

## Supporting Information

### AgSbF<sub>6</sub>-Catalyzed C3 *aza*-Friedel-Crafts Alkylation of *N,O* -Acetals with Indoles for Synthesis of *N*- Indole Substituted Pyrrolidine and Piperidine Derivatives

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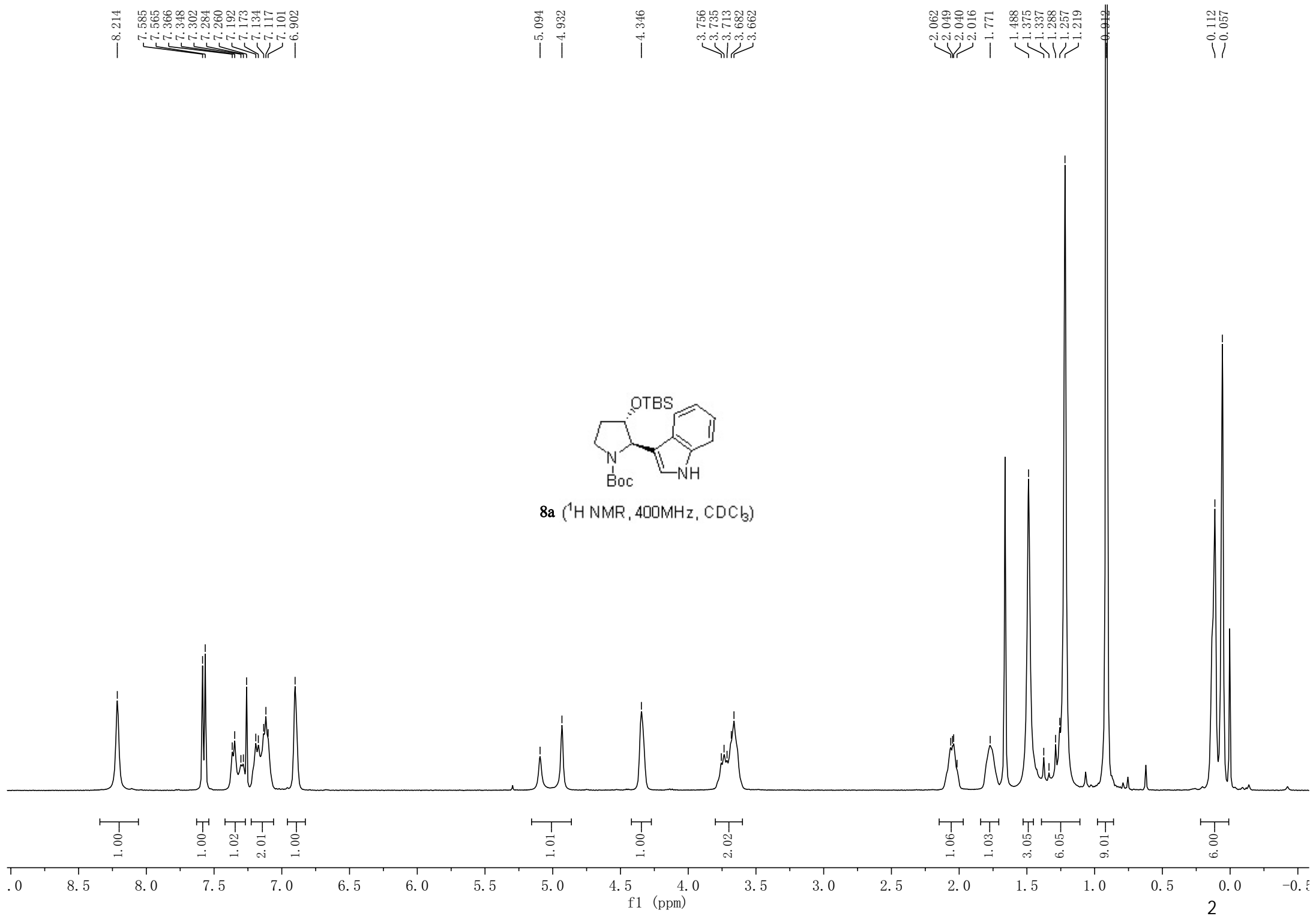
<sup>a</sup> School of Life Science and Engineering, Lanzhou University of Technology, Lanzhou 730050, China.

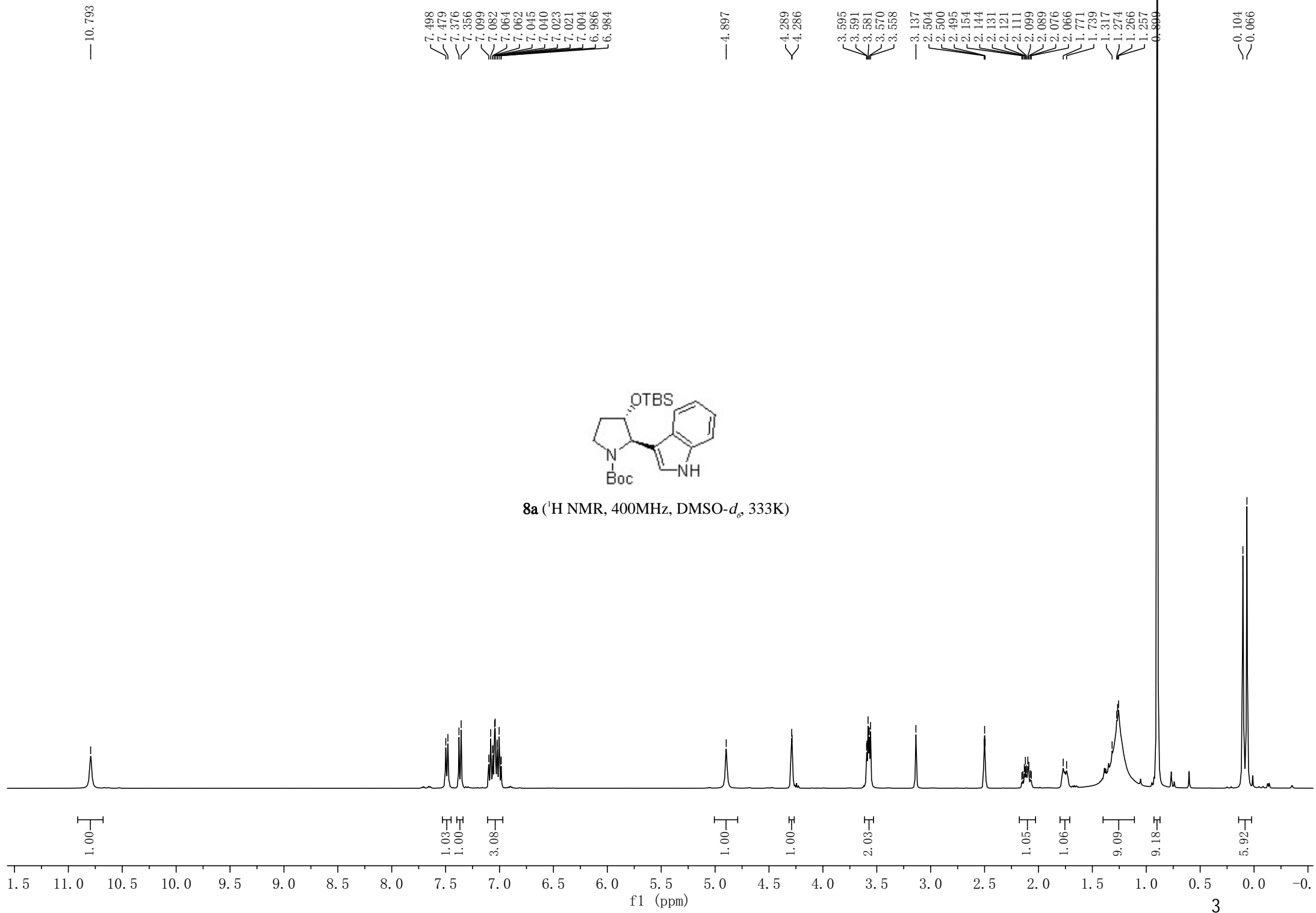
<sup>b</sup> Department of Natural Medicine, School of Pharmacy, Fudan University, 826 Zhangheng Road, Shanghai 201203, China.

<sup>§</sup> These authors contributed equally to this work.

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155.574  
155.212

136.994  
136.680

125.685  
122.072  
121.432  
119.564  
118.930  
117.354  
116.555  
111.436

79.216

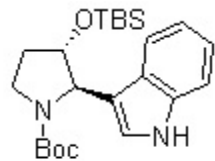
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44.990  
44.290

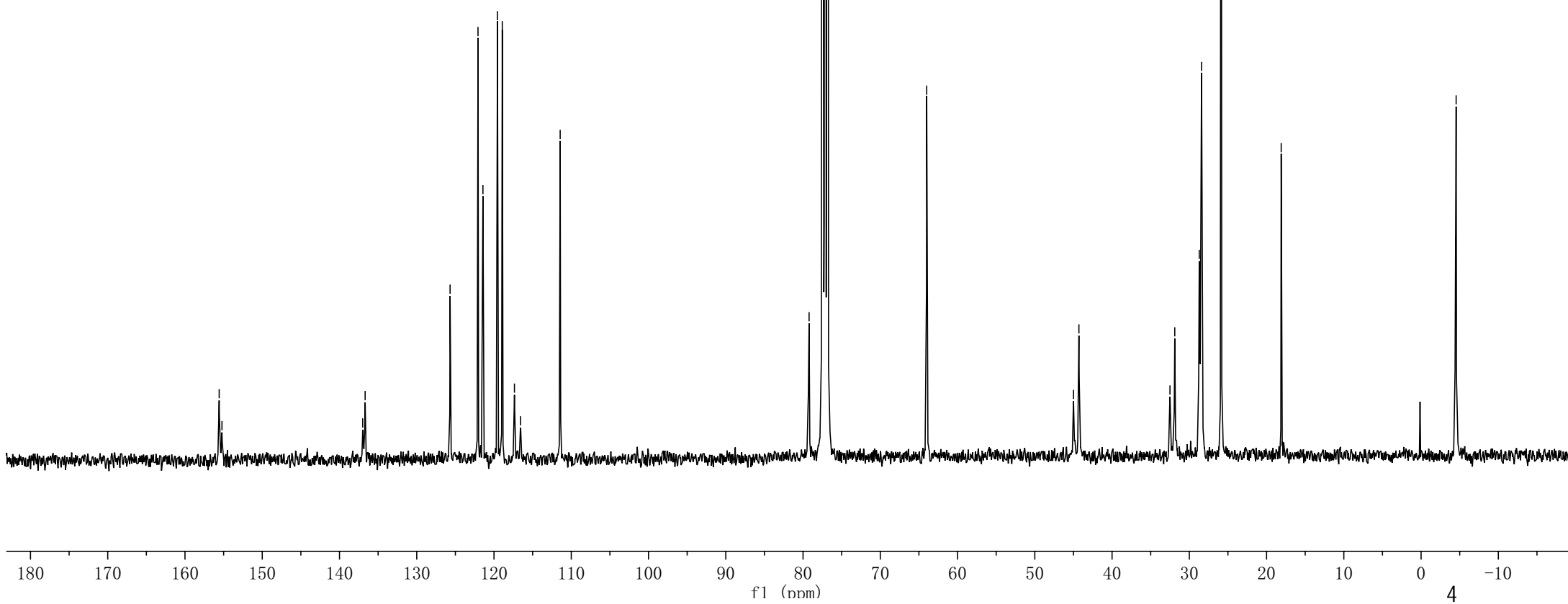
32.503  
31.883  
28.715  
28.418  
26.892

18.107

-4.468  
-4.538



8a (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



7.576  
7.556  
7.281  
7.247  
7.227  
7.209  
7.108  
7.092  
6.783

5.102  
4.939

4.327

3.727  
3.675  
3.653  
3.632

2.070  
2.047

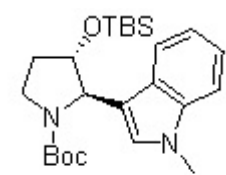
1.733

1.480

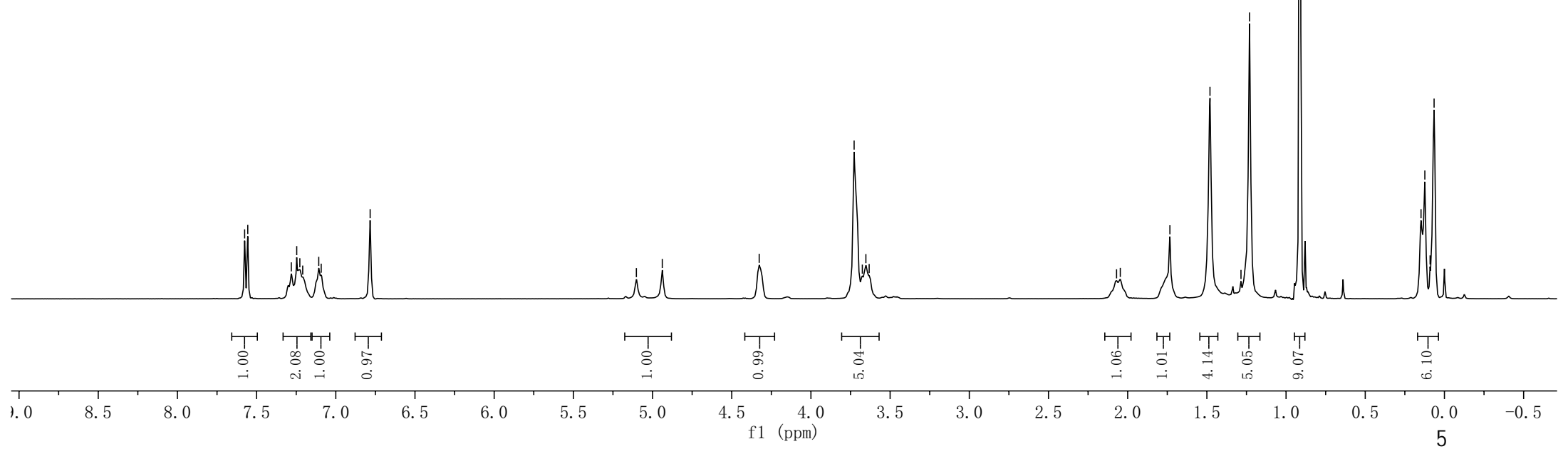
1.285  
1.231

0.912

0.148  
0.124  
0.091  
0.065



8b (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



155.535  
155.187

137.651  
137.330

126.096  
125.963

121.645  
119.057  
115.838  
115.125

109.449

79.130

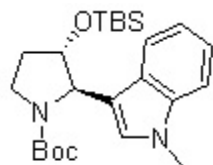
63.946

44.928  
44.226

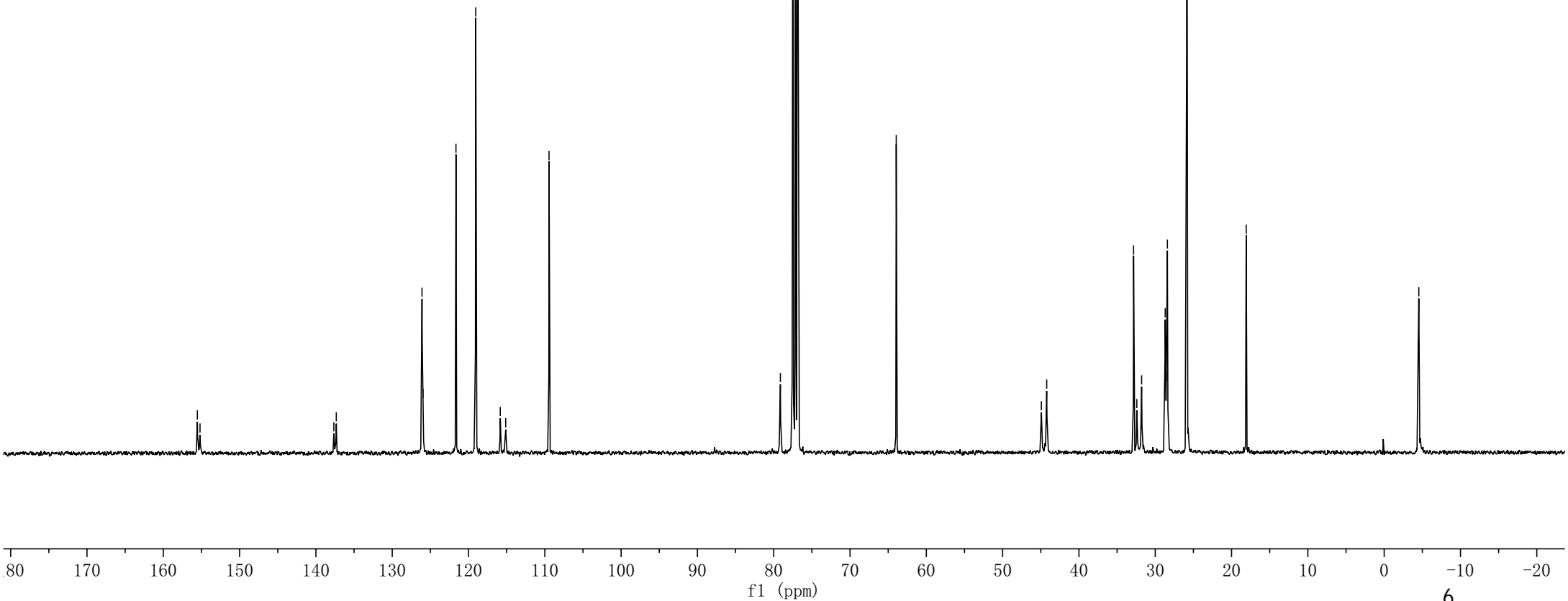
32.841  
32.413  
31.787  
28.694  
28.548  
28.410  
25.875

18.084

-4.457  
-4.540



**8b** (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



7.687  
7.667  
7.642  
7.606  
7.586  
7.574  
7.548  
7.530  
7.516  
7.393  
7.375  
7.360  
7.288  
7.271  
7.252  
7.234  
7.215  
7.198  
7.168  
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7.106

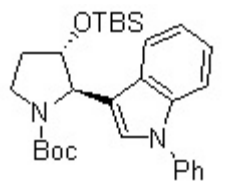
5.228  
5.151  
5.011

4.563  
4.550  
4.538  
4.525  
4.454

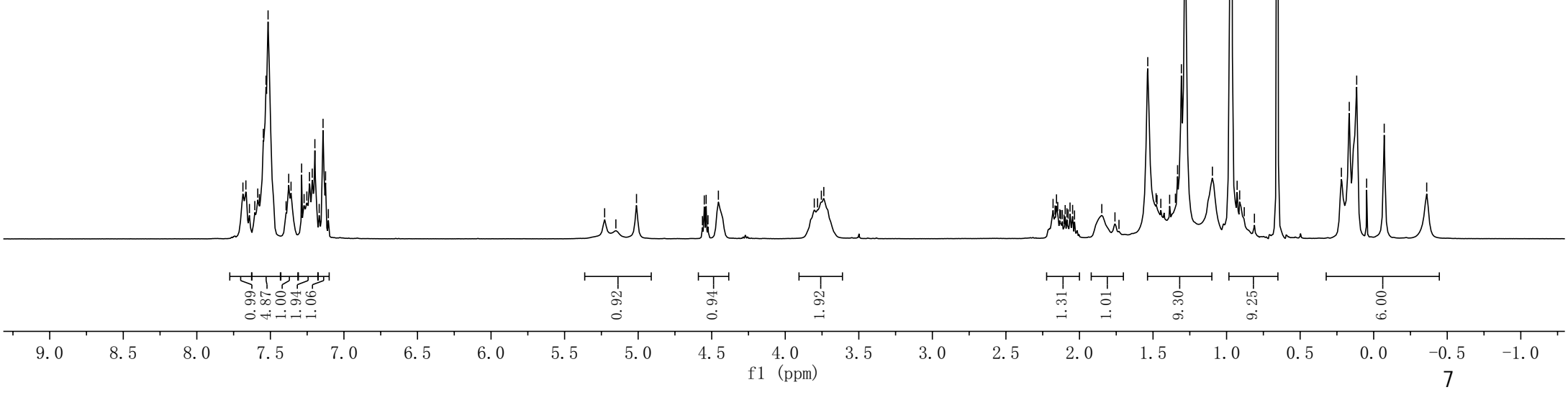
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3.755  
3.738

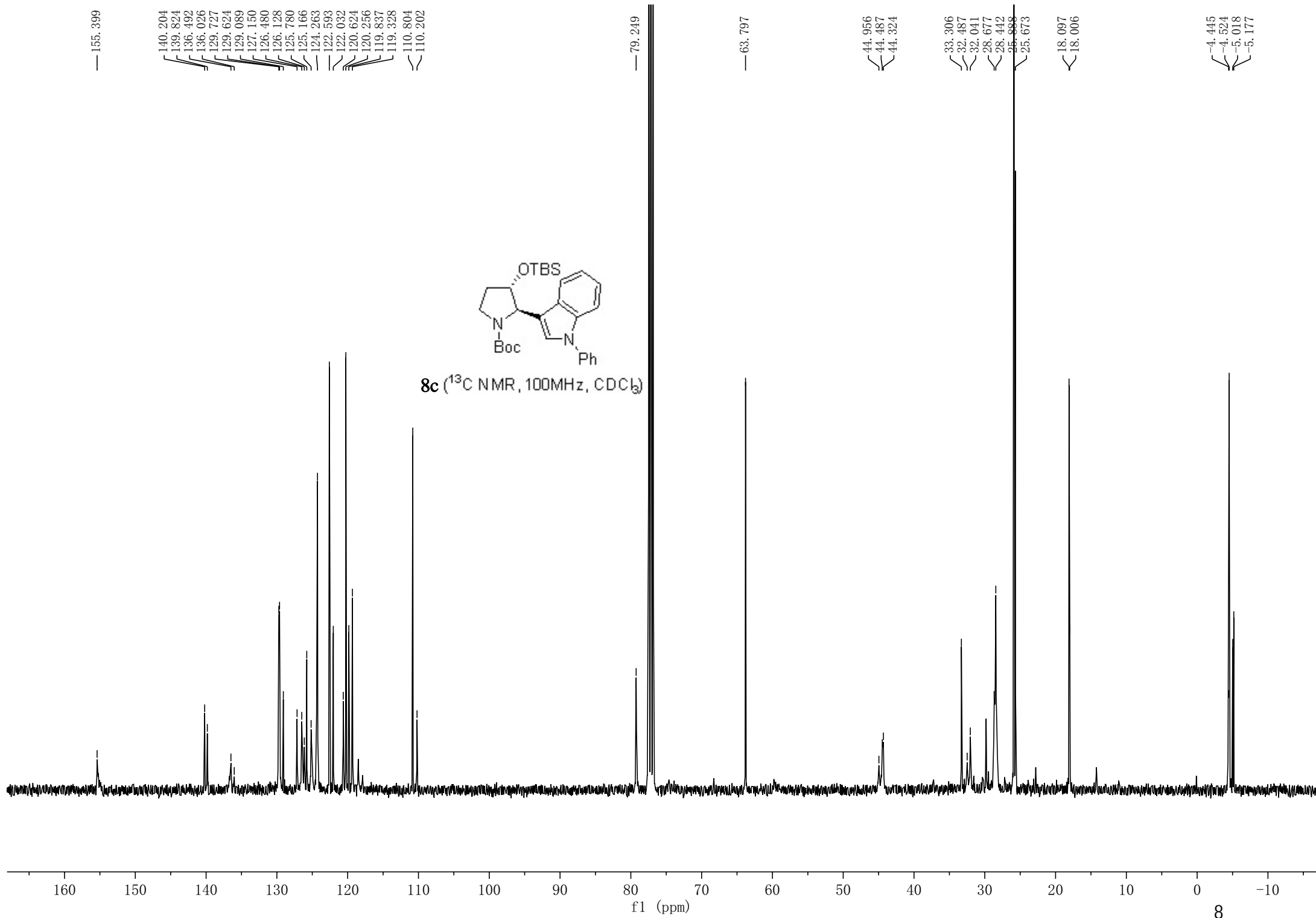
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2.156  
2.148  
2.134  
2.128  
2.116  
2.105  
2.097  
2.085  
2.077  
2.064  
2.047  
2.034  
1.848  
1.759  
1.731  
1.536  
1.479  
1.473  
1.447  
1.387  
1.348  
1.333  
1.307  
1.281  
1.096

0.970  
0.928  
0.911  
0.880  
0.811  
0.656  
0.220  
0.166  
0.116  
0.048  
-0.072  
-0.360



8c (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)







8.474  
8.318

7.526  
7.459  
7.245  
7.139  
7.122  
7.062  
7.025  
6.914  
6.808

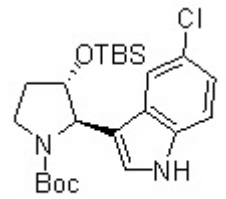
4.962  
4.838

4.293  
4.245  
3.753  
3.734  
3.710  
3.690  
3.659  
3.653  
3.632  
3.612  
3.606

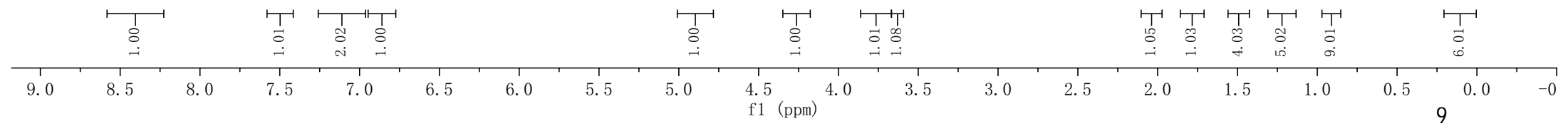
2.078  
2.068  
2.055  
2.046  
2.035  
2.023  
2.014  
2.001  
1.991  
1.788

1.496  
1.284  
1.252  
1.221

0.093  
0.047



8d (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



155.440  
155.311

135.239  
134.986

126.755  
126.476

125.279  
122.978

122.738  
122.415

122.227  
118.473

118.287  
117.230

115.917  
112.451

79.582  
79.437

63.887  
63.667

45.131  
44.338

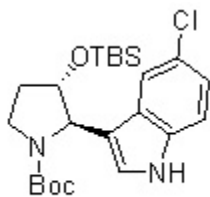
32.634  
32.038

30.275  
28.697

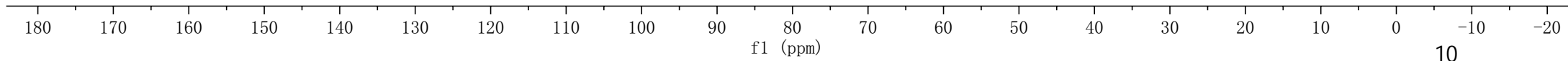
28.428  
25.887

18.118

-4.547



8d (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)





155.444  
155.343

135.455  
135.248  
127.432  
127.096  
124.953  
124.704  
122.804  
122.545  
121.604  
121.314  
117.099  
115.716  
112.913  
112.774

79.628  
79.451

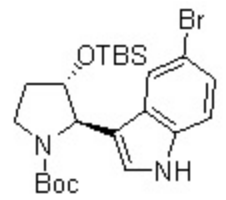
63.920  
63.665

45.160  
44.338

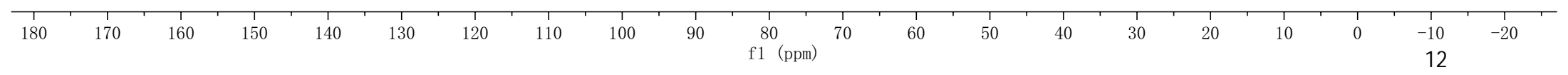
32.630  
32.012  
28.708  
28.437  
25.891

18.122

-4.541



8e (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



8.144  
8.076  
8.028

7.393  
7.361  
7.274  
7.254  
7.234  
7.214  
7.054  
7.035  
7.016  
6.937  
6.878  
6.744

5.107  
4.953

4.493  
4.479  
4.466  
4.452  
4.391

3.781  
3.762  
3.741  
3.676

2.510  
2.484  
2.431  
2.419

2.072  
2.059  
2.047

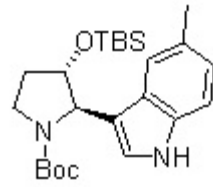
1.787

1.524

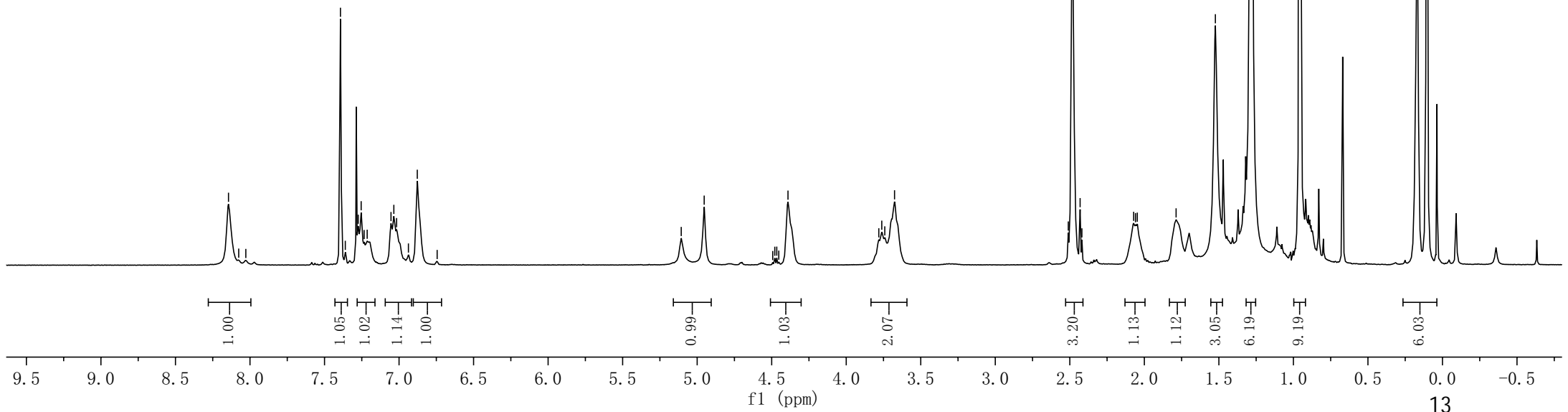
1.292  
1.280

0.957

0.169  
0.105



8f (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



— 155.520

— 134.960

~ 128.516

~ 125.853

~ 123.492

~ 122.960

~ 121.376

~ 118.590

~ 116.618

— 110.956

— 79.079

— 63.949

~ 44.872

~ 44.187

~ 32.373

~ 31.750

~ 29.708

~ 28.599

~ 28.344

~ 25.793

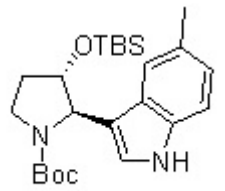
~ 25.583

— 21.552

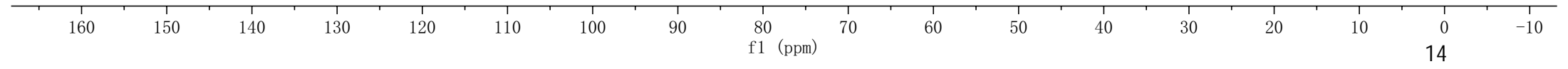
— 18.006

~ -4.592

~ -4.632



8f (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



8.350  
8.286

7.482  
7.463  
7.448  
7.427  
7.286  
7.110  
7.092  
7.073  
7.048  
7.032  
7.004  
6.948  
6.927  
6.910  
6.875

5.122  
5.003

4.392  
4.347

3.794  
3.775  
3.752  
3.714  
3.692

2.519  
2.370

2.086  
2.060

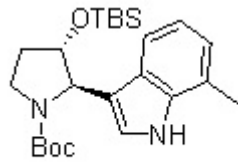
1.790

1.537  
1.478

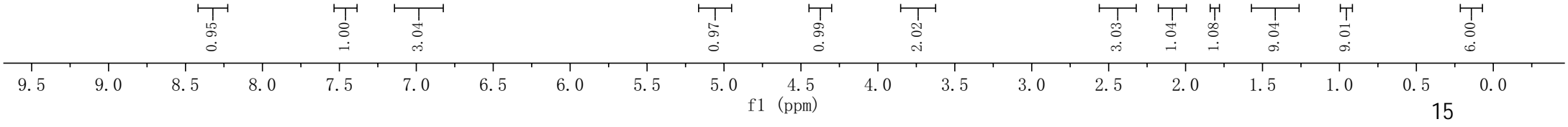
1.289

0.055

0.176  
0.105



8g (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



155.703  
155.213

136.467  
136.296  
125.186  
124.987  
122.572  
122.430  
121.287  
121.160  
120.708  
119.725  
117.621  
116.657  
116.553  
116.465  
116.397

79.247

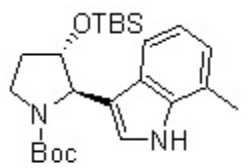
64.159

45.035  
44.291

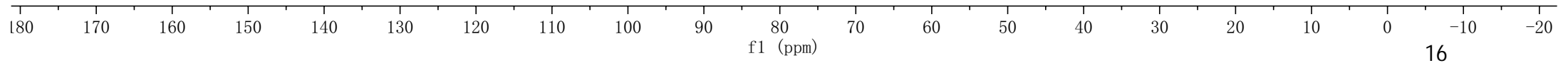
32.446  
31.729  
28.736  
28.456  
25.887  
25.743

18.091  
16.759  
16.642

-4.441  
-4.515



8g (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)









8.236  
8.168

7.480  
7.460  
7.450  
7.295  
7.234  
7.000  
6.954  
6.888  
6.869  
6.849

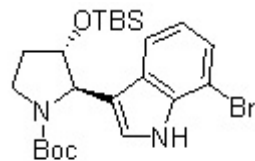
5.004  
4.824

4.420  
4.407  
4.393  
4.380  
4.250

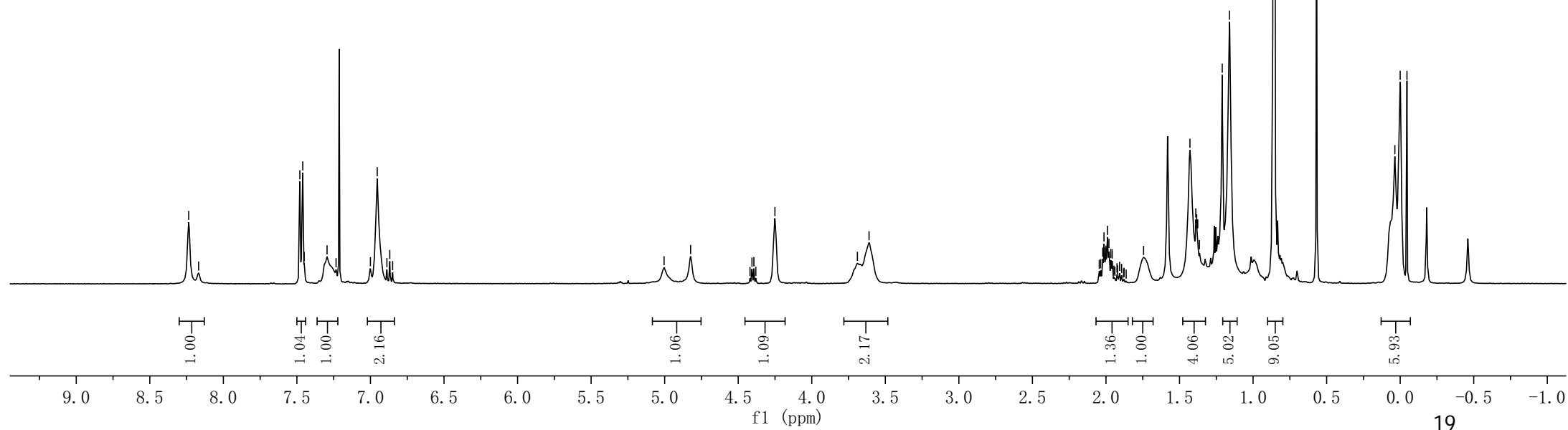
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3.611  
2.046  
2.036  
2.022  
2.013  
2.003  
1.999  
1.990  
1.980  
1.967  
1.958  
1.946  
1.939  
1.925  
1.921  
1.907  
1.894  
1.881  
1.877  
1.863  
1.744

1.429  
1.390  
1.383  
1.376  
1.365  
1.210  
1.161  
0.859

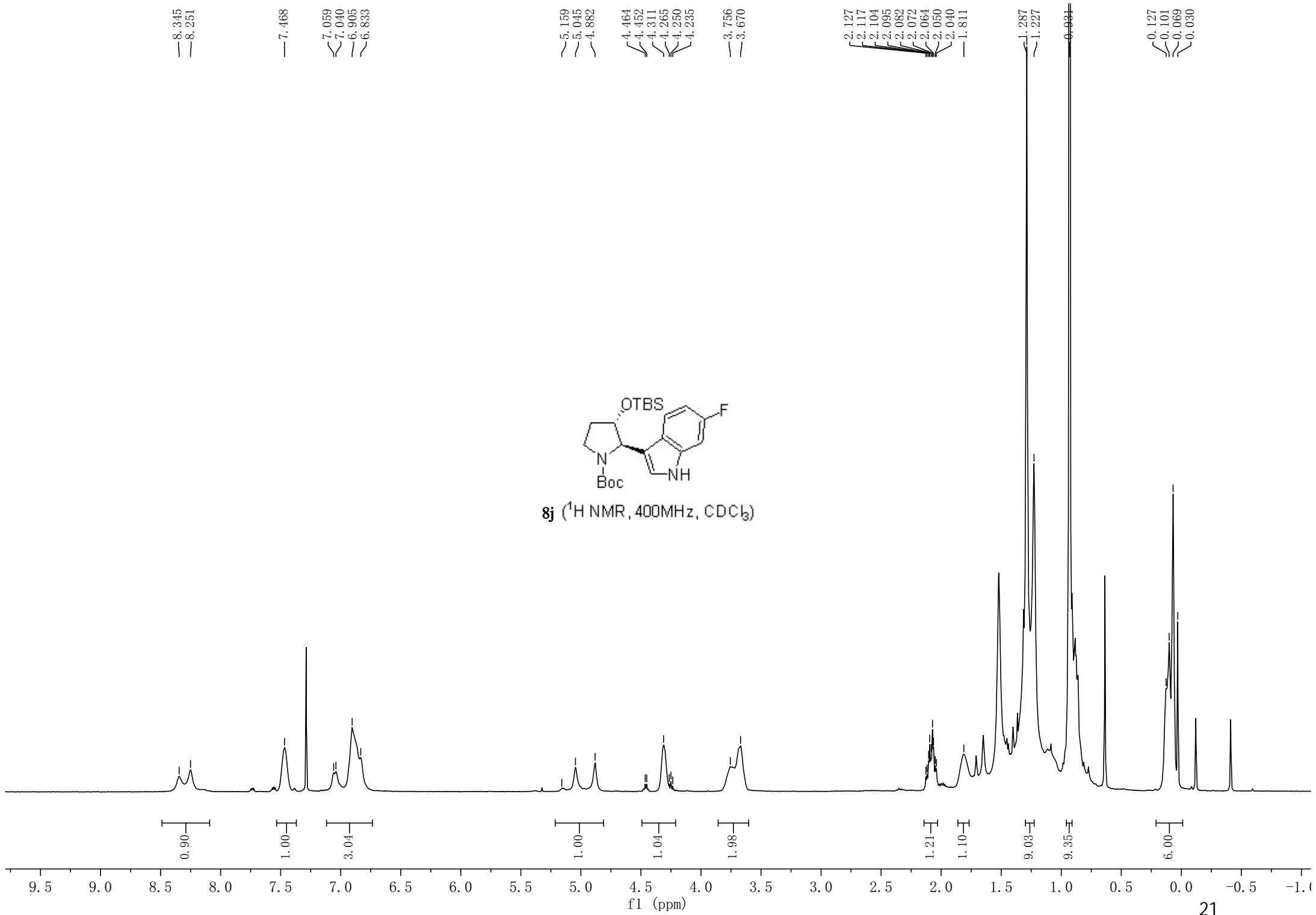
0.036  
0.000  
-0.046



**8i** ( $^1\text{H}$  NMR, 400MHz,  $\text{CDCl}_3$ )







161.061  
160.999  
158.689  
158.637  
155.527  
155.468  
155.443

137.028  
136.909  
136.886  
136.688  
136.633  
136.559

122.330  
122.063  
121.813  
119.276  
119.232  
119.045  
119.014  
117.086  
115.714  
108.194  
107.991

97.871  
97.615

79.565  
79.375

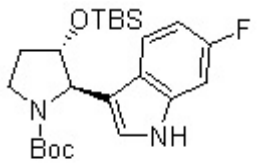
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63.853

45.096  
44.320

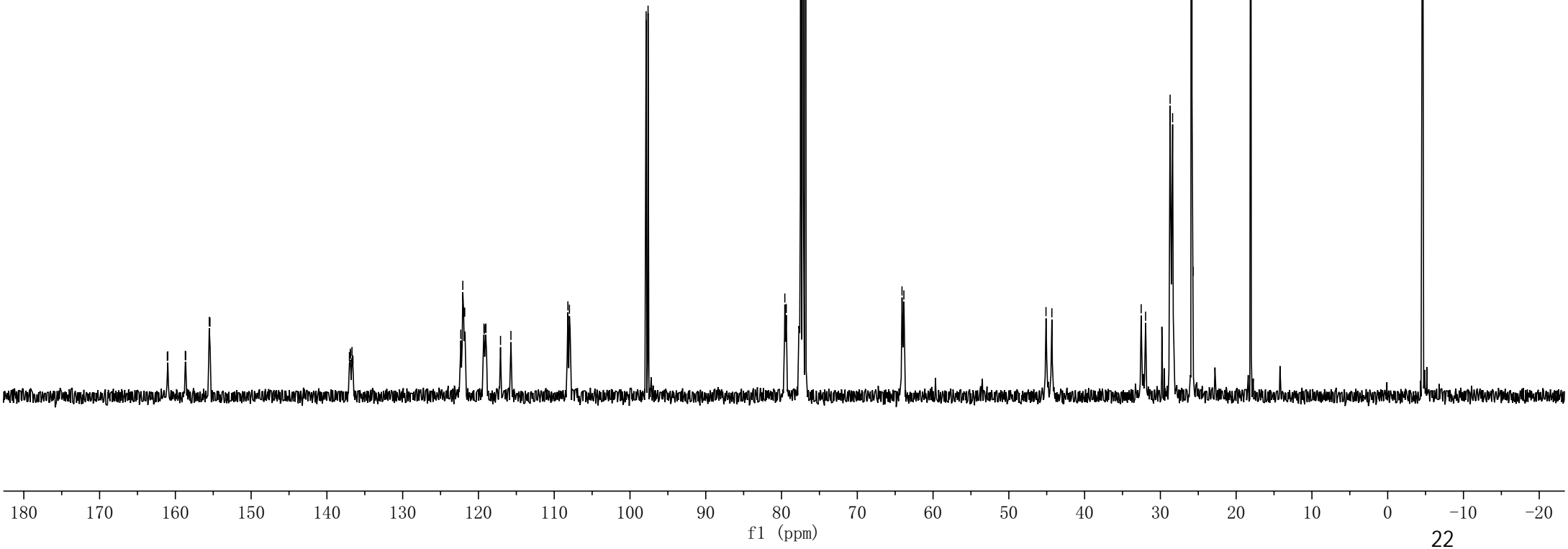
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31.949  
28.715  
28.387  
25.850  
25.676

18.076

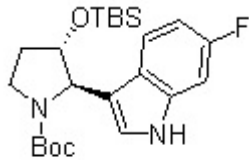
-4.532  
-4.601



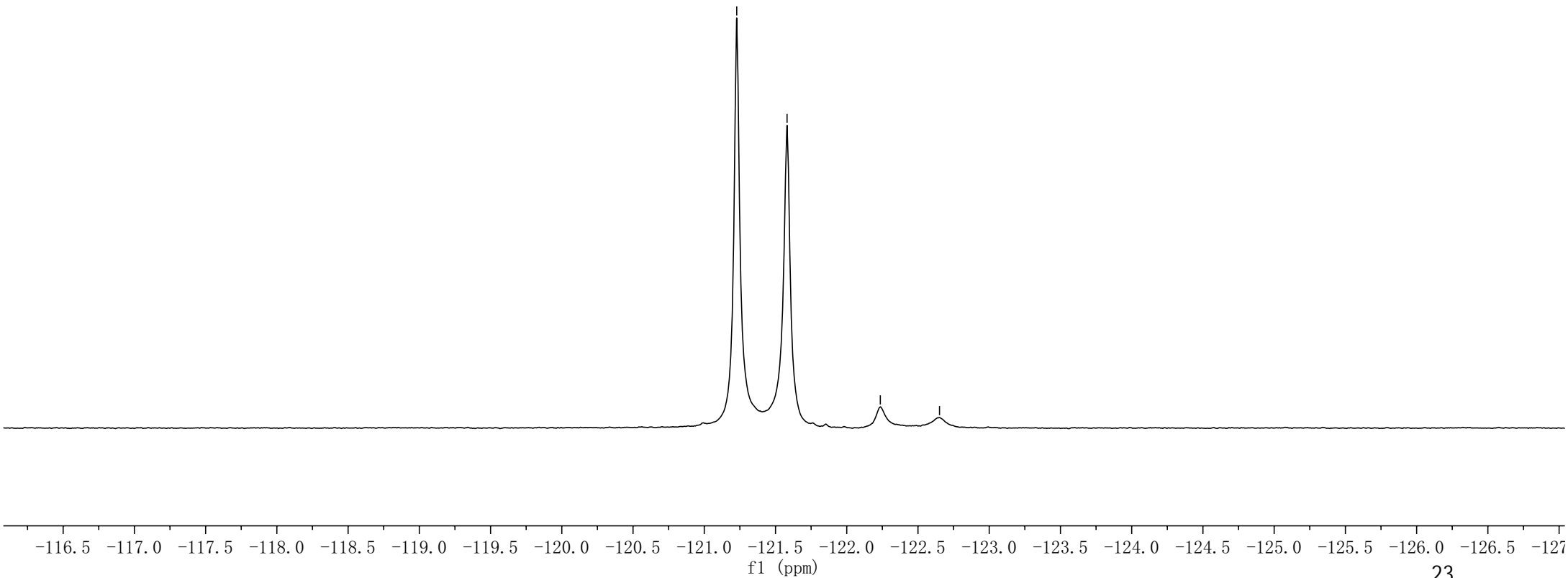
8j (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



-121.228  
-121.581  
-122.236  
-122.651



8j (<sup>19</sup>F NMR, 376MHz, CDCl<sub>3</sub>)



8.473  
8.313

7.467  
7.434  
7.357  
7.140  
7.115  
7.096  
7.054  
6.920  
6.802

5.024  
4.874

4.290

3.754  
3.738  
3.684  
3.664

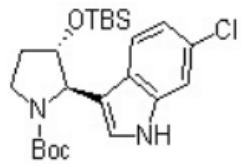
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2.072  
2.059  
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2.036  
2.027  
1.811

1.524

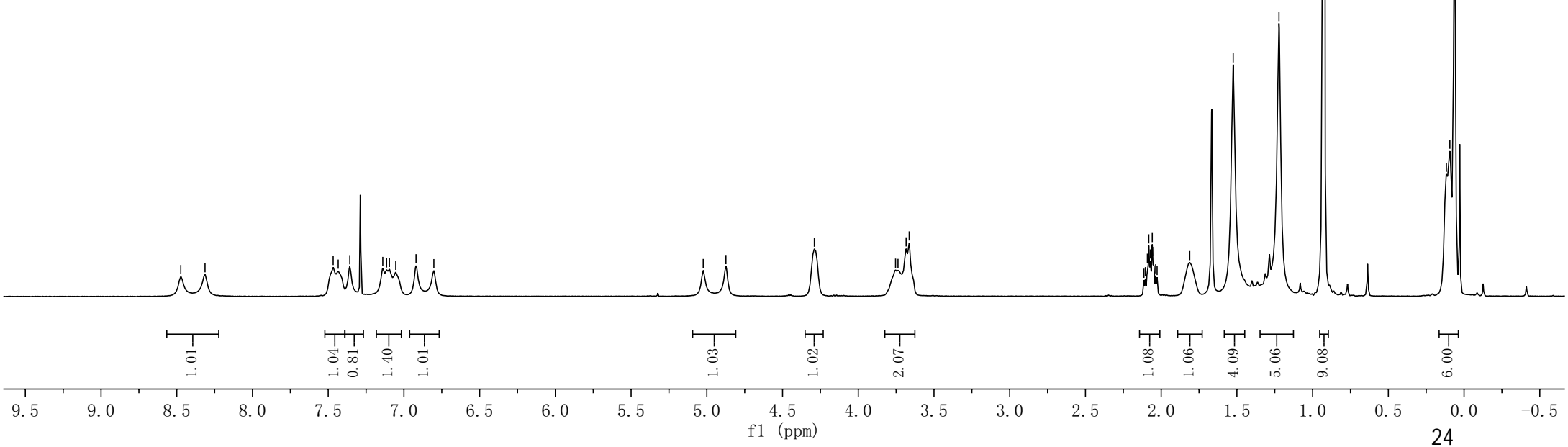
1.222

0.998

0.117  
0.094  
0.063



8k: (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)





— 155.380

137.264  
136.963

128.014  
124.306  
124.088  
122.233  
122.069  
120.325  
120.210  
119.678  
119.431  
117.715  
116.346  
111.401

79.550

79.368

63.903

63.711

45.073

44.353

32.576

32.027

28.721

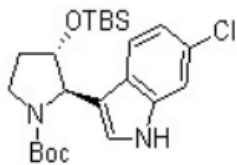
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25.885

