

## **Supporting Information**

### **Synthesis of Highly Fused Pyrano[2,3-*b*]pyridines via Rh(III)-Catalyzed C-H Activation and Intramolecular Cascade Annulation under Room Temperature**

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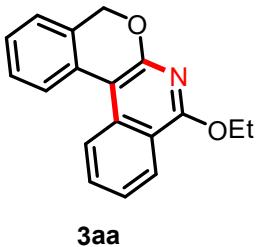
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## Table of Contents

<b>1.X-ray crystallography data .....</b>	<b>S2</b>
<b>1.1 X-ray Single Crystal Diffraction Data of compound 3aa .....</b>	<b>S2</b>
<b>1.2 X-ray Single Crystal Diffraction Data of compound 3na.....</b>	<b>S4</b>
<b>2.Mechanistic investigations.....</b>	<b>S7</b>
<b>2.1 H/D exchange experiment .....</b>	<b>S7</b>
<b>2.2 Intermolecular competition experiments.....</b>	<b>S7</b>
<b>2.3 Kinetic isotope effect (KIE) experiment .....</b>	<b>S9</b>
<b>3.NMR spectra data for desired compounds .....</b>	<b>S10</b>
<b>4.NMR spectra data for new compounds .....</b>	<b>S86</b>

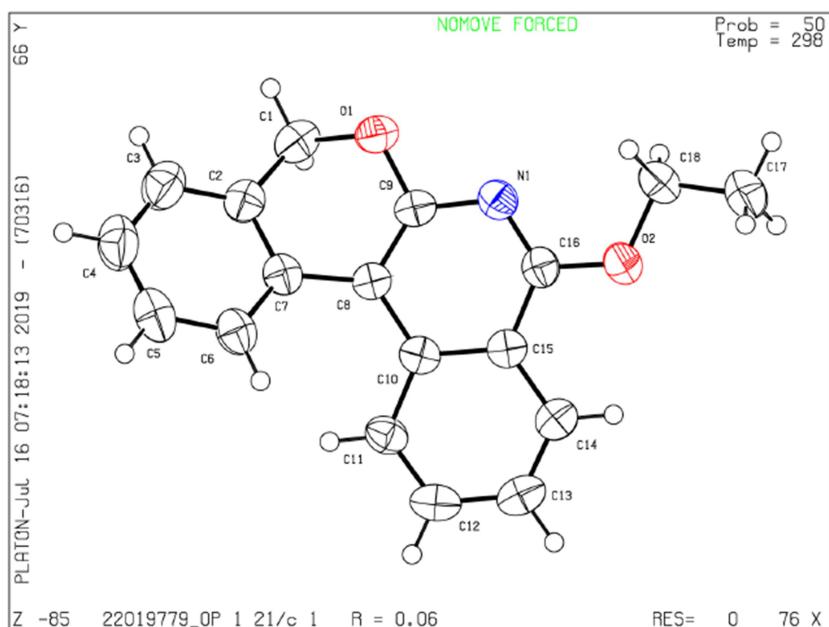
## 1. X-ray crystallography data

### 1.1 X-ray Single Crystal Diffraction Data of compound 3aa



**Sample preparation:** Compound **3aa** (19 mg) was dissolved in EtOAc (0.6 mL) and the mixture was sonicated until the solid was completely dissolved. The solution was filtered through a nylon-membrane syringe filter (13 mm\*0.22 µm, purchased from ANPEL Laboratory Tech. Shanghai, Inc.) and transferred into a clean 2 mL vial. The vial was sealed with a thin layer of parafilm on top of which 3-5 holes was made with a capillary (0.3 mm) to allow the solvent slowly violated at room temperature to afford the single crystal **3aa**.

**Single crystal structure of 3aa:** X-ray crystal structure of **3aa** was determined at room temperature (298K) with the ellipsoid contour at 50% probability levels.



**Crystal data and structure refinement for 22019779\_0m (3aa).**

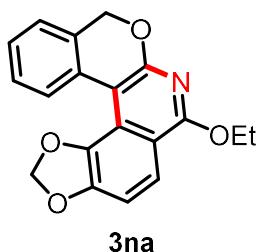
Identification code	22019779_0m
Empirical formula	C <sub>18</sub> H <sub>15</sub> NO <sub>2</sub>
Formula weight	277.31
Temperature/K	298
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /c
a/Å	3.999(2)
b/Å	18.448(10)
c/Å	18.493(11)
α/°	90
β/°	90.662(19)
γ/°	90
Volume/Å <sup>3</sup>	1364.3(13)
Z	4
ρ <sub>calc</sub> g/cm <sup>3</sup>	1.350
μ/mm <sup>-1</sup>	0.088
F(000)	584.0
Crystal size/mm <sup>3</sup>	0.15 × 0.12 × 0.08
Radiation	MoKα ( $\lambda = 0.71073$ )
2Θ range for data collection/°	4.928 to 50.044

Index ranges	$-4 \leq h \leq 4, -21 \leq k \leq 21, -21 \leq l \leq 22$
Reflections collected	11590
Independent reflections	2397 [ $R_{\text{int}} = 0.1037, R_{\text{sigma}} = 0.0776$ ]
Data/restraints/parameters	2397/0/191
Goodness-of-fit on $F^2$	1.074
Final R indexes [ $I >= 2\sigma(I)$ ]	$R_1 = 0.0590, wR_2 = 0.1253$
Final R indexes [all data]	$R_1 = 0.0986, wR_2 = 0.1434$
Largest diff. peak/hole / e Å <sup>-3</sup>	0.16/-0.18

### Crystal structure determination of [22019779\_0m] (3aa)

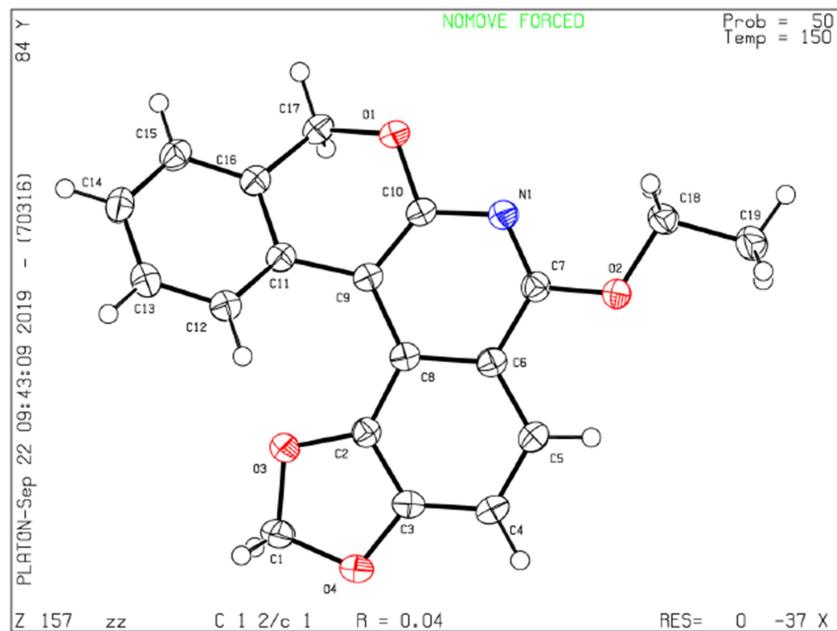
**Crystal Data** for C<sub>18</sub>H<sub>15</sub>NO<sub>2</sub> ( $M = 277.31$  g/mol): monoclinic, space group P2<sub>1</sub>/c (no. 14),  $a = 3.999(2)$  Å,  $b = 18.448(10)$  Å,  $c = 18.493(11)$  Å,  $\beta = 90.662(19)^\circ$ ,  $V = 1364.3(13)$  Å<sup>3</sup>,  $Z = 4$ ,  $T = 298$  K,  $\mu(\text{MoK}\alpha) = 0.088$  mm<sup>-1</sup>,  $D_{\text{calc}} = 1.350$  g/cm<sup>3</sup>, 11590 reflections measured ( $4.928^\circ \leq 2\Theta \leq 50.044^\circ$ ), 2397 unique ( $R_{\text{int}} = 0.1037$ ,  $R_{\text{sigma}} = 0.0776$ ) which were used in all calculations. The final  $R_1$  was 0.0590 ( $I > 2\sigma(I)$ ) and  $wR_2$  was 0.1434 (all data).

### 1.2 X-ray Single Crystal Diffraction Data of compound 3na



**Sample preparation:** The single crystal of **3na** was prepared in the same manner of how single crystal of **3aa** was prepared.

**Single crystal structure of 3na:** X-ray crystal structure of **3na** was determined at room temperature (298K) with the ellipsoid contour at 50% probability levels



#### Crystal data and structure refinement for ZZ (3na).

Identification code	ZZ
Empirical formula	C <sub>19</sub> H <sub>15</sub> NO <sub>4</sub>
Formula weight	321.32
Temperature/K	150.0
Crystal system	monoclinic
Space group	C2/c
a/Å	14.4200(17)
b/Å	19.703(2)
c/Å	10.3796(12)
α/°	90

$\beta/^\circ$	90.12(5)
$\gamma/^\circ$	90
Volume/ $\text{\AA}^3$	2949.0(6)
Z	8
$\rho_{\text{calc}} \text{g/cm}^3$	1.447
$\mu/\text{mm}^{-1}$	0.843
F(000)	1344.0
Crystal size/ $\text{mm}^3$	0.08 $\times$ 0.05 $\times$ 0.04
Radiation	CuK $\alpha$ ( $\lambda = 1.54178$ )
2 $\Theta$ range for data collection/ $^\circ$	7.598 to 149.94
Index ranges	-17 $\leq$ h $\leq$ 17, -24 $\leq$ k $\leq$ 24, -9 $\leq$ l $\leq$ 12
Reflections collected	16198
Independent reflections	3008 [ $R_{\text{int}} = 0.0402$ , $R_{\text{sigma}} = 0.0354$ ]
Data/restraints/parameters	3008/0/218
Goodness-of-fit on $F^2$	0.970
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.0368$ , $wR_2 = 0.1027$
Final R indexes [all data]	$R_1 = 0.0377$ , $wR_2 = 0.1035$
Largest diff. peak/hole / e $\text{\AA}^{-3}$	0.23/-0.22

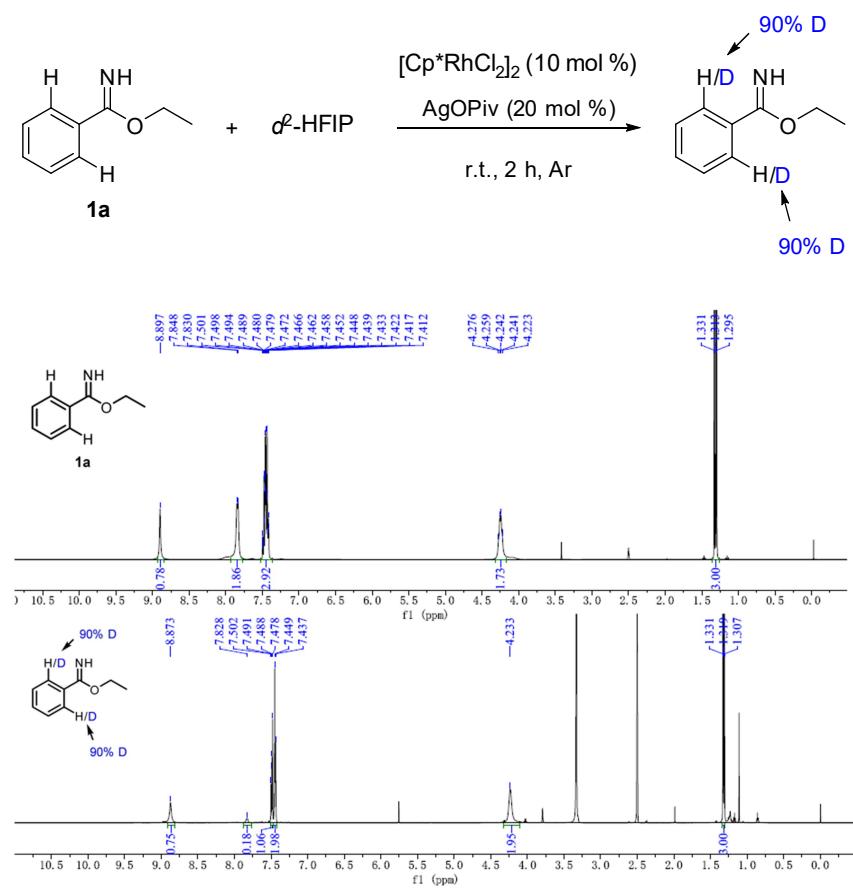
### Crystal structure determination of [ZZ] (3na)

**Crystal Data** for C<sub>19</sub>H<sub>15</sub>NO<sub>4</sub> ( $M=321.32$  g/mol): monoclinic, space group C2/c (no. 15),  $a = 14.4200(17)$   $\text{\AA}$ ,  $b = 19.703(2)$   $\text{\AA}$ ,  $c = 10.3796(12)$   $\text{\AA}$ ,  $\beta = 90.12(5)^\circ$ ,  $V =$

$2949.0(6) \text{ \AA}^3$ ,  $Z = 8$ ,  $T = 150.0 \text{ K}$ ,  $\mu(\text{CuK}\alpha) = 0.843 \text{ mm}^{-1}$ ,  $D_{\text{calc}} = 1.447 \text{ g/cm}^3$ , 16198 reflections measured ( $7.598^\circ \leq 2\Theta \leq 149.94^\circ$ ), 3008 unique ( $R_{\text{int}} = 0.0402$ ,  $R_{\text{sigma}} = 0.0354$ ) which were used in all calculations. The final  $R_1$  was 0.0368 ( $I > 2\sigma(I)$ ) and  $wR_2$  was 0.1035 (all data).

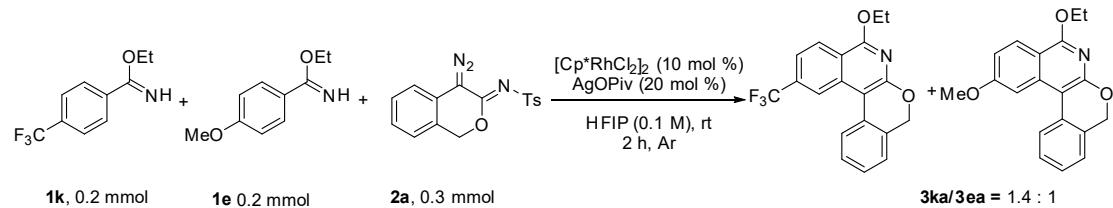
## 2. Mechanistic investigations

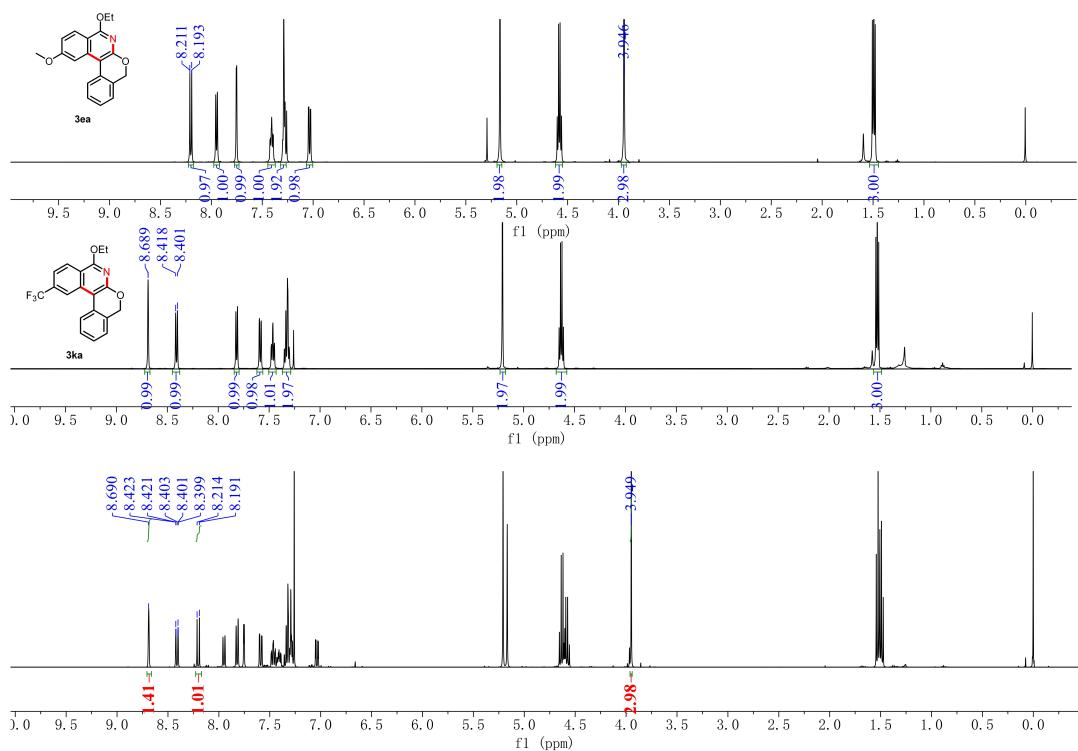
### 2.1 H/D exchange experiment



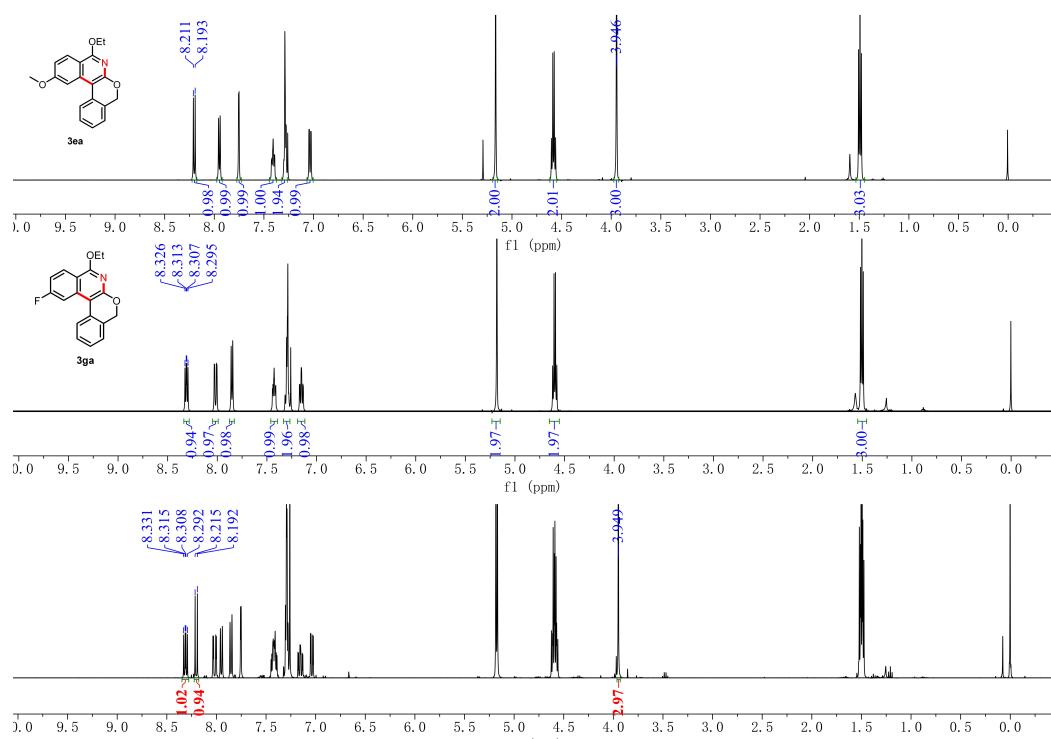
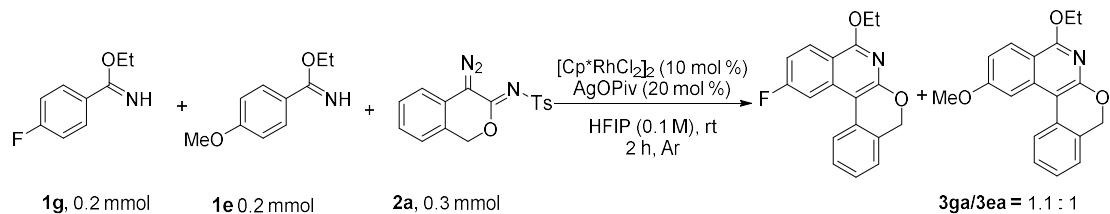
### 2.2 Intermolecular competition experiments

#### 2.2.1 Intermolecular competition experiments between **1k** and **1e** coupled with **2a**

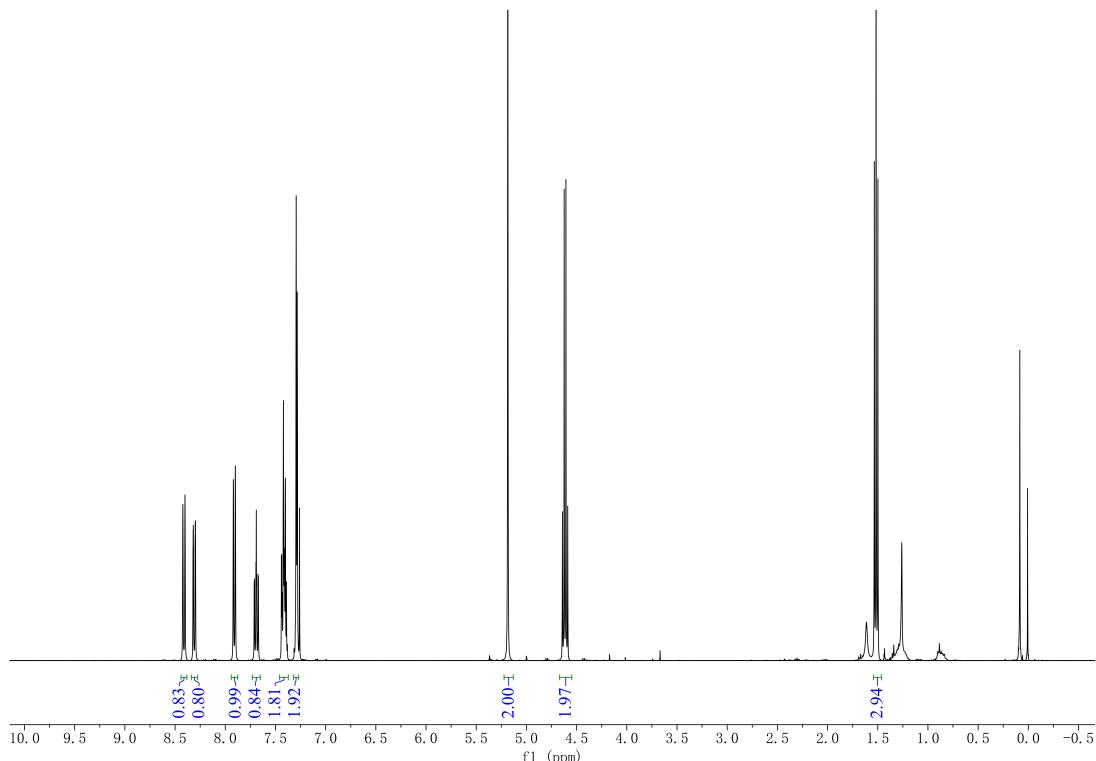
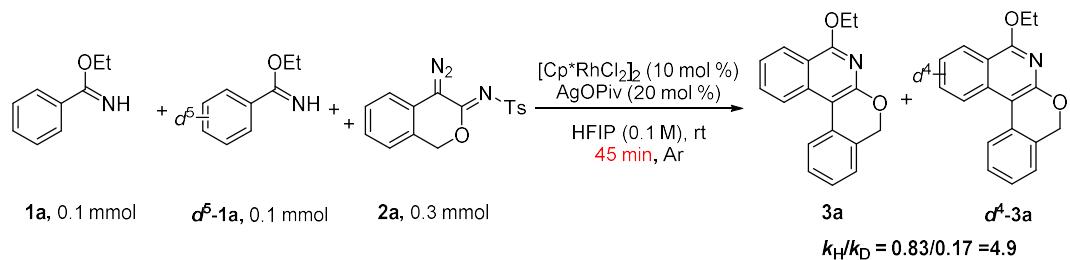




### 2.2.2 Intermolecular competition experiments between 1g and 1e coupled with 2a

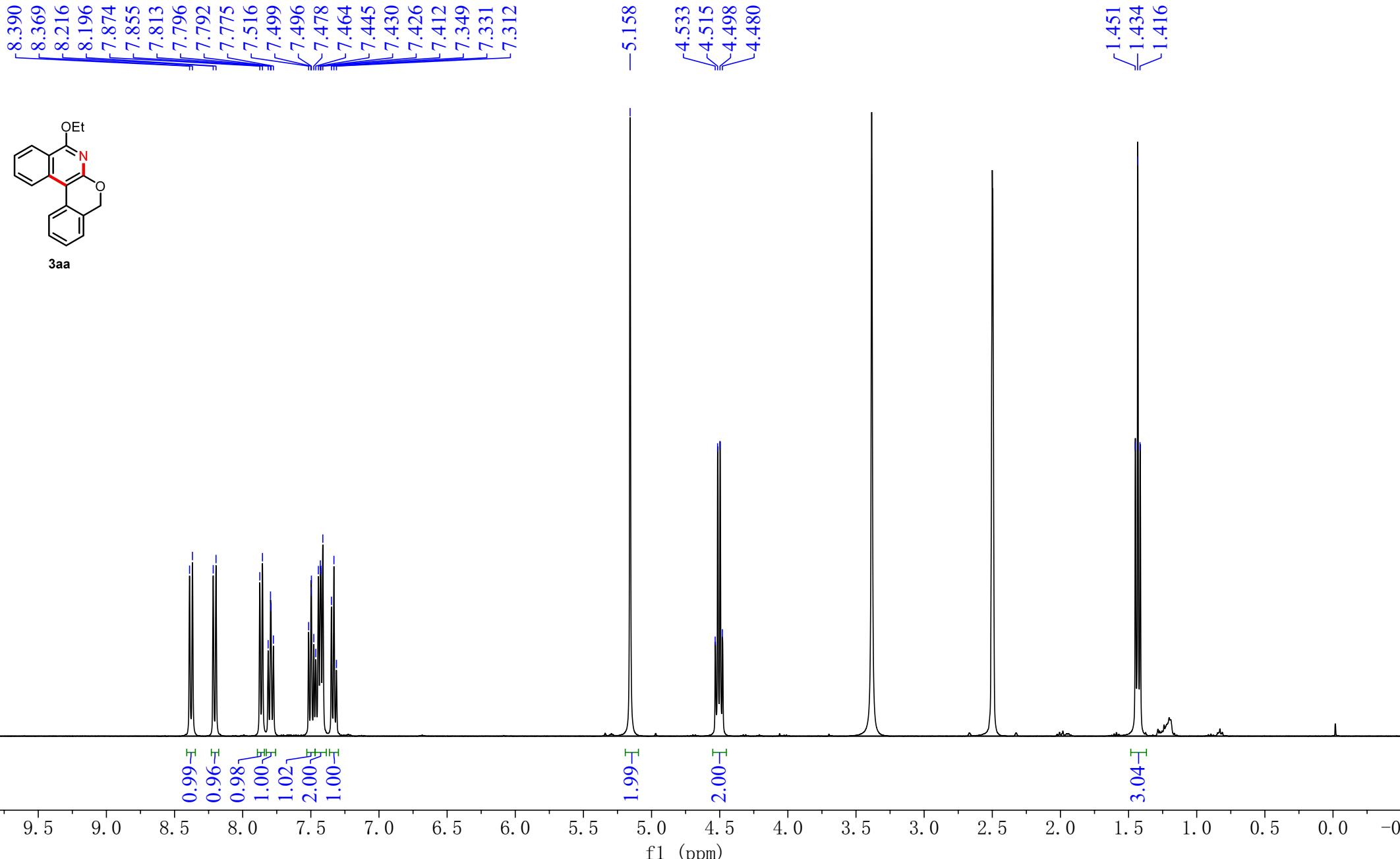


### 2.3 Kinetic isotope effect (KIE) experiment

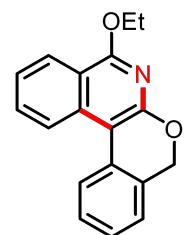


$$k_{\text{H}}/k_{\text{D}} = 0.83/(1-0.83) = 4.9$$

### 3. NMR spectra data for desired compounds



$^1\text{H}$  NMR spectrum of 3aa



**3aa**

—159.861  
—157.249

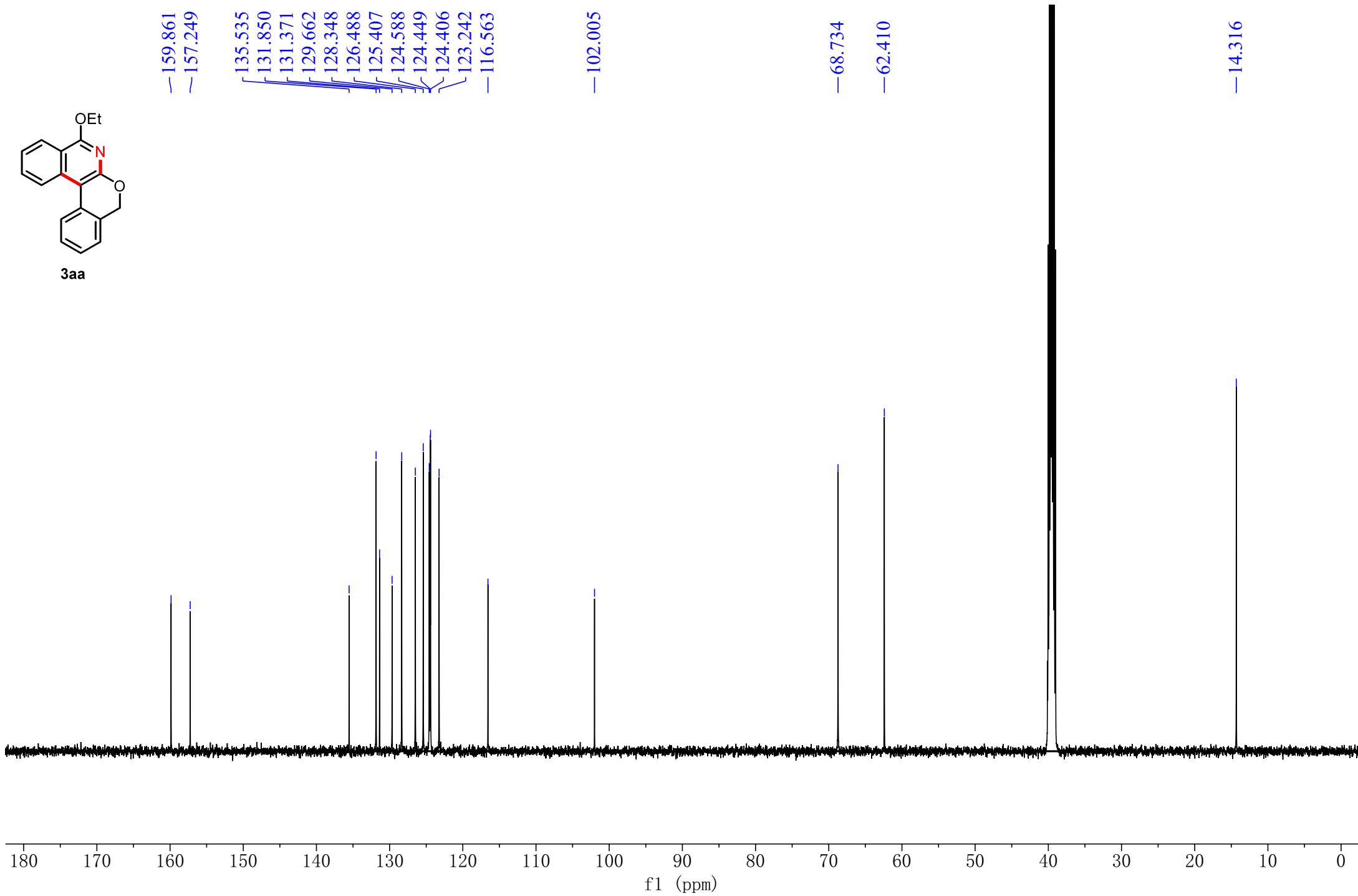
135.535  
131.850  
131.371  
129.662  
128.348  
126.488  
125.407  
125.407  
124.588  
124.449  
124.406  
123.242  
—116.563

—102.005

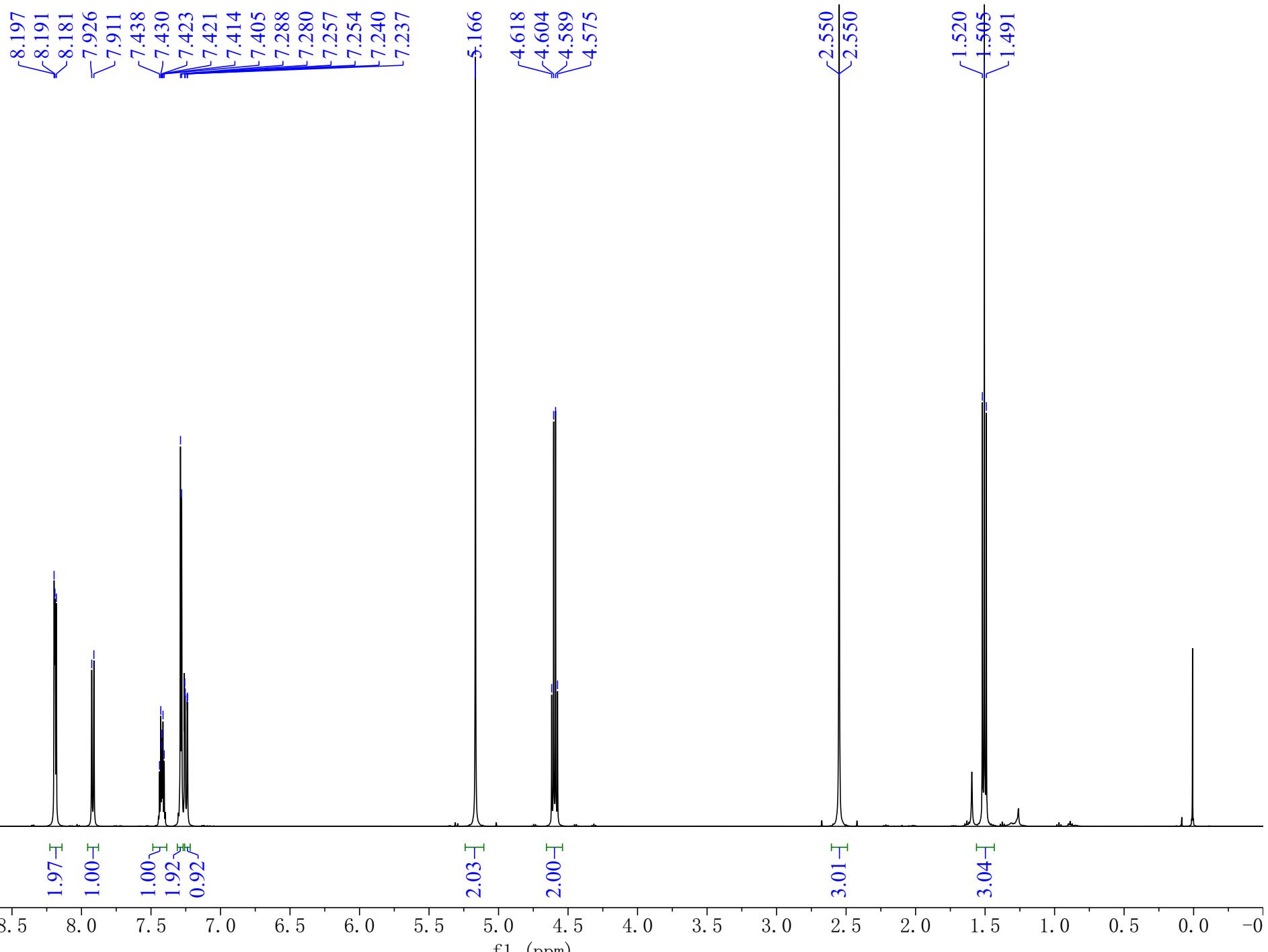
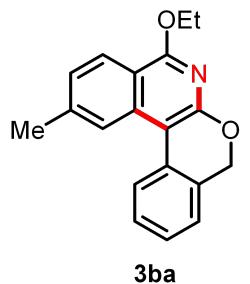
—68.734

—62.410

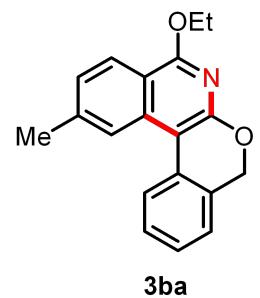
—14.316



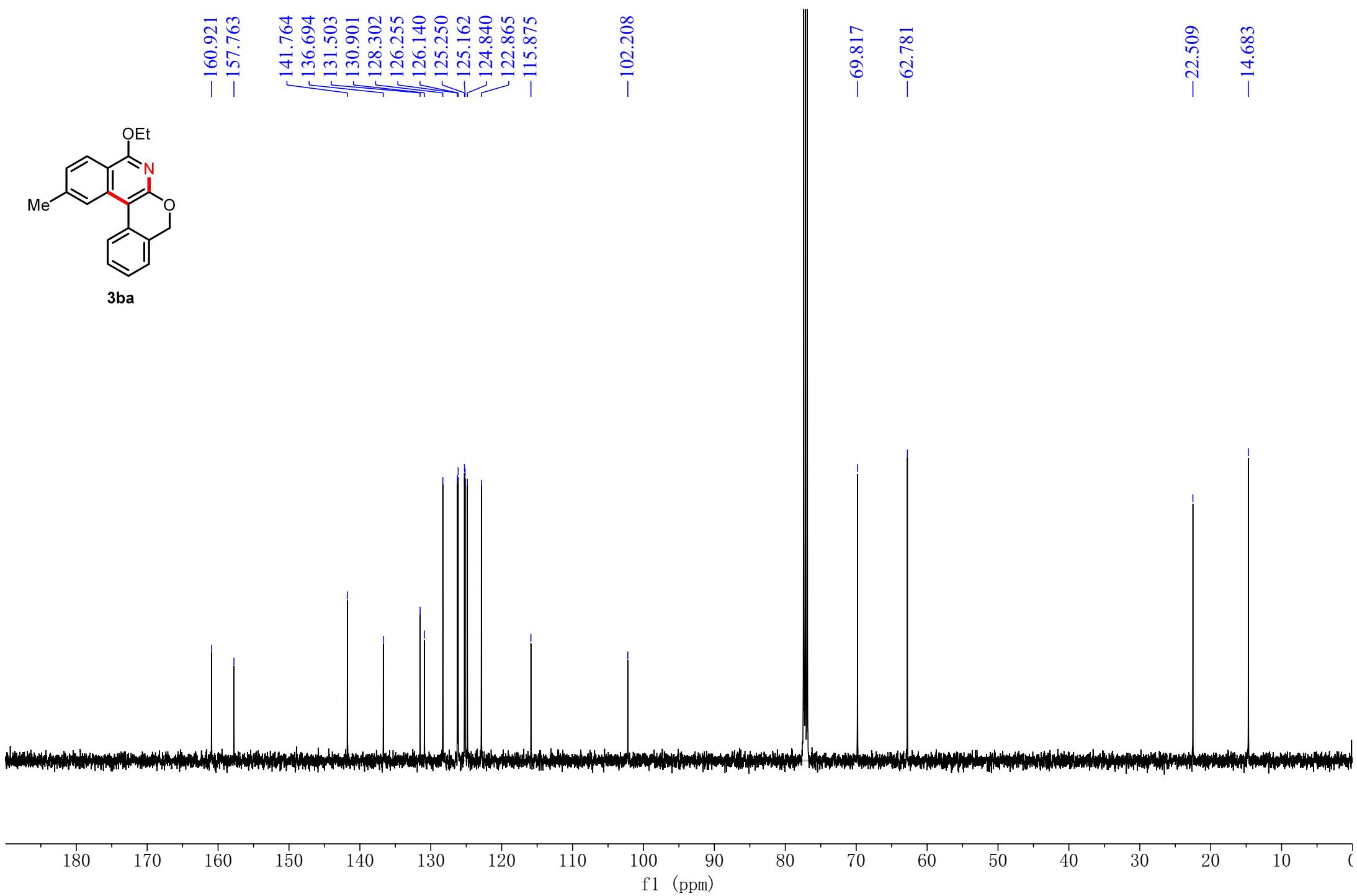
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3aa**



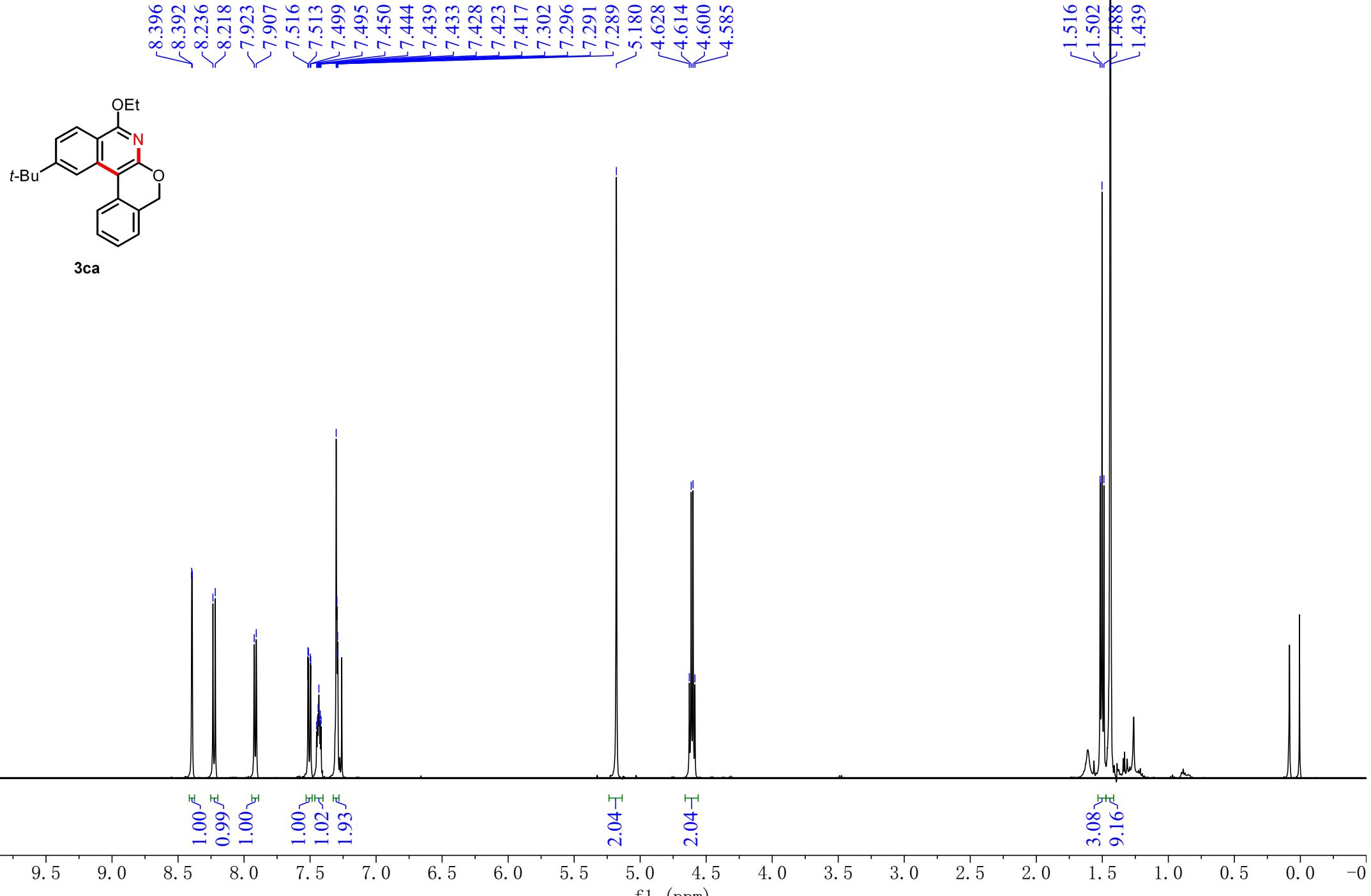
<sup>1</sup>H NMR spectrum of **3ba**



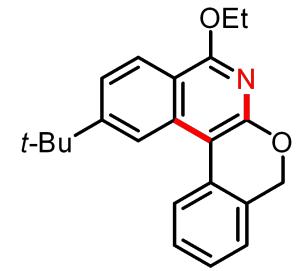
—160.921  
 —157.763  
 141.764  
 136.694  
 131.503  
 130.901  
 128.302  
 126.255  
 126.140  
 125.250  
 125.162  
 124.840  
 122.865  
 —115.875  
 —102.208  
 —69.817  
 —62.781  
 —22.509  
 —14.683



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3ba**



$^1\text{H}$  NMR spectrum of **3ca**



—160.848  
—157.799  
—154.573

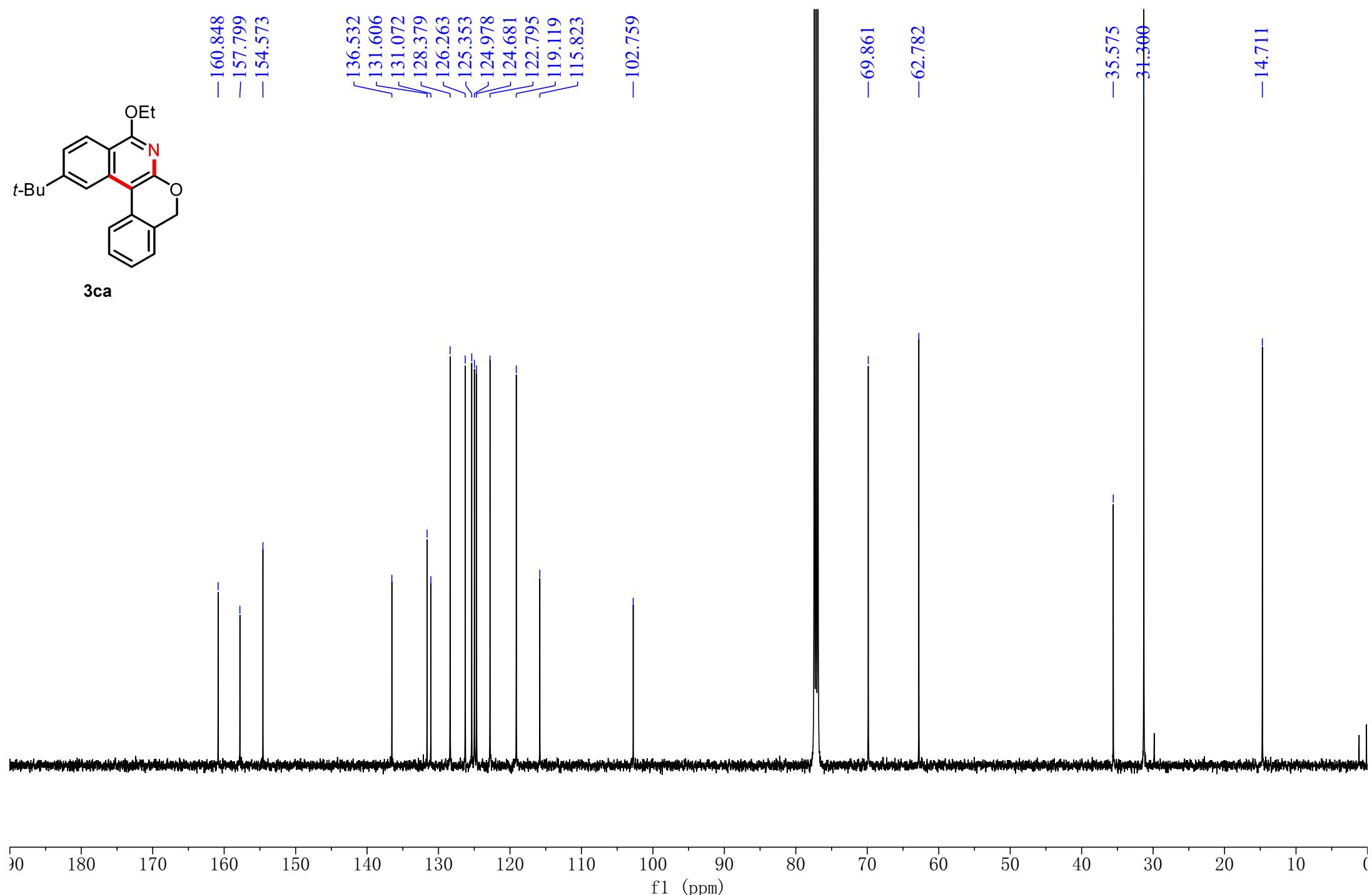
136.532  
131.606  
131.072  
128.379  
126.263  
125.353  
124.978  
124.681  
122.795  
119.119  
115.823

—102.759

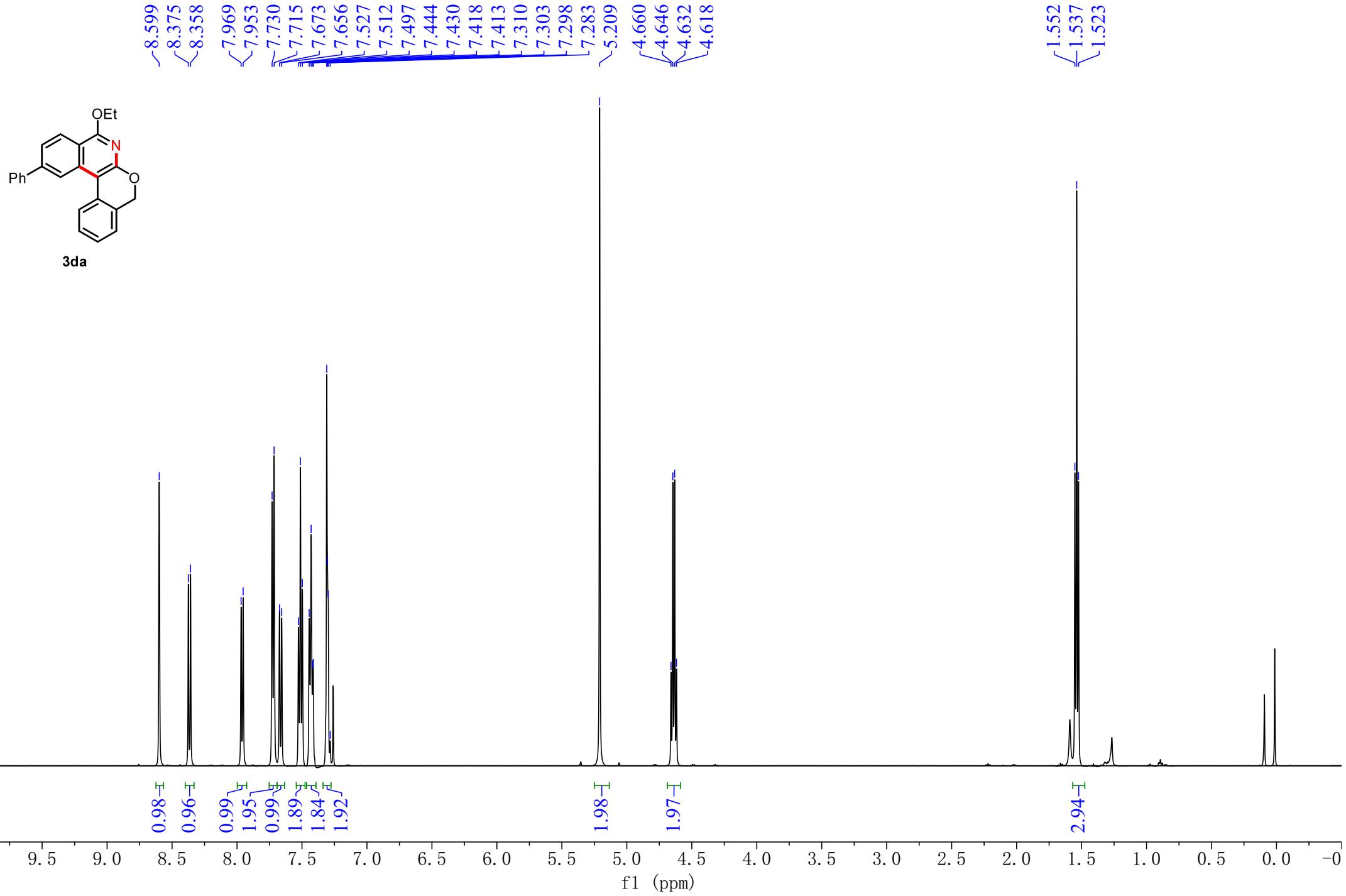
—69.861  
—62.782

—35.575  
31.300

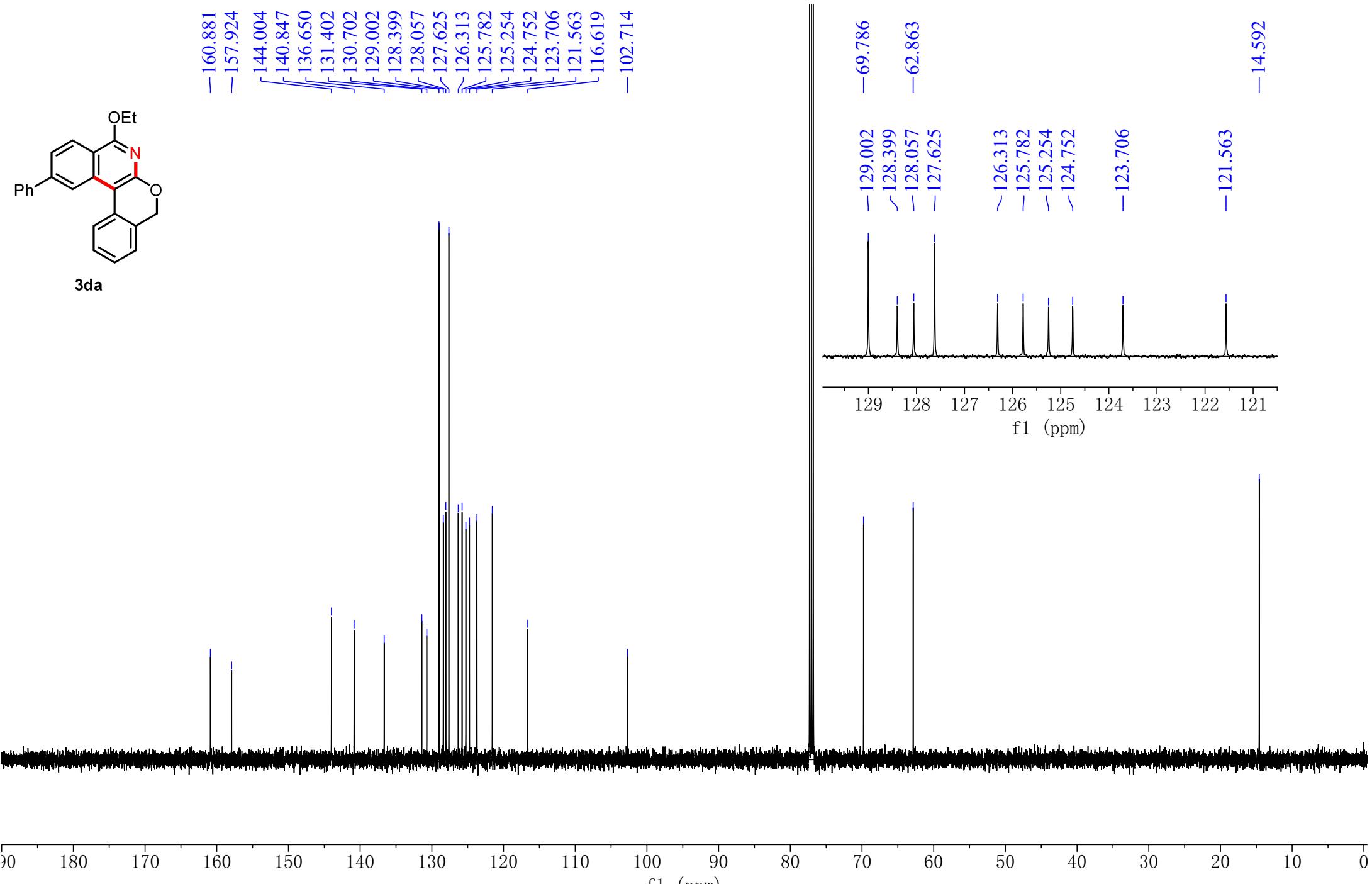
—14.711



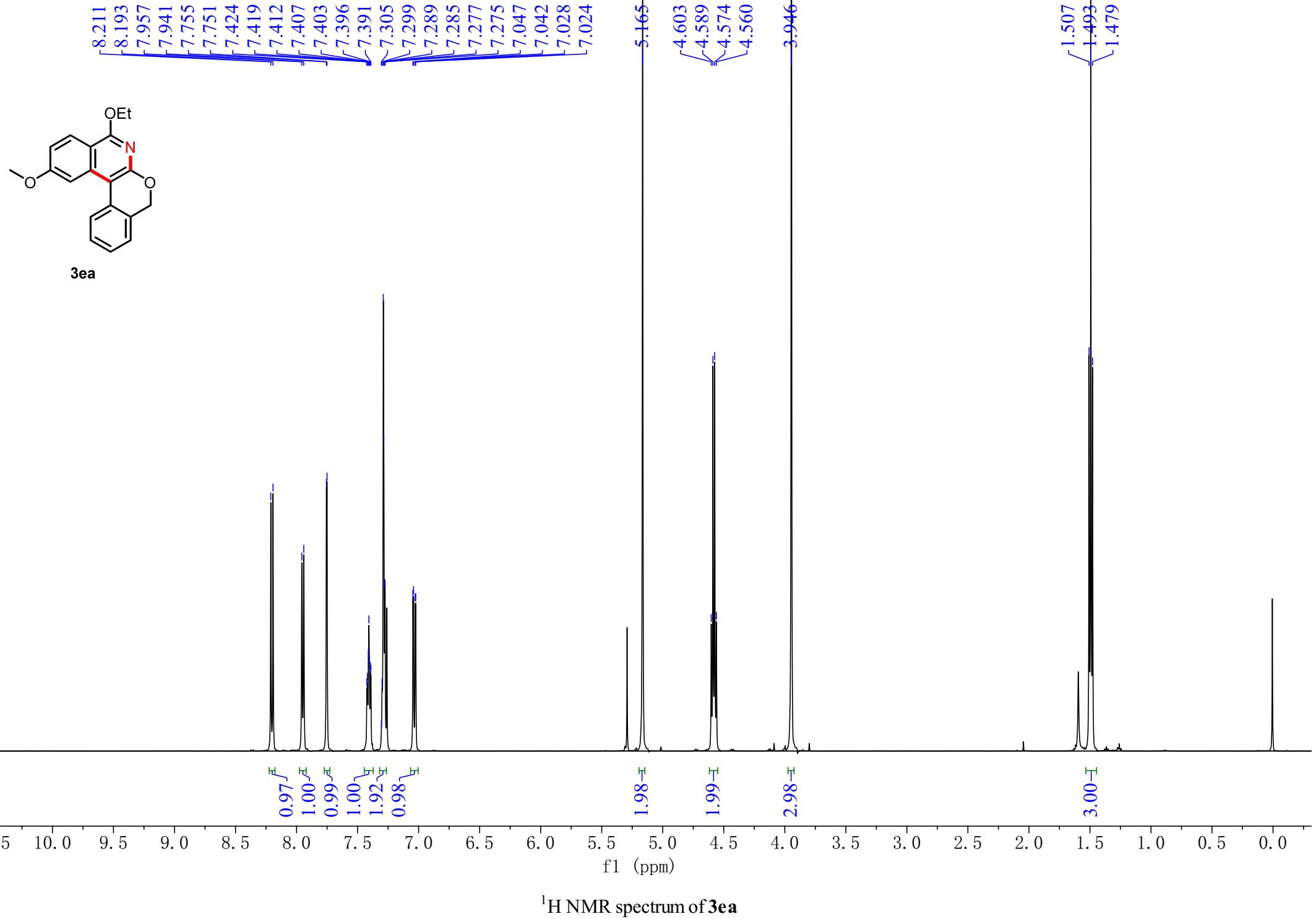
$^{13}\text{C}\{^1\text{H}\}$  NMR of 3ca

