1043
117.0185
116.8937
77.3304
77.0129
76.6954



¹³C NMR of 5m

—165.1528

—161.4092

—158.9137

132.9366

132.2979

132.2178

132.1365

131.7831

131.7648

130.7129

130.5715

128.9064

128.4115

128.2609

127.8274

125.4929

125.4558

123.3013

121.9742

121.7802

121.6209

121.3570

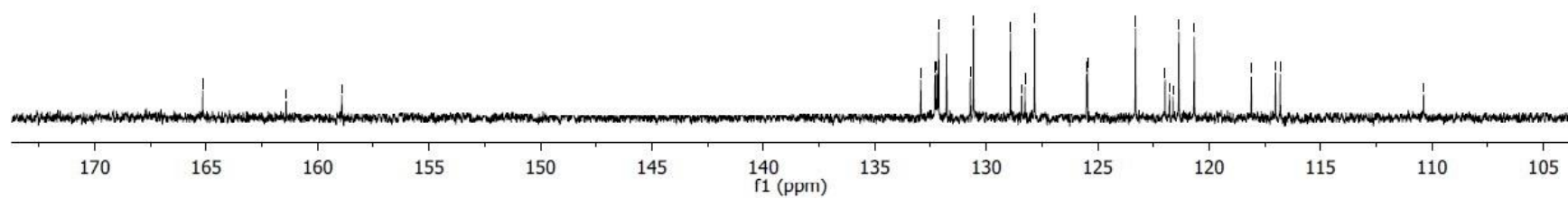
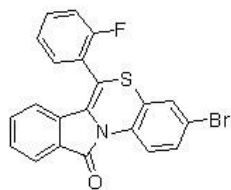
120.6634

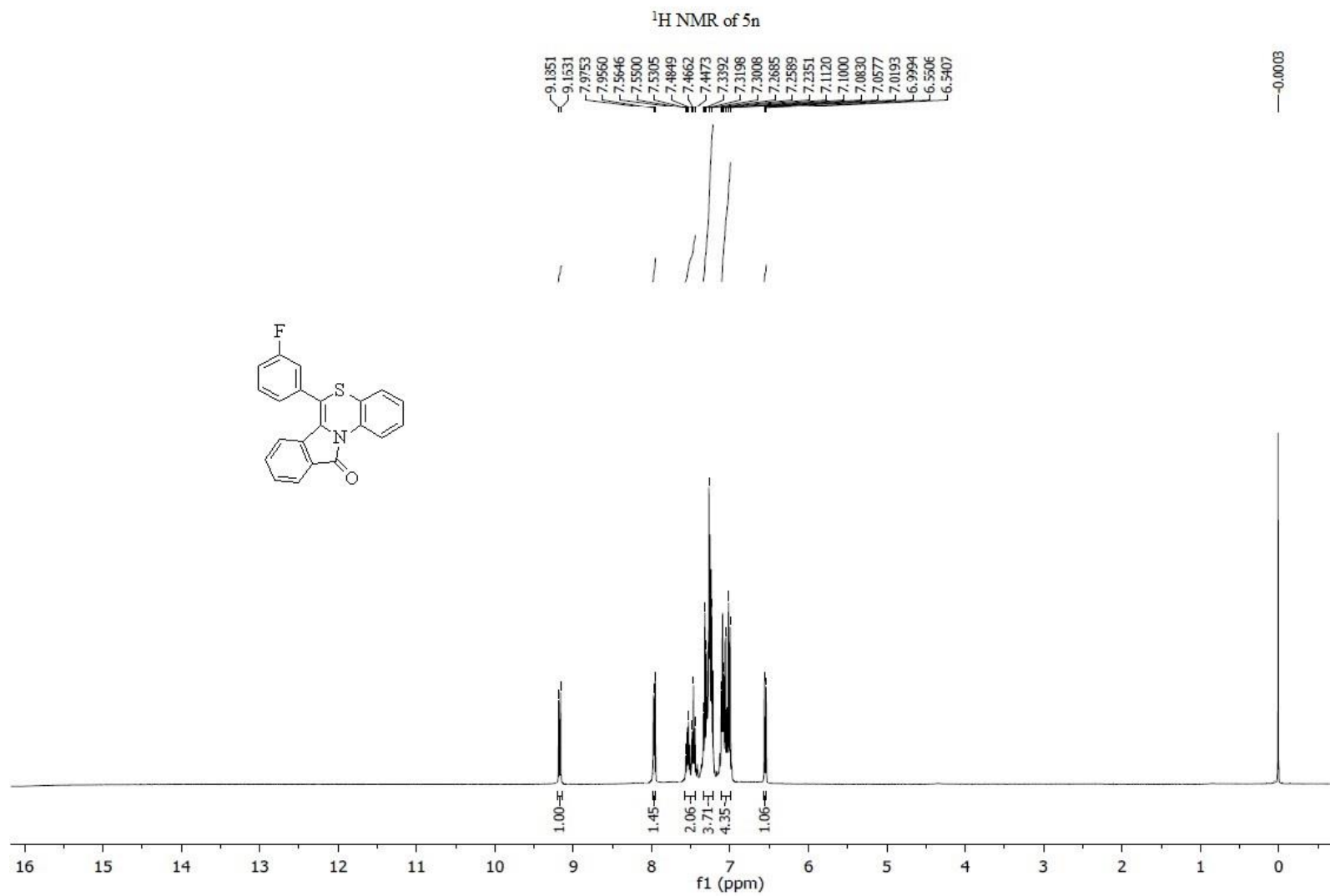
118.1043

117.0185

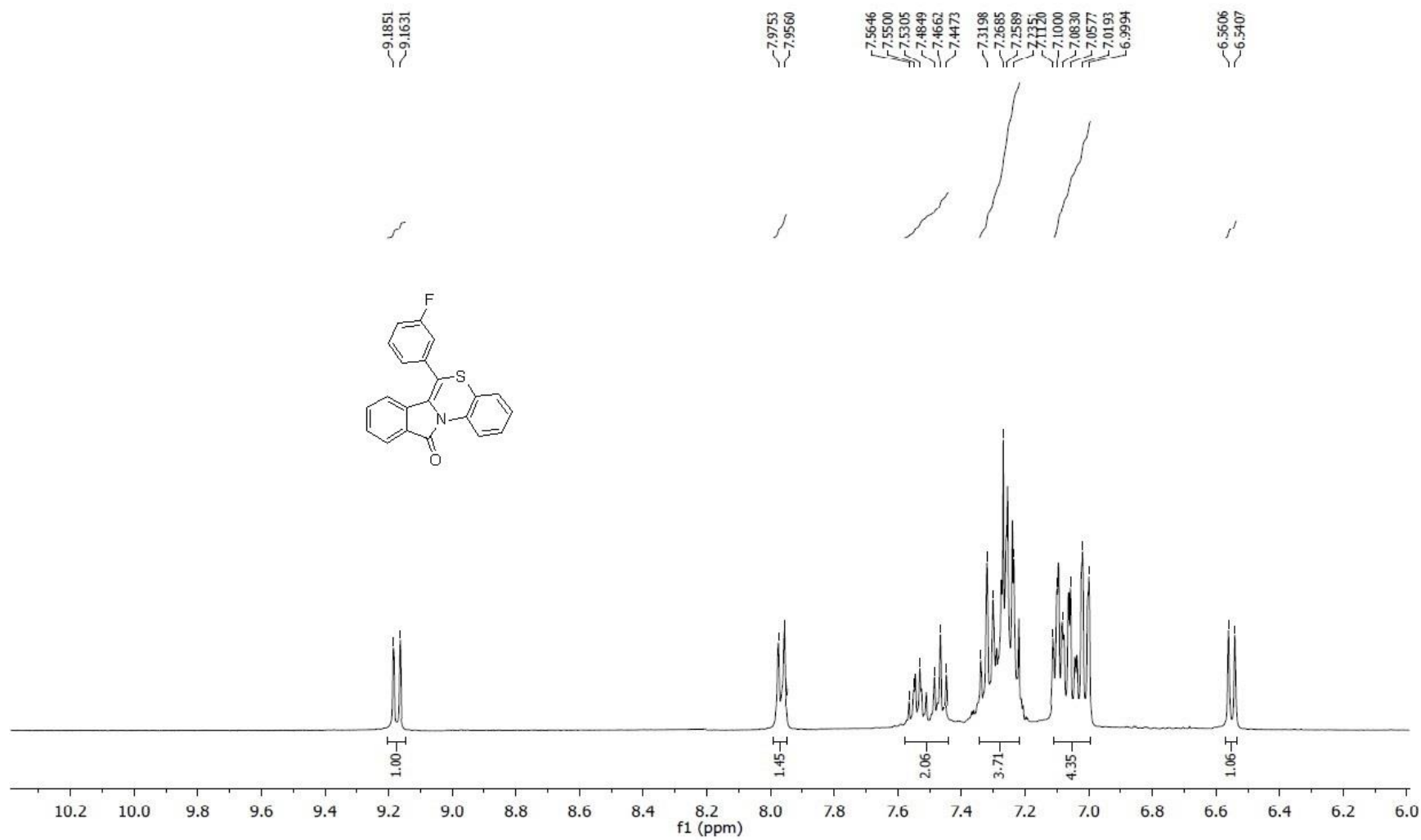
116.8077

—110.3737





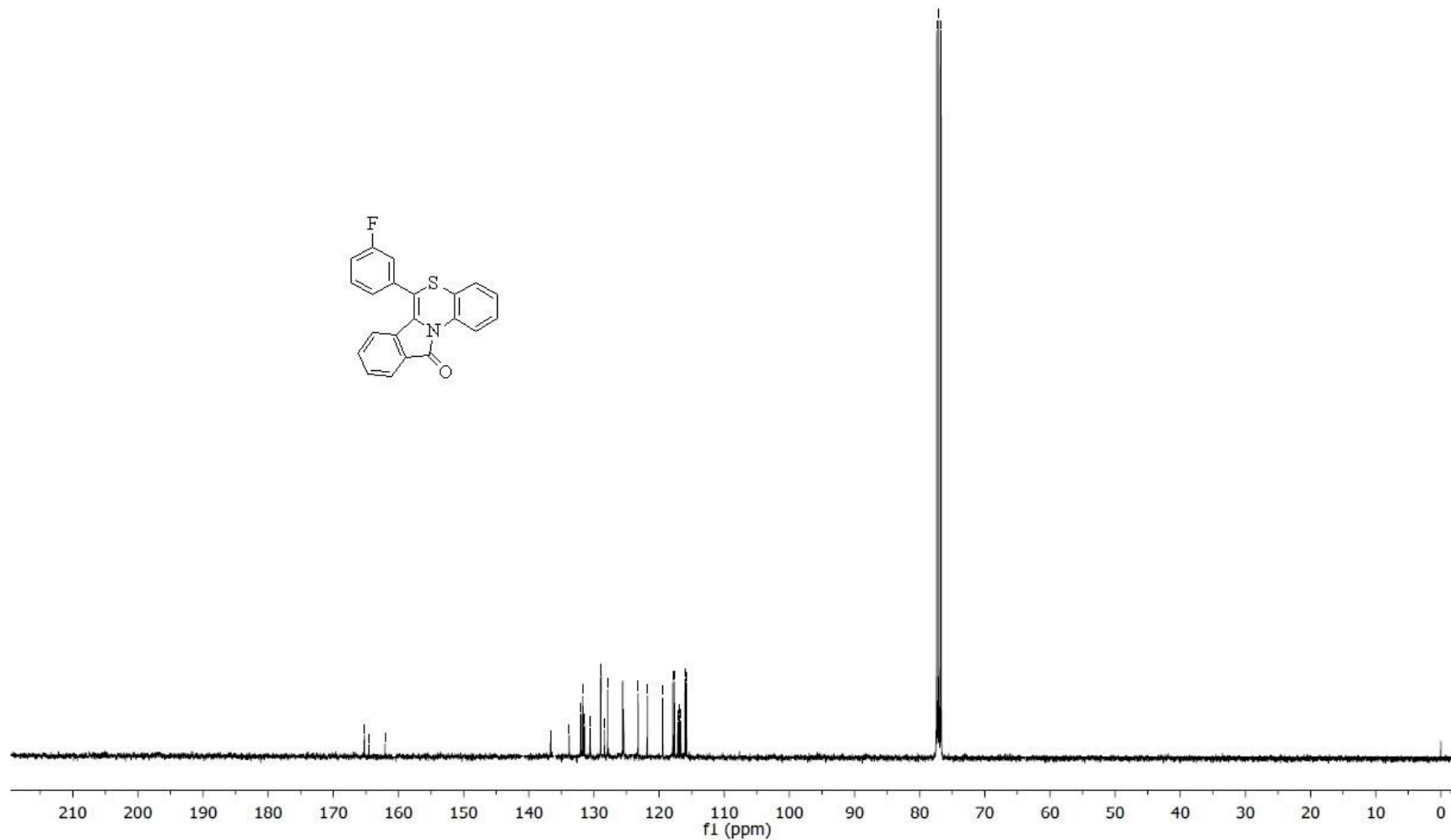
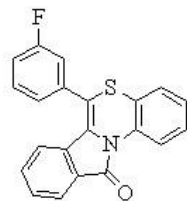
¹H NMR of 5n



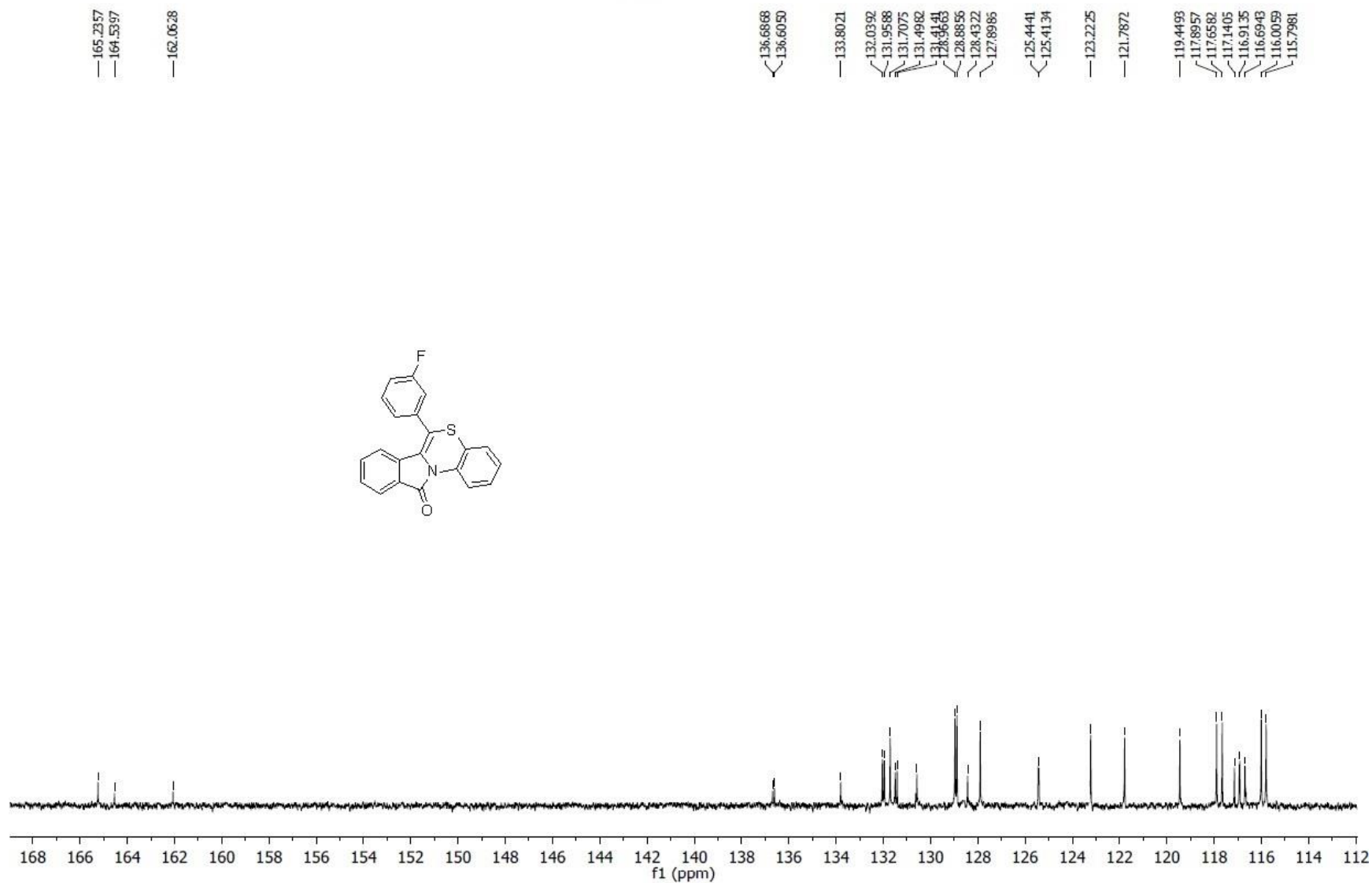
¹³C NMR of 5n

165.2357
164.5397
162.0628
136.6868
136.6050
133.8021
132.0392
131.9588
131.7075
131.4982
131.4141
130.5814
128.9663
128.8856
128.4322
127.8986
125.4441
125.4134
123.2225
121.7872
119.4493
117.8957
117.6582
117.1405
116.9135
116.6943
116.0059
115.7961