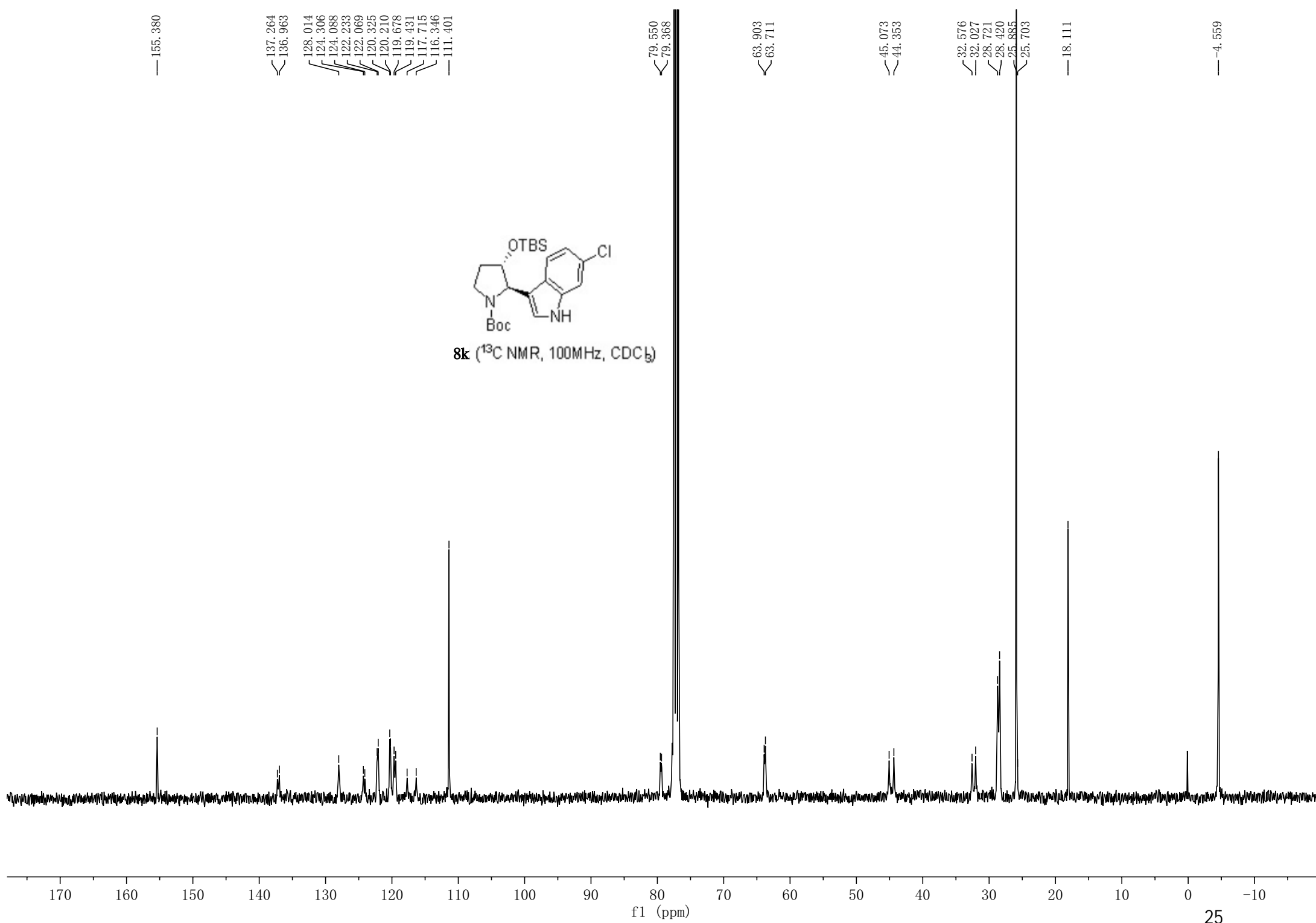
25.703

— 18.111

— -4.559



8k (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



— 8.650  
— 8.471

7.474  
7.414  
7.397  
7.325  
7.307  
7.260  
7.200  
7.133  
7.118  
6.852  
— 6.690

— 4.986  
— 4.852

4.262  
4.230

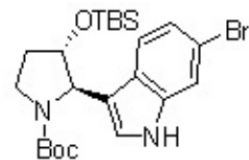
3.730  
3.711  
3.659  
3.637  
3.616

2.078  
2.068  
2.055  
2.046  
2.035  
2.023  
2.014  
2.000  
1.991  
1.779  
1.726

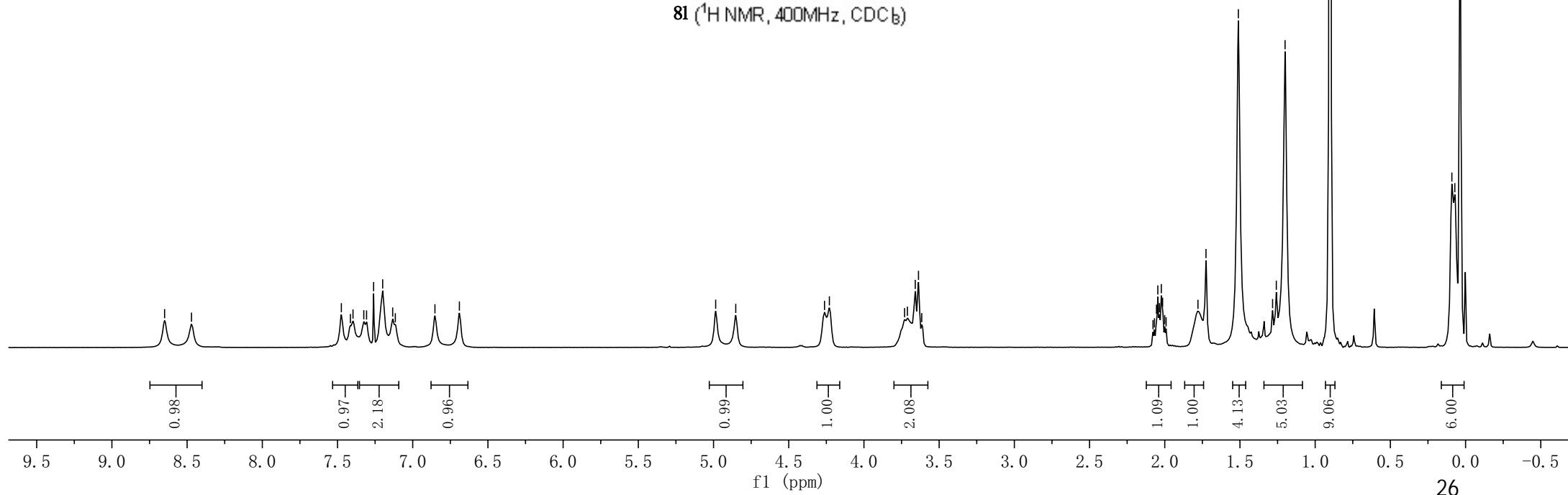
— 1.511  
1.283  
1.258  
1.200

0.991

0.091  
0.072  
0.036



81 ( $^1\text{H}$  NMR, 400MHz,  $\text{CDCl}_3$ )



— 155.427

137.652  
137.403

124.597  
124.147  
122.837  
122.603  
122.265  
122.012  
119.990  
119.576  
117.559  
116.033  
115.560  
114.437

79.641  
79.388

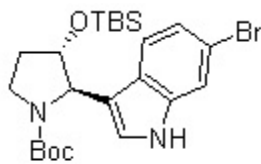
63.974  
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45.107  
44.347

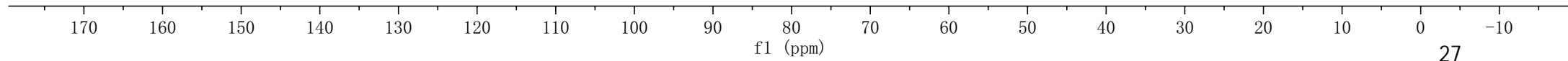
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25.878  
25.695

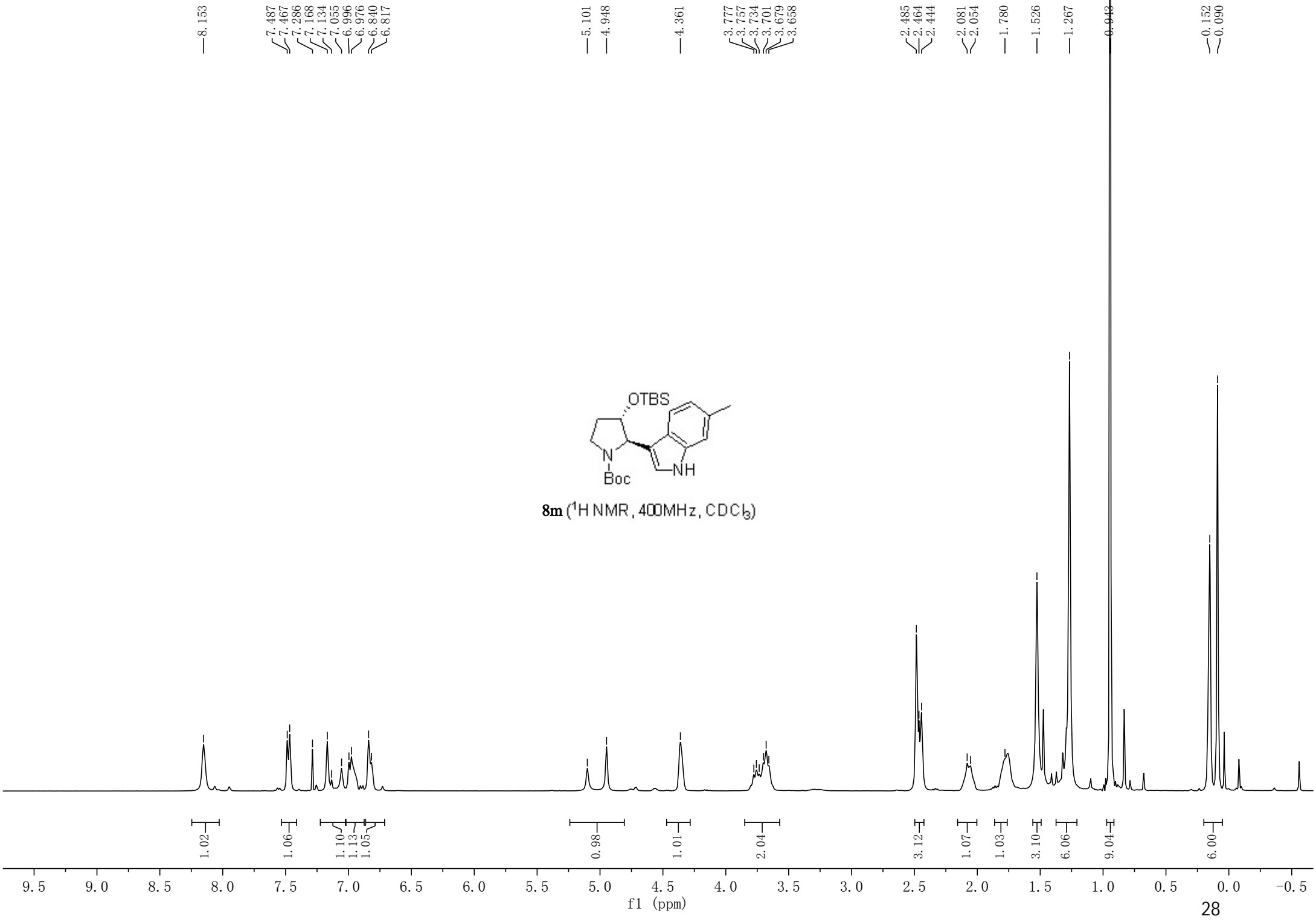
— 18.099

-4.496  
-4.568



**81** ( $^{13}\text{C}$  NMR, 100MHz,  $\text{CDCl}_3$ )





— 155.591

137.470

137.187

— 131.881

123.566

121.328

120.780

118.553

117.192

116.369

— 111.386

— 79.176

— 64.084

44.959

44.276

32.516

31.848

28.730

28.594

28.453

26.130

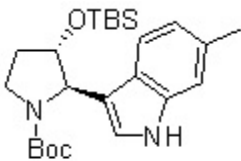
25.902

21.776

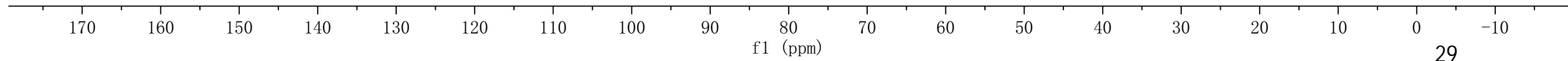
— 18.111

-4.442

-4.534



**8m** ( $^{13}\text{C}$  NMR, 100MHz,  $\text{CDCl}_3$ )





155.772  
155.460

138.516  
138.181

126.019  
125.519  
123.291  
122.971  
122.780  
122.624  
122.509  
120.464  
120.117  
118.188  
116.550  
110.161  
110.064

79.401  
79.292  
78.681

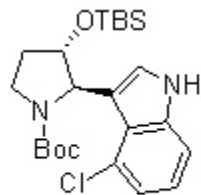
64.515

45.196  
44.542

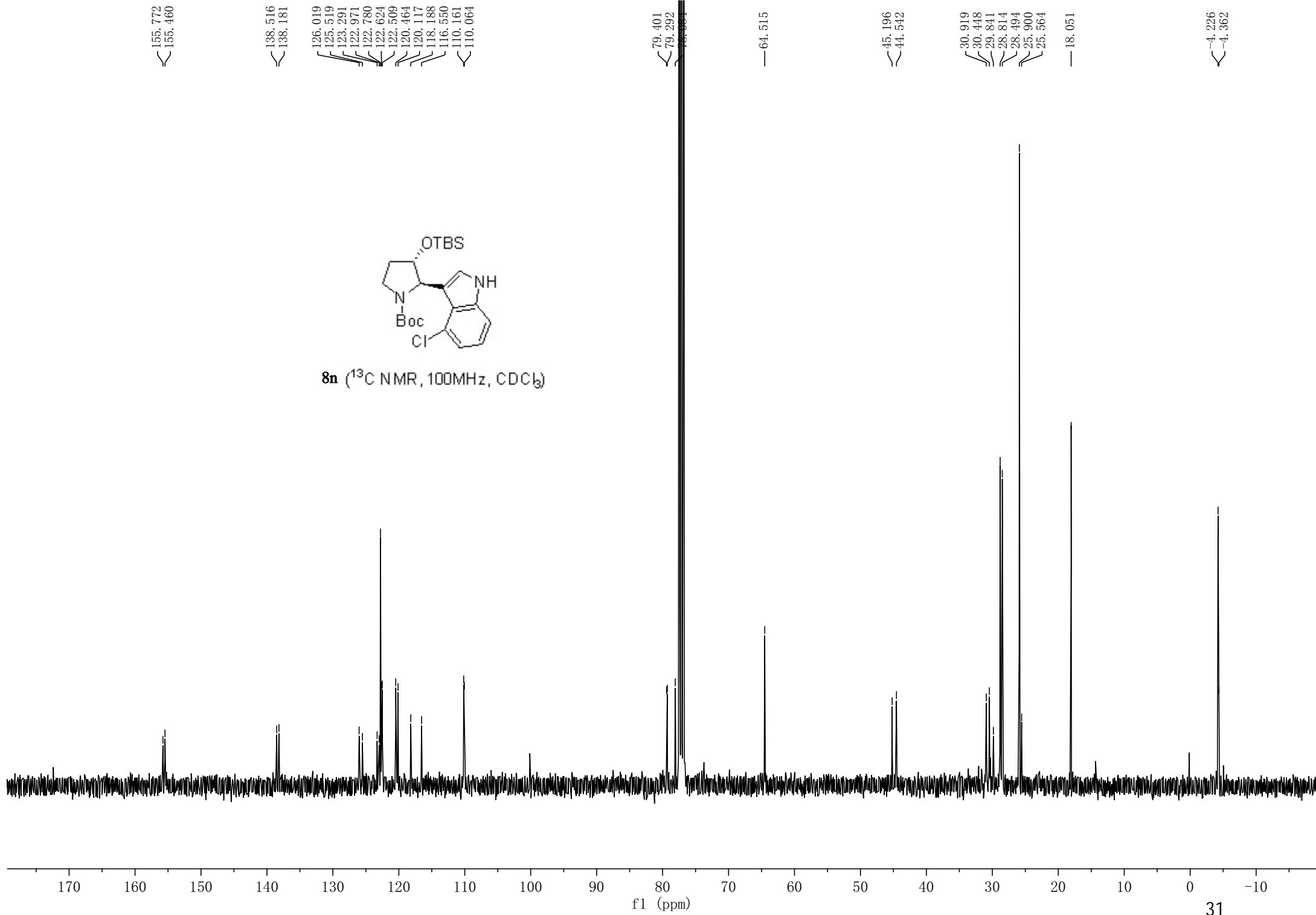
30.919  
30.448  
29.841  
28.814  
28.494  
25.900  
25.564

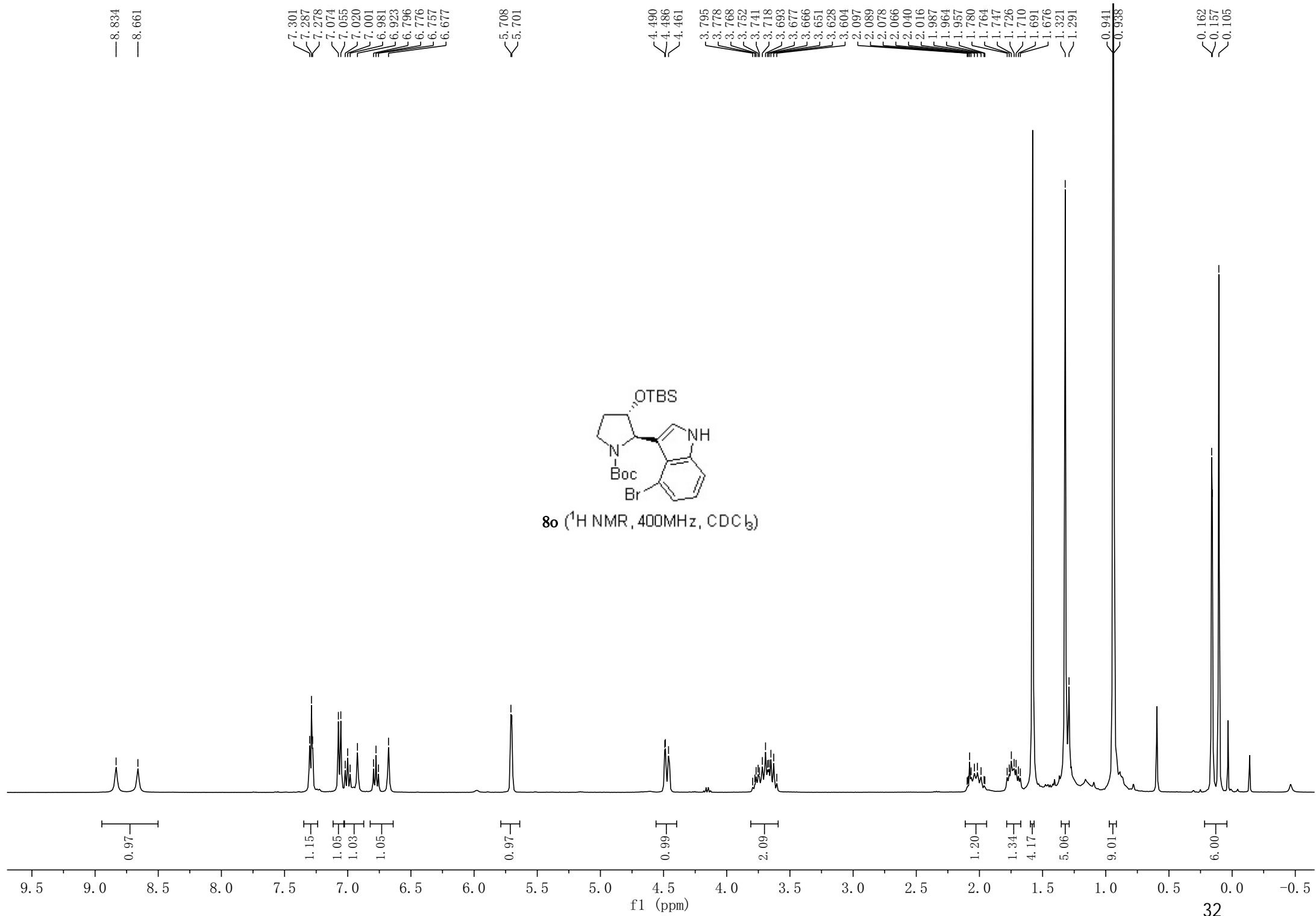
18.051

-4.226  
-4.362



**8n** ( $^{13}\text{C}$  NMR, 100MHz,  $\text{CDCl}_3$ )









8.271  
8.154

7.192  
7.172  
7.107  
7.086  
7.067  
7.047  
7.019  
7.000  
6.881  
6.862  
6.845

5.434  
5.314

4.343  
4.319

3.713  
3.690  
3.653  
3.633

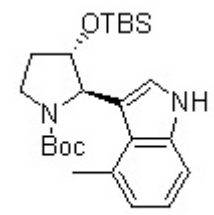
2.732

2.109  
2.086  
2.056

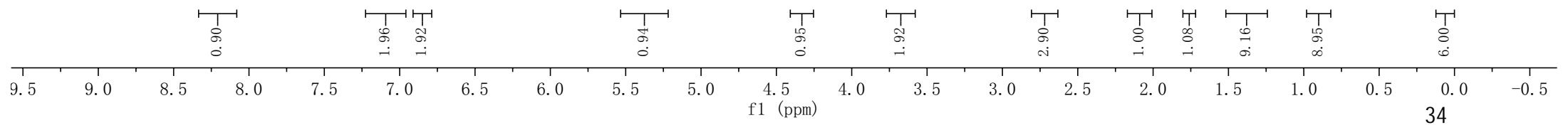
1.725  
1.512  
1.433  
1.383  
1.345  
1.295  
1.264

0.014

0.097  
0.080  
0.062  
0.011



8p (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)





—8.914  
—8.682

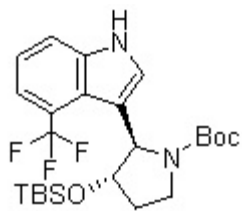
7.535  
7.515  
7.489  
7.470  
7.249  
7.225  
7.206  
7.185  
7.160  
7.034  
6.917  
6.897  
6.878  
6.777

—5.297  
—5.253

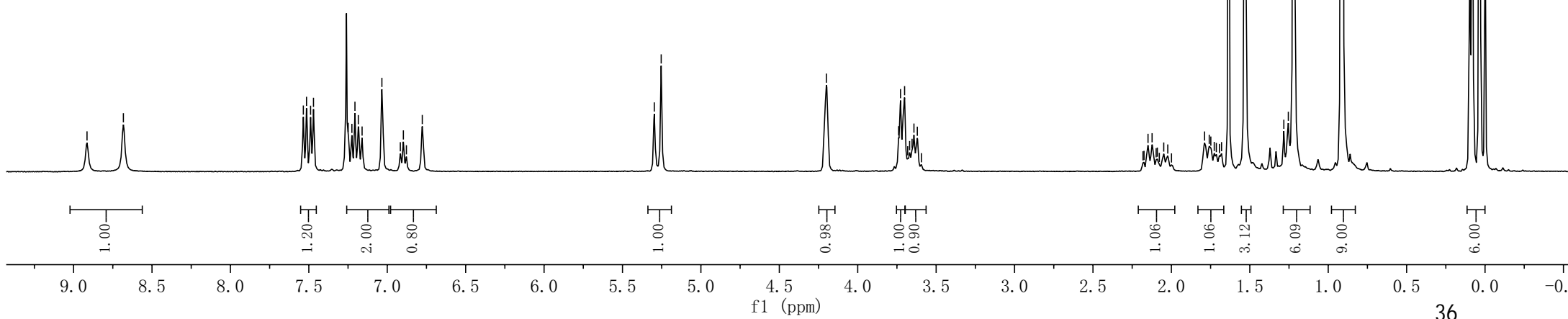
—4.200  
3.739  
3.727  
3.701  
3.681  
3.669  
3.653  
3.642  
3.620  
3.594

2.181  
2.174  
2.149  
2.123  
2.097  
2.089  
2.077  
2.049  
2.023  
1.999  
1.788  
1.759  
1.748  
1.727  
1.713  
1.694  
1.680  
1.531  
1.283  
1.254  
1.220  
0.912

0.097  
0.081  
0.035  
-0.001



8q (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



155.695  
155.438

138.088  
137.722

124.761  
124.561  
121.117  
120.846  
120.527  
120.369  
118.198  
116.173  
115.624

79.458  
79.298  
76.444

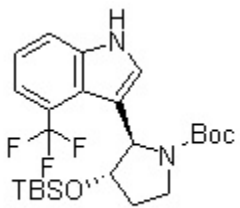
64.387  
64.351

45.059  
44.395

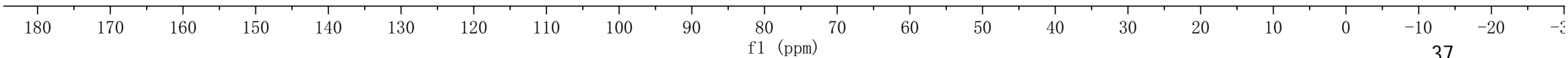
31.001  
30.420  
28.834  
28.366  
25.866

18.038

-4.193  
-4.320  
-4.849  
-4.977



8q (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)





7.944  
7.821  
7.407  
7.377  
7.357  
7.245  
7.230  
7.193  
7.173  
7.144  
7.138  
7.072  
7.053  
7.029  
7.027  
7.010  
6.992  
6.990  
6.970  
6.968  
6.951  
6.933

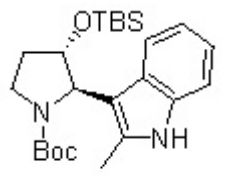
4.969  
4.686  
4.429  
4.328  
4.227

3.811  
3.728  
3.712  
3.701  
3.694  
3.685  
3.667

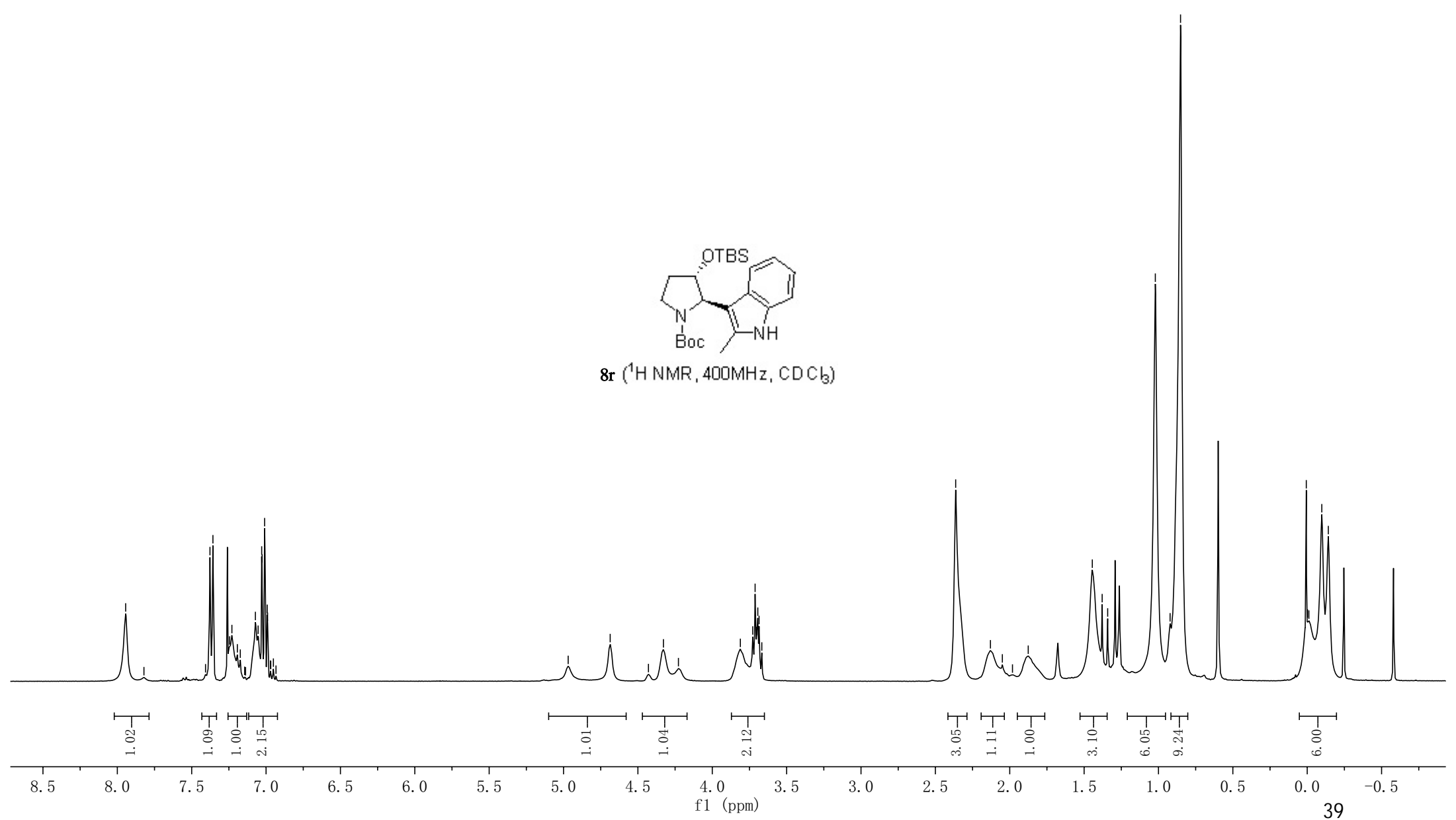
2.364  
2.130  
2.050  
1.982  
1.876

1.445  
1.379  
1.342  
1.021  
0.922  
0.852

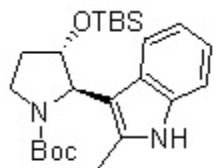
0.006  
-0.002  
-0.011  
-0.098  
-0.142



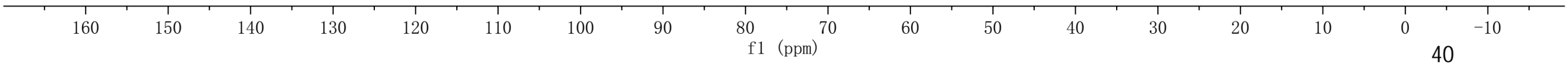
8r (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



155.175  
135.426  
131.311  
126.802  
120.842  
119.355  
118.364  
111.825  
110.349  
78.831  
78.833  
63.682  
62.824  
45.453  
44.776  
34.381  
33.157  
30.347  
29.825  
28.681  
28.183  
25.629  
25.687  
18.025  
12.131  
-4.826  
-5.477



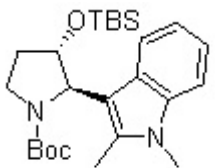
8r (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



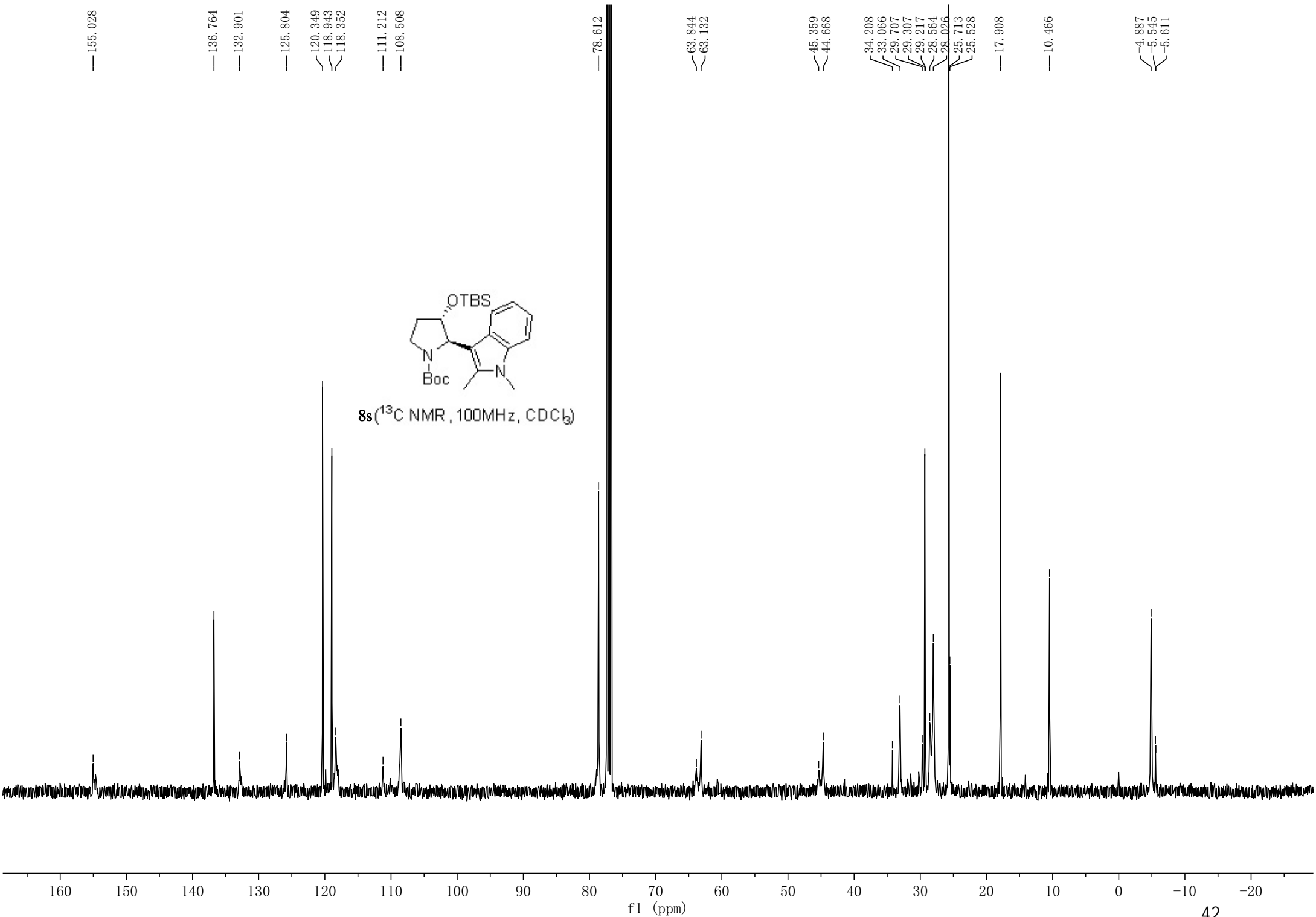




— 155.028  
— 136.764  
— 132.901  
— 125.804  
— 120.349  
— 118.943  
— 118.352  
— 111.212  
— 108.508  
— 78.612  
— 63.844  
— 63.132  
— 45.359  
— 44.668  
— 34.208  
— 33.066  
— 29.707  
— 29.307  
— 29.217  
— 28.564  
— 28.026  
— 25.713  
— 25.528  
— 17.908  
— 10.466  
— 4.887  
— 5.545  
— 5.611



8s (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



— 8.725  
— 8.474

7.260  
7.148  
7.089  
6.891  
6.788  
6.726

— 4.897  
— 4.779

— 4.242  
— 4.188

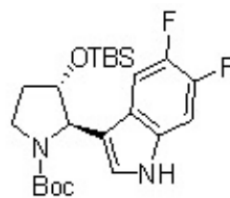
3.712  
3.660  
3.654  
3.633  
3.613  
3.606

2.088  
2.078  
2.065  
2.056  
2.046  
2.033  
2.024  
2.011  
2.001  
1.803  
1.508

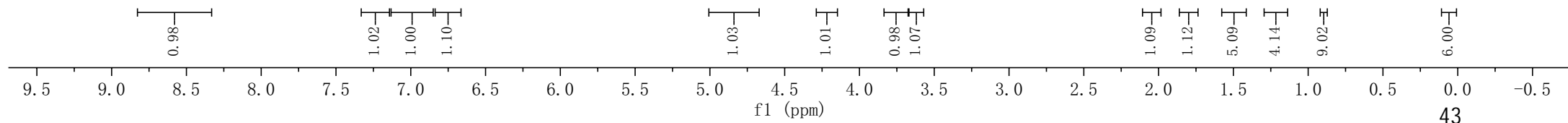
1.283  
1.254  
1.200

0.897

0.071  
0.032  
-0.002



8t (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



155.428  
149.098  
147.574  
146.685  
145.159

131.856  
131.518

123.116  
122.773  
120.895  
120.407  
117.589  
115.889

105.236  
104.919  
104.737  
99.397  
99.184

79.795  
79.461

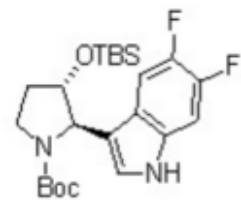
63.964  
63.584

45.190  
44.330

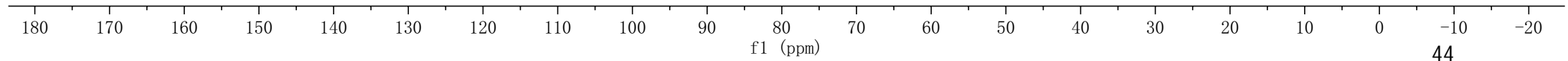
32.663  
32.062  
28.708  
28.388  
25.800

18.100

-4.592



8t (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)

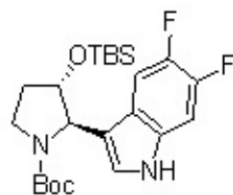


-143.817  
-143.871

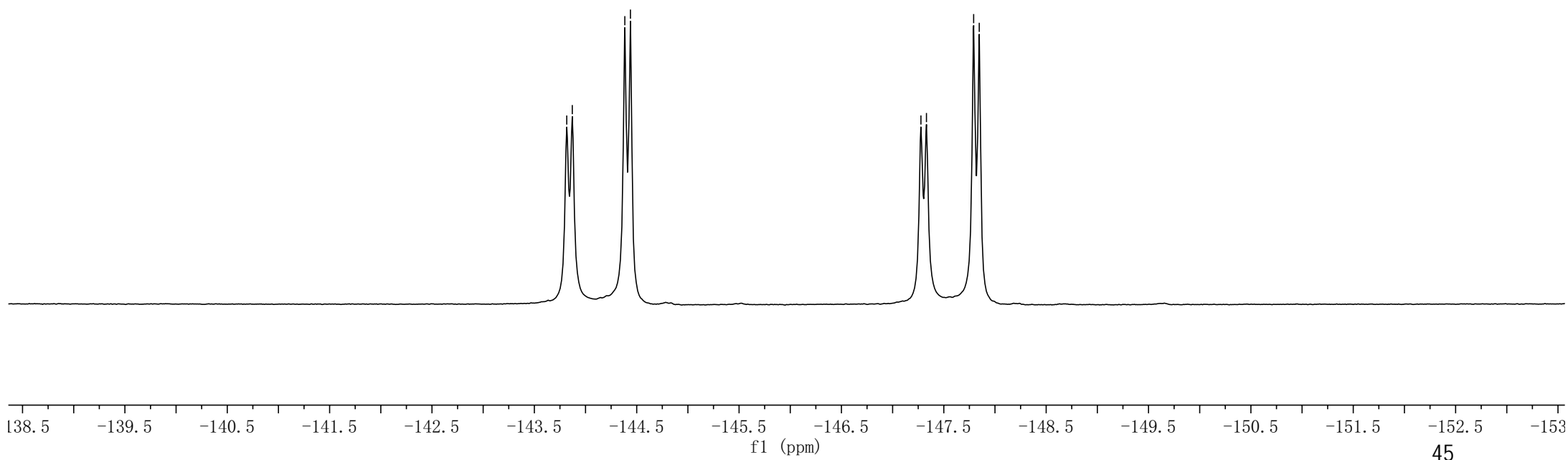
-144.384  
-144.439

-147.277  
-147.331

-147.792  
-147.846



8t (<sup>19</sup>F NMR, 376MHz, CDCl<sub>3</sub>)



8.998  
8.875  
8.663  
8.491  
8.453

7.613  
7.485  
7.443  
7.385  
7.324  
6.994  
6.863  
6.712  
6.613

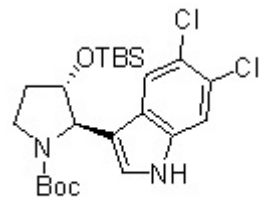
4.994  
4.879  
4.807

4.388  
4.248  
4.181

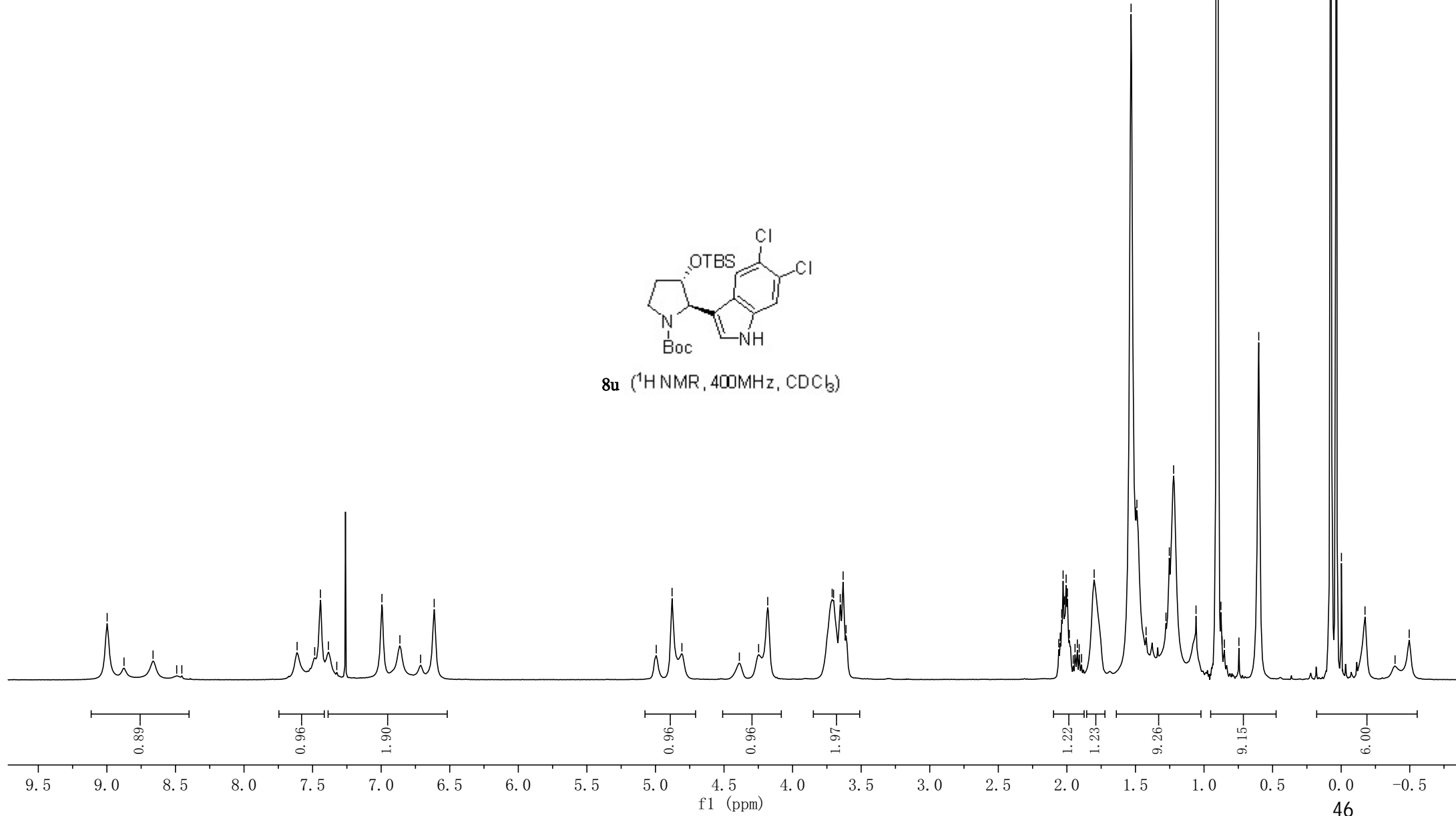
3.712  
3.701  
3.653  
3.631  
3.610

2.059  
2.049  
2.037  
2.027  
2.016  
2.005  
1.996  
1.982  
1.954  
1.940  
1.924  
1.910  
1.893  
1.801  
1.532  
1.498  
1.490  
1.423  
1.278  
1.253  
1.222  
1.068  
0.904  
0.877  
0.868  
0.851  
0.746  
0.601

0.076  
0.036  
-0.002  
-0.174  
-0.393  
-0.496



**8u** ( $^1\text{H NMR}$ , 400MHz,  $\text{CDCl}_3$ )



155.532  
155.214

135.565

125.591  
124.685  
123.714  
123.257  
119.857  
119.085  
117.062  
115.013  
112.891  
112.386

79.973  
79.601  
74.486

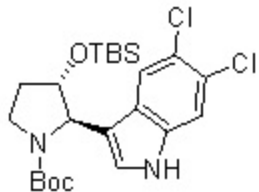
63.924  
63.487

45.232  
44.367

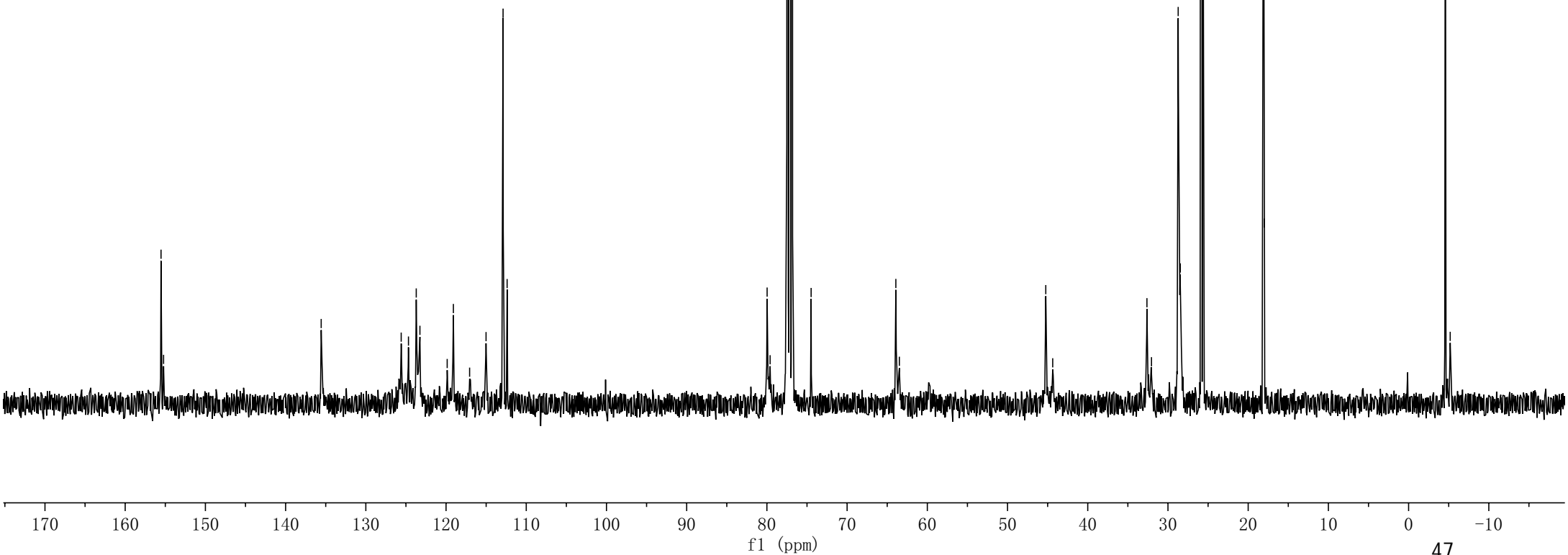
32.621  
32.053  
28.726  
28.463  
25.874  
25.647

18.107  
17.988

-4.577  
-5.186



**8u** (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



7.753  
7.668

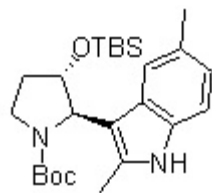
7.163  
7.101  
7.080  
6.932  
6.913  
6.863  
6.843

4.982  
4.697  
4.436  
4.427  
4.418  
4.338  
4.238  
3.832  
3.734  
3.718  
3.700  
3.674

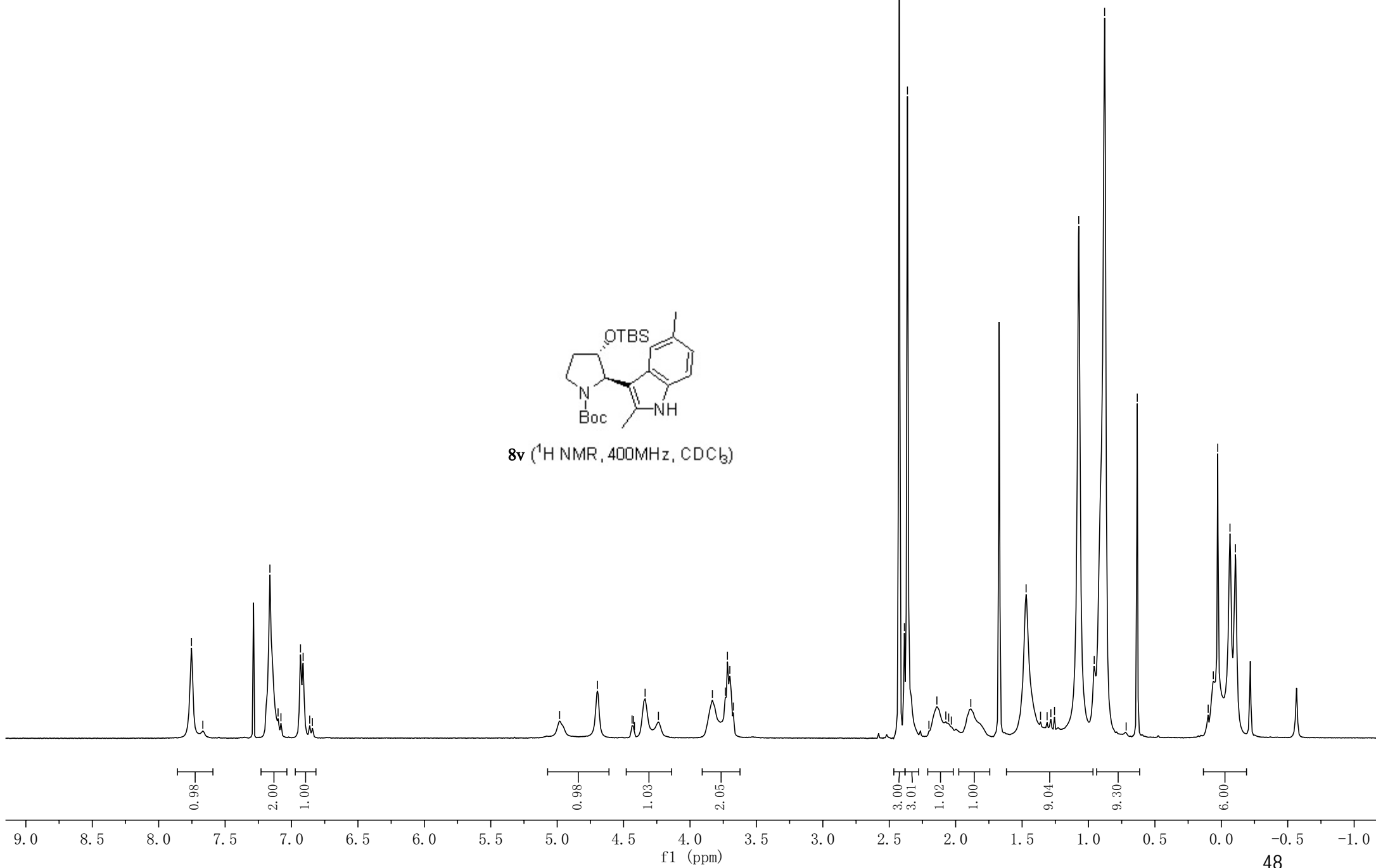
2.424  
2.386  
2.363  
2.201  
2.141  
2.074  
2.053  
2.033  
1.886

1.470  
1.361  
1.312  
1.283  
1.256  
1.073  
0.957  
0.879  
0.717  
0.633

0.099  
0.060  
0.027  
-0.065  
-0.106



8v (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)





