

Sc(OTf)₃-Catalyzed Chemodivergent Annulations of γ -Butyrolactone Fused Cyclopropanes with Anthranils

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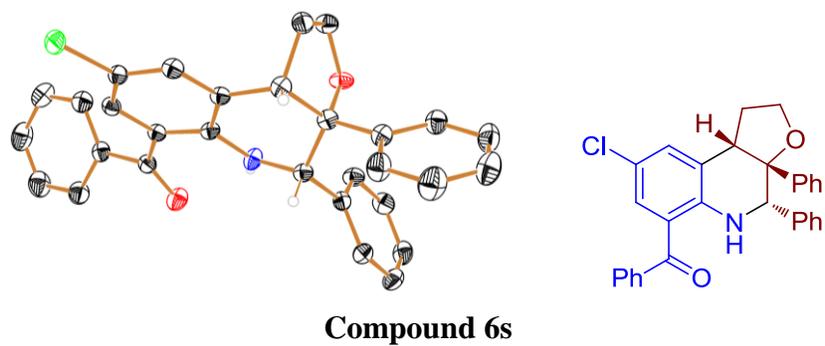
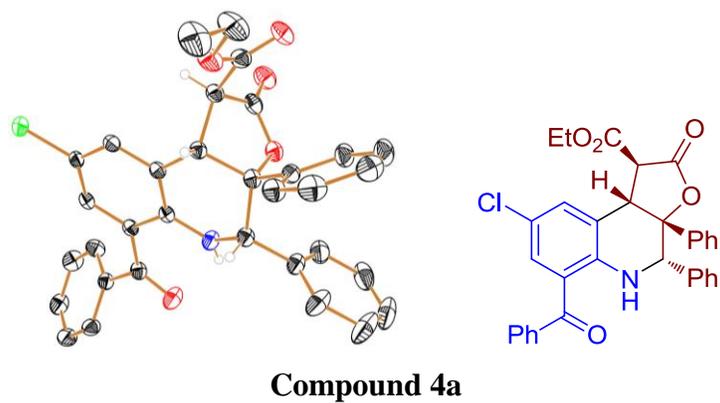
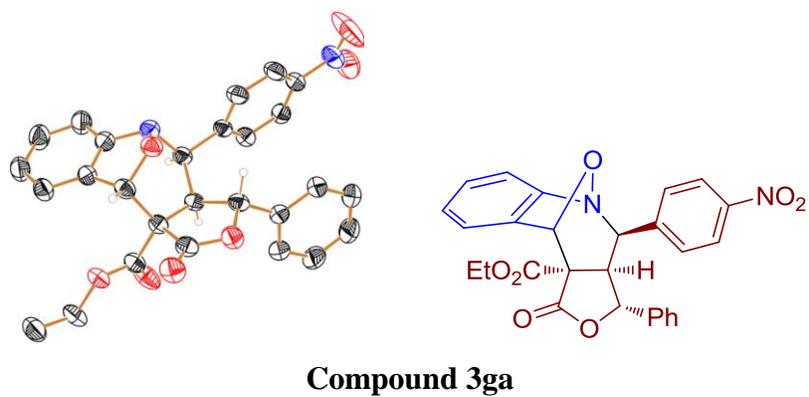
I. X-ray crystallographic analysis

The single crystals of **3ga**, **4a** and **6s** suitable for X-ray crystallographic analysis were obtained by recrystallization from a mixed solvent of dichloromethane and petroleum ether. The single crystal X-ray diffraction data for the six compounds were collected on a diffractometer with graphite monochromated Cu K α radiation ($\lambda = 1.54178 \text{ \AA}$) for **3ga** and **4a**, Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$) for **6s**. SAINT program and SADABS program carried out the data integration. The structure was solved by a direct method and refined on F² using SHELXTL suite of program. All non-hydrogen atoms were anisotropically refined by full-matrix least squares methods. All hydrogen atoms were geometrically generated and isotropically refined using a riding model. The details of the X-ray data collection, structure solution and structure refinements are given in Table S1.

Table S1 Crystallographic data and structural refinement details for compound **3ga**, **4a** and **6s**.

Compound	3ga	4a	6s
Formula	C ₂₇ H ₂₂ N ₂ O ₇	C ₃₃ H ₂₆ ClNO ₅	C ₃₀ H ₂₄ ClNO ₂
Formula weight	486.47	552.00	465.95
Temperature/K	273	273	293
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P21/c	P21	P21/n
<i>a</i> , Å	11.4226(11)	11.3905(2)	10.318(3)
<i>b</i> , Å	10.6852(11)	6.8267(2)	8.418(2)
<i>c</i> , Å	20.1313(18)	18.0192(4)	26.443(8)
α , deg	/	/	/
β , deg	104.995(5)	102.296(1)	93.828(4)
γ , deg	/	/	/
<i>V</i> / Å ³	2511.0(5)	1369.02(6)	2291.6(11)
<i>Z</i>	4	2	4
μ , mm ⁻¹	0.828	1.595	0.196
θ range for data collection, deg	4.5 to 80.1	2.5 to 68.2	1.5 to 25.0
Reflections collected	36521	36346	18663
Unique reflections/R _{int}	5020 / R(int) = 0.129	4950 / R(int) = 0.068	3863 / R(int) = 0.063
Goodness-of-fit on F ²	1.02	1.10	1.13
R, R _w [I > 2 σ (I)]	0.0659, 0.2020	0.0371, 0.0760	0.0711, 0.1505
Residual ρ /(e Å ⁻³)	0.19, -0.23	0.14, -0.24	0.35, -0.35
CCDC	1951589	1951590	1951591

Figure S1 X-ray structure (30 % probability ellipsoids) of **3ga**, **4a** and **6s**.



II. Copies of NMR spectra for 3

Compound 3aa

7.4404
7.2567
7.1205
7.1030
7.0762
6.7740
6.7599

5.7126

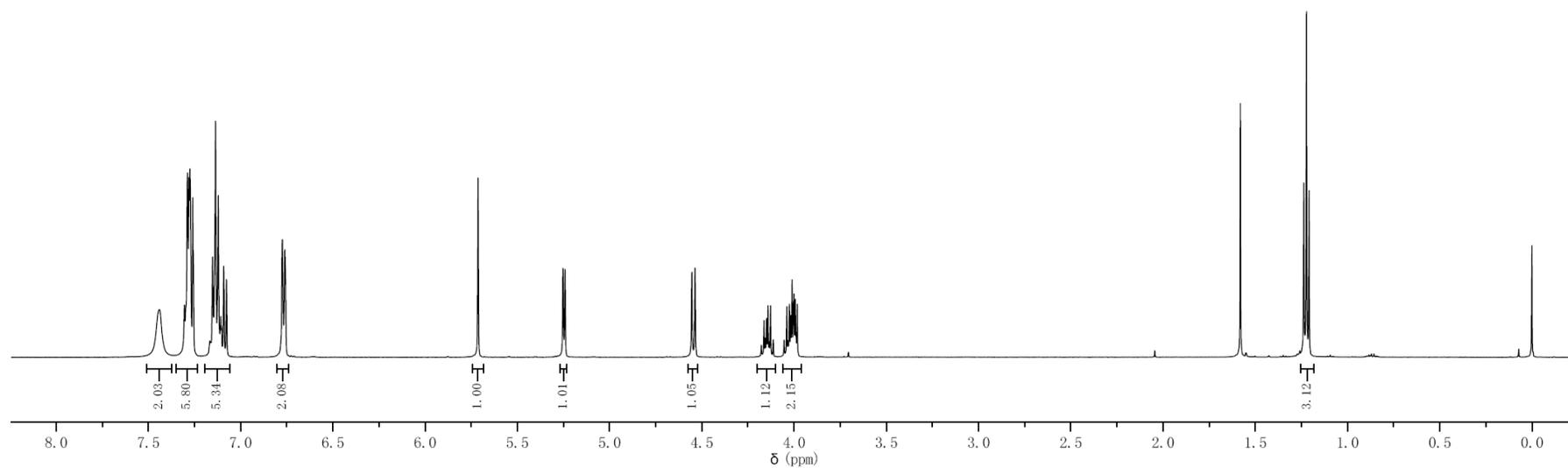
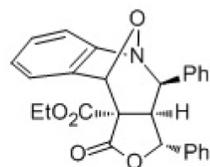
5.2522
5.2415

4.5542
4.5367
4.1771
4.1627
4.1556
4.1484
4.1413
4.1342
4.1270
4.1127
4.0534
4.0391
4.0248
4.0176
4.0108
4.0029
4.0002
3.9933
3.9893
3.9826

1.5808

1.2370
1.2227
1.2084

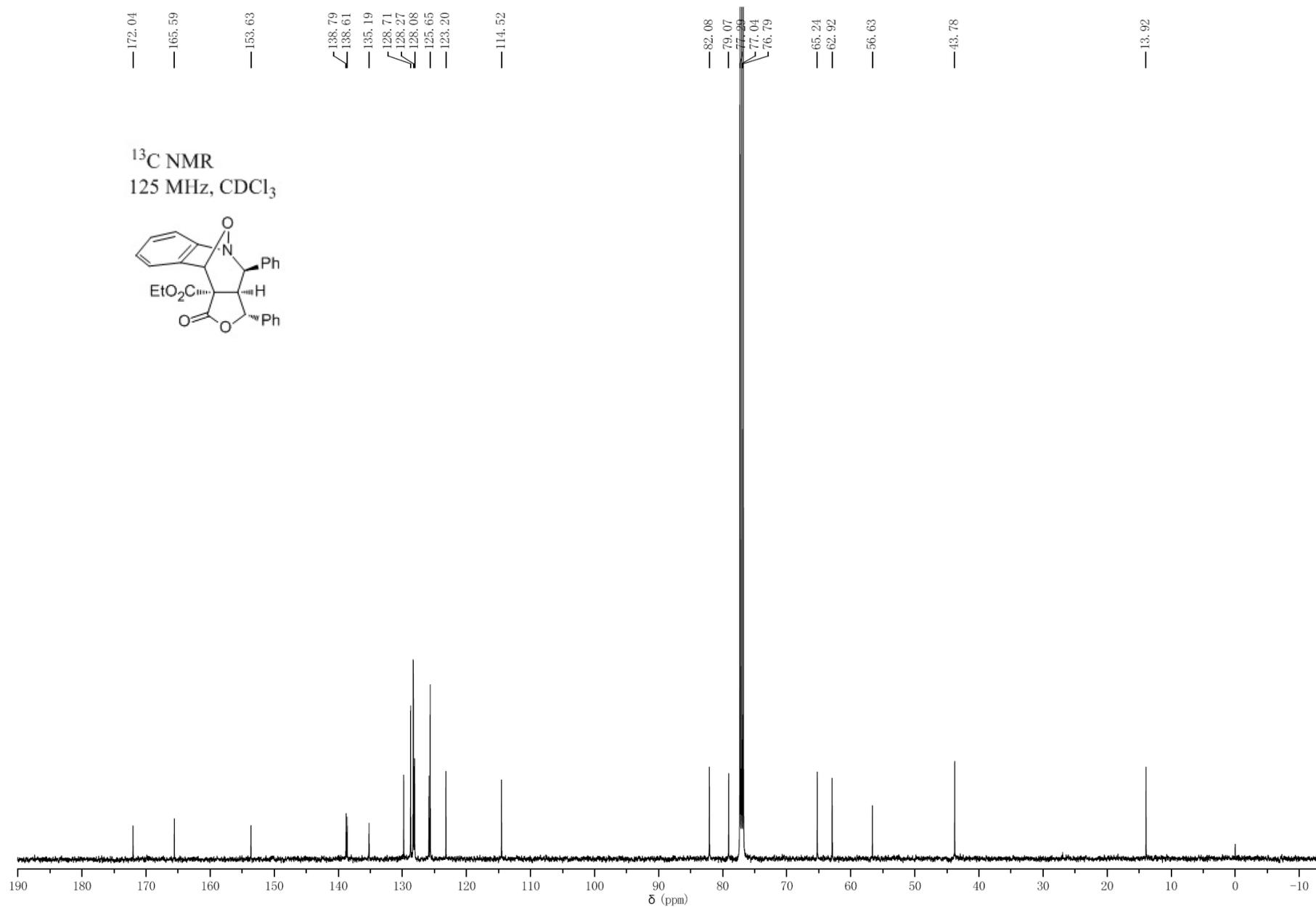
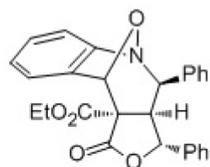
^1H NMR
500 MHz, CDCl_3



Compound 3aa

- 172.04
- 165.59
- 153.63
- 138.79
- 138.61
- 135.19
- 128.71
- 128.27
- 128.08
- 125.65
- 123.20
- 114.52
- 82.08
- 79.07
- 77.04
- 76.79
- 65.24
- 62.92
- 56.63
- 43.78
- 13.92

^{13}C NMR
125 MHz, CDCl_3



Compound 3ba

7.2581
7.2438
7.2292
7.1714
7.1572
7.1406
7.1286
7.1107
7.1088
7.1019
7.0926
7.0864
7.0775
6.8006
6.7869

5.7018

5.2389
5.2290

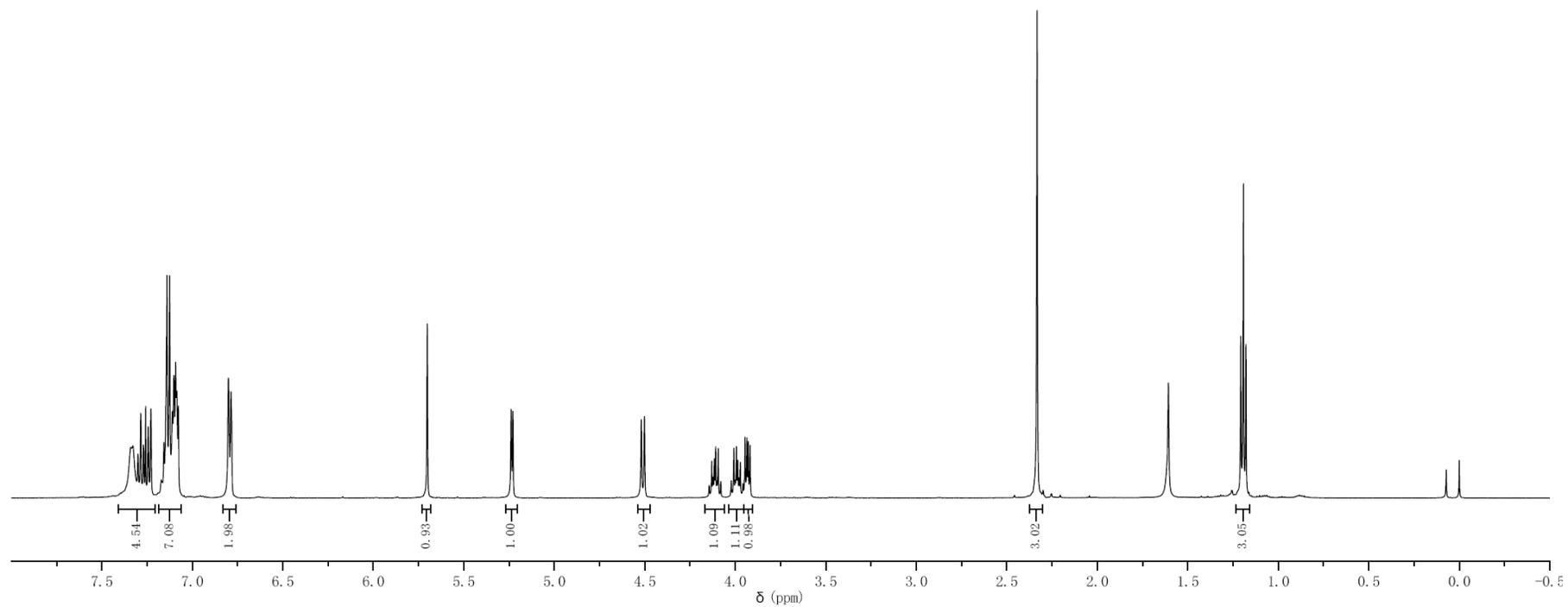
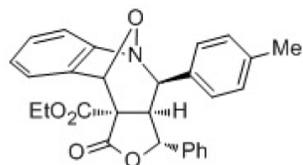
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4.5021
4.1085
4.0799
4.0221
4.0078
4.0005
3.9935
3.9863
3.9792
3.9720
3.9576
3.9460
3.9360
3.9284
3.9183

2.3327

1.6069

1.2070
1.1927
1.1785

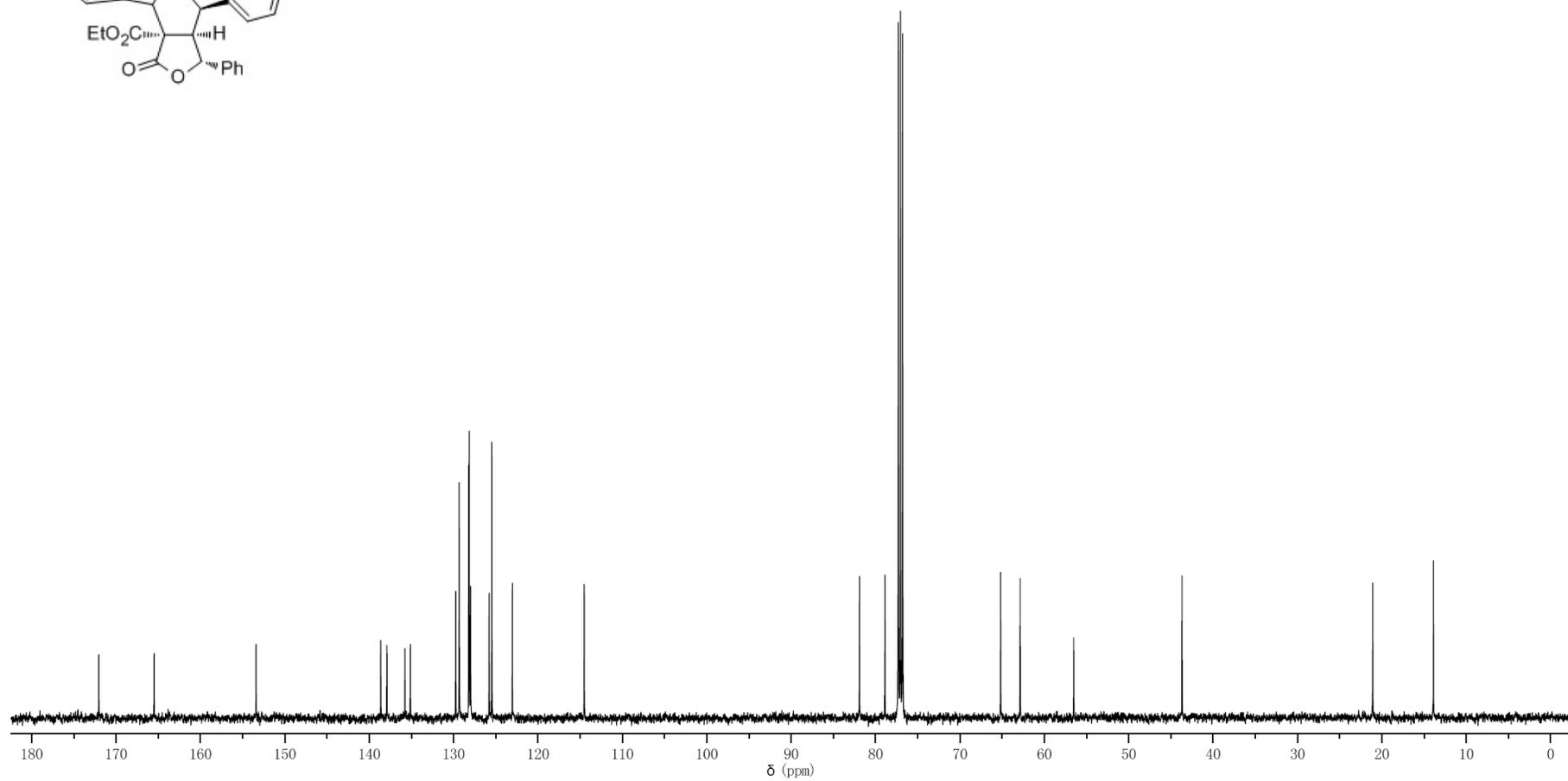
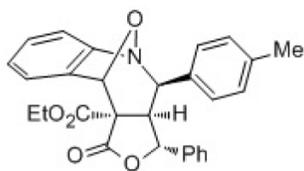
¹H NMR
500 MHz, CDCl₃



Compound 3ba



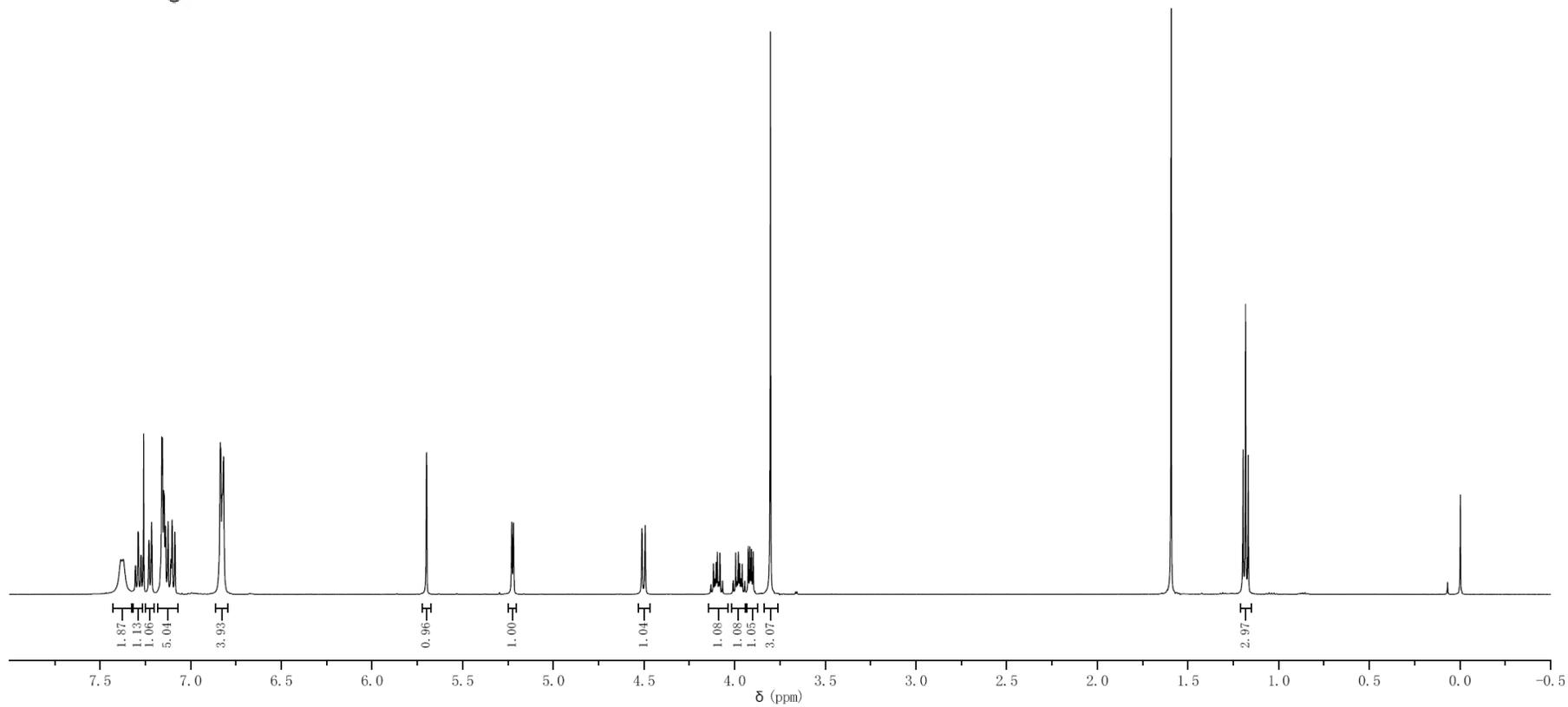
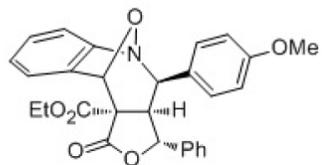
^{13}C NMR
125 MHz, CDCl_3



Compound 3ca



¹H NMR
500 MHz, CDCl₃



Compound 3ca

—172.03
—165.46
—159.48
—153.27

—138.67
—135.12
—129.54
—128.25
—128.03
—125.43
—123.01

—114.54
—114.10

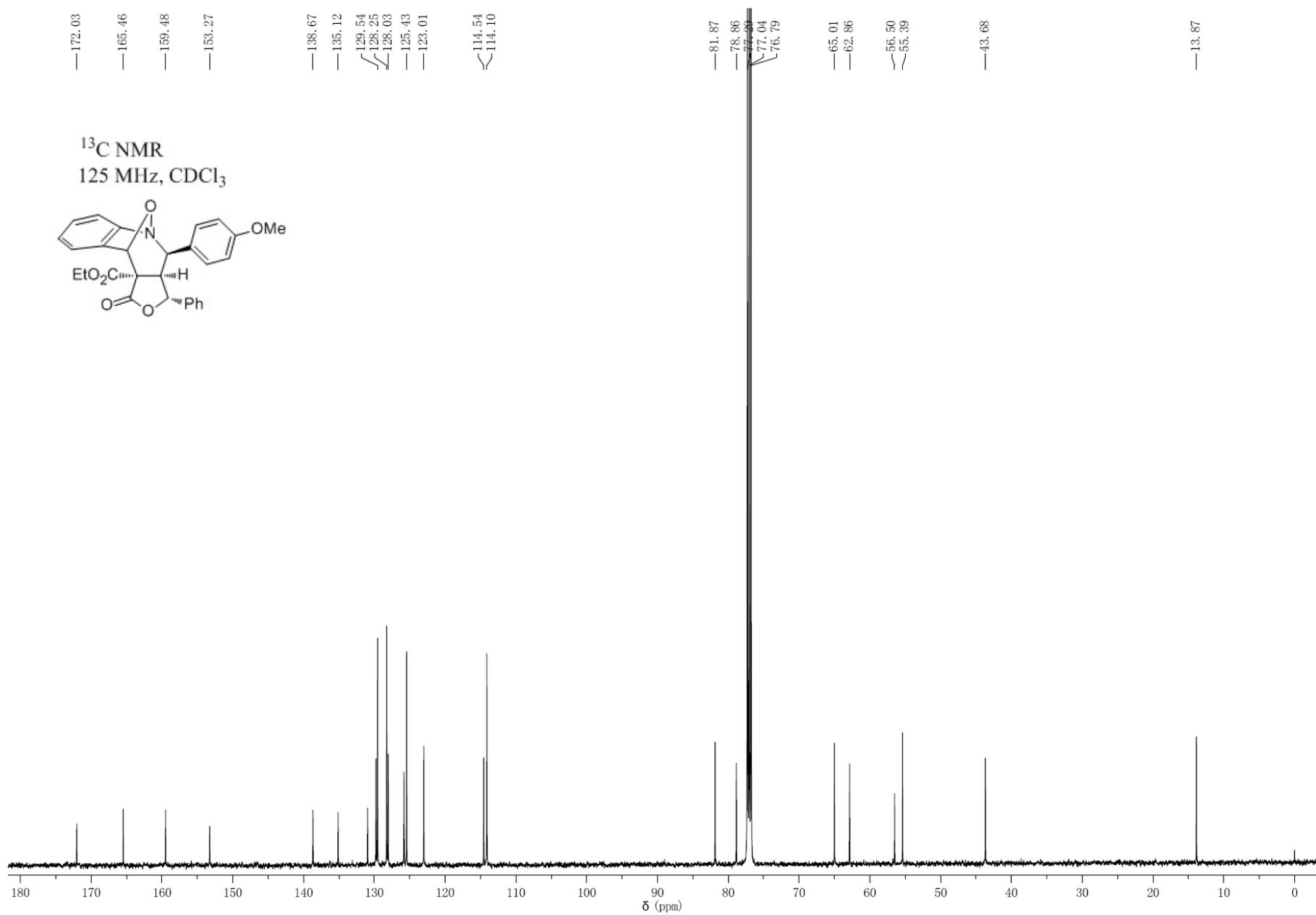
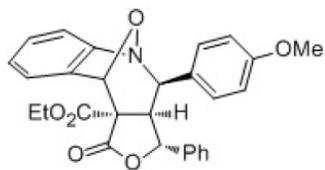
—81.87
—78.86
—77.04
—76.79

—65.01
—62.86
—56.50
—55.39

—43.68

—13.87

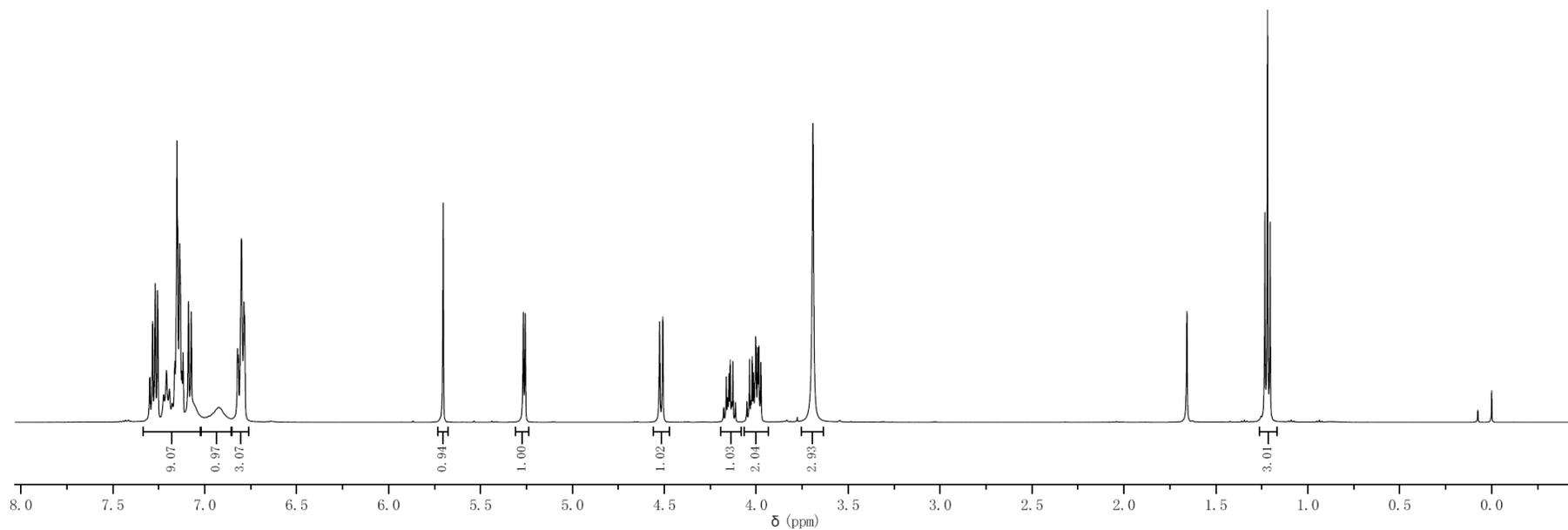
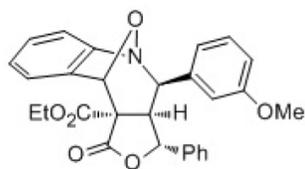
¹³C NMR
125 MHz, CDCl₃



Compound 3da



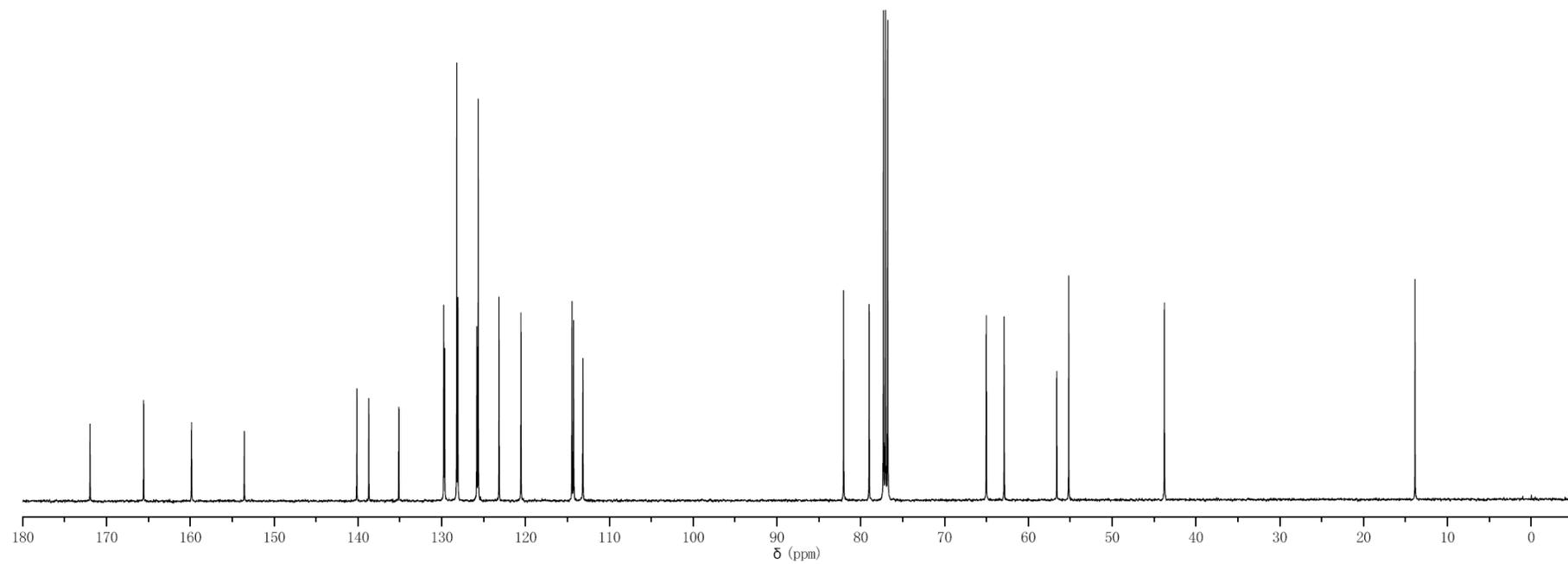
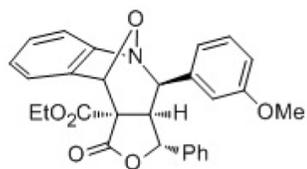
¹H NMR
500 MHz, CDCl₃



Compound 3da



^{13}C NMR
125 MHz, CDCl_3



Compound 3ea

8.0594
8.0567
8.0442
8.0416
7.2605
7.2206
7.1699
7.1498
7.1306
7.1253
7.1107
7.0991
7.0833
6.7658
6.7517
6.4438
6.4276

5.6932

5.2092
5.1964

4.8610
4.8443

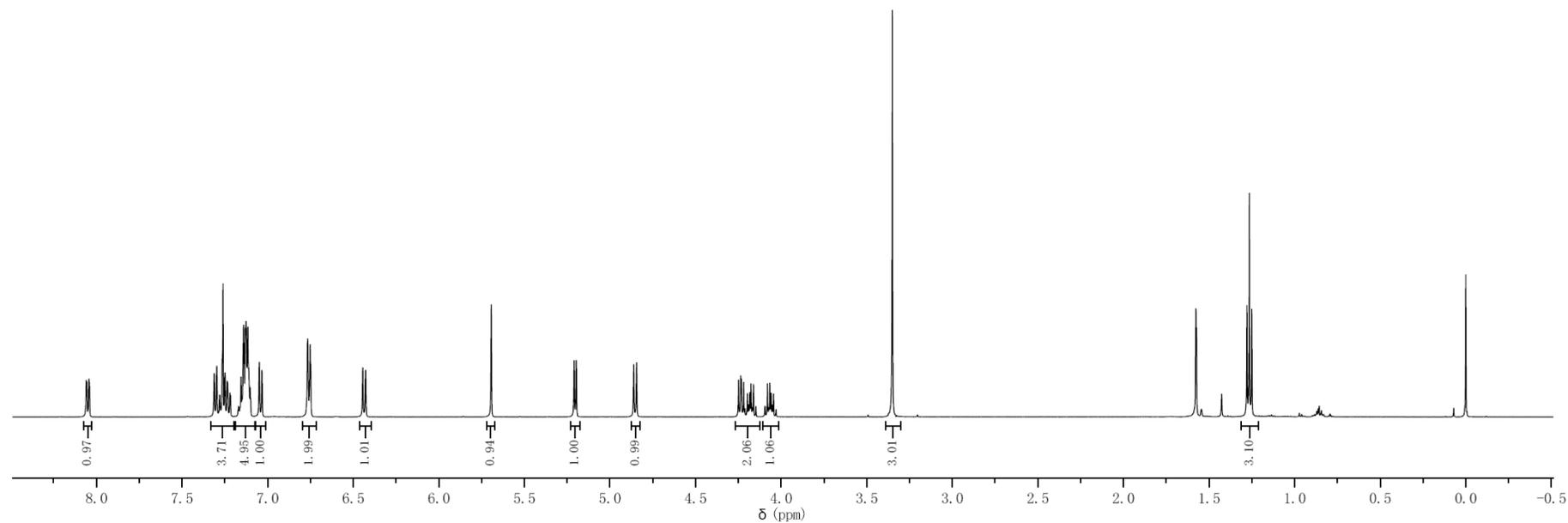
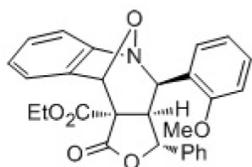
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4.2191
4.1973
4.1830
4.1686
4.1472
4.0799
4.0656
4.0513
4.0299

3.3499

1.5771

1.2786
1.2643
1.2500

¹H NMR
500 MHz, CDCl₃



Compound 3ea

172.43
166.00
155.70
154.49

138.61
135.44
129.09
128.05
127.55
125.59
123.41
121.04
114.48
109.48

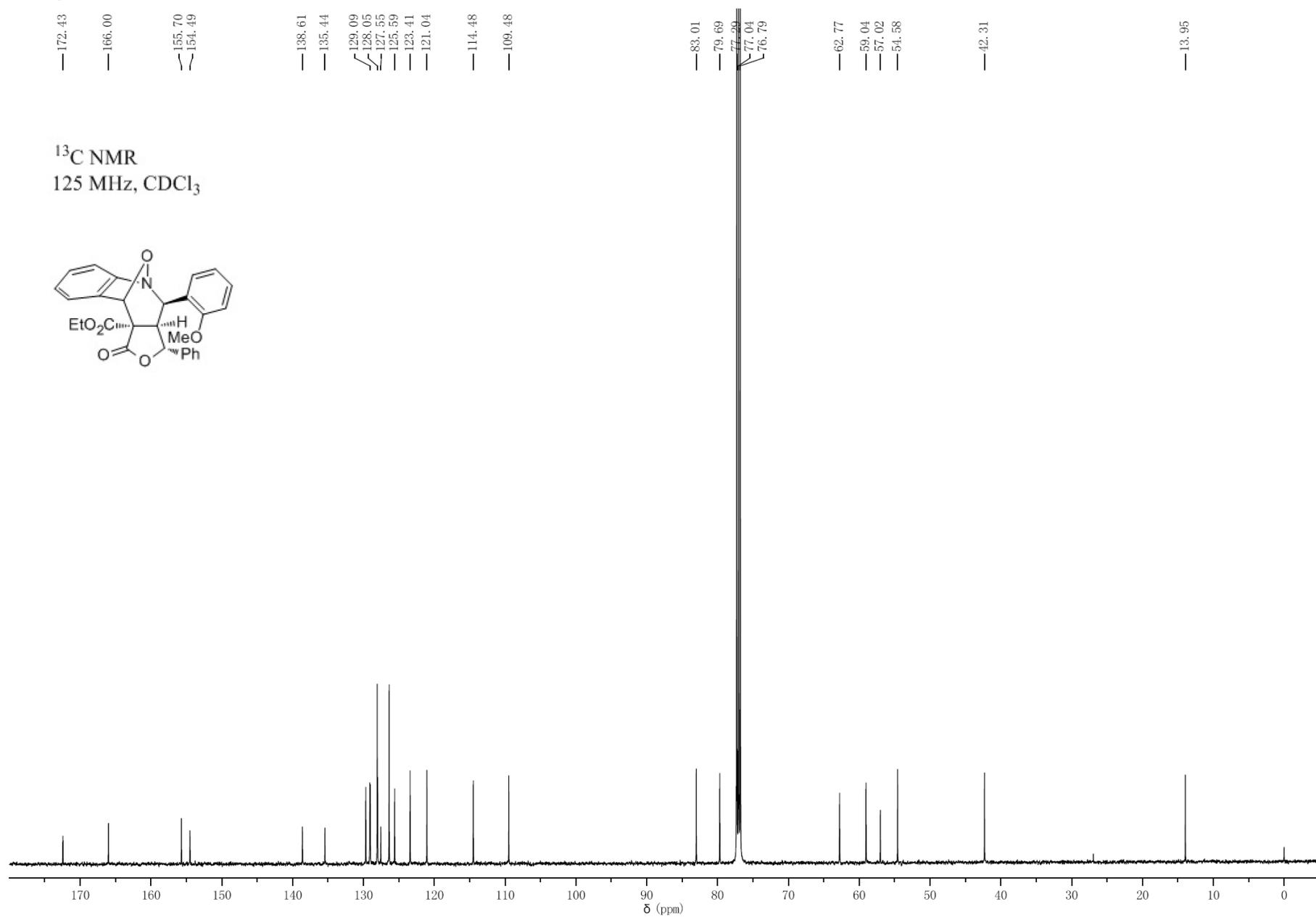
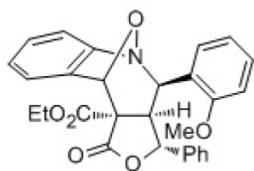
83.01
79.69
77.29
77.04
76.79

62.77
59.04
57.02
54.58

42.31

13.95

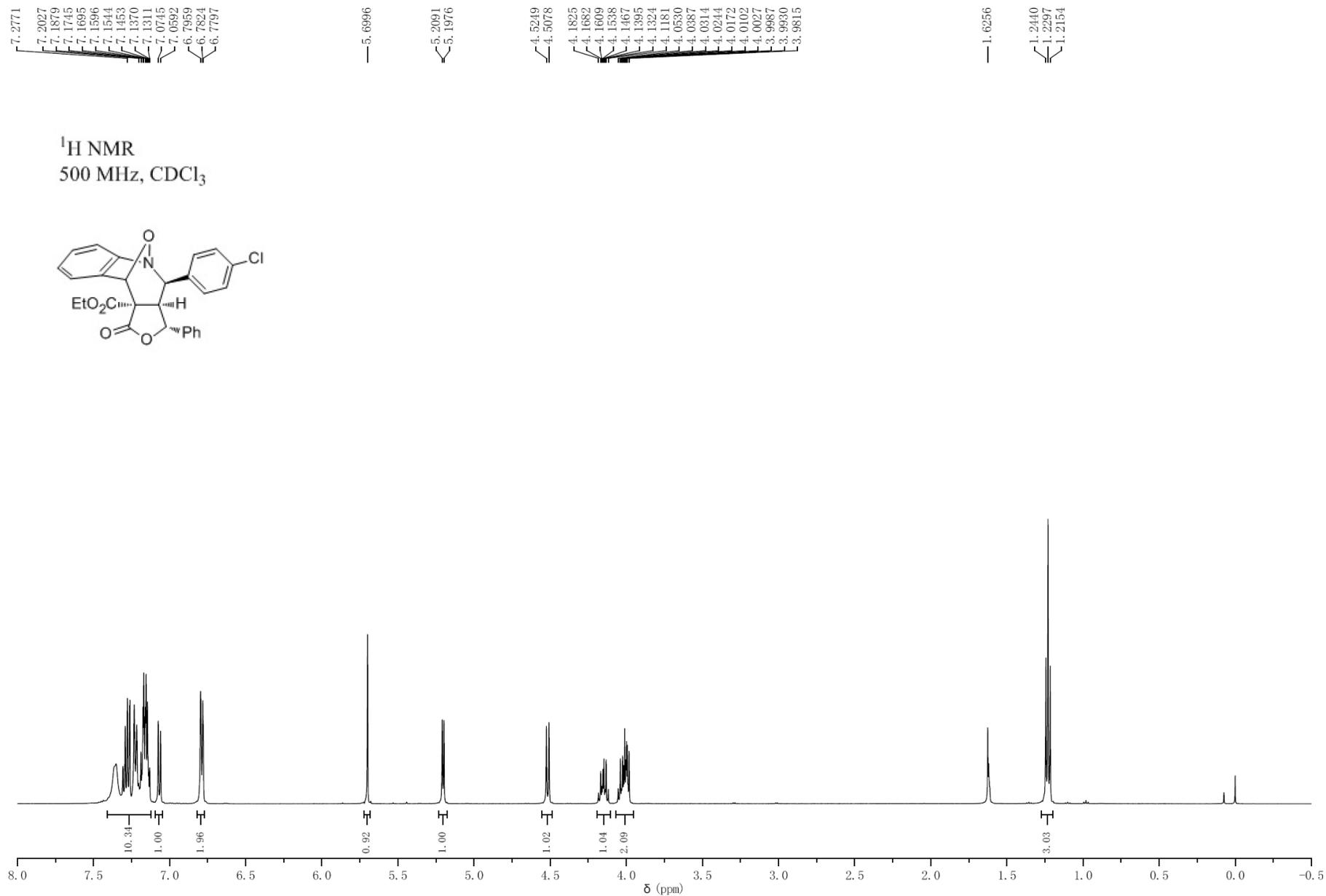
¹³C NMR
125 MHz, CDCl₃



Compound 3fa



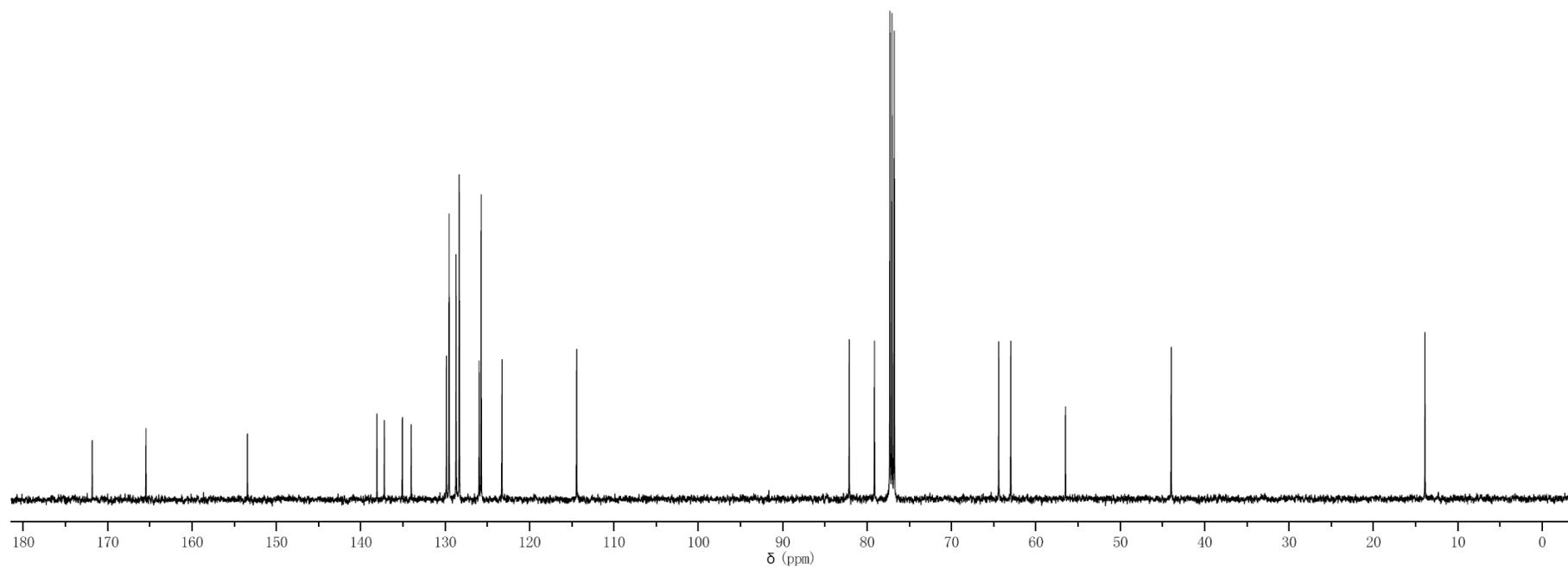
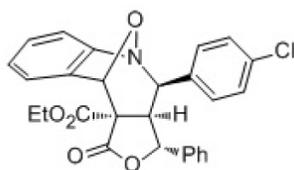
^1H NMR
500 MHz, CDCl_3