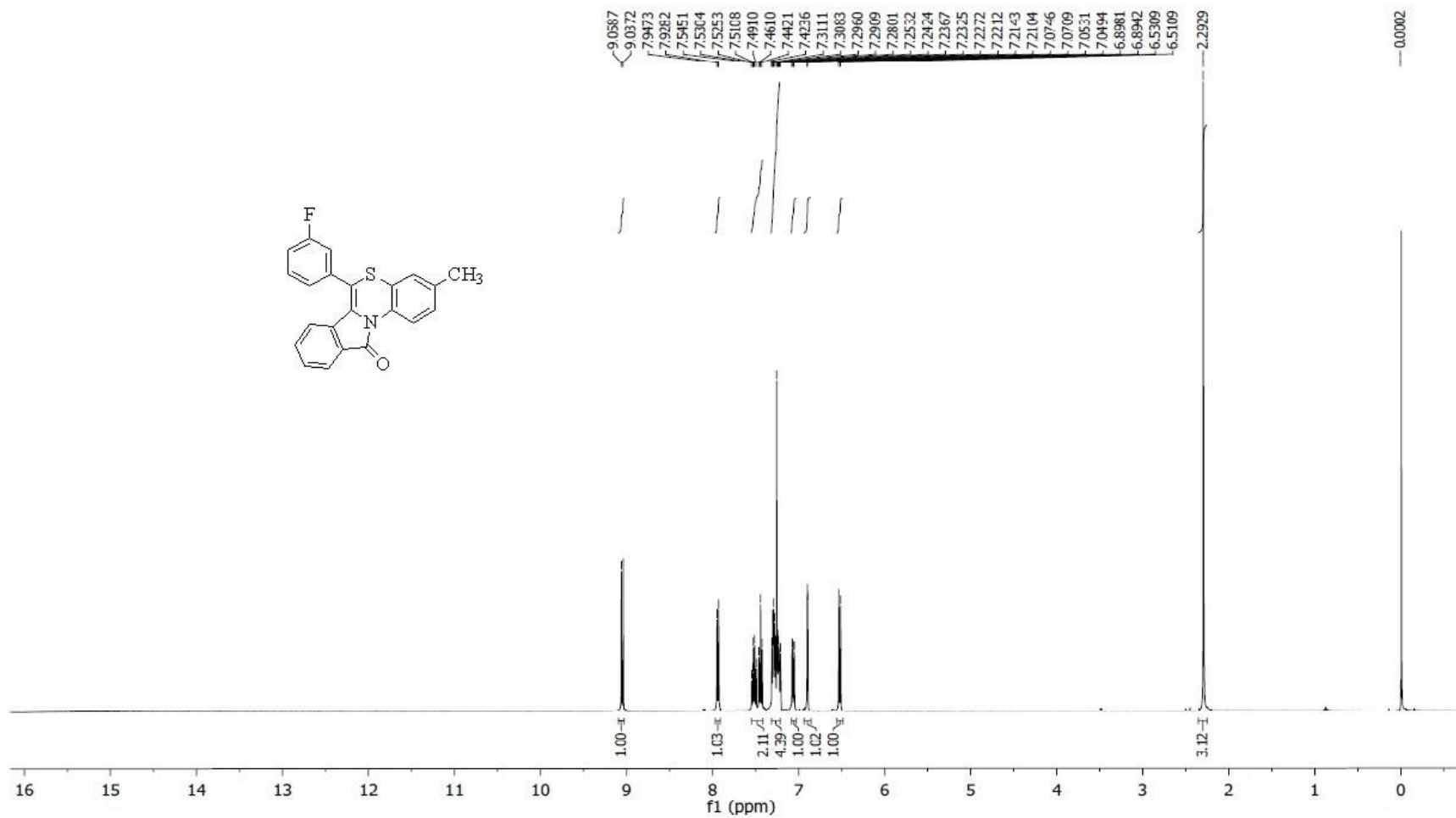
77.3643
77.0457
76.7290



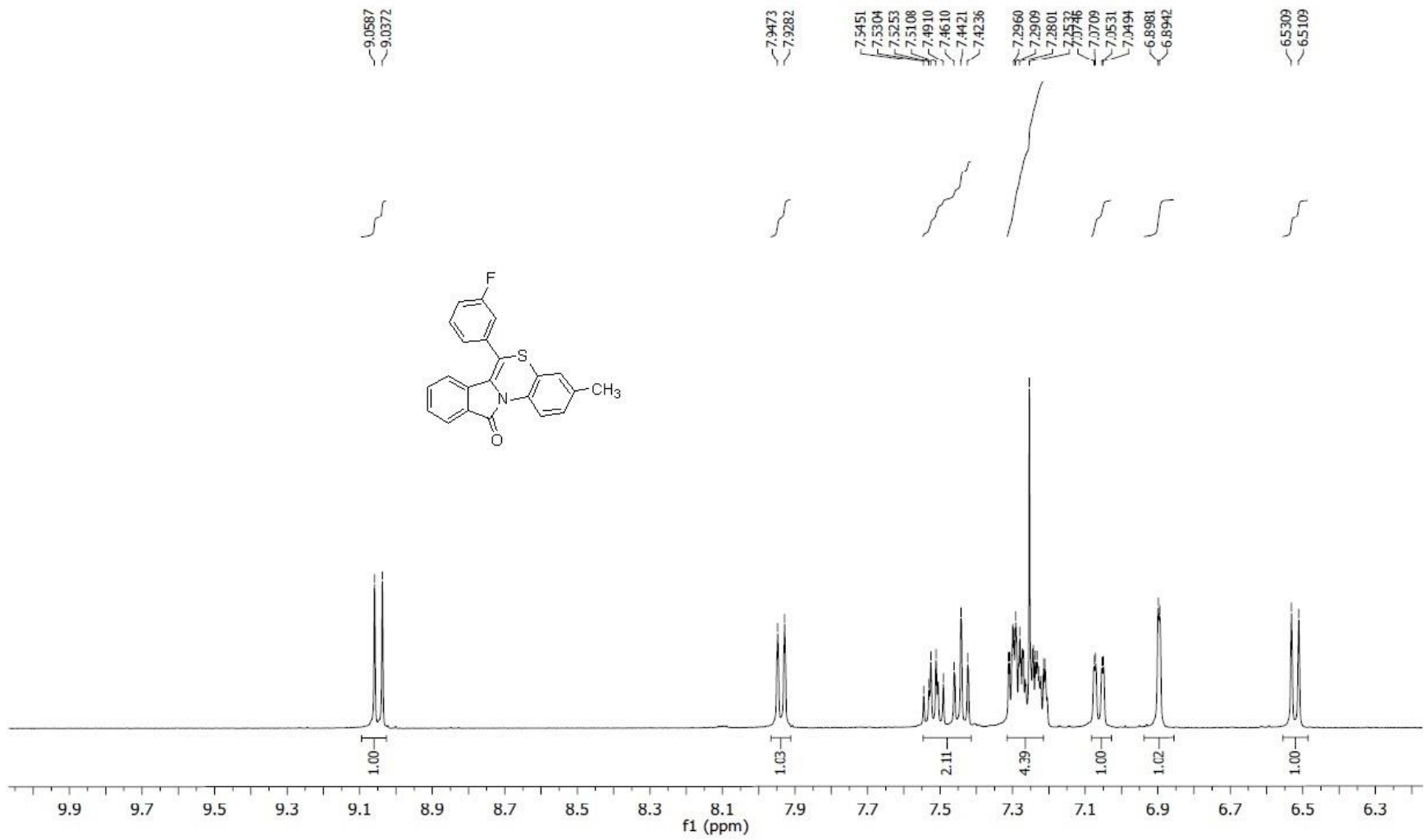
¹³C NMR of 5n



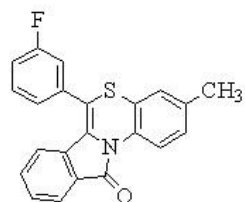
¹H NMR of 5o



¹H NMR of 5o



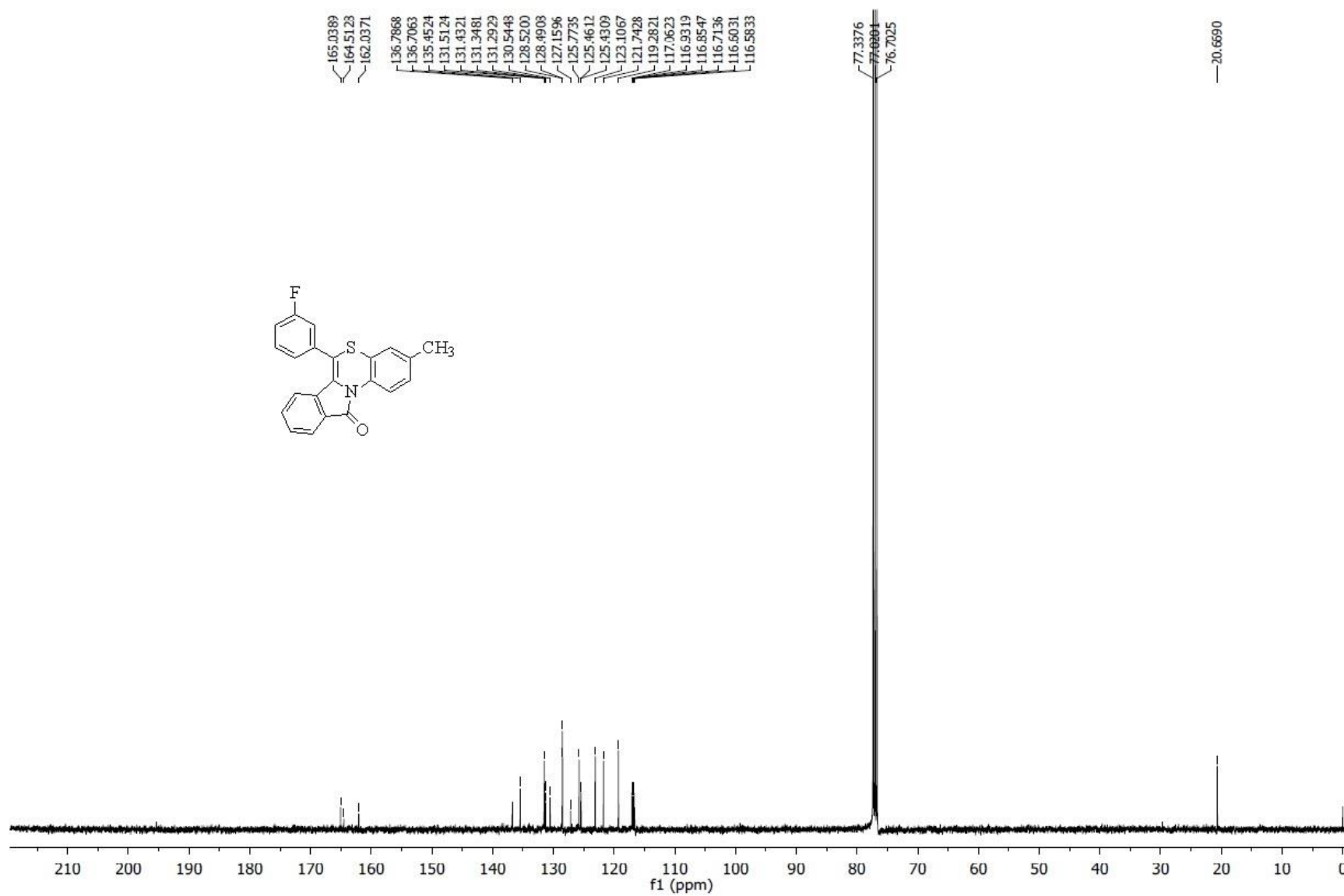
¹³C NMR of 5o



165.0389
164.5123
162.0371
136.7868
136.7063
135.4524
131.5124
131.4321
131.3481
131.2929
130.5448
128.5200
128.4903
127.1596
125.7735
125.4612
125.4309
123.1067
121.7428
119.2821
117.9623
116.9319
116.8547
116.7136
116.6031
116.5833

77.3376
77.0001
76.7025

20.6690



¹³C NMR of 5o

165.0389
164.5123

162.0371

136.7868
136.7063
135.4524

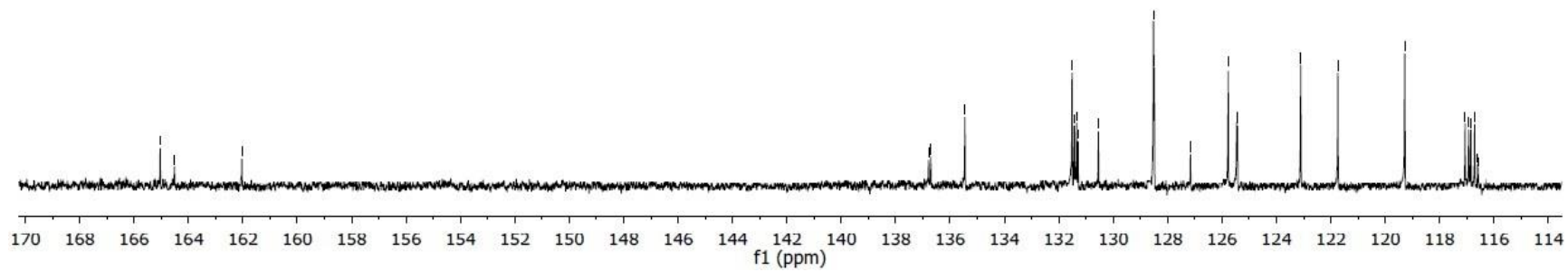
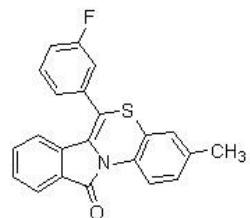
131.5124
131.4321
131.3481
131.2929
130.5448

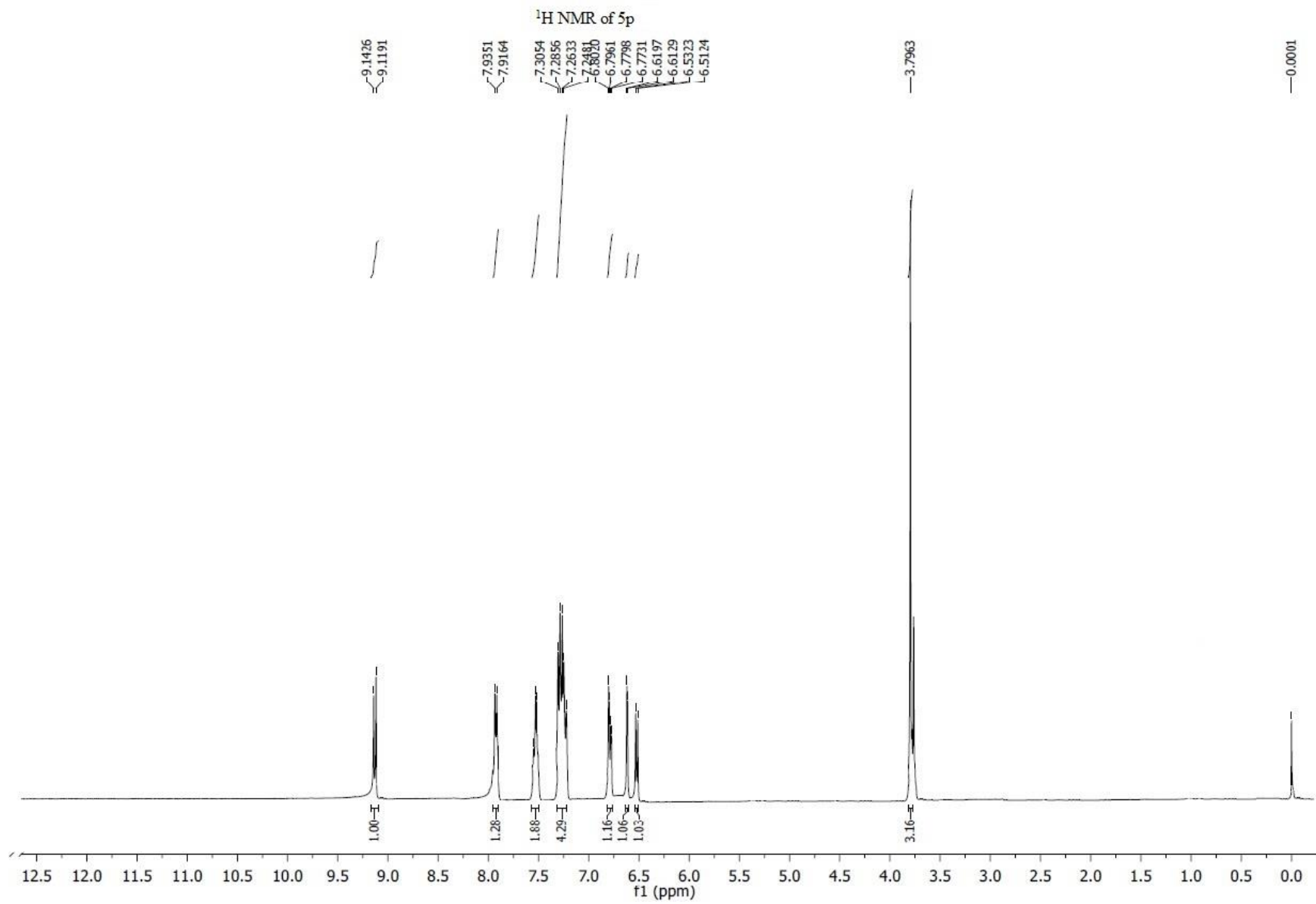
128.5200
128.4908
127.1596

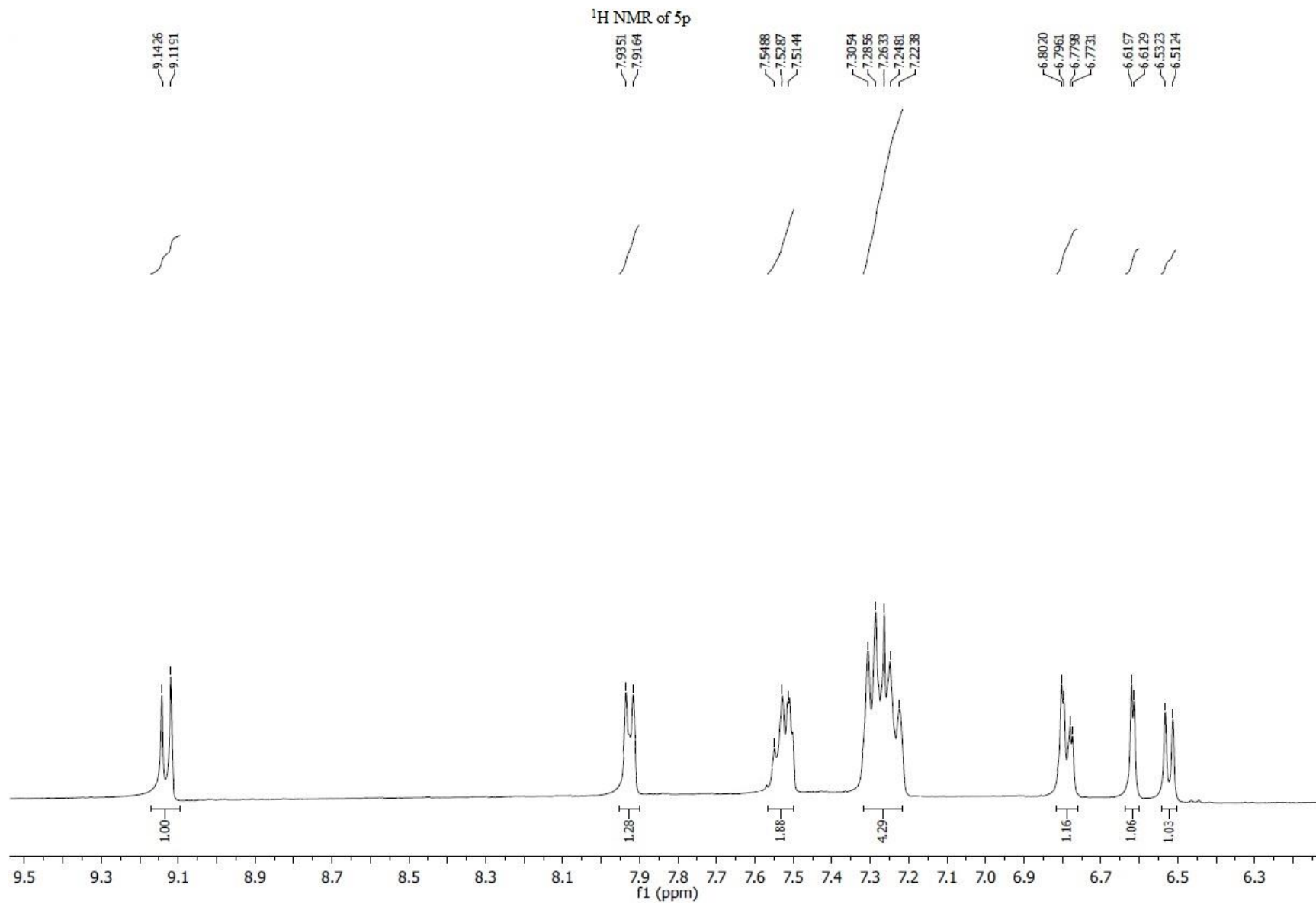
125.7735
125.4612
125.4309

123.1067
121.7428

119.2821
117.0623
116.9319
116.8547
116.7136
116.6031
116.5833

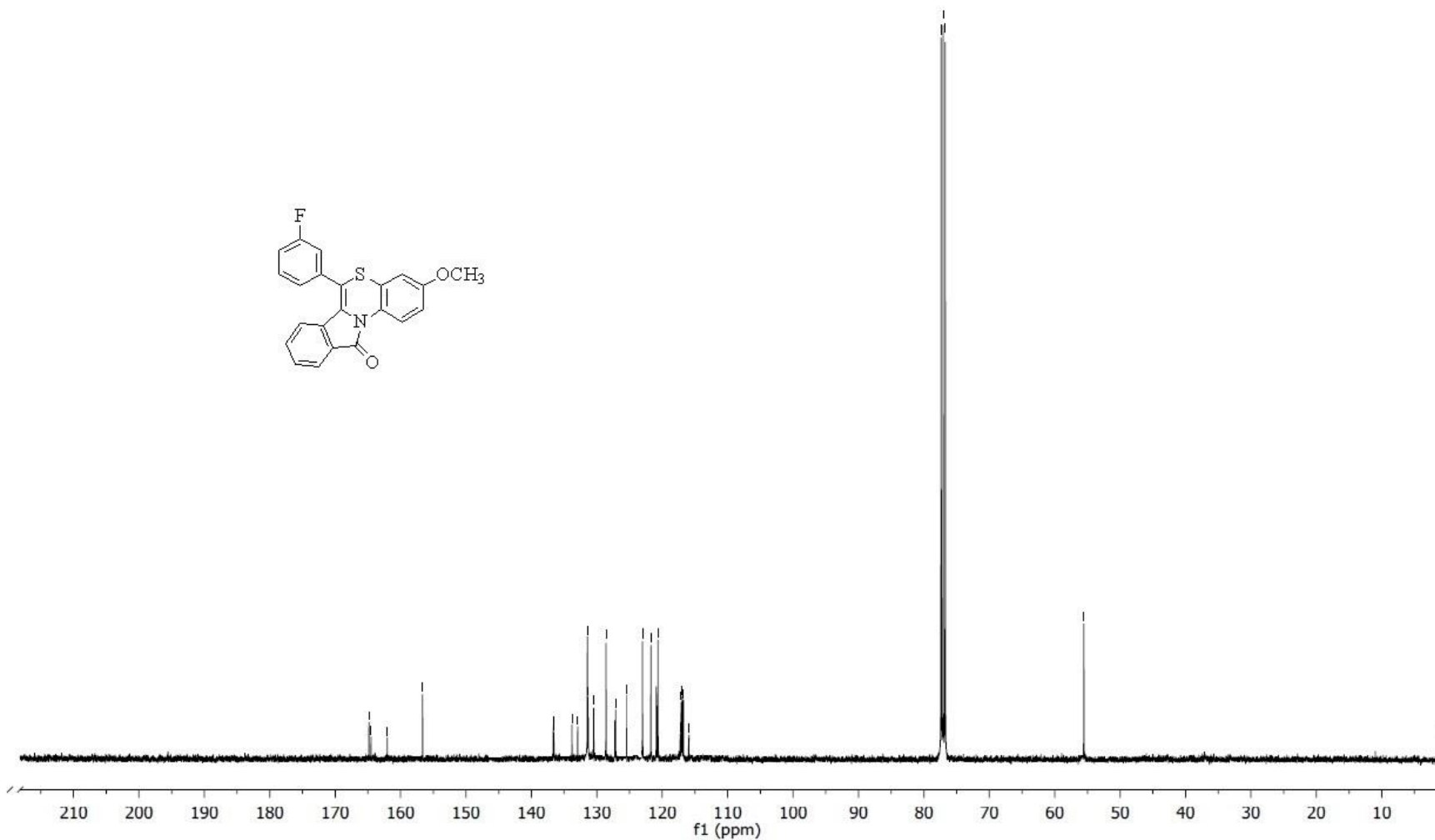
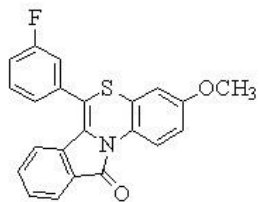