— 155.136

— 133.582

— 131.189

— 128.191

— 127.049

— 122.179

— 118.029

— 111.168

— 109.826

— 78.732

— 78.151

— 62.854

— 44.650

— 32.989

— 29.704

— 28.123

— 25.721

— 25.563

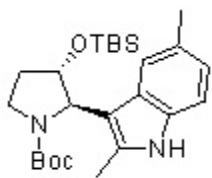
— 21.636

— 17.914

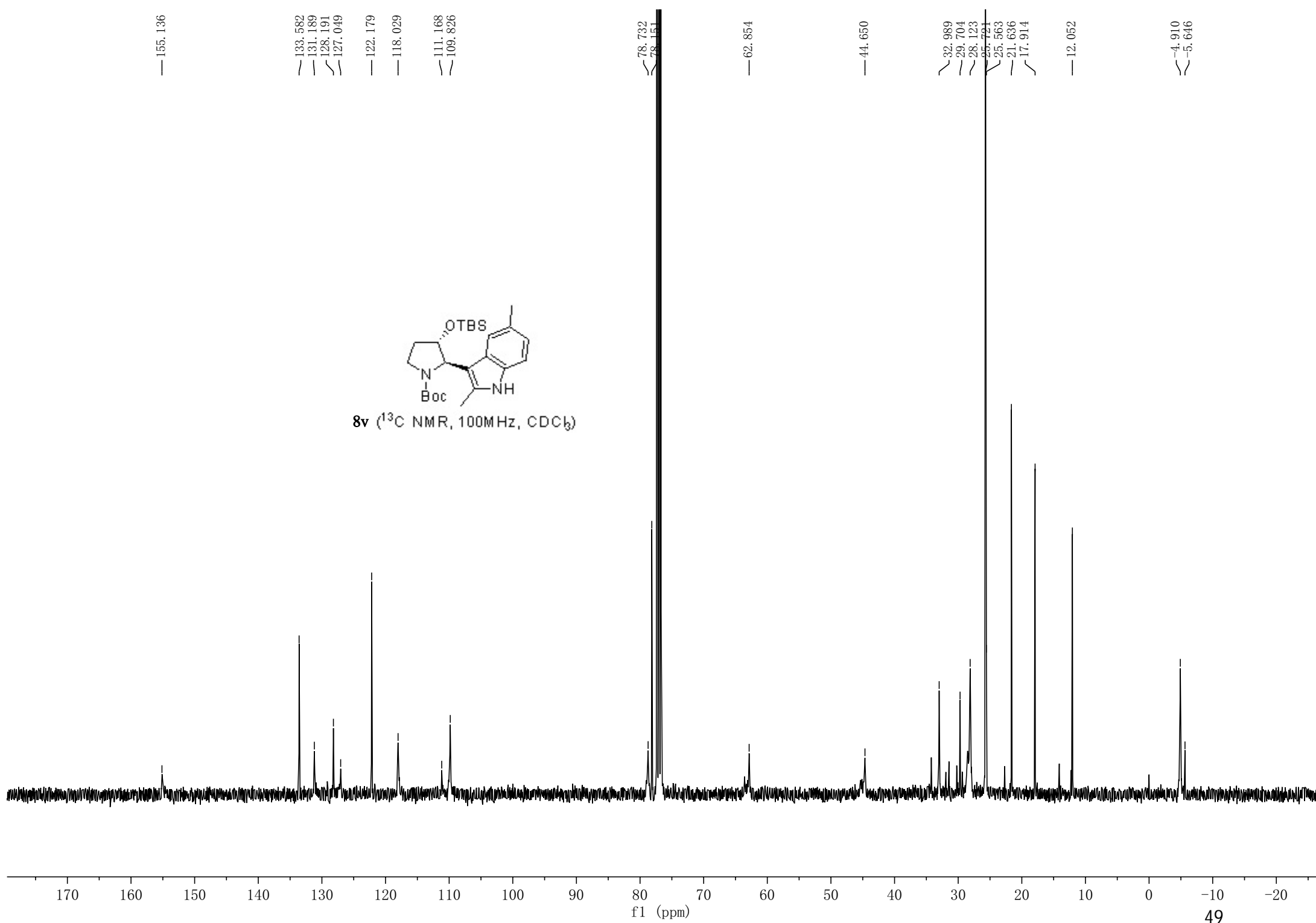
— 12.052

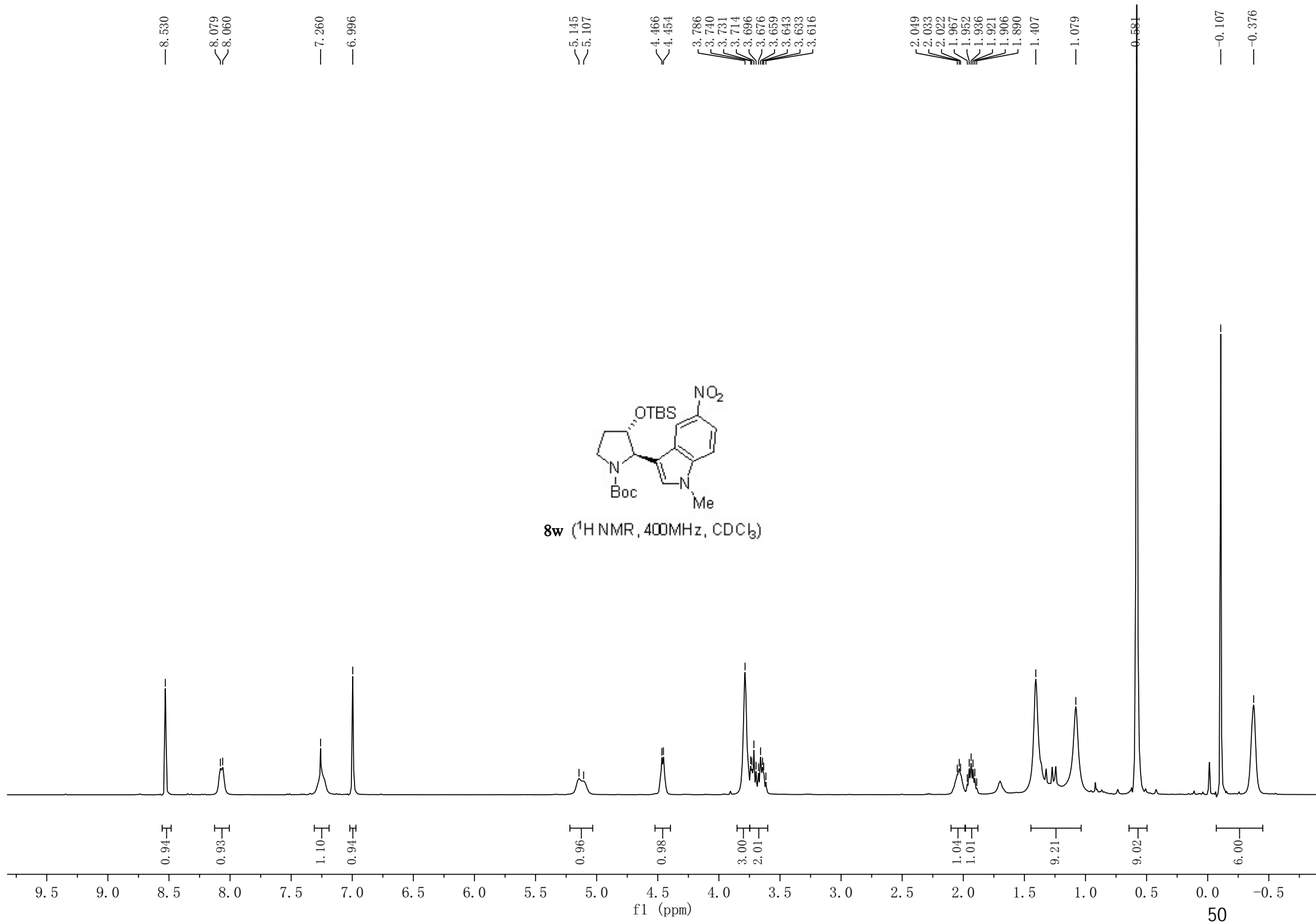
— 4.910

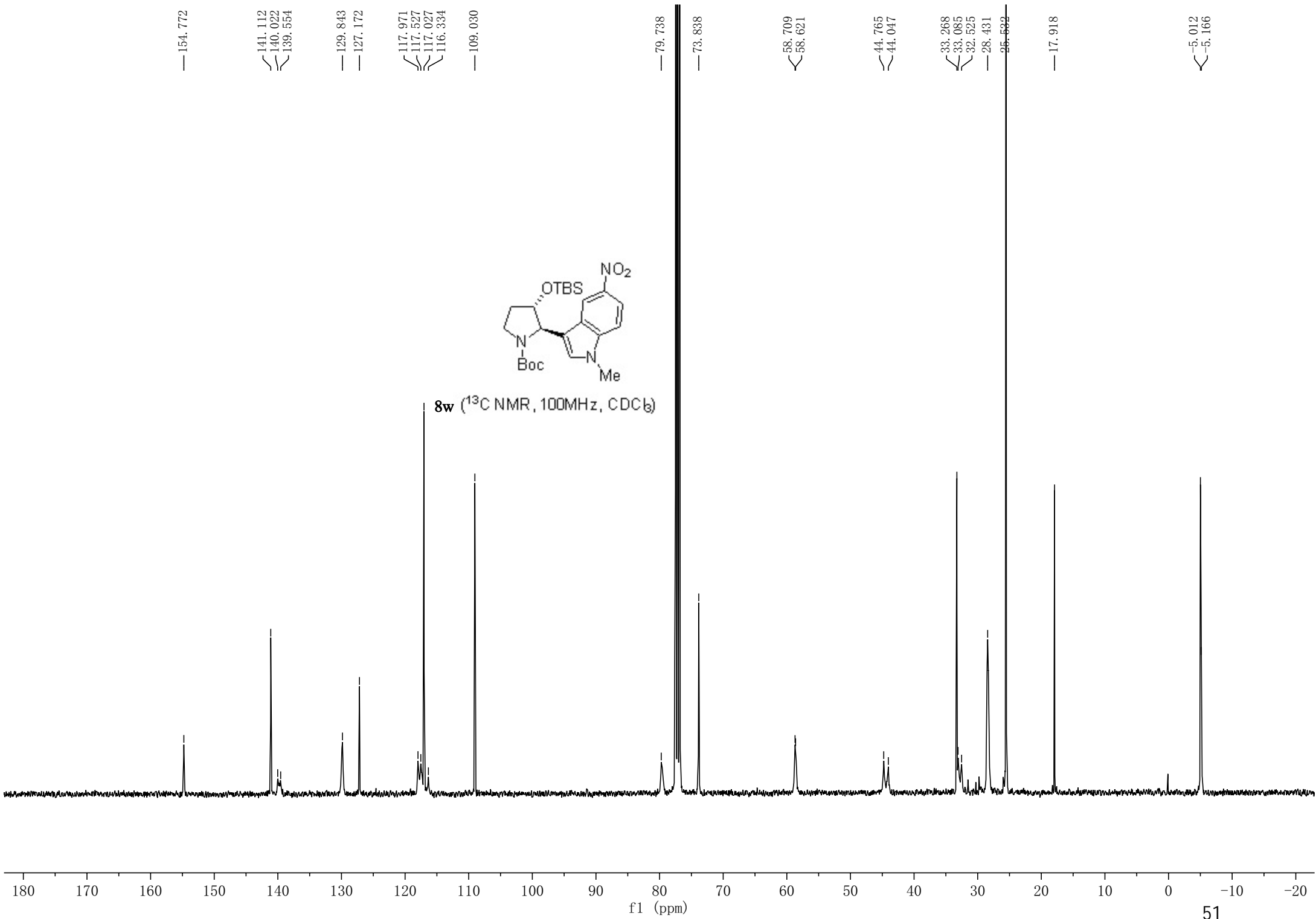
— 5.646



8v (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)







8.226  
8.194  
8.109  
8.001  
7.592  
7.573  
7.388  
7.362  
7.332  
7.311  
7.289  
7.256  
7.238  
7.220  
7.200  
7.158  
7.138  
7.111  
6.967  
6.950  
6.830  
6.800

5.293  
5.232  
5.201  
5.184  
5.149  
5.105  
5.060

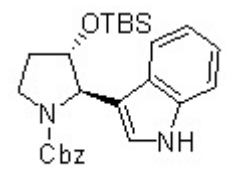
4.376

3.815  
3.801  
3.794  
3.772  
3.750  
3.725

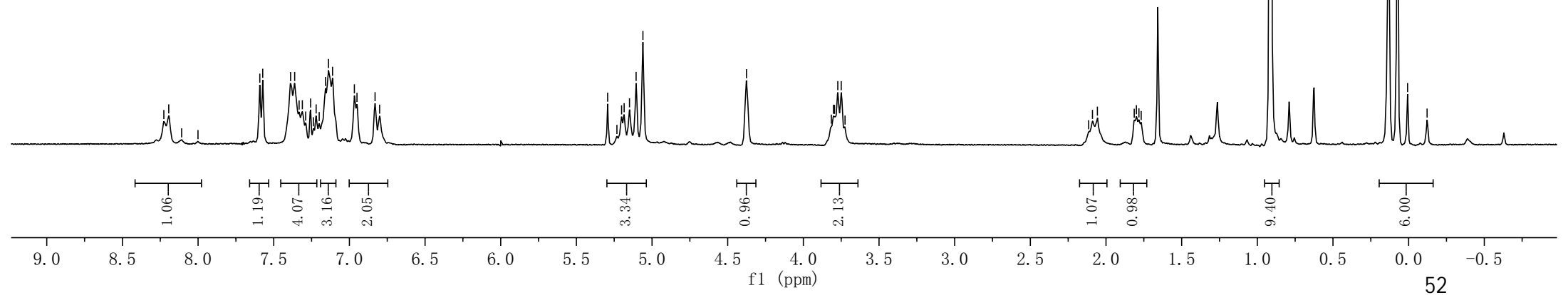
2.114  
2.089  
2.057  
1.814  
1.799  
1.782  
1.768

0.013

0.132  
0.074  
0.007  
-0.122



8x (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



155.823  
155.474  
137.333  
137.211  
136.957  
136.744  
128.609  
128.233  
128.141  
127.935  
127.753  
127.461  
127.120  
125.602  
122.243  
122.103  
121.624  
121.503  
119.747  
119.626  
119.280  
119.246  
118.803  
116.718  
115.763  
111.556  
111.310  
111.022

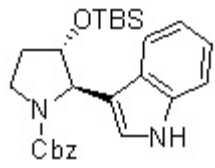
66.797  
66.453  
64.704  
64.103

44.928  
44.820

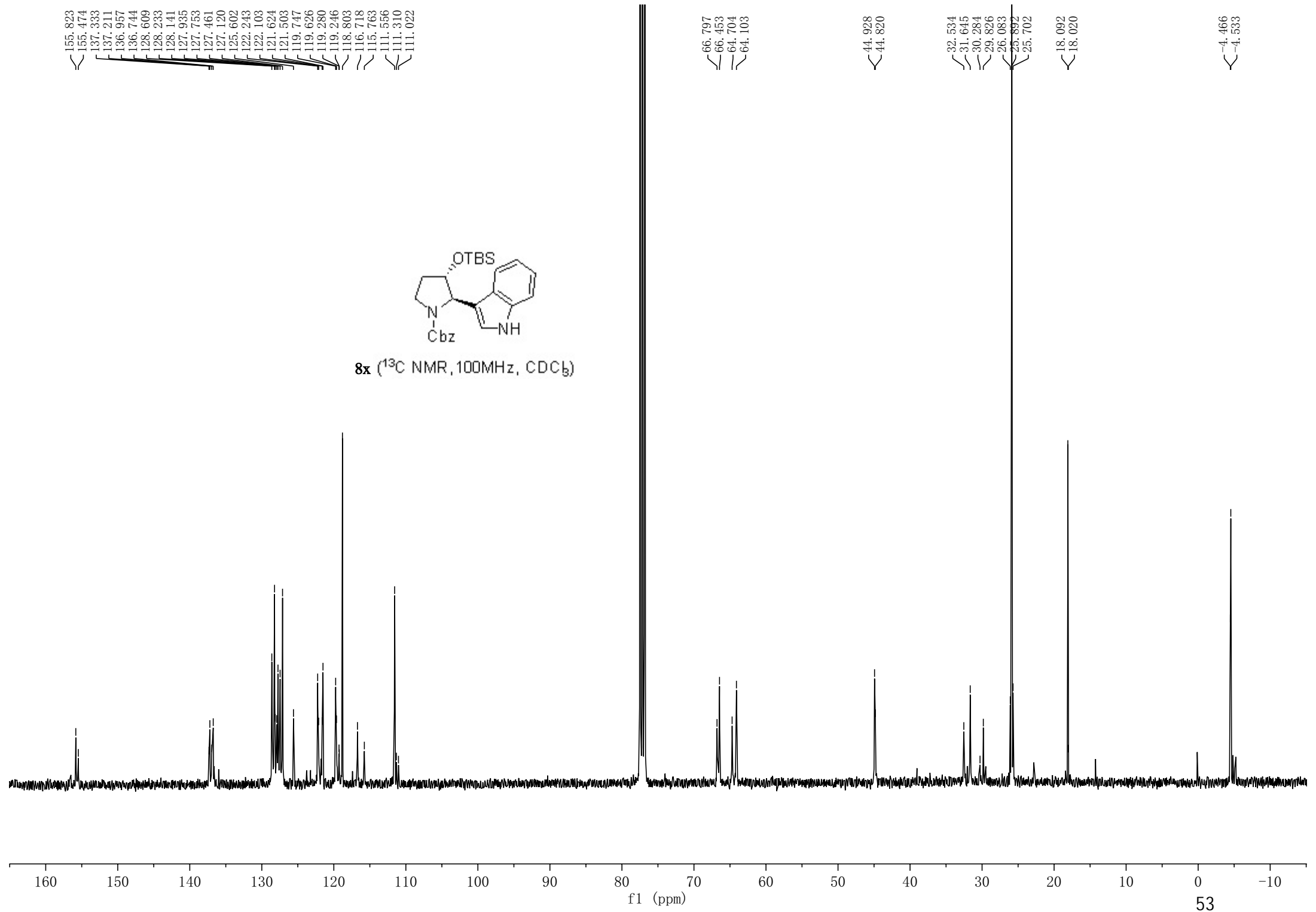
32.534  
31.645  
30.284  
29.826  
26.083  
25.892  
25.702

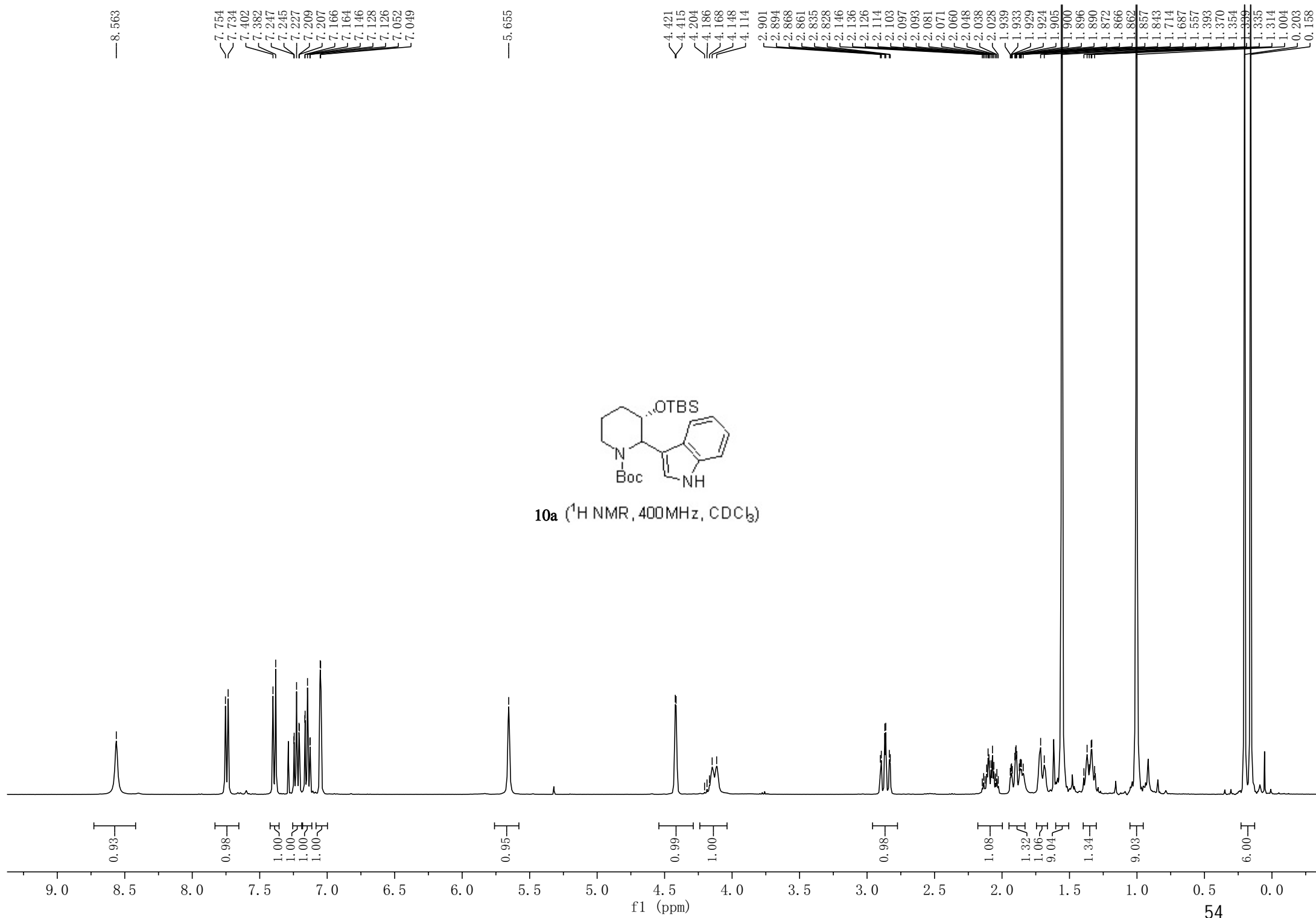
18.092  
18.020

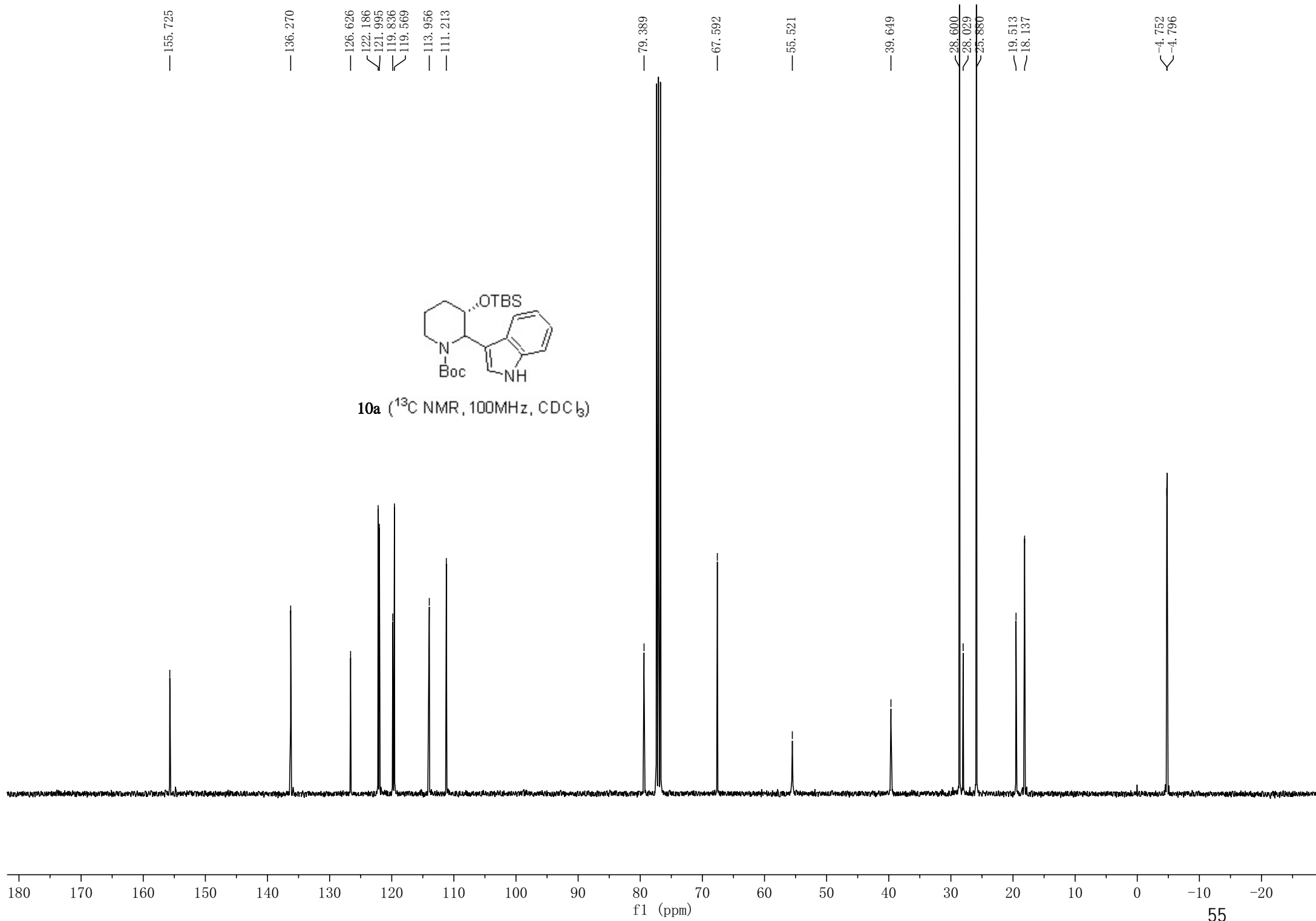
-4.466  
-4.533

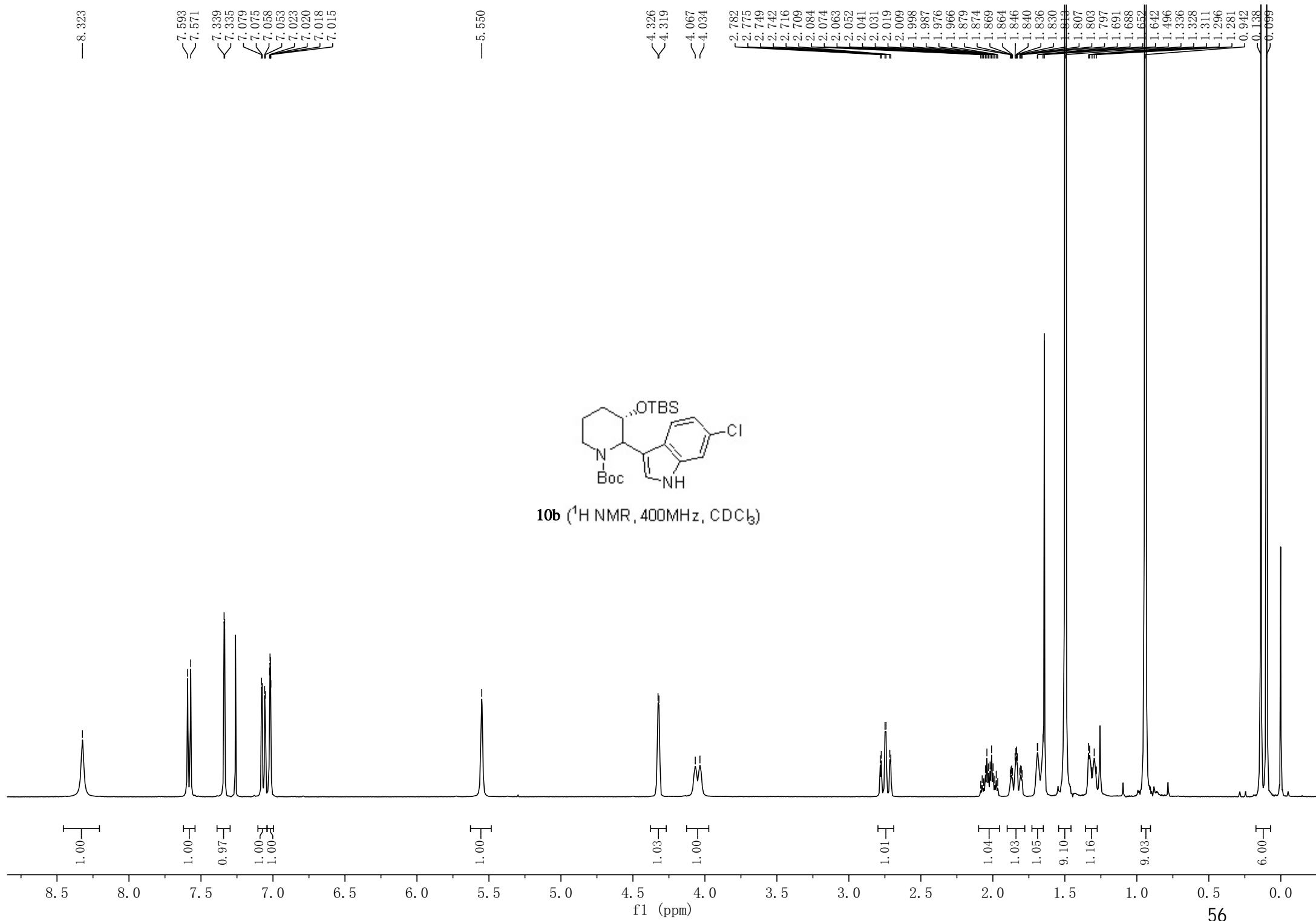


8x (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)

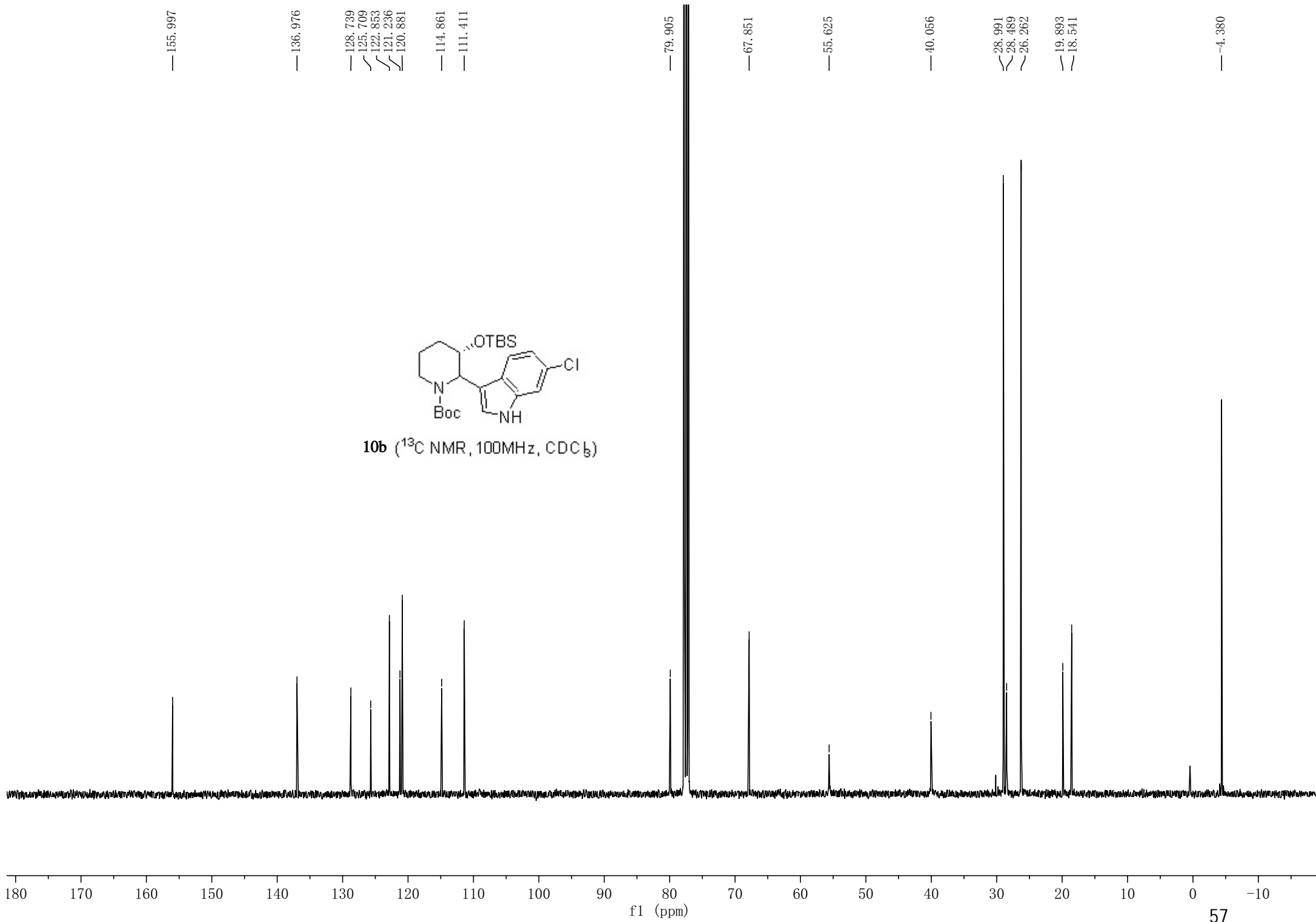


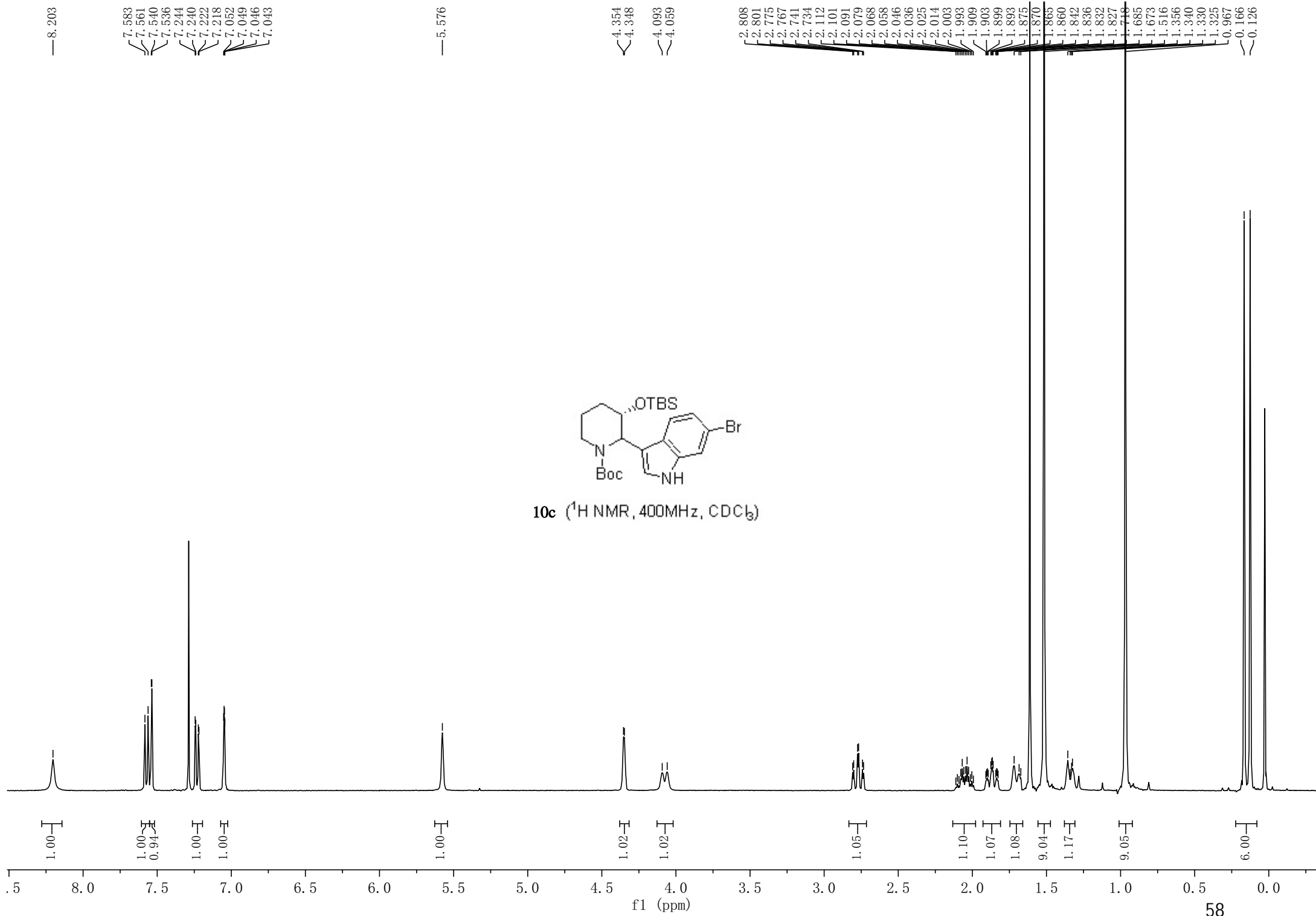


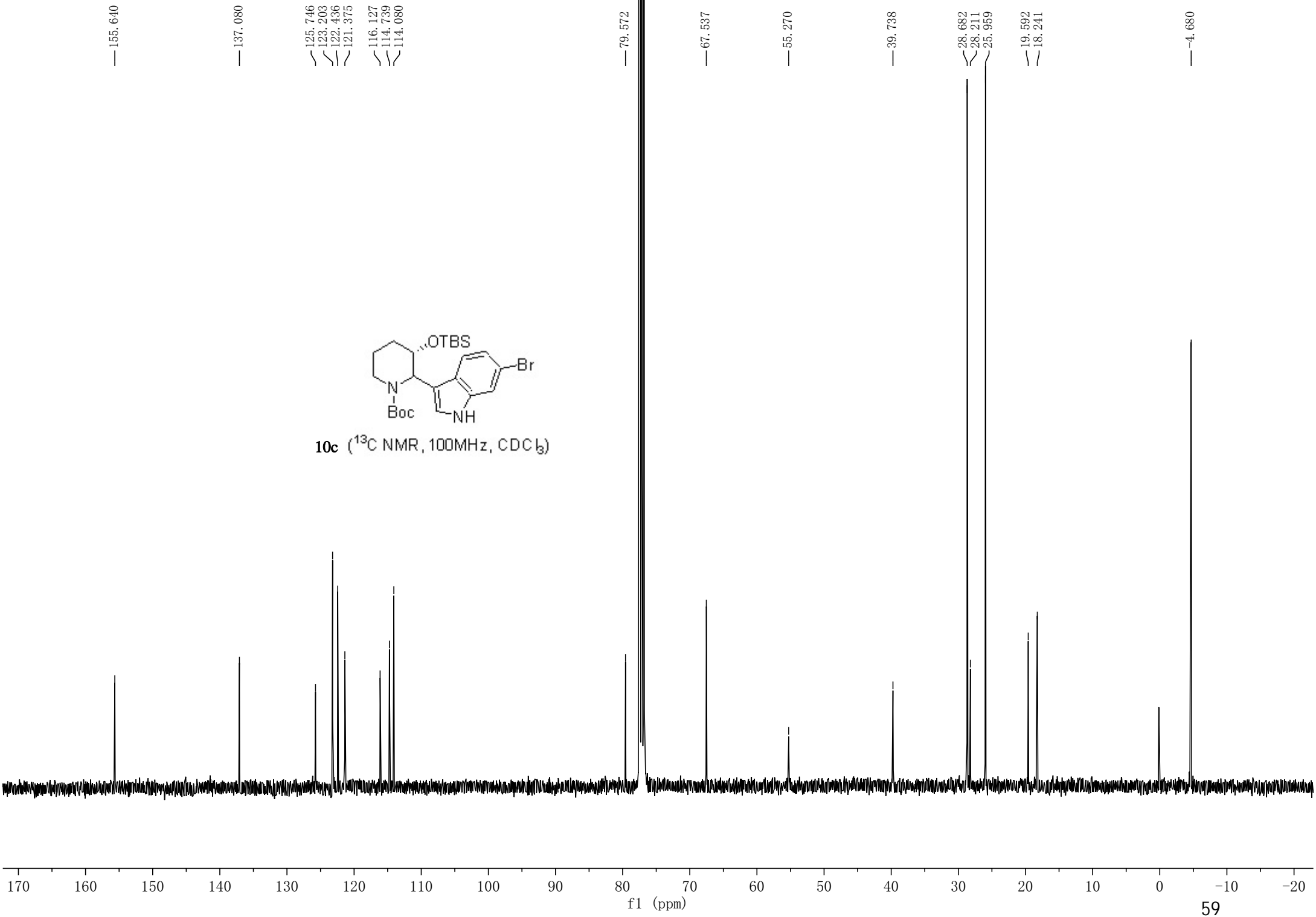


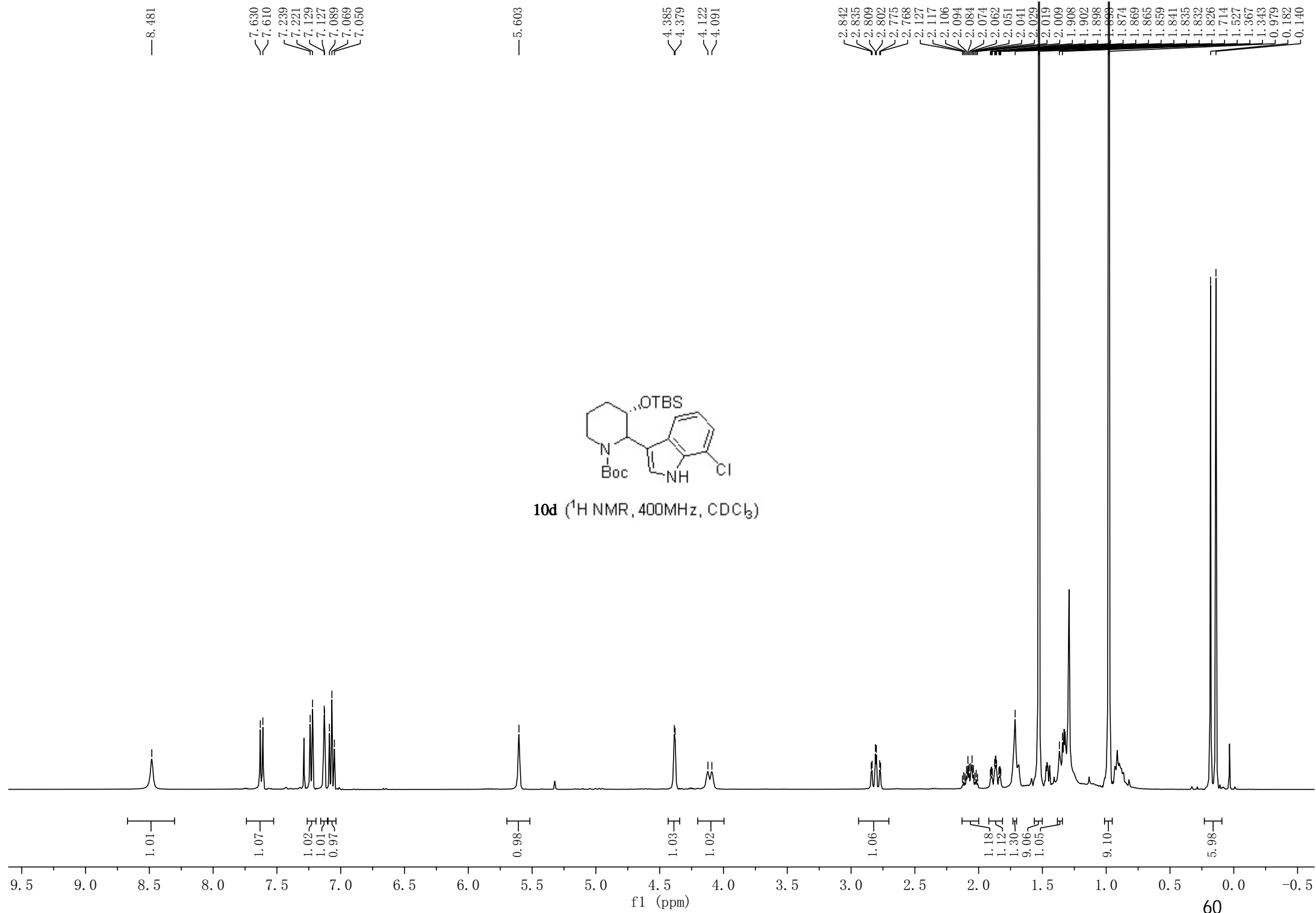












— 155.673

— 133.607

— 128.227

122.567

121.793

120.622

118.739

116.734

115.593

— 79.571

— 67.549

— 55.467

— 39.759

29.840

28.676

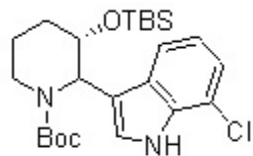
28.133

25.959

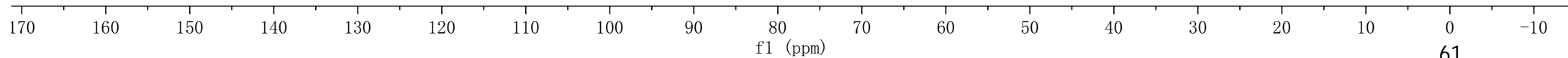
19.554

18.236

— -4.682



10d ( $^{13}\text{C}$  NMR, 100MHz,  $\text{CDCl}_3$ )

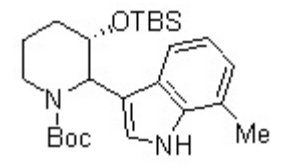


8.091  
7.580  
7.562  
7.087  
7.084  
7.081  
7.078  
7.072  
7.053  
7.047  
7.032

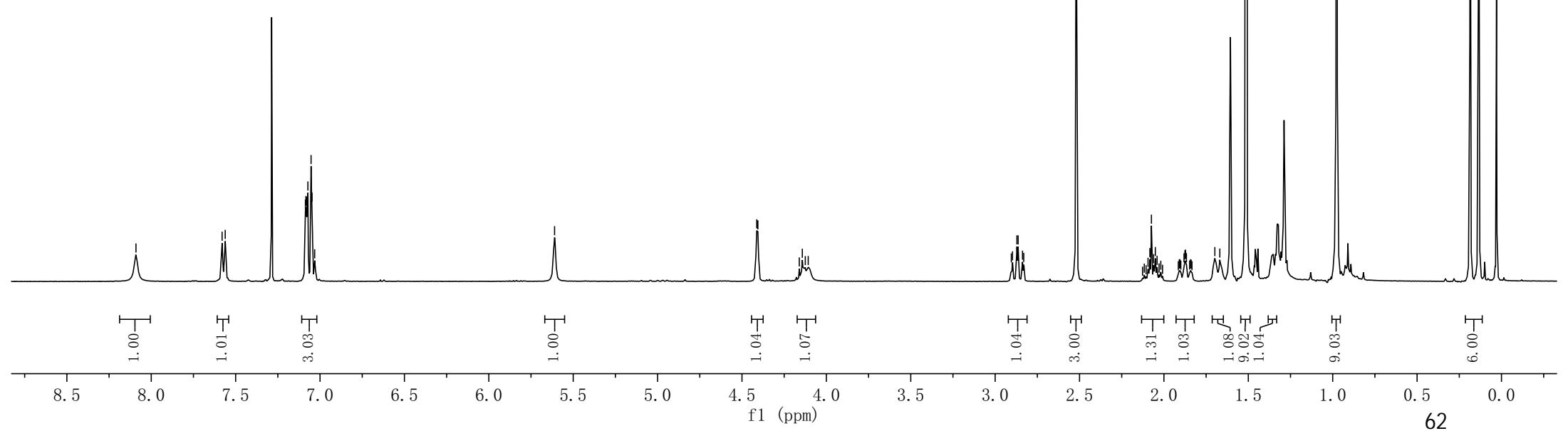
5.610

4.413  
4.406  
4.160  
4.142  
4.125  
4.108

2.904  
2.897  
2.871  
2.864  
2.838  
2.831  
2.519  
2.127  
2.116  
2.106  
2.094  
2.083  
2.074  
2.061  
2.051  
2.041  
2.029  
2.019  
2.008  
1.915  
1.909  
1.905  
1.900  
1.881  
1.876  
1.872  
1.867  
1.848  
1.842  
1.839  
1.834  
1.698  
1.669  
1.513  
0.976  
0.185  
0.135



10e (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



— 155.670

— 135.795

— 126.132  
— 122.780  
— 121.571  
— 120.260  
— 119.901  
— 117.631  
— 114.758

— 79.285

— 67.574

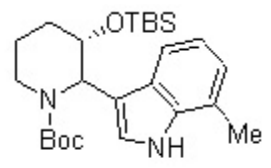
— 55.609

— 39.637

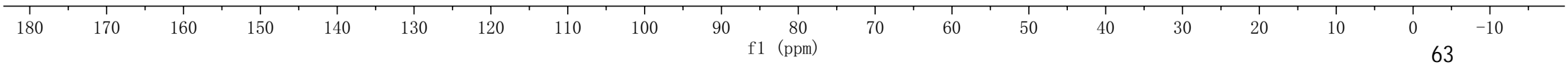
— 28.555  
— 27.957  
— 25.859

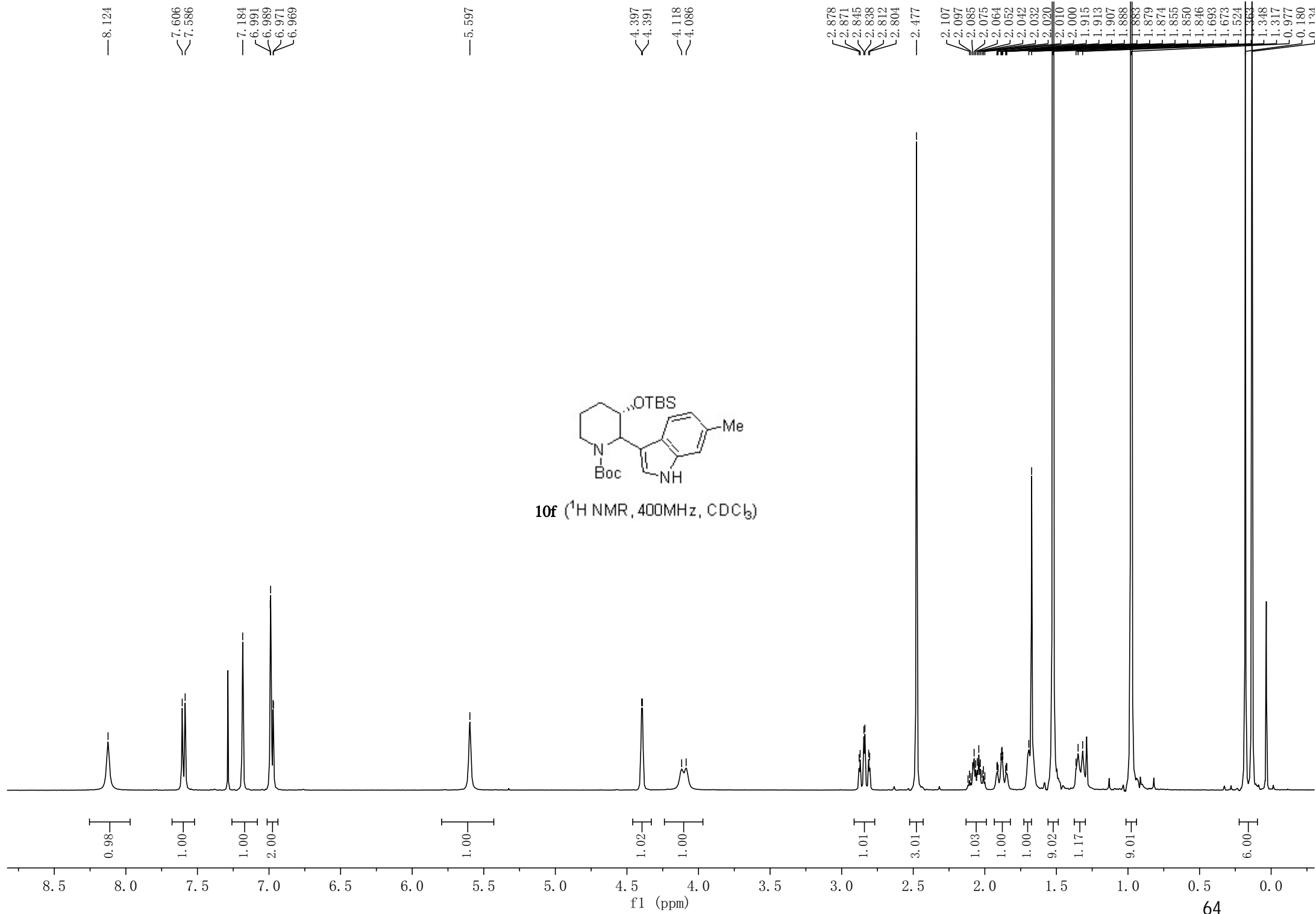
— 19.454  
— 18.120  
— 16.597

— -4.766  
— -4.814



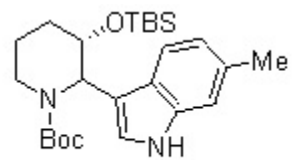
10e (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