Compound 3fa



^{13}C NMR
125 MHz, CDCl_3



Compound 3ga

8.0689
8.0519
7.5838
7.5752
7.3126
7.2627
7.1841
7.1244
7.0940
7.0520
6.7661
6.7512

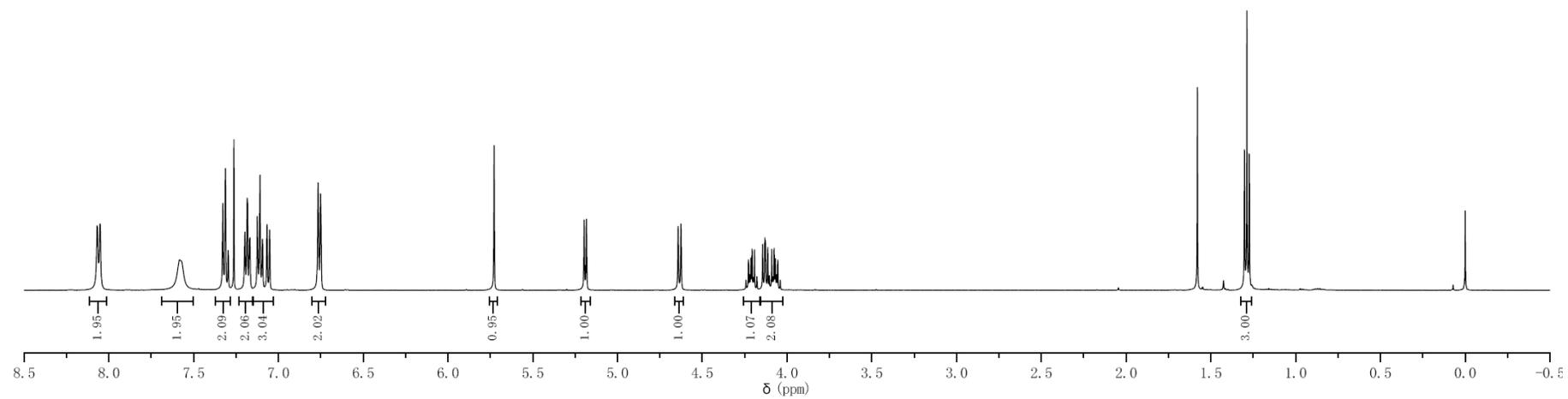
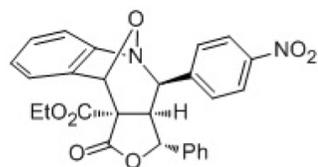
5.7277

5.1965
5.1832

4.6423
4.6256
4.2276
4.2133
4.2061
4.1990
4.1918
4.1775
4.1437
4.1303
4.1272
4.1137
4.1044
4.0901
4.0829
4.0758
4.0686
4.0615
4.0543
4.0400

1.5795
1.3018
1.2875
1.2732

^1H NMR
500 MHz, CDCl_3

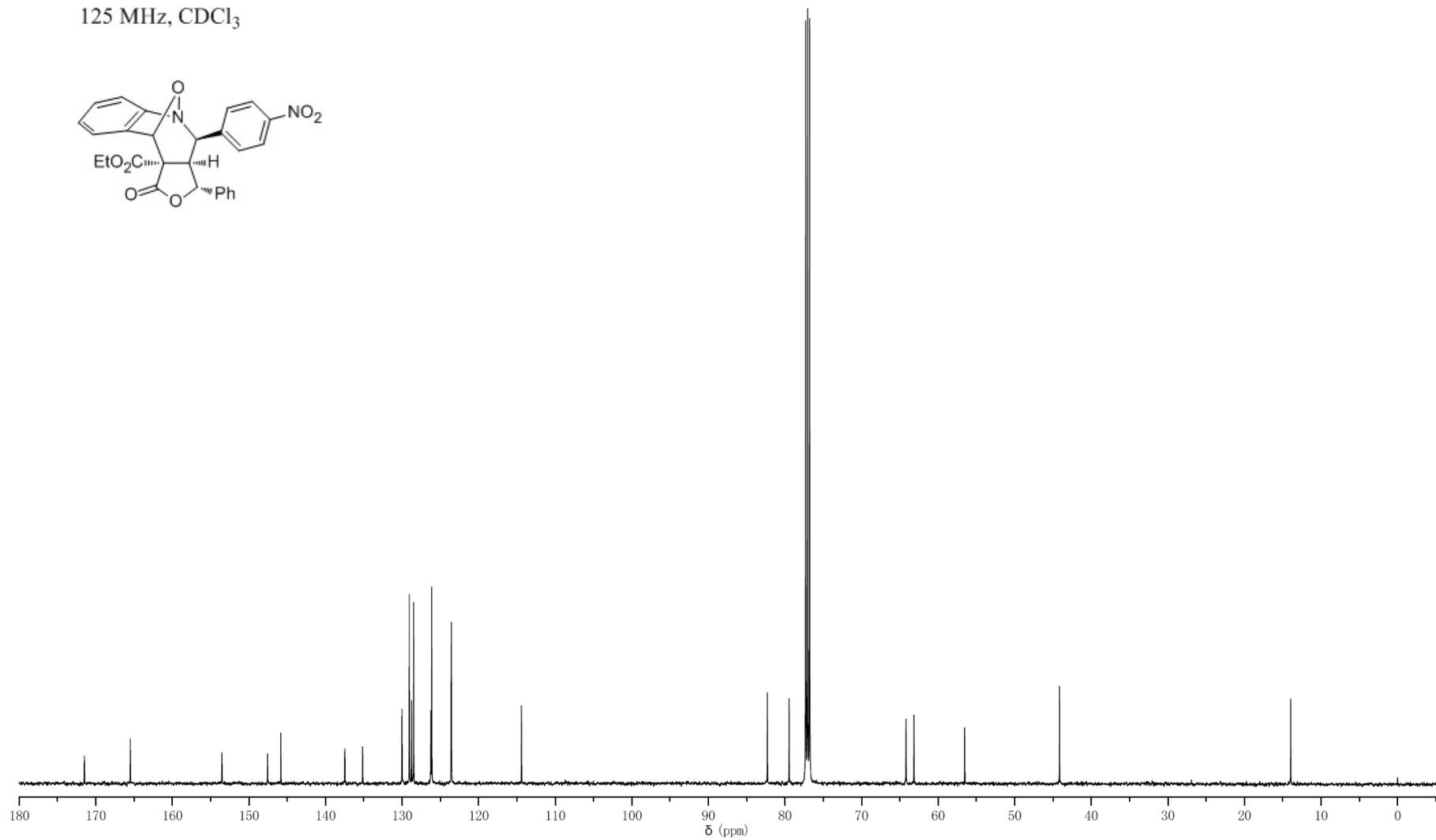
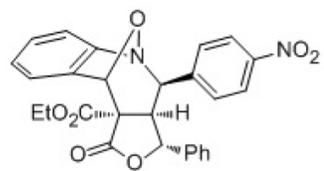


Compound 3ga

171.48
165.49
153.53
147.56
145.82
137.47
135.14
129.05
128.77
128.48
126.12
123.59
123.56
114.40

82.30
79.46
77.29
77.04
76.79
64.19
63.17
56.53
44.15
13.97

^{13}C NMR
125 MHz, CDCl_3



Compound 3ha

8.0842
8.0822
8.0661
8.0293
7.9266
7.4883
7.4729
7.4577
7.2597
7.1810
7.1513
7.1235
7.0945
7.0451
6.7492
6.7346

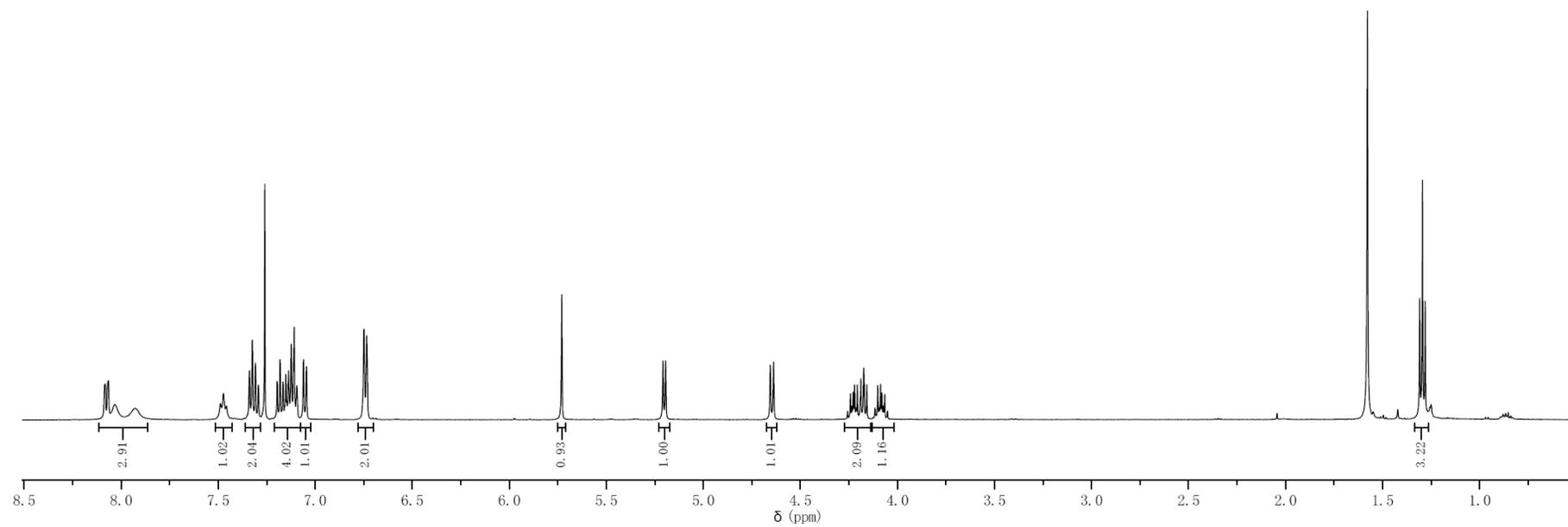
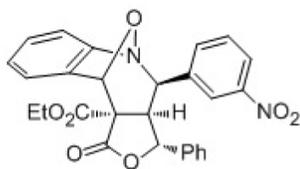
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5.2082
5.1942

4.6548
4.6383
4.2566
4.2423
4.2350
4.2280
4.2208
4.2137
4.2065
4.1884
4.1740
4.1579
4.1156
4.1013
4.0940
4.0870
4.0798
4.0727
4.0655
4.0512

1.5781
1.3090
1.2947
1.2804

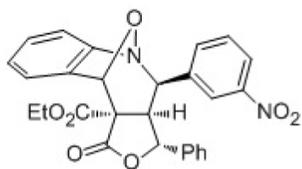
¹H NMR
500 MHz, CDCl₃



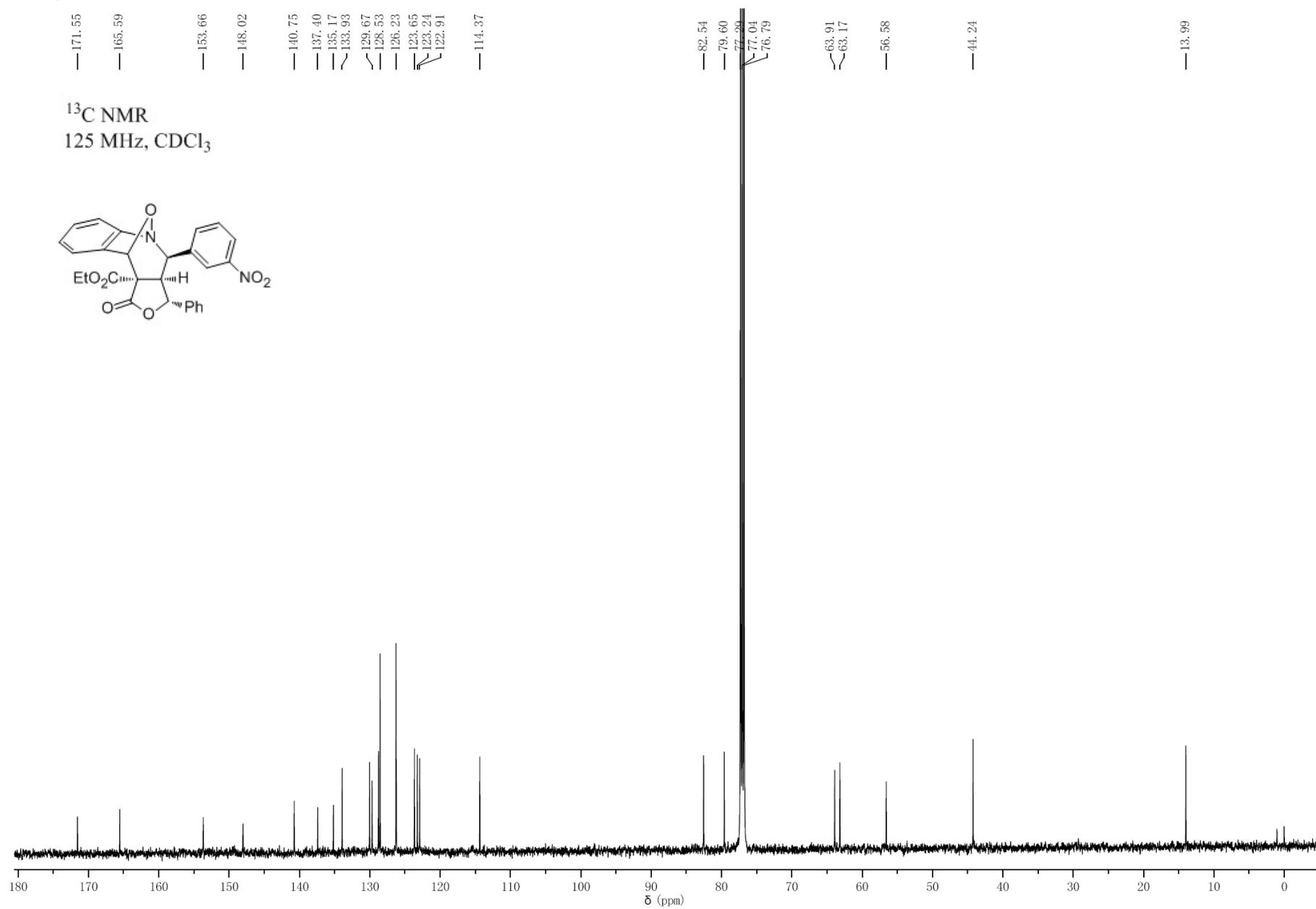
Compound 3ha

171.55
165.59
153.66
148.02
140.75
137.40
135.17
133.93
129.67
128.53
126.23
123.65
123.24
122.91
114.37

¹³C NMR
125 MHz, CDCl₃



82.54
79.60
77.20
77.04
76.79
63.91
63.17
56.58
44.24
13.99



Compound 3ia

8.5278
8.5120
7.8905
7.8501
7.8480
7.8345
7.8195
7.8174
7.5132
7.4963
7.3232
7.3081
7.2599
7.2036
7.1758
7.1657
7.1483
7.0586
7.0408
7.0257

5.7286

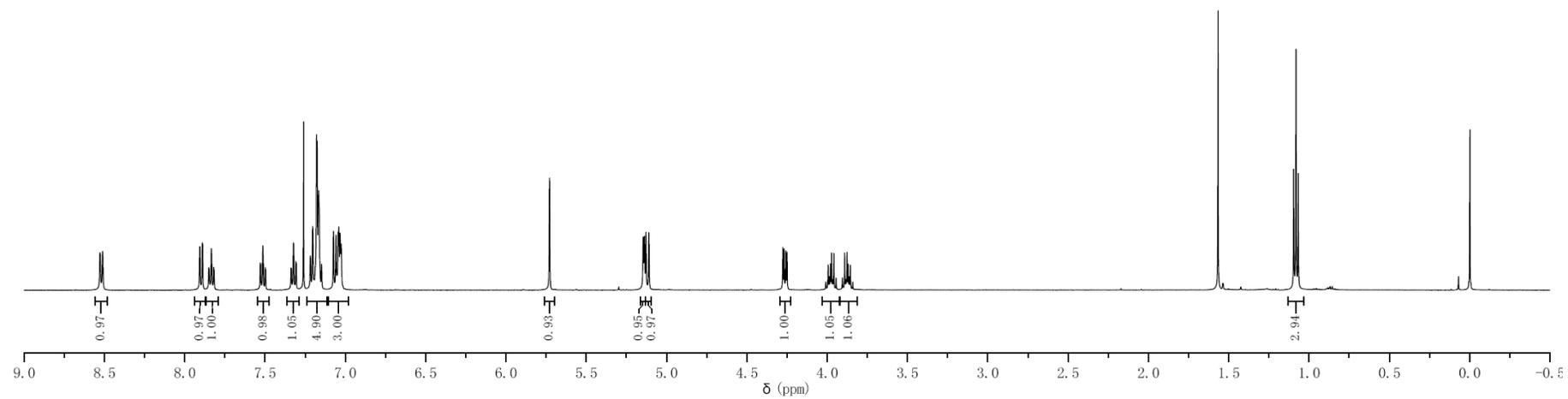
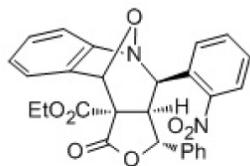
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5.1101

4.2759
4.2681
4.2575
4.2498
3.9942
3.9870
3.9799
3.9727
3.9656
3.9584
3.9442
3.9051
3.8908
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3.8550
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1.5660

1.0953
1.0810
1.0667

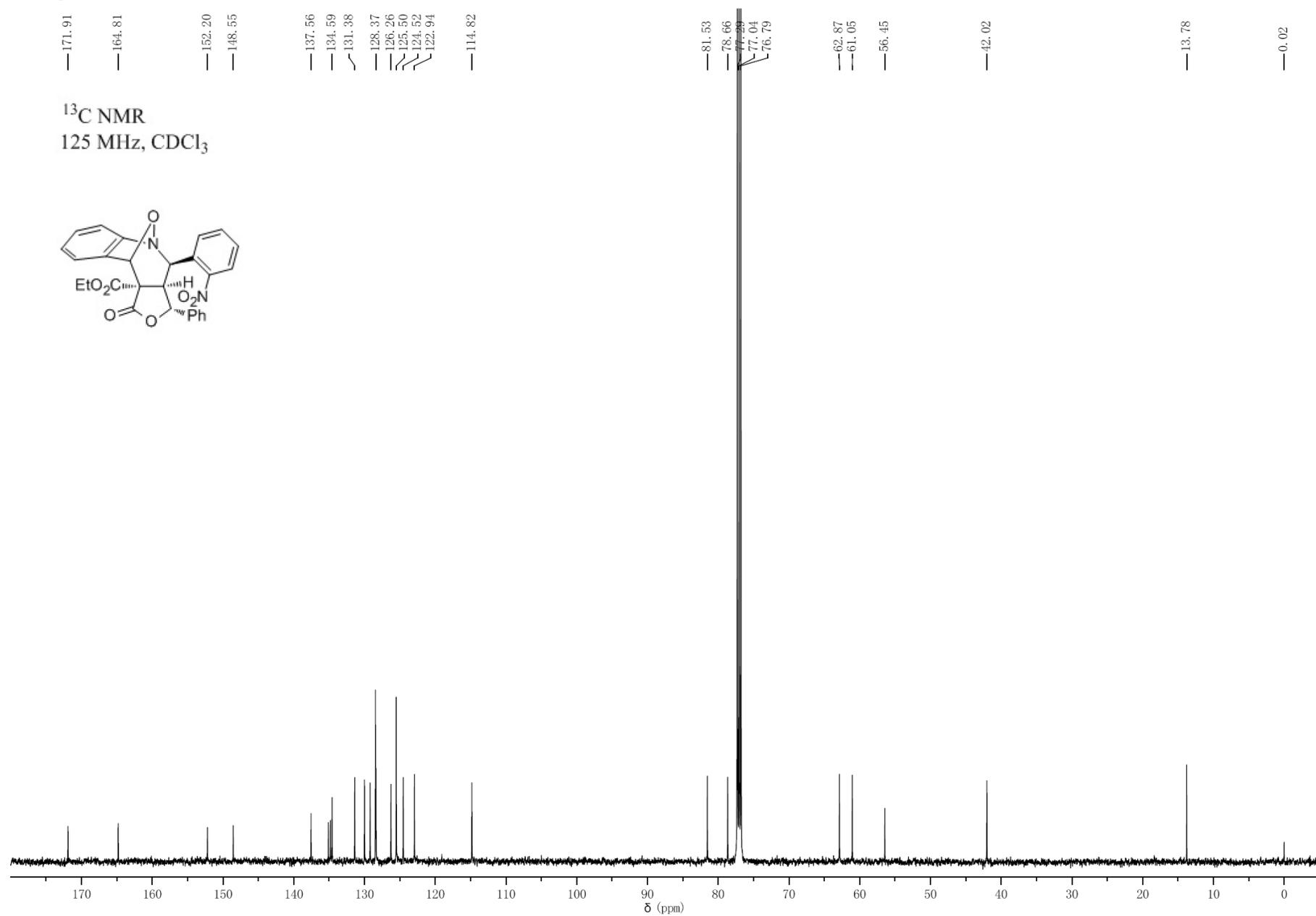
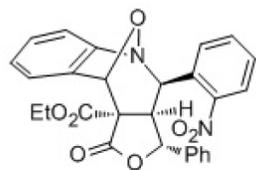
¹H NMR
500 MHz, CDCl₃



Compound 3ia

171.91
164.81
152.20
148.55
137.56
134.59
131.38
128.37
126.26
125.50
124.52
122.94
114.82

^{13}C NMR
125 MHz, CDCl_3



Compound 3ja

7.4387
7.2598
7.0707
6.9310
6.9151
6.6468
6.6307

5.7077

5.2266
5.2158

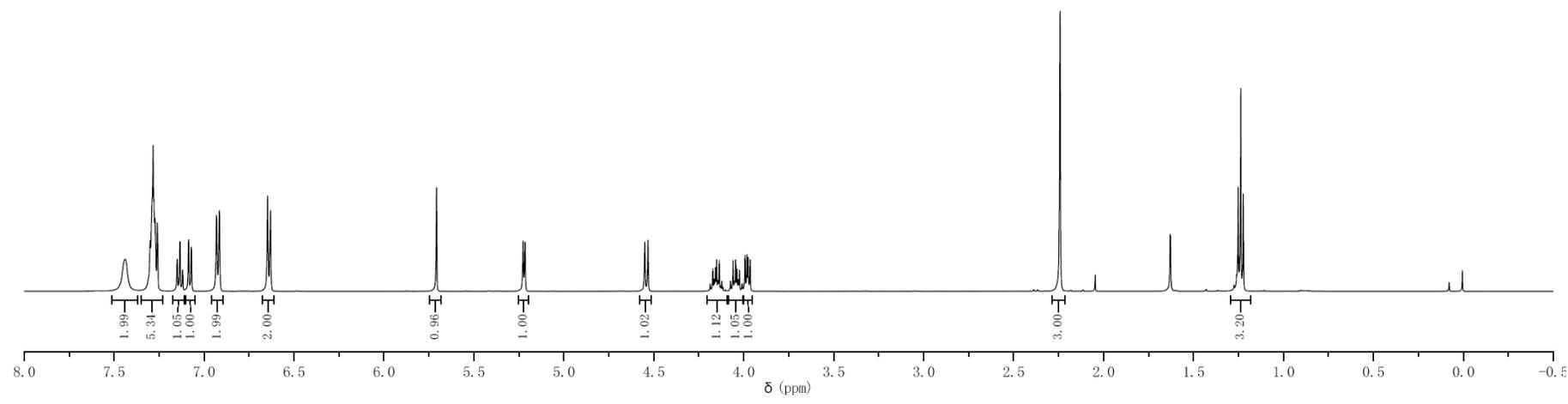
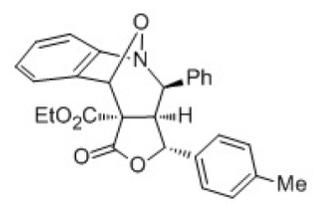
4.5500
4.5324
4.1507
4.1220
4.1156
4.0735
4.0592
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4.0449
4.0377
4.0305
4.0233
4.0090
3.9929
3.9820
3.9753
3.9645

2.2418

1.6289

1.2517
1.2374
1.2231

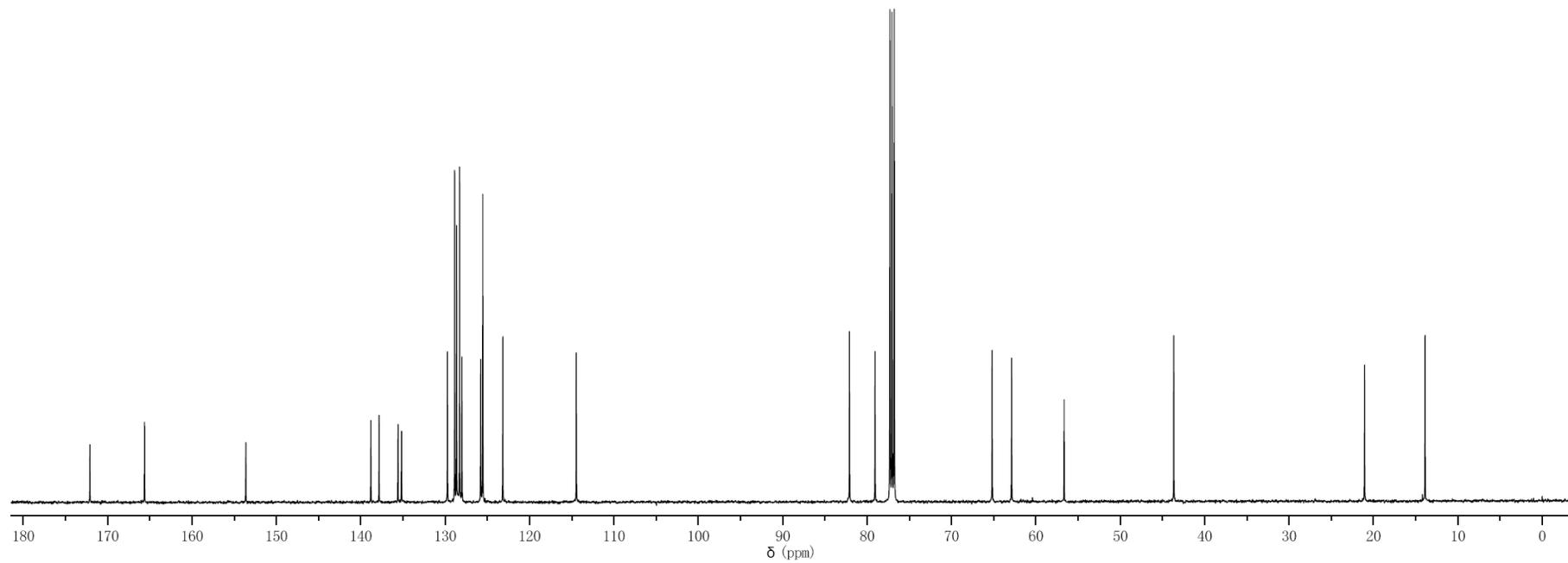
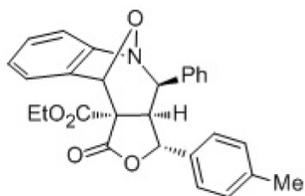
¹H NMR
500 MHz, CDCl₃



Compound 3ja



^{13}C NMR
125 MHz, CDCl_3



Compound 3ka

7.3843
7.3046
7.2898
7.2743
7.2573
7.2522
7.1491
7.1342
7.1193
7.0619
7.0464
6.6495
6.6430
6.6311
6.6273
6.6211
6.6147
6.6090

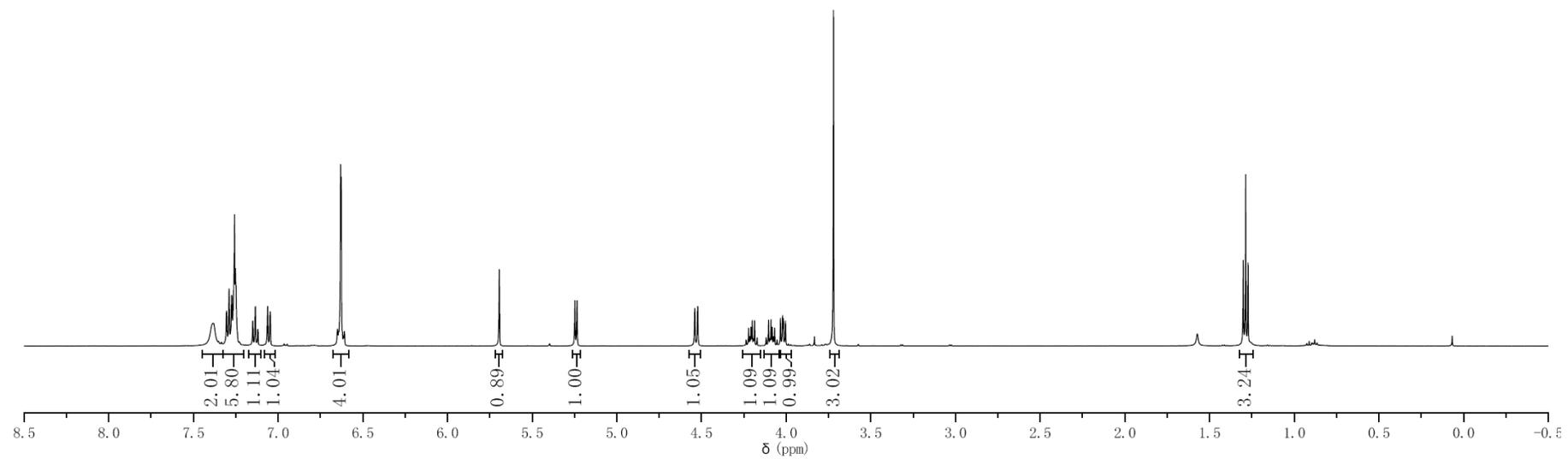
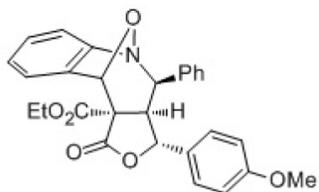
5.6939

5.2475
5.2349

4.5395
4.5225
4.1860
4.0967
4.0753
4.0335
4.0038
3.7205

1.3010
1.2867
1.2724

¹H NMR
500 MHz, CDCl₃



Compound 3ka

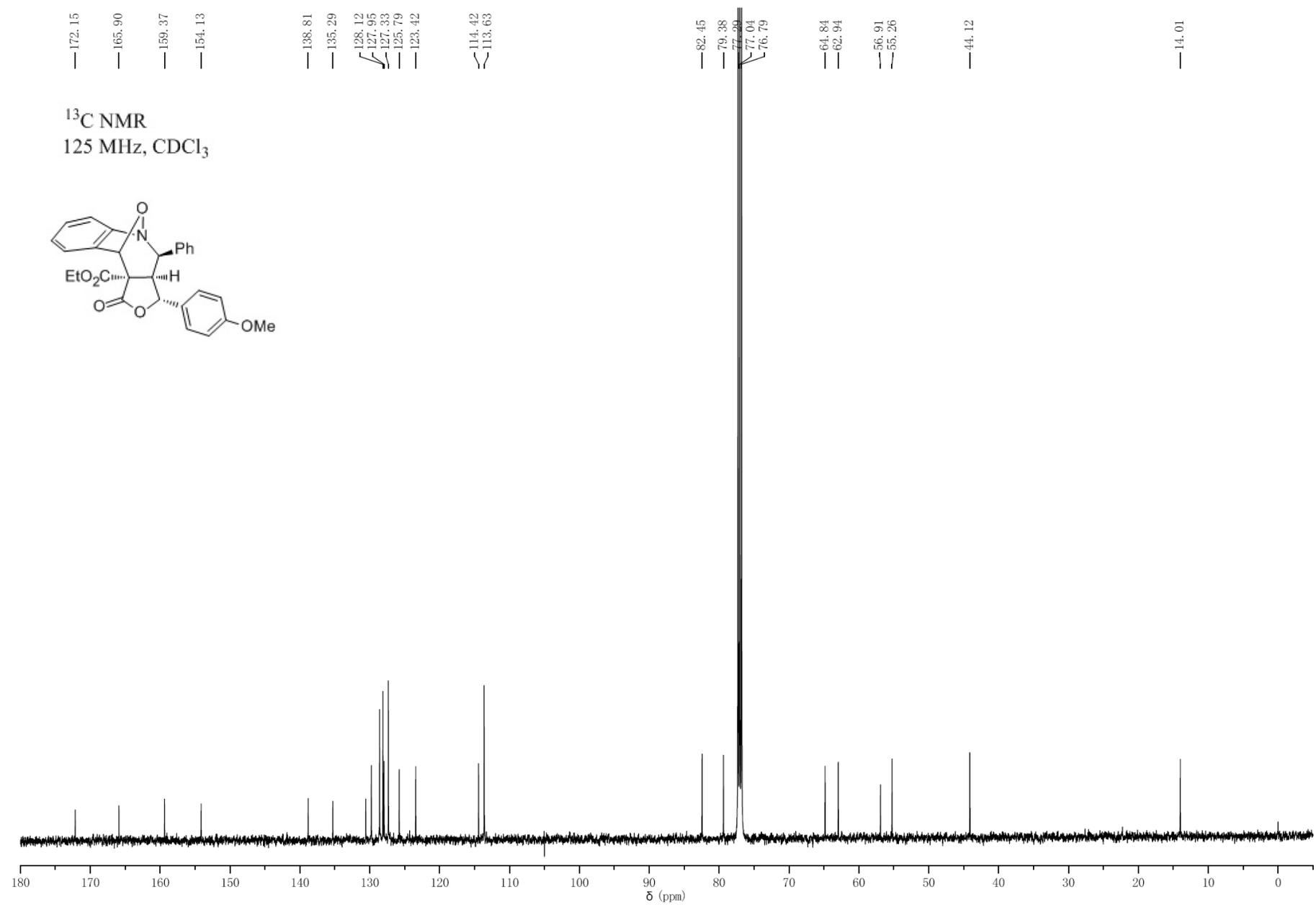
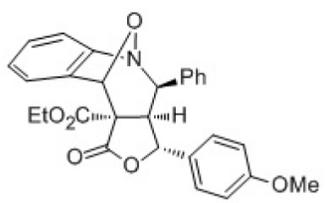
172.15
165.90
159.37
154.13

138.81
135.29
128.12
127.95
127.33
125.79
123.42
114.42
113.63

82.45
79.38
77.29
77.04
76.79
64.84
62.94
56.91
55.26
44.12

14.01

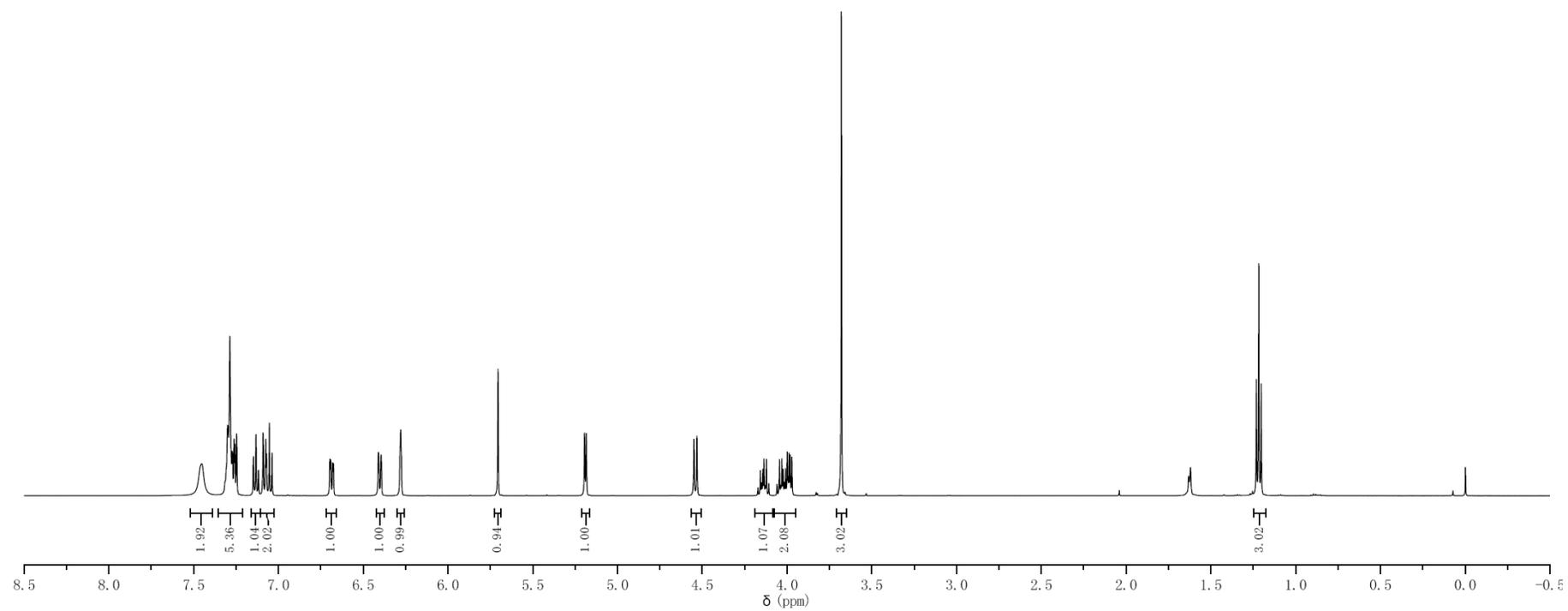
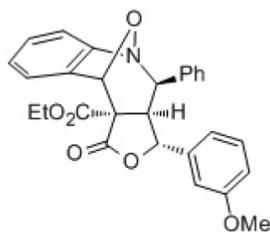
¹³C NMR
125 MHz, CDCl₃



Compound 3la

7.4524
7.2468
7.0902
7.0376
6.6964
6.6918
6.6801
6.6755
6.4099
6.3945
6.2819
6.2787
5.7046
5.1943
5.1839
4.5490
4.5314
4.1358
4.1072
4.0874
4.0161
3.9946
3.9711
3.6792
1.2316
1.2173
1.2030

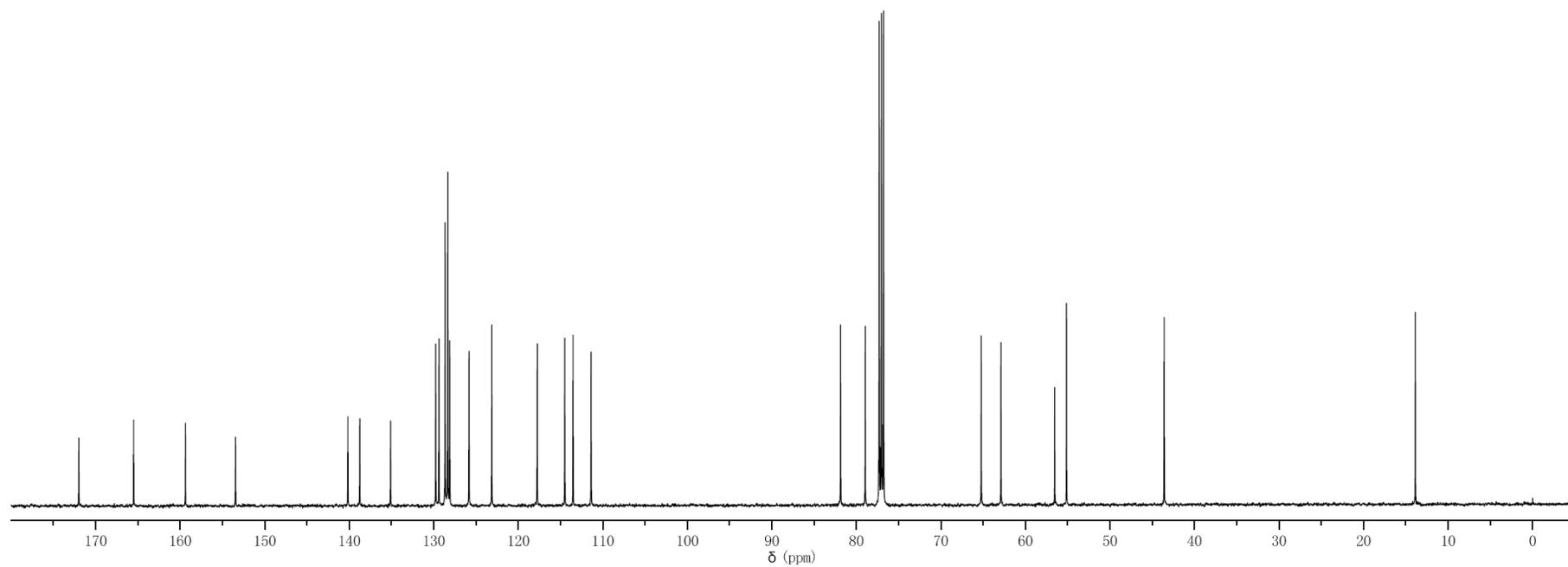
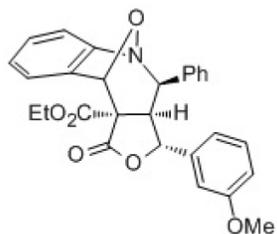
¹H NMR
500 MHz, CDCl₃



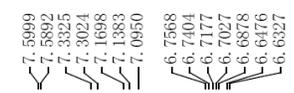
Compound 3la



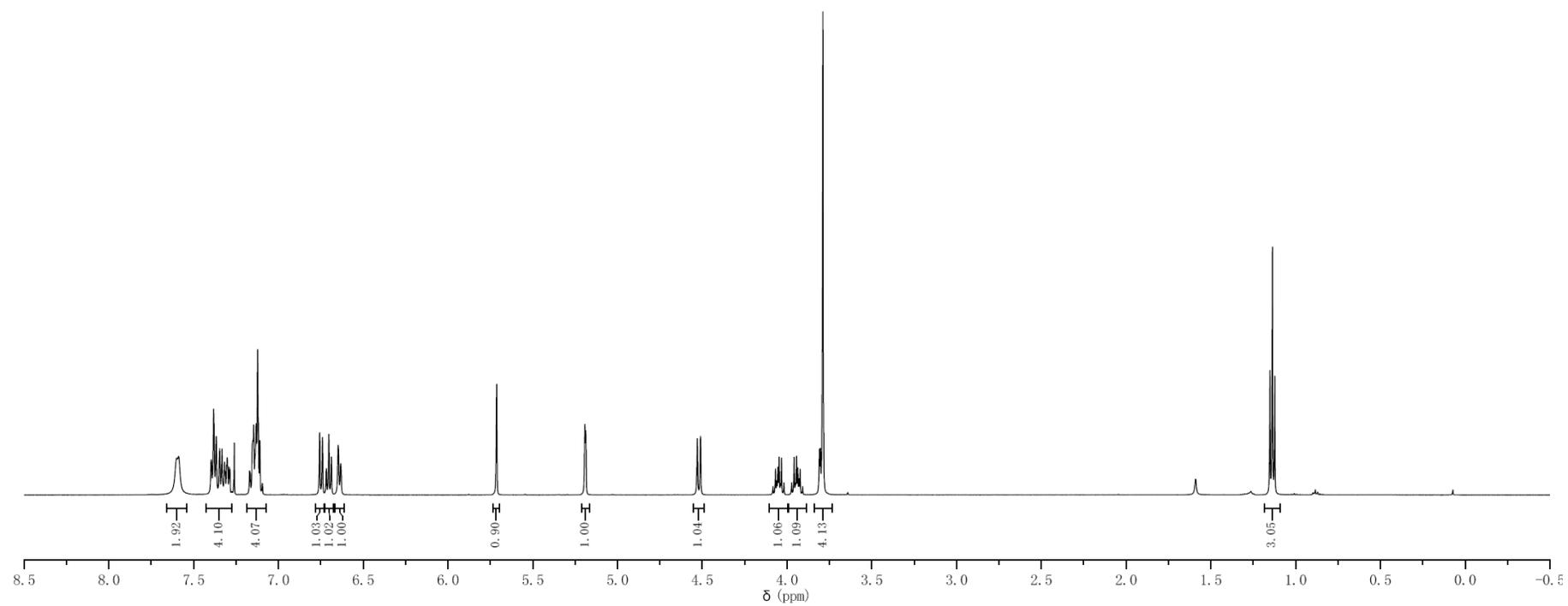
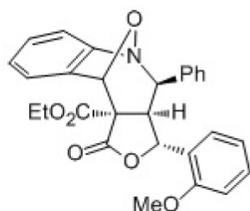
^{13}C NMR
125 MHz, CDCl_3



