

# Diastereoselective [3+2] cycloaddition of 3-ylideneoxindoles with *in situ* generated $\text{CF}_2\text{HCHN}_2$ : Syntheses of $\text{CF}_2\text{H}$ - containing spirooxindoles

Wen-Yong Han,\* Jia Zhao, Jian-Shu Wang, Guang-Yan Xiang, Ding-Lei Zhang, Mei Bai, Bao-Dong Cui, Nan-Wei Wan and Yong-Zheng Chen\*

*Generic Drug Research Center of Guizhou Province, School of Pharmacy, Zunyi Medical University, Zunyi, 563000, China.*

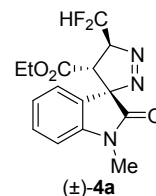
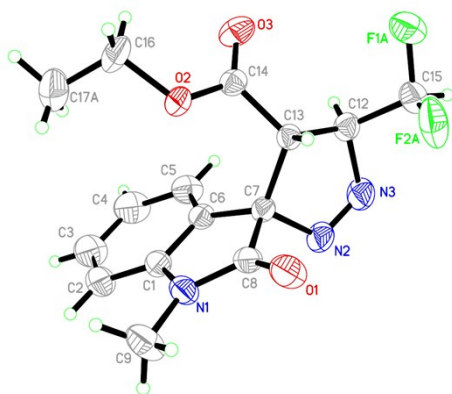
*hanwy@zmc.edu.cn; yzchen@zmc.edu.cn*

## Supporting Information

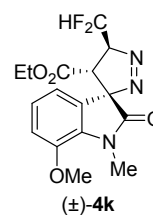
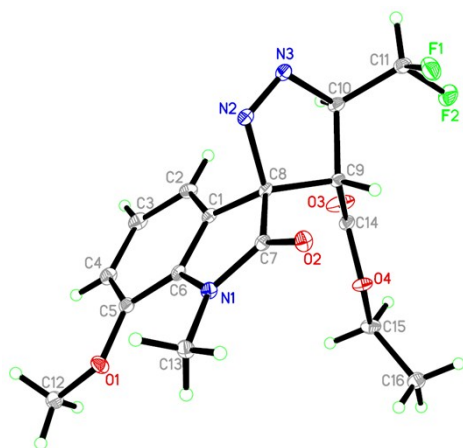
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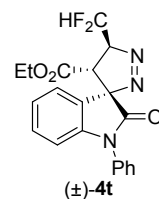
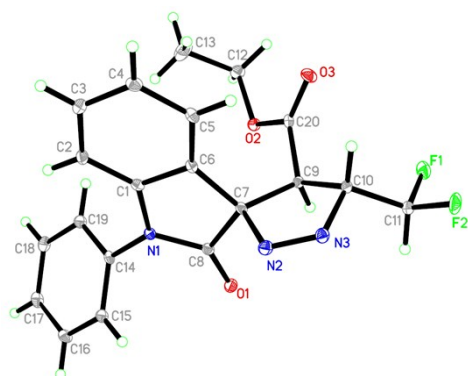
## 1. X-ray crystal data for compound (±)-4a, (±)-4k and (±)-4t



Compound	(±)-4a
Empirical formula	C <sub>15</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub> F <sub>2</sub>
Formula weight	323.30
Temperature/K	296.15
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a/Å	9.1037(4)
b/Å	18.2464(8)
c/Å	9.7398(5)
α/°	90.00
β/°	105.614(2)
γ/°	90.00
Volume/Å <sup>3</sup>	1558.17(13)
Z	4
ρ <sub>calc</sub> g/cm <sup>3</sup>	1.378
μ/mm <sup>-1</sup>	0.113
F(000)	672.0
Crystal size/mm <sup>3</sup>	0.22 × 0.2 × 0.18
Radiation	MoKα (λ = 0.71073)
θ range for data collection/°	3.110 to 27.550
Index ranges	-11 ≤ h ≤ 11, -23 ≤ k ≤ 23, -12 ≤ l ≤ 12
Reflections collected	23667
Independent reflections	3589 [R <sub>int</sub> = 0.0356, R <sub>sigma</sub> = 0.0277]
Data/restraints/parameters	3589/87/250
Goodness-of-fit on F <sup>2</sup>	1.021
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0483, wR <sub>2</sub> = 0.1174
Final R indexes [all data]	R <sub>1</sub> = 0.0879, wR <sub>2</sub> = 0.1355
Largest diff. peak/hole/e Å <sup>-3</sup>	0.20/-0.18

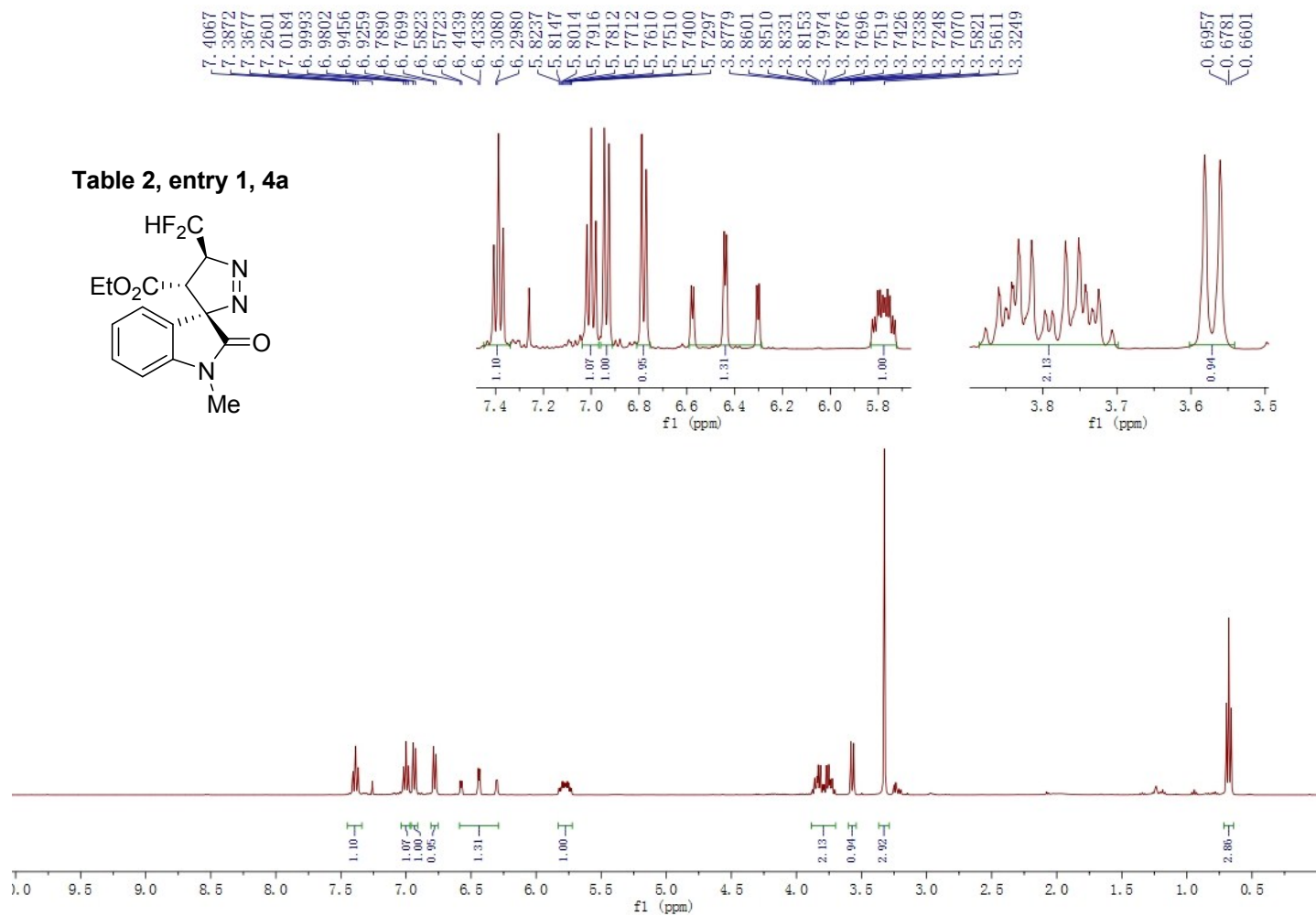


Compound	(±)- <b>4k</b>
Empirical formula	C <sub>16</sub> H <sub>17</sub> F <sub>2</sub> N <sub>3</sub> O <sub>4</sub>
Formula weight	353.32
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.1522(5)
b/Å	9.1400(6)
c/Å	12.4646(8)
α/°	89.726(5)
β/°	76.757(5)
γ/°	63.771(7)
Volume/Å <sup>3</sup>	806.00(10)
Z	2
ρ <sub>calc</sub> g/cm <sup>3</sup>	1.456
μ/mm <sup>-1</sup>	0.121
F(000)	368.0
Crystal size/mm <sup>3</sup>	0.28 × 0.2 × 0.18
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	3.379 to 29.538
Index ranges	-11 ≤ h ≤ 8, -12 ≤ k ≤ 11, -14 ≤ l ≤ 15
Reflections collected	7228
Independent reflections	3757 [R <sub>int</sub> = 0.0249, R <sub>sigma</sub> = 0.0439]
Data/restraints/parameters	3757/0/229
Goodness-of-fit on F <sup>2</sup>	1.052
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0467, wR <sub>2</sub> = 0.1074
Final R indexes [all data]	R <sub>1</sub> = 0.0566, wR <sub>2</sub> = 0.1151
Largest diff. peak/hole/e Å <sup>-3</sup>	0.36/-0.38



Compound	(±)-4t
Empirical formula	C <sub>20</sub> H <sub>17</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>
Formula weight	385.36
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a/Å	10.7505(5)
b/Å	12.0115(5)
c/Å	14.5754(7)
α/°	90
β/°	106.876(5)
γ/°	90
Volume/Å <sup>3</sup>	1801.05(14)
Z	4
ρ <sub>calc</sub> g/cm <sup>3</sup>	1.421
μ/mm <sup>-1</sup>	0.111
F(000)	800.0
Crystal size/mm <sup>3</sup>	0.3 × 0.25 × 0.2
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	3.257 to 29.502
Index ranges	-14 ≤ h ≤ 13, -16 ≤ k ≤ 16, -19 ≤ l ≤ 19
Reflections collected	15974
Independent reflections	4427 [R <sub>int</sub> = 0.0448, R <sub>sigma</sub> = 0.0446]
Data/restraints/parameters	4427/0/254
Goodness-of-fit on F <sup>2</sup>	1.030
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0461, wR <sub>2</sub> = 0.1027
Final R indexes [all data]	R <sub>1</sub> = 0.0580, wR <sub>2</sub> = 0.1117
Largest diff. peak/hole/e Å <sup>-3</sup>	0.38/-0.30

2.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{19}\text{F}$  NMR spectra of ( $\pm$ )-4a-u



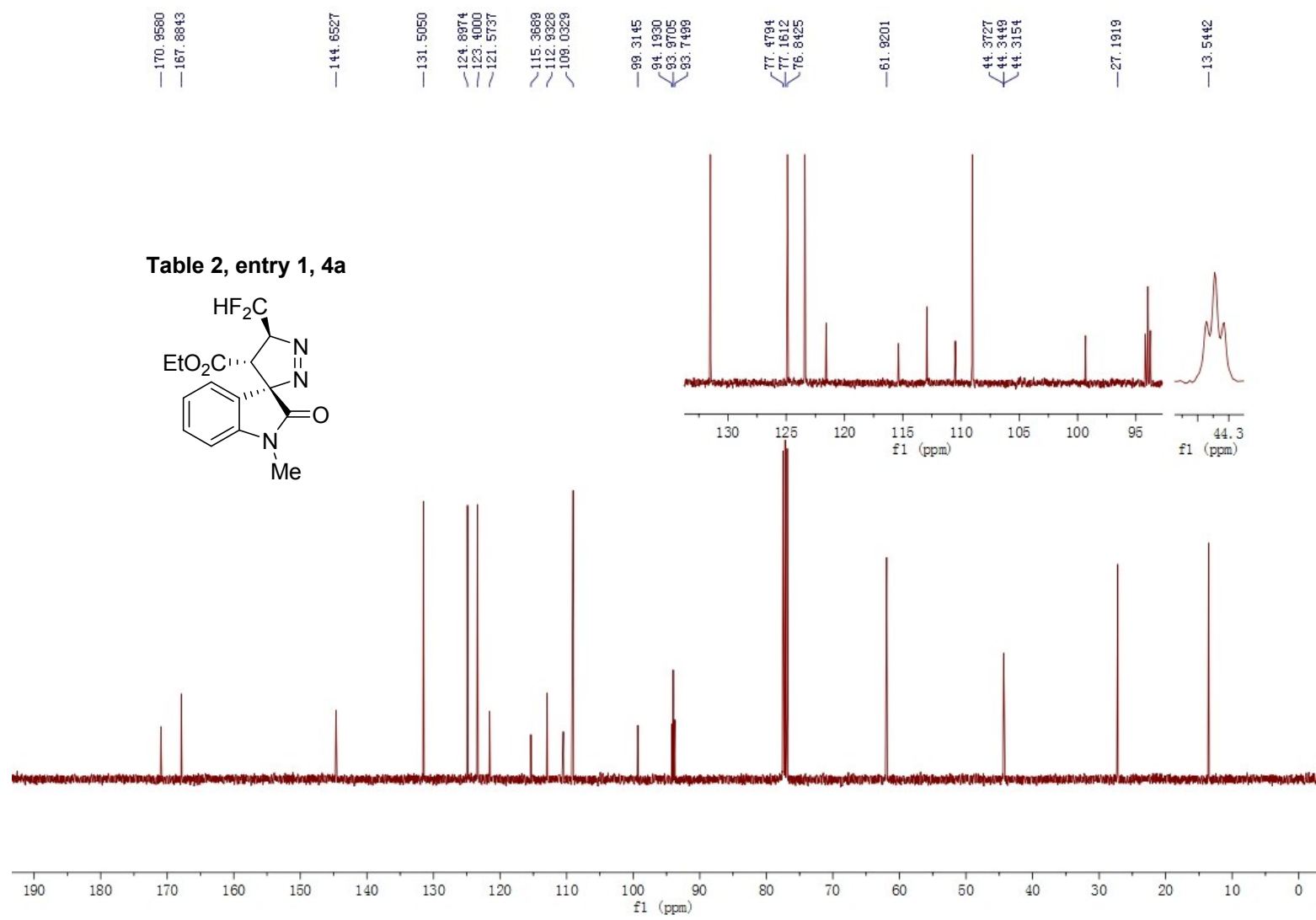
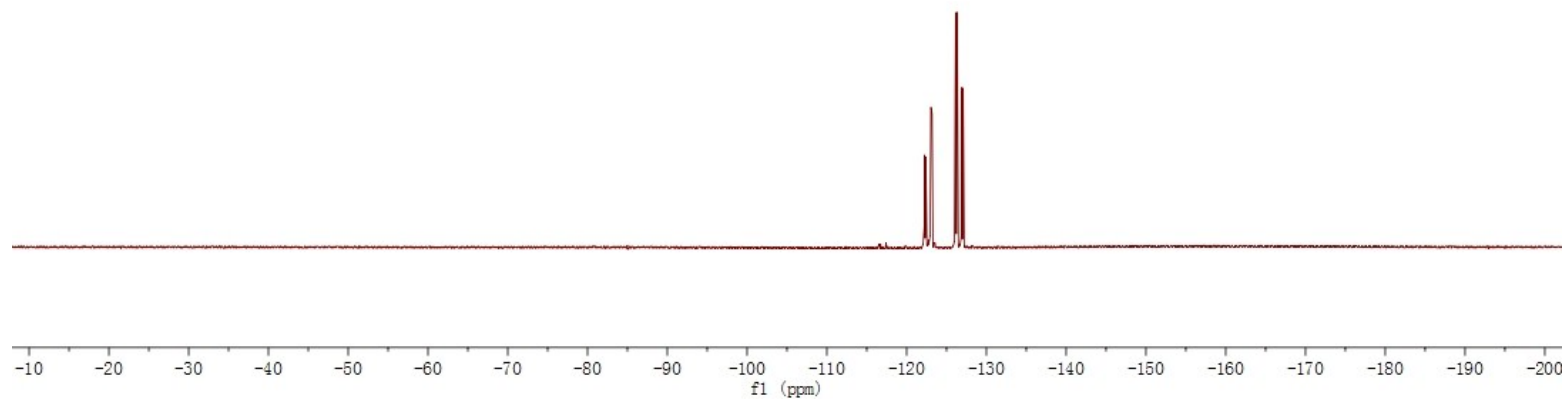
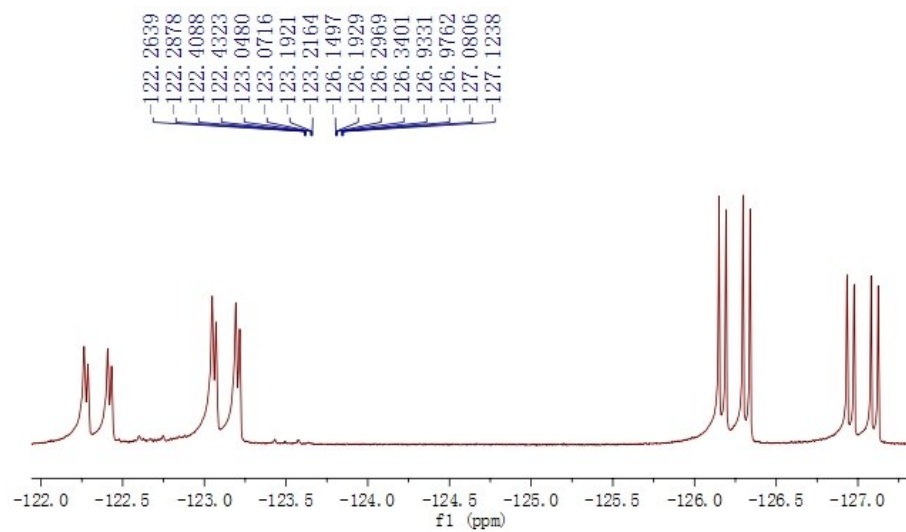
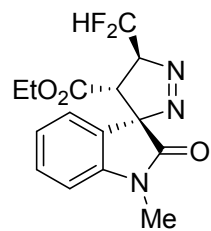
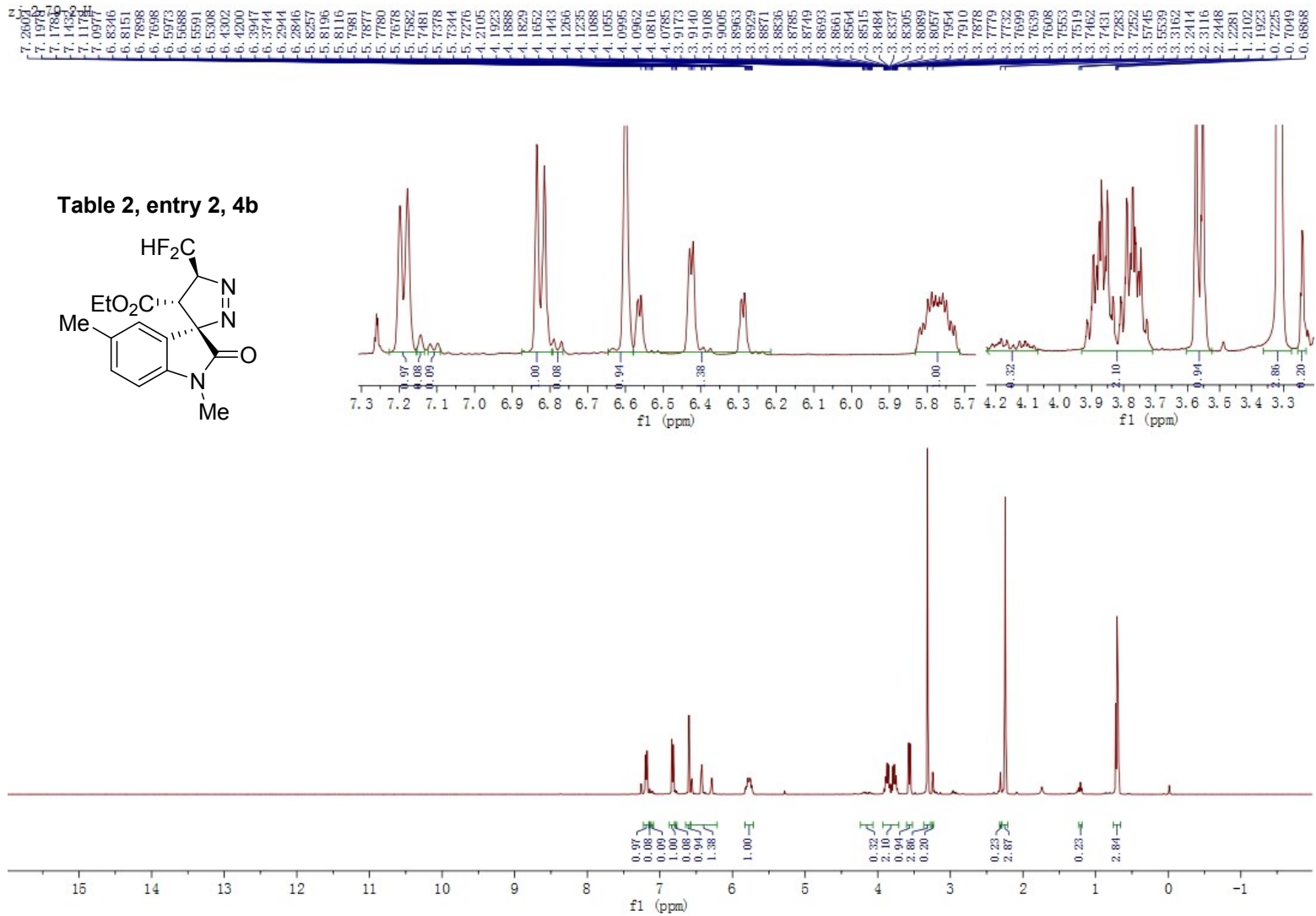


Table 2, entry 1, 4a







zj-2-79-2-C

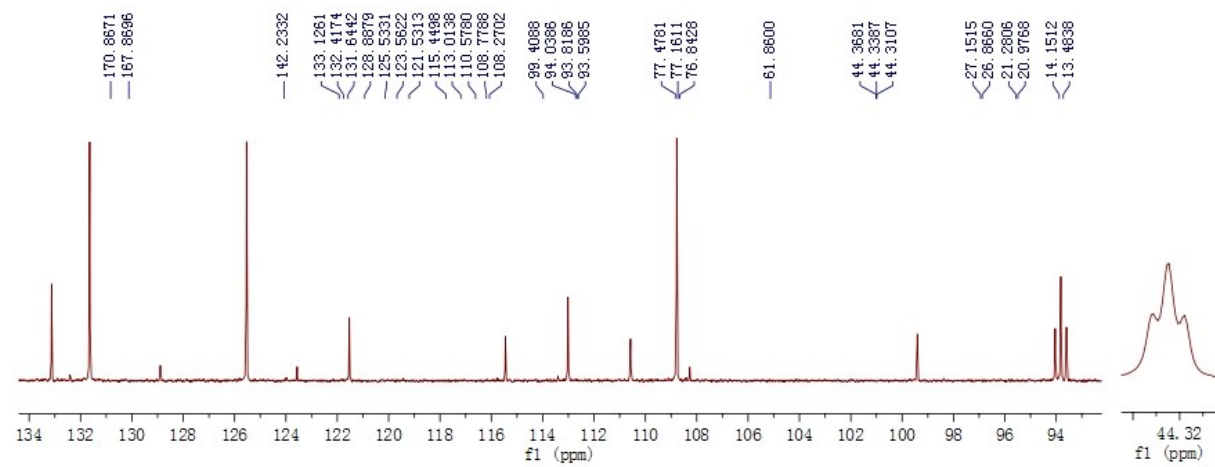
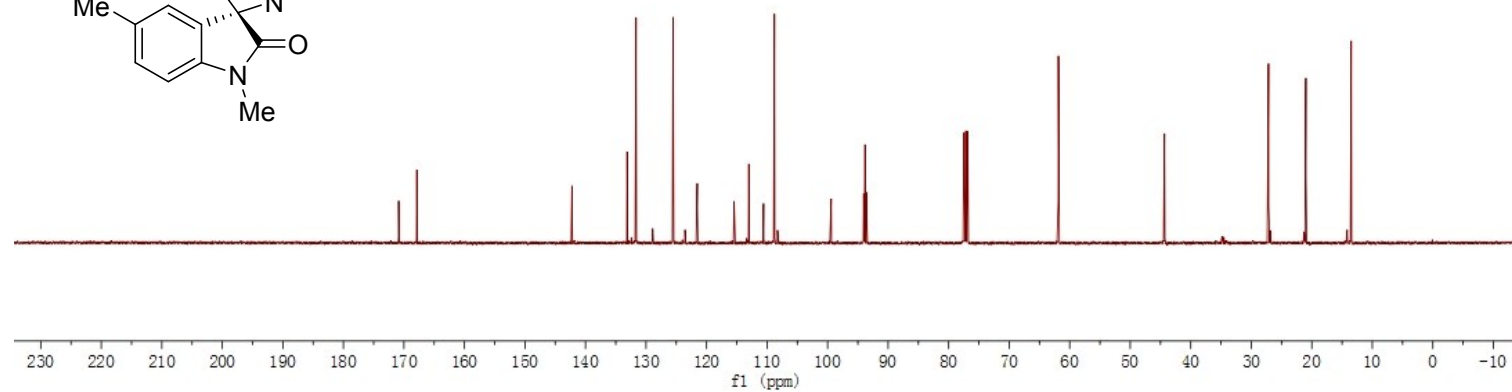
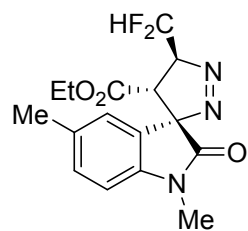


Table 2, entry 2, 4b



zj-2-20-2-F

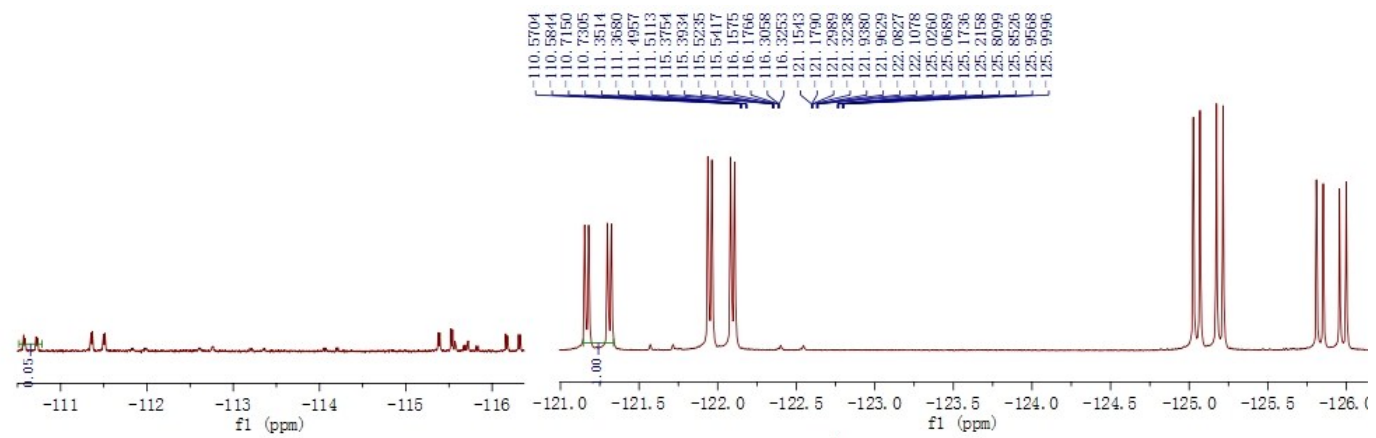
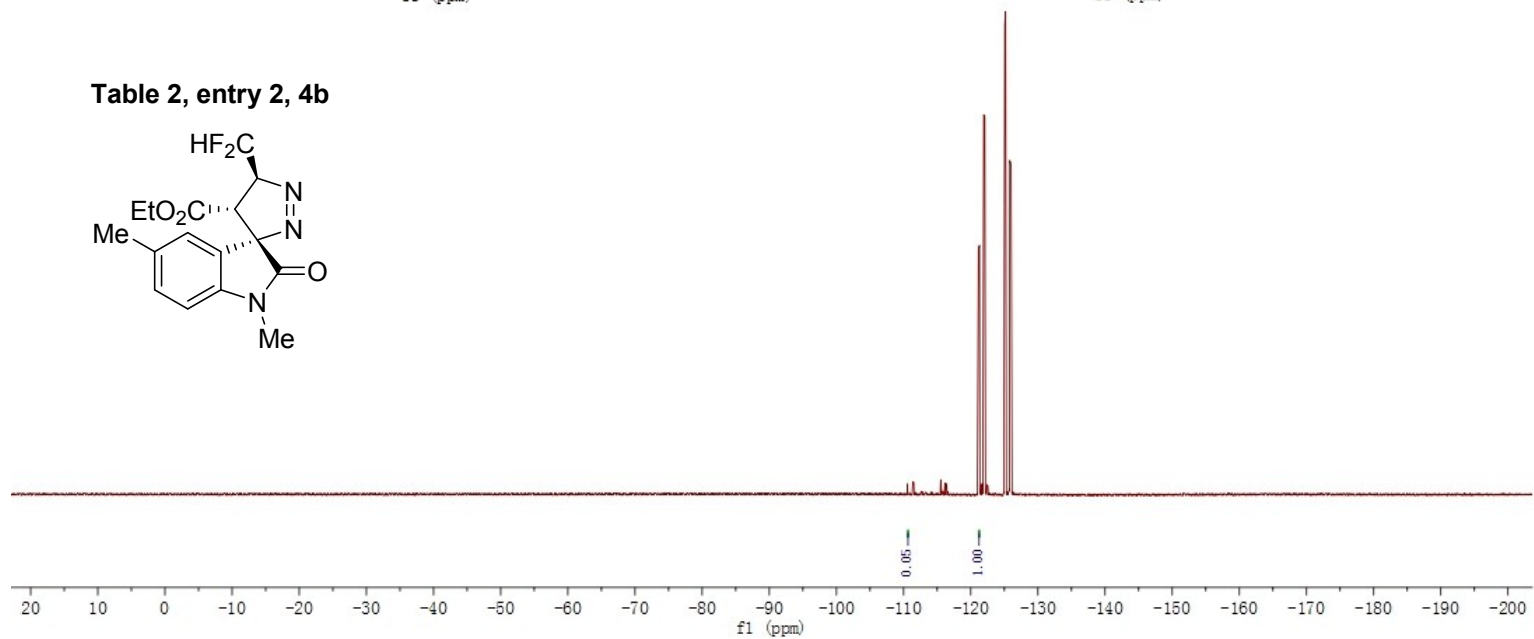
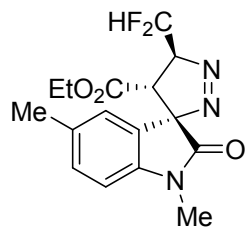
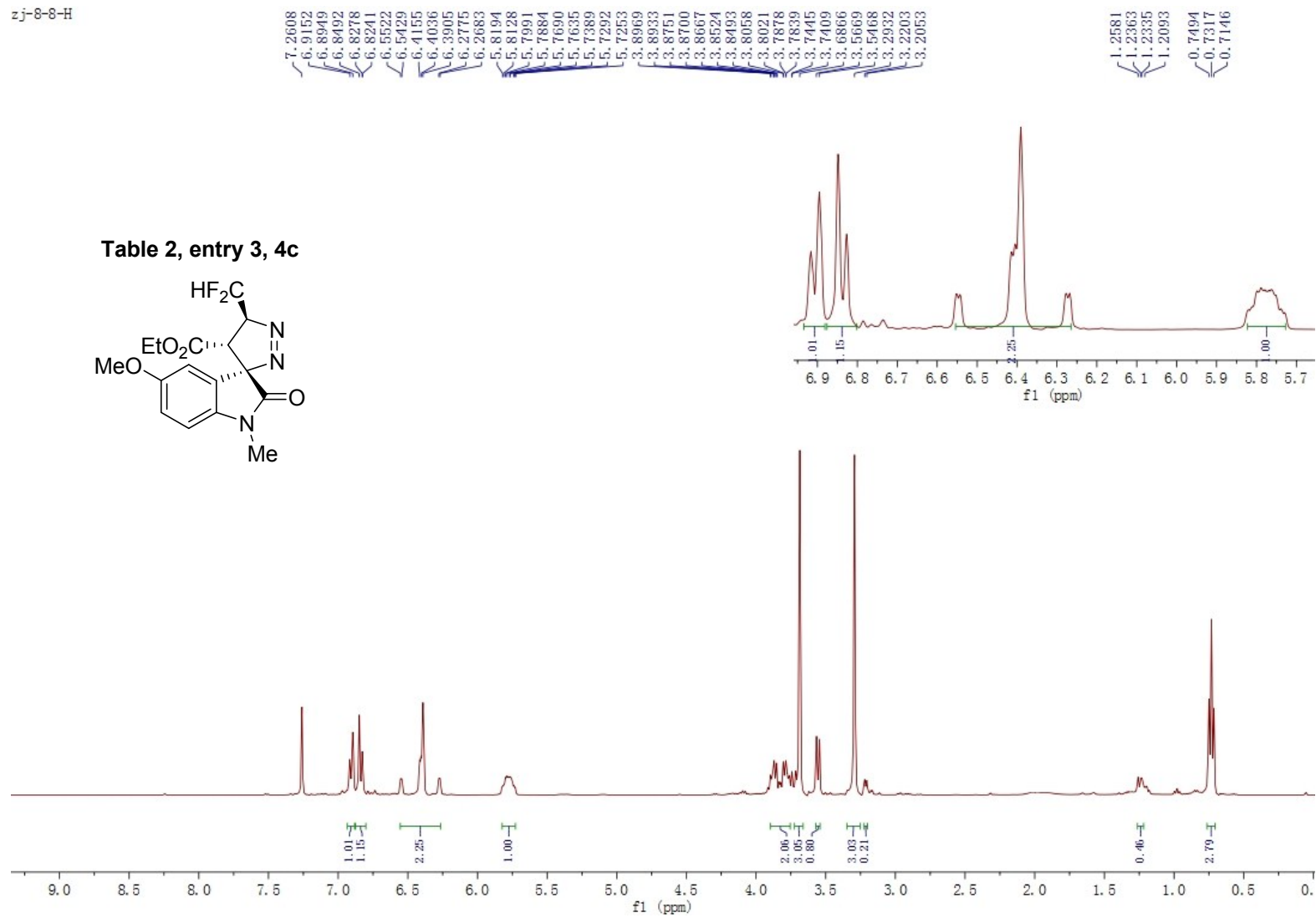
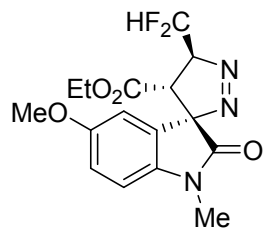