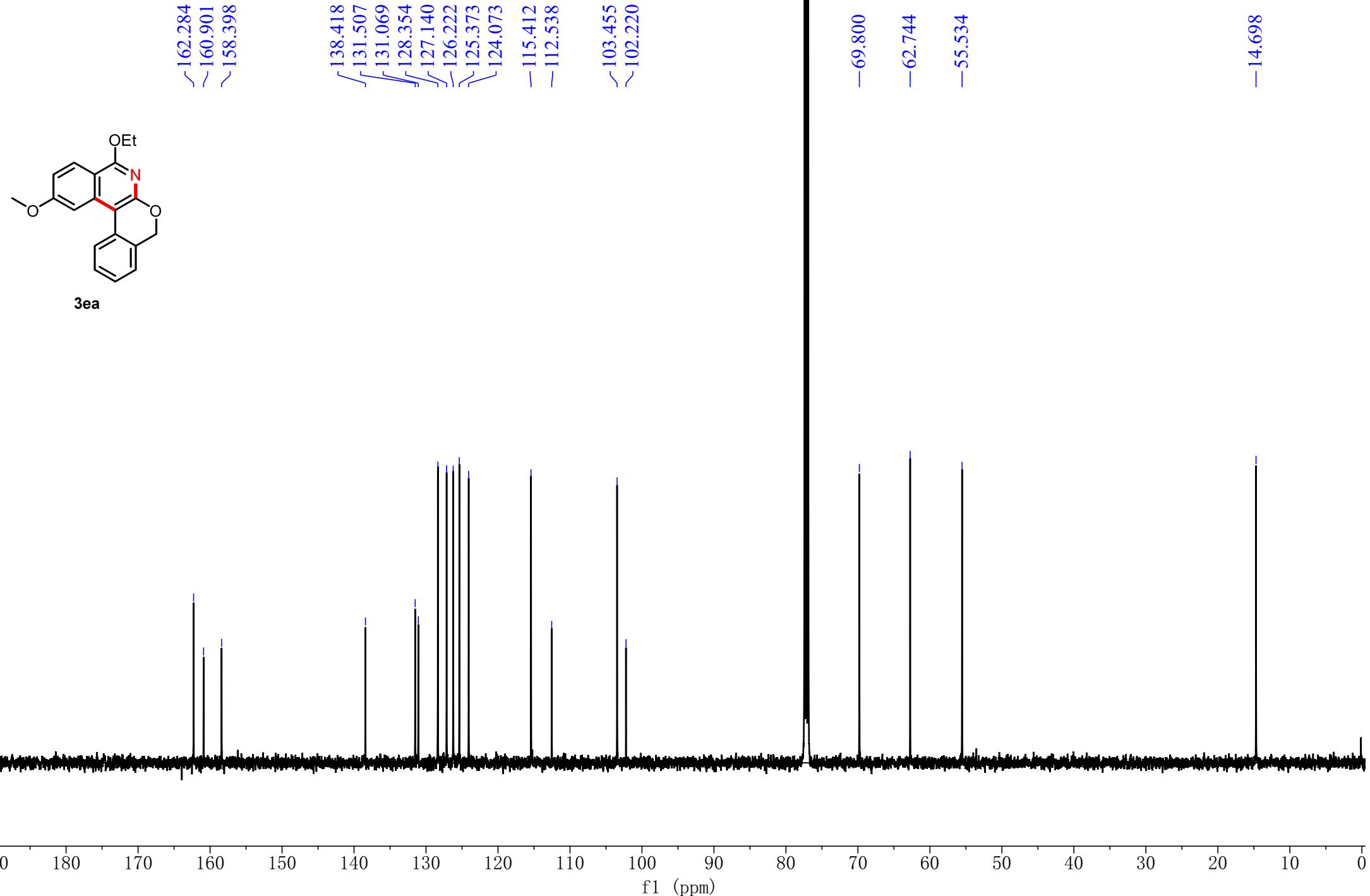


<sup>1</sup>H NMR spectrum of **3da**

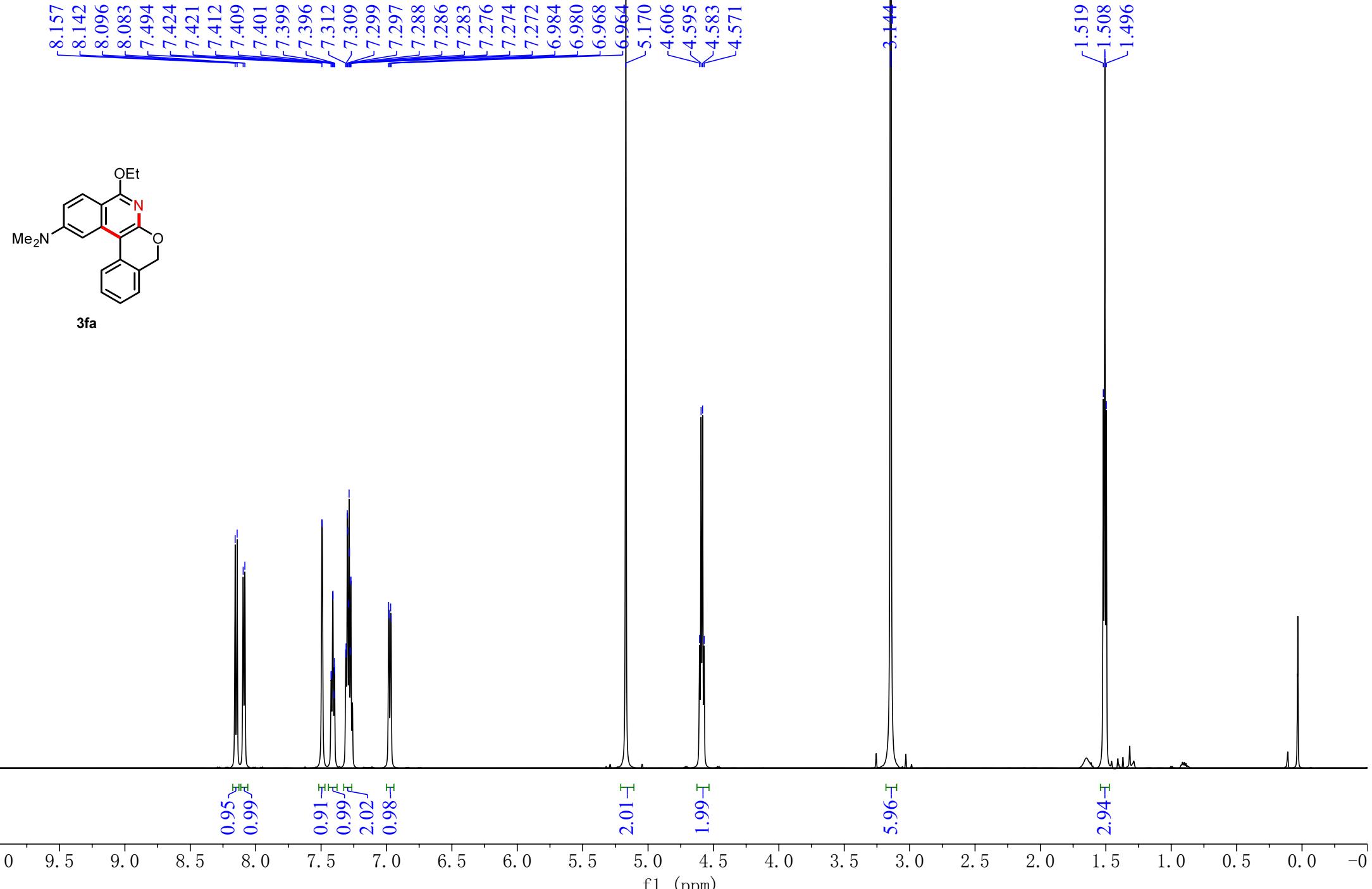


$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3da**

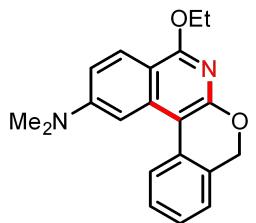




$^{13}\text{C}\{\text{H}\}$  NMR spectrum of **3ea**



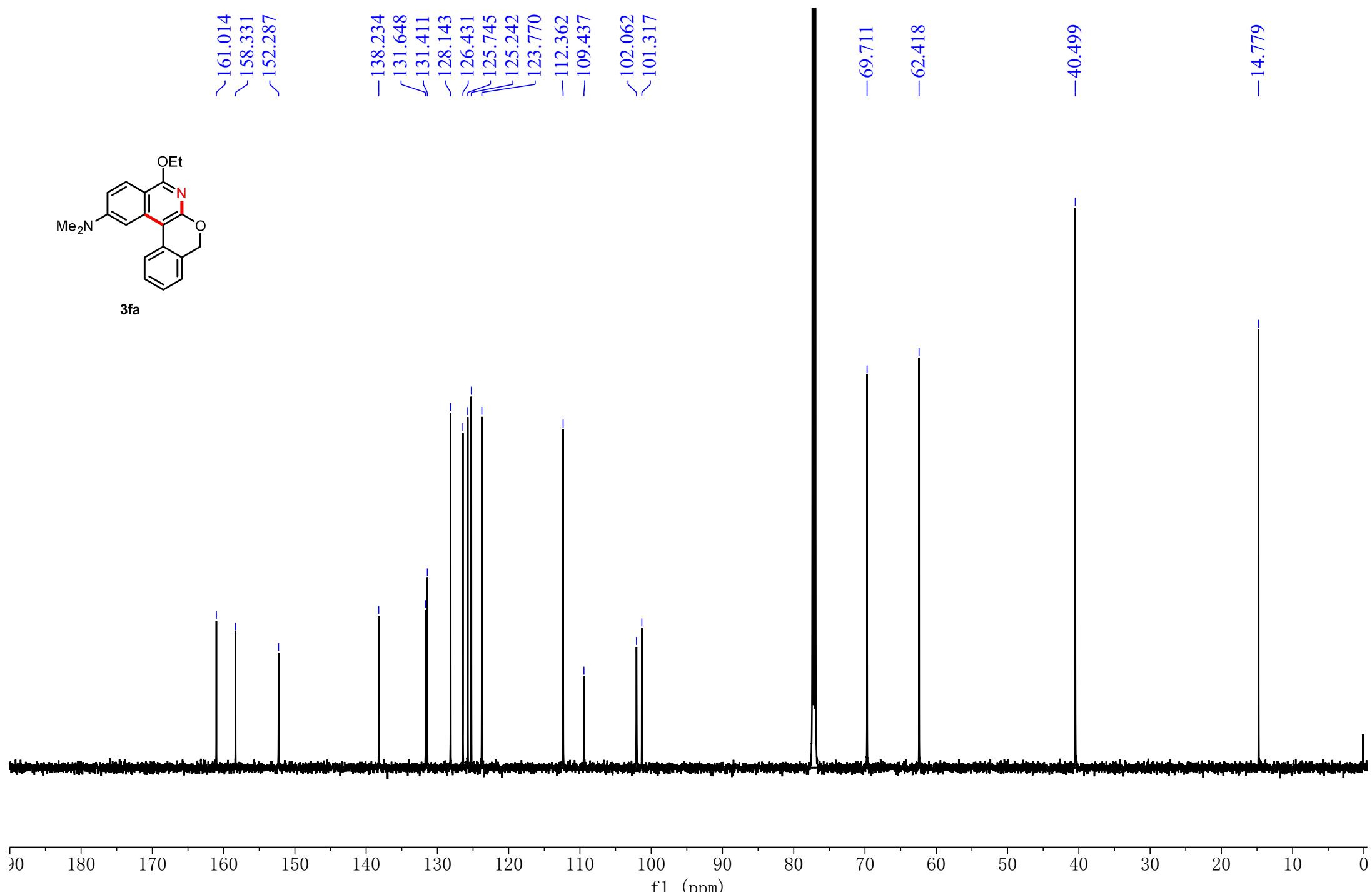
$^1\text{H}$  NMR spectrum of **3fa**



3fa

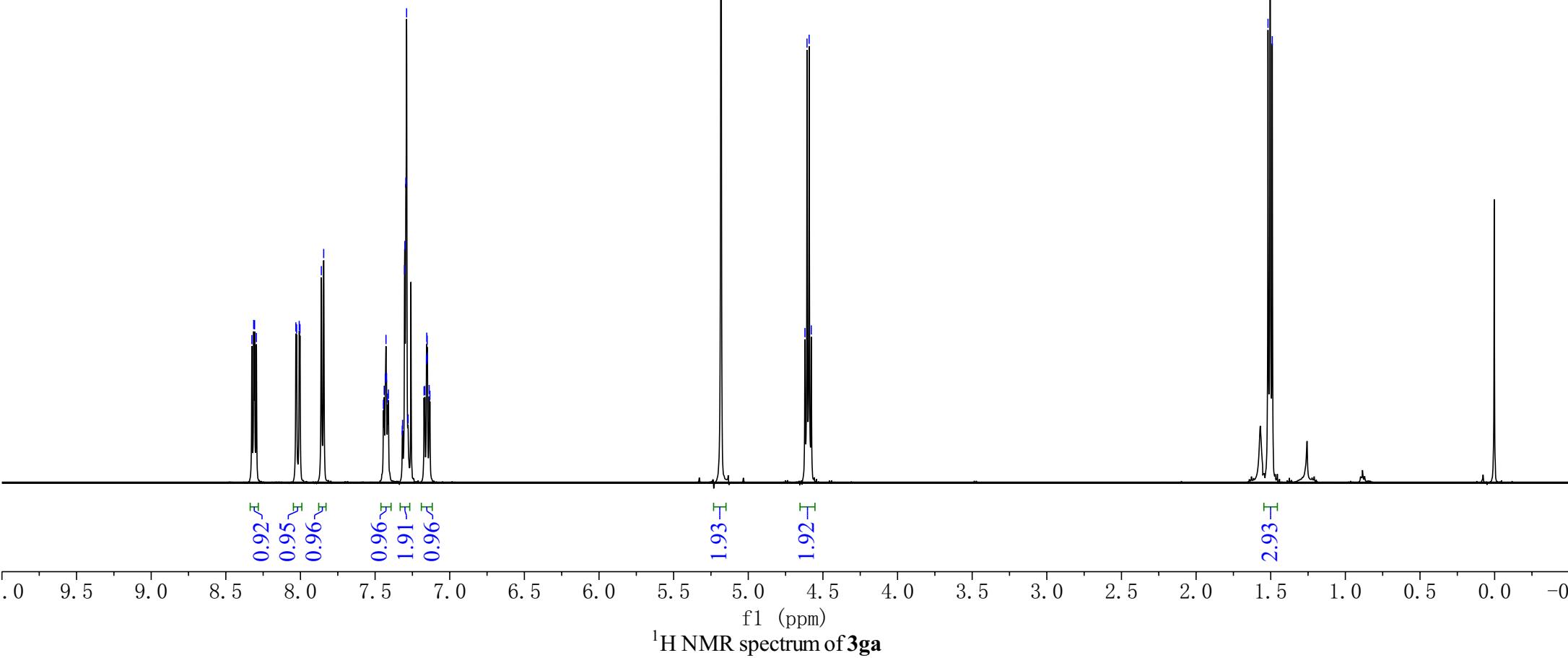
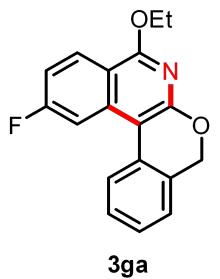
Peak assignments for the <sup>13</sup>C NMR spectrum of 3fa:

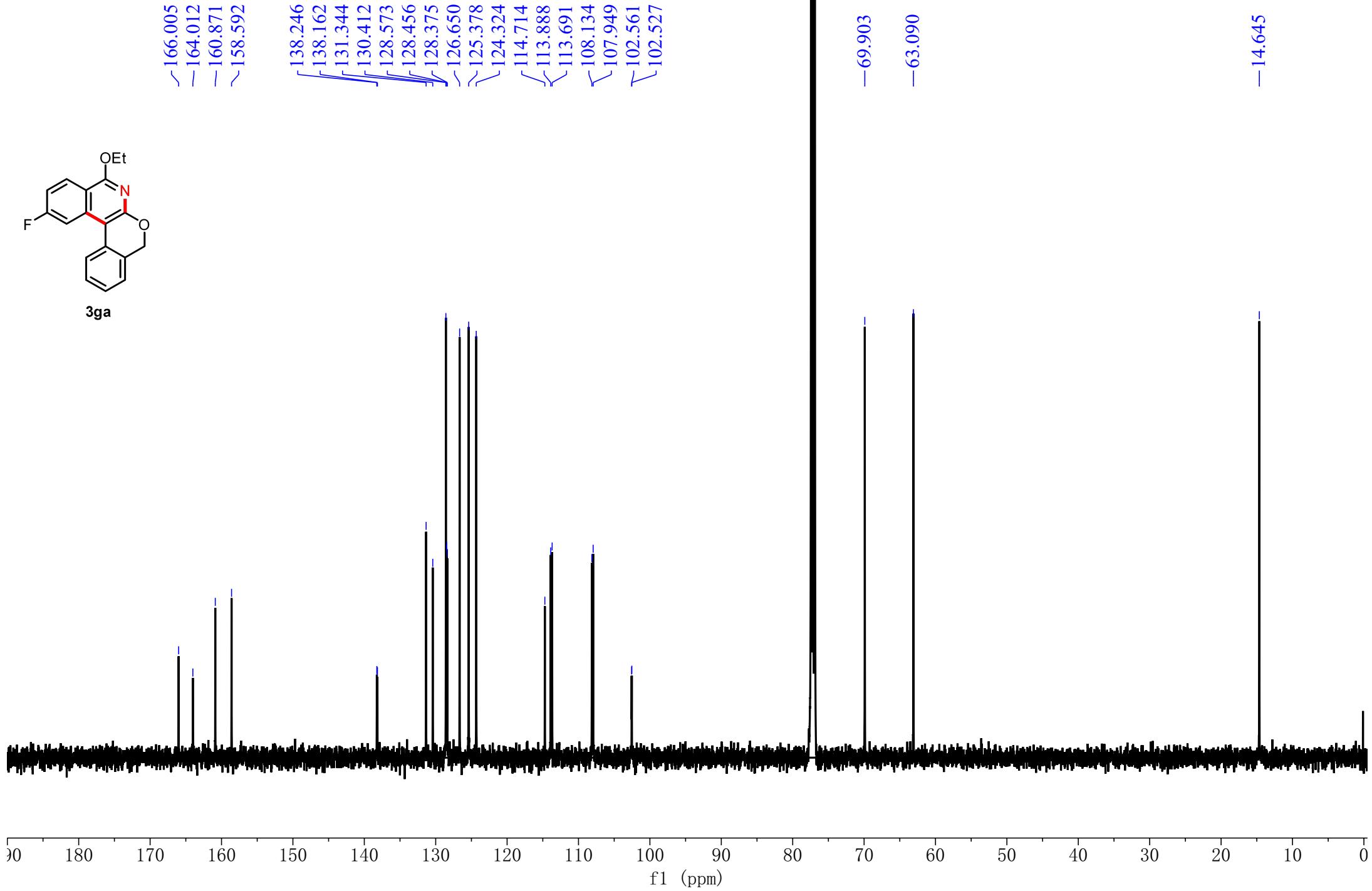
- ~161.014
- ~158.331
- ~152.287
- 138.234
- 131.648
- 131.411
- 128.143
- ~126.431
- 125.745
- 125.242
- 123.770
- 112.362
- 109.437
- 102.062
- 101.317
- 69.711
- 62.418
- 40.499
- 14.779



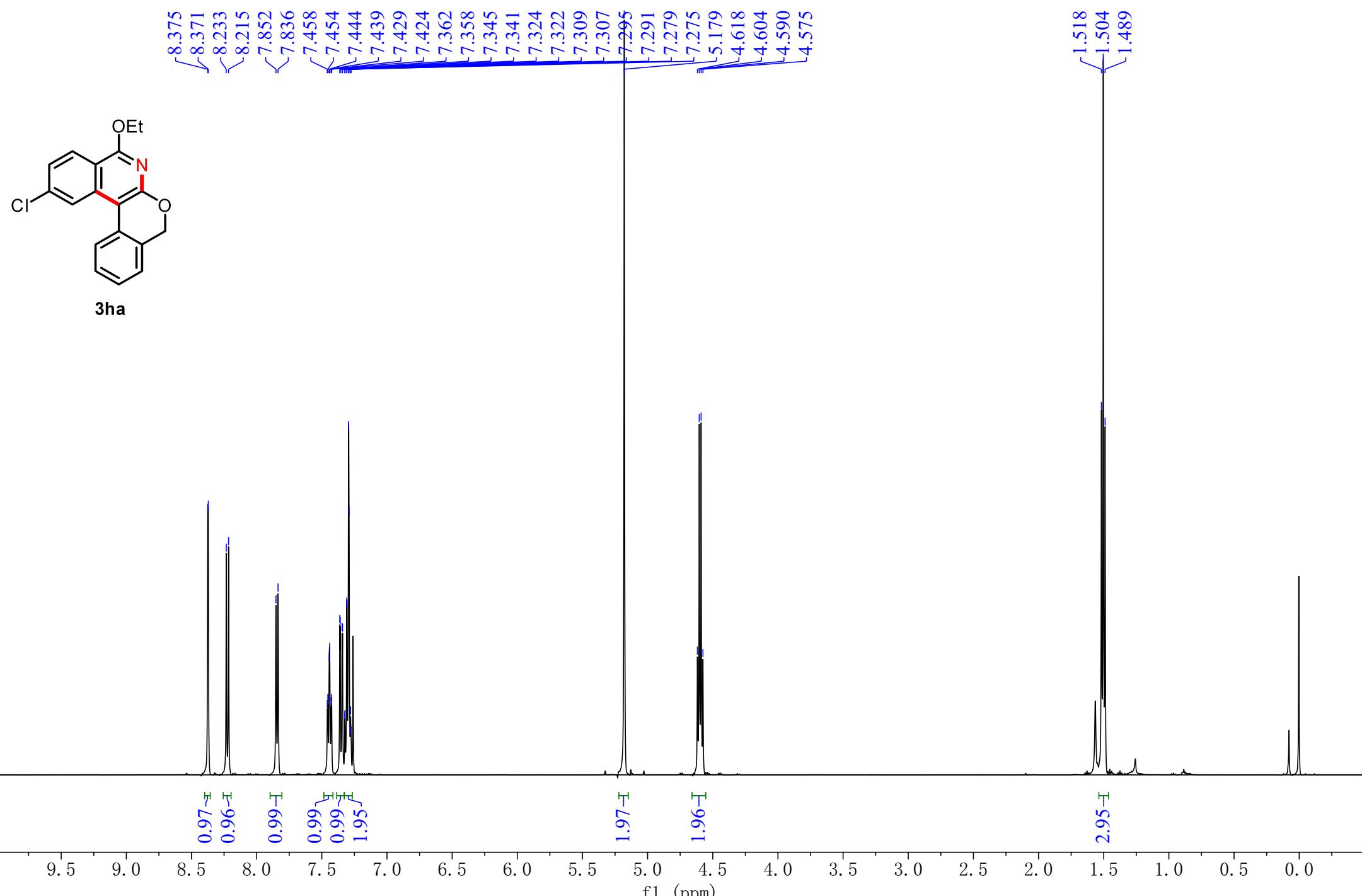
<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 3fa

8.326  
8.313  
8.307  
8.295  
8.031  
8.026  
8.008  
8.003  
7.860  
7.844  
7.444  
7.439  
7.432  
7.427  
7.423  
7.416  
7.411  
7.318  
7.316  
7.303  
7.301  
7.294  
7.289  
7.279  
7.172  
7.167  
7.156  
7.154  
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7.149  
7.138  
7.133  
5.183  
4.621  
4.606  
4.592  
4.578

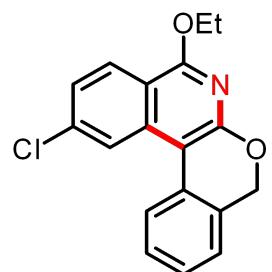




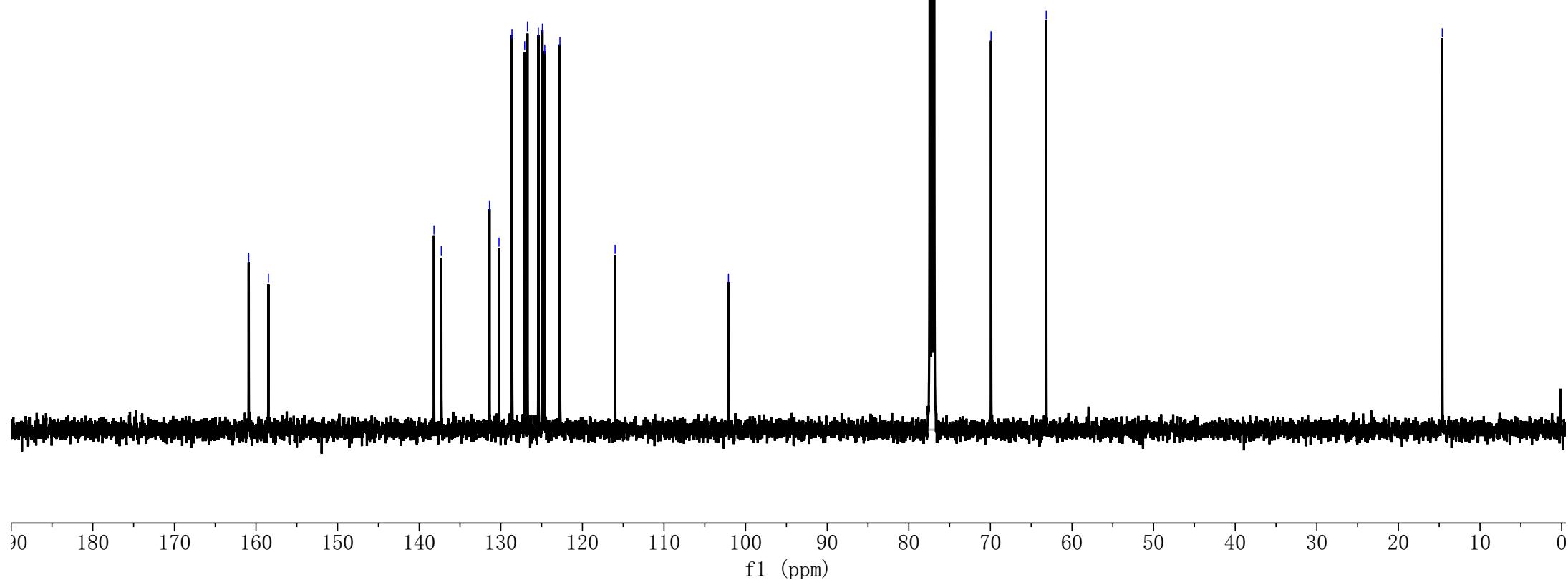
$^{13}\text{C}\{\text{H}\}$  NMR spectrum of **3ga**



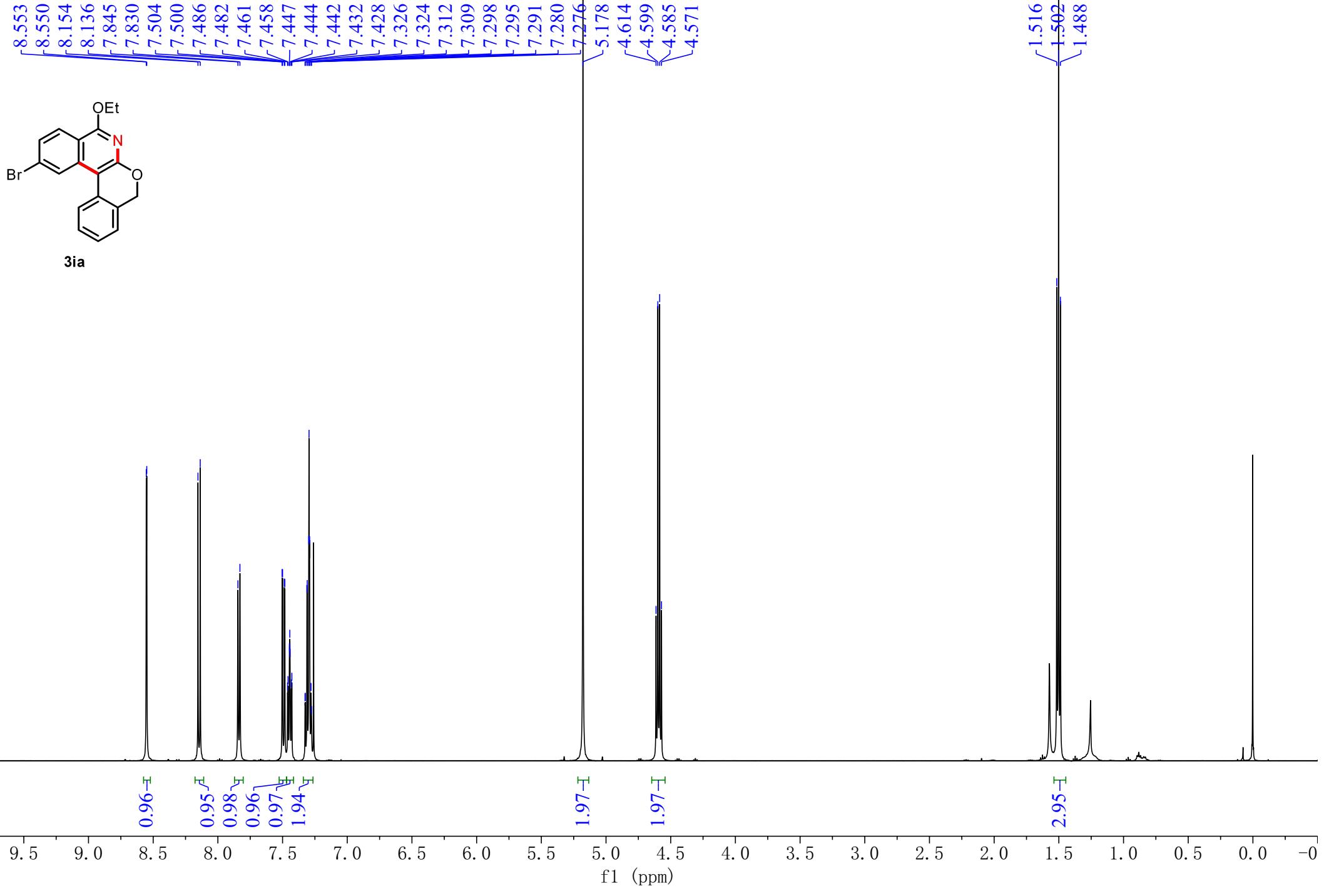
$^1\text{H}$  NMR spectrum of **3ha**



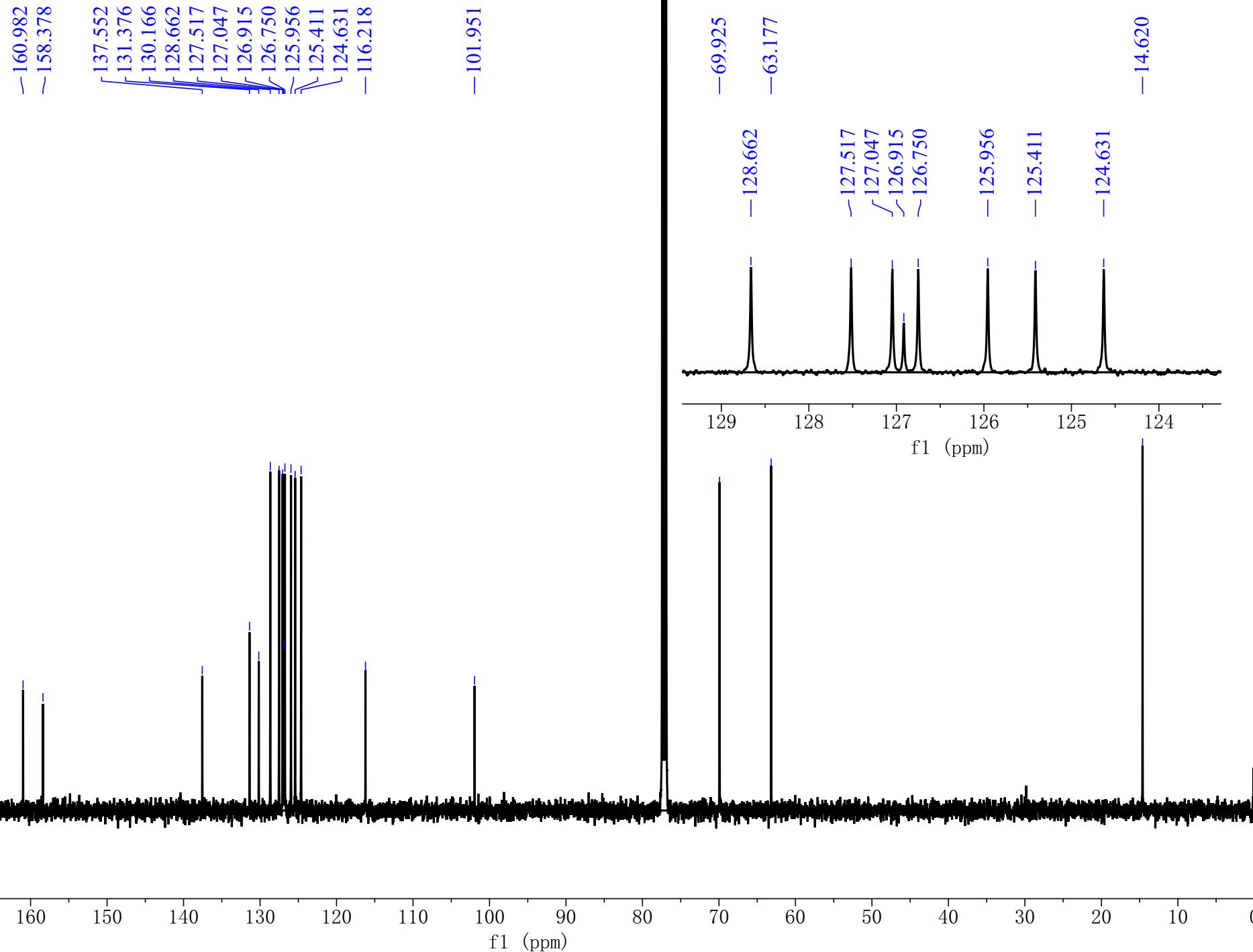
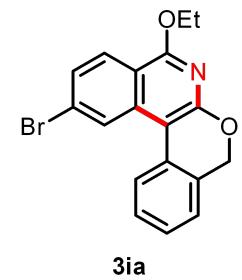
3ha

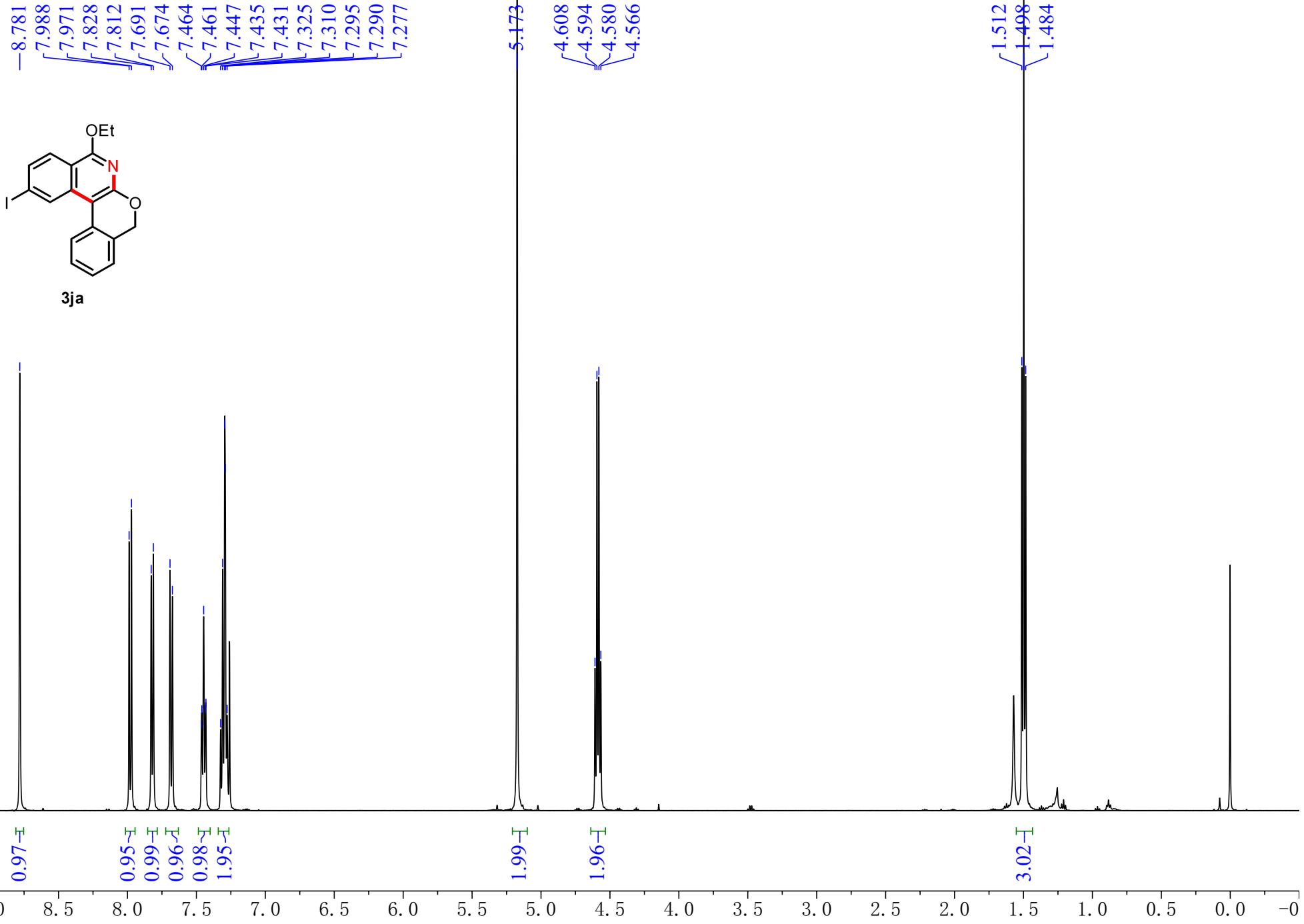


<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 3ha

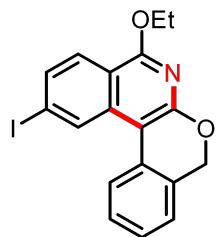


$^1\text{H}$  NMR spectrum of 3ia



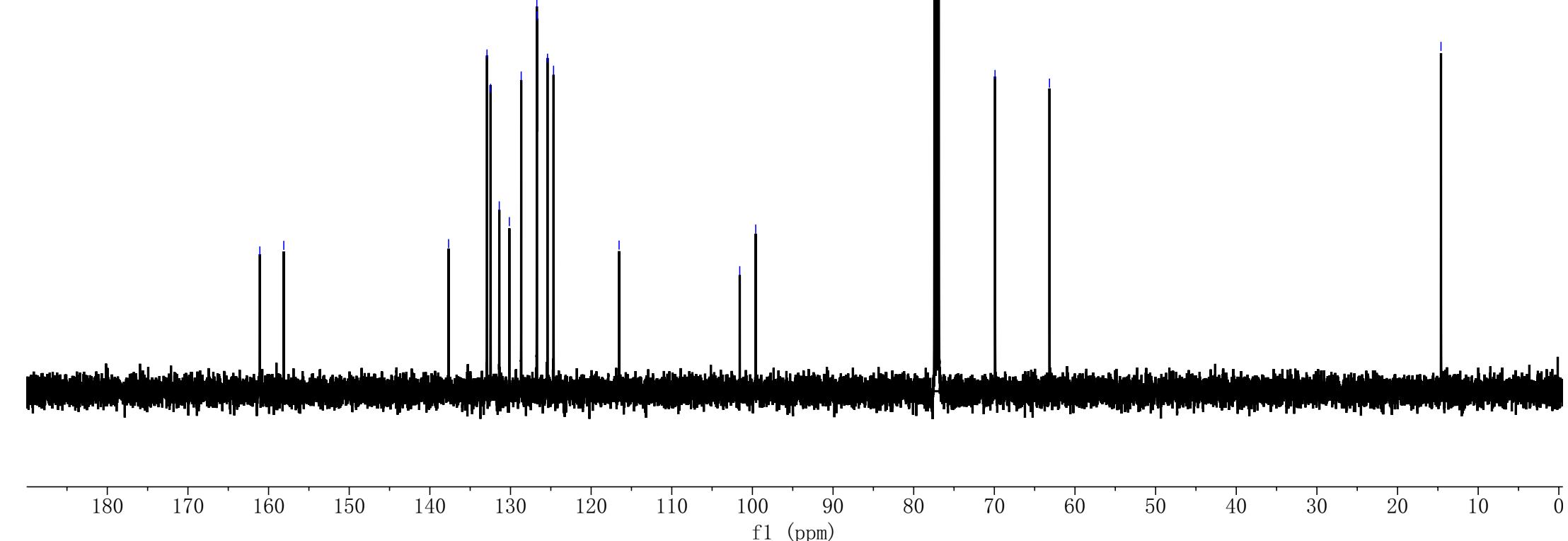


$^1\text{H}$  NMR spectrum of **3ja**

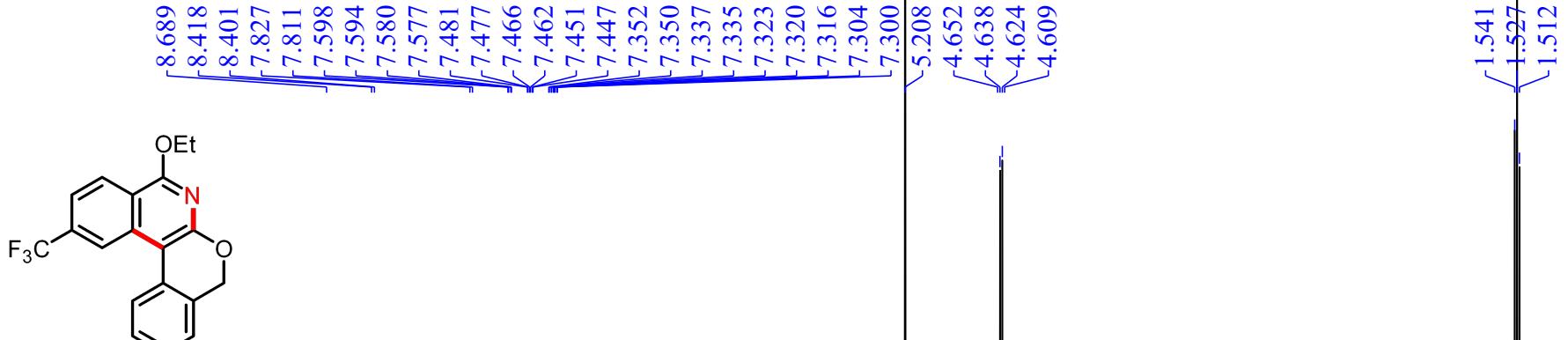


**3ja**

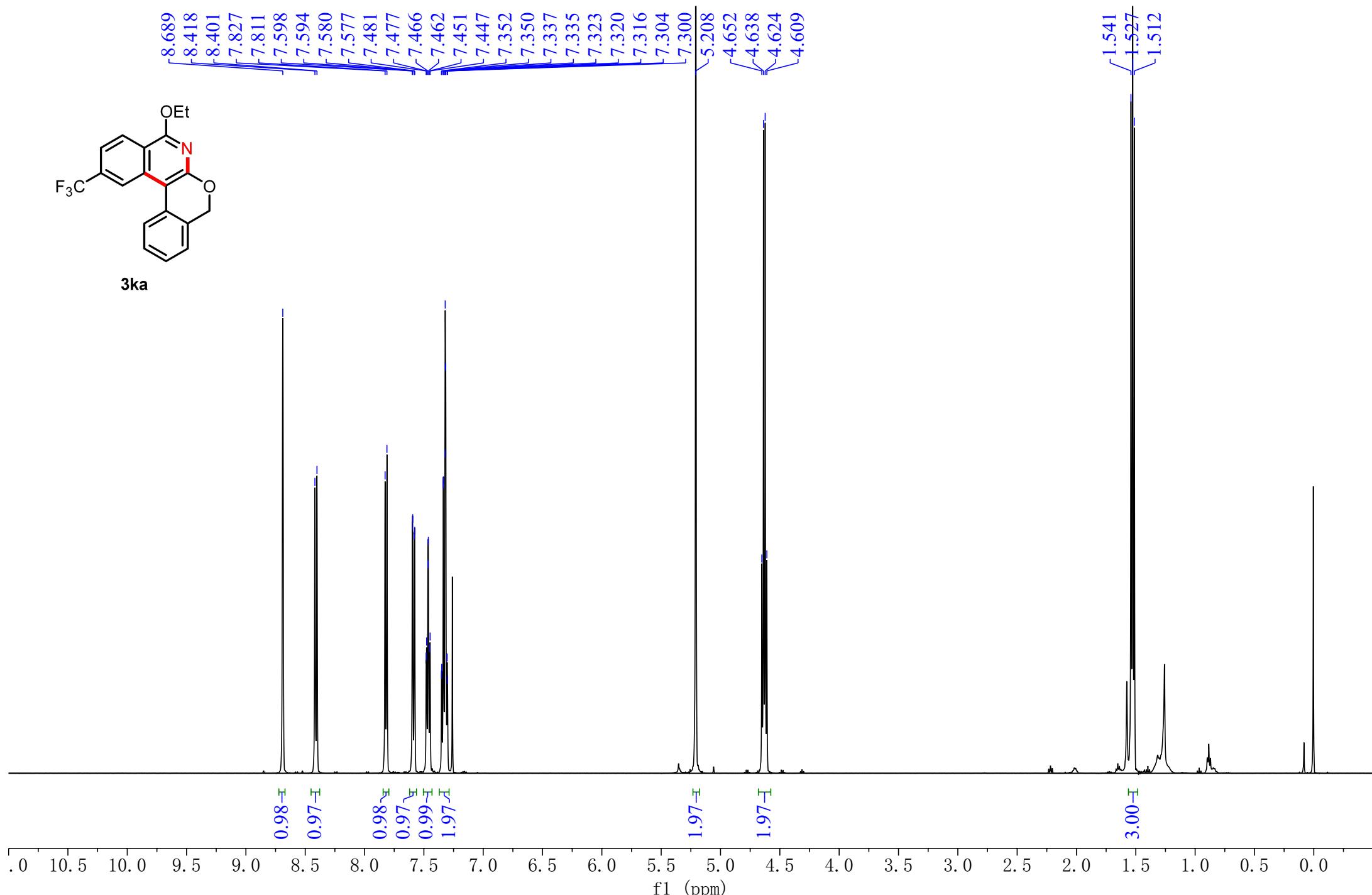
—161.080  
—158.115  
  
137.677  
132.917  
132.467  
131.392  
130.143  
128.674  
126.735  
126.718  
125.410  
124.661  
—116.537  
  
~101.571  
~99.592  
  
—69.917  
—63.163  
  
—14.615



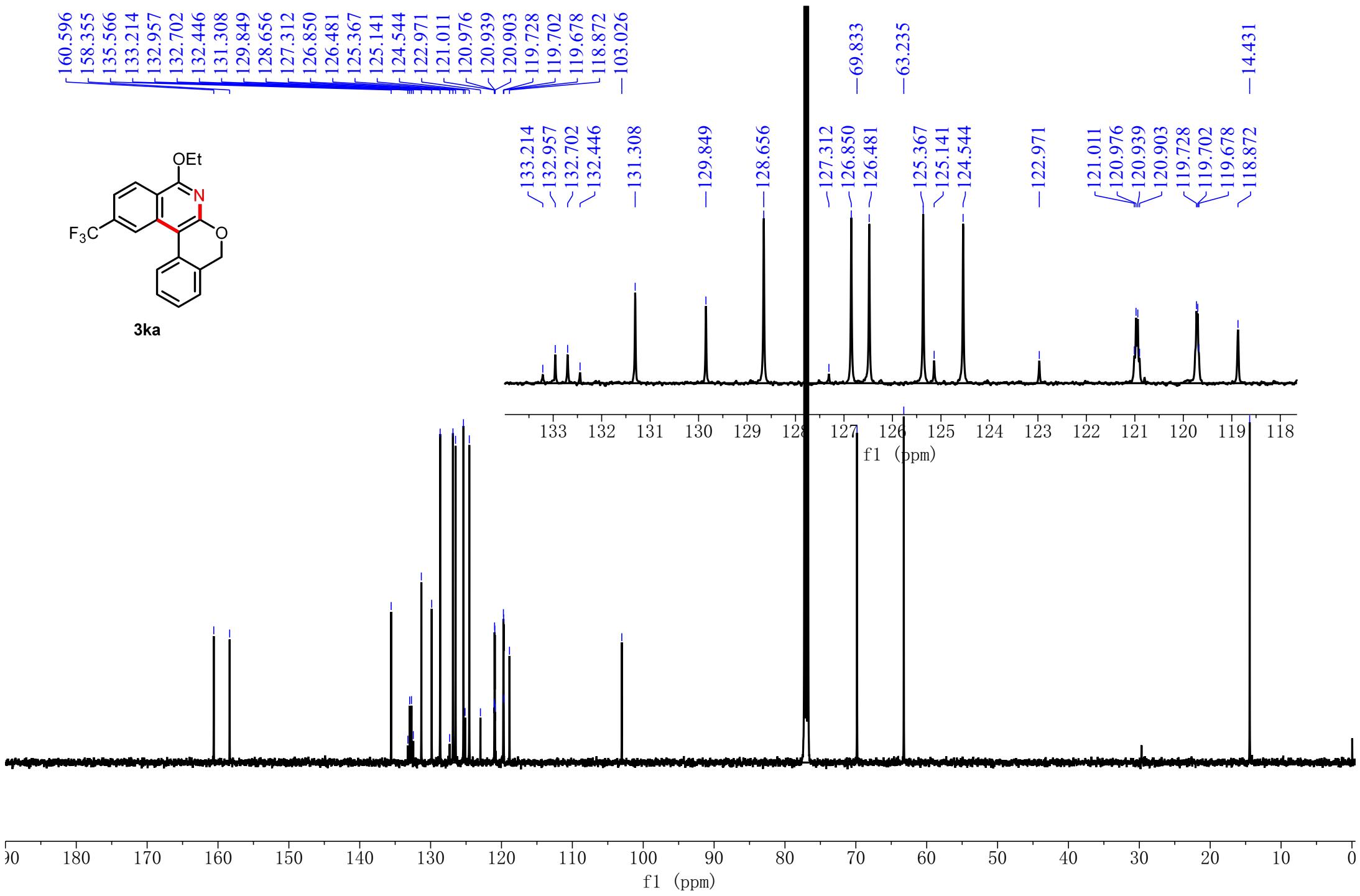
$^{13}\text{C}\{\text{H}\}$  NMR spectrum of **3ja**