Compound 3ma



¹H NMR
500 MHz, CDCl₃



Compound 3ma

— 172.45
— 165.13
— 155.46
— 152.34

— 139.02
— 135.05
— 129.10
— 128.69
— 127.16
— 125.34
— 122.24
— 120.11
— 114.77
— 110.24

78.95
78.36
77.29
77.04
76.79

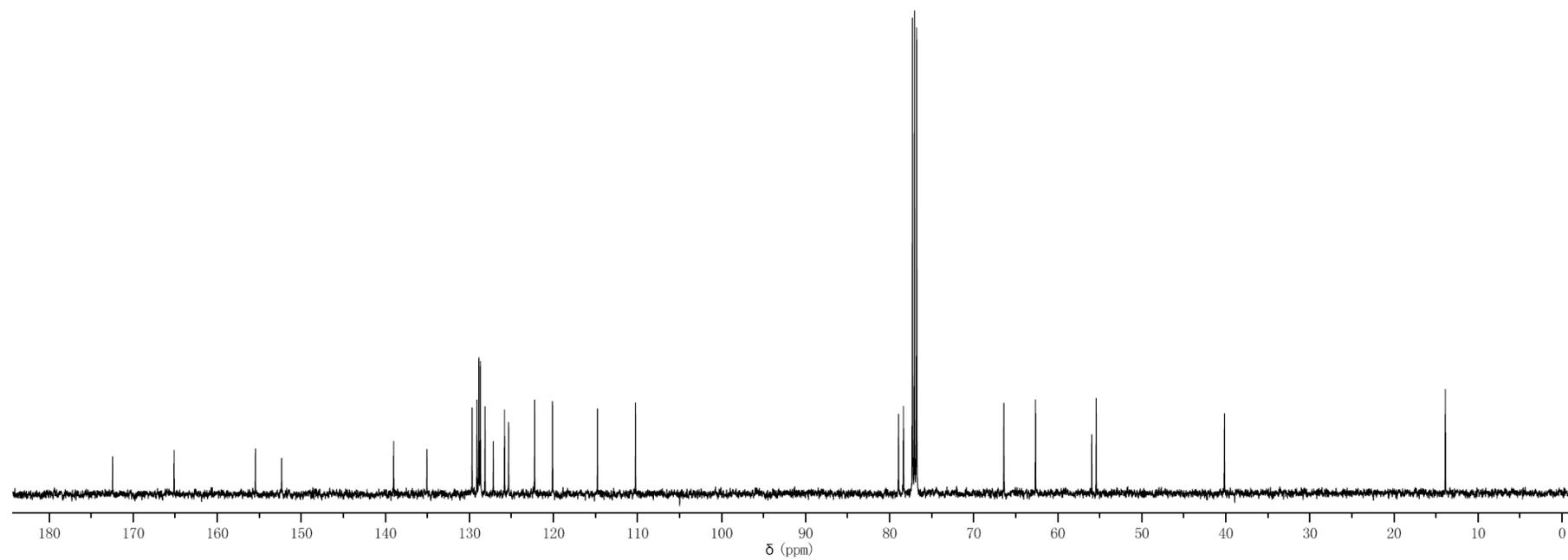
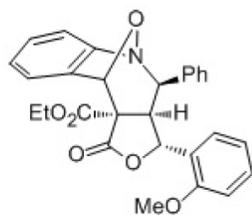
— 66.41
— 62.65

55.96
55.43

— 40.17

— 13.90

^{13}C NMR
125 MHz, CDCl_3



Compound 3na

7.3965
7.3955
7.2579
7.1433
7.1283
7.0838
7.0539
6.6498
6.6329

5.7004

5.2488
5.2365

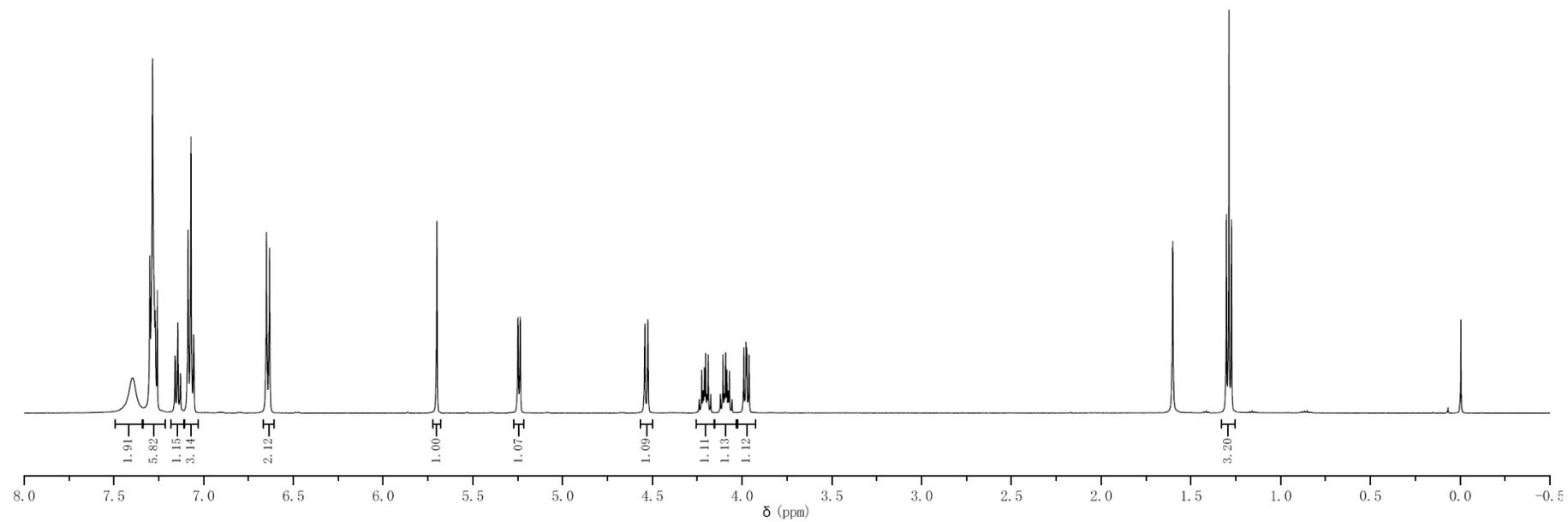
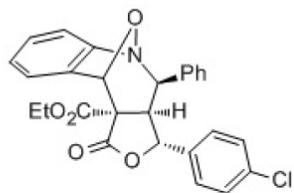
4.5419
4.5249

4.2249
4.2177
4.2106
4.2034
4.1962
4.1891
4.1748
4.1207
4.1064
4.0991
4.0921
4.0849
4.0778
4.0706
4.0563
3.9907
3.9784
3.9737
3.9614

1.6009

1.3022
1.2879
1.2736

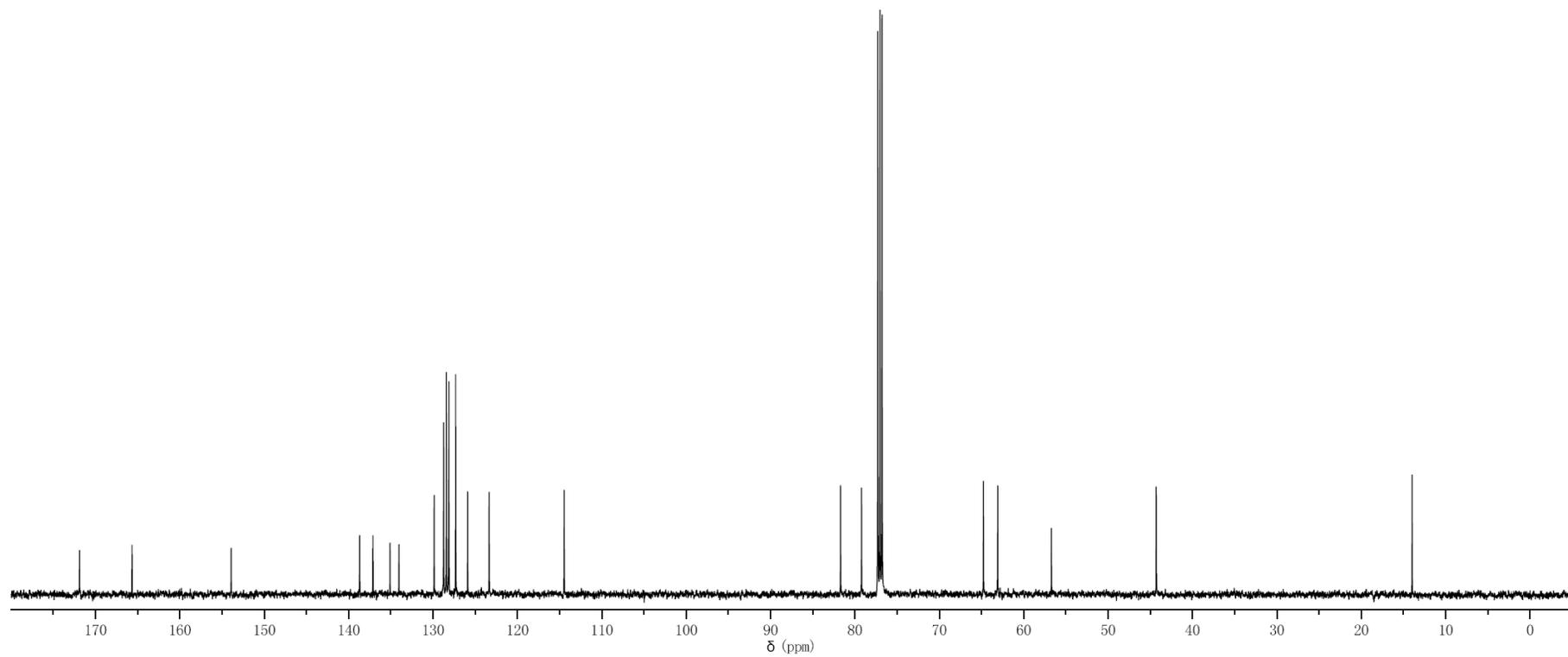
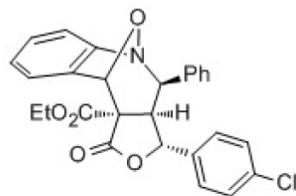
¹H NMR
500 MHz, CDCl₃



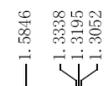
Compound 3na



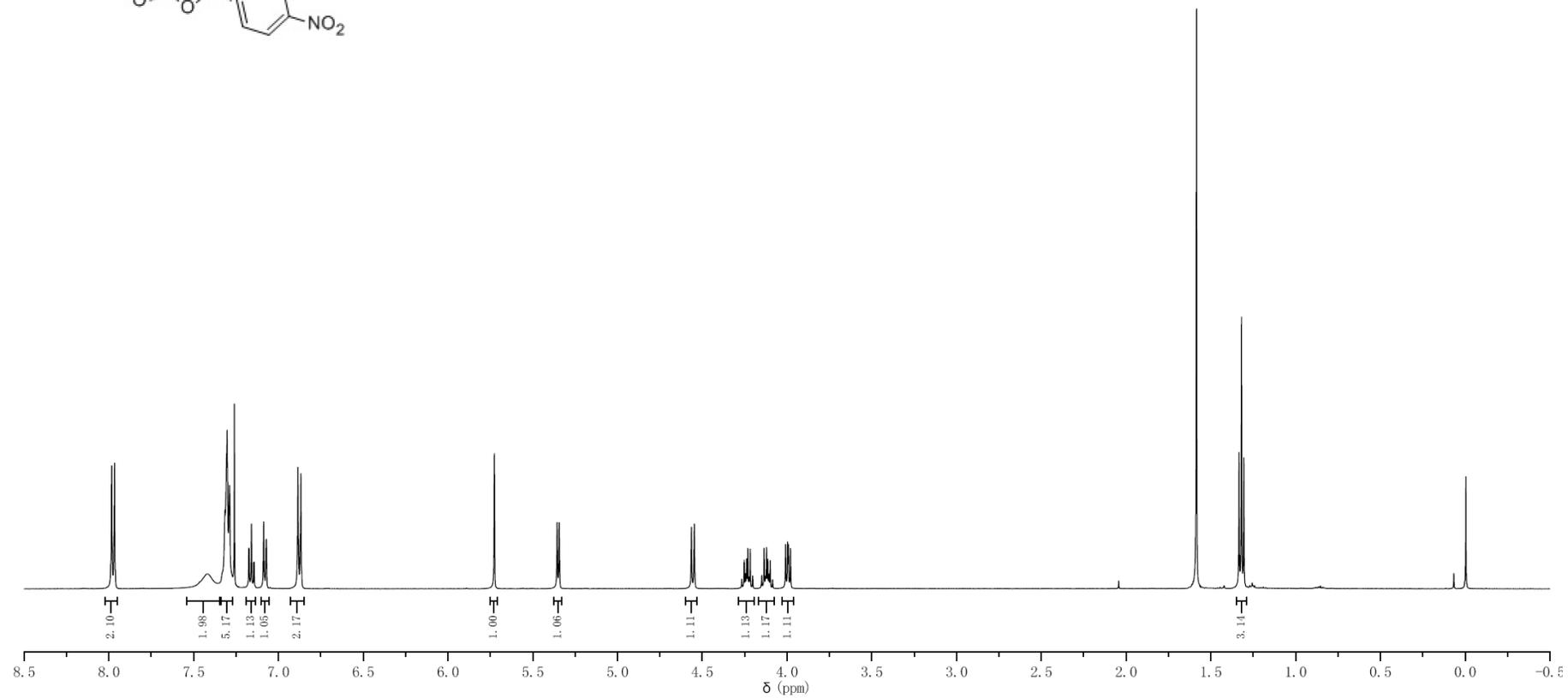
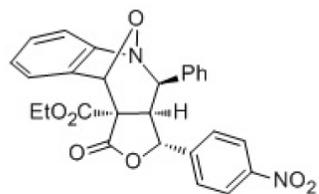
^{13}C NMR
125 MHz, CDCl_3



Compound 30a



¹H NMR
500 MHz, CDCl₃

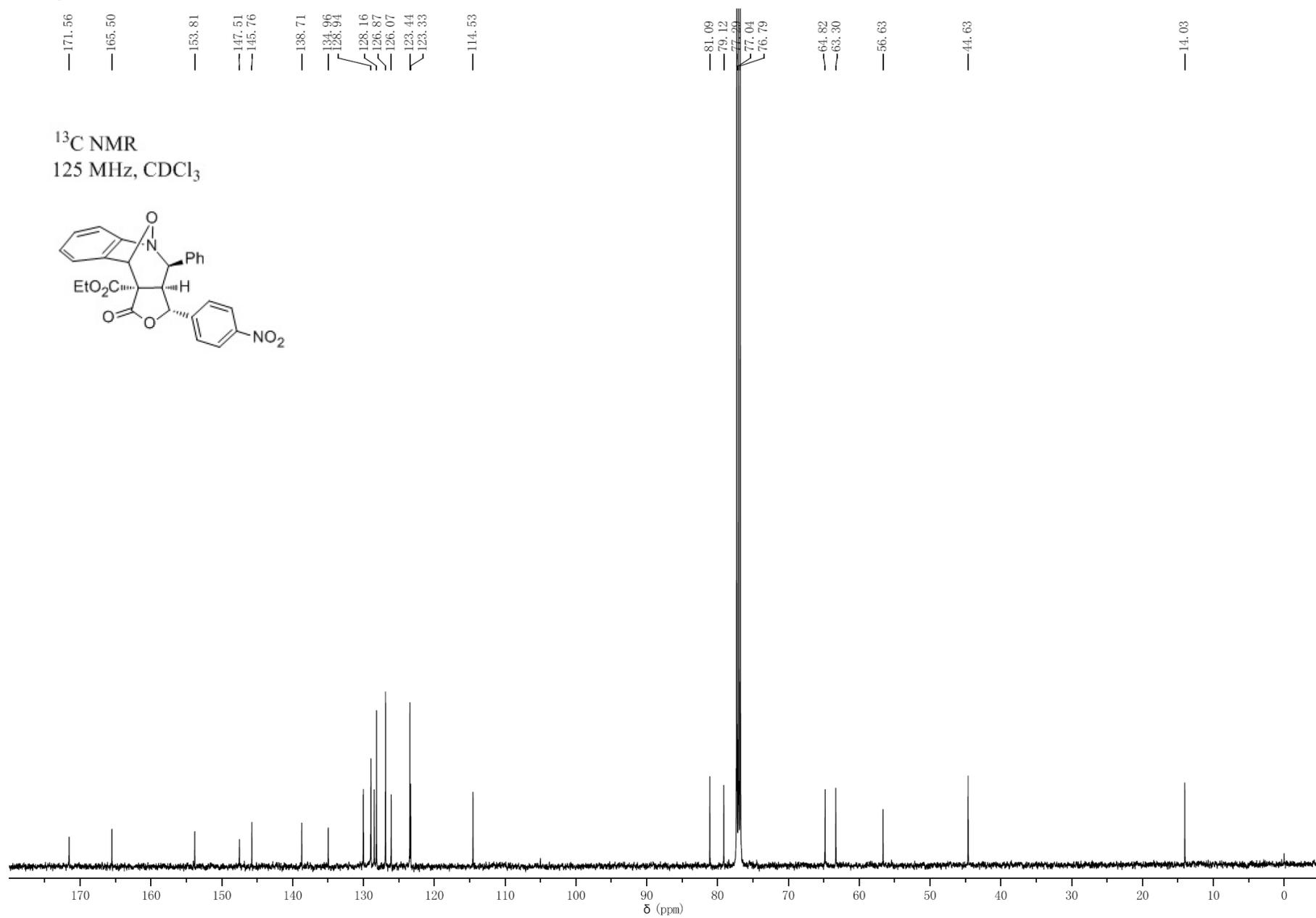
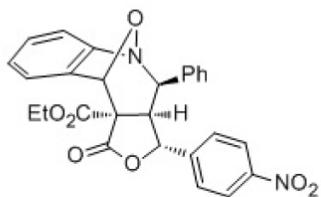


Compound 30a

171.56
165.50
153.81
147.51
145.76
138.71
134.96
128.91
128.16
126.87
126.07
123.44
123.33
114.53

81.09
79.12
77.20
77.04
76.79
64.82
63.30
56.63
44.63
14.03

¹³C NMR
125 MHz, CDCl₃



Compound 3pa

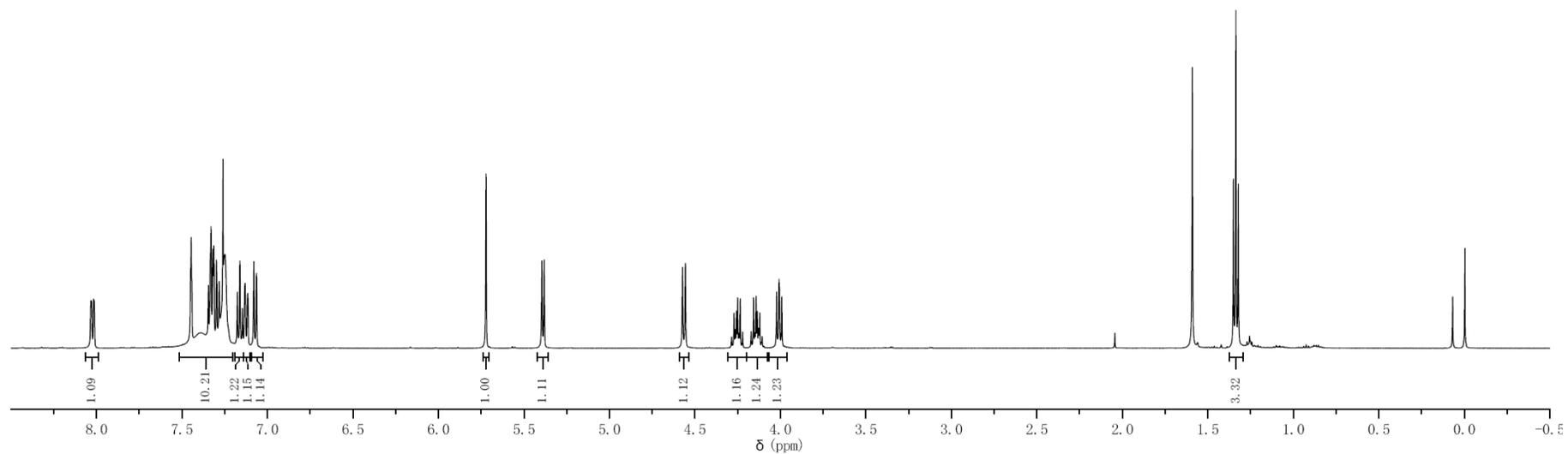
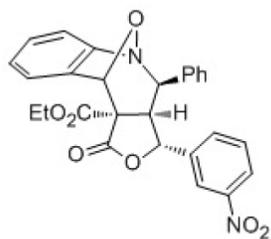
8.0331
8.0321
8.0294
8.0171
8.0157
8.0131
7.4462
7.2828
7.2601
7.2489
7.1762
7.1461
7.1310
7.1155
7.0795
7.0641

5.7215
5.3950
5.3815

4.5722
4.5556
4.2709
4.2566
4.2494
4.2423
4.2351
4.2208
4.1708
4.1565
4.1492
4.1422
4.1350
4.1279
4.1207
4.1064
4.0217
4.0080
4.0054
3.9917

1.5905
1.3503
1.3359
1.3217

¹H NMR
500 MHz, CDCl₃

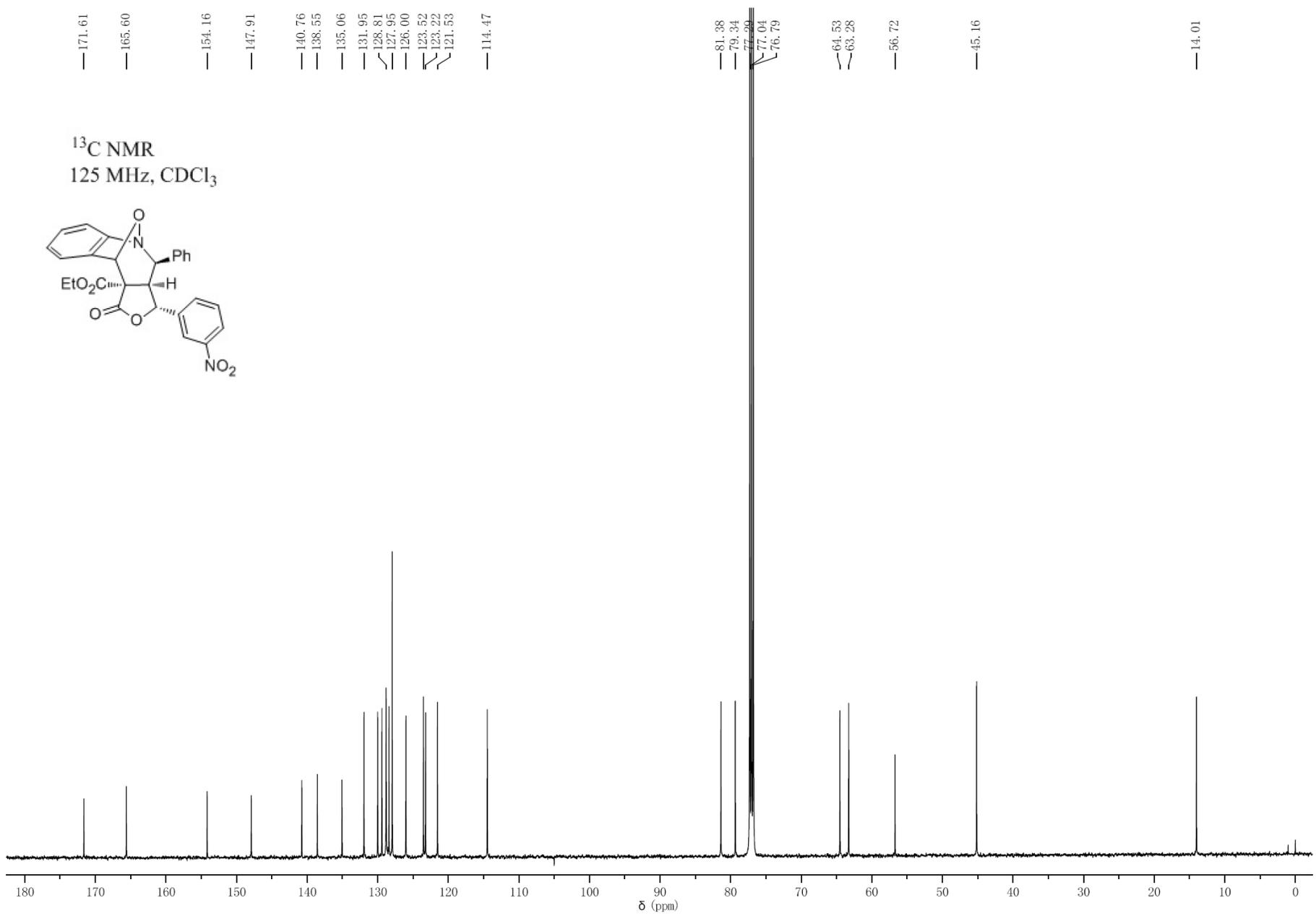
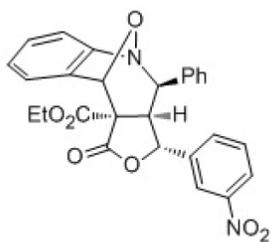


Compound 3pa

171.61
165.60
154.16
147.91
140.76
138.55
135.06
131.95
128.81
127.95
126.00
123.52
123.22
121.53
114.47

81.38
79.34
77.20
77.04
76.79
64.53
63.28
56.72
45.16
14.01

^{13}C NMR
125 MHz, CDCl_3



Compound 3qa

8.2260
8.2243
8.2095
7.8899
7.8770
7.4476
7.3980
7.3835
7.3688
7.3495
7.3341
7.3197
7.2599
7.2148
7.1994
7.1084
7.0935
7.0786
6.9991
6.9845

5.7561
5.6080

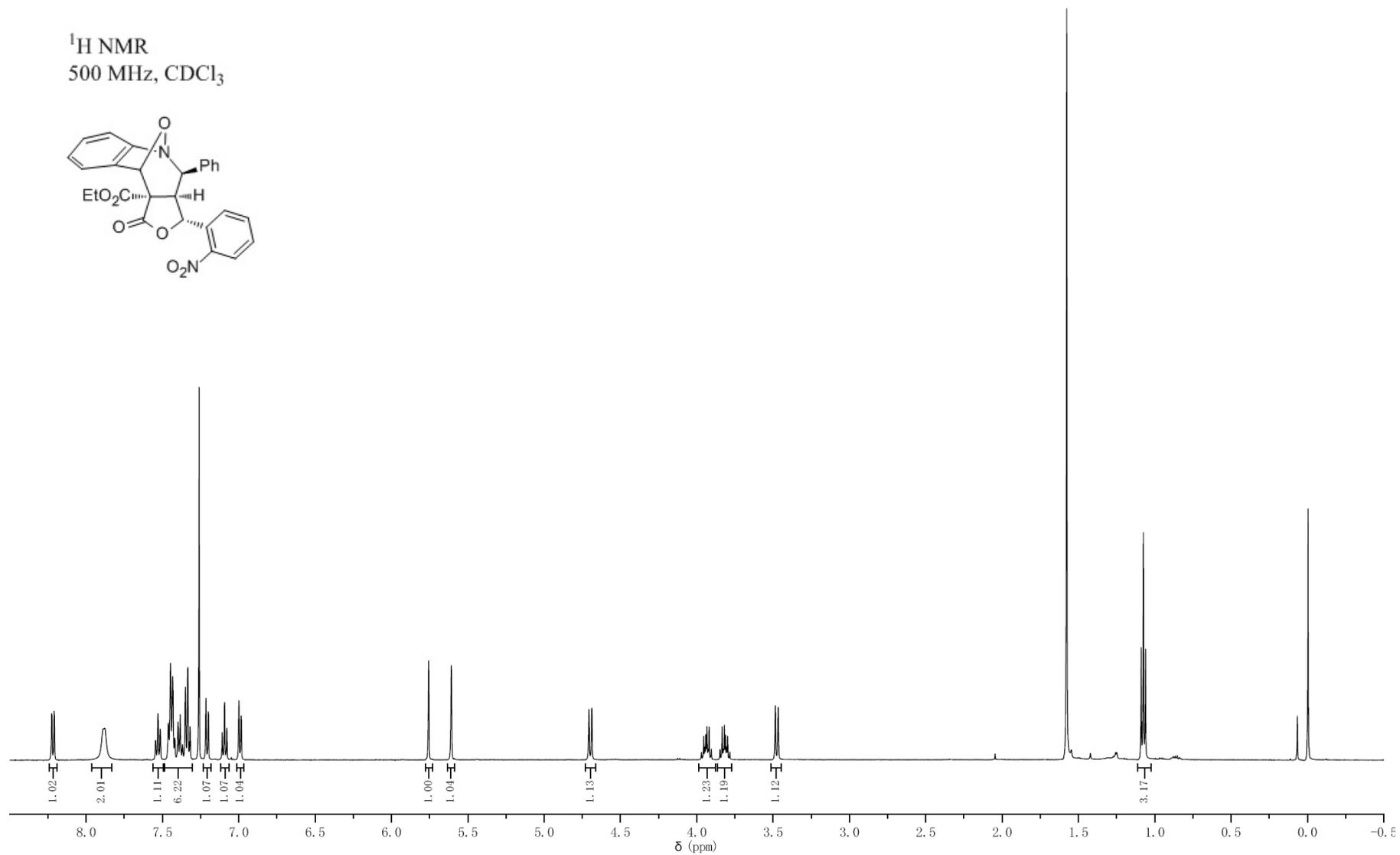
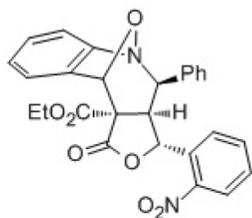
4.7062
4.6874

3.9549
3.9407
3.9264
3.9050
3.8835
3.8192
3.8049
3.7835
3.4854
3.4666

1.5765

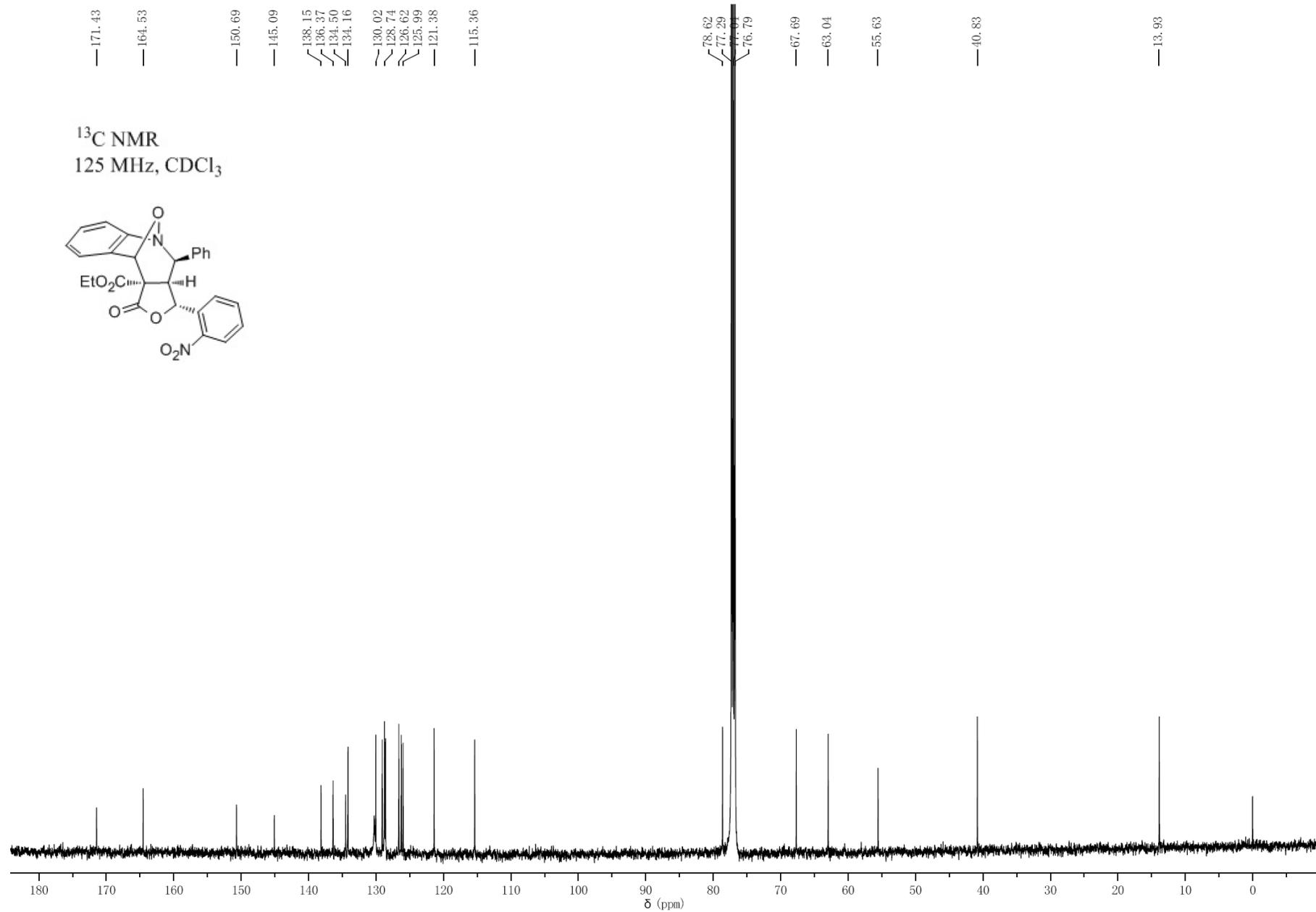
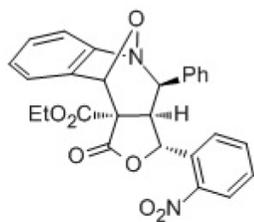
1.0888
1.0745
1.0603

¹H NMR
500 MHz, CDCl₃



Compound 3qa

^{13}C NMR
125 MHz, CDCl_3



Compound 3ra

7.4066
7.4009
7.2893
7.2445
7.1362
7.0941
7.0655
6.7208
6.7063

5.7136

5.2949
5.2827

4.5472
4.5301

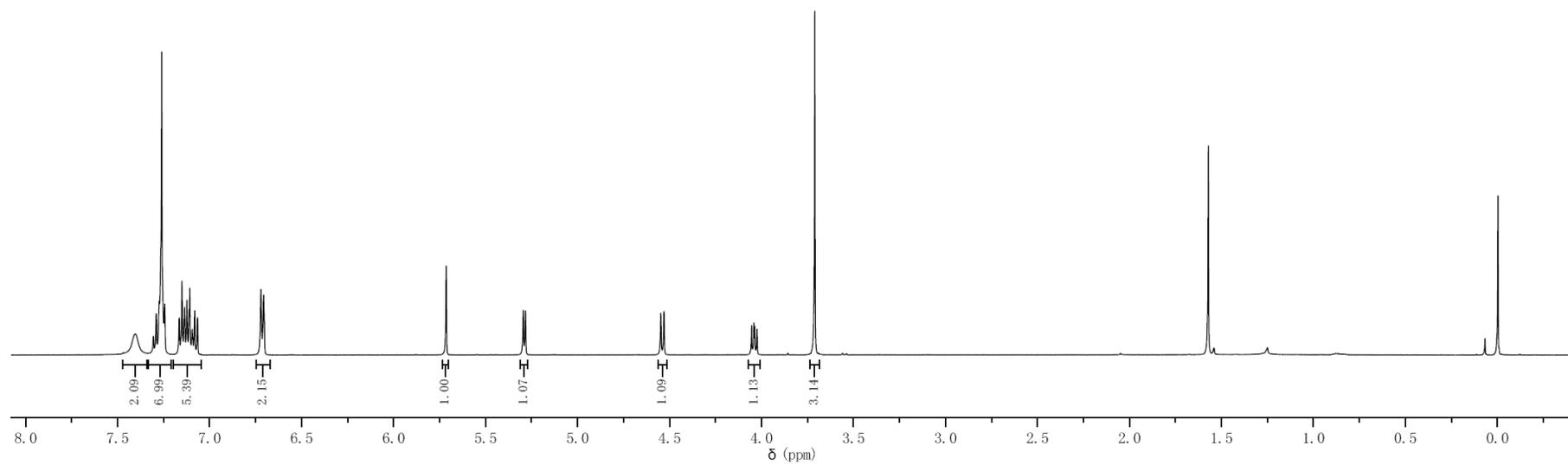
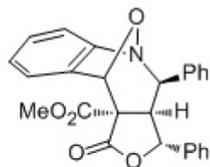
4.0537
4.0414
4.0366
4.0243

3.7102

1.5713

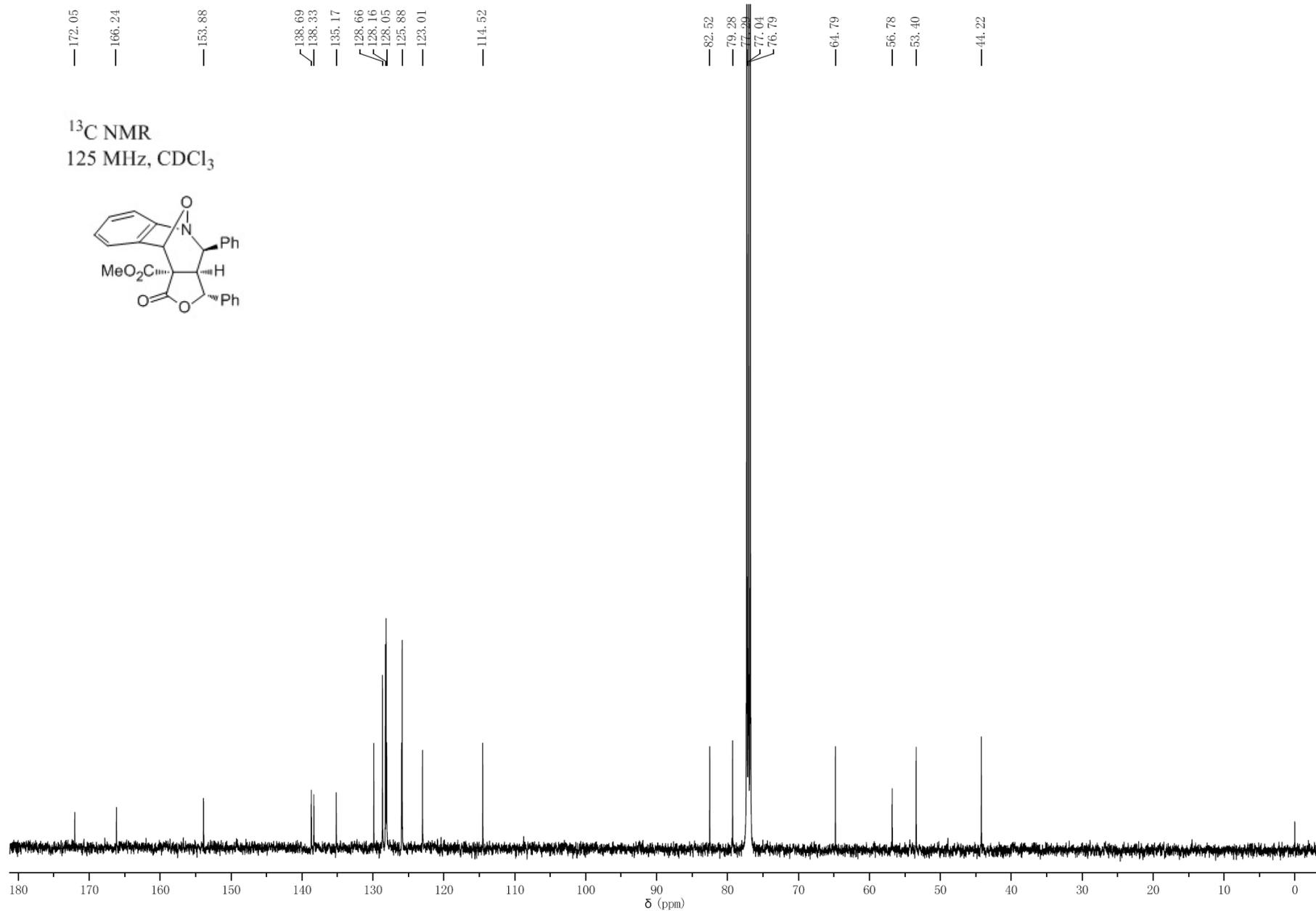
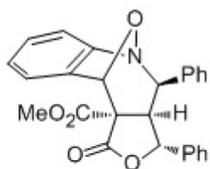
0.0031

^1H NMR
500 MHz, CDCl_3



Compound 3ra

^{13}C NMR
125 MHz, CDCl_3



Compound 3sa

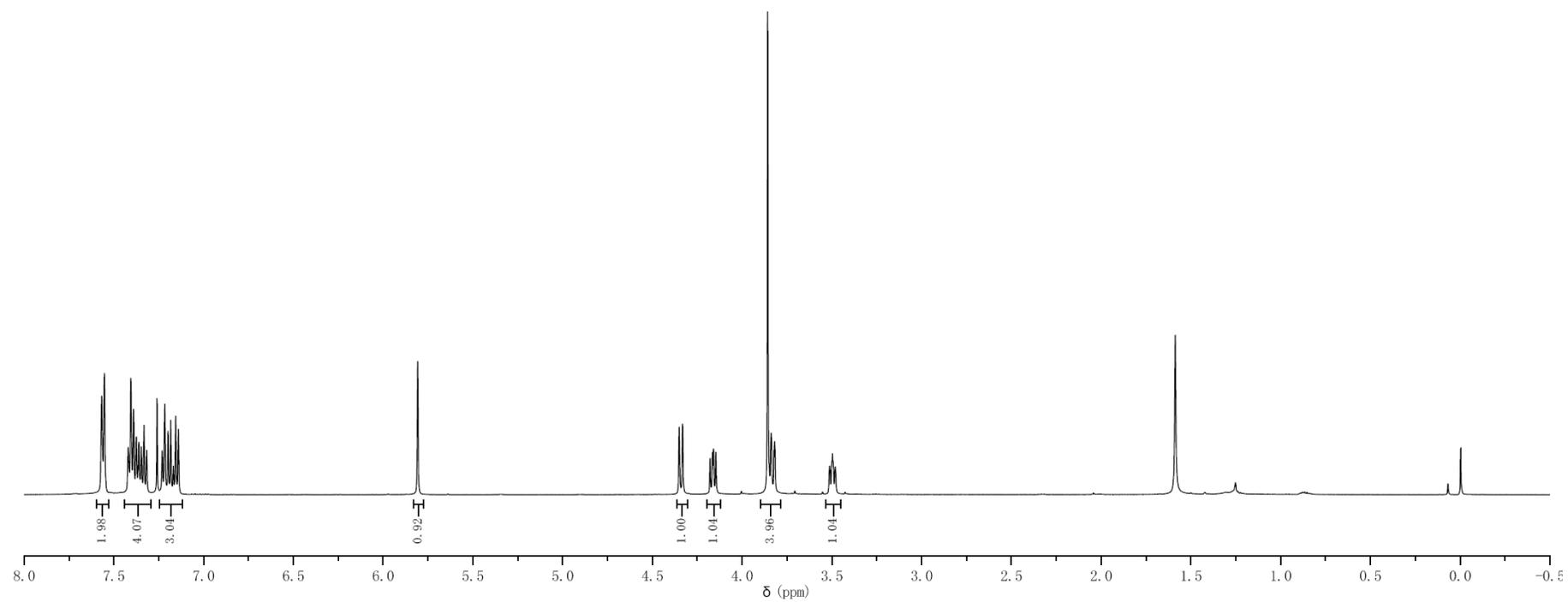
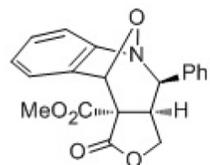
7.5681
7.5525
7.4054
7.3172
7.2603
7.2583
7.2309
7.2164
7.1980
7.1833
7.1685
7.1558
7.1404

5.8074

4.3507
4.3318
4.1645
4.1467
3.8584
3.8566
3.8384
3.8193
3.5128
3.4967
3.4812

1.5873

¹H NMR
500 MHz, CDCl₃



Compound 3sa

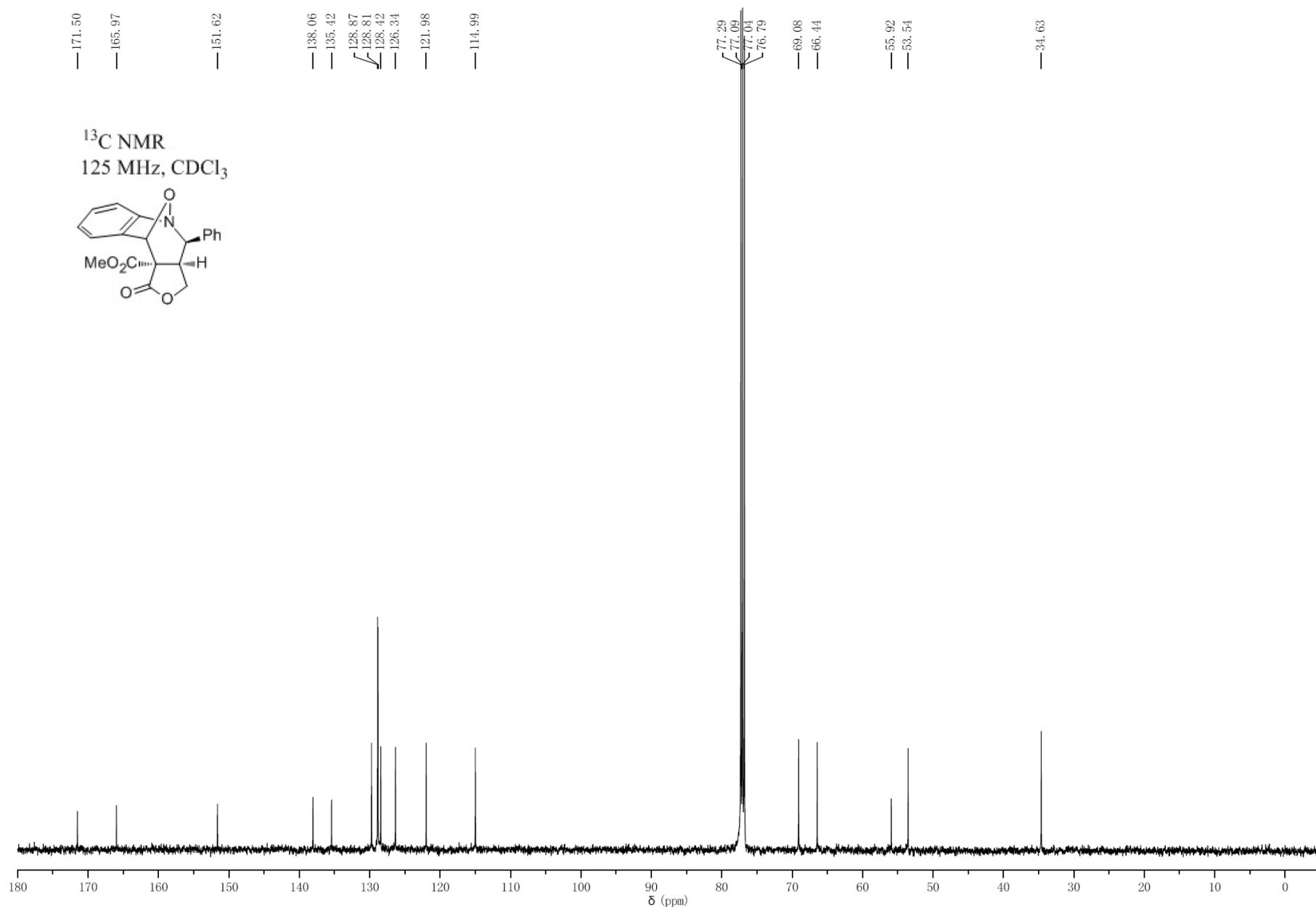
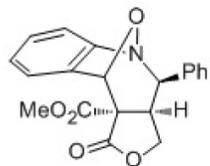
— 171.50
— 165.97
— 151.62