Table 2, entry 2, 4b



zj-8-8-H

Table 2, entry 3, 4c



zj-8-8-C

— 170.5663  
— 167.8079

— 156.3191

— 137.9256

— 122.4819  
— 115.9248  
— 115.4297  
— 112.9945  
— 111.9788  
— 110.5591  
— 109.4917

— 99.6107  
— 94.1799  
— 93.9597  
— 93.7393

— 77.4791  
— 77.1604  
— 76.8420

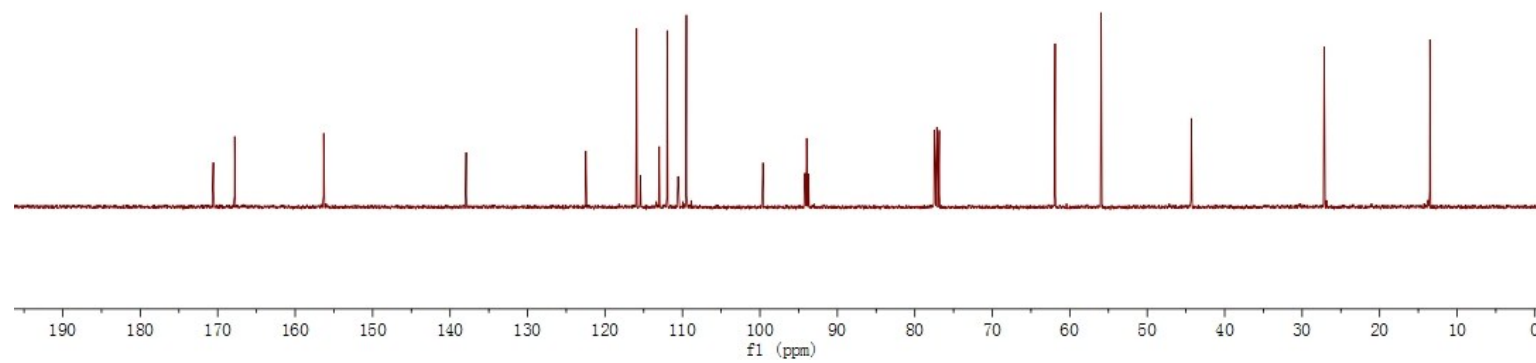
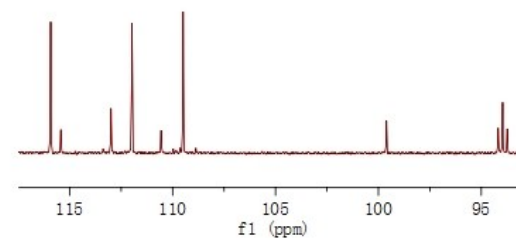
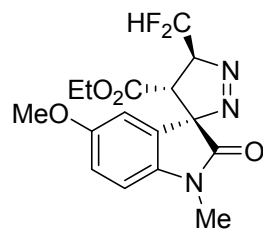
— 61.8888  
— 55.9418

— 44.3238  
— 44.2947  
— 44.2656

— 27.1478

— 13.5048

Table 2, entry 3, 4c



zj-2-76-2-F  
STANDARD FLUORINE PARAMETERS

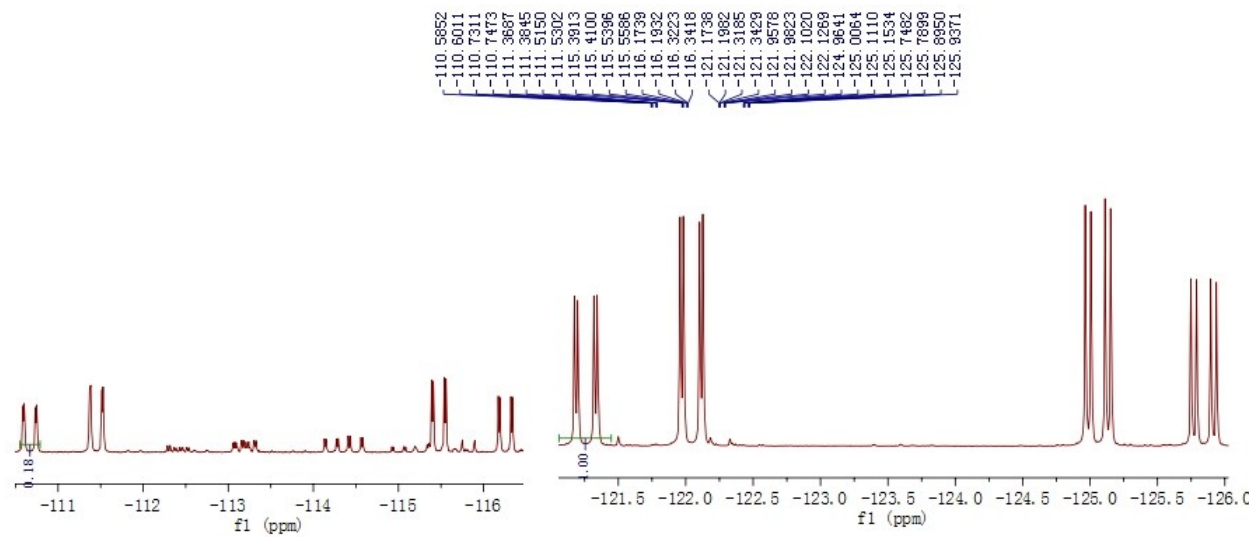
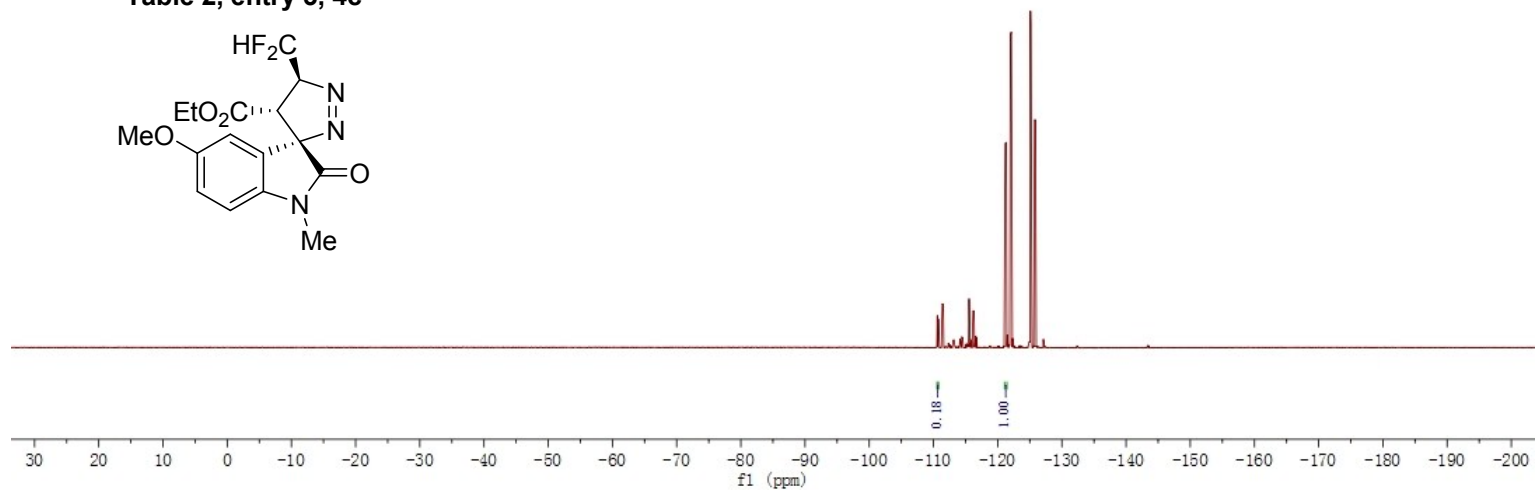
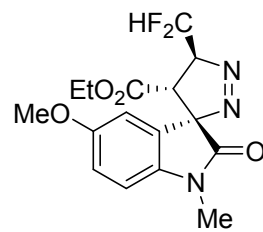


Table 2, entry 3, 4c

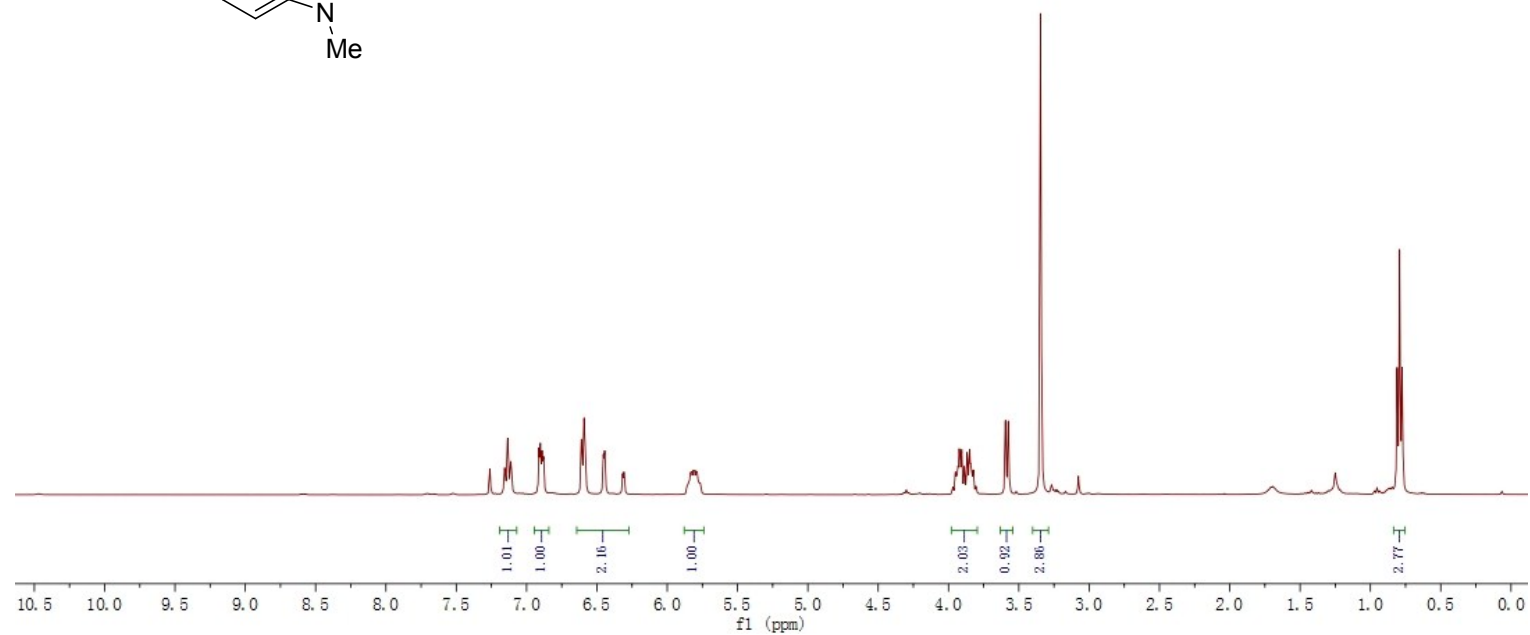
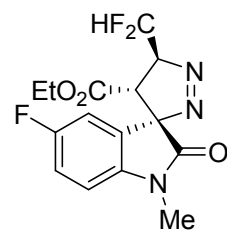


zj-2-22-2-H

7.2599  
7.1563  
7.1347  
7.1130  
6.8105  
6.8018  
6.8001  
6.8086  
6.8100  
6.8046  
6.5917  
6.4545  
6.4444  
6.3165  
6.3079  
5.8565  
5.8467  
5.8358  
5.8263  
5.8162  
5.8059  
5.7964  
5.7860  
5.7815  
5.7771  
5.7746  
5.7654  
3.9671  
3.9490  
3.9227  
3.9047  
3.8870  
3.8702  
3.8662  
3.8597  
3.8527  
3.8455  
3.8236  
3.8082  
3.8047  
3.5939  
3.5738  
3.3443

0.8104  
0.7926  
0.7749

Table 2, entry 4, 4d



zj-2-22-2-c

170.6224  
167.7488

160.3689  
157.9461

140.7364

122.8532  
122.7711  
117.9523  
117.7195  
115.2561  
113.4086  
113.1533  
112.8177  
110.3805  
109.7323  
109.6527  
99.3853  
94.7672  
94.5456  
94.3218

77.4777  
77.1602  
76.8417

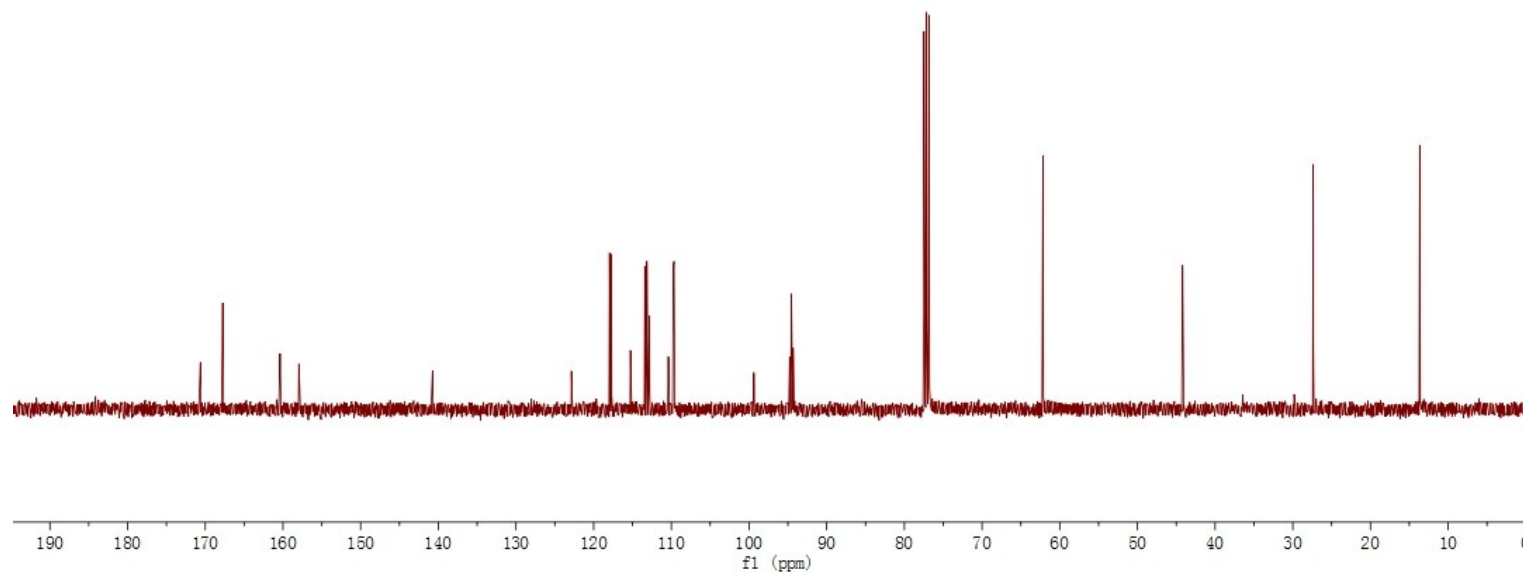
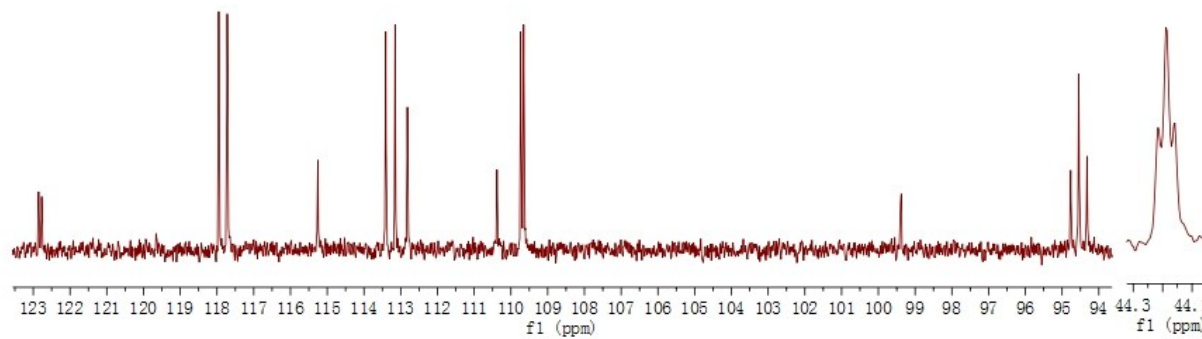
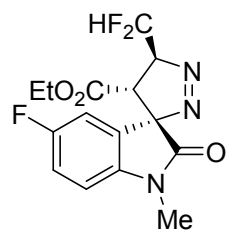
62.1573

44.2157  
44.1879  
44.1588

27.3645

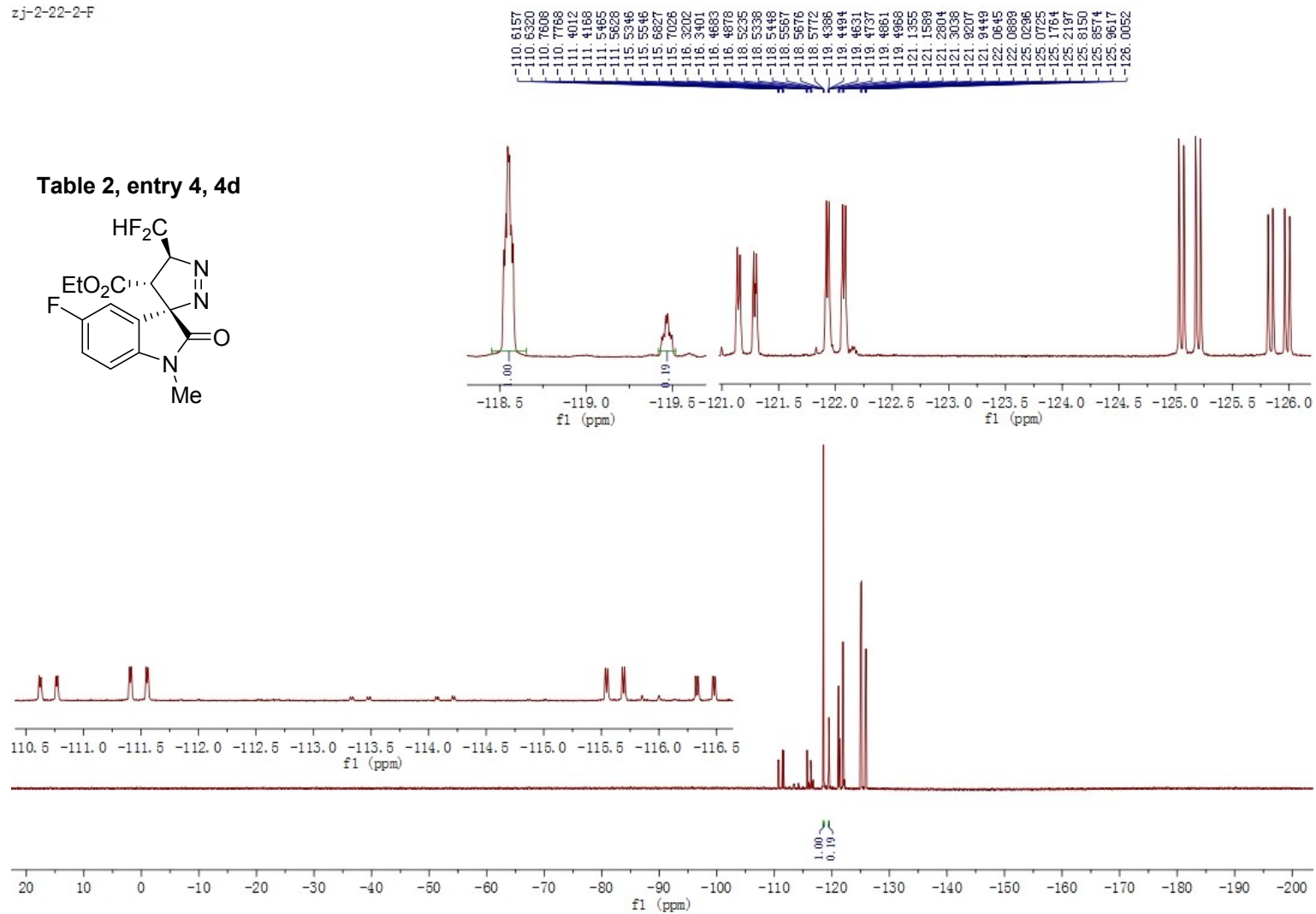
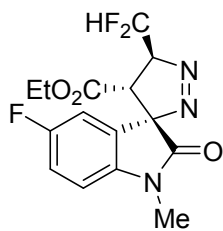
13.6578

Table 2, entry 4, 4d



zj-2-22-2-F

Table 2, entry 4, 4d



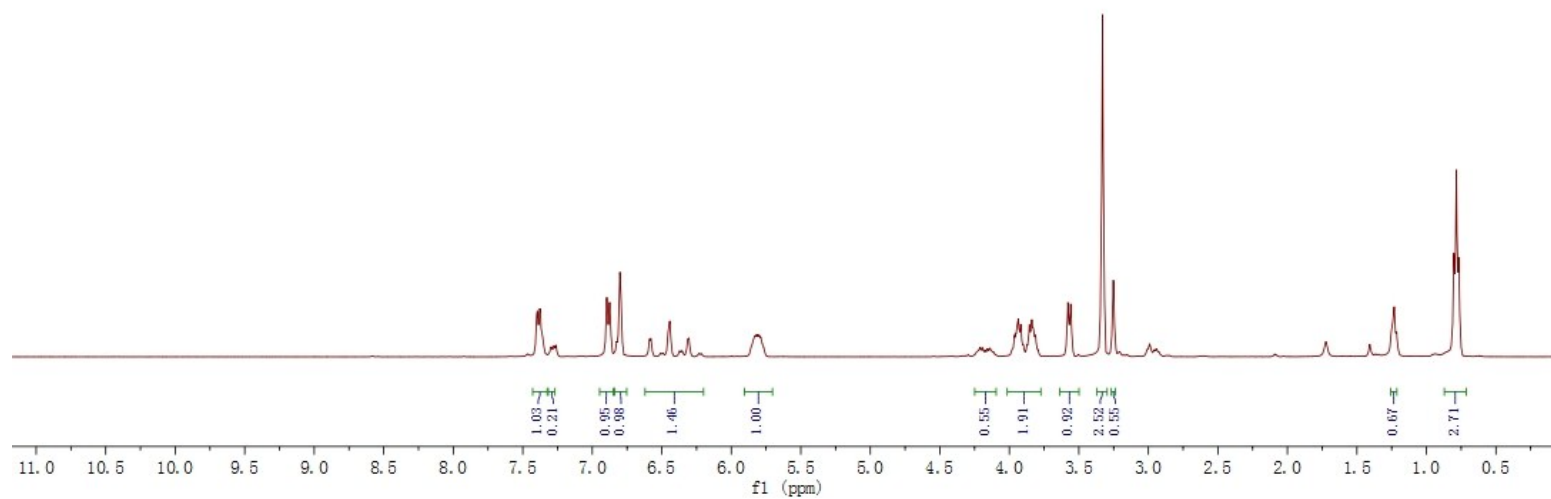
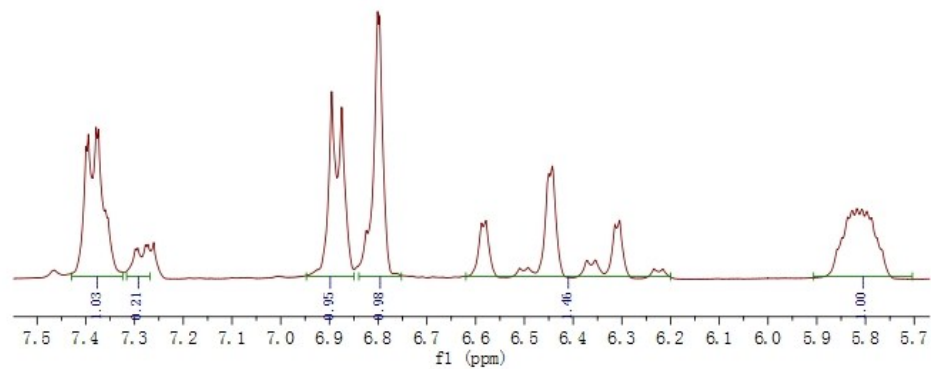
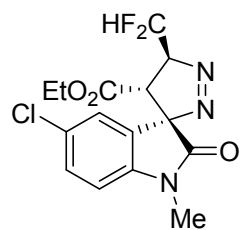


zj-2-132-1-H-6-C1

7.3899  
7.3843  
7.3791  
7.3740  
7.3594  
7.3542  
7.2887  
7.2831  
7.2779  
7.2724  
7.2612  
6.8951  
6.8745  
6.8247  
6.8017  
6.7954  
6.5882  
6.5782  
6.5094  
6.4823  
6.4518  
6.4417  
6.3717  
6.3542  
6.3143  
6.3042  
6.2337  
6.2160  
5.8580  
5.8484  
5.8324  
5.8170  
5.8074  
5.8014  
5.7973  
5.7876  
5.7652  
5.7103  
4.2556  
4.2263  
4.2086  
4.1904  
4.1565  
4.1387  
4.1119  
3.9629  
3.9537  
3.9356  
3.9180  
3.8562  
3.8470  
3.8382  
3.8379  
3.8203  
3.8112  
3.5783  
3.5585  
3.5503  
3.2514

1.2498  
1.2315  
0.8024  
0.7848  
0.7674

Table 2, entry 5, 4e



zj-2-104-2-2-C

—170.4961  
—167.6538

—143.2578

131.3714  
128.8092  
128.6114  
128.3391  
125.3980  
123.5213  
123.0740  
115.2385  
112.8013  
110.8626  
110.0067  
108.4259

—99.1398  
—94.7728  
—94.5505  
—94.3282

77.4778  
77.1600  
76.8426

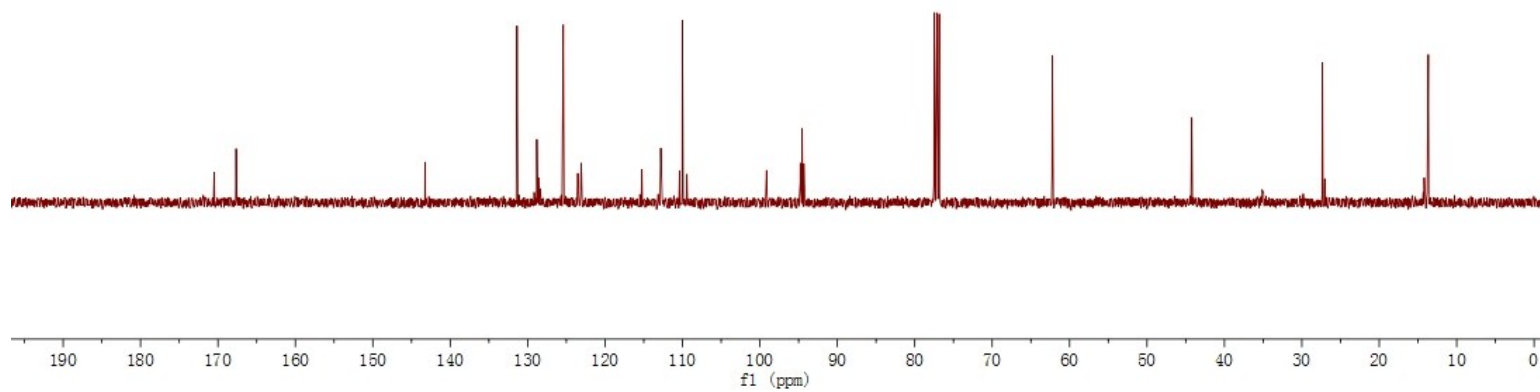
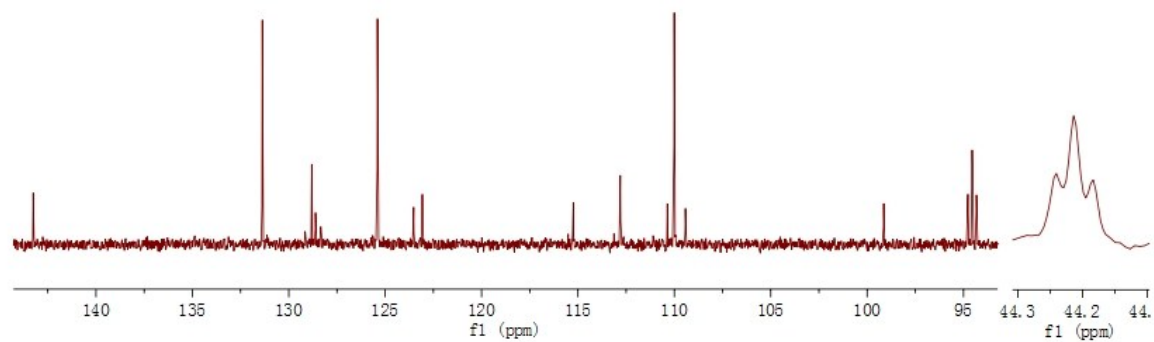
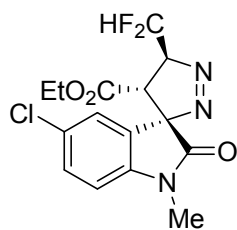
—62.2326

