

## **I<sub>2</sub>-Mediated Transition-Metal-Free Aromatic C–H Amination for the Synthesis of Benzimidazol-2-ones and Related Heterocycles**

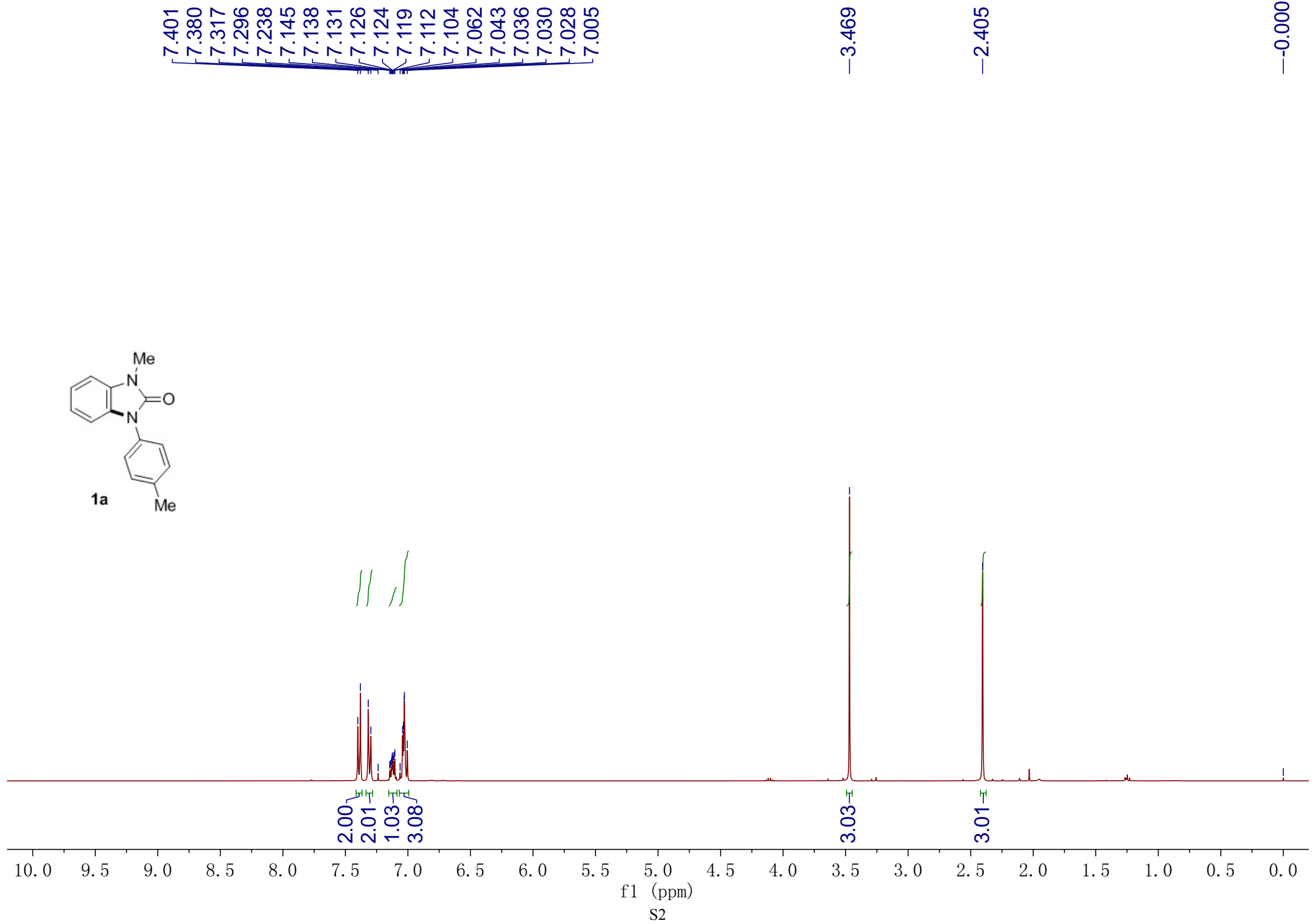
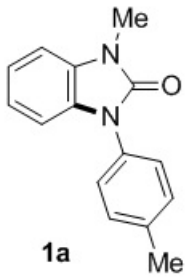
Yinggao Meng,<sup>a</sup> Bingnan Wang,<sup>a</sup> Linning Ren,<sup>a</sup> Qiongli Zhao,<sup>b</sup> Wenquan Yu,<sup>a,\*</sup> and Junbiao Chang<sup>a,b,\*</sup>

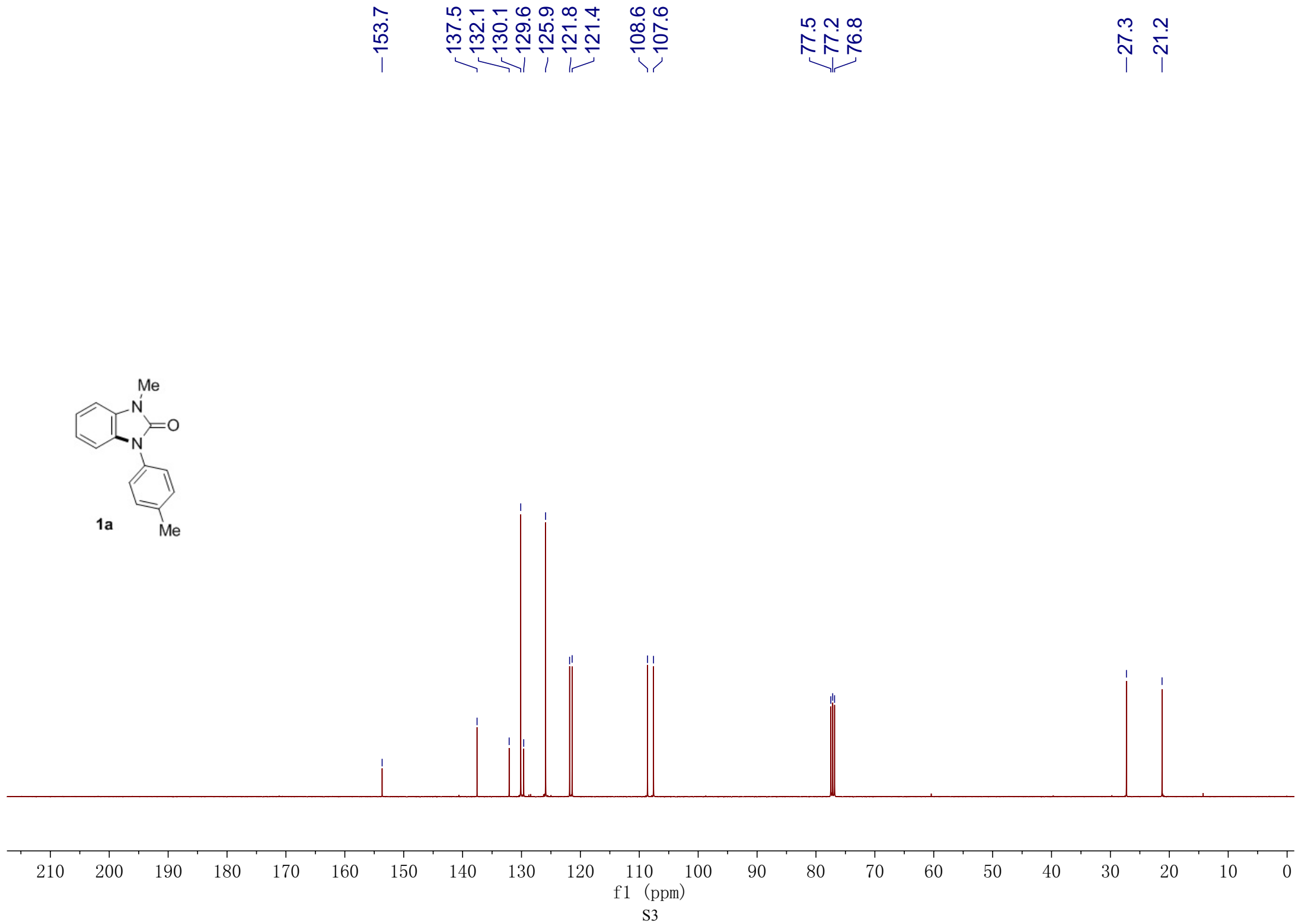
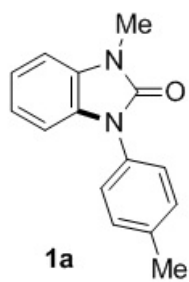
<sup>a</sup>*College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou, Henan Province 450001, China*

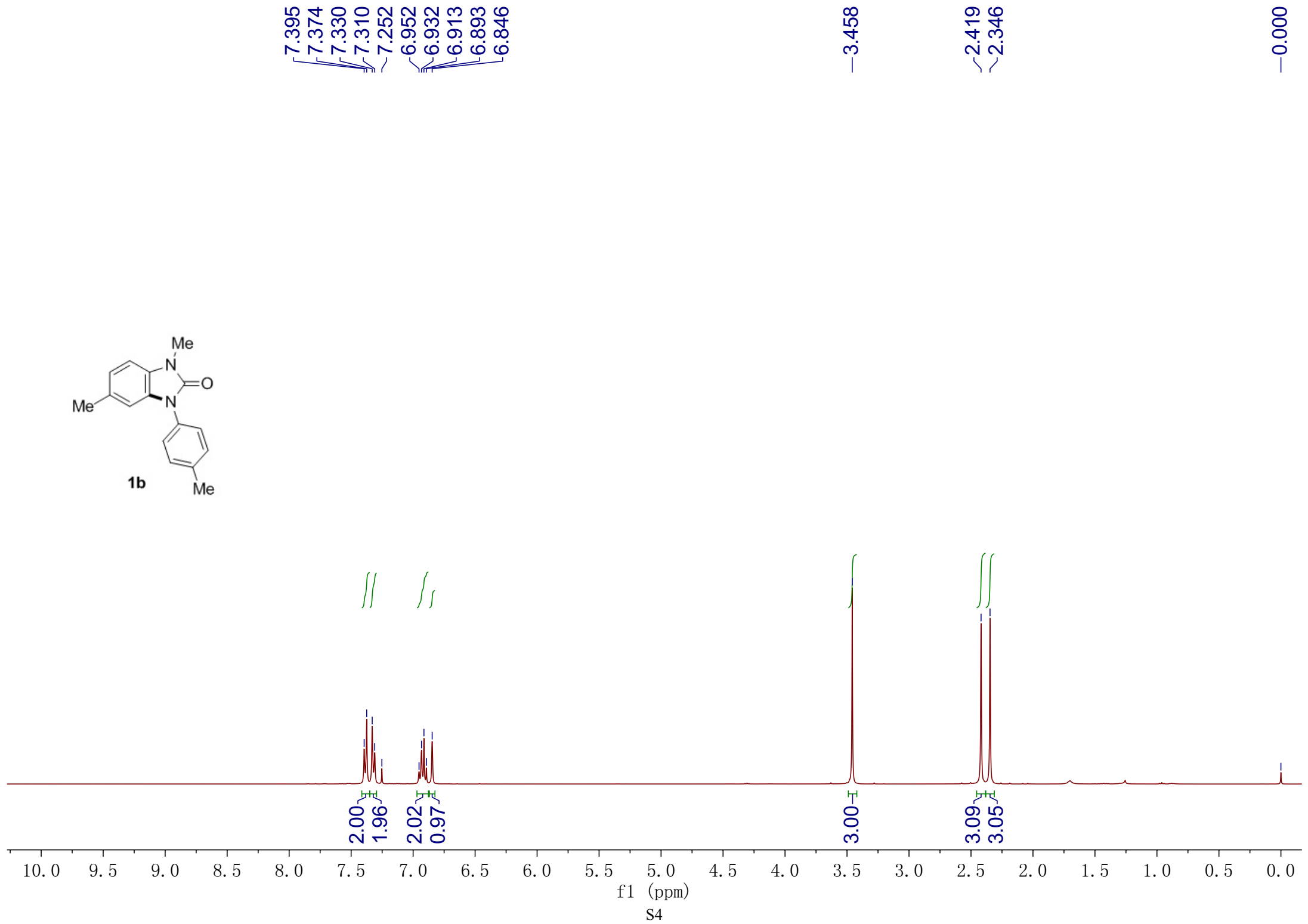
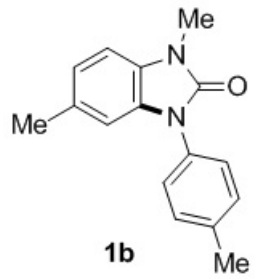
<sup>b</sup>*Collaborative Innovation Center of New Drug Research and Safety Evaluation, Henan Province, and School of Pharmaceutical Sciences, Zhengzhou University, Zhengzhou, Henan Province 450001, China*

1. <sup>1</sup>H NMR and <sup>13</sup>C NMR Spectra of Products **1**

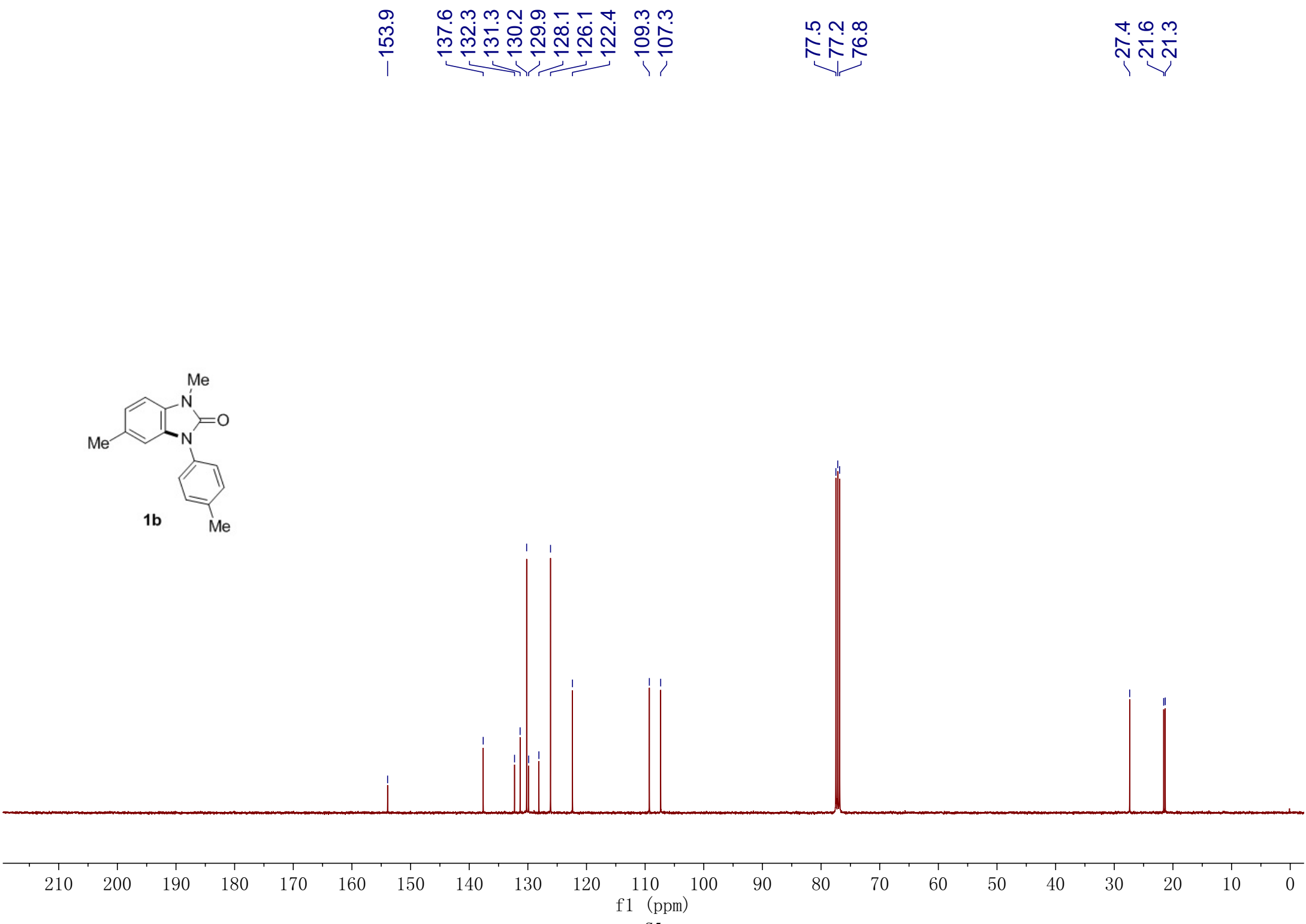
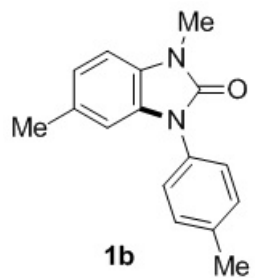
S2