— 138.06
— 135.42
— 128.87
— 128.81
— 128.42
— 126.34
— 121.98
— 114.99

77.29
77.09
76.79
— 69.08
— 66.44
— 55.92
— 53.54

— 34.63

^{13}C NMR
125 MHz, CDCl_3



Compound 3ab

7.4338
7.2529
7.1072
6.9809
6.7947
6.7780
6.7732
6.7651
6.7614
6.7563

5.6604

5.2310
5.2206

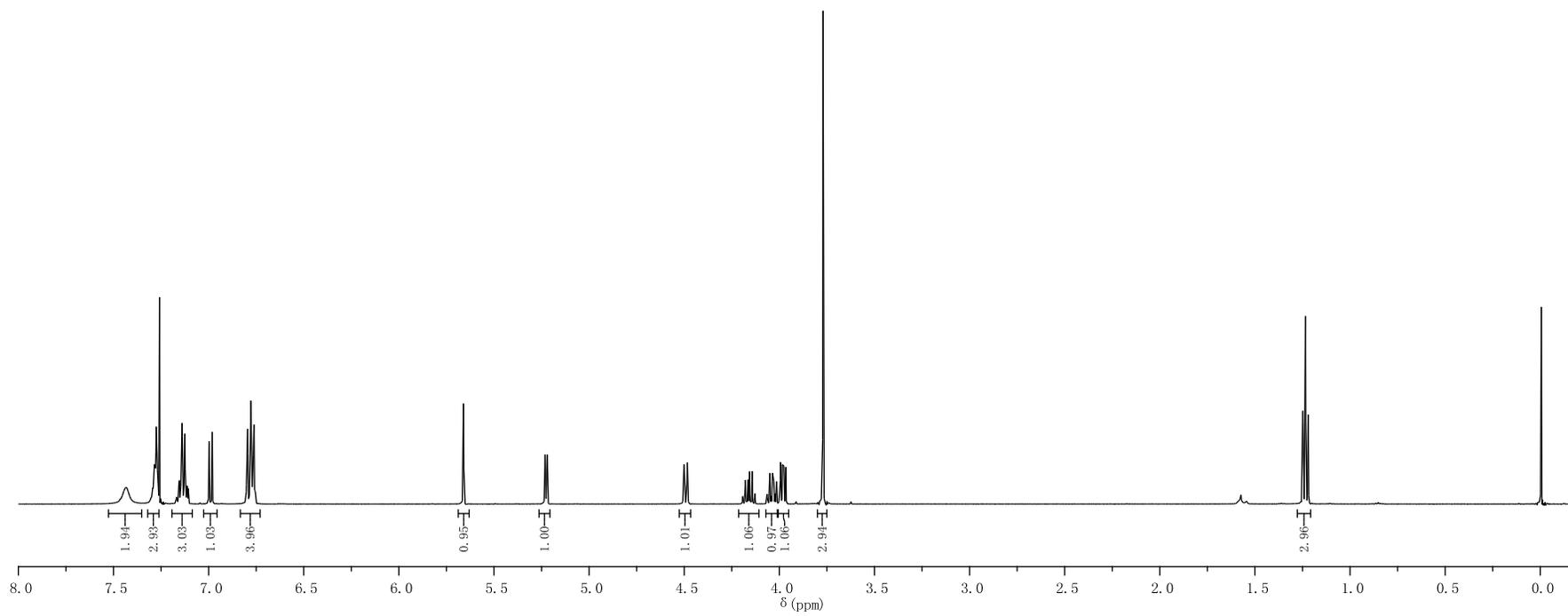
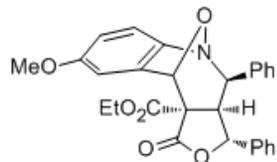
4.5010
4.4834

4.1567
4.1280
4.0429
4.0214
3.9937
3.9657
3.7701

1.2487
1.2344
1.2201

-0.0044
-0.0053

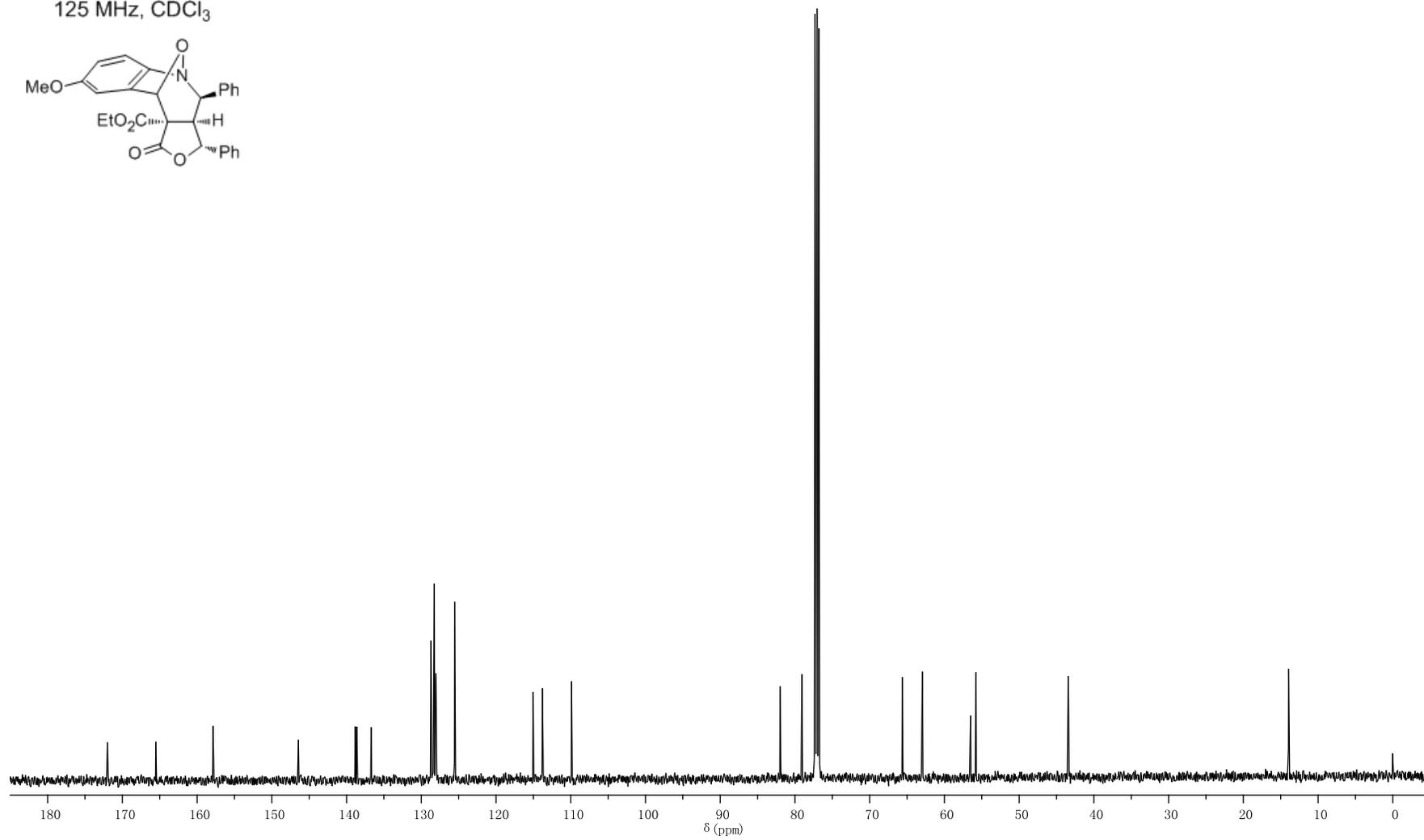
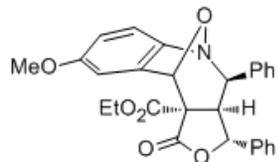
¹H NMR
500 MHz, CDCl₃



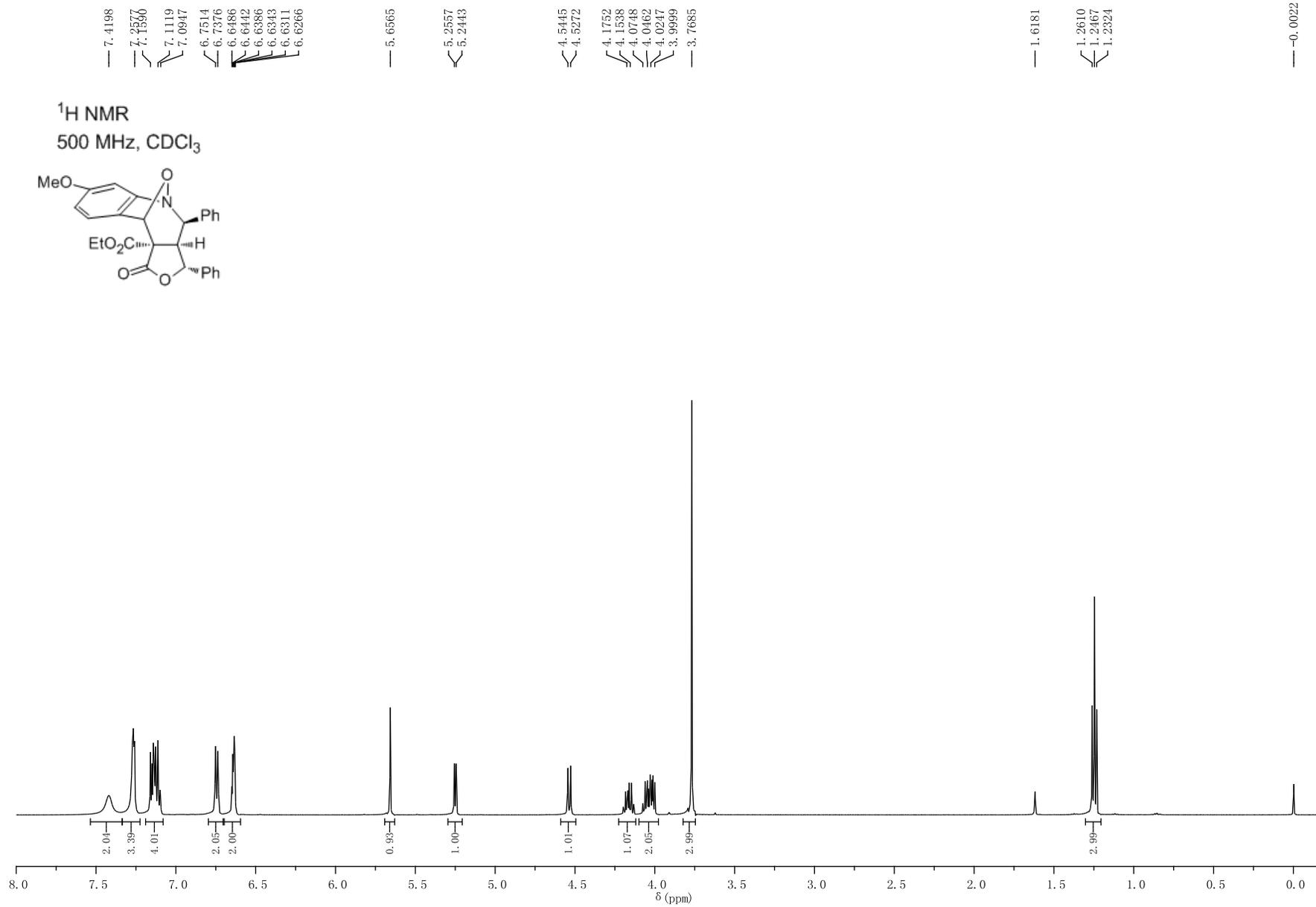
Compound 3ab

172.00
165.52
157.86
146.44
138.85
138.63
136.71
128.26
128.08
128.04
125.53
115.04
113.79
109.89
81.99
79.07
77.30
77.04
76.79
65.63
62.95
56.50
55.78
43.41
13.95
0.02

¹³C NMR
125 MHz, CDCl₃



Compound 3ac



Compound 3ac

— 172.11
— 165.72
— 161.14
— 155.43

— 138.72
— 138.53
— 128.23
— 128.20
— 128.06
— 126.76
— 125.72
— 123.76

— 111.05

— 100.88

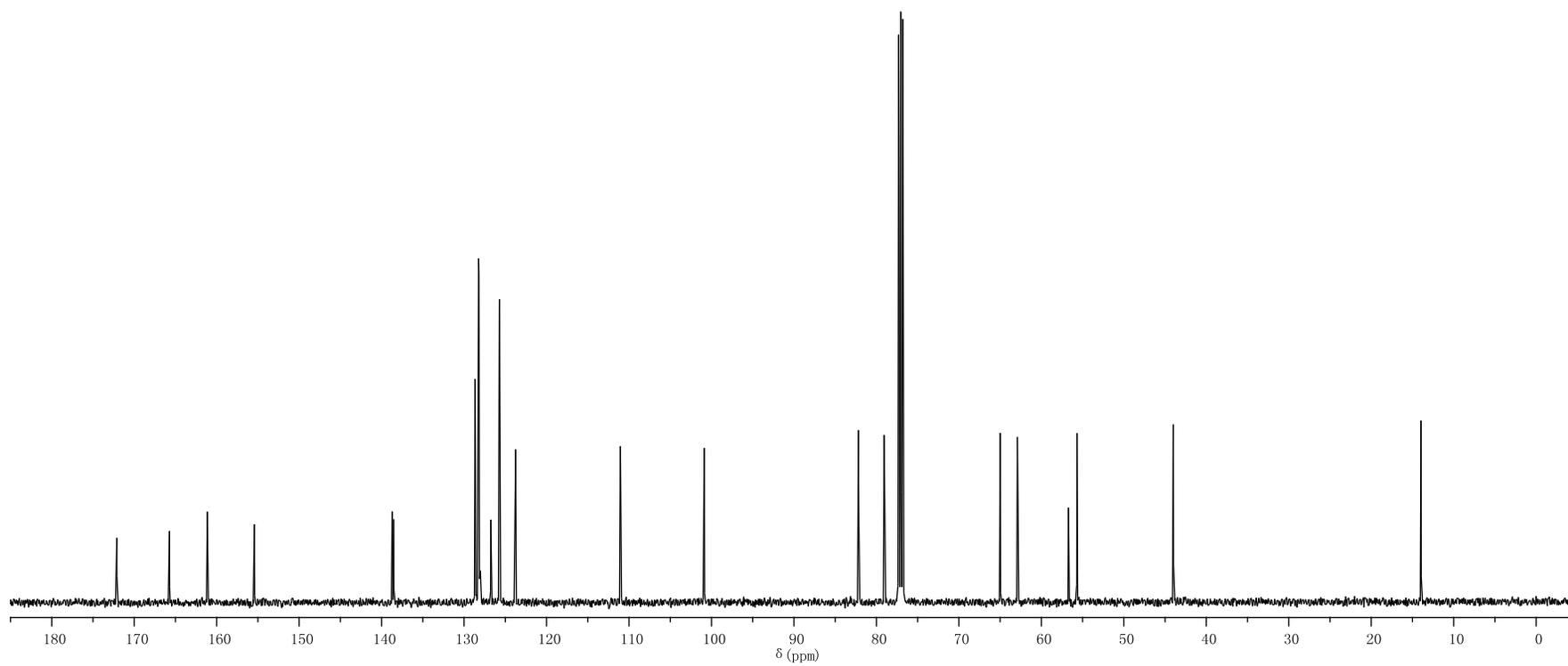
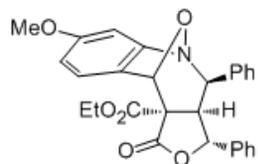
— 82.18
— 79.06
— 77.30
— 77.05
— 76.80

— 64.99
— 62.90
— 56.72
— 55.68

— 43.99

— 13.96

¹³C NMR
125 MHz, CDCl₃



Compound 3ad

7.5055
7.2723
7.2553
7.1456
7.0804
6.8437
6.8350
6.8277
6.8005
6.7857

5.7200

5.2050
5.1967

4.6042
4.5858

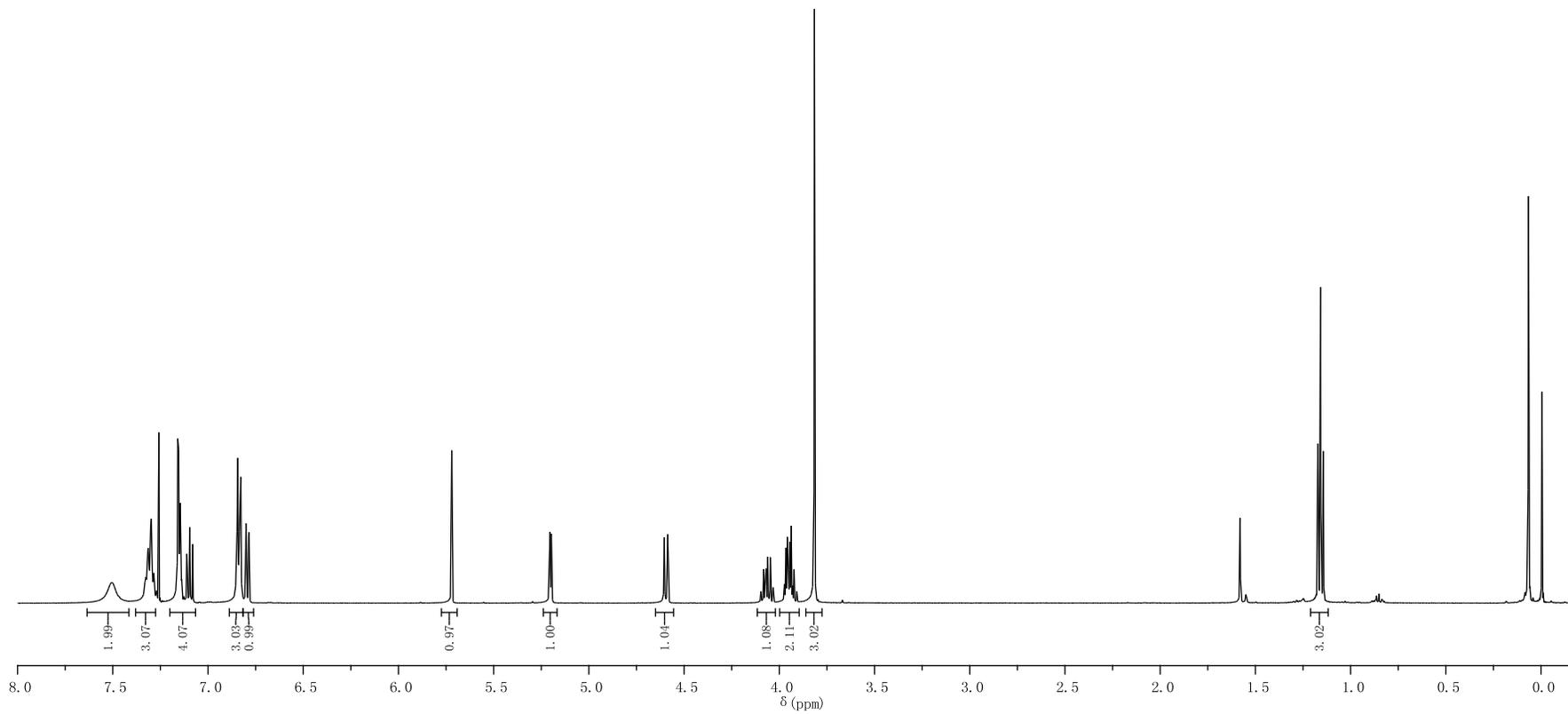
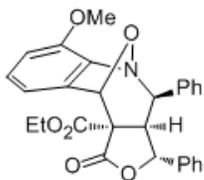
4.0611
3.9725
3.9575
3.9446
3.9297
3.9082
3.8159

1.5803

1.1723
1.1580
1.1437

0.0661
-0.0047

¹H NMR
500 MHz, CDCl₃



Compound 3ad

171.96
165.28

147.44

139.80

138.75

136.49

128.59

128.10

127.48

125.17

114.67

112.90

81.48

79.14

77.30

77.05

76.80

62.97

62.85

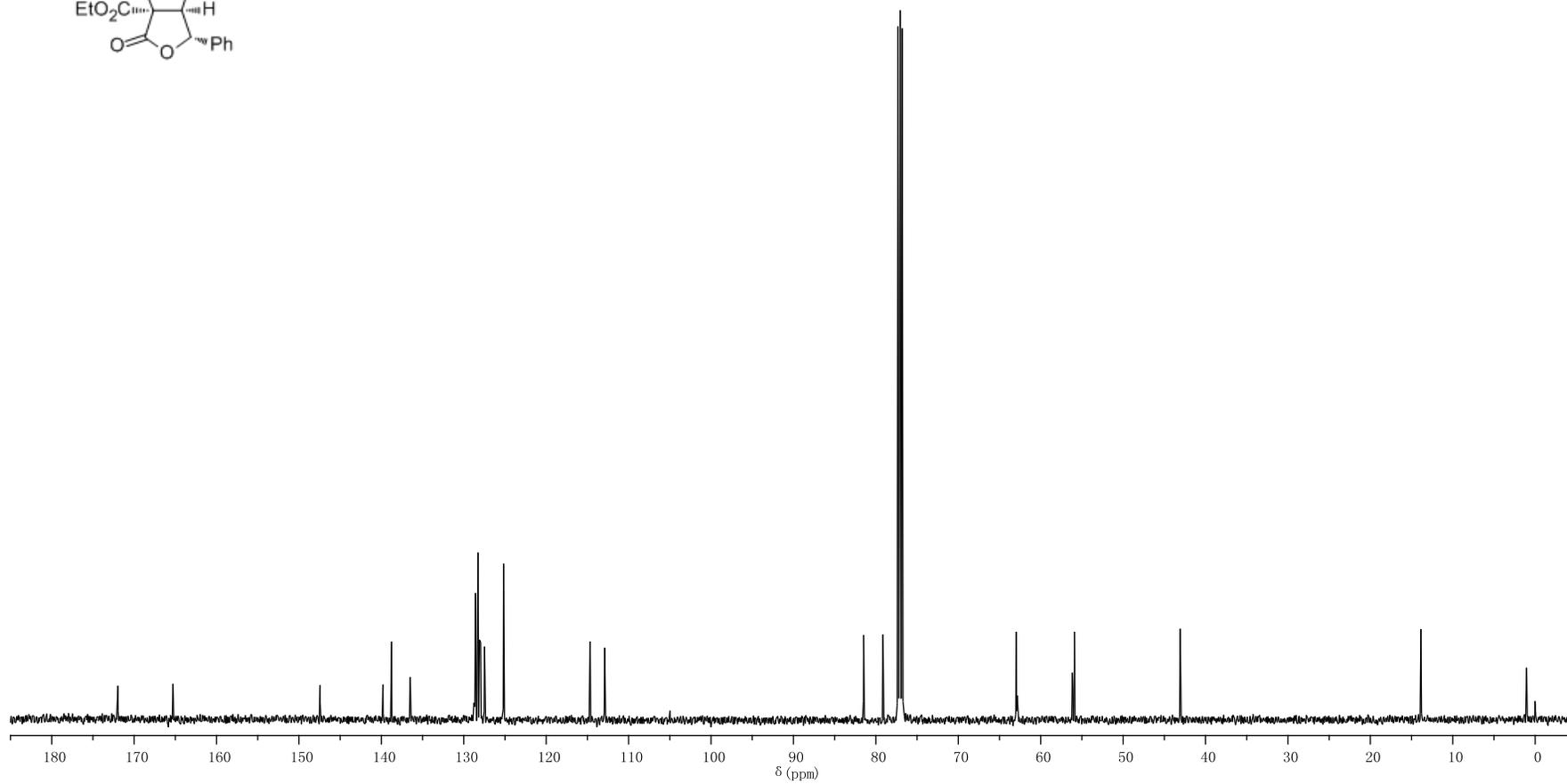
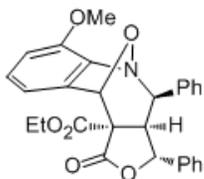
56.16

55.90

43.07

13.86

¹³C NMR
125 MHz, CDCl₃



Compound 3ae

7.6347
7.6225
7.4305
7.2640
7.2552
7.2491
7.2390
7.2263
7.2116
7.2003
7.1854
7.1656
7.1205
7.0432
7.0278

5.7575

5.0511

4.6146
4.5950

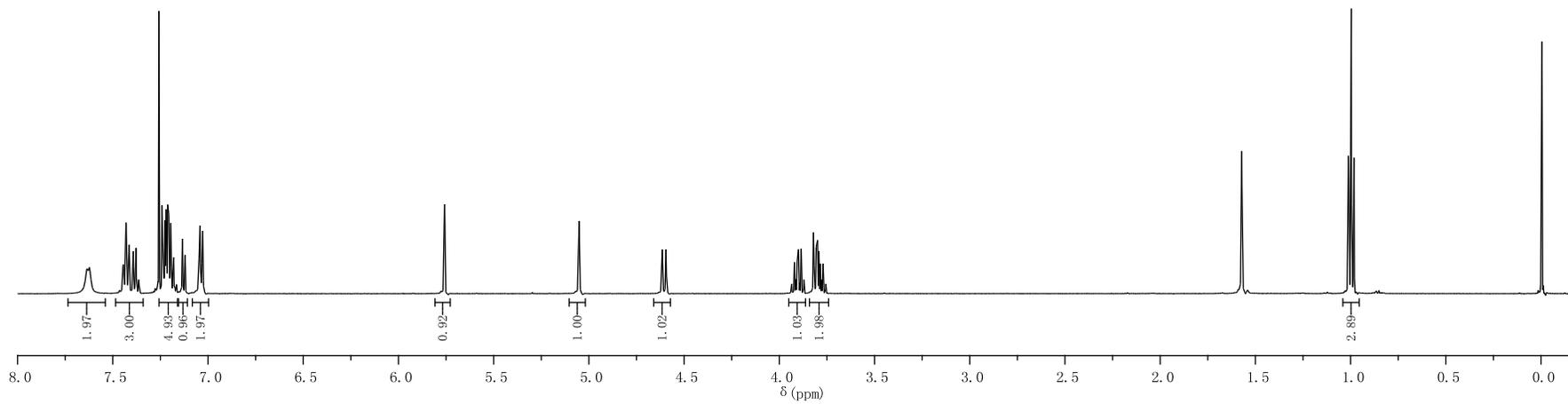
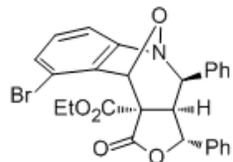
3.9352
3.9209
3.9137
3.9066
3.8994
3.8923
3.8851
3.8708
3.8207
3.8187
3.8062
3.8012
3.7990
3.7919
3.7848
3.7775
3.7703
3.7560

1.5715

1.0109
0.9965
0.9822

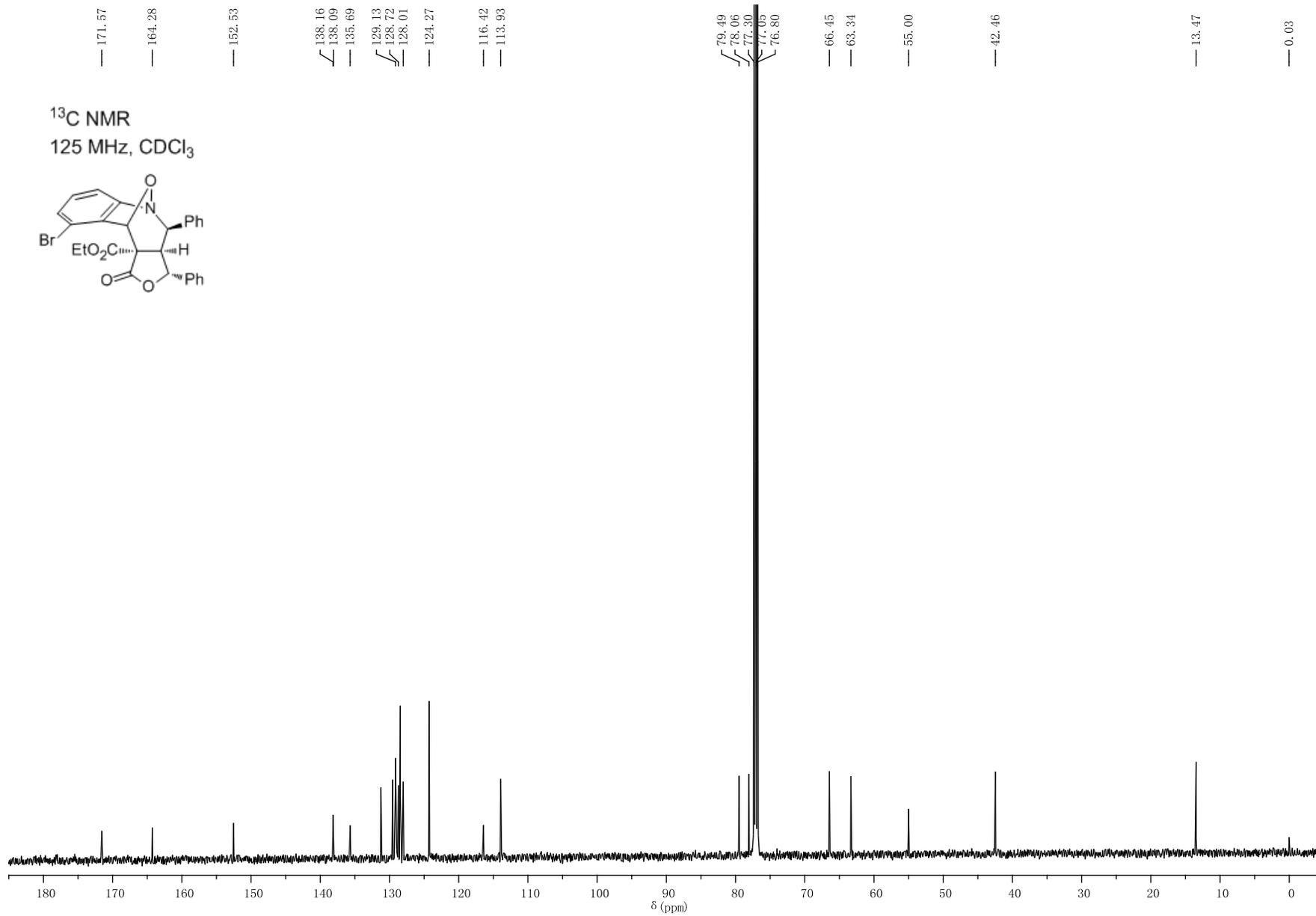
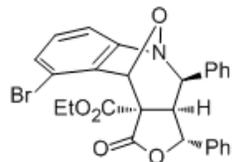
0.0047

¹H NMR
500 MHz, CDCl₃



Compound 3ae

¹³C NMR
125 MHz, CDCl₃



Compound 3af

7.4206
7.4169
7.4045
7.4007
7.3976
7.1443
7.1068
6.9510
6.7593
6.7454

5.6836

5.2455
5.2344

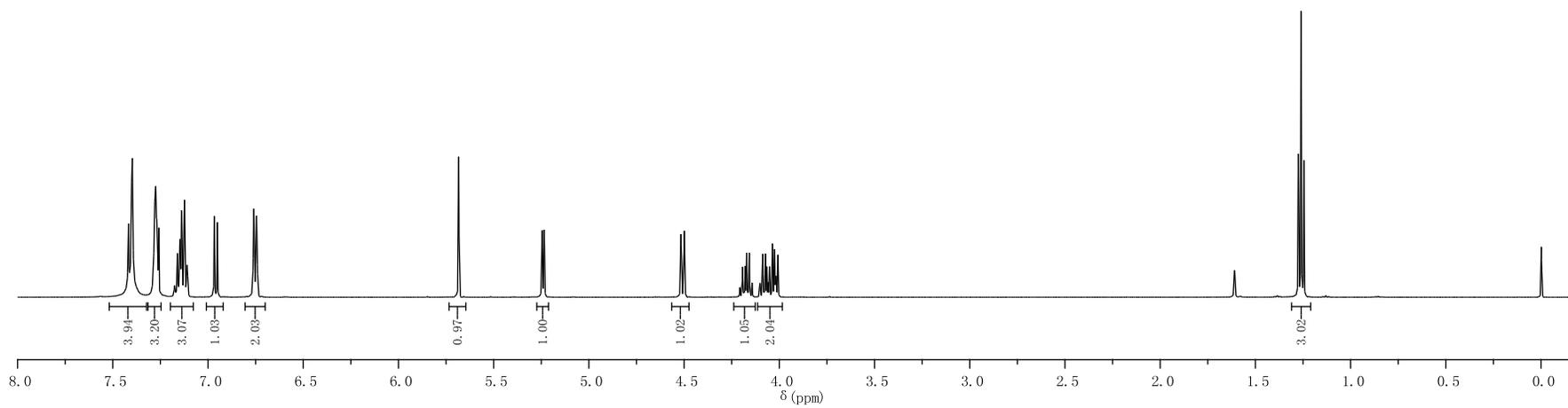
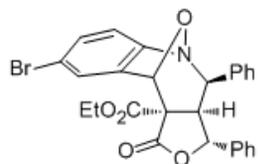
4.5164
4.4991
4.2074
4.1831
4.1859
4.1788
4.1716
4.1645
4.1572
4.1429
4.1014
4.0871
4.0799
4.0728
4.0656
4.0585
4.0513
4.0361
4.0248
4.0186
4.0074

1.6092

1.2744
1.2600
1.2457

0.0013

¹H NMR
500 MHz, CDCl₃



Compound 3af

171.71

165.46

152.78

138.28

137.61

133.94

128.17

128.15

126.65

125.66

118.76

116.01

82.16

78.82

77.30

77.05

76.80

65.06

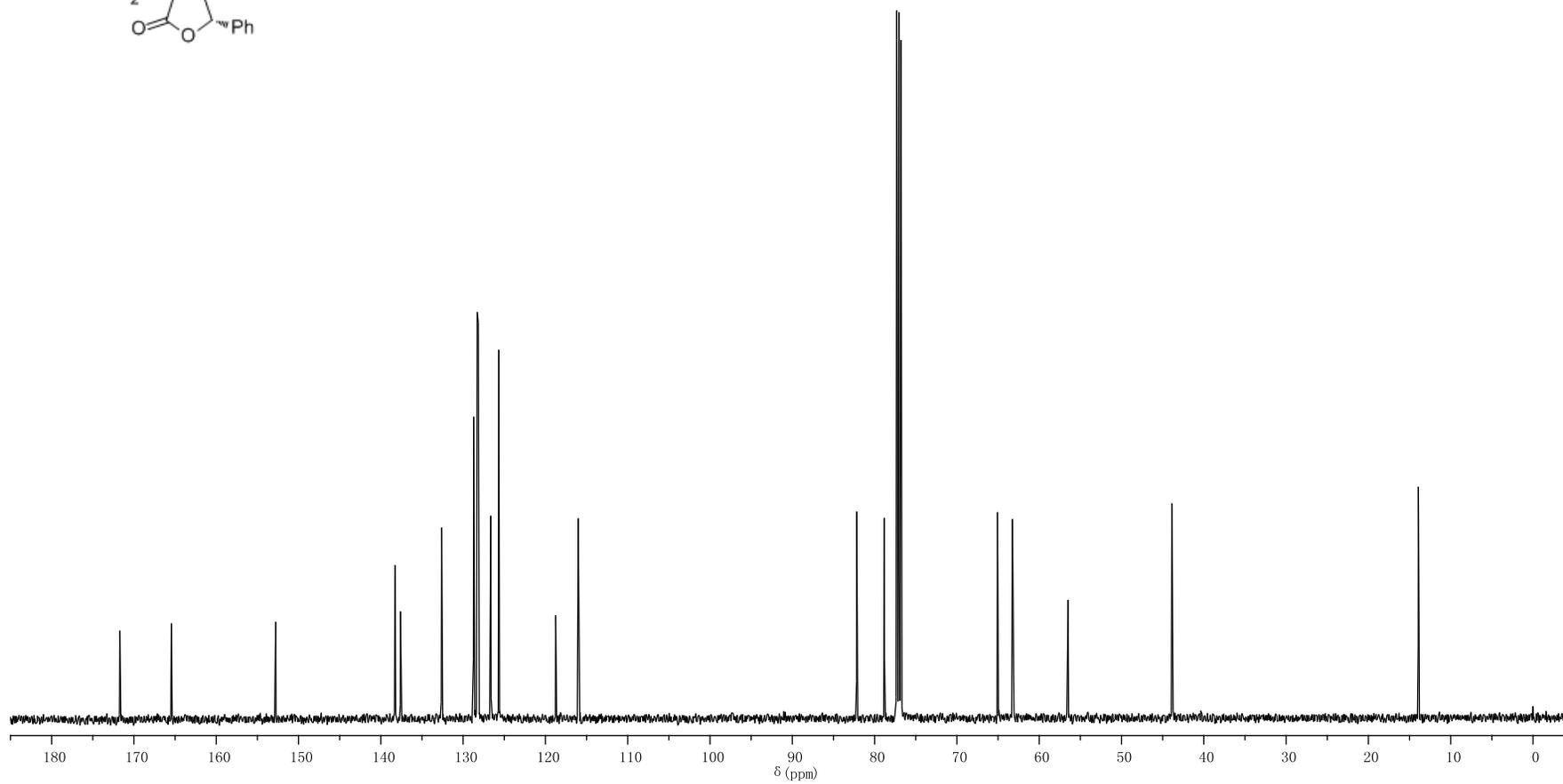
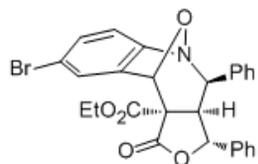
63.25

56.49

43.88

13.93

¹³C NMR
125 MHz, CDCl₃



Compound 3ag

7.4638
7.4052
7.2846
7.1746
7.1400
7.1077
6.7678
6.7666
6.7583
6.7501

5.6754

5.2393
5.2284

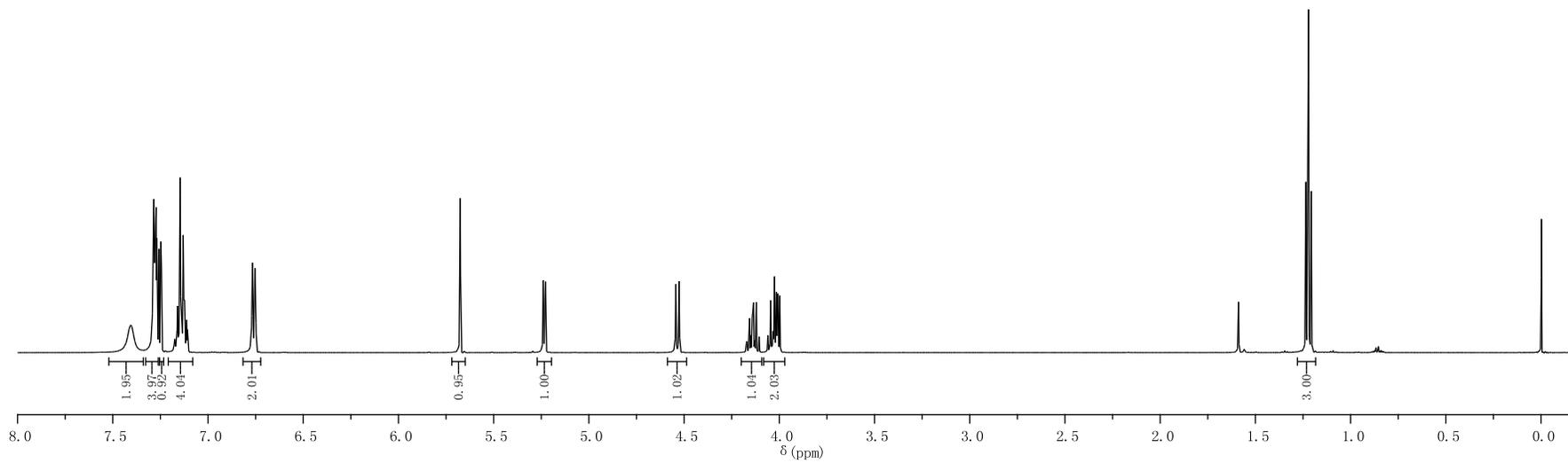
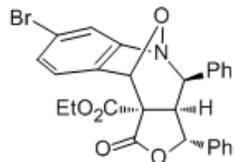
4.5434
4.5260
4.1708
4.1565
4.1493
4.1422
4.1350
4.1279
4.1207
4.1064
4.0601
4.0458
4.0386
4.0314
4.0254
4.0148
4.0094
4.0084
3.9973

1.5889

1.2351
1.2208
1.2065

0.0020

¹H NMR
500 MHz, CDCl₃



Compound 3ag

171.78
165.45
155.28

138.35
138.23
134.46
128.30
128.18
125.64
124.56
123.18
118.16

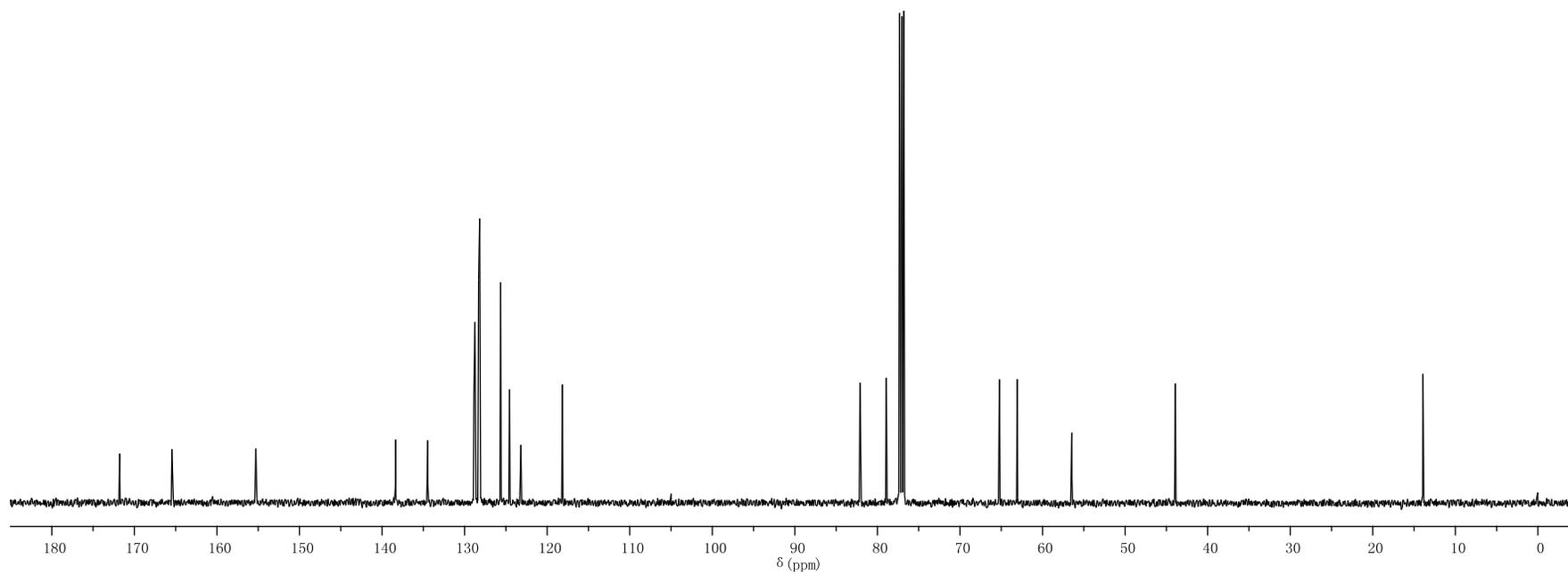
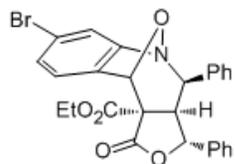
82.11
78.92
77.30
77.05
76.79
65.22
63.07
56.45

43.91

13.92

0.02

¹³C NMR
125 MHz, CDCl₃



Compound 3ah

7.4640
7.4039
7.2459
7.1499
7.1071
6.9982
6.7633
6.7495
6.7470

5.6815

5.2444
5.2333

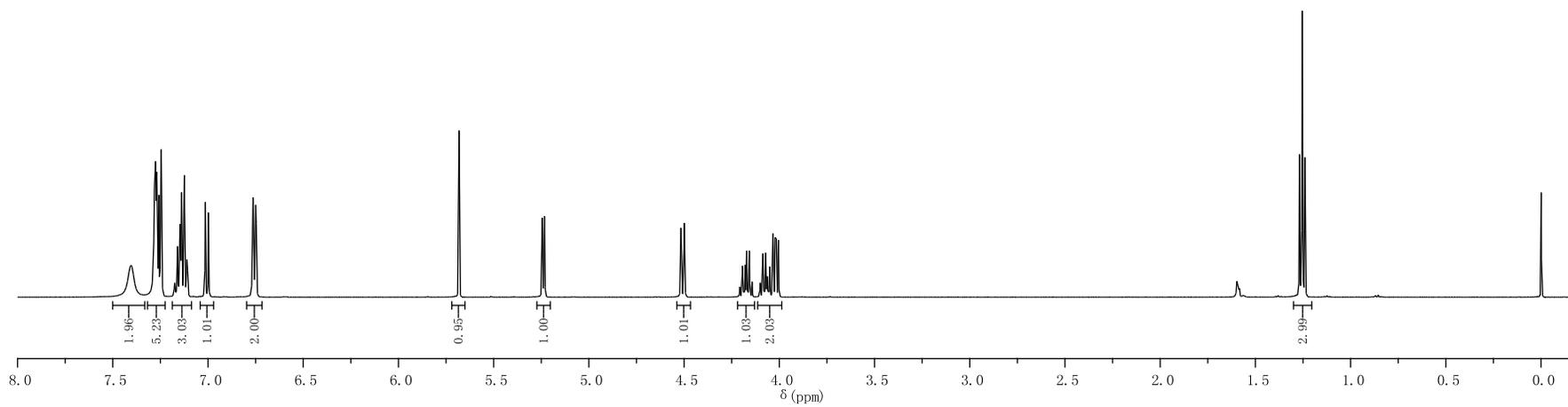
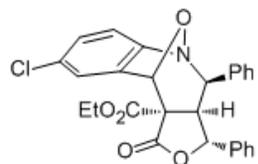
4.5163
4.4989
4.2077
4.1834
4.1861
4.1791
4.1718
4.1647
4.1575
4.1431
4.1004
4.0861
4.0788
4.0718
4.0646
4.0575
4.0502
4.0329
4.0218
4.0155
4.0044