44.2420  
44.2136  
44.1638

—27.3451  
—27.0346

14.1947  
13.6625

Table 2, entry 5, 4e



zj-2-104-2-2-F  
STANDARD FLUORINE PARAMETERS

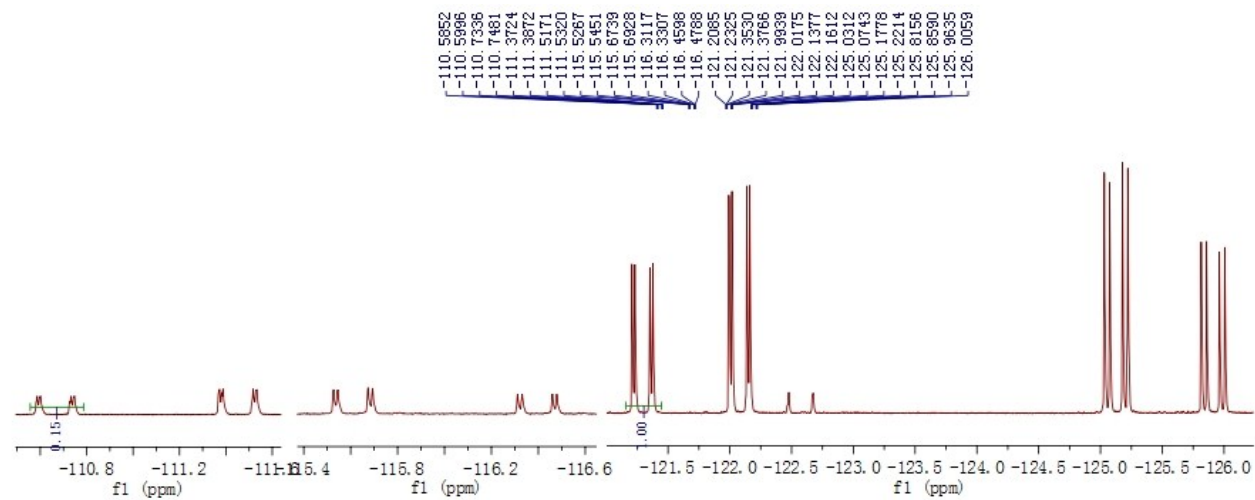
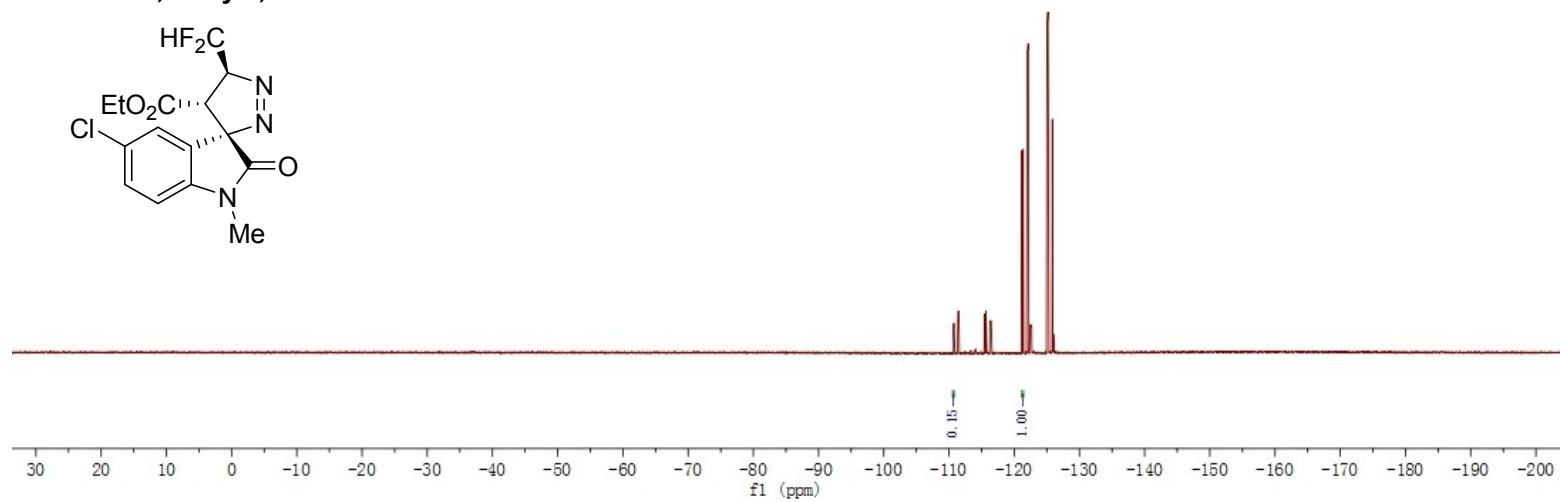
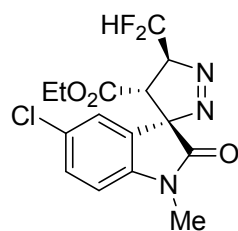
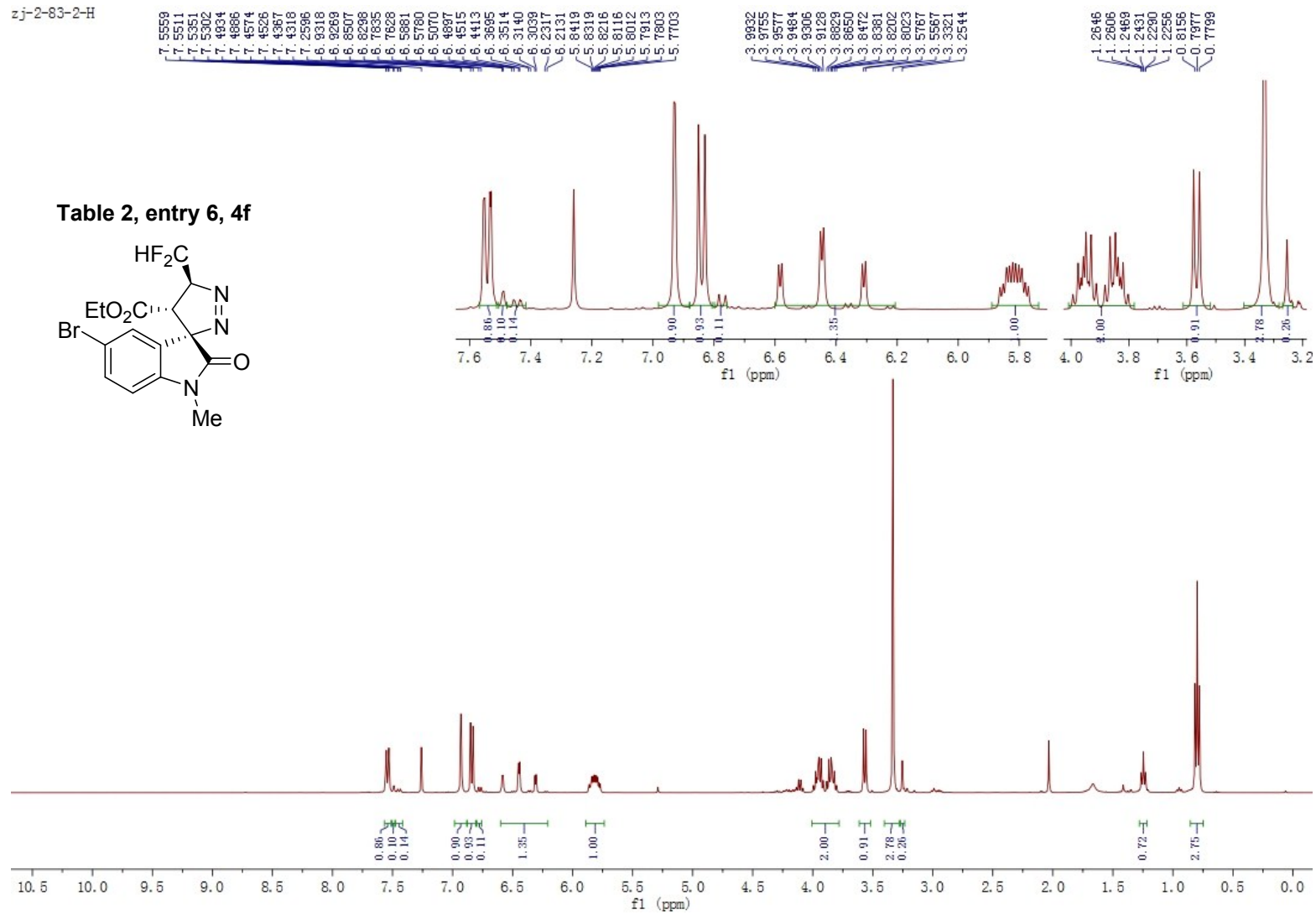
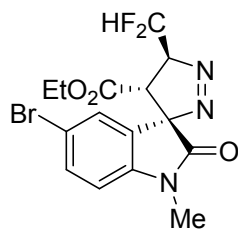


Table 2, entry 5, 4e



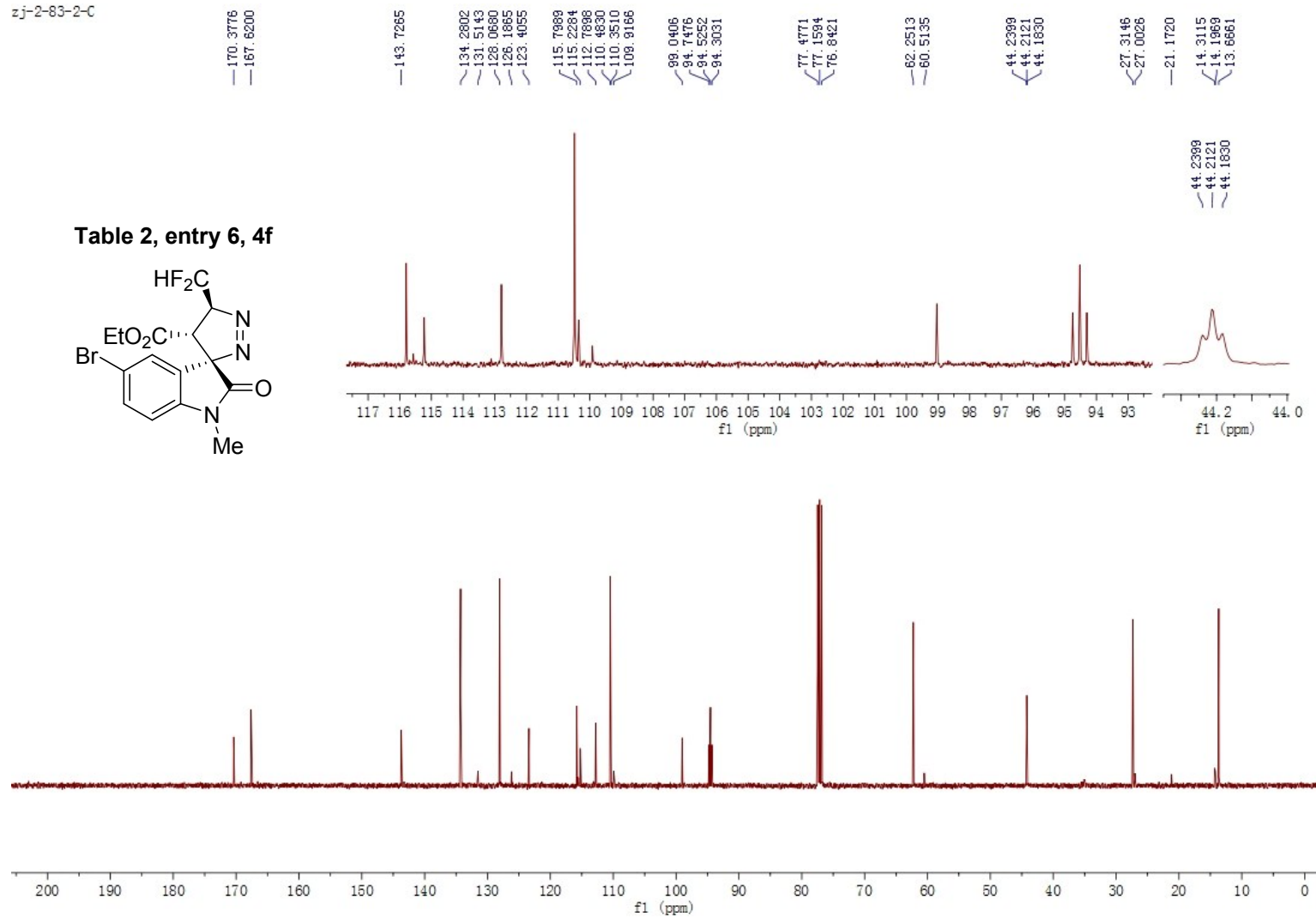
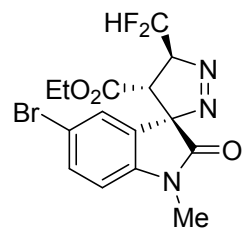
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Table 2, entry 6, 4f



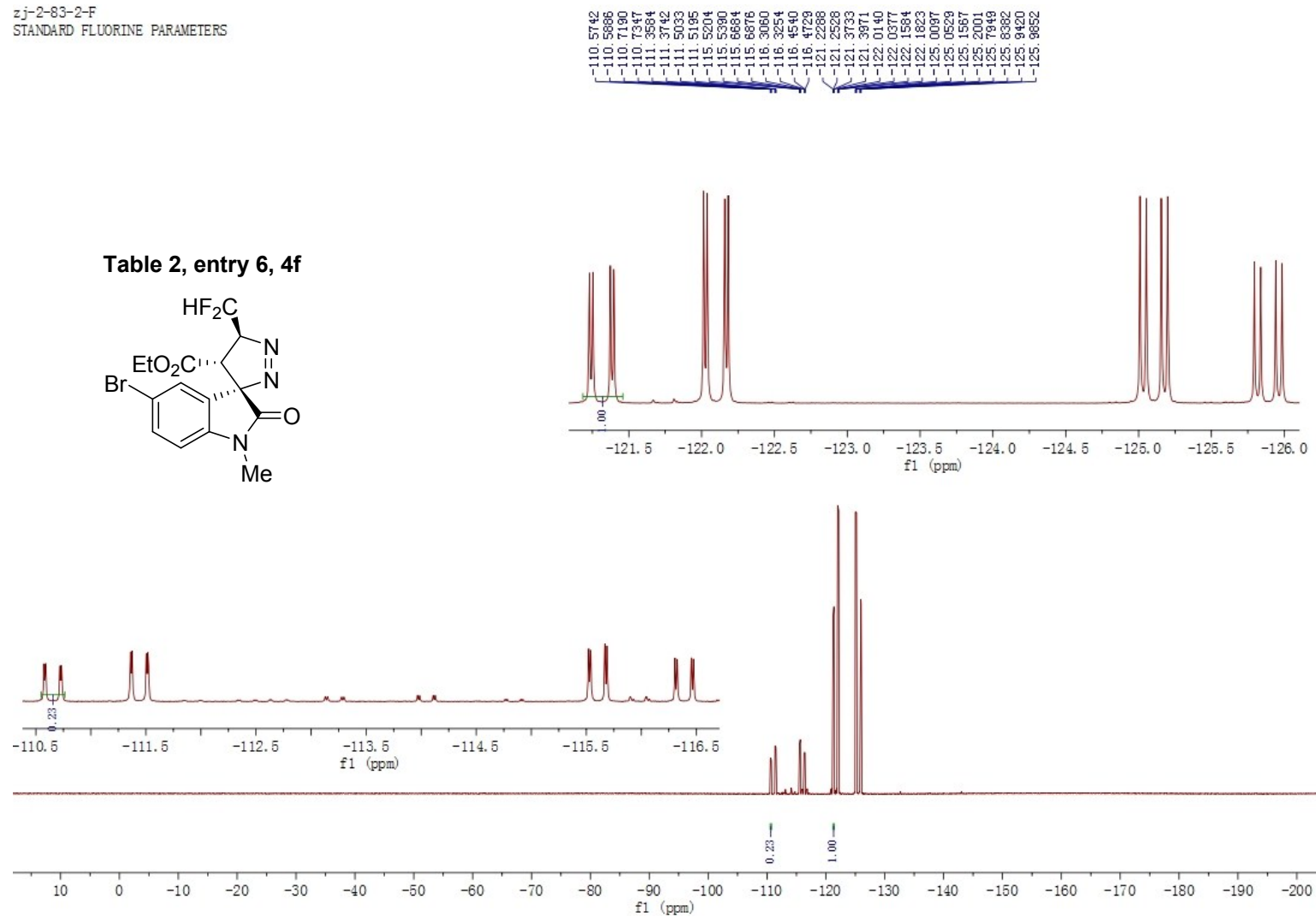
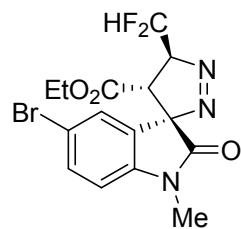
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Table 2, entry 6, 4f



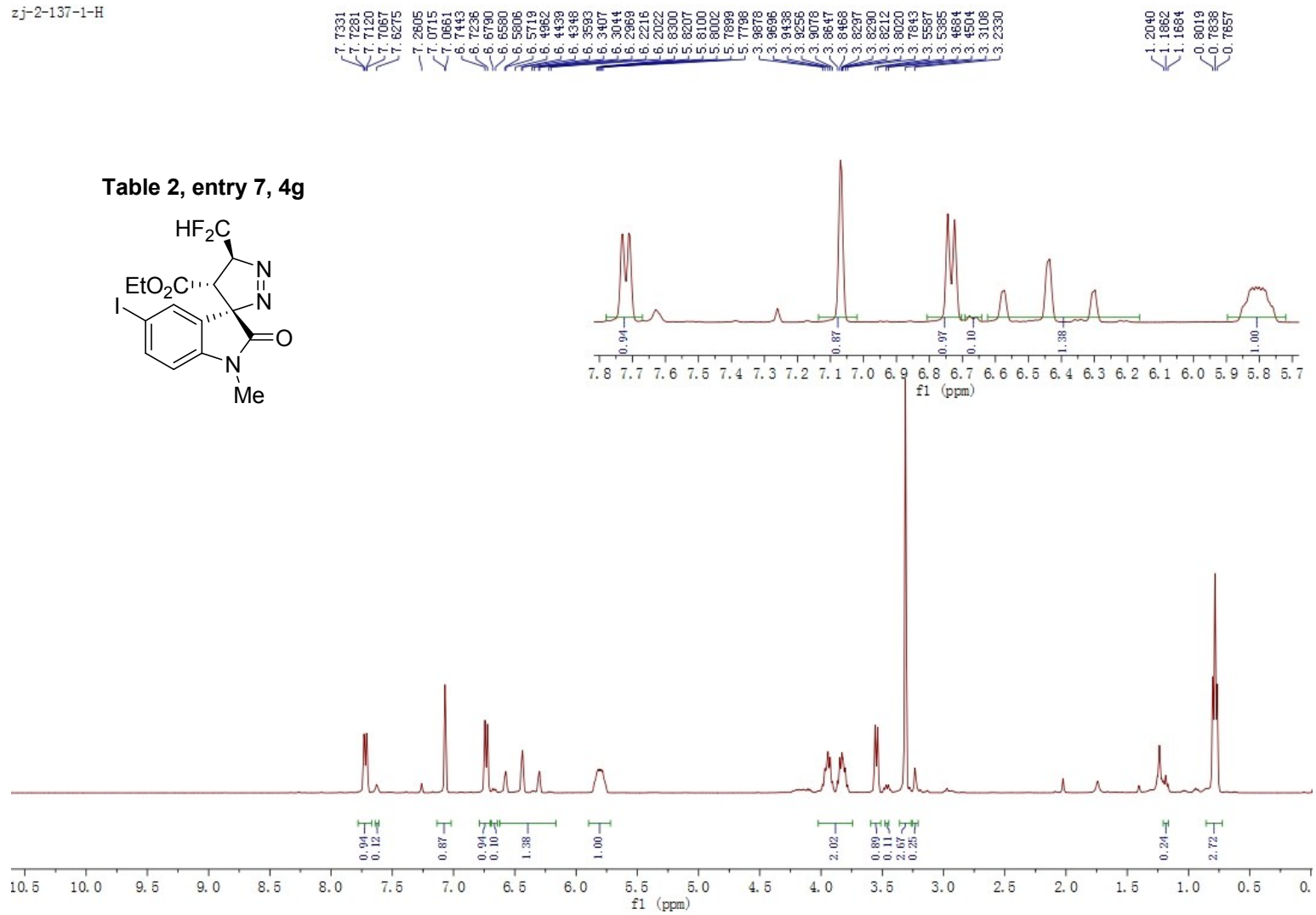
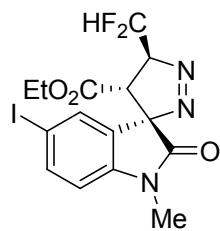
zj-2-83-2-F  
STANDARD FLUORINE PARAMETERS

Table 2, entry 6, 4f



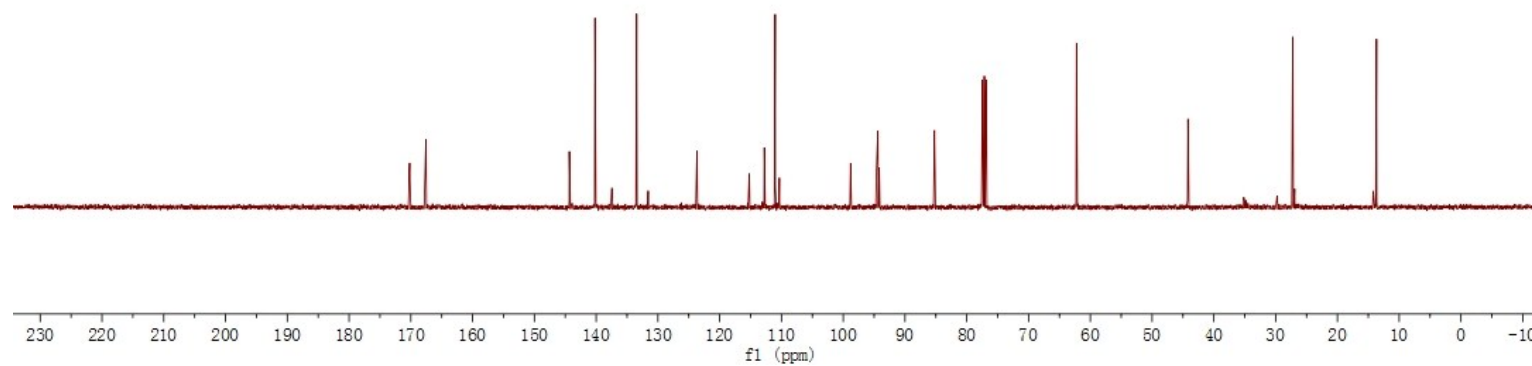
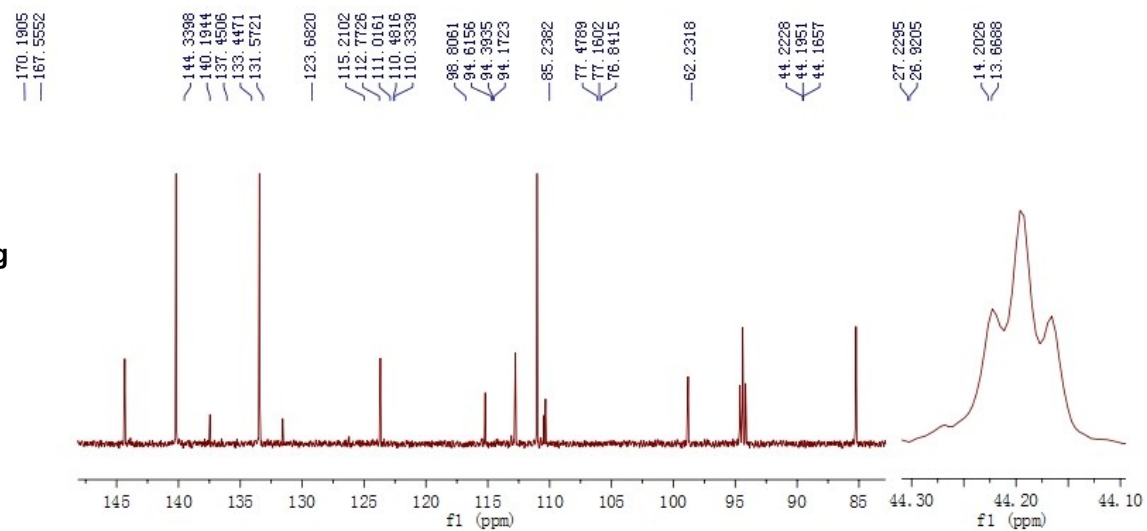
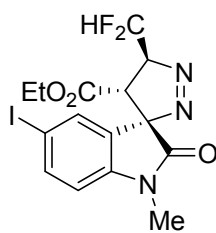
zj-2-137-1-H

Table 2, entry 7, 4g



zj-2-137-2-C

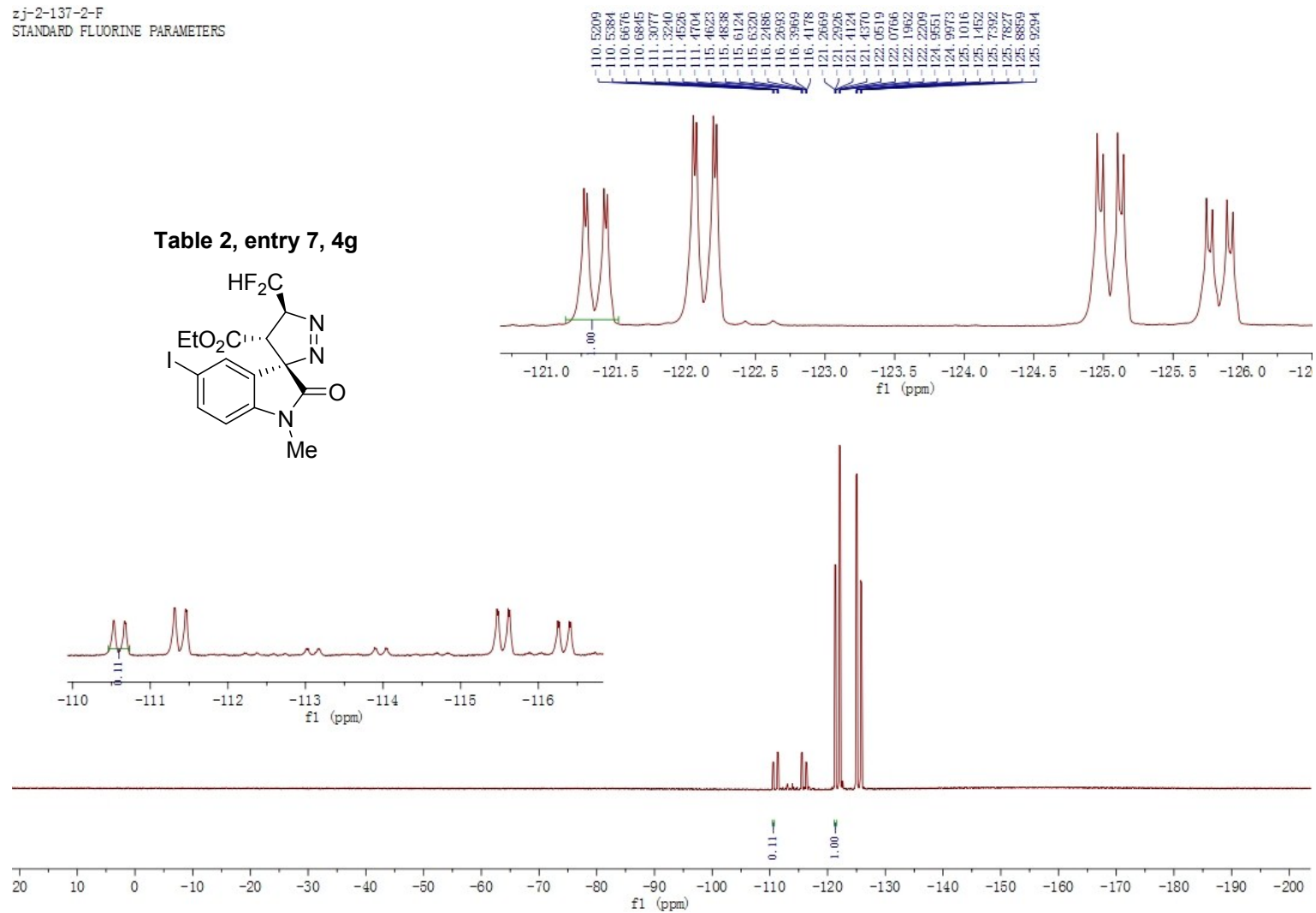
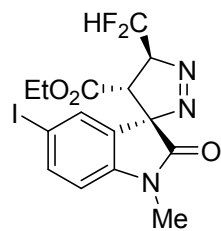
Table 2, entry 7, 4g





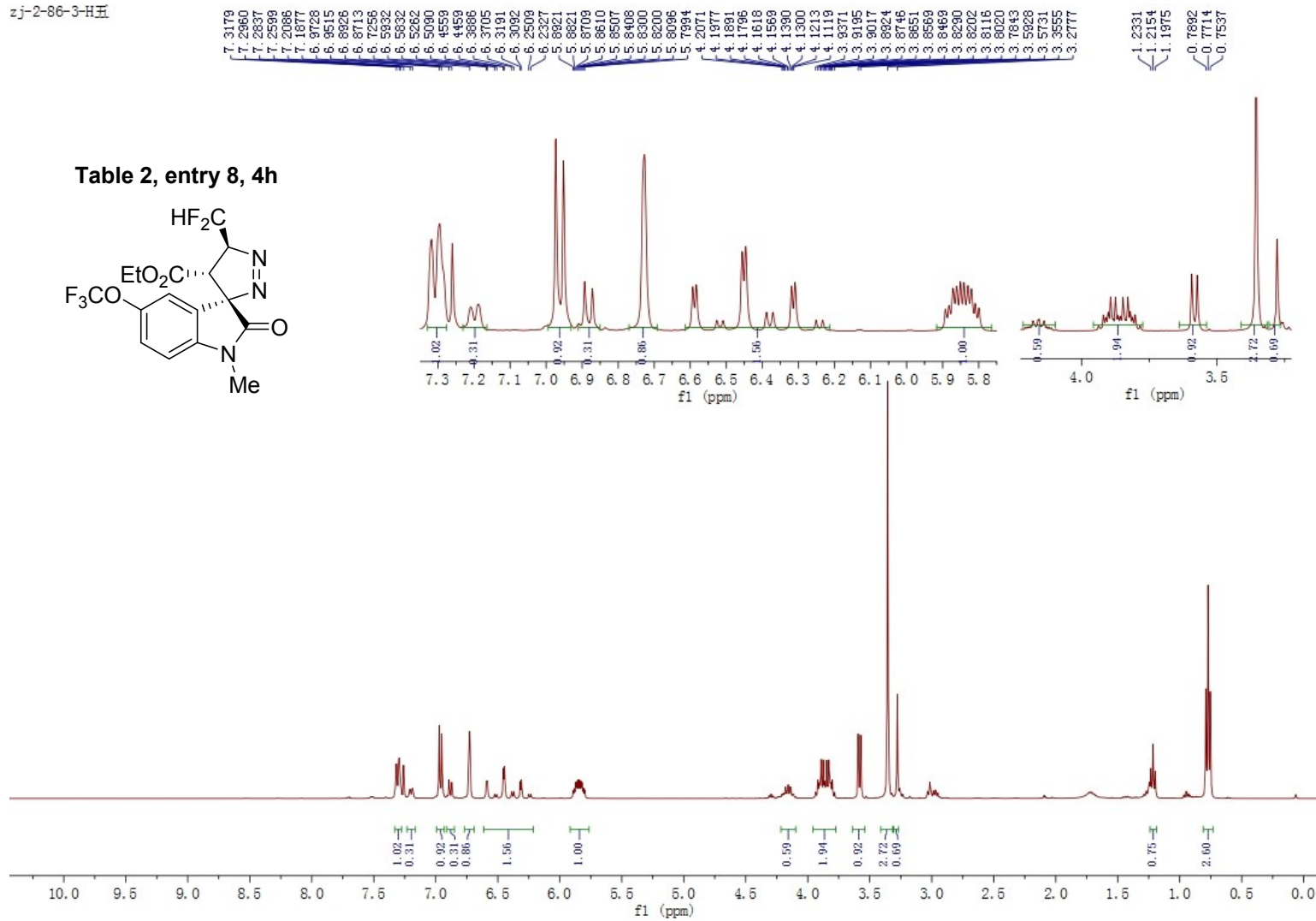
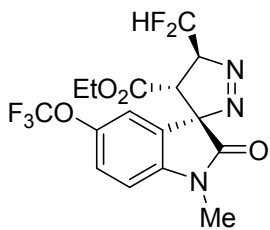
zj-2-137-2-F  
STANDARD FLUORINE PARAMETERS

Table 2, entry 7, 4g



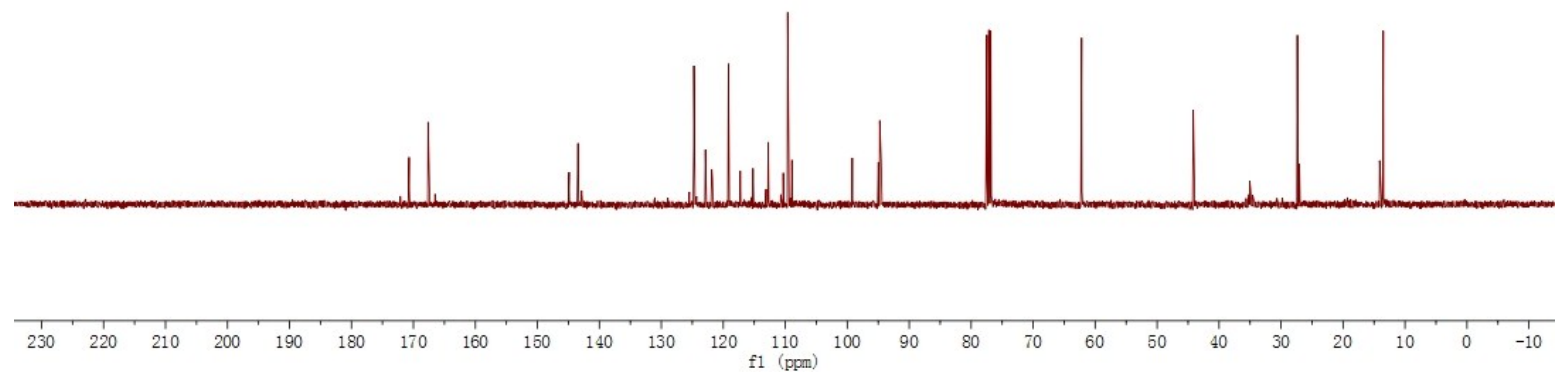
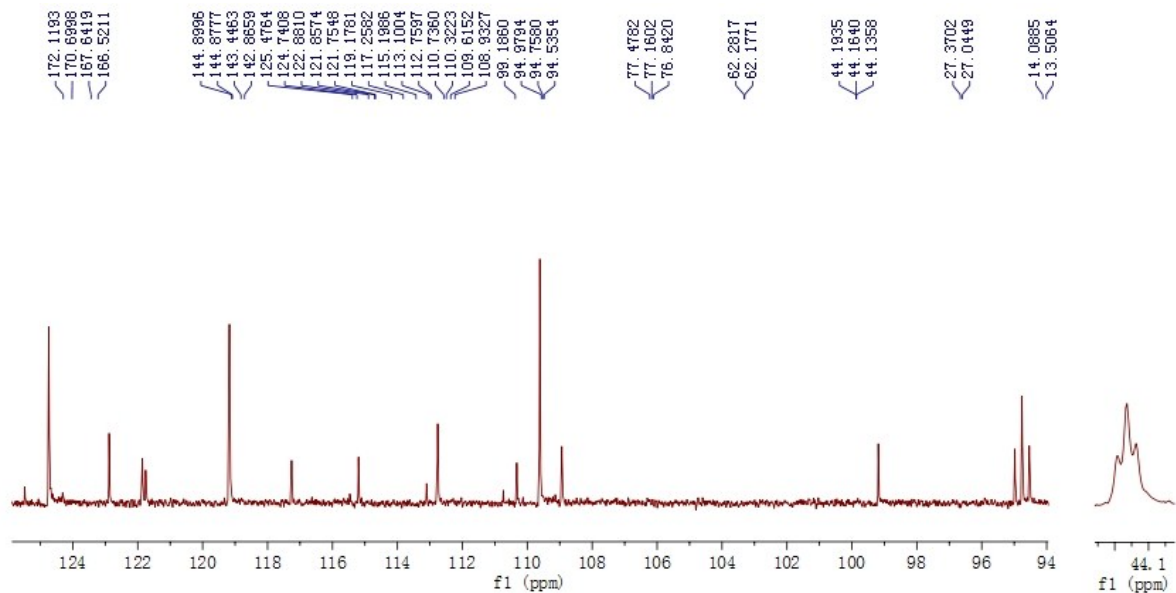
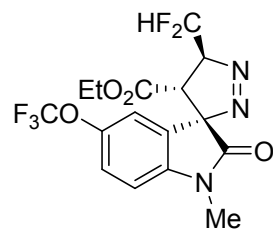
zj-2-86-3-HH