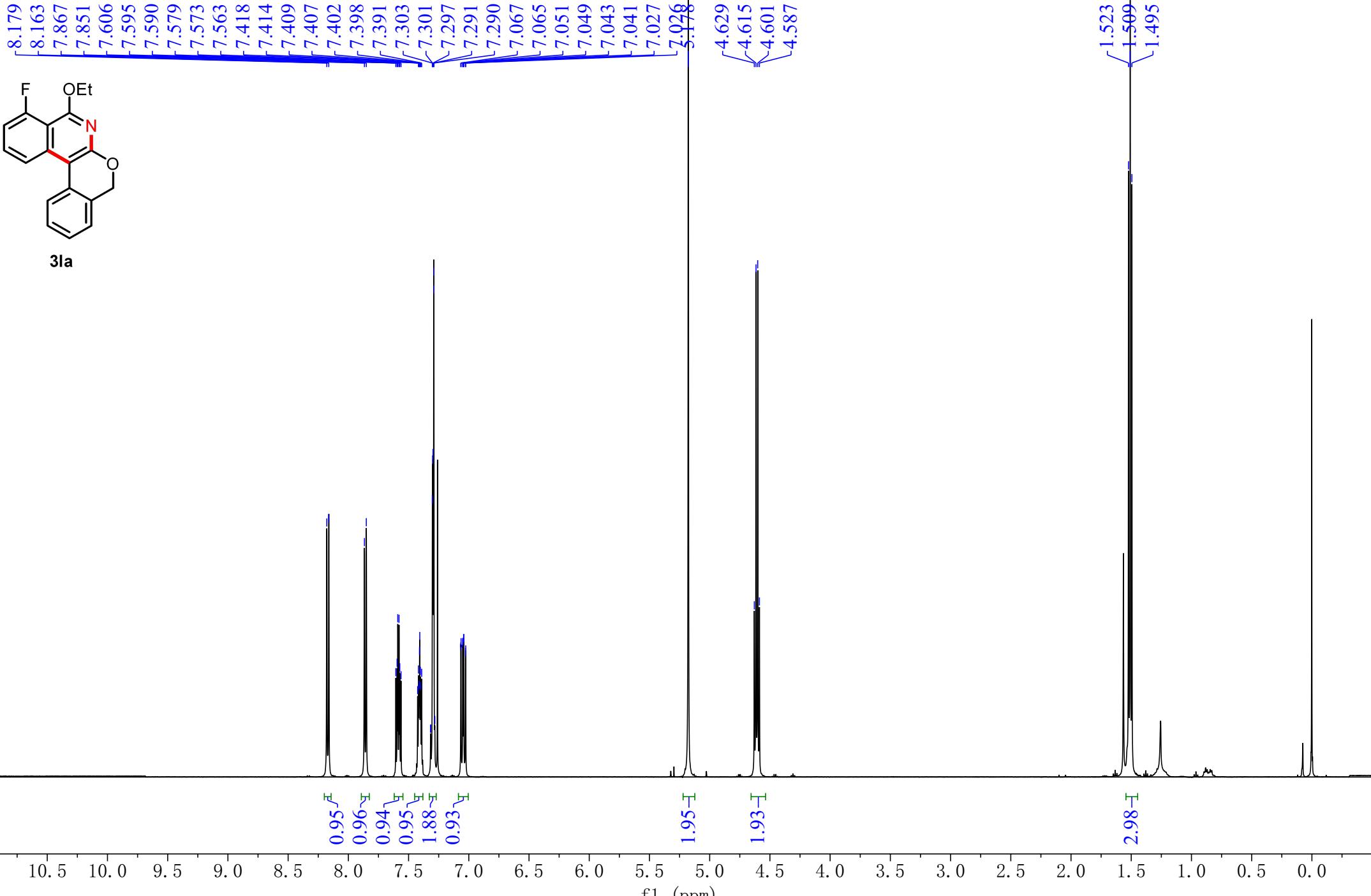
**3ka**



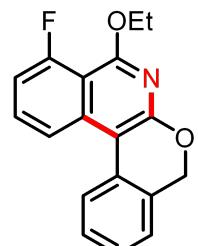
$^1\text{H}$  NMR spectrum of **3ka**



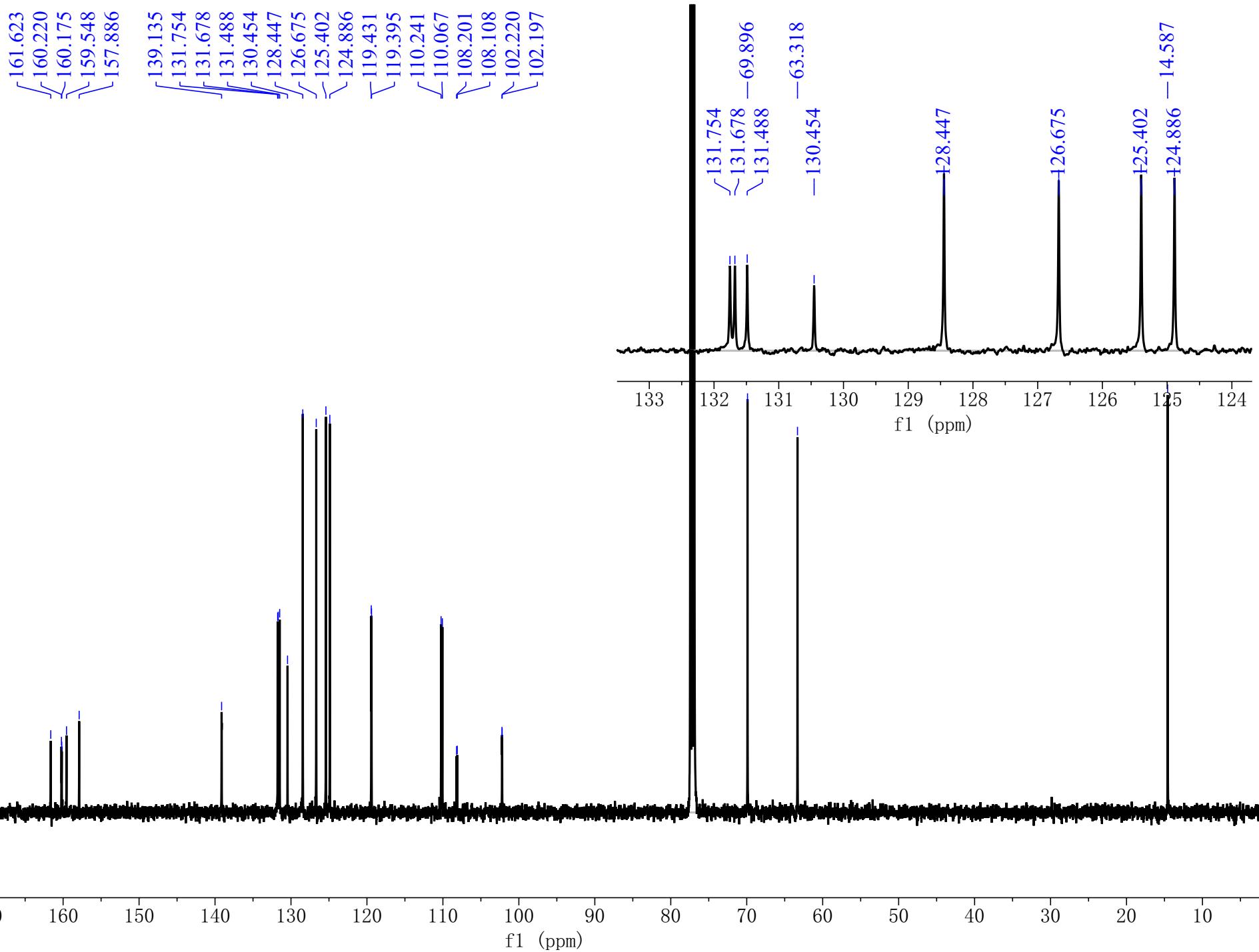
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3ka**



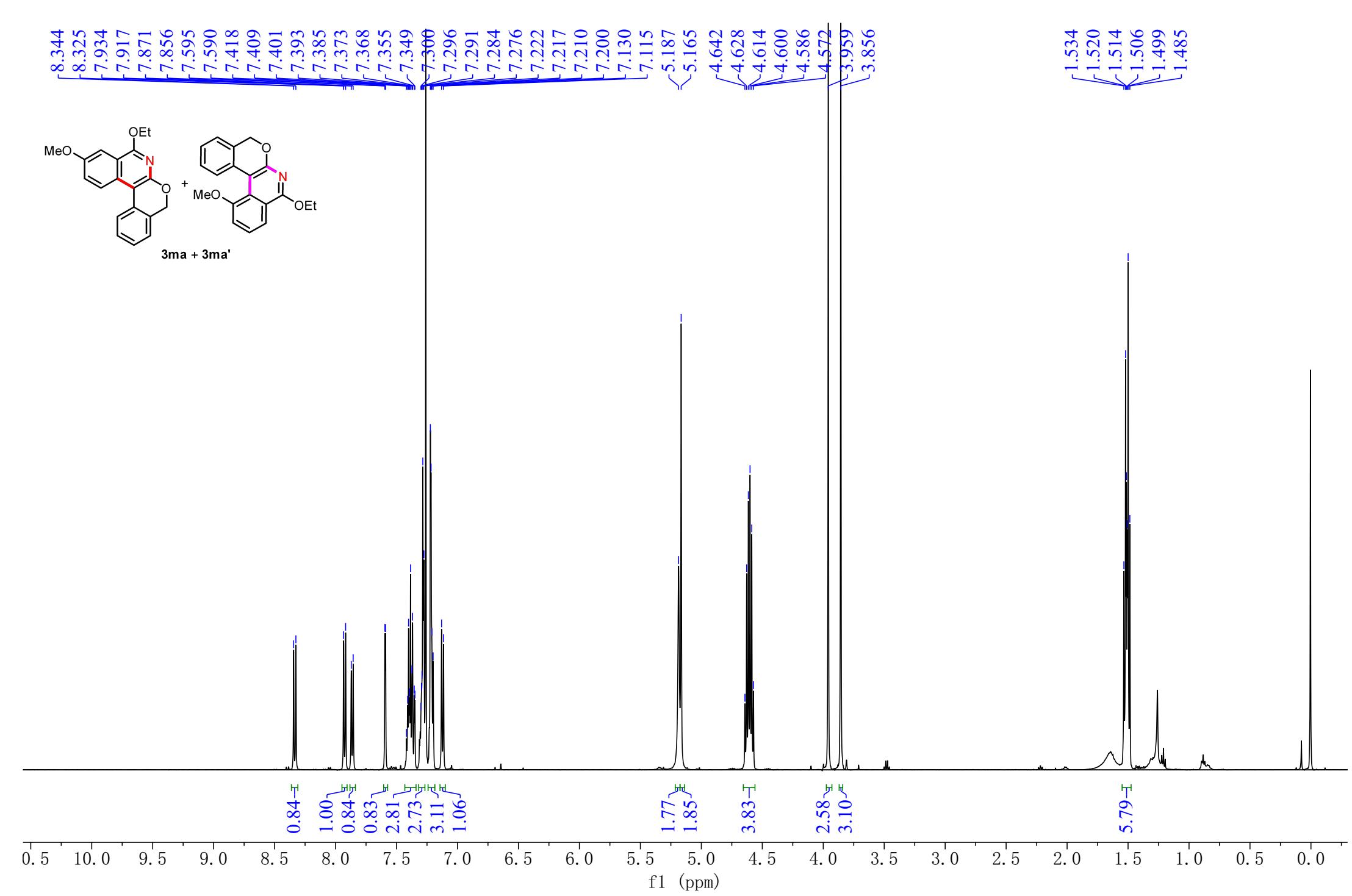
$^1\text{H}$  NMR spectrum of **3la**



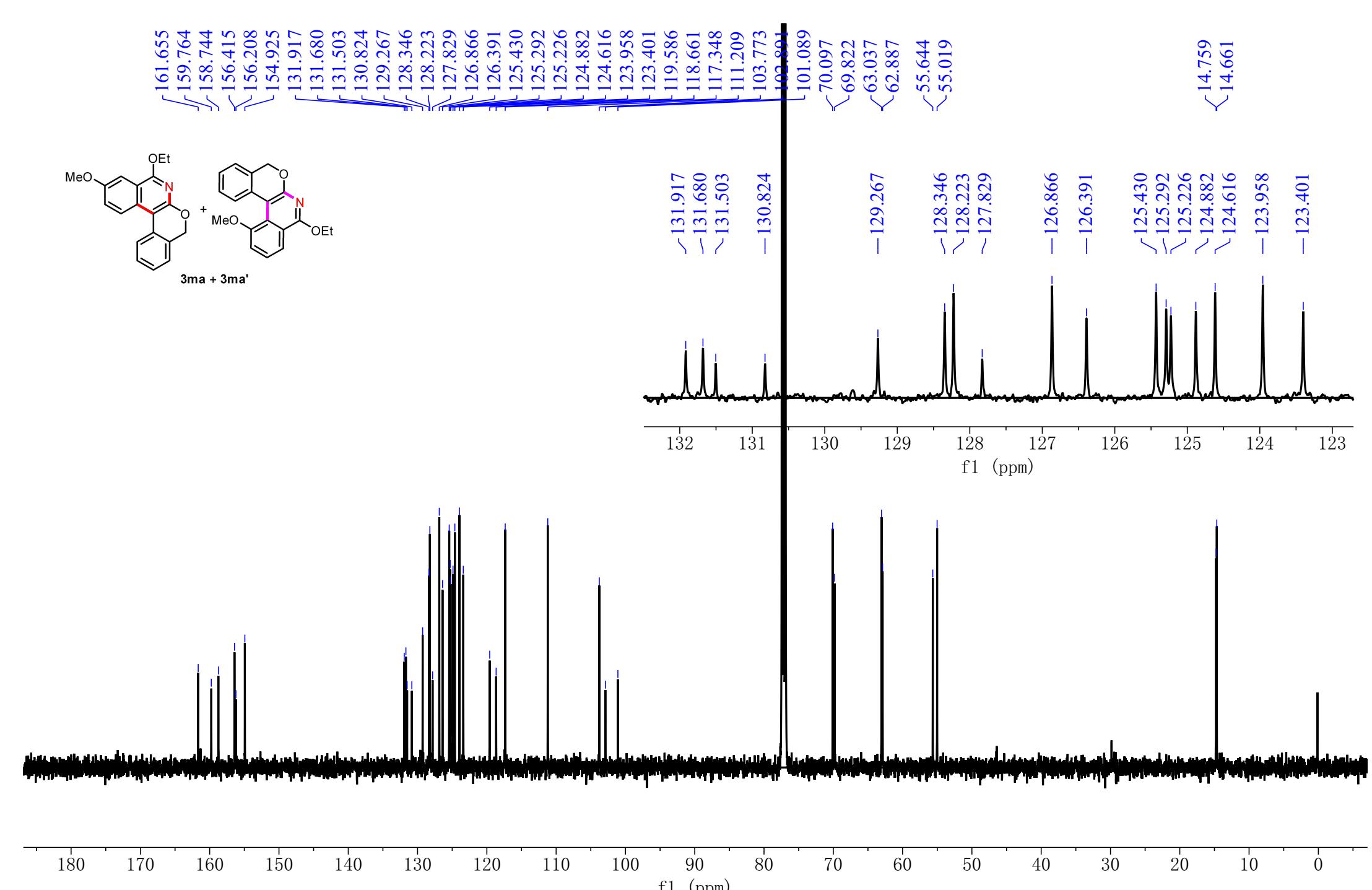
**3la**



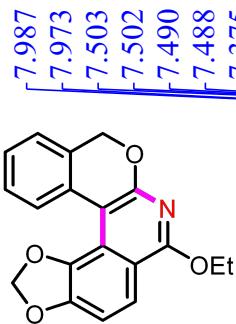
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3la**



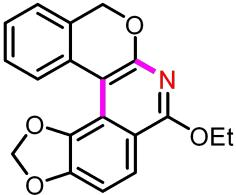
<sup>1</sup>H NMR spectrum of a mixture of **3ma** and **3ma'**



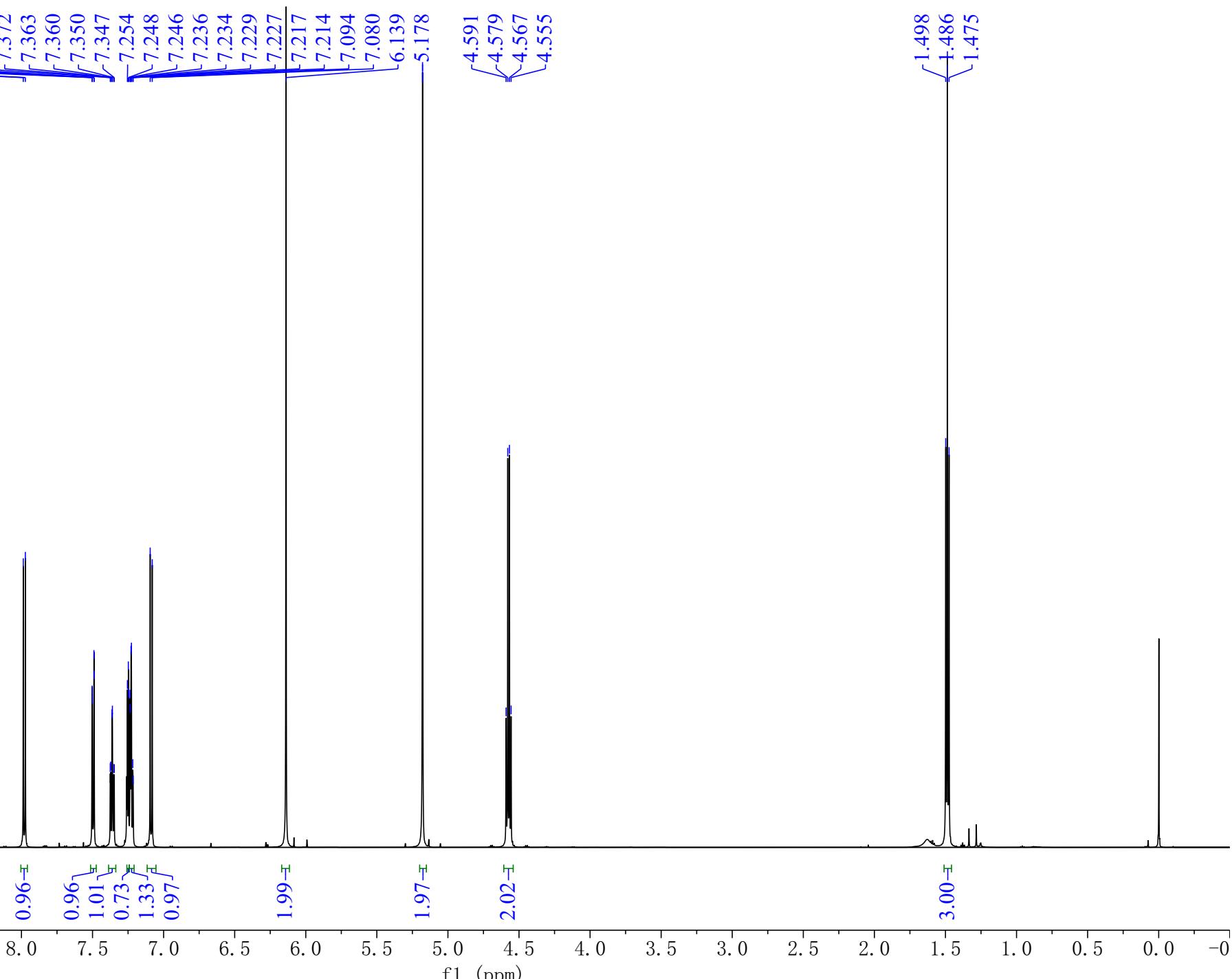
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of a mixture of **3ma** and **3ma'**



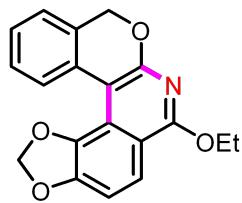
**3na**



**3na**



<sup>1</sup>H NMR spectrum of **3na**



**3na**

—161.750  
—158.921

—149.008

139.950  
130.302  
129.758  
127.622  
127.043  
125.976  
—124.340  
~121.948  
121.118  
—114.629

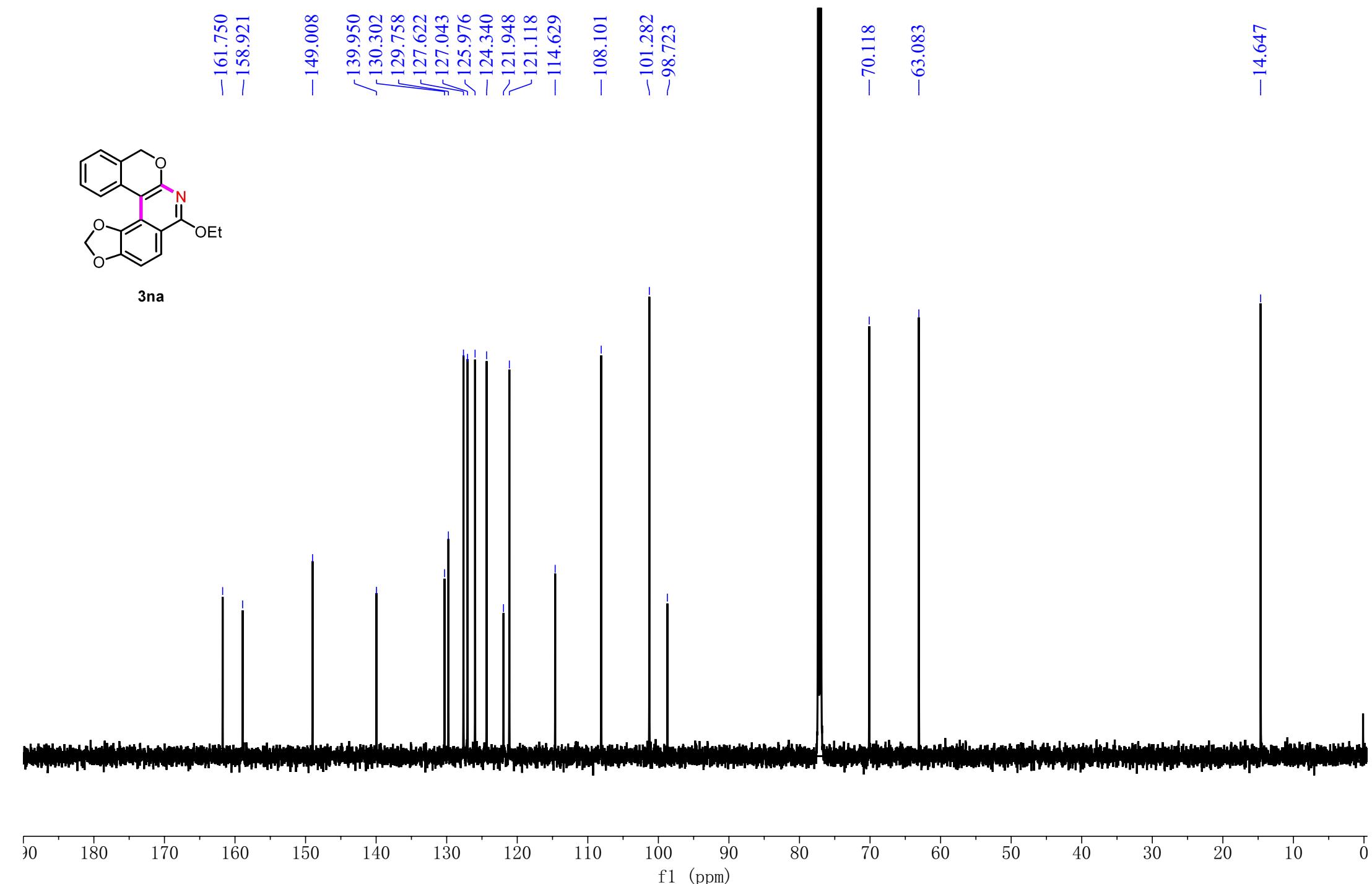
—108.101

—101.282  
—98.723

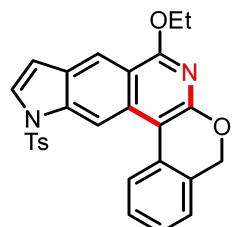
—70.118

—63.083

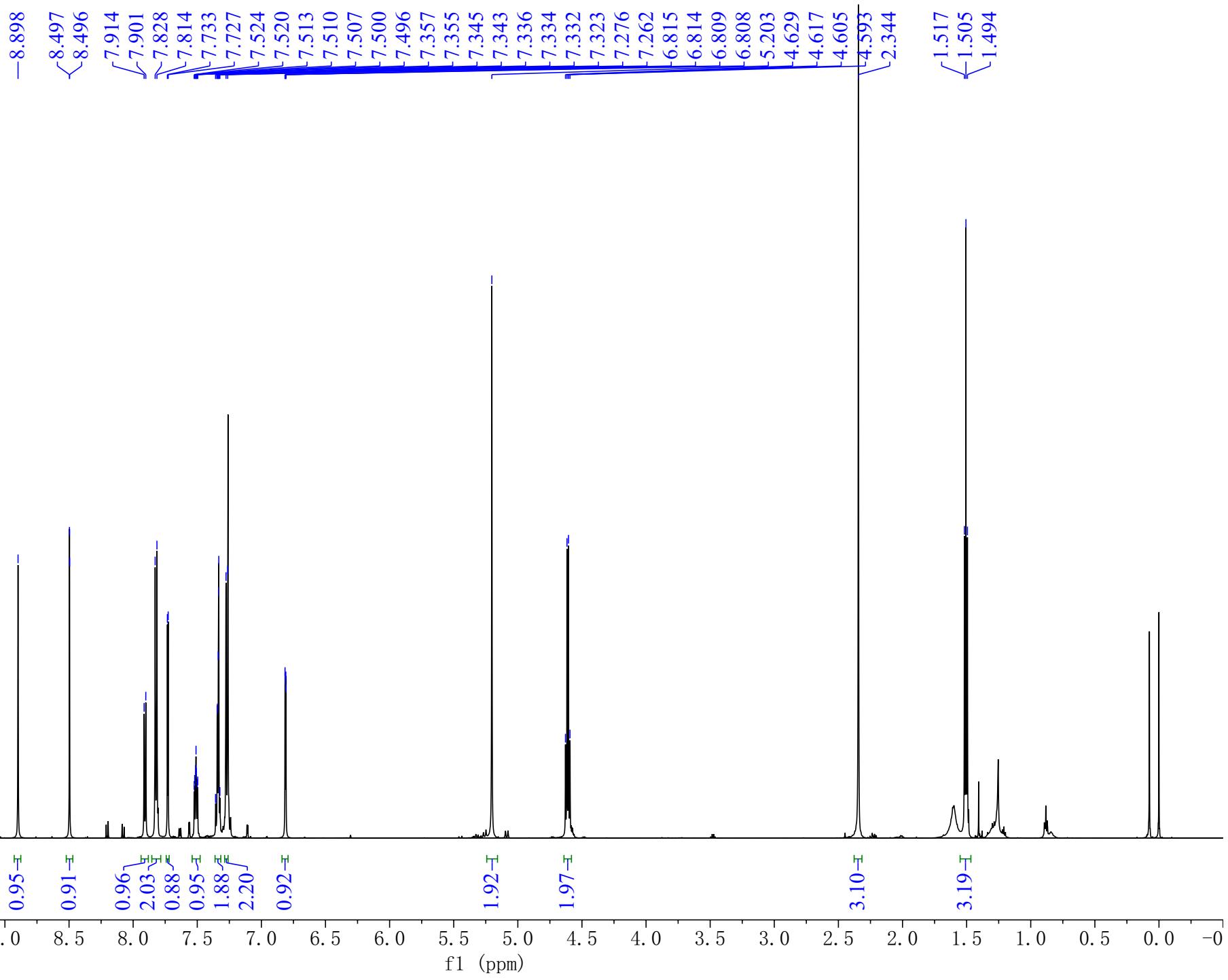
—14.647



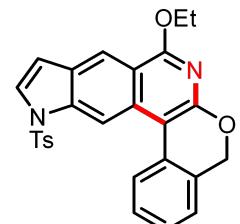
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3na**



**3oa**

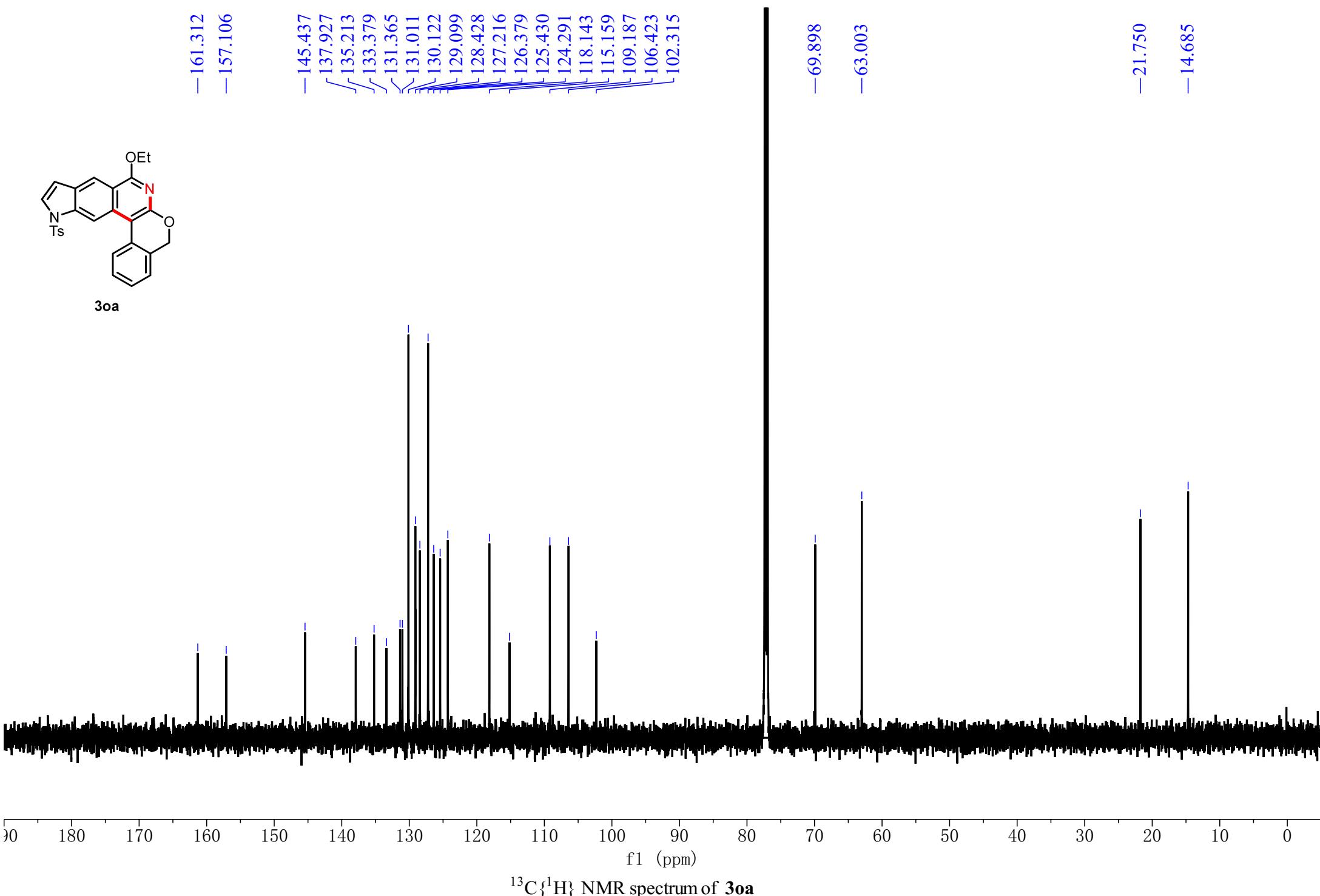


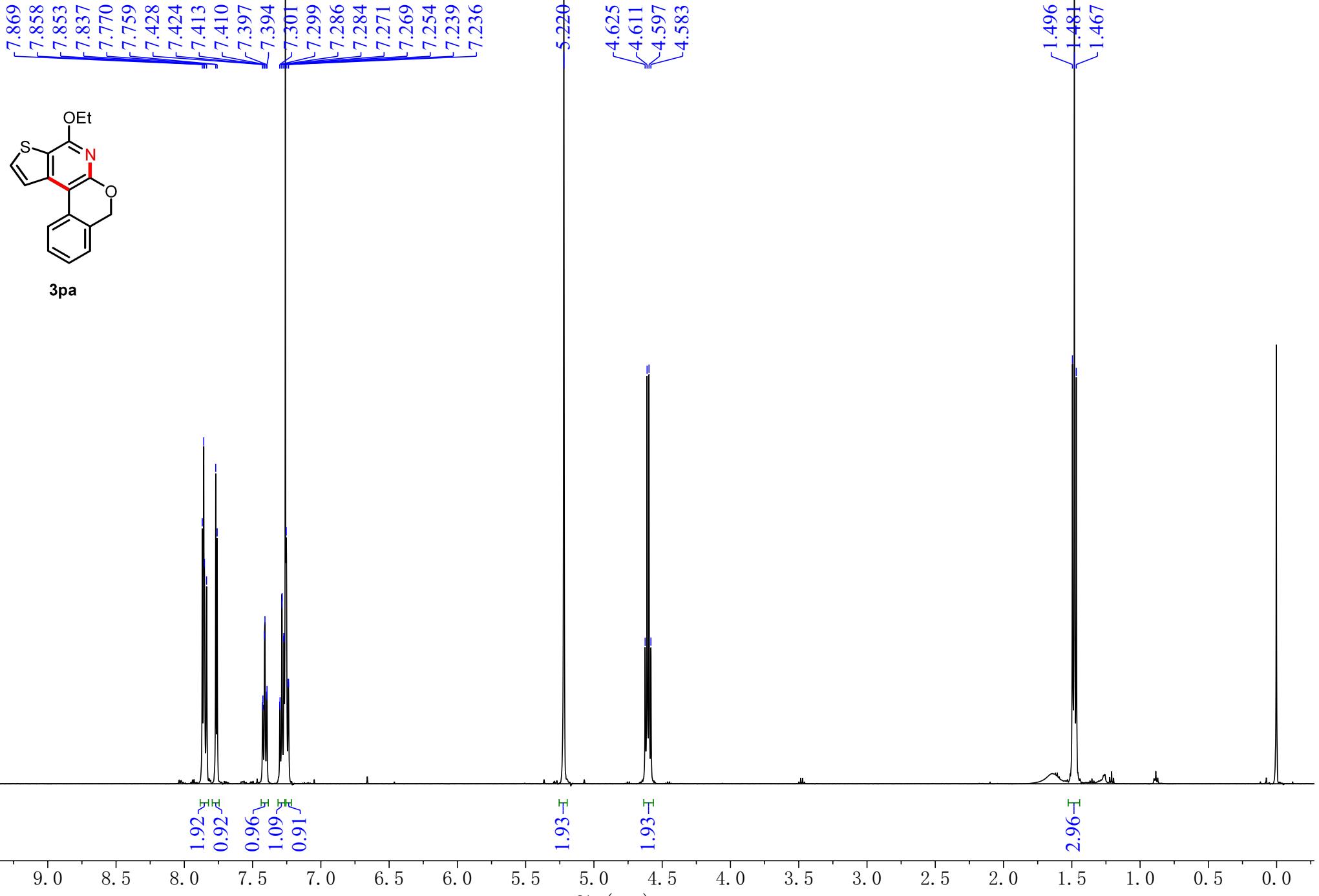
<sup>1</sup>H NMR spectrum of **3oa**



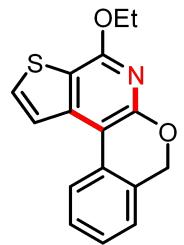
3oa

-161.312  
-157.106  
  
-145.437  
137.927  
135.213  
133.379  
131.365  
131.011  
130.122  
129.099  
128.428  
127.216  
126.379  
125.430  
124.291  
118.143  
115.159  
109.187  
106.423  
102.315

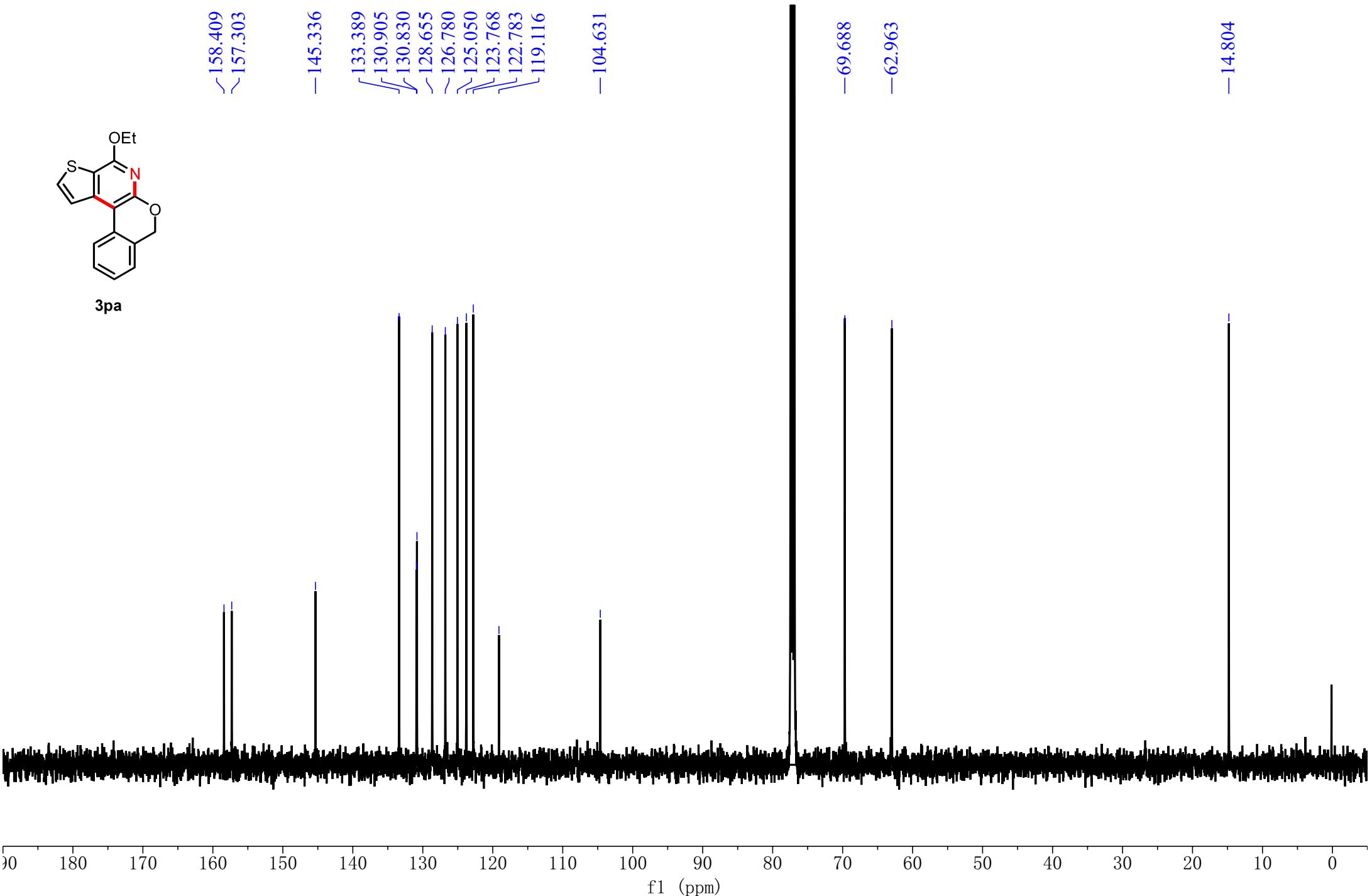




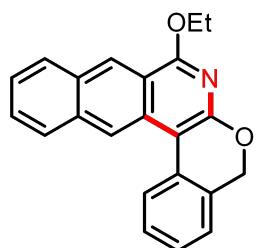
$^1\text{H}$  NMR spectrum of **3pa**



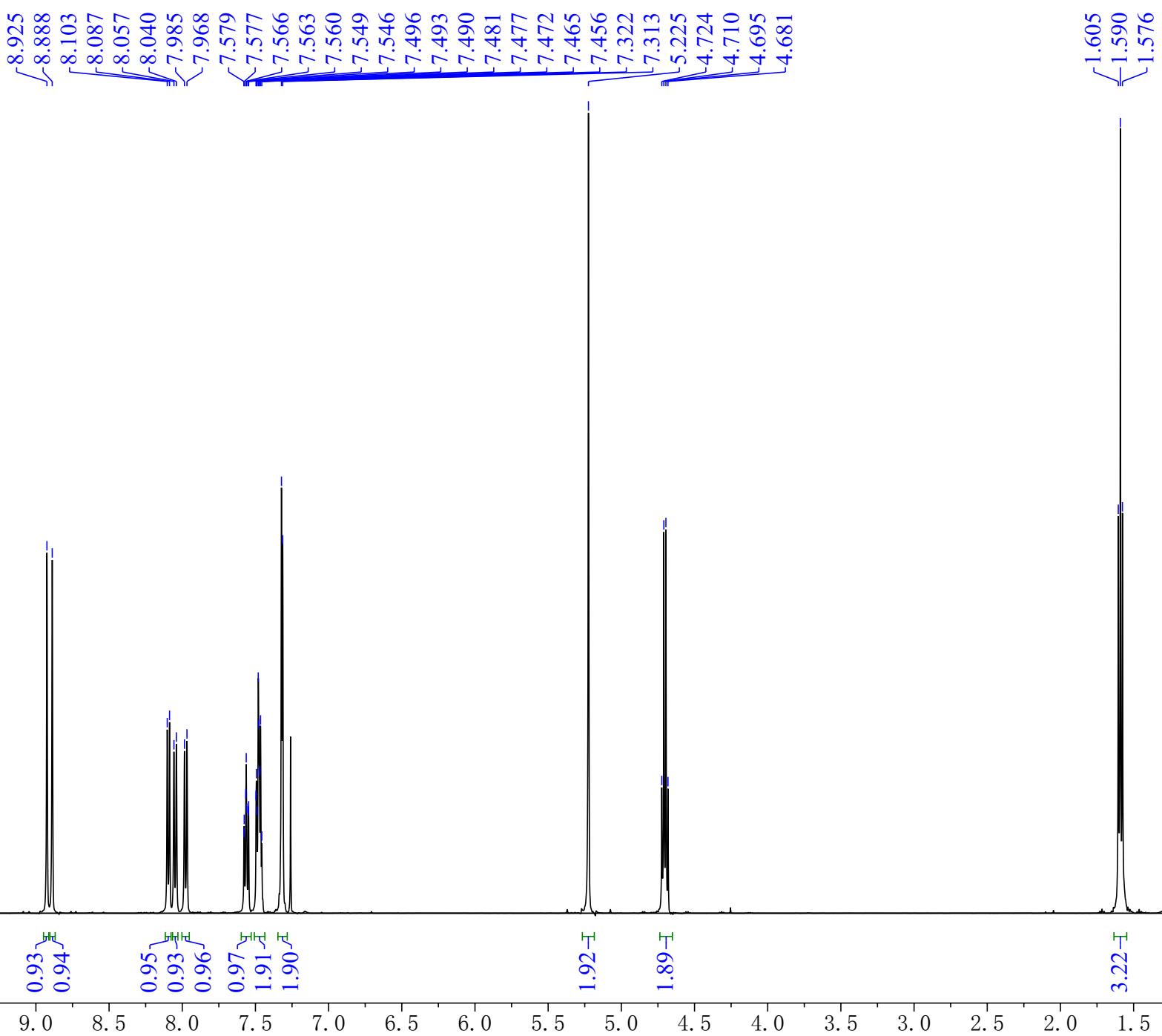
3pa



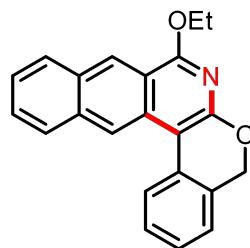
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 3pa



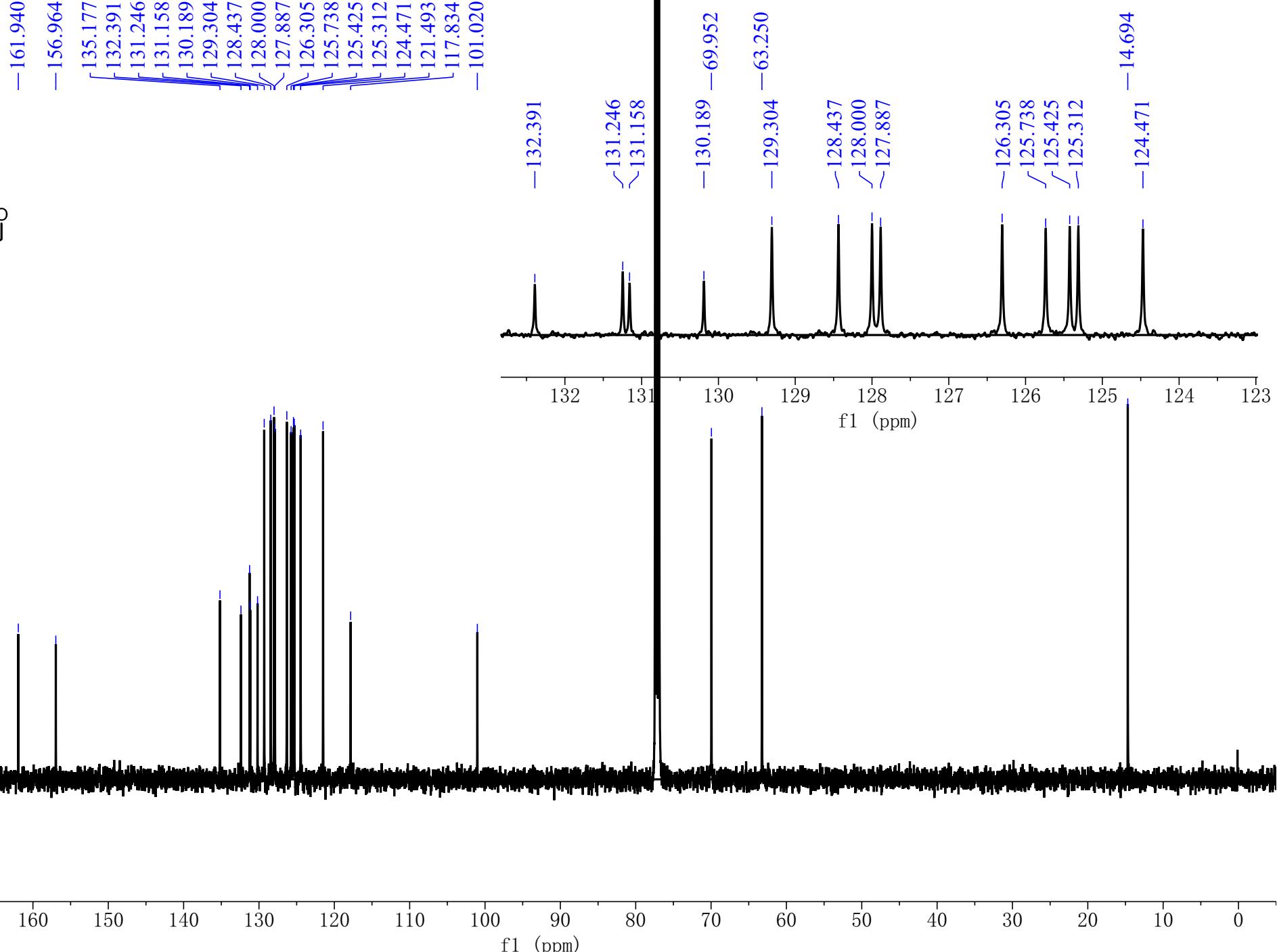
3qa



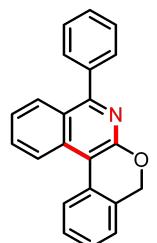
<sup>1</sup>H NMR spectrum of 3qa



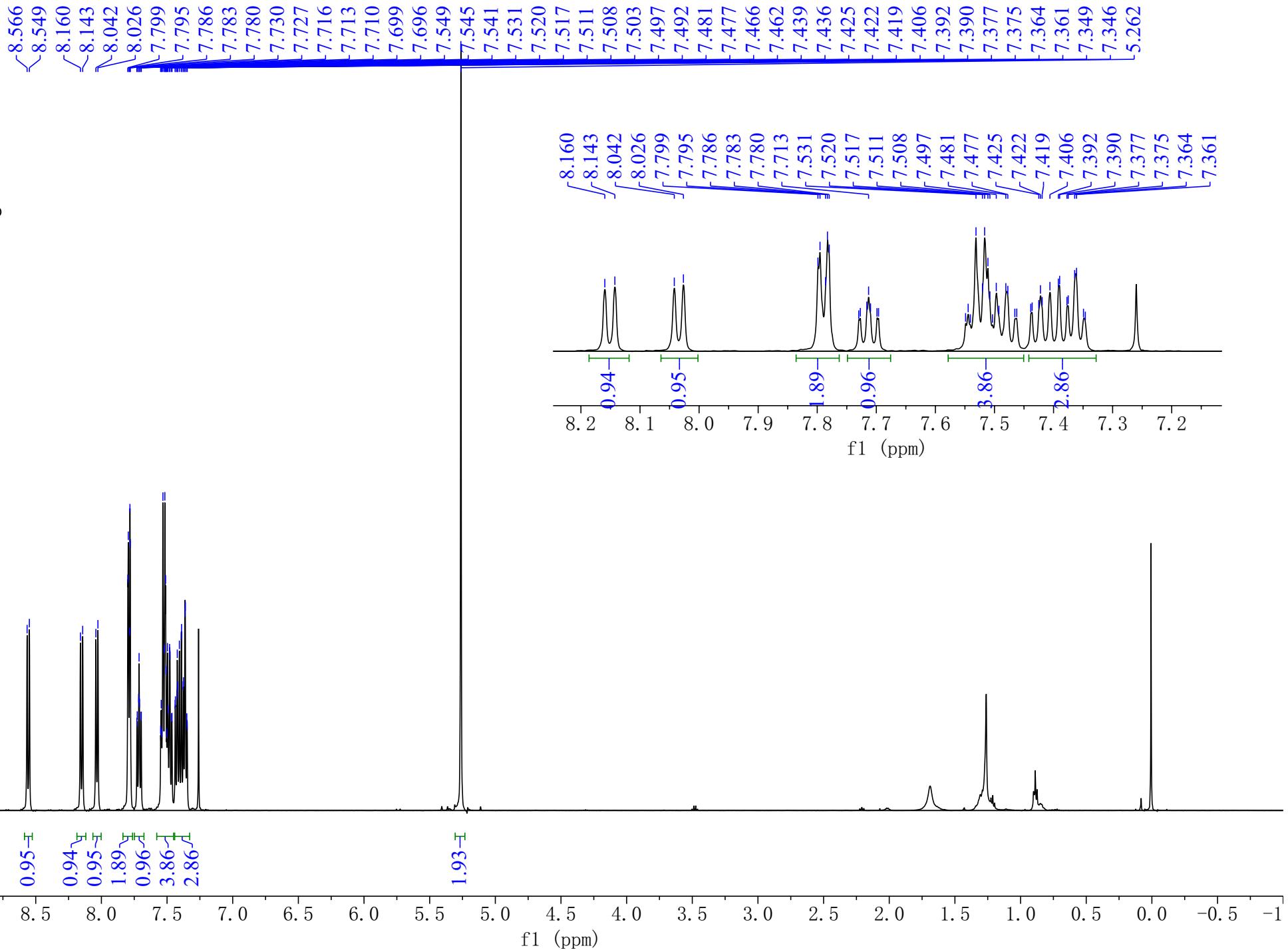
**3qa**



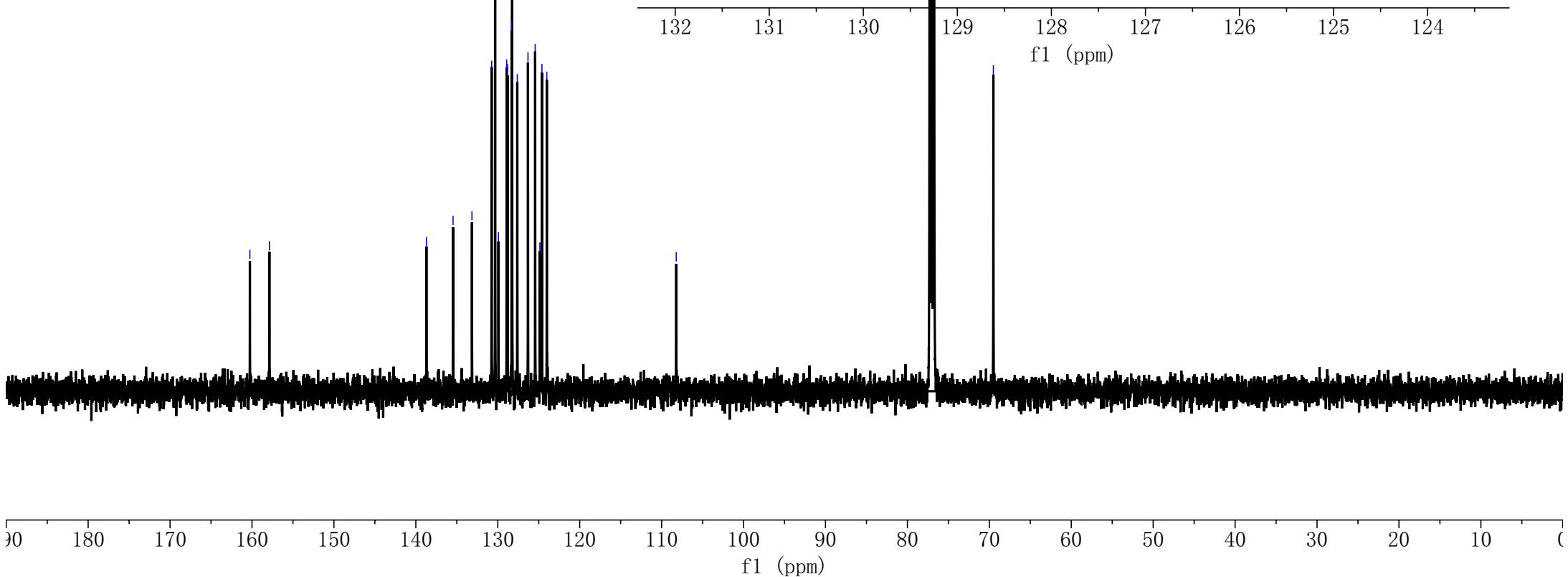
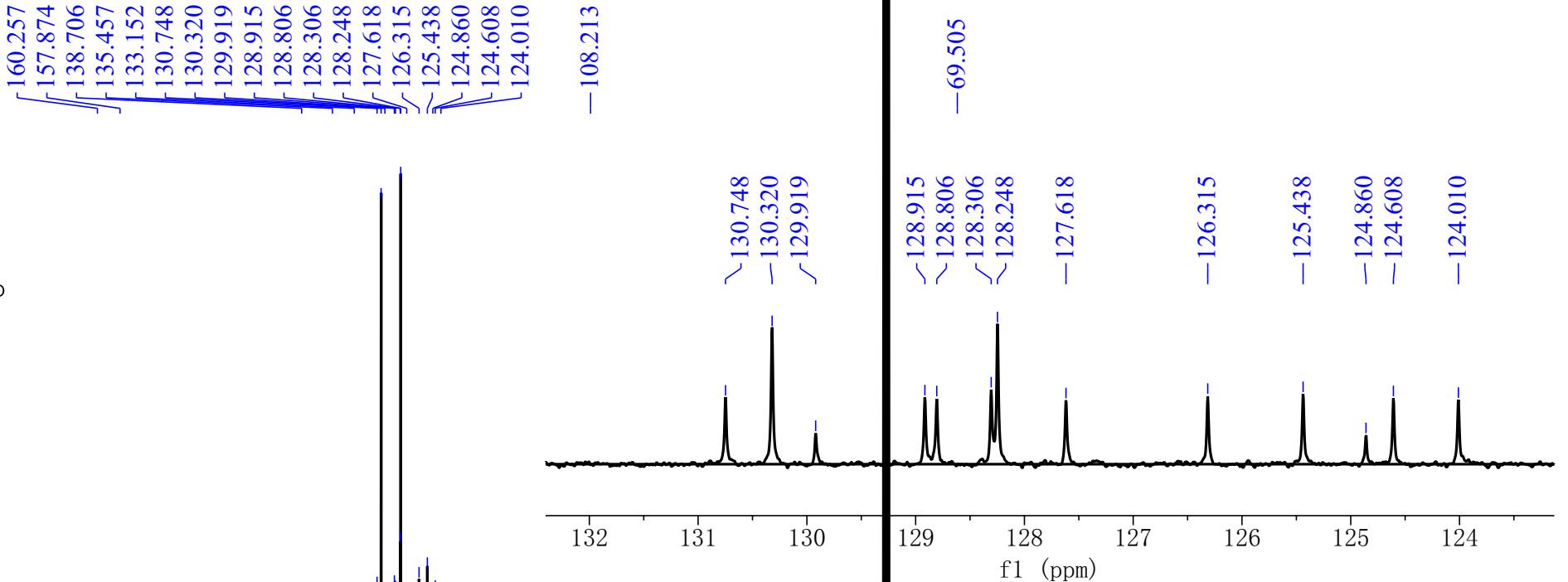
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3qa**