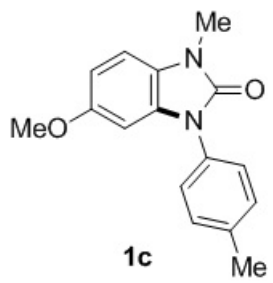










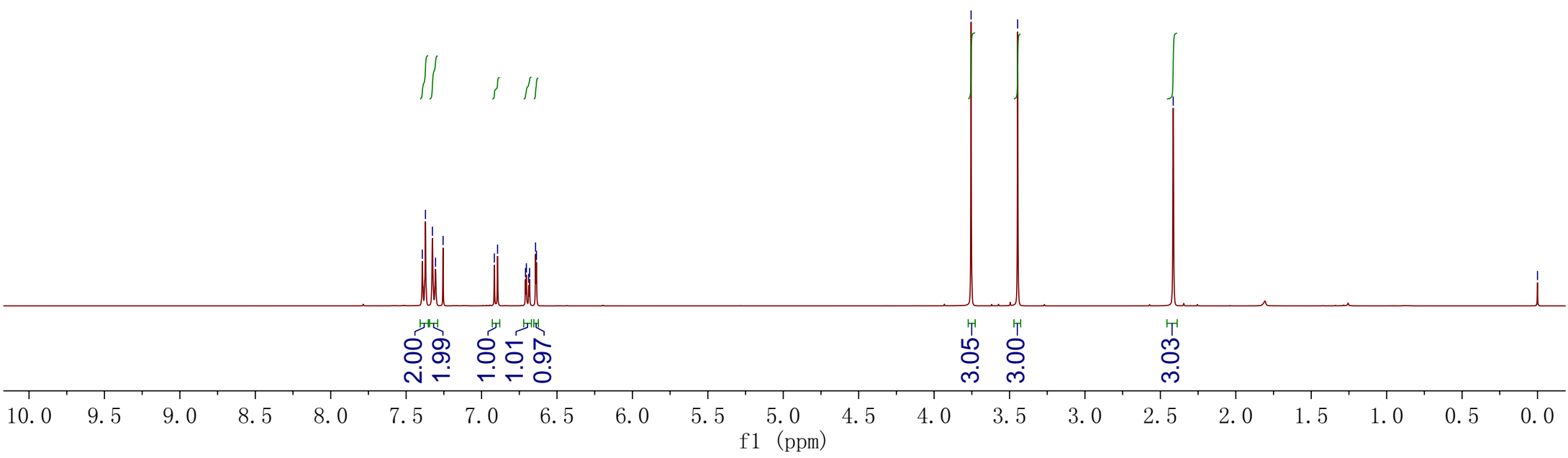


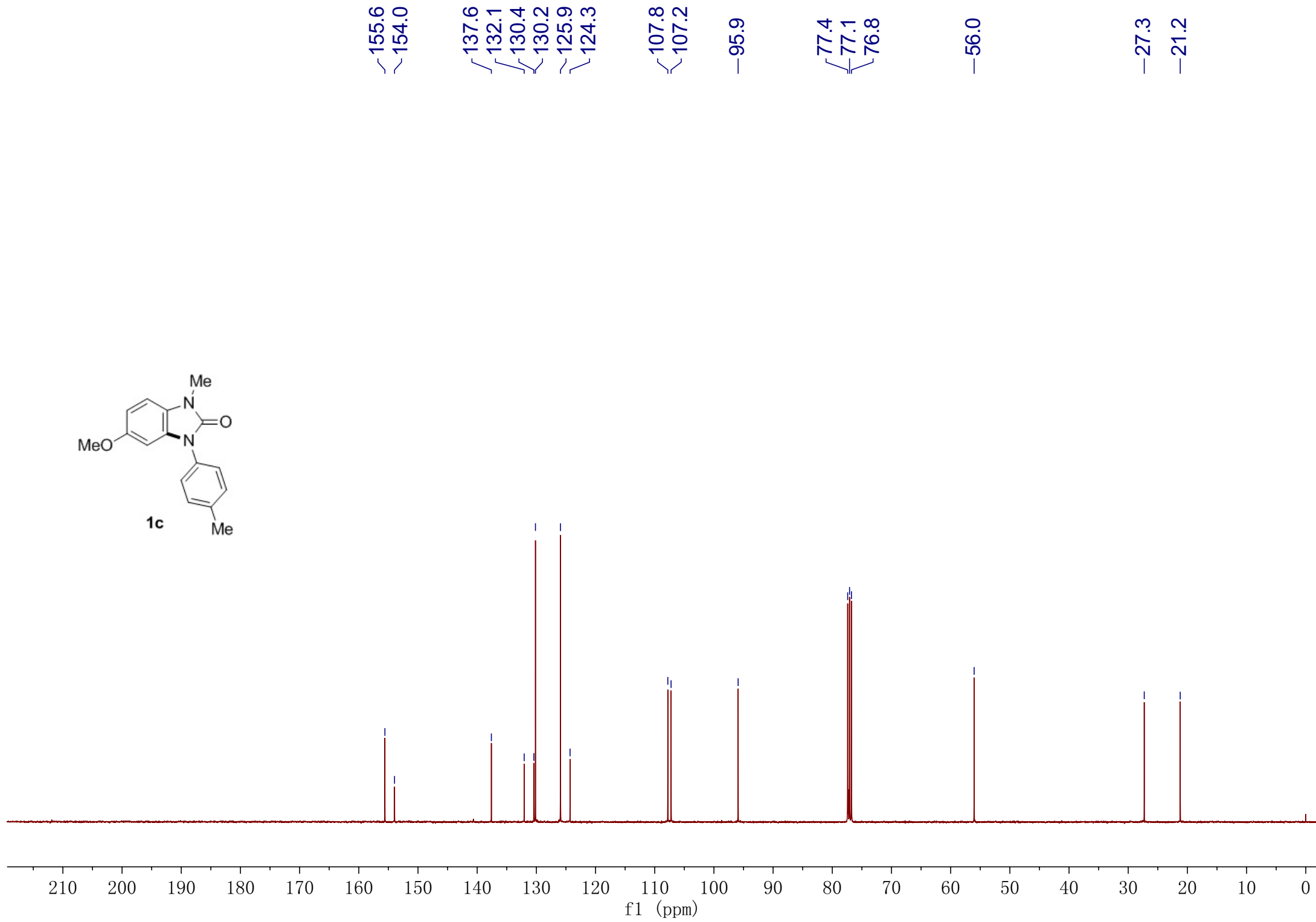
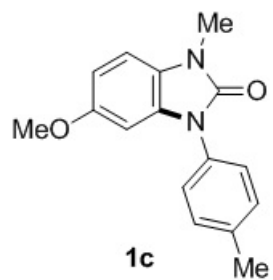
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7.372  
7.326  
7.305  
7.255  
6.915  
6.894  
6.709  
6.703  
6.688  
6.682  
6.642  
6.636

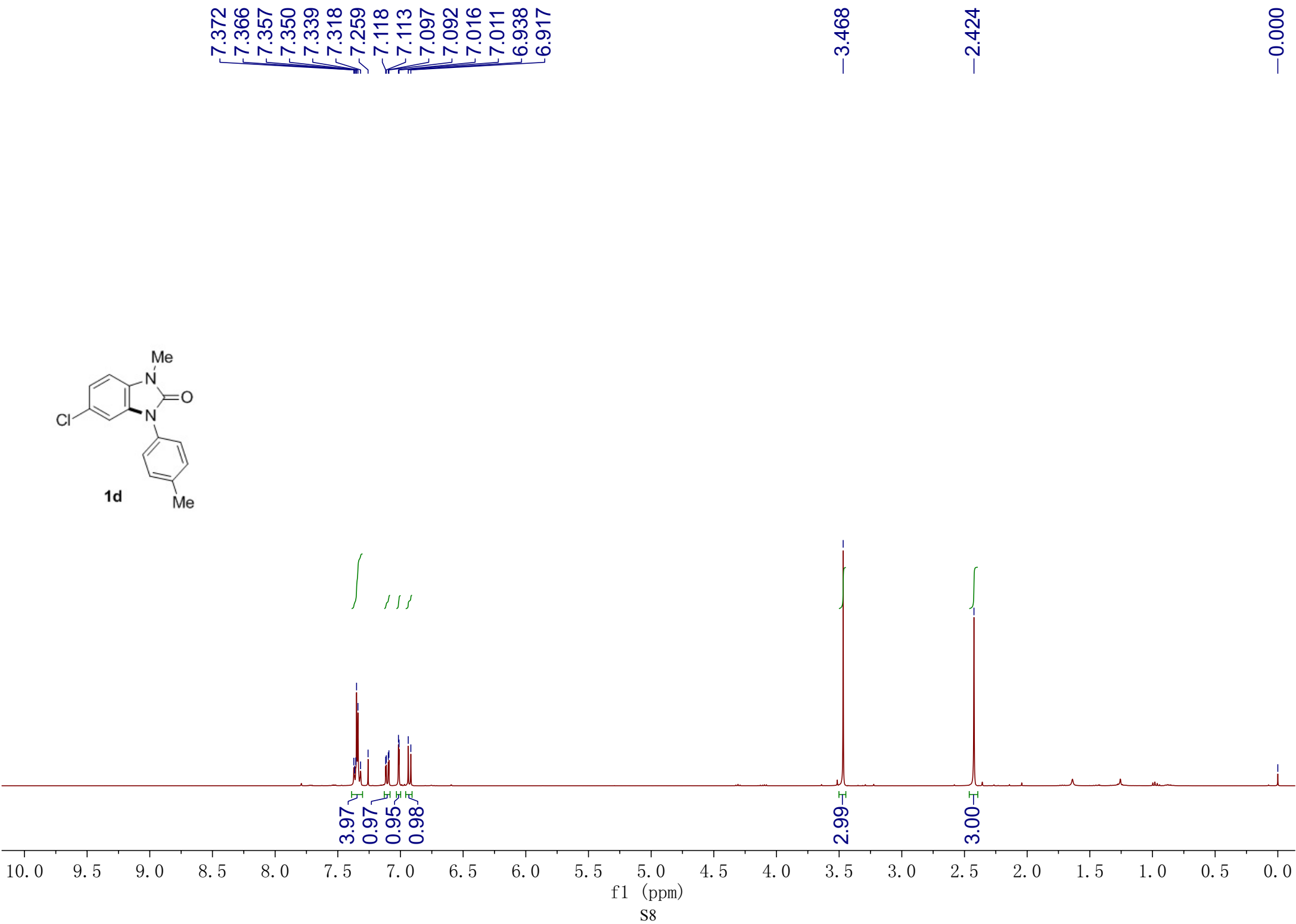
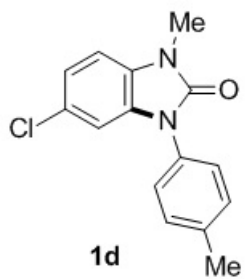
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-3.446

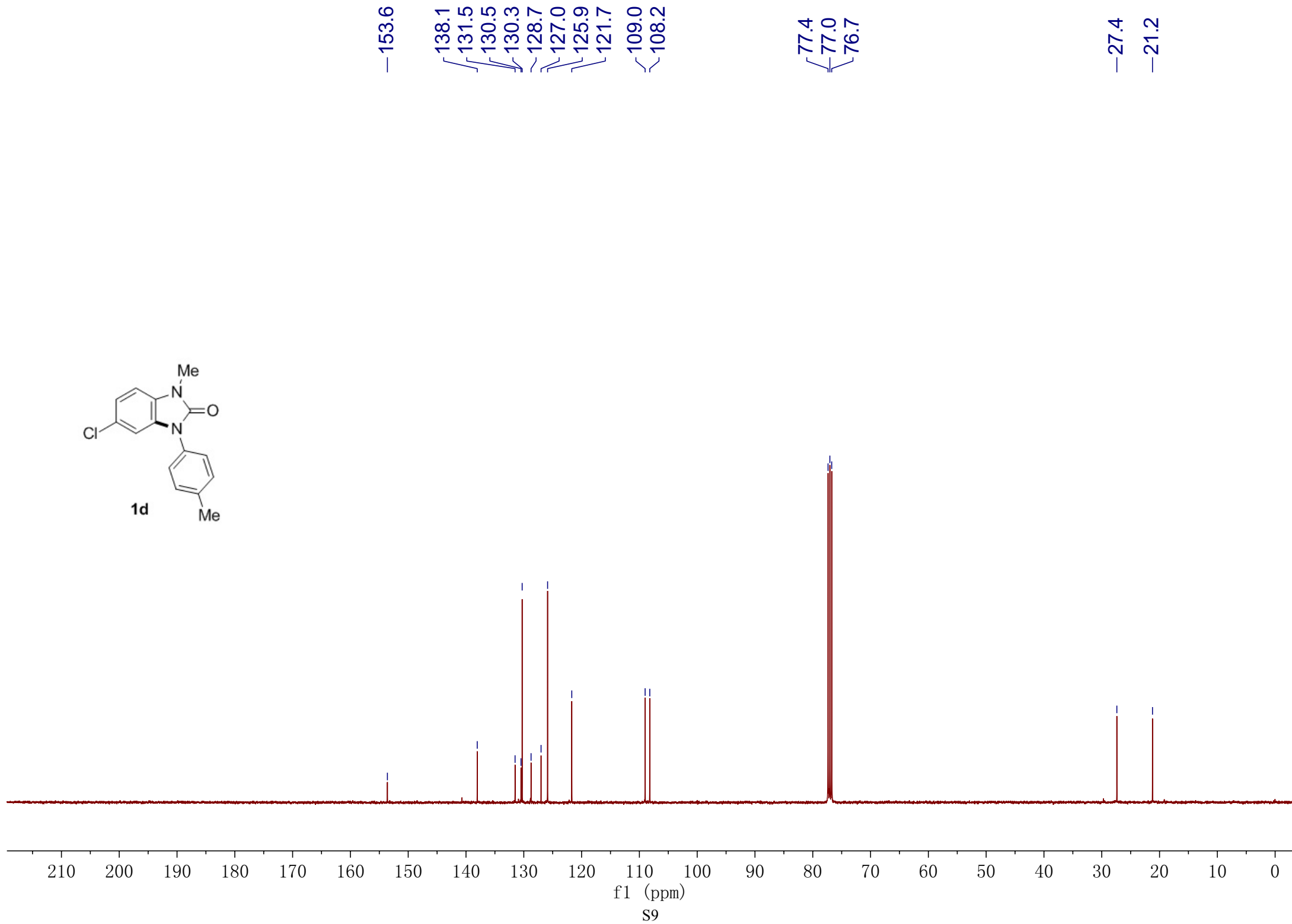
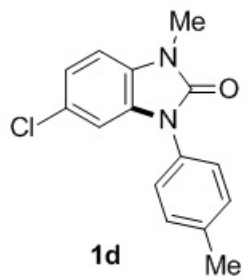
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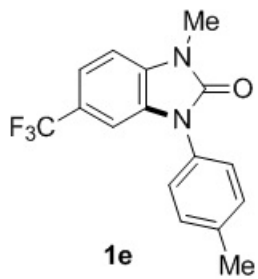
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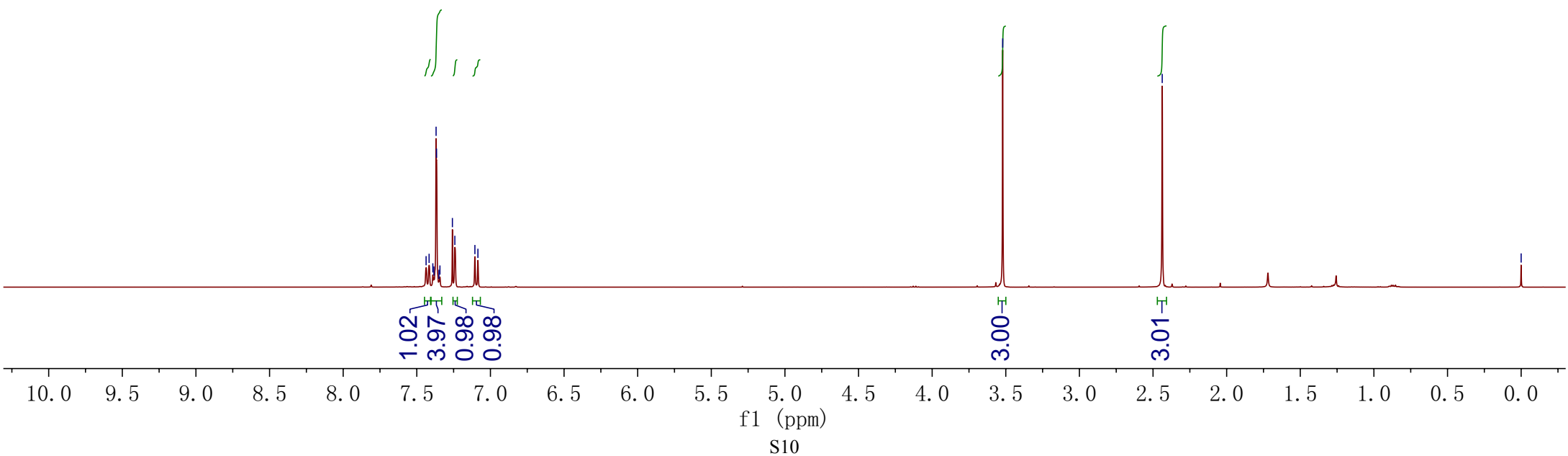


7.437  
7.416  
7.391  
7.384  
7.369  
7.366  
7.350  
7.343  
7.258  
7.242  
7.105  
7.085