¹³C NMR of 5p

164.8395
164.5171
162.0389
156.6333
136.6491
136.5695
133.7939
132.9225
131.4389
131.3764
131.2993
130.4703
129.9663
129.8854
128.5823
127.1183
125.5163
125.4863
123.0229
121.7398
120.6477
117.2526
117.1212
116.9753
116.9135
116.7567
115.8910
77.3740
77.0563
76.7386
55.5502



¹³C NMR of 5p

164.8395
164.5171

162.0389

156.6333

136.6491
136.5696

133.7939

132.9126

131.4389

131.3764

131.2993

130.4708

129.9668

129.8854

128.5823

127.1183

125.168

125.4863

123.0229

121.7398

120.6477

117.2526

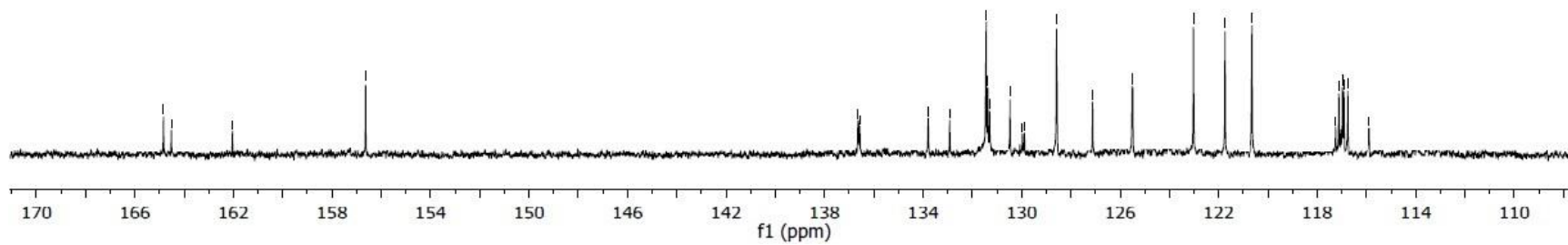
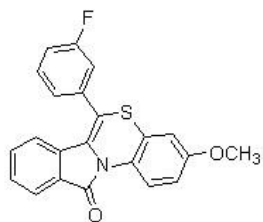
117.1212

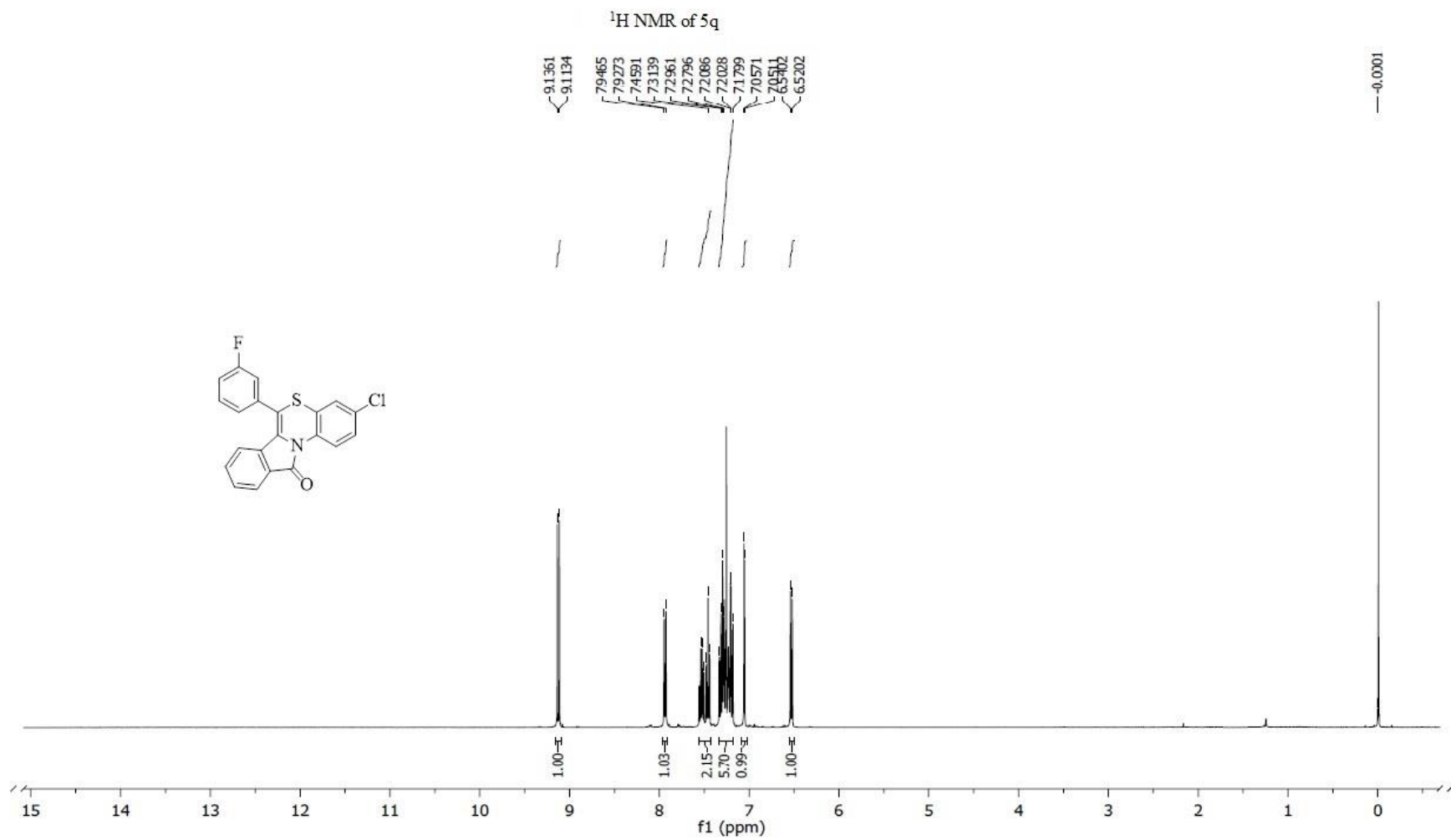
116.9753

116.9135

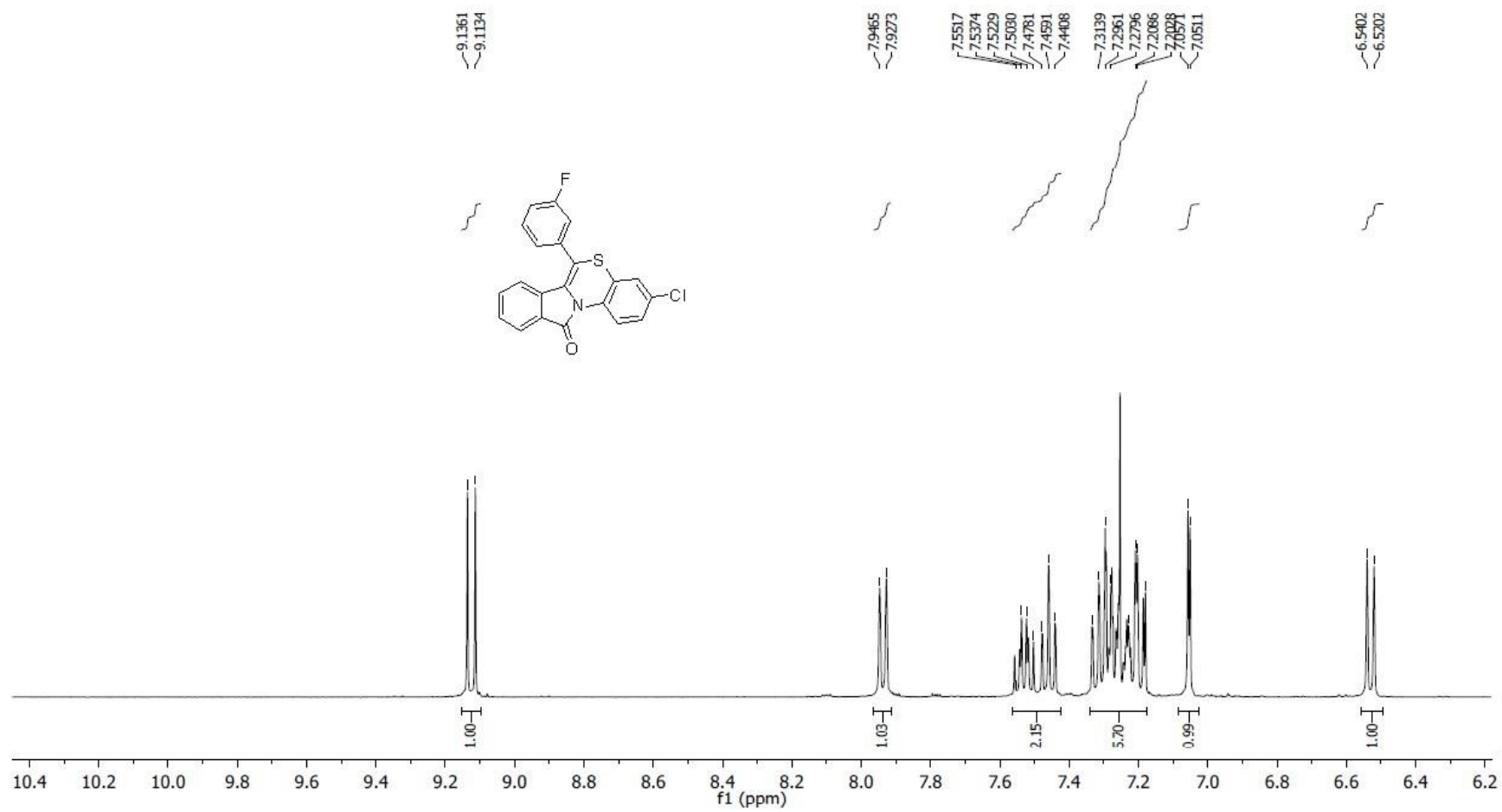
116.7367

115.8910

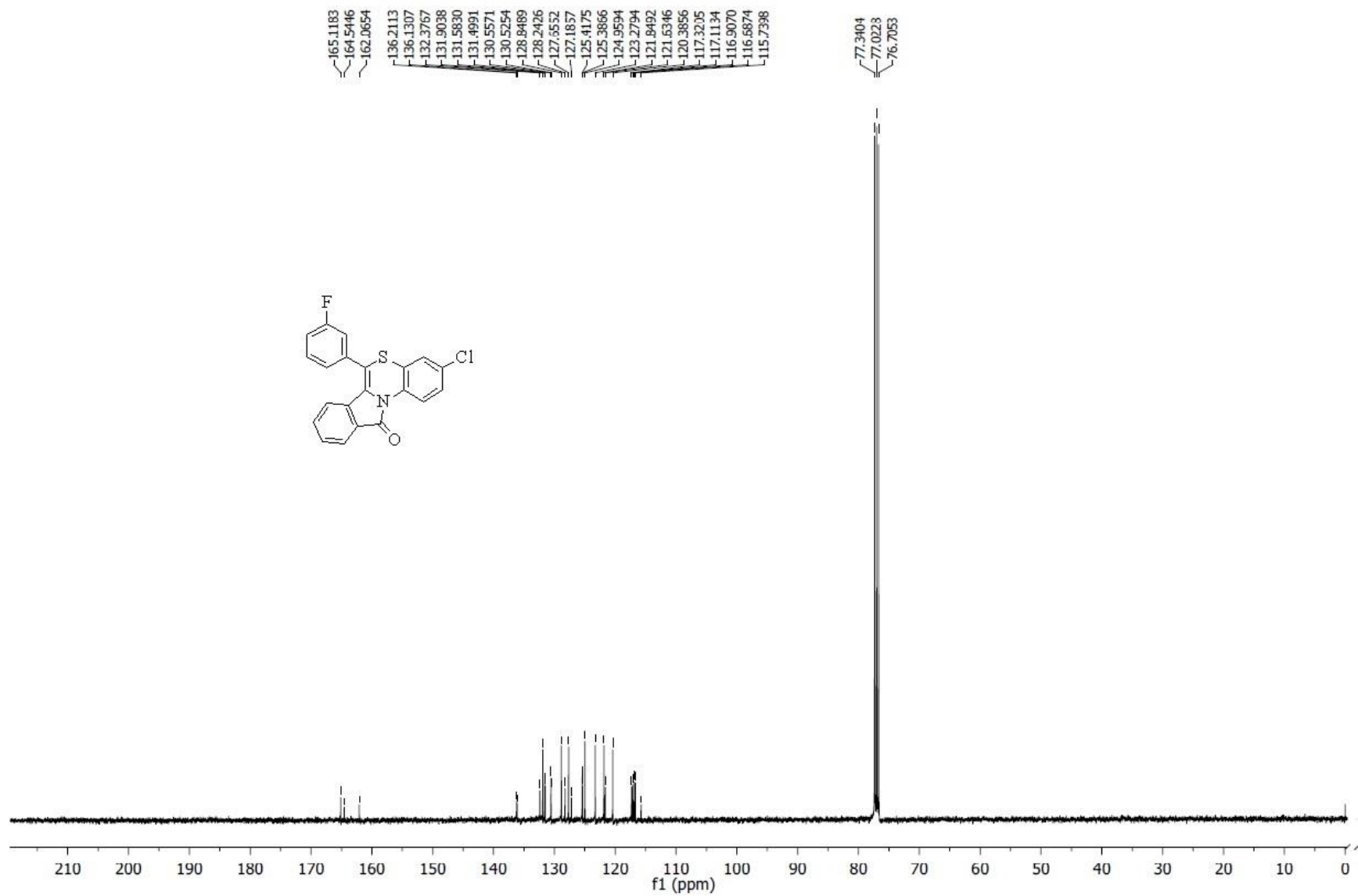




¹H NMR of 5q



¹³C NMR of 5q



¹³C NMR of 5q

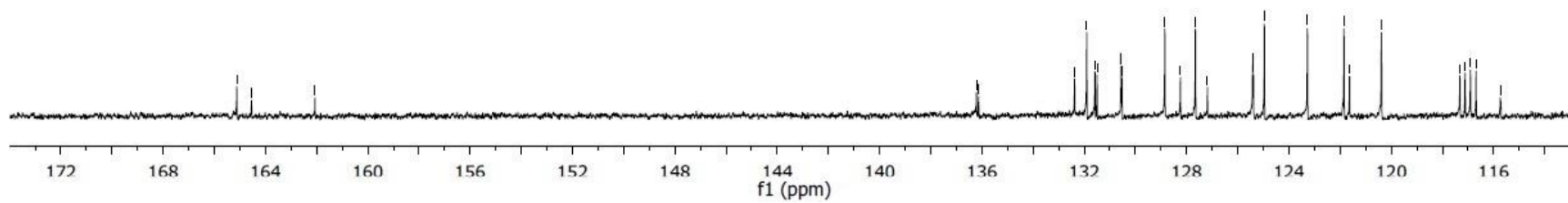
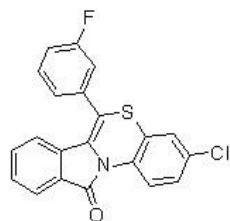
165.1183
164.5446
162.0654