Table 2, entry 8, 4h



zj-2-86-3-C

Table 2, entry 8, 4h



zj-2-86-3-F  
STANDARD FLUORINE PARAMETERS

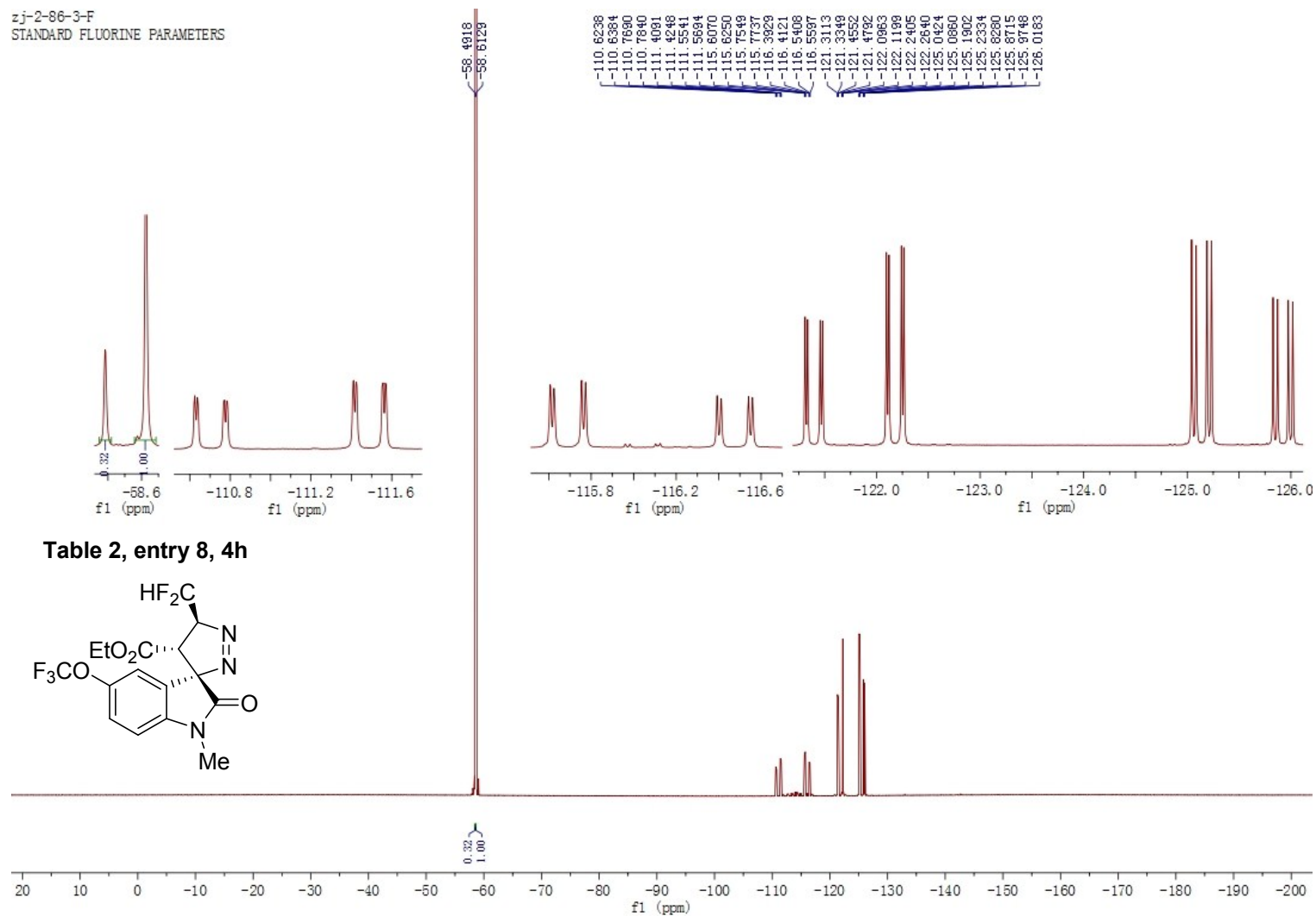
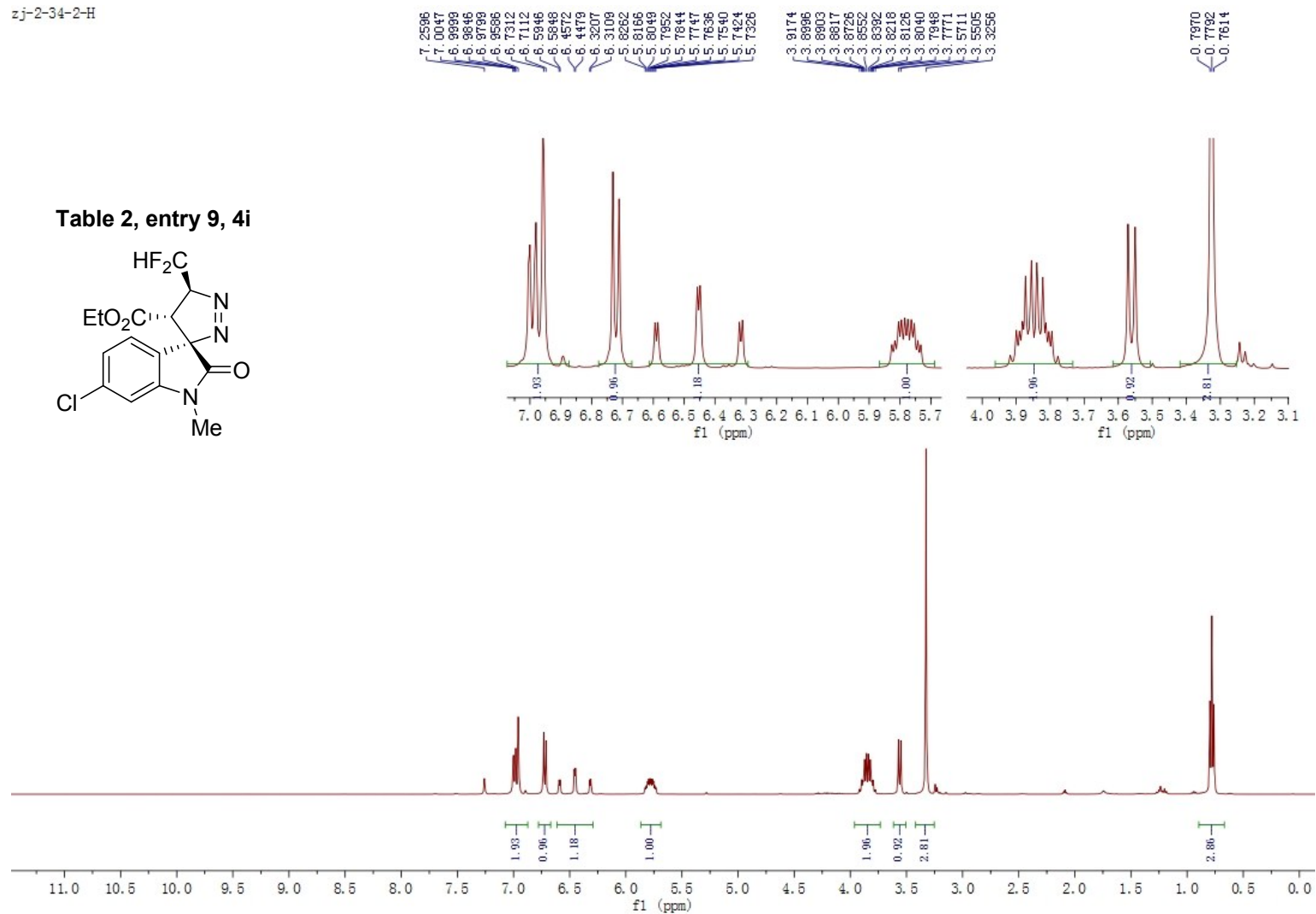
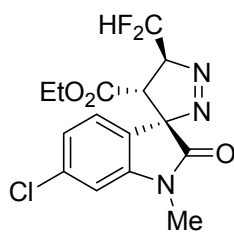


Table 2, entry 8, 4h

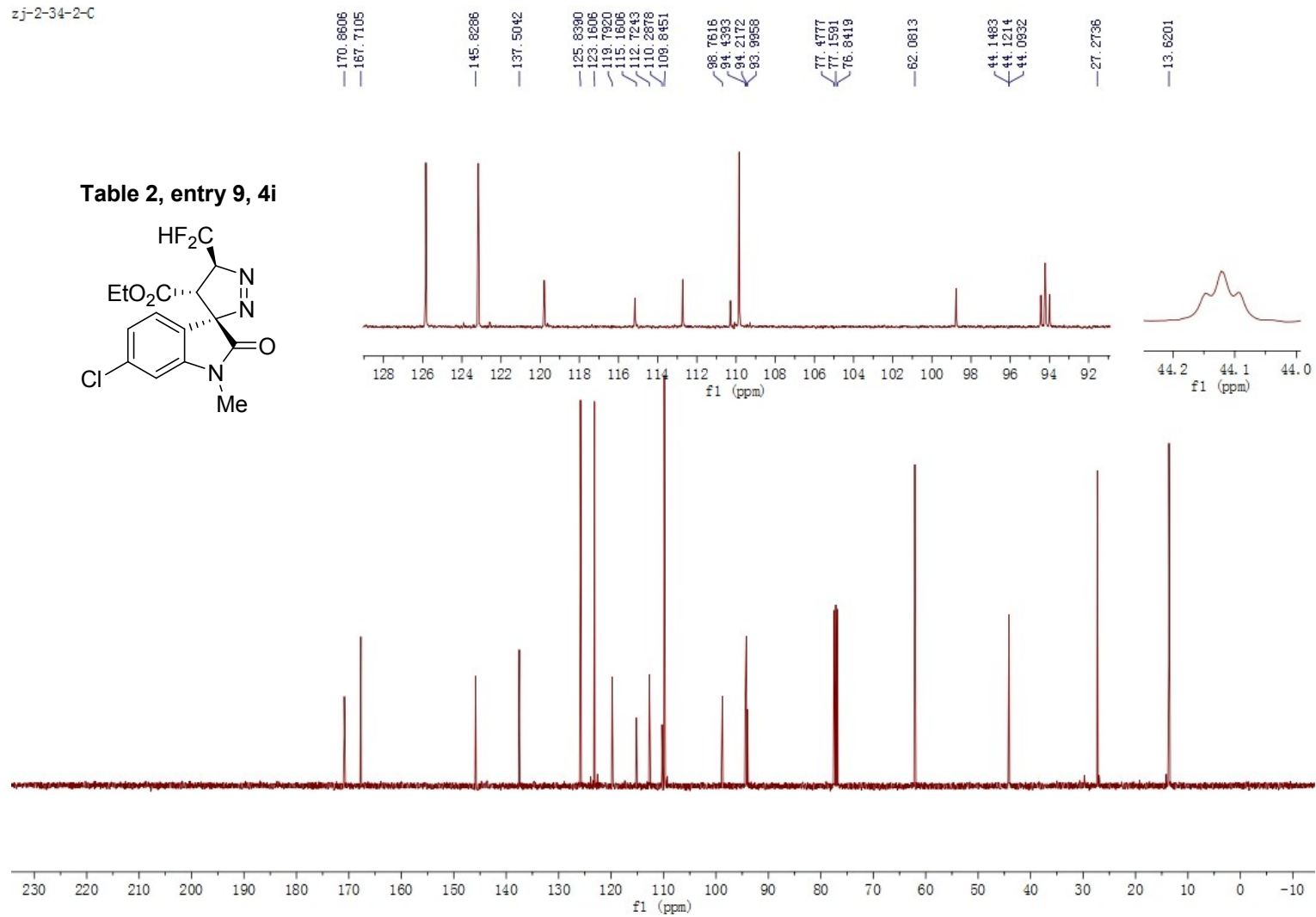
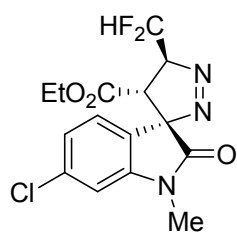
zj-2-34-2-H

Table 2, entry 9, 4i



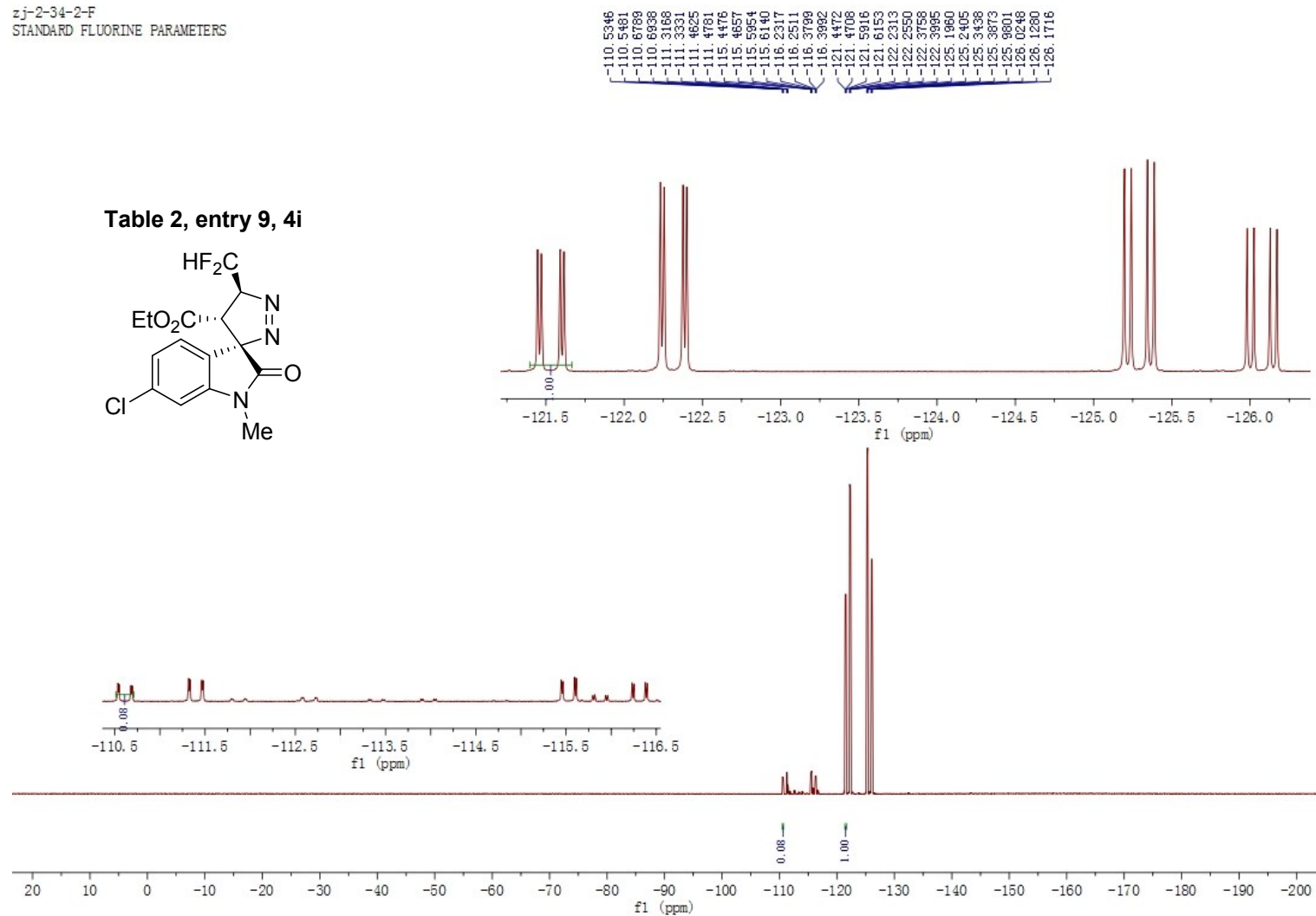
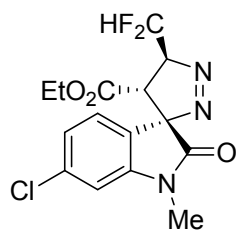
zj-2-34-2-C

Table 2, entry 9, 4i



zj-2-34-2-F  
STANDARD FLUORINE PARAMETERS

Table 2, entry 9, 4i



zj-2-99-2-H  
STANDARD PROTON

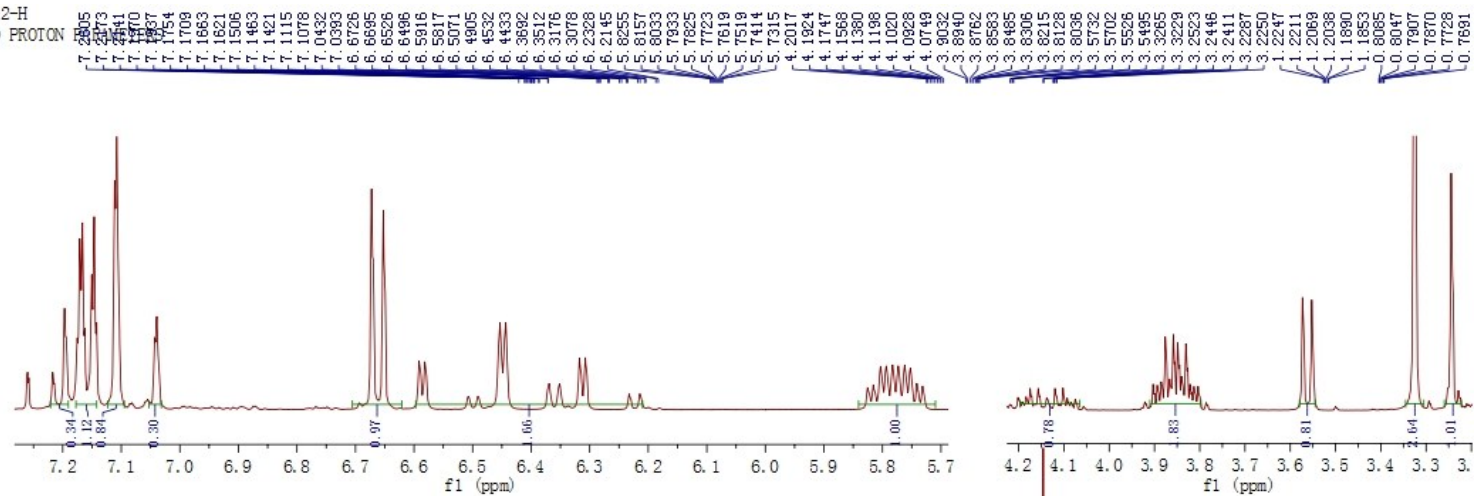
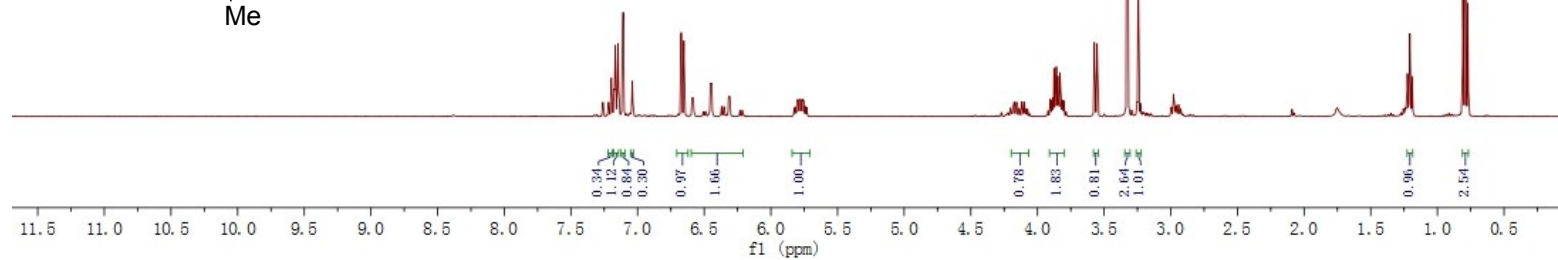
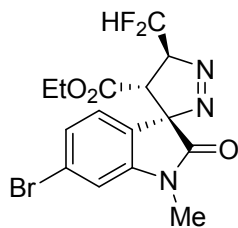


Table 2, entry 10, 4j





zj-2-99-2-C

172.1468  
170.7636  
167.7192  
166.6715  
166.6506

145.8911  
145.4244

126.1499  
126.1154  
125.5633  
125.3919  
124.2485  
122.8566  
122.4047  
120.3821  
115.4836  
115.1834  
113.1167  
112.7459  
112.6377  
112.0582  
110.7491  
110.3086

98.8656  
94.5403  
94.3174  
94.0863

77.4777  
77.1593  
76.8413

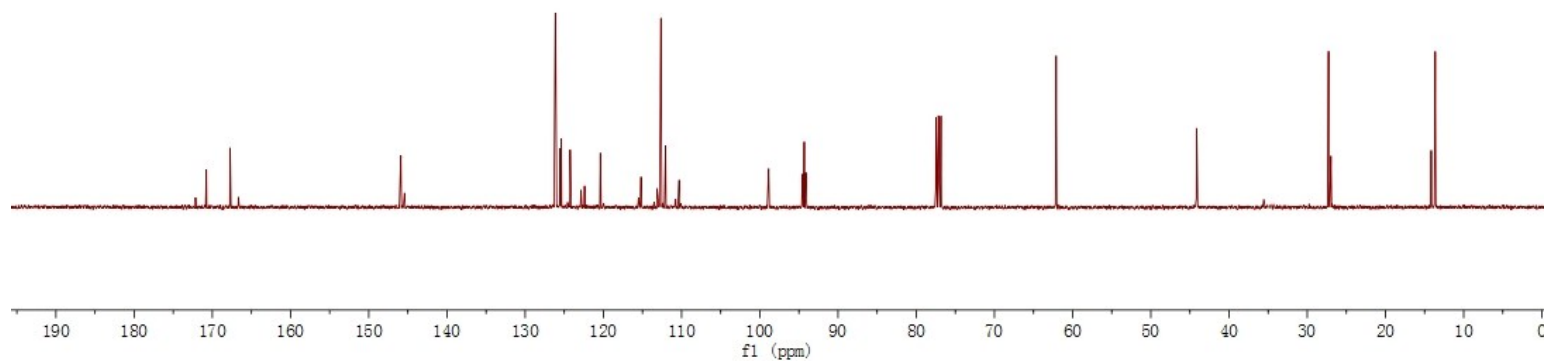
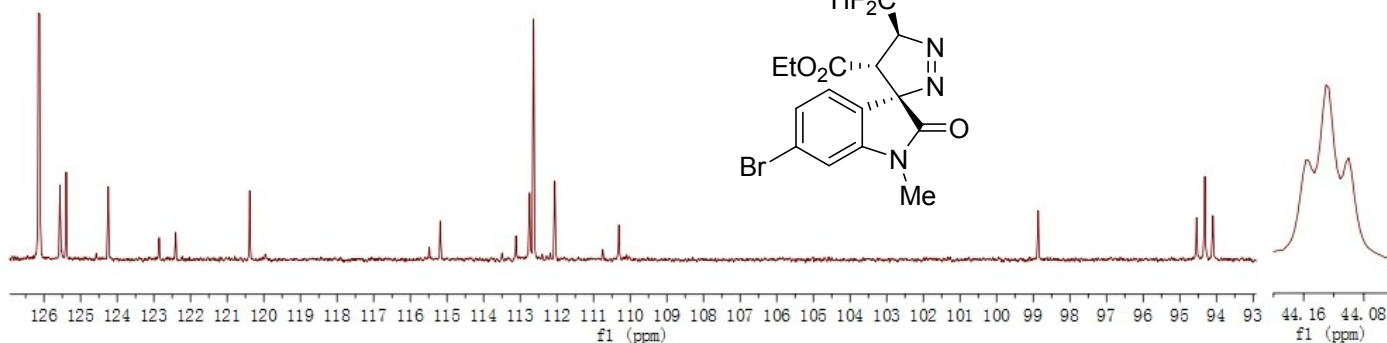
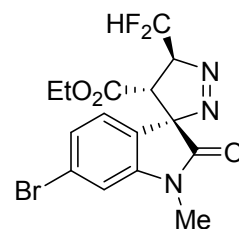
62.1051

44.1565  
44.1290  
44.1001

27.2803  
26.9702

14.1485  
13.6335

Table 2, entry 10, 4j



zj-2-99-2-F  
STANDARD FLUORINE PARAMETERS

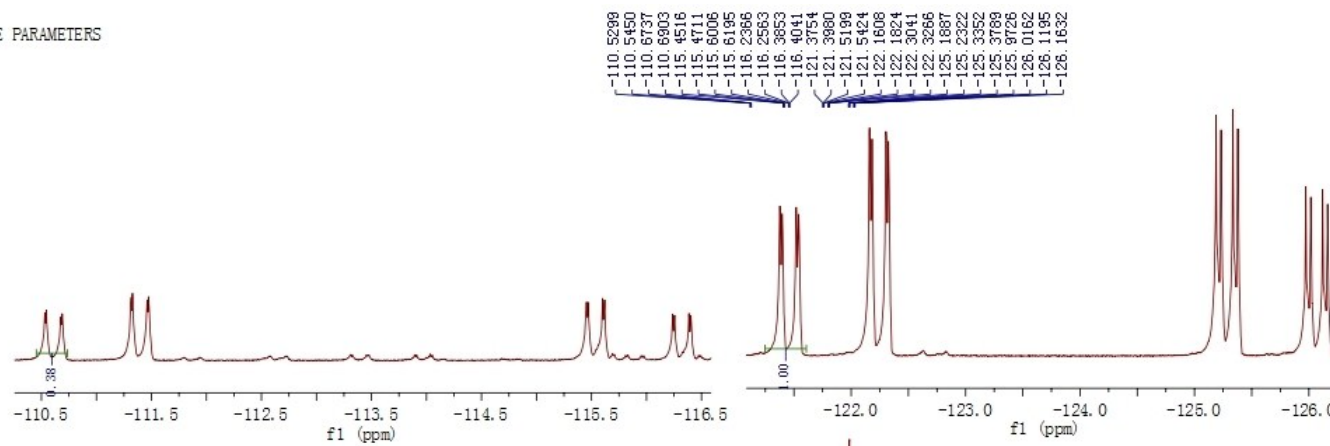
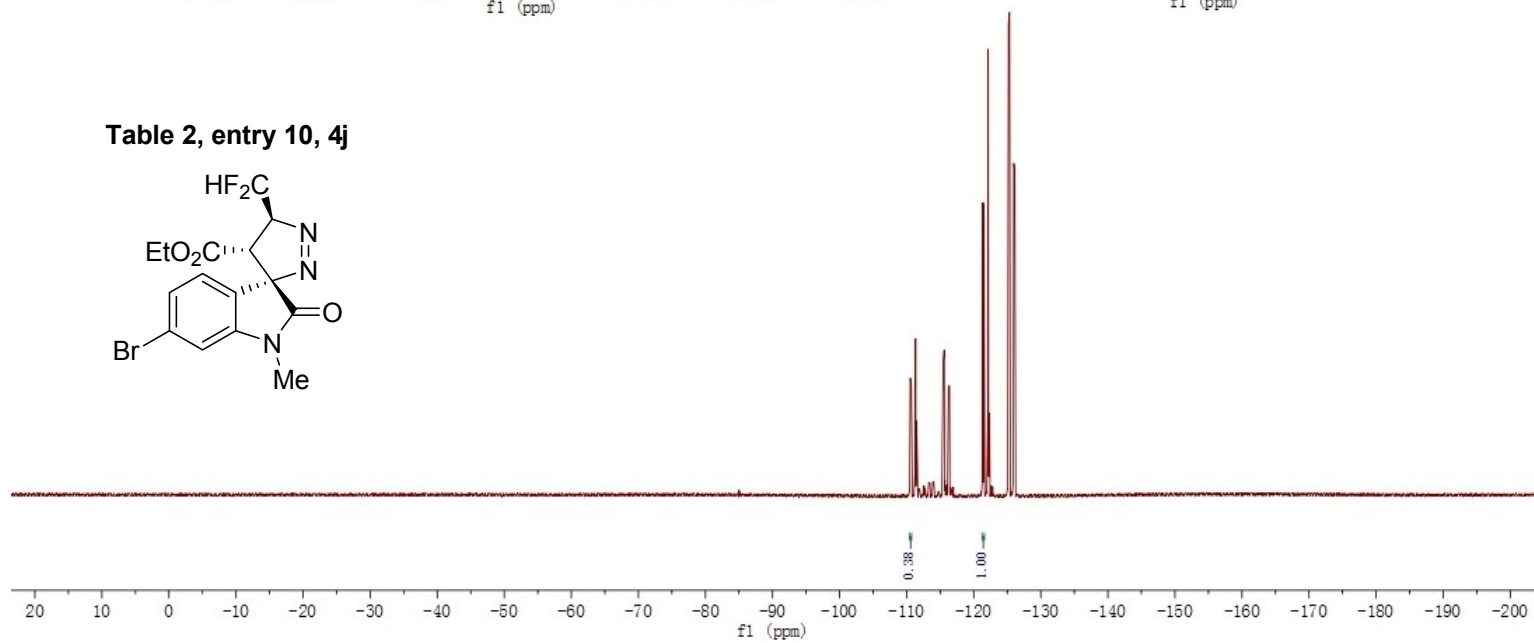
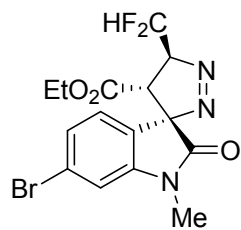
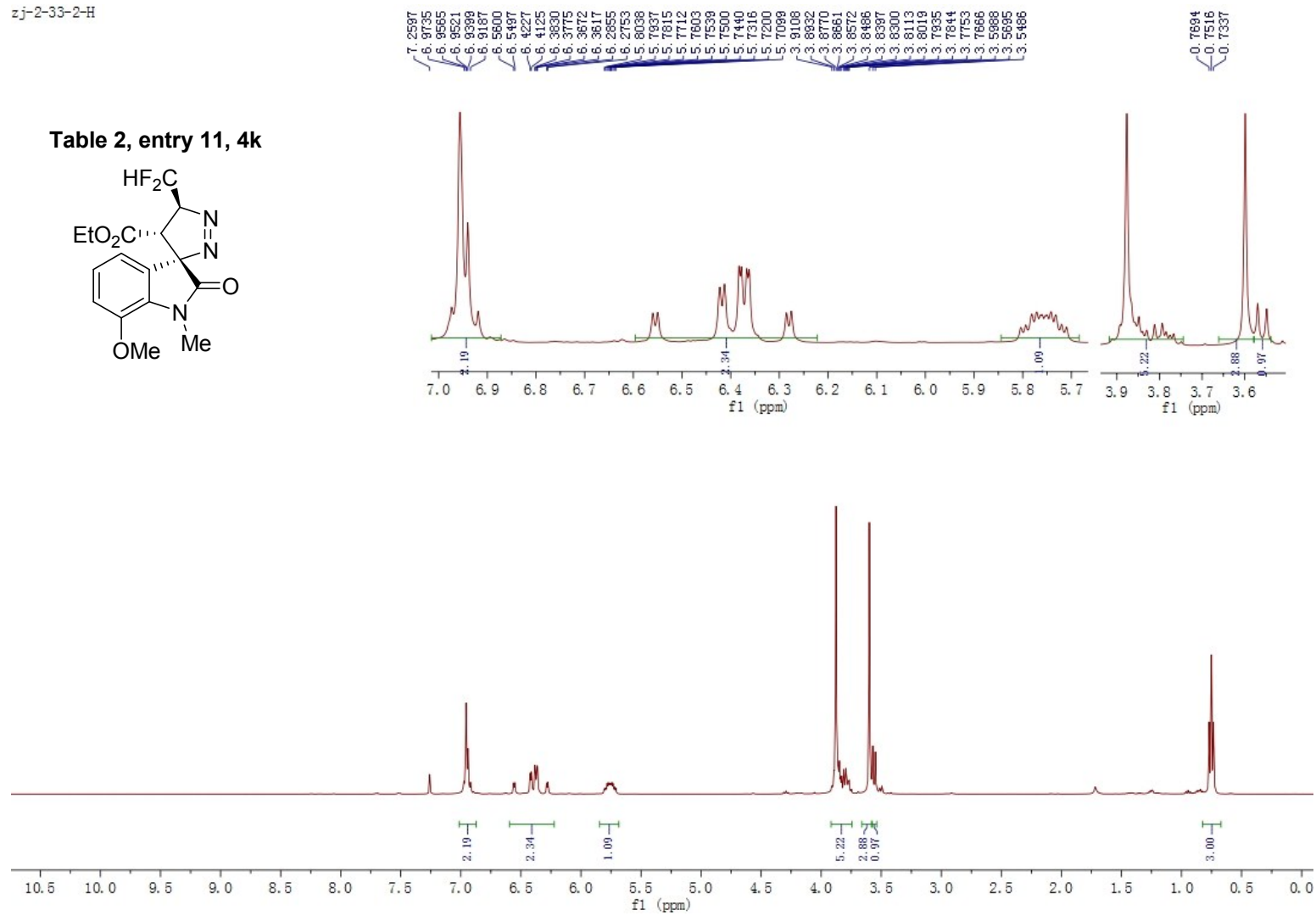
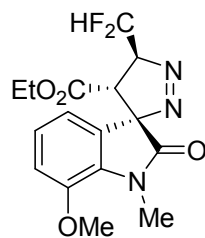