3.521

2.438

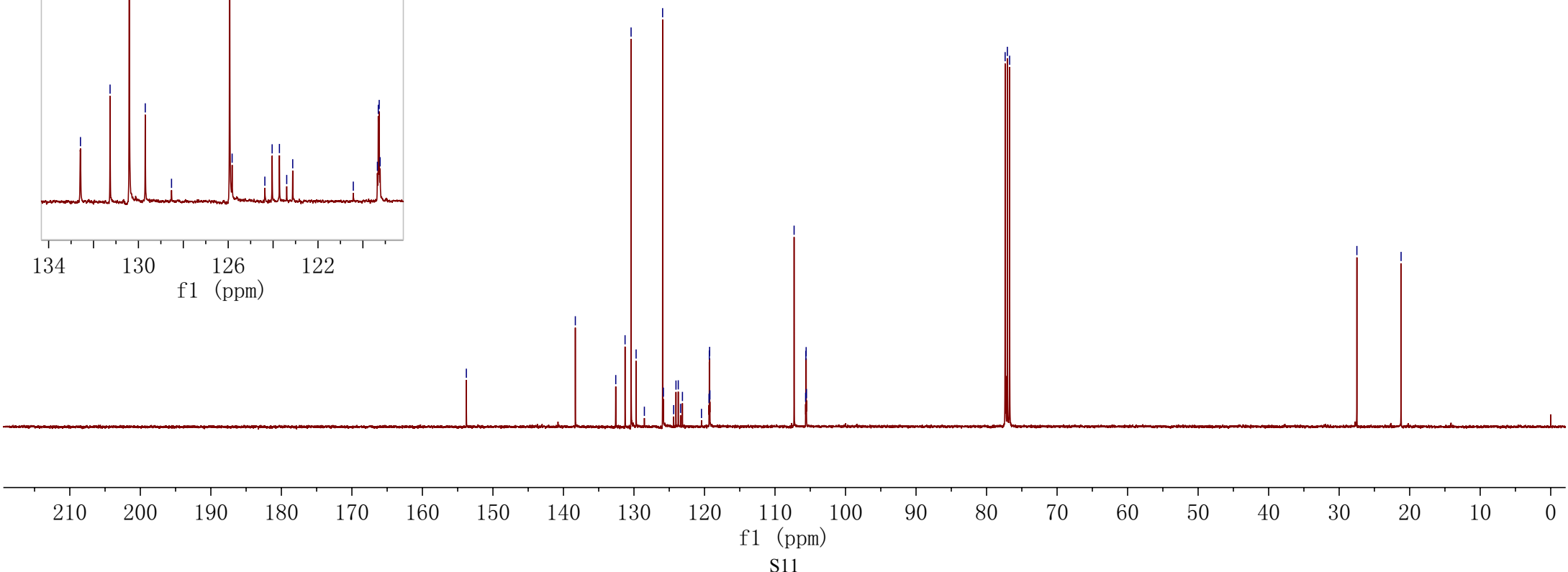
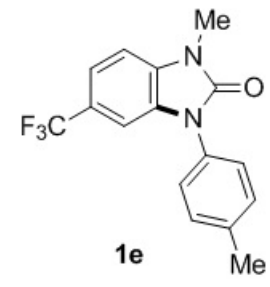
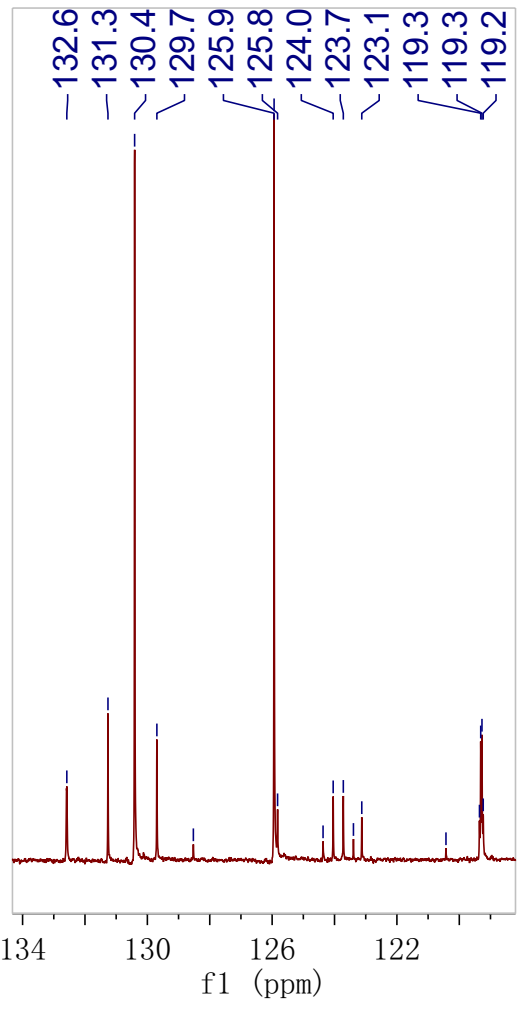
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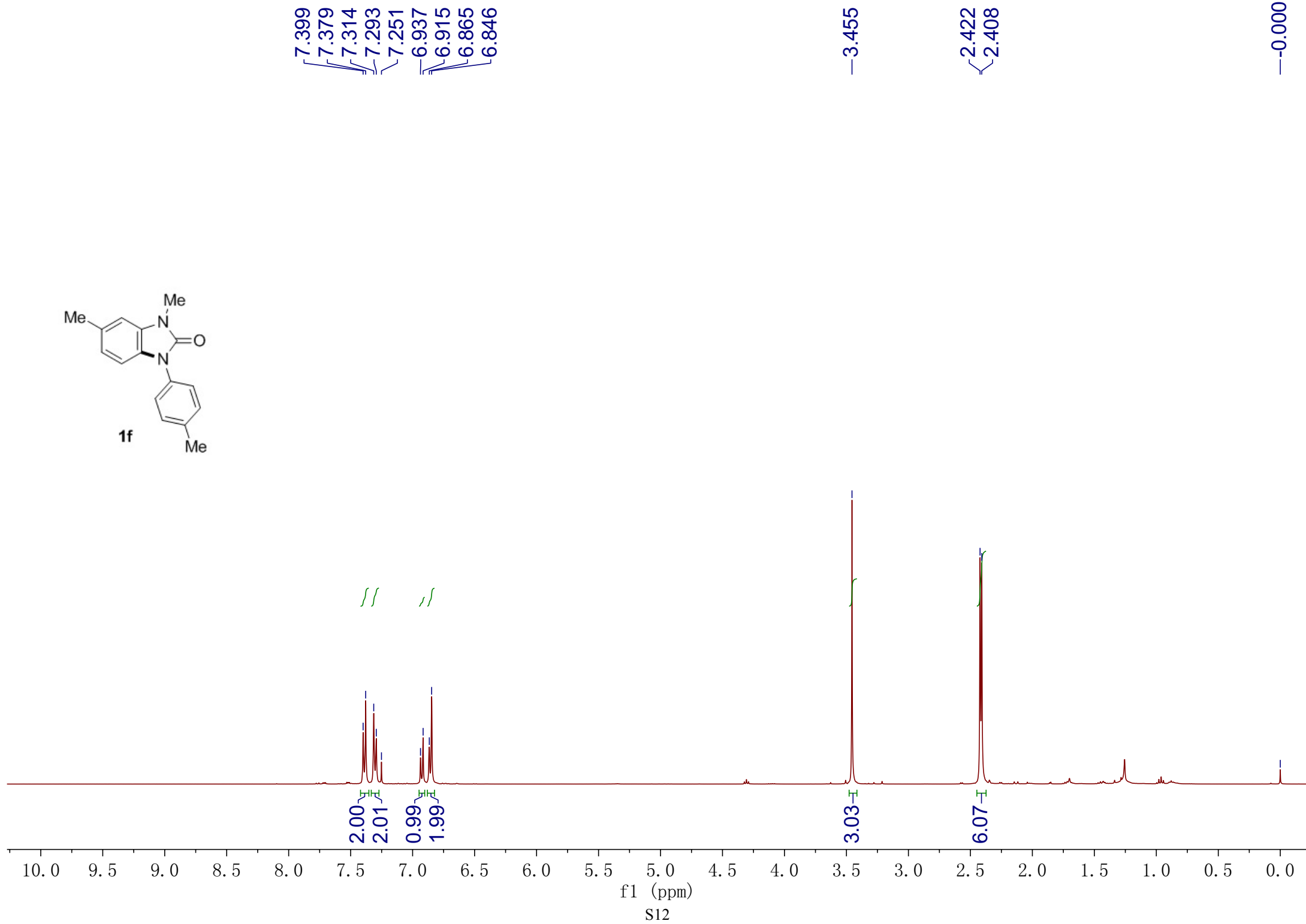
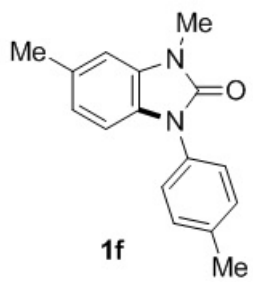


153.8  
138.3  
132.6  
131.3  
130.4  
129.7  
125.9  
125.8  
124.0  
123.7  
123.1  
119.3  
119.3  
119.2  
107.3  
105.7  
105.6  
105.6  
105.5

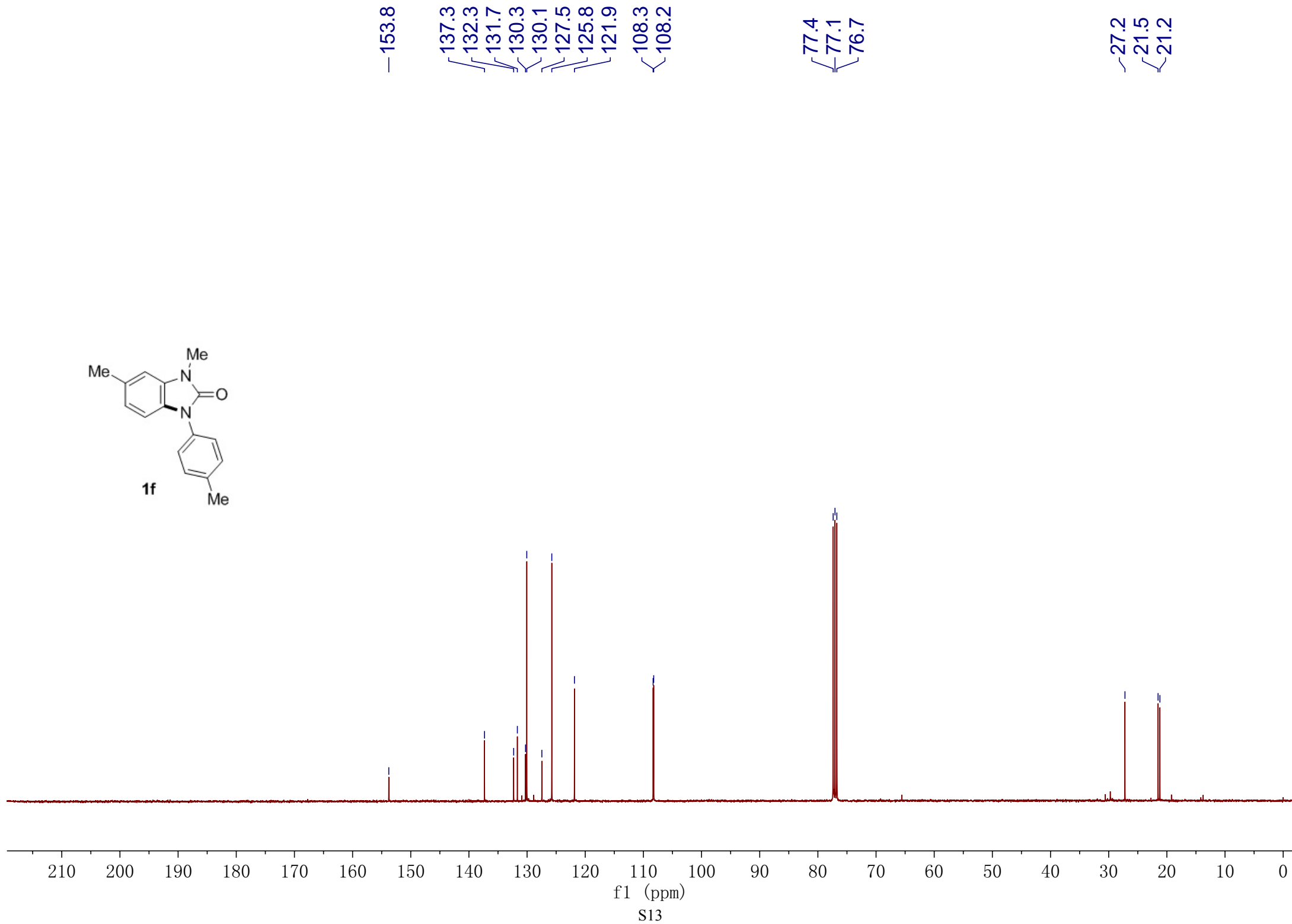
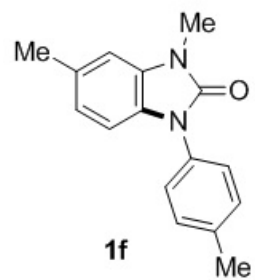
77.4  
77.0  
76.7

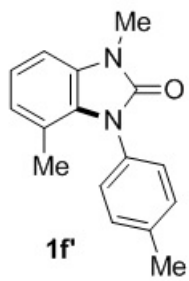
27.5  
21.2











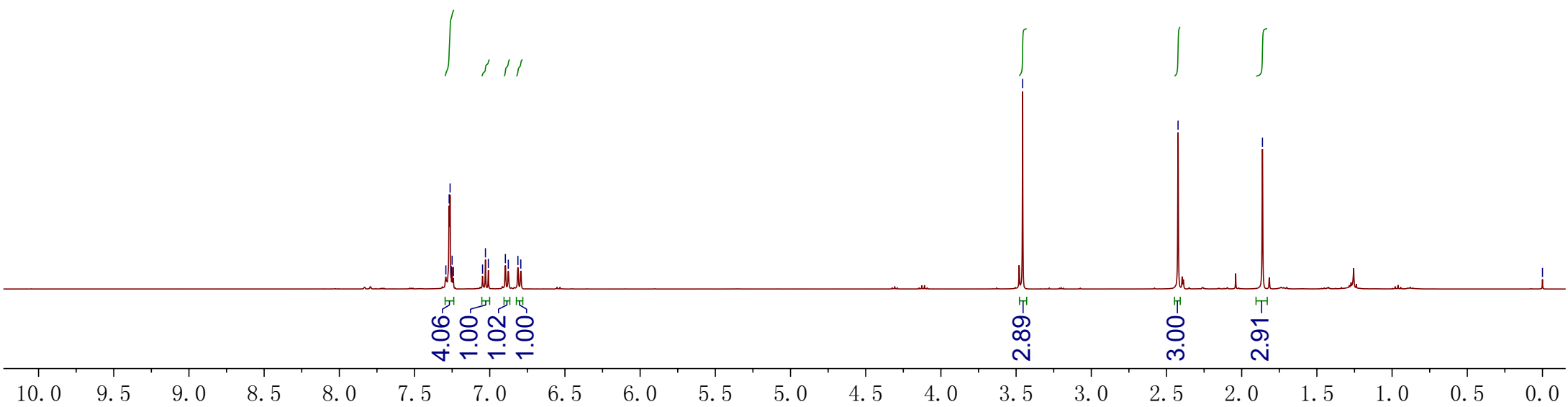
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7.270  
7.264  
7.257  
7.250  
7.242  
7.048  
7.029  
7.009  
6.896  
6.877  
6.813  
6.793

-3.457

-2.423

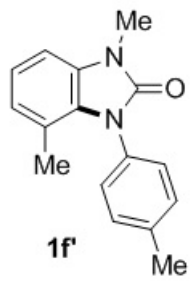
-1.862

-0.000



f1 (ppm)