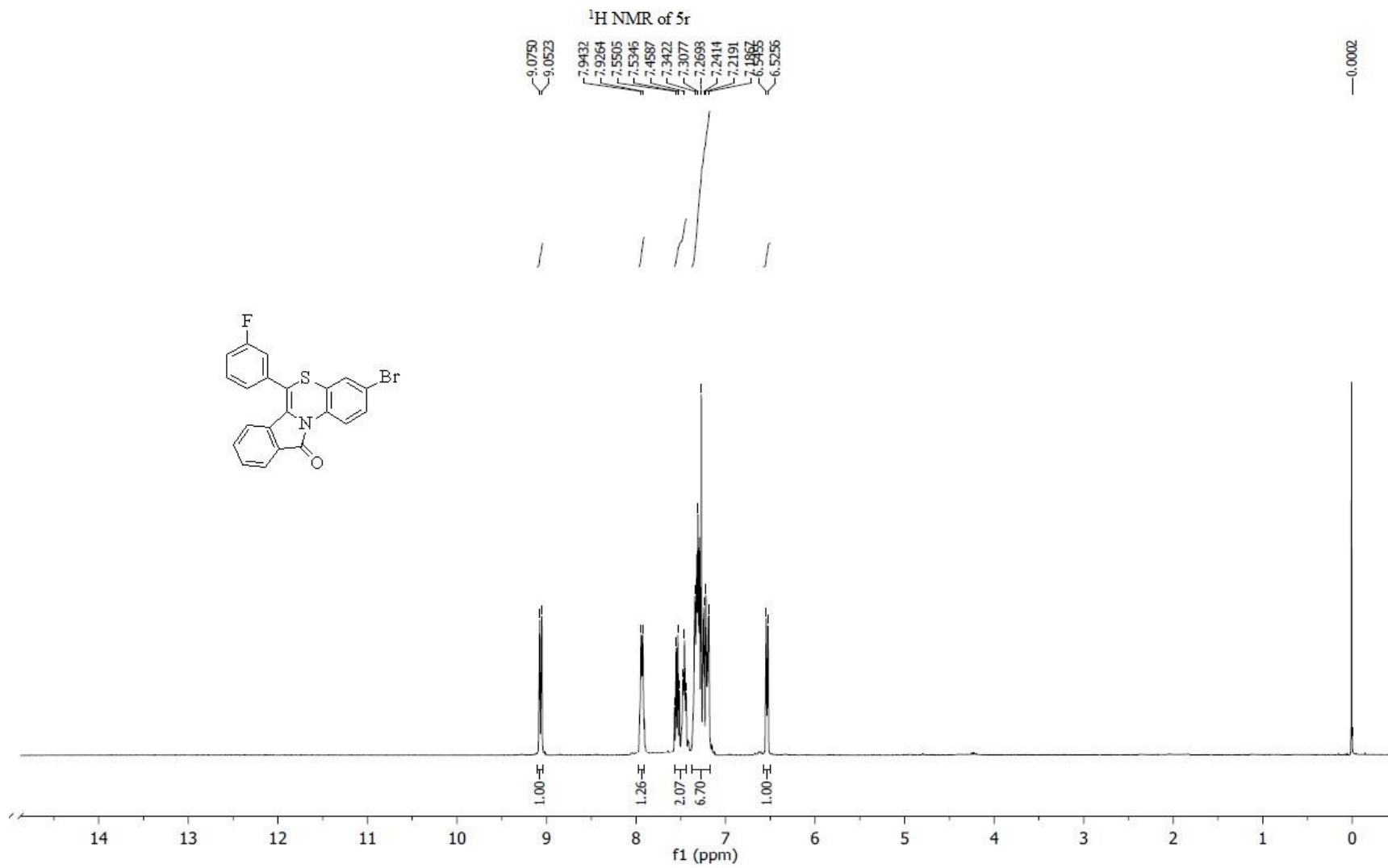
136.2113
136.1307

132.3767
131.9038
131.5830
131.4491
130.5571
130.5254
128.8489
128.2426
127.6552
127.1857

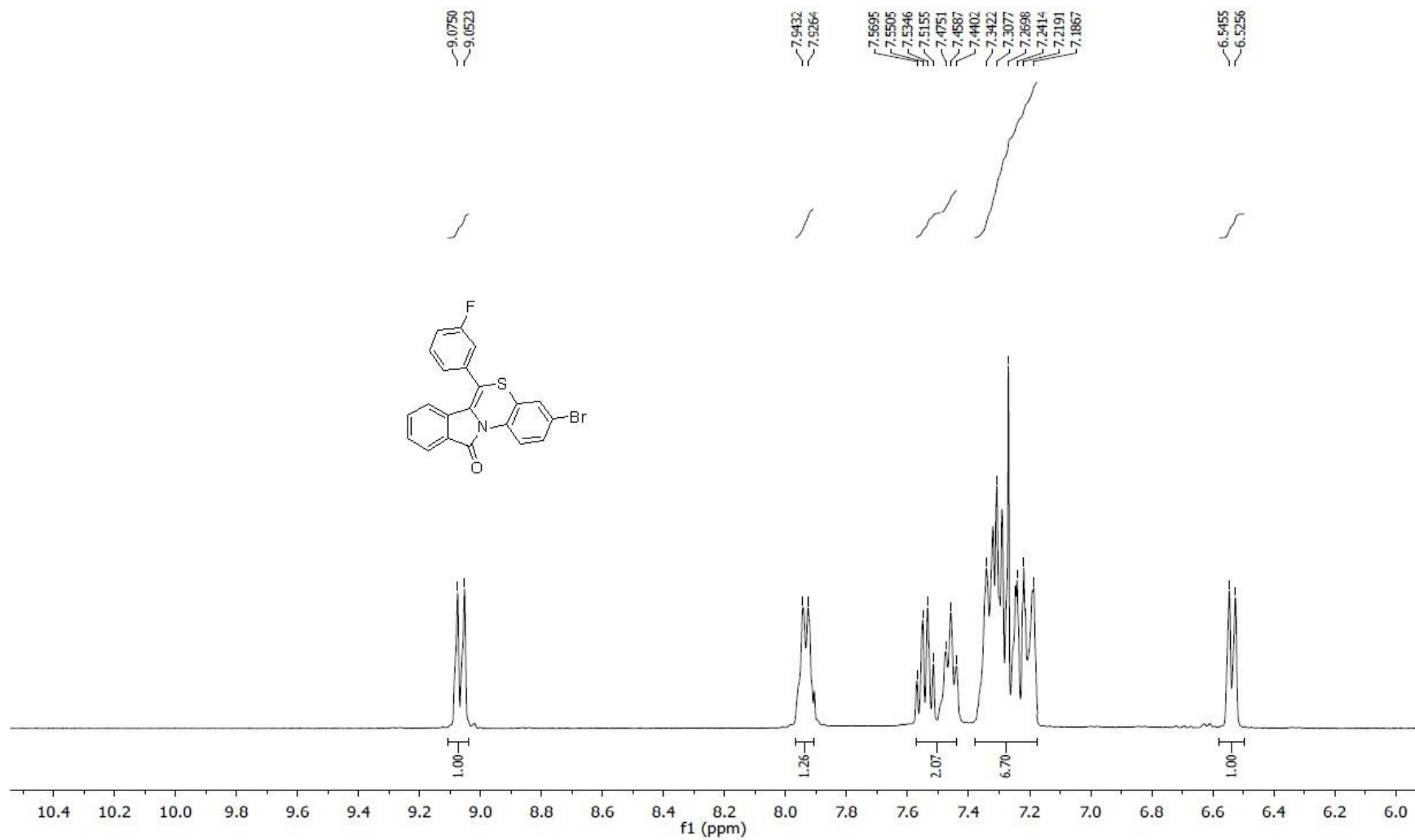
125.4175
125.3866
124.9594
123.2794
121.8492
121.6346
120.3856

117.3205
117.1134
116.9070
116.6874
115.7898



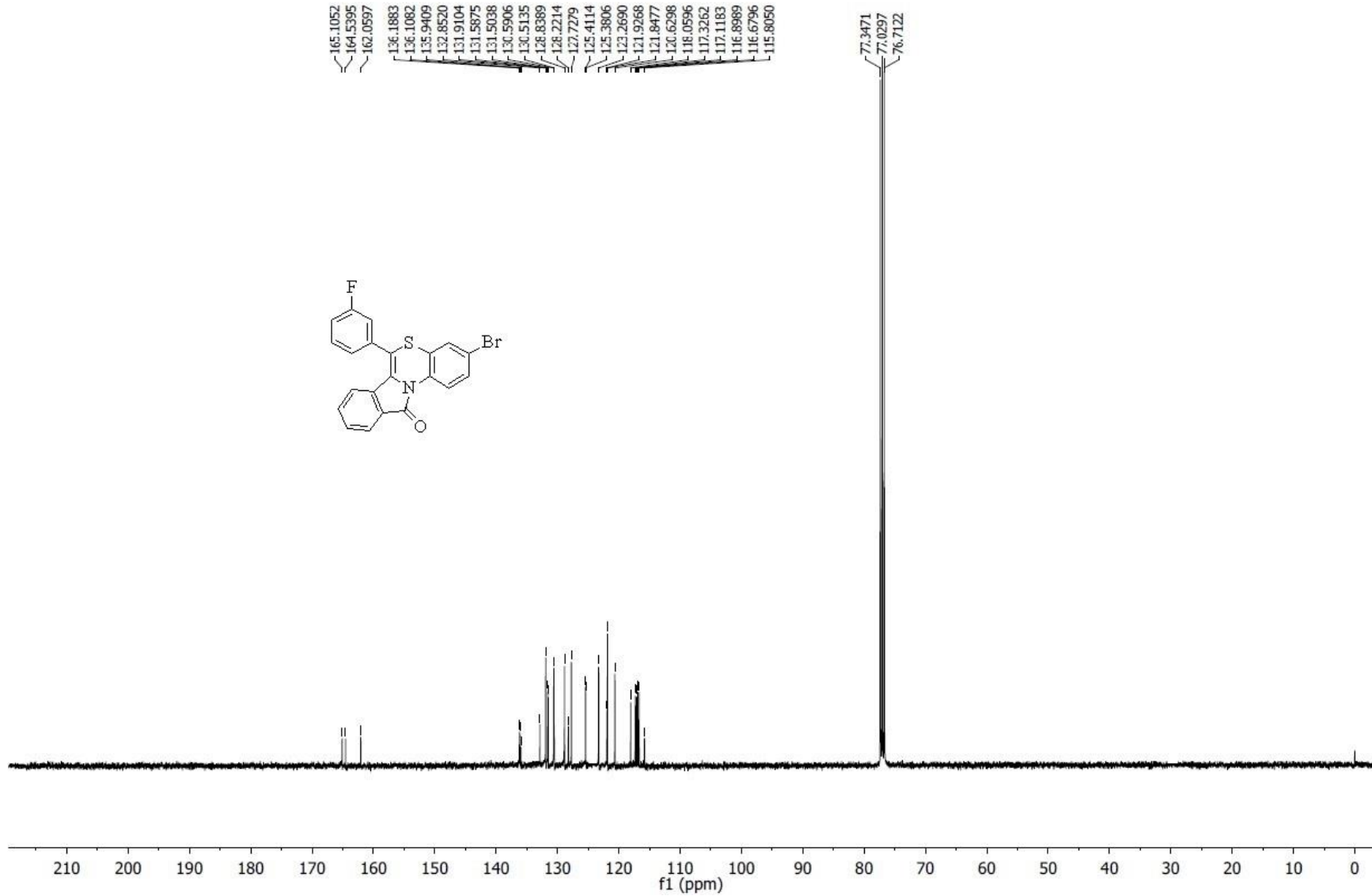
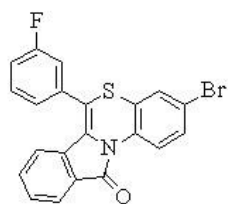


¹H NMR of 5r



¹³C NMR of 5r

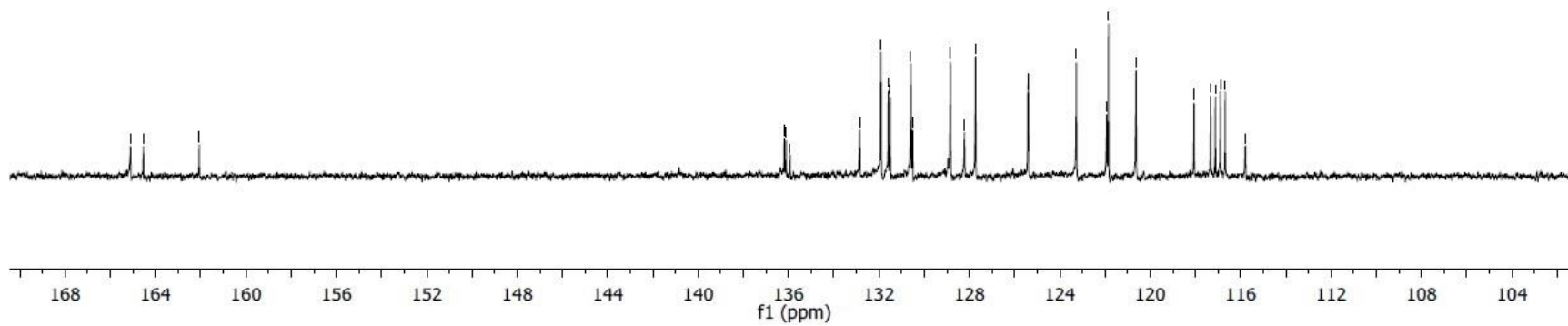
165.1052
164.5395
162.0597
136.1883
136.1082
135.9409
132.8520
131.9104
131.5875
131.5038
130.5906
130.5135
128.8389
128.2214
127.7279
125.4114
125.3806
123.2690
121.9268
121.8477
120.6298
118.0596
117.3262
117.1183
116.8989
116.6796
115.8050
77.3471
77.0297
76.7122



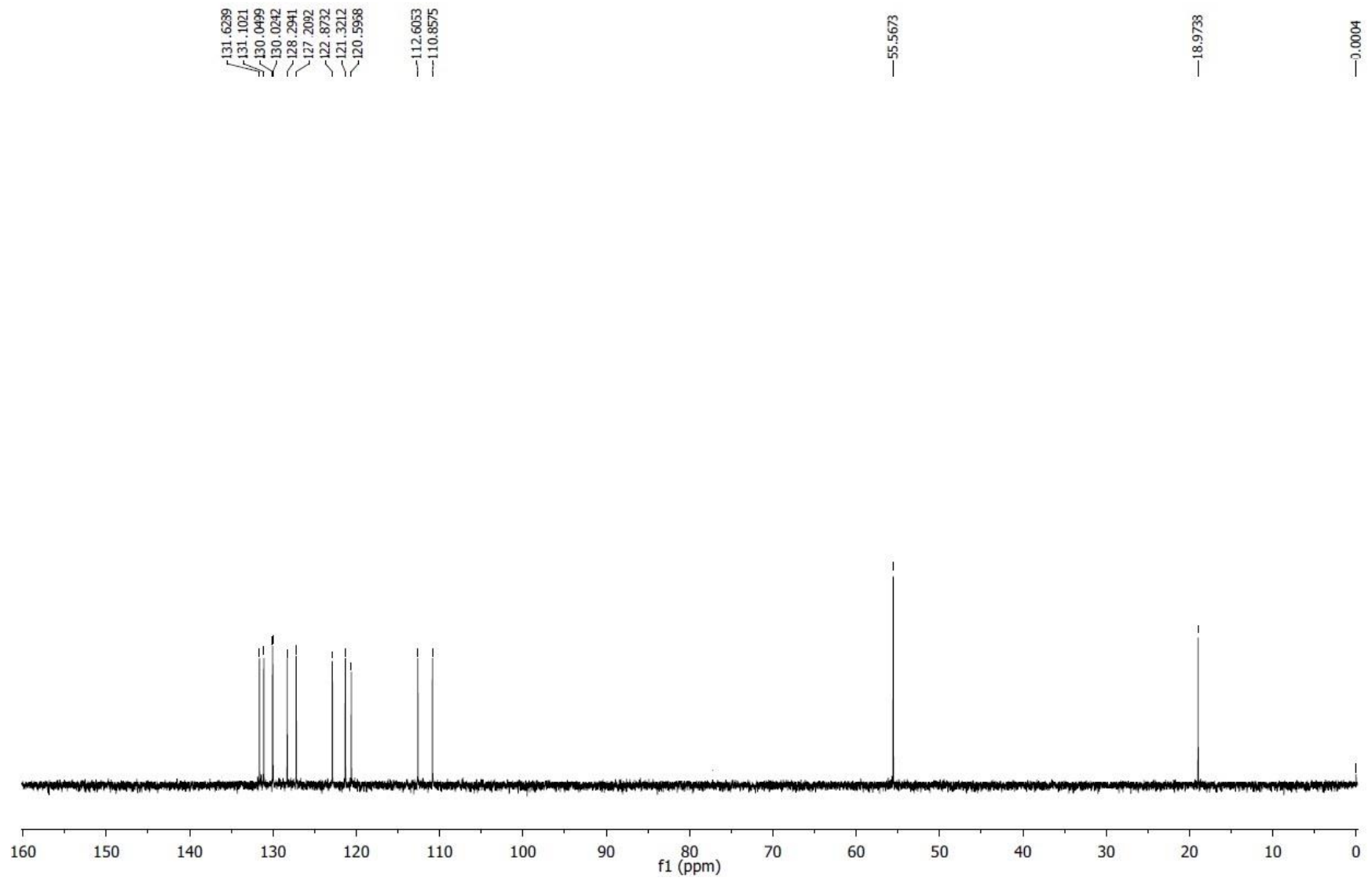
¹³C NMR of 5r

165.1052
164.5395
162.0697

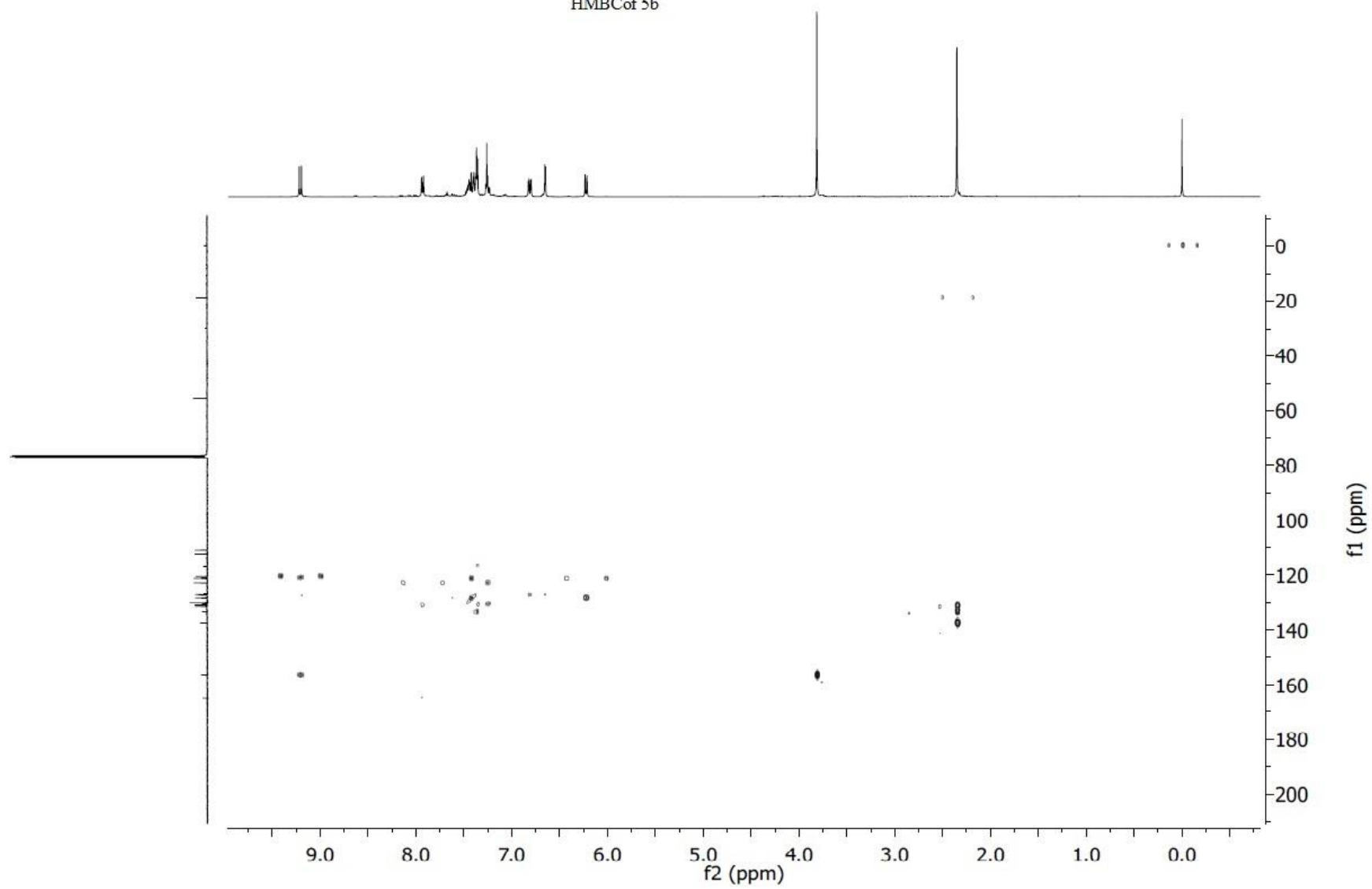
136.1883
136.1082
135.9409
132.8520
131.9104
131.5875
131.5038
130.5906
130.5135
128.8389
128.7214
127.7279
125.4114
125.3806
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118.0596
117.3262
117.1183
116.8889
116.6796
115.8050