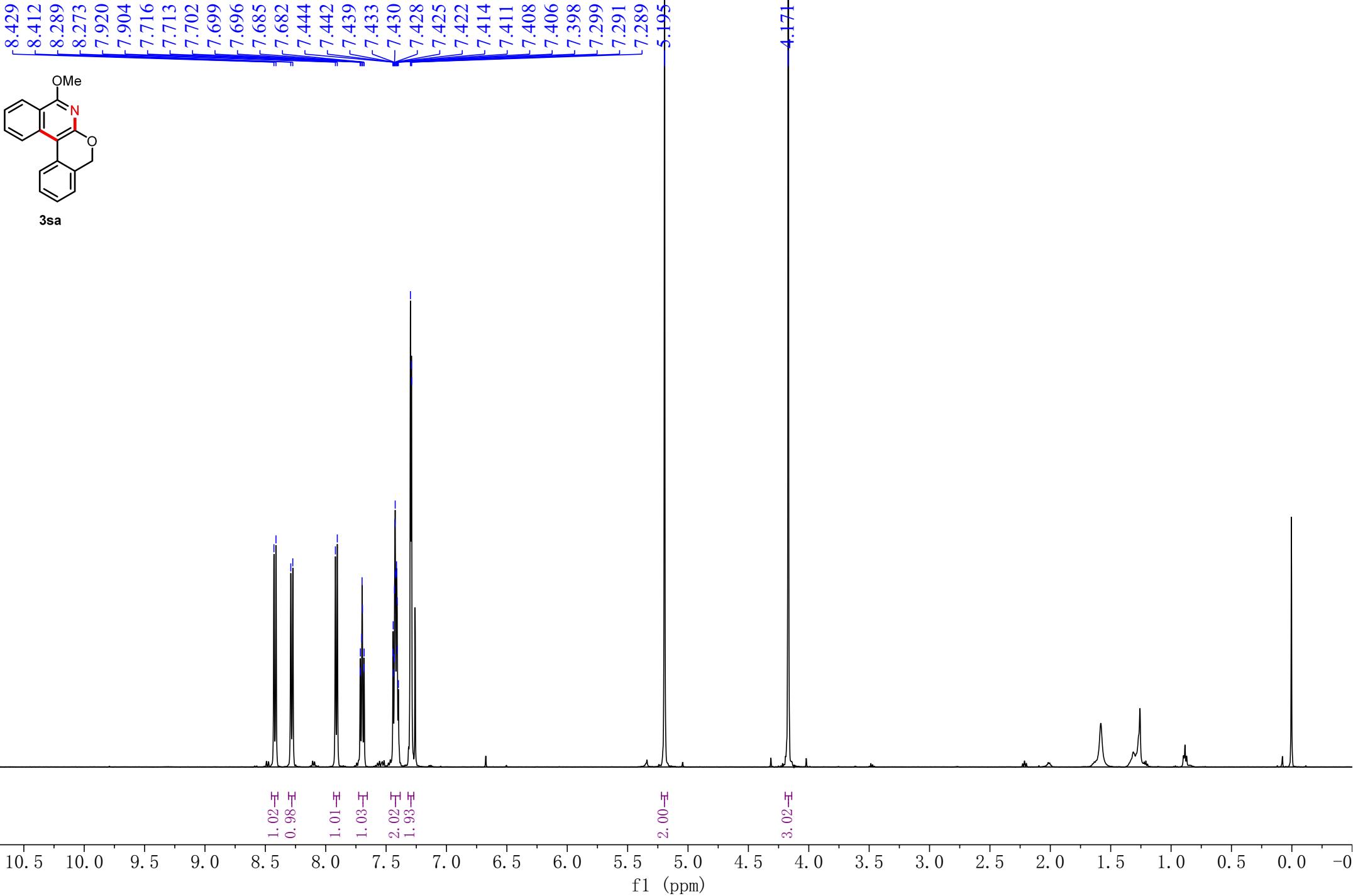
3ra



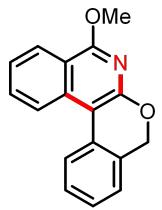
<sup>1</sup>H NMR spectrum of 3ra



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3ra**



$^1\text{H}$  NMR spectrum of **3sa**



3sa

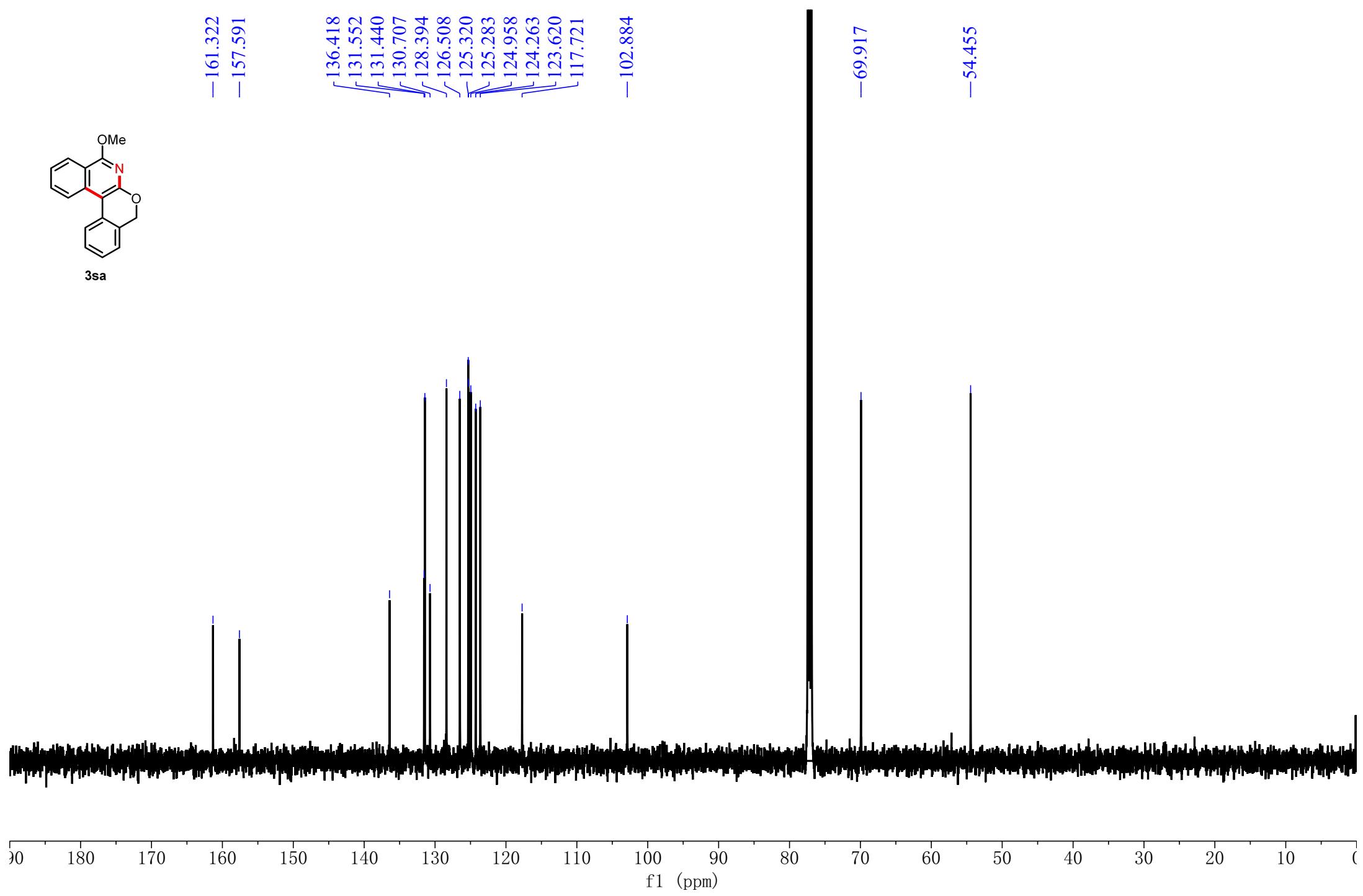
-161.322  
-157.591

136.418  
131.552  
131.440  
130.707  
128.394  
126.508  
125.320  
125.283  
124.958  
124.263  
123.620  
117.721

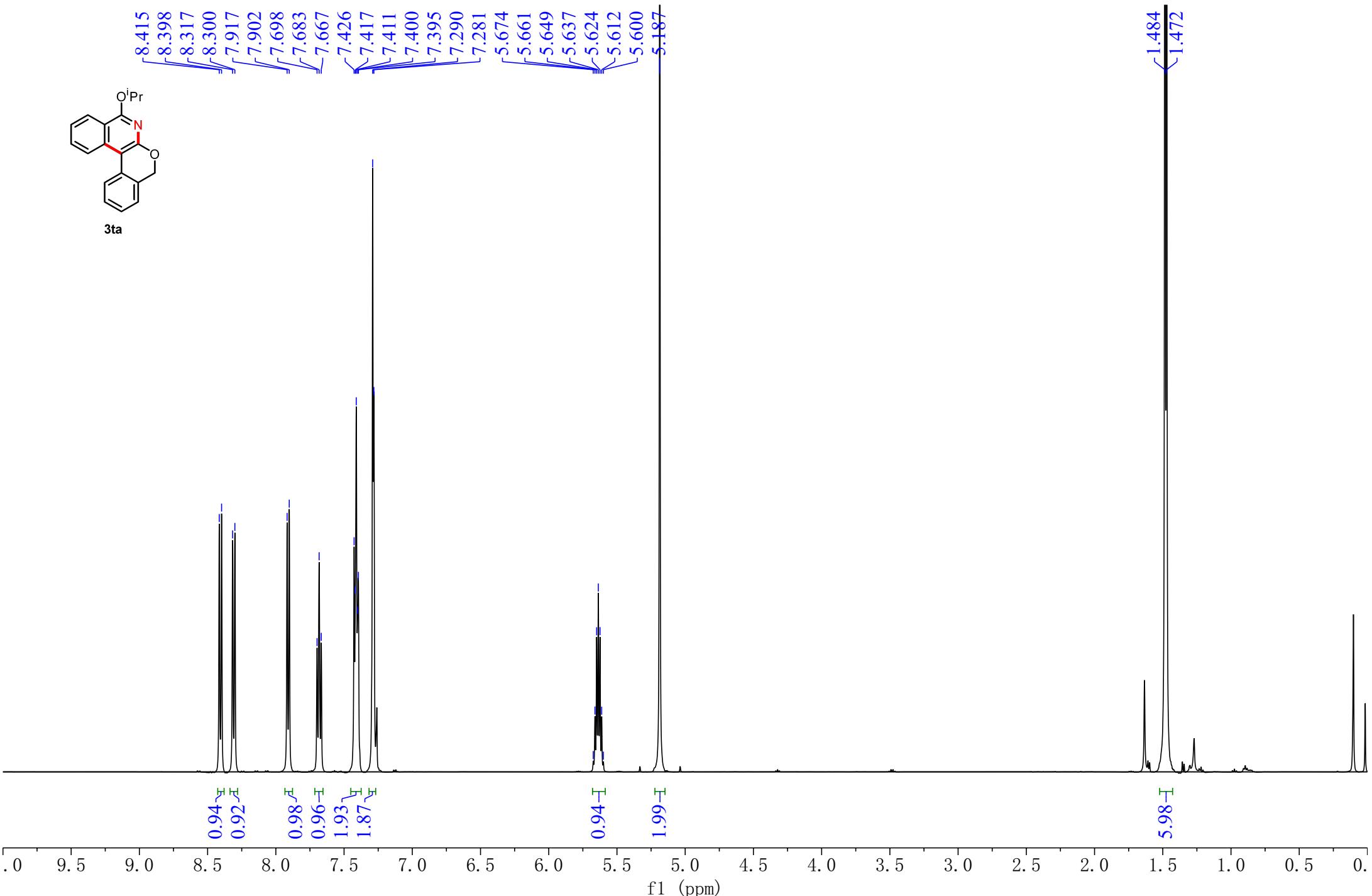
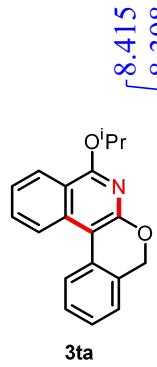
-102.884

-69.917

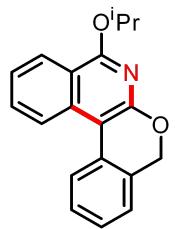
-54.455



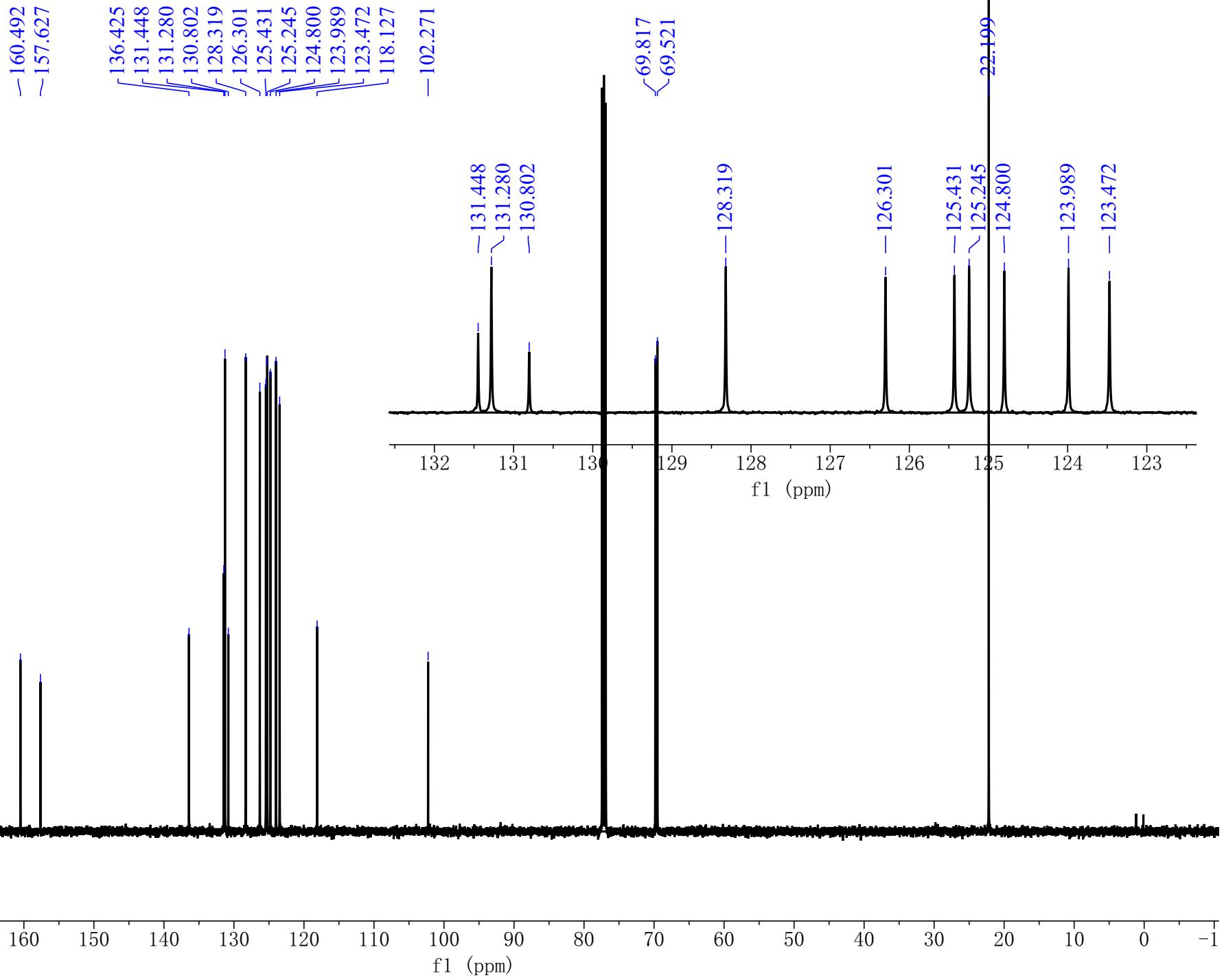
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 3sa

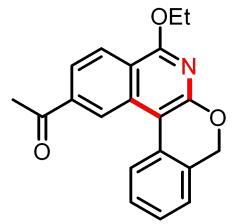


<sup>1</sup>H NMR spectrum of 3ta

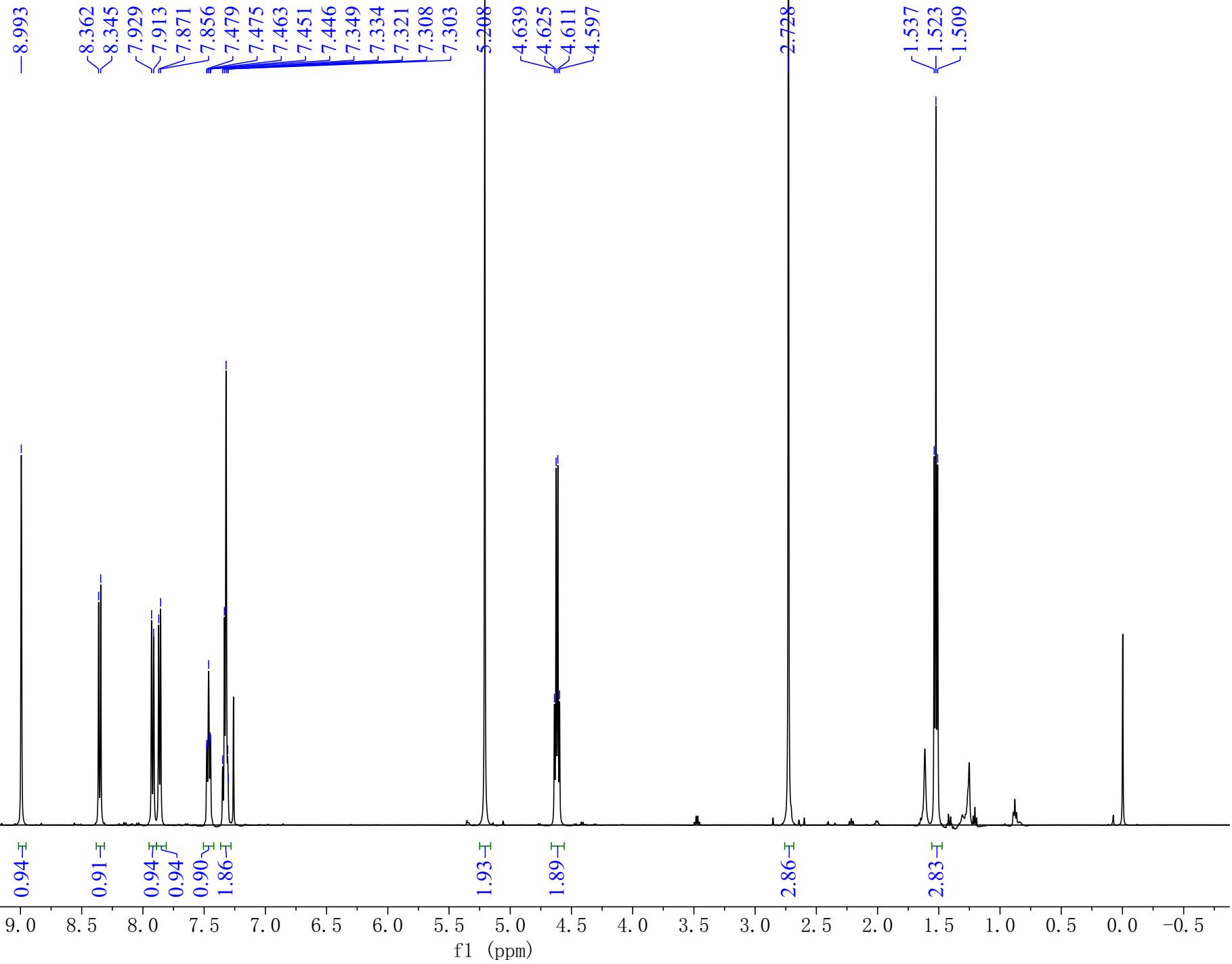


3ta

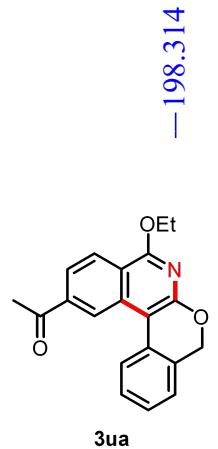




3ua



<sup>1</sup>H NMR spectrum of 3ua



-198.314

$\sim$ 160.772

$\sim$ 158.186

138.907

135.958

131.504

130.274

128.766

126.890

125.525

124.934

124.823

122.405

119.598

-131.504

-103.556

-130.274

-128.766

-126.890

-69.952

-63.308

>125.525

<124.934

<124.823

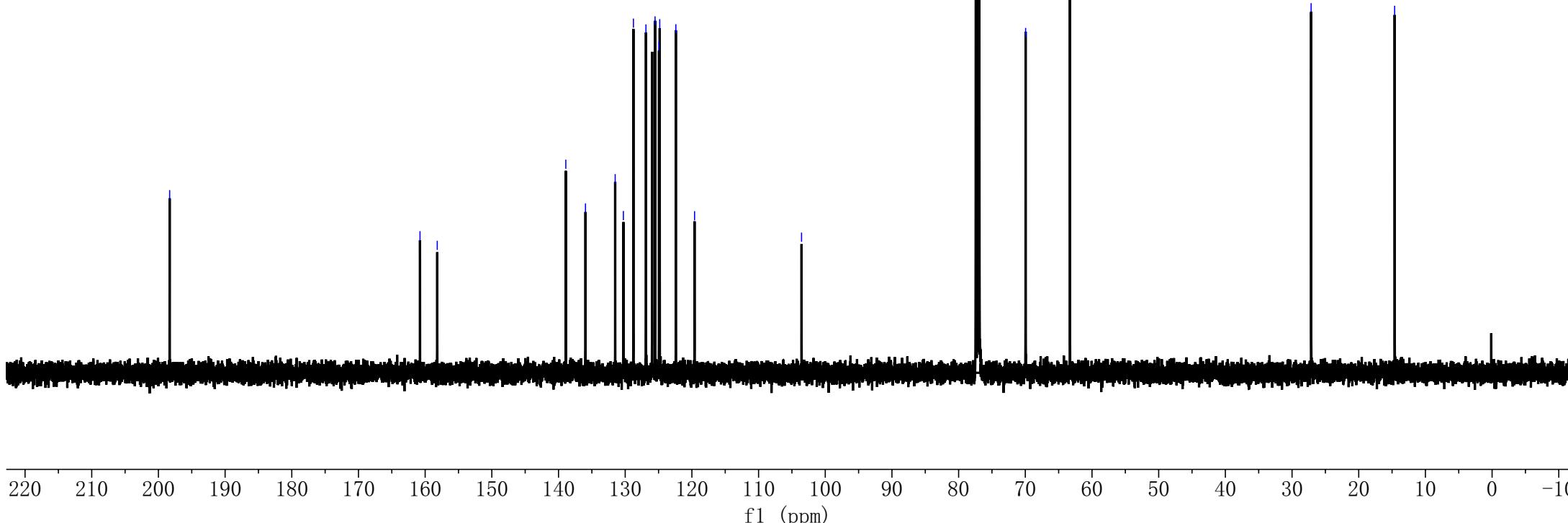
-122.405

-27.139

-14.613

-119.598

132 131 130 129 128 127 126 125 124 123 122 121 120 119 118  
f1 (ppm)



$^{13}\text{C}\{\text{H}\}$  NMR spectrum of 3ua

9.138  
9.136

8.344

8.330

8.001

7.999

7.987

7.984

7.99

7.98

7.984

7.984

7.910

7.897

7.897

7.897

7.475

7.472

7.462

7.459

7.450

7.447

7.339

7.337

7.326

7.325

7.315

7.313

7.311

7.308

7.298

7.295

5.206

4.637

4.626

4.614

4.602

4.477

4.465

4.453

4.441

1.535

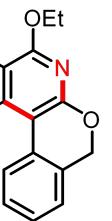
1.524

1.512

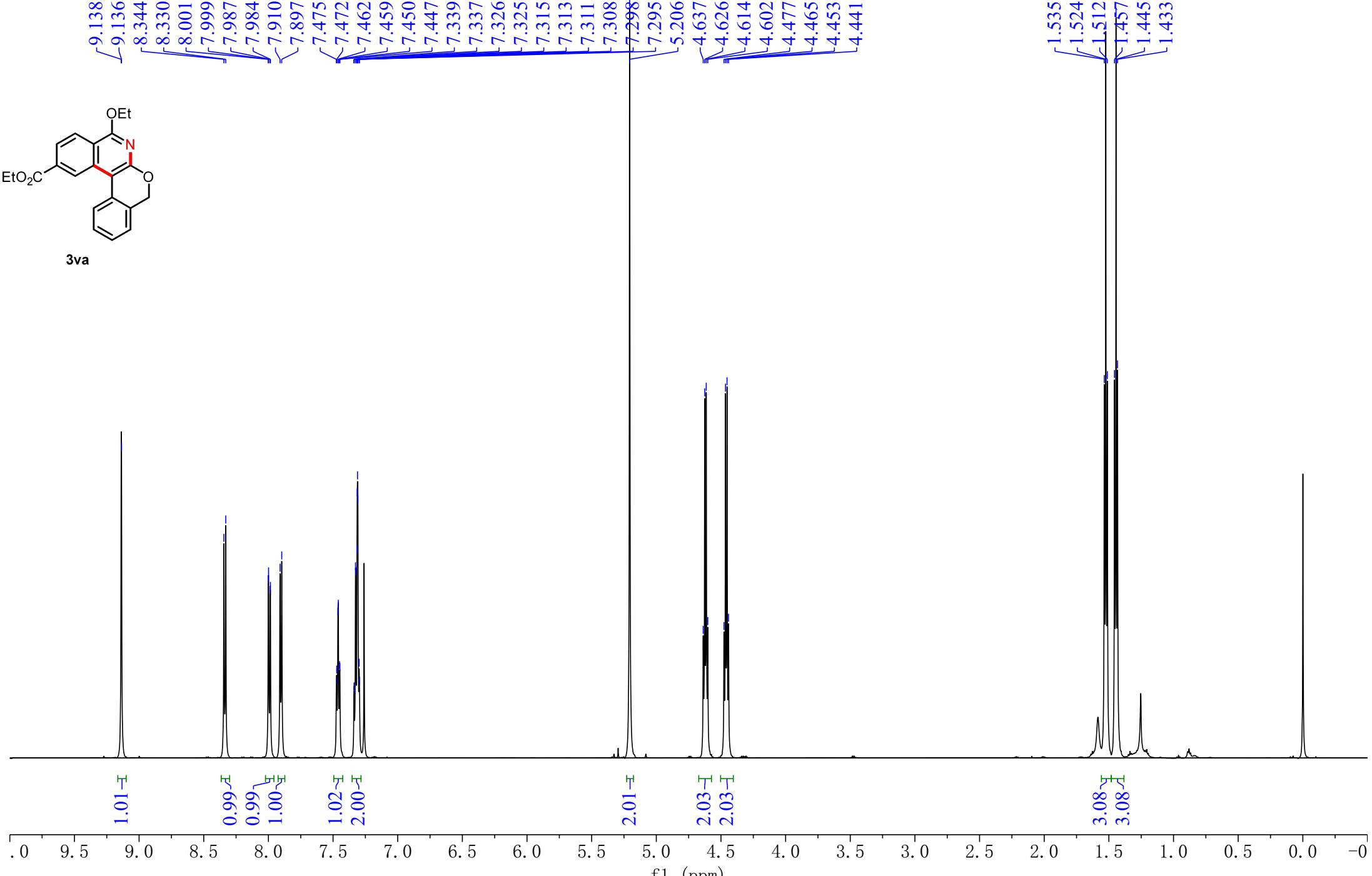
1.457

1.445

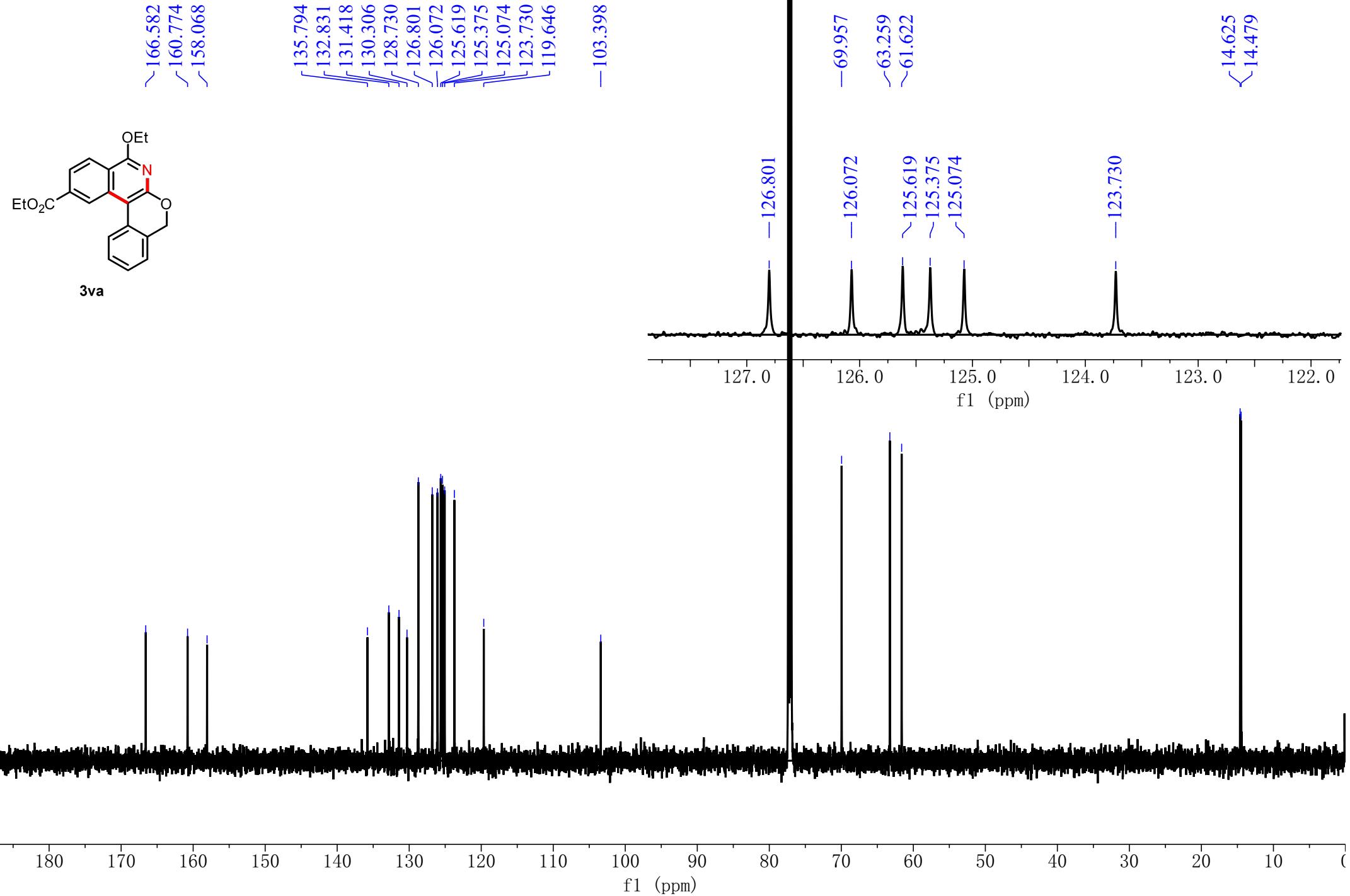
1.433



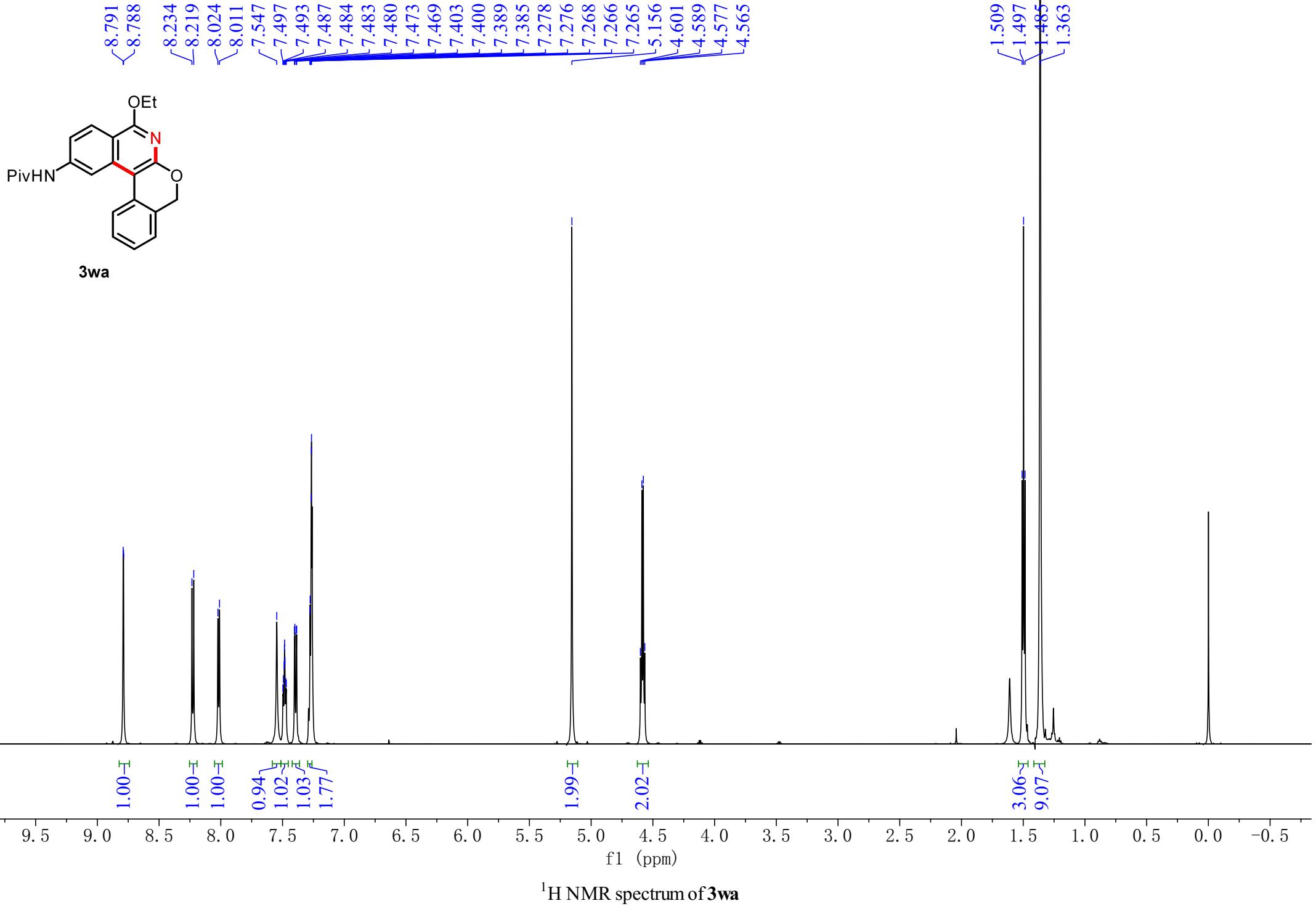
3va

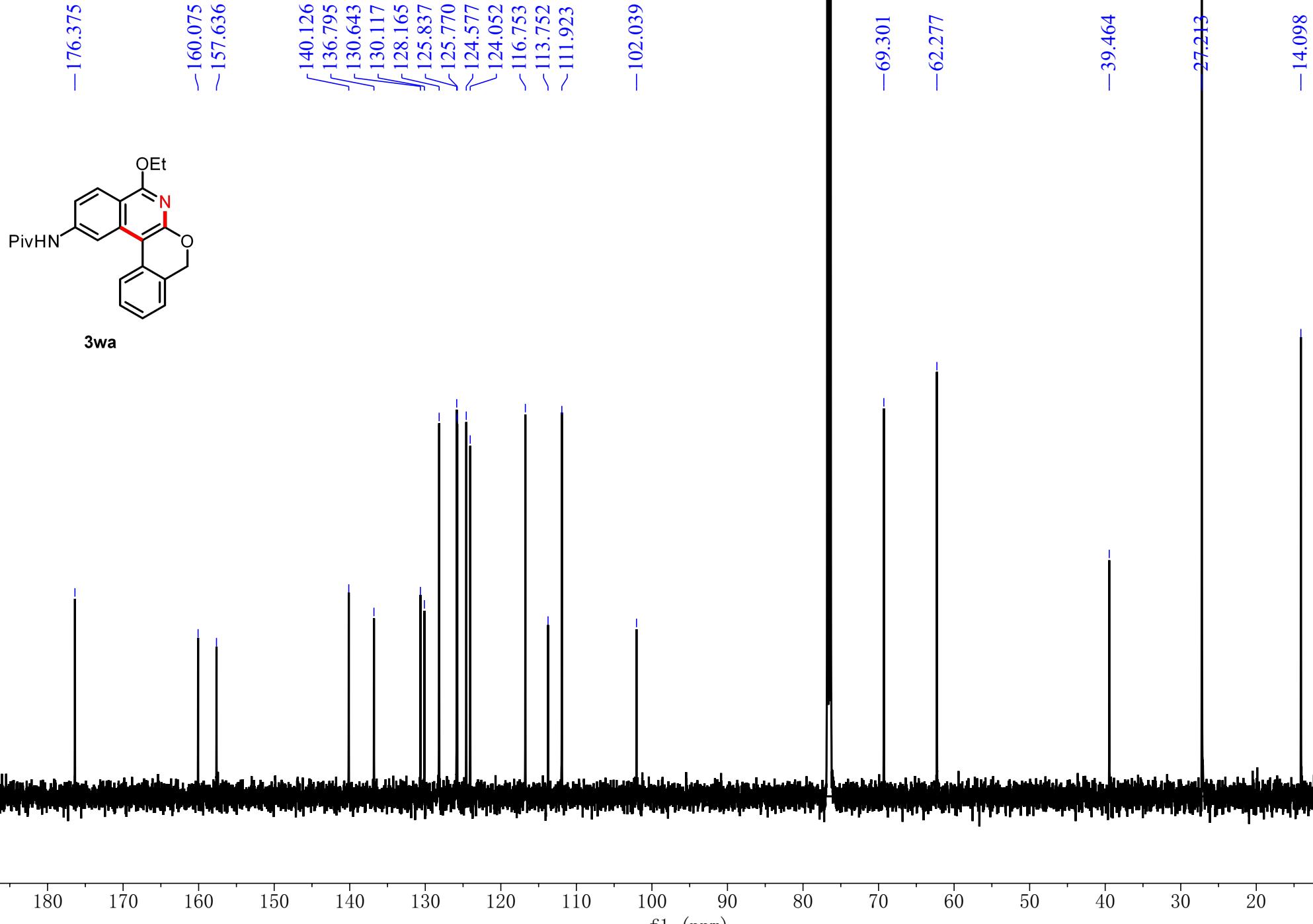


<sup>1</sup>H NMR spectrum of 3va

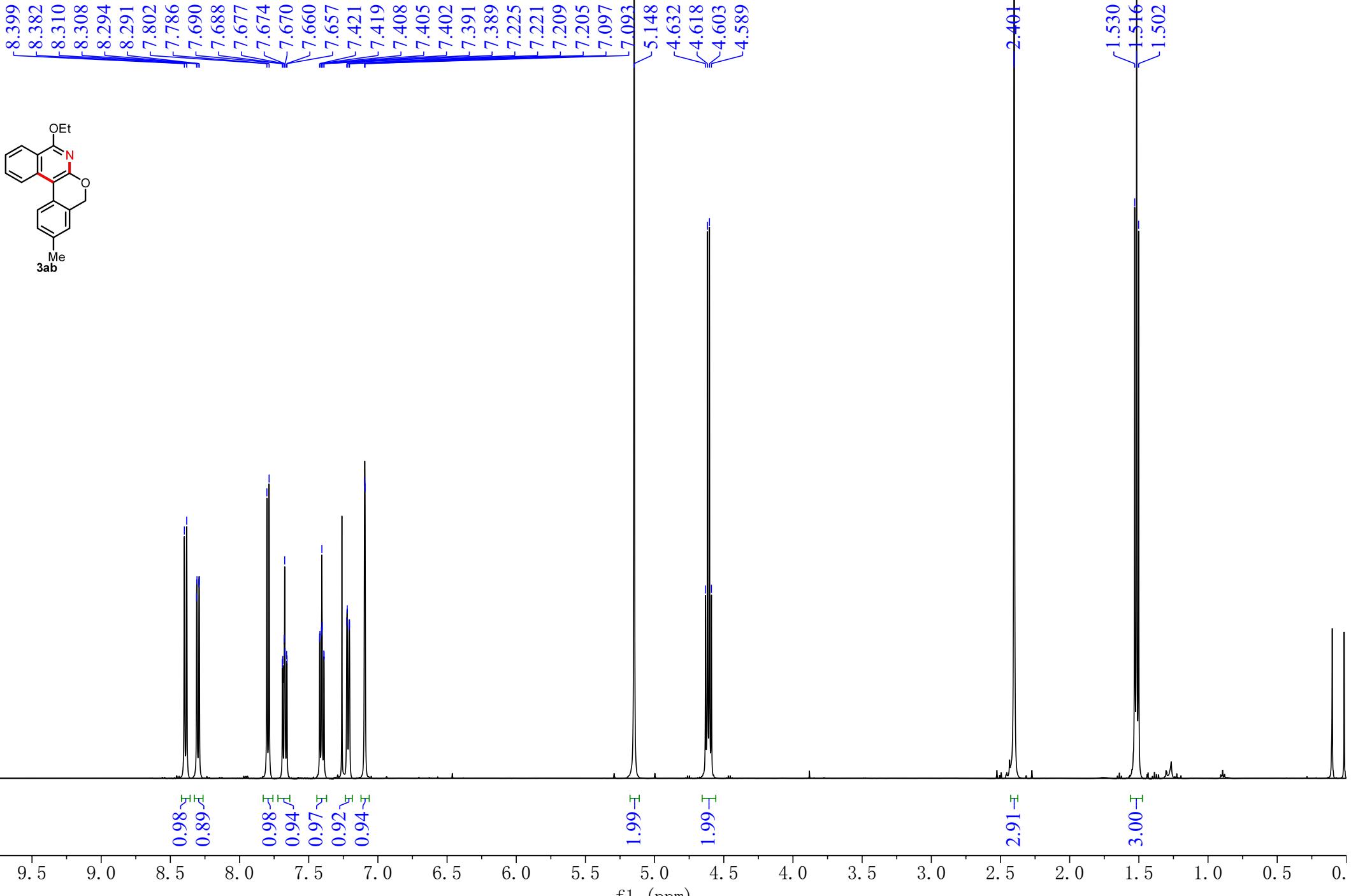


$^{13}\text{C}\{\text{H}\}$  NMR spectrum of **3va**





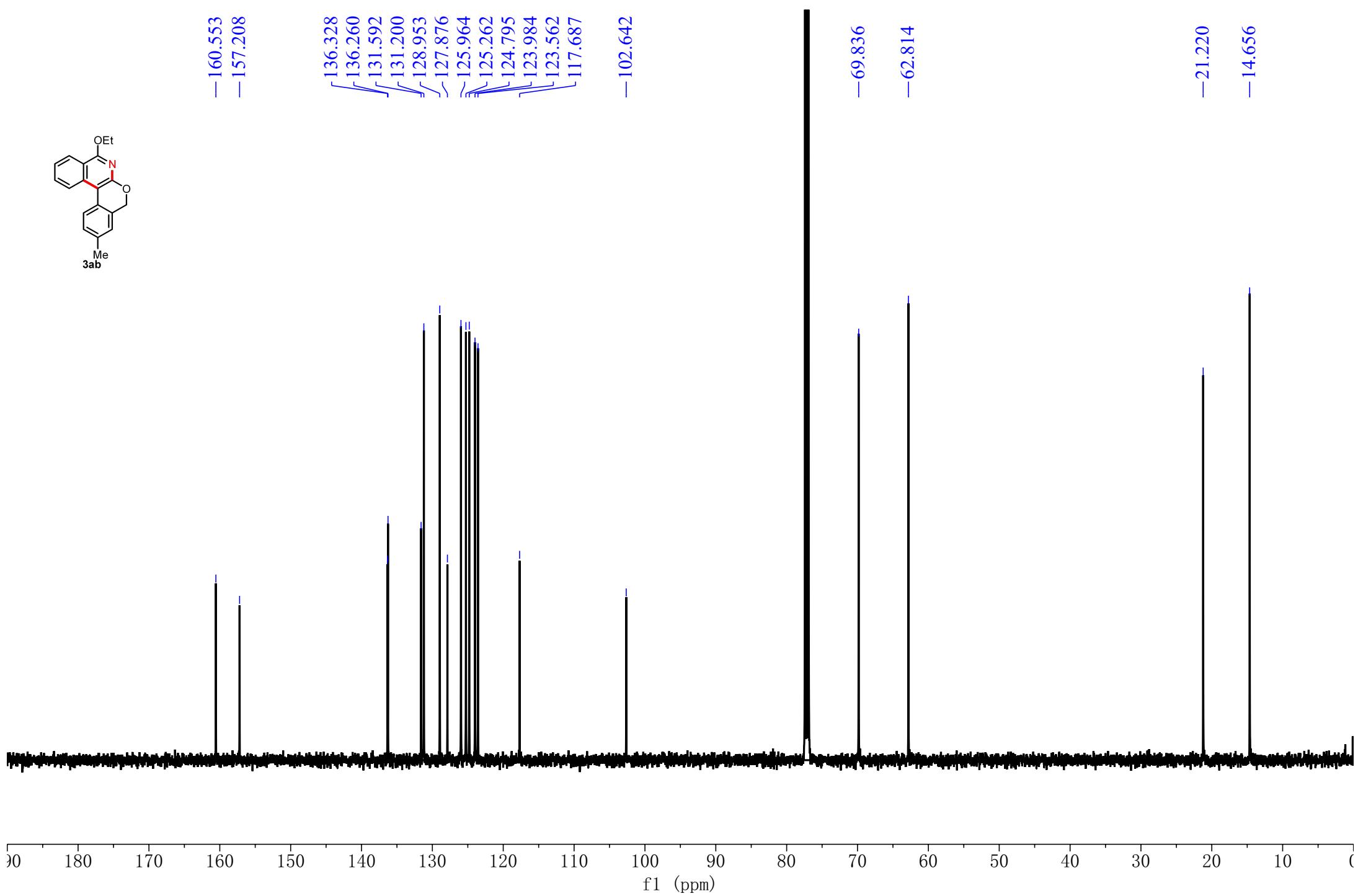
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 3wa



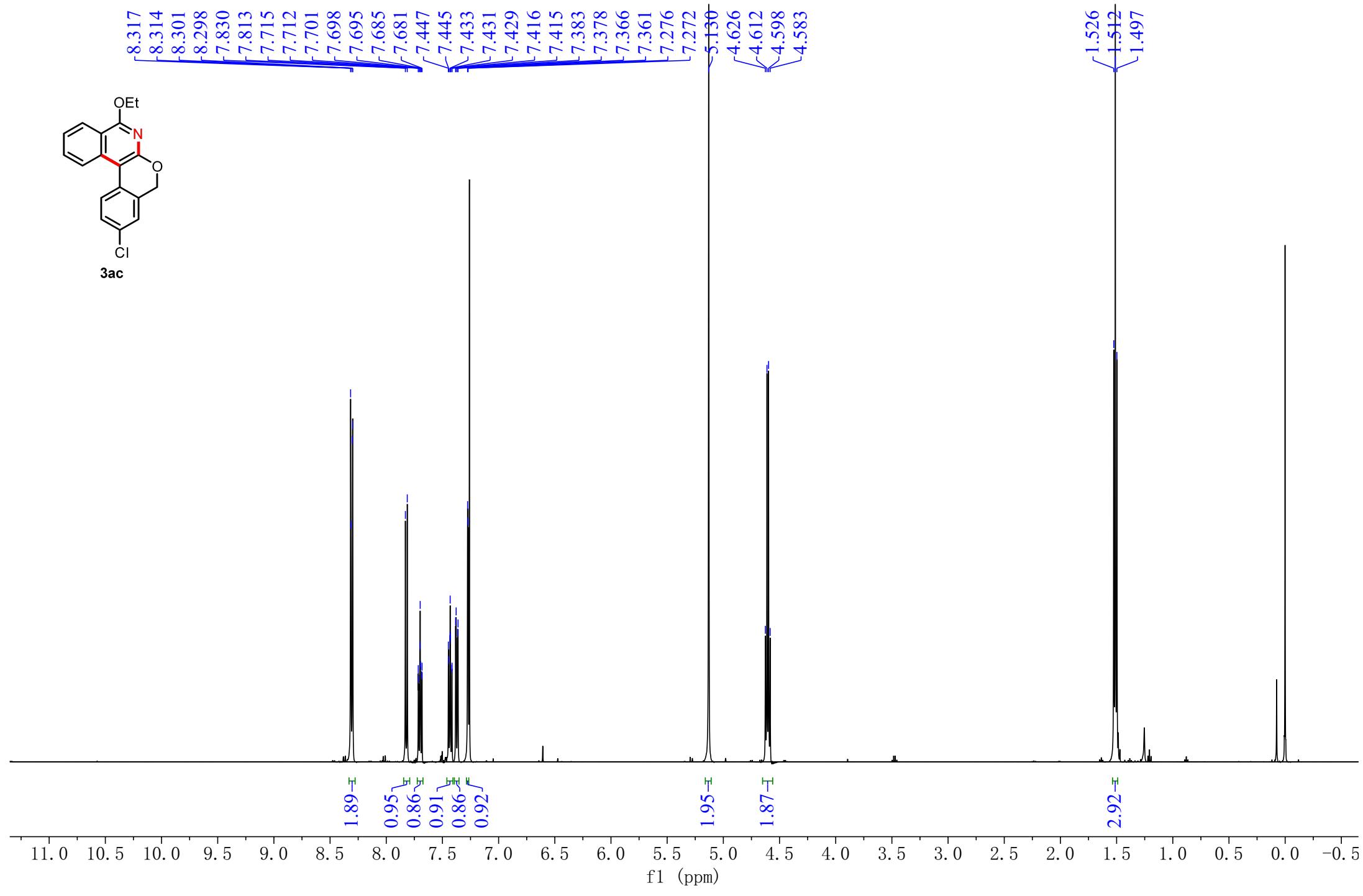
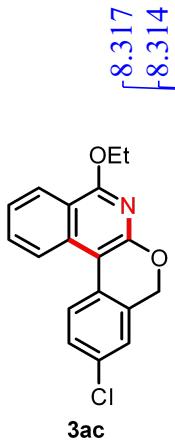
<sup>1</sup>H NMR spectrum of 3ab

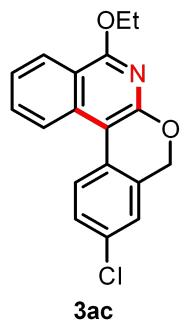


—160.553  
—157.208  
136.328  
136.260  
131.592  
131.200  
128.953  
127.876  
125.964  
125.262  
124.795  
123.984  
123.562  
117.687  
—102.642  
—69.836  
—62.814  
—21.220  
—14.656