S14



—154.7

138.6

133.5

130.5

129.7

128.9

127.8

124.6

121.4

120.1

—105.4

77.4

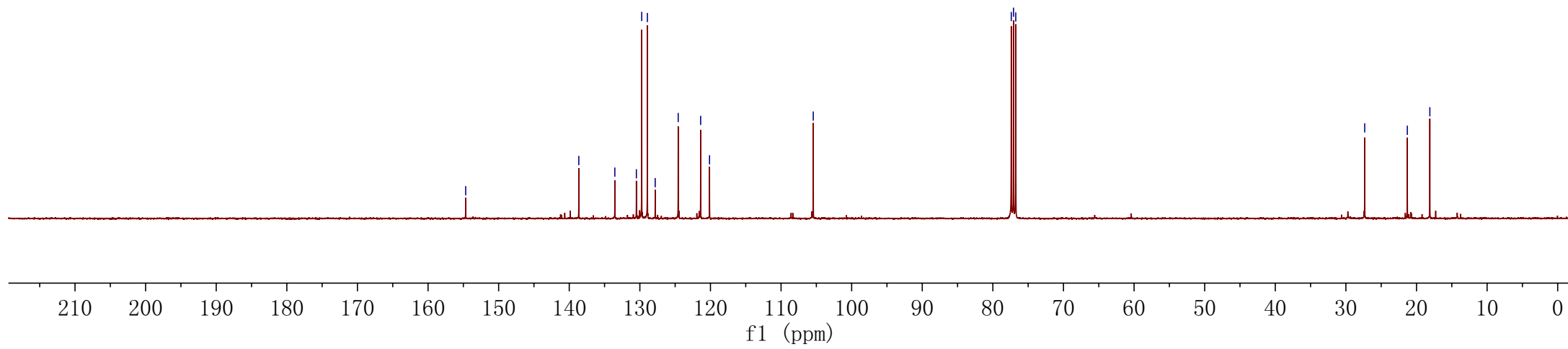
77.1

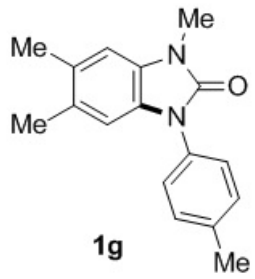
76.8

~27.3

~21.3

~18.1



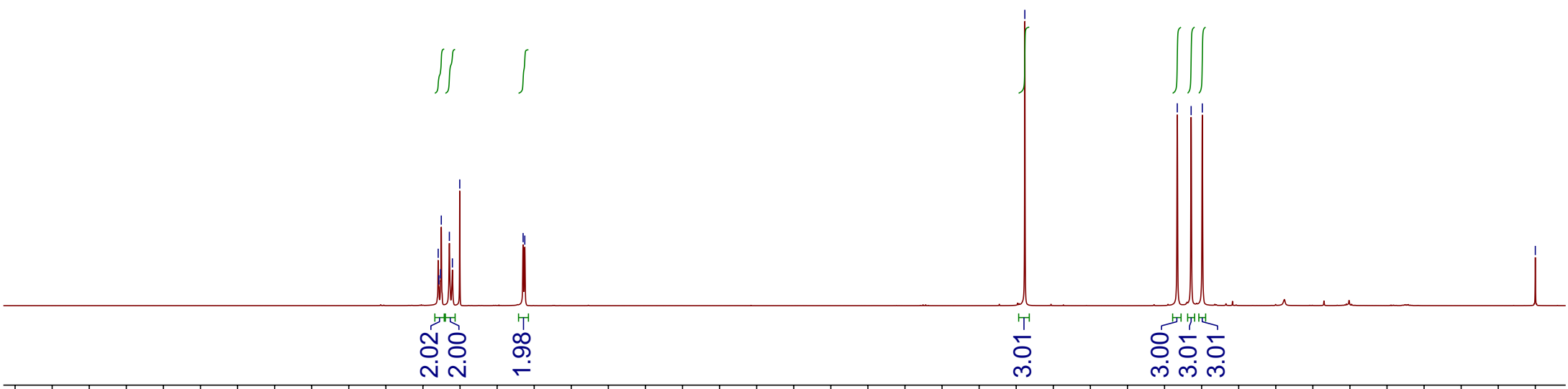


7.397  
7.393  
7.381  
7.376  
7.322  
7.301  
7.252  
6.825  
6.813

-3.442

2.414  
2.321  
2.245

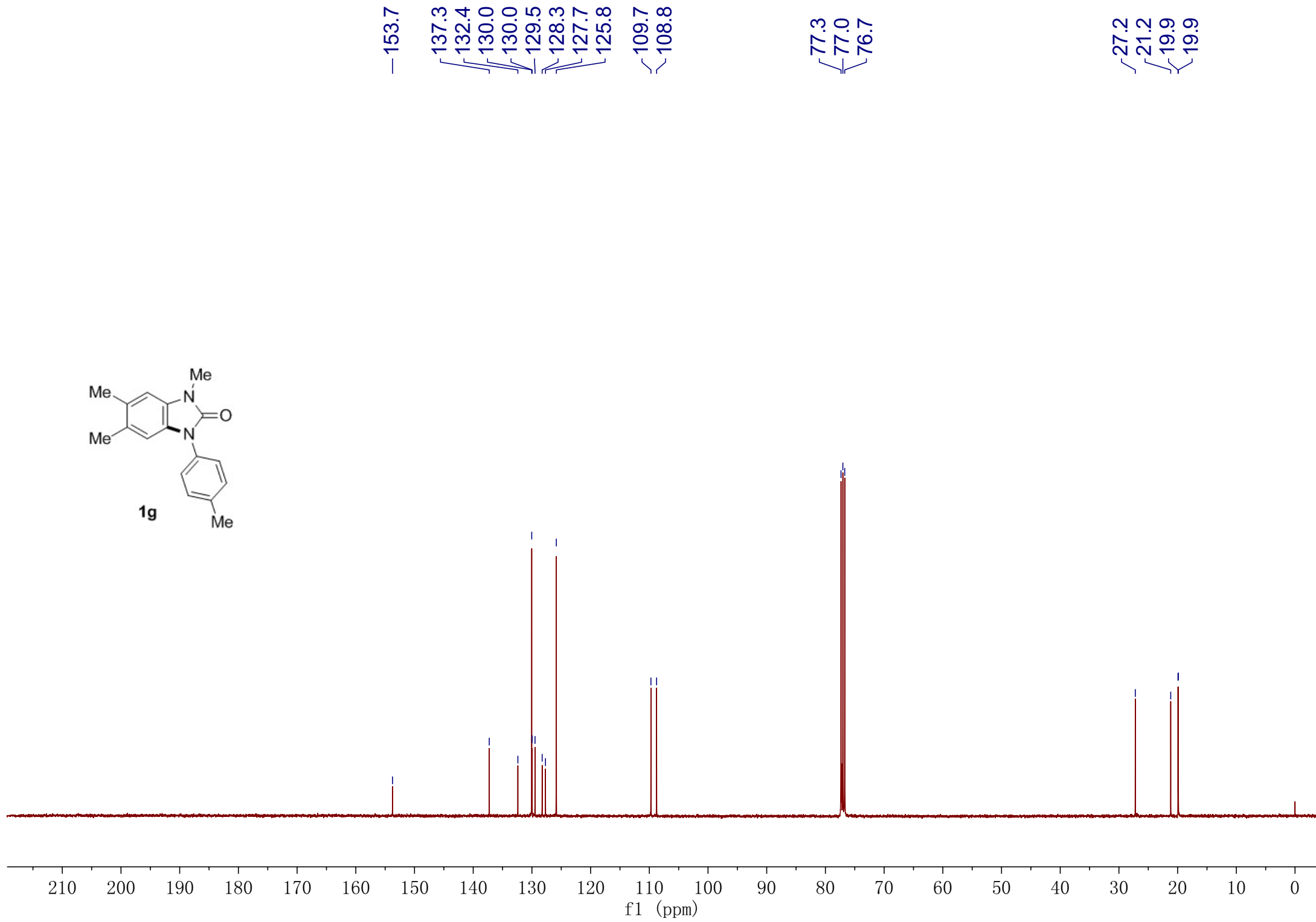
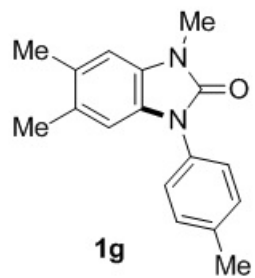
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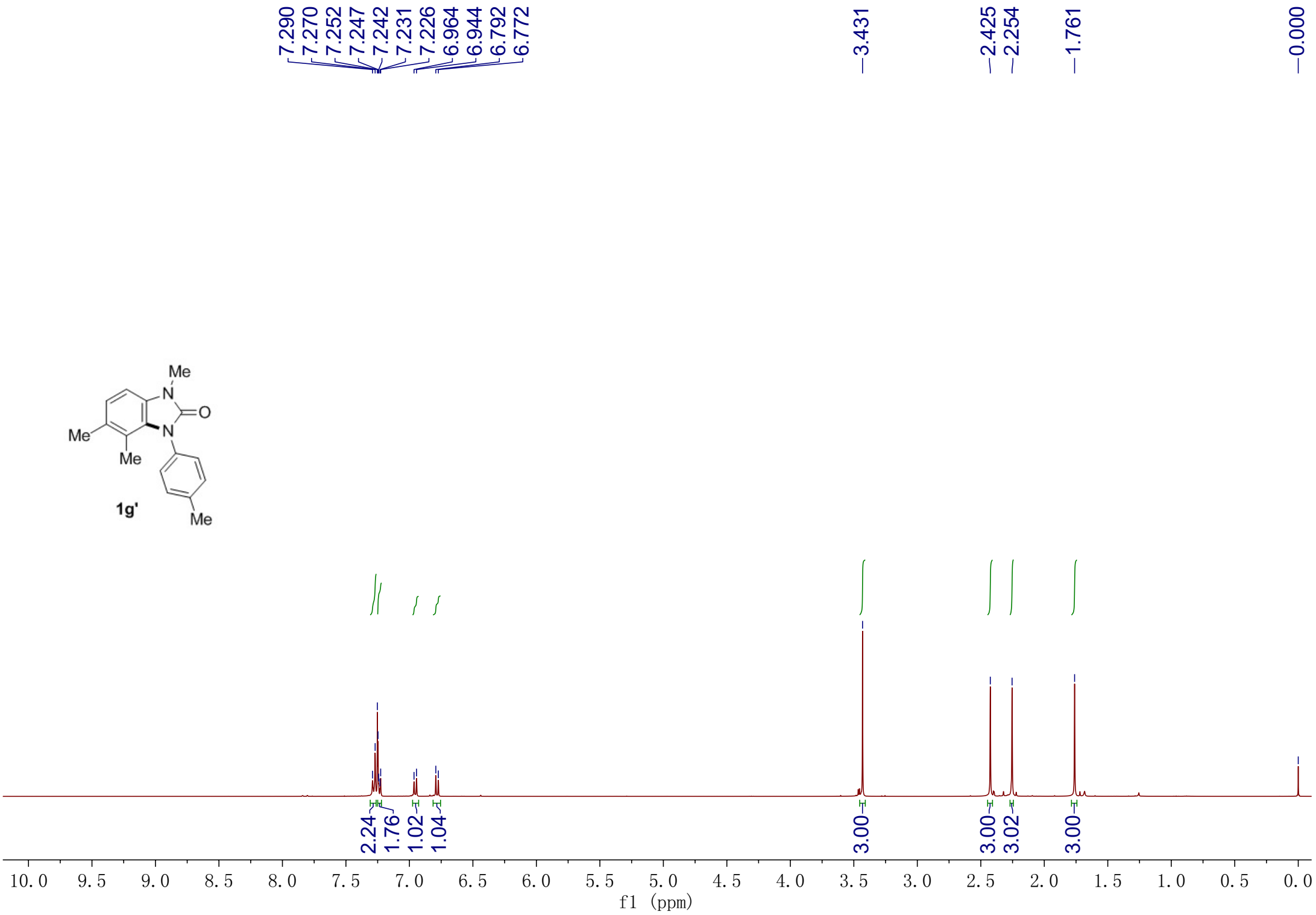
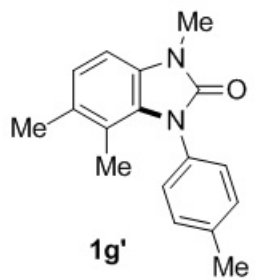


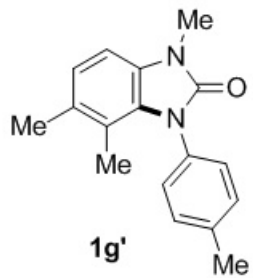
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)

S16







—154.9

138.4

134.1

130.8

129.8

129.0

128.7

128.2

122.9

119.0

—104.7

77.3

77.0

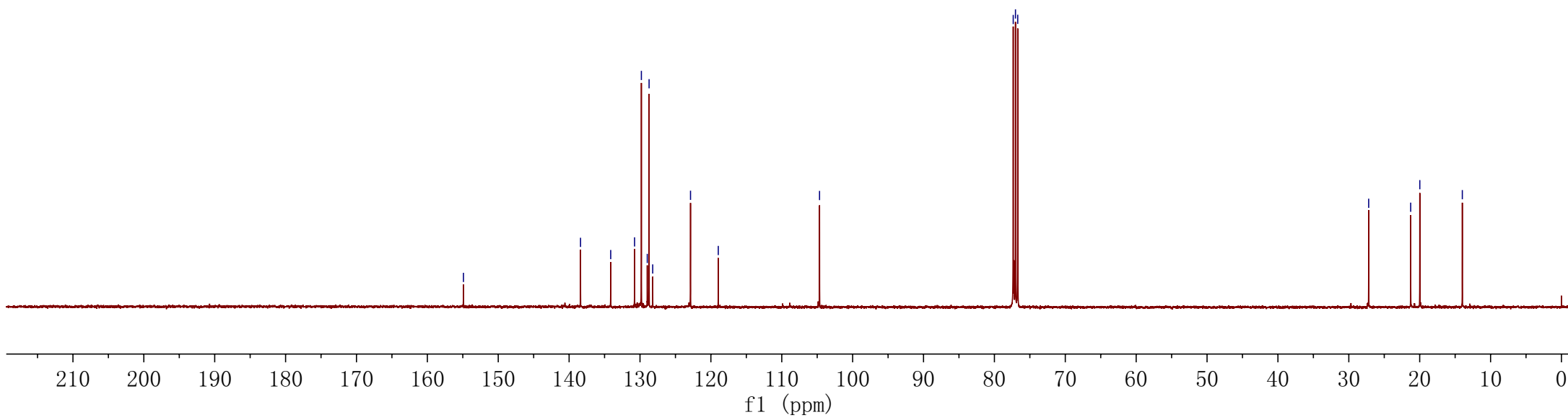
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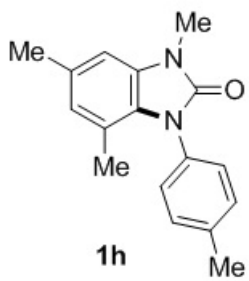
~27.2

~21.3

~20.0

~14.0





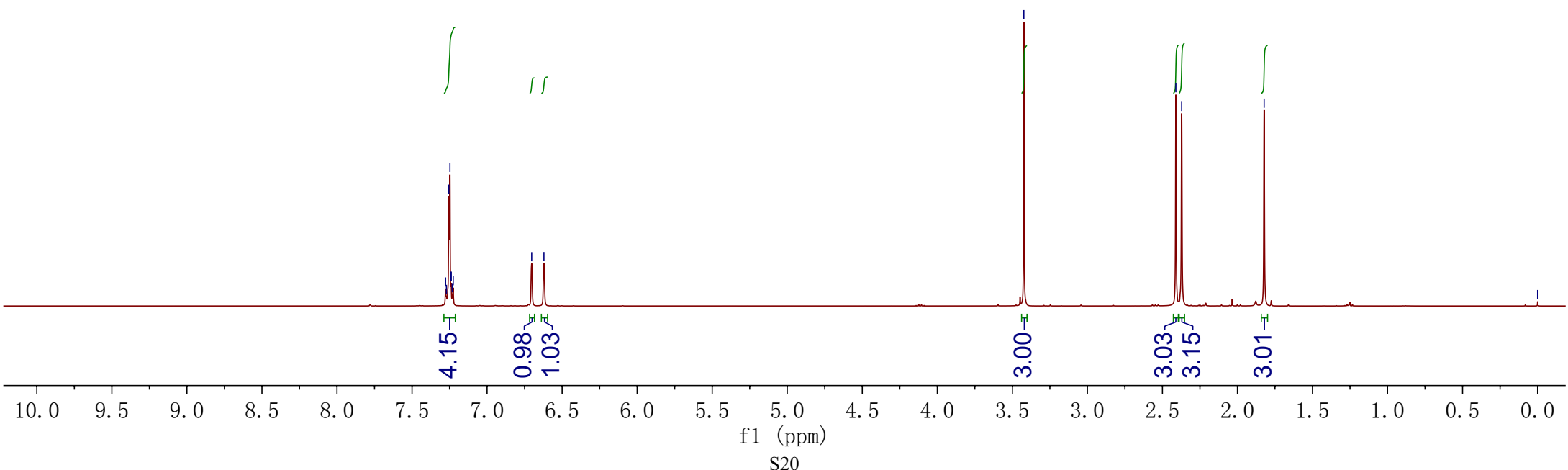
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7.271  
7.255  
7.247  
7.240  
7.239  
7.232  
7.226  
6.703  
6.621

3.423

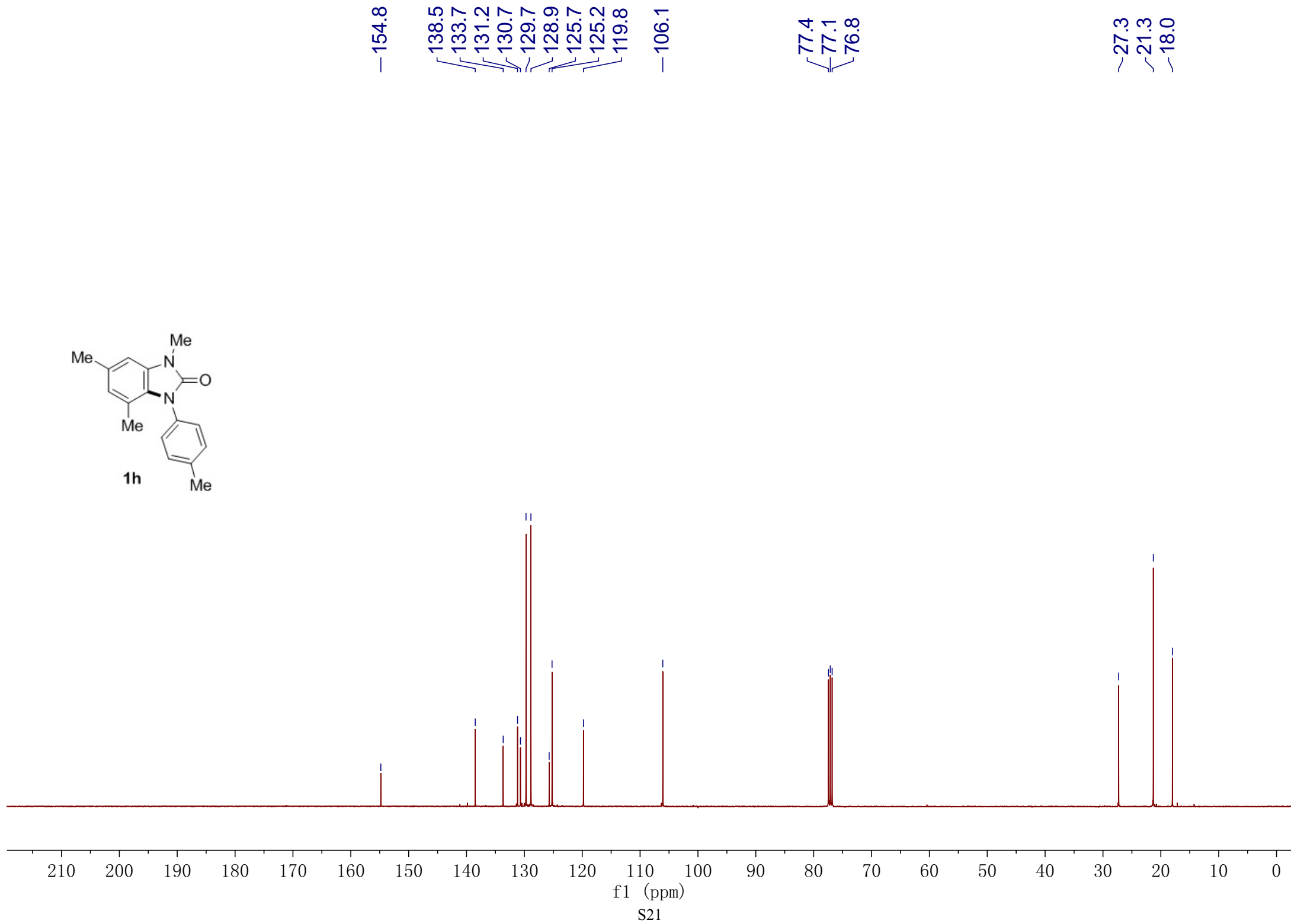
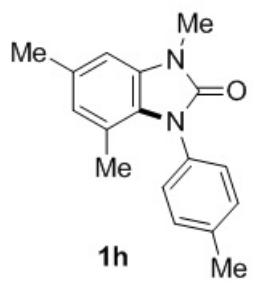
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2.372