Table 2, entry 10, 4j



zj-2-33-2-H

Table 2, entry 11, 4k



zj-2-33-2-C

171.0626  
167.8220

145.8050

132.4498

124.0226  
122.8132

117.1623  
115.4371  
115.1061  
113.0011  
110.5854

98.4290  
94.0253  
93.8051  
93.5846

77.4787  
77.1600  
76.8418

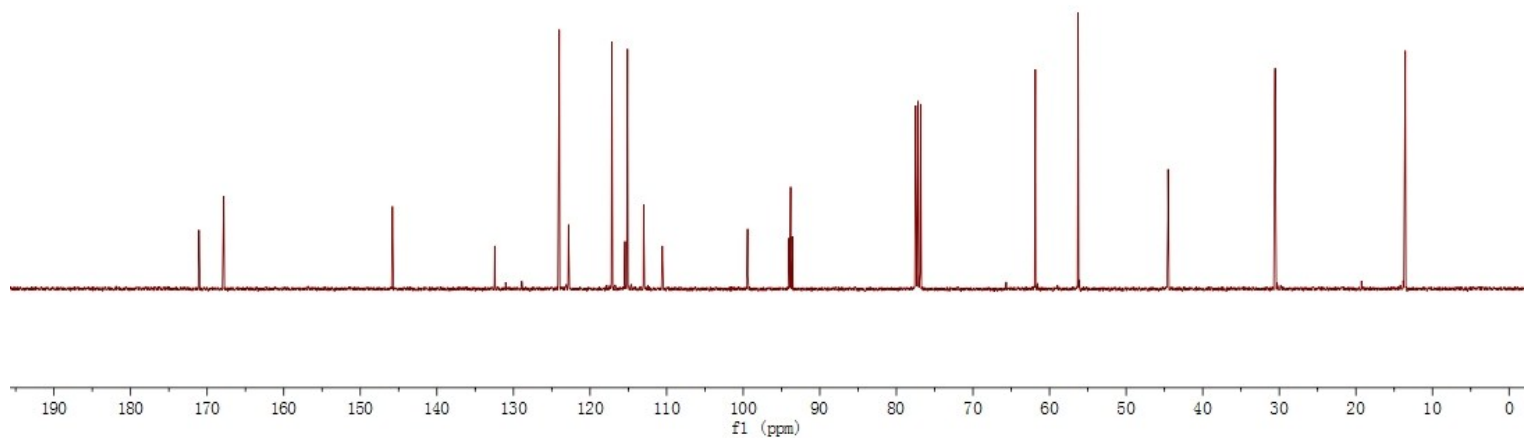
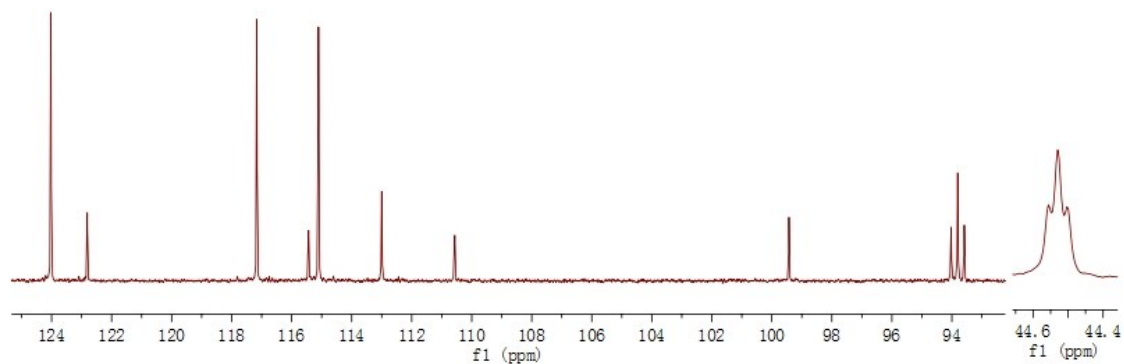
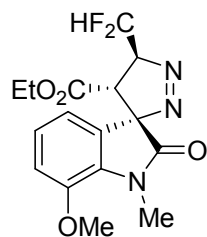
61.8547  
56.2656

44.5569  
44.5297  
44.5007

30.5520

13.5464

Table 2, entry 11, 4k



zj-2-33-2-F  
STANDARD FLUORINE PARAMETER

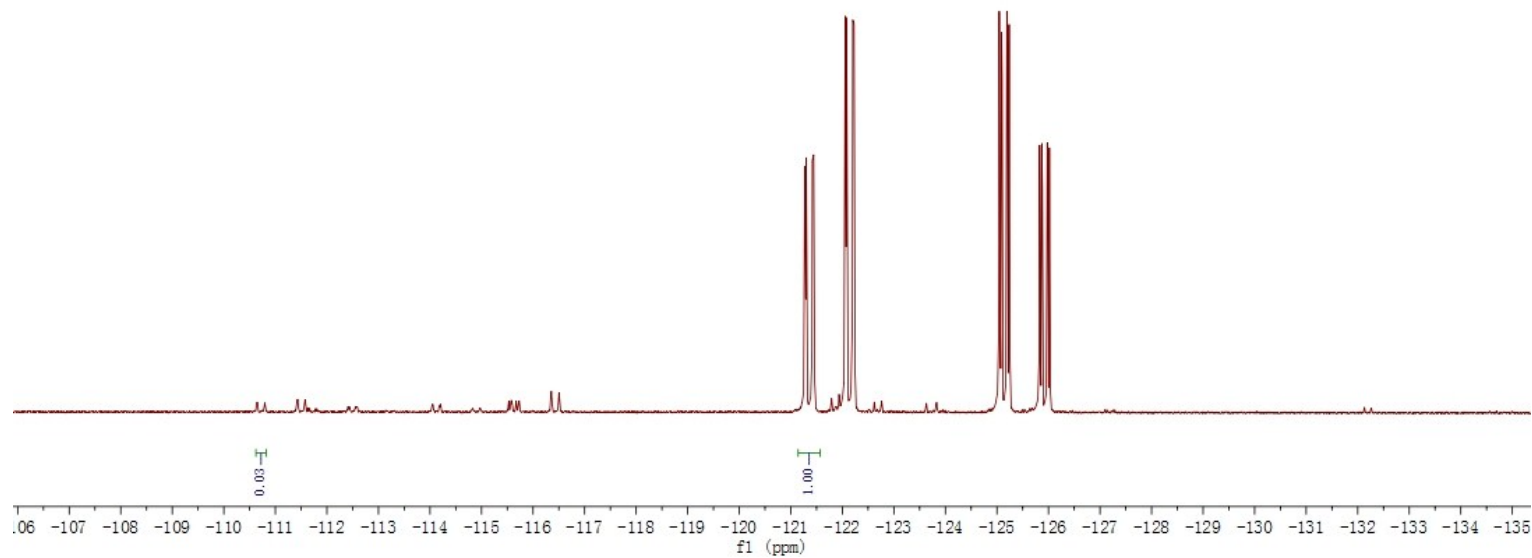
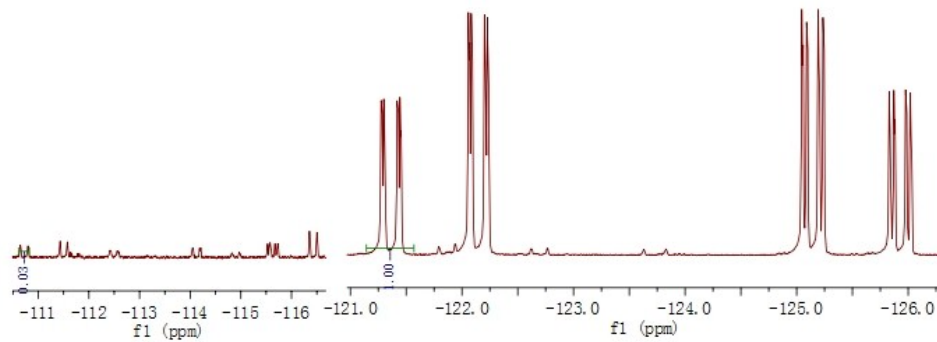
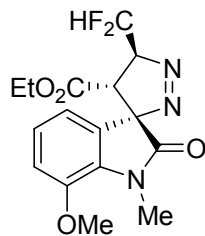
-110.6772  
-110.7823  
-111.4300  
-111.5745

-115.5271  
-115.6737  
-116.3548  
-116.4998

-121.2751  
-121.2898  
-121.4190  
-121.4444  
-122.0578  
-122.0829  
-122.2025  
-122.2277

-125.0458  
-125.0888  
-125.1952  
-125.2358  
-125.8288  
-125.8718  
-125.9767  
-126.0189

Table 2, entry 11, 4k



zj-9-9-H

7.2605  
7.1641  
7.1570  
7.1412  
7.1360  
7.1148  
7.1075  
6.9775  
6.9607  
6.9510  
6.9416  
6.9204  
6.5848  
6.5771  
6.5668  
6.4411  
6.3038  
5.8189  
5.7977  
5.7876  
5.7775  
5.7671  
5.7570  
5.7372  
4.2275  
4.2108  
4.2023  
4.1904  
4.1745  
3.8903  
3.8721  
3.8536  
3.8464  
3.8294  
3.8045  
3.7867  
3.5887  
3.5810  
3.5598  
3.5485  
3.4847  
3.4782  
3.4735  
3.4532  
3.4404  
1.2702  
1.2603  
1.2523  
1.2418  
1.2344  
1.2177  
0.7875  
0.7803  
0.7697  
0.7619  
0.7513  
0.7442

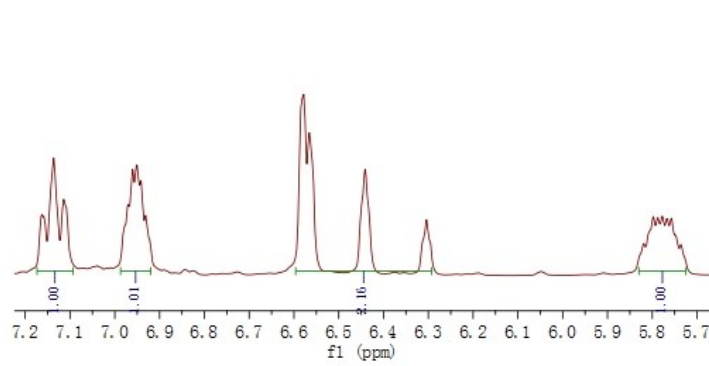
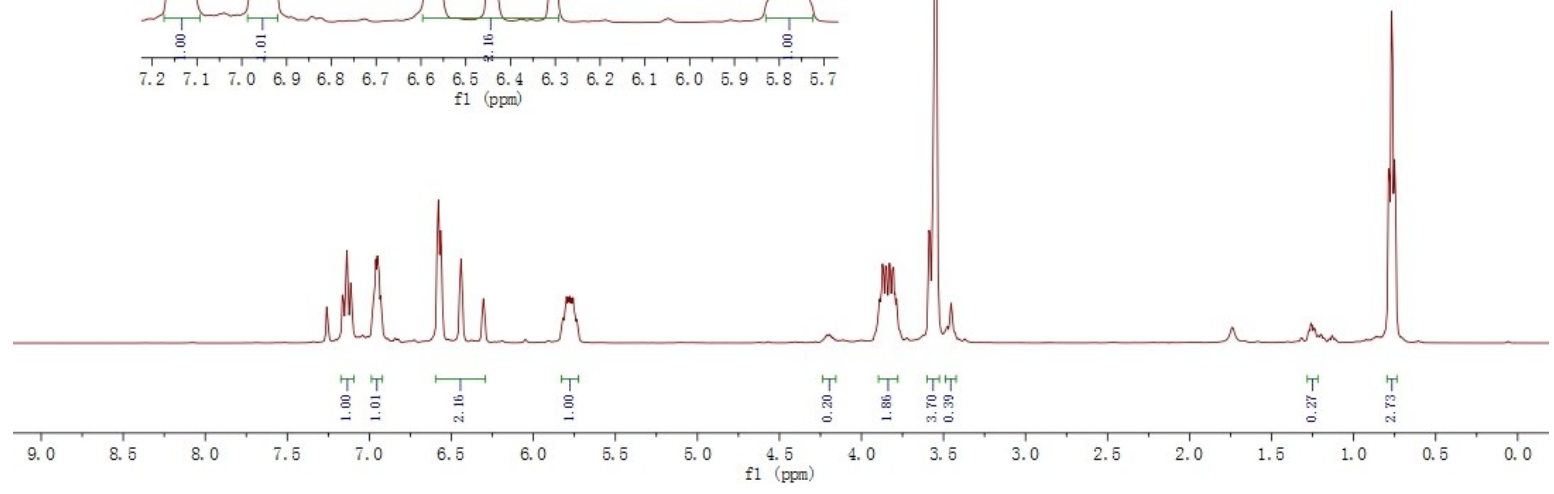
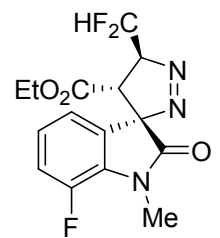


Table 2, entry 12, 4l



zj-9-9-C

170.5434  
167.6142

149.0796  
146.6395

131.3872  
131.2990  
124.1525  
124.1200  
124.0518  
123.9879  
120.7676  
120.7327  
119.5208  
119.3290  
115.2187  
112.7806  
110.3440

99.1466  
94.3718  
94.1499  
93.9277

77.4781  
77.1597  
76.8407

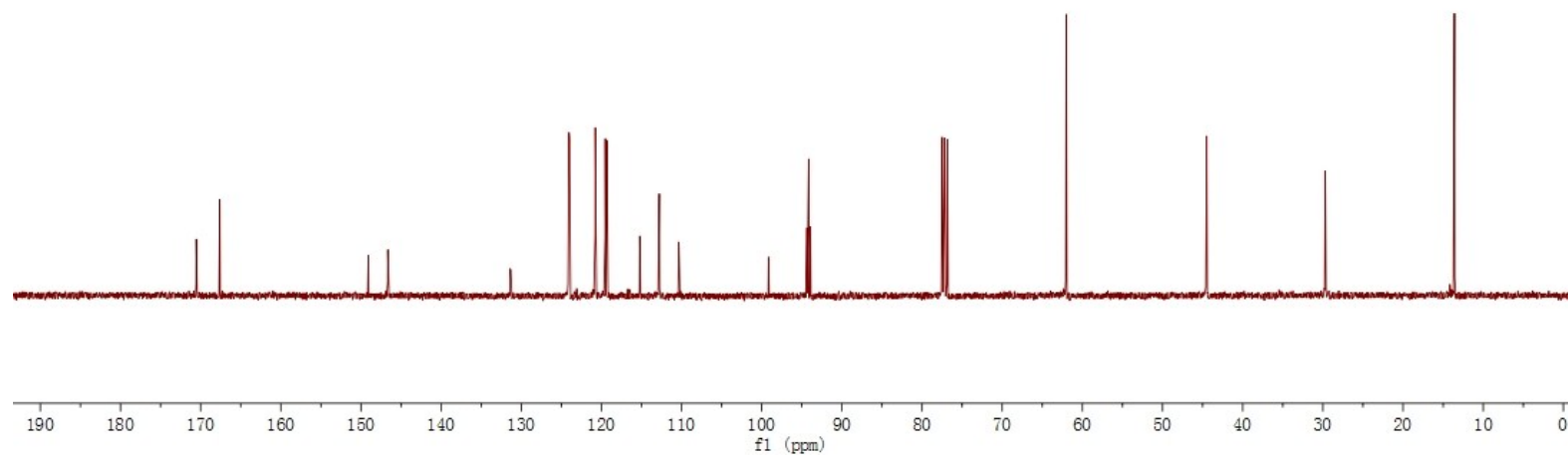
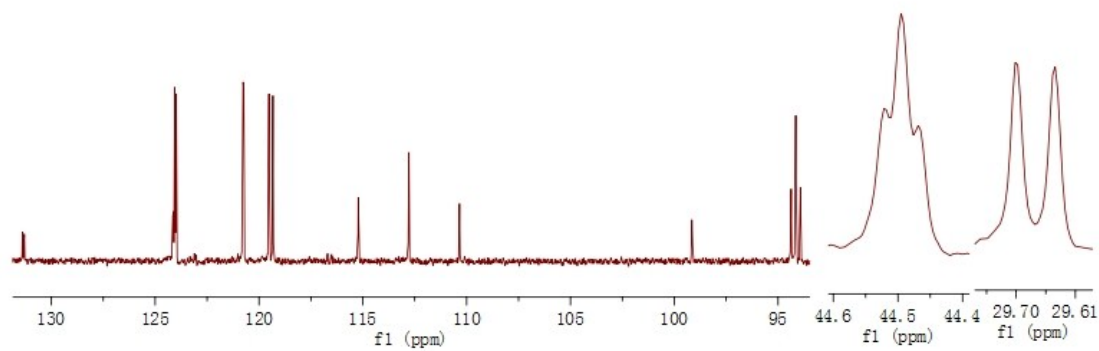
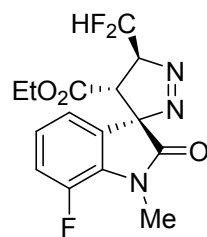
62.0205

44.5224  
44.4949  
44.4664

29.7002  
29.6418

13.5816

Table 2, entry 12, 4I



zj-2-68-2-F  
STANDARD FLUORINE PARAMETERS

-110.6075  
-110.6216  
-110.7503  
-110.7644  
-111.3947  
-111.4107  
-111.5358  
-111.5511  
-115.6407  
-115.6610  
-115.7800  
-115.8087  
-116.4288  
-116.4454  
-116.5759  
-116.5924  
-121.3544  
-121.3782  
-121.4982  
-121.5218  
-122.1389  
-122.1626  
-122.2823  
-122.3066  
-125.2159  
-125.2594  
-125.3627  
-125.4062  
-126.0002  
-126.0437  
-126.1467  
-126.1802  
-135.1666  
-135.1760  
-135.1863  
-135.1958  
-135.2063  
-135.2174  
-135.2323  
-135.4279  
-135.4351  
-135.4404  
-135.4475  
-135.4584  
-135.4669  
-135.4773  
-135.4842

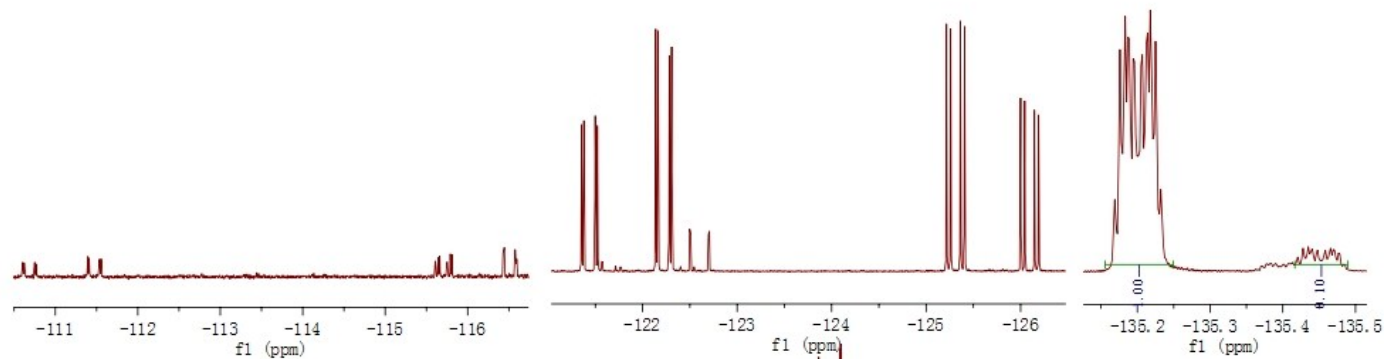
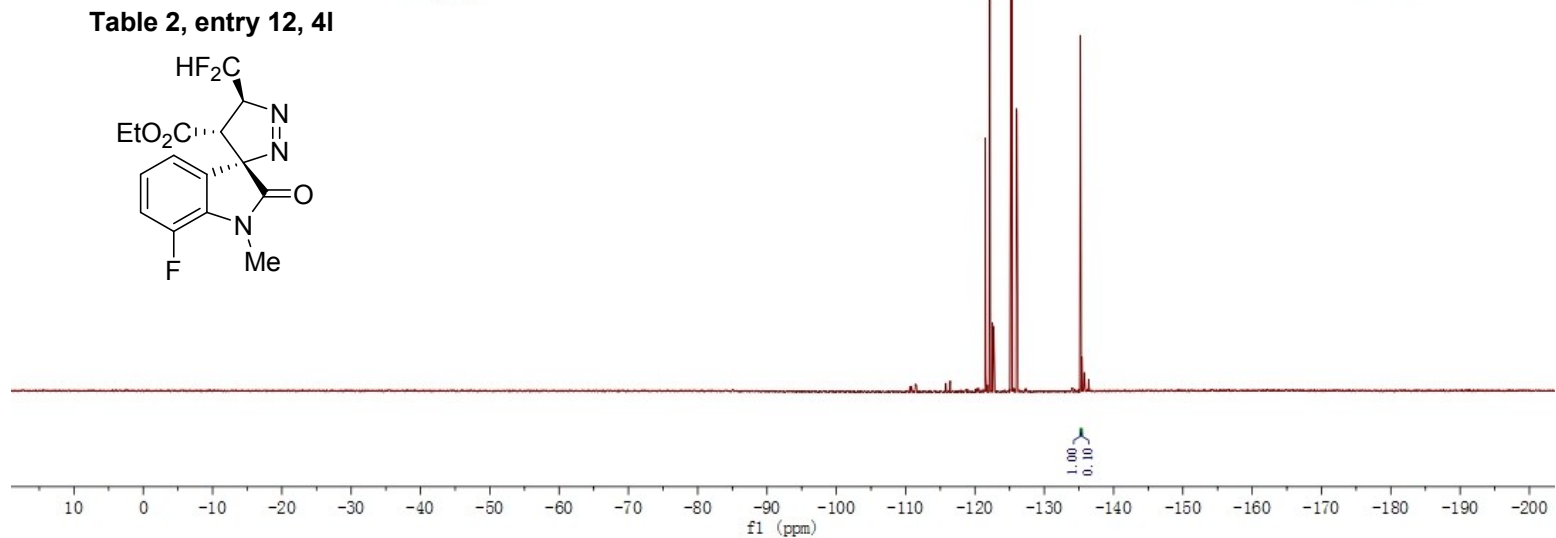
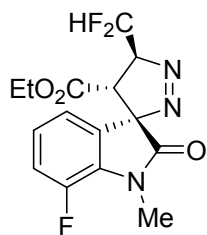


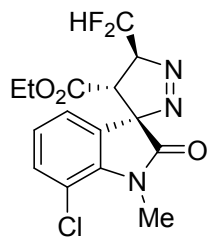
Table 2, entry 12, 4l





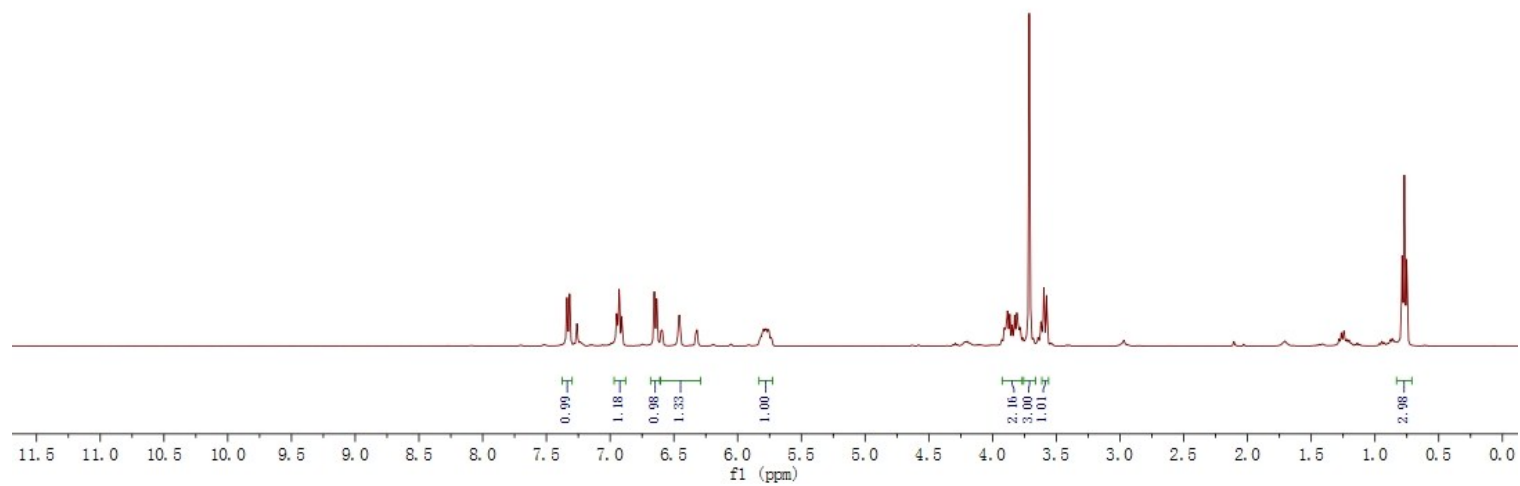
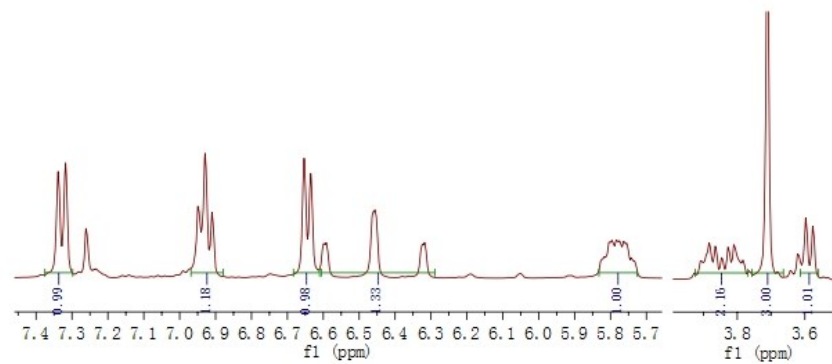
zj-2-31-2\_3-H

Table 2, entry 13, 4m



7.3385  
7.3178  
7.2812  
6.9464  
6.9300  
6.9089  
6.8533  
6.8347  
6.5982  
6.5817  
6.4631  
6.3271  
6.3190  
5.8052  
5.8008  
5.7857  
5.7815  
5.7833  
5.7737  
5.7639  
5.7597  
5.7555  
5.7428  
5.7402  
5.7335  
3.9273  
3.9090  
3.8831  
3.8781  
3.8651  
3.8608  
3.8464  
3.8278  
3.8232  
3.8101  
3.8049  
3.7979  
3.7833  
3.7124  
3.5978  
3.5772

0.7868  
0.7680  
0.7521



zj-7-7-C

171.2574  
167.5272

140.5016  
133.6109  
130.9168  
124.0355  
123.3292  
116.4325  
115.1576  
112.7210  
110.2843

98.6781  
94.2733  
94.0520  
93.8293

77.4778  
77.1607  
76.8422

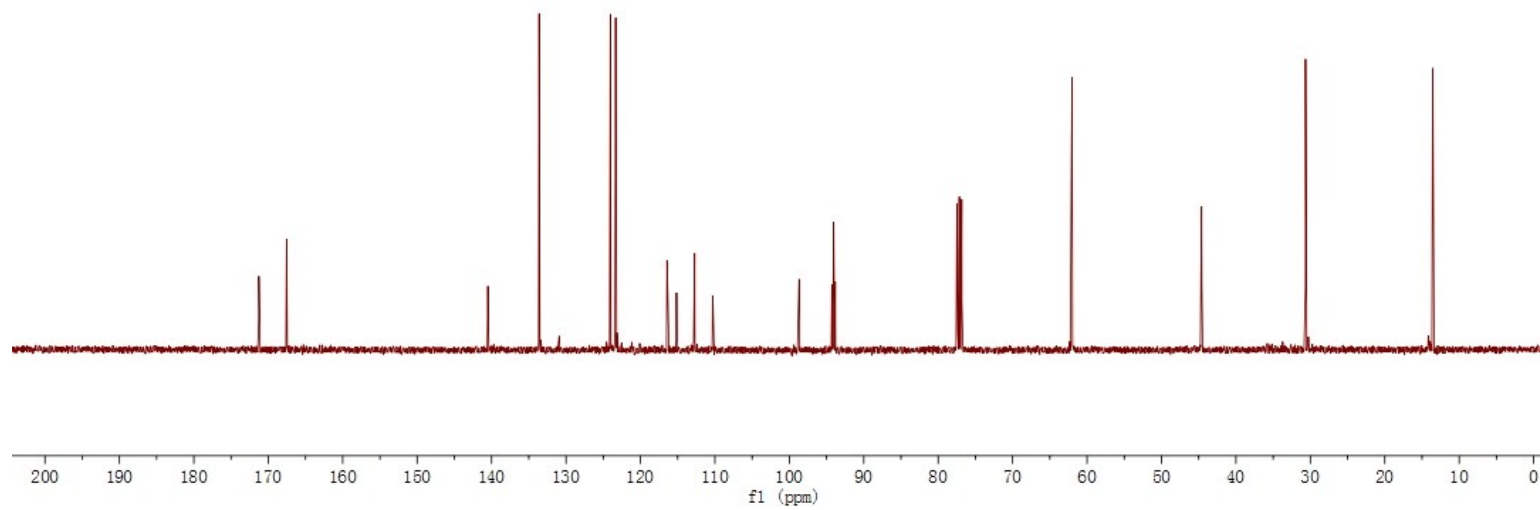
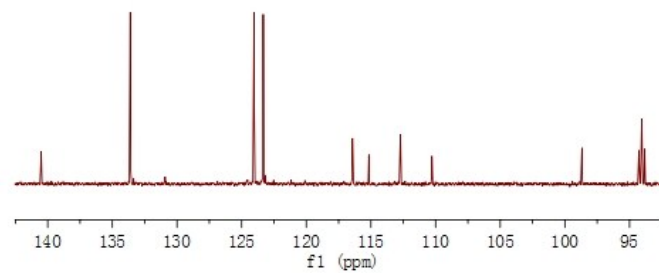
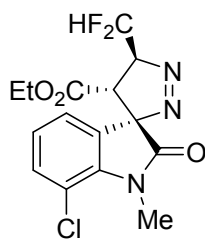
62.0198