1.5973

1.2688
1.2545
1.2402

0.0010

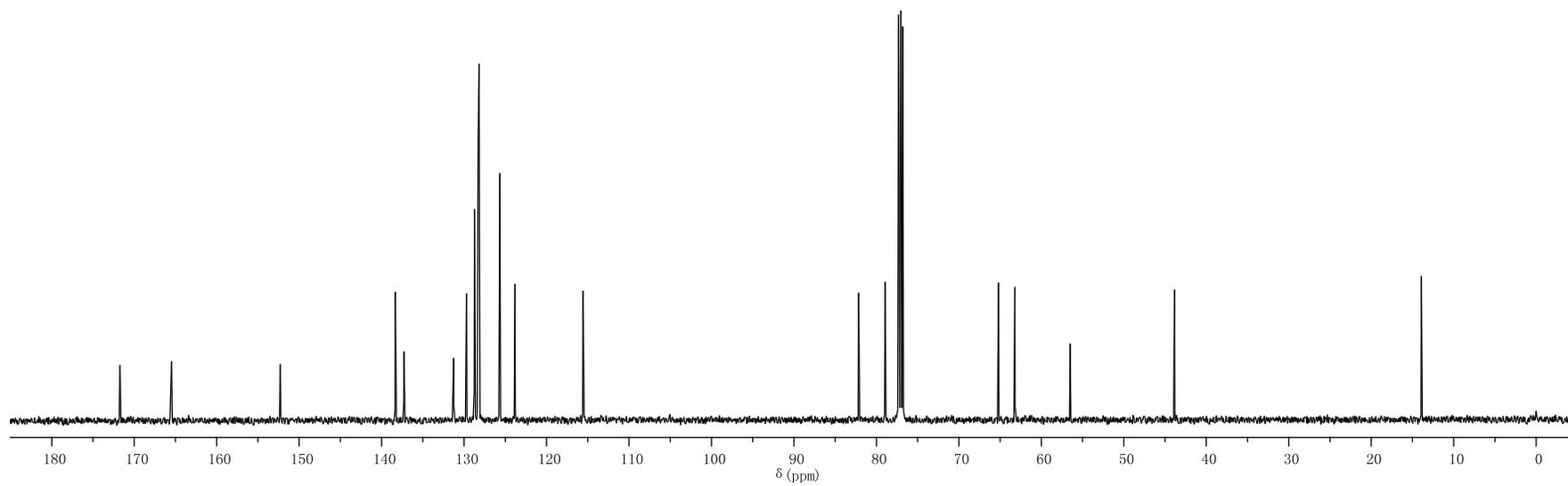
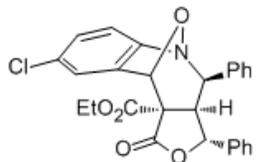
¹H NMR
500 MHz, CDCl₃



Compound 3ah



¹³C NMR
125 MHz, CDCl₃



Compound 3ai

7.4641
7.4178
7.2575
7.1626
7.1192
7.0206
6.9508
6.7752
6.7619
6.7597

5.6816

5.2425
5.2317

4.5232
4.5057

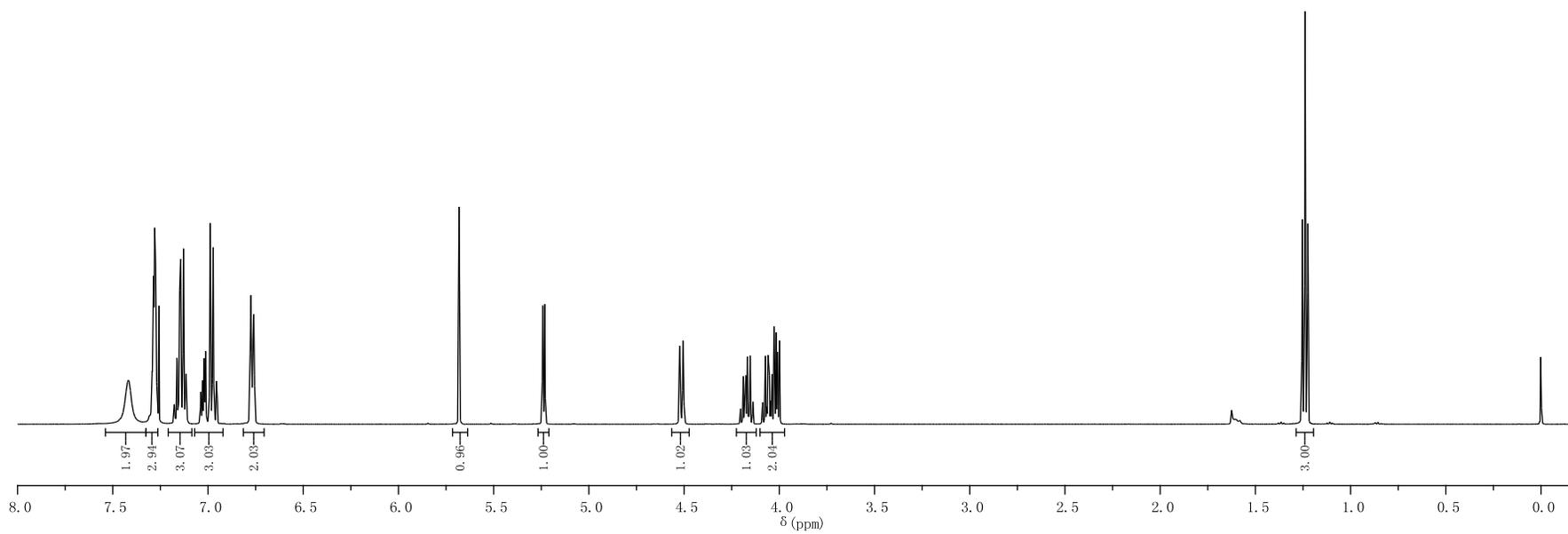
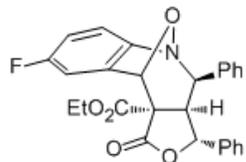
4.1890
4.1818
4.1747
4.1675
4.1604
4.1532
4.1388
4.0876
4.0733
4.0660
4.0590
4.0517
4.0447
4.0374
4.0275
4.0232
4.0167
4.0100
3.9992

1.6250

1.2533
1.2390
1.2247

0.0018

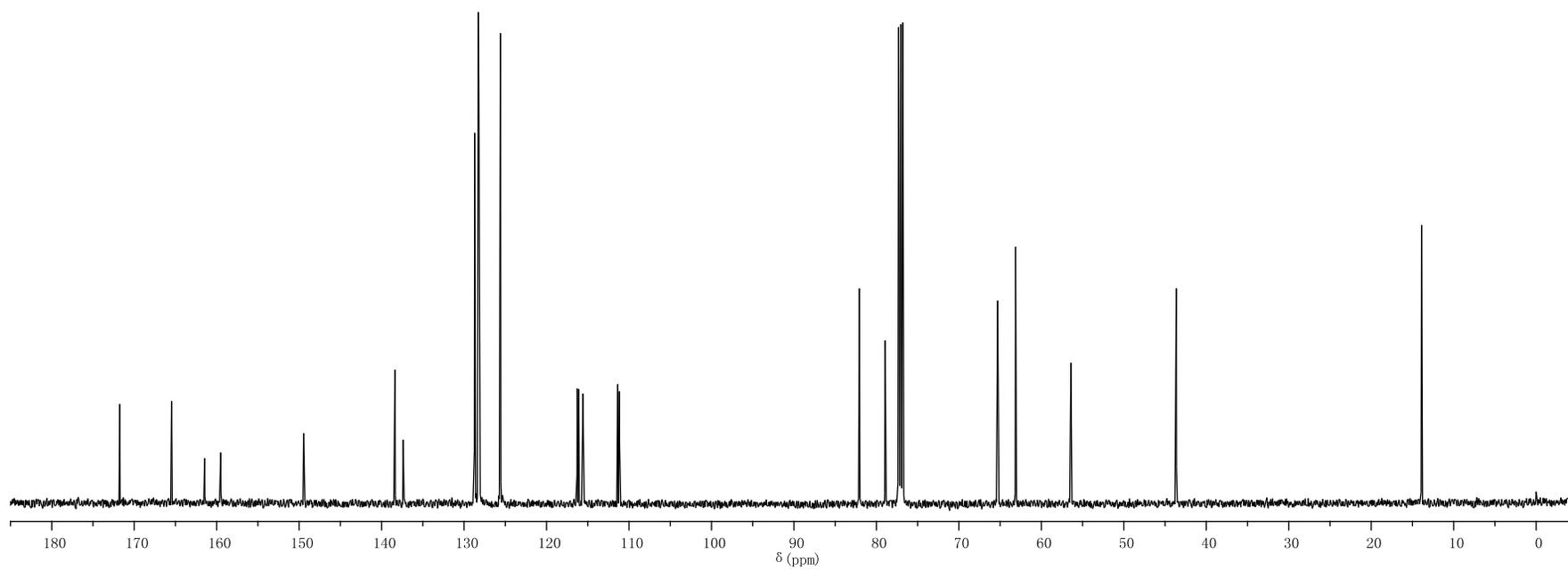
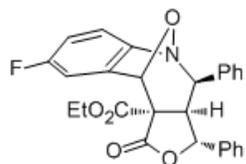
¹H NMR
500 MHz, CDCl₃



Compound 3ai



¹³C NMR
125 MHz, CDCl₃



Compound 3aj

7.4644
7.4080
7.2853
7.1742
7.1428
6.8993
6.8863
6.8827
6.8268
6.8225
6.8155
6.8106
6.8066
6.7619
6.7482

5.6816

5.2420
5.2311

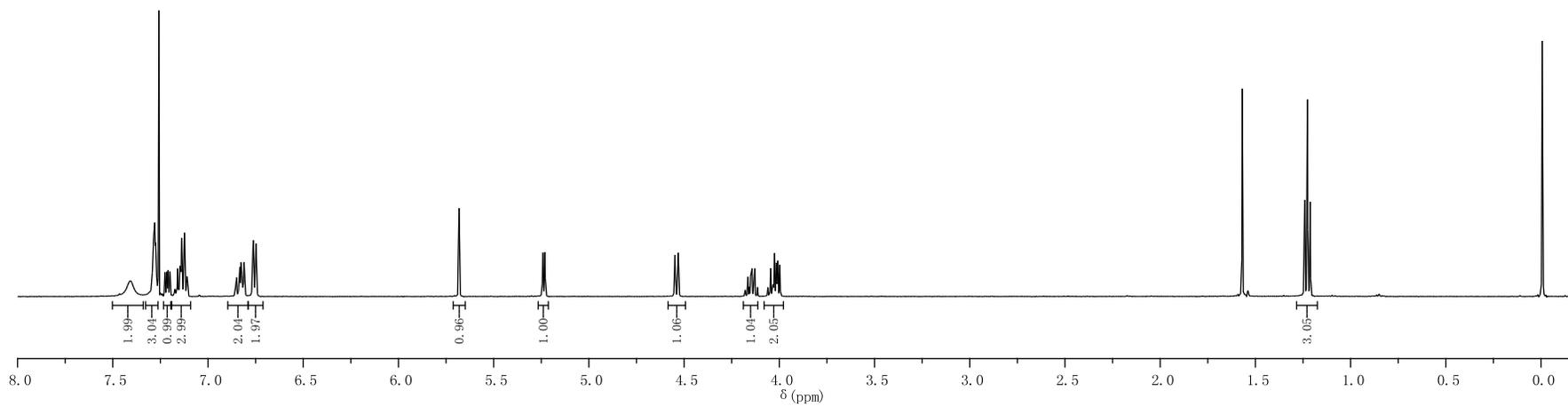
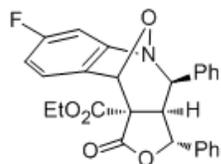
4.5480
4.5306
4.1790
4.1648
4.1575
4.1505
4.1432
4.1361
4.1289
4.1146
4.0602
4.0459
4.0386
4.0315
4.0251
4.0147
4.0085
3.9871

1.5688

1.2410
1.2267
1.2124

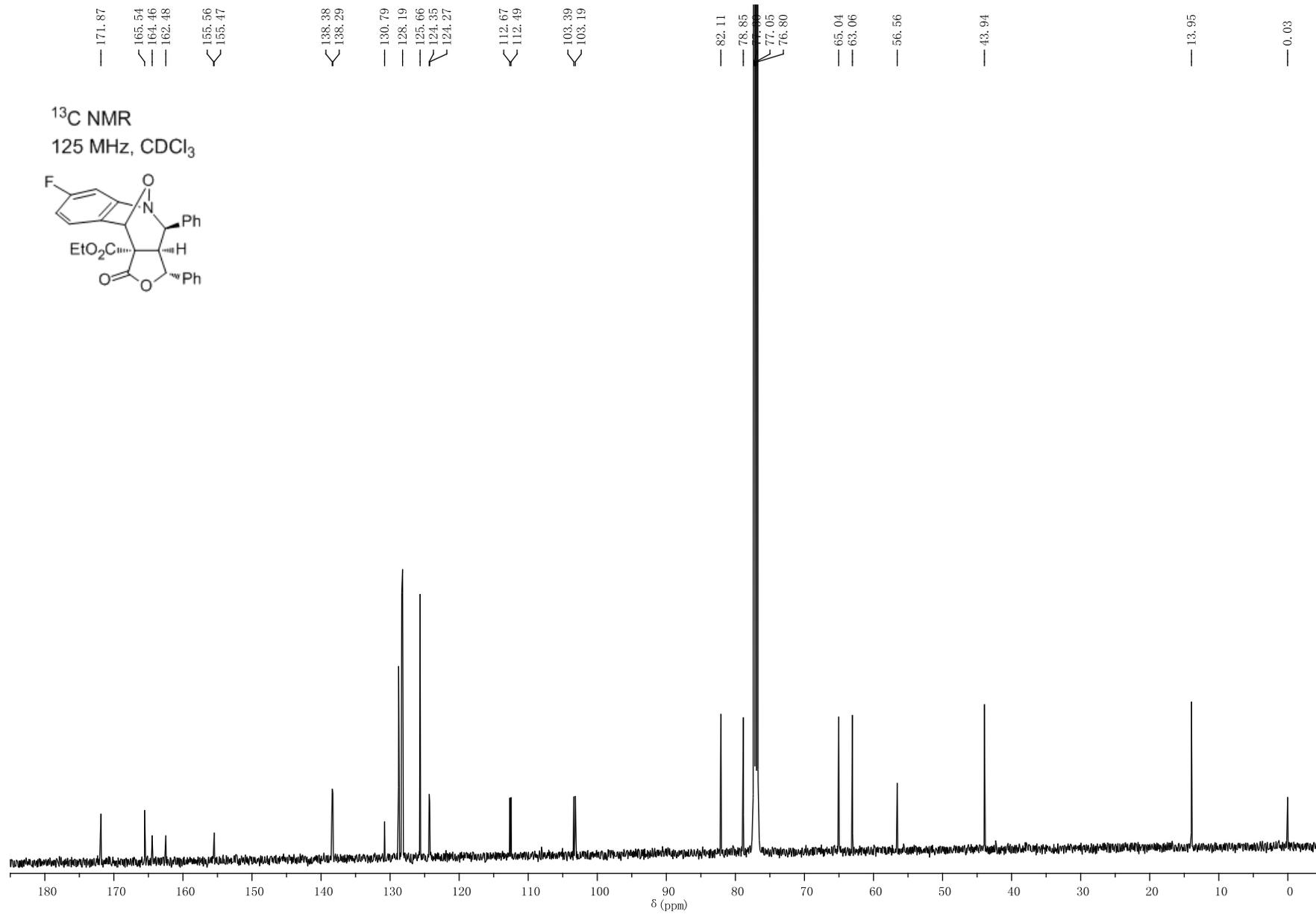
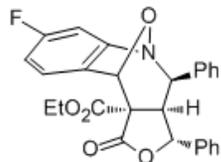
0.0061

¹H NMR
500 MHz, CDCl₃



Compound 3aj

¹³C NMR
125 MHz, CDCl₃



Compound 3ak

7.4240
7.2639
7.2580
7.1829
7.1759
7.1684
7.1628
7.1547
7.1481
7.1331
7.1236
7.1199
7.1162
6.7779
6.7646
6.7615

5.7596

5.2642
5.2534

4.5818
4.5644

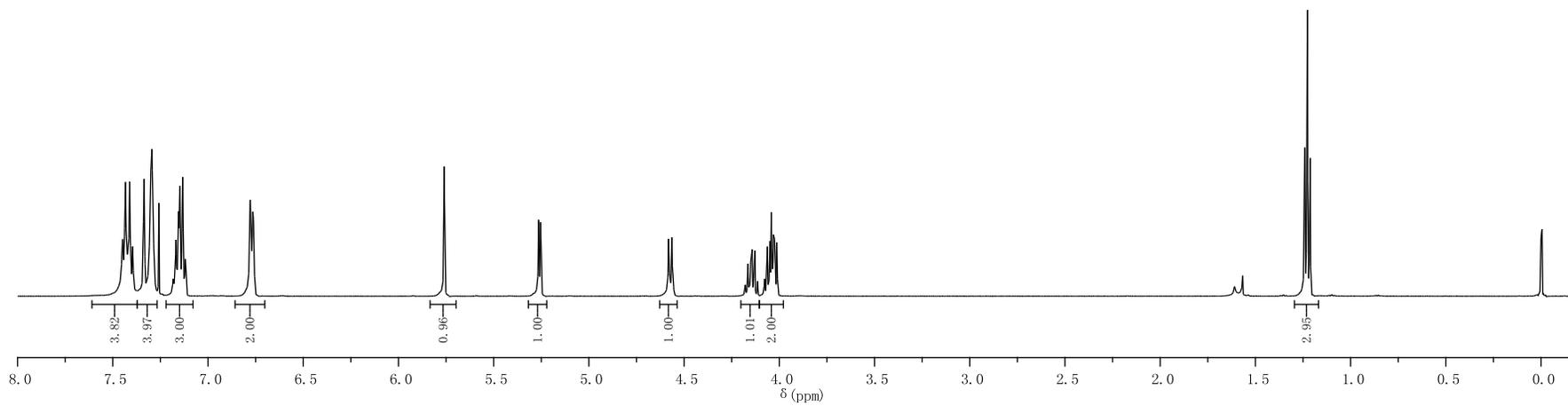
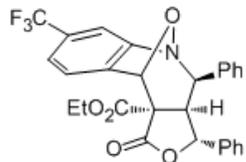
4.1786
4.1643
4.1570
4.1500
4.1428
4.1356
4.1285
4.1142
4.0772
4.0629
4.0554
4.0486
4.0418
4.0310
4.0268
4.0247
4.0135

1.6095

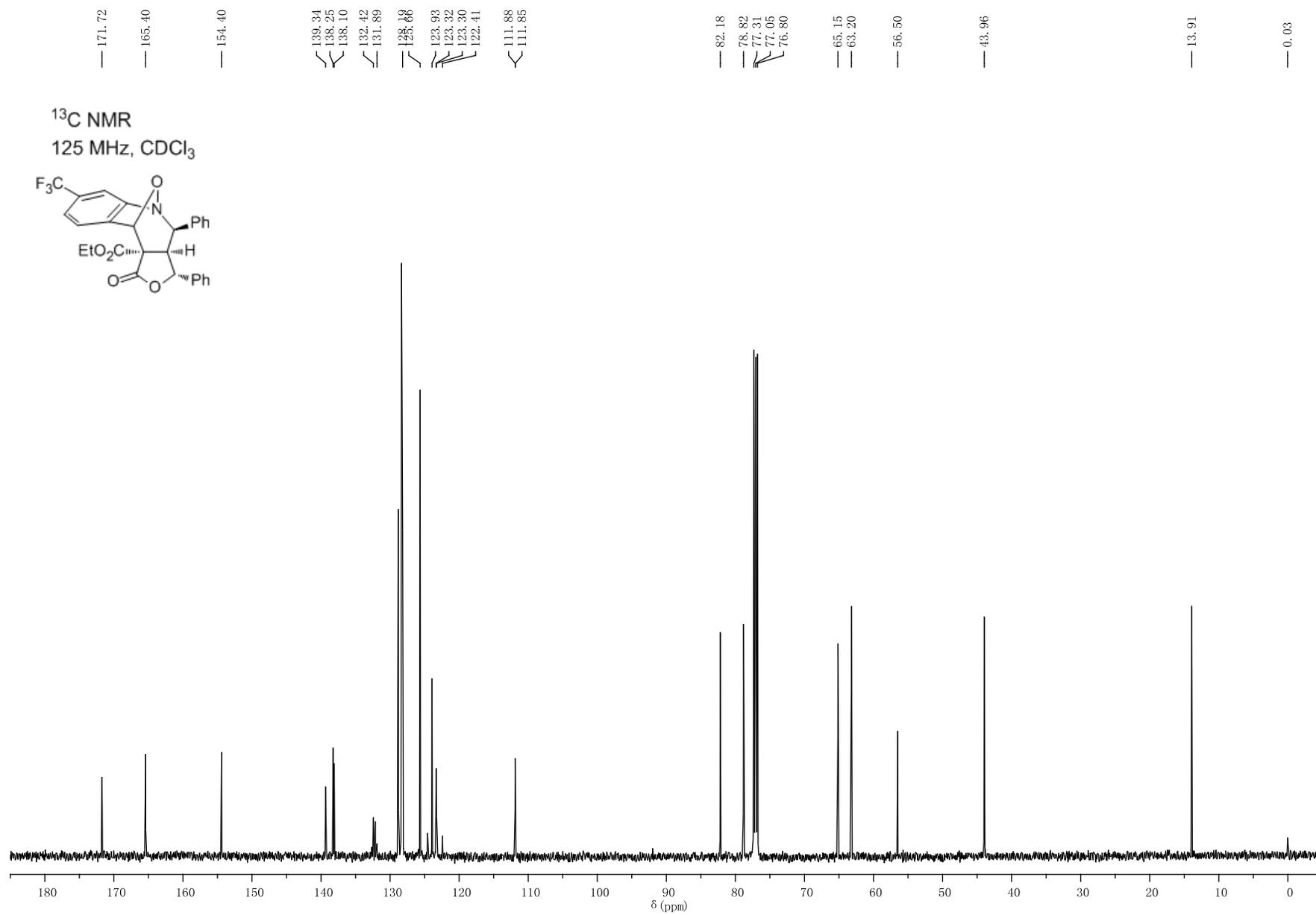
1.2411
1.2268
1.2125

0.0004
-0.0051

¹H NMR
500 MHz, CDCl₃

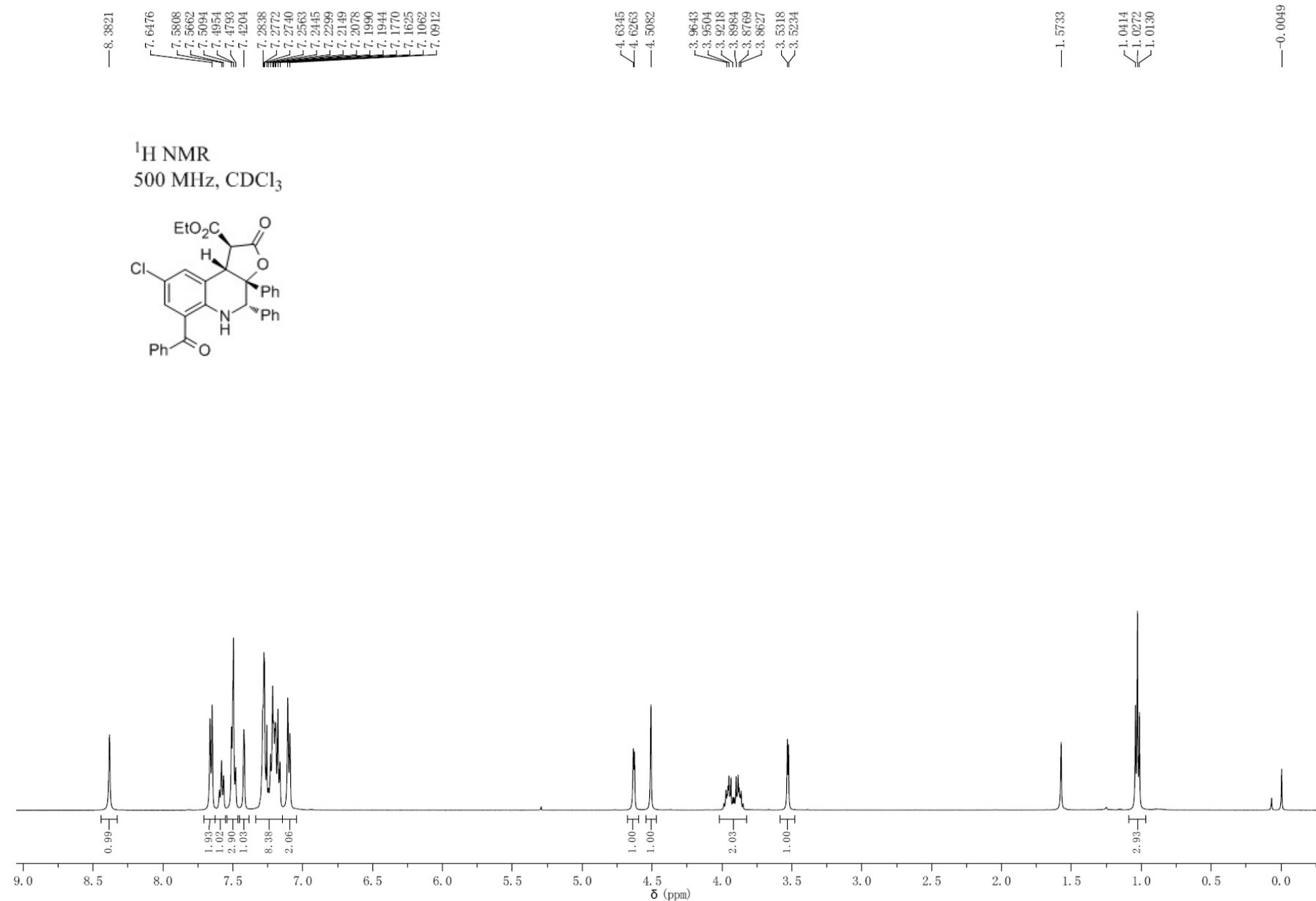


Compound 3ak



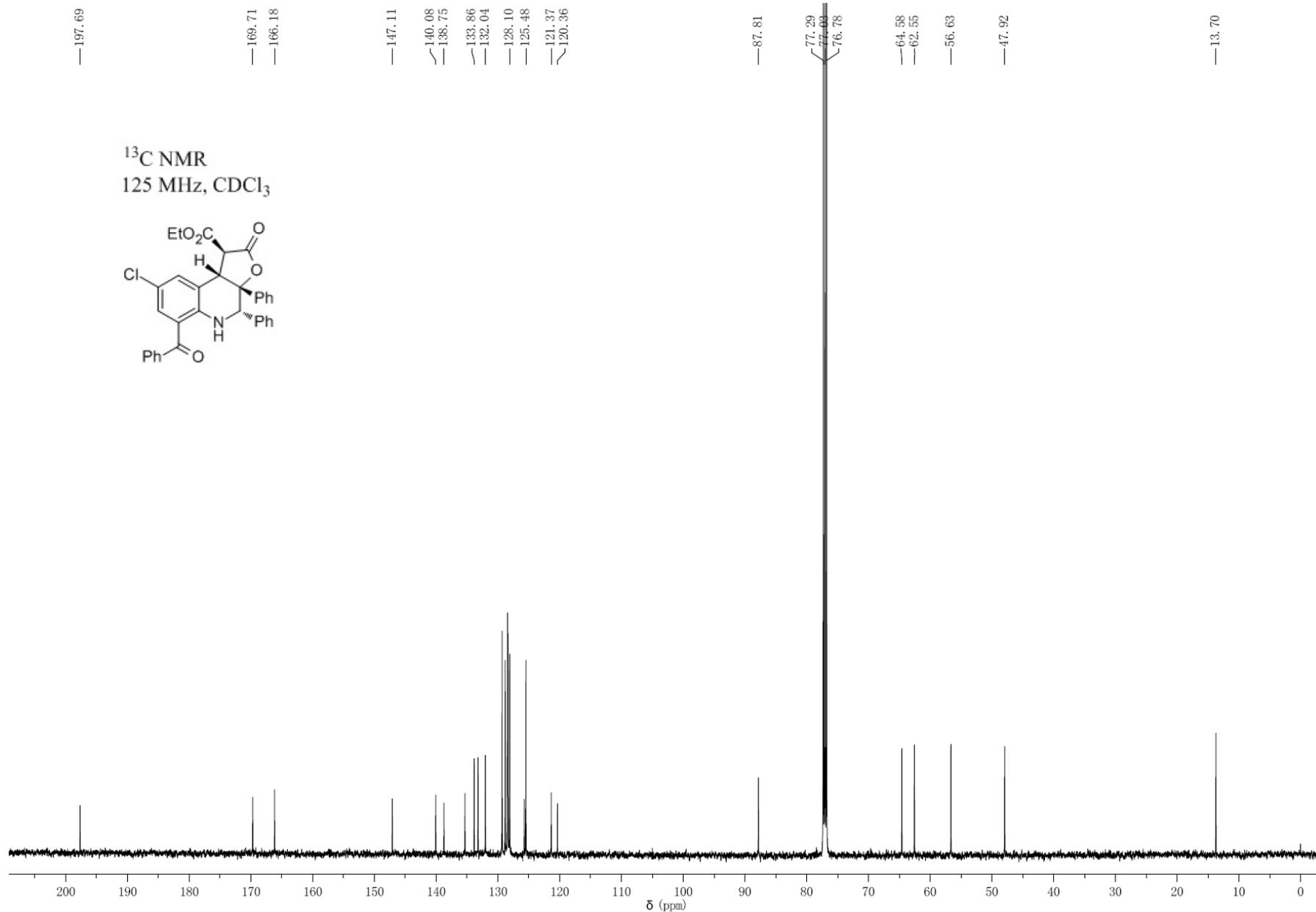
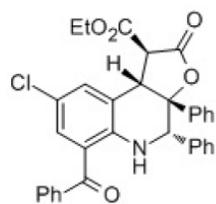
III. Copies of NMR spectra for 4

Compound 4a



Compound 4a

^{13}C NMR
125 MHz, CDCl_3



Compound 4b

8.3489
7.6414
7.5813
7.5625
7.4930
7.4764
7.3039
7.2841
7.2716
7.2318
7.2124
6.9852

4.6081
4.5986
4.4906
3.9784
3.9426
3.9236
3.9093
3.8950
3.8735
3.5235
3.5140

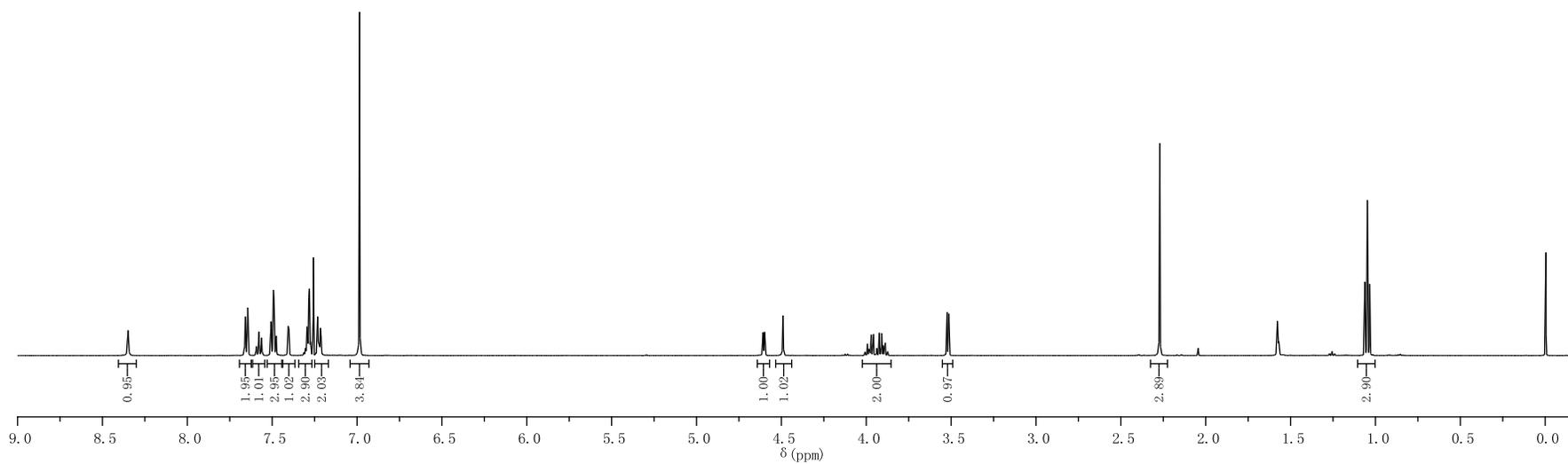
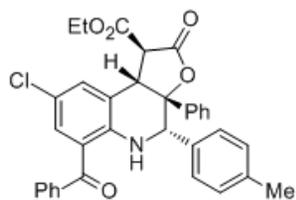
2.2705

1.5781

1.0622
1.0479
1.0337

-0.0040

¹H NMR
500 MHz, CDCl₃



Compound 4b

197.64

169.74
166.28

147.18
140.35
138.79
138.21

132.01
128.37
125.48
121.25
120.29

87.78

77.30
77.05
76.80

64.30
62.56
56.53

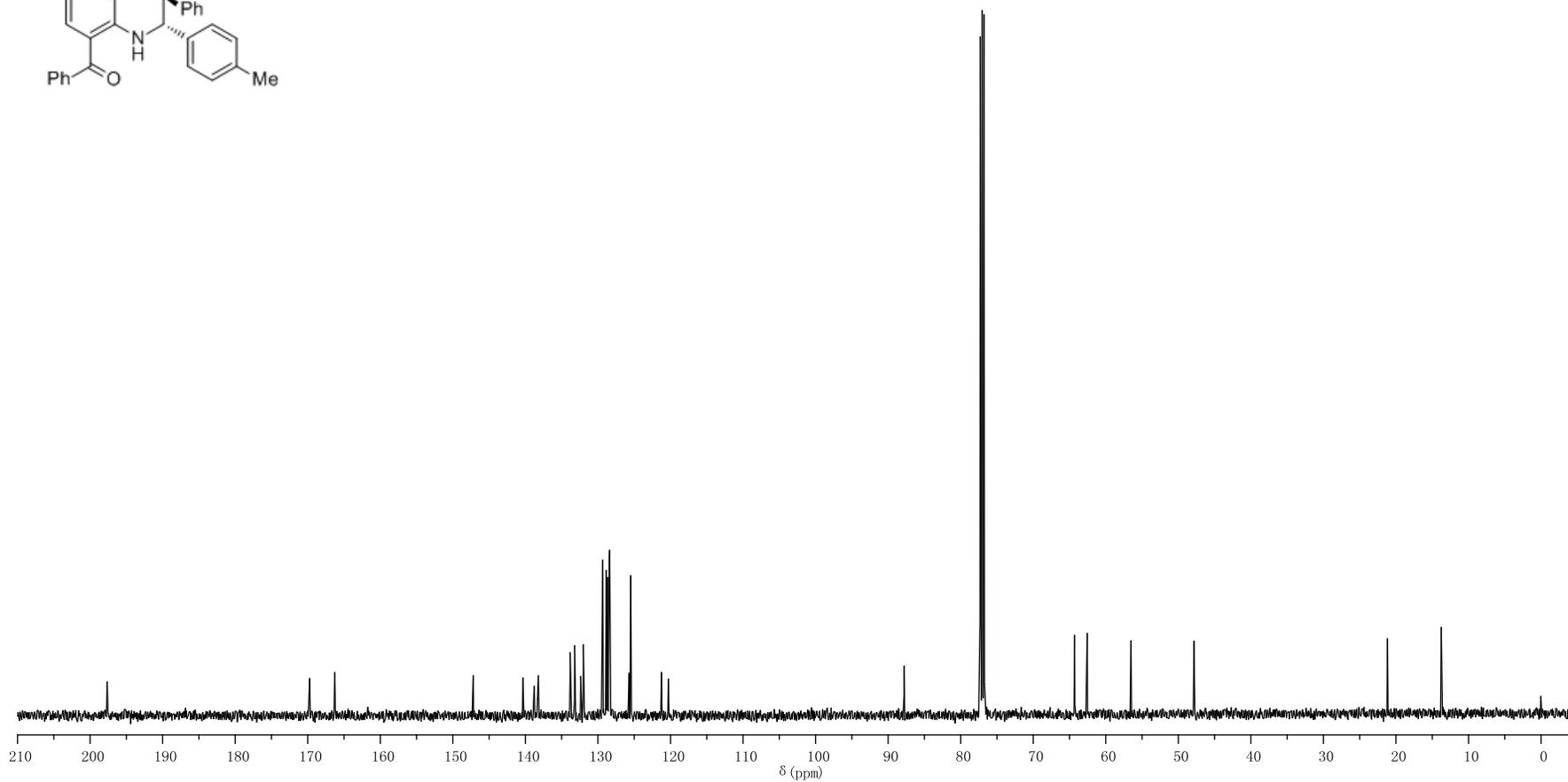
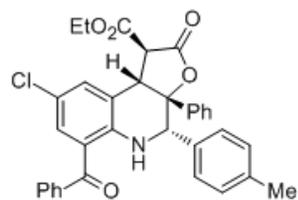
47.85

21.17

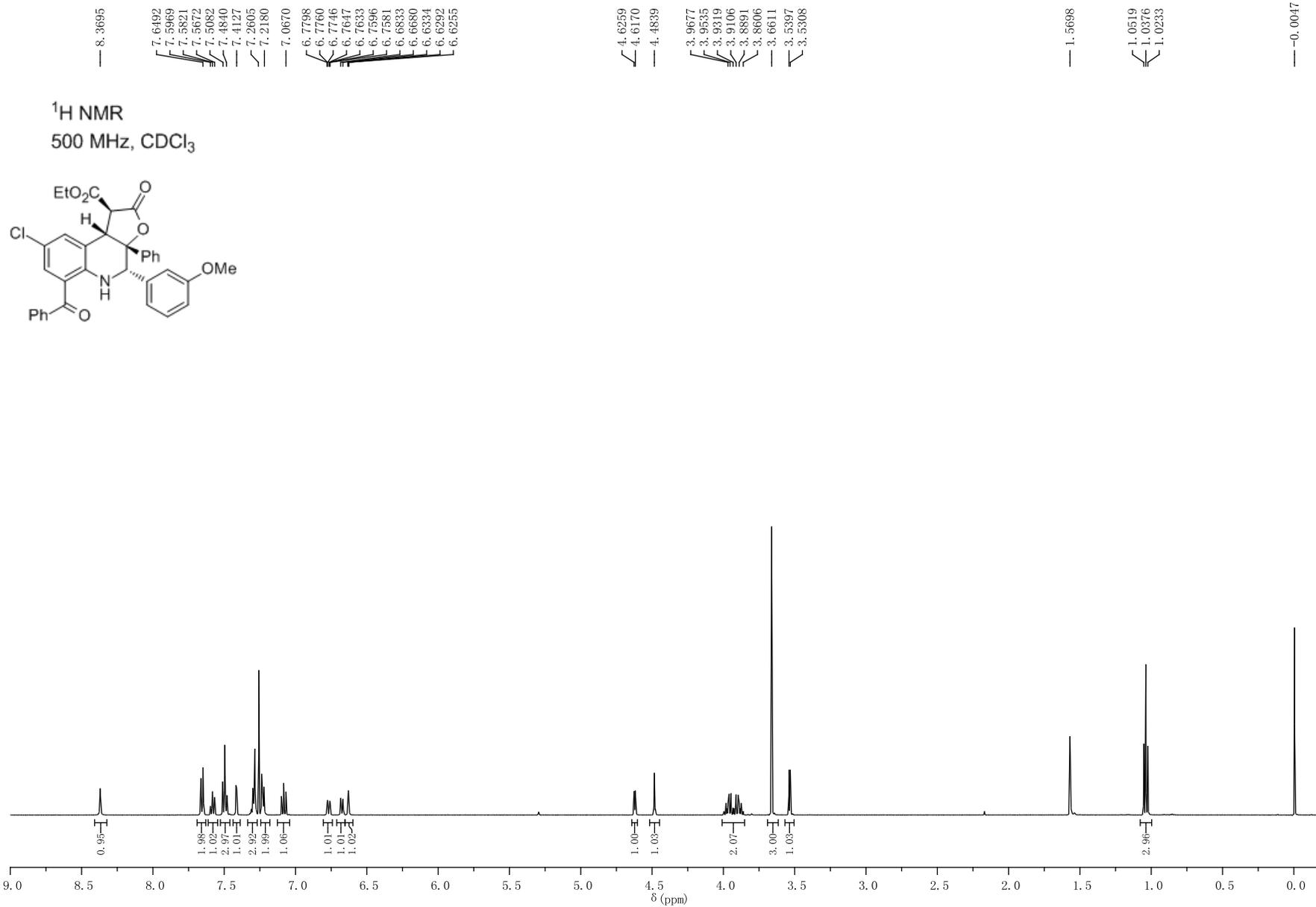
13.75

0.03

¹³C NMR
125 MHz, CDCl₃

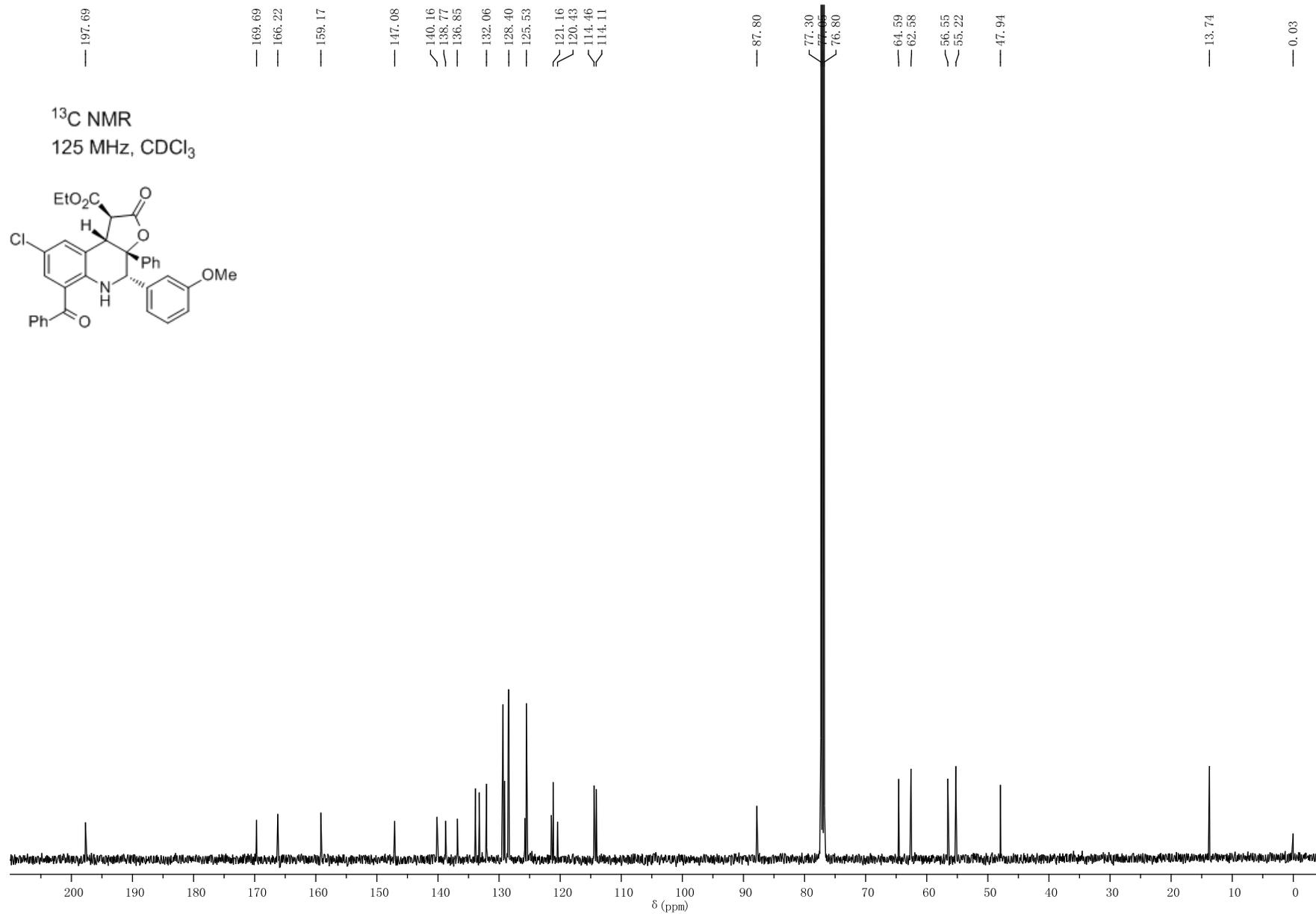
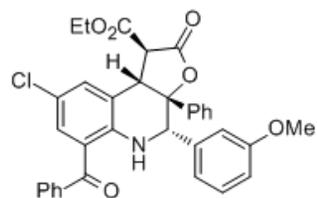


Compound 4c



Compound 4c

¹³C NMR
125 MHz, CDCl₃



Compound 4d

8.2943
7.6428
7.5864
7.5715
7.5089
7.4846
7.4206
7.3179
7.1711
6.9742
6.9694
6.9660
6.9558
6.9525
6.9476