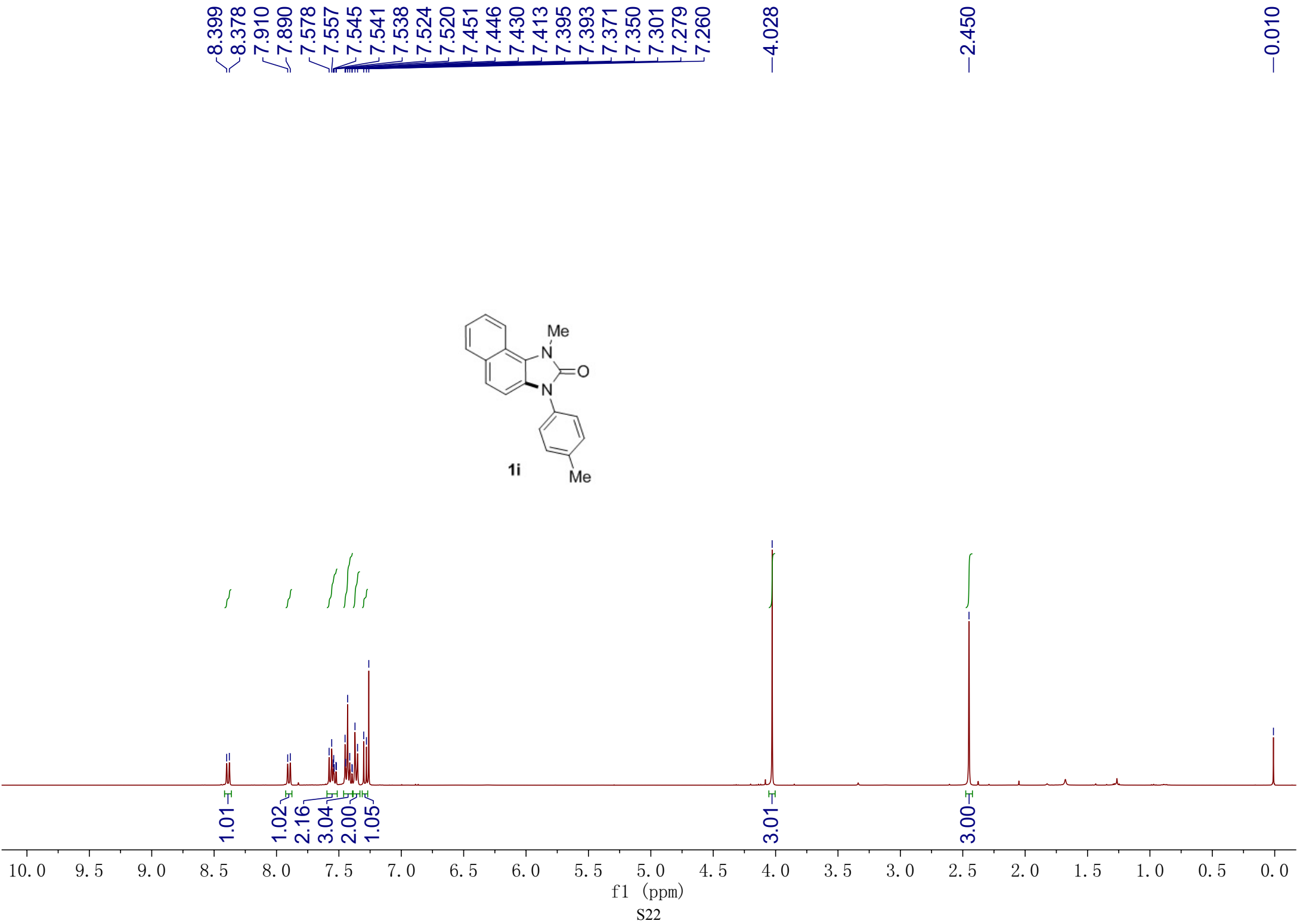
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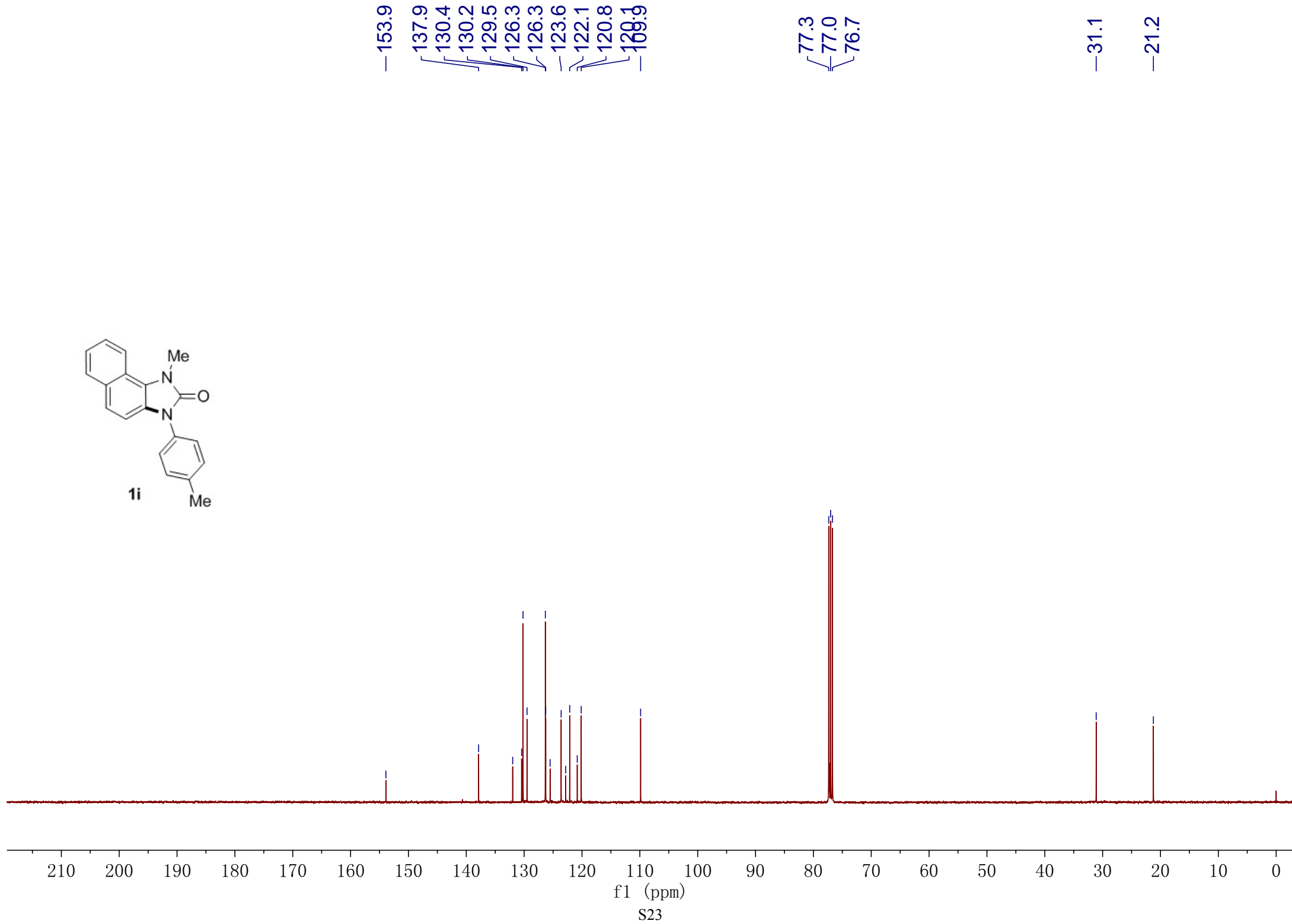
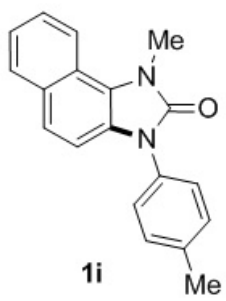
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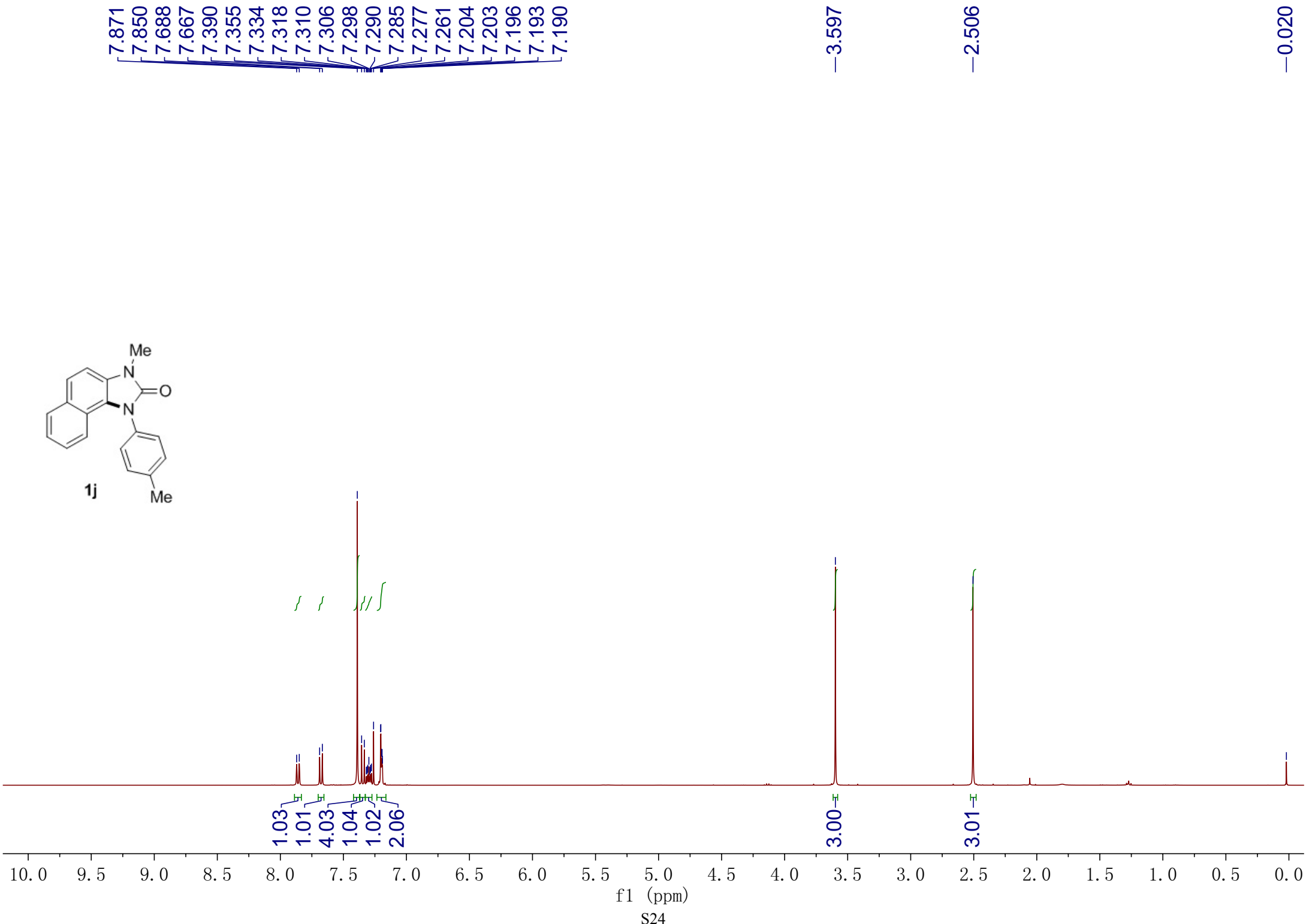
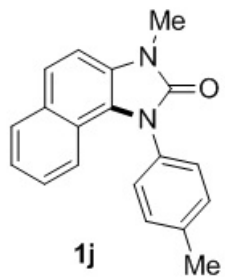


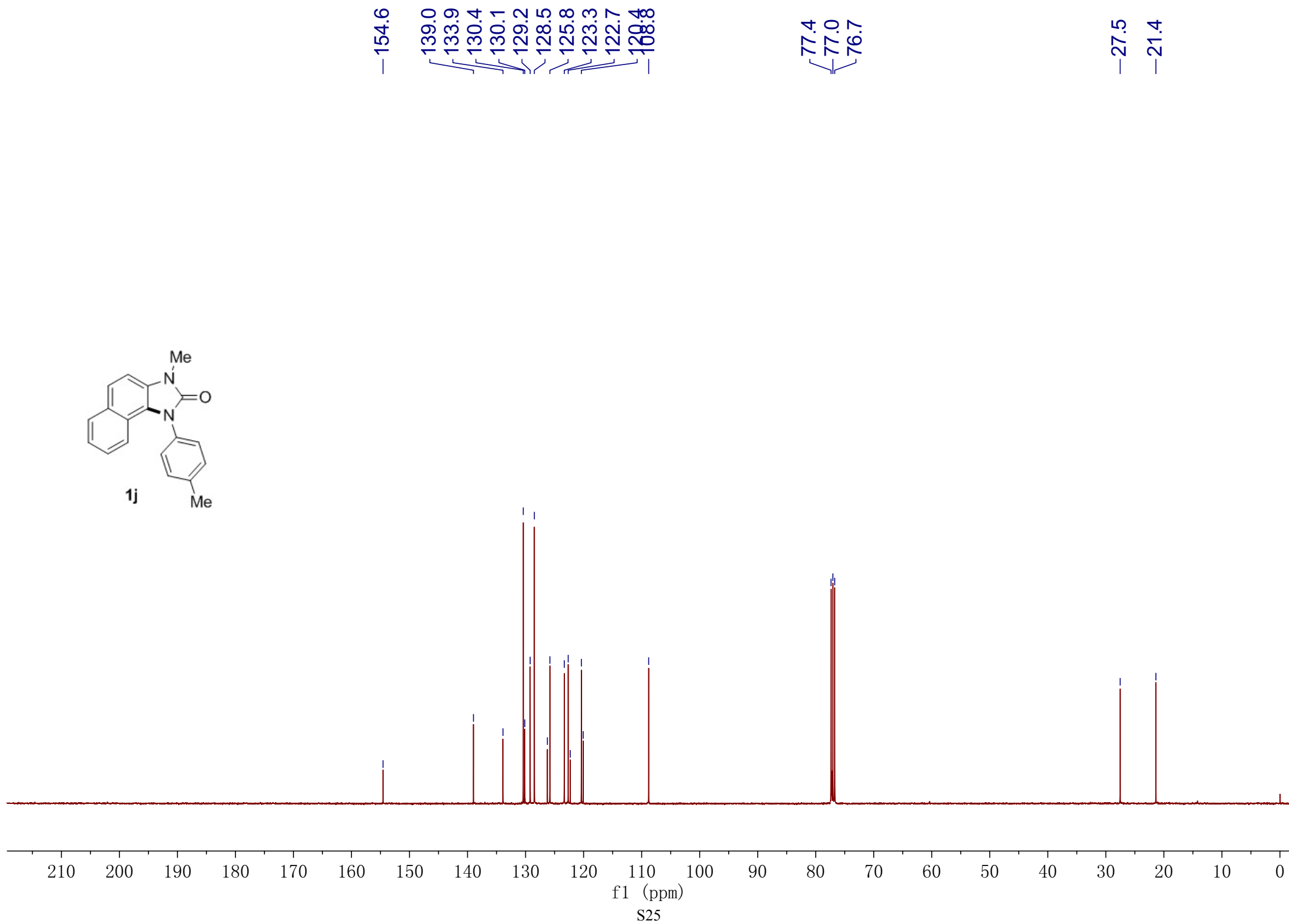
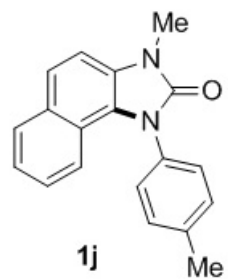


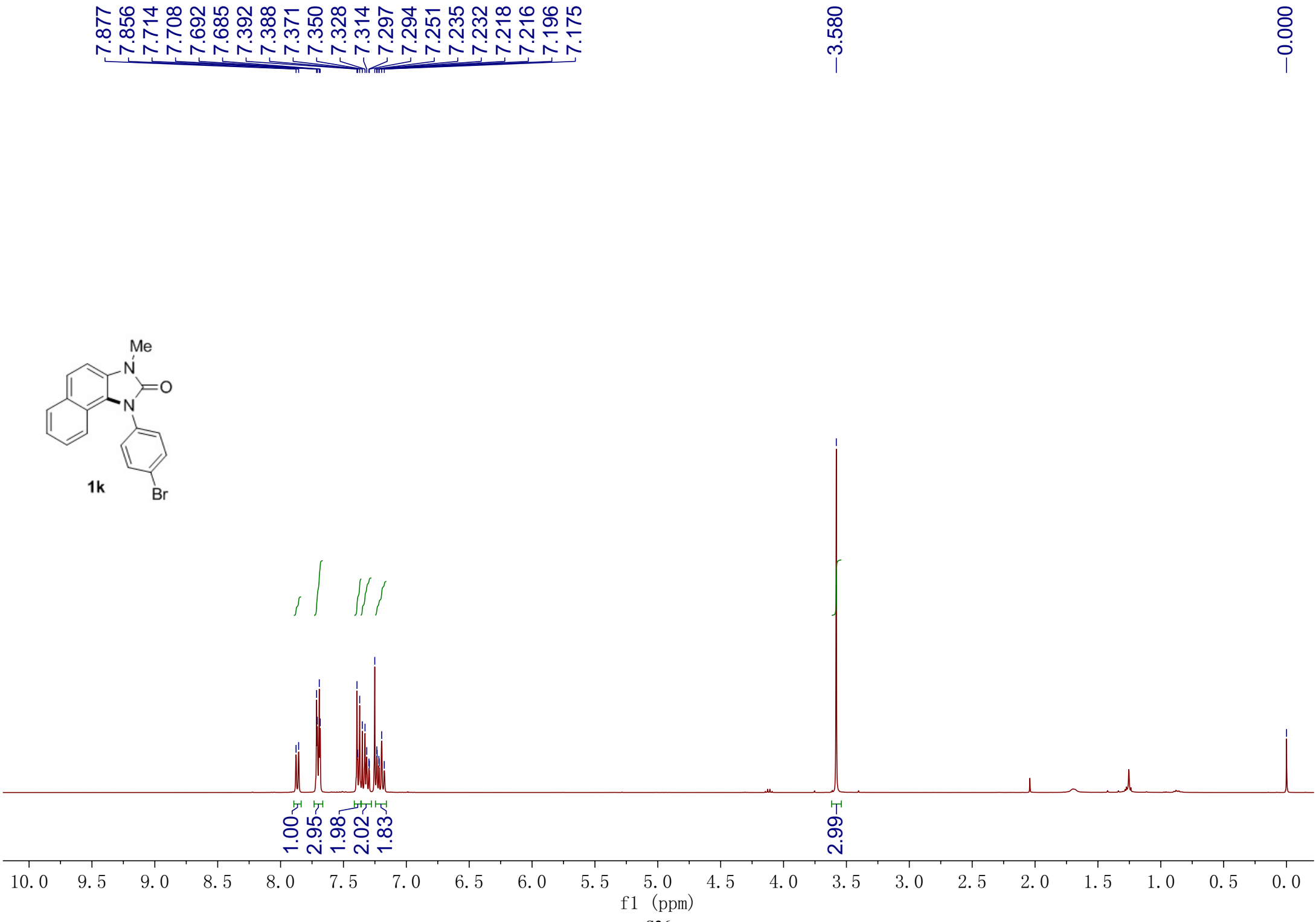
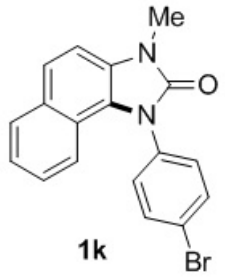