$^{13}\text{C}\{\text{H}\}$  NMR spectrum of **3ab**





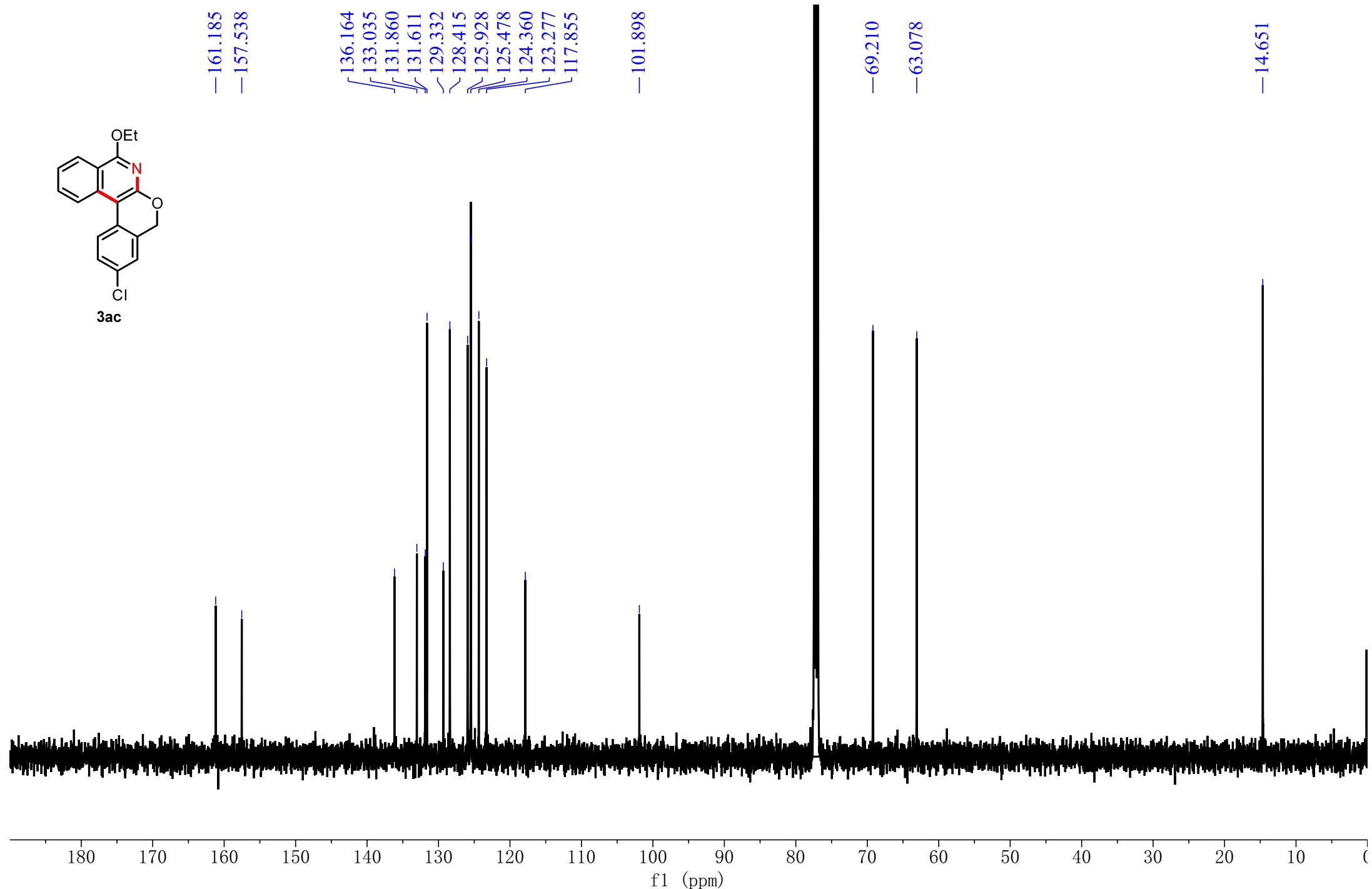
—161.185  
—157.538

136.164  
133.035  
131.860  
131.611  
129.332  
128.415  
125.928  
125.478  
124.360  
123.277  
117.855

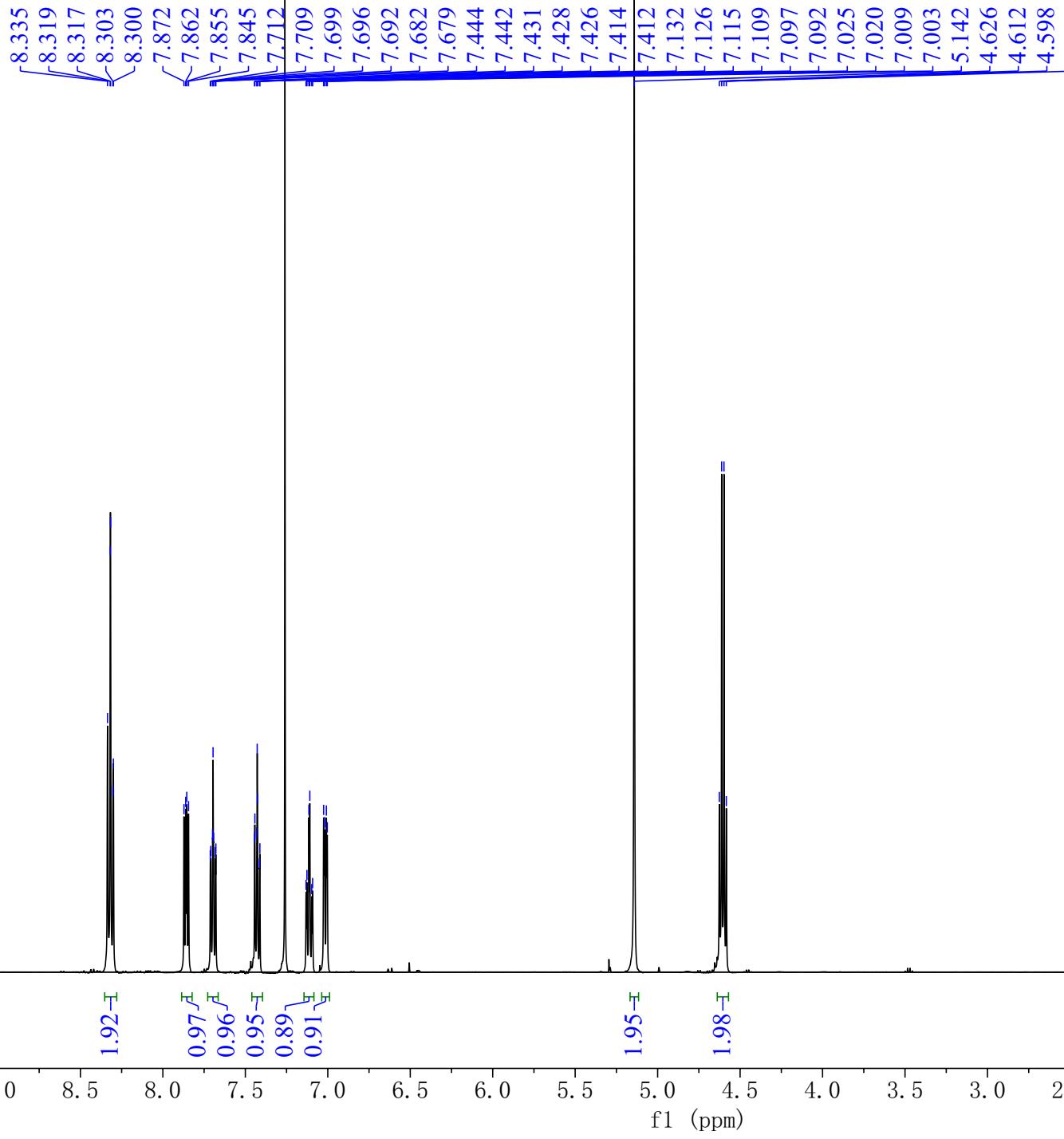
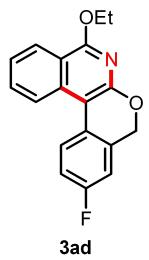
—101.898

—69.210  
—63.078

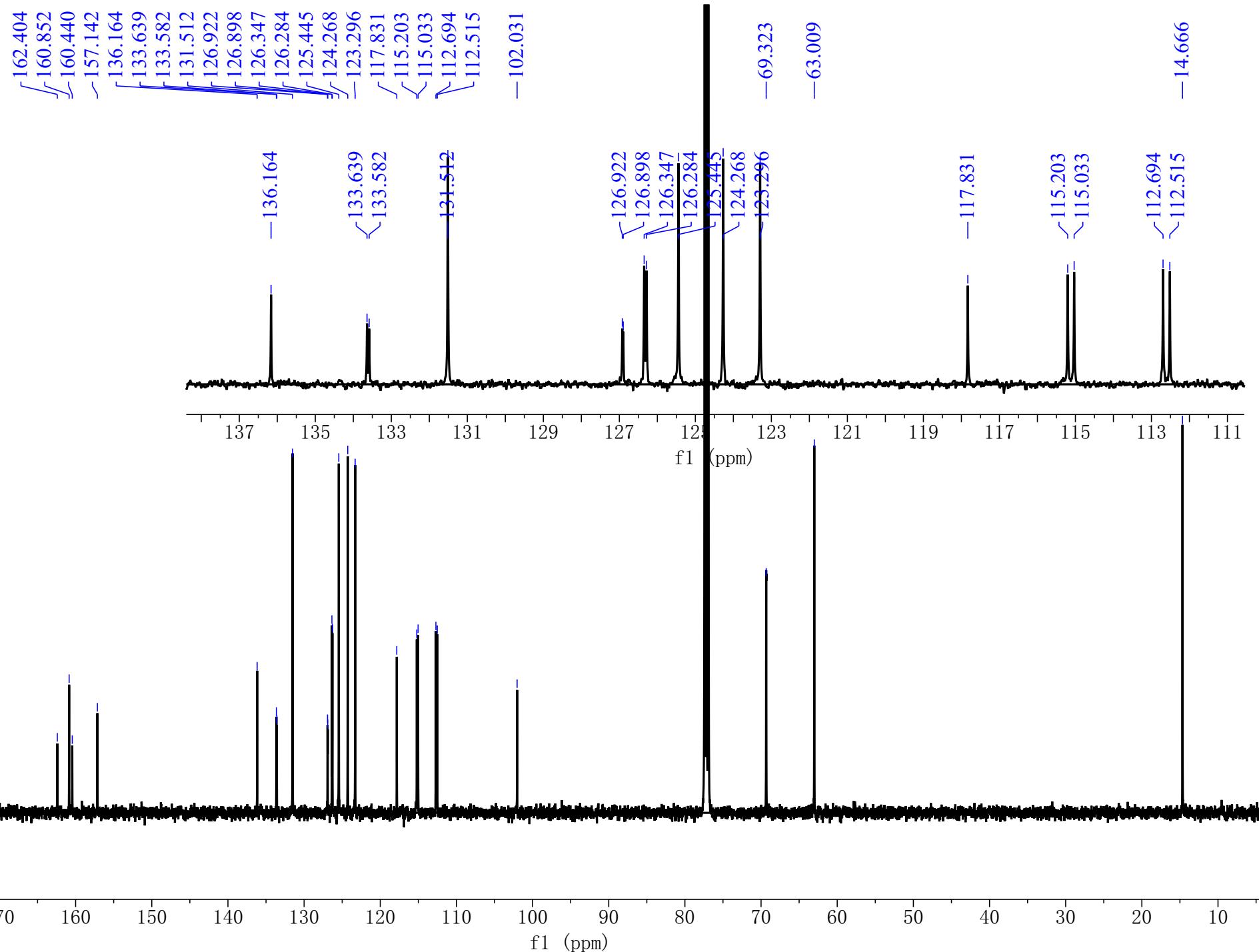
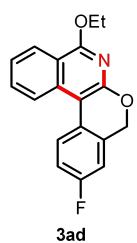
—14.651



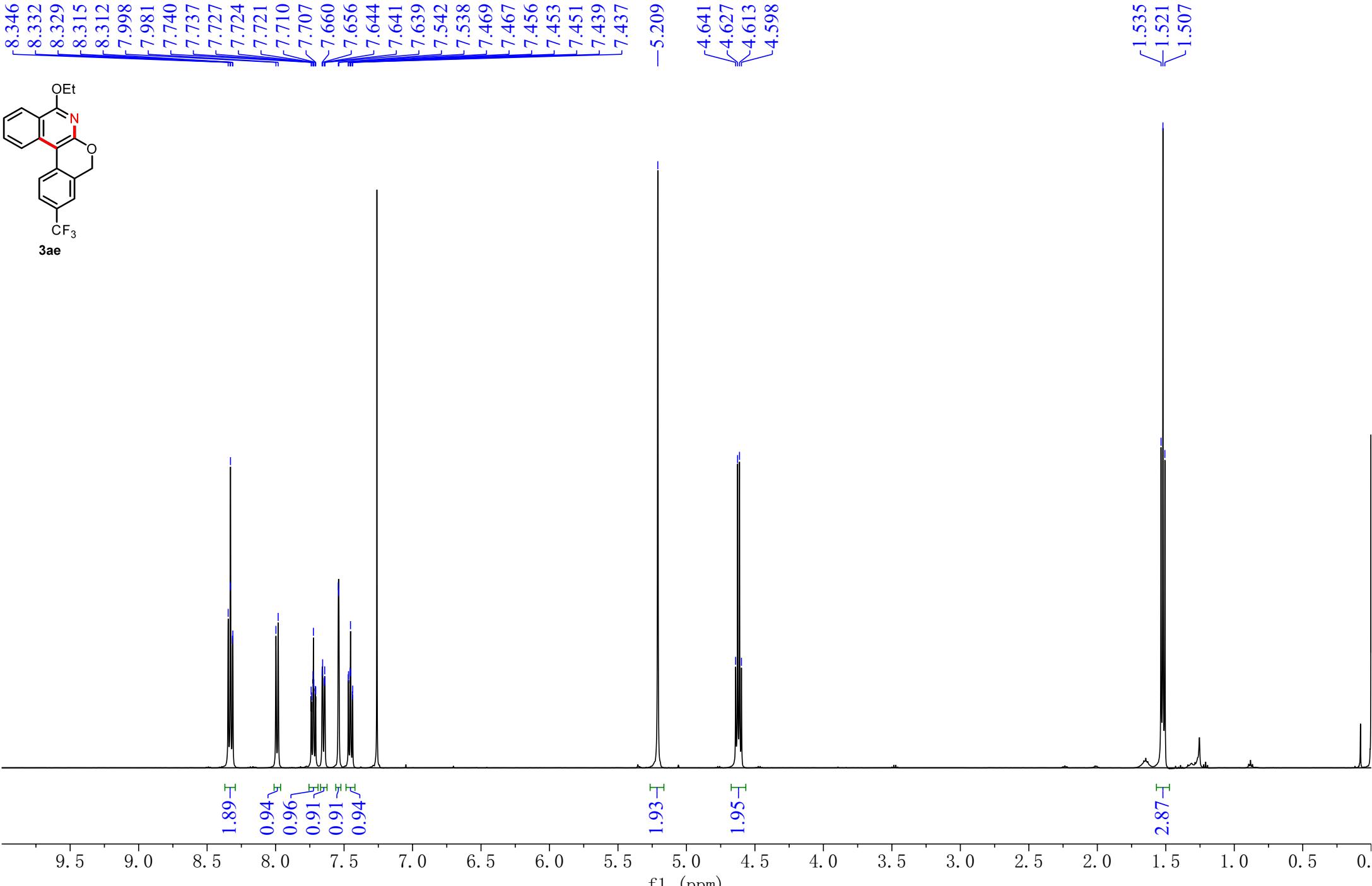
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3ac**



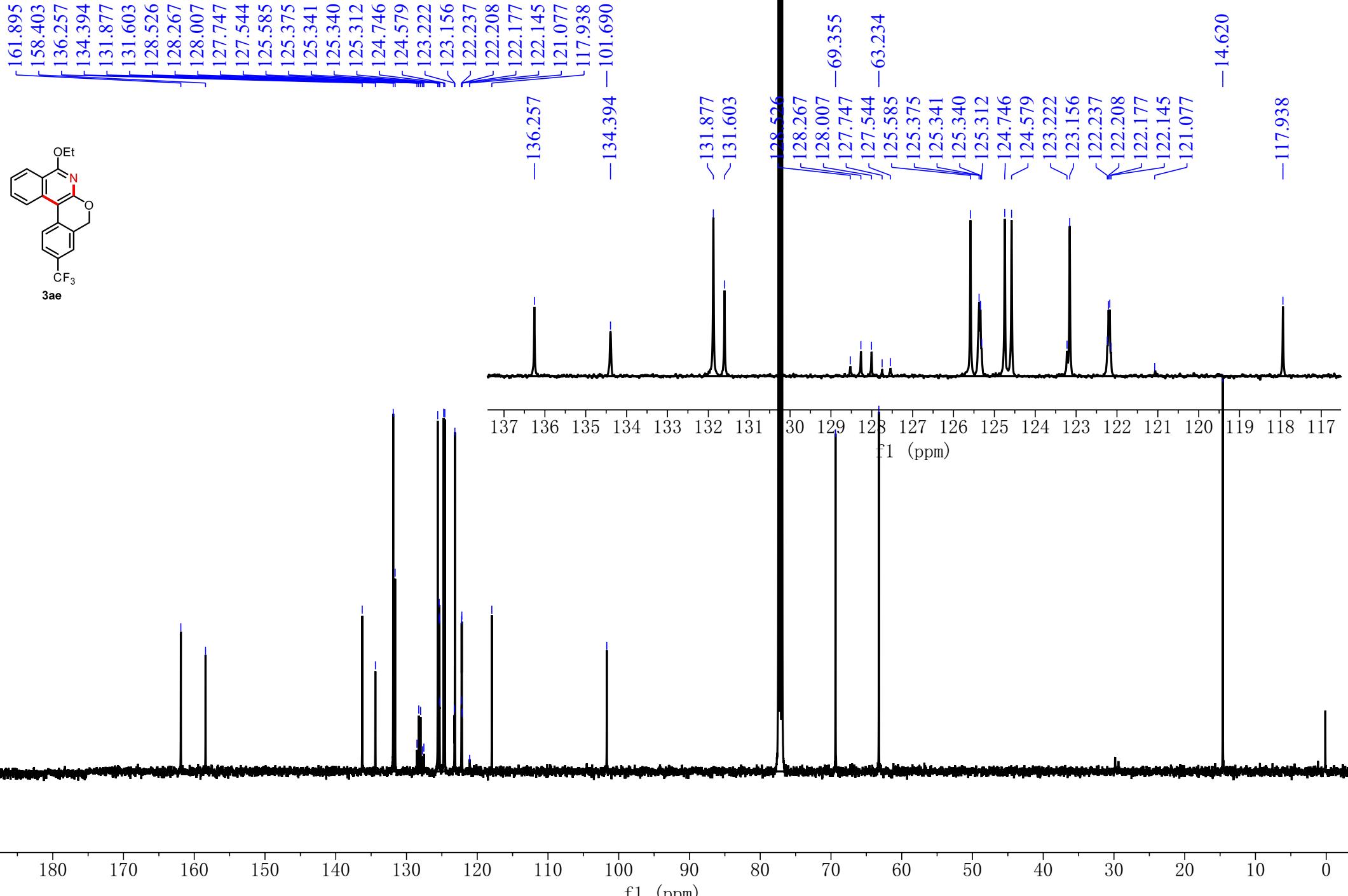
<sup>1</sup>H NMR spectrum of **3ad**



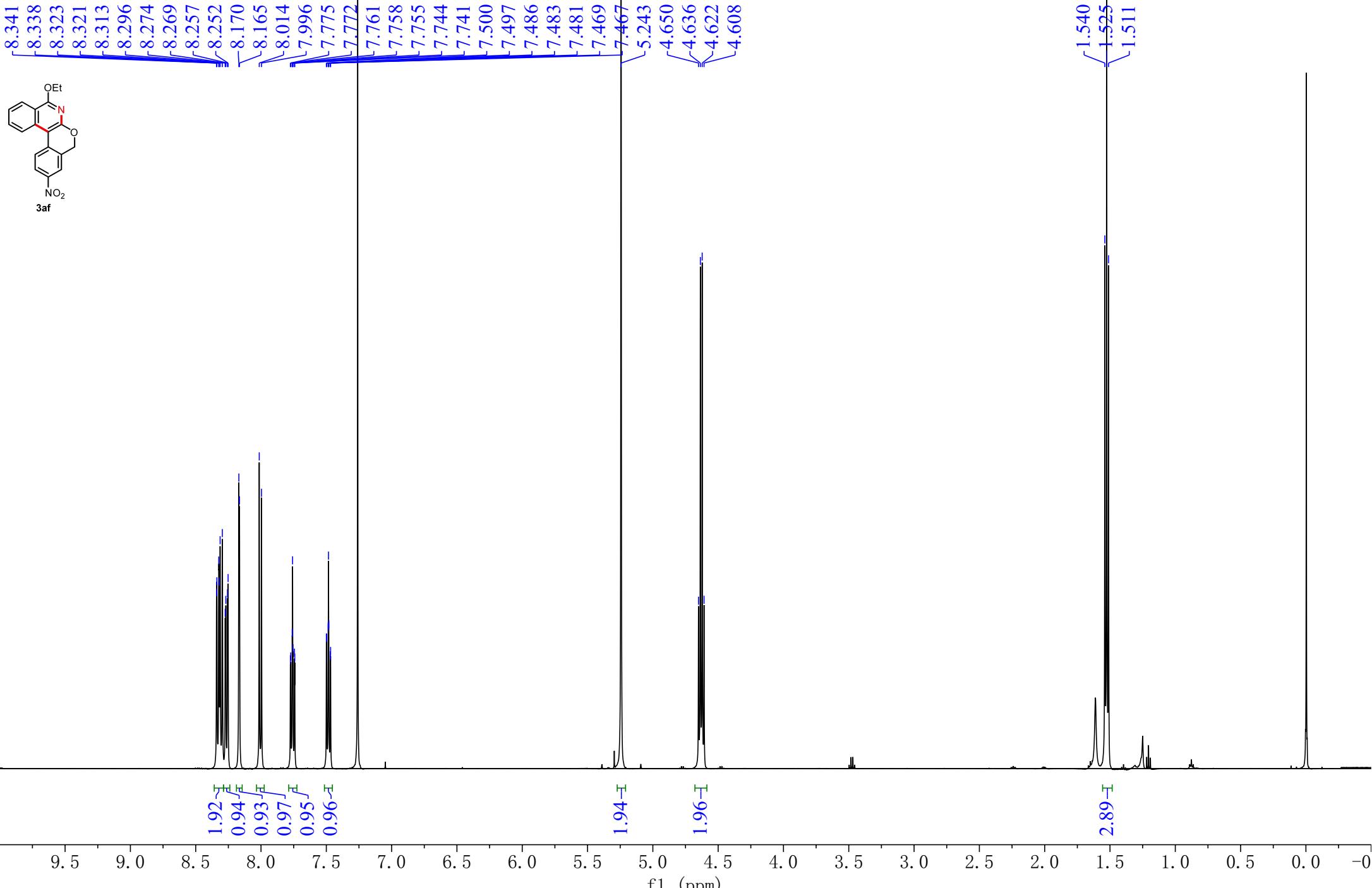
<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 3ad



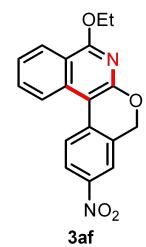
$^1\text{H}$  NMR spectrum of 3ae



<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **3ae**



$^1\text{H}$  NMR spectrum of **3af**



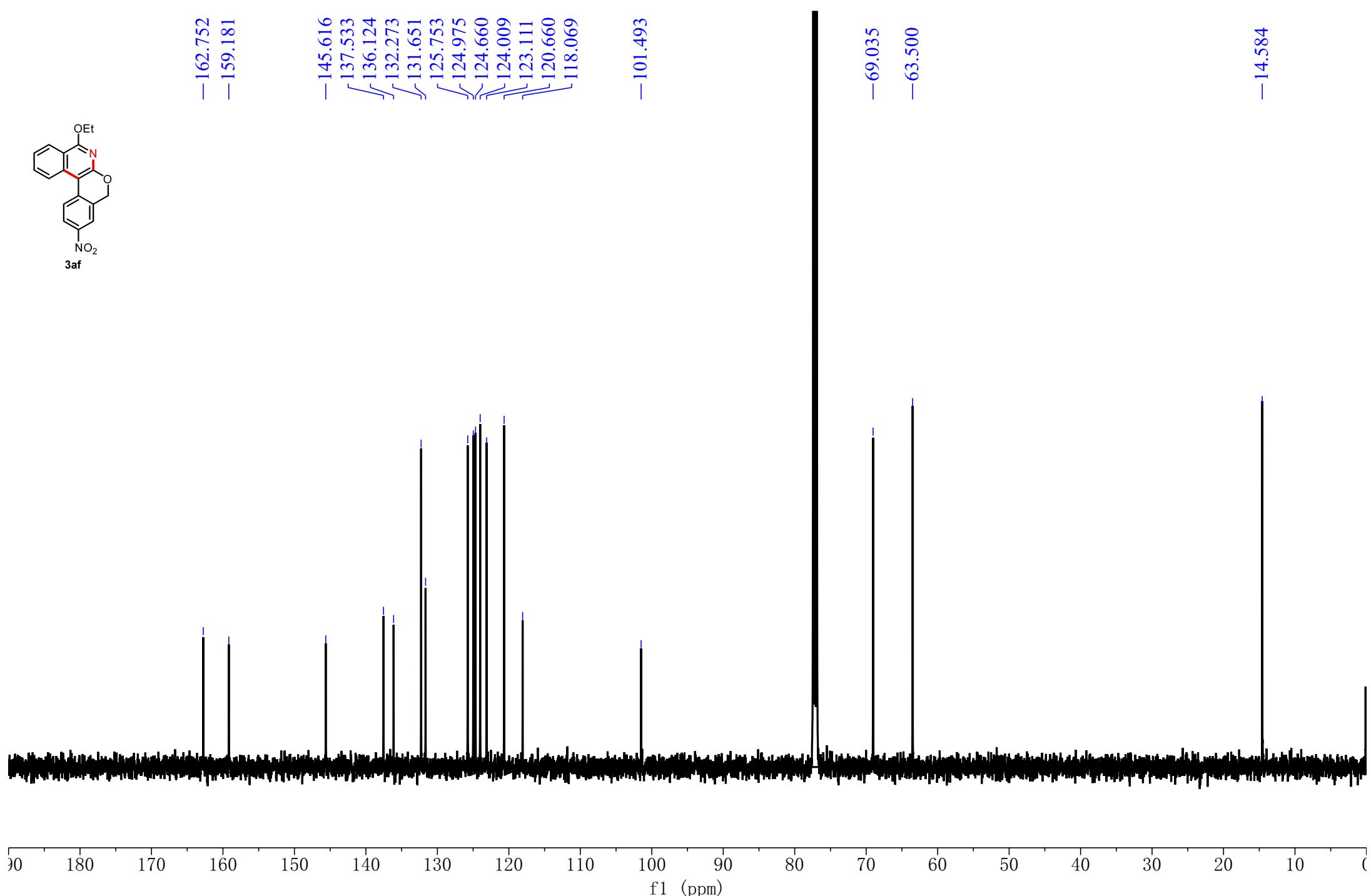
—162.752  
—159.181

—145.616  
—137.533  
—136.124  
—132.273  
—131.651  
—125.753  
—124.975  
—124.660  
—124.009  
—123.111  
—120.660  
—118.069

—101.493

—69.035  
—63.500

—14.584



<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **3af**

8.372  
8.358

8.306  
8.304

8.292  
8.290

8.298  
8.288

8.244  
7.824

7.689  
7.687

7.678  
7.675

7.675  
7.672

7.663  
7.420

7.410  
7.407

7.395  
7.395

6.969  
6.964

6.955  
6.848

6.950  
6.848

5.150  
4.617

4.605  
4.593

4.582  
4.582

3.865



3ag

0.96  
0.94

0.98  
0.98

0.98  
1.01

0.95  
0.95

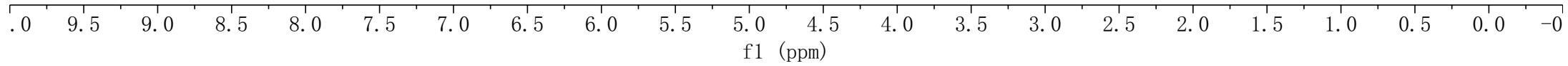
1.98

2.01

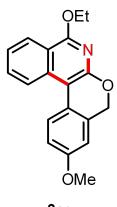
2.97

3.01

1.519  
1.507  
1.496



<sup>1</sup>H NMR spectrum of 3ag



**3ag**

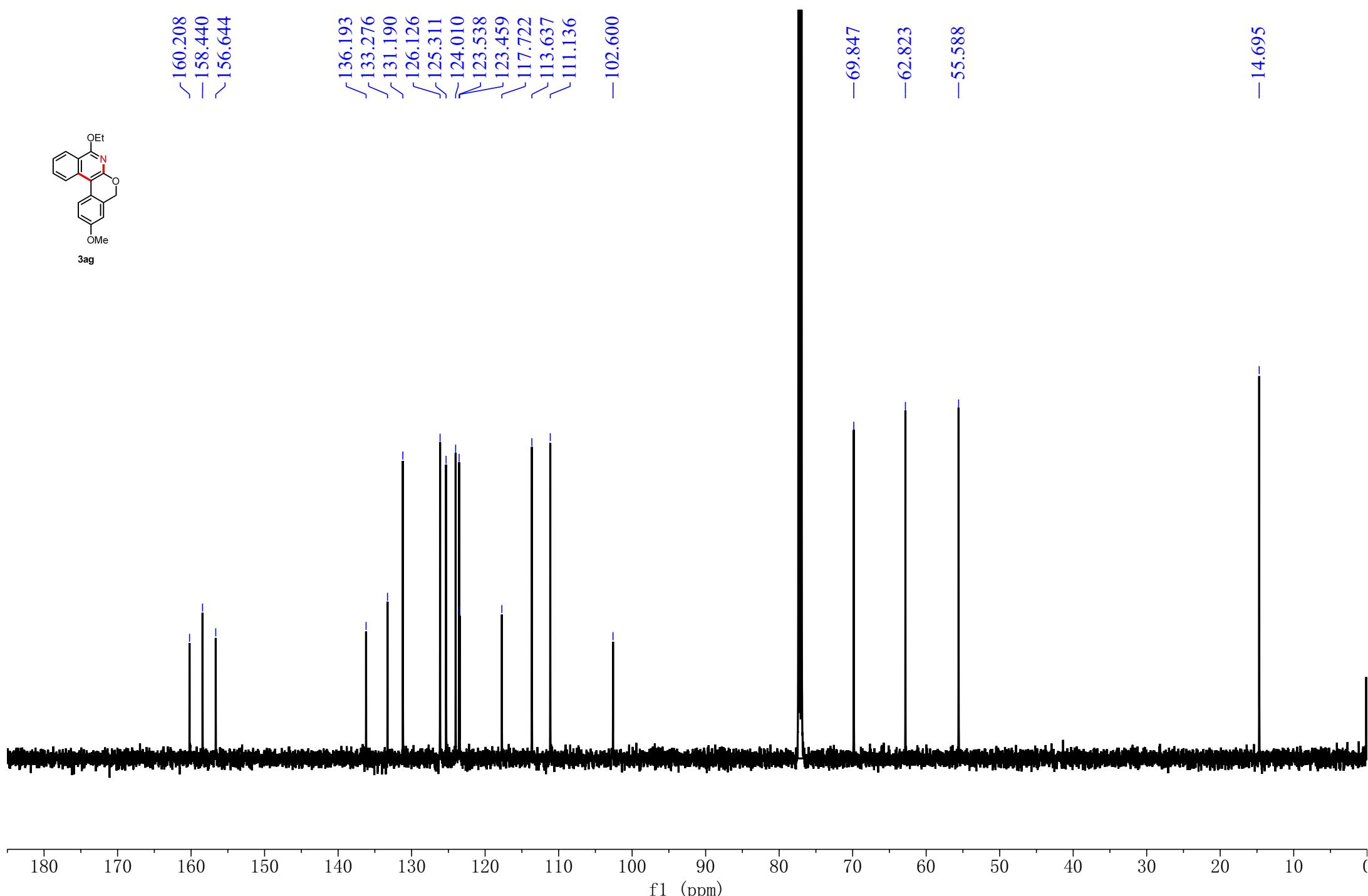
✓ 160.208  
— 158.440  
~ 156.644

✓ 136.193  
✓ 133.276  
✓ 131.190  
✓ 126.126  
✓ 125.311  
✓ 124.010  
✓ 123.538  
✓ 123.459  
✓ 117.722  
✓ 113.637  
✓ 111.136

— 102.600

— 69.847  
— 62.823  
— 55.588

— 14.695



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3ag**

8.432

8.418

8.311

8.297

7.705

7.702

7.693

7.691

7.679

7.688

7.677

7.466

7.462

7.431

7.429

7.419

7.417

7.415

7.406

7.404

7.216

7.202

6.834

6.830

6.820

6.816

5.133

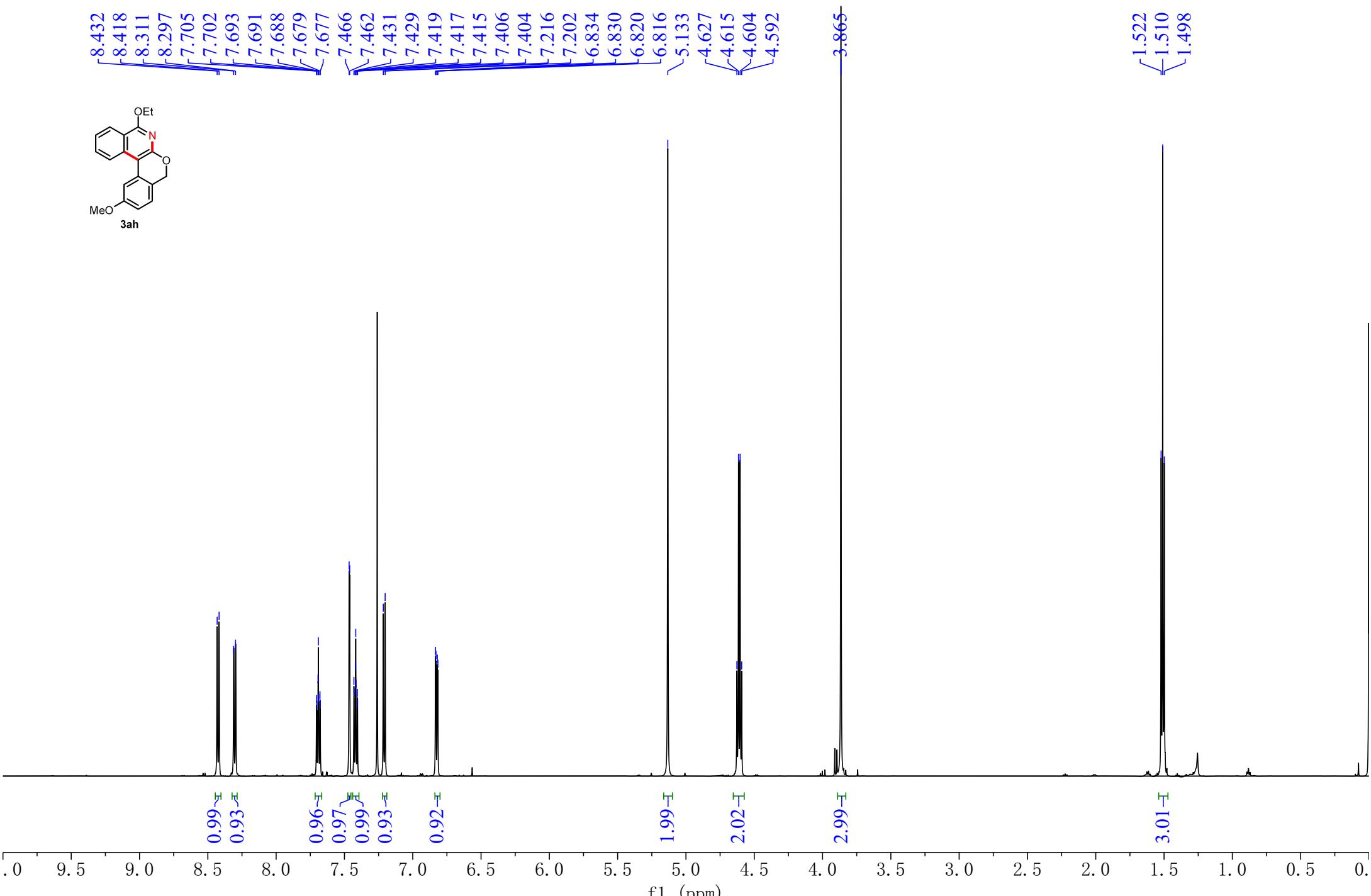
4.627

4.615

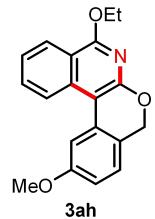
4.604

4.592

3.865



<sup>1</sup>H NMR spectrum of **3ah**



✓ 161.063  
✓ 159.826  
✓ 157.838

✓ 136.411  
✓ 132.007  
✓ 131.466  
✓ 126.164  
✓ 125.392  
✓ 124.130  
✓ 124.021  
✓ 123.460  
✓ 117.771  
✓ 111.507  
✓ 110.967

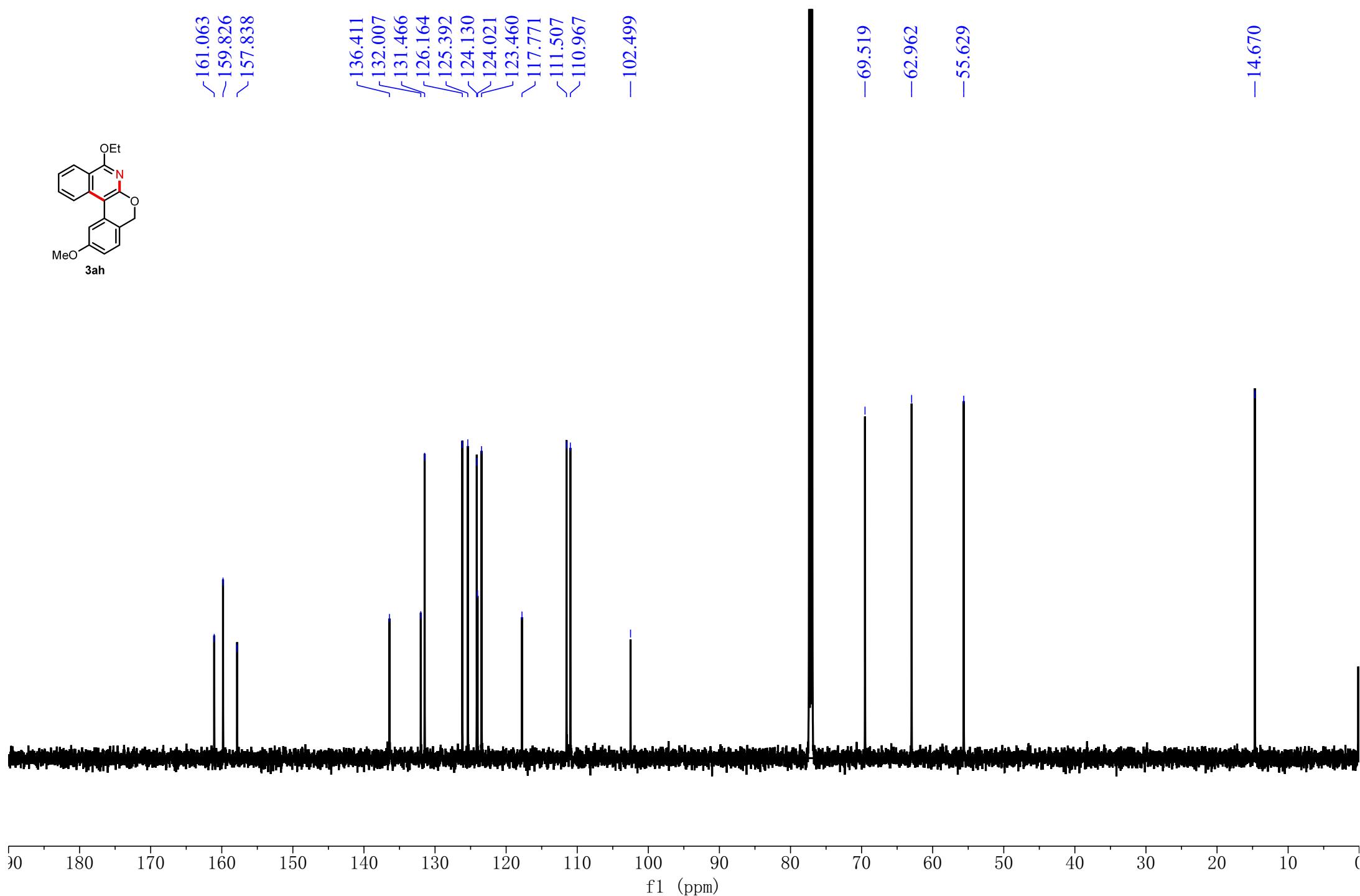
- 102.499

- 69.519

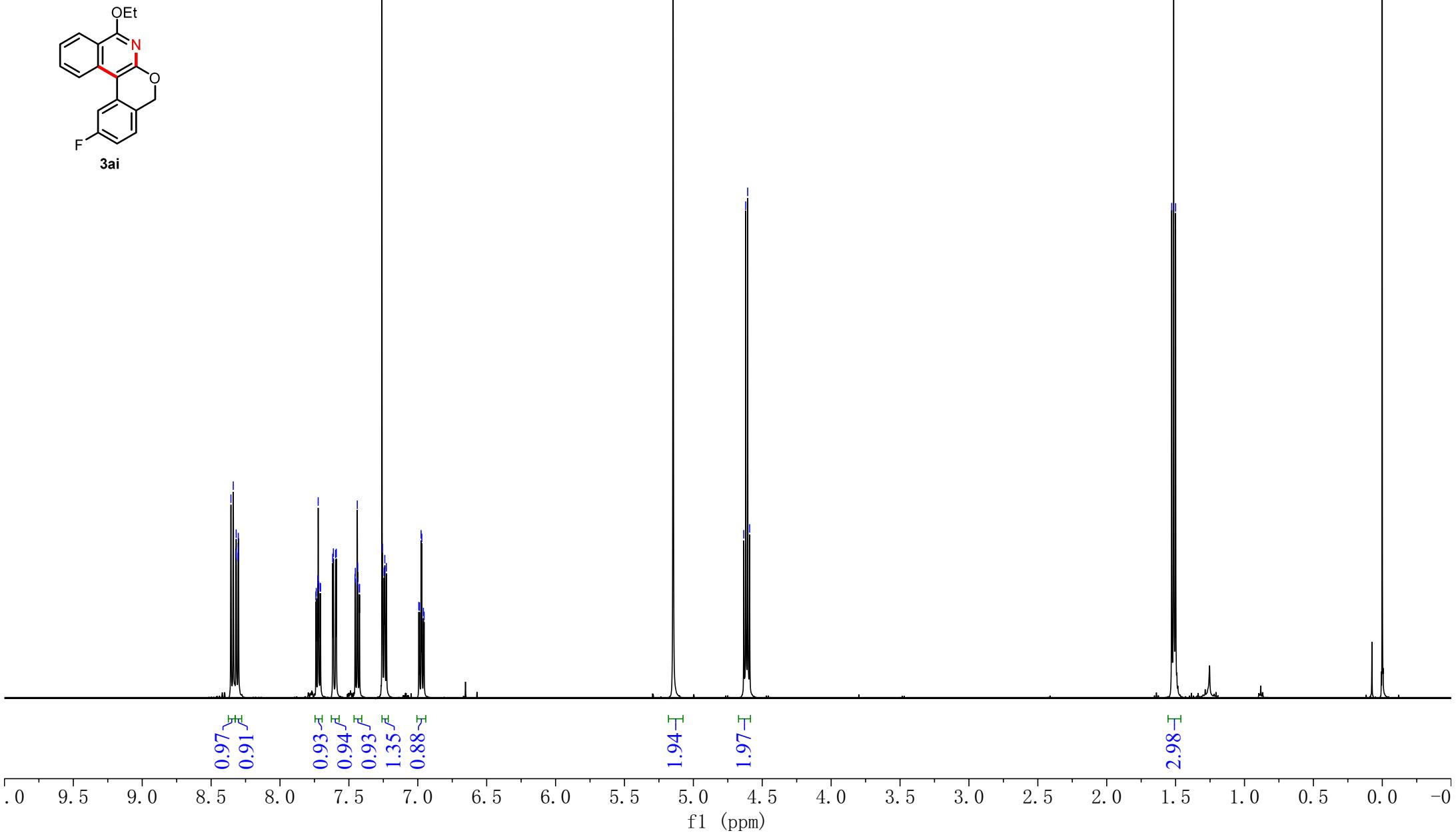
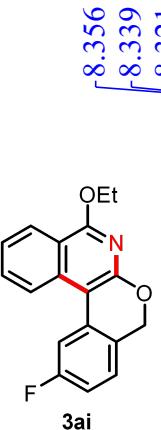
- 62.962

- 55.629

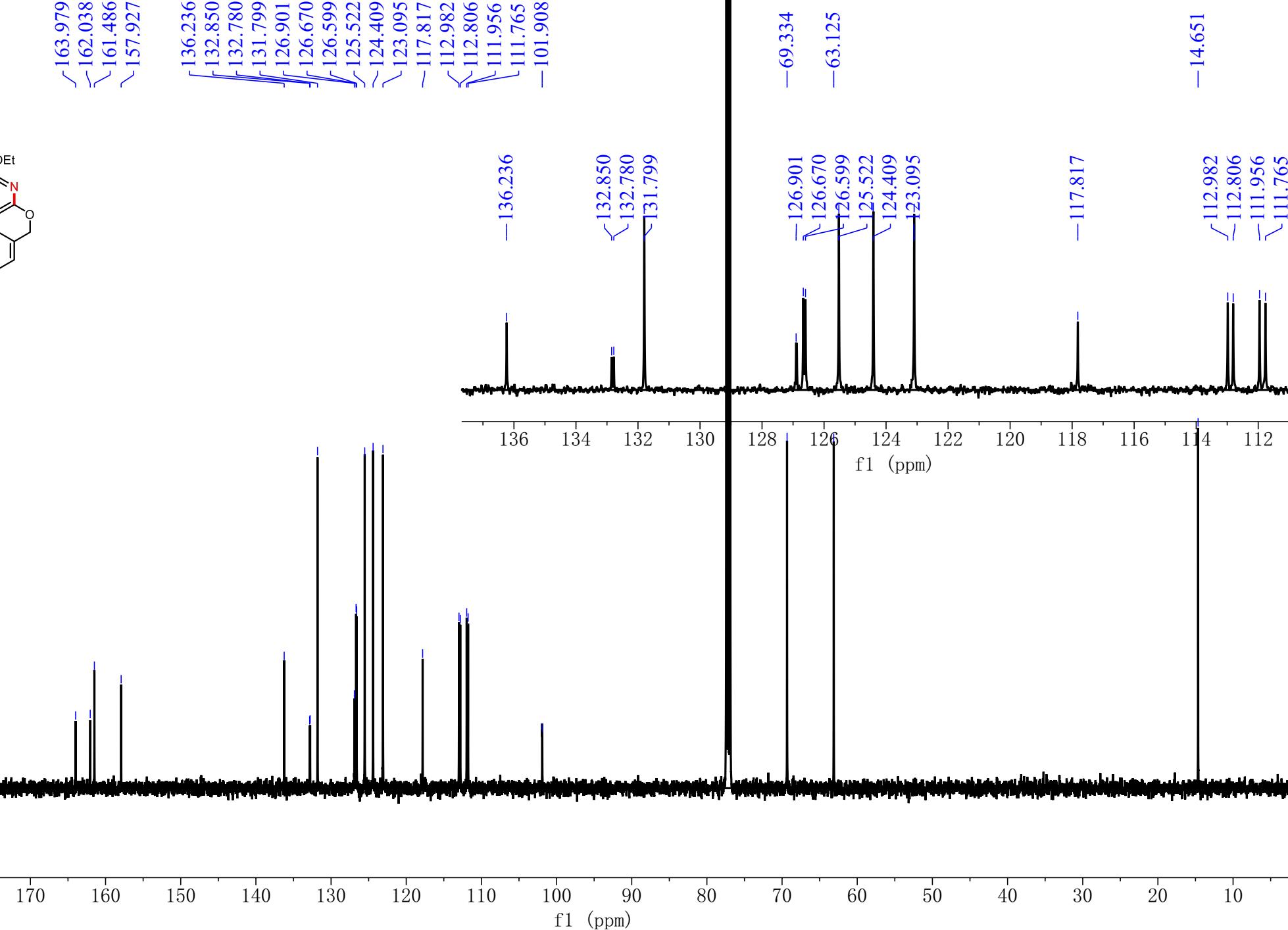
- 14.670



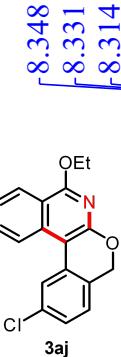
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **3ah**



<sup>1</sup>H NMR spectrum of 3ai



<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 3ai



1.01  
0.98

0.98  
1.00

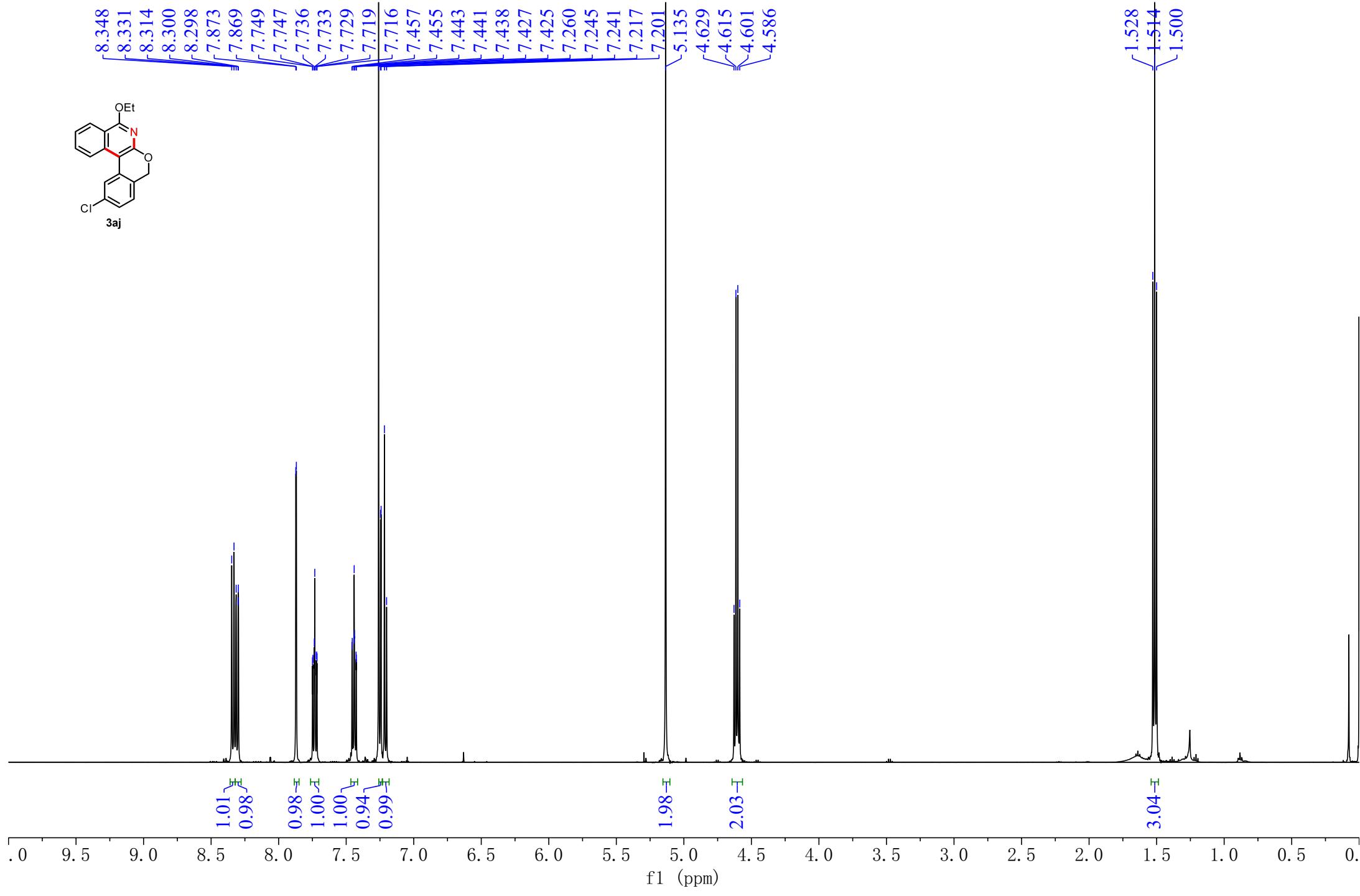
1.00  
0.94

0.99  
0.99

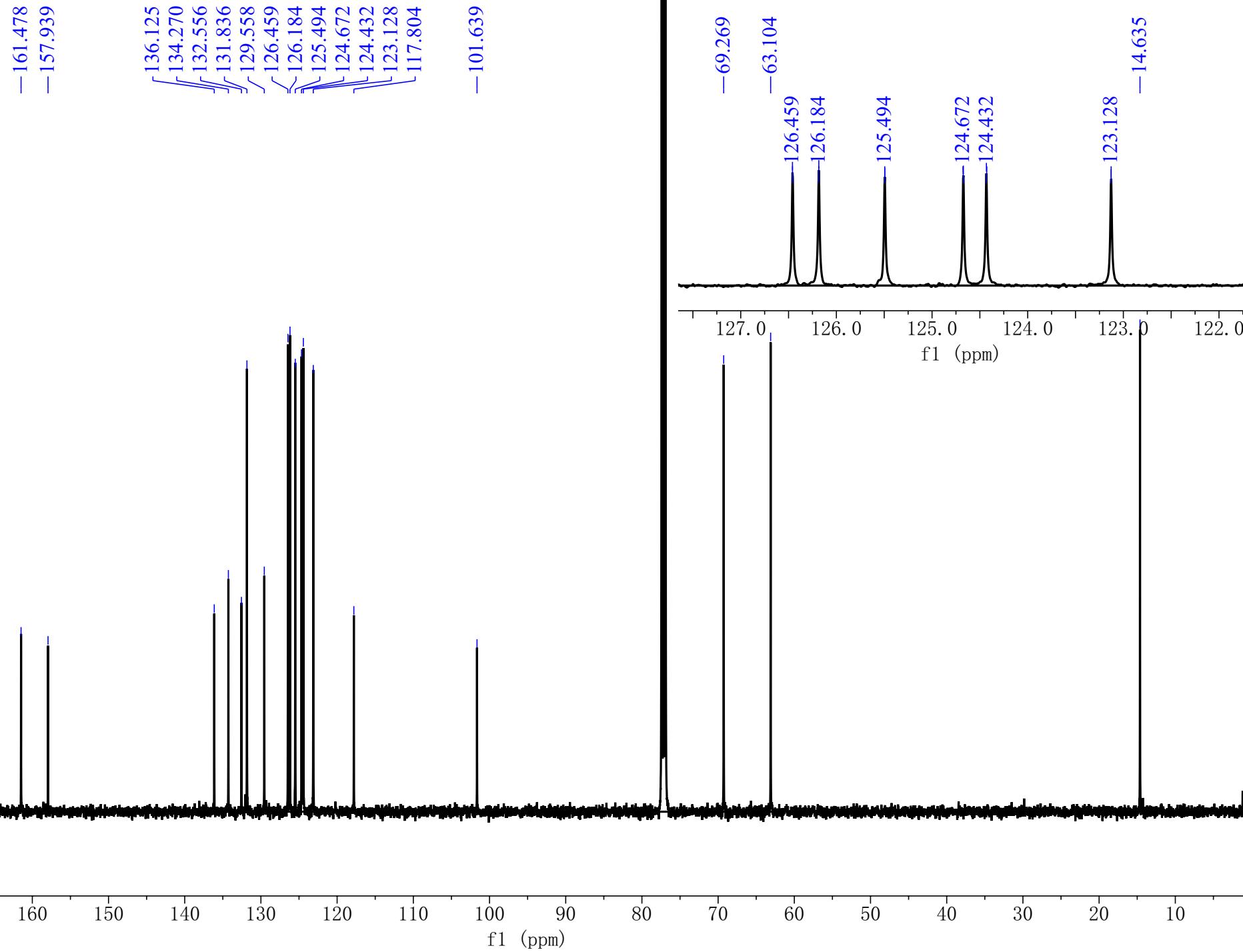
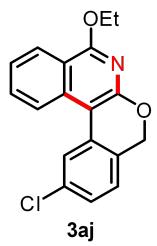
1.98  
2.03