5.2937

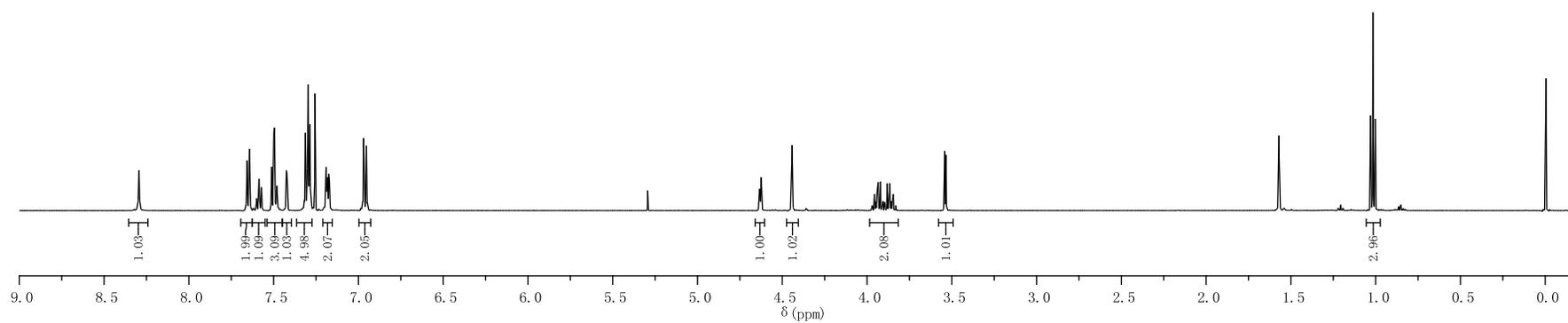
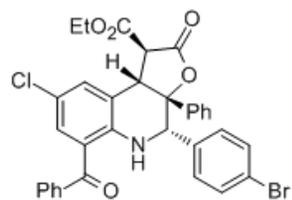
4.6320
4.6246
4.4425
3.9418
3.9060
3.8810
3.8668
3.8525
3.8310
3.5414
3.5339

1.5704

1.0304
1.0161
1.0018

-0.0049

¹H NMR
500 MHz, CDCl₃



Compound 4d

197.76

169.58

166.00

146.95

139.64

138.62

132.17

129.37

128.49

125.46

122.68

121.80

120.59

87.84

77.30

77.05

76.80

64.28

62.62

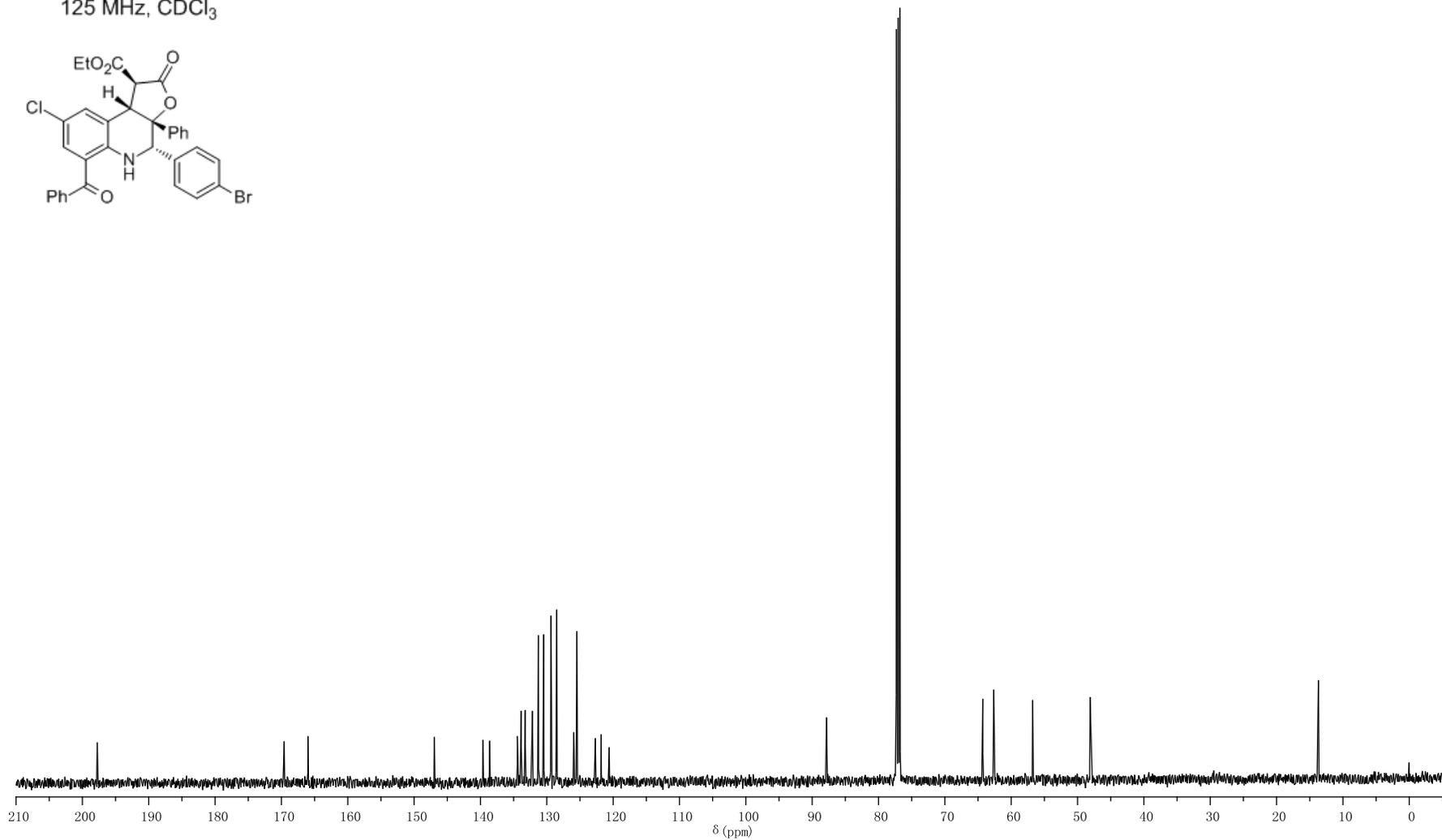
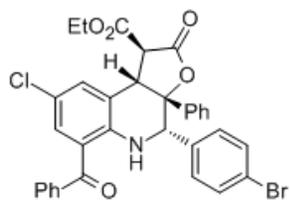
56.77

48.11

13.70

0.03

¹³C NMR
125 MHz, CDCl₃



Compound 4e

197.73

169.58

165.96

146.91

139.60

138.60

132.13

128.54

128.27

125.43

121.72

120.52

87.83

77.30

77.05

76.80

64.11

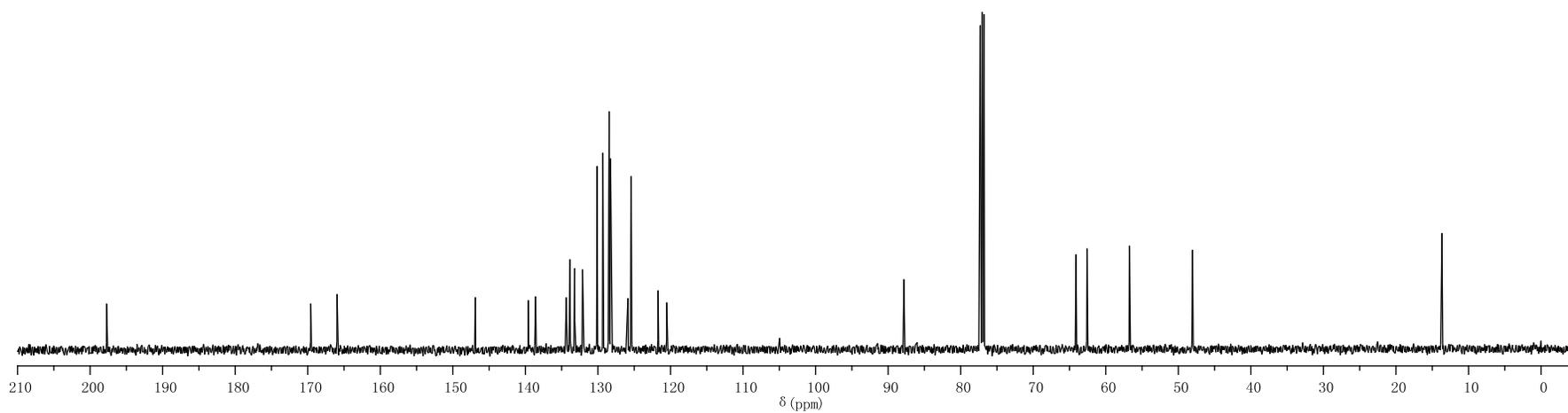
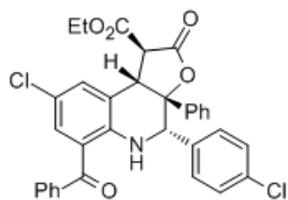
62.58

56.75

48.05

13.66

¹³C NMR
125 MHz, CDCl₃



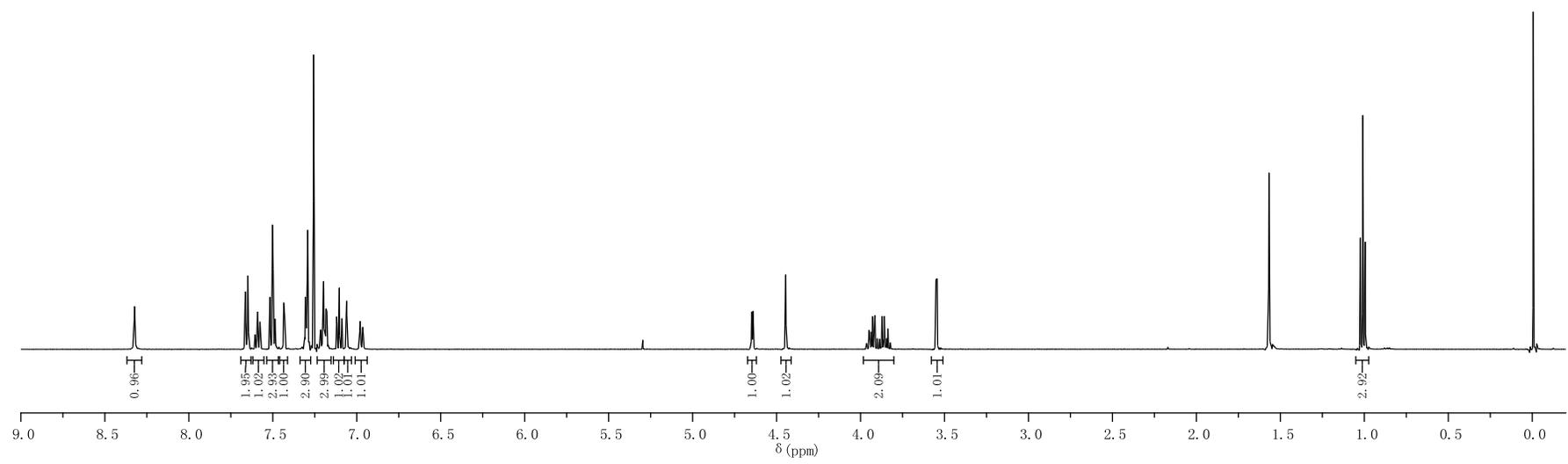
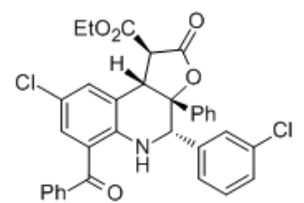
Compound 4f

8.3230
7.6492
7.6060
7.5911
7.5762
7.5142
7.4900
7.4303
7.2966
7.2843
7.2711
7.2599
7.2365
7.2174
7.2133
7.2035
7.1976
7.1907
7.1829
7.1708
7.1040
7.0642
7.0570
6.9640

4.6477
4.6405
4.4458
3.9358
3.9000
3.8723
3.8580
3.8438
3.8223
3.5508
3.5435

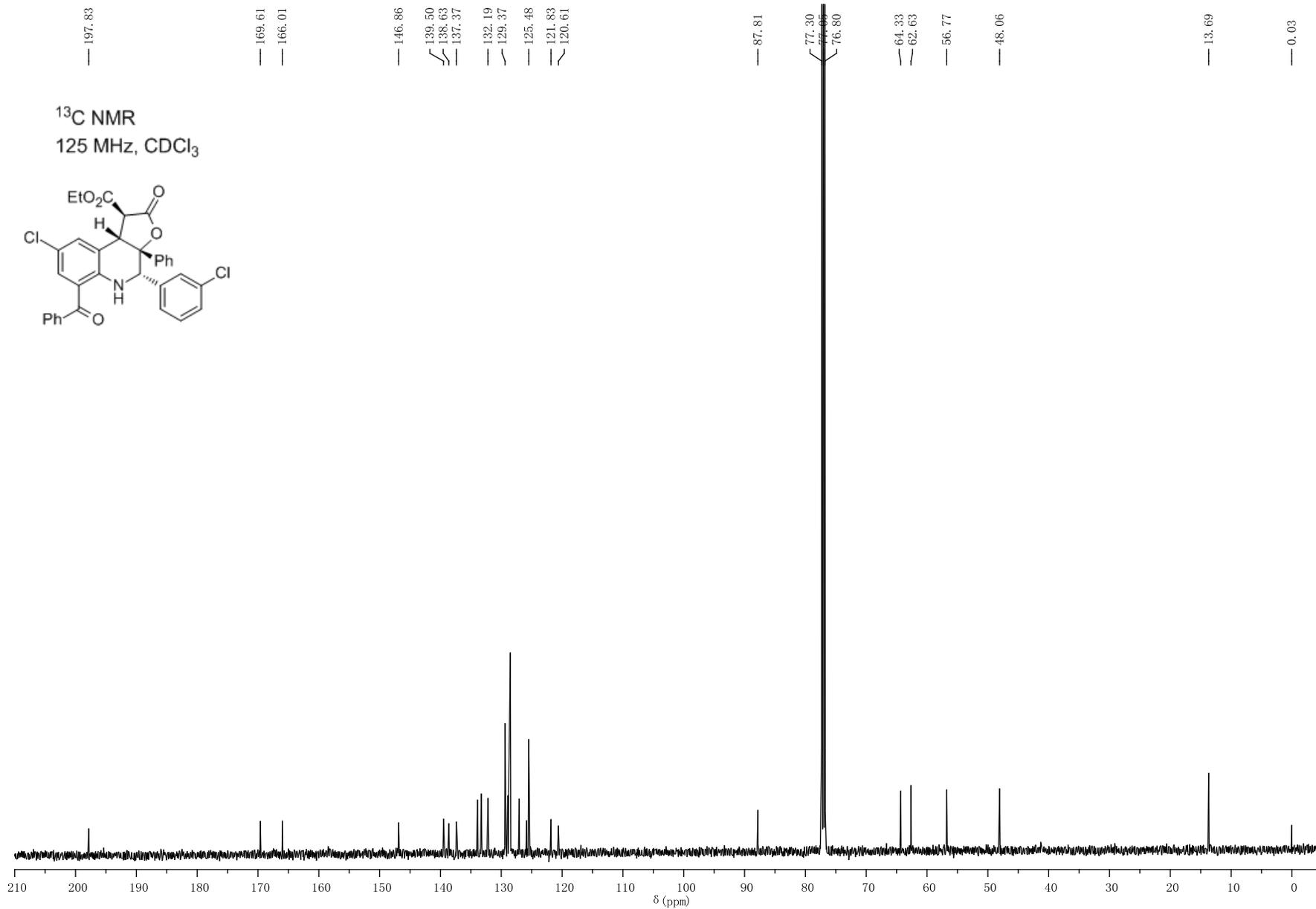
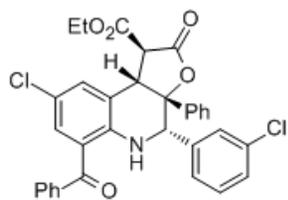
1.5680
1.0233
1.0090
0.9948
-0.0059

¹H NMR
500 MHz, CDCl₃



Compound 4f

¹³C NMR
125 MHz, CDCl₃



Compound 4g

8.2160
7.8869
7.8844
7.8712
7.8686
7.5795
7.5047
7.4544
7.3049
7.2805
7.2753
7.2693
7.2630
7.2551
7.2454
7.2354
7.2045
7.1886
7.1738
7.1217
7.1056

5.1335

4.7179
4.7098

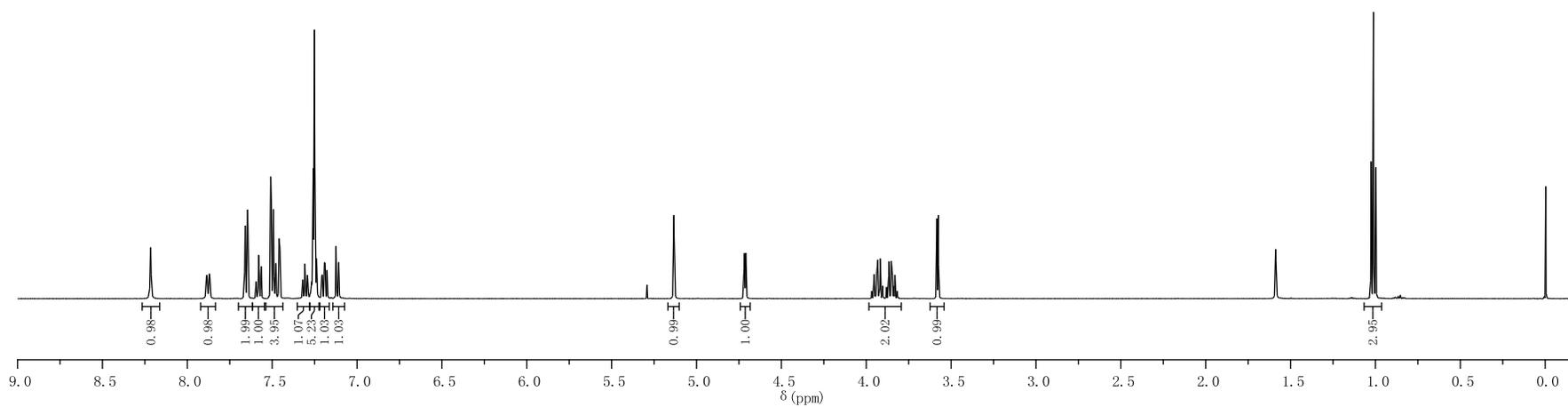
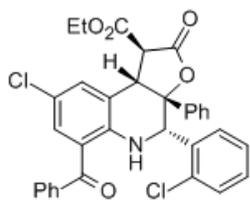
3.9392
3.9249
3.9034
3.8667
3.8525
3.8382
3.8167
3.5834
3.5753

1.5879

1.0261
1.0118
0.9975

0.0030

¹H NMR
500 MHz, CDCl₃



Compound 4g

197.74

169.58

166.10

147.01

139.04

138.70

133.42

130.78

129.19

128.22

123.58

121.60

120.39

87.67

77.30

77.05

76.80

62.58

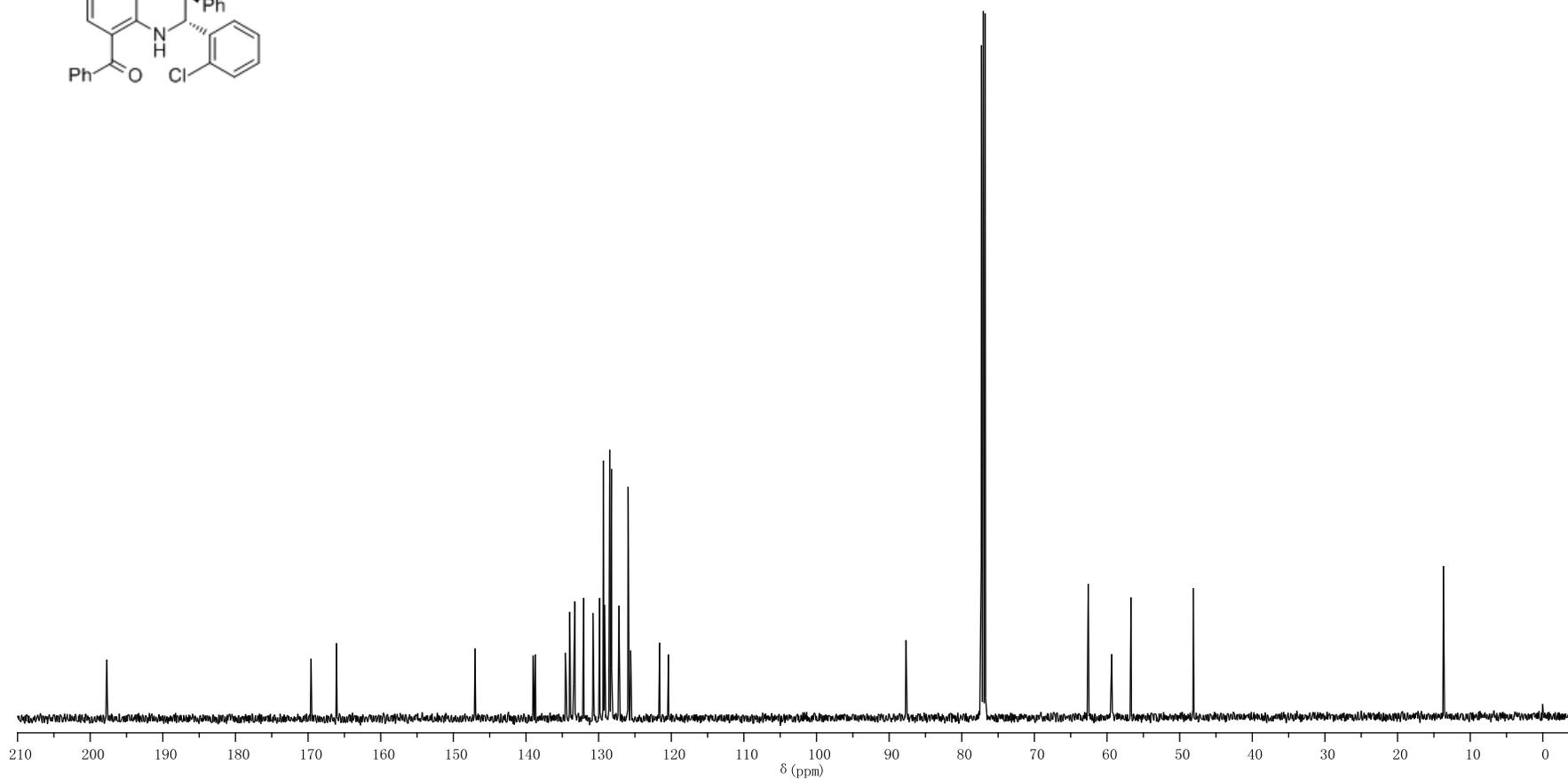
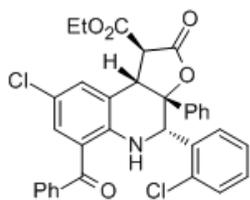
59.36

56.71

48.13

13.68

¹³C NMR
125 MHz, CDCl₃



Compound 4h

8.3547
8.0395
8.0361
8.0119
8.0172
7.5950
7.5237
7.4971
7.4508
7.3122
7.2608
7.2593
7.2589
7.2534
7.2497
7.1867
7.1838
7.1787
7.1739
7.1694
7.1666
7.1639
7.1614
7.1594

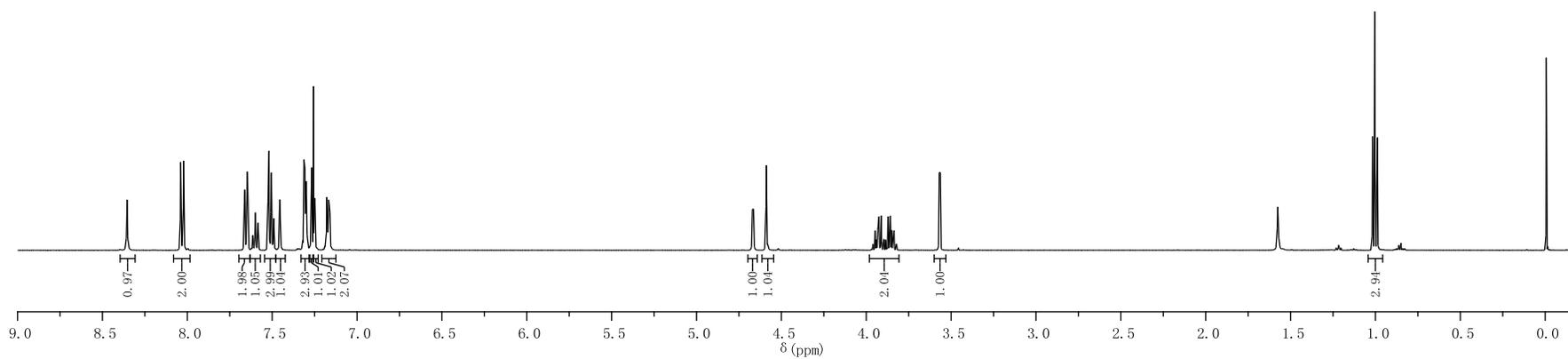
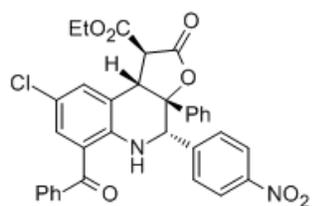
4.6708
4.6641
4.5885
3.9325
3.8967
3.8717
3.8574
3.8431
3.8216
3.5701
3.5634

1.5752

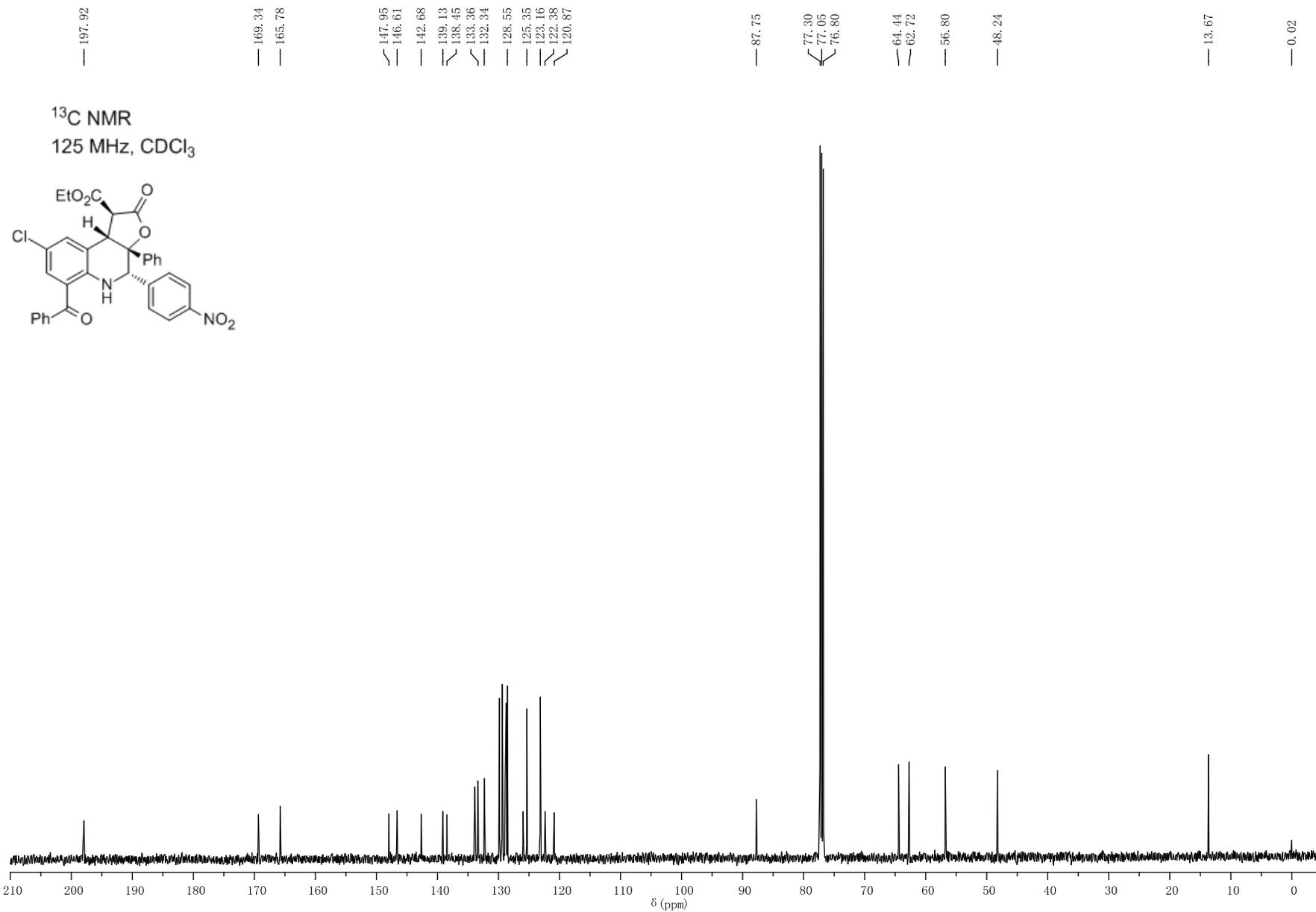
1.0171
1.0028
0.9885

-0.0064

¹H NMR
500 MHz, CDCl₃



Compound 4h



Compound 4i

8.3789
8.1160
8.1116
8.0995
8.0952
7.8526
7.6104
7.5857
7.5177
7.4603
7.4068
7.3094
7.3045
7.2977
7.2916
7.2838
7.2571
7.1830
7.1745
7.1677
7.1638
7.1606
7.1553

5.2941

4.6847
4.6784
4.5914

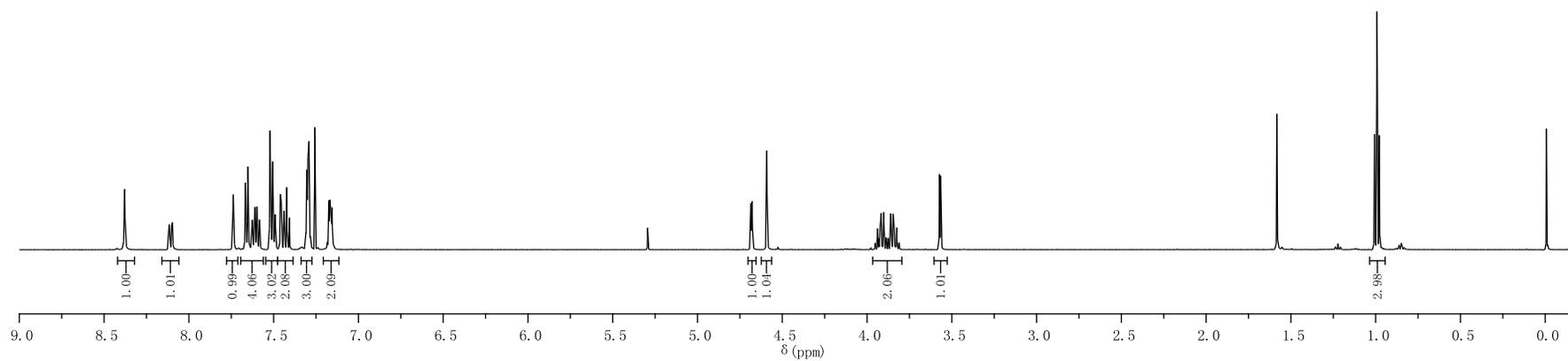
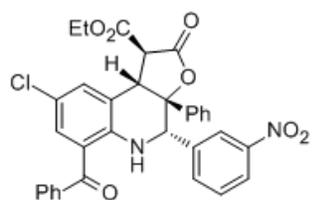
3.9238
3.8879
3.8611
3.8468
3.8326
3.8110
3.5728
3.5663

1.5829

1.0070
0.9927
0.9785

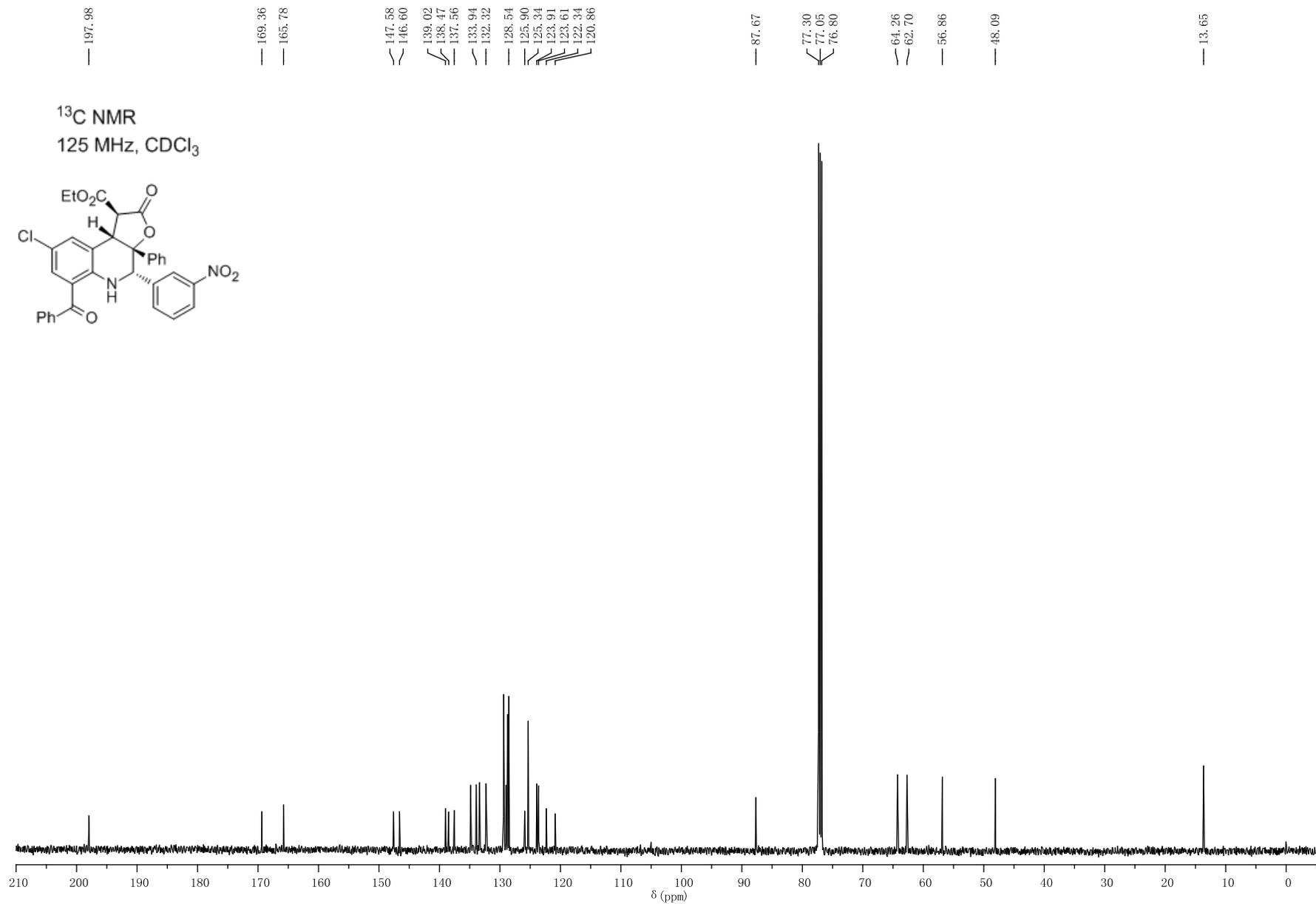
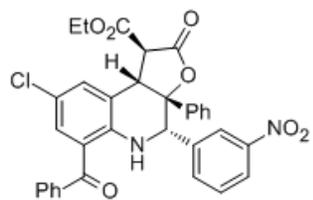
-0.0072

¹H NMR
500 MHz, CDCl₃

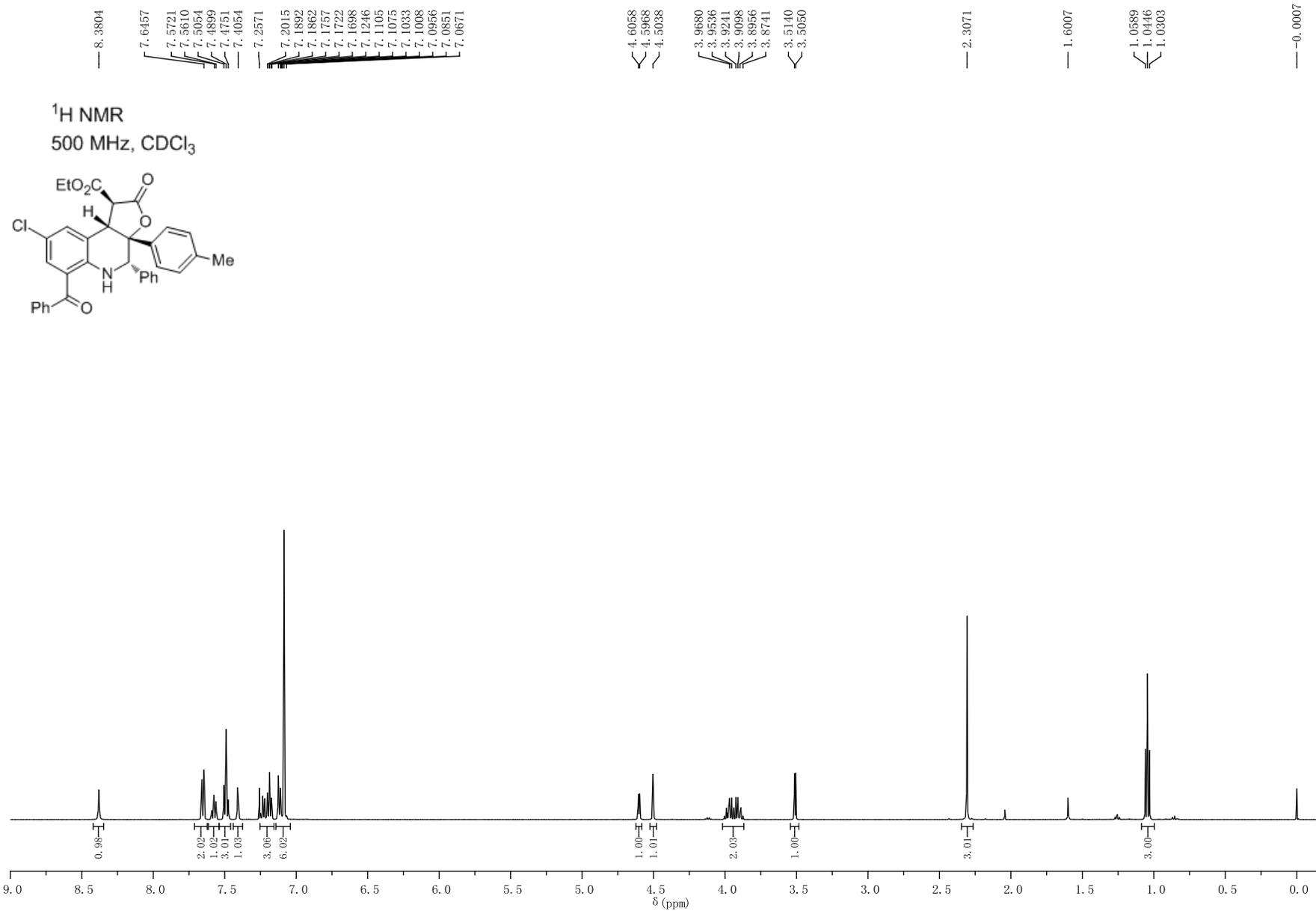


Compound 4i

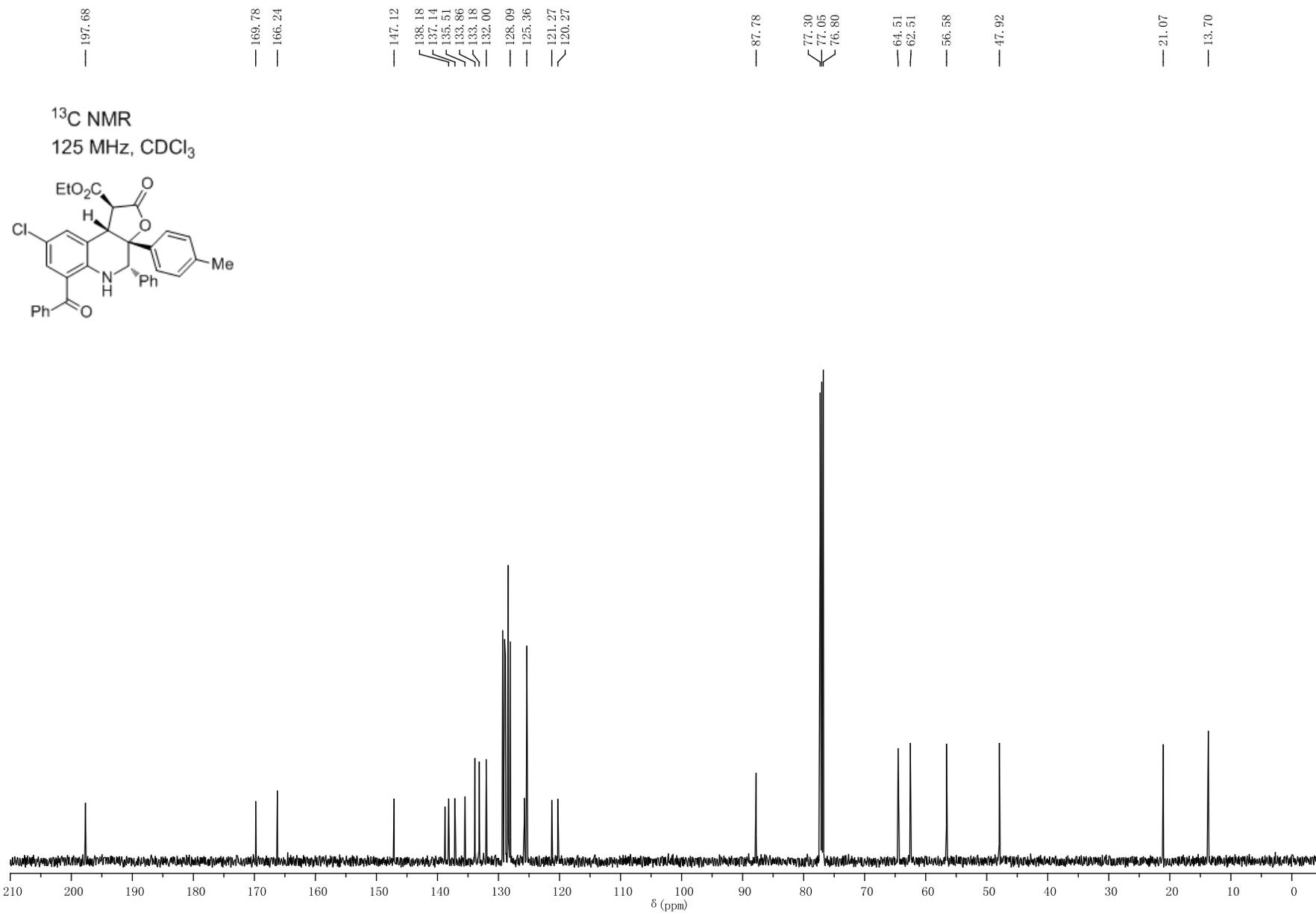
¹³C NMR
125 MHz, CDCl₃



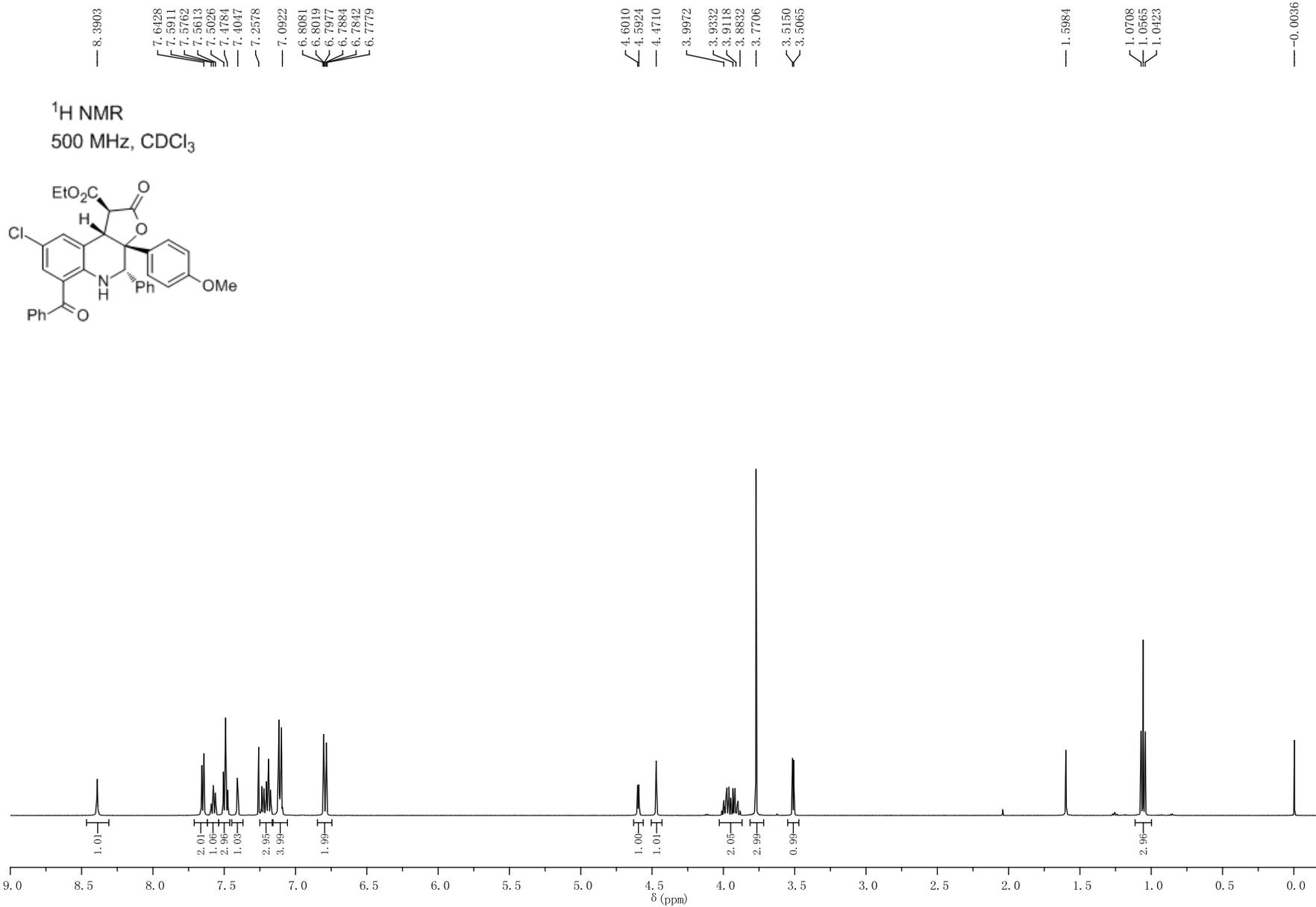
Compound 4j



Compound 4j



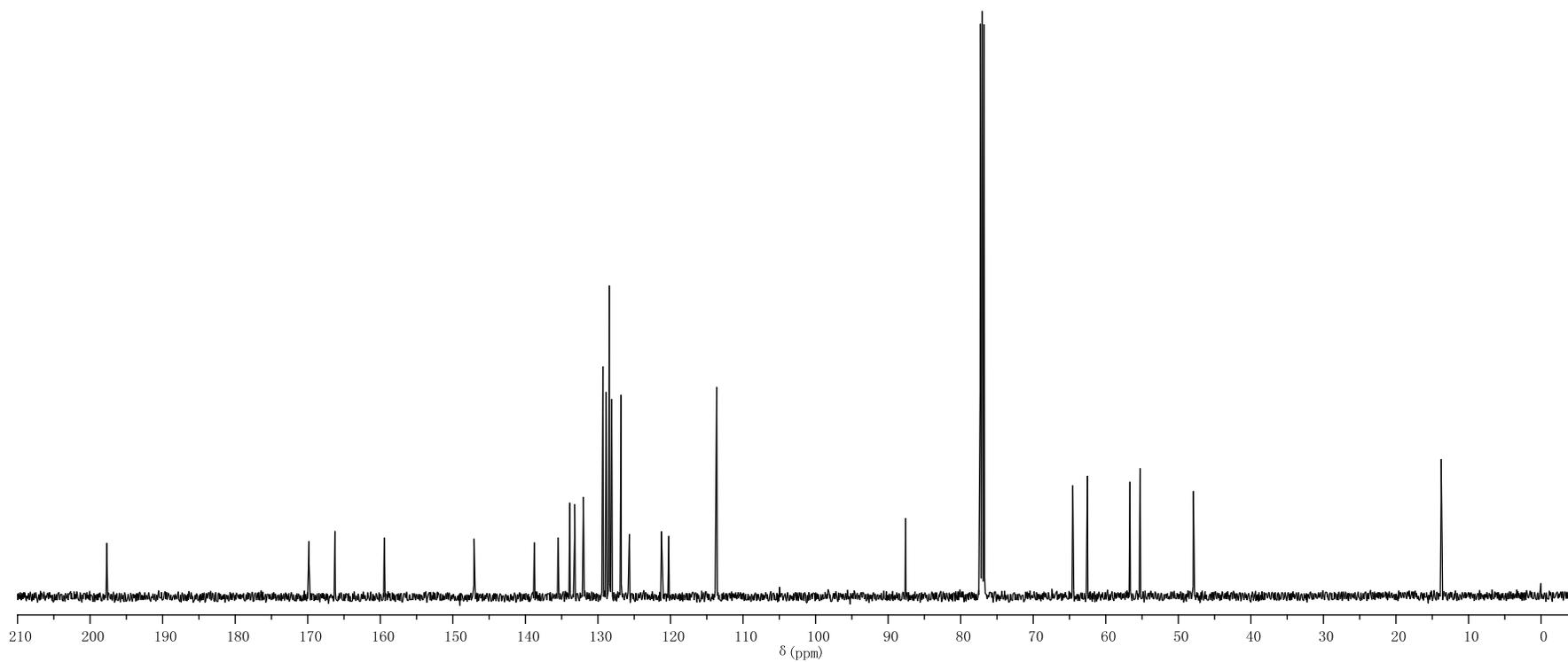
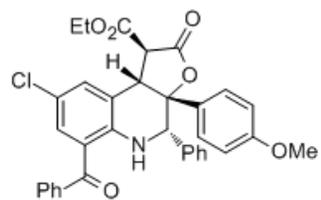
Compound 4k