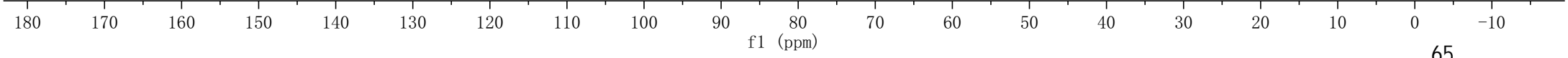


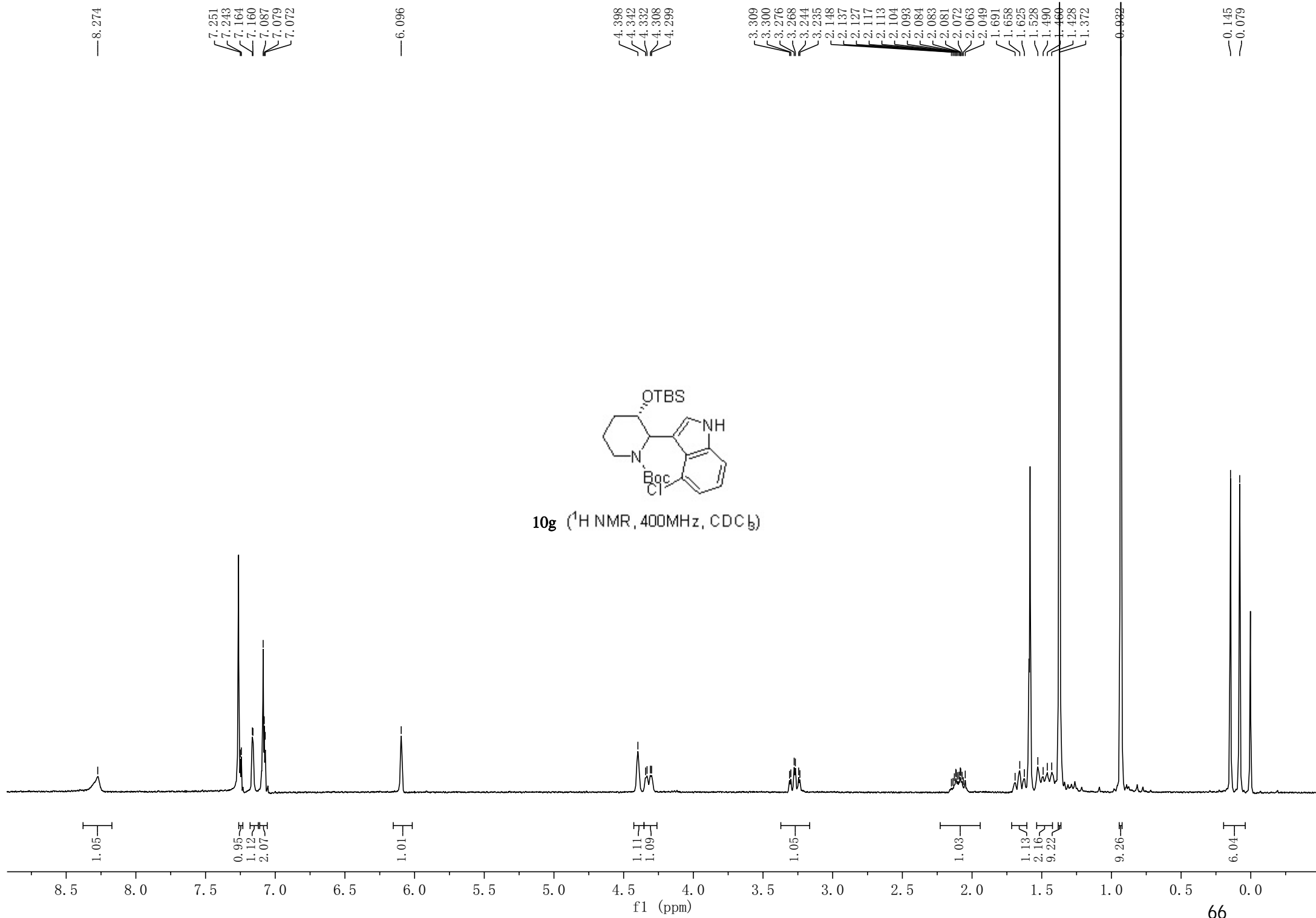


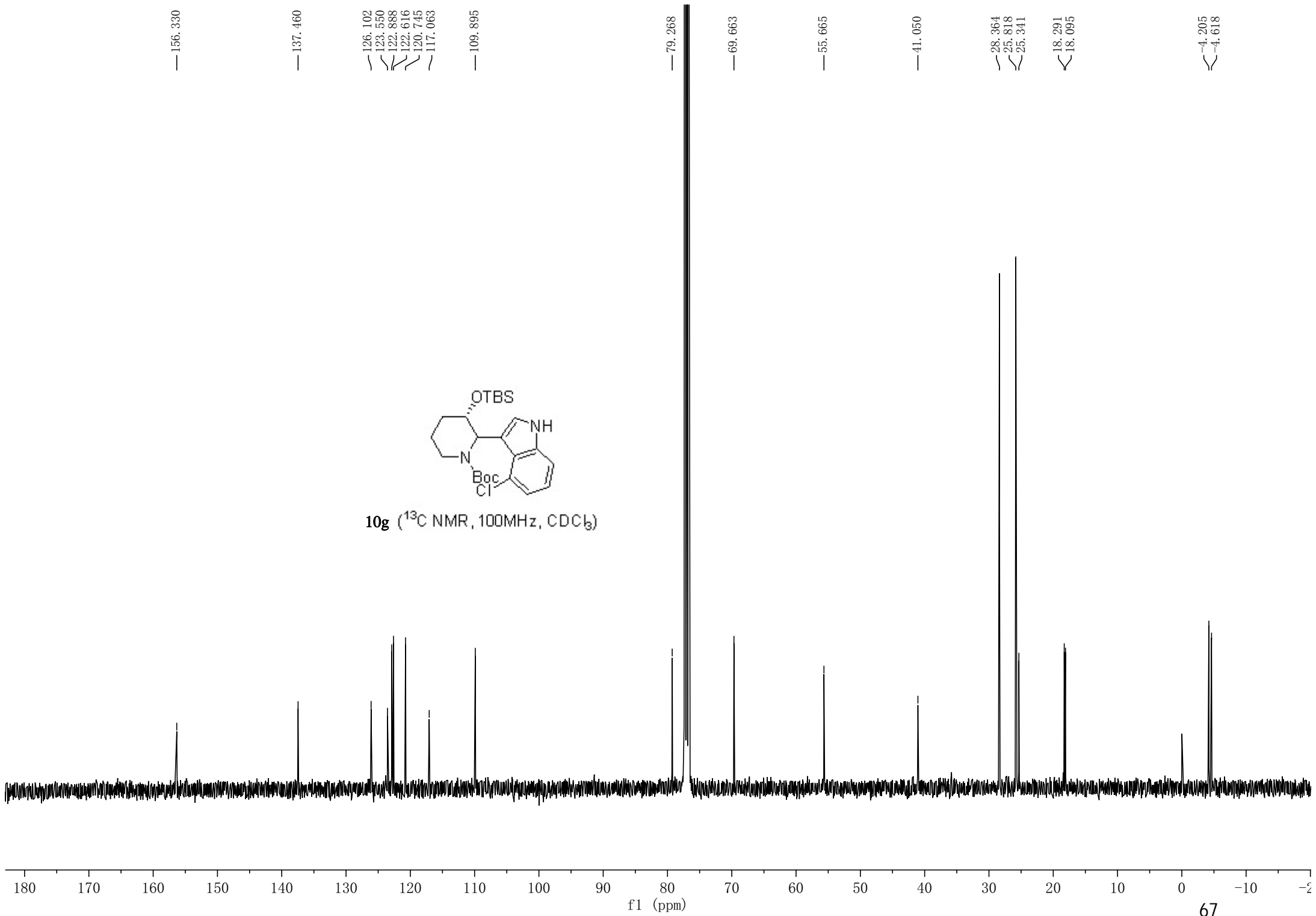
— 155.612  
— 136.644  
— 132.123  
— 124.444  
— 121.447  
— 121.178  
— 119.575  
— 114.057  
— 110.992  
— 79.241  
— 67.520  
— 55.483  
— 39.555  
— 28.553  
— 28.012  
— 25.847  
— 21.604  
— 19.481  
— 18.113  
— 4.791  
— 4.832



10f (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)







— 8.829

7.250  
7.241  
7.231  
7.132  
7.127  
6.963  
6.943  
6.923

6.238  
6.216

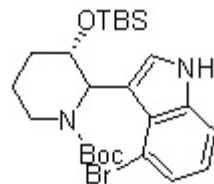
4.392  
4.344  
4.332  
4.310  
4.299

3.317  
3.307  
3.284  
3.274  
3.251  
3.242

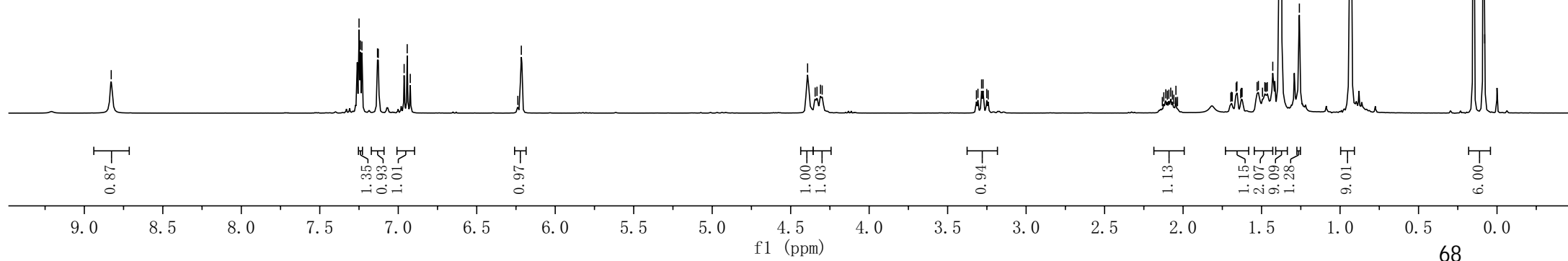
2.132  
2.123  
2.110  
2.100  
2.091  
2.079  
2.068  
2.059  
2.045  
2.036

1.696  
1.691  
1.687  
1.662  
1.657  
1.633  
1.629  
1.624  
1.528  
1.520

1.494  
1.479  
1.472  
1.463  
1.429  
1.388  
1.379  
1.259  
0.933  
0.150  
0.086  
0.079



10h (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



— 156.759

— 137.478

124.894  
124.175  
124.115  
123.468  
122.817

117.053  
113.885  
110.772

— 79.629

— 70.007

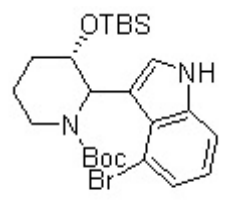
— 55.342

— 41.348

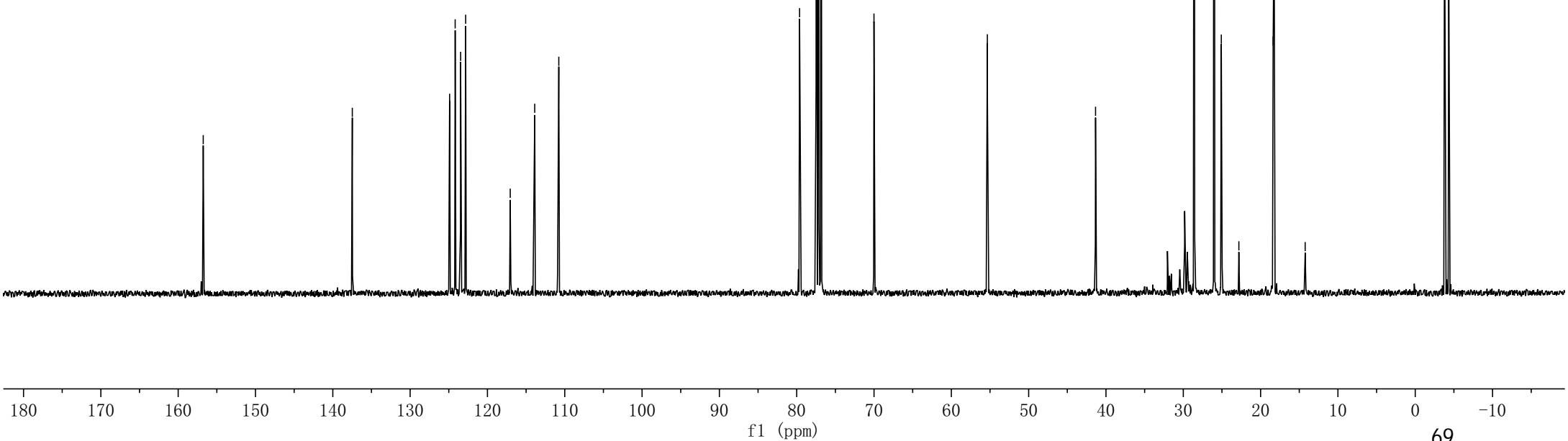
28.562  
26.018  
25.083

22.812  
18.381  
18.256  
14.236

— 3.789  
— 4.331



10h (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



8.457

7.794  
7.791

7.565  
7.287  
7.276  
7.272  
7.255  
7.251  
7.242  
7.220

5.782

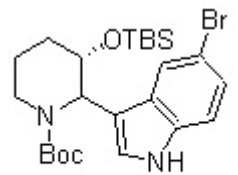
4.057  
4.045  
4.030  
4.016  
4.004  
3.863  
3.857  
3.852  
3.849  
3.843

2.505  
2.483  
2.478  
2.471  
2.466  
2.451  
2.431  
2.155  
2.125  
2.106  
2.100  
2.081  
2.049  
1.870  
1.861  
1.850  
1.838

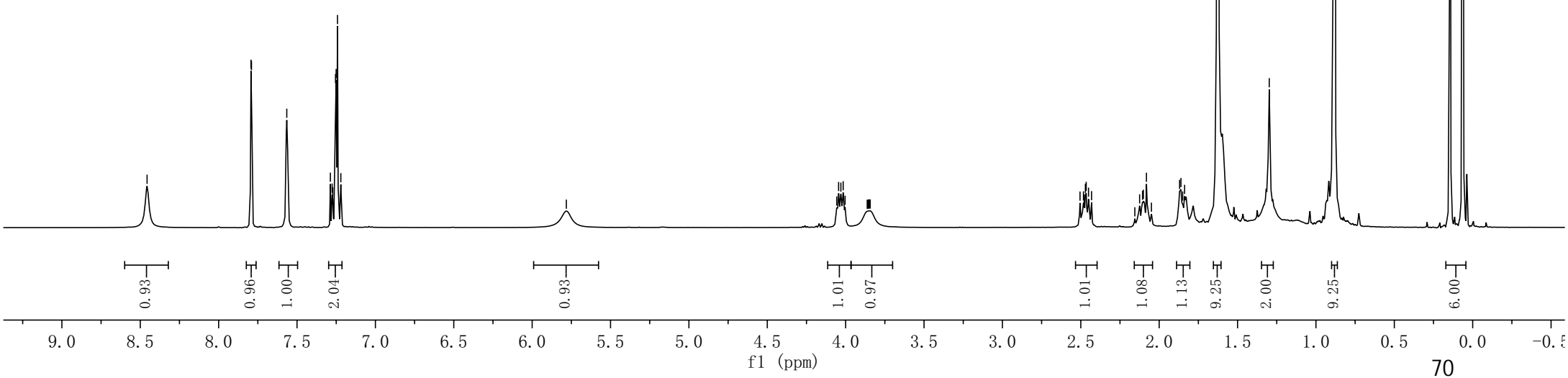
1.298

0.884

0.145  
0.064



10i-1 (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



— 154.714

— 134.564

— 129.513

— 125.732

— 124.726

— 122.592

— 112.982

— 112.391

— 110.835

— 80.249

— 71.379

— 29.824

— 29.610

— 28.776

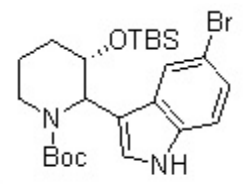
— 25.924

— 24.877

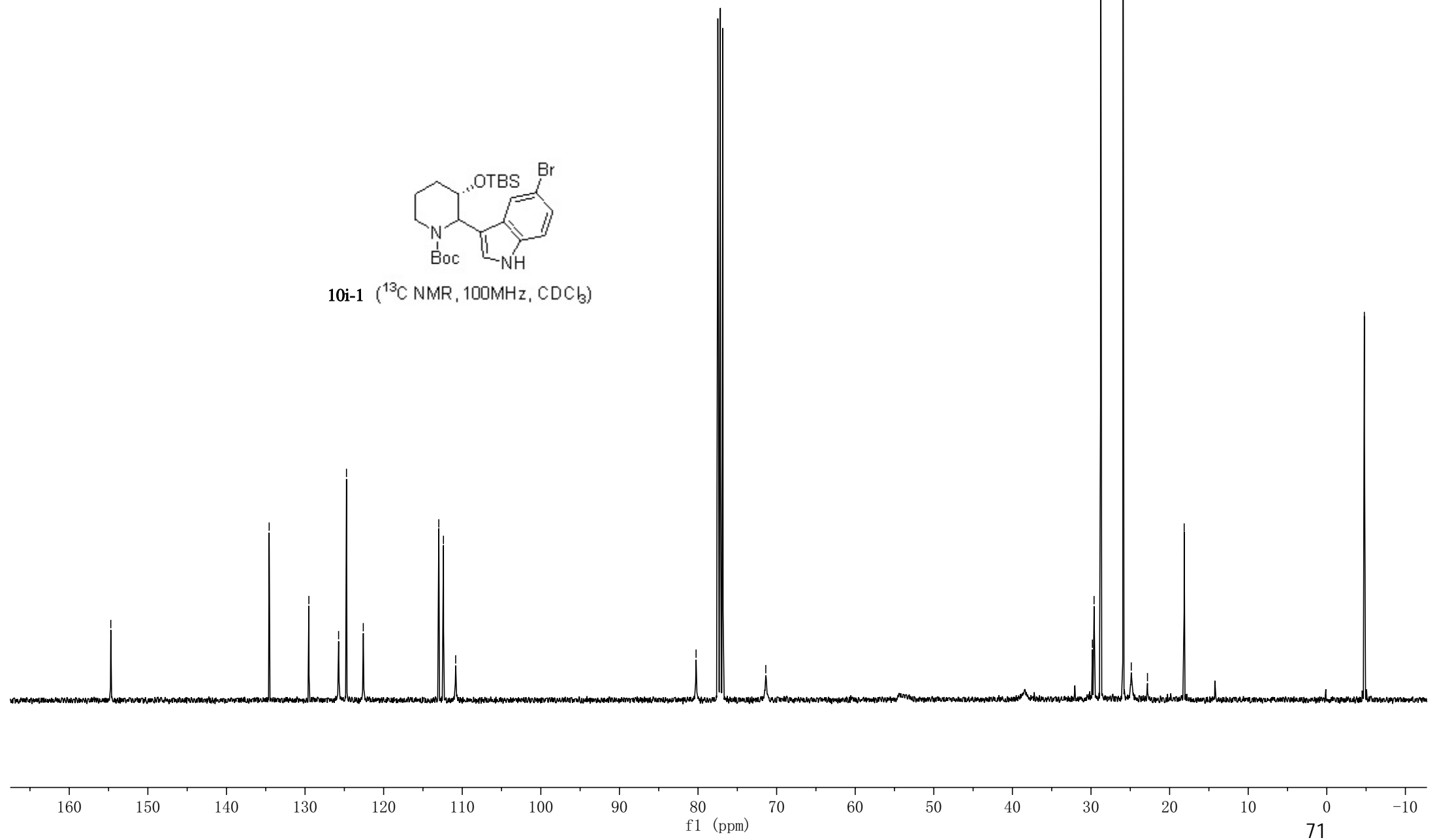
— 22.814

— 18.145

— -4.779



10i-1 (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



— 8.281

7.904  
7.901

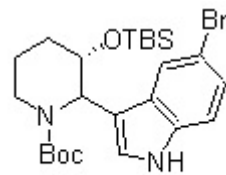
7.315  
7.311  
7.293  
7.288  
7.261  
7.239  
7.074

— 5.552

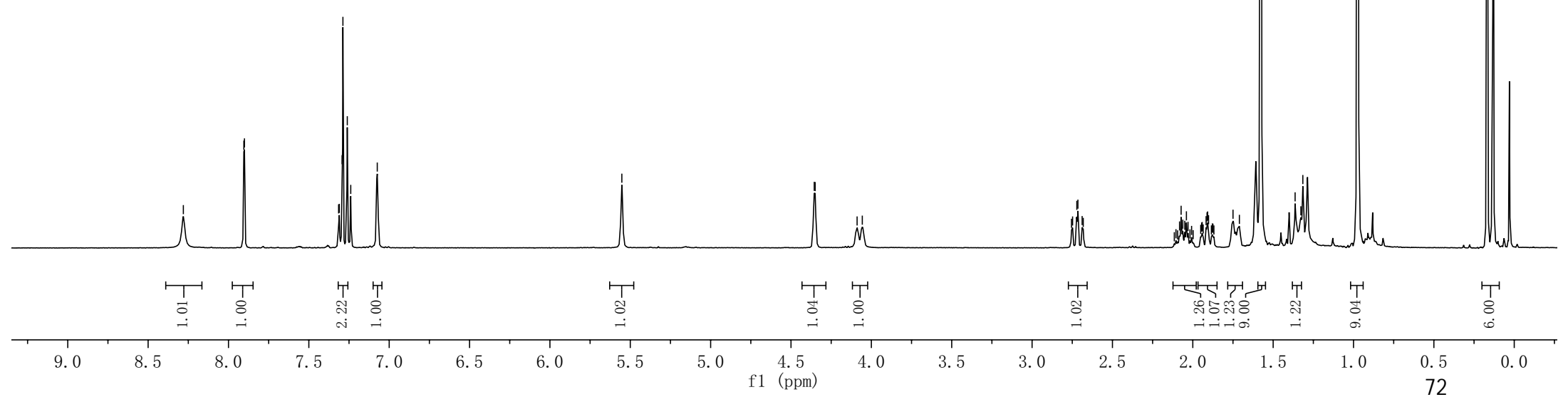
4.355  
4.350

4.089  
4.056

2.755  
2.748  
2.722  
2.715  
2.689  
2.682  
2.115  
2.105  
2.094  
2.082  
2.073  
2.062  
2.050  
2.040  
2.030  
2.018  
2.007  
1.998  
1.951  
1.945  
1.942  
1.935  
1.917  
1.911  
1.908  
1.902  
1.884  
1.878  
1.875  
1.869  
1.750  
1.710  
1.577  
1.363  
1.328  
1.315  
0.975  
0.169  
0.131



10i-2 (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)





— 155.396

— 134.743

— 128.532

— 125.267

— 122.953

— 122.732

— 114.066

— 113.131

— 112.401

— 79.689

— 67.255

— 55.030

— 39.418

— 28.586

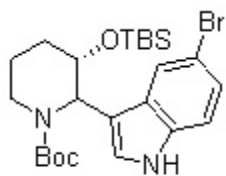
— 28.357

— 25.831

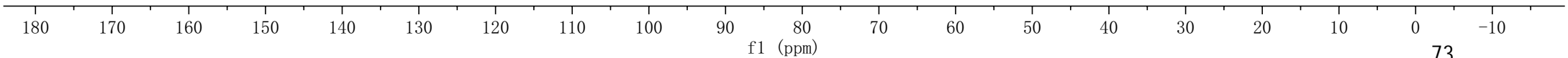
— 19.565

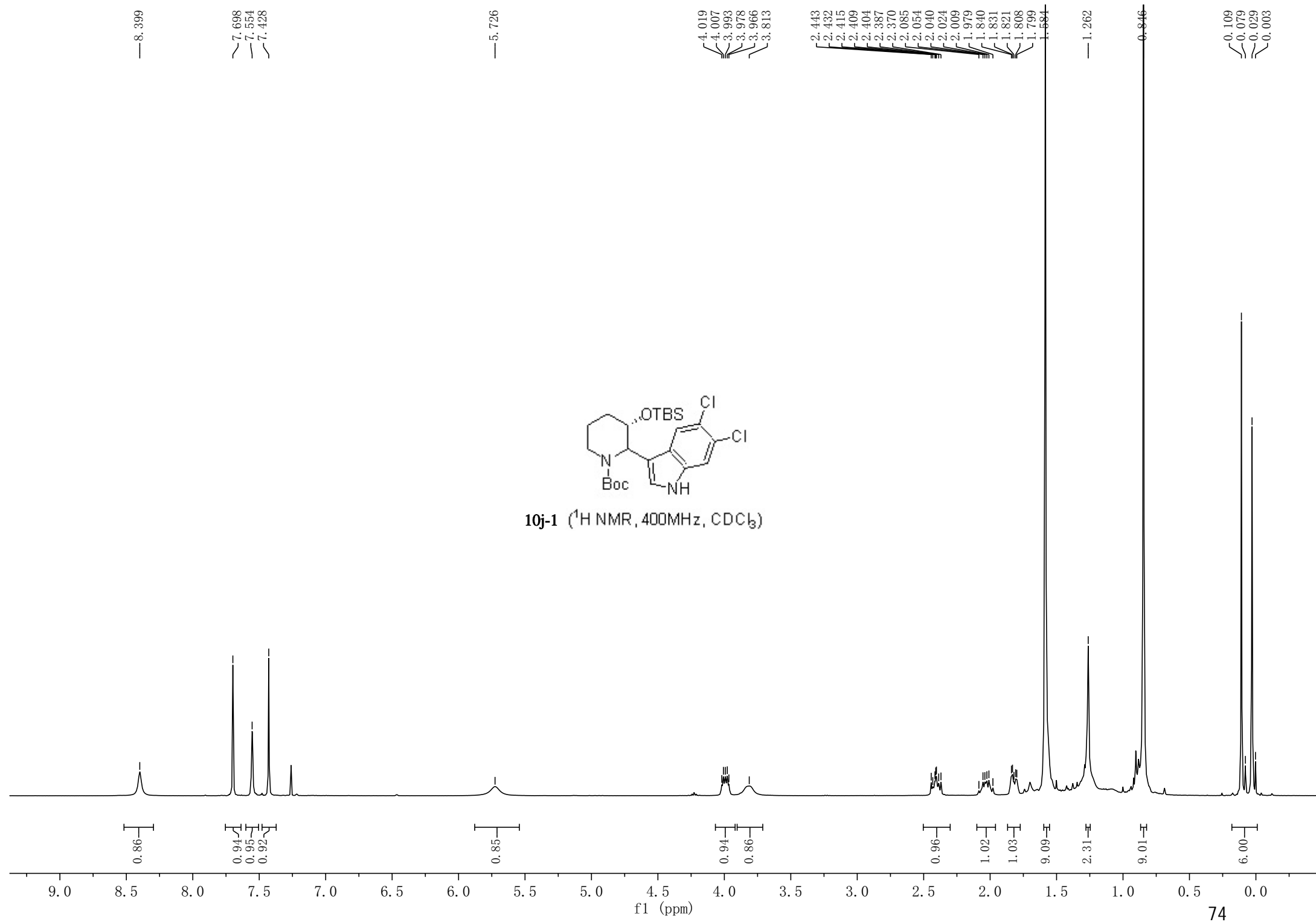
— 18.102

— -4.832



10i-2 (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)





— 154.618

— 134.630

— 127.404

— 126.260

— 125.624

— 123.582

— 120.946

— 112.268

— 110.978

— 80.242

— 71.147

— 29.707

— 29.442

— 29.369

— 28.623

— 25.782

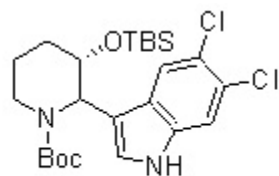
— 24.702

— 22.697

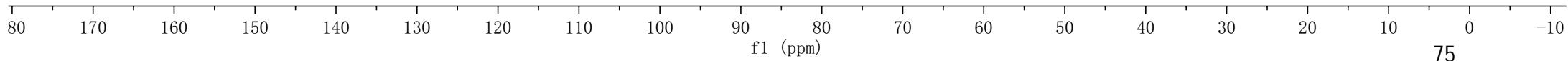
— 18.008

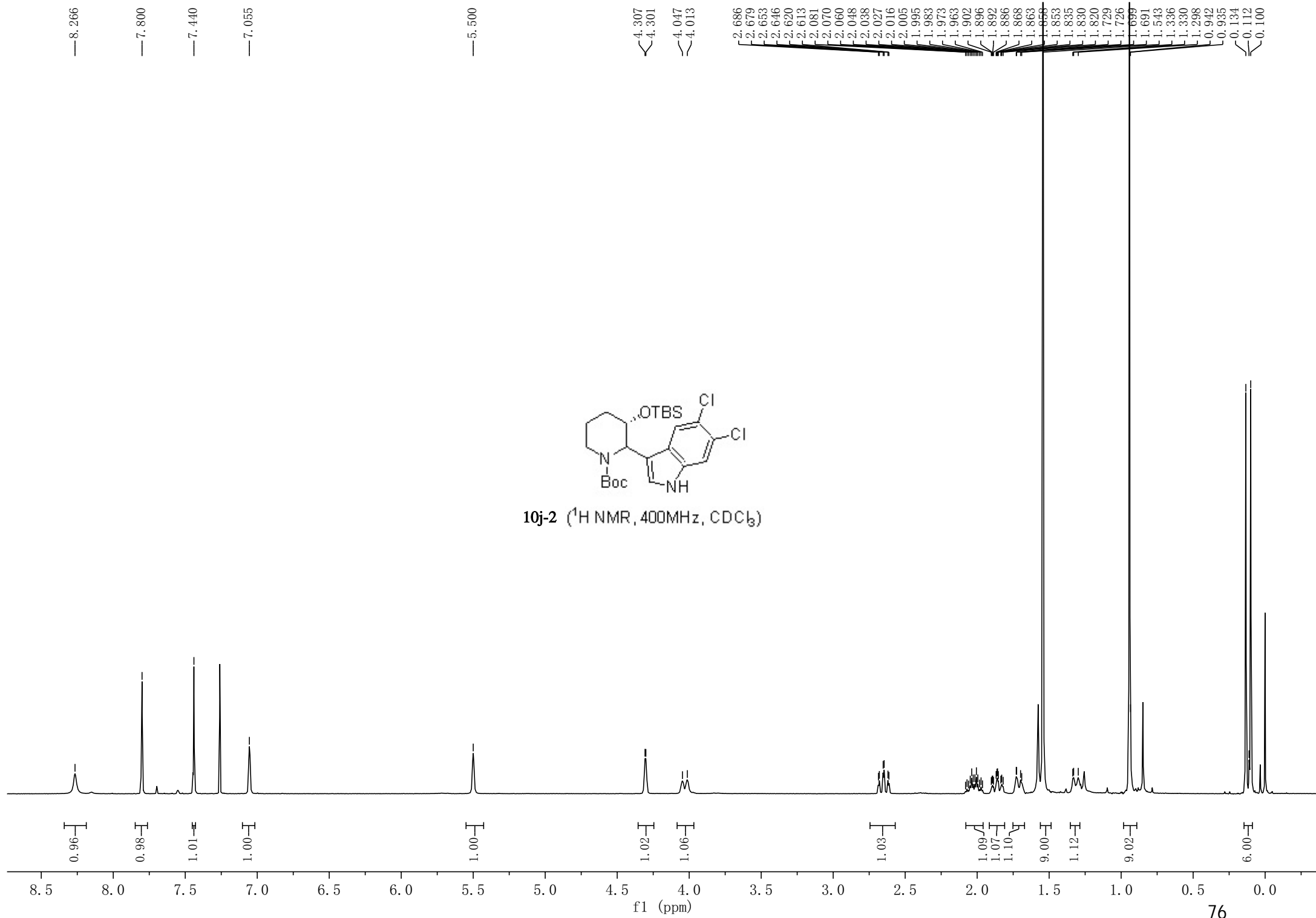
— 4.893

— 4.918



10j-1 (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)





— 155.528

— 135.039

126.697

126.482

124.115

123.747

121.327

114.342

112.548

— 79.935

— 67.276

— 55.023

— 39.603

28.757

28.712

28.448

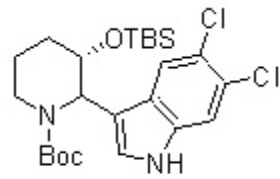
25.953

19.675

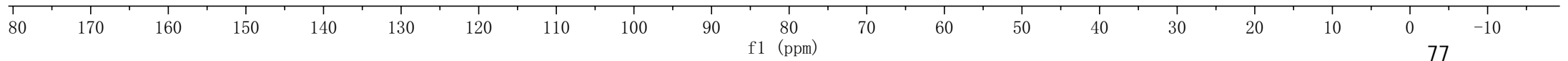
18.236

— 4.681

— 4.710



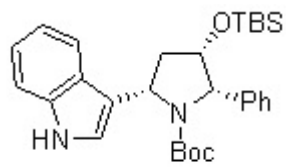
10j-2 (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



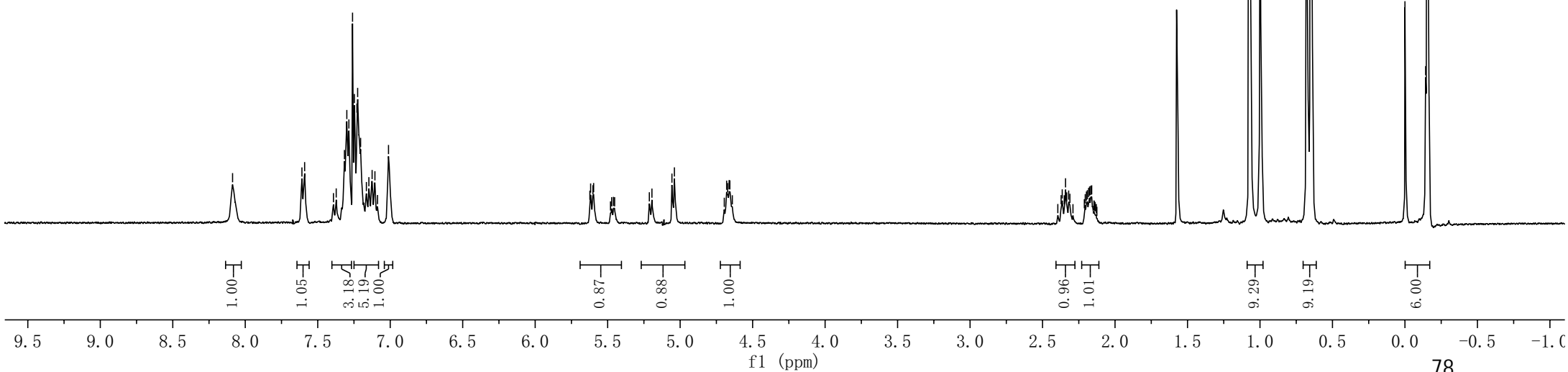
8.087  
7.609  
7.590  
7.392  
7.372  
7.316  
7.299  
7.285  
7.260  
7.247  
7.230  
7.225  
7.204  
7.164  
7.147  
7.125  
7.105  
7.087  
7.012  
5.623  
5.617  
5.602  
5.597  
5.480  
5.472  
5.460  
5.452  
5.212  
5.195  
5.057  
5.040  
4.695  
4.679  
4.672  
4.662  
4.657  
4.640

2.395  
2.372  
2.364  
2.350  
2.341  
2.333  
2.320  
2.311  
2.290  
2.212  
2.205  
2.197  
2.191  
2.182  
2.175  
2.168  
2.161  
2.145  
2.144  
2.140  
2.138  
2.129  
2.125  
1.074  
1.000

0.679  
0.651  
-0.000  
-0.143  
-0.153



12a (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



154.496  
154.384

140.468  
138.970  
137.146  
136.566

128.525  
127.902  
127.780  
127.702  
127.554  
126.920  
126.760  
126.638  
126.329  
125.703  
125.384  
122.042  
121.931  
121.675  
121.590  
120.994  
120.508  
120.413  
119.486  
119.294  
119.147  
119.016  
118.841  
118.716  
118.683  
118.594  
118.539  
111.562  
111.381  
111.233  
79.727  
79.549  
79.339

72.031  
71.472

66.110  
65.004

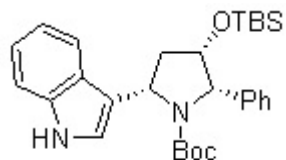
53.440  
53.316

40.350  
39.538

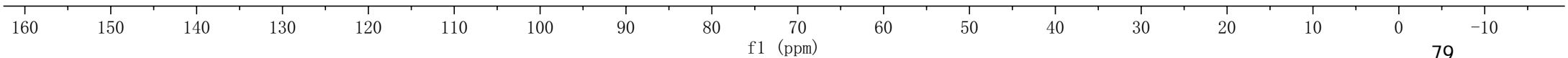
29.830  
28.278  
28.149  
25.744  
25.671  
25.446

18.025  
17.931  
17.807

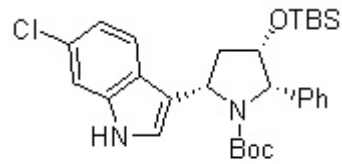
-4.680  
-4.794  
-4.951  
-5.149



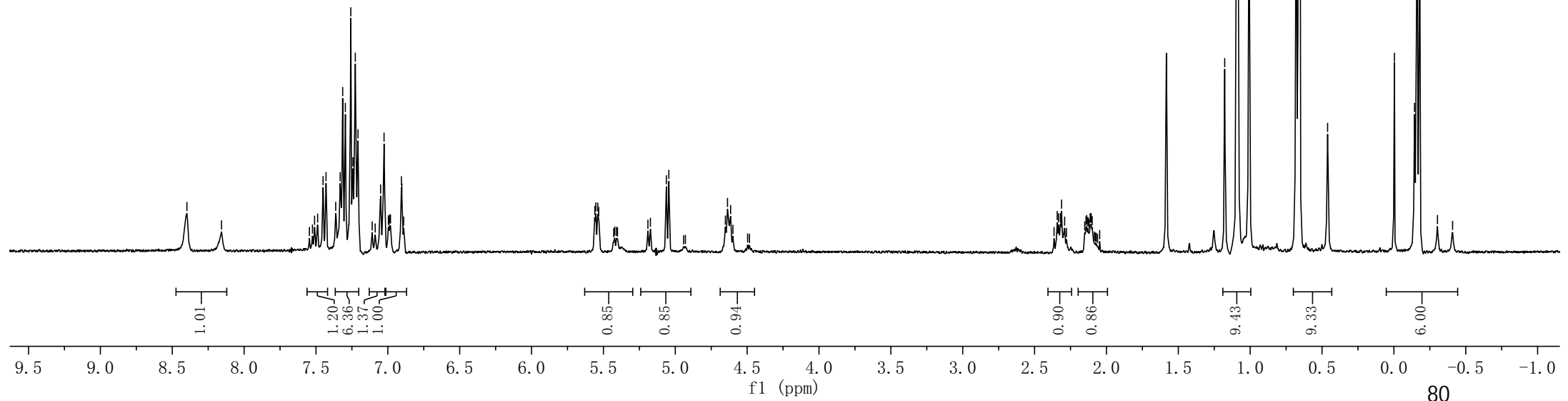
12a (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



8.398  
8.157  
7.545  
7.524  
7.510  
7.488  
7.451  
7.430  
7.363  
7.332  
7.314  
7.296  
7.258  
7.243  
7.226  
7.208  
7.109  
7.088  
7.050  
7.026  
6.996  
6.993  
6.986  
6.981  
6.905  
6.902  
6.890  
5.560  
5.553  
5.539  
5.533  
5.533  
5.428  
5.421  
5.409  
5.402  
5.190  
5.173  
5.173  
5.062  
5.045  
5.045  
4.942  
4.930  
4.651  
4.637  
4.615  
4.599  
4.497  
4.484  
2.365  
2.343  
2.334  
2.320  
2.312  
2.291  
2.279  
2.151  
2.142  
2.138  
2.129  
2.128  
2.120  
2.113  
2.112  
2.108  
2.107  
2.099  
2.084  
2.076  
2.071  
2.062  
2.047  
2.047  
1.177  
1.089  
1.008  
0.680  
0.660  
0.461  
-0.004  
-0.143  
-0.163  
-0.180  
-0.303  
-0.408



12b ( $^1\text{H}$  NMR, 400MHz,  $\text{CDCl}_3$ )





156.169  
154.853  
154.797  
154.353

140.162  
139.824  
138.724  
137.475  
136.870  
128.432  
127.893  
127.815  
127.623  
127.558  
127.382  
126.998  
126.886  
126.717  
124.605  
124.252  
123.368  
122.409  
122.195  
122.127  
121.251  
120.415  
120.151  
119.723  
119.530  
119.452  
118.935  
118.873  
117.752  
111.505  
111.164

79.953  
79.926  
79.493  
72.014  
71.963  
71.425  
66.466  
66.370  
65.023

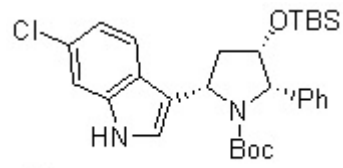
54.613  
53.579  
53.519  
53.269

40.908  
40.457  
40.124  
39.991

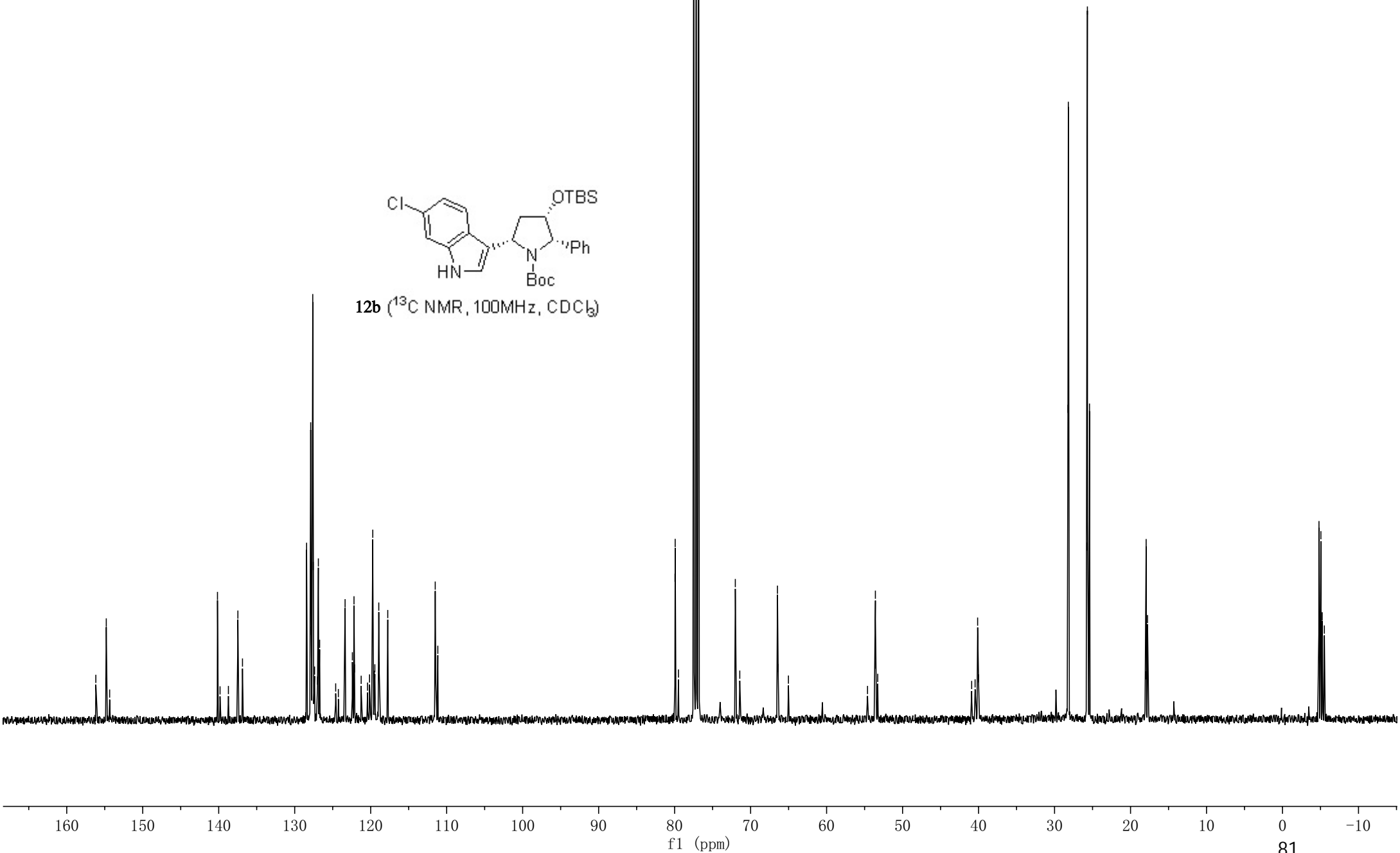
28.238  
28.188  
25.729  
25.679  
25.401