3.04  
3.04

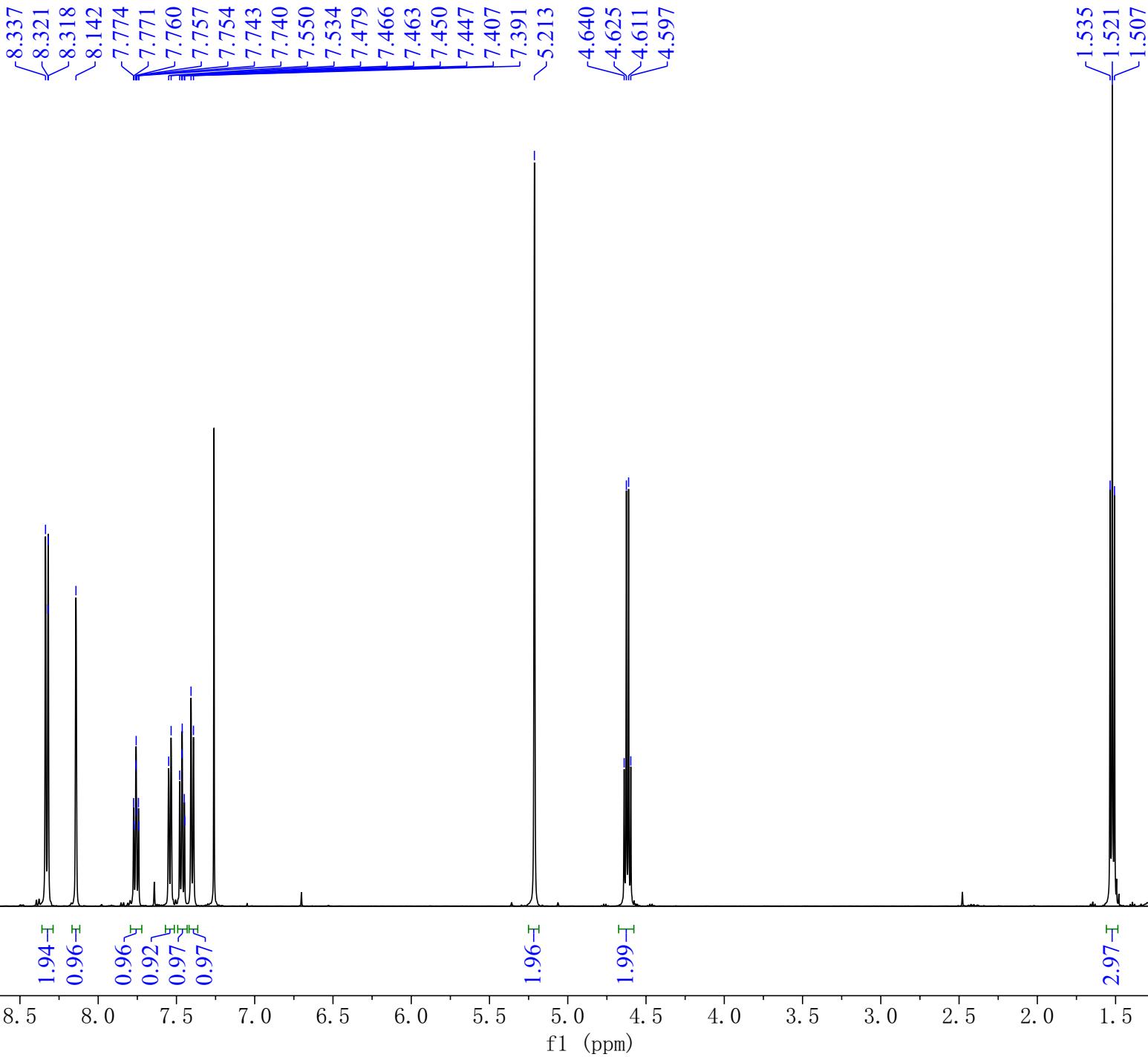
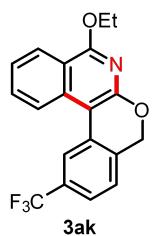
1.528  
1.514  
1.500



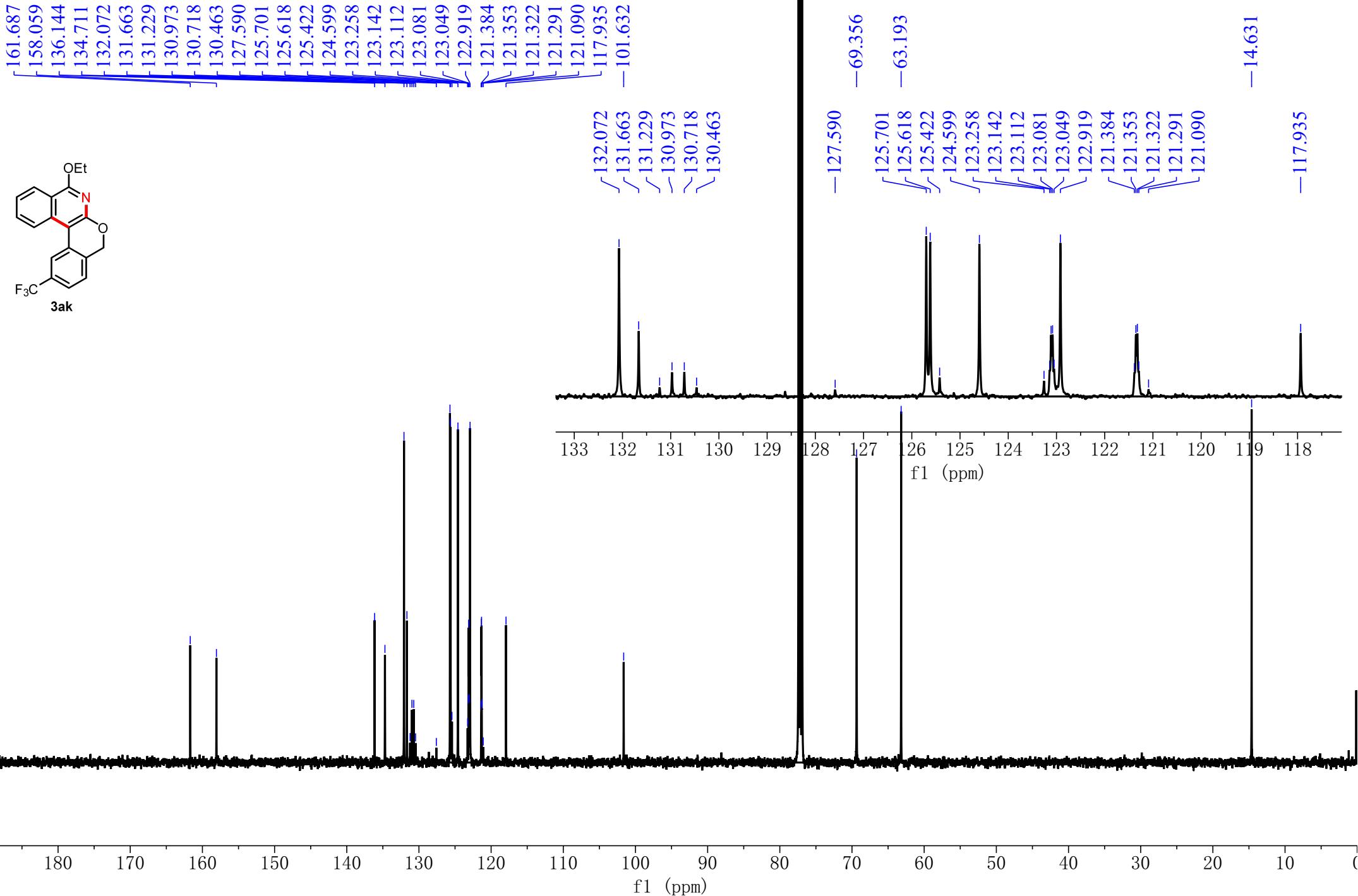
<sup>1</sup>H NMR spectrum of 3aj



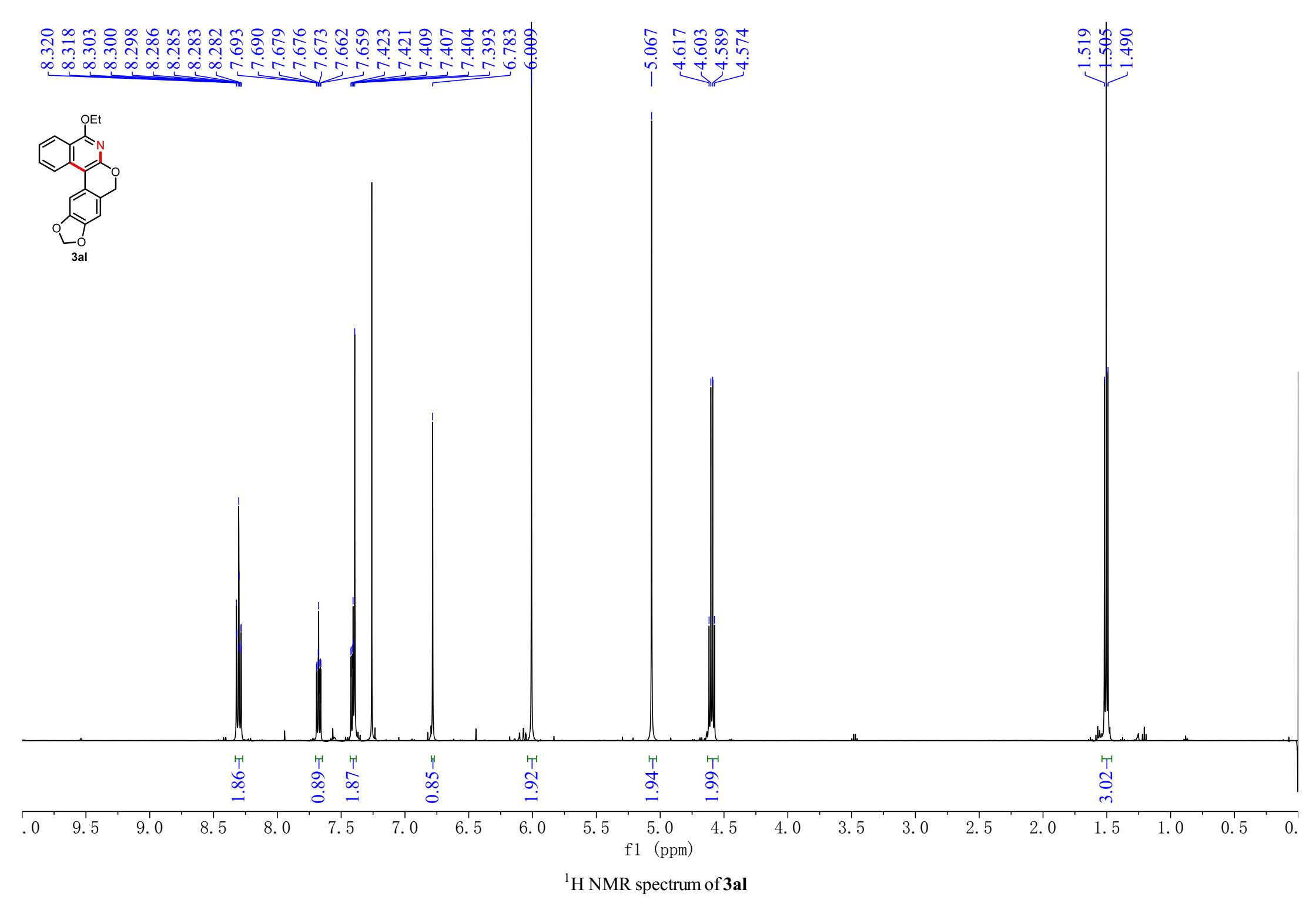
<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 3aj



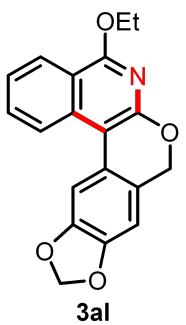
<sup>1</sup>H NMR spectrum of **3ak**



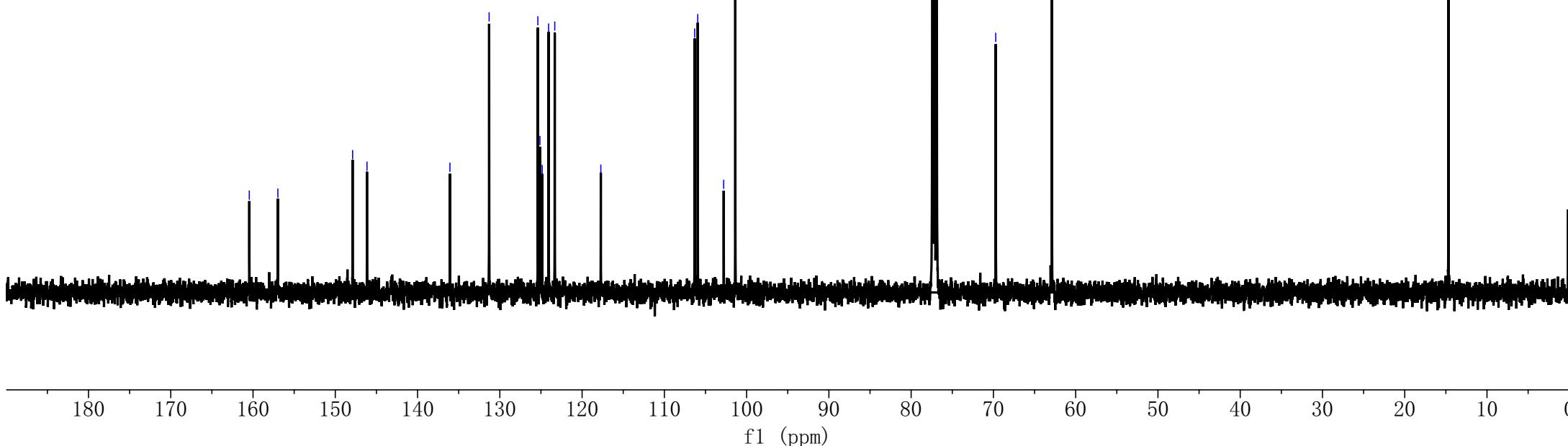
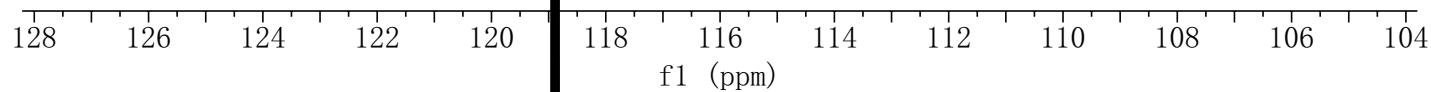
<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **3ak**



<sup>1</sup>H NMR spectrum of **3al**

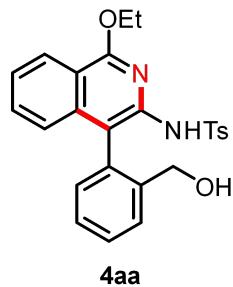


-160.455  
 -156.982  
 ~147.894  
 ~146.146  
 136.065  
 131.300  
 125.378  
 125.121  
 124.844  
 124.071  
 123.322  
 ~117.724  
 125.378  
 ~125.121  
 124.844  
 ~124.071  
 ~123.322  
 106.315  
 105.942  
 102.785  
 ~101.380  
 -117.724  
 -69.717  
 -62.889  
 106.315  
 ~105.942  
 -14.685



<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **3al**

9.690  
8.081  
8.067  
8.064  
7.845  
7.828  
7.721  
7.705  
7.586  
7.584  
7.573  
7.570  
7.567  
7.562  
7.560  
7.556  
7.553  
7.547  
7.545  
7.532  
7.529  
7.473  
7.471  
7.460  
7.457  
7.454  
7.447  
7.444  
7.440  
7.432  
7.429  
7.397  
7.381  
7.369  
7.138  
7.123  
7.121  
6.989  
6.972  
4.309  
4.281  
4.056  
4.049  
4.041  
4.036  
4.028  
4.022  
4.013  
4.008  
3.999  
3.994  
2.387  
2.367  
1.222  
1.207  
1.193



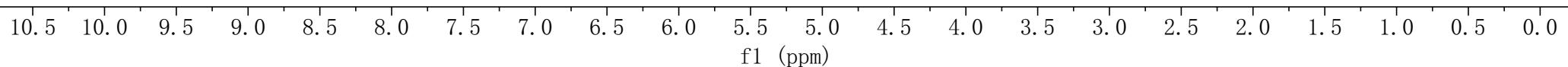
1.00 -

1.02  
2.07  
1.42  
2.11  
2.14  
2.26  
1.03  
1.02

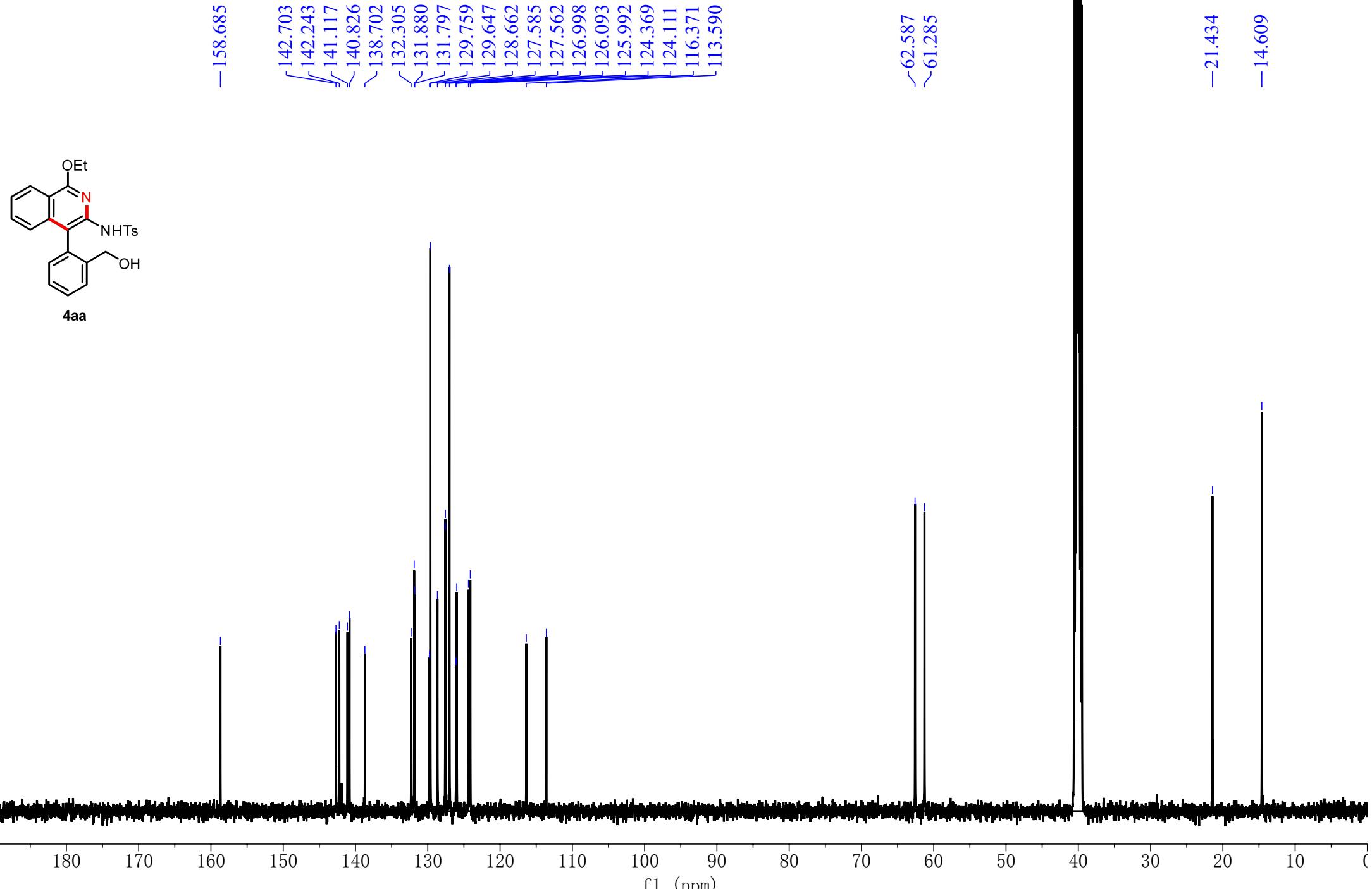
1.02 -  
3.11 -

3.02  
0.63

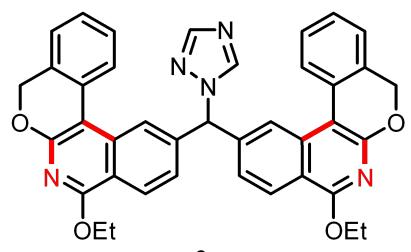
3.44 -



<sup>1</sup>H NMR spectrum of **4aa**

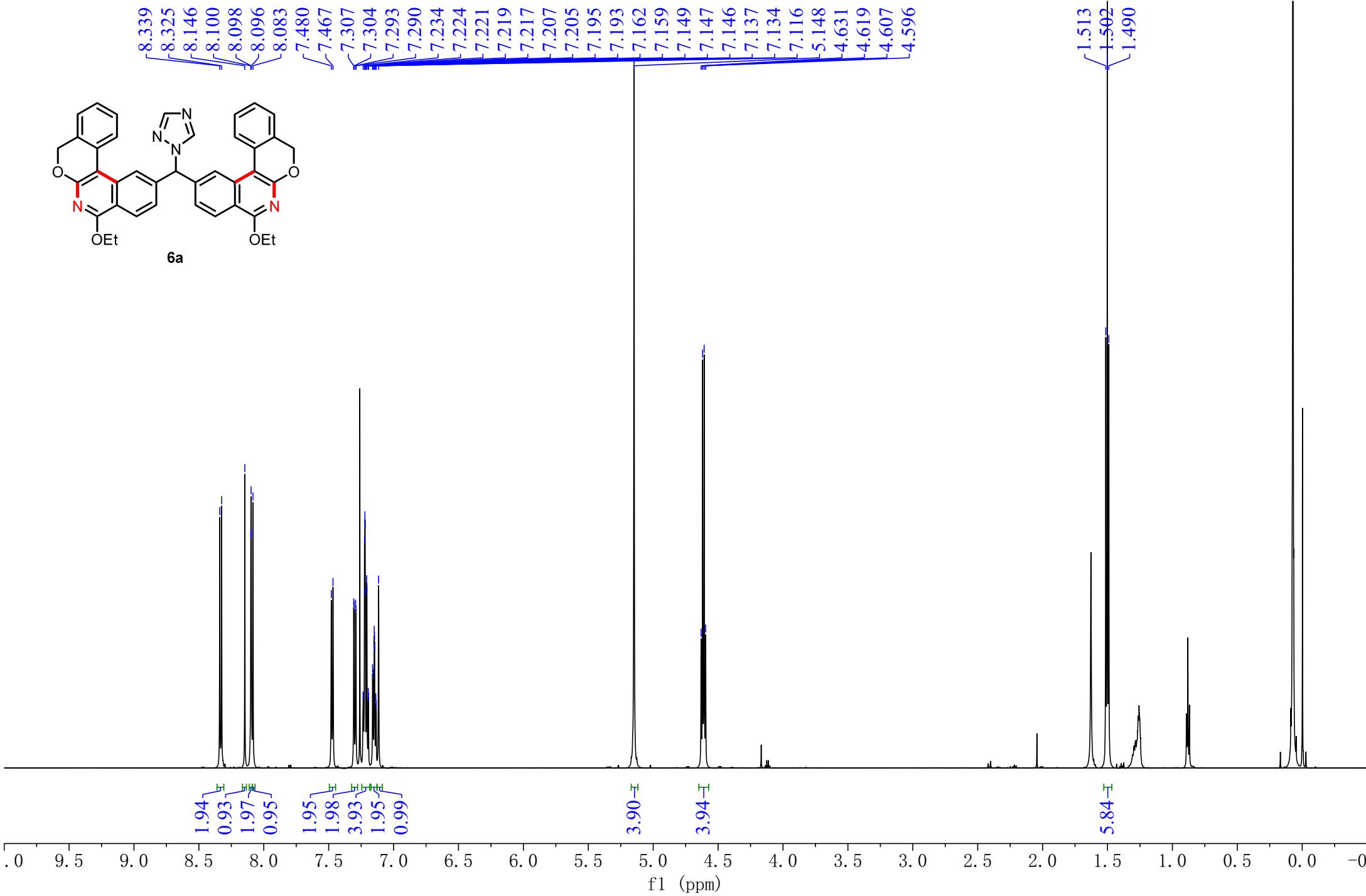


$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **4aa**

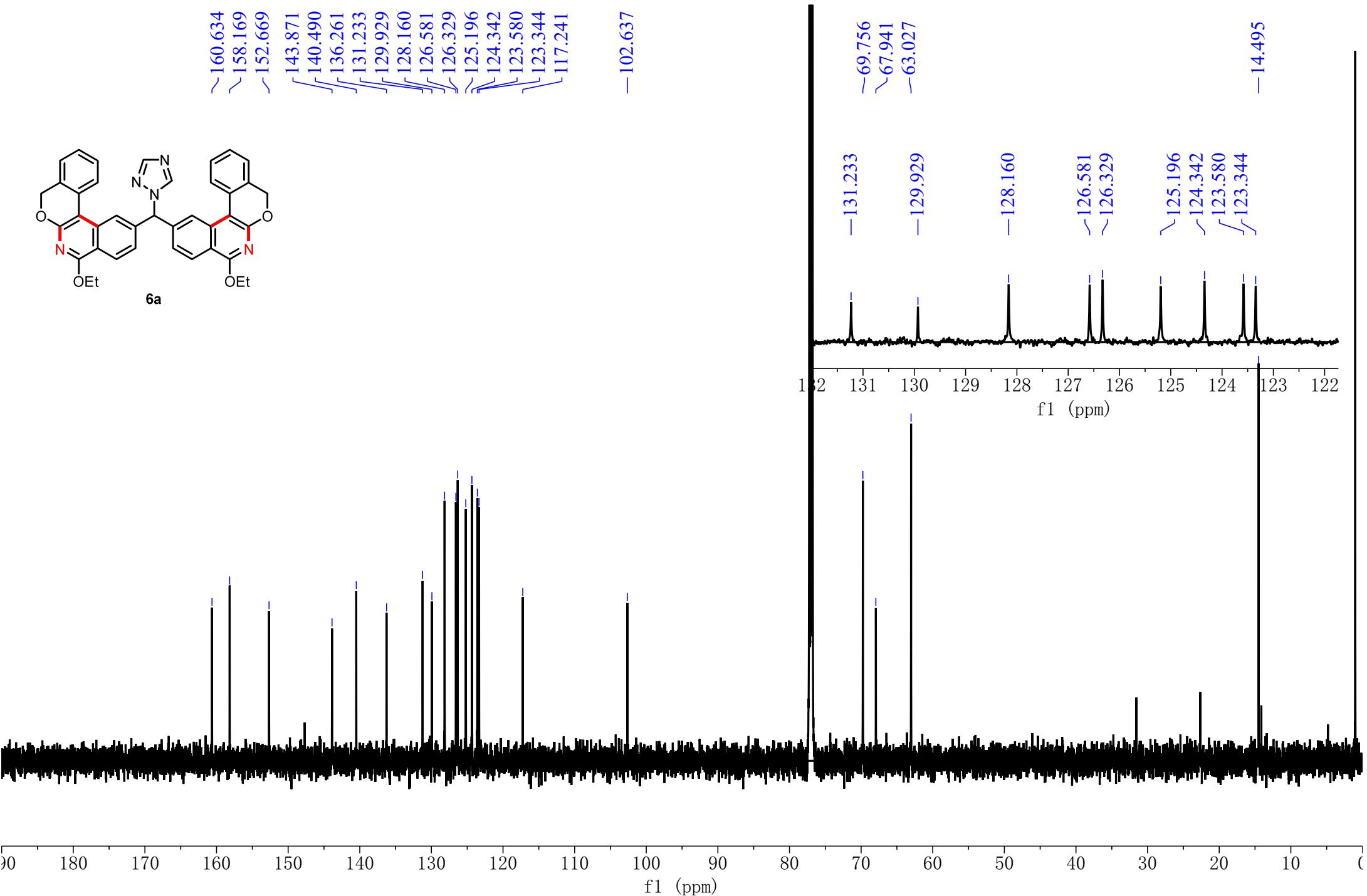


8.339  
8.325  
8.146  
8.100  
8.098  
8.096  
8.083  
7.480  
7.467  
7.307  
7.304  
7.293  
7.290  
7.234  
7.224  
7.221  
7.219  
7.217  
7.207  
7.205  
7.195  
7.193  
7.159  
7.149  
7.147  
7.137  
7.134  
7.116  
5.148  
4.631  
4.619  
4.607  
4.596

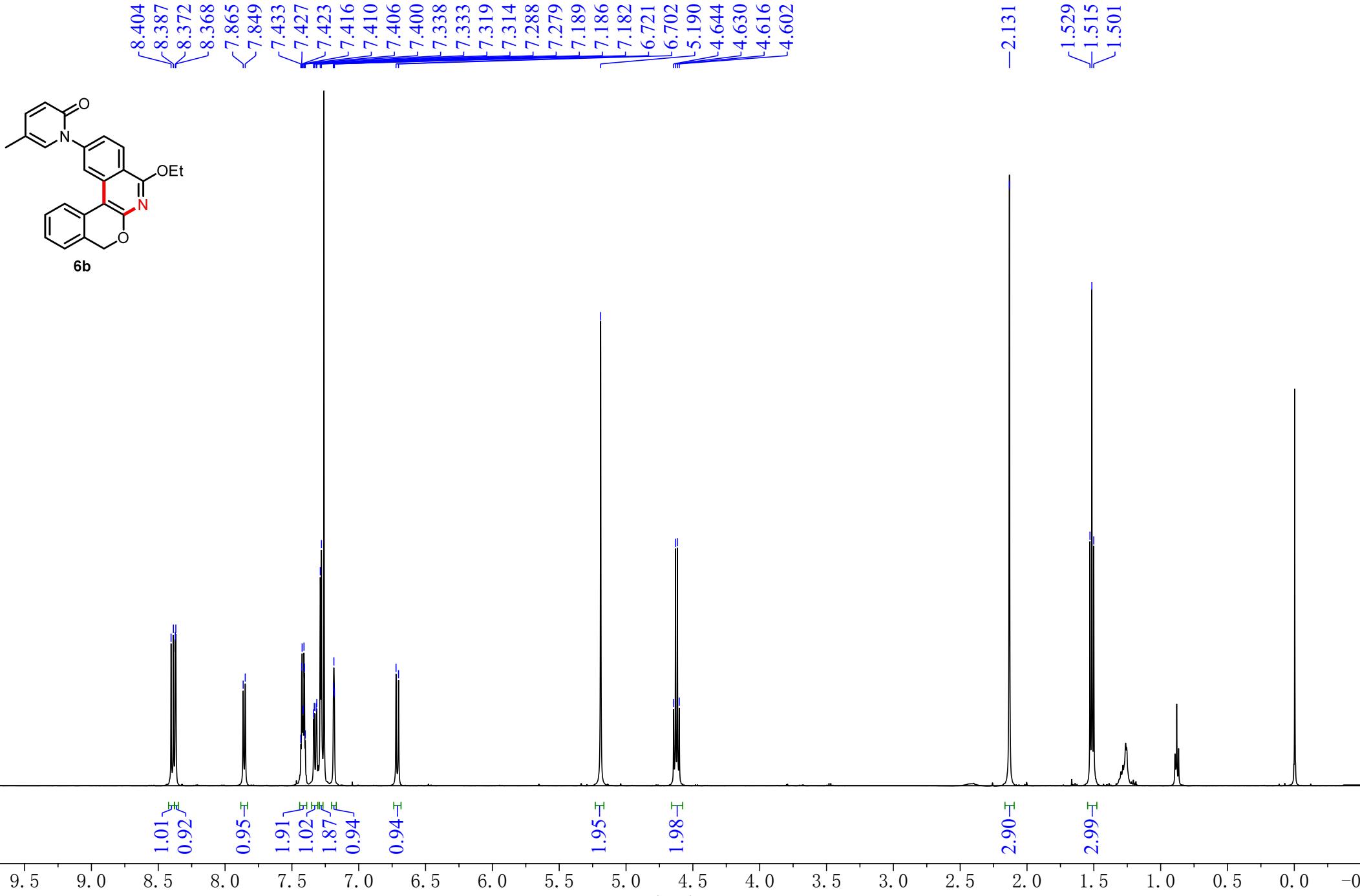
1.513  
1.502  
1.490



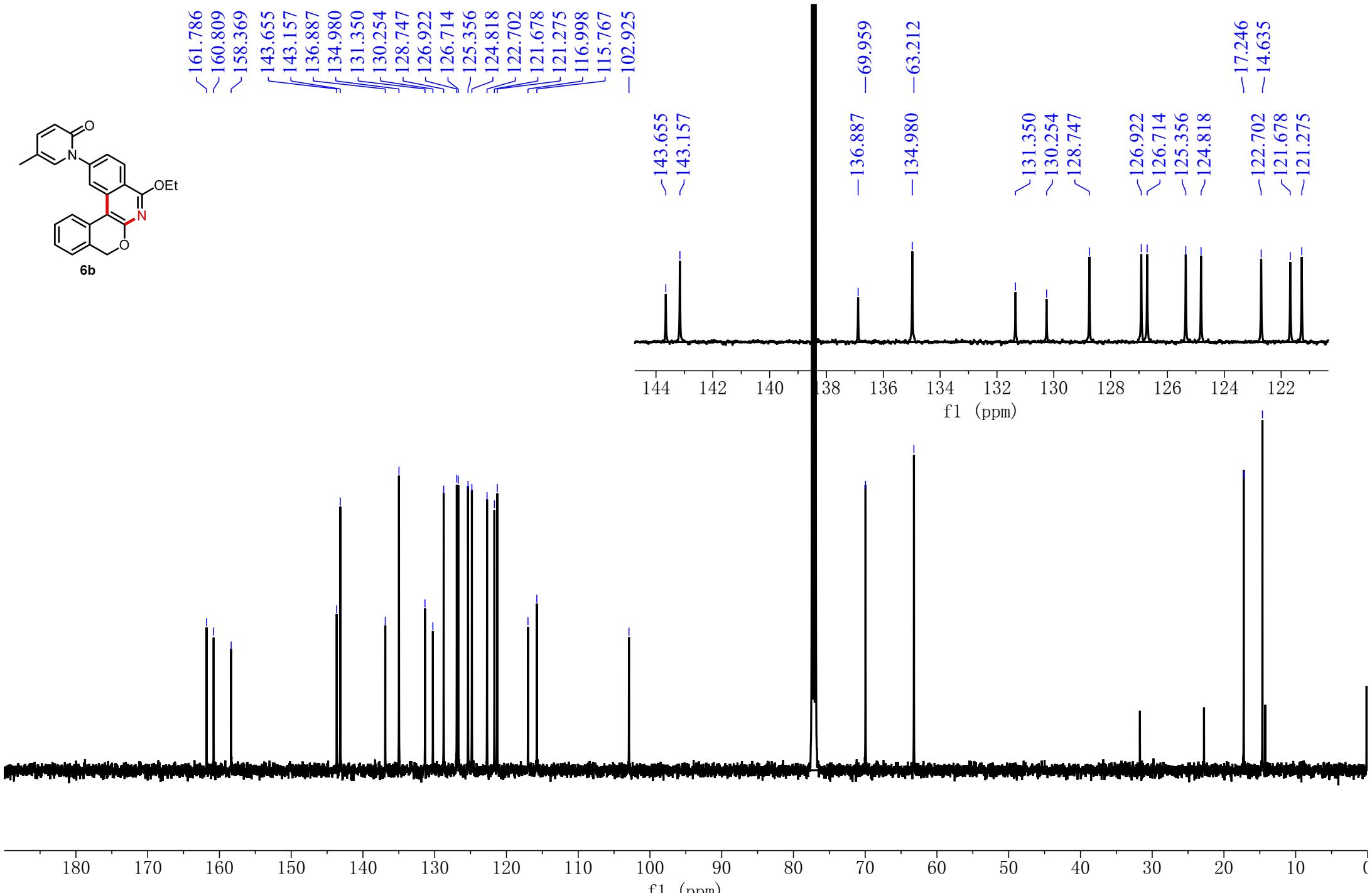
<sup>1</sup>H NMR spectrum of **6a**



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **6a**

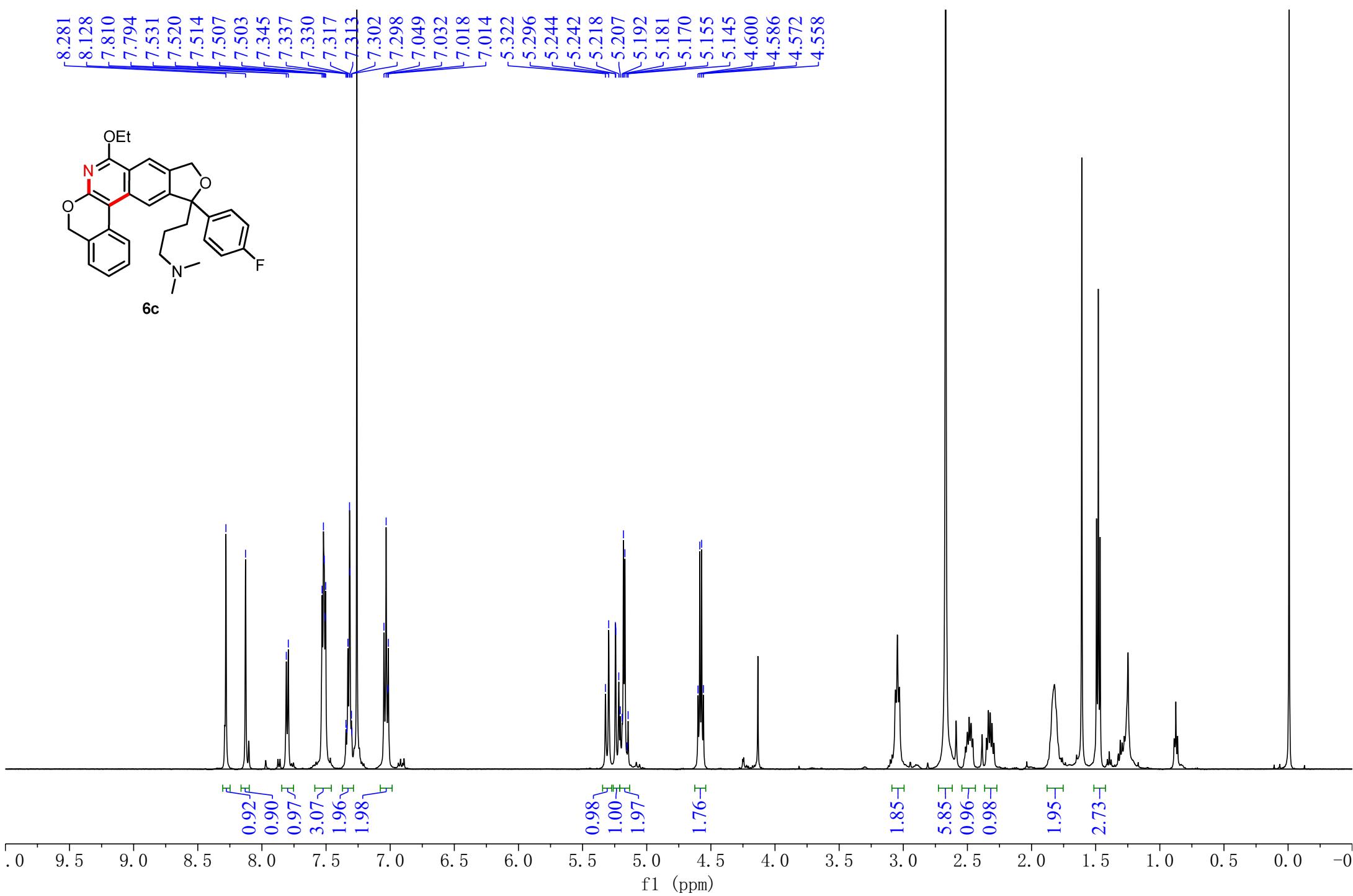
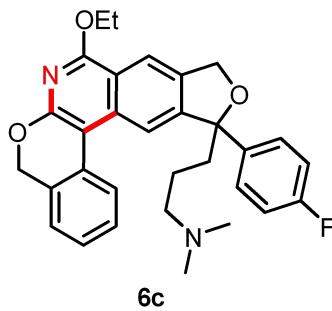


$^1\text{H}$  NMR spectrum of **6b**

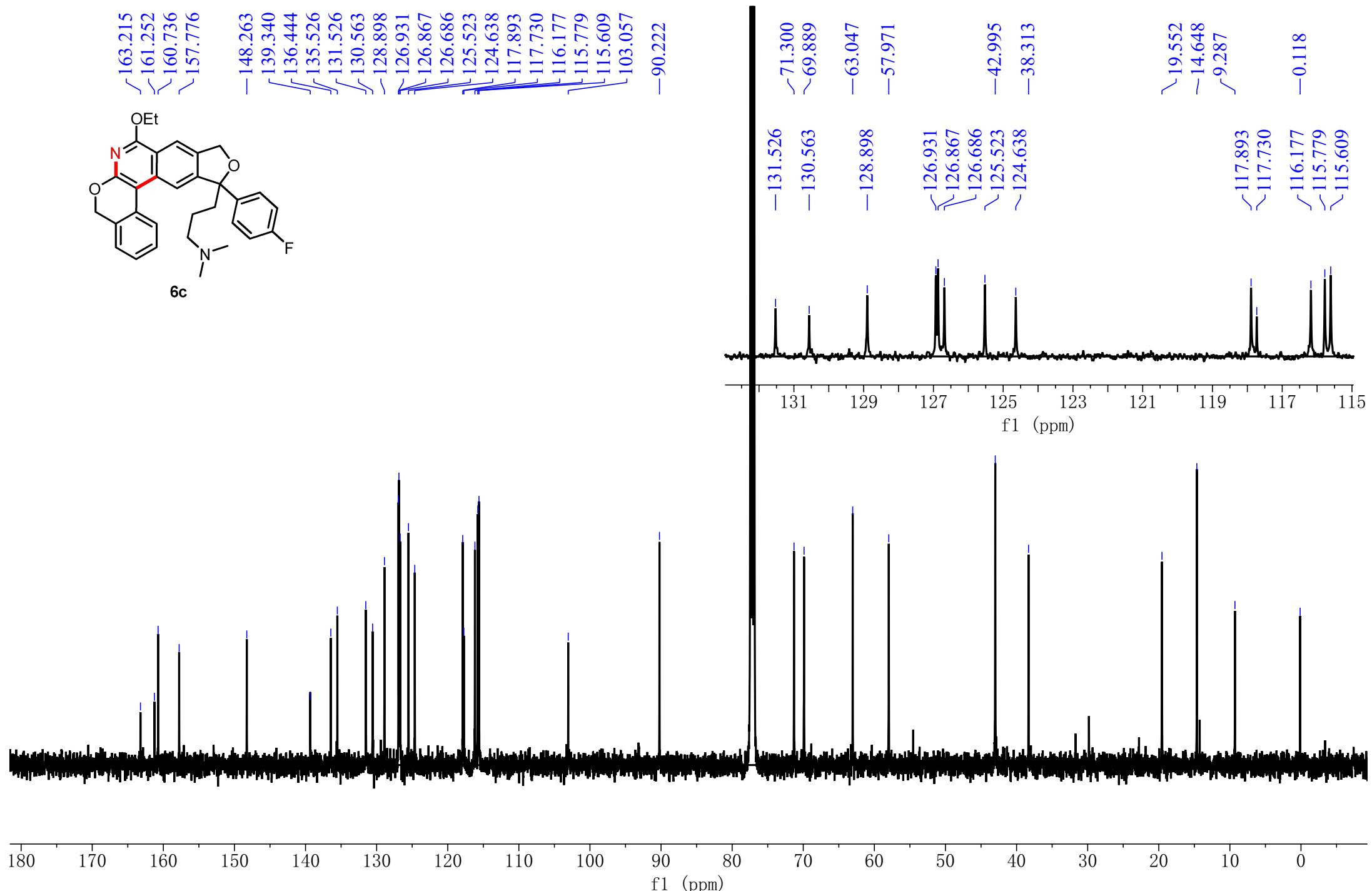


<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **6b**

8.281  
8.128  
7.810  
7.794  
7.531  
7.520  
7.514  
7.507  
7.503  
7.345  
7.337  
7.330  
7.317  
7.313  
7.302  
7.298  
7.049  
7.032  
7.018  
7.014  
5.322  
5.296  
5.244  
5.242  
5.218  
5.207  
5.192  
5.181  
5.170  
5.155  
5.145  
4.600  
4.586  
4.572  
4.558

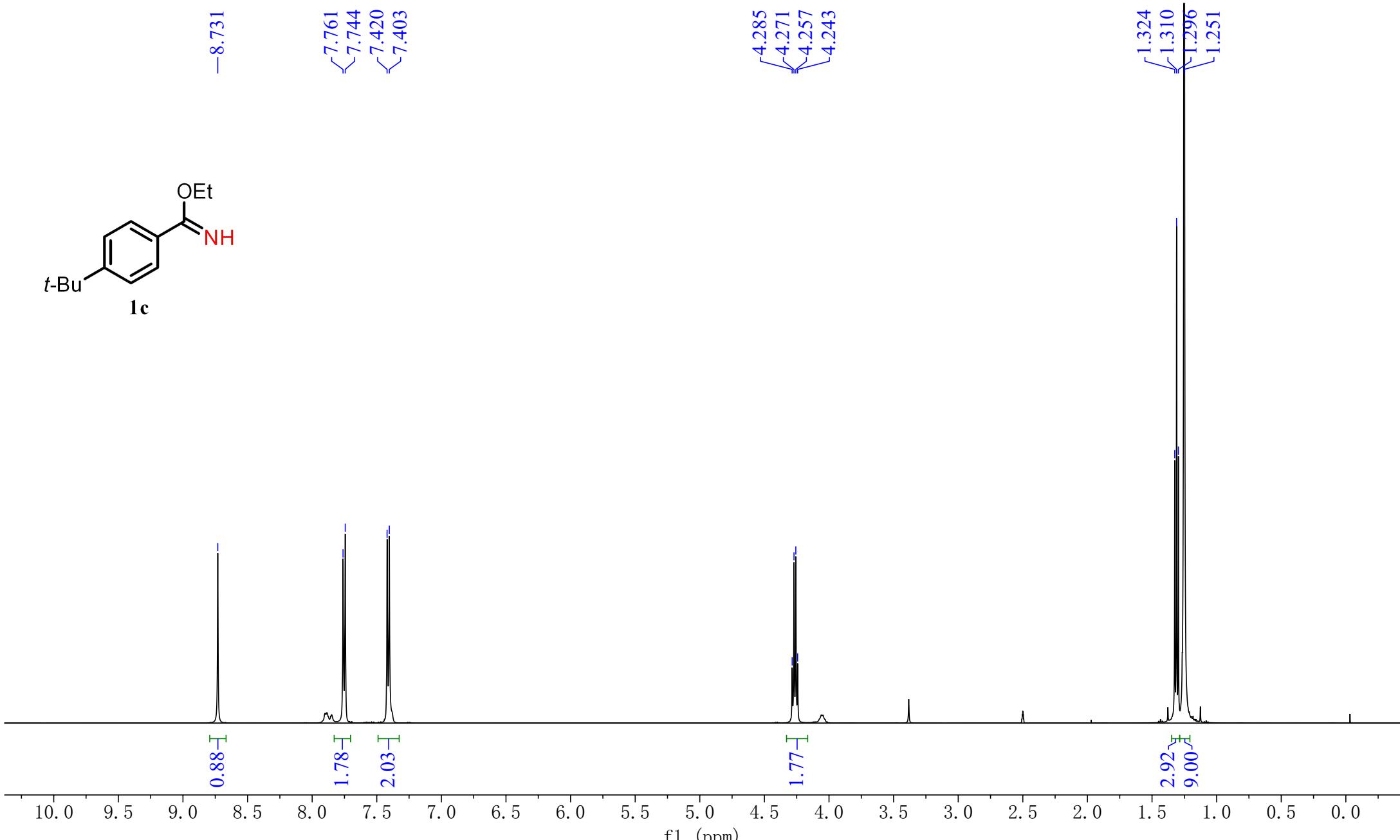
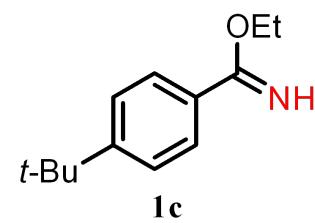


<sup>1</sup>H NMR spectrum of **6c**



<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **6c**

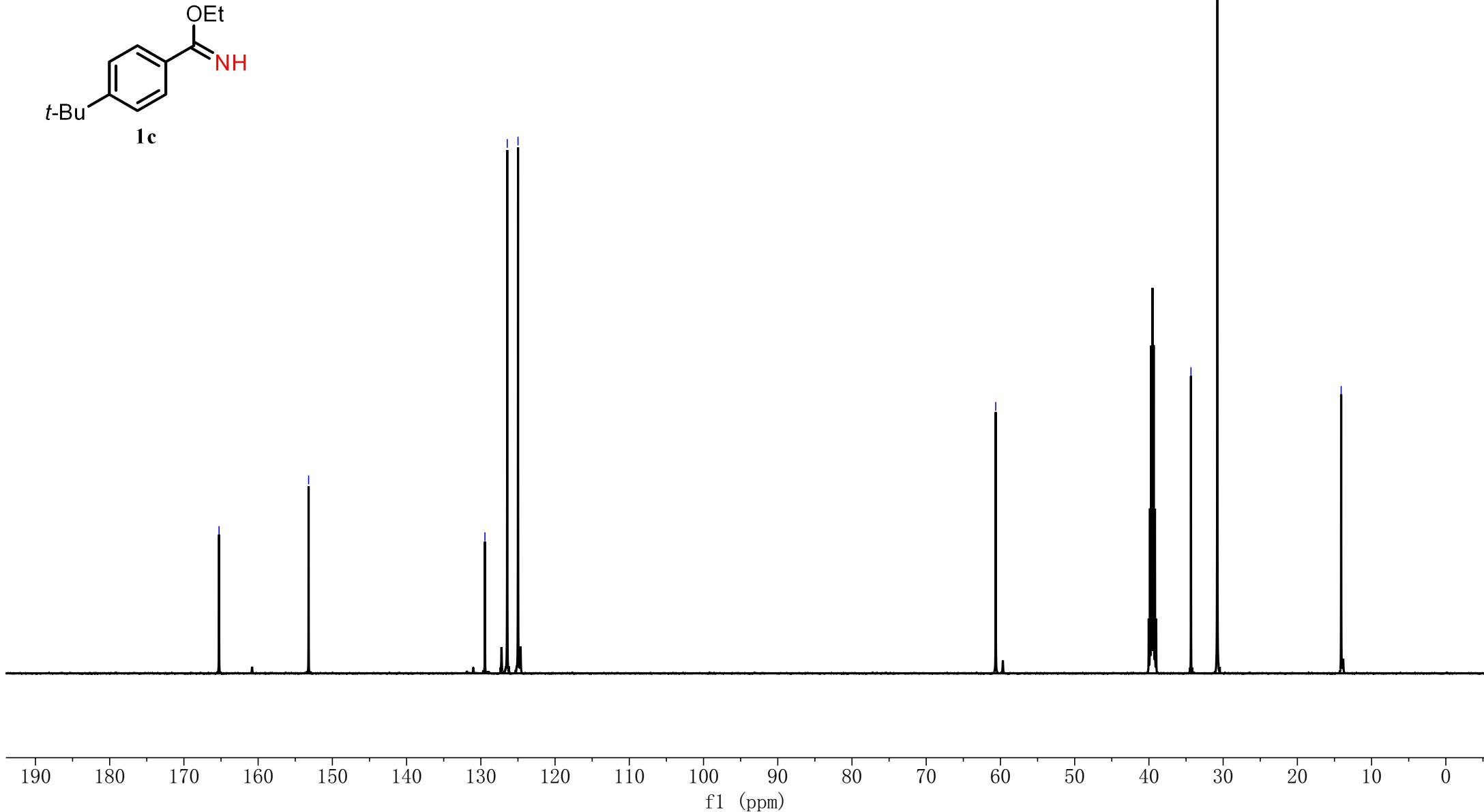
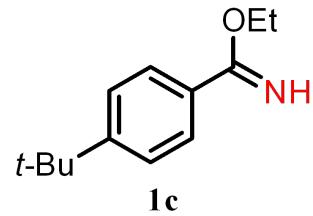
#### 4. NMR spectra data for new compounds