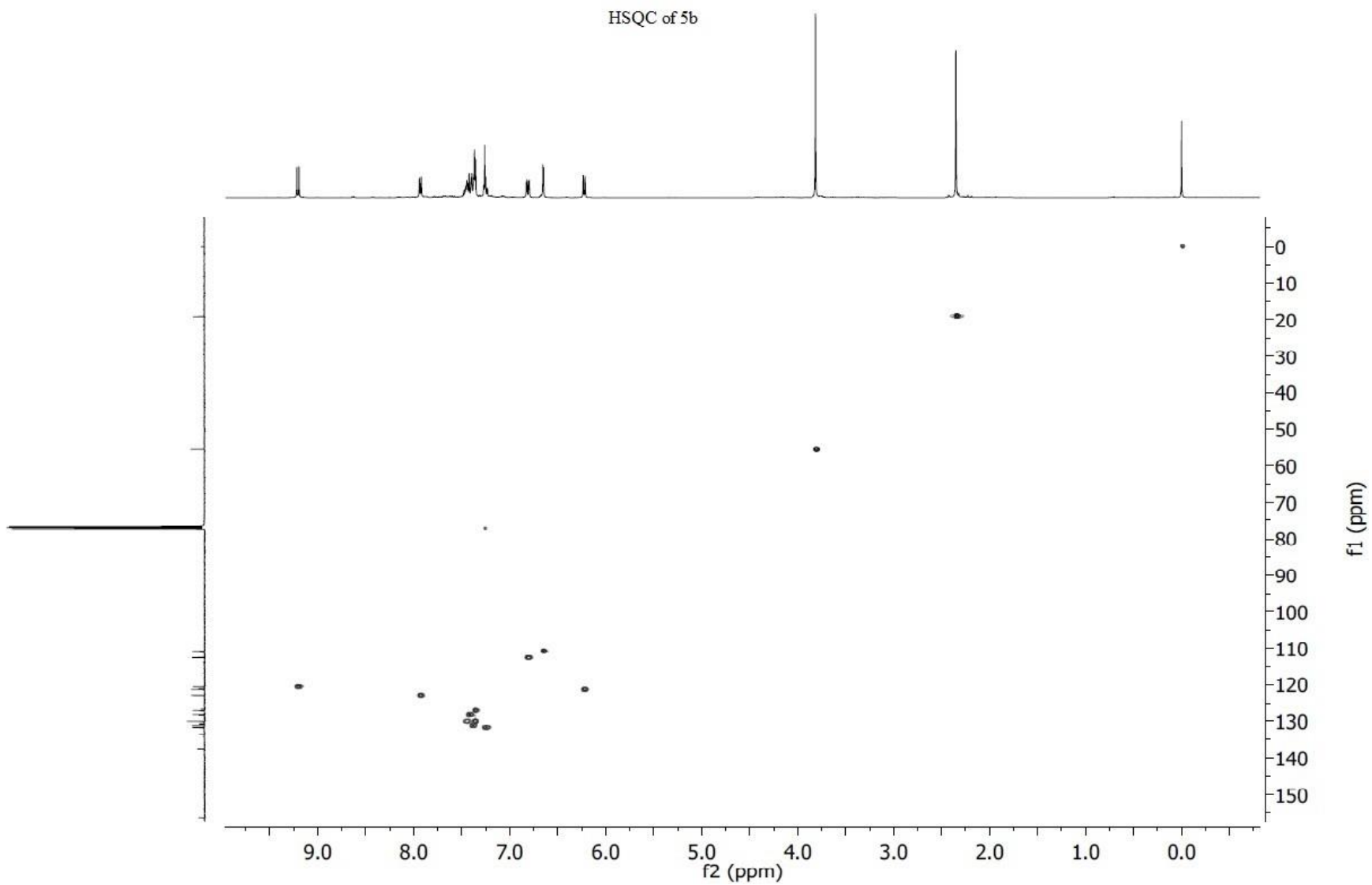


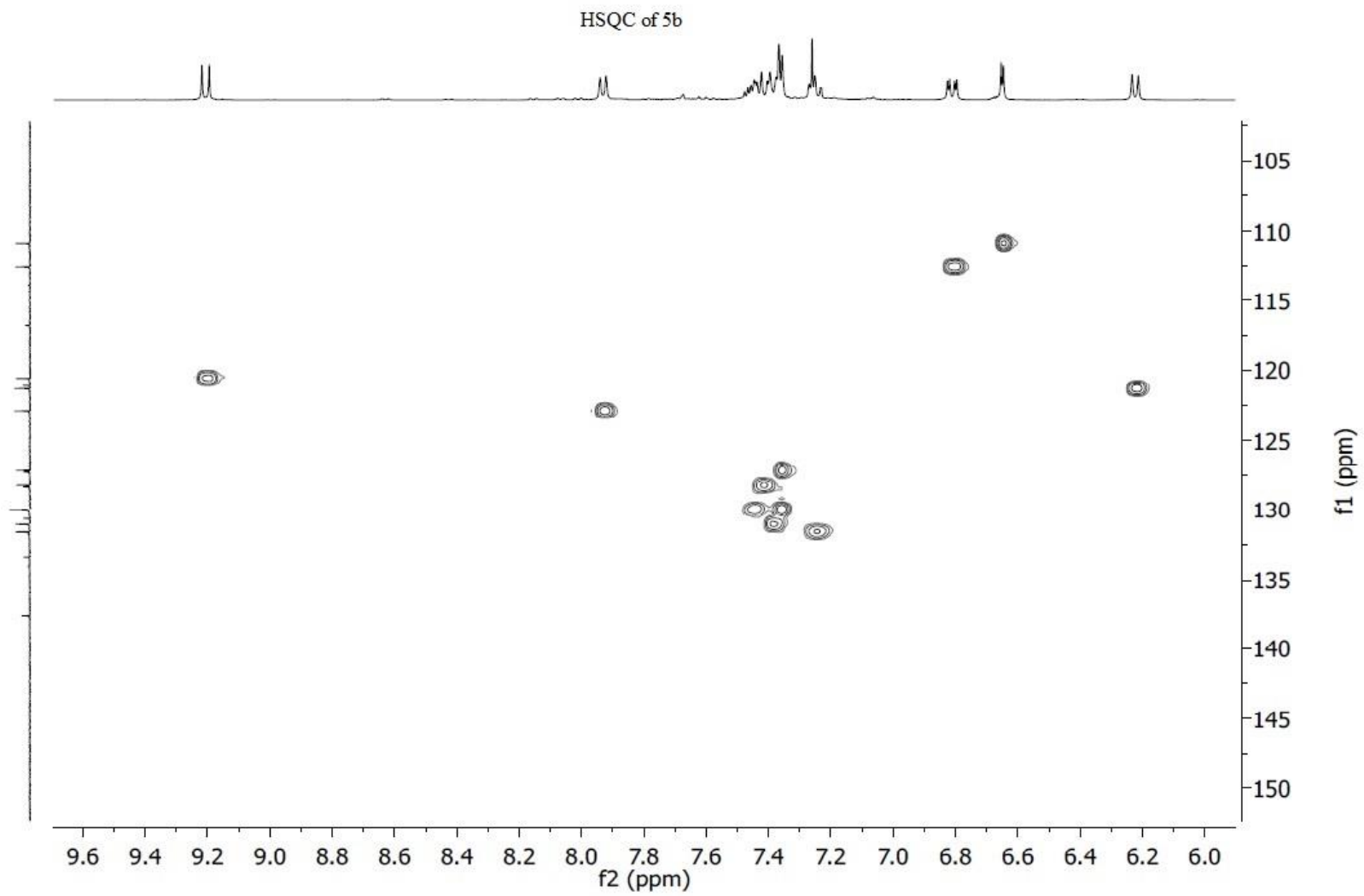
DEPT of 5b

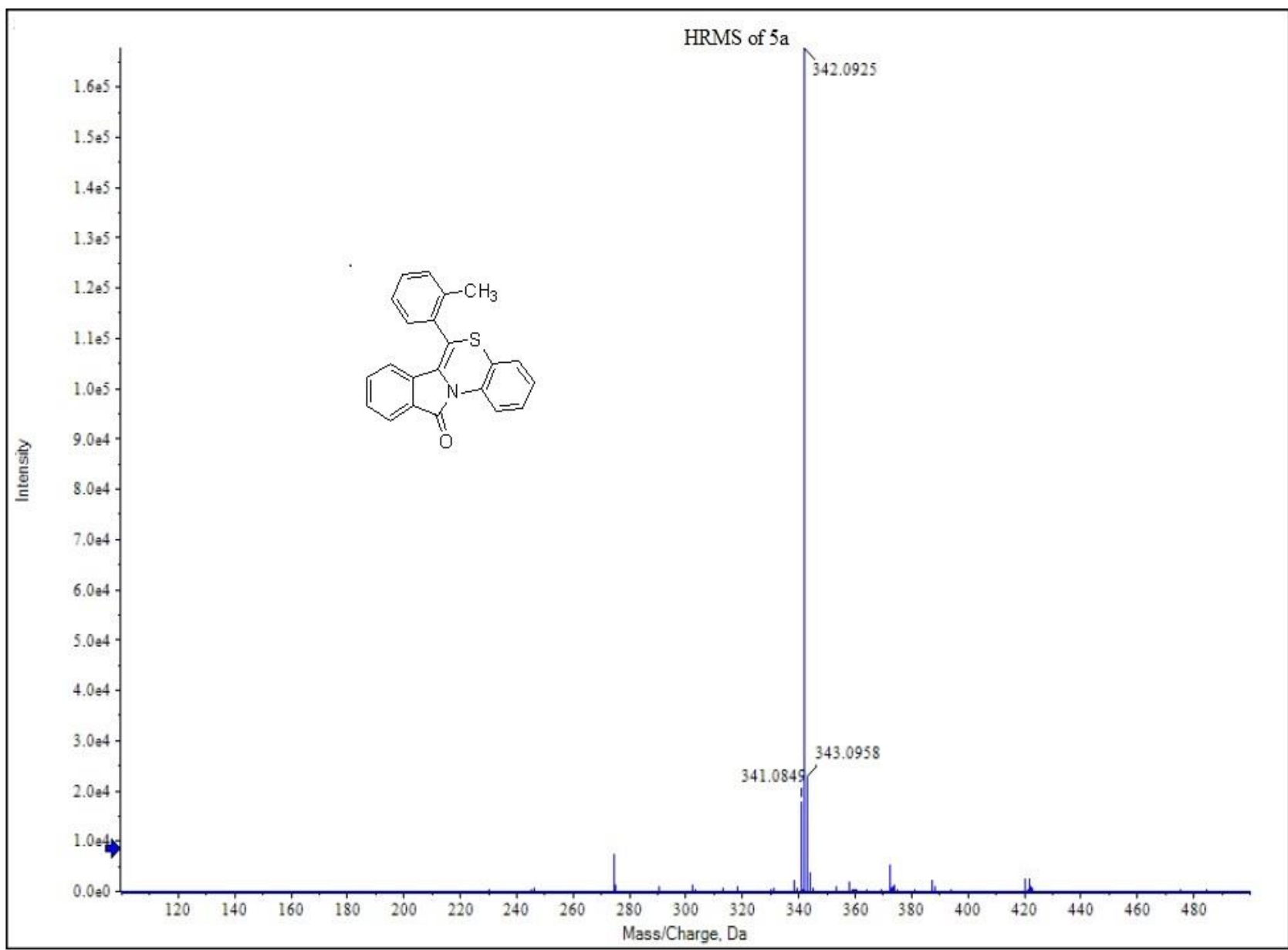


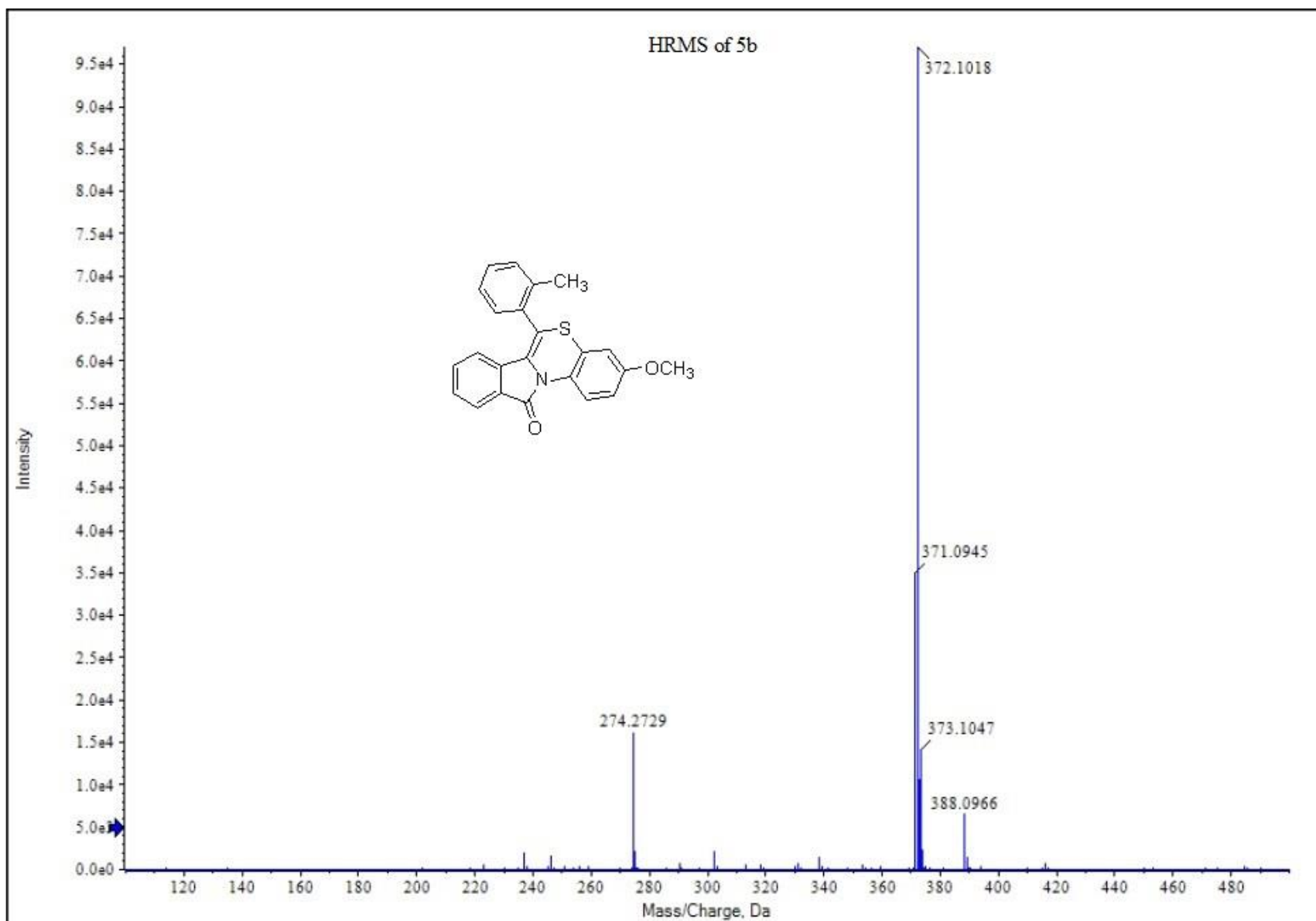
HMBC of 5b

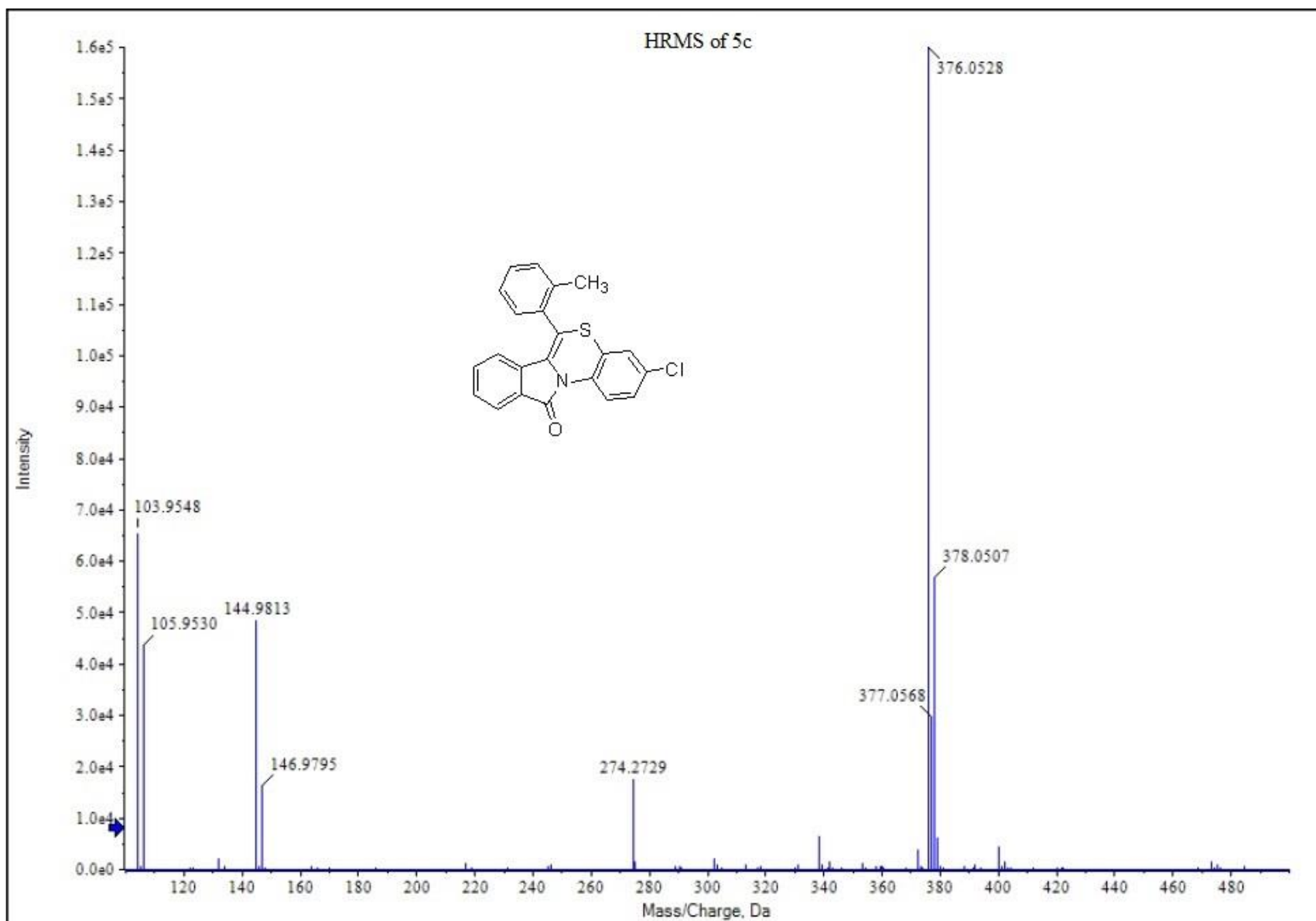


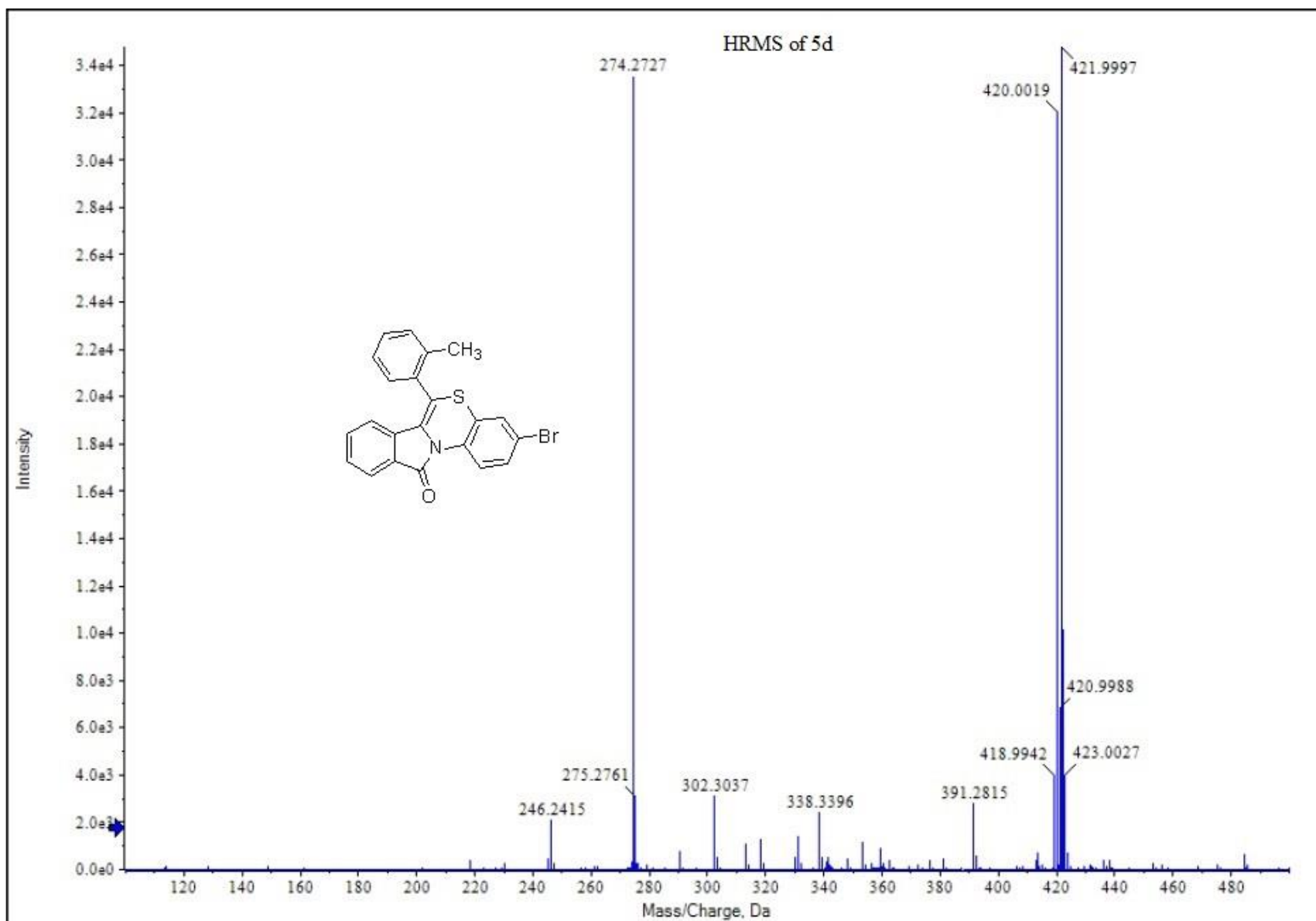


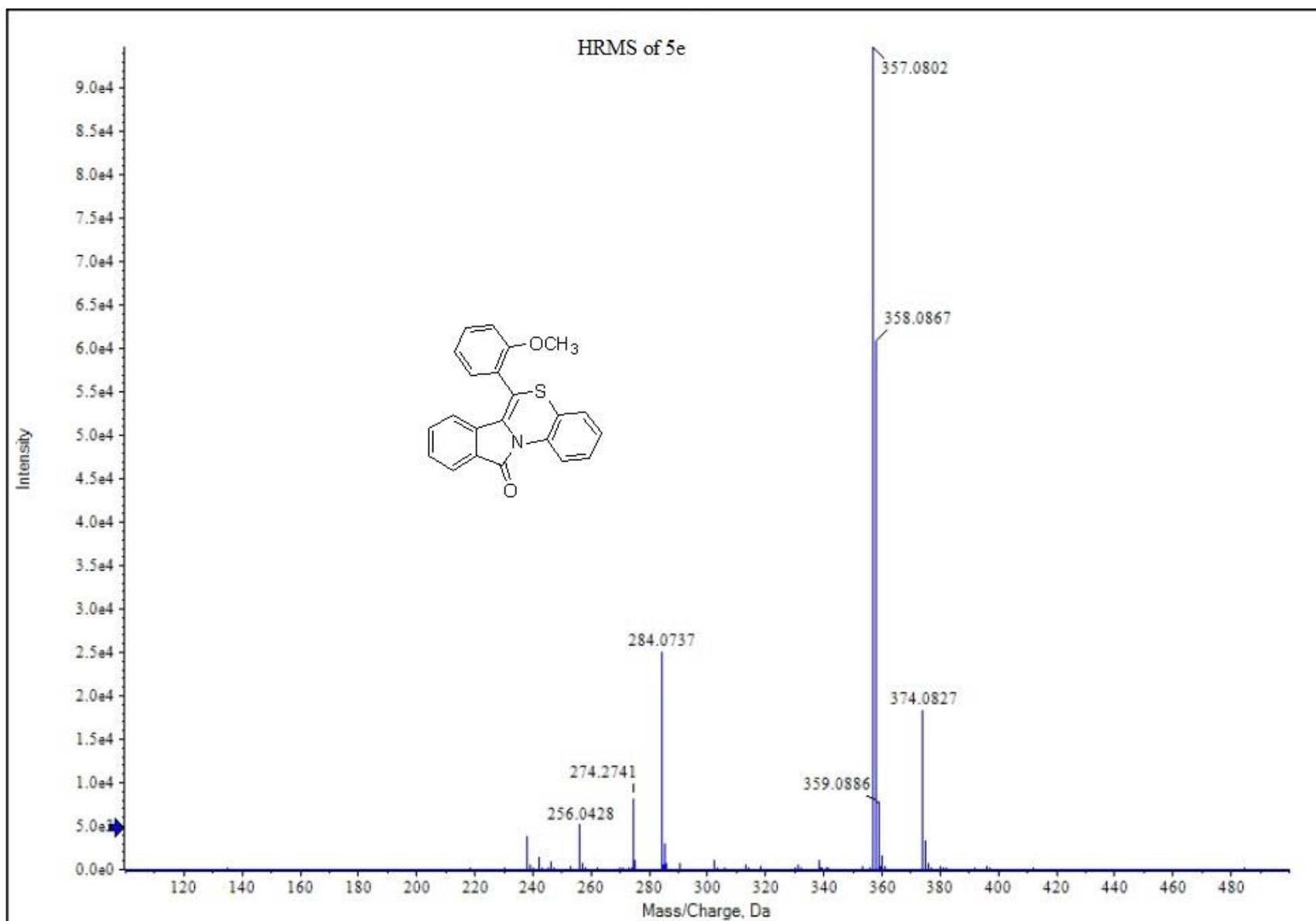


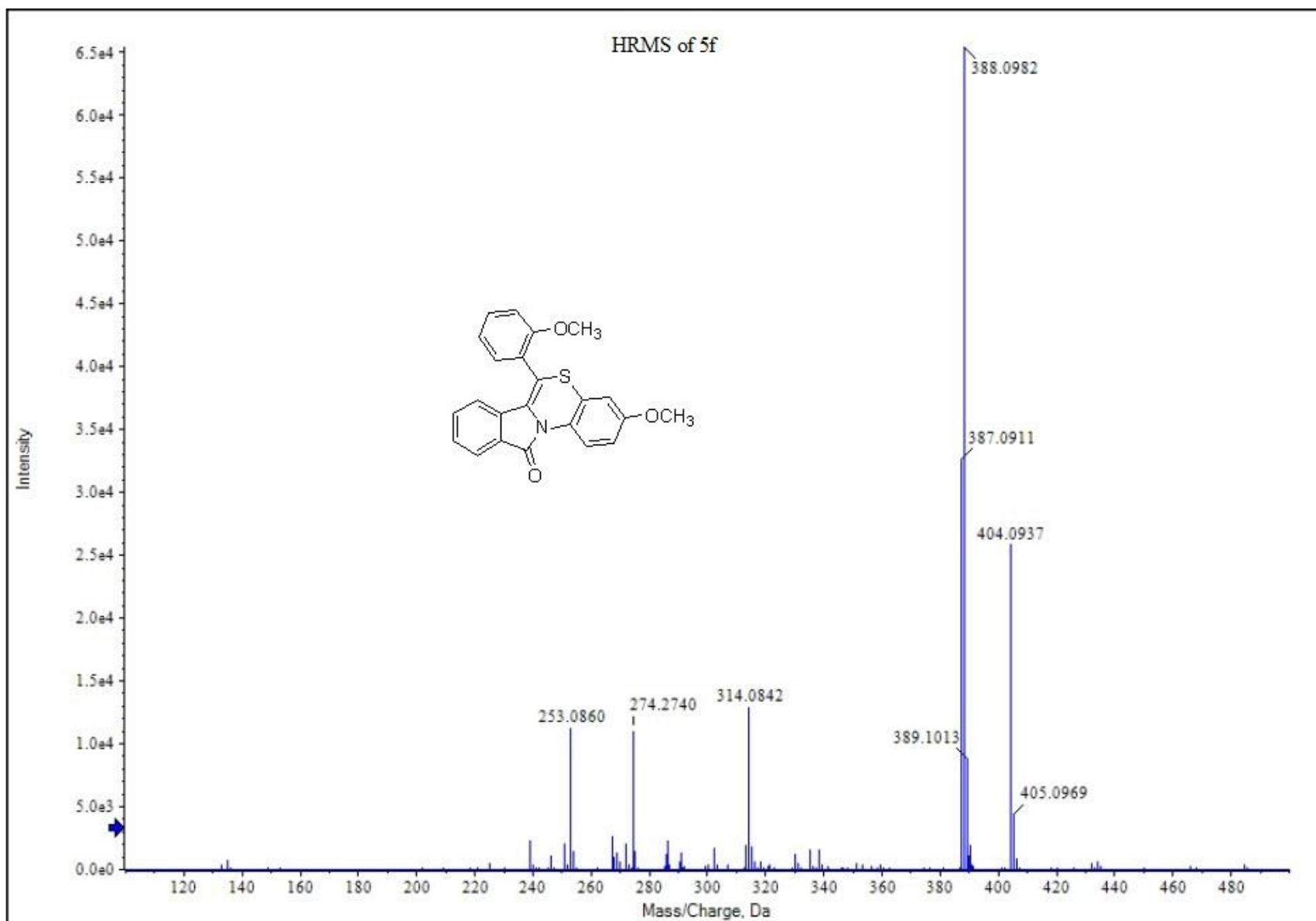


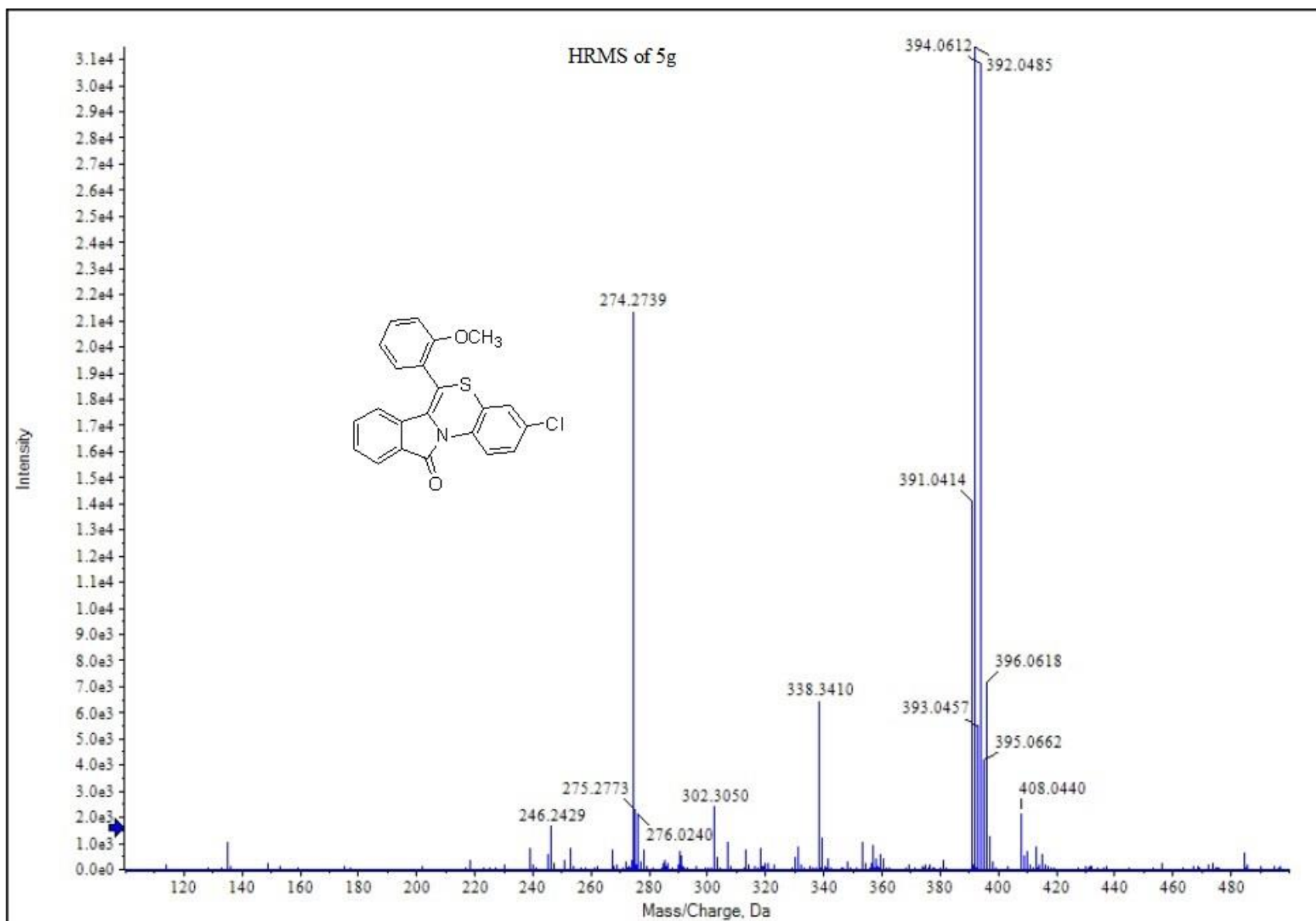


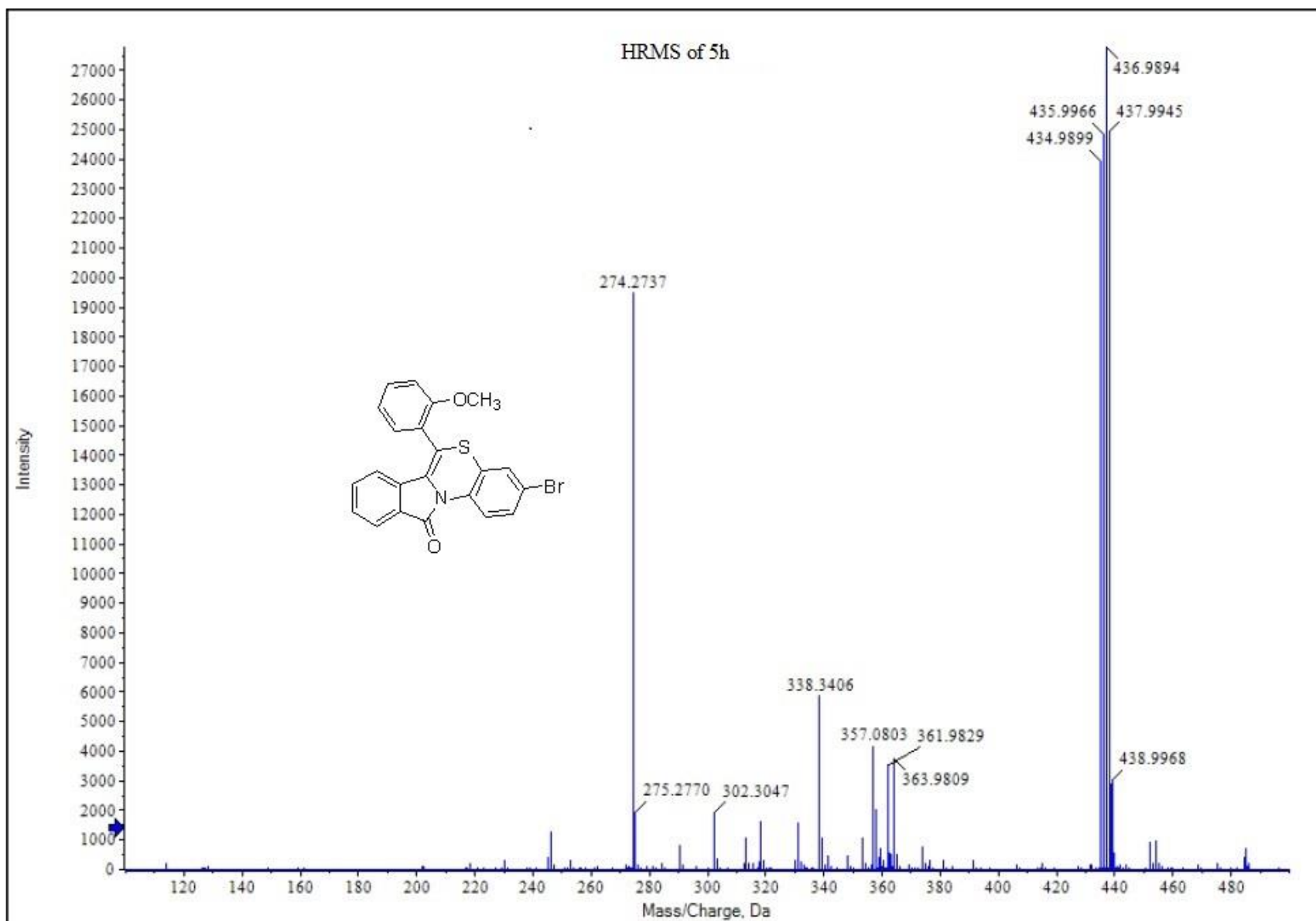


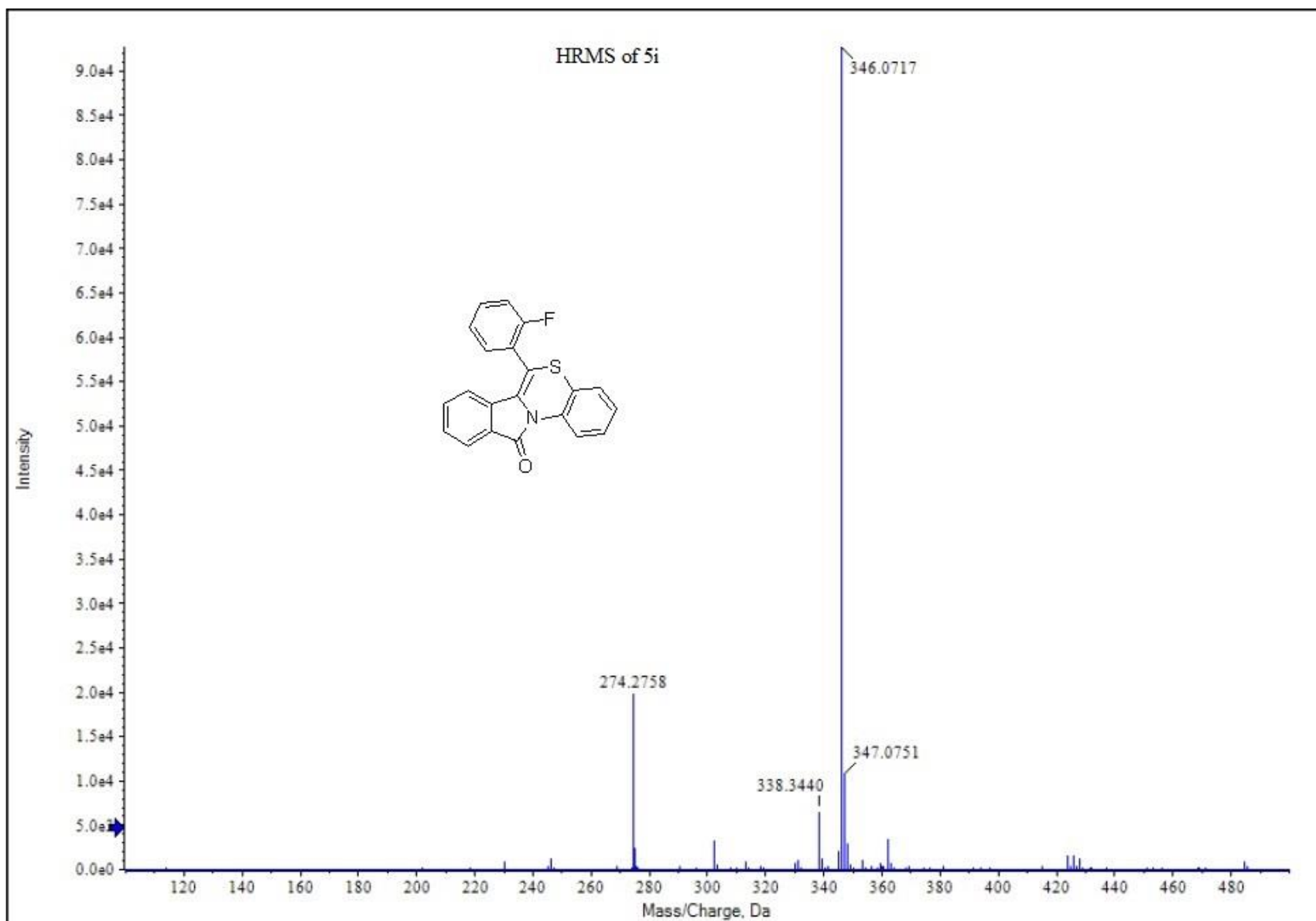


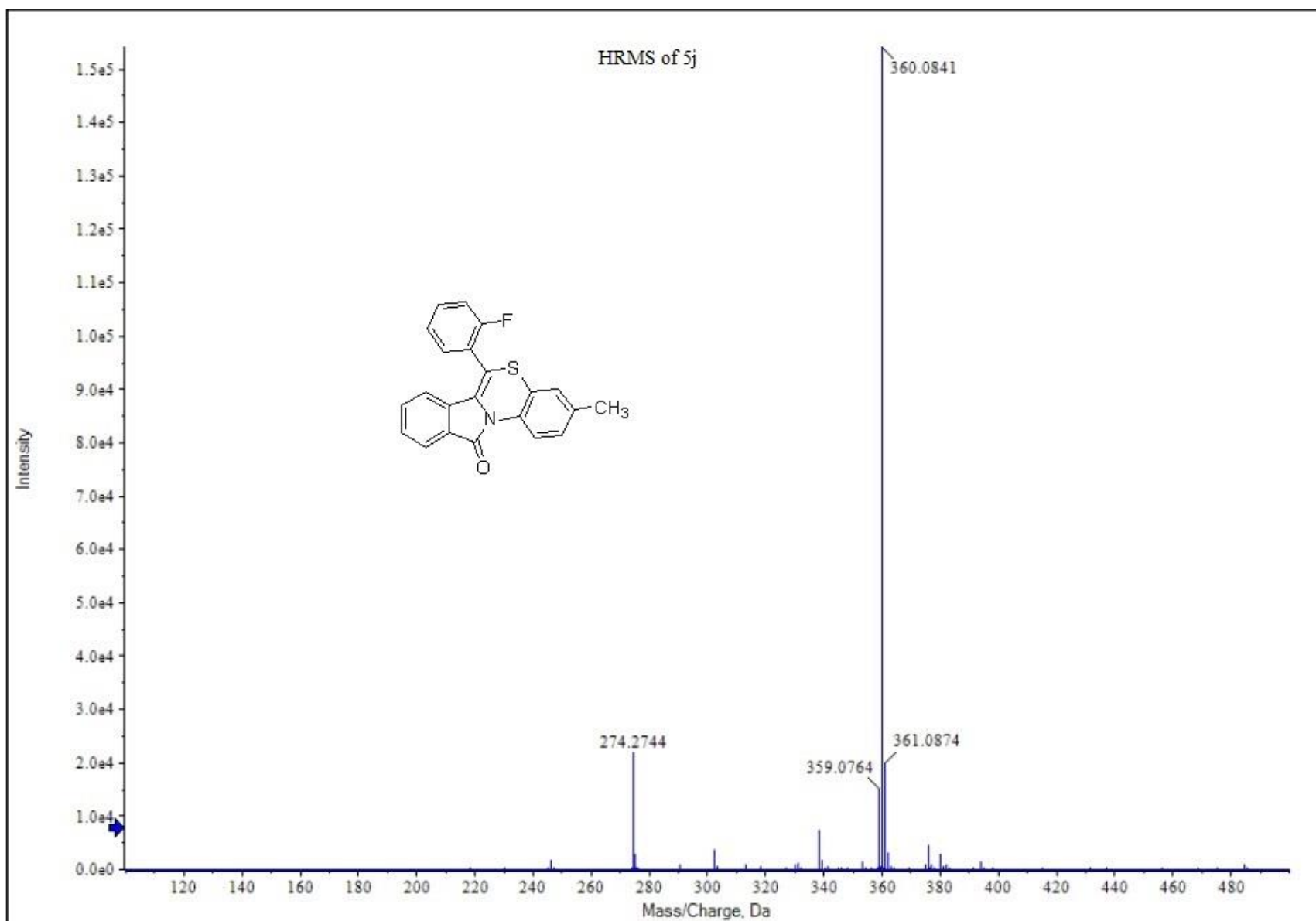


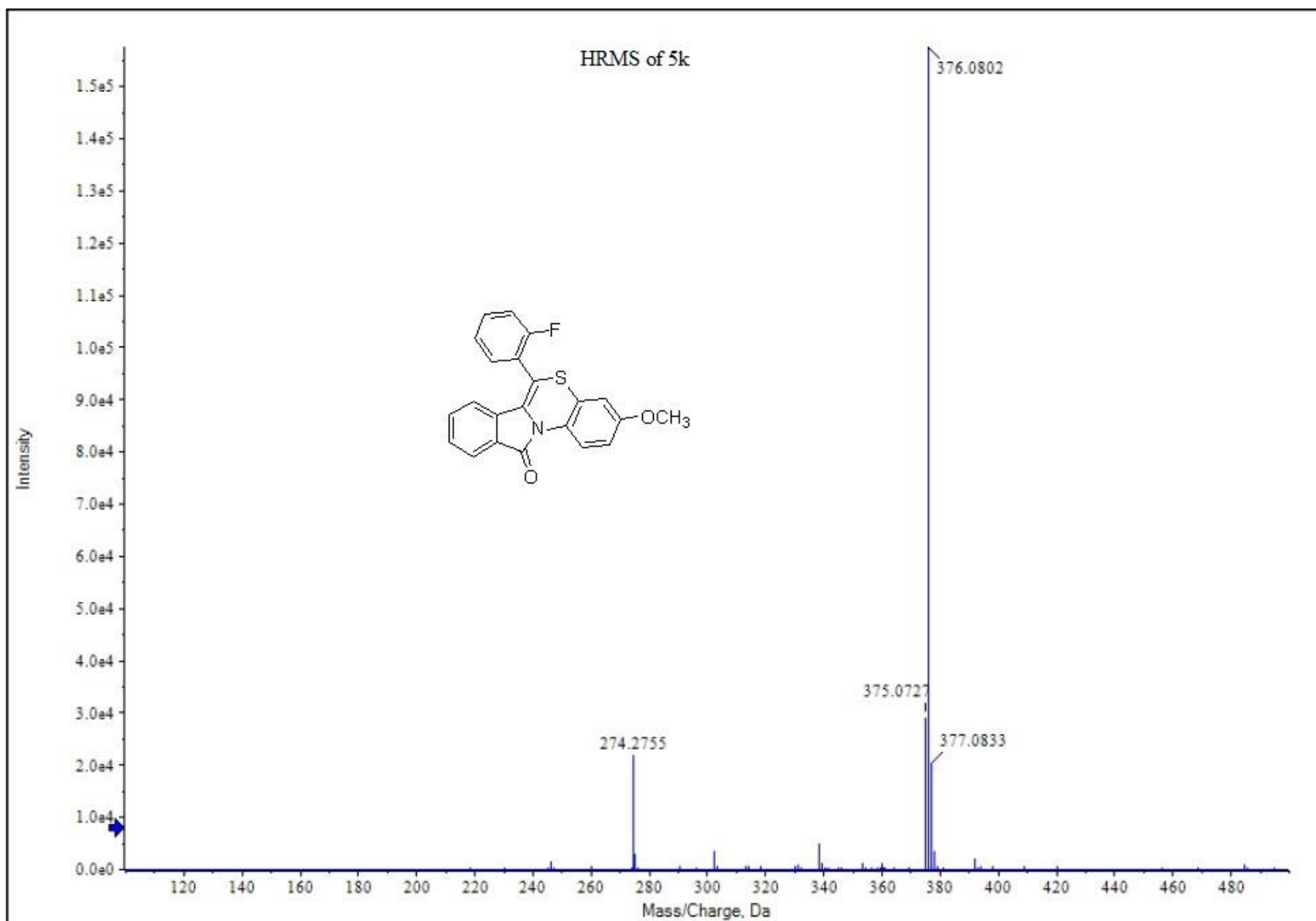


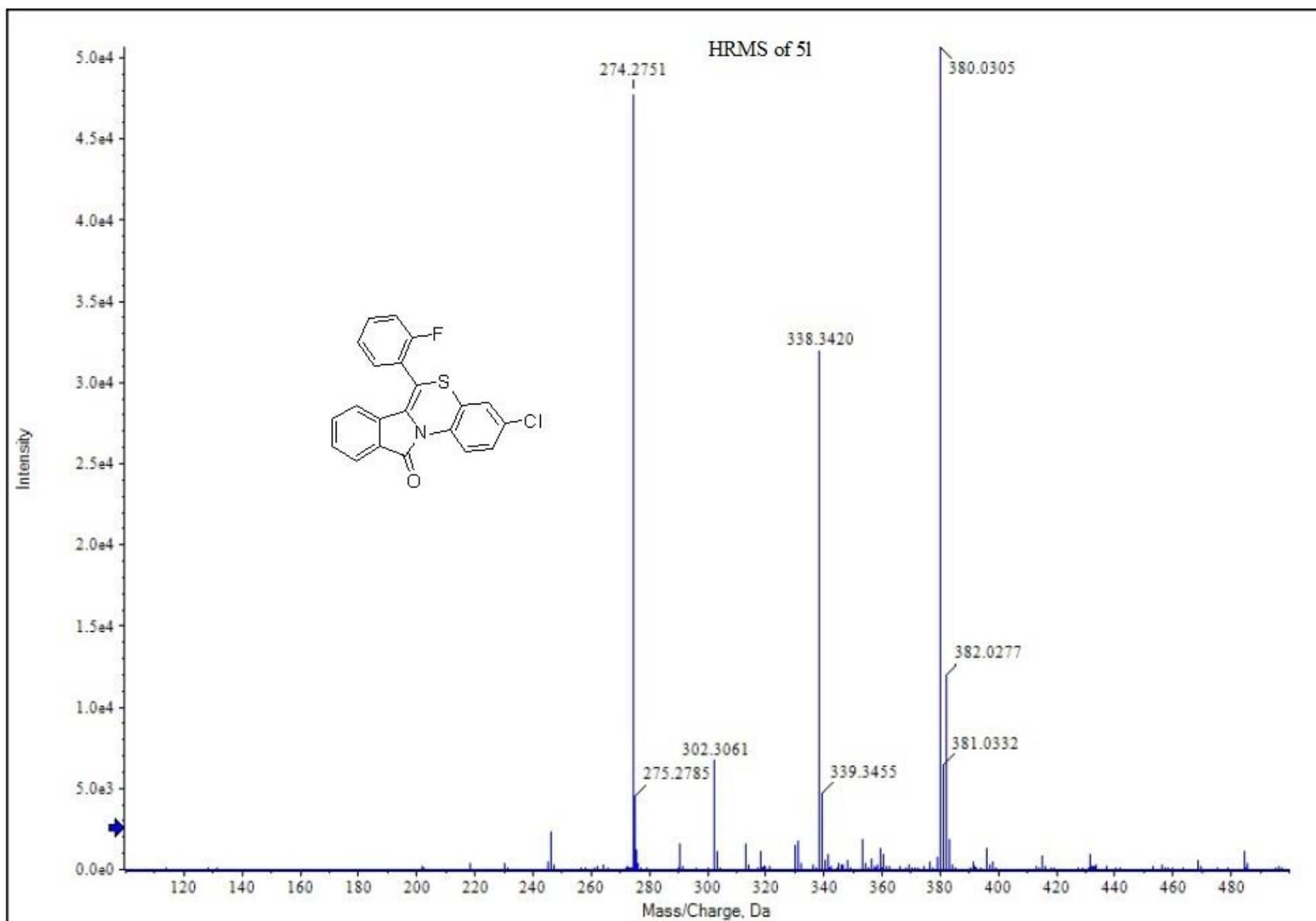


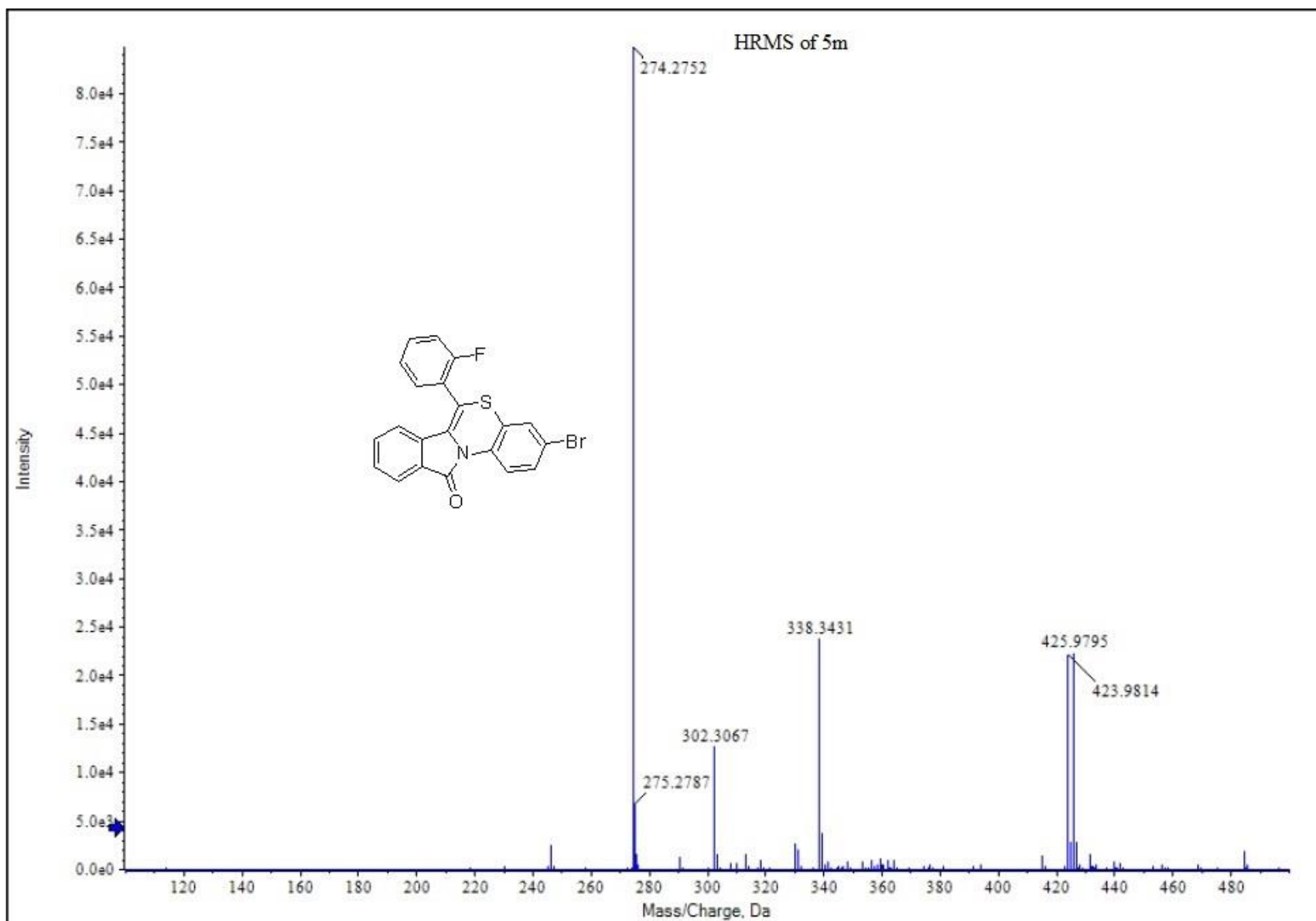


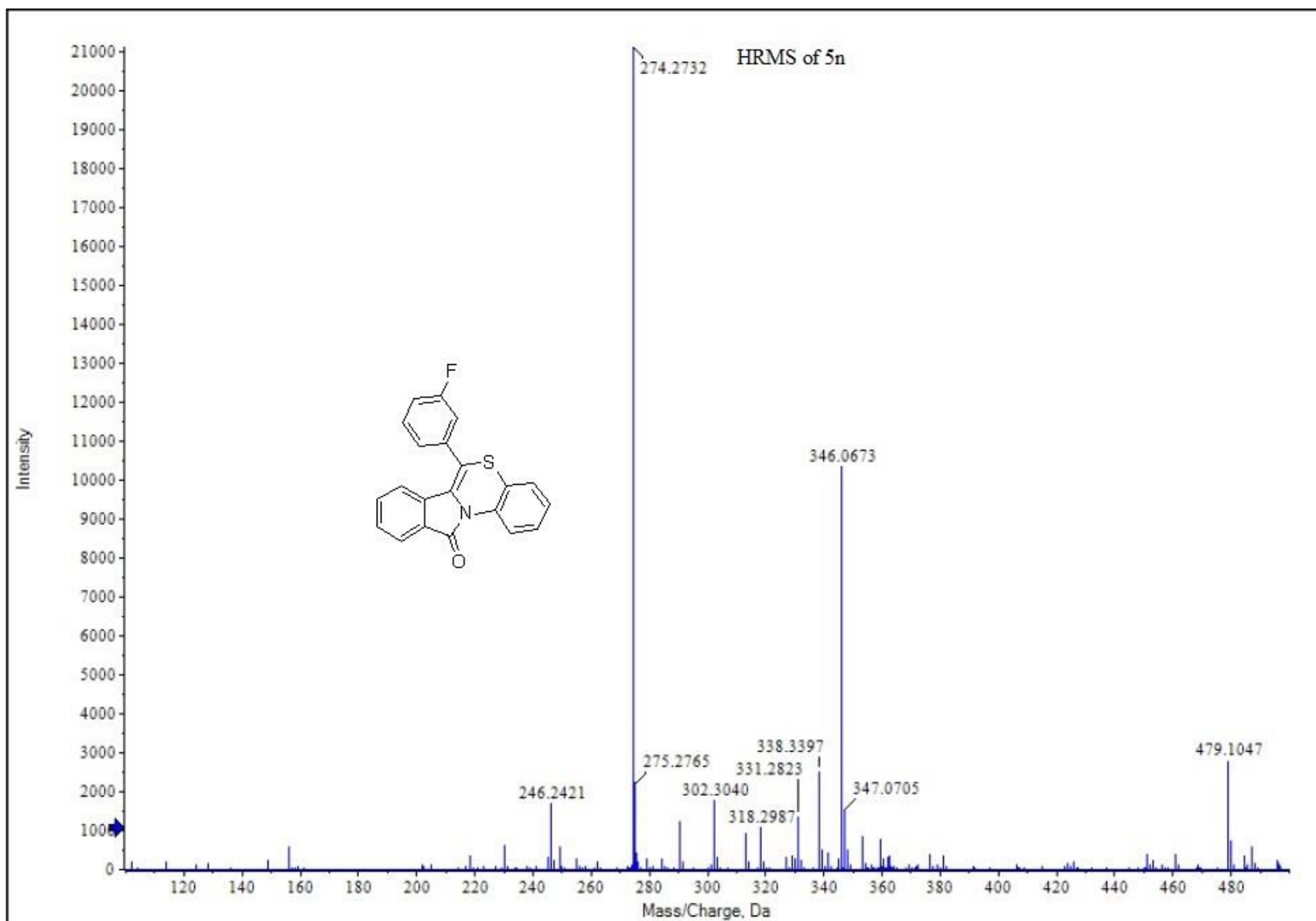


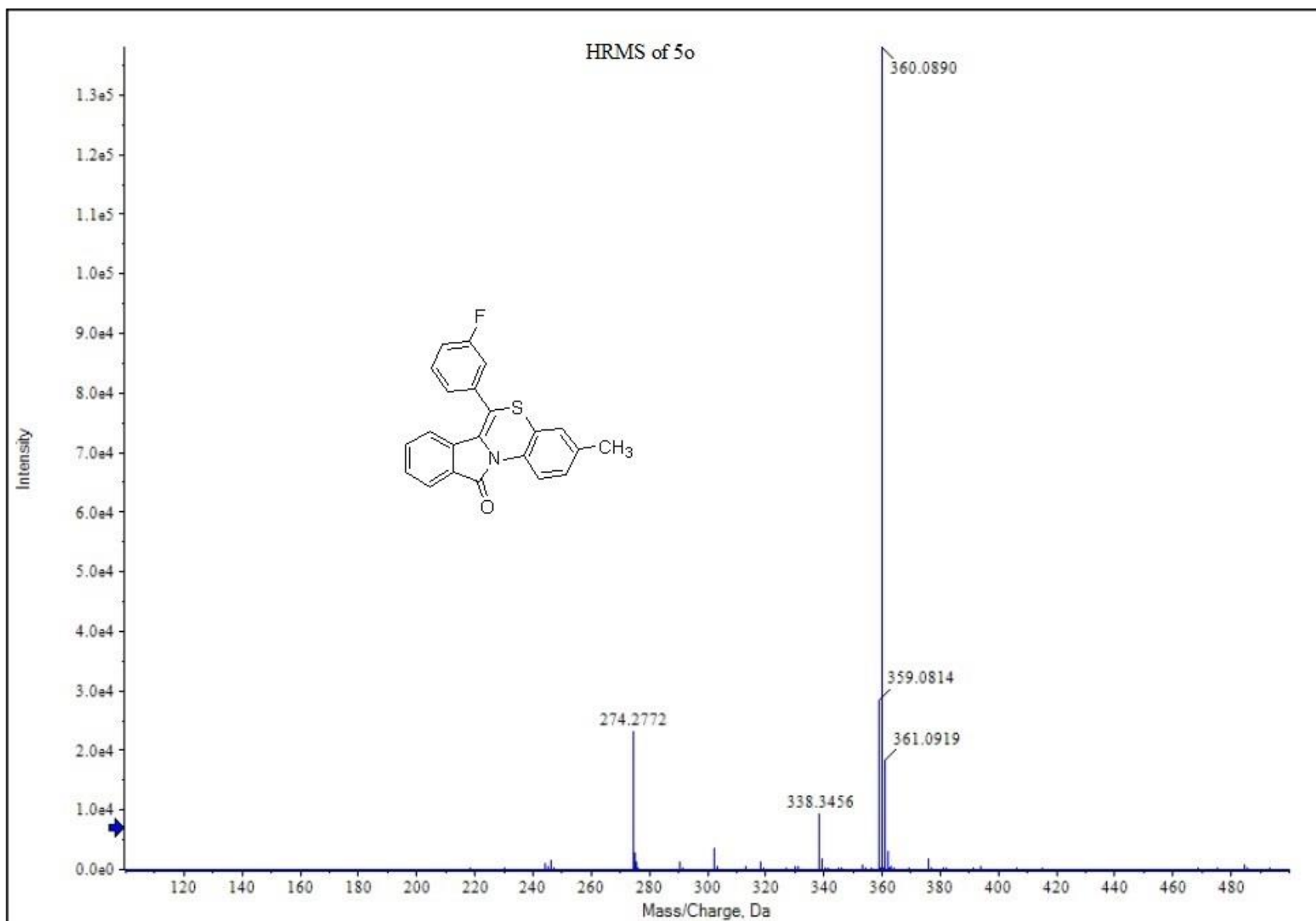


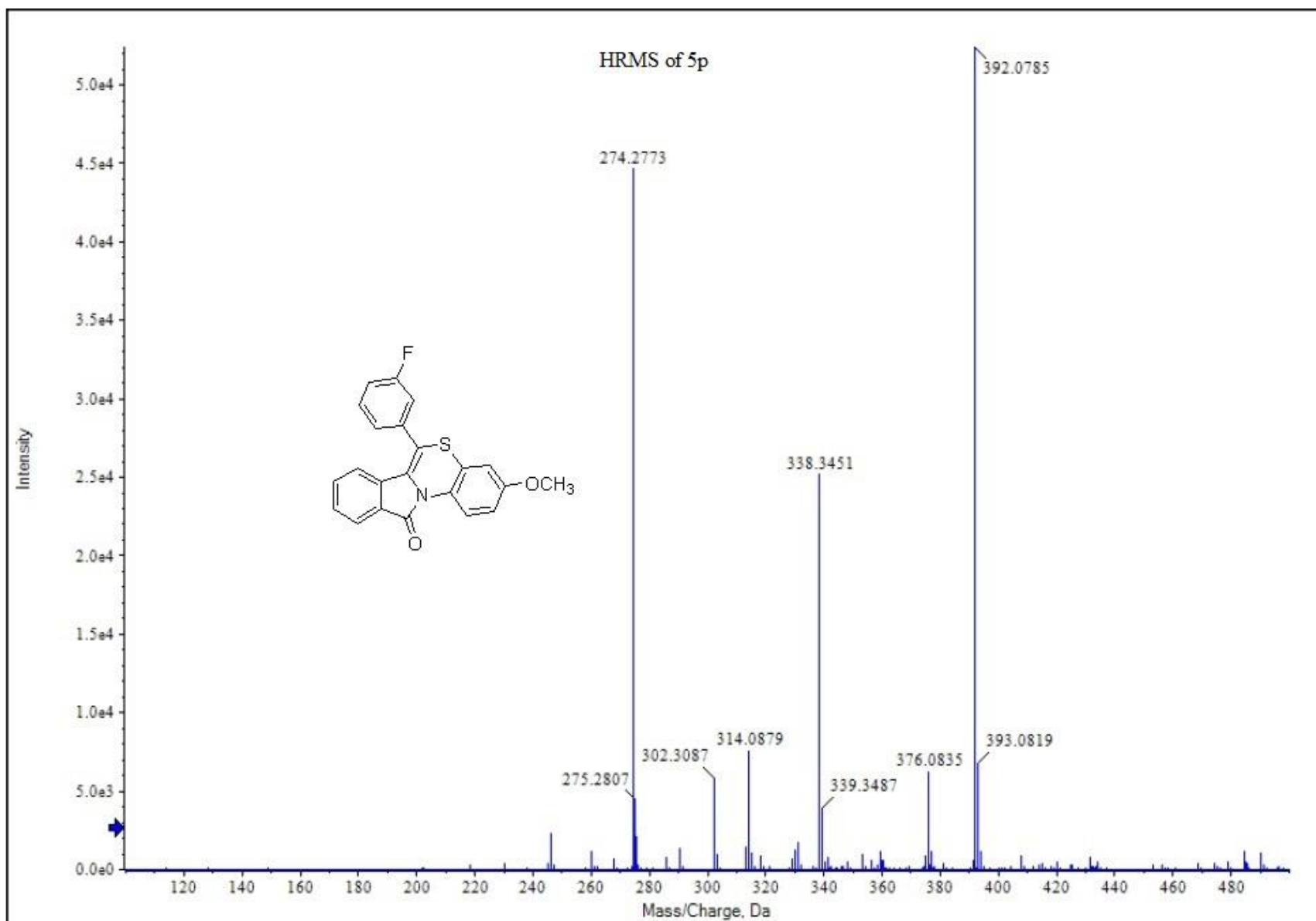