18.013  
17.945  
17.764

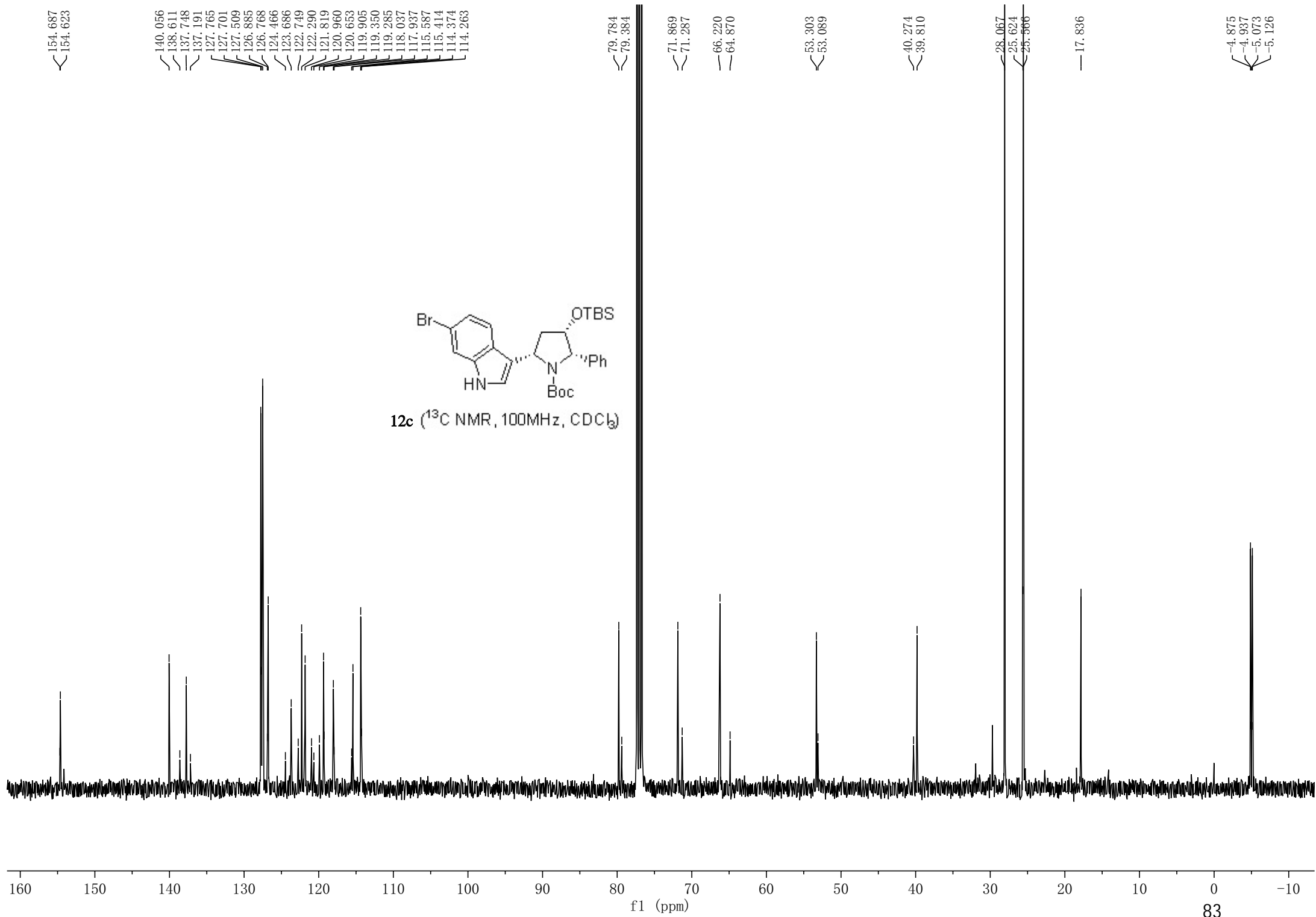
-4.800  
-5.050  
-5.223  
-5.506

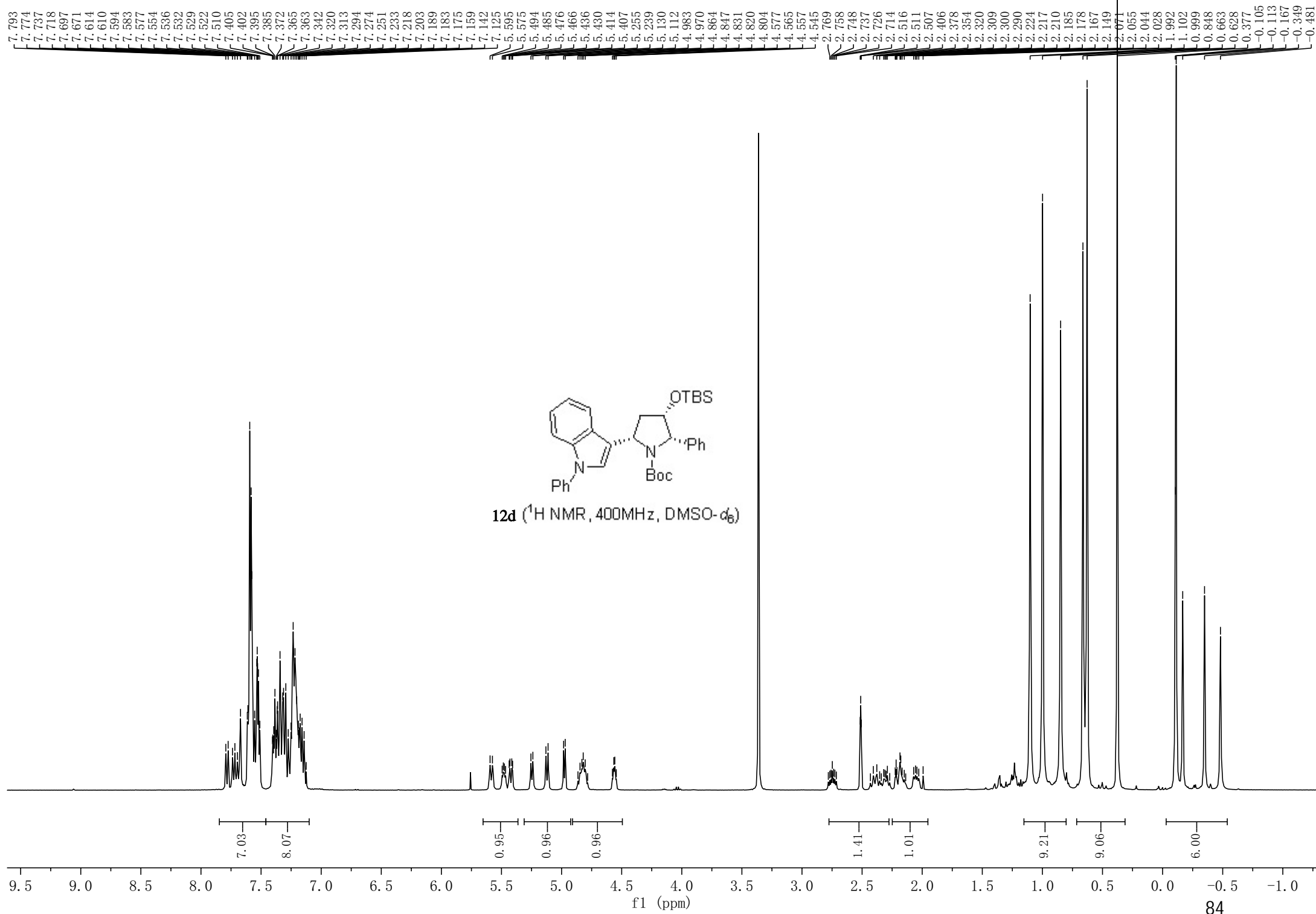


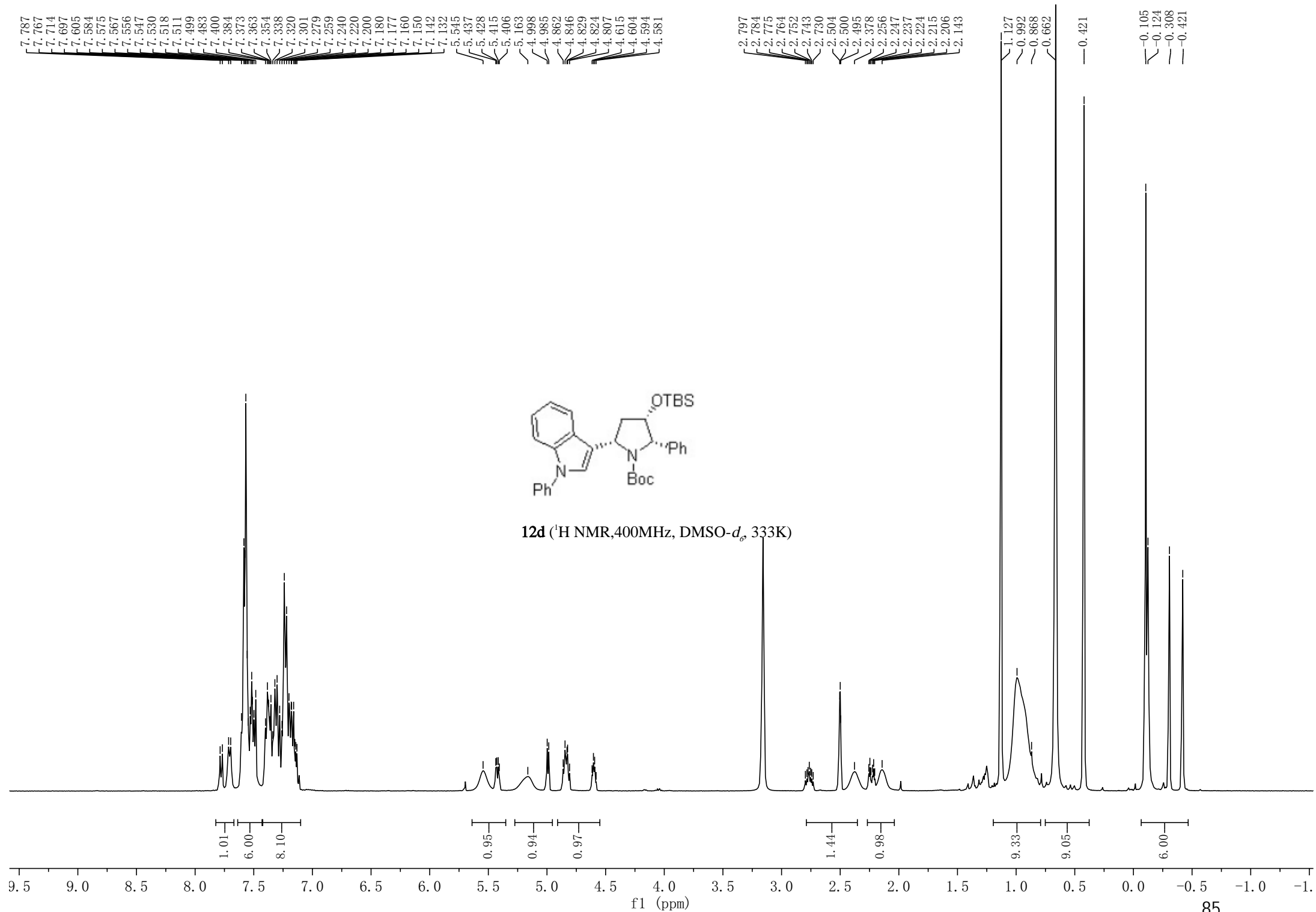
12b (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)







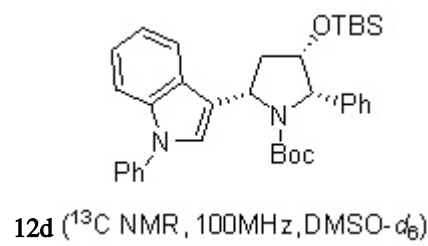
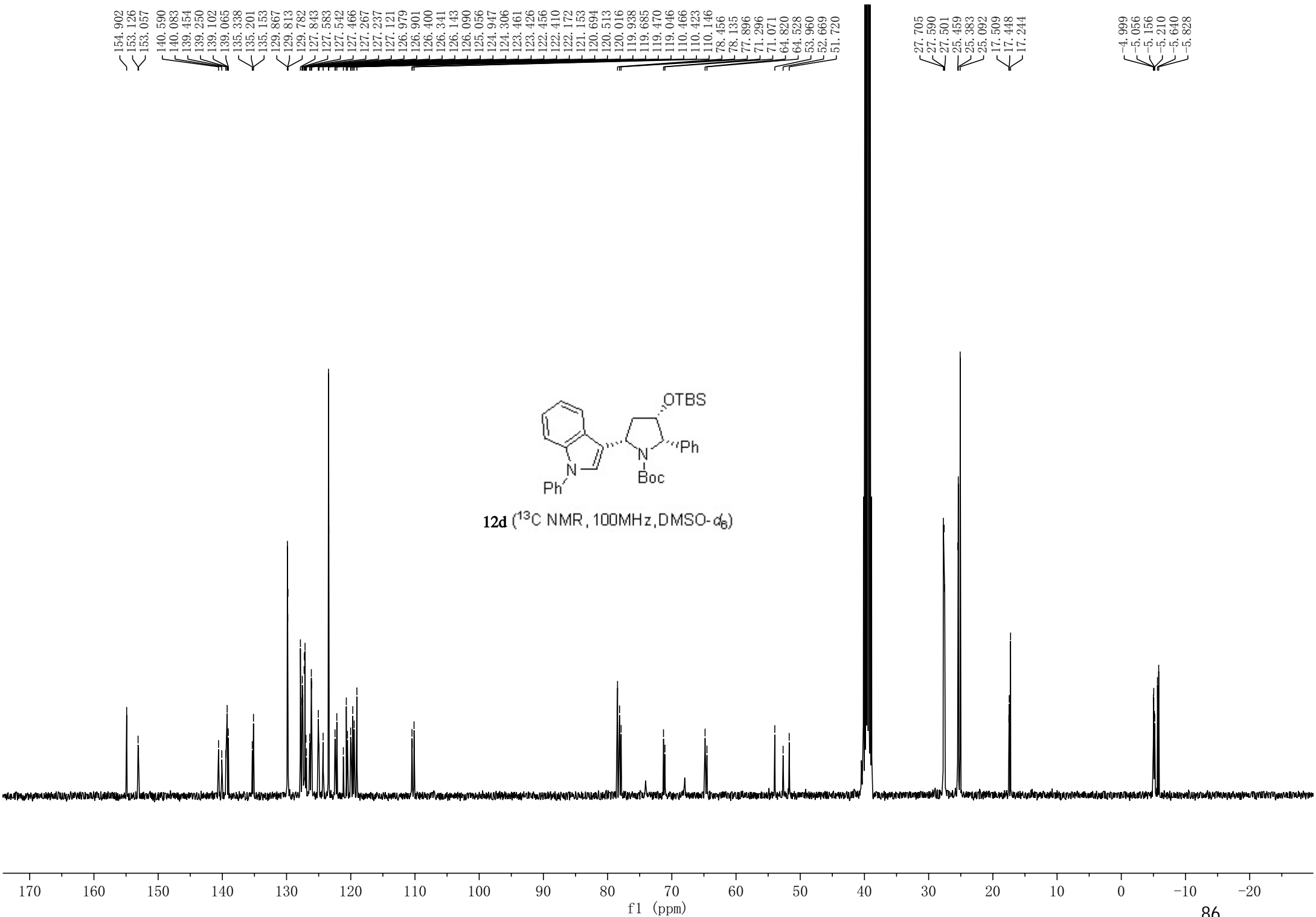


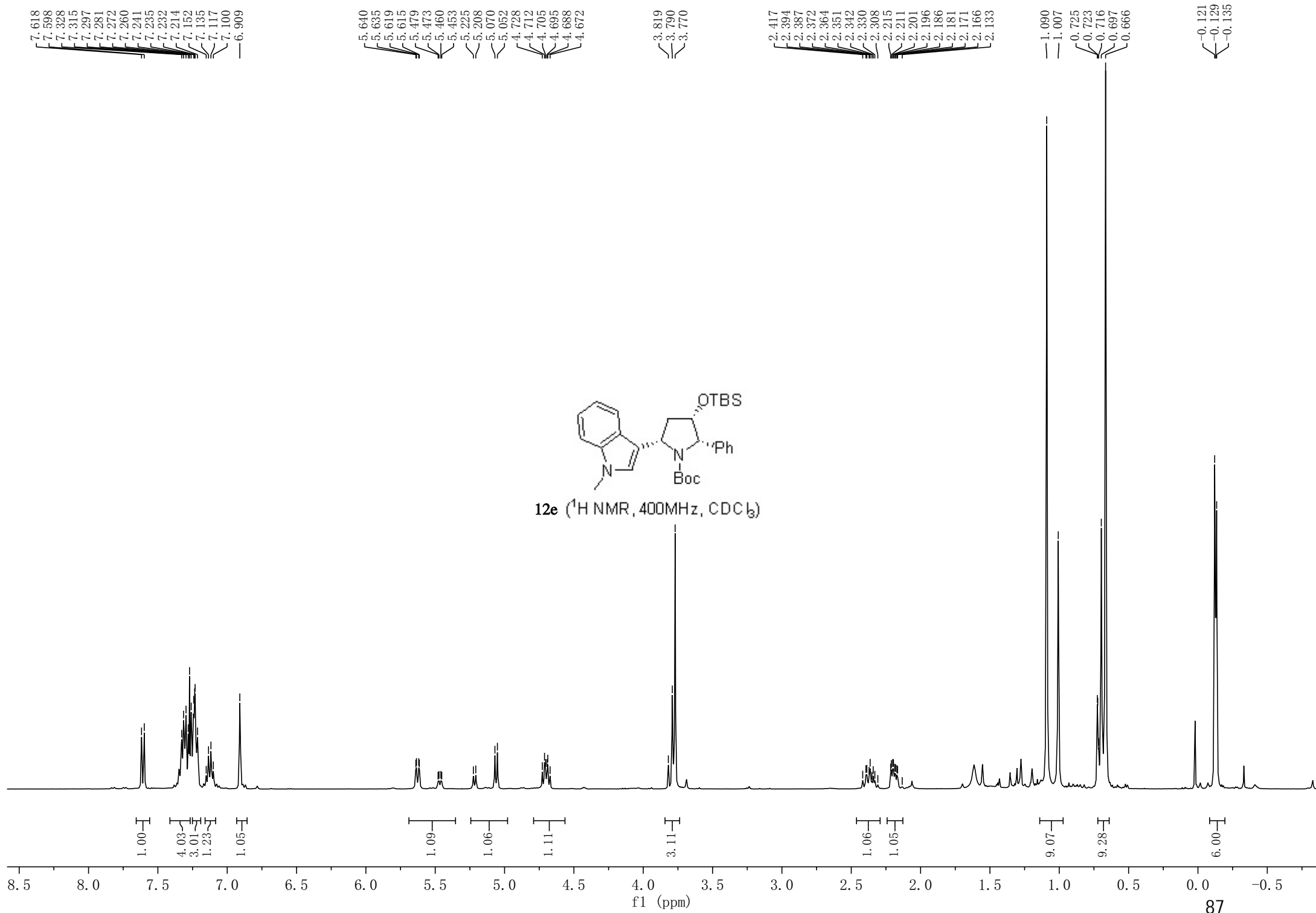


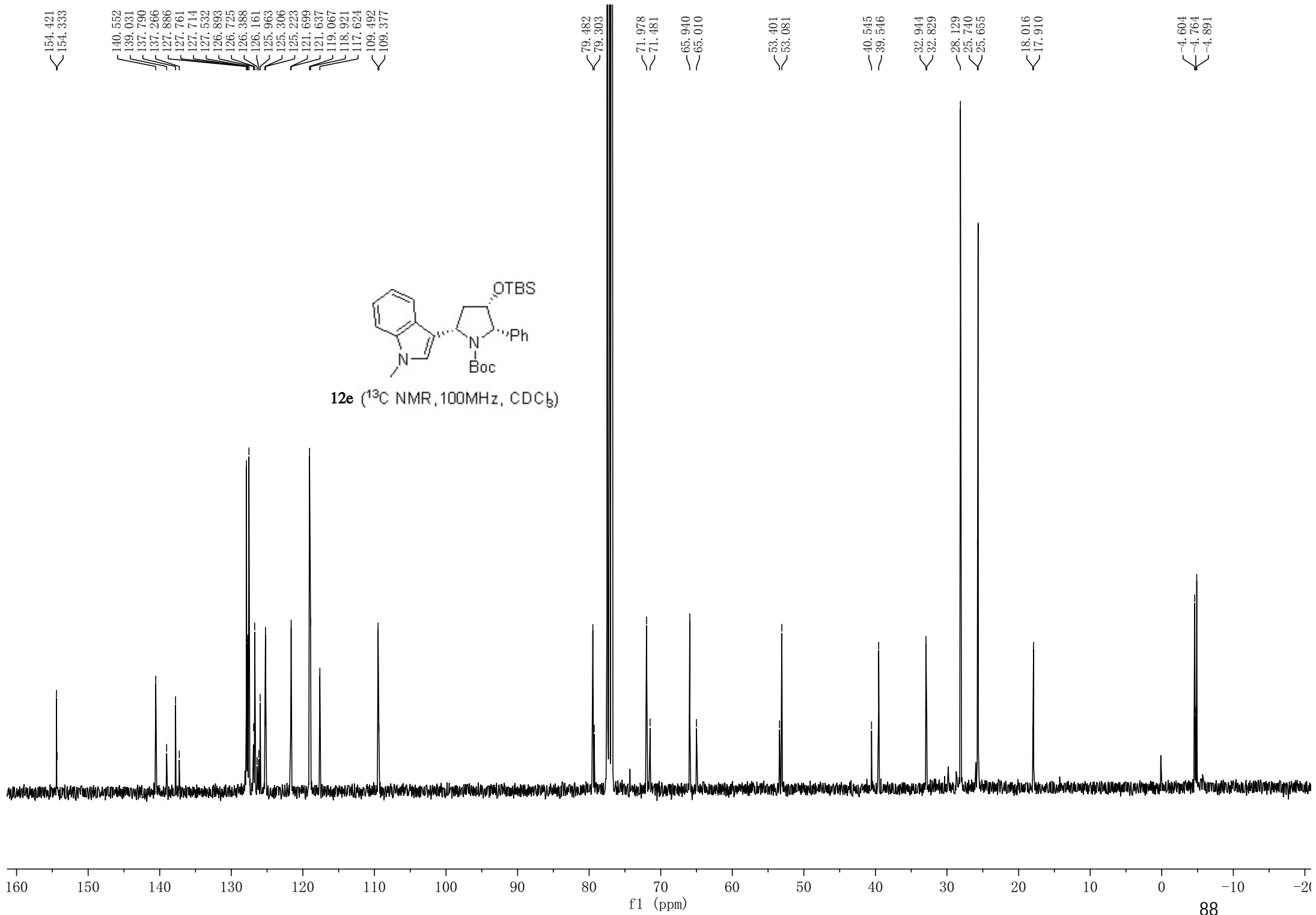
154.902  
153.126  
153.057  
140.590  
140.083  
139.454  
139.250  
139.102  
139.065  
135.338  
135.201  
135.153  
129.867  
129.813  
129.782  
127.843  
127.583  
127.542  
127.466  
127.267  
127.237  
127.121  
126.979  
126.901  
126.400  
126.341  
126.143  
126.090  
125.056  
124.947  
124.306  
123.461  
123.426  
122.456  
122.410  
122.172  
121.153  
120.694  
120.513  
120.016  
119.938  
119.685  
119.470  
119.046  
110.466  
110.423  
110.146  
78.456  
78.135  
77.896  
71.296  
71.071  
64.820  
64.528  
53.960  
52.669  
51.720

27.705  
27.590  
27.501  
25.459  
25.383  
25.092  
17.509  
17.448  
17.244

-4.999  
-5.056  
-5.156  
-5.210  
-5.640  
-5.828

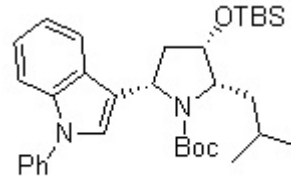




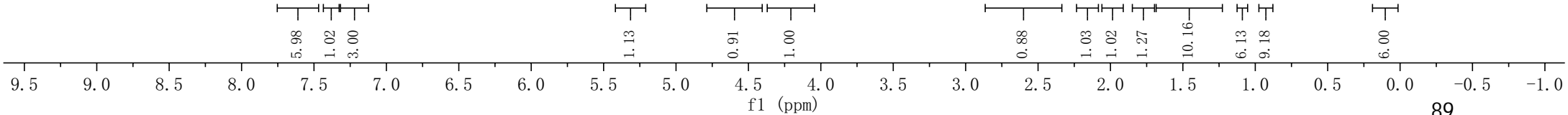




7.705  
7.686  
7.664  
7.645  
7.603  
7.581  
7.558  
7.539  
7.534  
7.517  
7.394  
7.378  
7.366  
7.361  
7.288  
7.278  
7.260  
7.242  
7.226  
7.225  
7.207  
7.189  
7.171  
5.313  
4.695  
4.496  
4.479  
4.473  
4.462  
4.456  
4.439  
4.302  
4.286  
4.275  
4.210  
4.193  
4.175  
4.157  
2.800  
2.782  
2.768  
2.753  
2.735  
2.450  
2.428  
2.420  
2.398  
2.374  
2.177  
2.155  
2.125  
2.101  
2.033  
2.017  
2.001  
1.984  
1.967  
1.951  
1.935  
1.803  
1.781  
1.768  
1.761  
1.747  
1.734  
1.727  
1.714  
1.665  
1.552  
1.495  
1.474  
1.457  
1.447  
1.419  
1.396  
1.376  
1.359  
1.336  
1.318  
1.300  
1.099  
0.855  
1.068  
1.055  
0.966  
0.955  
0.942  
0.935  
0.900  
0.149  
0.094  
0.074



12f (<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>)



155.594  
154.378

140.097  
139.909  
136.527  
136.156  
129.647  
127.303  
127.212  
126.183  
124.266  
123.747  
122.529  
122.375  
120.124  
119.889  
119.479  
119.240  
110.677  
110.634

79.538  
78.805

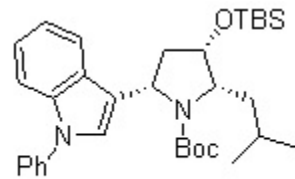
71.652  
70.866

58.852

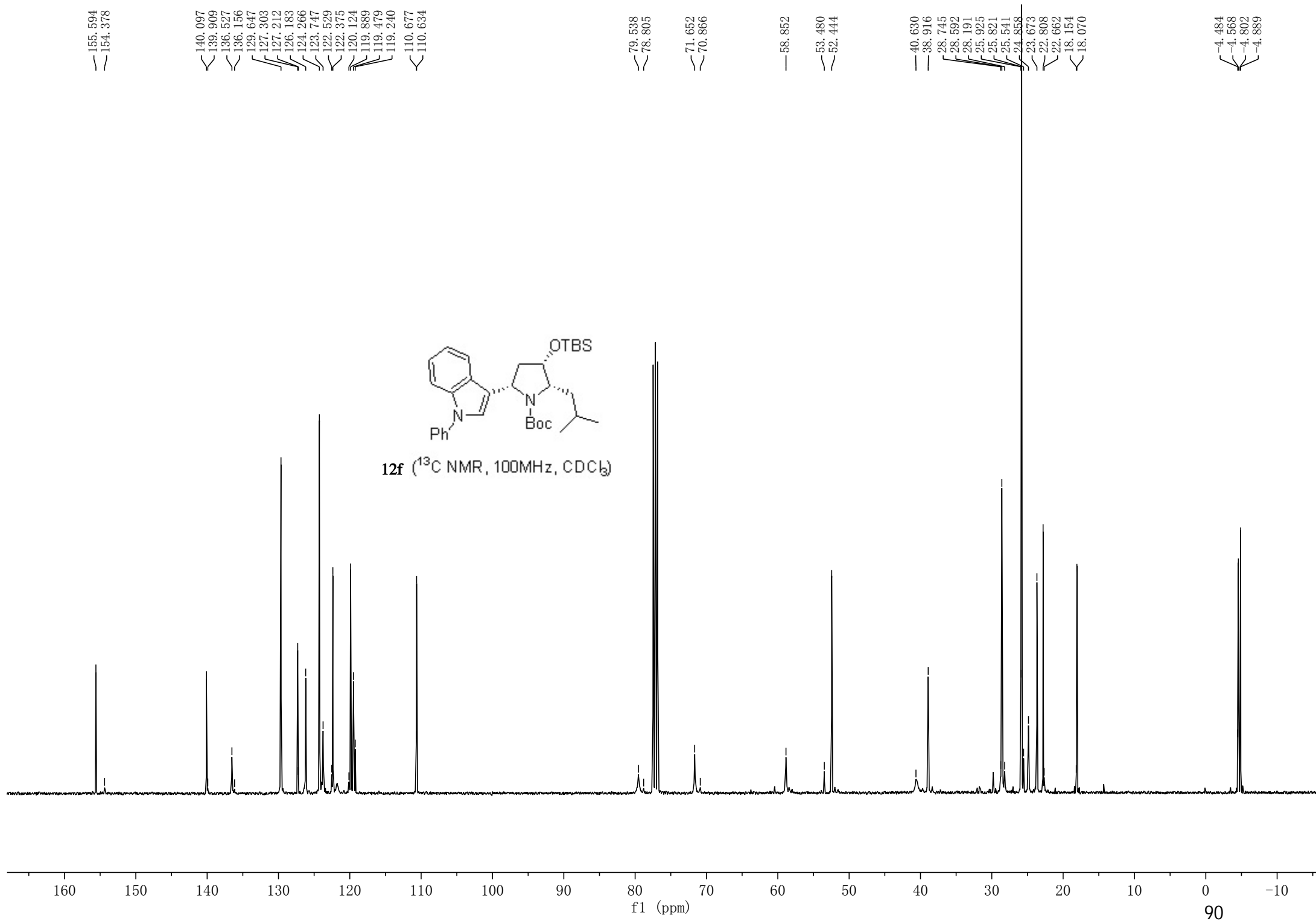
53.480  
52.444

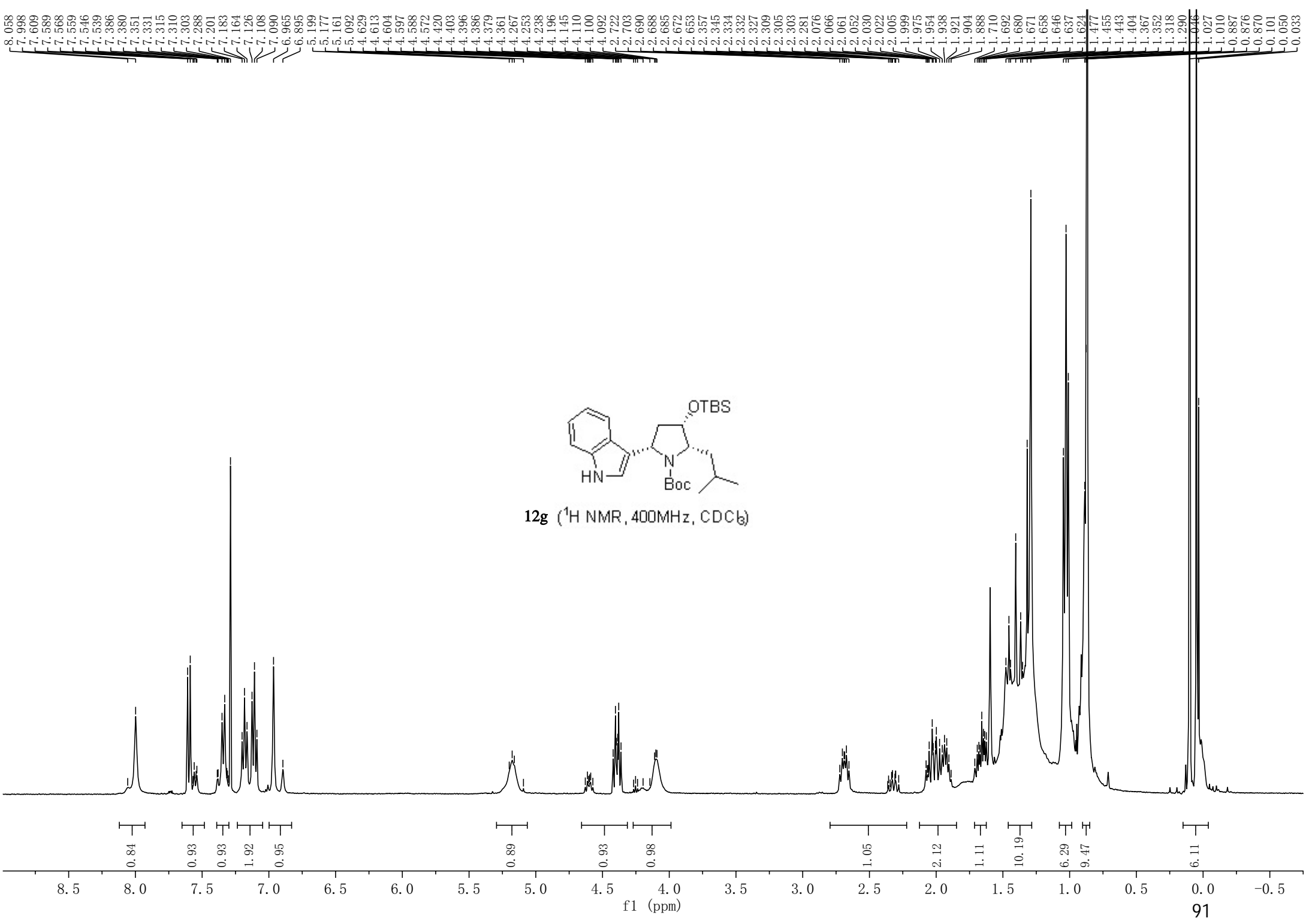
40.630  
38.916  
28.745  
28.592  
28.191  
25.925  
25.821  
25.541  
24.858  
23.673  
22.808  
22.662  
18.154  
18.070

-4.484  
-4.568  
-4.802  
-4.889



12f (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)





— 155.669

— 136.750

— 125.777

— 121.831

— 120.011

— 119.304

— 119.151

— 119.051

— 118.763

— 111.268

— 79.516

— 71.558

— 58.647

— 58.174

— 52.460

— 38.941

— 28.591

— 25.922

— 25.849

— 24.818

— 23.750

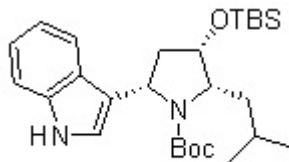
— 22.787

— 18.109

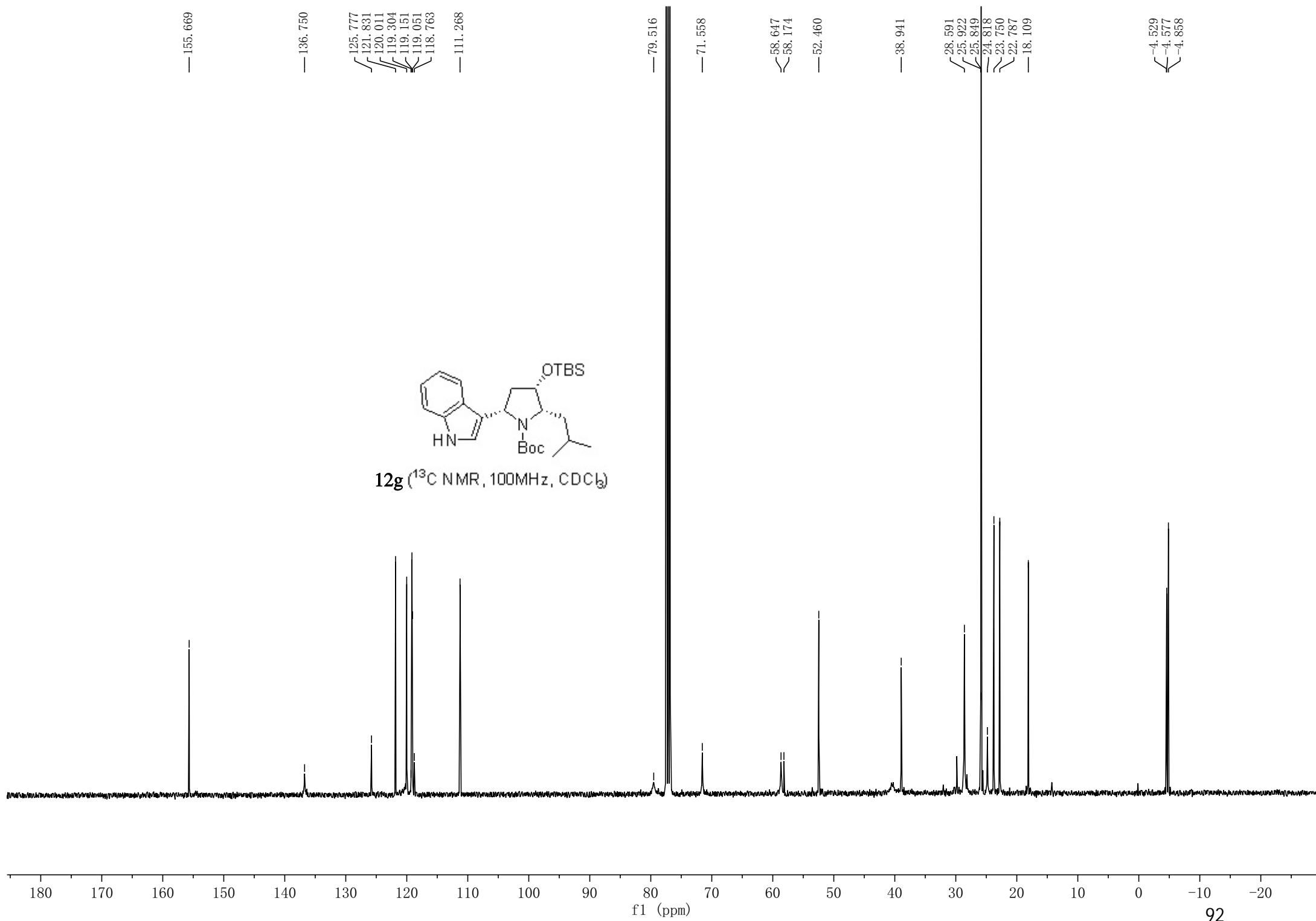
— 4.529

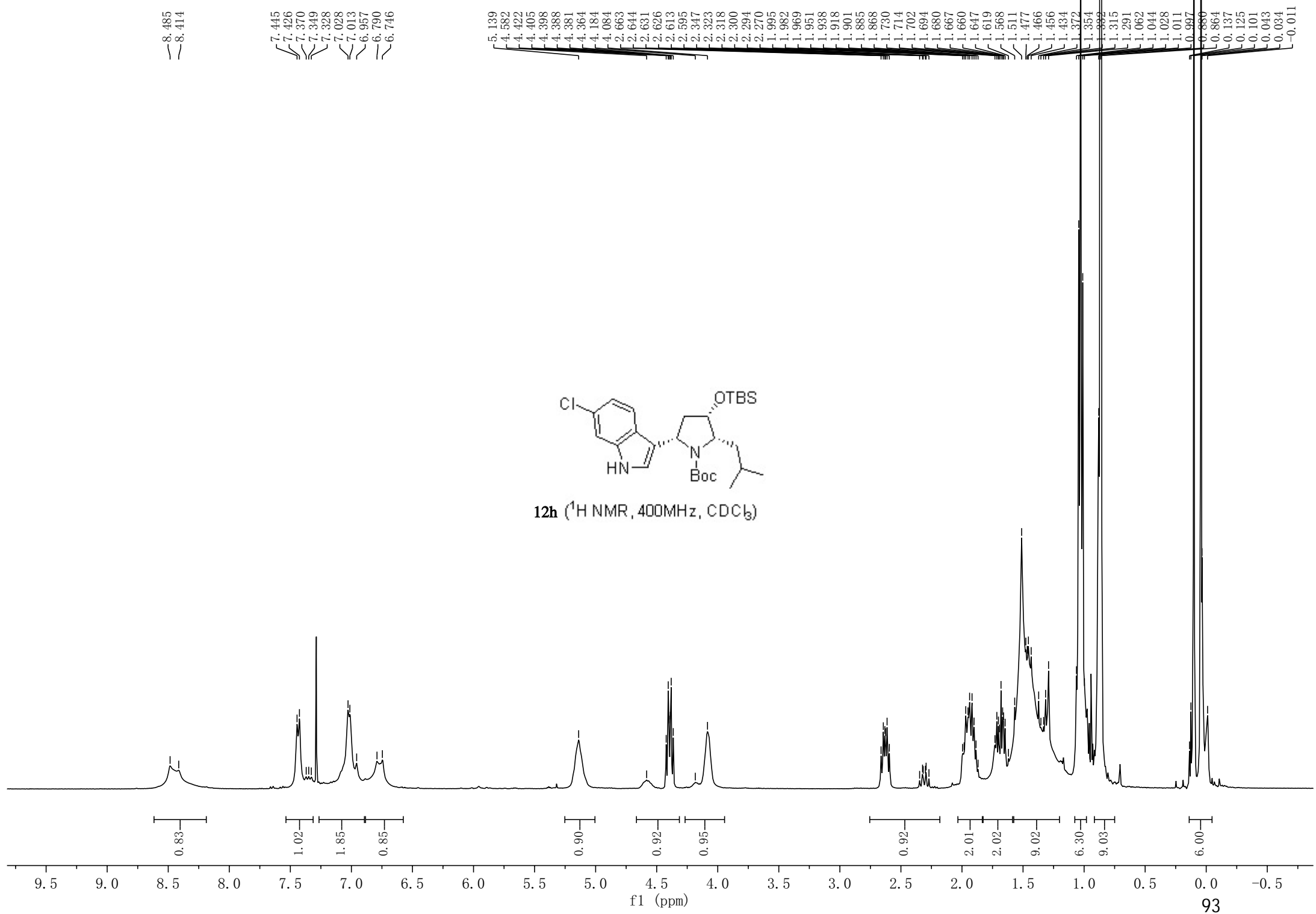
— 4.577

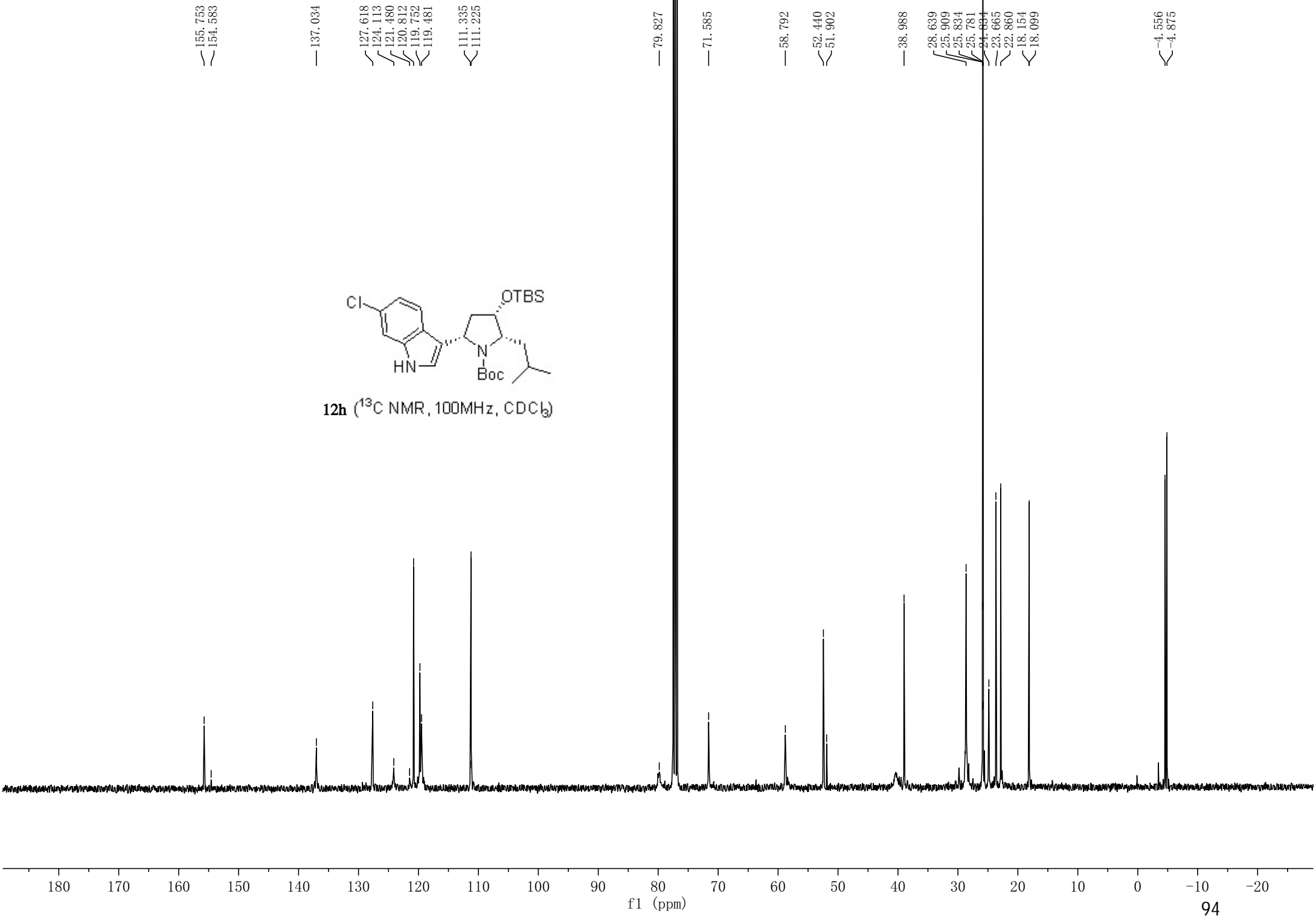
— 4.858

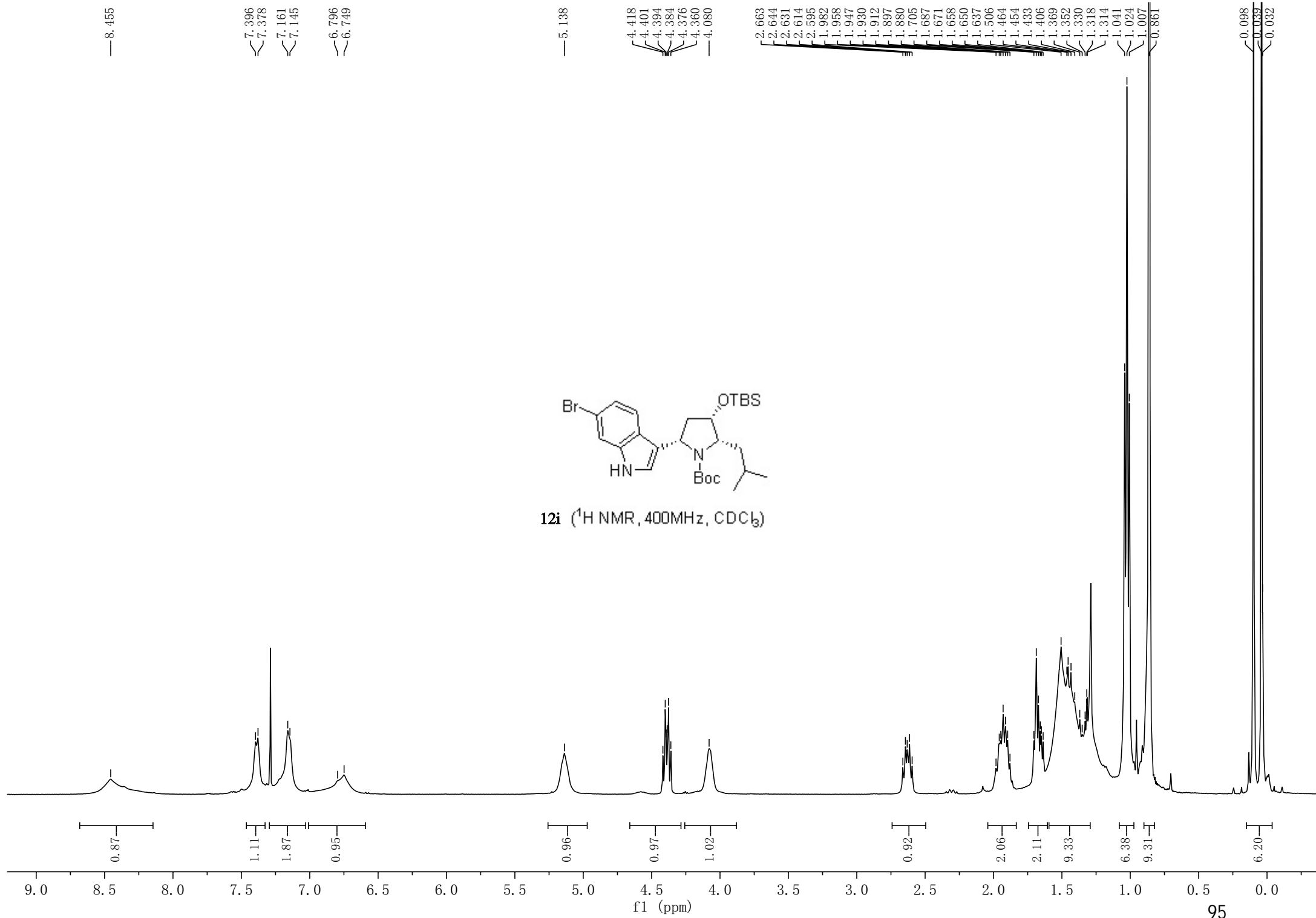


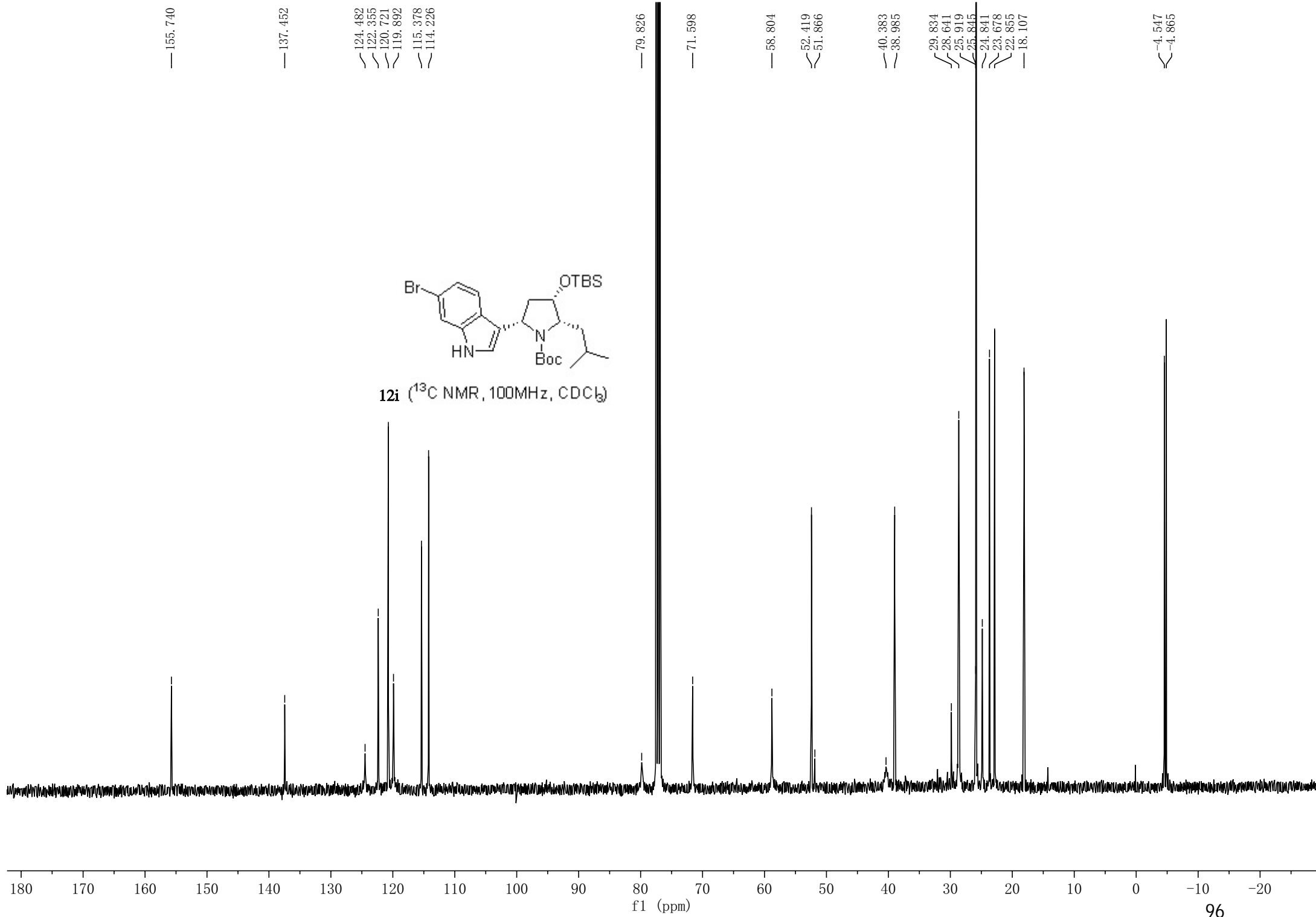
12g (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