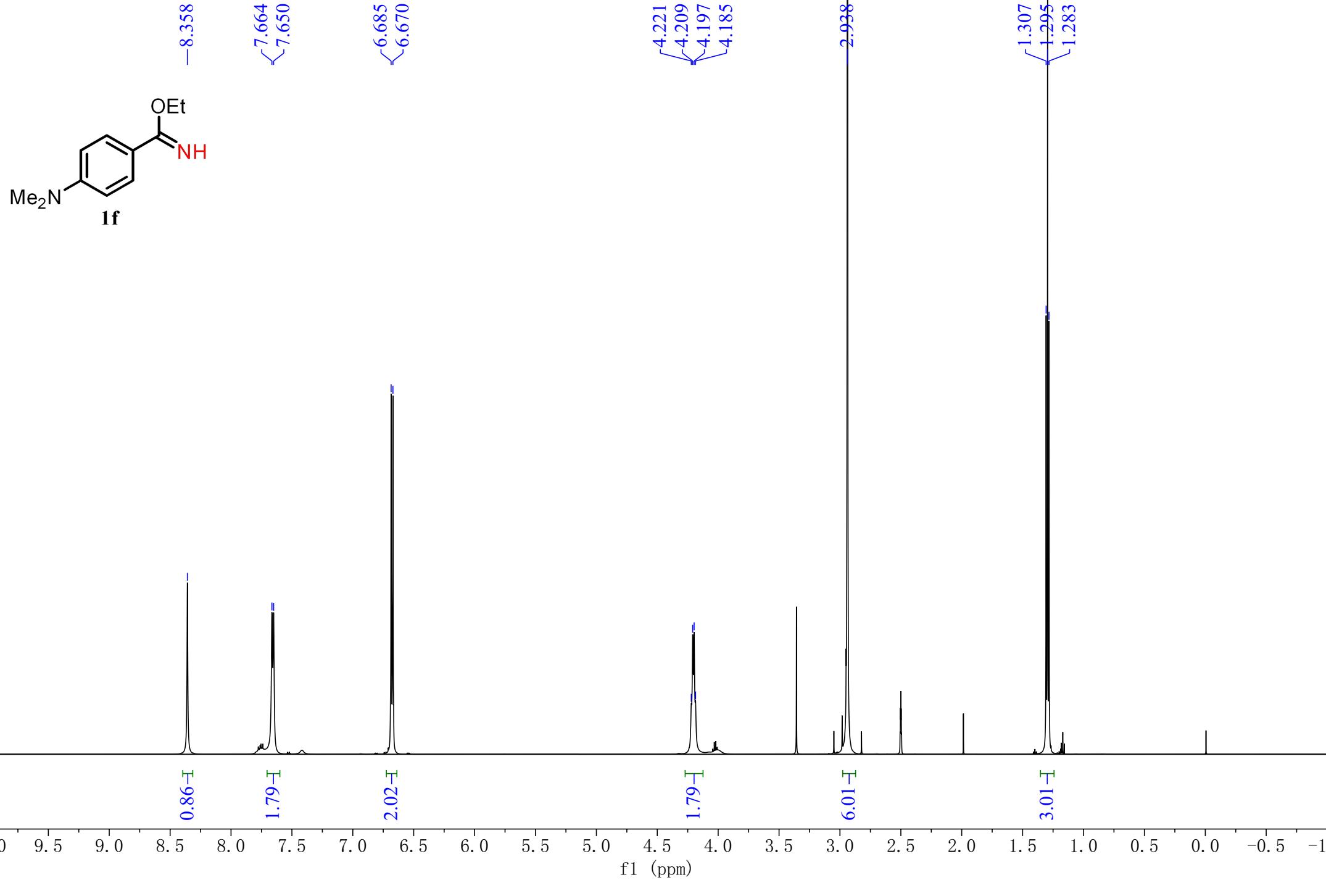


<sup>1</sup>H NMR spectrum of **1c**

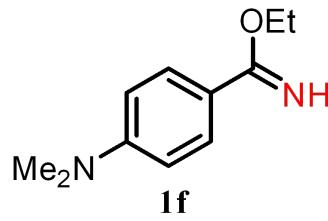
\*c1ccc(C(=N)C(=O)OC)c(\*)cc1

—165.267  
—153.201  
  
✓129.446  
✓126.442  
~124.990  
  
—60.637  
—34.333  
—30.783  
—14.099

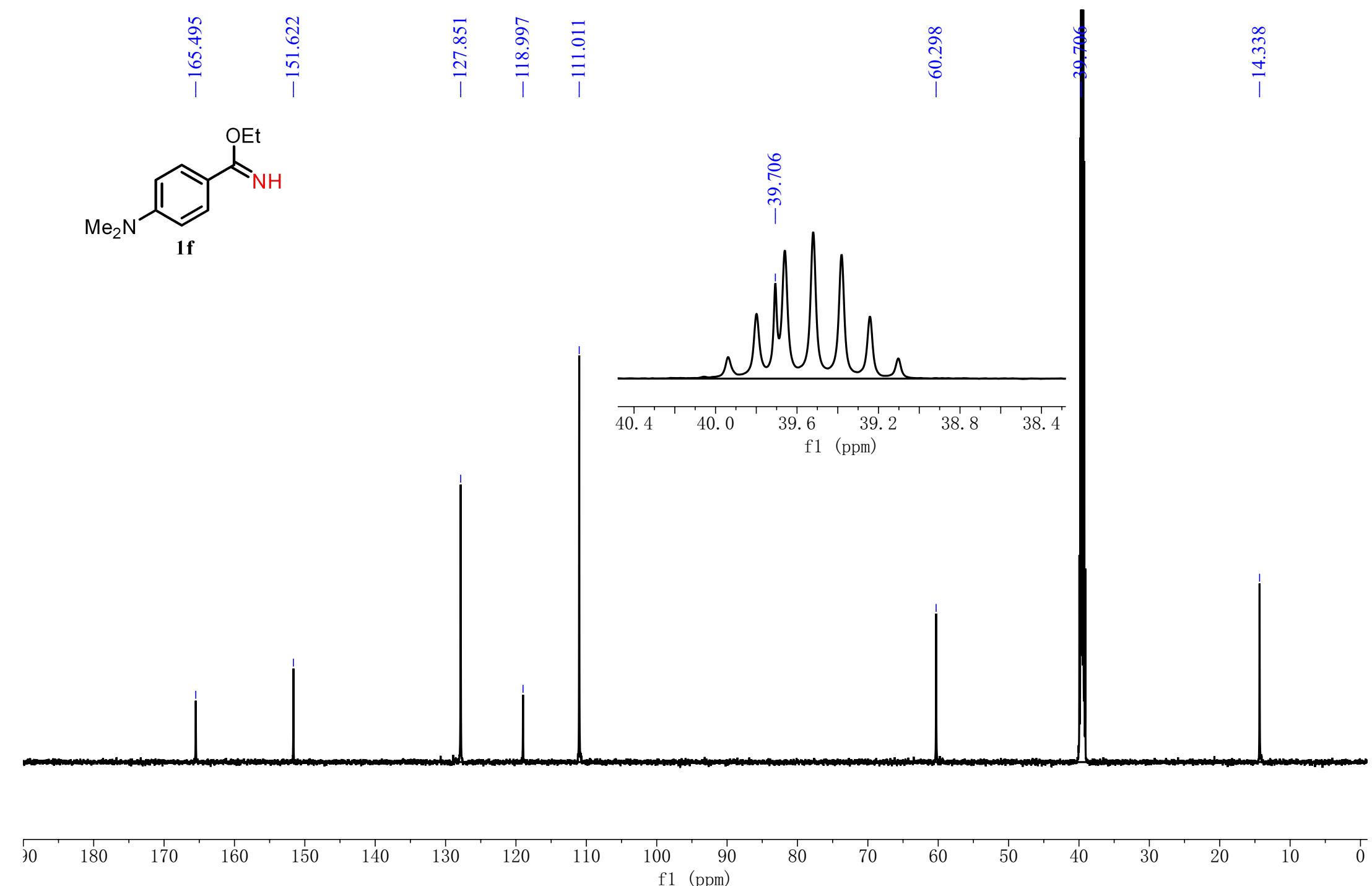




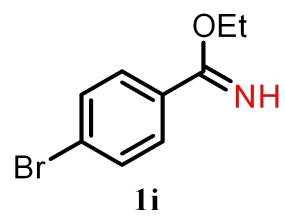
<sup>1</sup>H NMR spectrum of **1f**



-165.495    -151.622    -127.851    -118.997    -111.011    -60.298    -39.706    -14.338



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1f**

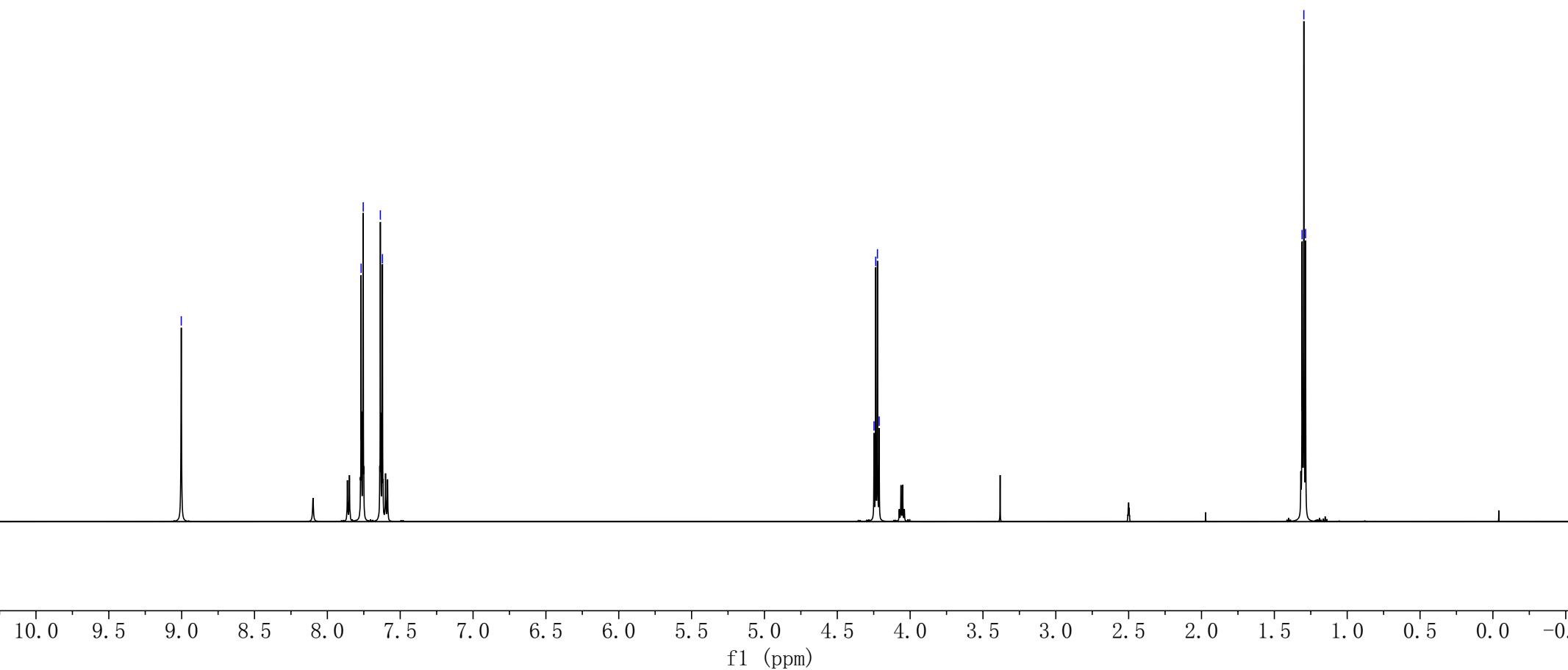


-9.003

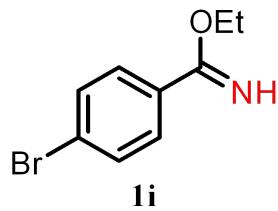
7.768  
7.754  
7.636  
7.622

4.248  
4.236  
4.224  
4.212

1.310  
1.298  
1.286



$^1\text{H}$  NMR spectrum of **1i**

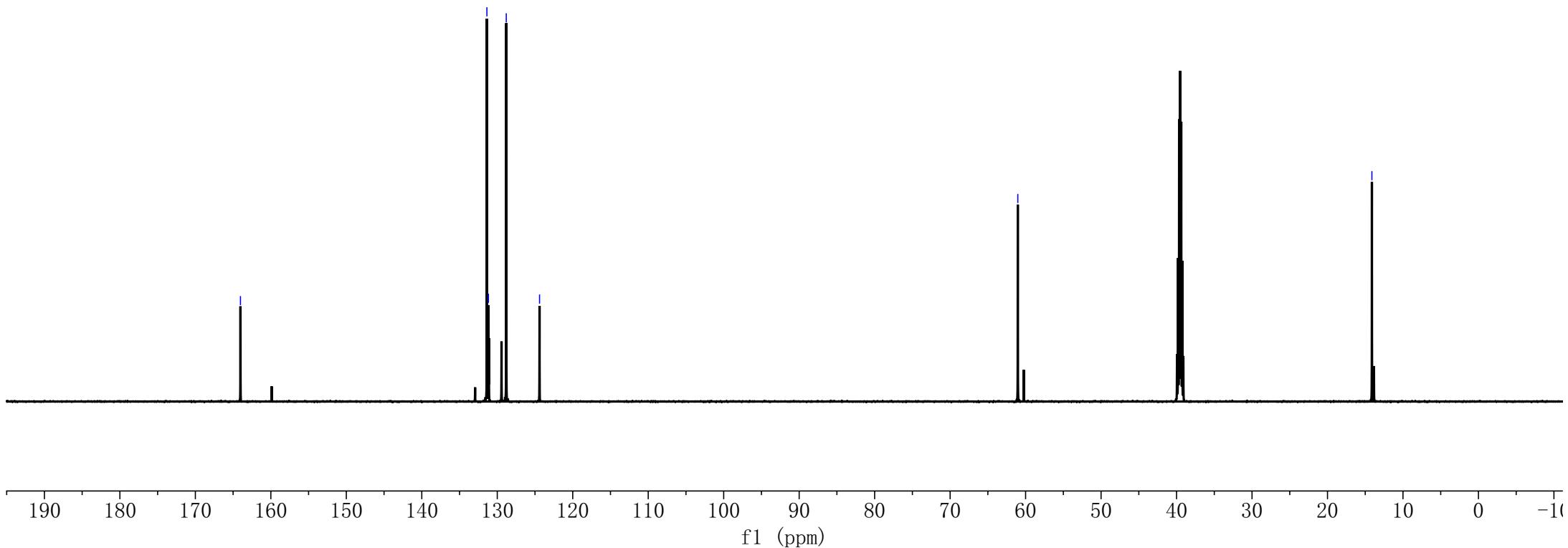


-164.024

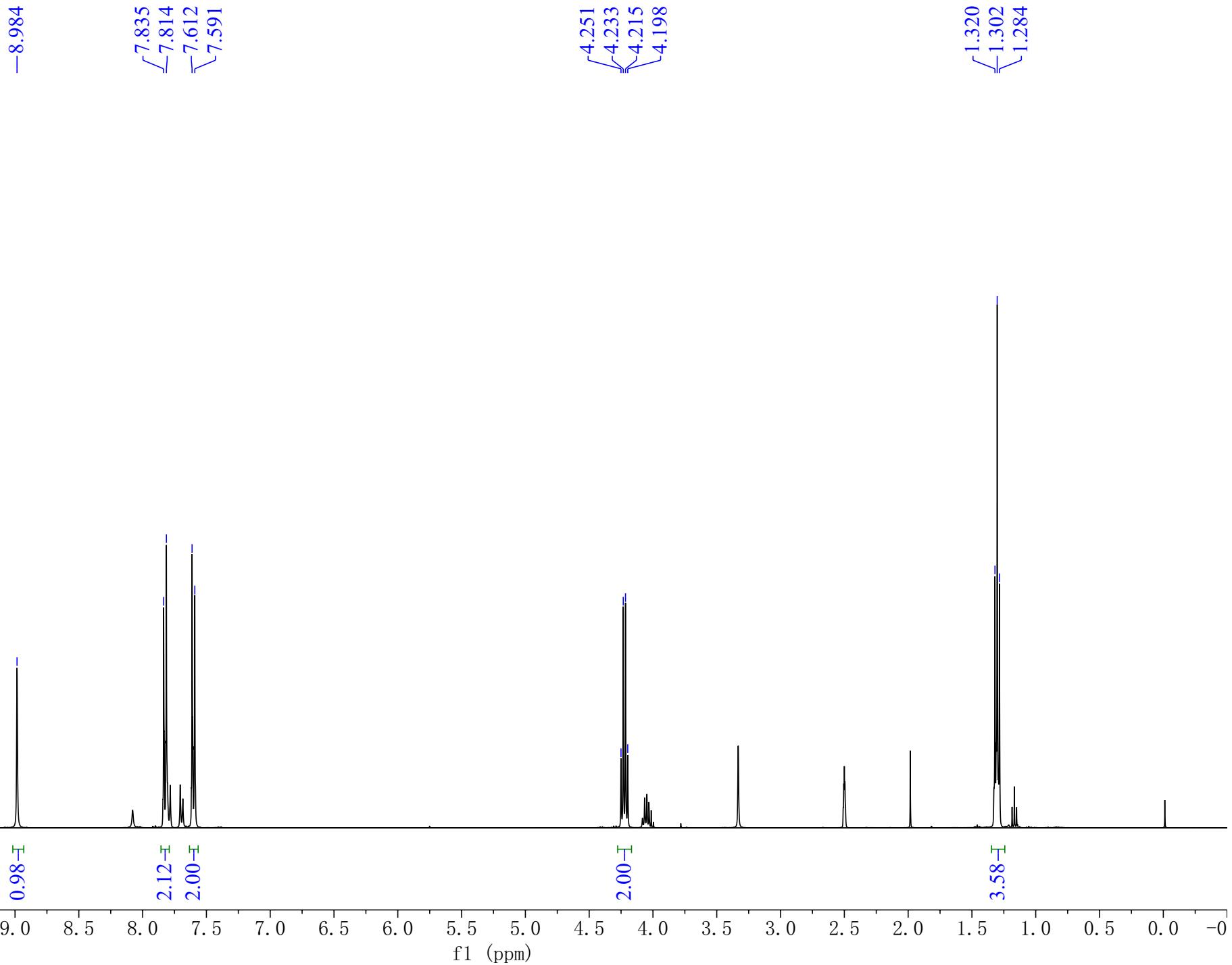
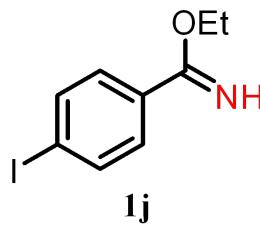
131.374  
131.169  
128.808  
124.399

-61.031

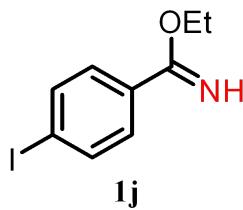
-14.116



<sup>13</sup>C{<sup>1</sup>H} NMR spectrum of **1i**



$^1\text{H}$  NMR spectrum of **1j**  
S92



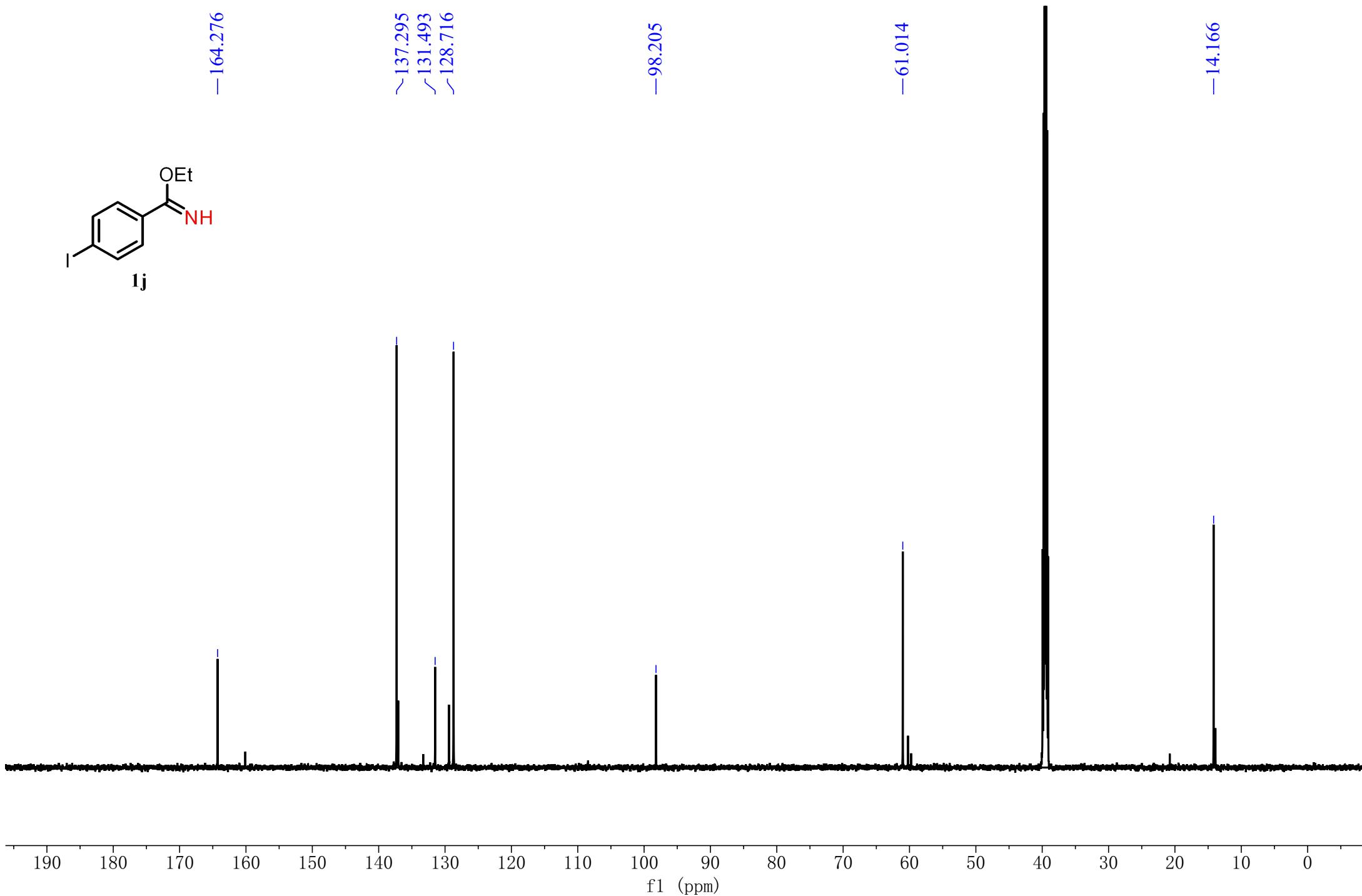
-164.276

~137.295  
✓ 131.493  
✓ 128.716

-98.205

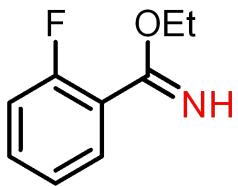
-61.014

-14.166

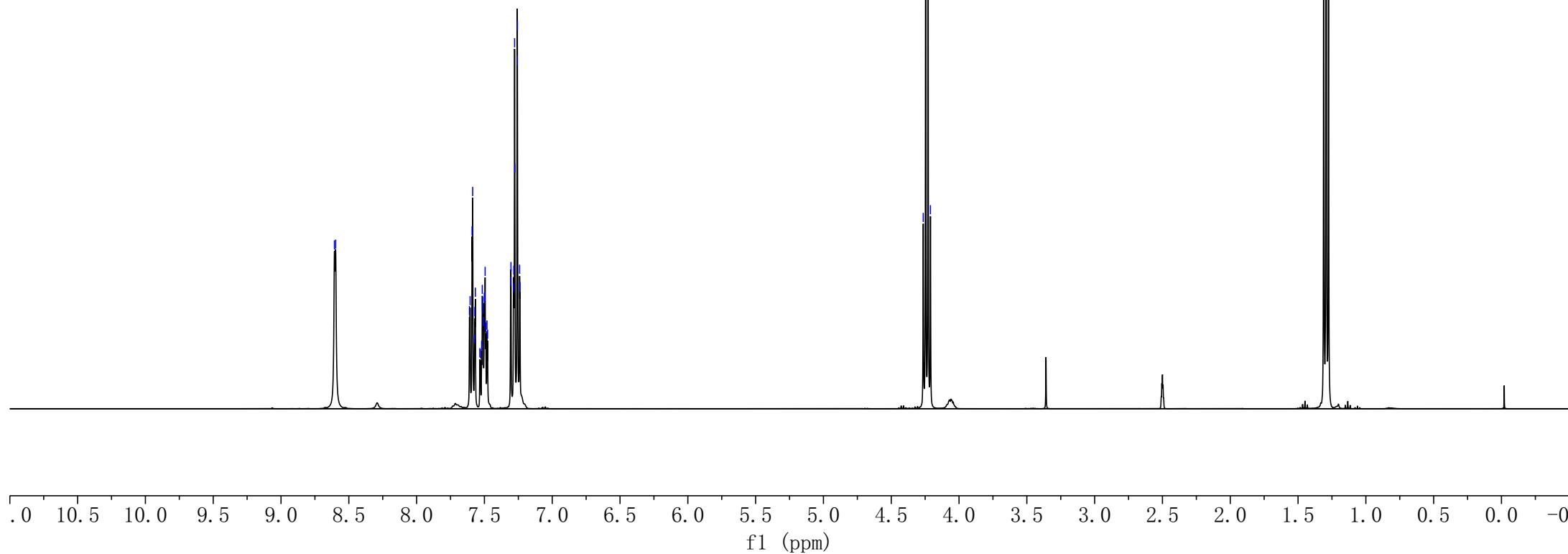


$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1j**

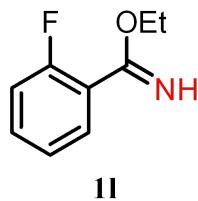
8.606  
8.597  
7.610  
7.606  
7.591  
7.586  
7.573  
7.571  
7.567  
7.534  
7.529  
7.521  
7.516  
7.513  
7.511  
7.508  
7.501  
7.498  
7.495  
7.490  
7.481  
7.477  
7.307  
7.304  
7.286  
7.283  
7.278  
7.275  
7.259  
7.257  
7.241  
7.238



4.264  
4.246  
4.228  
4.211  
1.311  
1.293  
1.275



<sup>1</sup>H NMR spectrum of 1l

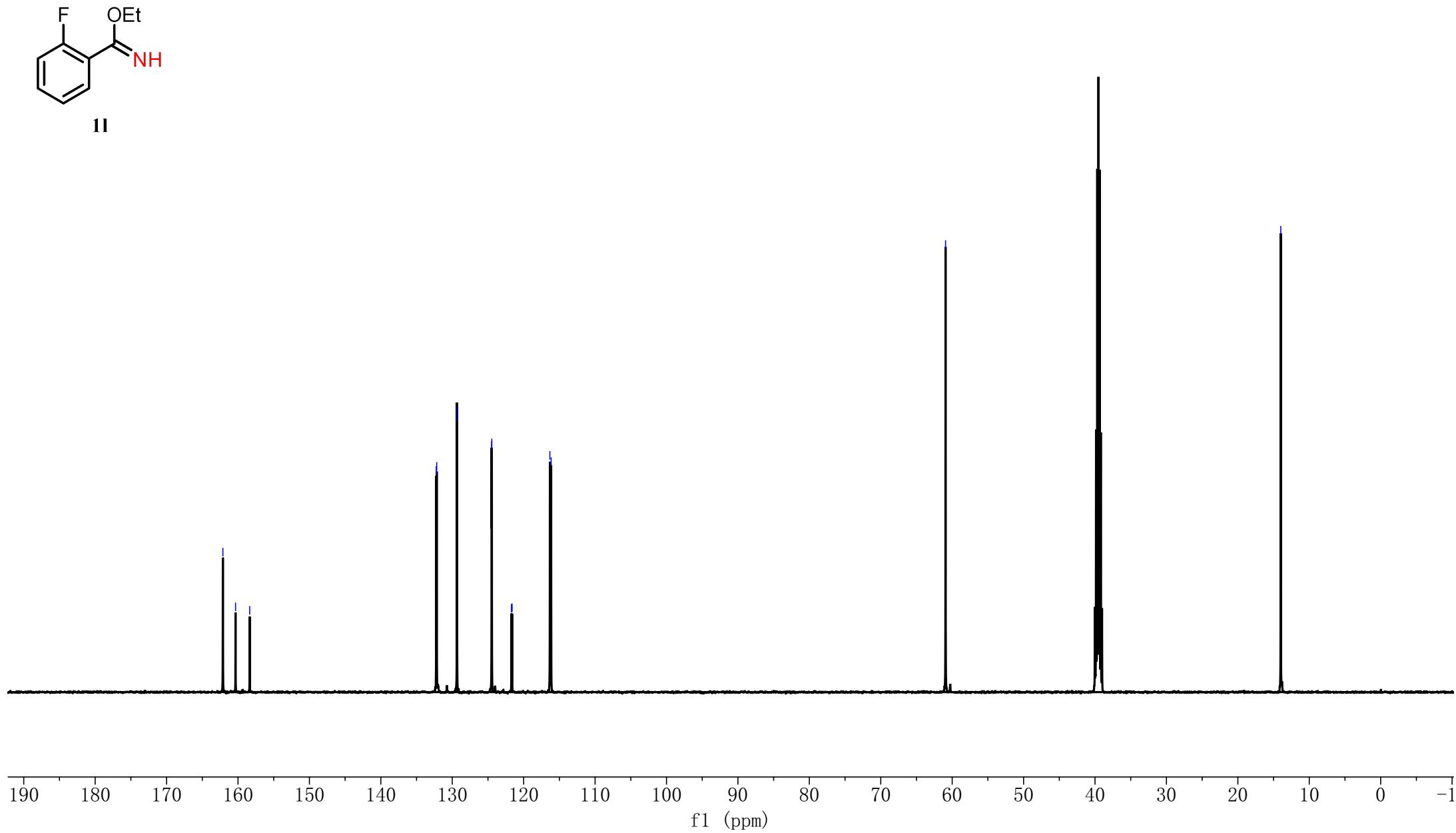


✓ 162.115  
— 160.343  
~ 158.357

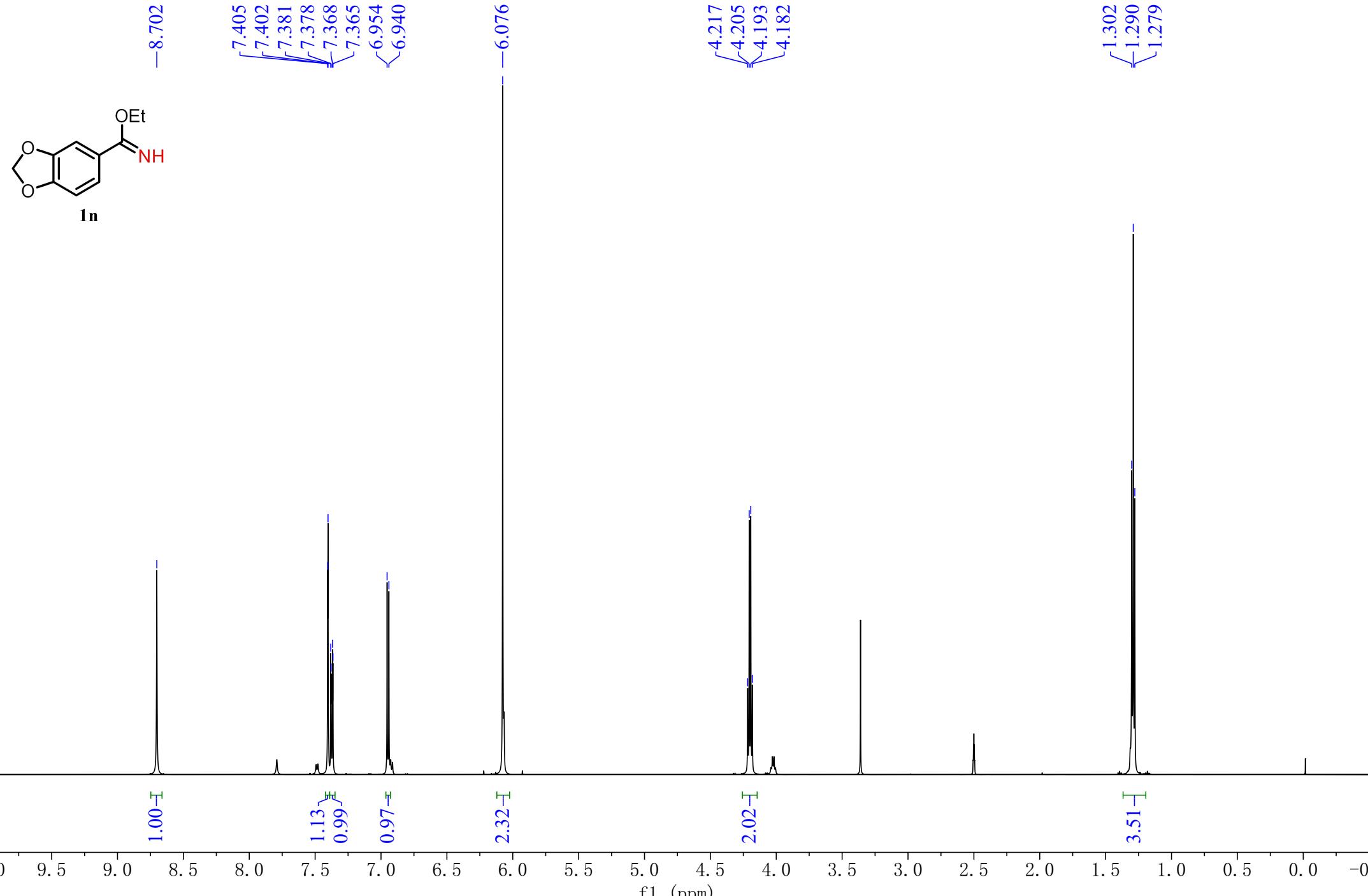
✓ 132.242  
✓ 132.172  
✓ 129.349  
✓ 129.330  
✓ 124.486  
✓ 124.458  
✓ 121.711  
✓ 121.620  
✓ 116.328  
✓ 116.153

— 60.926

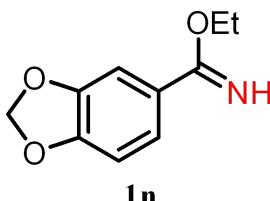
— 13.992



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **11**  
S95



<sup>1</sup>H NMR spectrum of **1n**



-164.302

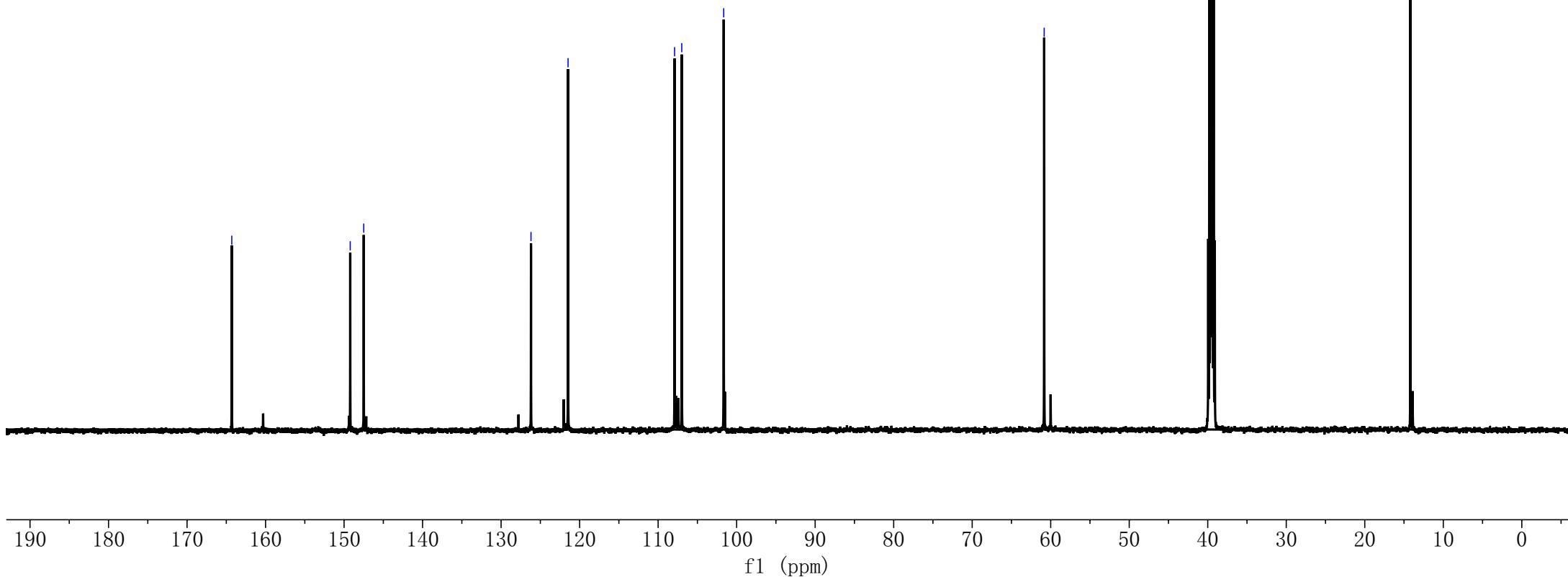
~149.217  
~147.495

-126.193  
-121.473

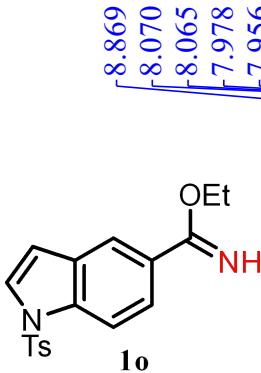
107.904  
106.992  
-101.648

-60.832

-14.194



$^{13}\text{C}\{\text{H}\}$  NMR spectrum of **1n**



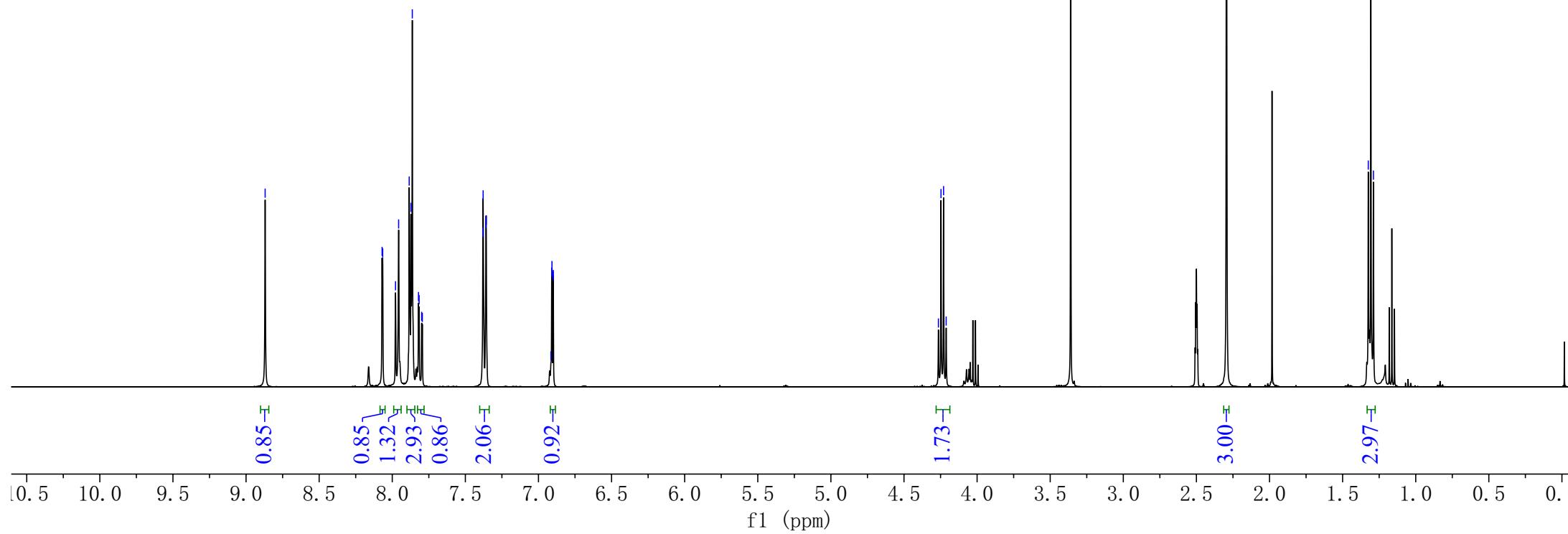
8.869  
8.070  
8.065  
7.978  
7.956  
7.884  
7.872  
7.863  
7.821  
7.816  
7.799  
7.794  
7.381  
7.378  
7.359  
7.357  
6.915  
6.910  
6.908  
6.900  
6.898

4.265  
4.247  
4.229  
4.212

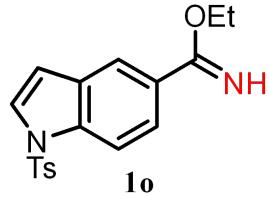
3.360

-2.294

1.324  
1.307  
1.289



$^1\text{H}$  NMR spectrum of **1o**



-165.495

-146.177

135.626

134.489

130.777

128.554

128.248

127.220

123.865

120.919

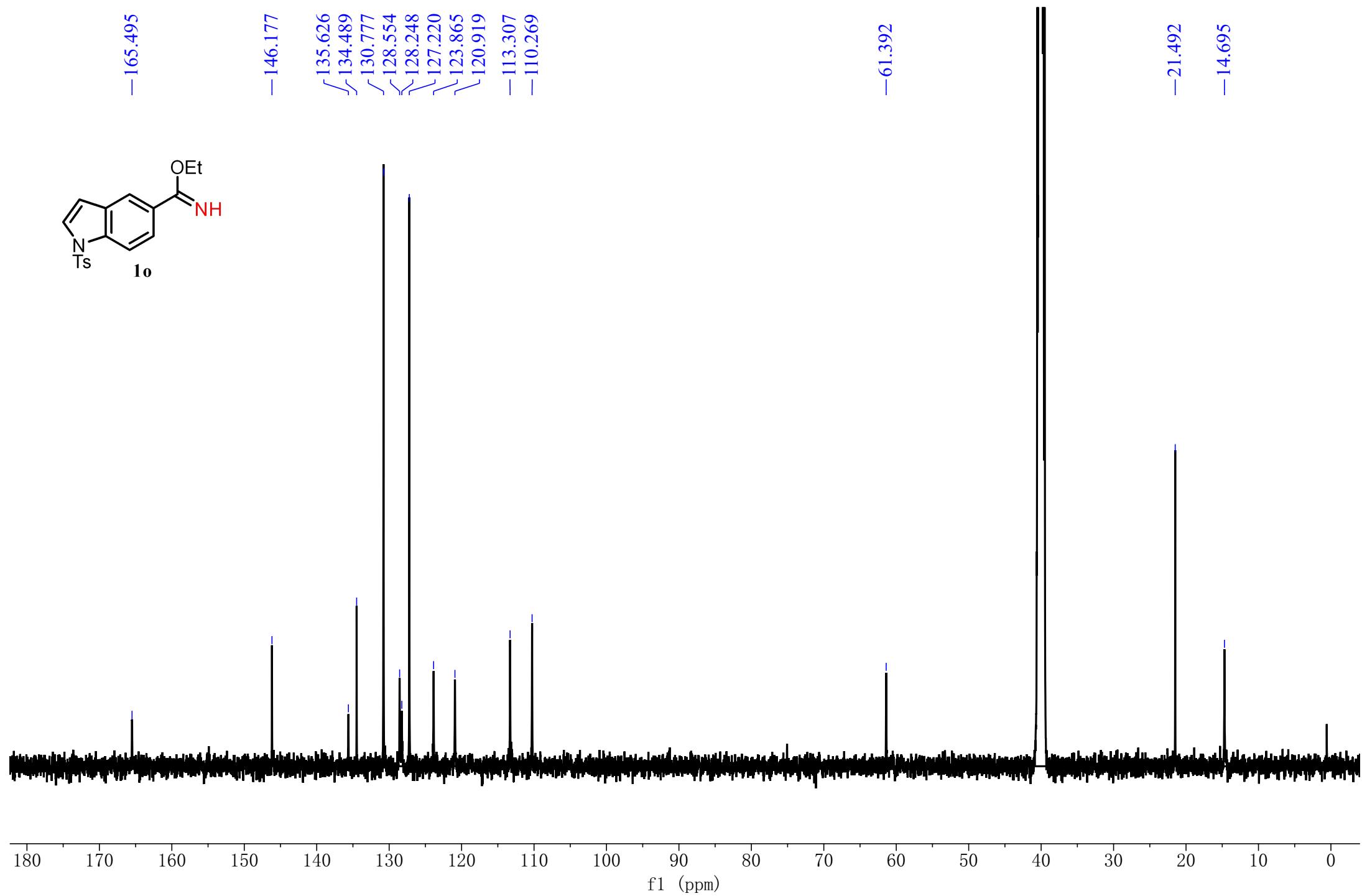
-113.307

-110.269

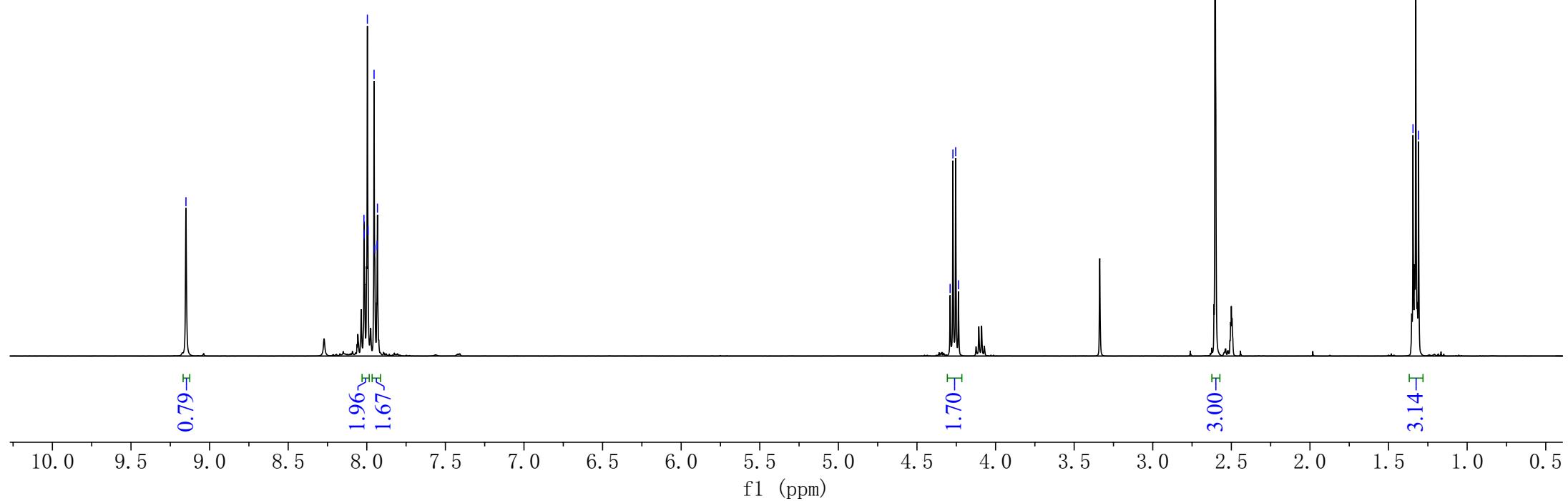
-61.392

-21.492

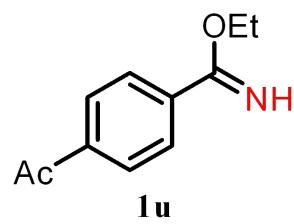
-14.695



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1o**



$^1\text{H}$  NMR spectrum of **1u**



-197.612

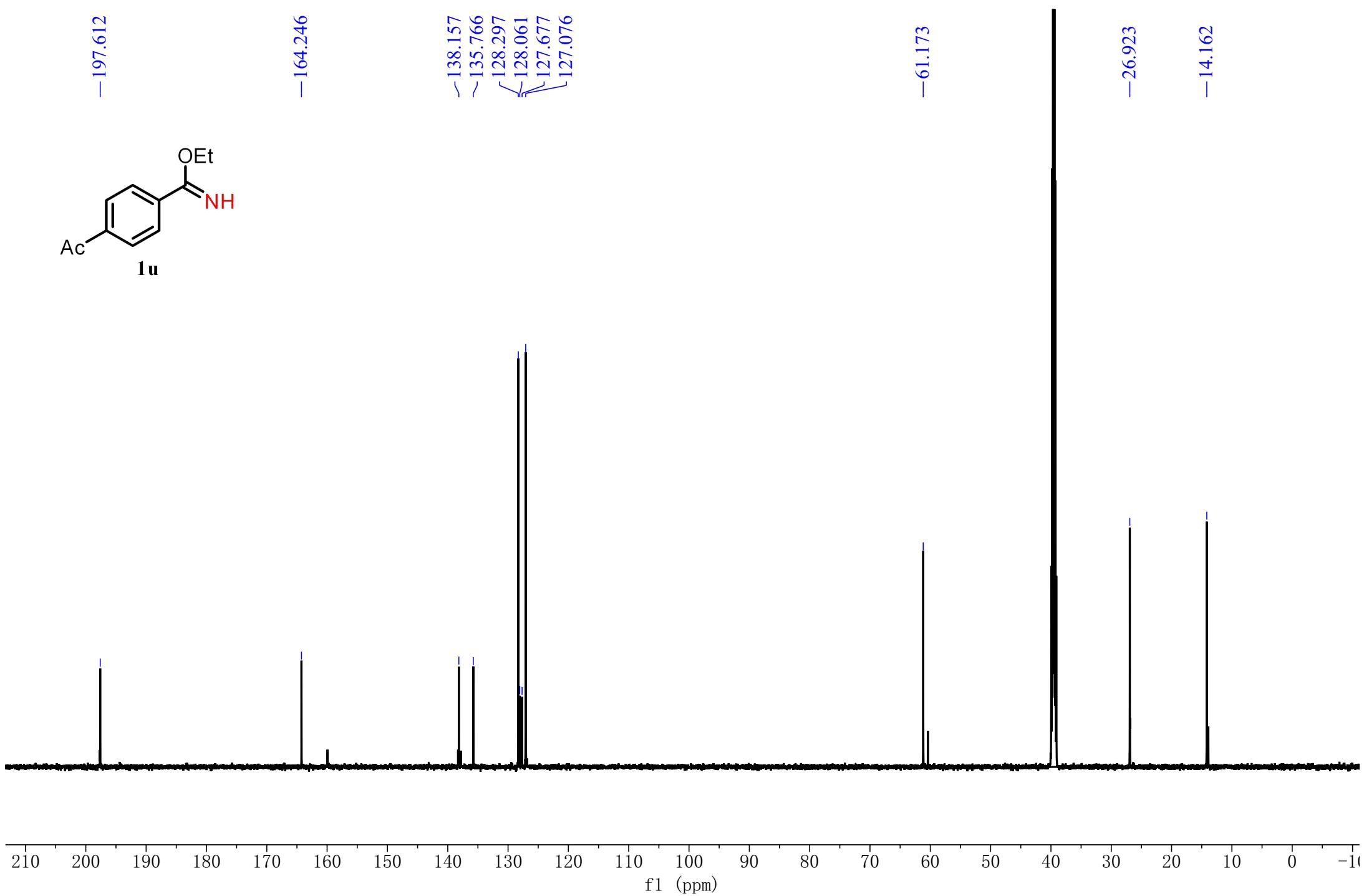
-164.246

~138.157  
~135.766  
128.297  
128.061  
127.677  
127.076

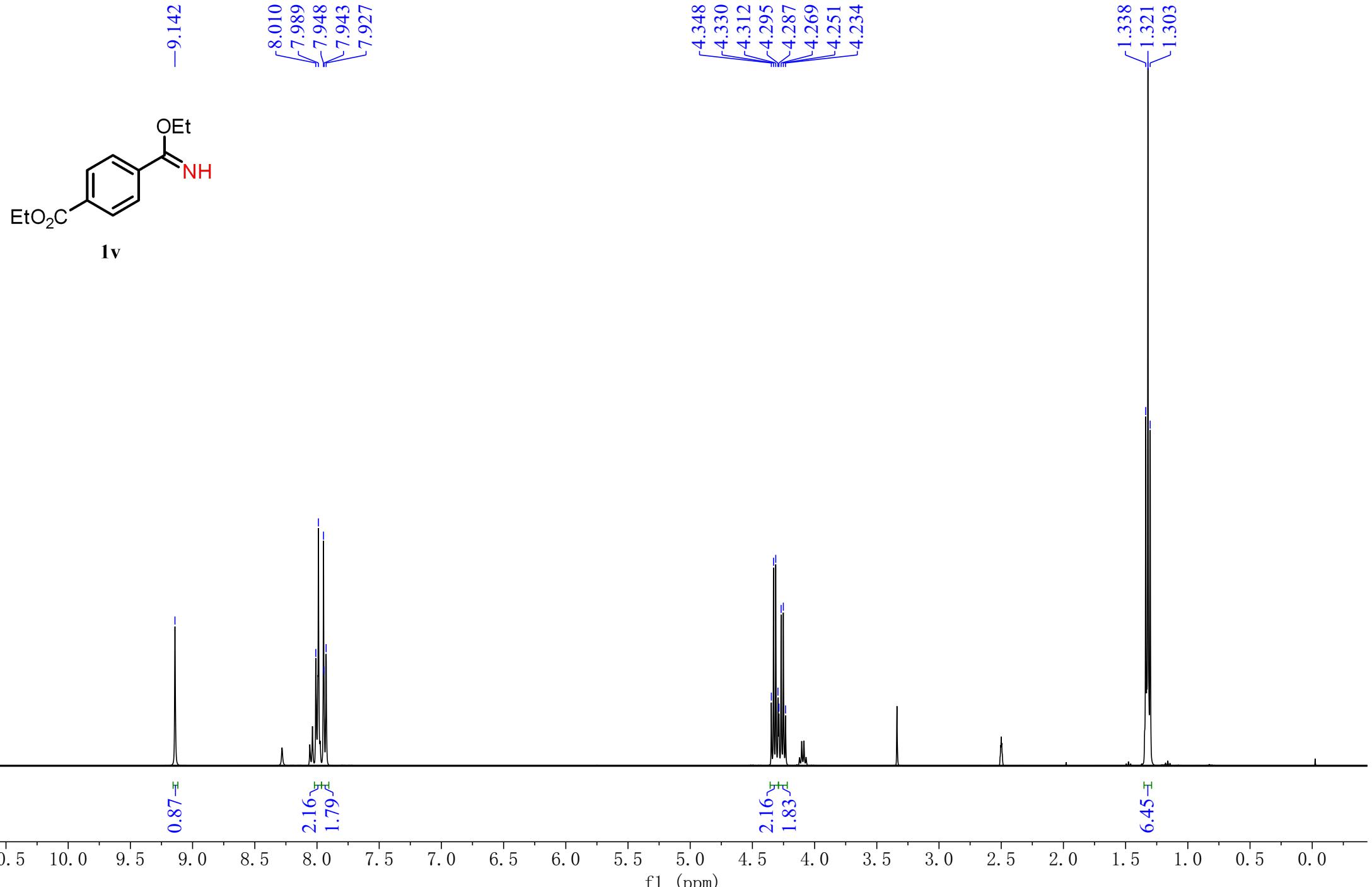
-61.173

-26.923

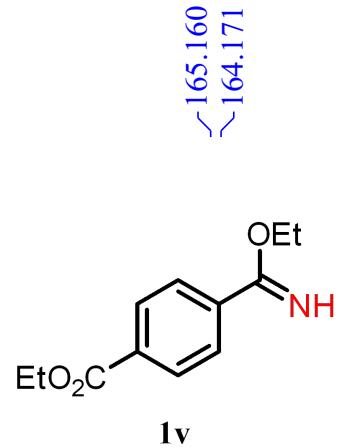
-14.162



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1u**



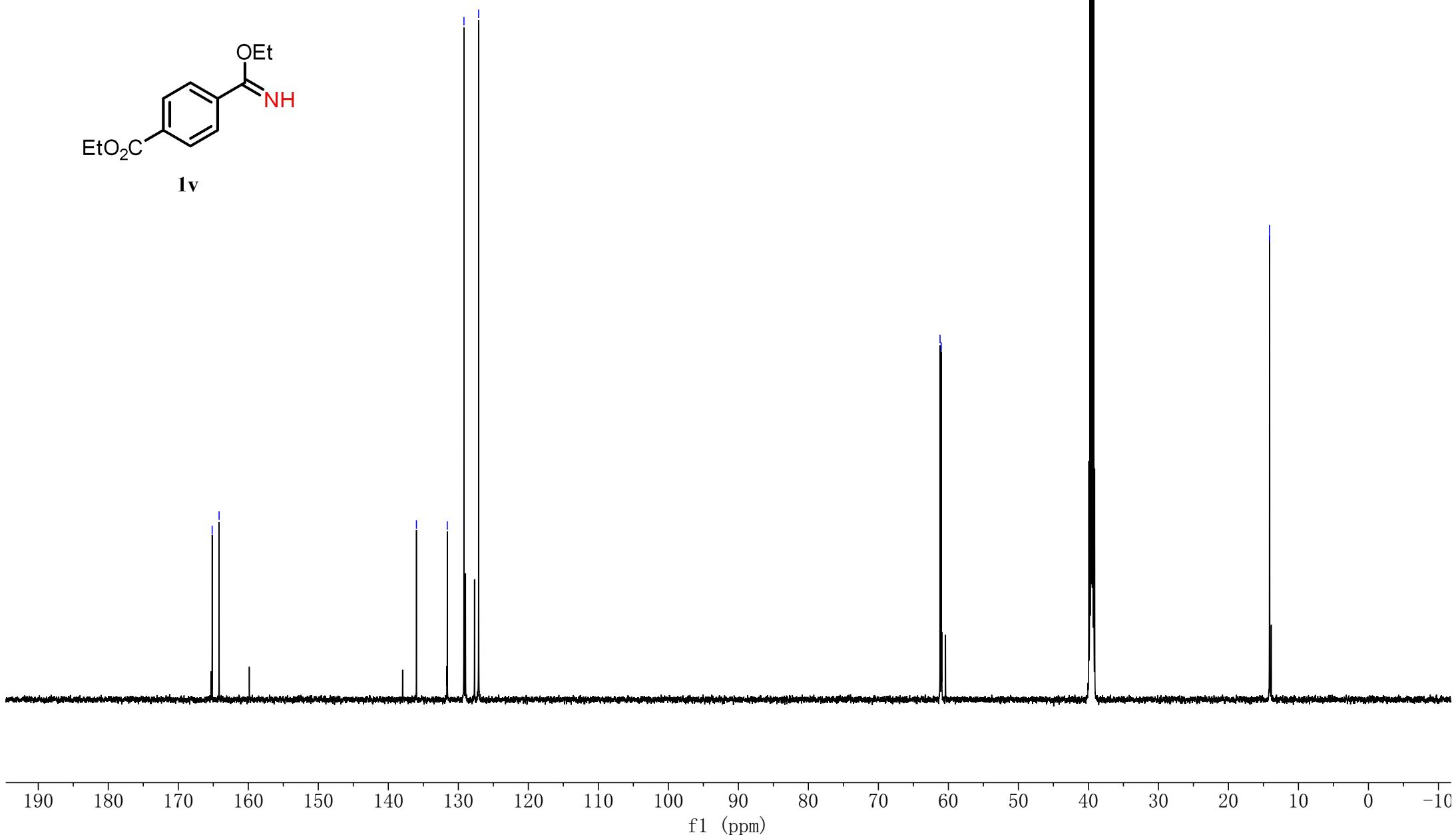
<sup>1</sup>H NMR spectrum of **1v**



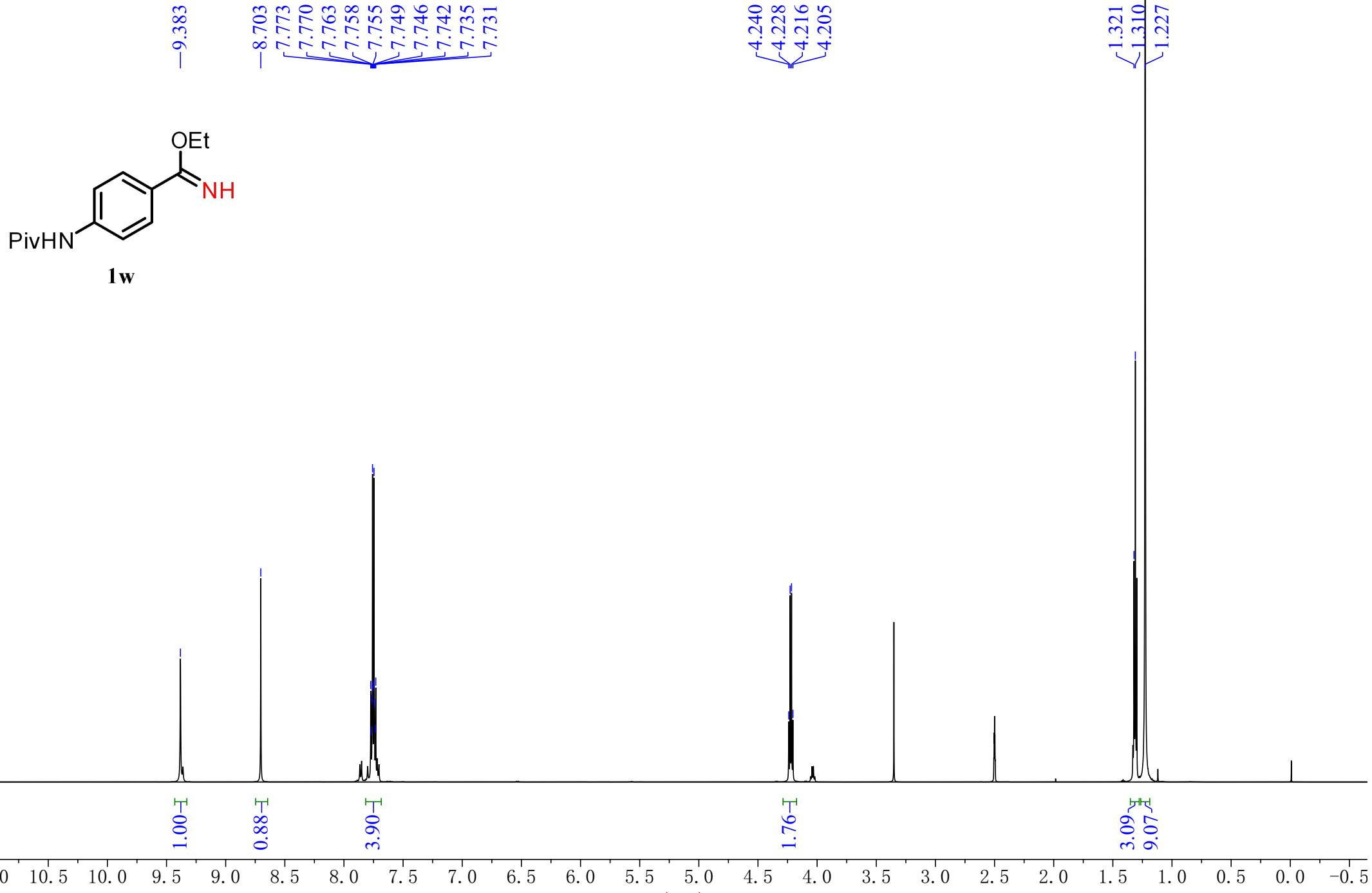
$\sim$ 165.160  
 $\sim$ 164.171  
 $\sim$ 135.982  
 $\sim$ 131.574  
 $\sim$ 129.195  
 $\sim$ 127.094