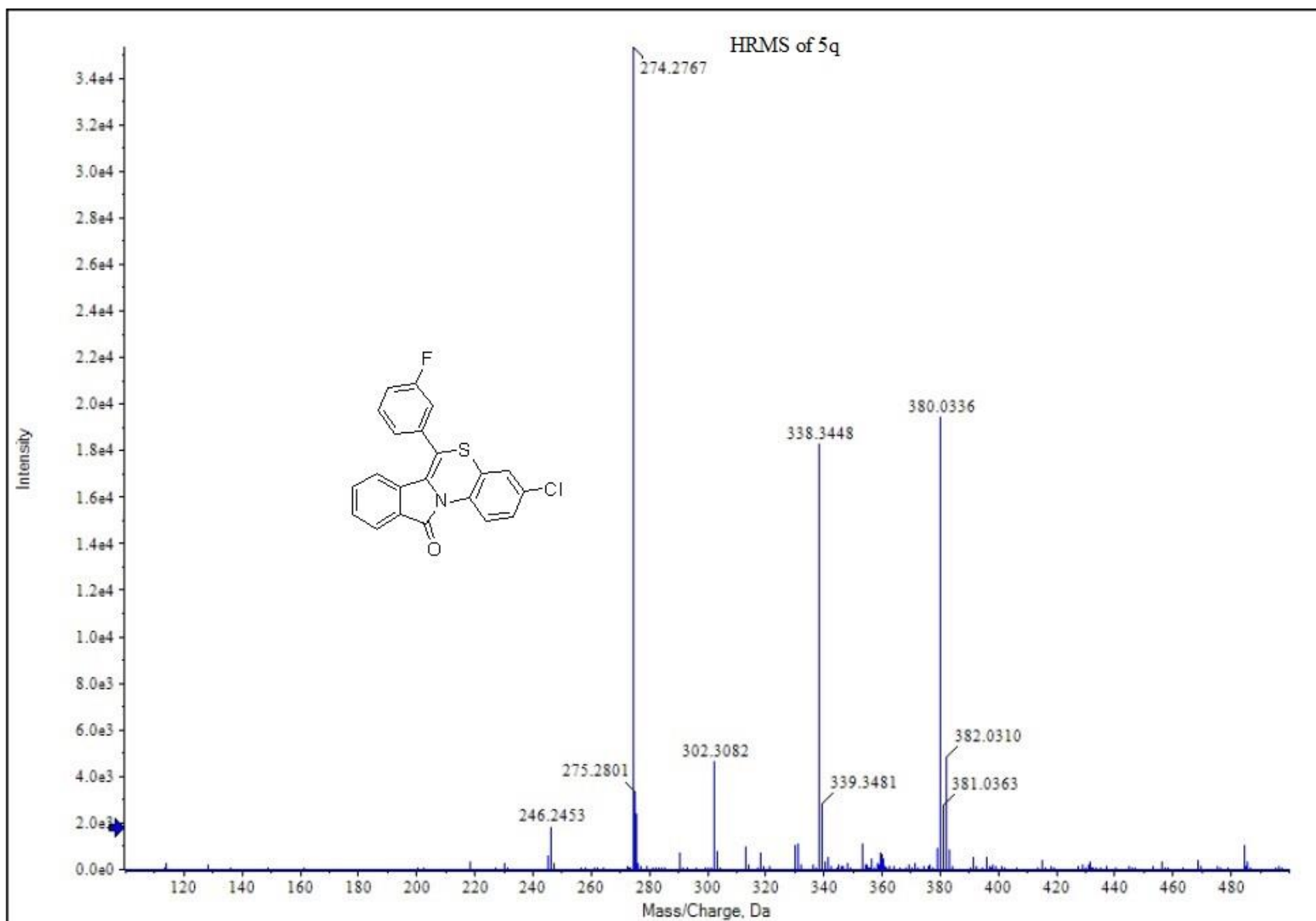


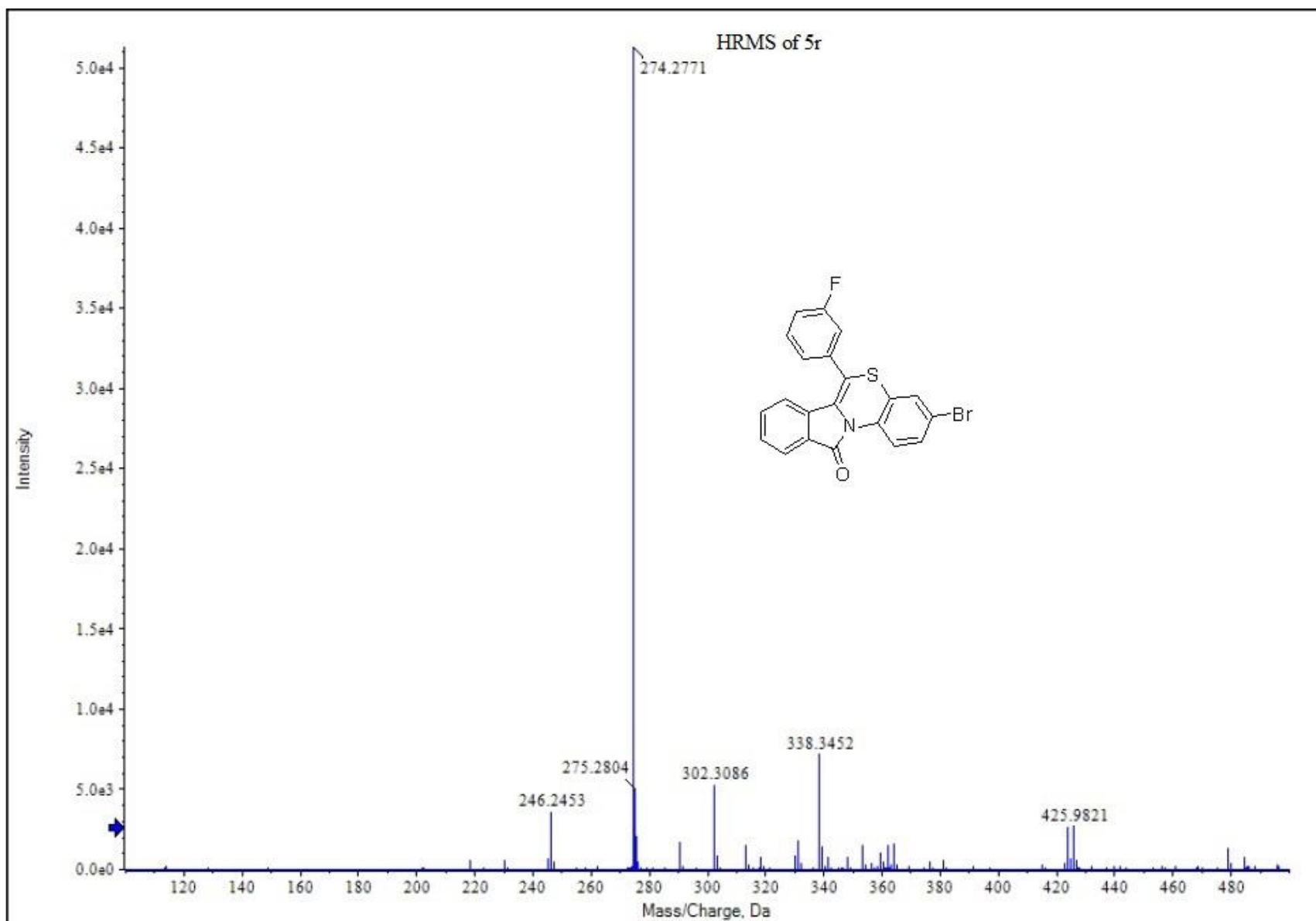












Crystal data of 5b

Table 3 Selected bond distances, bond angles and torsion angles of **5b** (standard uncertainties (s.u.) are given in parentheses)

Bond	Bond distance (Å)	Bond	Bond distance (Å)
C3-C4	1.457(2)	C6-C21	1.396(2)
C3-C18	1.391(2)	C6-S1	1.7521(17)
C4-N1	1.434(2)	C17-O2	1.221(2)
C4-C5	1.343(2)	C17-C18	1.462(3)
C5-C10	1.492(2)	C17-N1	1.398(2)
C5-S1	1.7387(19)	C21-N1	1.419(2)
Bond	Bond angle (°)	Bond	Bond angle (°)
C2-C3-C4	133.10(16)	C6-C21-N1	121.17(15)
C2-C3-C18	119.21(17)	C6-C21-C22	117.60(16)
C3-C4-C5	129.25(16)	C7-C6-C21	120.82(16)
C3-C4-N1	106.36(14)	C7-C6-S1	115.03(13)
C3-C18-C17	109.65(15)	C10-C5-S1	112.79(12)
C3-C18-C19	122.46(18)	C17-N1-C21	126.08(14)
C4-C3-C18	107.67(15)	C17-C18-C19	127.88(17)