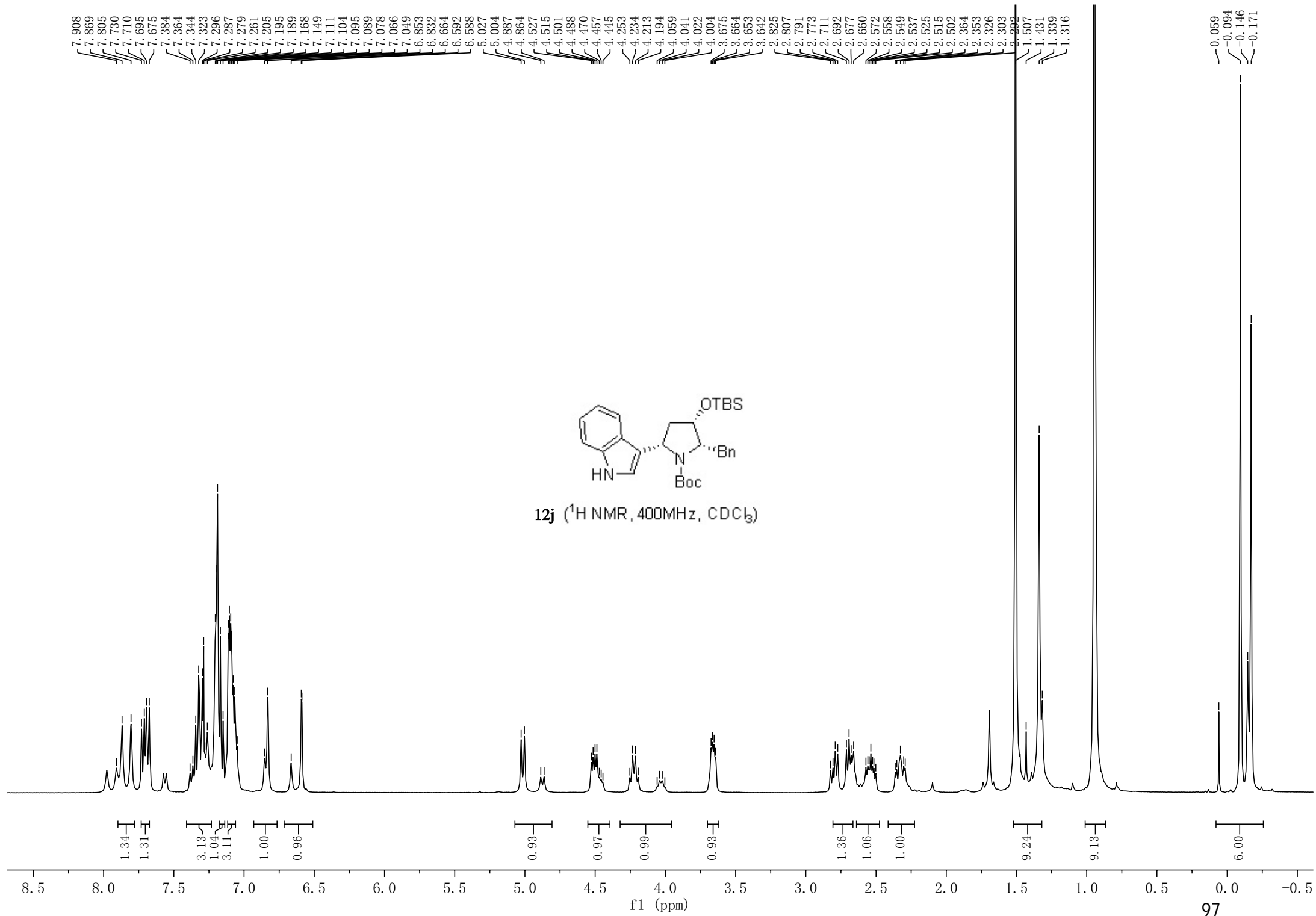












155.951

139.368  
139.003  
136.872  
136.682  
129.423  
128.420  
128.281  
126.959  
126.673  
126.138  
125.986  
122.125  
121.865  
121.674  
121.436  
120.418  
120.099  
119.825  
119.634  
119.248  
119.204  
118.547  
118.097  
111.379  
111.267  
111.078

79.824

79.266

71.802

71.154

55.705

53.960

39.724

39.147

31.049

30.806

28.641

28.319

26.161

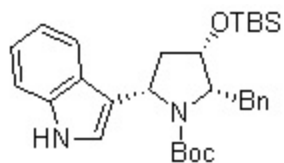
26.075

18.247

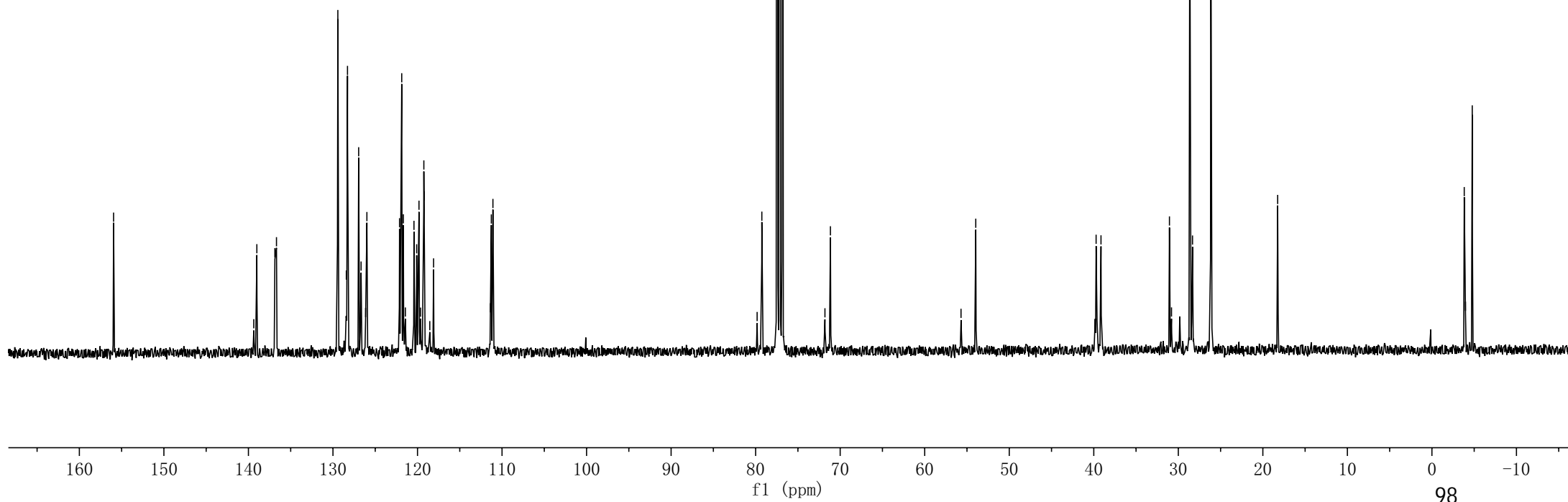
-3.824

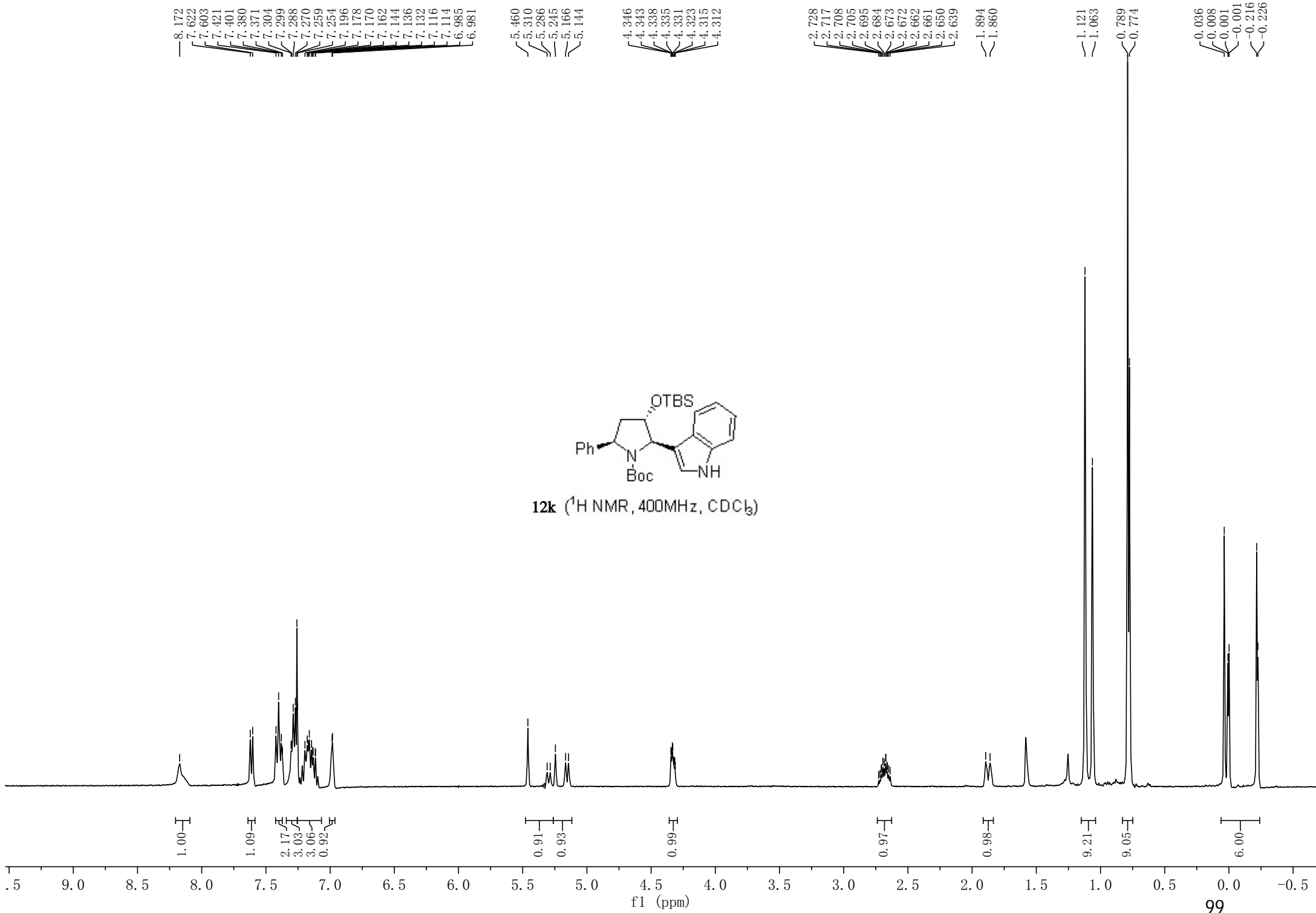
-3.972

-4.769



12j (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)





154.815  
154.349  
145.524  
144.372  
137.103  
136.545  
128.133  
127.802  
126.737  
126.326  
126.242  
125.884  
125.640  
122.220  
122.167  
121.112  
120.816  
119.723  
119.630  
118.856  
118.157  
116.505  
111.567  
111.426

79.550  
79.310  
78.554  
77.944

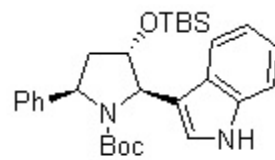
65.959  
65.919  
62.045  
61.158

41.761  
41.293

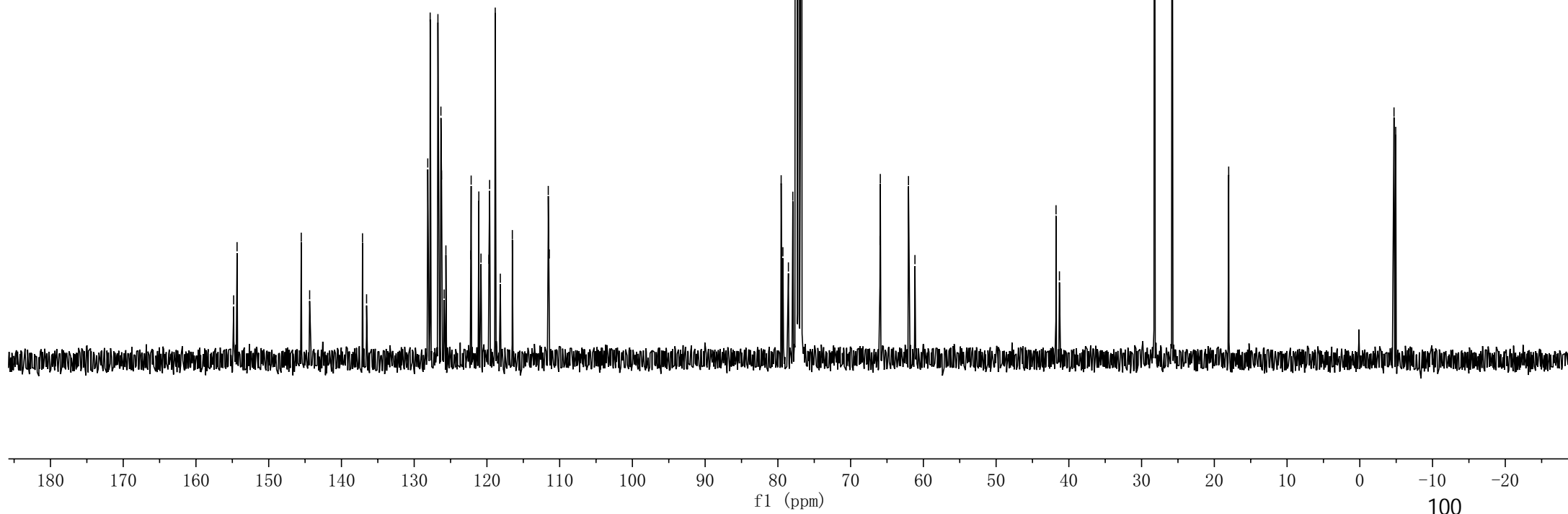
28.229  
25.799

18.026

-4.703  
-4.936



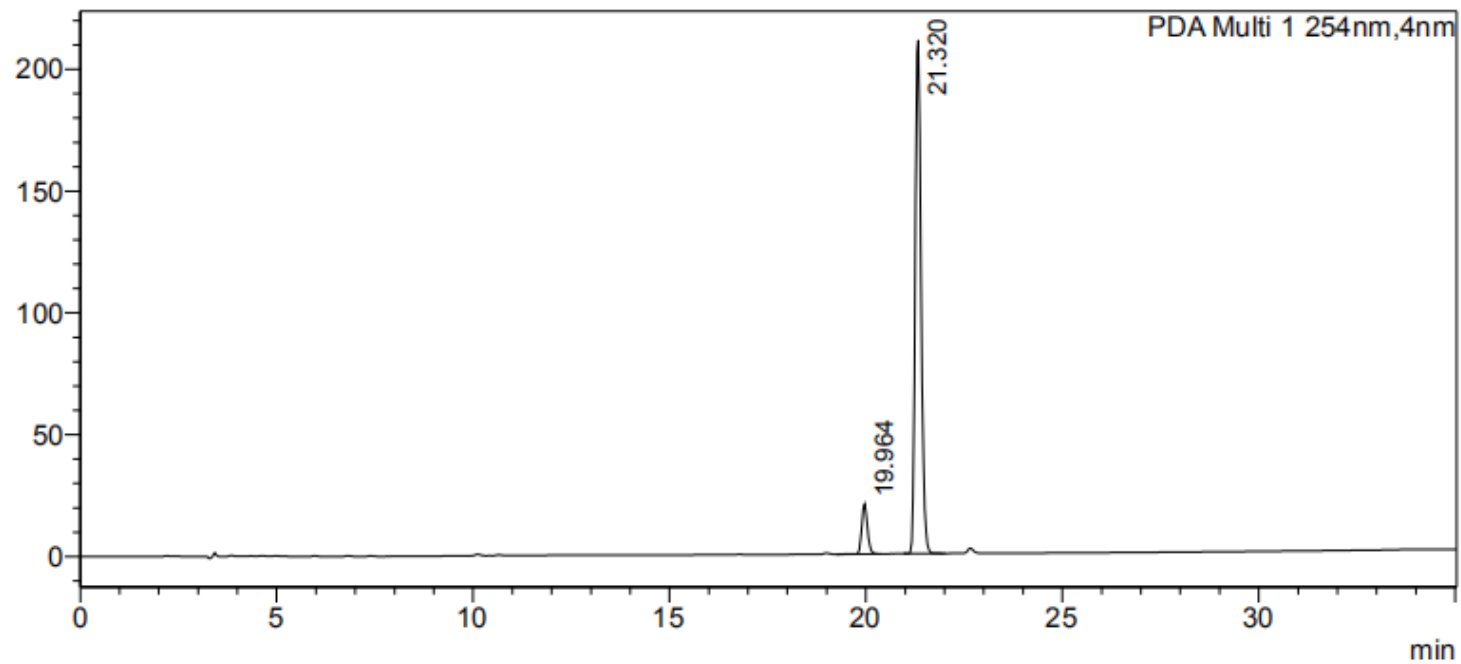
12k (<sup>13</sup>C NMR, 100MHz, CDCl<sub>3</sub>)



HPLC data of **8b**

### <Chromatogram>

mAU



### <Peak Table>

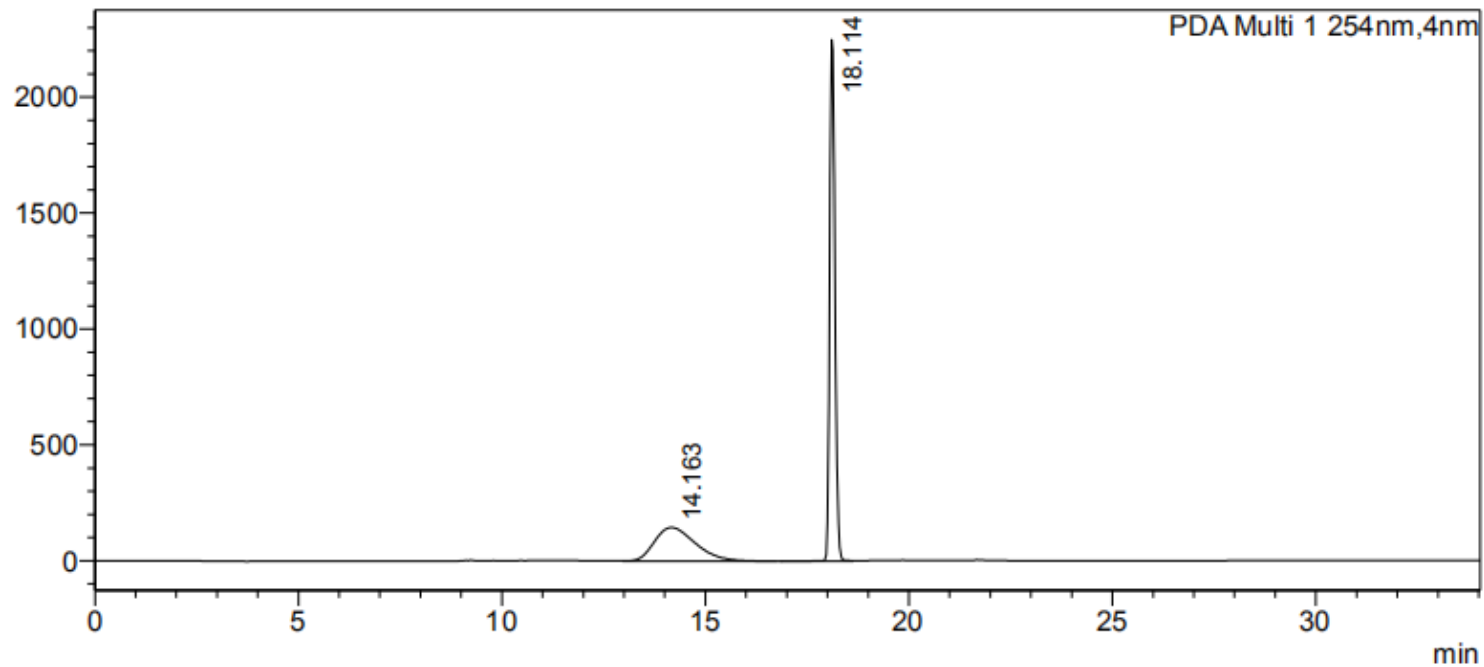
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	19.964	202607	20504	8.474
2	21.320	2188340	210798	91.526
Total		2390947	231302	

HPLC data of 8c

### <Chromatogram>

mAU



### <Peak Table>

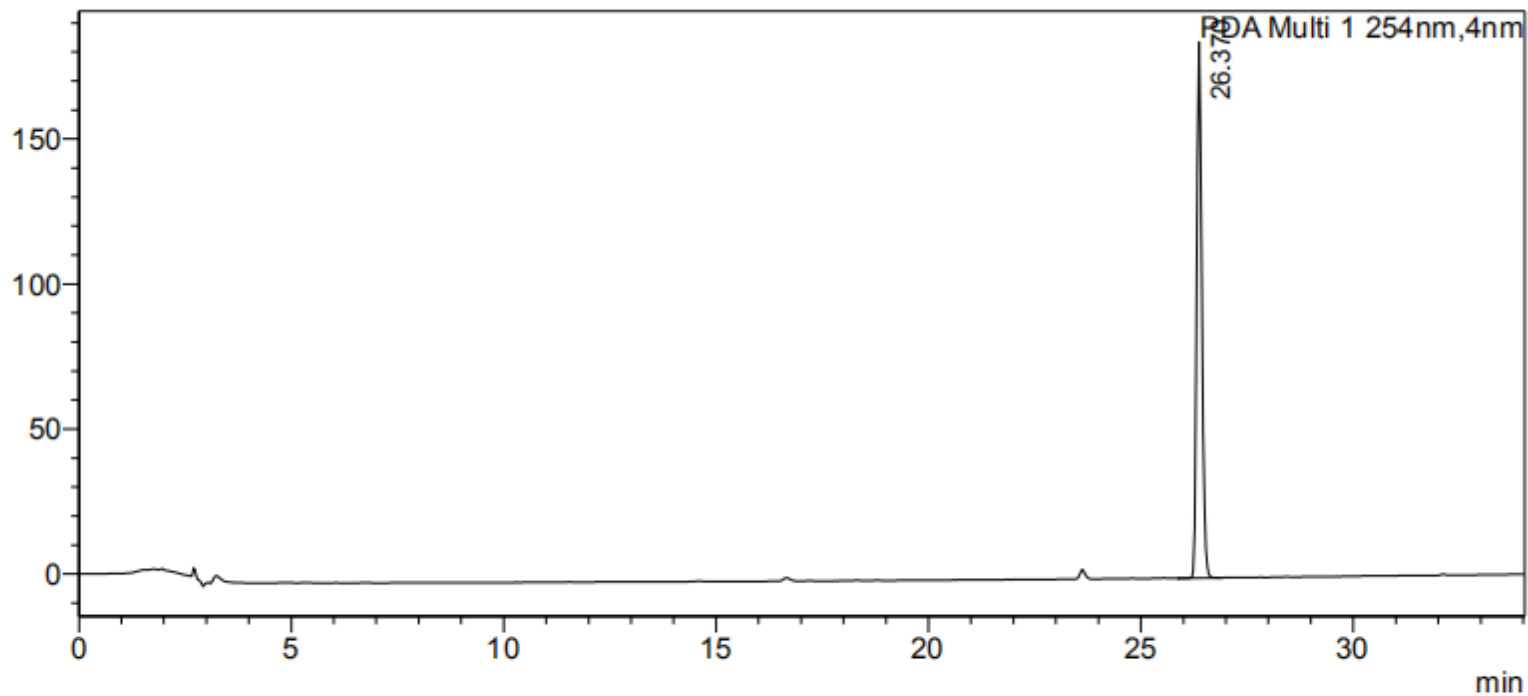
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	14.163	10186719	145836	33.222
2	18.114	20475690	2251122	66.778
Total		30662409	2396958	

HPLC data of 8d

### <Chromatogram>

mAU



### <Peak Table>

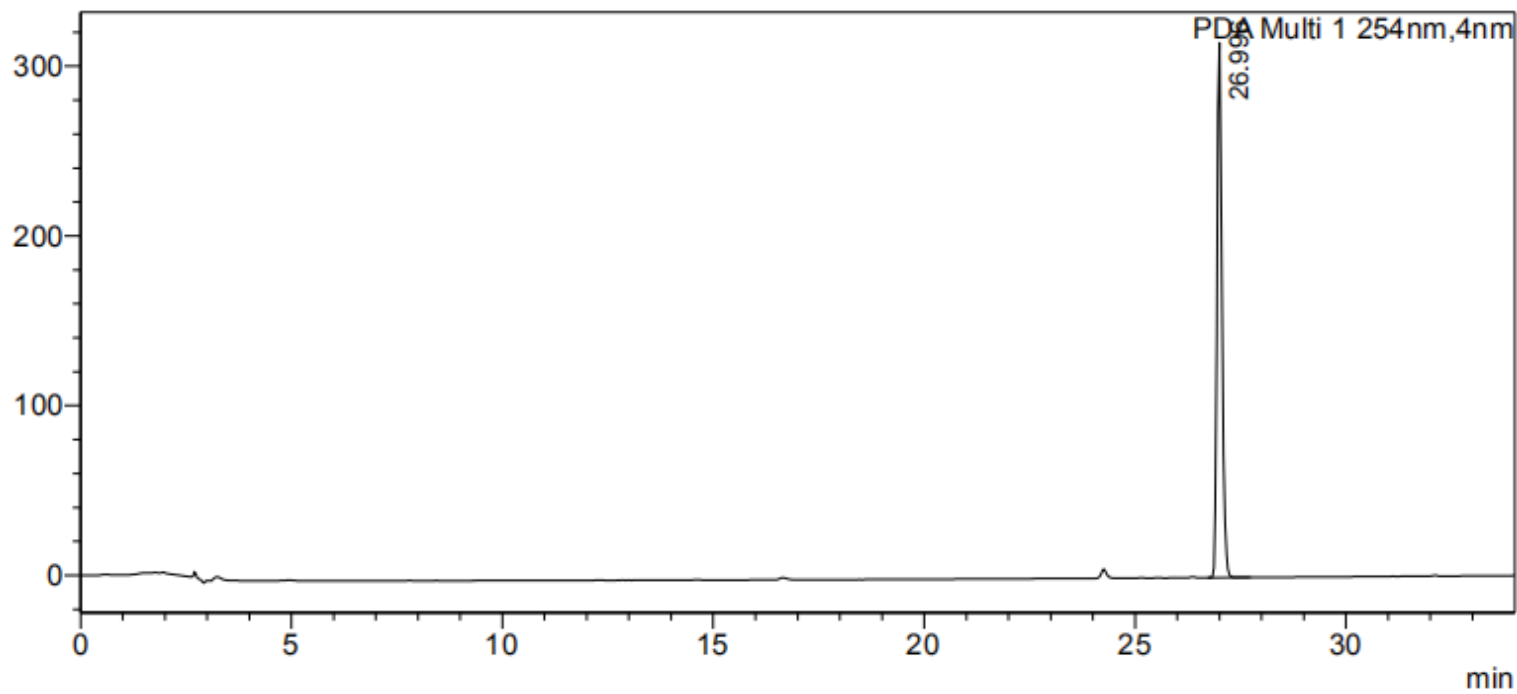
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	26.370	1527804	184947	100.000
Total		1527804	184947	

HPLC data of 8e

### <Chromatogram>

mAU



### <Peak Table>

PDA Ch1 254nm

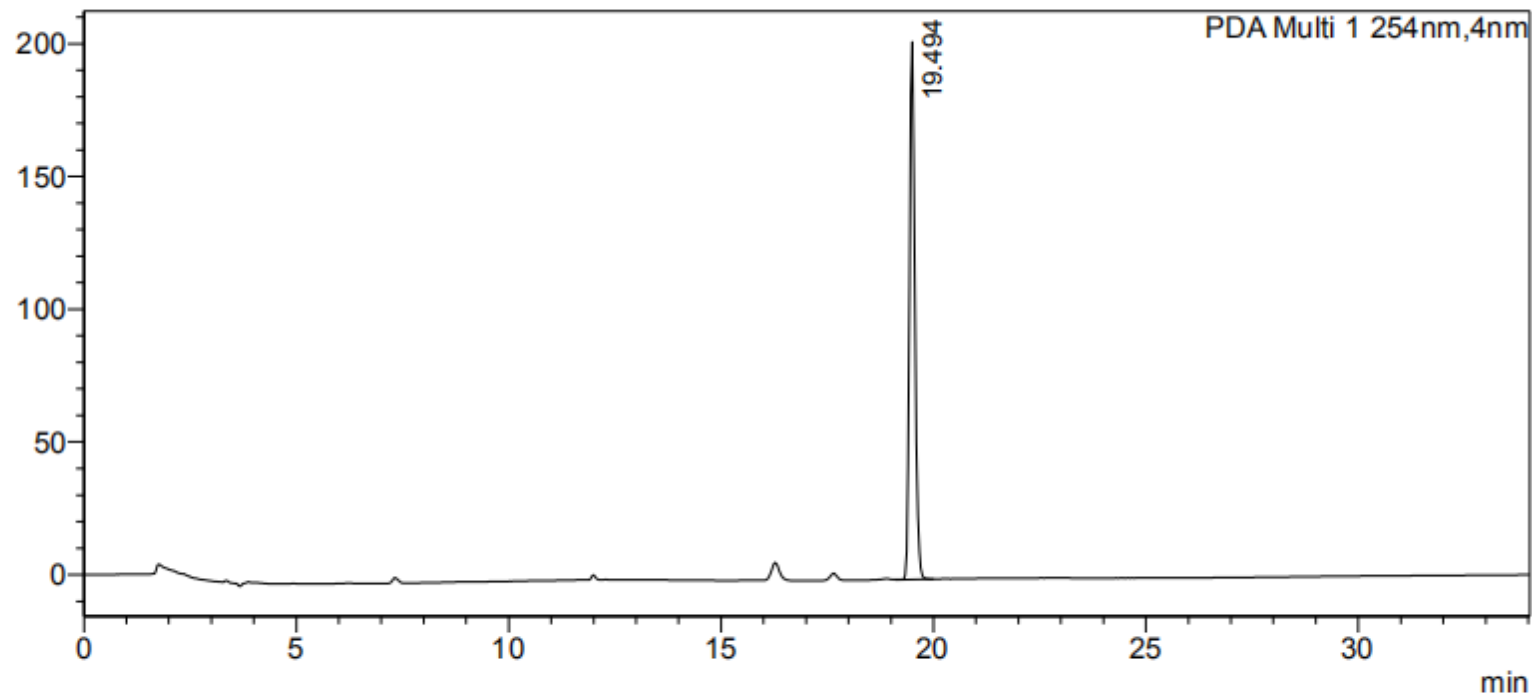
Peak#	Ret. Time	Area	Height	Conc.
1	26.996	2599864	315364	100.000
Total		2599864	315364	



HPLC data of 8f

### <Chromatogram>

mAU



### <Peak Table>

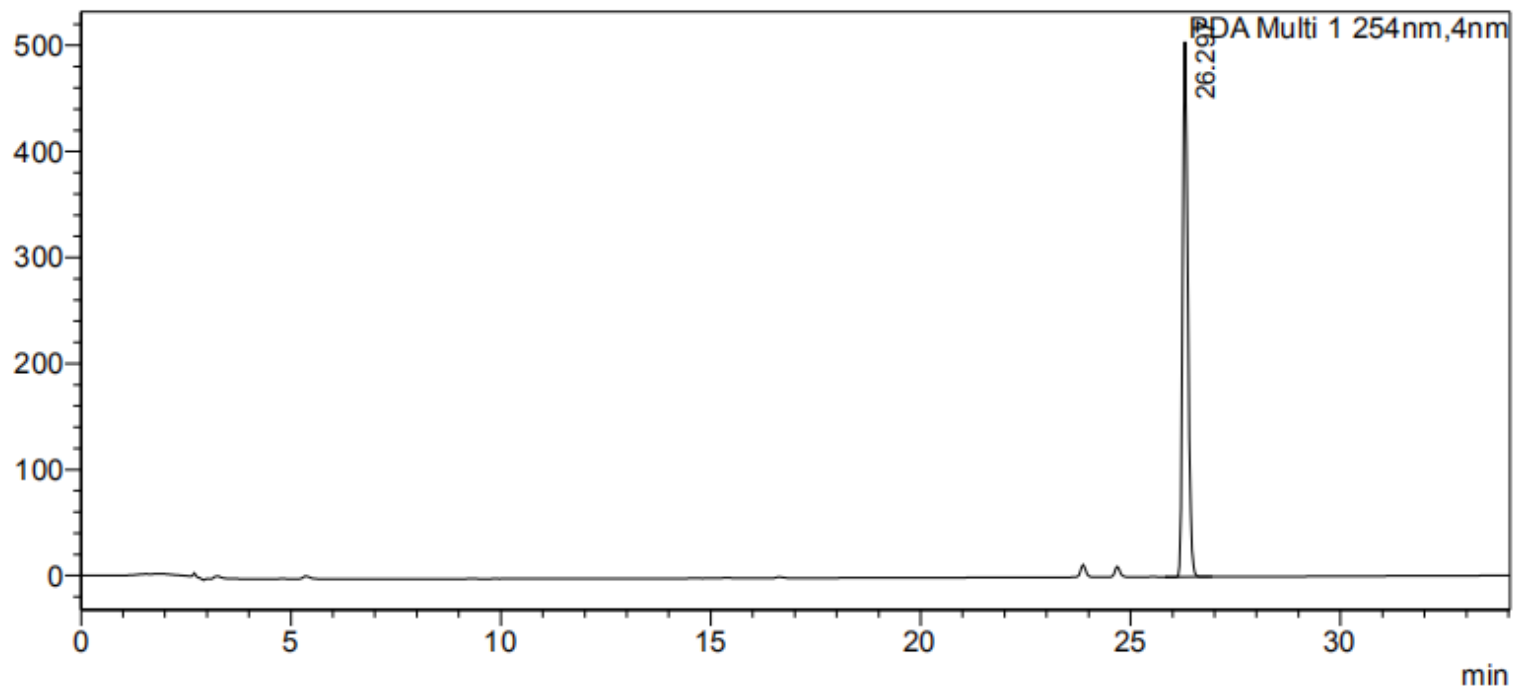
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	19.494	1812528	202585	100.000
Total		1812528	202585	

HPLC data of 8g

### <Chromatogram>

mAU



### <Peak Table>

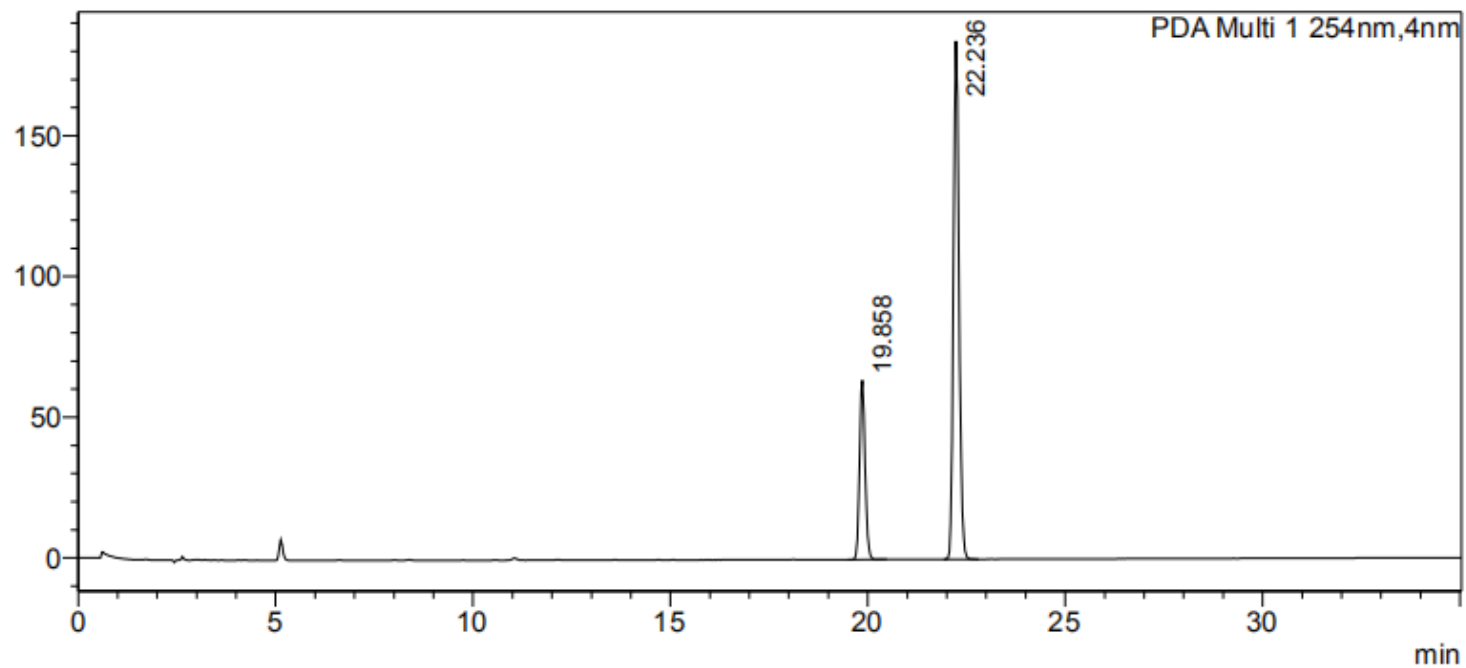
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	26.297	4265935	504599	100.000
Total		4265935	504599	

HPLC data of 8h

### <Chromatogram>

mAU



### <Peak Table>

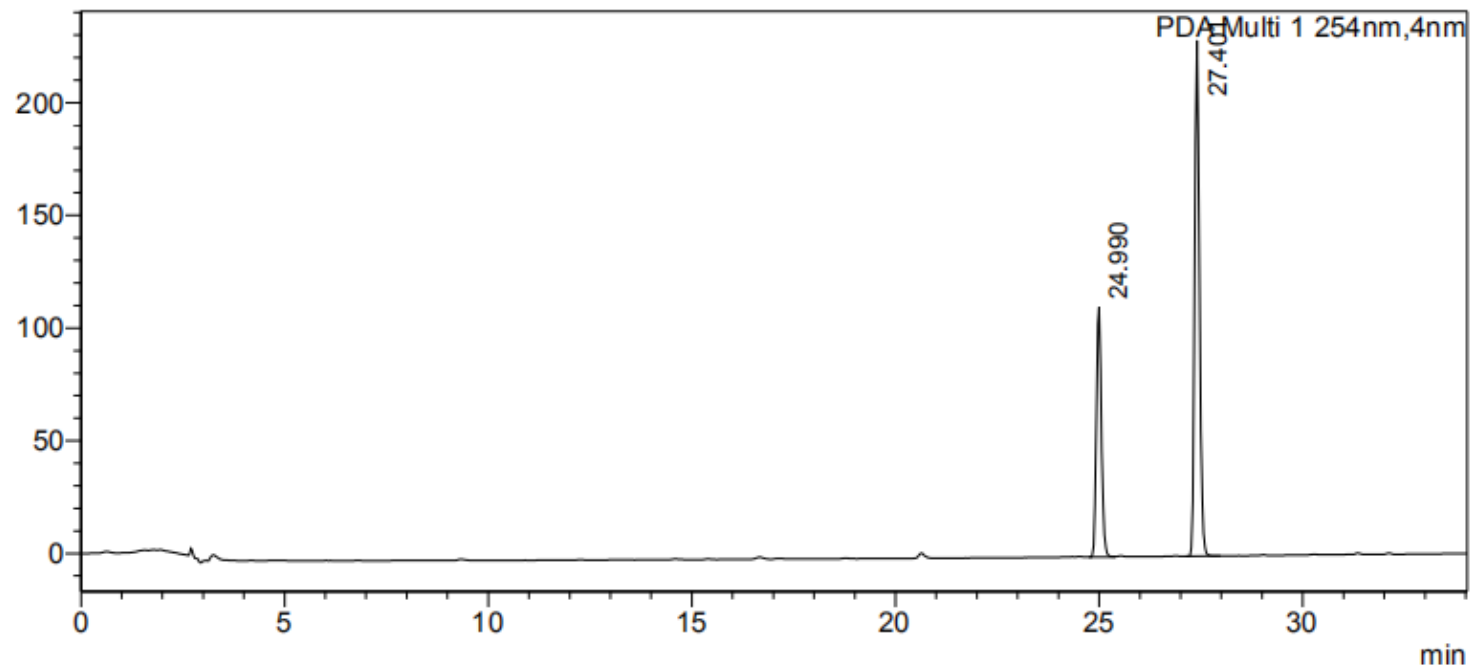
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	19.858	626505	63755	25.512
2	22.236	1829255	184118	74.488
Total		2455760	247873	

HPLC data of 8i

### <Chromatogram>

mAU



### <Peak Table>

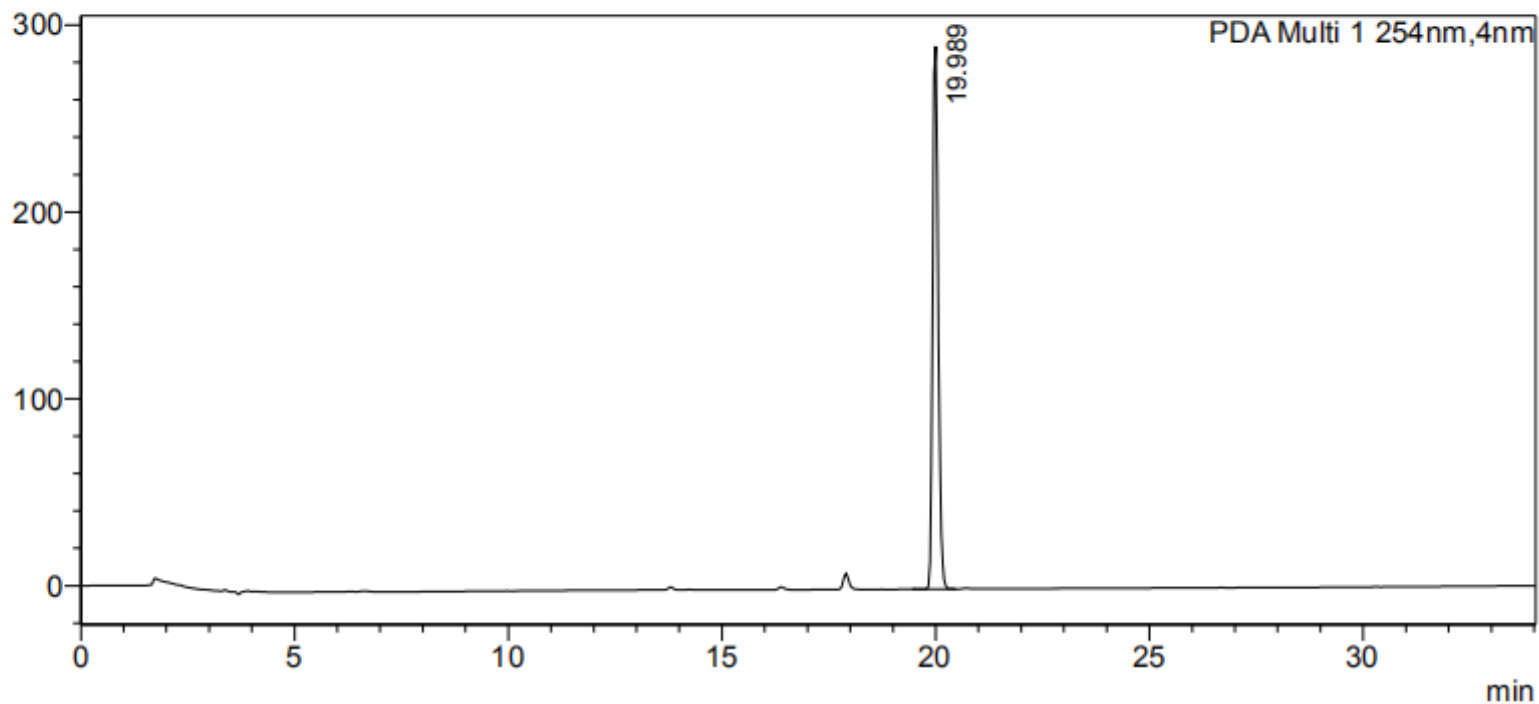
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	24.990	948305	110861	33.782
2	27.401	1858819	228861	66.218
Total		2807125	339721	

HPLC data of 8j

### <Chromatogram>

mAU



### <Peak Table>

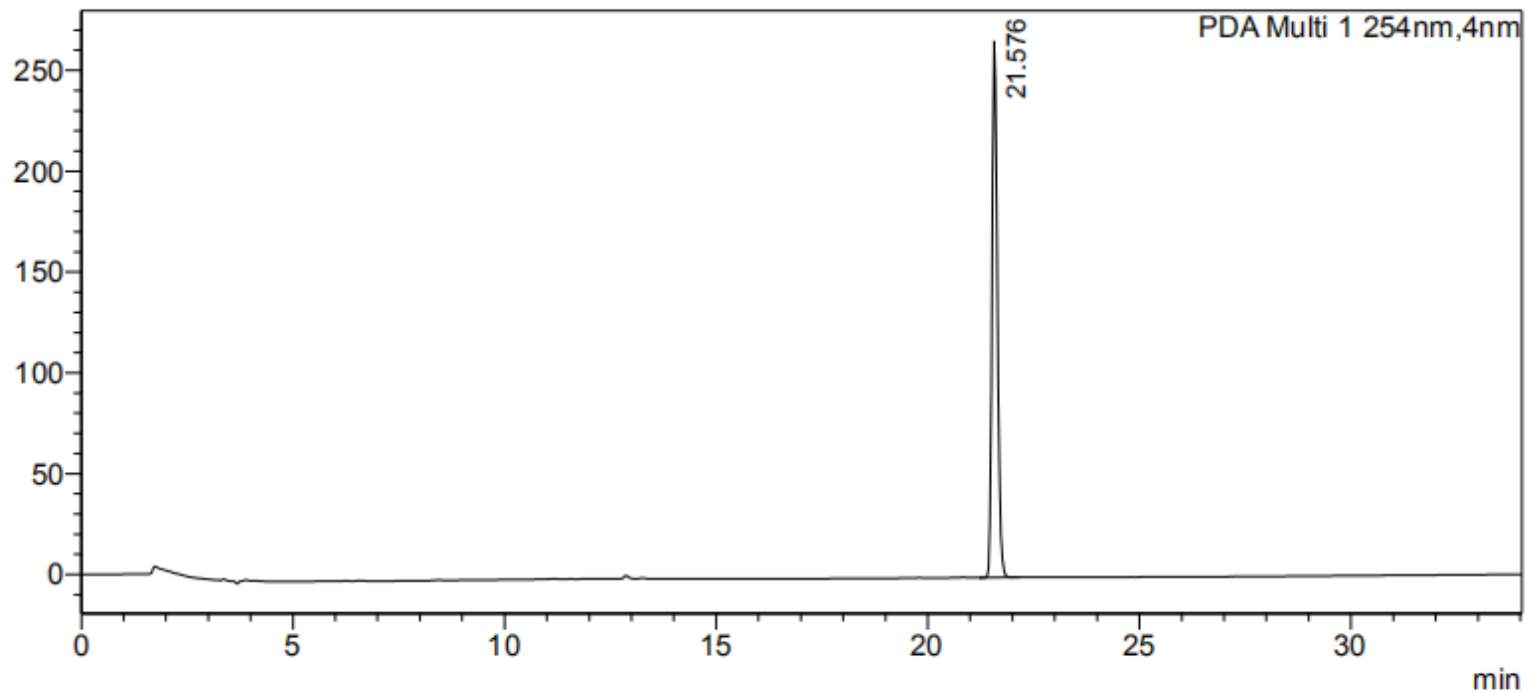
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	19.989	2580039	290415	100.000
Total		2580039	290415	

HPLC data of 8o

### <Chromatogram>

mAU



### <Peak Table>

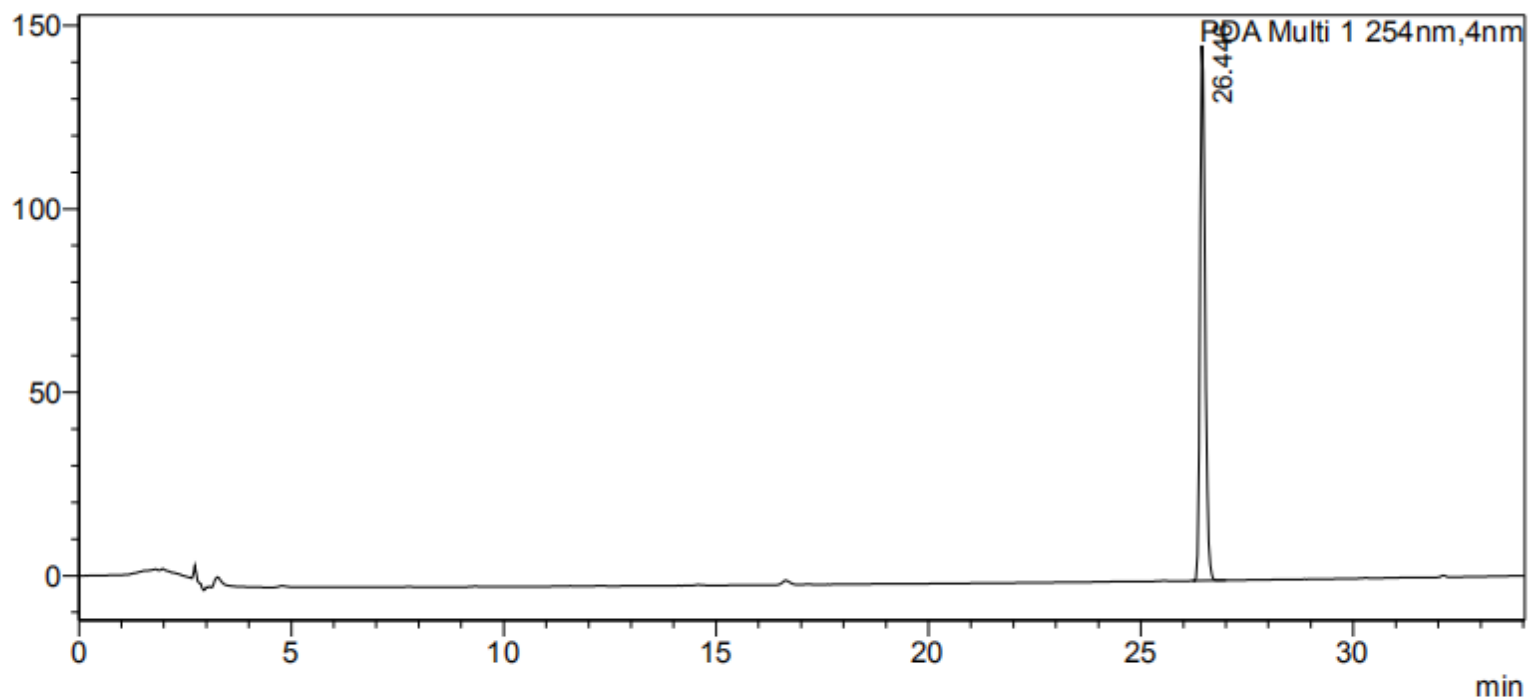
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	21.576	2366172	266067	100.000
Total		2366172	266067	