$\sim$ 61.186  
 $\sim$ 61.020

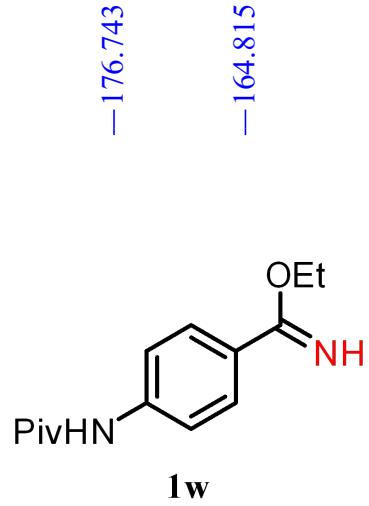
$\sim$ 14.135  
 $\sim$ 14.102



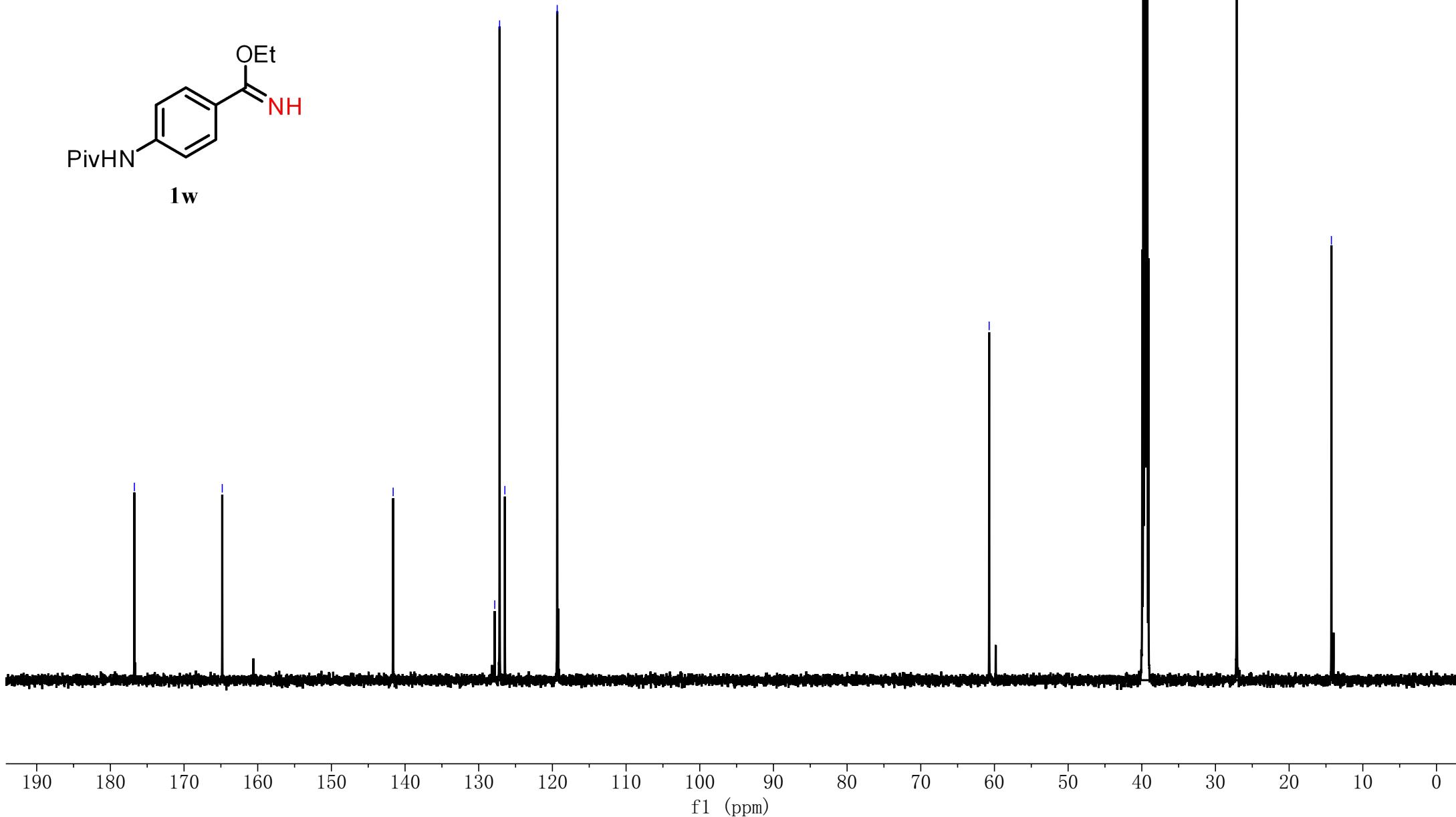
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1v**



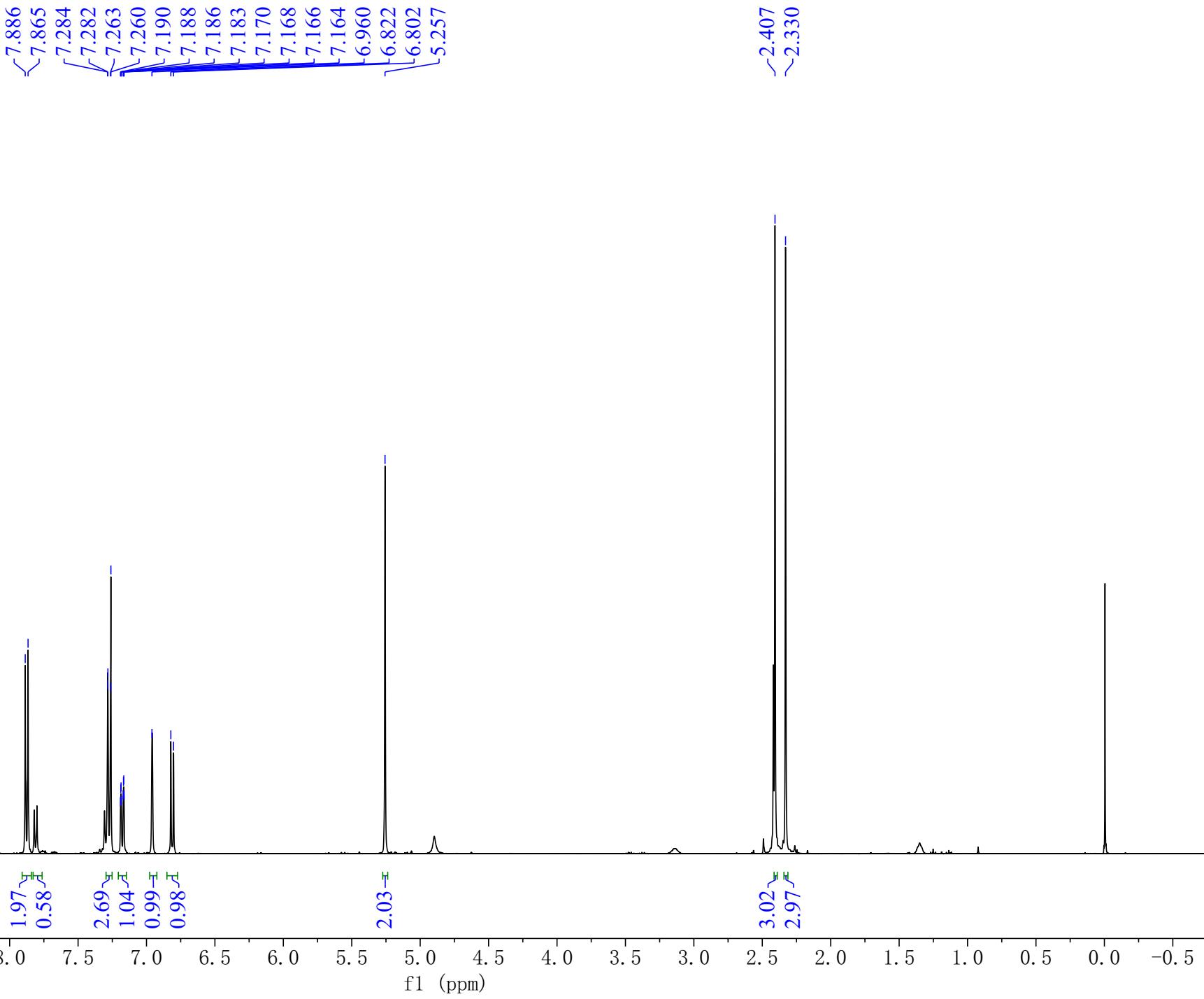
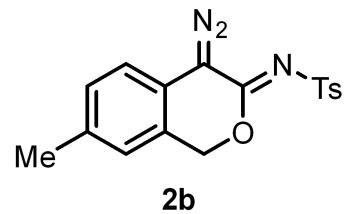
$^1\text{H}$  NMR spectrum of **1w**



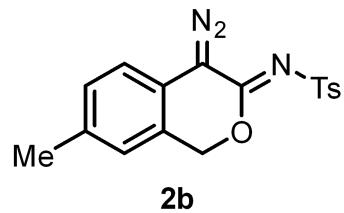
-176.743      -164.815      -141.619  
 127.828      127.167      126.452  
 \      \      \  
 -119.347  
 -60.717      27.110  
 -14.262



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1w**



<sup>1</sup>H NMR spectrum of **2b**



-164.050

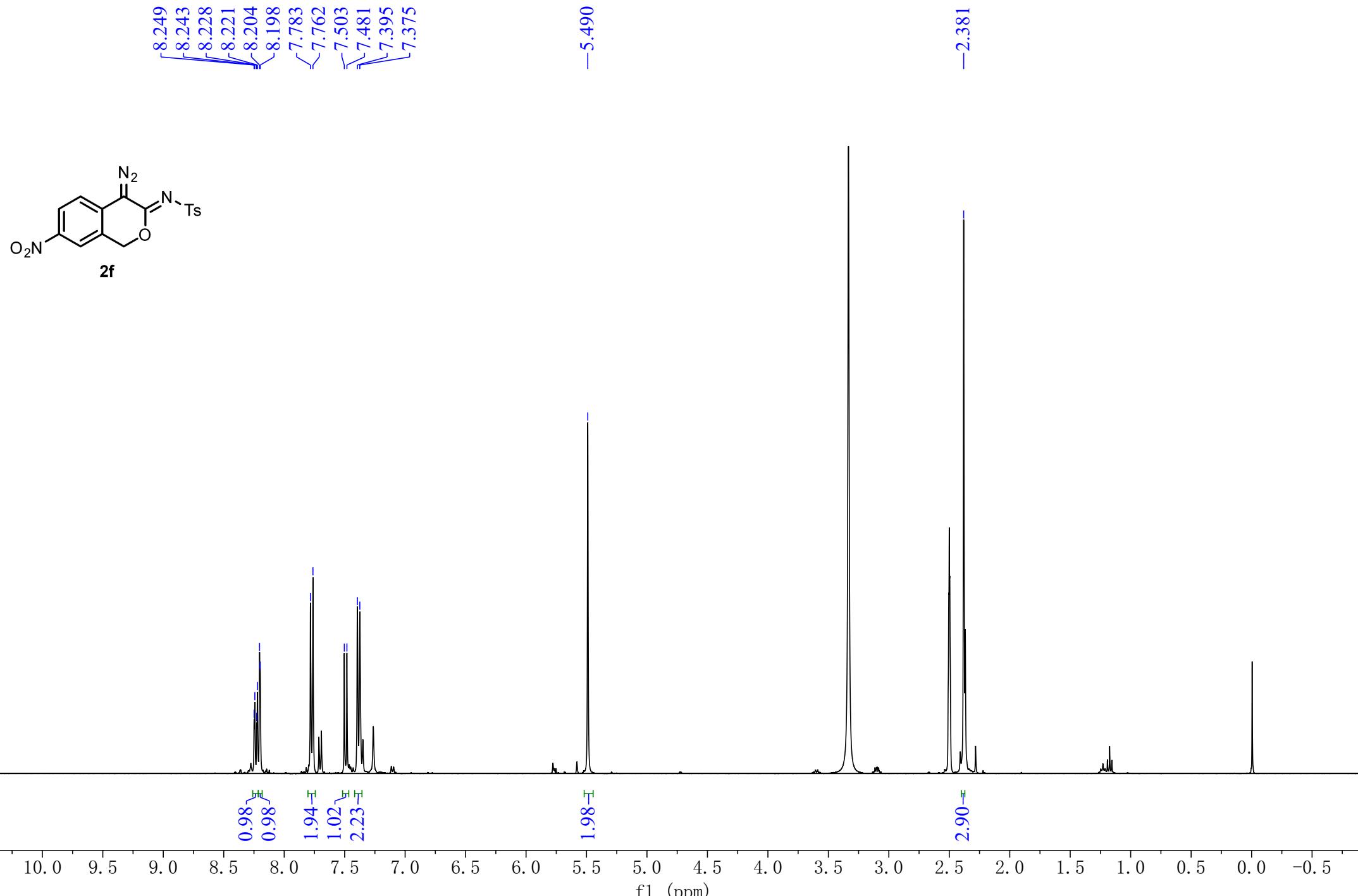
143.633  
143.066  
139.359  
136.614  
130.362  
129.815  
129.267  
127.372  
126.581  
125.618  
124.622  
118.971  
117.385

-71.421

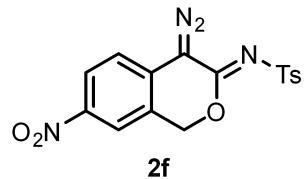
21.676  
21.197

f1 (ppm)

$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2b**



<sup>1</sup>H NMR spectrum of **2f**

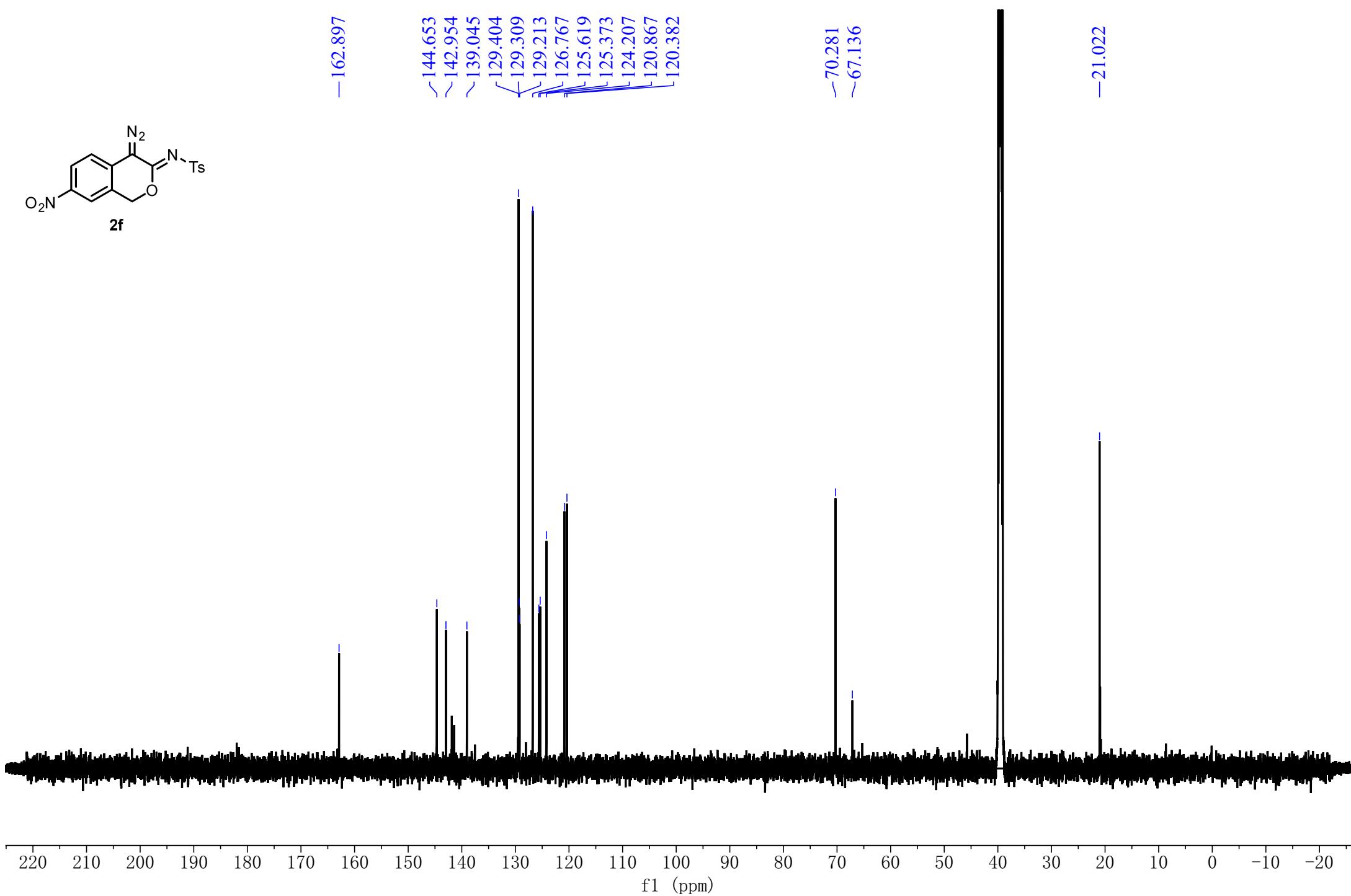


-162.897

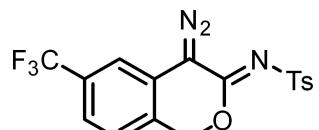
$\sim$ 144.653  
 $\sim$ 142.954  
 $\sim$ 139.045  
129.404  
 $\begin{cases} \sim 129.309 \\ \sim 129.213 \\ \sim 126.767 \end{cases}$   
125.619  
125.373  
124.207  
120.867  
120.382

-70.281  
-67.136

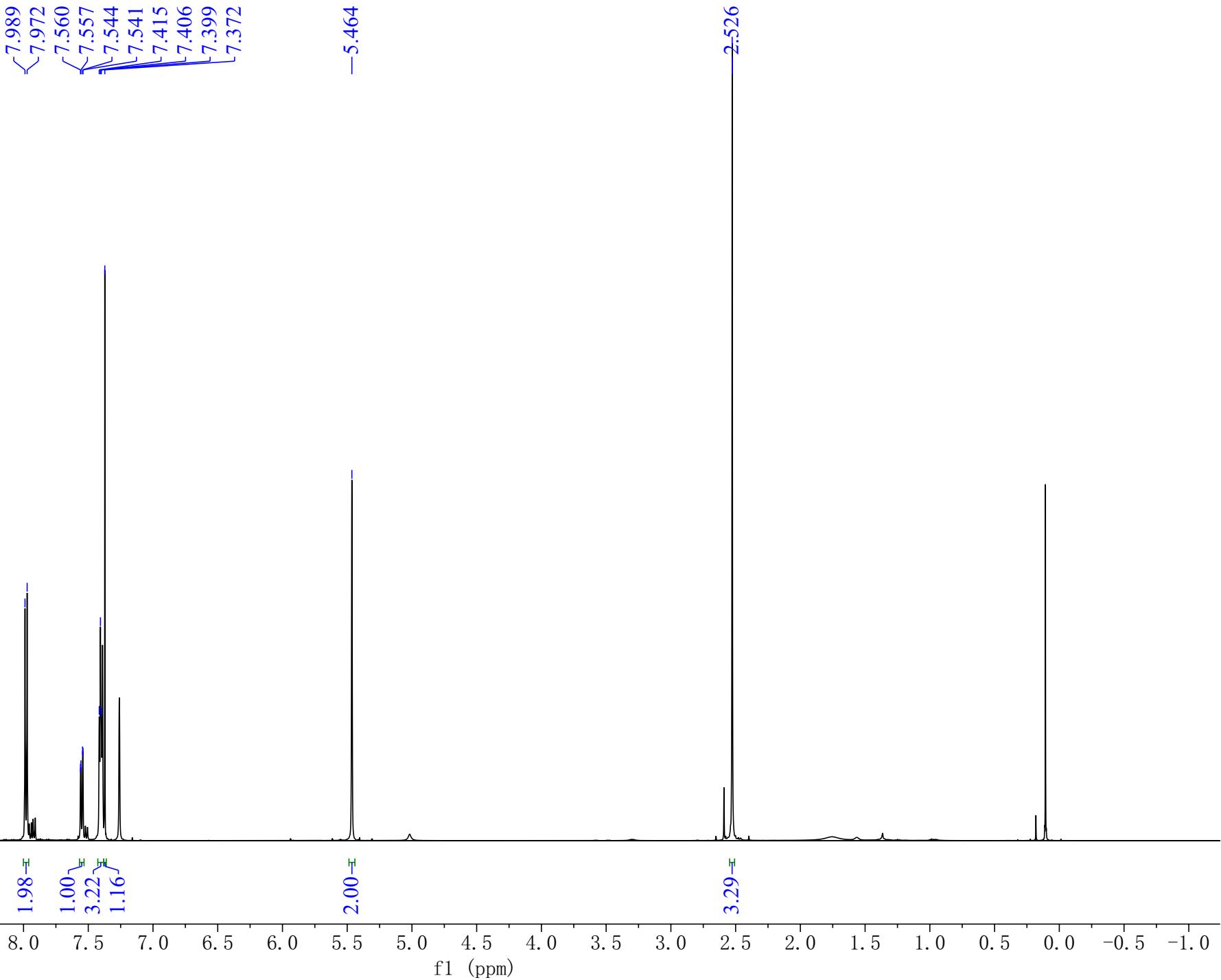
-21.022



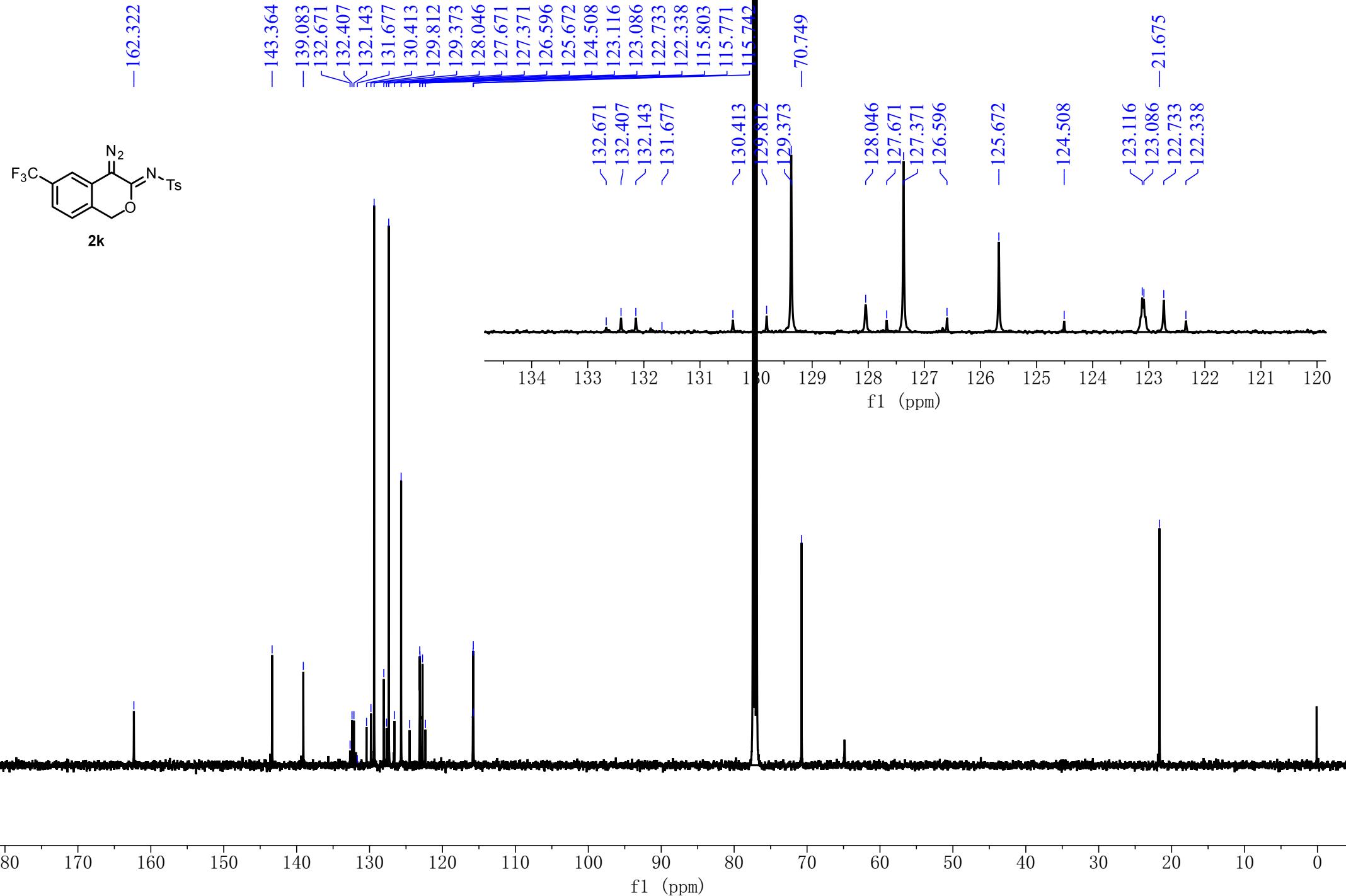
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2f**



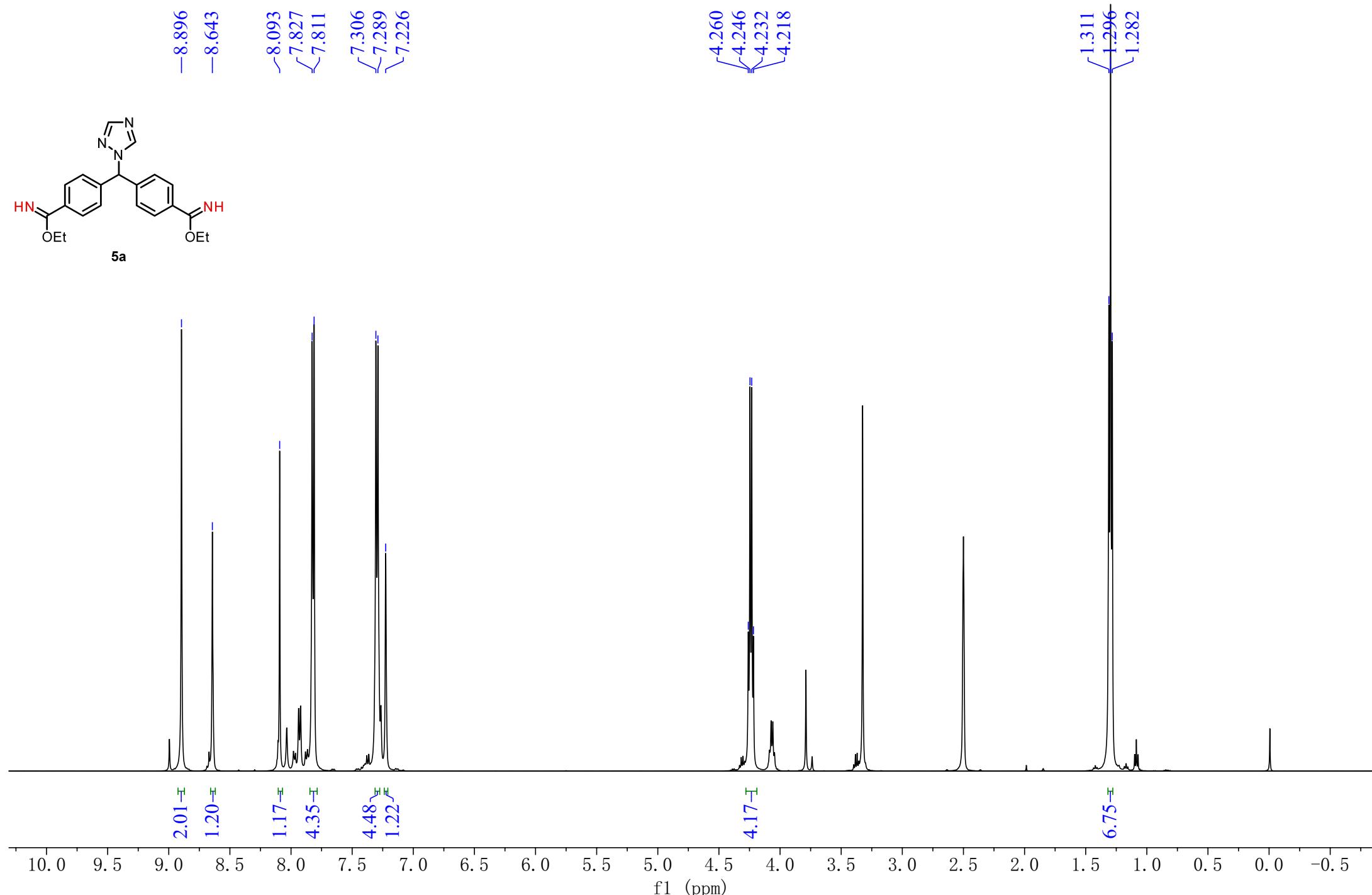
**2k**



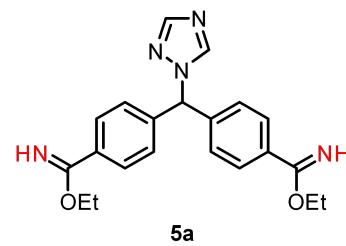
$^1\text{H}$  NMR spectrum of **2k**



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2k**



$^1\text{H}$  NMR spectrum of **5a**



—164.678

—152.077

—144.626

—141.028

~131.930

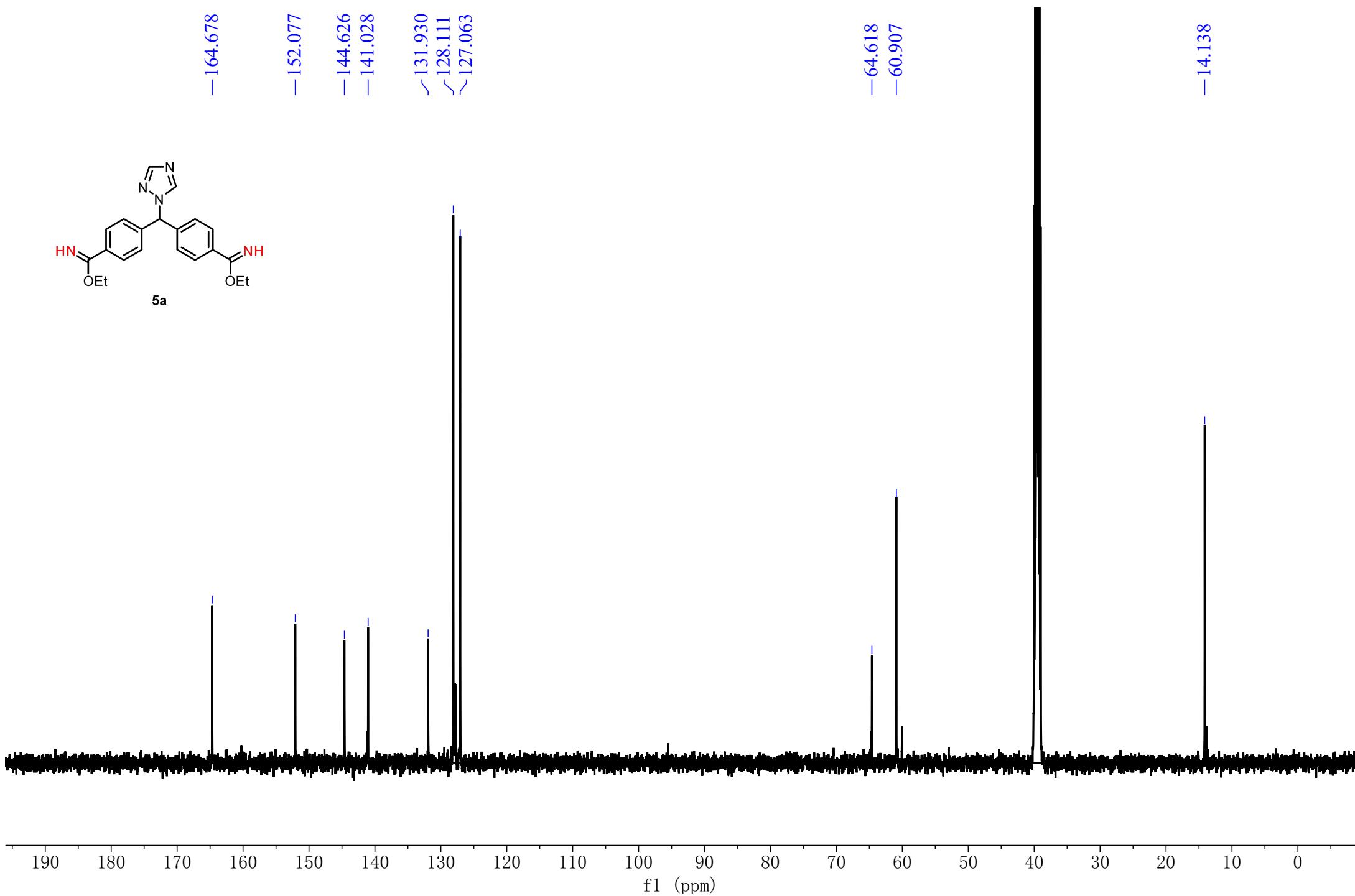
~128.111

~127.063

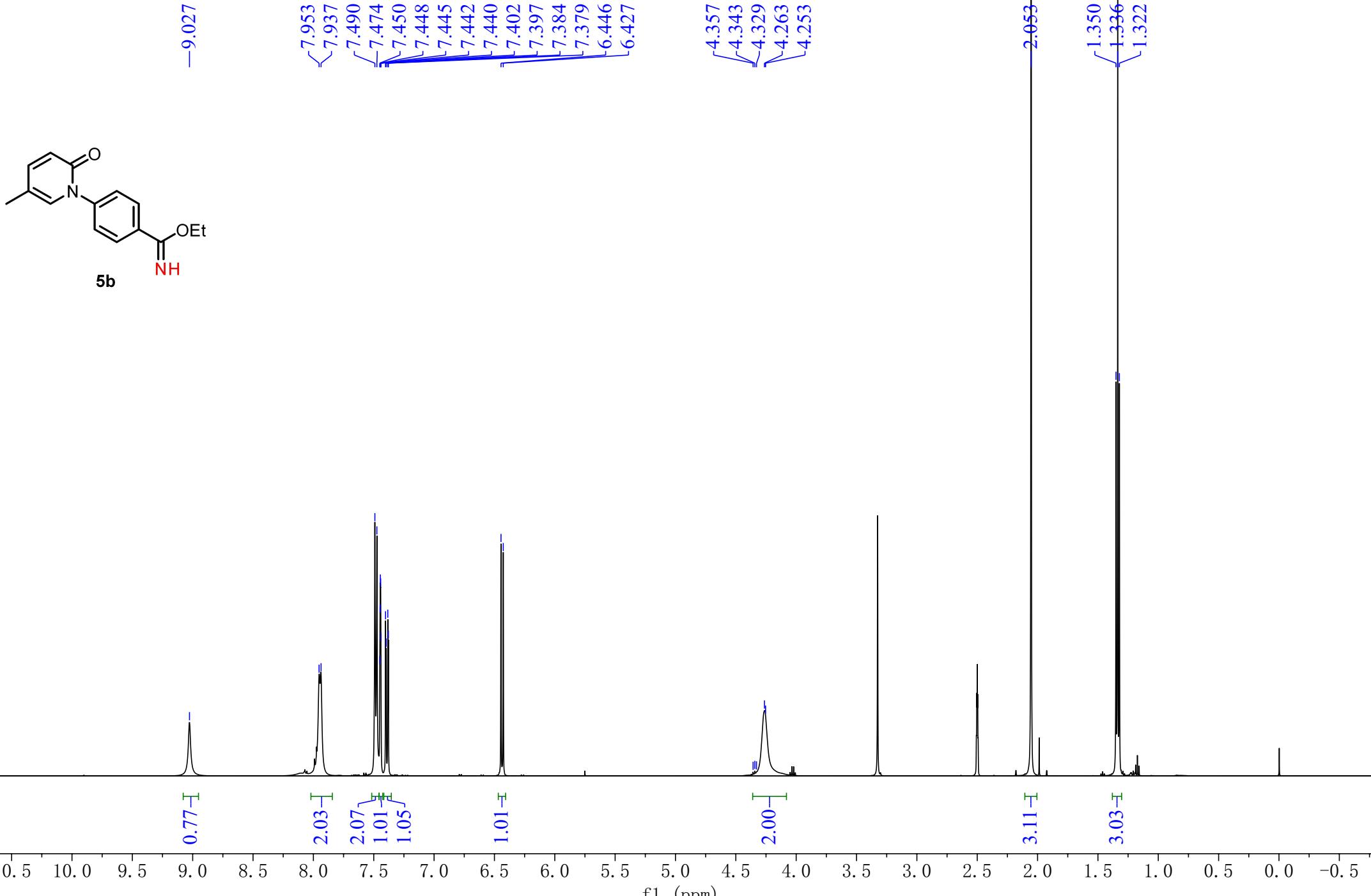
—64.618

—60.907

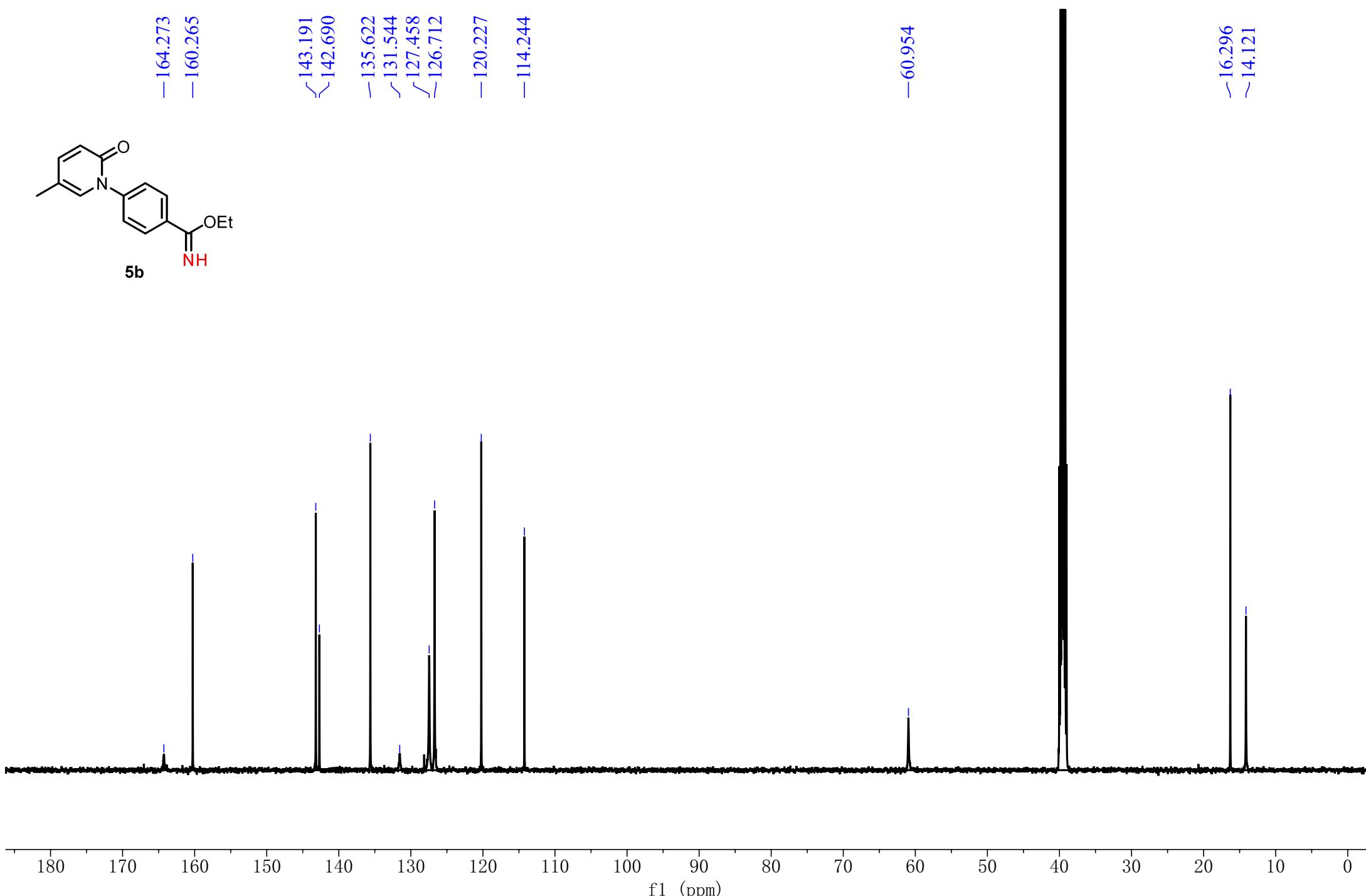
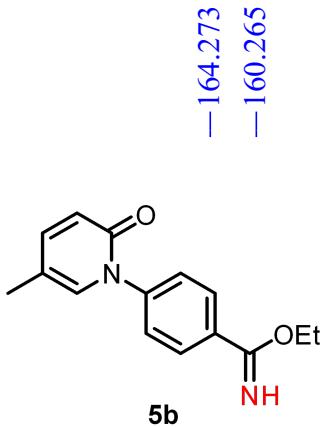
—14.138



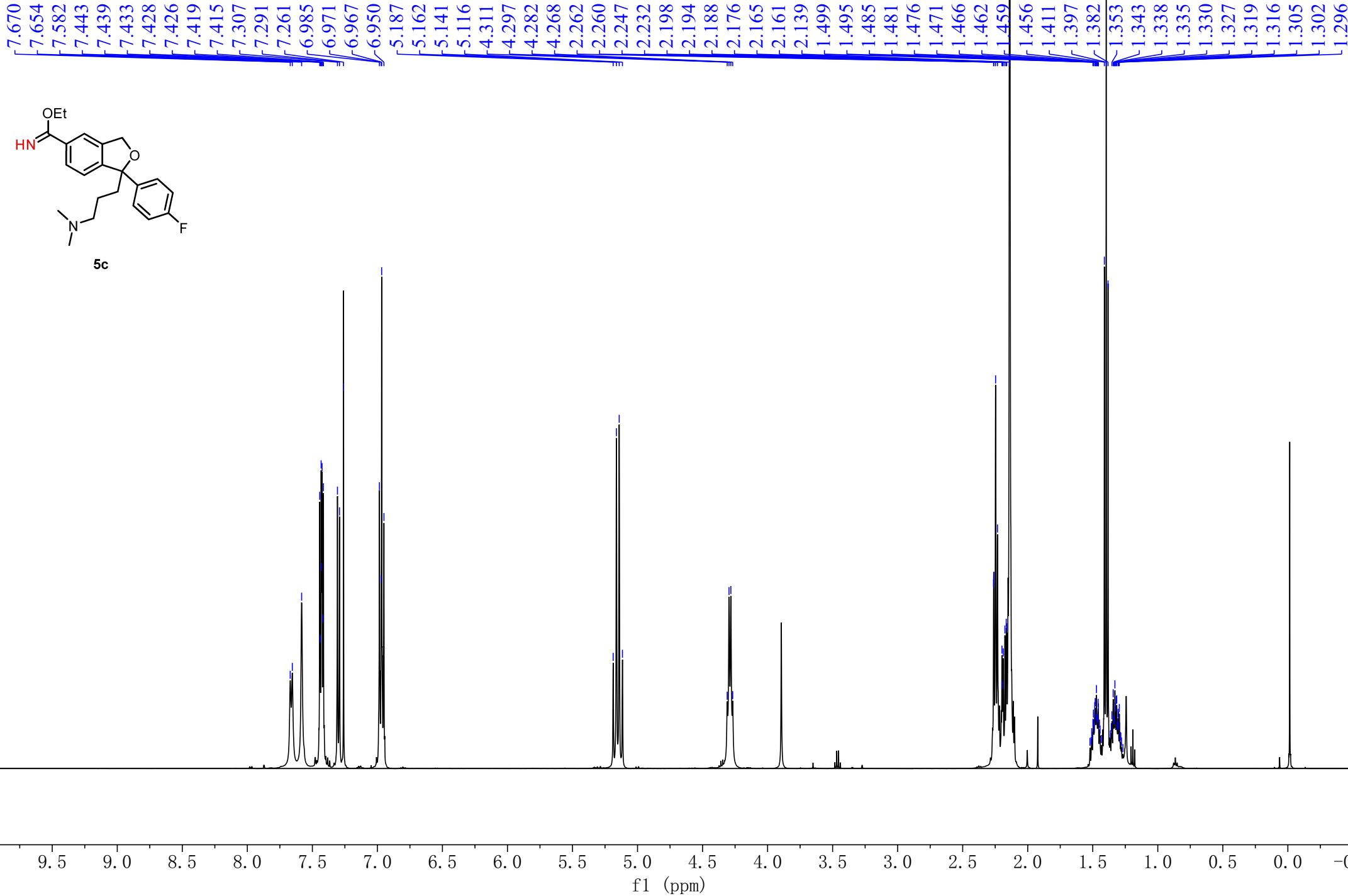
$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **5a**  
S113



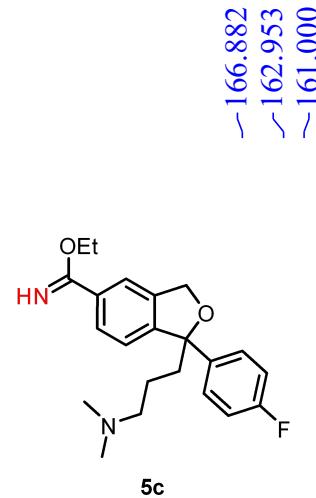
$^1\text{H}$  NMR spectrum of **5b**



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **5b**

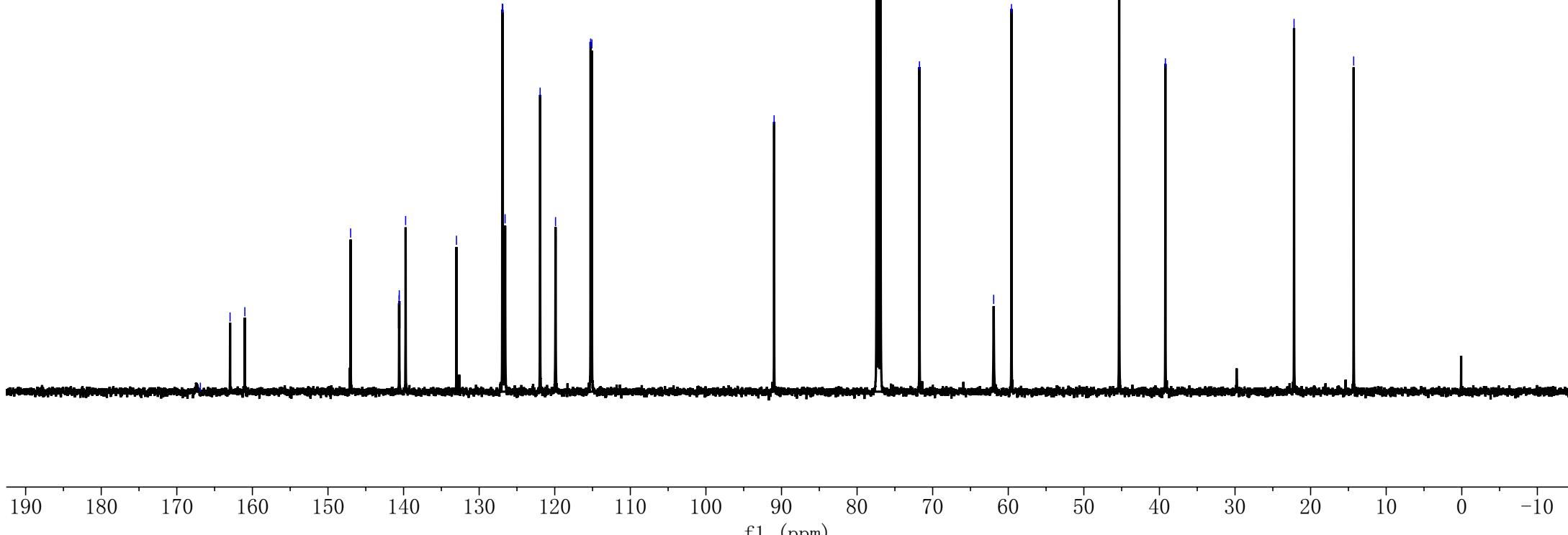


$^1\text{H}$  NMR spectrum of **5c**



147.003  
 140.594  
 140.567  
 139.728  
 133.004  
 126.939  
 126.876  
 126.567  
 -121.934  
 ~119.895  
 115.254  
 115.085

-90.977  
 -71.751  
 -61.931  
 ~59.578  
 -45.327  
 -39.217  
 -22.189  
 -14.303



$^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **5c**