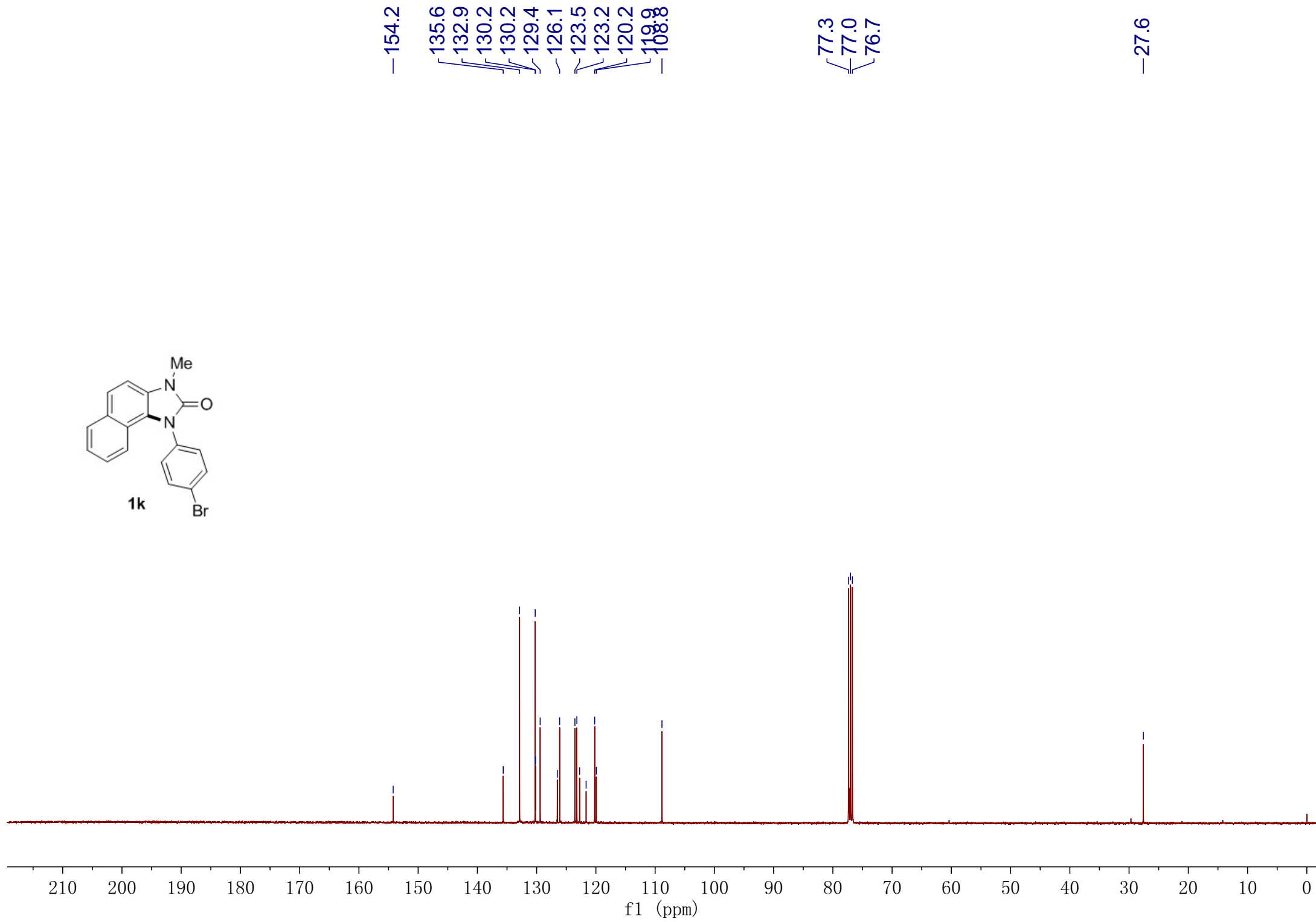
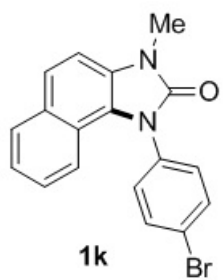


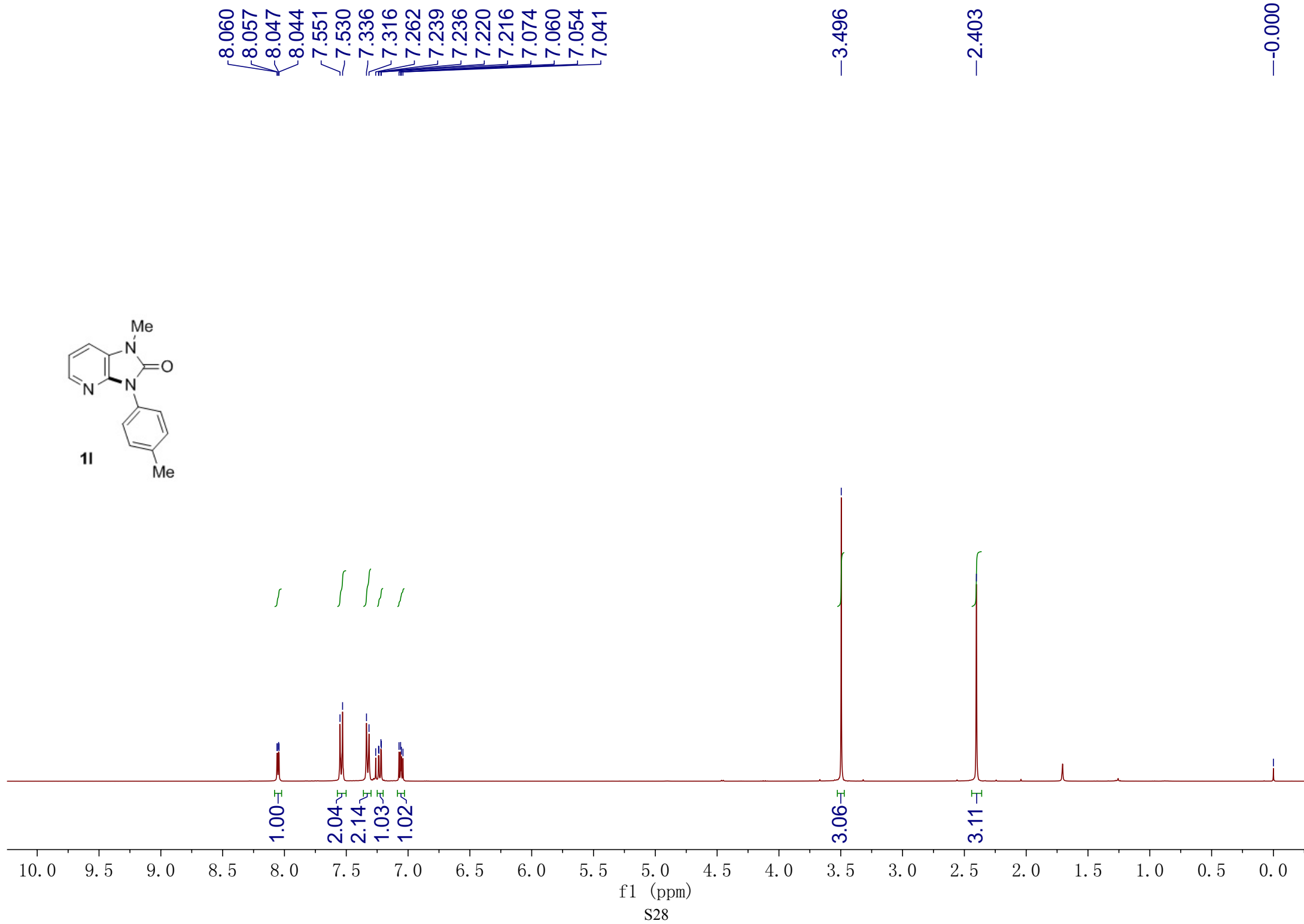
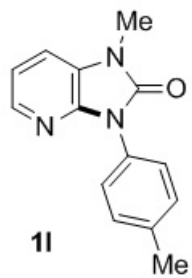




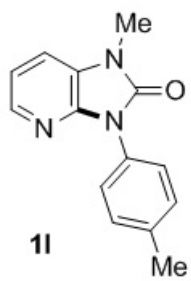








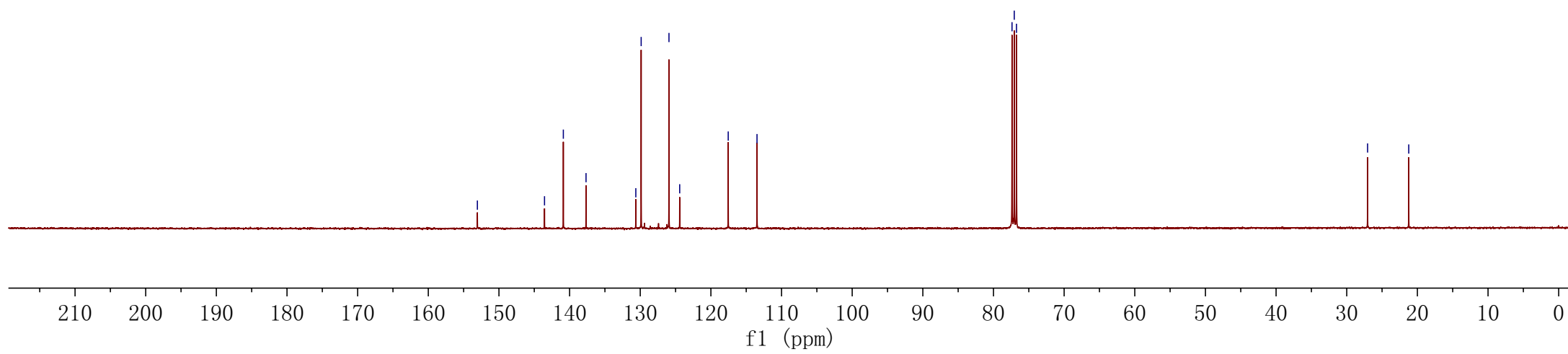


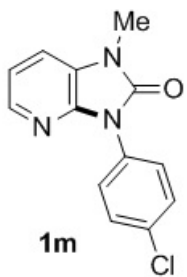


— 153.1  
~ 143.5  
~ 140.9  
~ 137.7  
~ 130.6  
~ 129.9  
~ 125.9  
~ 124.4  
~ 117.5  
~ 113.5

77.4  
77.1  
76.7

— 27.0  
— 21.2

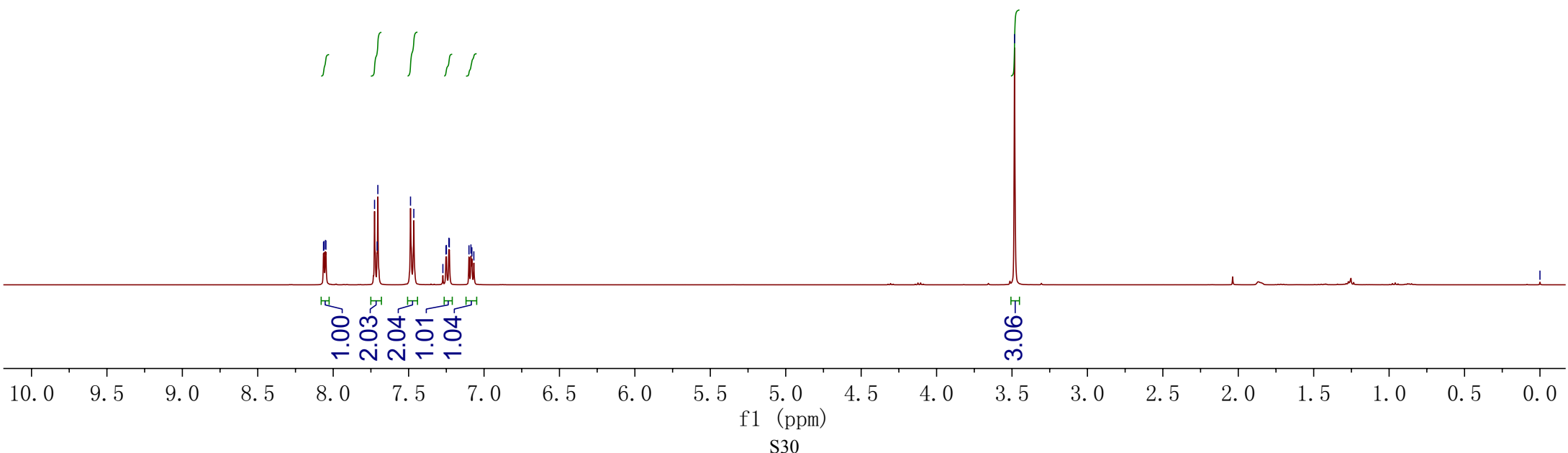


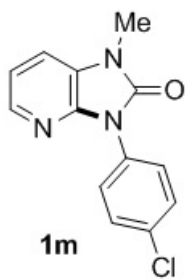


8.064  
8.061  
8.051  
8.048  
7.726  
7.708  
7.704  
7.487  
7.466  
7.273  
7.252  
7.250  
7.233  
7.230  
7.100  
7.087  
7.081  
7.068

—3.483

—0.000

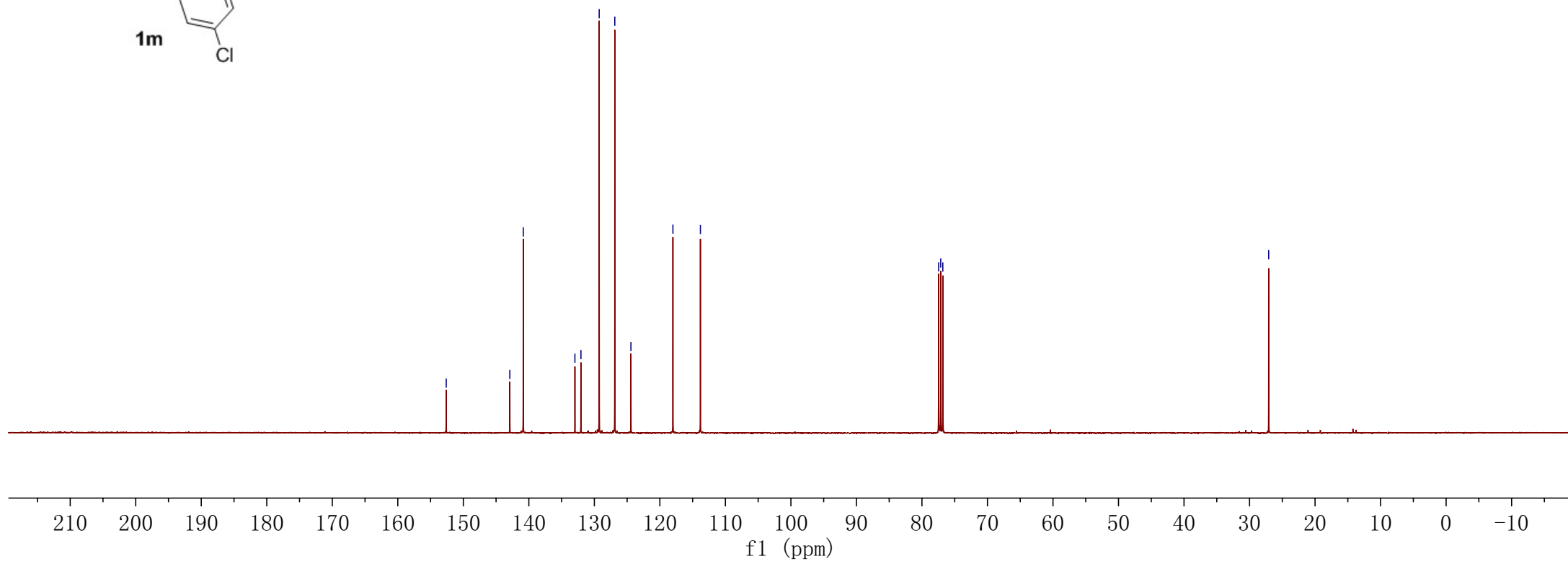




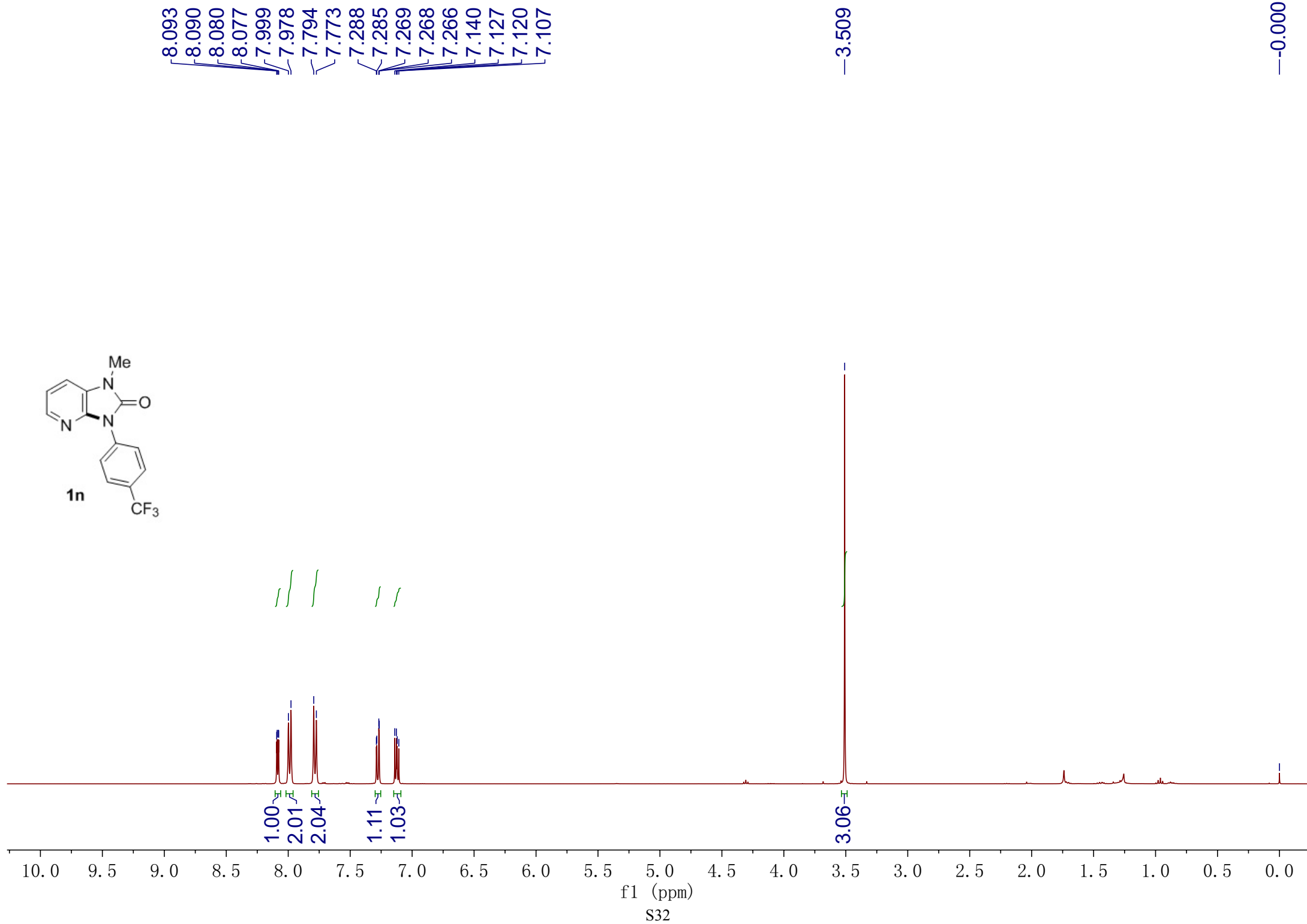
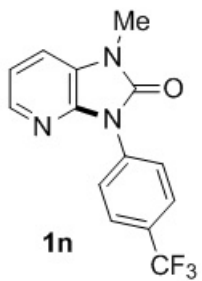
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132.0  
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126.9  
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118.0  
113.8