HPLC data of 8q

### <Chromatogram>

mAU



### <Peak Table>

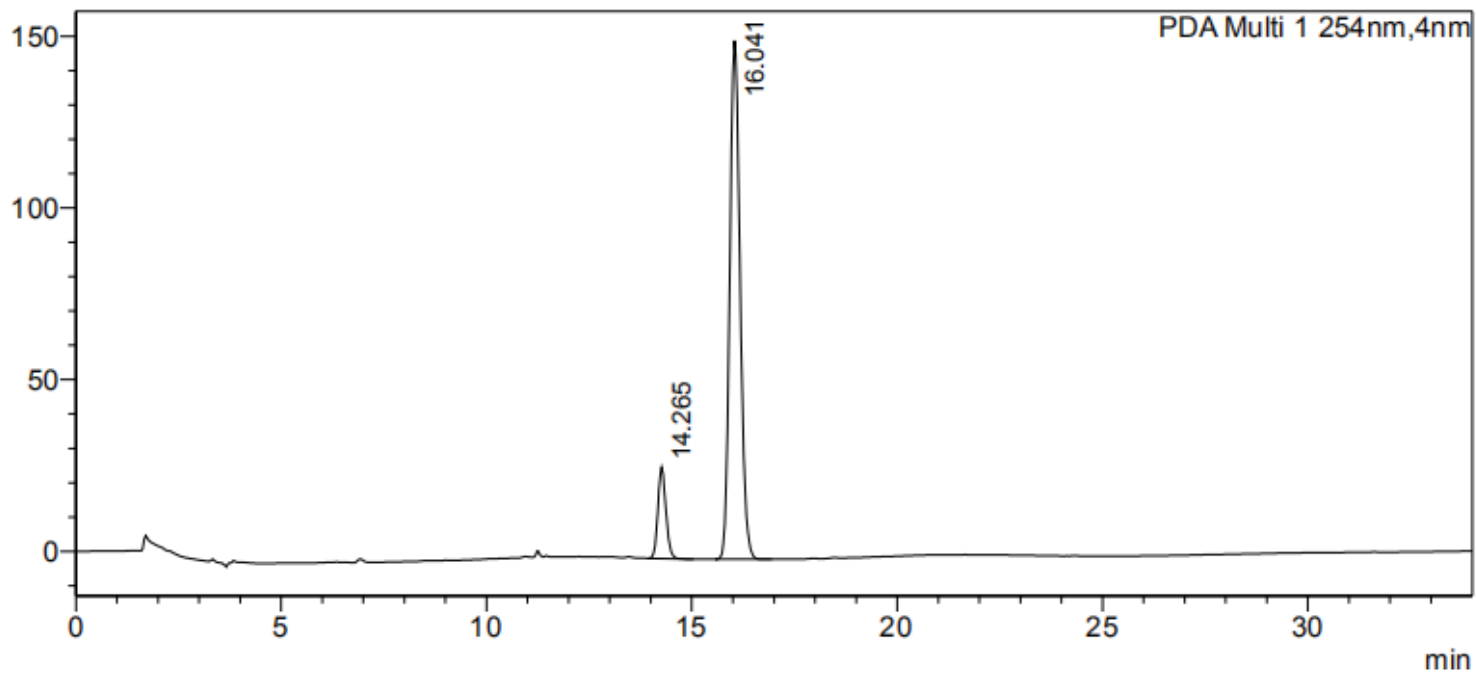
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	26.446	1230264	145890	100.000
Total		1230264	145890	

HPLC data of 8r

### <Chromatogram>

mAU



### <Peak Table>

PDA Ch1 254nm

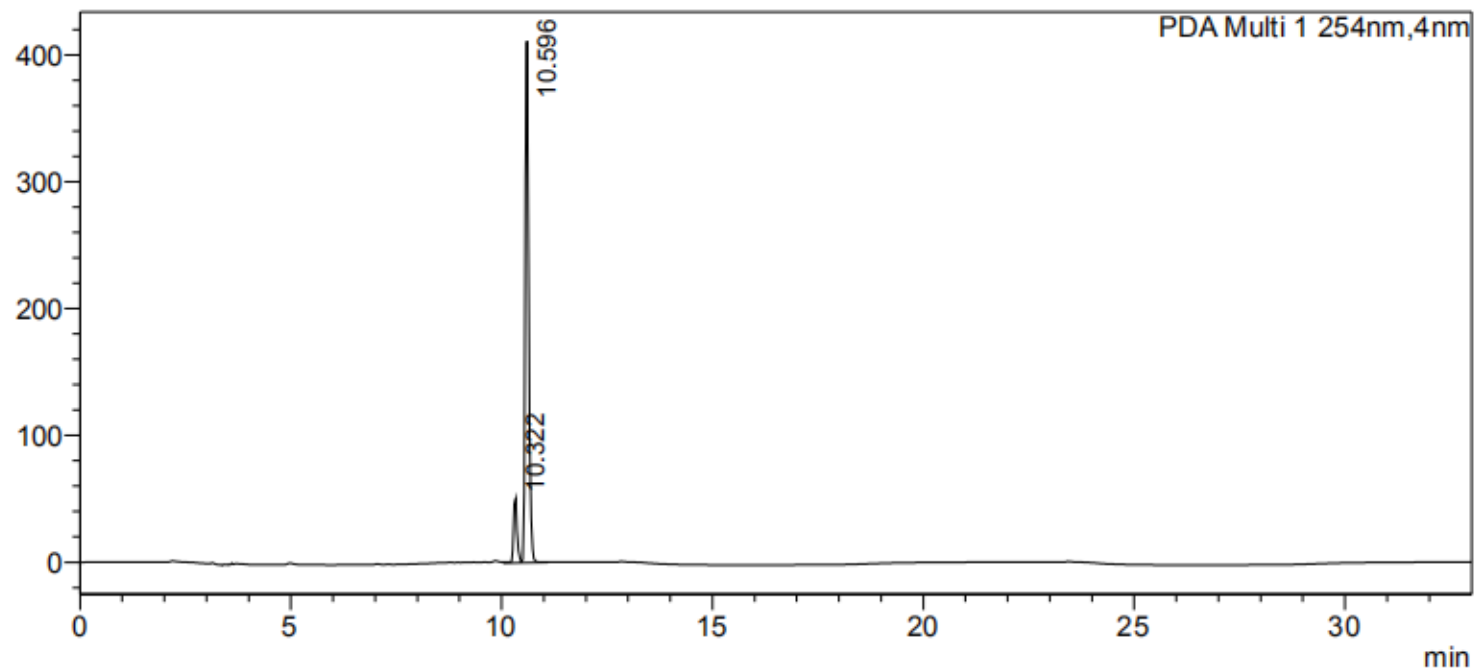
Peak#	Ret. Time	Area	Height	Conc.
1	14.265	361193	26587	12.082
2	16.041	2628437	151014	87.918
Total		2989631	177601	



HPLC data of 8s

**<Chromatogram>**

mAU



**<Peak Table>**

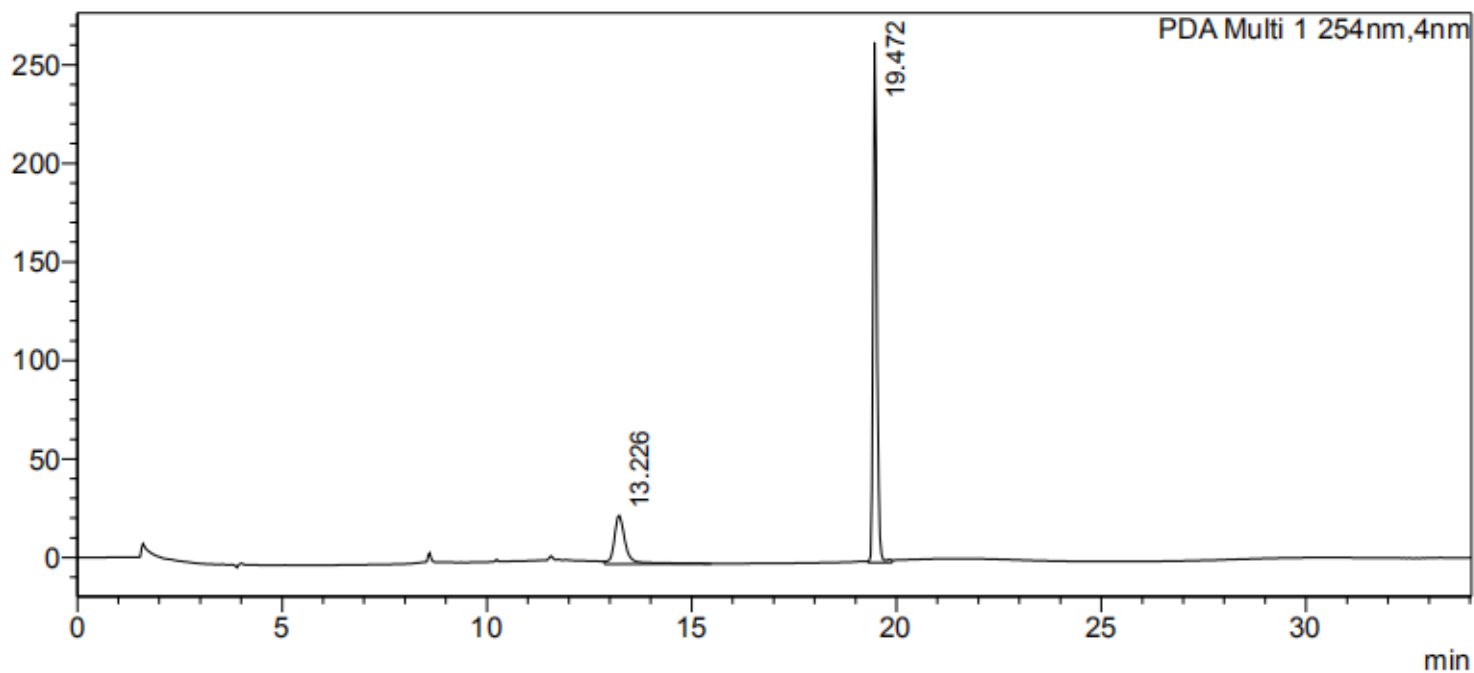
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	10.322	303715	50778	11.508
2	10.596	2335408	411193	88.492
Total		2639124	461971	

HPLC data of 8t

### <Chromatogram>

mAU



### <Peak Table>

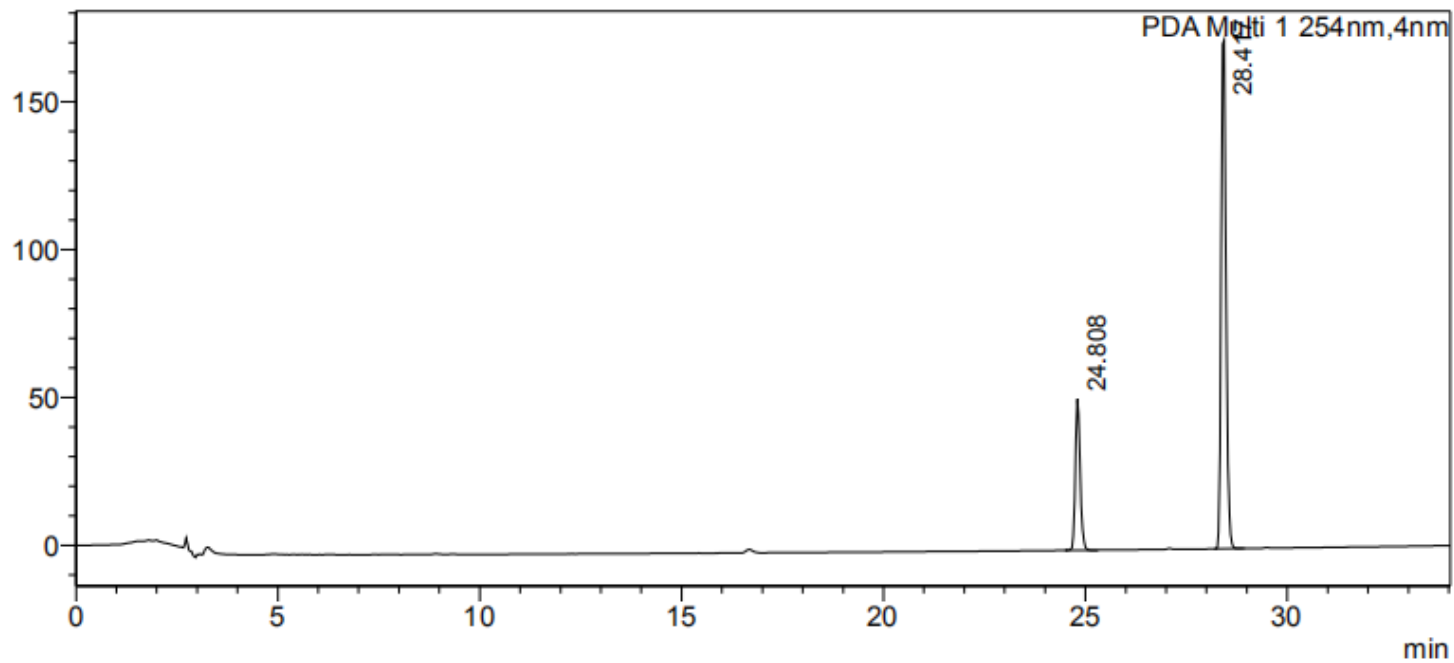
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	13.226	465705	24557	21.631
2	19.472	1687295	264054	78.369
Total		2153000	288610	

HPLC data of 8u

### <Chromatogram>

mAU



### <Peak Table>

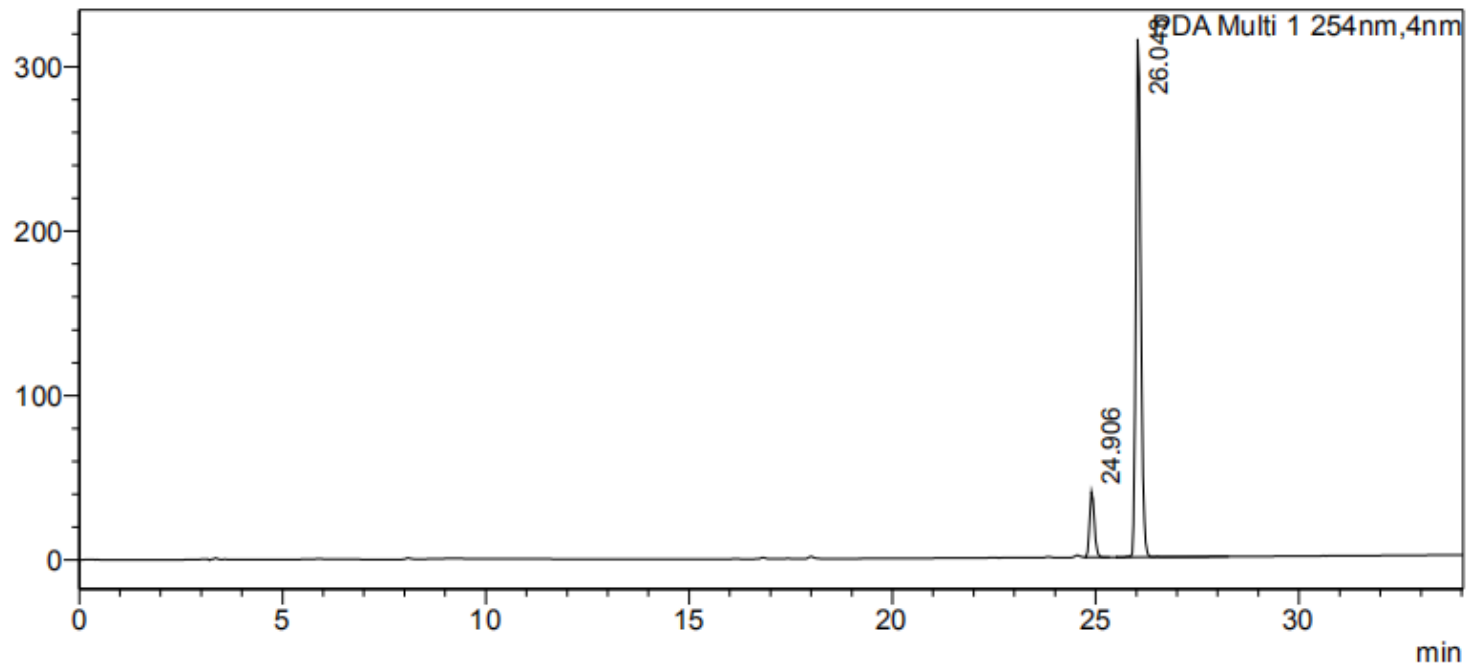
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	24.808	429187	51164	23.106
2	28.417	1428250	172030	76.894
Total		1857437	223194	

HPLC data of 8v

### <Chromatogram>

mAU



### <Peak Table>

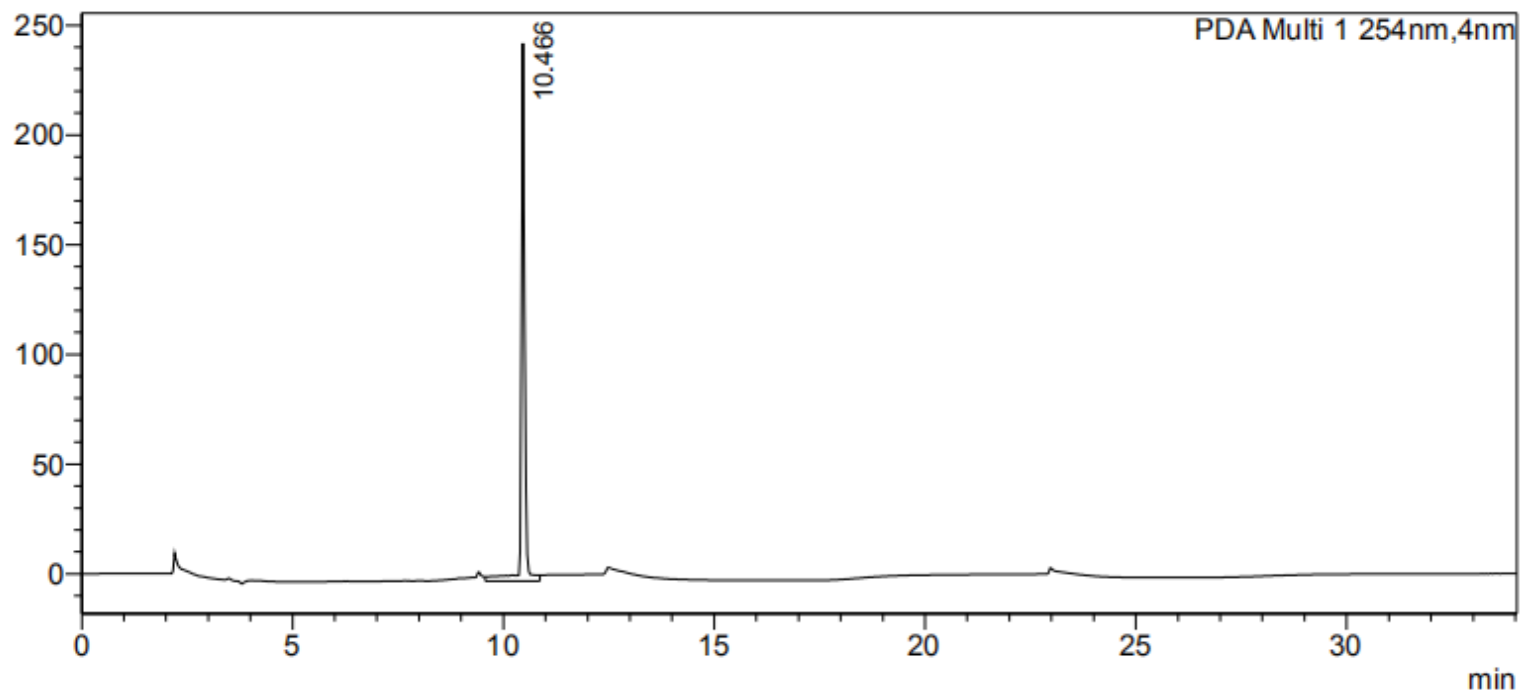
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	24.906	322326	39884	10.803
2	26.043	2661224	315428	89.197
Total		2983550	355312	

HPLC data of 10a

### <Chromatogram>

mAU



### <Peak Table>

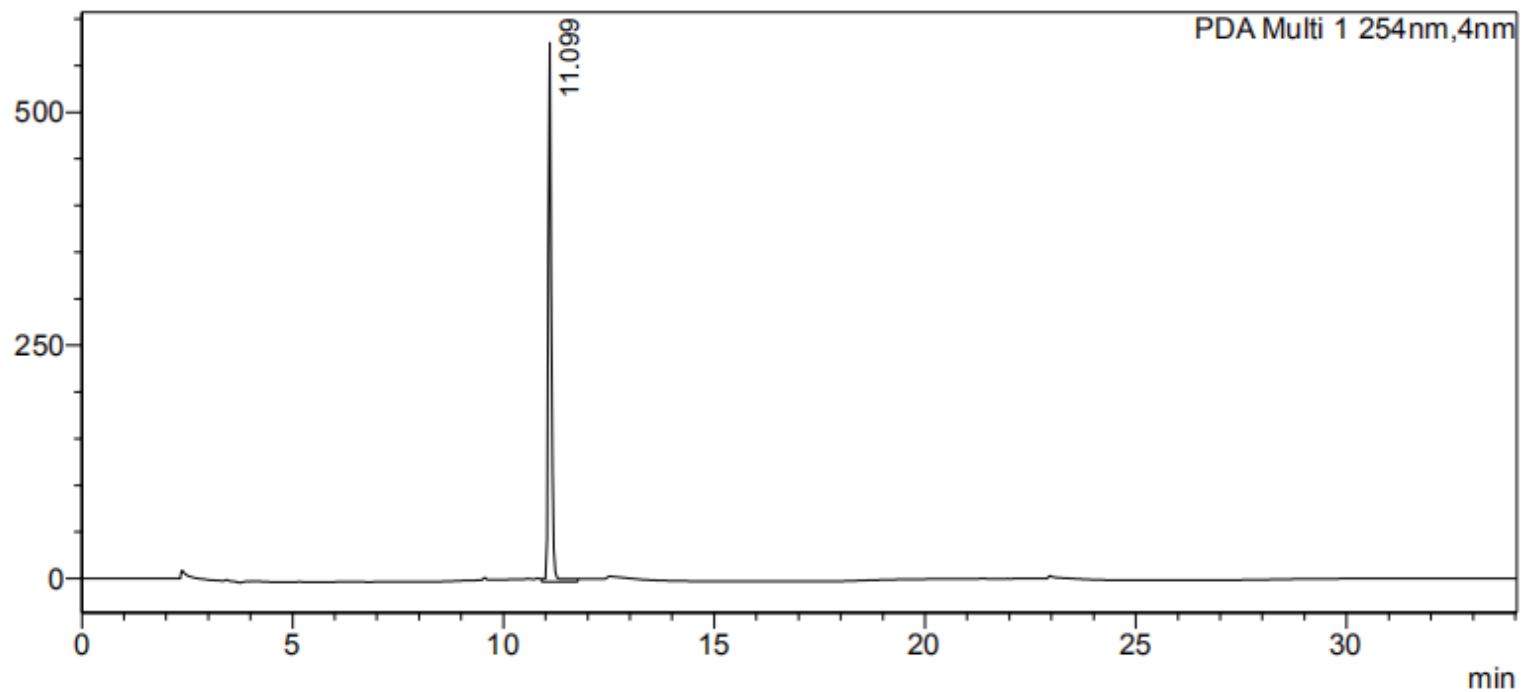
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	10.466	1318244	244996	100.000
Total		1318244	244996	

HPLC data of 10b

### <Chromatogram>

mAU



### <Peak Table>

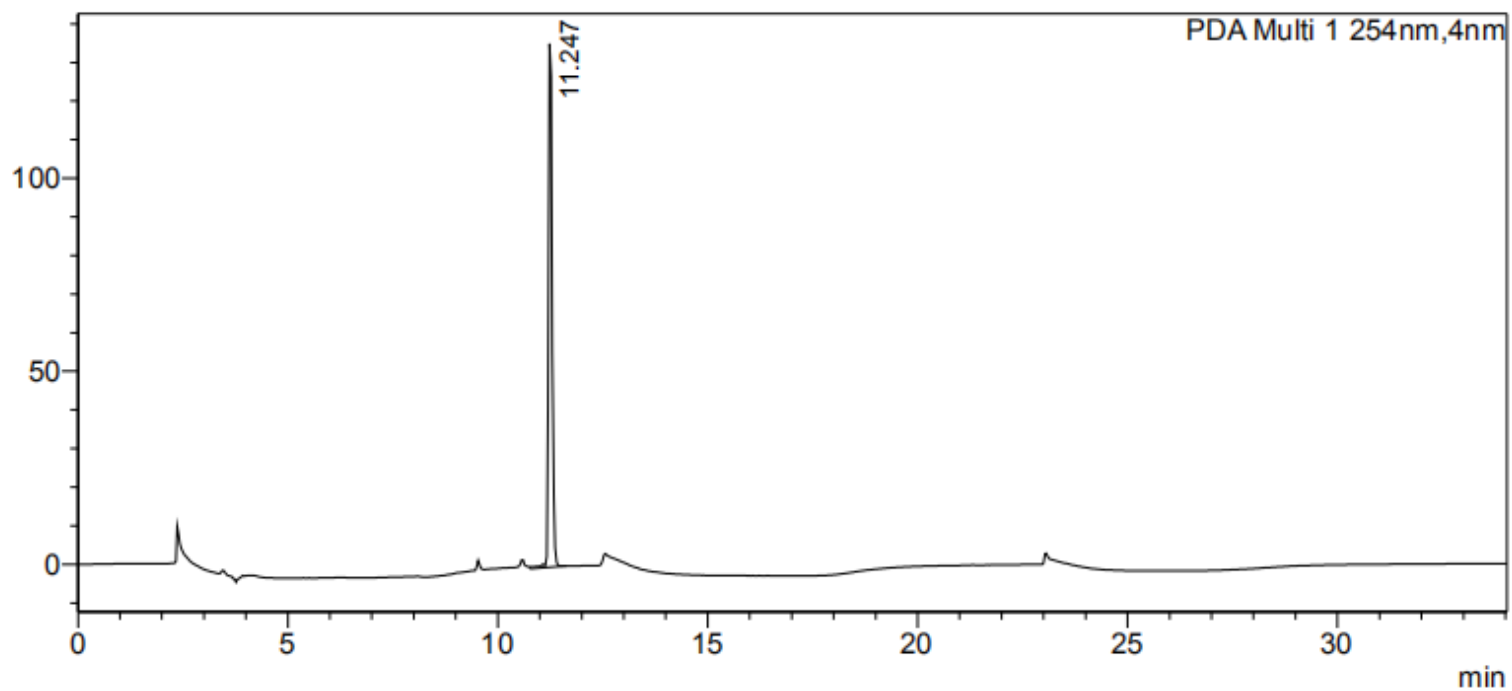
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	11.099	3056200	578097	100.000
Total		3056200	578097	

HPLC data of 10c

### <Chromatogram>

mAU



### <Peak Table>

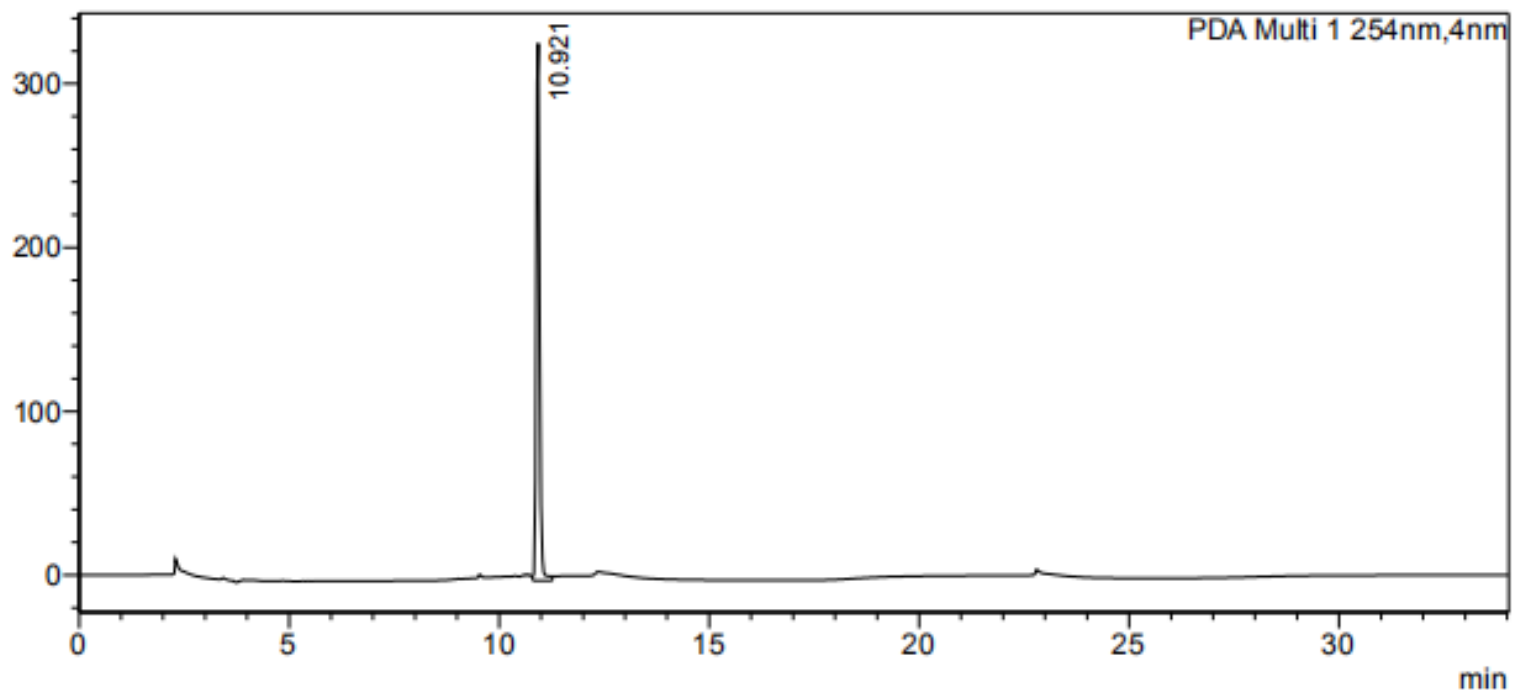
PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	11.247	787842	135567	100.000
Total		787842	135567	

HPLC data of 10f

### <Chromatogram>

mAU



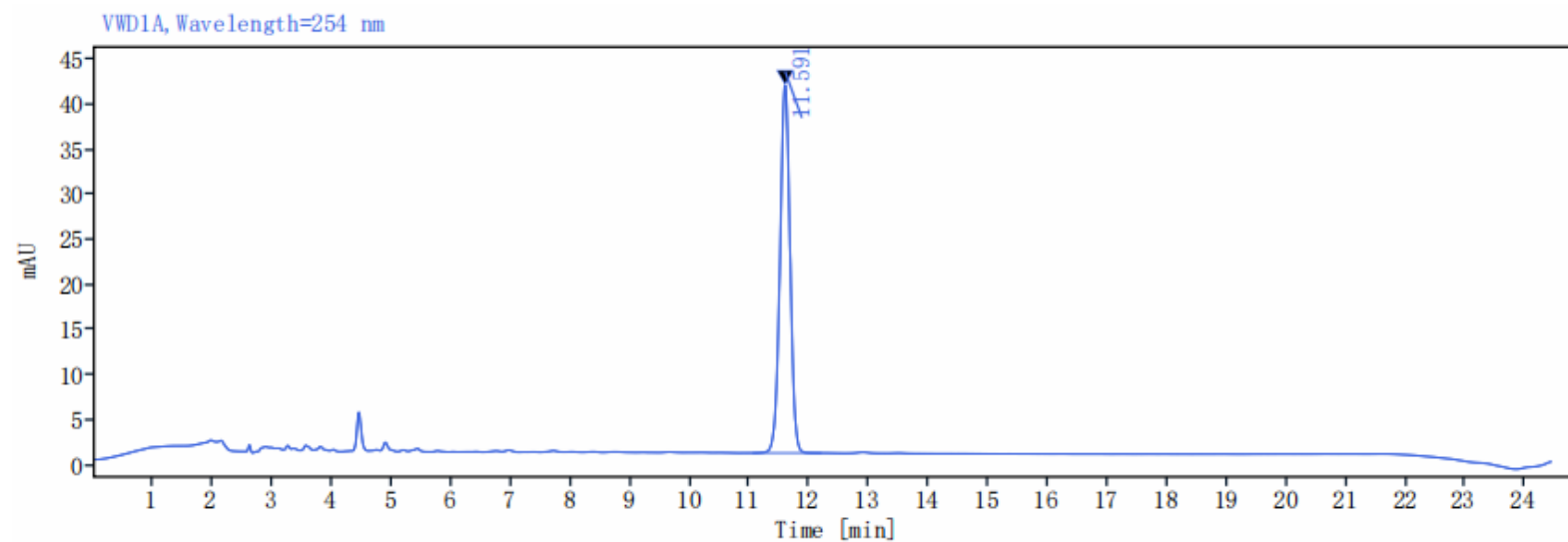
### <Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.
1	10.921	1846185	328029	100.000
Total		1846185	328029	



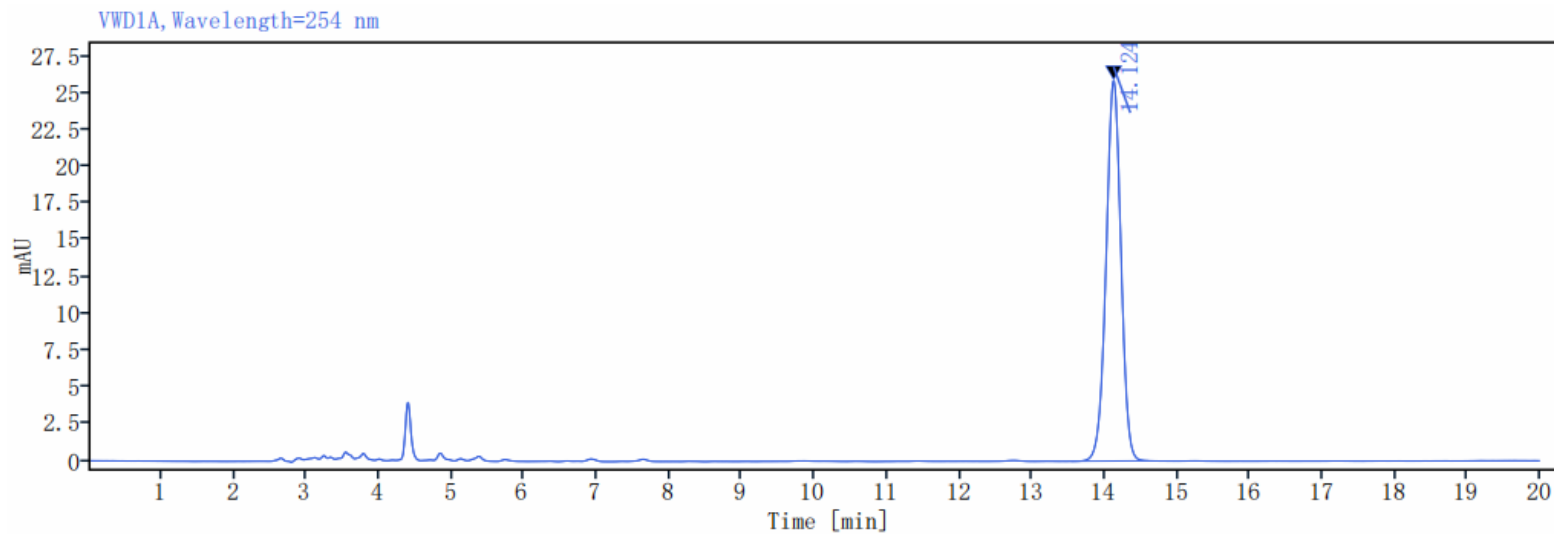
HPLC data of **12a**



Signal: VWD1A, Wavelength=254 nm

Retention time [min]	Type	Peak width [min]	Peak area	Height	Peak area (%)	Name
11.591	BB	1.15	479.34	40.82	100.00	
	sum	1.15	479.34			

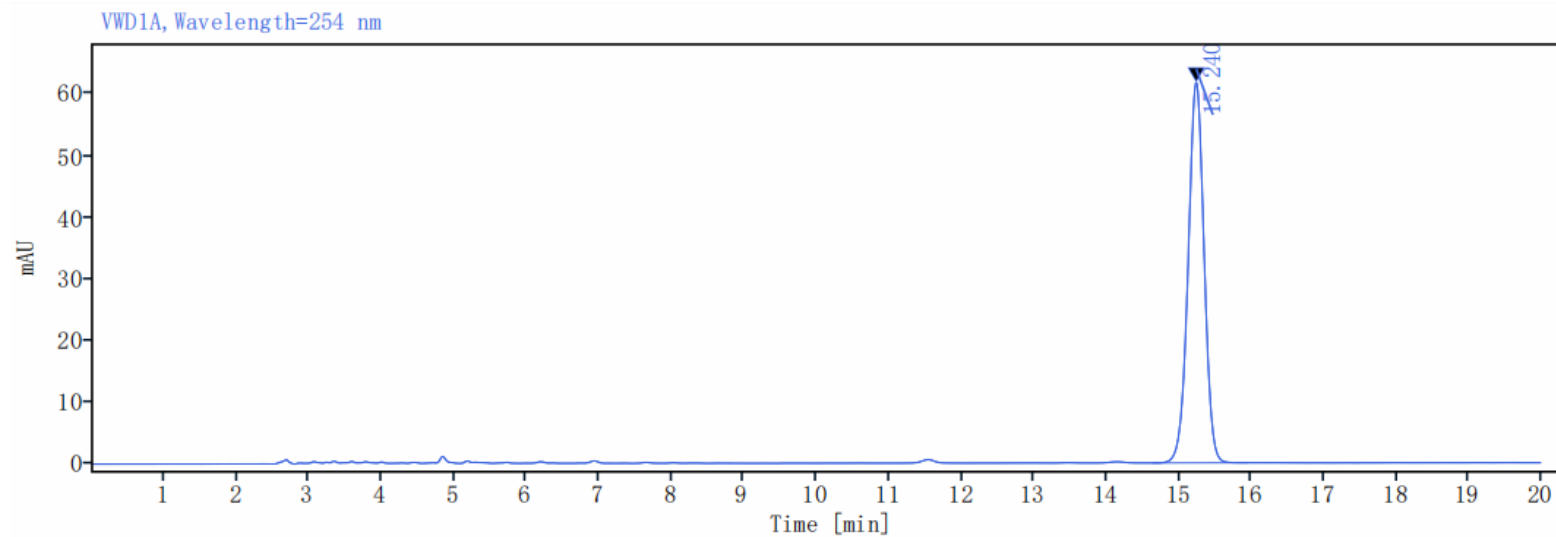
HPLC data of **12b**



Signal: VWD1A, Wavelength=254 nm

Retention time [min]	Type	Peak width [min]	Peak area	Height	Peak area (%)	Name
14.124	BM m	1.06	368.43	25.86	100.00	
	sum	1.06	368.43			

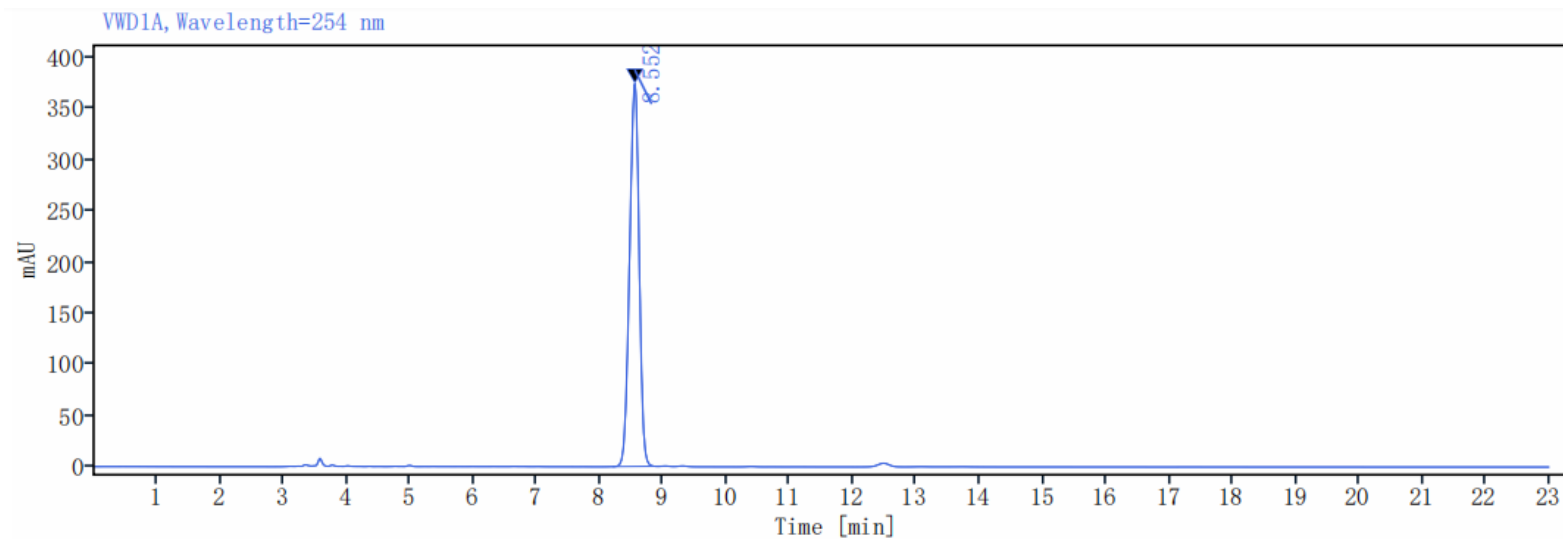
HPLC data of **12c**



Signal: VWD1A, Wavelength=254 nm

Retention time [min]	Type	Peak width [min]	Peak area	Height	Peak area (%)	Name
15.240	BB	1.31	945.02	61.71	100.00	
	sum	1.31	945.02			

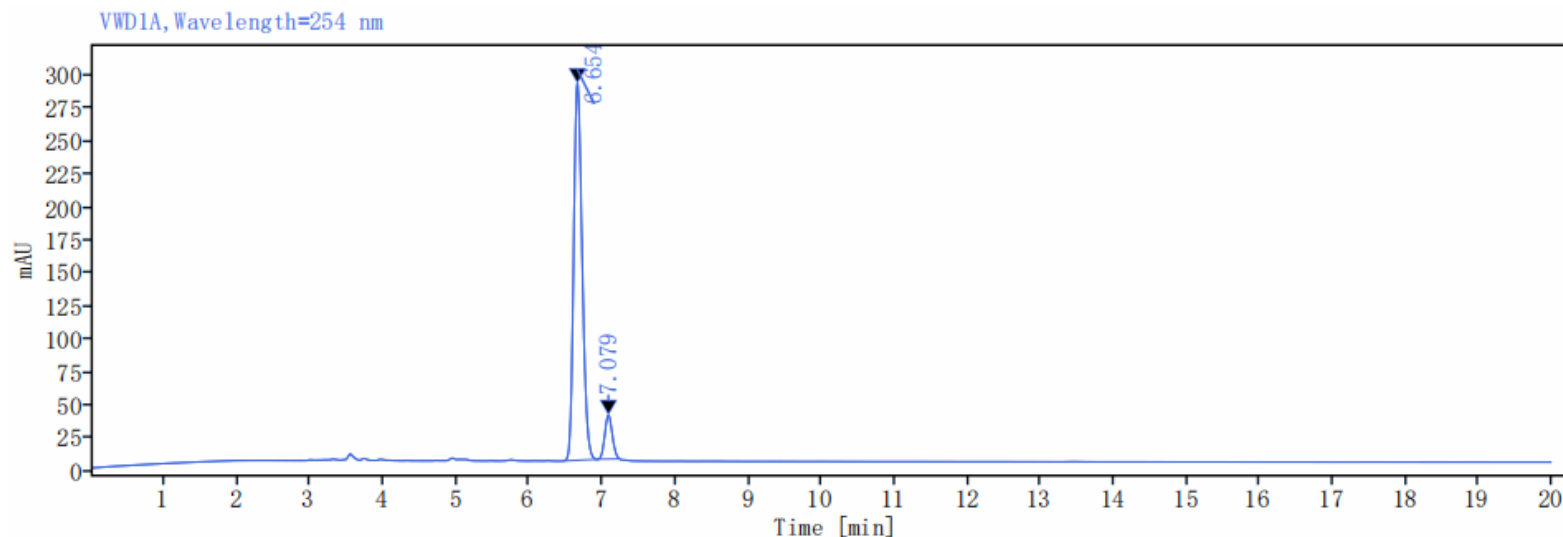
HPLC data of **12d**



Signal: VWD1A, Wavelength=254 nm

Retention time [min]	Type	Peak width [min]	Peak area	Height	Peak area (%)	Name
8.552	MM m	0.79	3937.50	374.76	100.00	
	sum	0.79	3937.50			

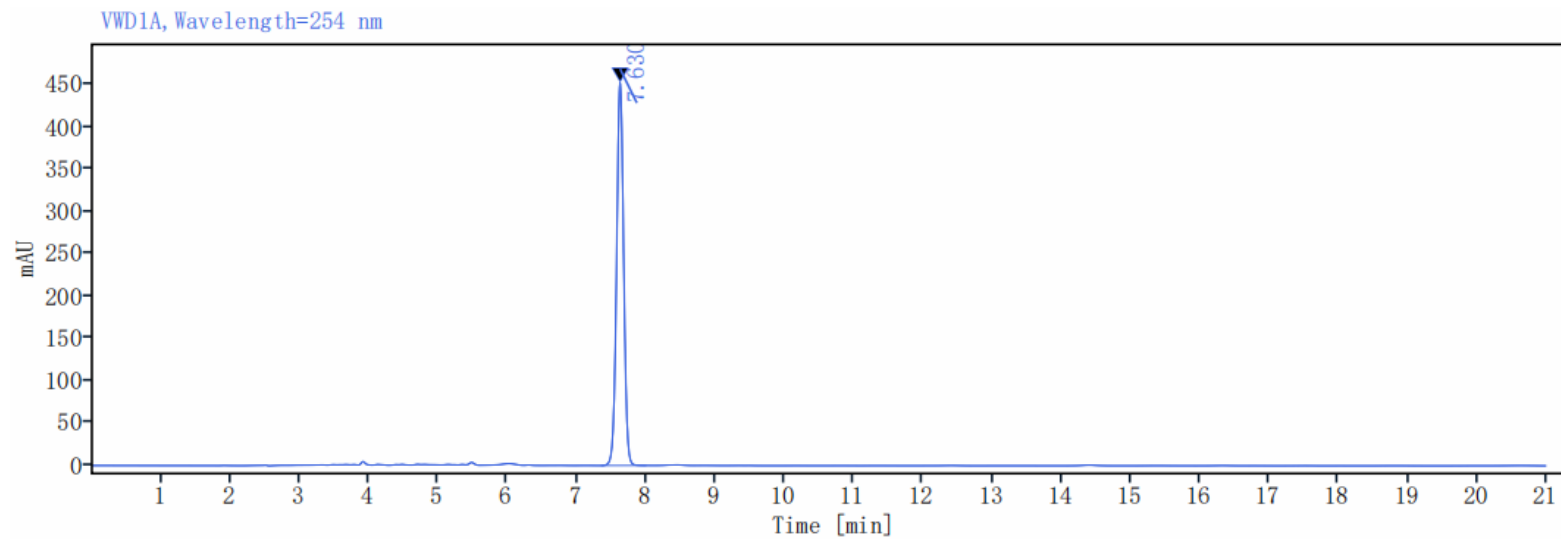
HPLC data of 12e



Signal: VWD1A, Wavelength=254 nm

Retention time [min]	Type	Peak width [min]	Peak area	Height	Peak area (%)	Name
6.654	MM m	0.48	2307.94	285.77	90.63	
7.079	MM m	0.29	238.50	33.34	9.37	
	sum	0.77	2546.43			

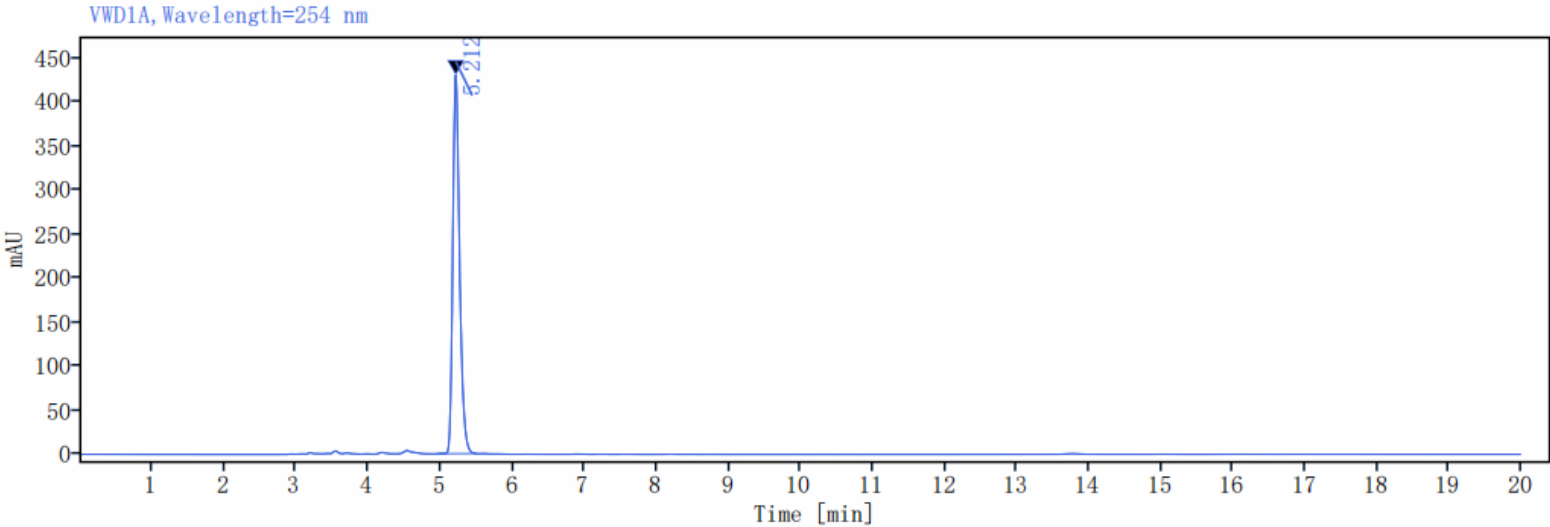
HPLC data of 12g



Signal: VWD1A, Wavelength=254 nm

Retention time [min]	Type	Peak width [min]	Peak area	Height	Peak area (%)	Name
7.630	MM m	0.65	3194.74	452.63	100.00	
	sum	0.65	3194.74			

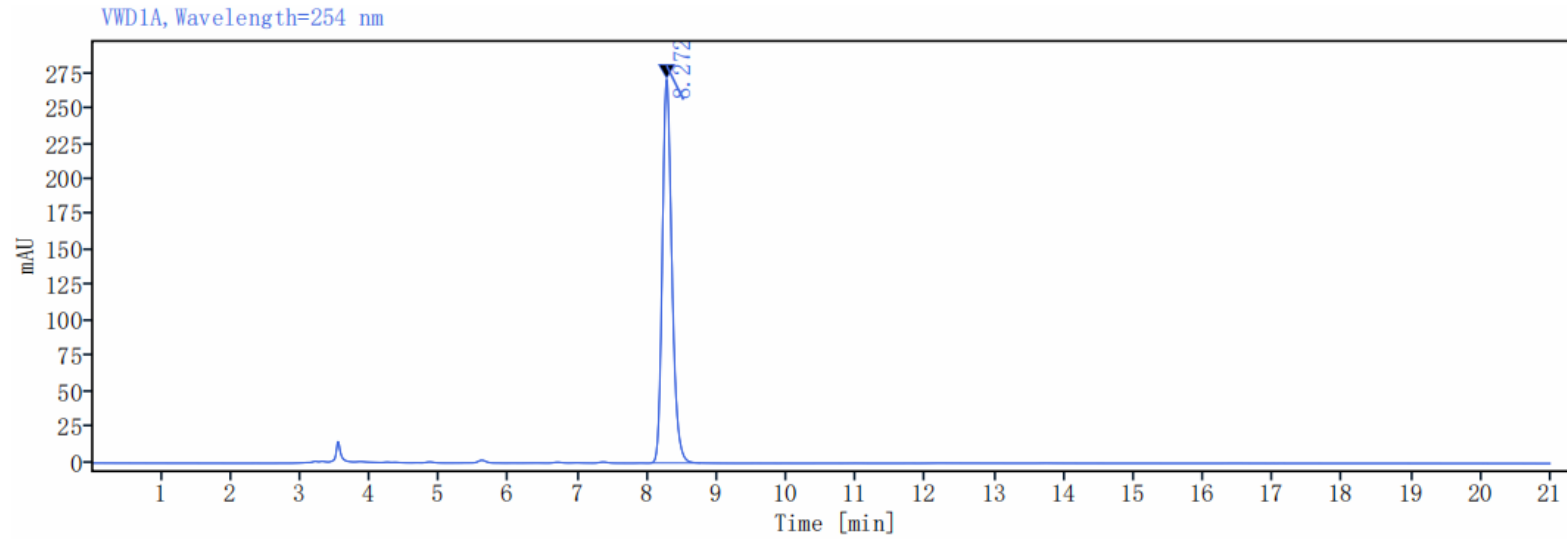
HPLC data of 12j



Signal: VWD1A, Wavelength=254 nm

Retention time [min]	Type	Peak width [min]	Peak area	Height	Peak area (%)	Name
5.212	MM m	0.52	2822.87	429.71	100.00	
	sum	0.52	2822.87			

HPLC data of 12k



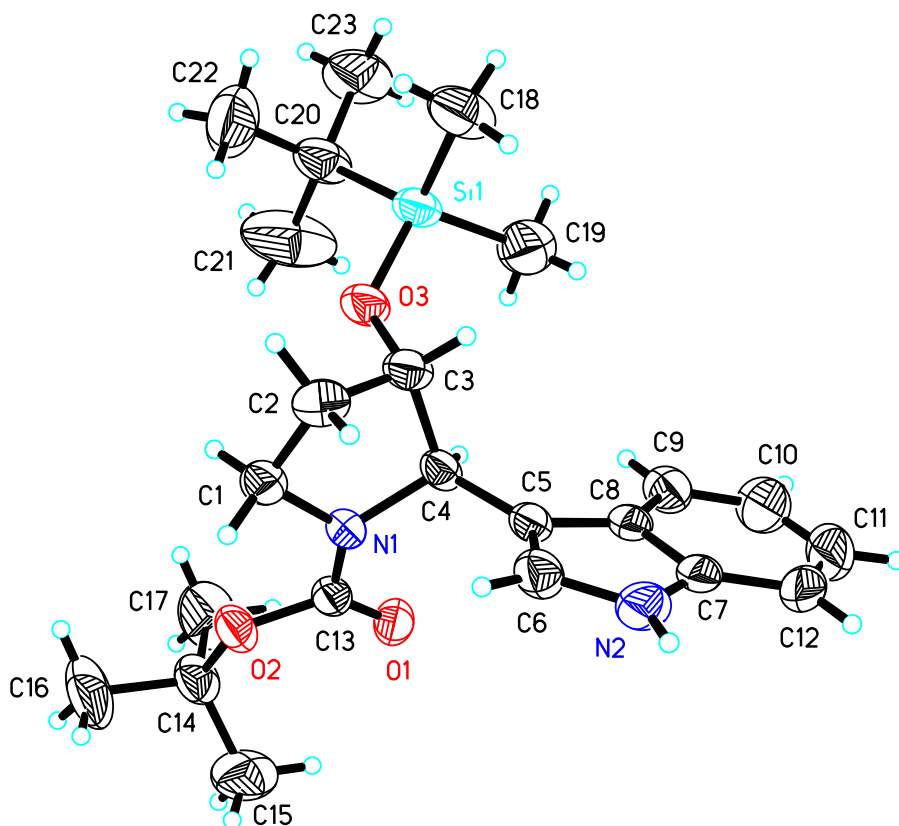
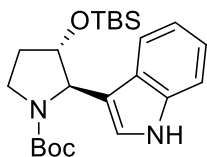
Signal: VWD1A, Wavelength=254 nm

Retention time [min]	Type	Peak width [min]	Peak area	Height	Peak area (%)	Name
8.272	MM m	0.71	2589.26	270.50	100.00	
	sum	0.71	2589.26			



ORTEP drawing of the X-ray crystallographic structure of compound **8a** (50% probability ellipsoids, **mo\_dd21076\_0m** is the original test number for **8a**):

The single crystal of compound **8a** was prepared from its solution in petroleum ether/ethylacetate (5:1) by slow evaporation of the solvent.