C4-N1-C17	110.37(14)	C18-C17-N1	105.91(14)
C4-C5-C10	123.73(16)	C18-C17-O2	127.55(17)
C4-C5-S1	123.46(14)	C21-C6-S1	124.16(14)
C4-N1-C21	123.55(14)	C22-C21-N1	121.23(15)
C5-S1-C6	103.01(9)	N1-C17-O2	126.53(17)
C5-C4-N1	124.34(16)	O1-C8-C23	115.66(16)
Bond	Torsion angle (°)	Bond	Torsion angle (°)
C2-C3-C4-C5	-1.8(3)	O2-C17-C18-C19	-3.6(3)
C3-C4-C5-S1	-174.27(15)	O2-C17-N1-C21	1.1(3)
S1-C6-C7-C8	179.93(16)	C22-C21-N1-C17	-3.8(3)
C3-C4-C5-C10	4.3(3)	C22-C21-N1-C4	175.30(17)

Table 4 X-ray crystallographic data of **5b**

Chemical formula	C ₂₃ H ₁₇ NO ₂ S
Formula weight	371.44
Crystal system, Space group	Triclinic, P-1
Temperature (K)	296(2)
Radiation type, wavelength (Å)	Mo K α , 0.71073
<i>a</i> , <i>b</i> , <i>c</i> (Å)	8.0068(7), 9.5362(10), 12.2550(9)
α , β , γ (°)	95.494(3), 98.424(3), 97.562(4)
<i>V</i> (Å ³)	911.24(14)
<i>Z</i>	2
Density (calc) (Mg m ⁻³)	1.354
<i>F</i> (000)	388
μ (mm ⁻¹)	0.196
Crystal size (mm)	0.30 × 0.20 × 0.20
Completeness to $\theta = 28.34$	89.9%
θ_{\min} , θ_{\max} (°)	2.60, 28.34
Data collection	
Measured reflections	7513
Independent reflections	4092
Reflections with $I > 2\sigma(I)$	3077
R _{int}	0.0182
Limiting indices (h, k, l)	-10→10; -11→12; -12→16
Absorption correction	Multi-scan SADABS (Bruker, 1999)
<i>T</i> _{min} , <i>T</i> _{max}	0.9436, 0.9619
Refinement	
Refinement method	Full-matrix least-squares on F ²
<i>R</i> [F ² > 2 σ (F ²)]	0.0470
w <i>R</i> (F ²)	0.1305
S(F ²)	1.046

No. of reflections	4092
No. of parameters	246
No. of restraints	0.0
Max. Shift, Av. Shift	0.024, 0.000
$\Delta\rho_{\min}, \Delta\rho_{\max}$ ($e \text{ \AA}^{-3}$)	-0.292, 0.230