44.6451  
44.6181  
44.5887

30.6451  
30.2756

14.1382  
13.5600

Table 2, entry 13, 4m



zj-2-31-2\_3-F  
STANDARD FLUORINE PARAMETERS

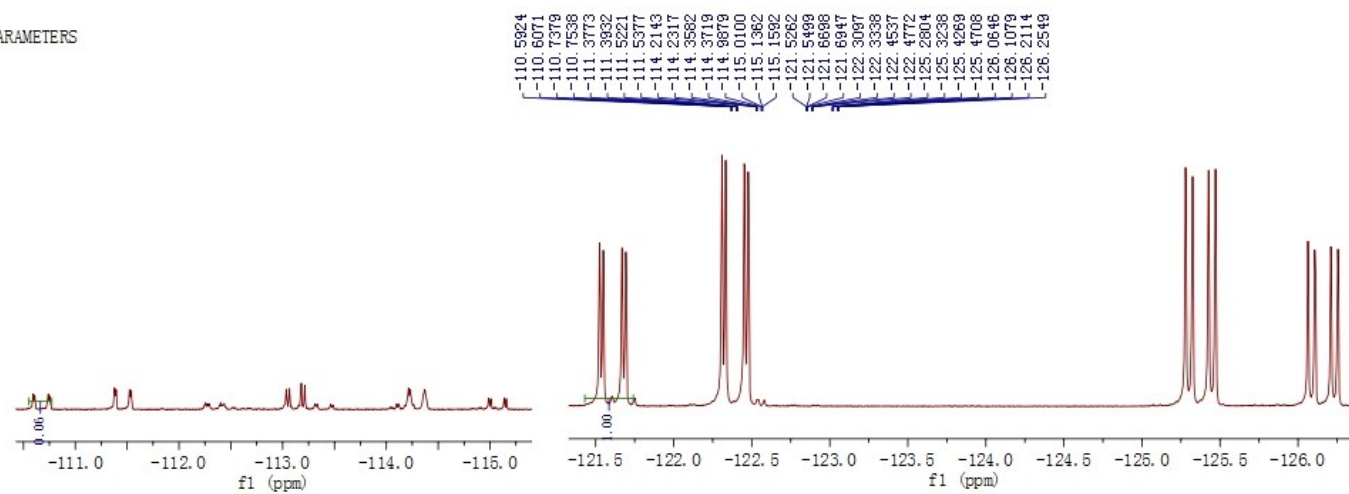
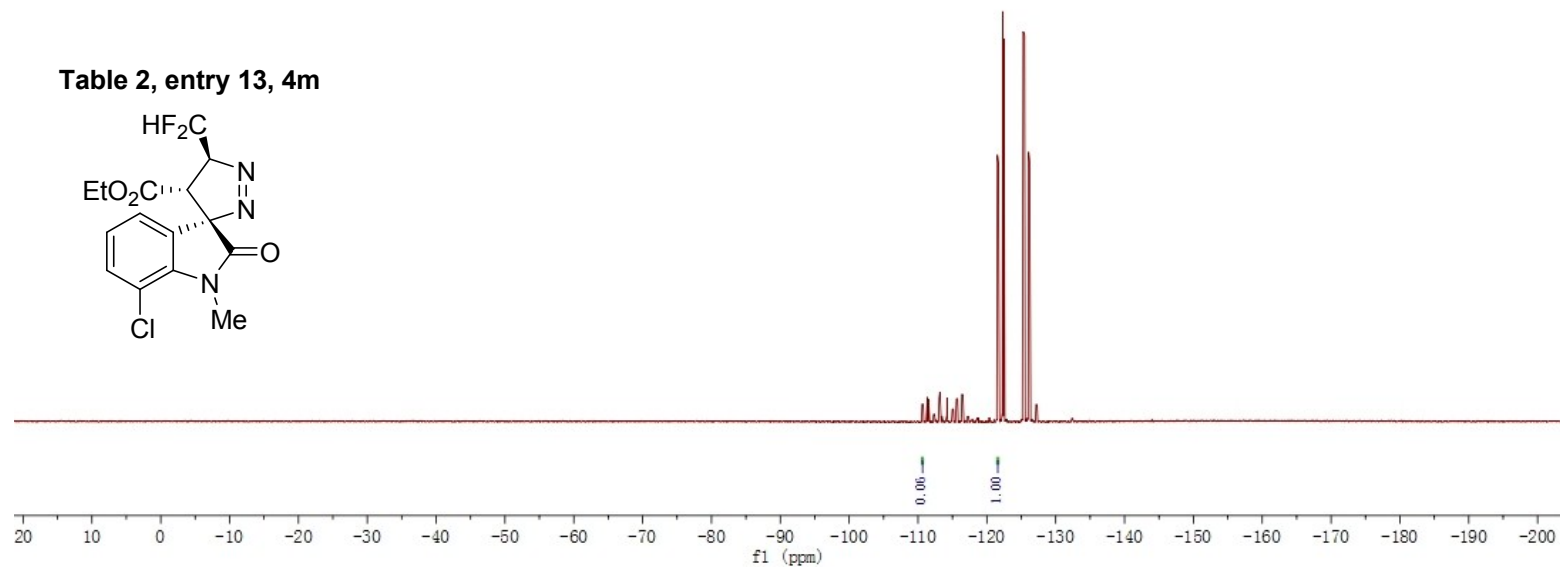
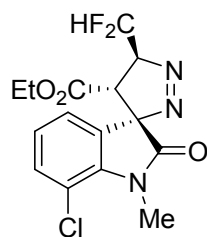
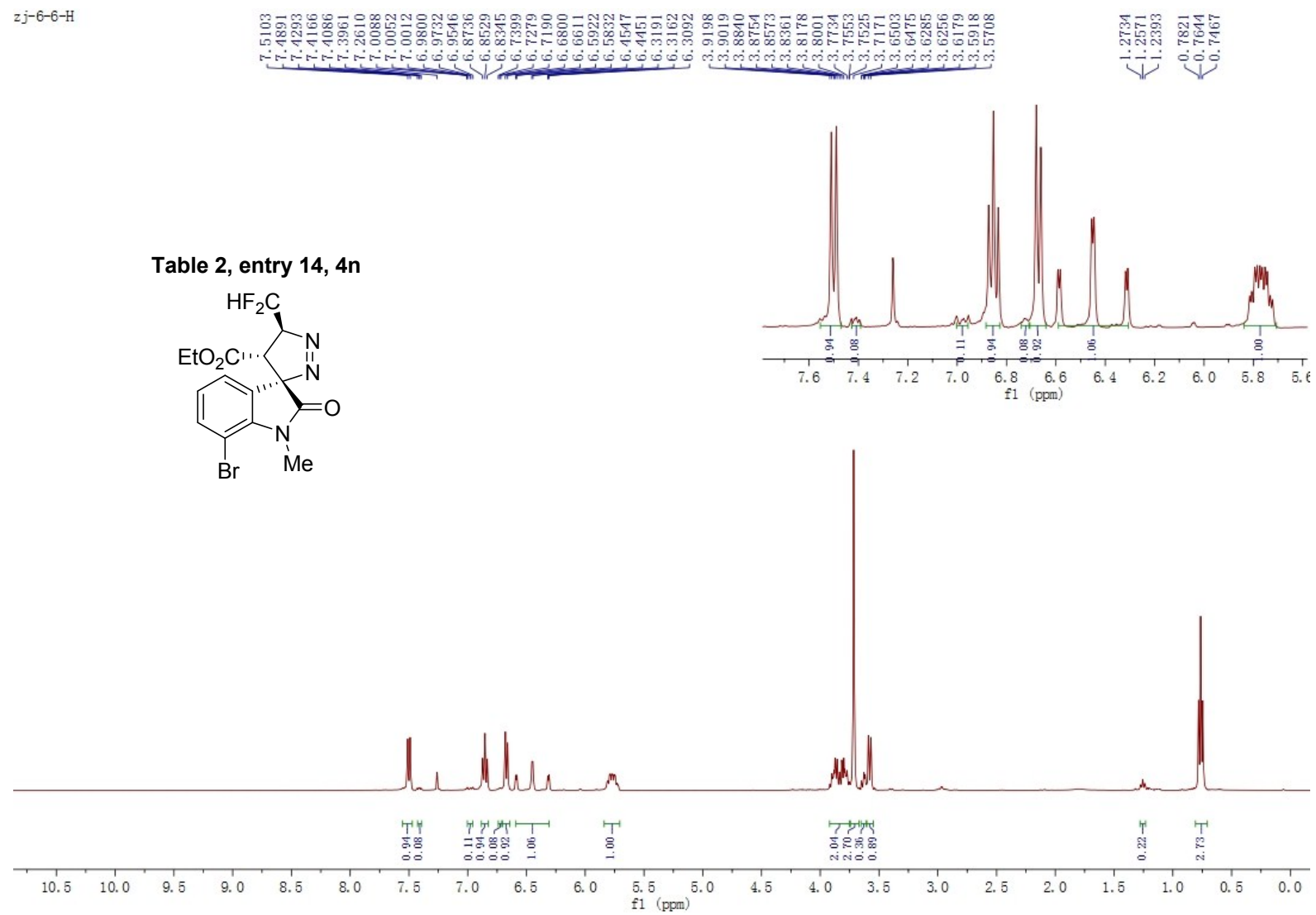
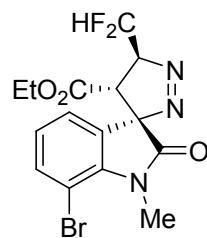


Table 2, entry 13, 4m



zj-6-6-H

Table 2, entry 14, 4n



zj-6-6-C

— 171.4778  
— 167.5138

— 141.9499  
— 136.9475  
— 134.2822

124.3737  
123.8538  
123.5291

— 115.1422  
— 112.7051  
— 110.2673

— 103.1233  
98.6283  
94.2551  
94.0320  
93.8111

77.4800  
77.1613  
76.8433

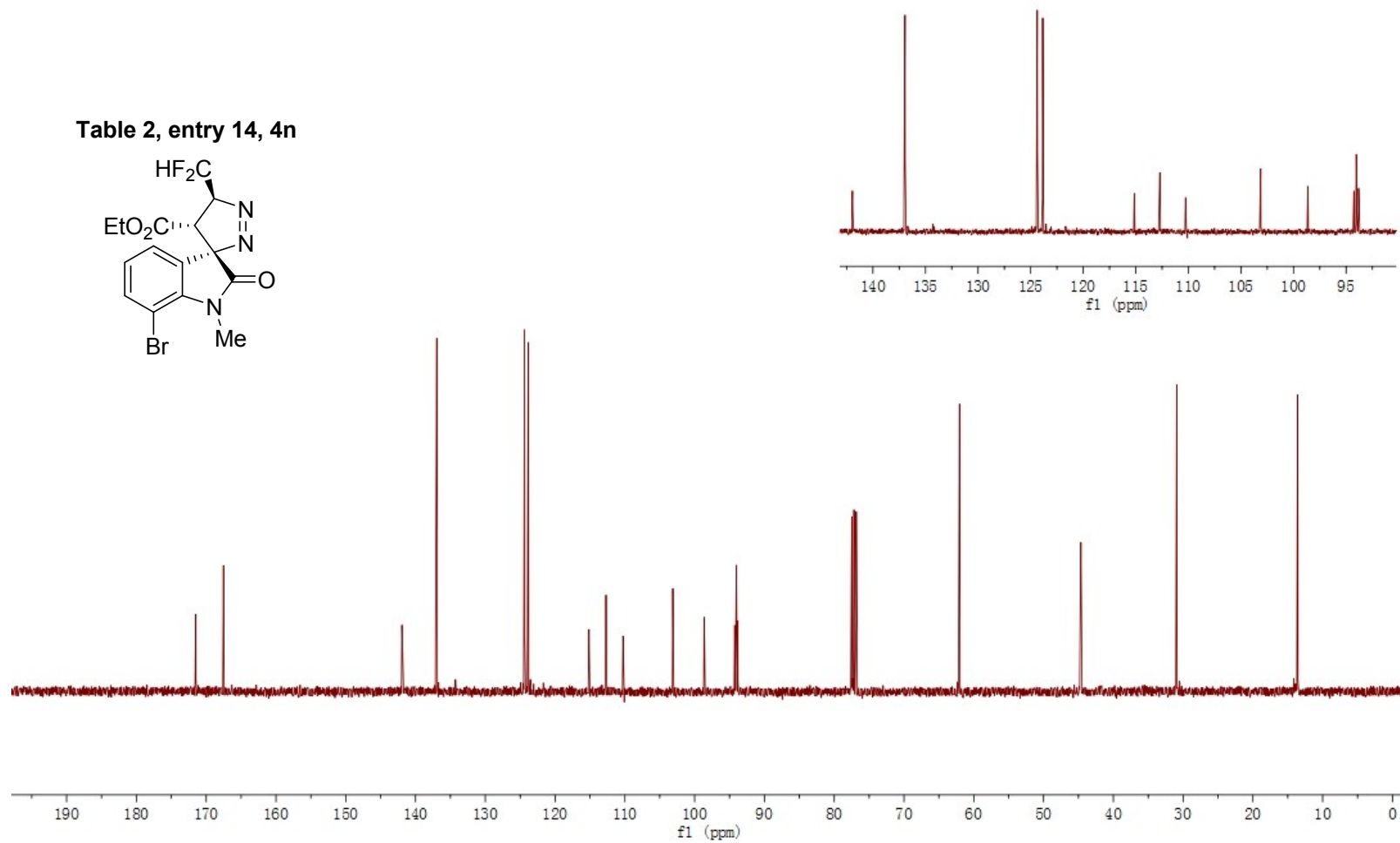
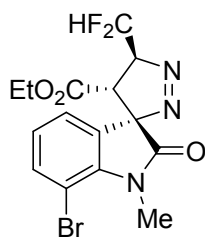
— 62.0351

44.6769  
44.6493  
44.6214

— 30.9125

14.1495  
13.5720

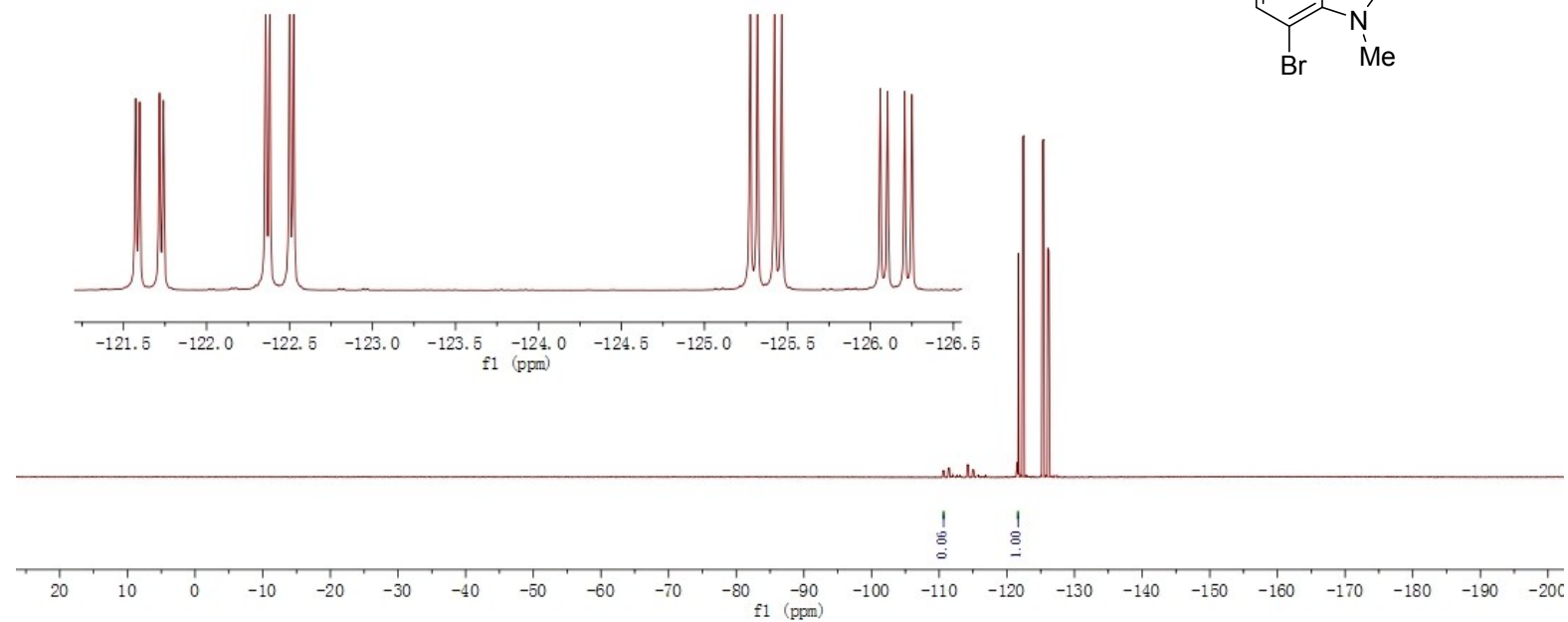
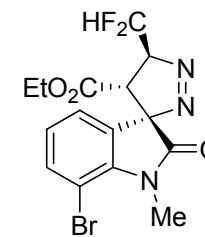
Table 2, entry 14, 4n



zj-6-6-F  
STANDARD FLUORINE PARAMETERS

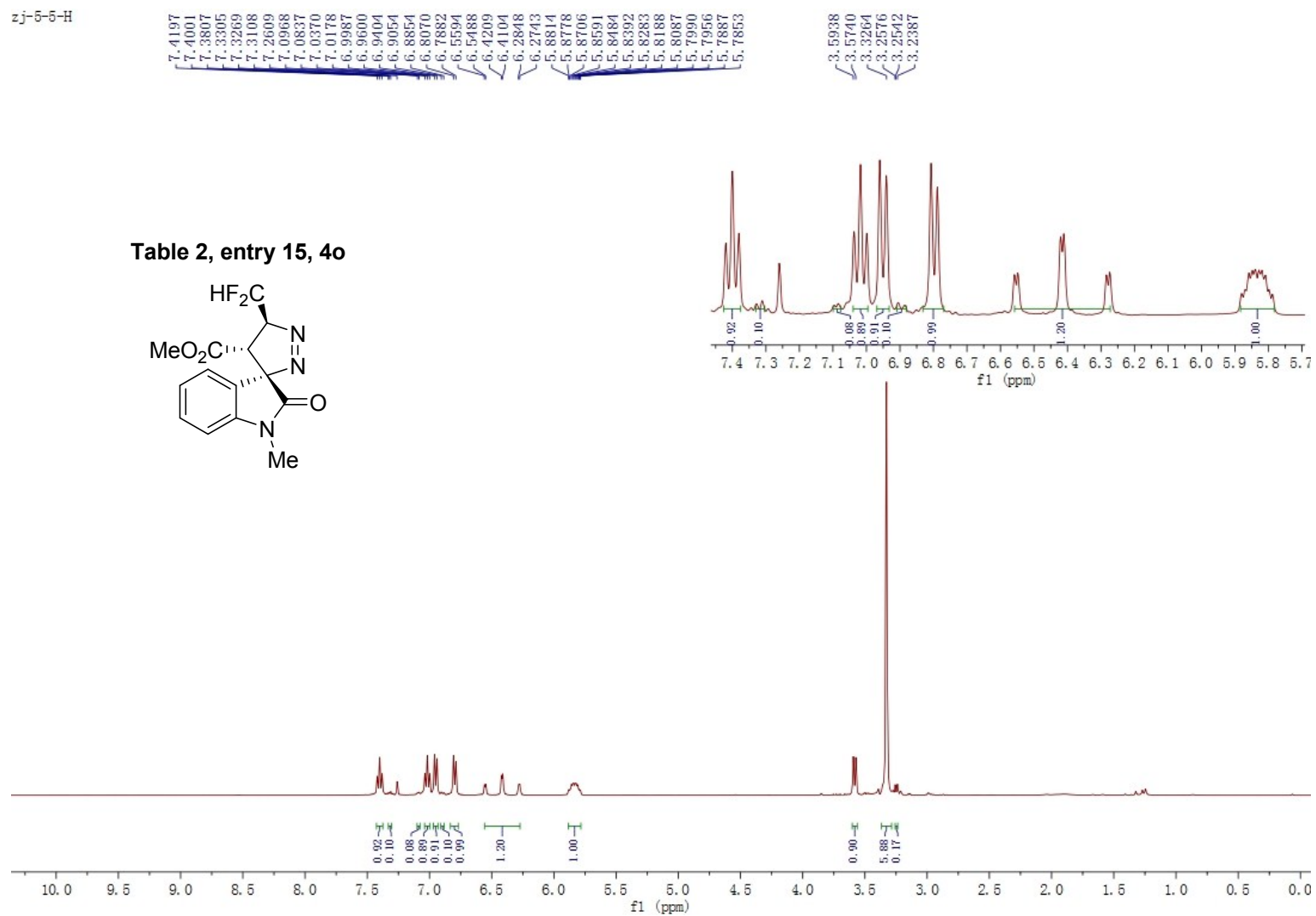
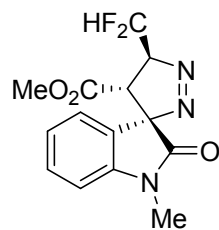
110.5767  
110.5922  
110.7210  
110.7374  
111.3614  
111.3771  
111.5070  
111.5229  
114.1656  
114.1818  
114.3131  
114.3256  
114.9423  
114.9640  
115.0903  
115.1127  
121.5725  
121.5965  
121.7168  
121.7406  
122.3564  
122.3801  
122.5009  
122.5246  
125.2754  
125.3189  
125.4222  
125.4657  
126.0593  
126.1029  
126.2062  
126.2497

Table 2, entry 14, 4n



zj-5-5-H

Table 2, entry 15, 4o



zj-5-5-C

—170.7697  
—168.5274

—144.5150

—131.4885  
—128.6855  
—124.6851  
—123.3773  
—122.8197  
—122.7514  
—121.4844  
—115.4283  
—112.9919  
—110.5560  
—109.1757

—99.5418  
—94.6737  
—94.4530  
—94.2327

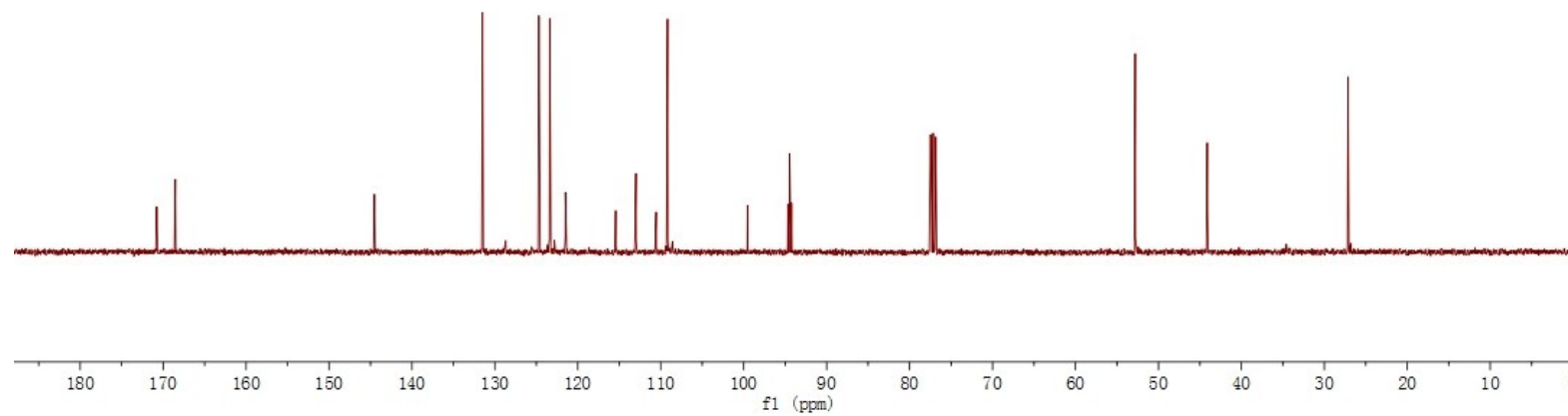
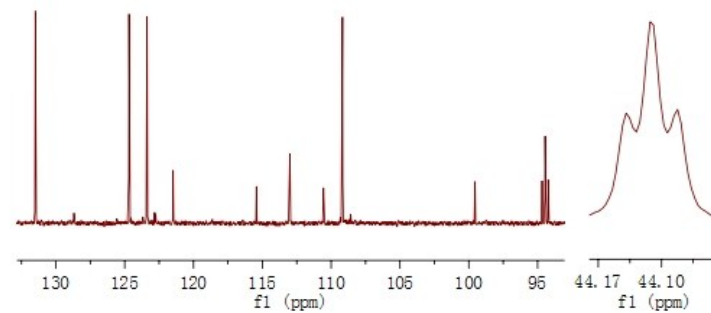
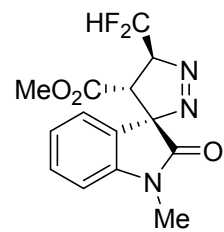
—77.4784  
—77.1598  
—76.8415

—52.8047

—44.1392  
—44.1101  
—44.0813

—27.1431

Table 2, entry 15, 4o





zj-2-84-2-F  
STANDARD FLUORINE PARAMETERS

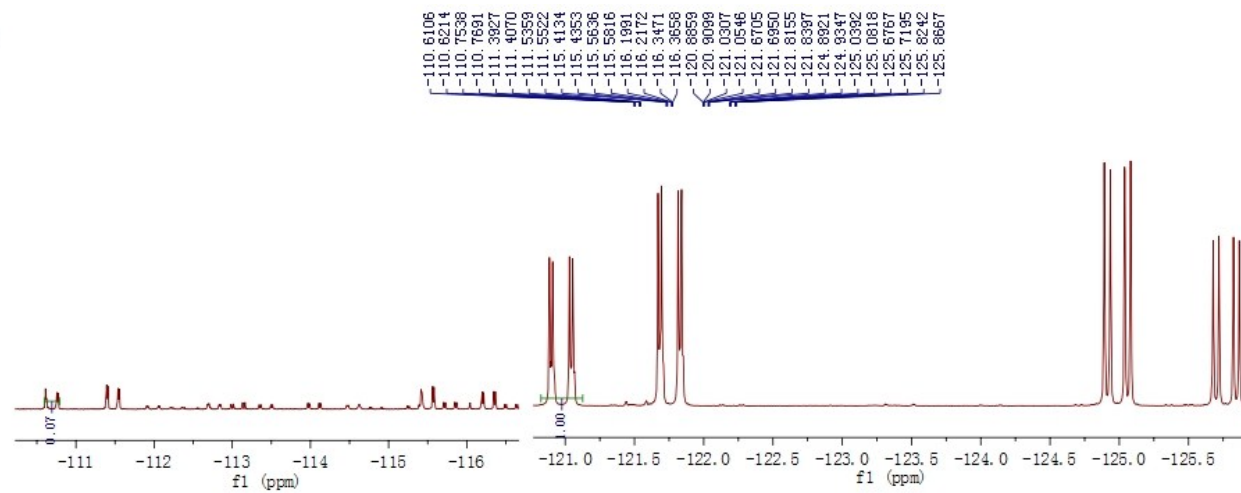
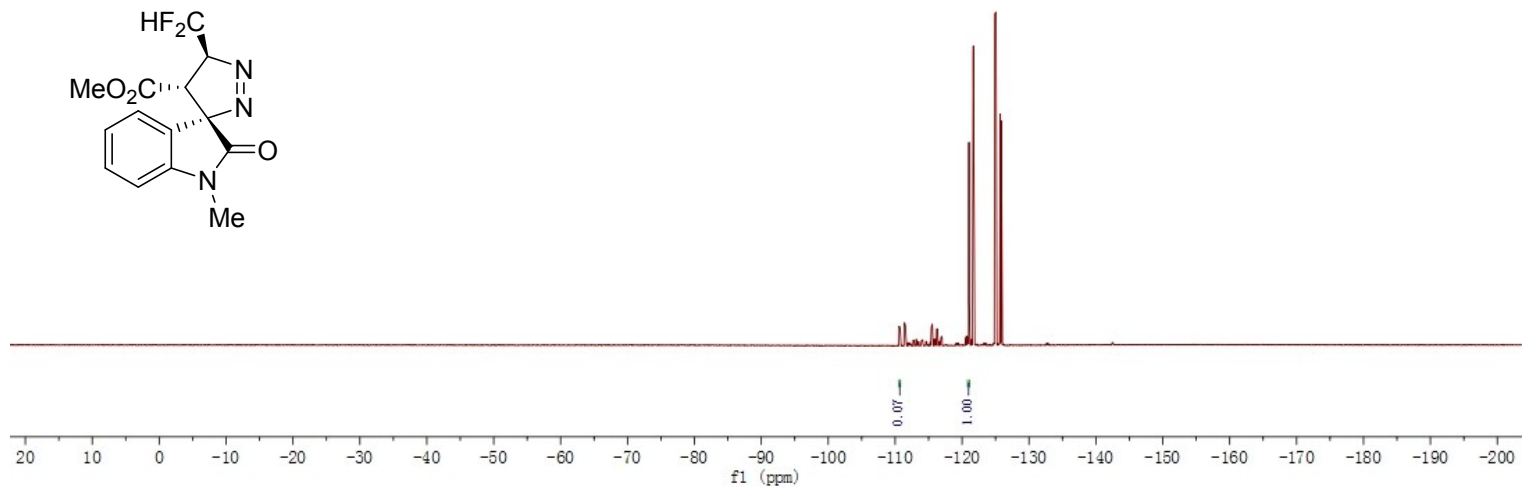
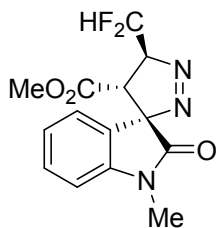


Table 2, entry 15, 4o



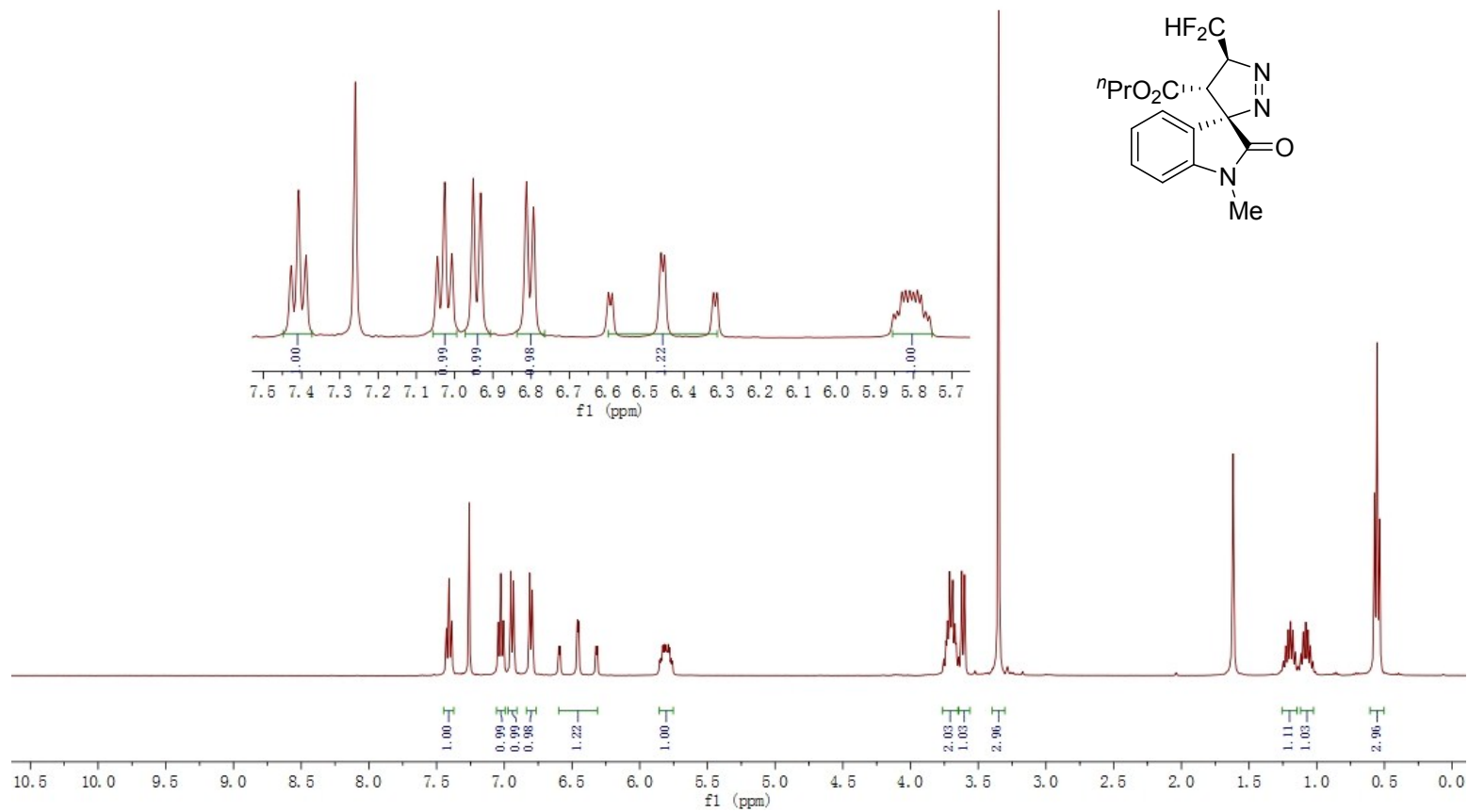
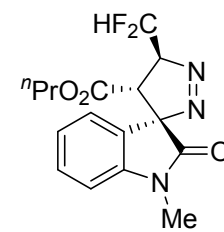
zj-4-4-H

7.4278  
7.4083  
7.3888  
7.2595  
7.0452  
7.0262  
7.0071  
6.9516  
6.9319  
6.8124  
6.7936  
6.5976  
6.5879  
6.4605  
6.4506  
6.3234  
6.3136  
5.8522  
5.8424  
5.8305  
5.8204  
5.8099  
5.8000  
5.7897  
5.7799  
5.7681  
5.7583

3.7541  
3.7378  
3.7271  
3.7111  
3.6883  
3.6773  
3.6720  
3.6618  
3.6452  
3.6221  
3.6214  
3.6014  
3.3497

1.6178  
1.2465  
1.2285  
1.2109  
1.1933  
1.1757  
1.1579  
1.1168  
1.0994  
1.0818  
1.0643  
1.0467  
1.0293  
0.5730  
0.5544  
0.5360