Compound 4k

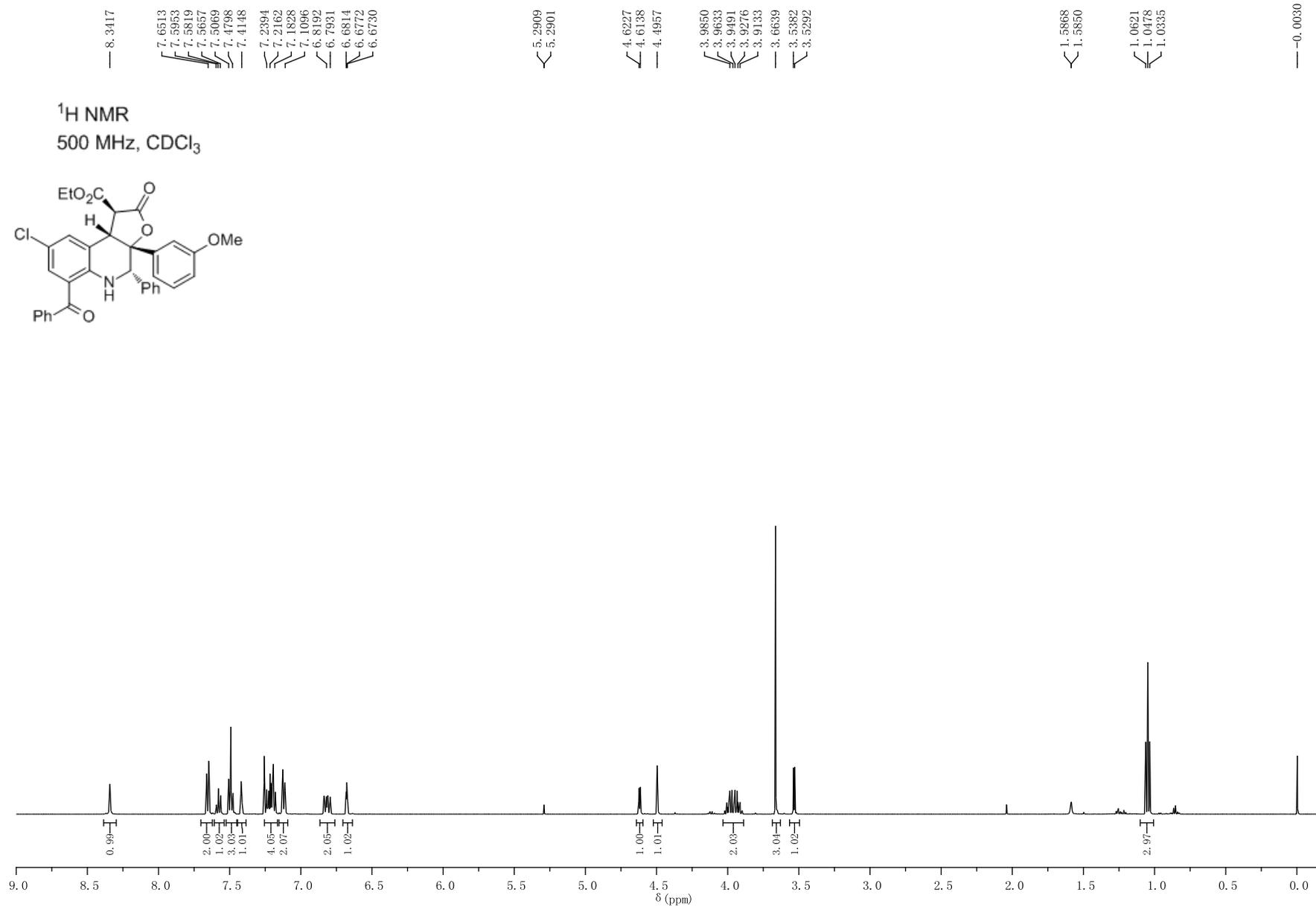
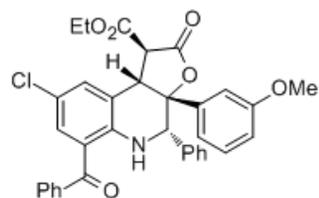


¹³C NMR
125 MHz, CDCl₃



Compound 4l

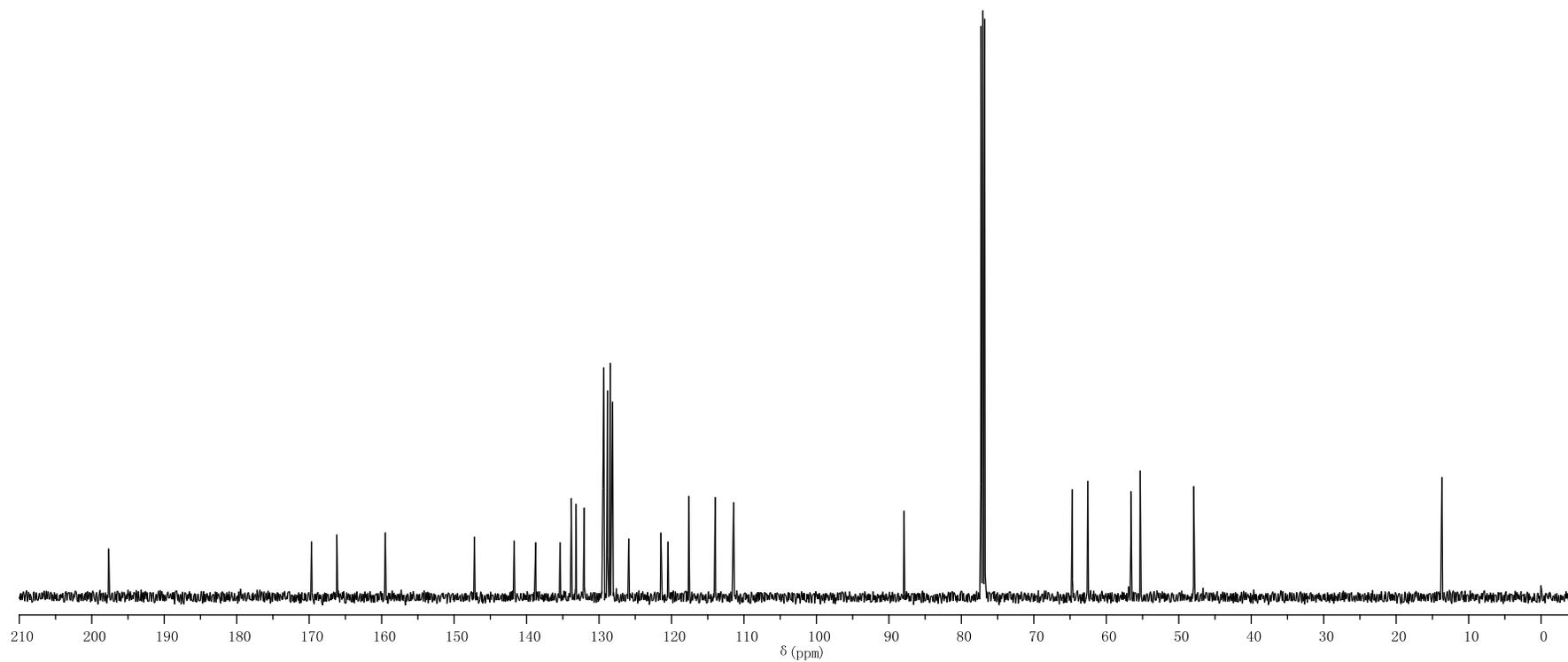
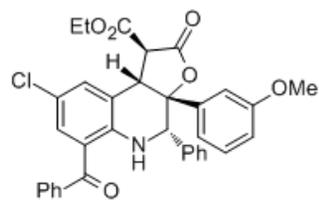
¹H NMR
500 MHz, CDCl₃



Compound 4l



¹³C NMR
125 MHz, CDCl₃



Compound 4m

8.2520
7.5879
7.5706
7.5533
7.4730
7.3504
7.2414
7.1832
7.1662
7.1221
7.0729
6.8923
6.7316
6.7239
6.7163
6.7150
6.7013
6.6995

4.9770
4.8729
4.8671

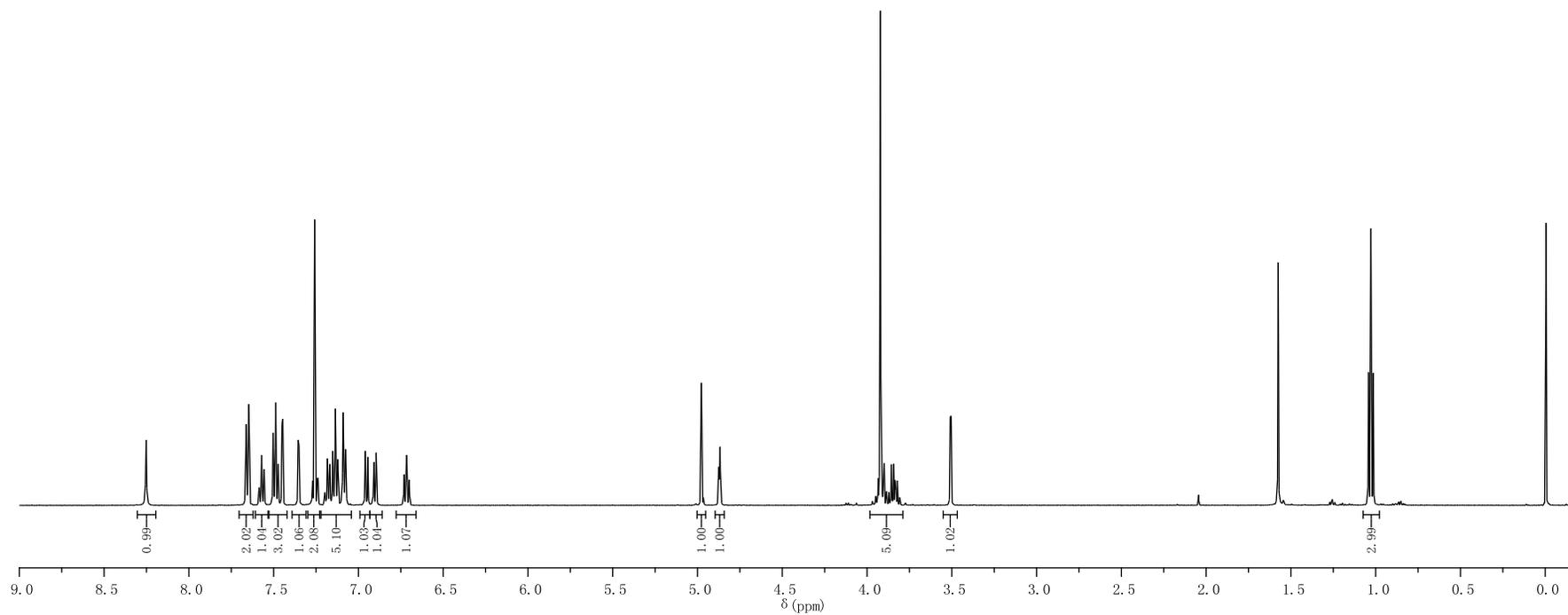
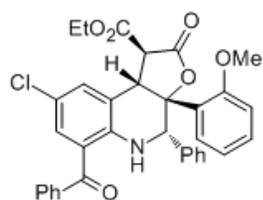
3.9207
3.8568
3.8495
3.8426
3.8354
3.8282
3.8211
3.8068
3.5096
3.5038

1.5751

1.0423
1.0280
1.0137

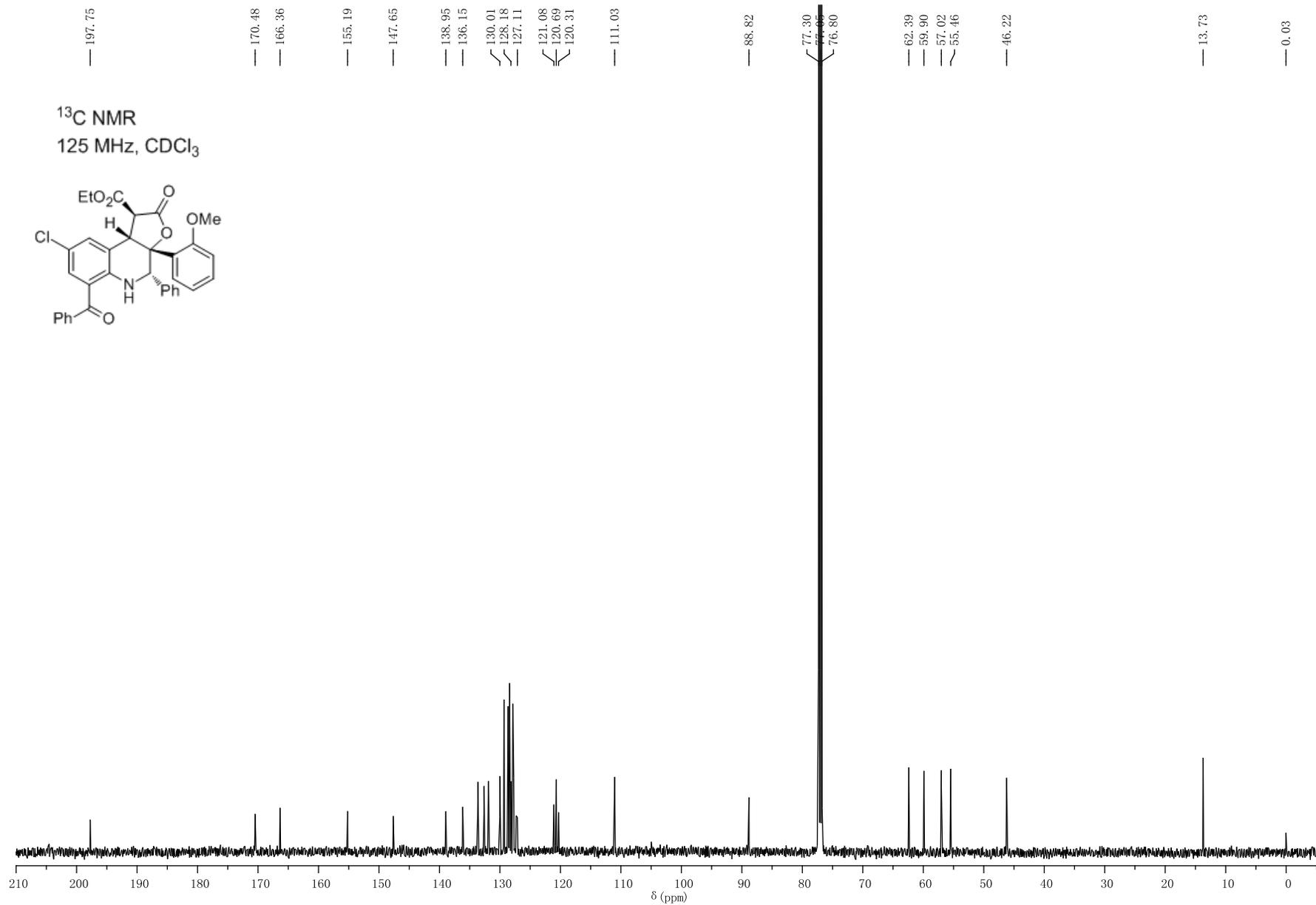
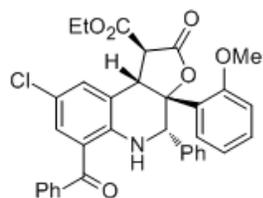
-0.0053

¹H NMR
500 MHz, CDCl₃



Compound 4m

¹³C NMR
125 MHz, CDCl₃



Compound 4n

8.2961
7.6573
7.5917
7.5754
7.5132
7.4859
7.4212
7.2865
7.1710
6.9695
6.9525

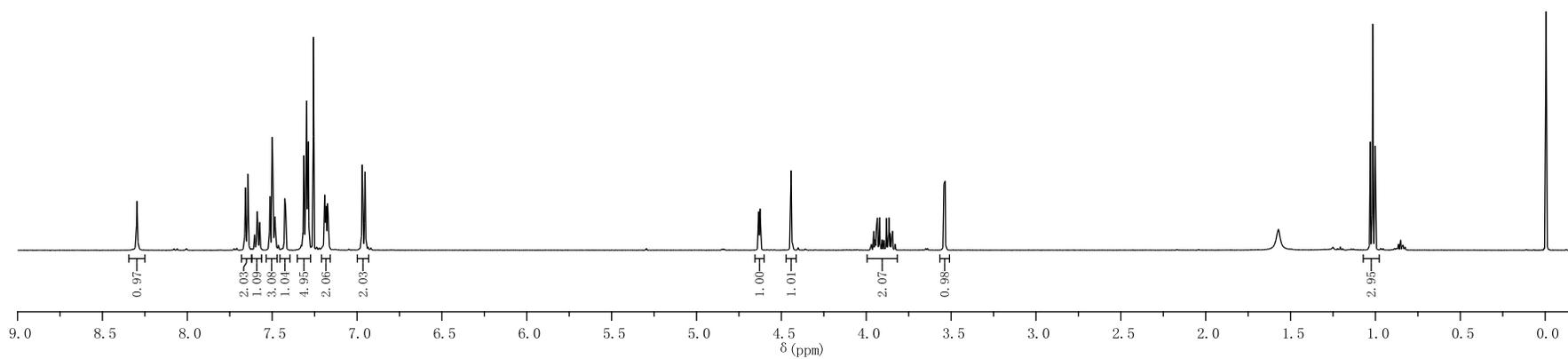
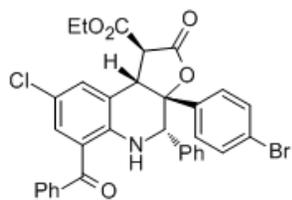
4.6330
4.6256
4.4428
3.9418
3.9061
3.8806
3.8663
3.8521
3.8306
3.5422
3.5347

1.5721

1.0304
1.0161
1.0019

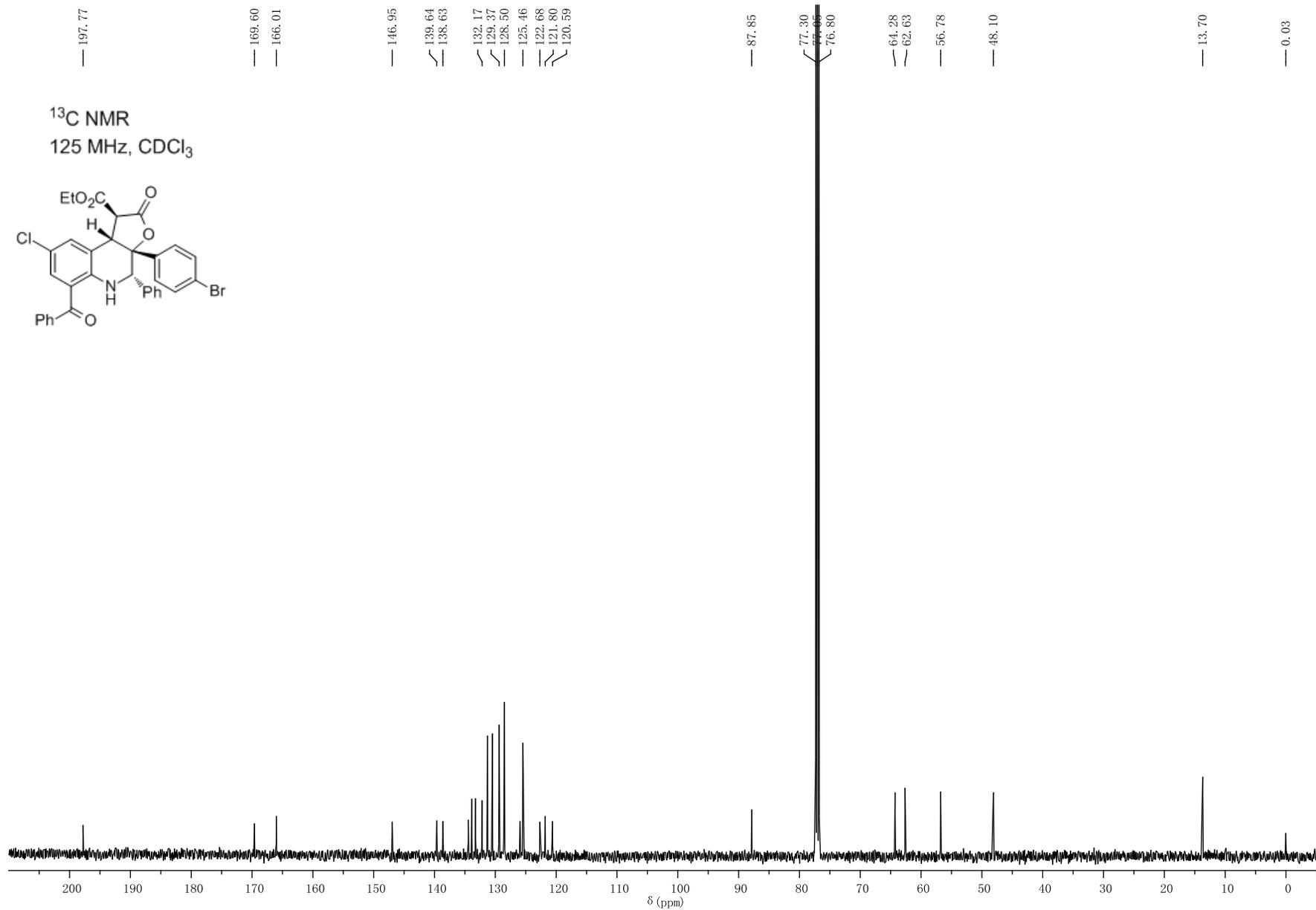
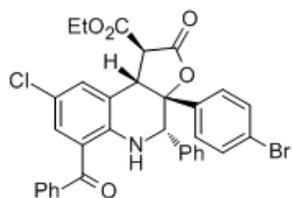
-0.0051

¹H NMR
500 MHz, CDCl₃



Compound 4n

^{13}C NMR
125 MHz, CDCl_3



Compound 4o

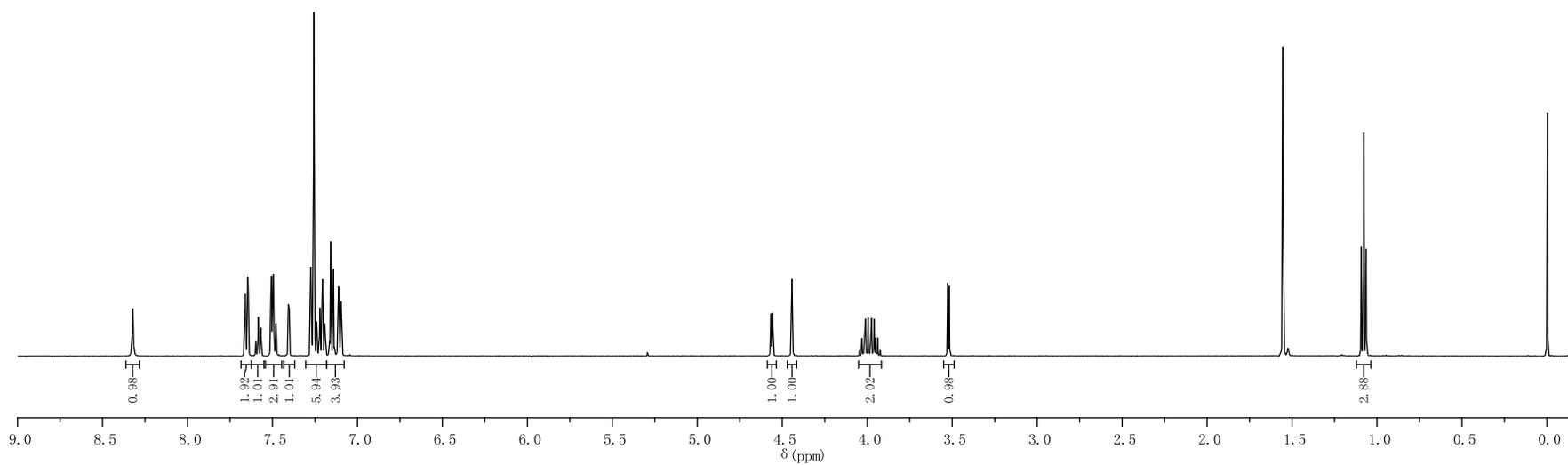
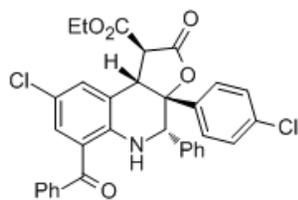
8.3213
7.6153
7.5976
7.5827
7.5678
7.5056
7.4821
7.2970
7.2211
7.2088
7.2057
7.1951
7.1917
7.1892
7.1632
7.1581
7.1540
7.1446
7.1408
7.1354
7.1107
7.0965
7.0936

4.5661
4.5571
4.4427
4.0166
3.9885
3.9743
3.9600
3.9458
3.9242
3.5260
3.5169

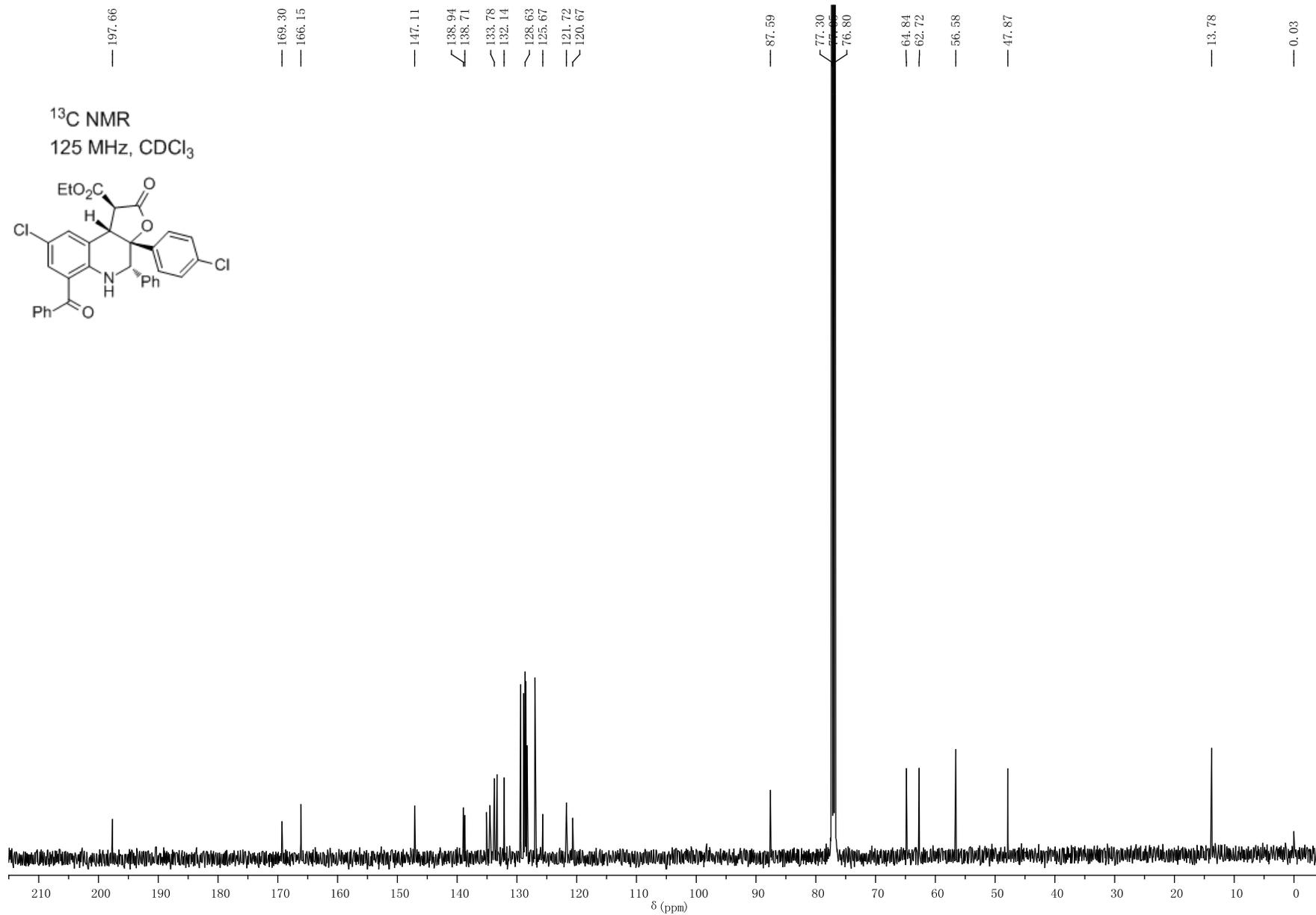
1.5543
1.0922
1.0780
1.0637

-0.0031

¹H NMR
500 MHz, CDCl₃



Compound 4o



Compound 4p

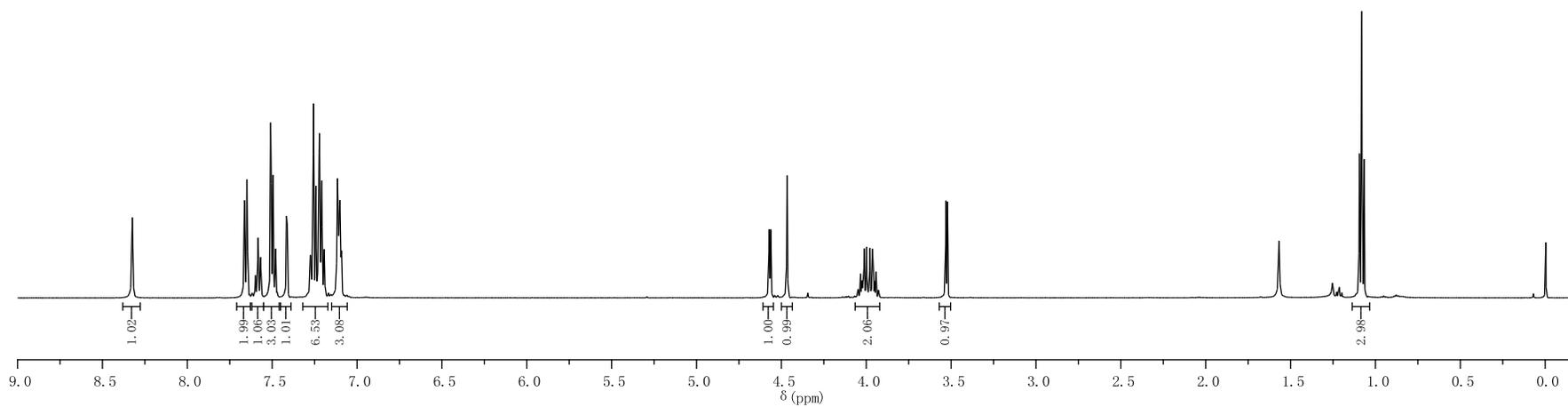
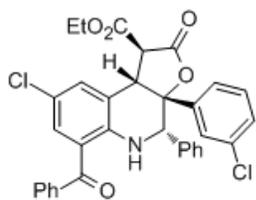
8.3237
7.5095
7.5047
7.4944
7.4795
7.4719
7.4155
7.4111
7.2751
7.2725
7.2622
7.2565
7.2427
7.2267
7.2219
7.2110
7.2075
7.1934
7.1156
7.1060
7.1013
7.0942
7.0913

4.5714
4.5623
4.4659
4.0195
3.9924
3.9781
3.9639
3.9496
3.9281
3.5305
3.5215

1.5681
1.2529
1.0945
1.0802
1.0660

-0.0034

¹H NMR
500 MHz, CDCl₃



Compound 4p

197.64

169.25

166.08

147.08

142.43

138.68

133.79

132.13

128.28

125.78

125.59

123.72

121.73

120.67

87.44

77.30

77.05

76.80

64.75

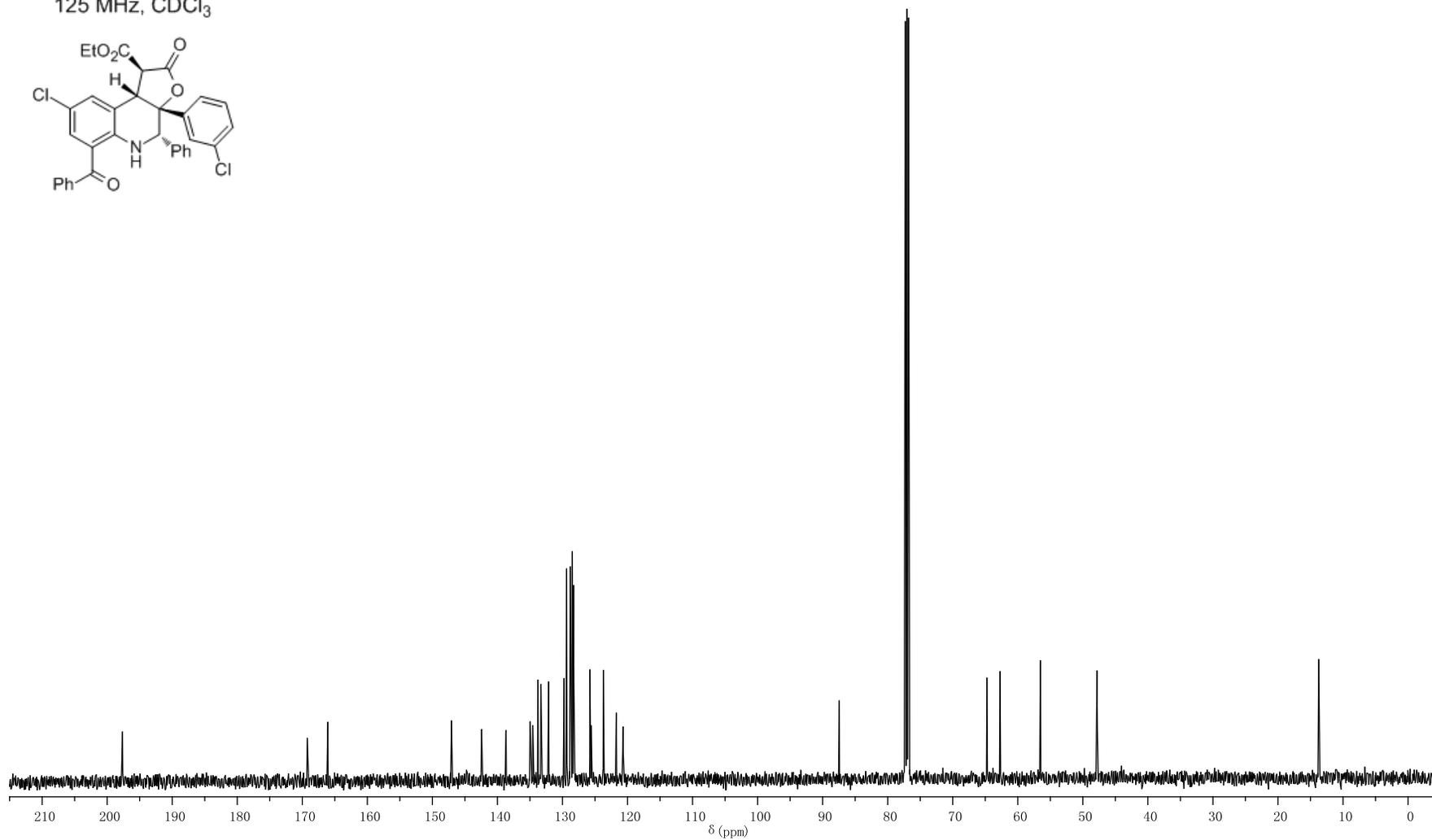
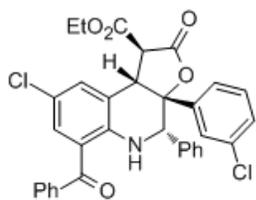
62.73

56.52

47.82

13.74

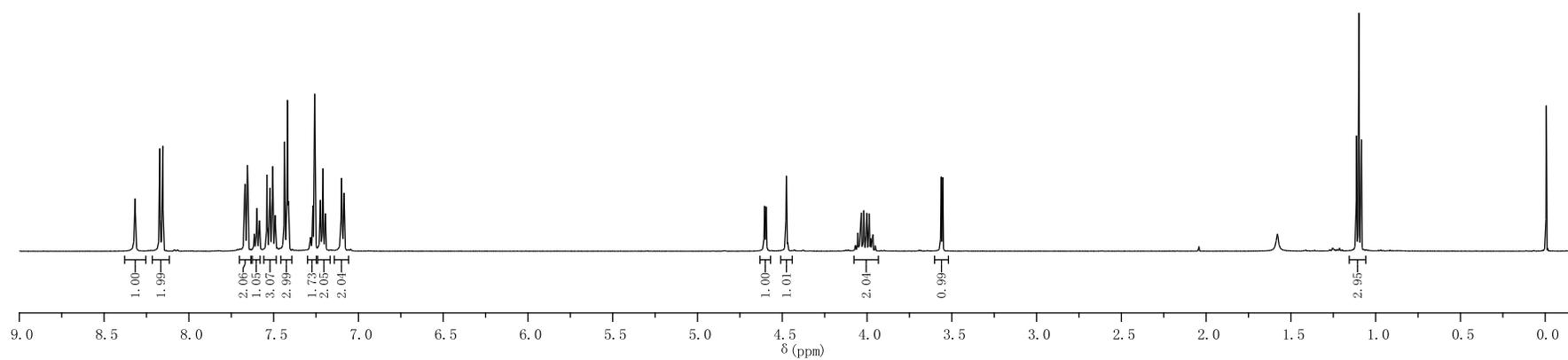
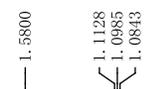
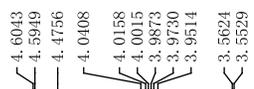
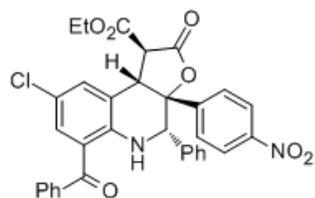
¹³C NMR
125 MHz, CDCl₃



Compound 4q

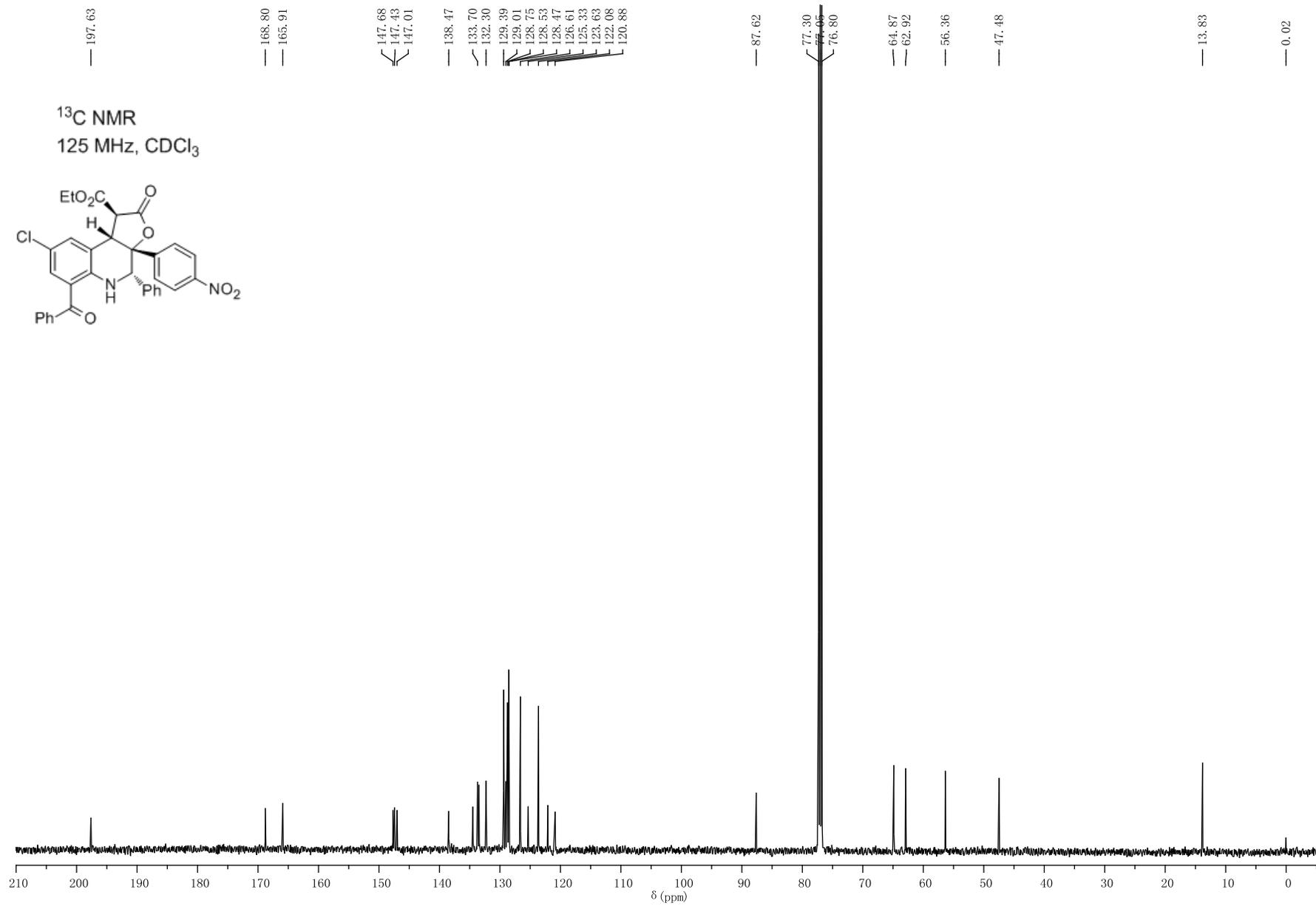
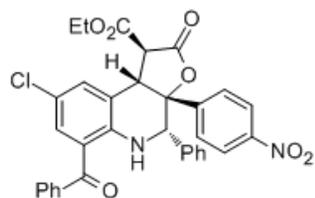


¹H NMR
500 MHz, CDCl₃



Compound 4q

^{13}C NMR
125 MHz, CDCl_3



Compound 4r

8.3367
8.1681
8.1546
7.6562
7.5360
7.5149
7.4821
7.4482
7.4251
7.2715
7.2569
7.2425
7.2184
7.2080
7.1886
7.1103
7.0955

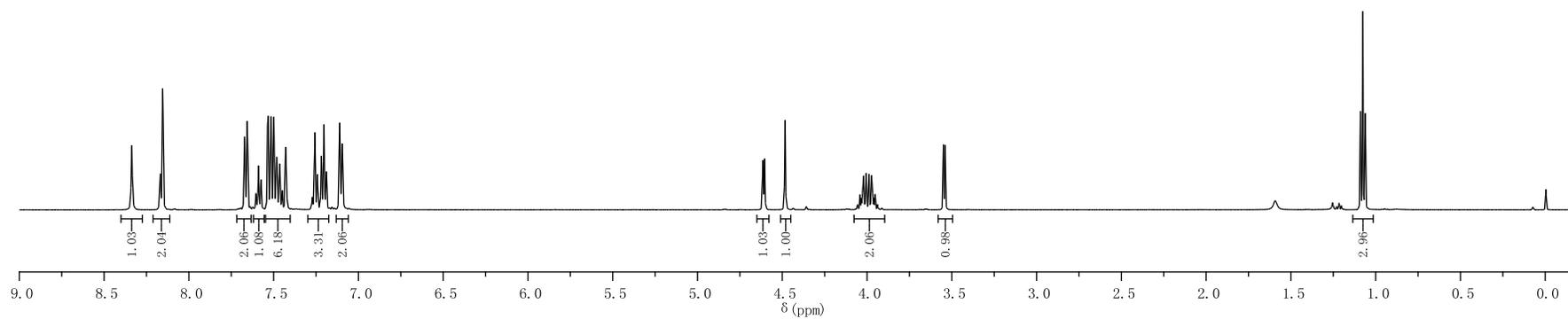
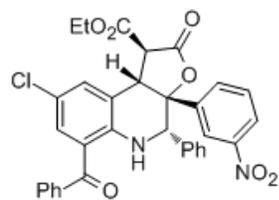
4.6142
4.6048
4.4832
4.0273
4.0130
3.9880
3.9737
3.9594
3.9378
3.5493
3.5399