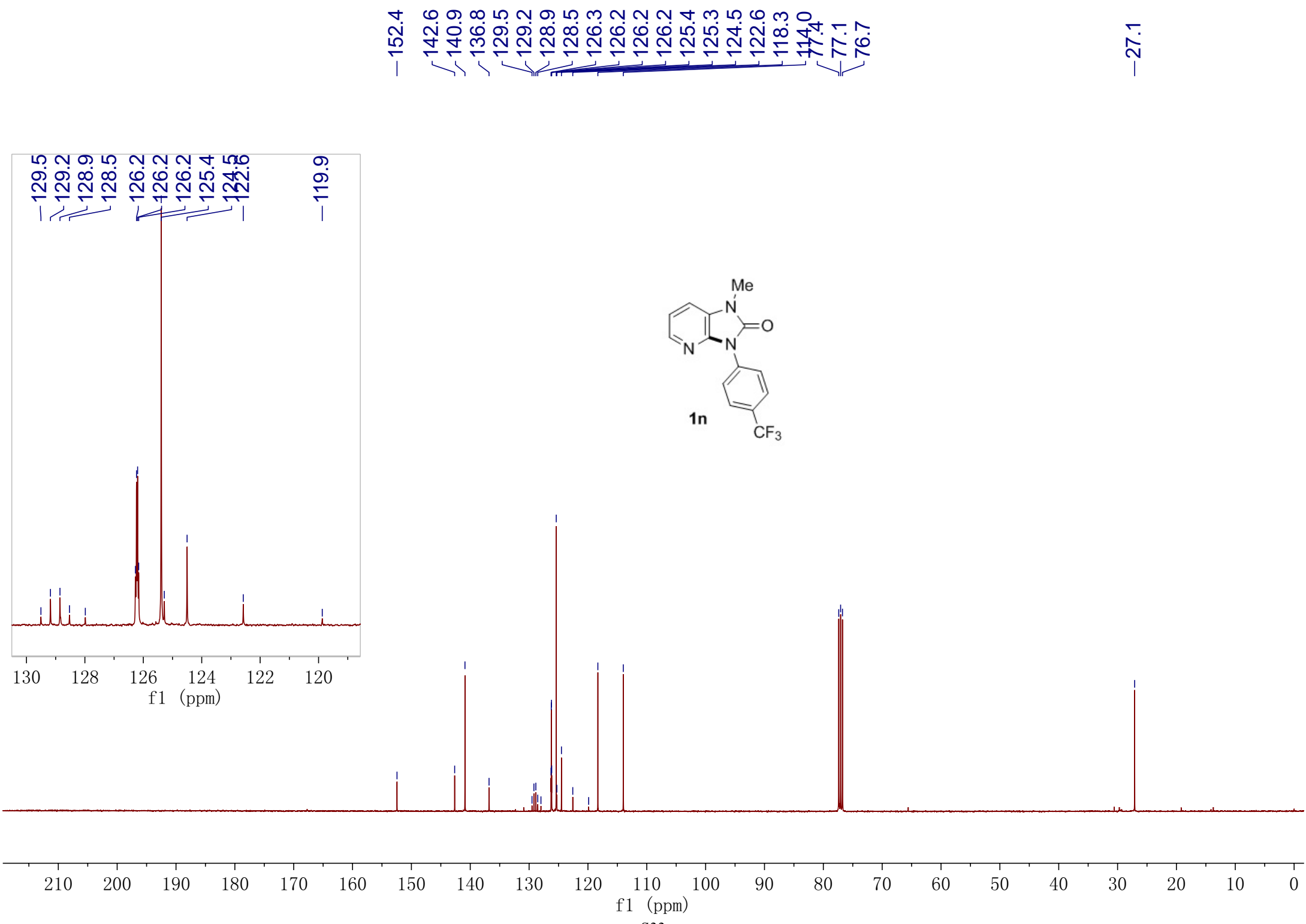
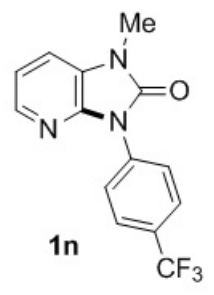
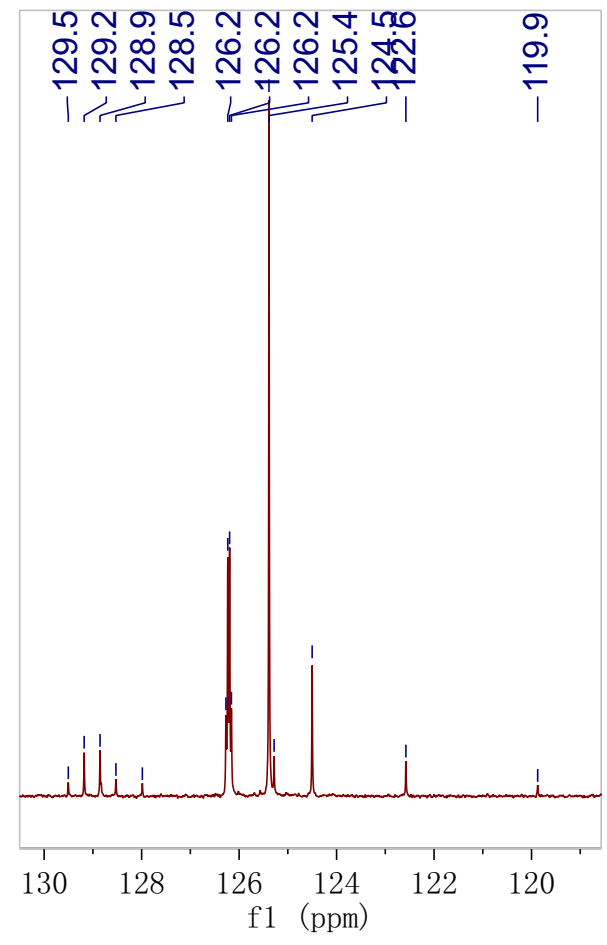
77.5  
77.1  
76.8

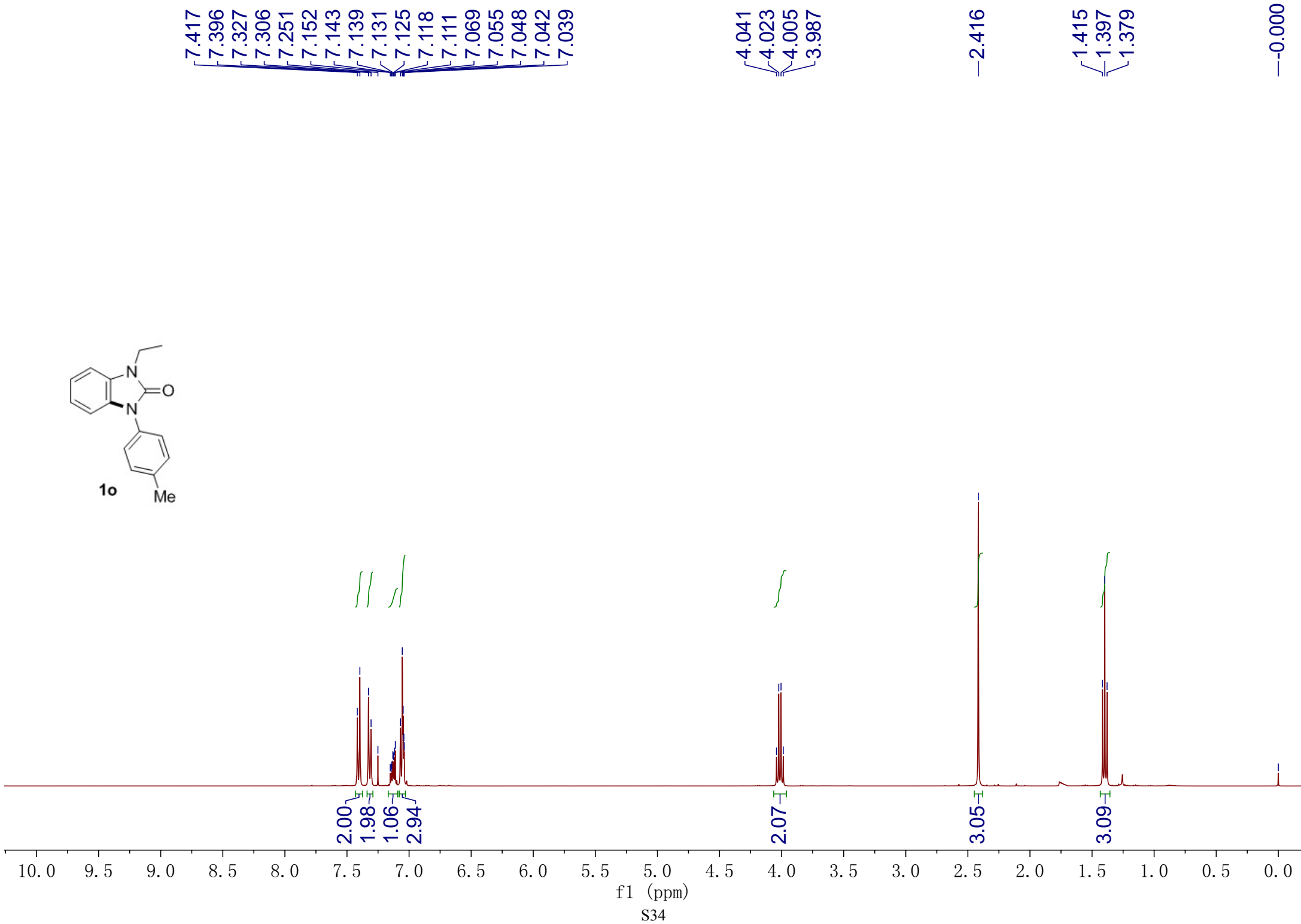
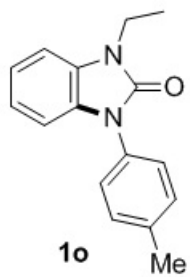
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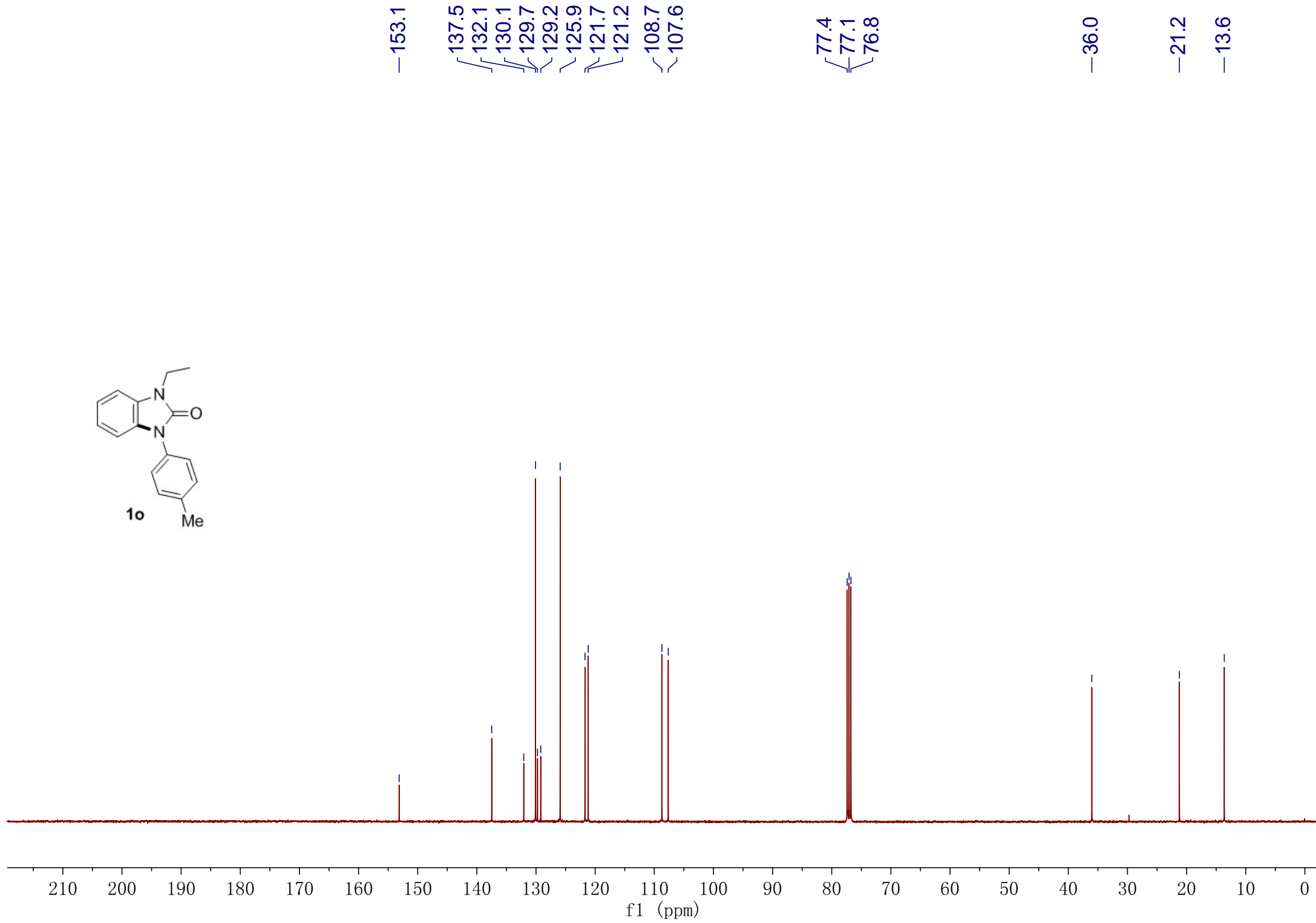
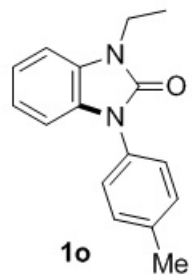