CCDC2171349 contains the supplementary crystallographic data for this paper.  
These data can be obtained free of charge from

The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

Table 1. Crystal data and structure refinement for mo\_dd21076\_0m.

Identification code	mo_dd21076_0m	
Empirical formula	C <sub>23</sub> H <sub>36</sub> N <sub>2</sub> O <sub>3</sub> Si	
Formula weight	416.63	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.786(2) Å	α = 90 °
	b = 15.114(5) Å	β = 90 °
	c = 24.774(8) Å	γ = 90 °
Volume	2541.0(14) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.089 Mg/m <sup>3</sup>	
Absorption coefficient	0.115 mm <sup>-1</sup>	
F(000)	904	
Crystal size	0.200 x 0.130 x 0.080 mm <sup>3</sup>	
Theta range for data collection	2.811 to 25.999 °	
Index ranges	-7 ≤ h ≤ 8, -16 ≤ k ≤ 18, -30 ≤ l ≤ 26	
Reflections collected	12595	
Independent reflections	4958 [R(int) = 0.0344]	
Completeness to theta = 25.242 °	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6708	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	4958 / 0 / 271	
Goodness-of-fit on F <sup>2</sup>	1.016	
Final R indices [I > 2σ(I)]	R1 = 0.0489, wR2 = 0.1138	
R indices (all data)	R1 = 0.0788, wR2 = 0.1339	
Absolute structure parameter	-0.01(7)	
Extinction coefficient	0.023(5)	
Largest diff. peak and hole	0.286 and -0.180 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mo\_dd21076\_0m.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
Si(1)	4814(2)	4627(1)	2868(1)	70(1)
O(1)	7425(4)	5226(2)	5033(1)	66(1)
O(2)	5076(4)	4280(2)	5356(1)	71(1)
O(3)	3987(5)	4661(2)	3491(1)	80(1)
N(1)	4378(4)	5133(2)	4657(1)	53(1)
N(2)	3942(6)	8050(2)	4552(1)	82(1)
C(1)	2502(5)	4670(3)	4585(1)	68(1)
C(2)	1568(6)	5155(3)	4118(2)	78(1)
C(3)	3325(6)	5420(3)	3777(1)	68(1)
C(4)	4870(6)	5705(2)	4194(1)	54(1)
C(5)	4845(6)	6678(2)	4312(1)	55(1)
C(6)	3452(7)	7169(3)	4570(1)	74(1)
C(7)	5662(7)	8144(2)	4280(1)	67(1)
C(8)	6293(5)	7289(2)	4125(1)	57(1)
C(9)	8098(6)	7207(3)	3855(2)	76(1)
C(10)	9185(9)	7941(5)	3752(2)	112(2)
C(11)	8531(12)	8769(5)	3904(3)	130(3)
C(12)	6803(11)	8890(3)	4169(2)	100(2)
C(13)	5778(6)	4910(2)	5015(1)	56(1)
C(14)	6382(7)	3762(3)	5699(2)	79(1)
C(15)	7384(10)	4323(4)	6119(2)	125(2)
C(16)	4971(11)	3112(4)	5958(2)	138(2)
C(17)	7853(11)	3280(4)	5352(3)	133(2)
C(18)	3017(9)	5141(4)	2399(2)	115(2)
C(19)	7145(10)	5287(4)	2814(2)	135(2)
C(20)	5236(9)	3442(3)	2738(2)	95(2)
C(21)	6563(17)	3046(5)	3162(3)	210(5)
C(22)	3143(13)	2972(4)	2758(3)	169(3)
C(23)	6065(10)	3277(4)	2175(2)	129(2)

Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for mo\_dd21076\_0m.

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Si(1)-O(3)	1.644(2)
Si(1)-C(20)	1.842(4)
Si(1)-C(18)	1.854(5)
Si(1)-C(19)	1.875(6)
O(1)-C(13)	1.216(4)
O(2)-C(13)	1.358(4)
O(2)-C(14)	1.457(5)
O(3)-C(3)	1.421(4)
N(1)-C(13)	1.343(4)
N(1)-C(1)	1.464(4)
N(1)-C(4)	1.474(4)
N(2)-C(7)	1.356(5)
N(2)-C(6)	1.373(5)
N(2)-H(2)	0.8600
C(1)-C(2)	1.508(5)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.516(6)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.535(5)
C(3)-H(3)	0.9800
C(4)-C(5)	1.499(4)
C(4)-H(4)	0.9800
C(5)-C(6)	1.362(5)
C(5)-C(8)	1.426(5)
C(6)-H(6)	0.9300
C(7)-C(12)	1.395(7)
C(7)-C(8)	1.414(5)
C(8)-C(9)	1.401(5)
C(9)-C(10)	1.357(7)
C(9)-H(9)	0.9300
C(10)-C(11)	1.380(9)
C(10)-H(10)	0.9300

C(11)-C(12)	1.356(9)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(14)-C(15)	1.505(6)
C(14)-C(17)	1.506(7)
C(14)-C(16)	1.514(7)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-C(21)	1.508(8)
C(20)-C(23)	1.525(6)
C(20)-C(22)	1.589(9)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
O(3)-Si(1)-C(20)	104.32(17)
O(3)-Si(1)-C(18)	110.5(2)

C(20)-Si(1)-C(18)	113.6(2)
O(3)-Si(1)-C(19)	109.8(2)
C(20)-Si(1)-C(19)	111.9(3)
C(18)-Si(1)-C(19)	106.7(3)
C(13)-O(2)-C(14)	121.7(3)
C(3)-O(3)-Si(1)	126.9(2)
C(13)-N(1)-C(1)	125.2(3)
C(13)-N(1)-C(4)	120.0(3)
C(1)-N(1)-C(4)	112.5(3)
C(7)-N(2)-C(6)	109.0(3)
C(7)-N(2)-H(2)	125.5
C(6)-N(2)-H(2)	125.5
N(1)-C(1)-C(2)	103.1(3)
N(1)-C(1)-H(1A)	111.1
C(2)-C(1)-H(1A)	111.1
N(1)-C(1)-H(1B)	111.1
C(2)-C(1)-H(1B)	111.1
H(1A)-C(1)-H(1B)	109.1
C(1)-C(2)-C(3)	103.0(3)
C(1)-C(2)-H(2A)	111.2
C(3)-C(2)-H(2A)	111.2
C(1)-C(2)-H(2B)	111.2
C(3)-C(2)-H(2B)	111.2
H(2A)-C(2)-H(2B)	109.1
O(3)-C(3)-C(2)	108.2(3)
O(3)-C(3)-C(4)	110.3(3)
C(2)-C(3)-C(4)	103.6(3)
O(3)-C(3)-H(3)	111.5
C(2)-C(3)-H(3)	111.5
C(4)-C(3)-H(3)	111.5
N(1)-C(4)-C(5)	114.9(2)
N(1)-C(4)-C(3)	101.8(3)
C(5)-C(4)-C(3)	113.5(3)
N(1)-C(4)-H(4)	108.8
C(5)-C(4)-H(4)	108.8
C(3)-C(4)-H(4)	108.8

C(6)-C(5)-C(8)	106.1(3)
C(6)-C(5)-C(4)	129.4(4)
C(8)-C(5)-C(4)	124.3(3)
C(5)-C(6)-N(2)	110.2(4)
C(5)-C(6)-H(6)	124.9
N(2)-C(6)-H(6)	124.9
N(2)-C(7)-C(12)	131.3(5)
N(2)-C(7)-C(8)	107.5(3)
C(12)-C(7)-C(8)	121.1(5)
C(9)-C(8)-C(7)	118.4(4)
C(9)-C(8)-C(5)	134.5(4)
C(7)-C(8)-C(5)	107.1(3)
C(10)-C(9)-C(8)	119.5(5)
C(10)-C(9)-H(9)	120.2
C(8)-C(9)-H(9)	120.2
C(9)-C(10)-C(11)	121.0(6)
C(9)-C(10)-H(10)	119.5
C(11)-C(10)-H(10)	119.5
C(12)-C(11)-C(10)	122.2(5)
C(12)-C(11)-H(11)	118.9
C(10)-C(11)-H(11)	118.9
C(11)-C(12)-C(7)	117.8(5)
C(11)-C(12)-H(12)	121.1
C(7)-C(12)-H(12)	121.1
O(1)-C(13)-N(1)	125.2(3)
O(1)-C(13)-O(2)	125.0(3)
N(1)-C(13)-O(2)	109.8(3)
O(2)-C(14)-C(15)	112.1(4)
O(2)-C(14)-C(17)	109.3(4)
C(15)-C(14)-C(17)	111.6(5)
O(2)-C(14)-C(16)	102.2(4)
C(15)-C(14)-C(16)	111.0(4)
C(17)-C(14)-C(16)	110.3(4)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5

C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
Si(1)-C(18)-H(18A)	109.5
Si(1)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
Si(1)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
Si(1)-C(19)-H(19A)	109.5
Si(1)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
Si(1)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(23)	110.6(5)
C(21)-C(20)-C(22)	109.5(6)
C(23)-C(20)-C(22)	106.6(5)
C(21)-C(20)-Si(1)	110.9(4)
C(23)-C(20)-Si(1)	112.1(4)
C(22)-C(20)-Si(1)	106.9(4)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5



C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mo\_dd21076\_0m. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Si(1)	94(1)	74(1)	43(1)	-3(1)	-1(1)	6(1)
O(1)	68(2)	57(2)	74(2)	5(1)	-5(1)	-9(1)
O(2)	81(2)	73(2)	58(1)	20(1)	0(1)	-6(2)
O(3)	131(2)	62(2)	46(1)	-7(1)	9(1)	3(2)
N(1)	62(2)	54(2)	43(1)	4(1)	4(1)	-3(1)
N(2)	122(3)	58(2)	66(2)	-11(2)	0(2)	21(2)
C(1)	68(2)	80(3)	55(2)	-3(2)	9(2)	-13(2)
C(2)	76(2)	89(3)	69(2)	-8(2)	-11(2)	2(2)
C(3)	101(3)	57(2)	47(2)	-3(2)	-4(2)	13(2)
C(4)	68(2)	53(2)	42(2)	4(1)	12(2)	6(2)
C(5)	70(2)	54(2)	41(1)	2(1)	4(2)	7(2)
C(6)	95(3)	65(3)	61(2)	-1(2)	19(2)	8(2)
C(7)	102(3)	57(2)	44(2)	2(2)	-21(2)	-1(2)
C(8)	71(2)	60(2)	40(2)	3(2)	-13(2)	1(2)
C(9)	66(3)	93(3)	68(2)	9(2)	-6(2)	-11(2)
C(10)	100(4)	134(5)	102(4)	10(4)	-11(3)	-50(4)
C(11)	164(6)	125(6)	101(4)	32(4)	-42(4)	-88(5)
C(12)	163(5)	64(3)	73(3)	8(2)	-49(4)	-25(3)
C(13)	72(2)	47(2)	48(2)	0(2)	5(2)	2(2)
C(14)	97(3)	68(3)	71(2)	21(2)	-1(2)	7(2)
C(15)	174(6)	116(4)	85(3)	7(3)	-53(4)	22(4)
C(16)	155(5)	129(4)	131(4)	81(4)	-6(5)	-25(5)
C(17)	167(6)	84(4)	148(5)	17(4)	33(5)	47(4)
C(18)	158(5)	117(4)	70(3)	8(3)	-10(3)	34(4)
C(19)	147(5)	159(6)	98(4)	-3(4)	6(4)	-54(5)
C(20)	148(5)	82(3)	57(2)	-5(2)	3(3)	32(3)
C(21)	357(13)	154(6)	120(5)	-14(4)	-77(7)	151(8)
C(22)	247(9)	108(5)	150(6)	-24(4)	53(6)	-68(6)
C(23)	178(6)	126(4)	84(3)	-33(3)	23(4)	40(4)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for mo\_dd21076\_0m.

	x	y	z	U(eq)
H(2)	3267	8474	4691	98
H(1A)	1693	4711	4907	81
H(1B)	2712	4051	4498	81
H(2A)	847	5671	4242	94
H(2B)	682	4772	3919	94
H(3)	2996	5905	3530	82
H(4)	6180	5543	4061	65
H(6)	2330	6941	4735	88
H(9)	8547	6653	3747	91
H(10)	10389	7886	3576	135
H(11)	9301	9260	3822	156
H(12)	6391	9451	4273	120
H(15A)	8122	4784	5945	187
H(15B)	8260	3961	6329	187
H(15C)	6410	4581	6352	187
H(16A)	4040	3428	6177	207
H(16B)	5696	2705	6179	207
H(16C)	4282	2792	5681	207
H(17A)	7169	2955	5076	199
H(17B)	8599	2877	5571	199
H(17C)	8727	3699	5186	199
H(18A)	1825	4799	2397	173
H(18B)	3564	5157	2042	173
H(18C)	2731	5732	2517	173
H(19A)	6862	5900	2877	202
H(19B)	7691	5218	2459	202
H(19C)	8075	5081	3077	202
H(21A)	7766	3379	3181	315
H(21B)	6855	2444	3070	315
H(21C)	5913	3064	3506	315

H(22A)	2429	3176	3069	253
H(22B)	3319	2343	2781	253
H(22C)	2416	3114	2437	253
H(23A)	5240	3560	1911	194
H(23B)	6102	2652	2106	194
H(23C)	7374	3514	2152	194

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Table 6. Torsion angles [ ° ] for mo\_dd21076\_0m.

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C(20)-Si(1)-O(3)-C(3)	-176.0(4)
C(18)-Si(1)-O(3)-C(3)	-53.5(4)
C(19)-Si(1)-O(3)-C(3)	63.9(4)
C(13)-N(1)-C(1)-C(2)	-176.9(3)
C(4)-N(1)-C(1)-C(2)	-14.2(4)
N(1)-C(1)-C(2)-C(3)	33.3(4)
Si(1)-O(3)-C(3)-C(2)	141.8(3)
Si(1)-O(3)-C(3)-C(4)	-105.6(3)
C(1)-C(2)-C(3)-O(3)	76.6(4)
C(1)-C(2)-C(3)-C(4)	-40.5(4)
C(13)-N(1)-C(4)-C(5)	-83.8(4)
C(1)-N(1)-C(4)-C(5)	112.6(3)
C(13)-N(1)-C(4)-C(3)	153.1(3)
C(1)-N(1)-C(4)-C(3)	-10.5(3)
O(3)-C(3)-C(4)-N(1)	-84.6(3)
C(2)-C(3)-C(4)-N(1)	31.0(4)
O(3)-C(3)-C(4)-C(5)	151.3(3)
C(2)-C(3)-C(4)-C(5)	-93.1(4)
N(1)-C(4)-C(5)-C(6)	-47.9(5)
C(3)-C(4)-C(5)-C(6)	68.7(4)
N(1)-C(4)-C(5)-C(8)	137.4(3)
C(3)-C(4)-C(5)-C(8)	-105.9(4)
C(8)-C(5)-C(6)-N(2)	0.3(4)
C(4)-C(5)-C(6)-N(2)	-175.1(3)
C(7)-N(2)-C(6)-C(5)	0.2(4)
C(6)-N(2)-C(7)-C(12)	-177.4(4)
C(6)-N(2)-C(7)-C(8)	-0.6(4)
N(2)-C(7)-C(8)-C(9)	-177.3(3)
C(12)-C(7)-C(8)-C(9)	-0.1(5)
N(2)-C(7)-C(8)-C(5)	0.8(4)
C(12)-C(7)-C(8)-C(5)	178.0(3)
C(6)-C(5)-C(8)-C(9)	177.0(4)
C(4)-C(5)-C(8)-C(9)	-7.3(6)
C(6)-C(5)-C(8)-C(7)	-0.7(4)

C(4)-C(5)-C(8)-C(7)	175.0(3)
C(7)-C(8)-C(9)-C(10)	0.2(5)
C(5)-C(8)-C(9)-C(10)	-177.3(4)
C(8)-C(9)-C(10)-C(11)	-0.6(7)
C(9)-C(10)-C(11)-C(12)	1.0(9)
C(10)-C(11)-C(12)-C(7)	-0.9(8)
N(2)-C(7)-C(12)-C(11)	176.9(4)
C(8)-C(7)-C(12)-C(11)	0.5(6)
C(1)-N(1)-C(13)-O(1)	170.7(3)
C(4)-N(1)-C(13)-O(1)	9.3(5)
C(1)-N(1)-C(13)-O(2)	-9.4(4)
C(4)-N(1)-C(13)-O(2)	-170.8(3)
C(14)-O(2)-C(13)-O(1)	-15.1(5)
C(14)-O(2)-C(13)-N(1)	165.0(3)
C(13)-O(2)-C(14)-C(15)	65.9(5)
C(13)-O(2)-C(14)-C(17)	-58.3(5)
C(13)-O(2)-C(14)-C(16)	-175.2(4)
O(3)-Si(1)-C(20)-C(21)	-54.4(6)
C(18)-Si(1)-C(20)-C(21)	-174.8(6)
C(19)-Si(1)-C(20)-C(21)	64.3(6)
O(3)-Si(1)-C(20)-C(23)	-178.6(4)
C(18)-Si(1)-C(20)-C(23)	61.0(5)
C(19)-Si(1)-C(20)-C(23)	-59.9(5)
O(3)-Si(1)-C(20)-C(22)	64.9(4)
C(18)-Si(1)-C(20)-C(22)	-55.5(4)
C(19)-Si(1)-C(20)-C(22)	-176.4(4)

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Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo\_dd21076\_0m [ $\text{\AA}$  and  $^\circ$ ].

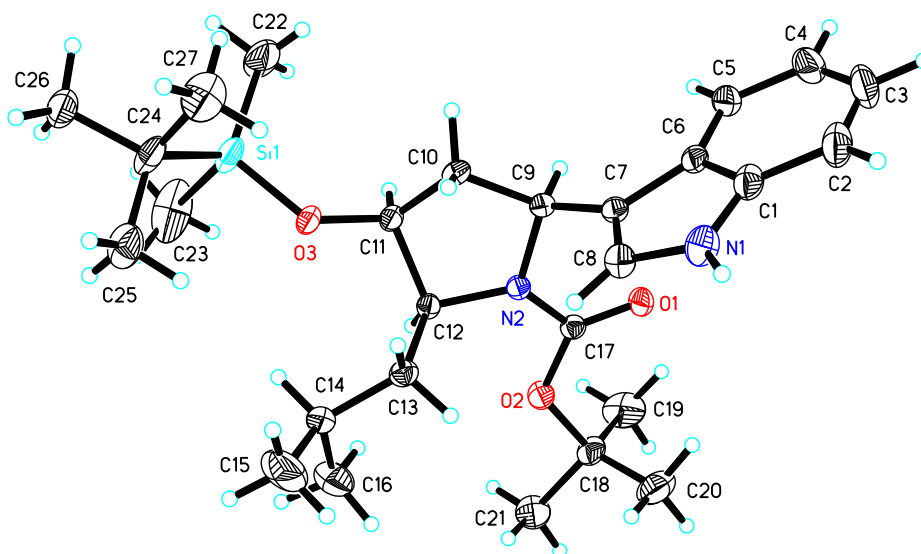
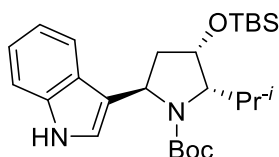
D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
C(17)-H(17C)...O(1)	0.96	2.50	3.059(6)	117.1
C(15)-H(15A)...O(1)	0.96	2.40	3.017(6)	121.4
N(2)-H(2)...O(1)#1	0.86	2.16	2.984(4)	161.2

Symmetry transformations used to generate equivalent atoms:

#1  $x-1/2, -y+3/2, -z+1$

ORTEP drawing of the X-ray crystallographic structure of compound **12g** (50% probability ellipsoids, **mo\_ddz21073\_0m** is the original test number for **12g**):

The single crystal of compound **12g** was prepared from its solution in petroleum ether/ethylacetate (5:1) by slow evaporation of the solvent.



CCDC2171350 contains the supplementary crystallographic data for this paper.  
These data can be obtained free of charge from

The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).



Table 1. Crystal data and structure refinement for mo\_ddz21073\_0m.

Identification code	mo_ddz21073_0m	
Empirical formula	C <sub>27</sub> H <sub>44</sub> N <sub>2</sub> O <sub>3</sub> Si	
Formula weight	472.73	
Temperature	213(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.2060(5) Å	α = 90 °
	b = 11.4624(6) Å	β = 106.937(2) °
	c = 12.4467(6) Å	γ = 90 °
Volume	1392.92(12) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.127 Mg/m <sup>3</sup>	
Absorption coefficient	0.113 mm <sup>-1</sup>	
F(000)	516	
Crystal size	0.200 x 0.160 x 0.120 mm <sup>3</sup>	
Theta range for data collection	2.466 to 25.999 °	
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15	
Reflections collected	22950	
Independent reflections	5418 [R(int) = 0.0323]	
Completeness to theta = 25.242 °	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6882	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	5418 / 119 / 368	
Goodness-of-fit on F <sup>2</sup>	1.044	
Final R indices [I > 2σ(I)]	R1 = 0.0400, wR2 = 0.1032	
R indices (all data)	R1 = 0.0435, wR2 = 0.1071	
Absolute structure parameter	0.03(4)	
Extinction coefficient	0.025(10)	
Largest diff. peak and hole	0.314 and -0.242 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mo\_ddz21073\_0m.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
Si(1)	3631(1)	3840(1)	3696(1)	50(1)
O(1)	2784(2)	3568(2)	9216(1)	36(1)
O(2)	886(2)	4185(2)	7861(2)	39(1)
O(3)	3313(2)	4474(2)	4782(1)	40(1)
N(1)	6160(3)	6315(2)	9817(2)	48(1)
N(2)	2917(2)	4212(2)	7536(2)	29(1)
C(1)	6789(3)	5373(3)	10407(2)	43(1)
C(2)	7769(3)	5303(4)	11456(3)	60(1)
C(3)	8192(4)	4225(4)	11867(3)	69(1)
C(4)	7679(4)	3212(4)	11265(3)	64(1)
C(5)	6701(3)	3260(3)	10228(2)	45(1)
C(6)	6242(2)	4359(3)	9788(2)	34(1)
C(7)	5240(2)	4755(2)	8781(2)	31(1)
C(8)	5237(3)	5936(3)	8840(2)	41(1)
C(9)	4412(2)	3995(2)	7840(2)	30(1)
C(10)	4711(2)	4199(3)	6715(2)	36(1)
C(11)	3367(2)	3949(2)	5826(2)	32(1)
C(12)	2276(2)	4448(2)	6334(2)	28(1)
C(13)	1954(3)	5740(2)	6086(2)	35(1)
C(14)	831(4)	5980(3)	4995(3)	52(1)
C(15)	862(6)	7239(4)	4660(4)	94(2)
C(16)	-588(4)	5670(4)	5088(4)	73(1)
C(17)	2231(2)	3954(2)	8283(2)	28(1)
C(18)	-34(3)	4137(3)	8585(2)	41(1)
C(19)	-46(4)	2933(4)	9063(4)	70(1)
C(20)	397(4)	5066(4)	9481(3)	69(1)
C(21)	-1411(3)	4424(4)	7772(3)	66(1)
C(22)	4638(17)	2553(12)	4015(10)	106(5)
C(23)	1831(11)	3282(10)	2743(8)	103(4)
C(24)	4106(15)	4999(17)	2881(15)	54(2)
C(25)	3214(9)	6059(6)	2678(7)	64(2)

C(26)	4220(20)	4614(12)	1735(14)	57(3)
C(27)	5607(11)	5317(11)	3684(9)	78(2)
C(22')	5516(15)	3152(13)	4314(10)	104(5)
C(23')	2560(20)	2609(15)	3142(13)	105(5)
C(24')	3980(20)	5030(30)	2790(20)	58(2)
C(25')	2542(15)	5672(13)	2425(11)	80(3)
C(26')	4240(30)	4343(19)	1780(20)	55(3)
C(27')	5256(13)	5781(9)	3346(9)	75(2)

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Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for mo\_ddz21073\_0m.

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Si(1)-O(3)	1.6470(18)
Si(1)-C(22)	1.776(10)
Si(1)-C(23')	1.794(13)
Si(1)-C(24)	1.82(2)
Si(1)-C(24')	1.87(4)
Si(1)-C(23)	1.980(9)
Si(1)-C(22')	2.014(11)
O(1)-C(17)	1.216(3)
O(2)-C(17)	1.346(3)
O(2)-C(18)	1.480(3)
O(3)-C(11)	1.419(3)
N(1)-C(1)	1.357(4)
N(1)-C(8)	1.374(4)
N(1)-H(1)	0.8700
N(2)-C(17)	1.350(3)
N(2)-C(12)	1.473(3)
N(2)-C(9)	1.482(3)
C(1)-C(2)	1.397(4)
C(1)-C(6)	1.416(4)
C(2)-C(3)	1.359(6)
C(2)-H(2)	0.9400
C(3)-C(4)	1.398(6)
C(3)-H(3)	0.9400
C(4)-C(5)	1.383(4)
C(4)-H(4)	0.9400
C(5)-C(6)	1.398(4)
C(5)-H(5)	0.9400
C(6)-C(7)	1.441(3)
C(7)-C(8)	1.356(4)
C(7)-C(9)	1.506(3)
C(8)-H(8)	0.9400
C(9)-C(10)	1.535(3)
C(9)-H(9)	0.9900
C(10)-C(11)	1.518(3)

C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(11)-C(12)	1.542(3)
C(11)-H(11)	0.9900
C(12)-C(13)	1.529(3)
C(12)-H(12)	0.9900
C(13)-C(14)	1.524(4)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(14)-C(15)	1.505(6)
C(14)-C(16)	1.529(5)
C(14)-H(14)	0.9900
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(15)-H(15C)	0.9700
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(16)-H(16C)	0.9700
C(18)-C(19)	1.505(5)
C(18)-C(21)	1.509(4)
C(18)-C(20)	1.511(5)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(19)-H(19C)	0.9700
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(20)-H(20C)	0.9700
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(21)-H(21C)	0.9700
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(22)-H(22C)	0.9700
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(23)-H(23C)	0.9700

C(24)-C(25)	1.495(17)
C(24)-C(26)	1.529(17)
C(24)-C(27)	1.608(14)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(25)-H(25C)	0.9700
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(26)-H(26C)	0.9700
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(27)-H(27C)	0.9700
C(22')-H(22D)	0.9700
C(22')-H(22E)	0.9700
C(22')-H(22F)	0.9700
C(23')-H(23D)	0.9700
C(23')-H(23E)	0.9700
C(23')-H(23F)	0.9700
C(24')-C(27')	1.54(2)
C(24')-C(26')	1.58(2)
C(24')-C(25')	1.59(2)
C(25')-H(25D)	0.9700
C(25')-H(25E)	0.9700
C(25')-H(25F)	0.9700
C(26')-H(26D)	0.9700
C(26')-H(26E)	0.9700
C(26')-H(26F)	0.9700
C(27')-H(27D)	0.9700
C(27')-H(27E)	0.9700
C(27')-H(27F)	0.9700
O(3)-Si(1)-C(22)	115.0(4)
O(3)-Si(1)-C(23')	114.8(5)
O(3)-Si(1)-C(24)	106.5(5)
C(22)-Si(1)-C(24)	120.0(7)
O(3)-Si(1)-C(24')	106.8(8)

C(23')-Si(1)-C(24')	123.0(9)
O(3)-Si(1)-C(23)	105.3(4)
C(22)-Si(1)-C(23)	103.9(7)
C(24)-Si(1)-C(23)	104.6(5)
O(3)-Si(1)-C(22')	104.7(4)
C(23')-Si(1)-C(22')	104.2(9)
C(24')-Si(1)-C(22')	100.8(8)
C(17)-O(2)-C(18)	120.70(19)
C(11)-O(3)-Si(1)	126.89(16)
C(1)-N(1)-C(8)	108.7(2)
C(1)-N(1)-H(1)	125.6
C(8)-N(1)-H(1)	125.6
C(17)-N(2)-C(12)	125.03(18)
C(17)-N(2)-C(9)	119.32(18)
C(12)-N(2)-C(9)	114.17(17)
N(1)-C(1)-C(2)	130.4(3)
N(1)-C(1)-C(6)	108.0(2)
C(2)-C(1)-C(6)	121.5(3)
C(3)-C(2)-C(1)	117.8(4)
C(3)-C(2)-H(2)	121.1
C(1)-C(2)-H(2)	121.1
C(2)-C(3)-C(4)	121.7(3)
C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(5)-C(4)-C(3)	121.5(4)
C(5)-C(4)-H(4)	119.2
C(3)-C(4)-H(4)	119.2
C(4)-C(5)-C(6)	118.0(3)
C(4)-C(5)-H(5)	121.0
C(6)-C(5)-H(5)	121.0
C(5)-C(6)-C(1)	119.5(2)
C(5)-C(6)-C(7)	134.1(3)
C(1)-C(6)-C(7)	106.4(3)
C(8)-C(7)-C(6)	106.2(2)
C(8)-C(7)-C(9)	127.6(2)
C(6)-C(7)-C(9)	126.2(2)

C(7)-C(8)-N(1)	110.6(3)
C(7)-C(8)-H(8)	124.7
N(1)-C(8)-H(8)	124.7
N(2)-C(9)-C(7)	113.82(19)
N(2)-C(9)-C(10)	101.85(18)
C(7)-C(9)-C(10)	114.0(2)
N(2)-C(9)-H(9)	109.0
C(7)-C(9)-H(9)	109.0
C(10)-C(9)-H(9)	109.0
C(11)-C(10)-C(9)	104.99(19)
C(11)-C(10)-H(10A)	110.7
C(9)-C(10)-H(10A)	110.7
C(11)-C(10)-H(10B)	110.7
C(9)-C(10)-H(10B)	110.7
H(10A)-C(10)-H(10B)	108.8
O(3)-C(11)-C(10)	111.9(2)
O(3)-C(11)-C(12)	112.24(19)
C(10)-C(11)-C(12)	103.76(18)
O(3)-C(11)-H(11)	109.6
C(10)-C(11)-H(11)	109.6
C(12)-C(11)-H(11)	109.6
N(2)-C(12)-C(13)	112.9(2)
N(2)-C(12)-C(11)	100.86(17)
C(13)-C(12)-C(11)	114.5(2)
N(2)-C(12)-H(12)	109.4
C(13)-C(12)-H(12)	109.4
C(11)-C(12)-H(12)	109.4
C(14)-C(13)-C(12)	114.6(2)
C(14)-C(13)-H(13A)	108.6
C(12)-C(13)-H(13A)	108.6
C(14)-C(13)-H(13B)	108.6
C(12)-C(13)-H(13B)	108.6
H(13A)-C(13)-H(13B)	107.6
C(15)-C(14)-C(13)	110.4(4)
C(15)-C(14)-C(16)	109.9(3)
C(13)-C(14)-C(16)	112.0(3)



C(15)-C(14)-H(14)	108.1
C(13)-C(14)-H(14)	108.1
C(16)-C(14)-H(14)	108.1
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(1)-C(17)-O(2)	125.5(2)
O(1)-C(17)-N(2)	123.2(2)
O(2)-C(17)-N(2)	111.25(19)
O(2)-C(18)-C(19)	110.8(2)
O(2)-C(18)-C(21)	102.5(2)
C(19)-C(18)-C(21)	110.6(3)
O(2)-C(18)-C(20)	108.9(2)
C(19)-C(18)-C(20)	112.9(3)
C(21)-C(18)-C(20)	110.8(3)
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5

C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
Si(1)-C(22)-H(22A)	109.5
Si(1)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
Si(1)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
Si(1)-C(23)-H(23A)	109.5
Si(1)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
Si(1)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-C(26)	106.5(15)
C(25)-C(24)-C(27)	110.1(12)
C(26)-C(24)-C(27)	109.1(13)
C(25)-C(24)-Si(1)	116.0(11)
C(26)-C(24)-Si(1)	114.5(12)
C(27)-C(24)-Si(1)	100.3(11)
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

C(24)-C(27)-H(27A)	109.5
C(24)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(24)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
Si(1)-C(22')-H(22D)	109.5
Si(1)-C(22')-H(22E)	109.5
H(22D)-C(22')-H(22E)	109.5
Si(1)-C(22')-H(22F)	109.5
H(22D)-C(22')-H(22F)	109.5
H(22E)-C(22')-H(22F)	109.5
Si(1)-C(23')-H(23D)	109.5
Si(1)-C(23')-H(23E)	109.5
H(23D)-C(23')-H(23E)	109.5
Si(1)-C(23')-H(23F)	109.5
H(23D)-C(23')-H(23F)	109.5
H(23E)-C(23')-H(23F)	109.5
C(27')-C(24')-C(26')	109(2)
C(27')-C(24')-C(25')	118(2)
C(26')-C(24')-C(25')	111(2)
C(27')-C(24')-Si(1)	114.9(16)
C(26')-C(24')-Si(1)	102.8(18)
C(25')-C(24')-Si(1)	100.7(16)
C(24')-C(25')-H(25D)	109.5
C(24')-C(25')-H(25E)	109.5
H(25D)-C(25')-H(25E)	109.5
C(24')-C(25')-H(25F)	109.5
H(25D)-C(25')-H(25F)	109.5
H(25E)-C(25')-H(25F)	109.5
C(24')-C(26')-H(26D)	109.5
C(24')-C(26')-H(26E)	109.5
H(26D)-C(26')-H(26E)	109.5
C(24')-C(26')-H(26F)	109.5
H(26D)-C(26')-H(26F)	109.5
H(26E)-C(26')-H(26F)	109.5

C(24')-C(27')-H(27D)	109.5
C(24')-C(27')-H(27E)	109.5
H(27D)-C(27')-H(27E)	109.5
C(24')-C(27')-H(27F)	109.5
H(27D)-C(27')-H(27F)	109.5
H(27E)-C(27')-H(27F)	109.5

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mo\_ddz21073\_0m. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Si(1)	86(1)	38(1)	38(1)	-1(1)	36(1)	8(1)
O(1)	39(1)	43(1)	29(1)	8(1)	13(1)	3(1)
O(2)	27(1)	59(1)	34(1)	7(1)	14(1)	0(1)
O(3)	54(1)	44(1)	28(1)	4(1)	20(1)	14(1)
N(1)	56(2)	42(1)	44(1)	-10(1)	12(1)	-12(1)
N(2)	24(1)	38(1)	26(1)	2(1)	9(1)	2(1)
C(1)	34(1)	62(2)	34(1)	-4(1)	13(1)	-10(1)
C(2)	52(2)	91(3)	34(2)	-9(2)	9(1)	-15(2)
C(3)	52(2)	113(4)	33(2)	4(2)	-3(1)	2(2)
C(4)	58(2)	87(3)	44(2)	21(2)	11(2)	21(2)
C(5)	43(2)	56(2)	36(1)	8(1)	13(1)	8(1)
C(6)	27(1)	50(2)	28(1)	0(1)	13(1)	0(1)
C(7)	25(1)	39(1)	29(1)	0(1)	10(1)	1(1)
C(8)	44(2)	41(2)	37(1)	0(1)	10(1)	-2(1)
C(9)	28(1)	34(1)	29(1)	1(1)	10(1)	5(1)
C(10)	31(1)	49(2)	34(1)	-1(1)	17(1)	6(1)
C(11)	39(1)	32(1)	25(1)	1(1)	13(1)	6(1)
C(12)	28(1)	32(1)	25(1)	1(1)	8(1)	0(1)
C(13)	41(1)	31(1)	36(1)	1(1)	16(1)	5(1)
C(14)	63(2)	57(2)	38(2)	10(1)	19(1)	30(2)
C(15)	106(4)	80(3)	99(4)	53(3)	36(3)	40(3)
C(16)	52(2)	85(3)	73(2)	5(2)	4(2)	19(2)
C(17)	30(1)	27(1)	30(1)	1(1)	11(1)	1(1)
C(18)	35(1)	56(2)	39(1)	0(1)	21(1)	-2(1)
C(19)	60(2)	69(2)	97(3)	20(2)	49(2)	-7(2)
C(20)	56(2)	86(3)	71(2)	-28(2)	28(2)	2(2)
C(21)	31(1)	110(3)	61(2)	5(2)	22(1)	6(2)
C(22)	172(13)	96(9)	68(6)	22(6)	63(8)	92(8)
C(23)	129(9)	114(8)	75(6)	-22(5)	41(6)	-83(7)
C(24)	76(3)	57(3)	43(3)	-4(3)	38(3)	1(3)
C(25)	104(5)	42(3)	58(3)	11(3)	41(3)	0(3)

C(26)	77(4)	58(5)	42(3)	2(4)	28(3)	8(5)
C(27)	78(5)	85(6)	73(5)	-12(4)	26(4)	-19(5)
C(22')	144(11)	119(10)	74(7)	47(7)	70(8)	94(8)
C(23')	144(12)	110(10)	78(8)	-46(7)	61(8)	-57(8)
C(24')	82(4)	57(3)	44(4)	2(3)	35(3)	3(3)
C(25')	108(6)	79(6)	59(5)	17(5)	35(5)	37(5)
C(26')	83(5)	59(7)	39(4)	0(5)	43(4)	-1(6)
C(27')	107(6)	59(5)	67(5)	2(4)	40(4)	-26(4)

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Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for mo\_ddz21073\_0m.

	x	y	z	U(eq)
H(1)	6316	7040	10023	57
H(2)	8123	5980	11864	72
H(3)	8847	4158	12573	83
H(4)	8006	2482	11571	76
H(5)	6355	2575	9831	53
H(8)	4680	6427	8289	49
H(9)	4591	3166	8057	36
H(10A)	5002	5005	6658	44
H(10B)	5431	3671	6634	44
H(11)	3240	3095	5726	38
H(12)	1423	3987	6065	34
H(13A)	1678	6080	6709	42
H(13B)	2792	6138	6054	42
H(14)	1011	5491	4398	62
H(15A)	687	7734	5235	141
H(15B)	164	7372	3953	141
H(15C)	1755	7422	4577	141
H(16A)	-589	4868	5338	110
H(16B)	-1261	5760	4360	110
H(16C)	-816	6185	5625	110
H(19A)	-247	2365	8459	105
H(19B)	-743	2892	9451	105
H(19C)	843	2766	9587	105
H(20A)	1318	4903	9952	103
H(20B)	-228	5067	9937	103
H(20C)	379	5823	9128	103
H(21A)	-1372	5187	7446	98
H(21B)	-2102	4427	8168	98
H(21C)	-1645	3843	7181	98
H(22A)	5476	2717	4606	159

H(22B)	4862	2289	3349	159
H(22C)	4127	1950	4264	159
H(23A)	1338	2914	3211	155
H(23B)	1969	2720	2203	155
H(23C)	1305	3937	2347	155
H(25A)	2343	5877	2135	96
H(25B)	3659	6682	2390	96
H(25C)	3061	6304	3378	96
H(26A)	3385	4216	1325	85
H(26B)	4991	4089	1840	85
H(26C)	4353	5293	1314	85
H(27A)	6020	5904	3324	117
H(27B)	6174	4621	3819	117
H(27C)	5534	5617	4393	117
H(22D)	6135	3740	4741	157
H(22E)	5844	2885	3699	157
H(22F)	5478	2498	4799	157
H(23D)	2516	2102	3754	157
H(23E)	2944	2183	2631	157
H(23F)	1649	2878	2742	157
H(25D)	2387	6058	3071	120
H(25E)	1824	5103	2129	120
H(25F)	2534	6246	1851	120
H(26D)	4217	4882	1170	83
H(26E)	3529	3759	1515	83
H(26F)	5126	3965	2018	83
H(27D)	6077	5329	3402	112
H(27E)	5239	6014	4091	112
H(27F)	5253	6470	2893	112

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Table 6. Torsion angles [ ° ] for mo\_ddz21073\_0m.

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C(22)-Si(1)-O(3)-C(11)	-21.2(7)
C(23')-Si(1)-O(3)-C(11)	58.8(8)
C(24)-Si(1)-O(3)-C(11)	-156.7(5)
C(24')-Si(1)-O(3)-C(11)	-161.1(7)
C(23)-Si(1)-O(3)-C(11)	92.6(4)
C(22')-Si(1)-O(3)-C(11)	-54.8(5)
C(8)-N(1)-C(1)-C(2)	-178.0(3)
C(8)-N(1)-C(1)-C(6)	-0.4(3)
N(1)-C(1)-C(2)-C(3)	177.8(3)
C(6)-C(1)-C(2)-C(3)	0.4(5)
C(1)-C(2)-C(3)-C(4)	0.4(5)
C(2)-C(3)-C(4)-C(5)	-0.9(6)
C(3)-C(4)-C(5)-C(6)	0.5(5)
C(4)-C(5)-C(6)-C(1)	0.3(4)
C(4)-C(5)-C(6)-C(7)	-178.1(3)
N(1)-C(1)-C(6)-C(5)	-178.6(2)
C(2)-C(1)-C(6)-C(5)	-0.7(4)
N(1)-C(1)-C(6)-C(7)	0.1(3)
C(2)-C(1)-C(6)-C(7)	178.0(3)
C(5)-C(6)-C(7)-C(8)	178.7(3)
C(1)-C(6)-C(7)-C(8)	0.2(3)
C(5)-C(6)-C(7)-C(9)	-3.5(4)
C(1)-C(6)-C(7)-C(9)	178.0(2)
C(6)-C(7)-C(8)-N(1)	-0.4(3)
C(9)-C(7)-C(8)-N(1)	-178.2(2)
C(1)-N(1)-C(8)-C(7)	0.5(3)
C(17)-N(2)-C(9)-C(7)	-66.3(3)
C(12)-N(2)-C(9)-C(7)	126.9(2)
C(17)-N(2)-C(9)-C(10)	170.6(2)
C(12)-N(2)-C(9)-C(10)	3.8(3)
C(8)-C(7)-C(9)-N(2)	-54.8(3)
C(6)-C(7)-C(9)-N(2)	127.9(2)
C(8)-C(7)-C(9)-C(10)	61.5(3)
C(6)-C(7)-C(9)-C(10)	-115.9(3)

N(2)-C(9)-C(10)-C(11)	-25.7(3)
C(7)-C(9)-C(10)-C(11)	-148.7(2)
Si(1)-O(3)-C(11)-C(10)	98.2(3)
Si(1)-O(3)-C(11)-C(12)	-145.65(19)
C(9)-C(10)-C(11)-O(3)	159.3(2)
C(9)-C(10)-C(11)-C(12)	38.1(3)
C(17)-N(2)-C(12)-C(13)	90.3(3)
C(9)-N(2)-C(12)-C(13)	-103.8(2)
C(17)-N(2)-C(12)-C(11)	-147.0(2)
C(9)-N(2)-C(12)-C(11)	18.9(3)
O(3)-C(11)-C(12)-N(2)	-155.1(2)
C(10)-C(11)-C(12)-N(2)	-34.1(2)
O(3)-C(11)-C(12)-C(13)	-33.5(3)
C(10)-C(11)-C(12)-C(13)	87.5(2)
N(2)-C(12)-C(13)-C(14)	-157.1(2)
C(11)-C(12)-C(13)-C(14)	88.2(3)
C(12)-C(13)-C(14)-C(15)	-164.0(3)
C(12)-C(13)-C(14)-C(16)	73.2(3)
C(18)-O(2)-C(17)-O(1)	8.9(4)
C(18)-O(2)-C(17)-N(2)	-170.8(2)
C(12)-N(2)-C(17)-O(1)	166.8(2)
C(9)-N(2)-C(17)-O(1)	1.5(4)
C(12)-N(2)-C(17)-O(2)	-13.5(3)
C(9)-N(2)-C(17)-O(2)	-178.8(2)
C(17)-O(2)-C(18)-C(19)	-60.9(3)
C(17)-O(2)-C(18)-C(21)	-178.9(3)
C(17)-O(2)-C(18)-C(20)	63.8(3)
O(3)-Si(1)-C(24)-C(25)	-45.9(10)
C(22)-Si(1)-C(24)-C(25)	-178.7(9)
C(23')-Si(1)-C(24)-C(25)	93.4(13)
C(24')-Si(1)-C(24)-C(25)	49(16)
C(23)-Si(1)-C(24)-C(25)	65.4(11)
C(22')-Si(1)-C(24)-C(25)	-153.5(10)
O(3)-Si(1)-C(24)-C(26)	-170.6(11)
C(22)-Si(1)-C(24)-C(26)	56.6(15)
C(23')-Si(1)-C(24)-C(26)	-31.4(17)

C(24')-Si(1)-C(24)-C(26)	-75(16)
C(23)-Si(1)-C(24)-C(26)	-59.4(13)
C(22')-Si(1)-C(24)-C(26)	81.8(13)
O(3)-Si(1)-C(24)-C(27)	72.7(8)
C(22)-Si(1)-C(24)-C(27)	-60.1(11)
C(23')-Si(1)-C(24)-C(27)	-148.0(10)
C(24')-Si(1)-C(24)-C(27)	168(17)
C(23)-Si(1)-C(24)-C(27)	-176.1(8)
C(22')-Si(1)-C(24)-C(27)	-34.9(9)
O(3)-Si(1)-C(24')-C(27')	63.1(15)
C(22)-Si(1)-C(24')-C(27')	-72.9(18)
C(23')-Si(1)-C(24')-C(27')	-160.9(13)
C(24)-Si(1)-C(24')-C(27')	-23(15)
C(23)-Si(1)-C(24')-C(27')	172.8(14)
C(22')-Si(1)-C(24')-C(27')	-46.0(16)
O(3)-Si(1)-C(24')-C(26')	-178.8(15)
C(22)-Si(1)-C(24')-C(26')	45.2(19)
C(23')-Si(1)-C(24')-C(26')	-43(2)
C(24)-Si(1)-C(24')-C(26')	95(17)
C(23)-Si(1)-C(24')-C(26')	-69.1(17)
C(22')-Si(1)-C(24')-C(26')	72.1(17)
O(3)-Si(1)-C(24')-C(25')	-64.2(12)
C(22)-Si(1)-C(24')-C(25')	159.7(10)
C(23')-Si(1)-C(24')-C(25')	71.8(16)
C(24)-Si(1)-C(24')-C(25')	-150(17)
C(23)-Si(1)-C(24')-C(25')	45.5(13)
C(22')-Si(1)-C(24')-C(25')	-173.4(11)

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Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo\_ddz21073\_0m [ $\text{\AA}$  and  $^\circ$ ].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
N(1)-H(1)...O(1)#1	0.87	2.07	2.920(3)	163.6
C(19)-H(19C)...O(1)	0.97	2.35	2.931(4)	117.9
C(20)-H(20A)...O(1)	0.97	2.49	3.075(4)	118.4

Symmetry transformations used to generate equivalent atoms:

#1  $-x+1, y+1/2, -z+2$