1.5927

1.0899
1.0756
1.0614

-0.0044

¹H NMR
500 MHz, CDCl₃



Compound 4r

197.62

168.76
165.93

148.20
146.89

142.80

138.54

133.75

128.98

128.44

125.19

123.41

122.04

120.84

120.51

87.17

77.29
77.04
76.78

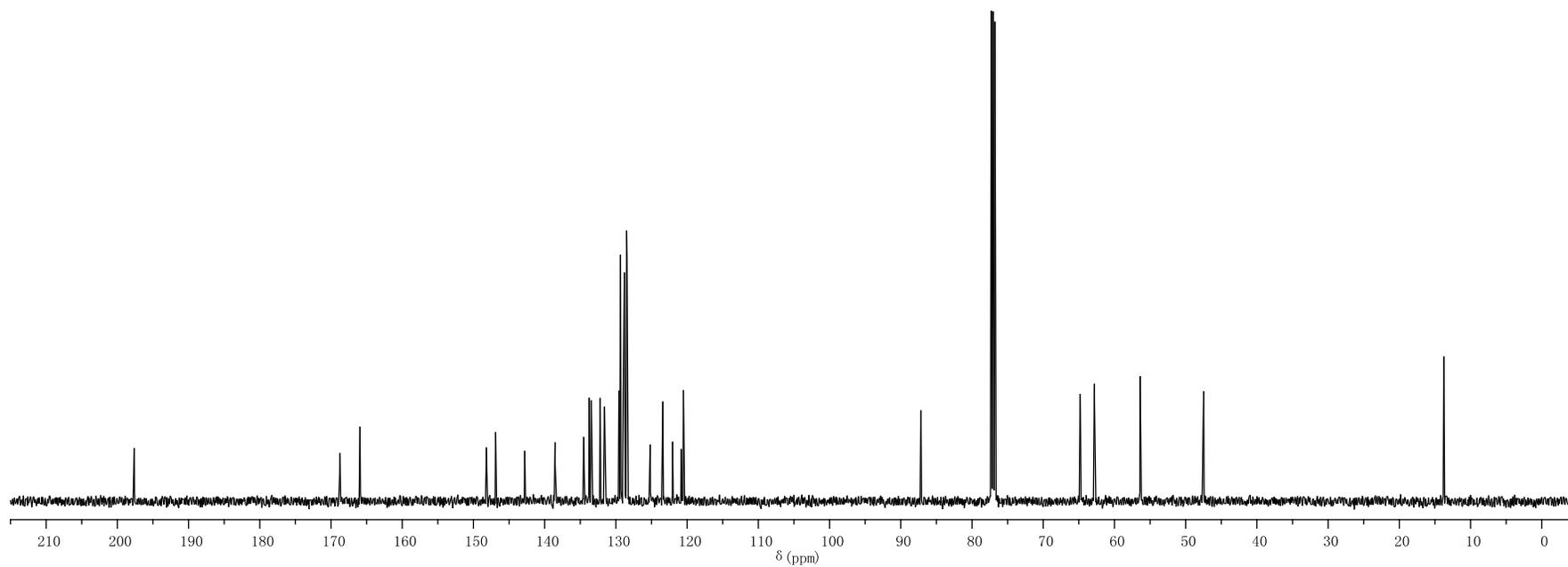
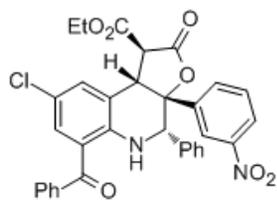
64.80
62.81

56.39

47.48

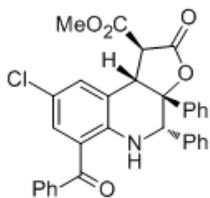
13.75

¹³C NMR
125 MHz, CDCl₃



Compound 4s

¹H NMR
500 MHz, CDCl₃



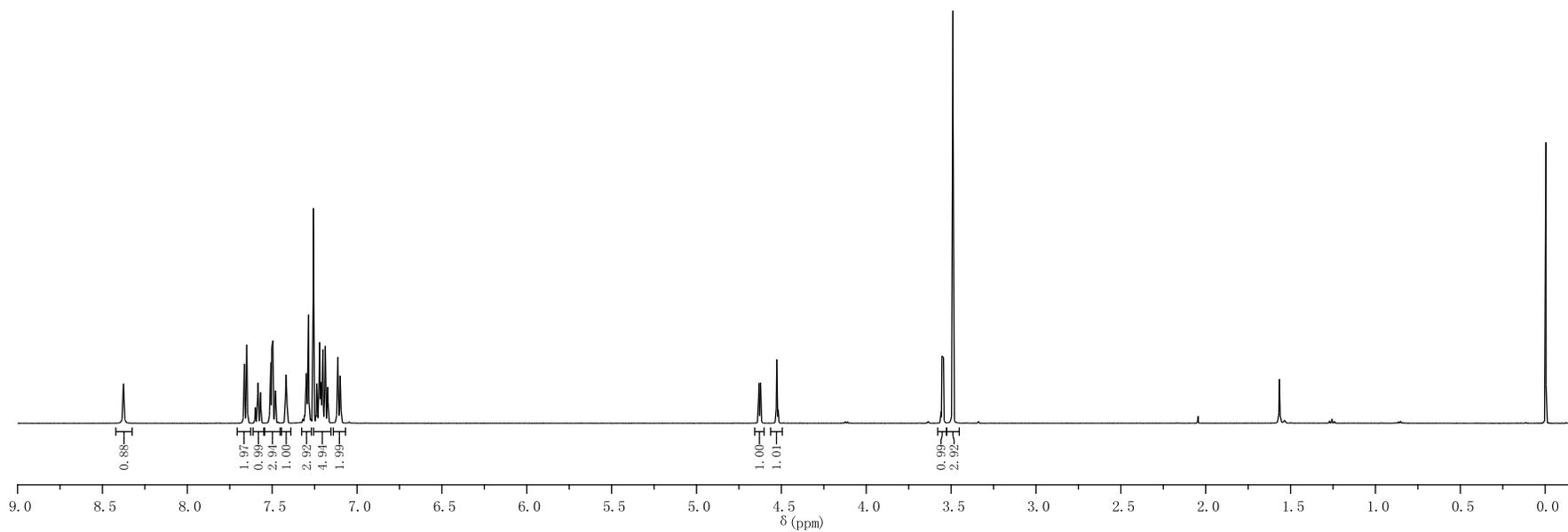
8.3762
7.6497
7.5984
7.5836
7.5687
7.5070
7.4845
7.4146
7.2574
7.2228
7.2204
7.2145
7.2118
7.2046
7.2013
7.1898
7.1868
7.1761
7.1727
7.1703
7.1135
7.0993
7.0964

4.6320
4.6226
4.5268

3.5539
3.5445
3.4891

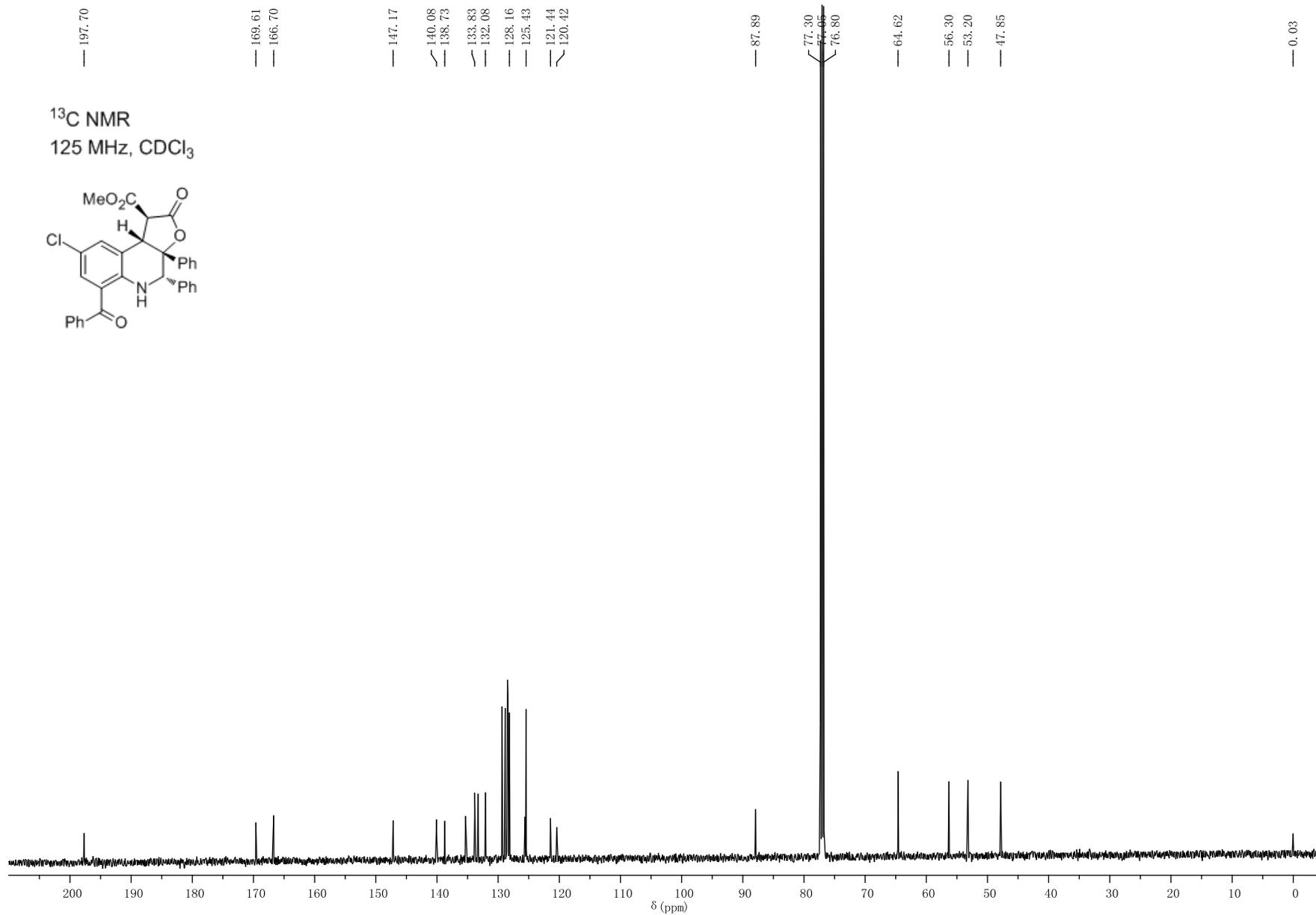
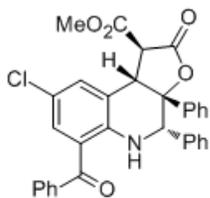
1.5663

-0.0042



Compound 4s

¹³C NMR
125 MHz, CDCl₃



Compound 4t

8.5000
7.6692
7.6550
7.6523
7.5335
7.4396
7.2622
7.2360
7.2086
7.1240
6.8170
6.8017
6.7862

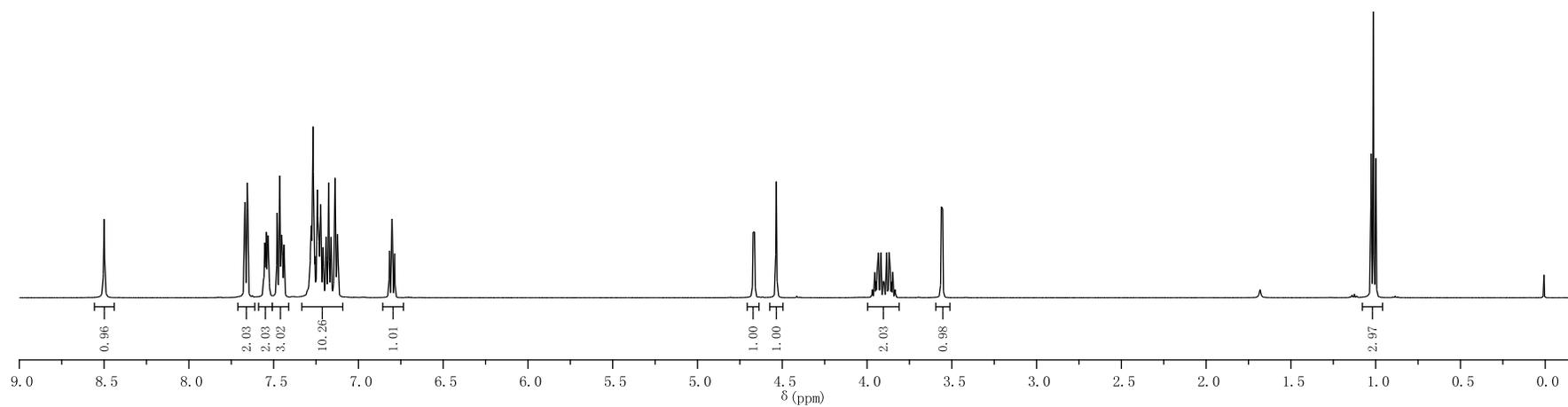
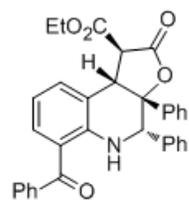
4.6717
4.6633
4.5354
3.9404
3.9046
3.8840
3.8697
3.8555
3.8340
3.5618
3.5533

1.6819

1.0271
1.0128
0.9985

0.0071

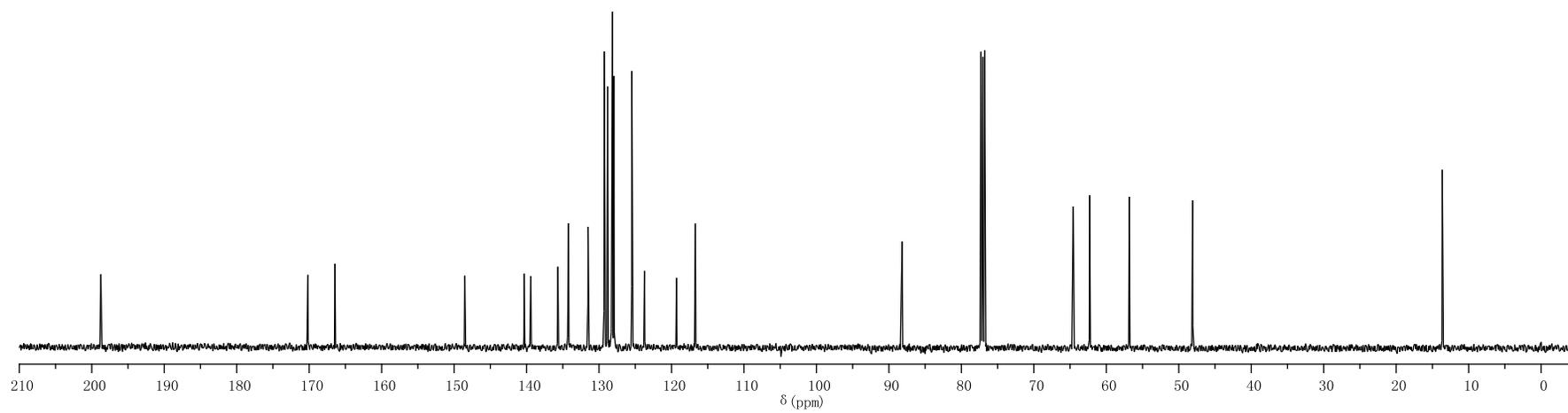
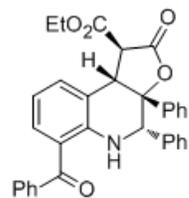
¹H NMR
500 MHz, CDCl₃



Compound 4t

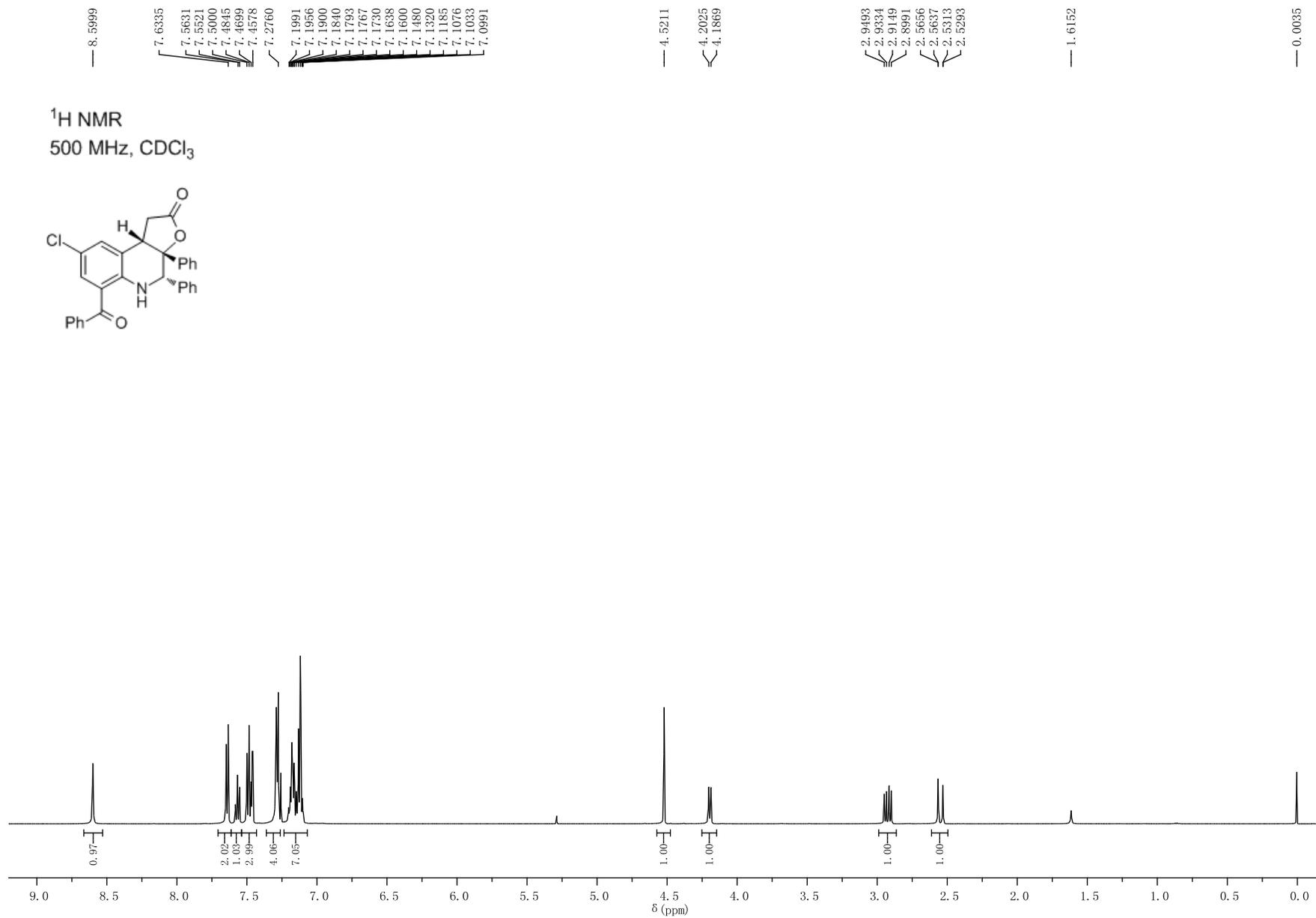


¹³C NMR
125 MHz, CDCl₃



IV. Copies of NMR spectra for 5s, 6s

Compound 5s



Compound 5s

197.87
175.00

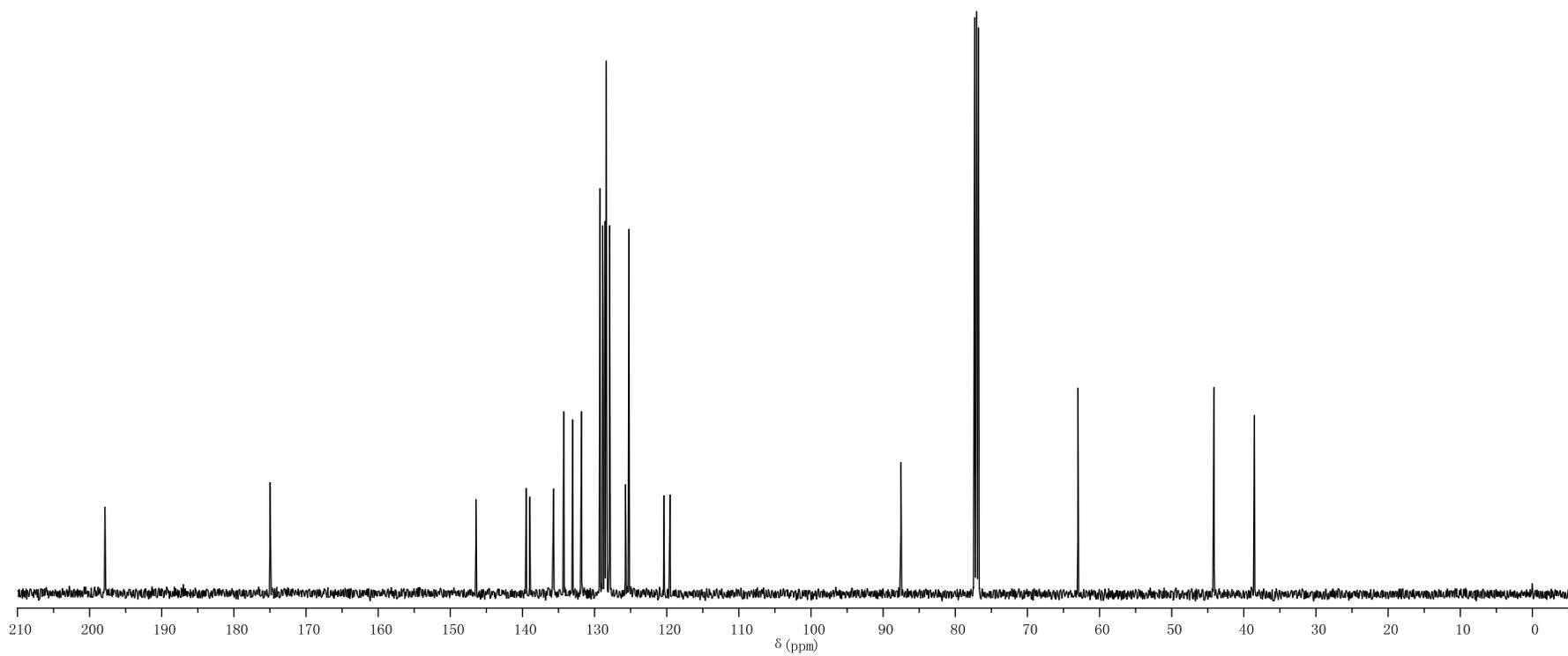
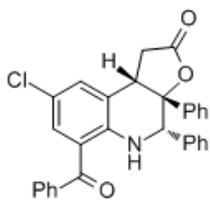
146.45
139.49
138.99
134.28
131.82
127.92
125.23
120.38
119.52

87.53
77.30
77.05
76.80

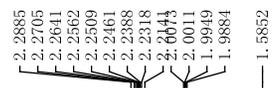
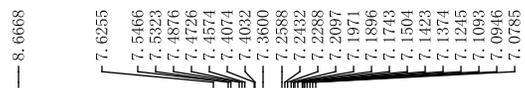
62.99

44.12
38.53

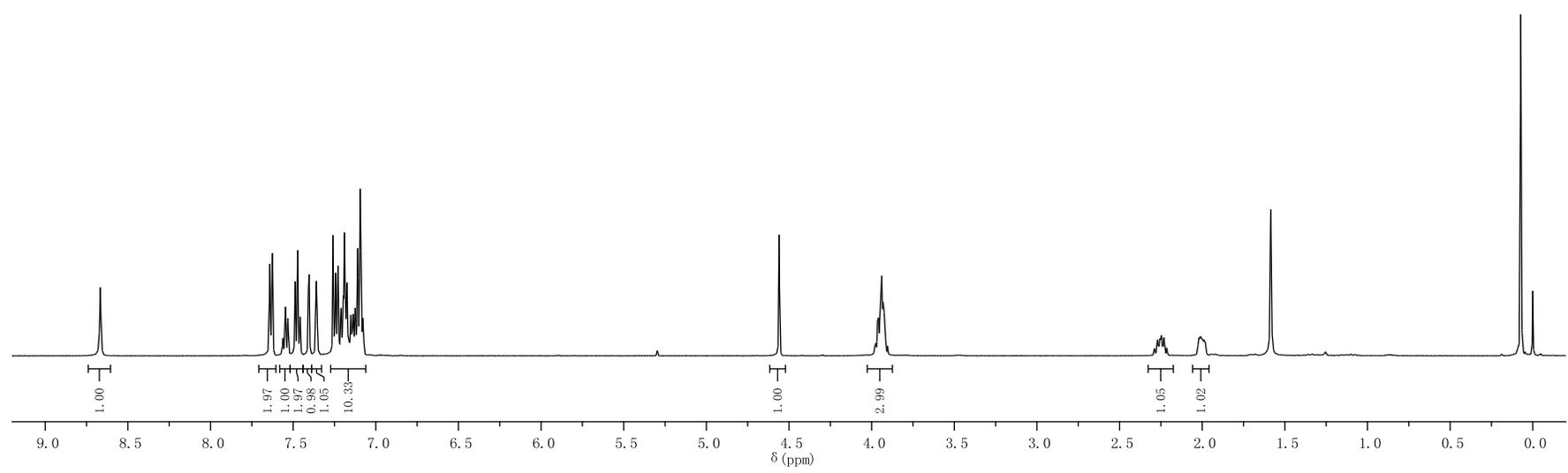
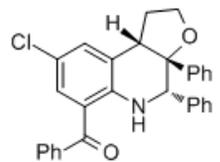
¹³C NMR
125 MHz, CDCl₃



Compound 6s

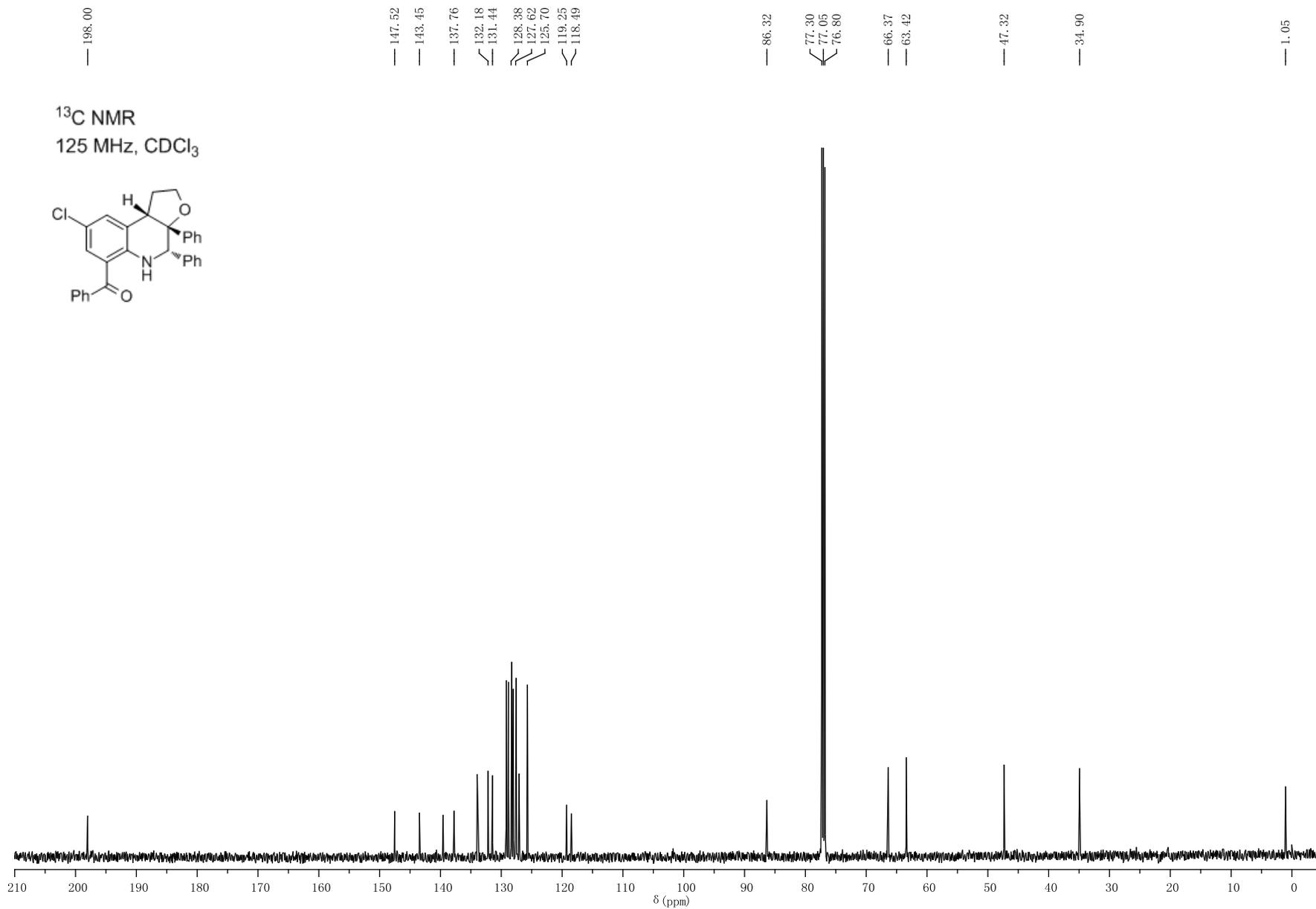
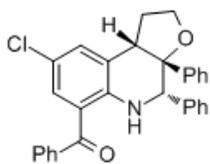


¹H NMR
500 MHz, CDCl₃



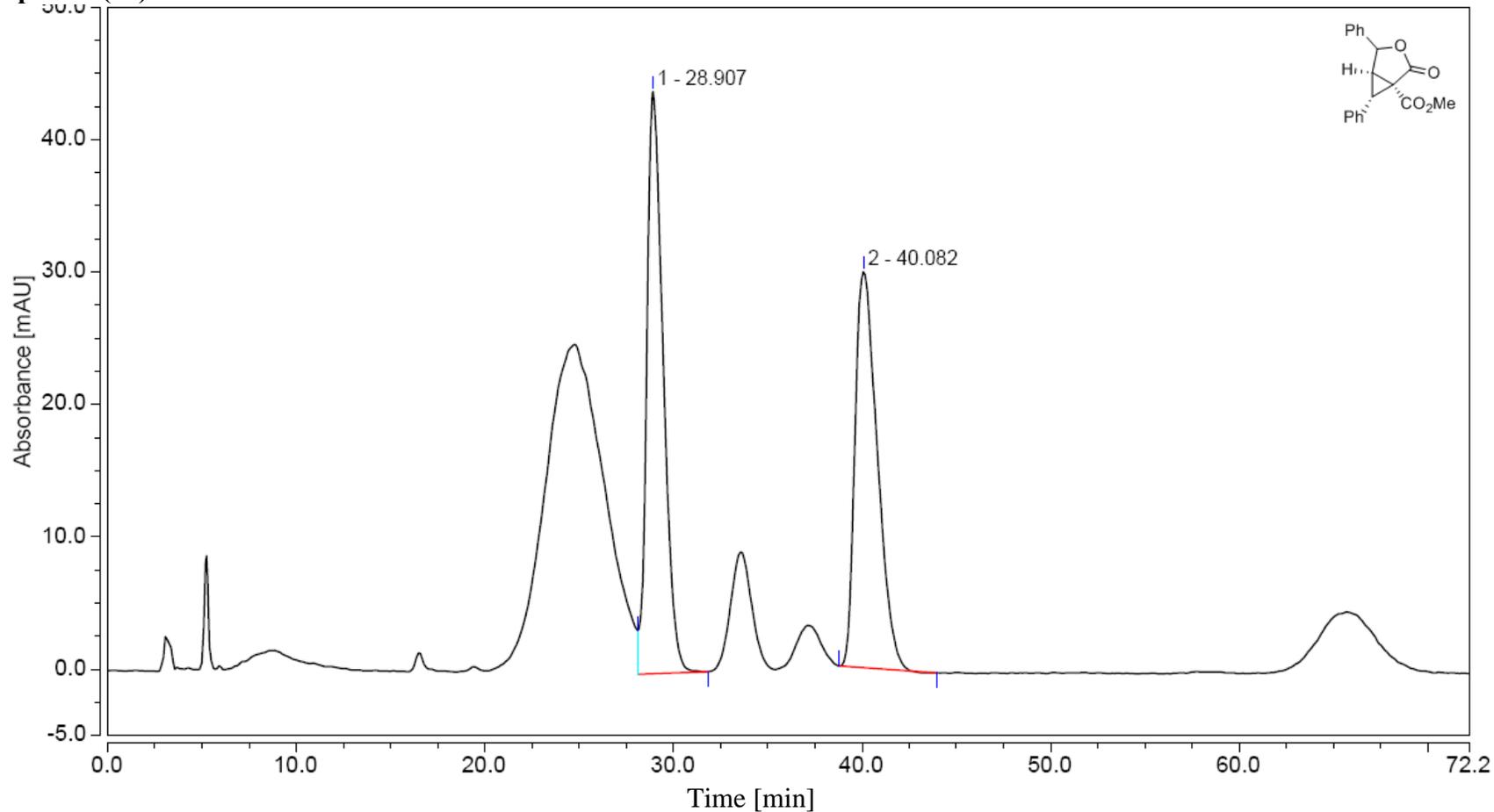
Compound 6s

¹³C NMR
125 MHz, CDCl₃



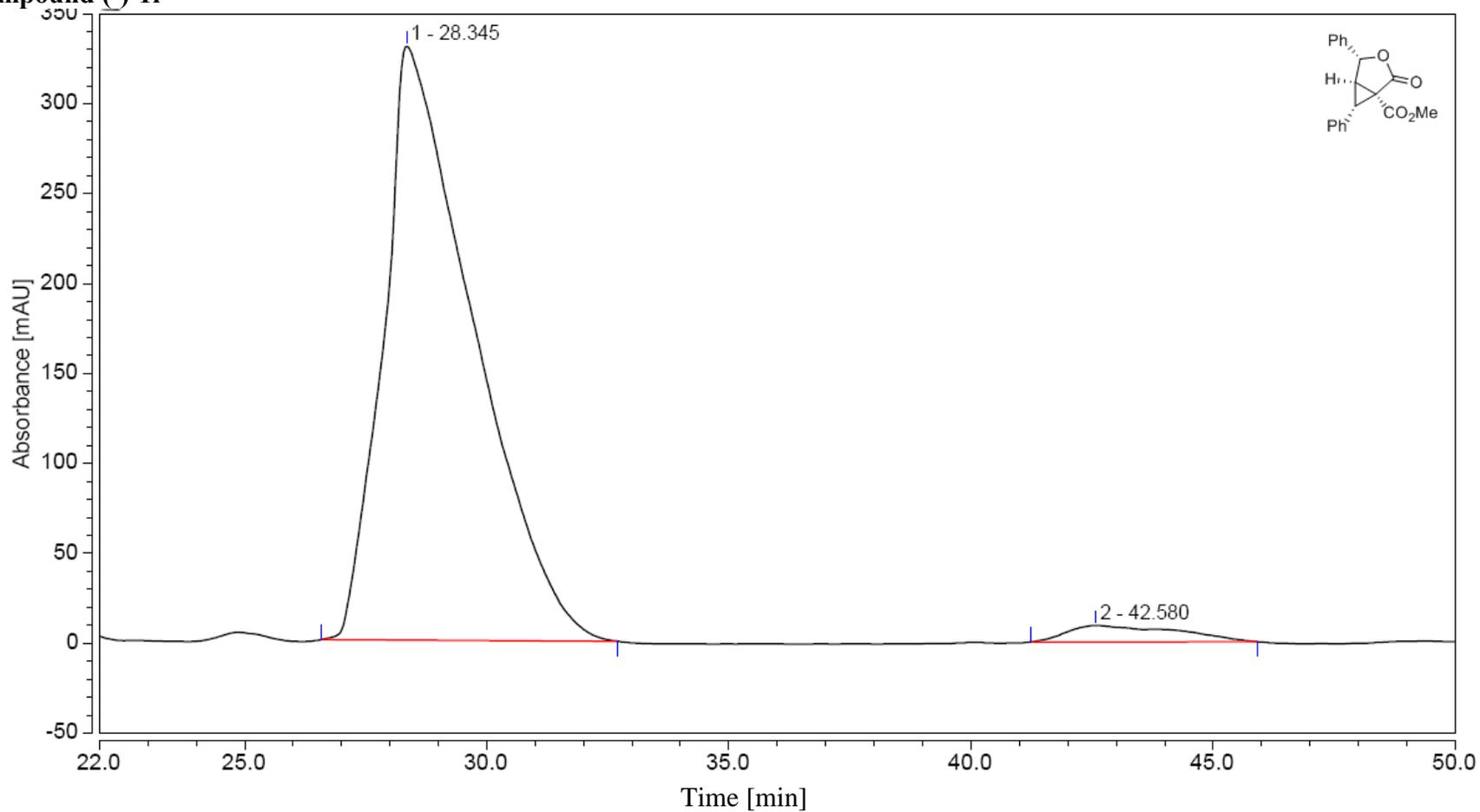
V. HPLC traces for compound 1r, 3ra

Compound (±)-1r



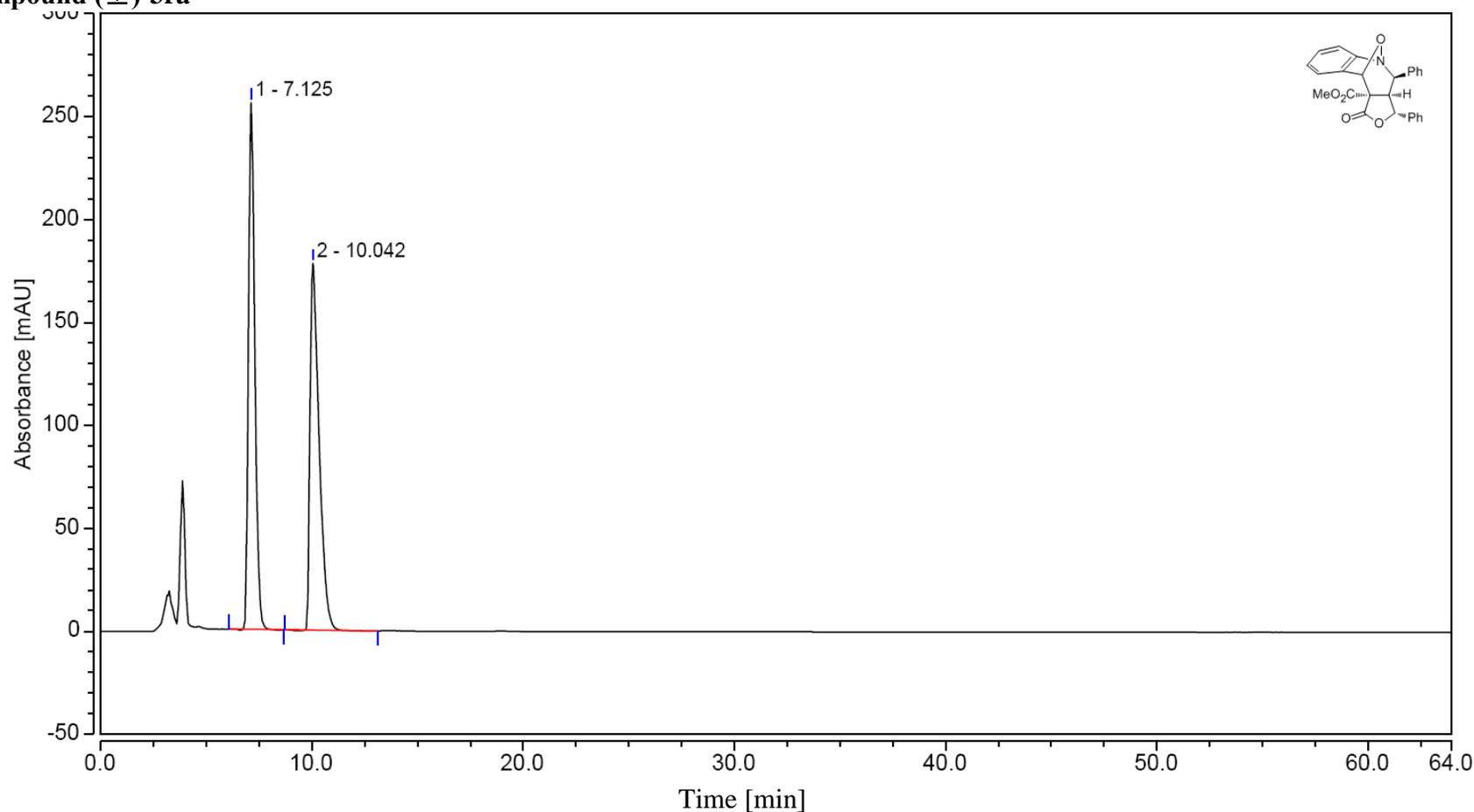
Area Percent Report					
Peak #	RetTime [min]	Area [mAU*min]	Height [mAU]	Area %	Height %
1	28.907	44.189	43.950	51.90	59.49
2	40.082	40.945	29.923	48.10	40.51
Total		85.134	73.873	100.00	100.00

Compound (-)-1r



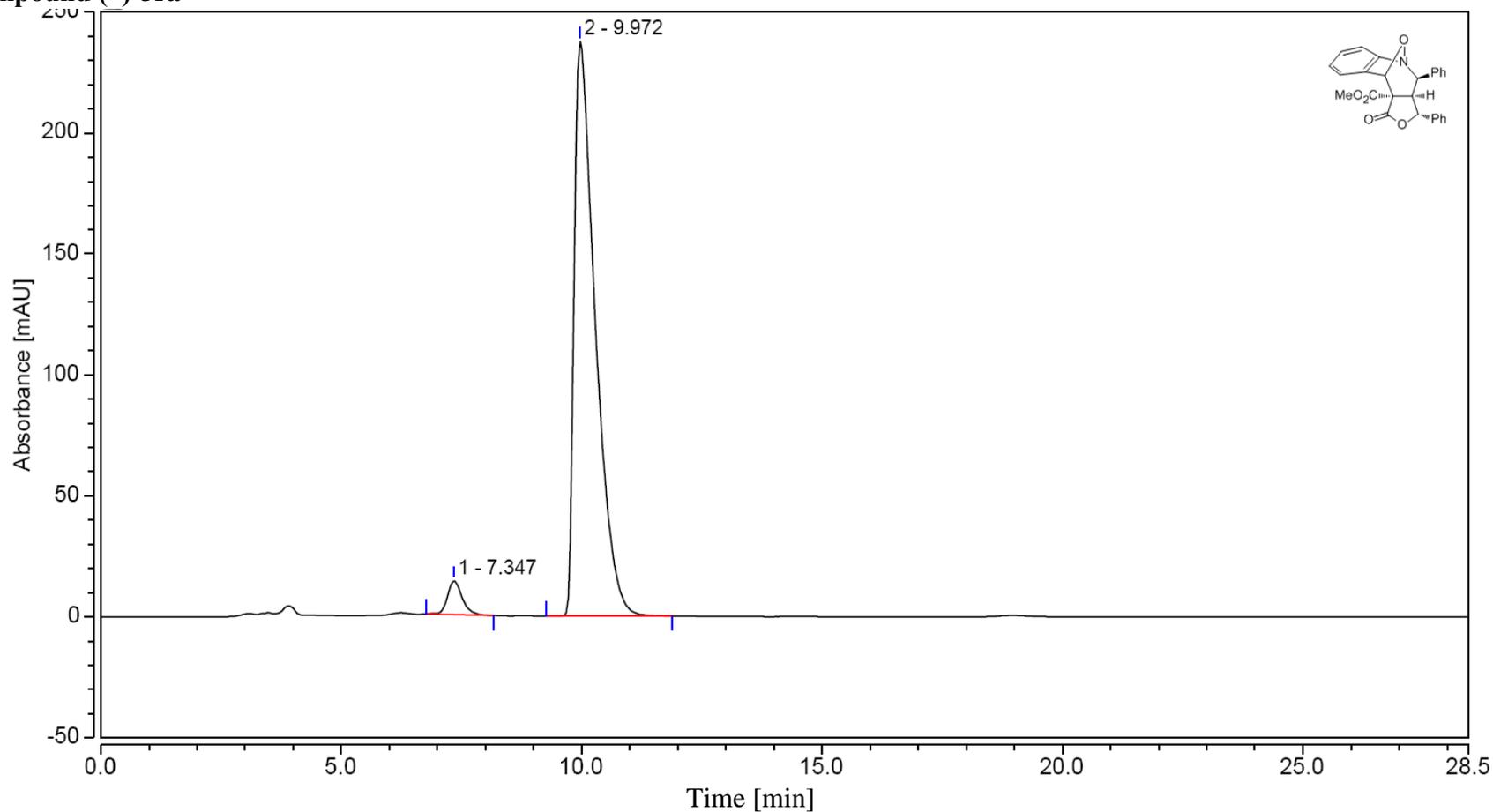
Area Percent Report					
Peak #	RetTime [min]	Area [mAU*min]	Height [mAU]	Area %	Height %
1	28.345	711.428	330.234	96.71	97.31
2	42.580	24.213	9.116	3.29	2.69
Total		735.641	339.350	100.00	100.00

Compound (±)-3ra



Area Percent Report					
Peak #	RetTime [min]	Area [mAU*min]	Height [mAU]	Area %	Height %
1	7.125	88.667	255.876	50.15	58.97
2	10.042	88.144	178.055	49.85	41.03
Total		176.811	433.931	100.00	100.00

Compound (+)-3ra



Area Percent Report					
Peak #	RetTime [min]	Area [mAU*min]	Height [mAU]	Area %	Height %
1	7.347	4.956	13.985	3.95	5.56
2	9.972	120.644	237.573	96.05	94.44
Total		125.600	251.558	100.00	100.00