Table 2, entry 16, 4p



zj-4-4-C

— 170.9817  
— 168.0486

— 144.6347

— 131.5124

— 124.9252

— 123.4672

— 121.6218

— 115.3819

— 112.9460

— 110.5101

— 109.1072

— 99.3908

— 94.3649

— 94.1423

— 93.9216

— 77.4774

— 77.1596

— 76.8416

— 67.6009

— 44.3780

— 44.3503

— 44.3226

— 27.1817

— 21.4290

— 10.0003

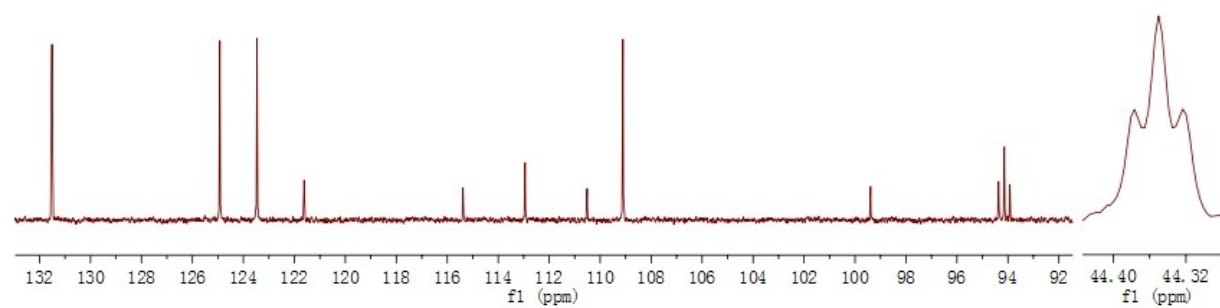
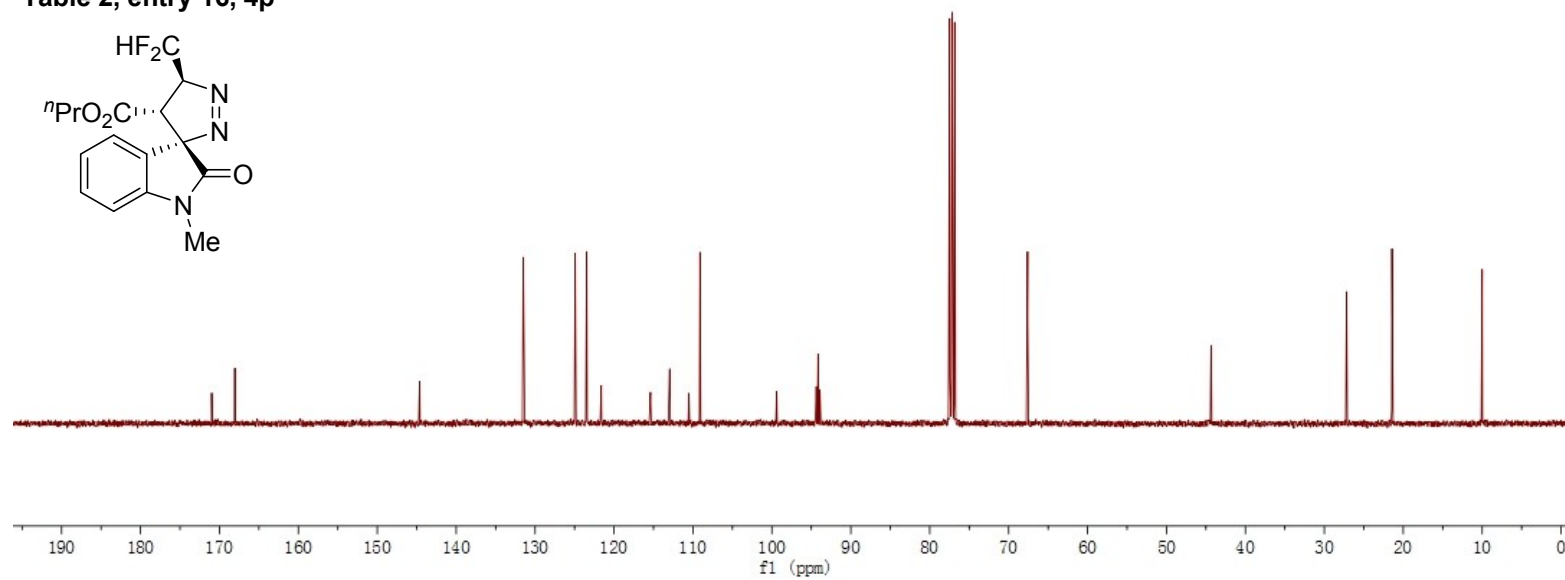
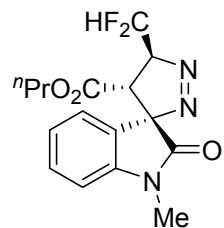
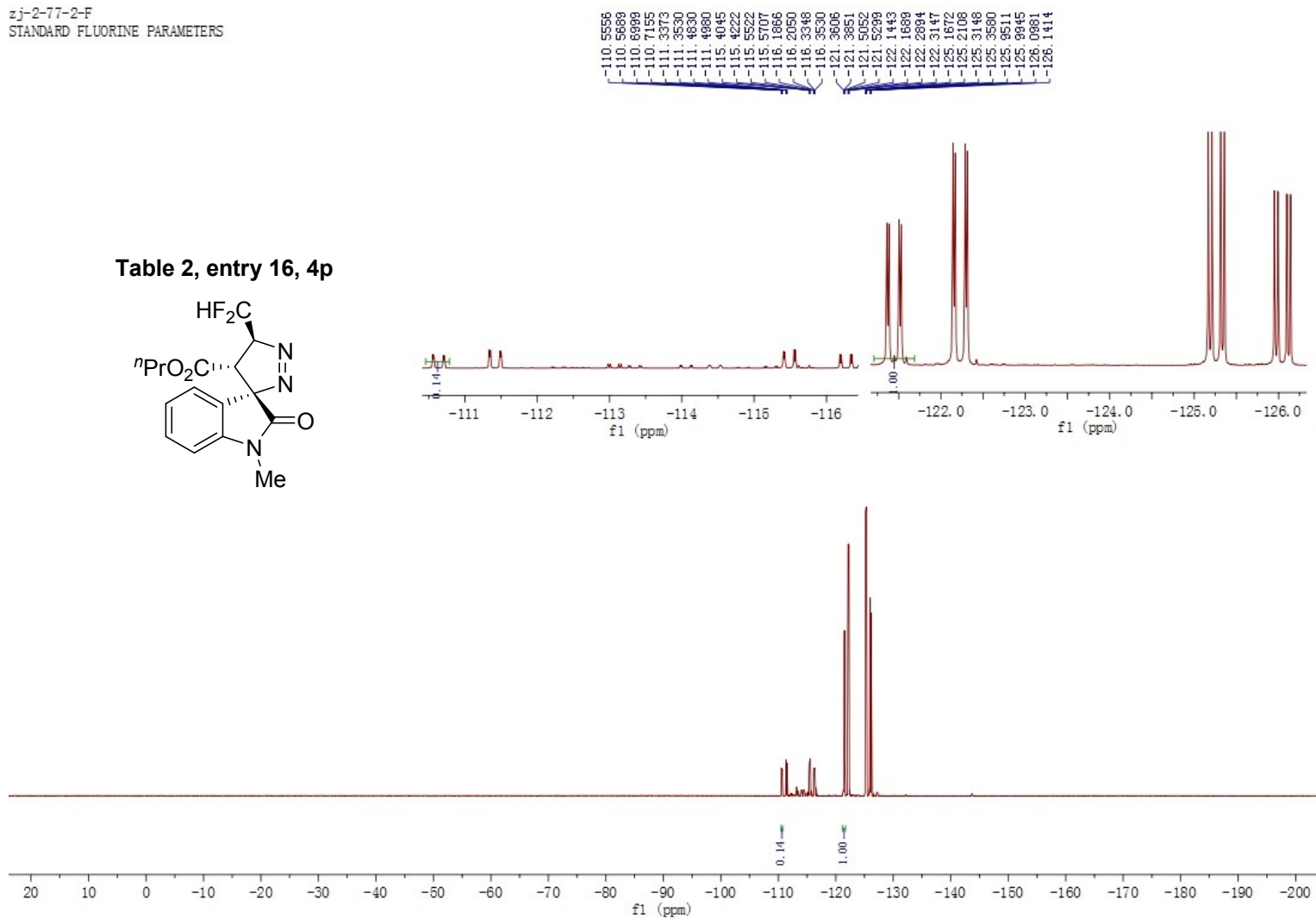
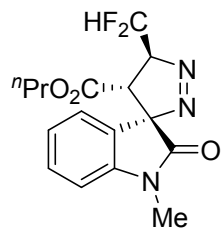


Table 2, entry 16, 4p



zj-2-77-2-F  
STANDARD FLUORINE PARAMETERS

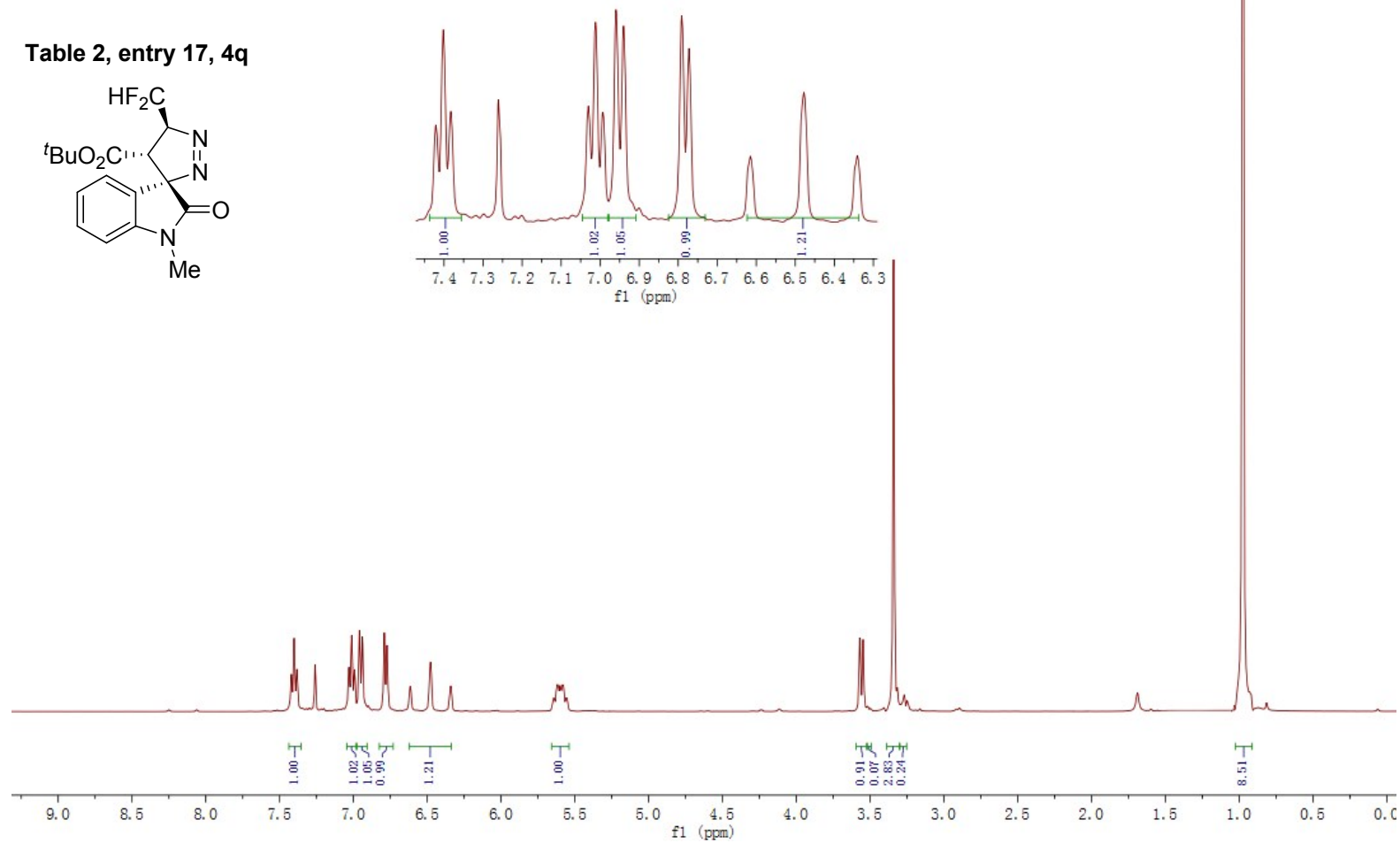
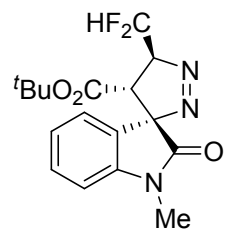
Table 2, entry 16, 4p



zj-3-H

7.4228  
7.4184  
7.4035  
7.3997  
7.3848  
7.3804  
7.2611  
7.0303  
7.0130  
6.9944  
6.9592  
6.9397  
6.7925  
6.7740  
6.6151  
6.4771  
6.3413  
5.6484  
5.6424  
5.6399  
5.6250  
5.6184  
5.6110  
5.6019  
5.5959  
5.5861  
5.5782  
5.5612  
5.5548  
  
3.5713  
3.5486  
3.5166  
3.4989  
3.3417  
3.2696

Table 2, entry 17, 4q



zj-3-C

—171.2857  
—166.3806

—144.7135

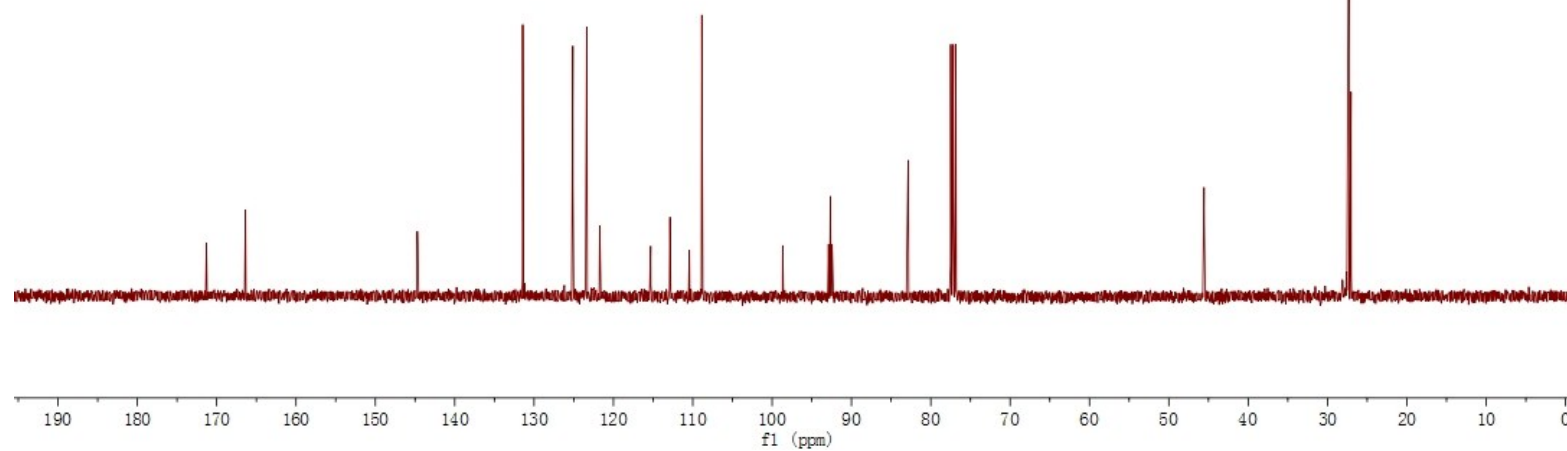
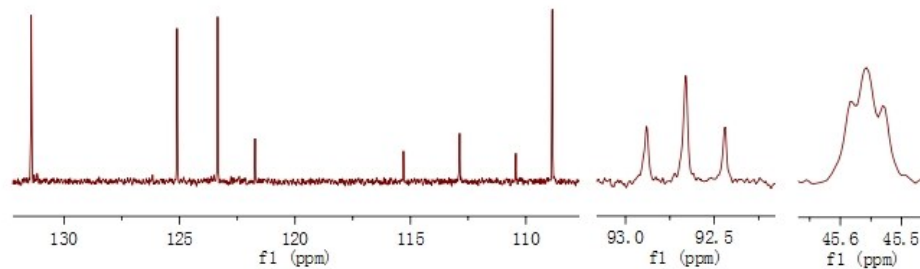
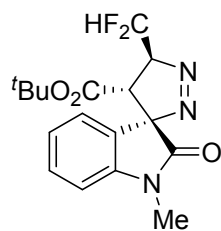
—131.4265  
—125.1063  
—123.3543  
—121.7320  
—115.3036  
—112.8703  
—110.4354  
—108.8560

—98.6572  
—92.8826  
—92.6623  
—92.4412  
—82.8517  
—77.4783  
—77.1600  
—76.8422

—45.5841  
—45.5573  
—45.5279

—27.3676  
—27.0341

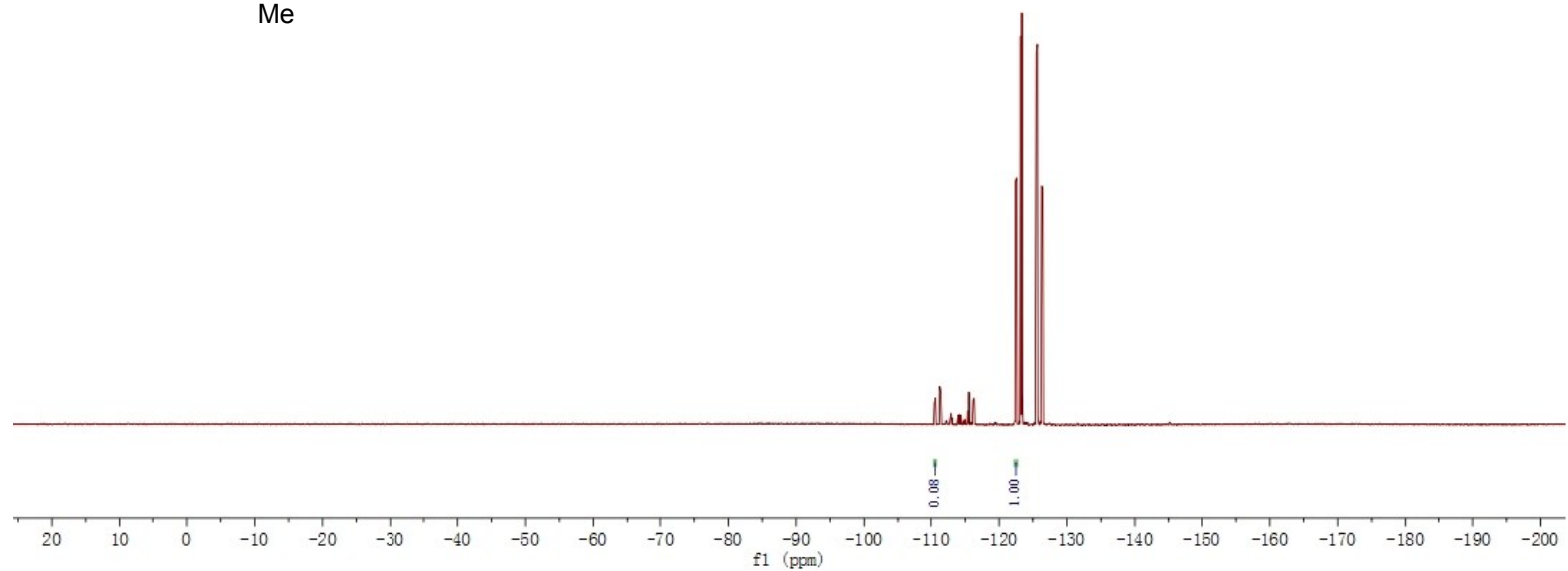
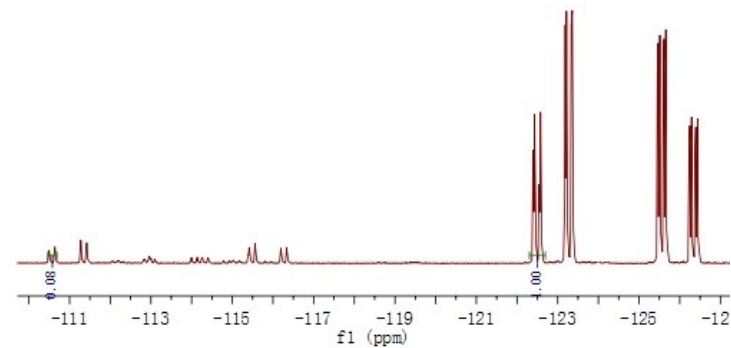
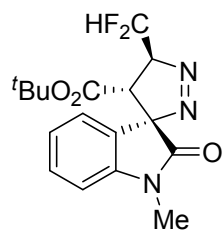
Table 2, entry 17, 4q



zj-3-F  
STANDARD FLUORINE PARAMETERS

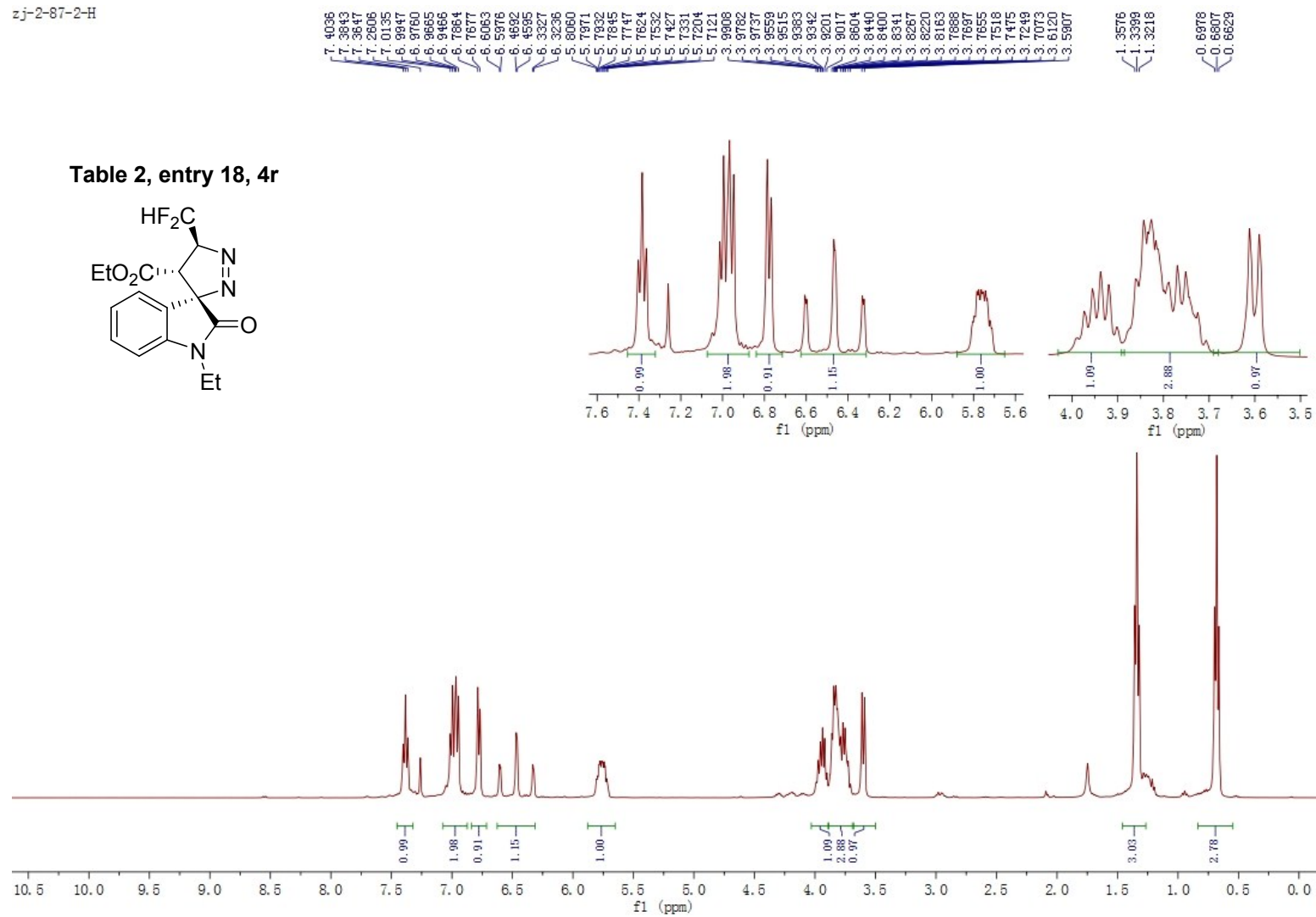
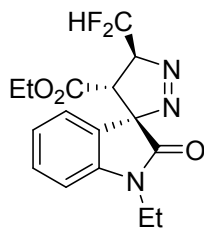


Table 2, entry 17, 4q



zj-2-87-2-H

Table 2, entry 18, 4r





zj-2-87-2-C五

—170.6445  
—167.8084

—143.6848

—131.4048

—125.0078  
—123.1562  
—121.7953

—115.3123  
—112.8777  
—110.4418  
—109.1442

—89.1440  
—83.8107  
—83.5880  
—83.3685

77.4777  
77.1600  
76.8419

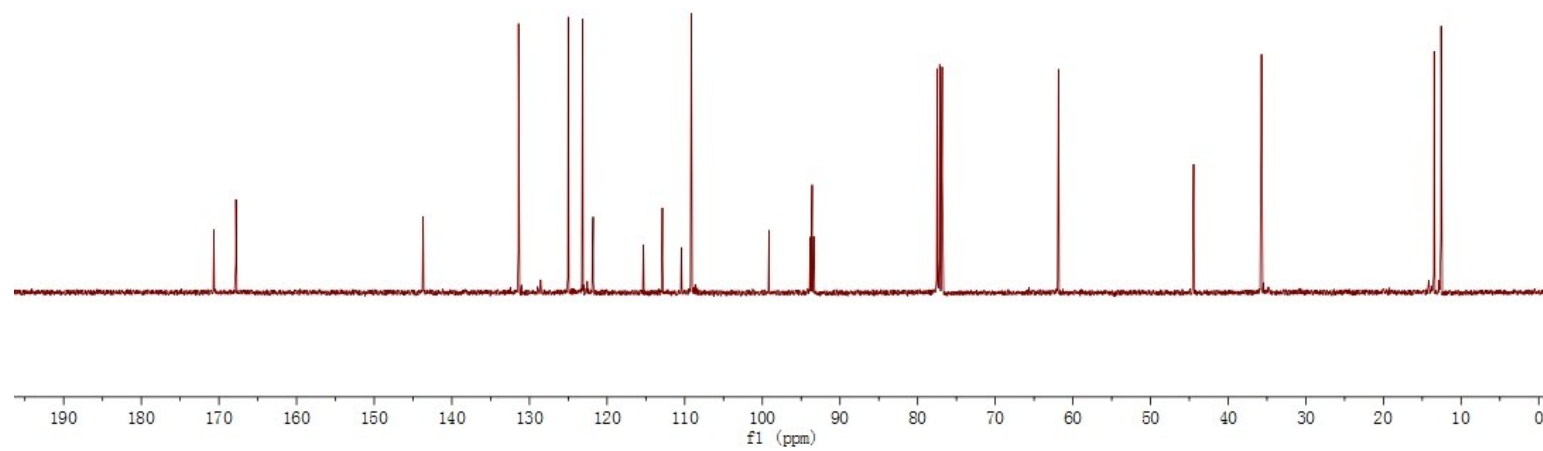
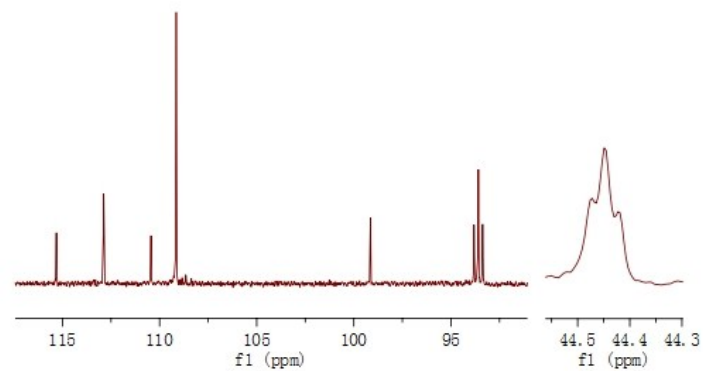
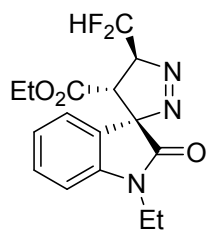
—61.8475

44.4757  
44.4487  
44.4202

—35.7048

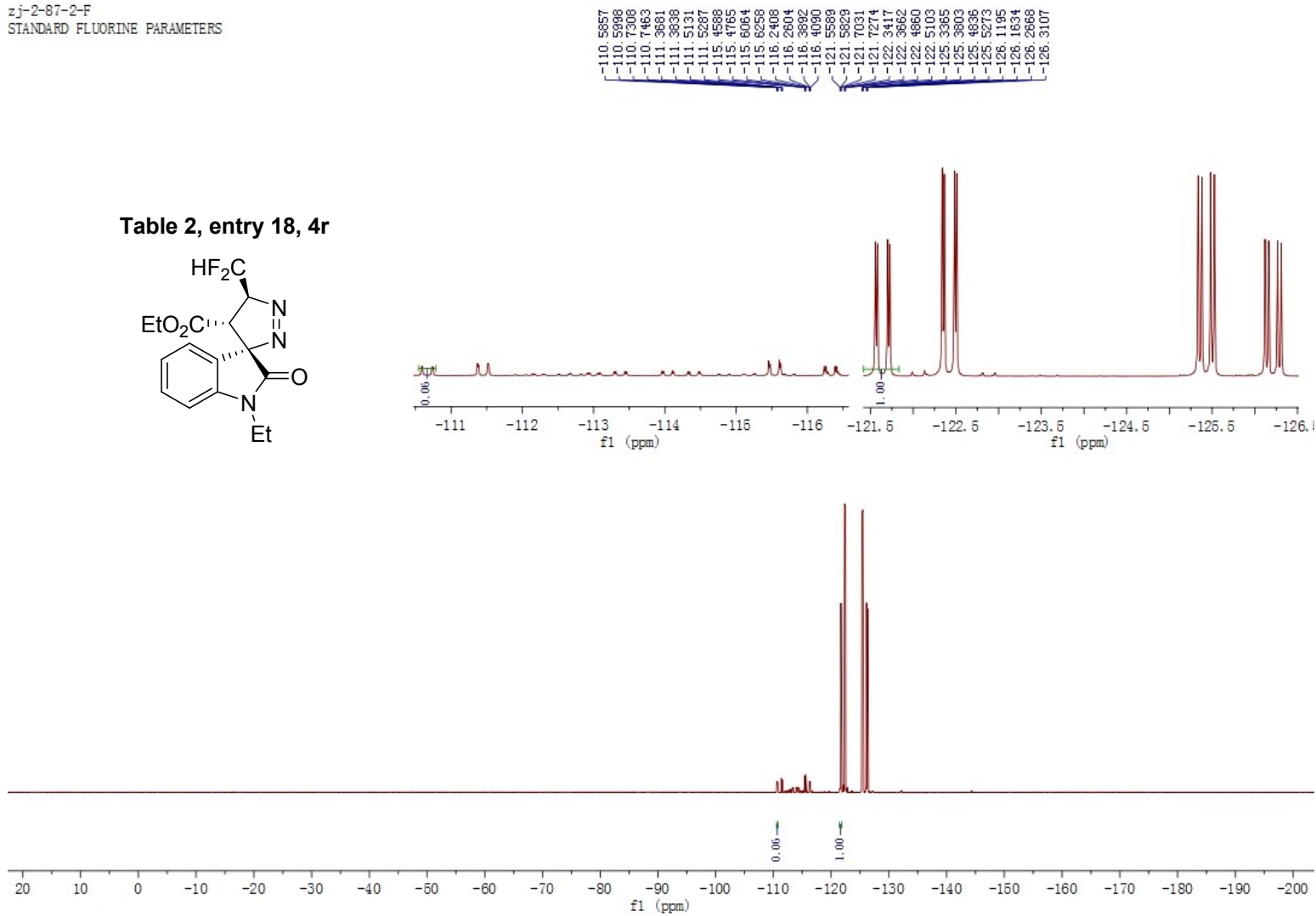
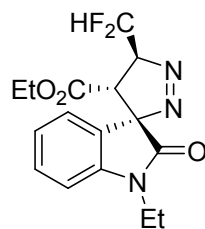
13.4618  
12.5747

Table 2, entry 18, 4r



zj-2-87-2-F  
STANDARD FLUORINE PARAMETERS

Table 2, entry 18, 4r

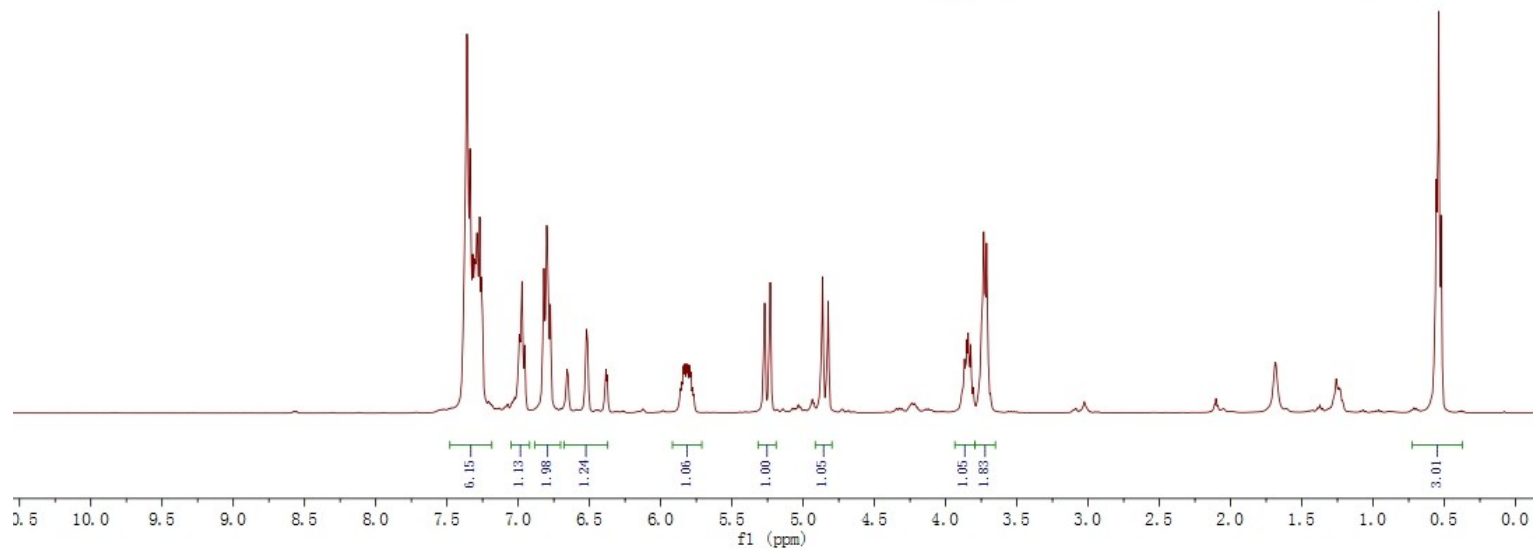
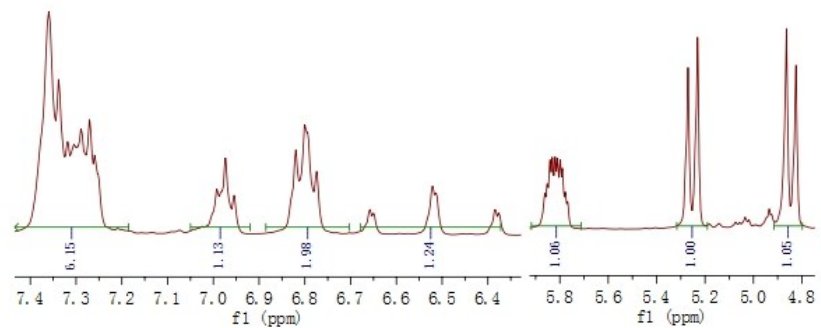
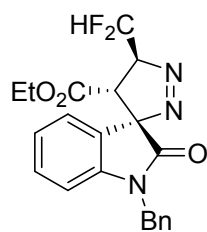


zj-2-85-2-HH

7.3763  
7.3698  
7.3373  
7.3188  
7.3045  
7.2880  
7.2702  
7.2585  
7.0031  
6.9925  
6.9896  
6.9794  
6.8545  
6.8201  
6.8007  
6.7927  
6.7741  
6.6584  
6.6491  
6.5215  
6.5121  
6.3847  
6.3753  
5.8826  
5.8526  
5.8407  
5.8310  
5.8196  
5.8099  
5.7984  
5.7889  
5.7765  
5.7671  
5.2703  
5.2311  
4.8242  
4.8242  
3.8861  
3.8784  
3.8683  
3.8595  
3.8507  
3.8414  
3.8334  
3.8254  
3.8057  
3.7896  
3.7573  
3.7466  
3.7335  
3.7214  
3.7125  
3.7031  
3.6947

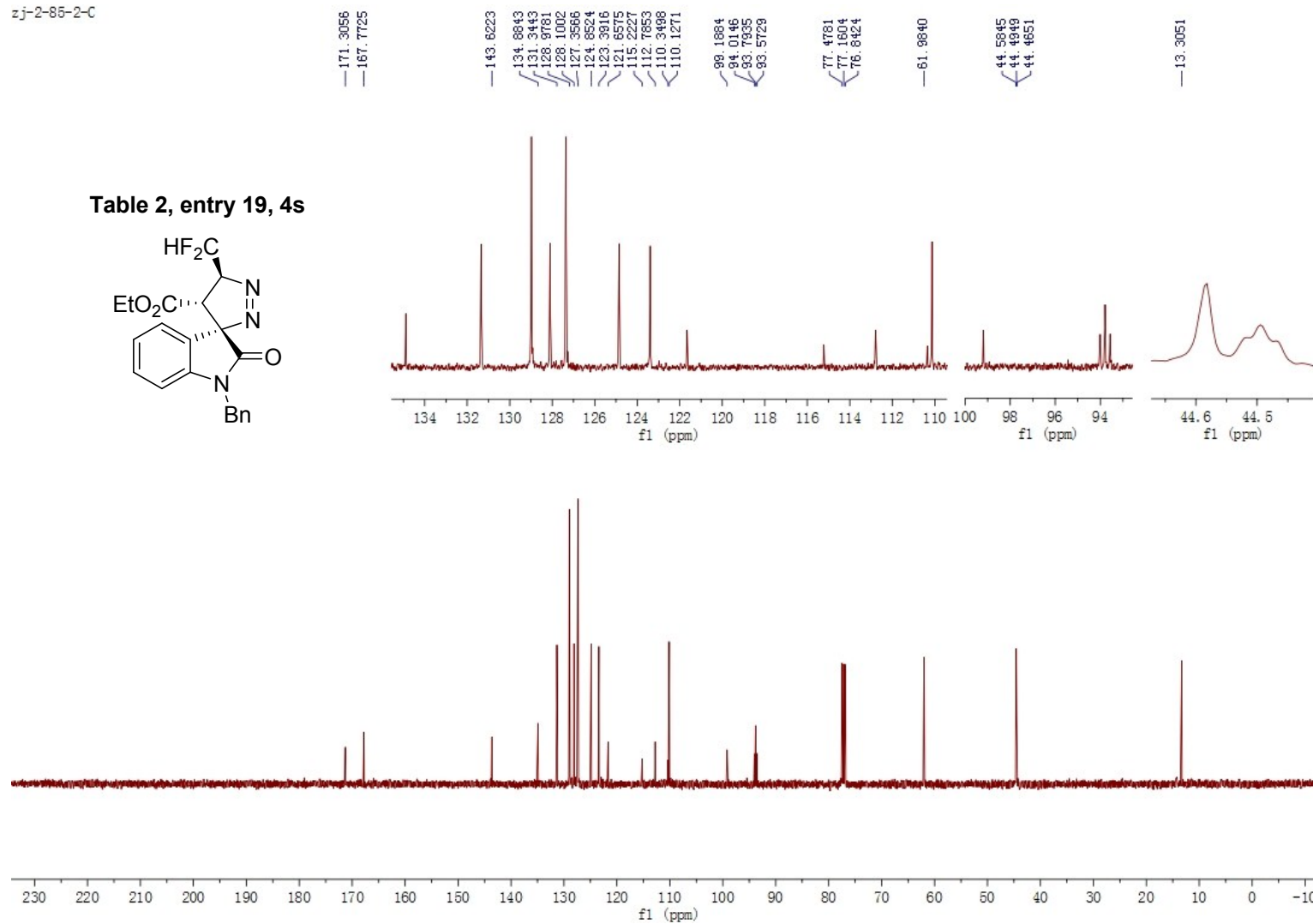
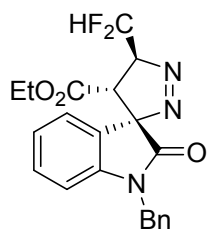
-0.5574  
-0.5397  
-0.5223

Table 2, entry 19, 4s



zj-2-85-2-C

Table 2, entry 19, 4s



zj-2-85-2-F  
STANDARD FLUORINE PARAMETERS

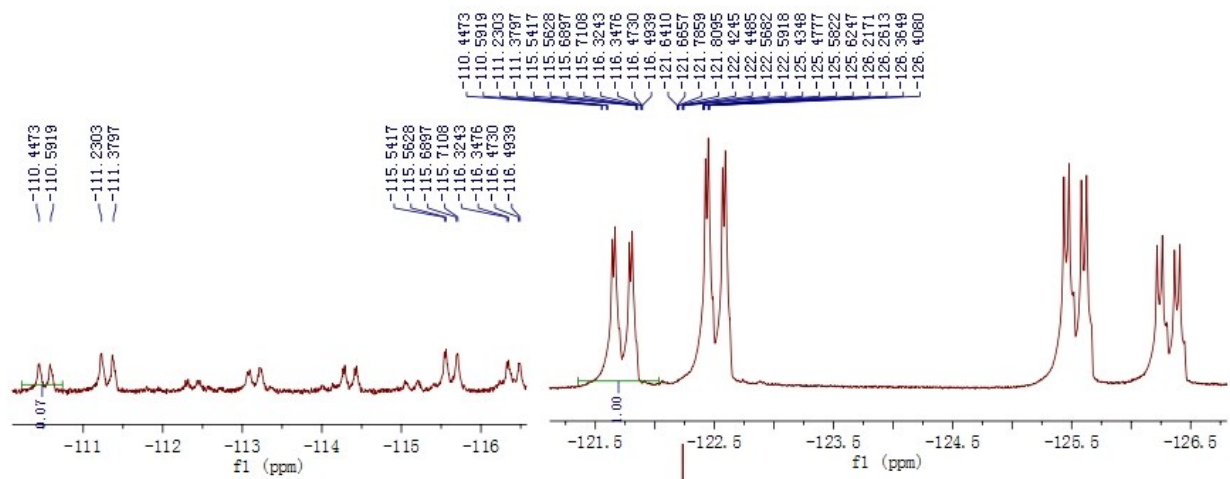
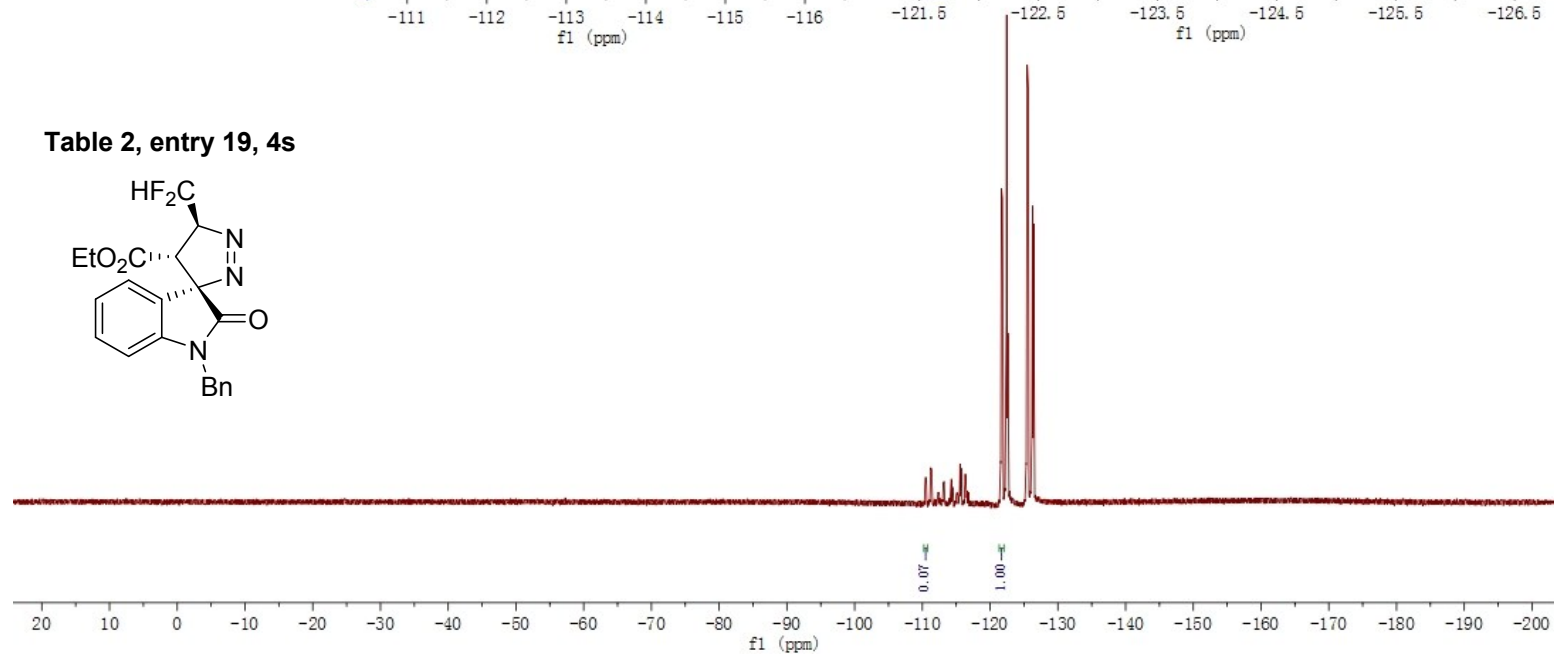
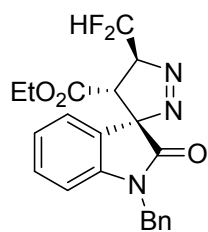


Table 2, entry 19, 4s

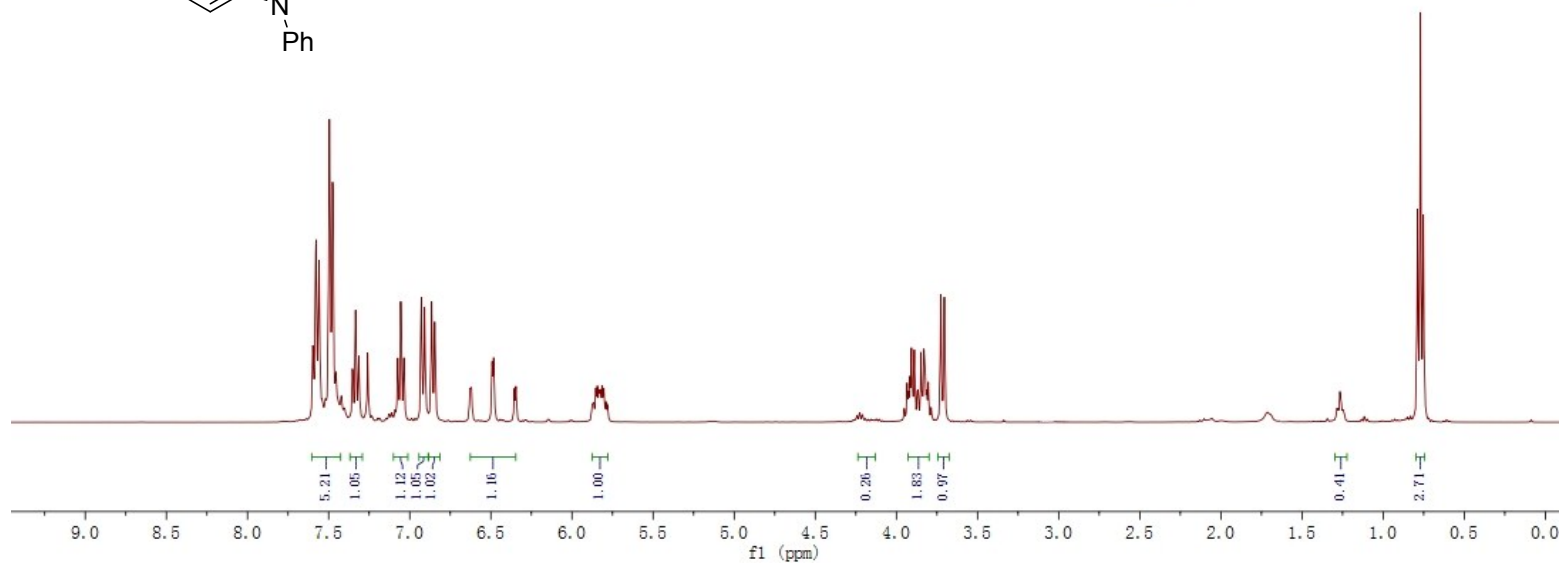
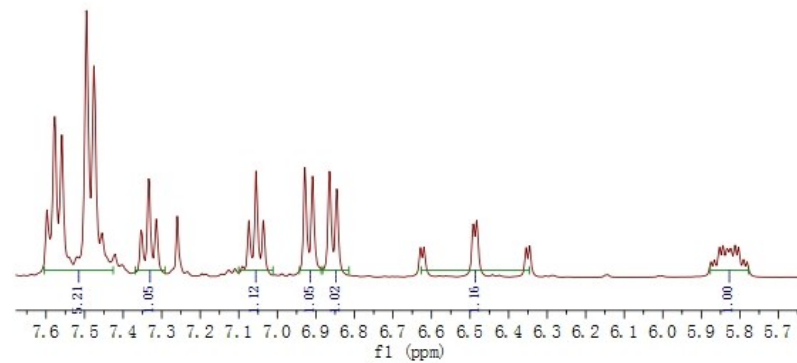
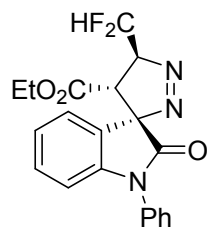


zj-2-2-H

7.5974  
7.5764  
7.5591  
7.4950  
7.4756  
7.4552  
7.3542  
7.3334  
7.3139  
7.2595  
7.0738  
7.0549  
7.0362  
6.9284  
6.9085  
6.8646  
6.8458  
6.6288  
6.6192  
6.4921  
6.4825  
6.3549  
6.3452  
5.8752  
5.8659  
5.8533  
5.8437  
5.8243  
5.8128  
5.8032  
5.7907  
5.7807  
4.2426  
4.2251  
4.2095  
4.1925  
4.1739  
4.1561  
4.1467  
4.1241  
4.1063  
3.9342  
3.9166  
3.9073  
3.8894  
3.8715  
3.8661  
3.8483  
3.8304  
3.8035  
3.7857  
3.7261  
3.7048

1.2887  
1.2843  
1.2765  
1.2663  
1.2586  
1.2485  
1.2405  
0.7880  
0.7701  
0.7523

Table 2, entry 20, 4t



zj-2-2-C

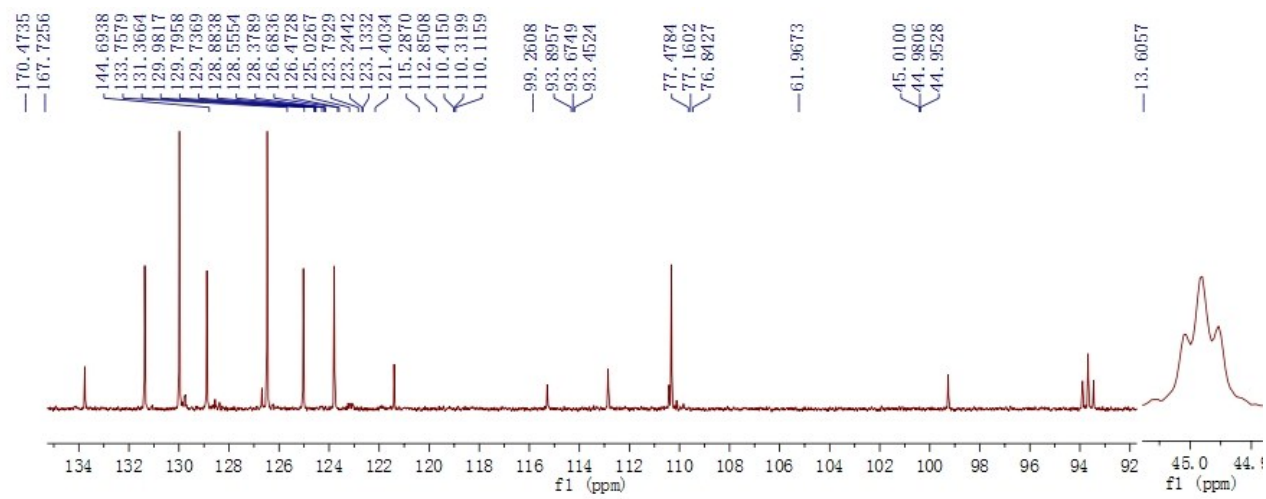
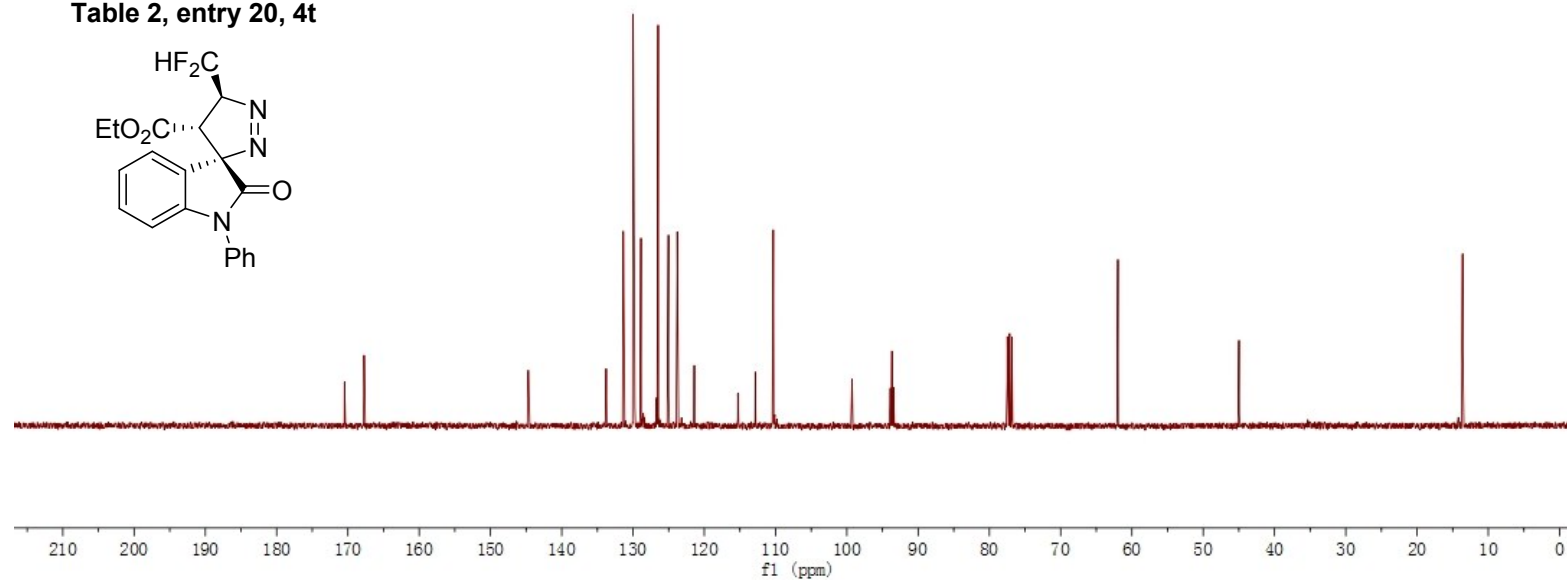
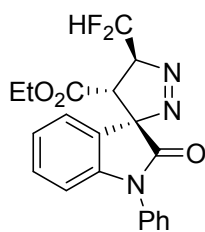


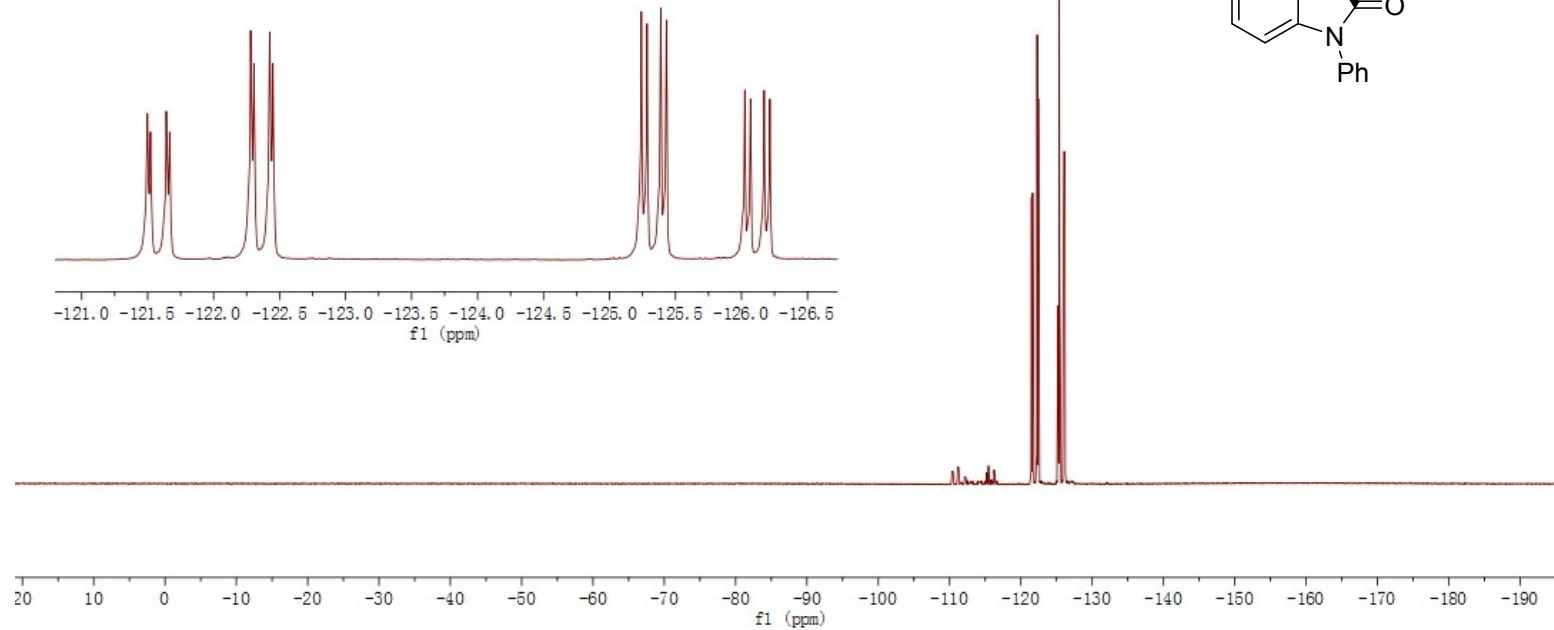
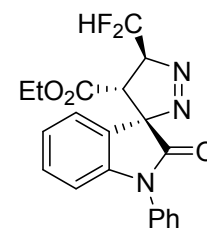
Table 2, entry 20, 4t



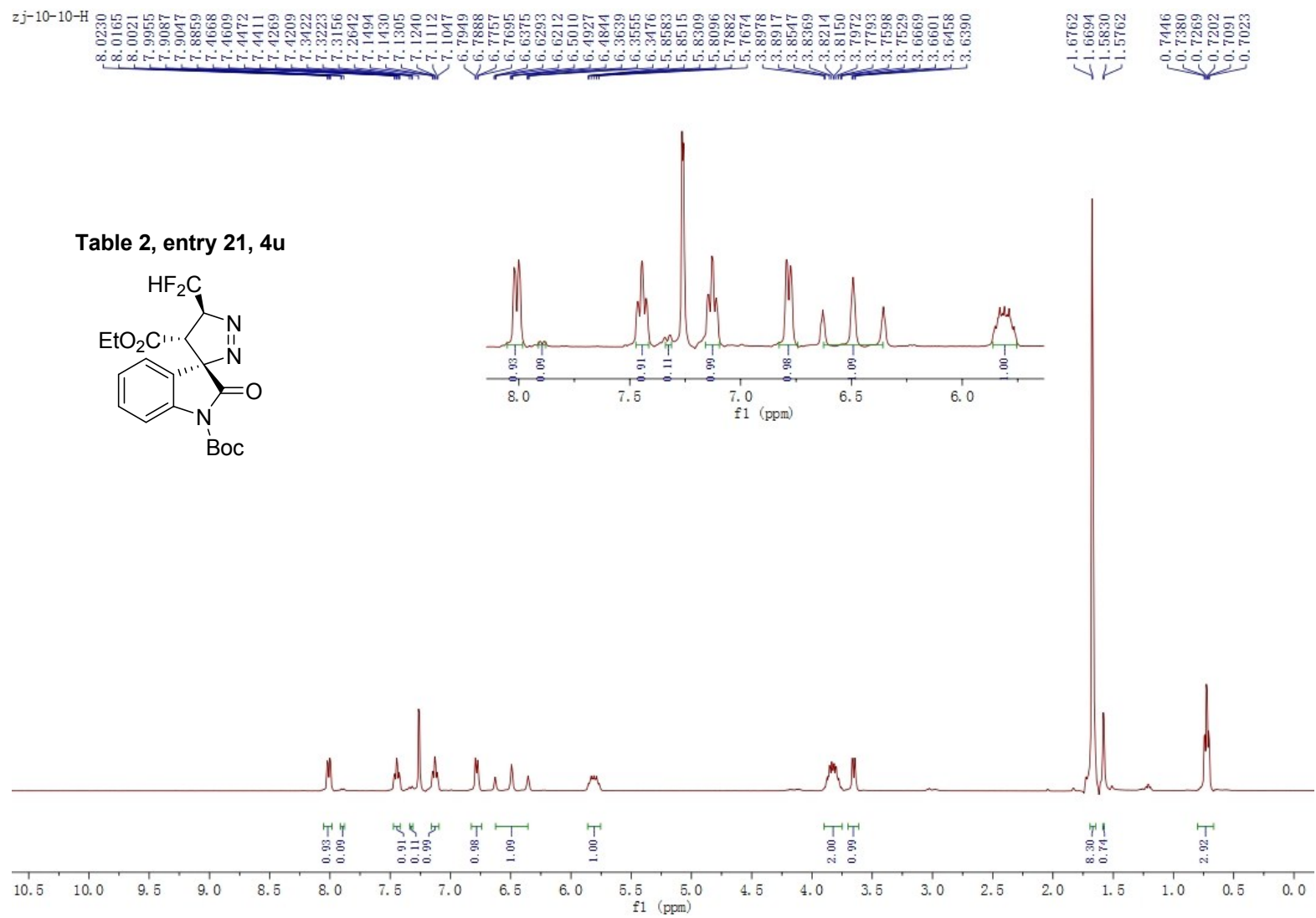
zj-2-2-F  
STANDARD FLUORINE PARAMETERS

-110.3452  
-110.3604  
-110.4905  
-110.5058  
-111.1284  
-111.1448  
-111.2751  
-111.2913  
-115.4543  
-115.4732  
-115.6016  
-115.6218  
-116.2385  
-116.2576  
-116.3863  
-116.4068  
-121.4980  
-121.5217  
-121.6416  
-121.6659  
-122.2809  
-122.3050  
-122.4256  
-122.4493  
-125.2412  
-125.2847  
-125.3881  
-125.4314  
-126.0248  
-126.0681  
-126.1717  
-126.2150

Table 2, entry 20, 4t







zj-10-10-C

169.3887  
167.5219

148.7289

140.8837

131.6788

128.9570

125.0736

124.6656

124.4640

122.4695

120.7280

115.9400

115.2177

115.0465

112.6067

110.1699

99.7951

94.3696

94.1466

93.9246

85.7022

77.4778

77.1603

76.8429

62.2032

45.0602

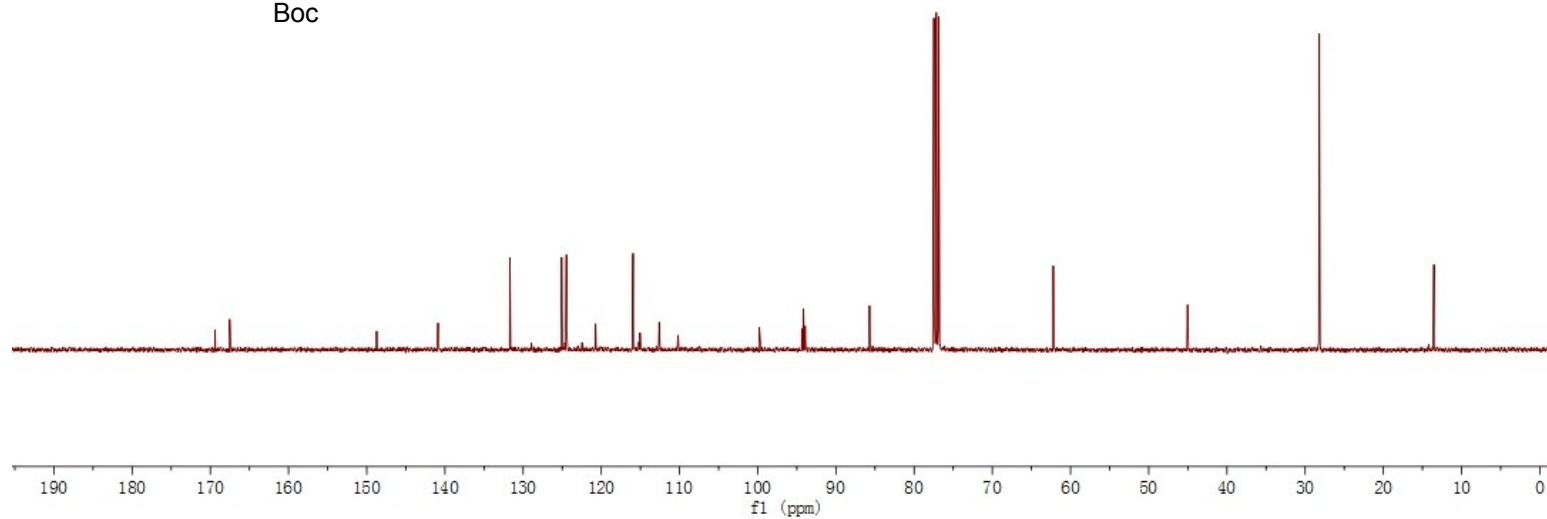
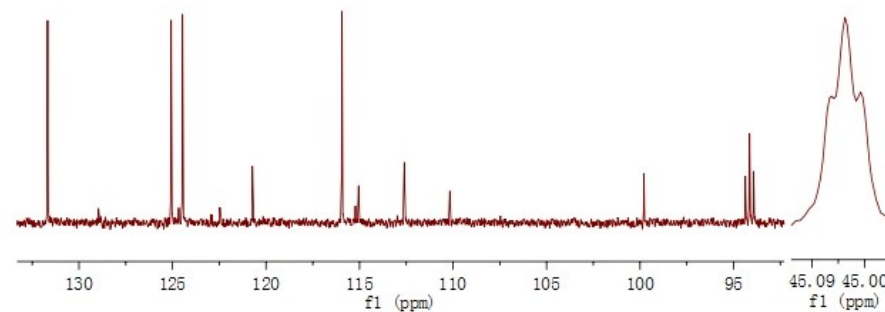
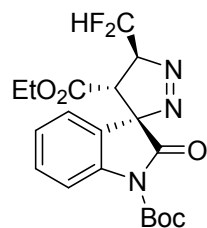
45.0335

45.0042

28.1842

13.5340

Table 2, entry 21, 4u



zj-2-73-2-F

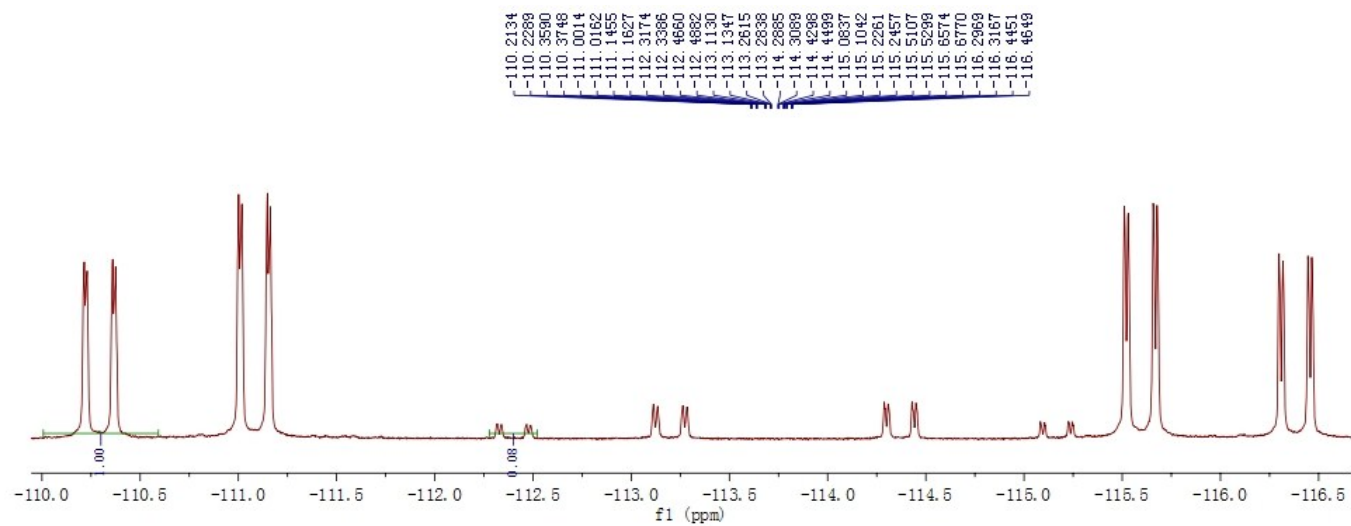


Table 2, entry 21, 4u