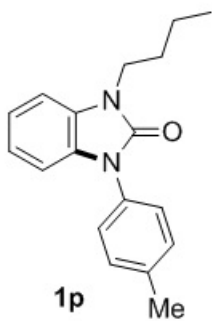
S31









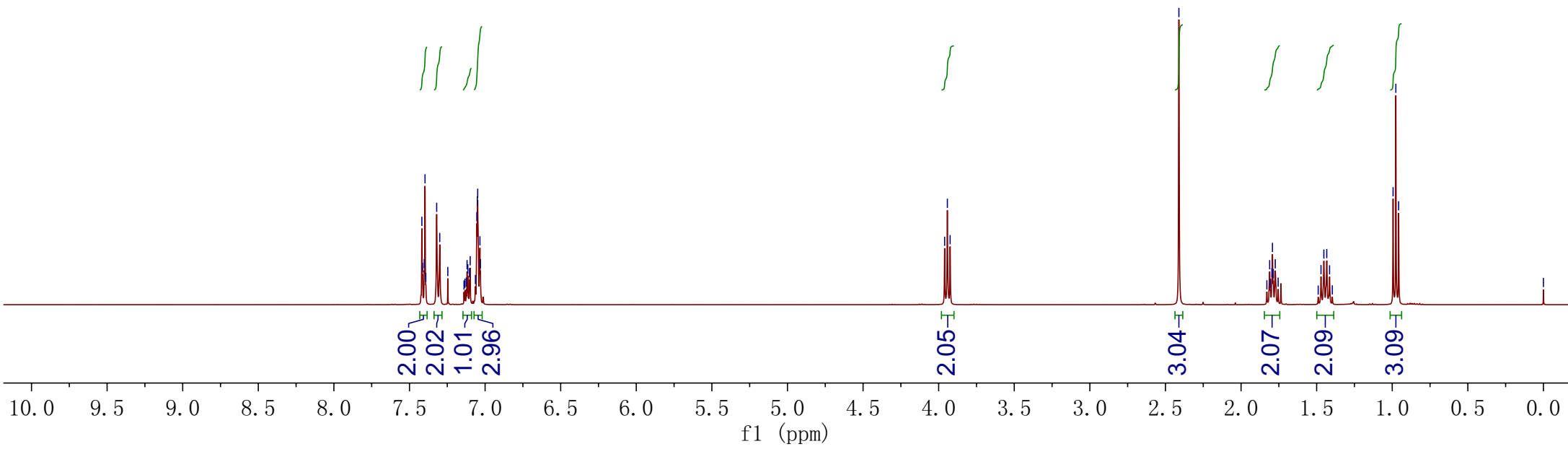


7.418  
7.414  
7.402  
7.397  
7.392  
7.320  
7.300  
7.247  
7.139  
7.133  
7.124  
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7.034  
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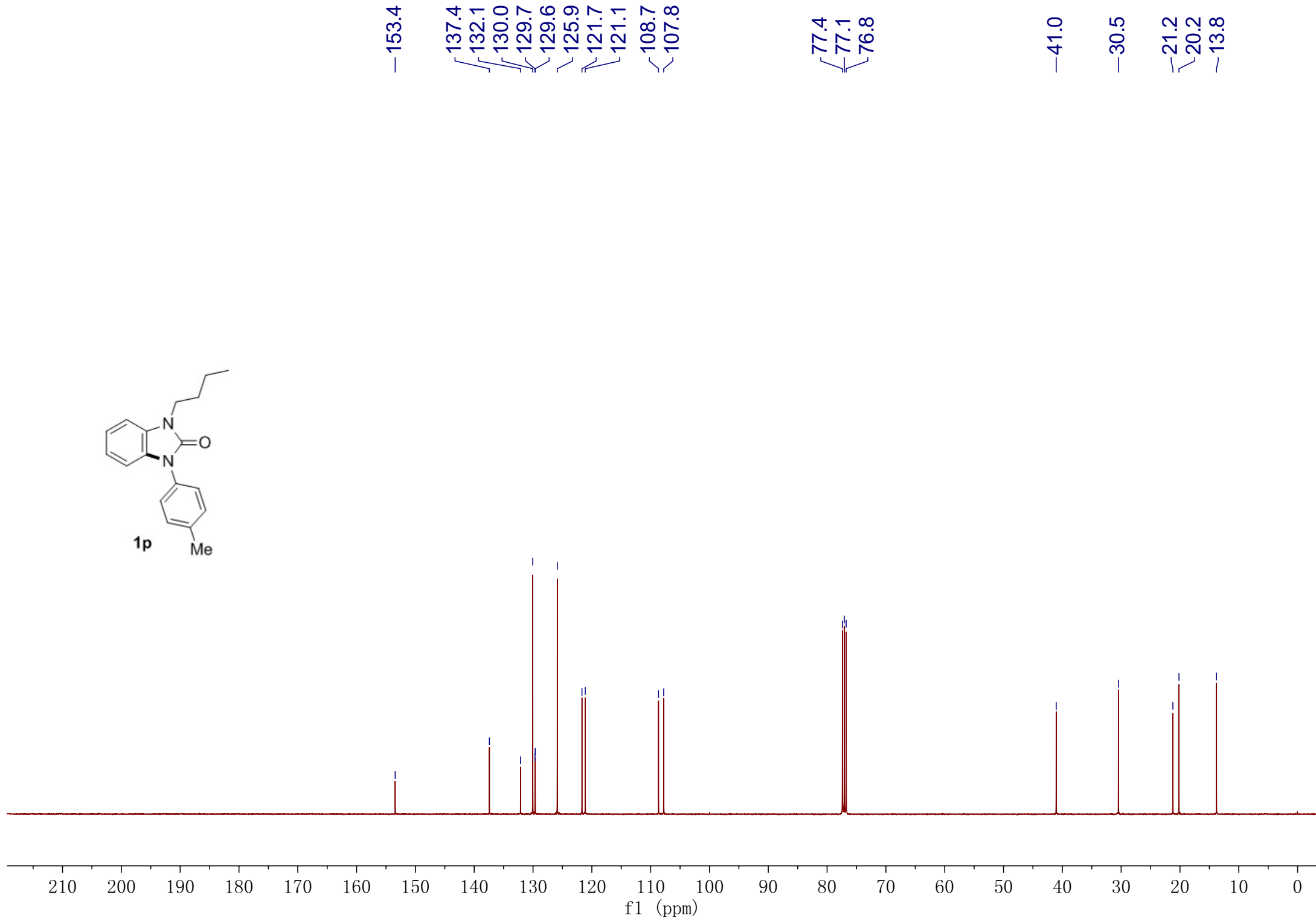
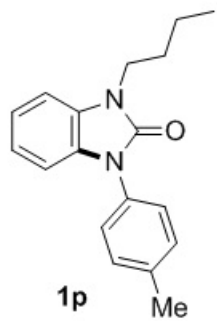
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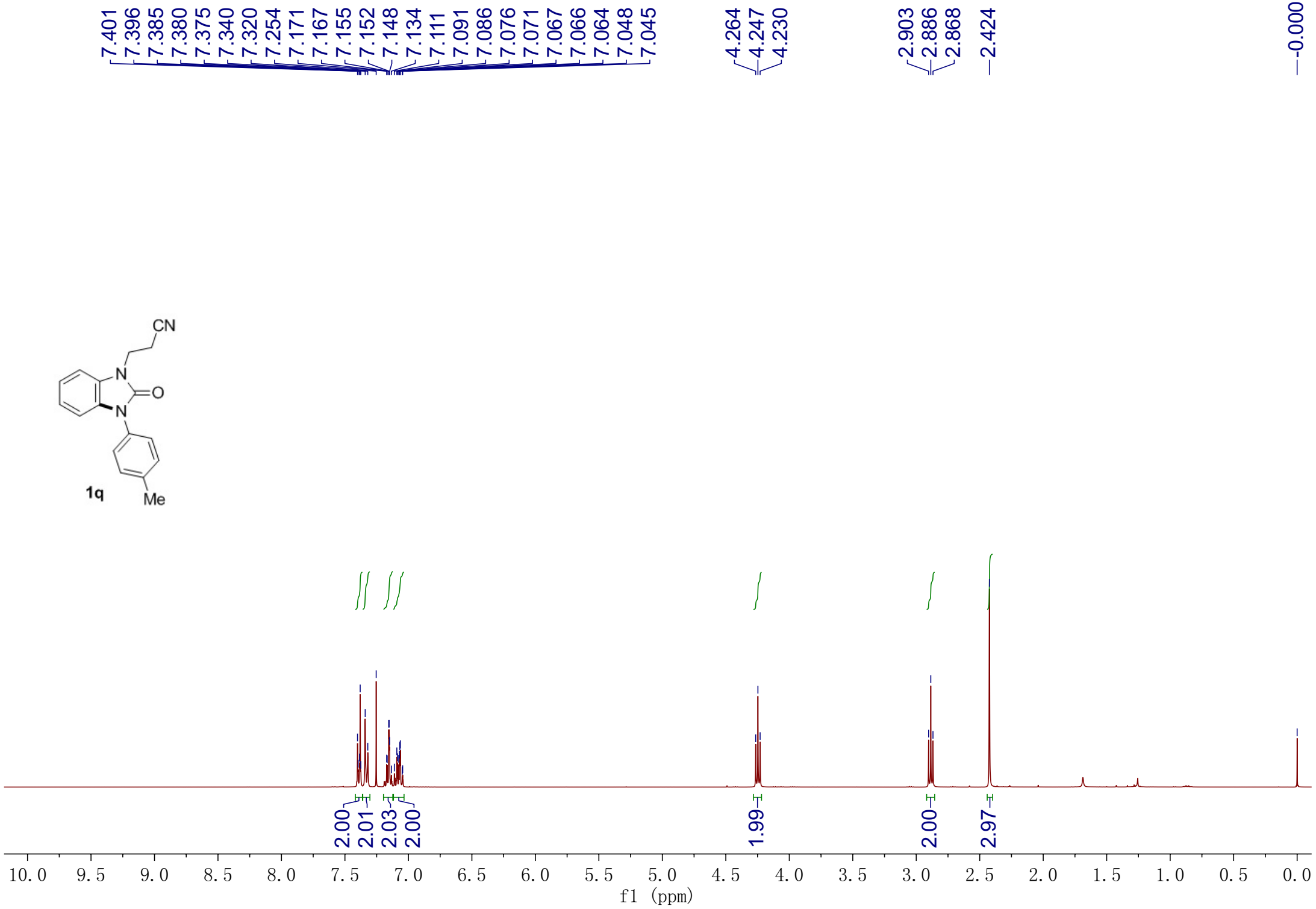
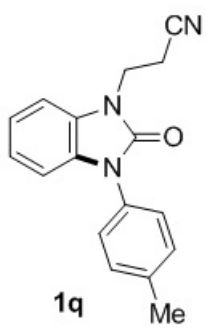
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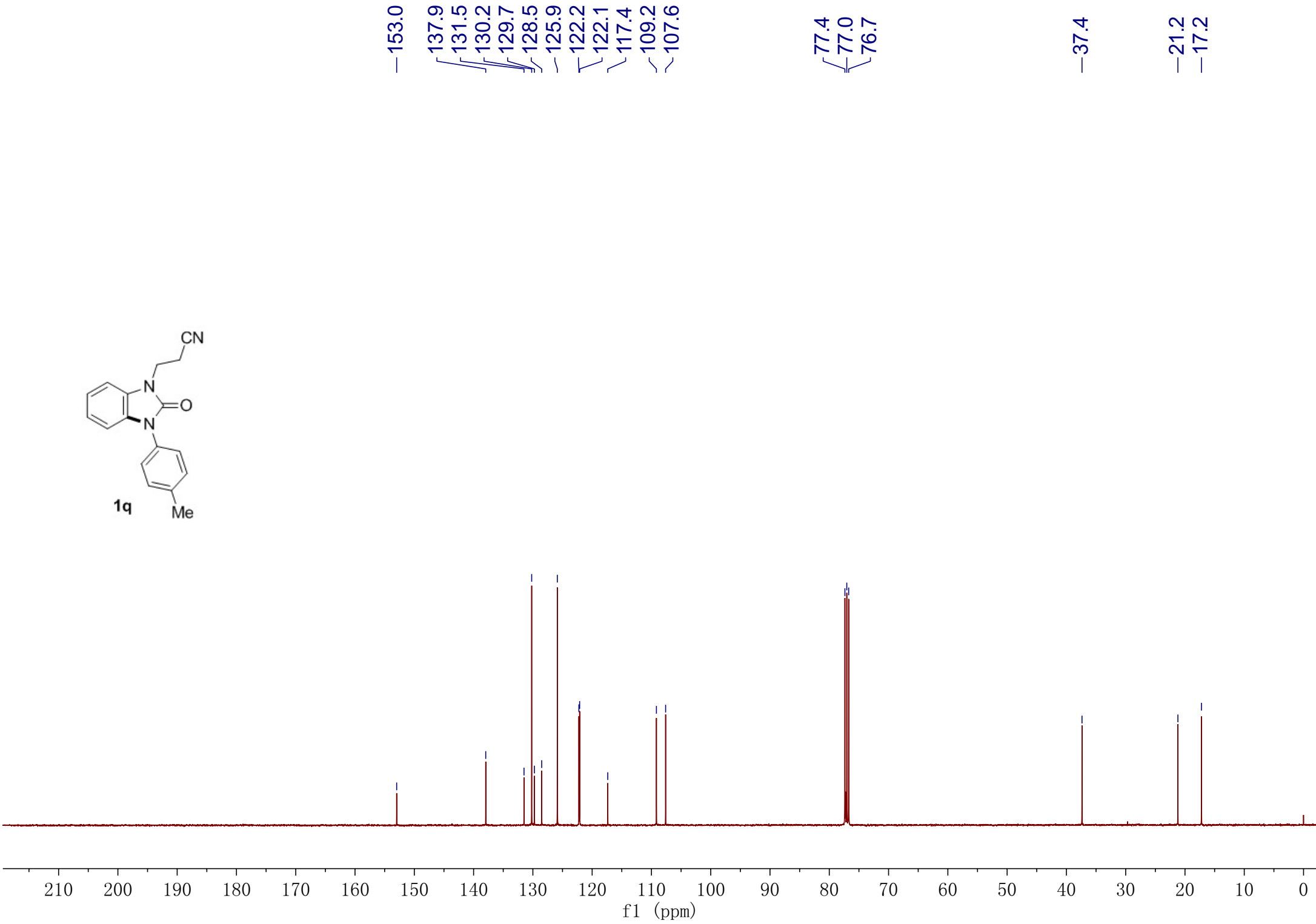
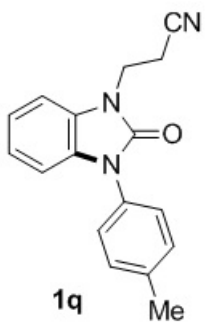
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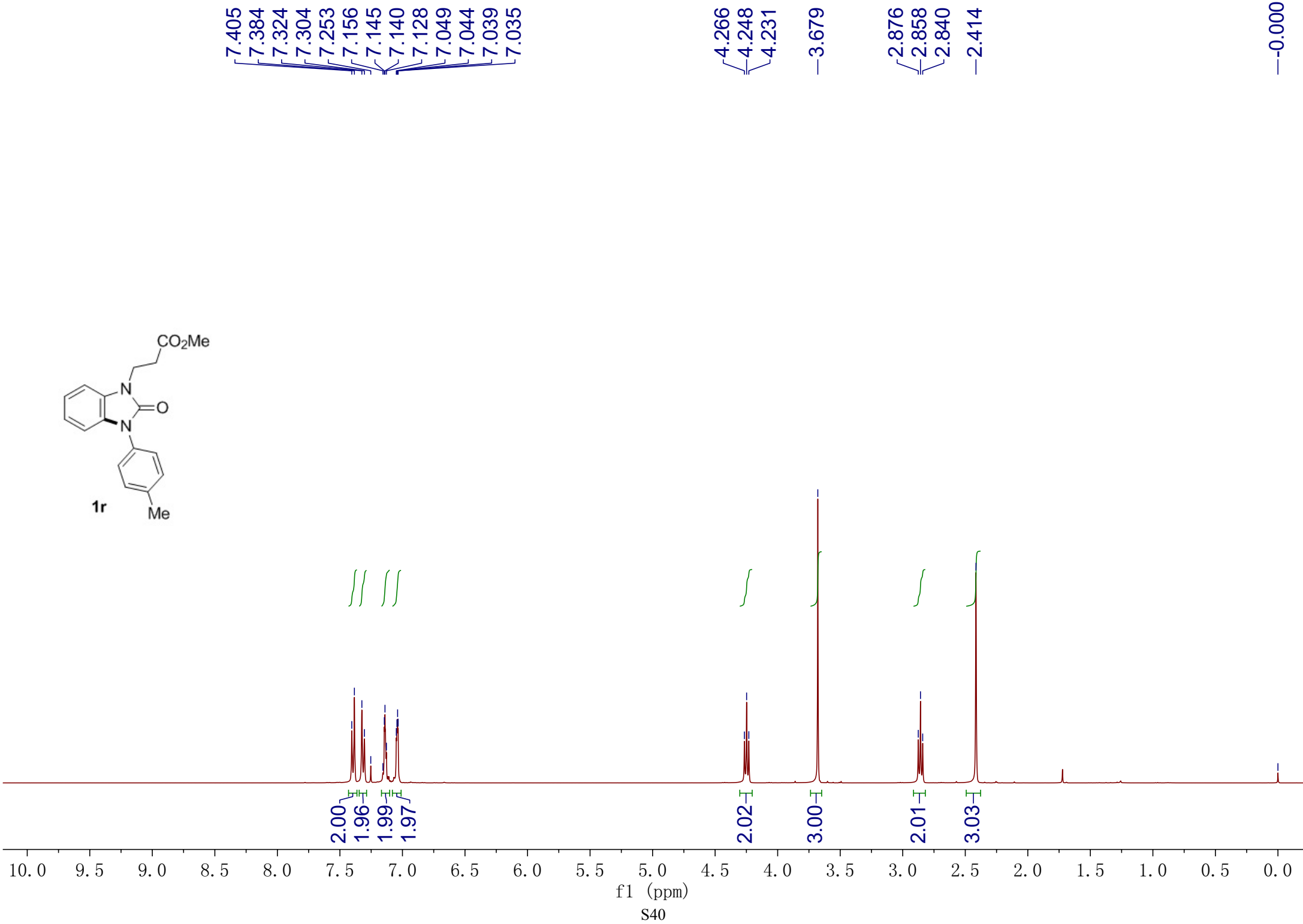
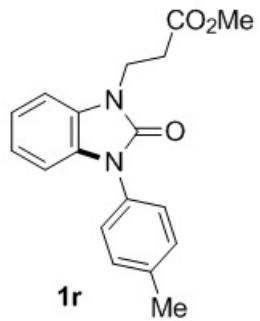


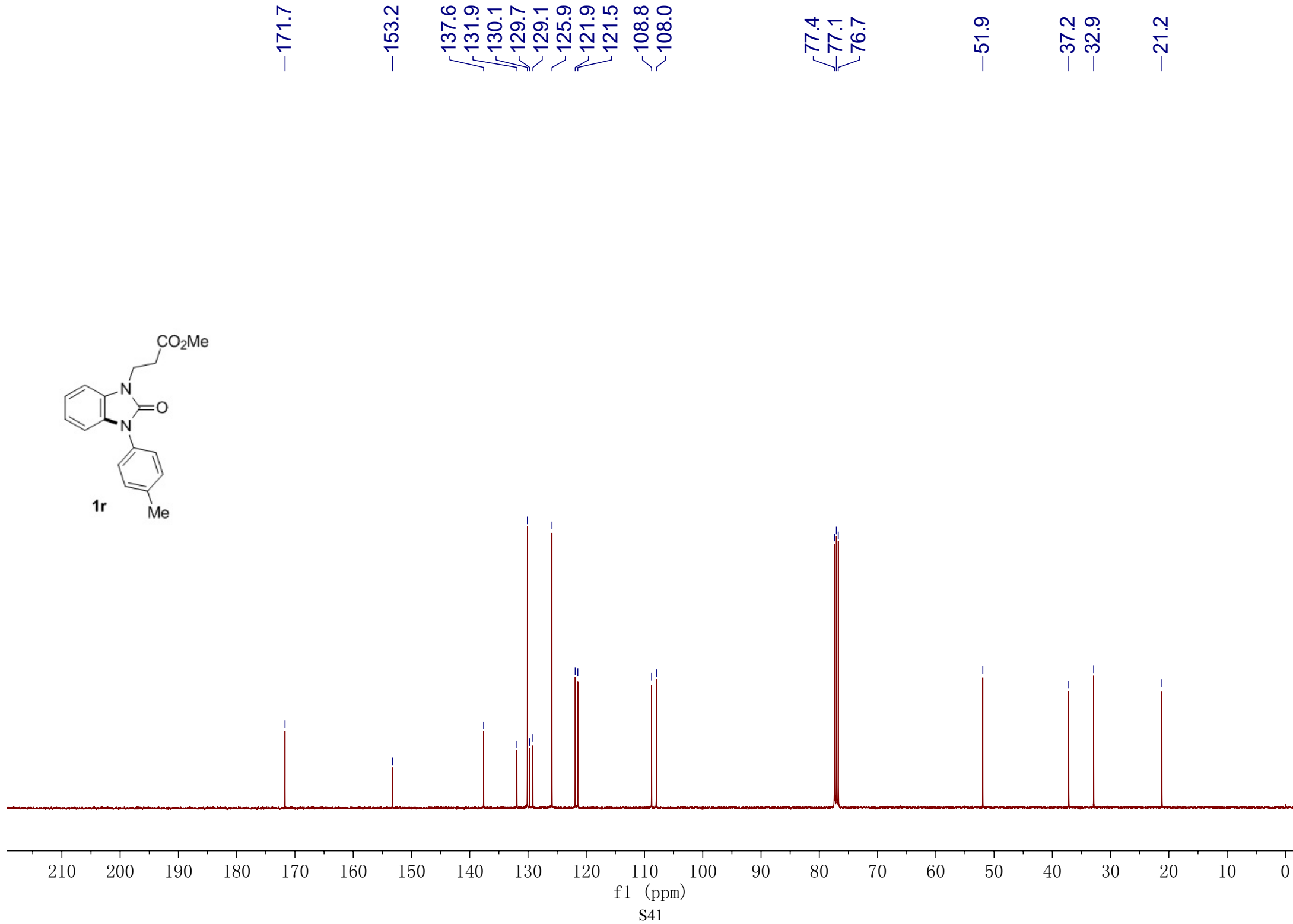
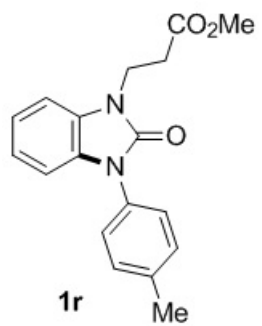


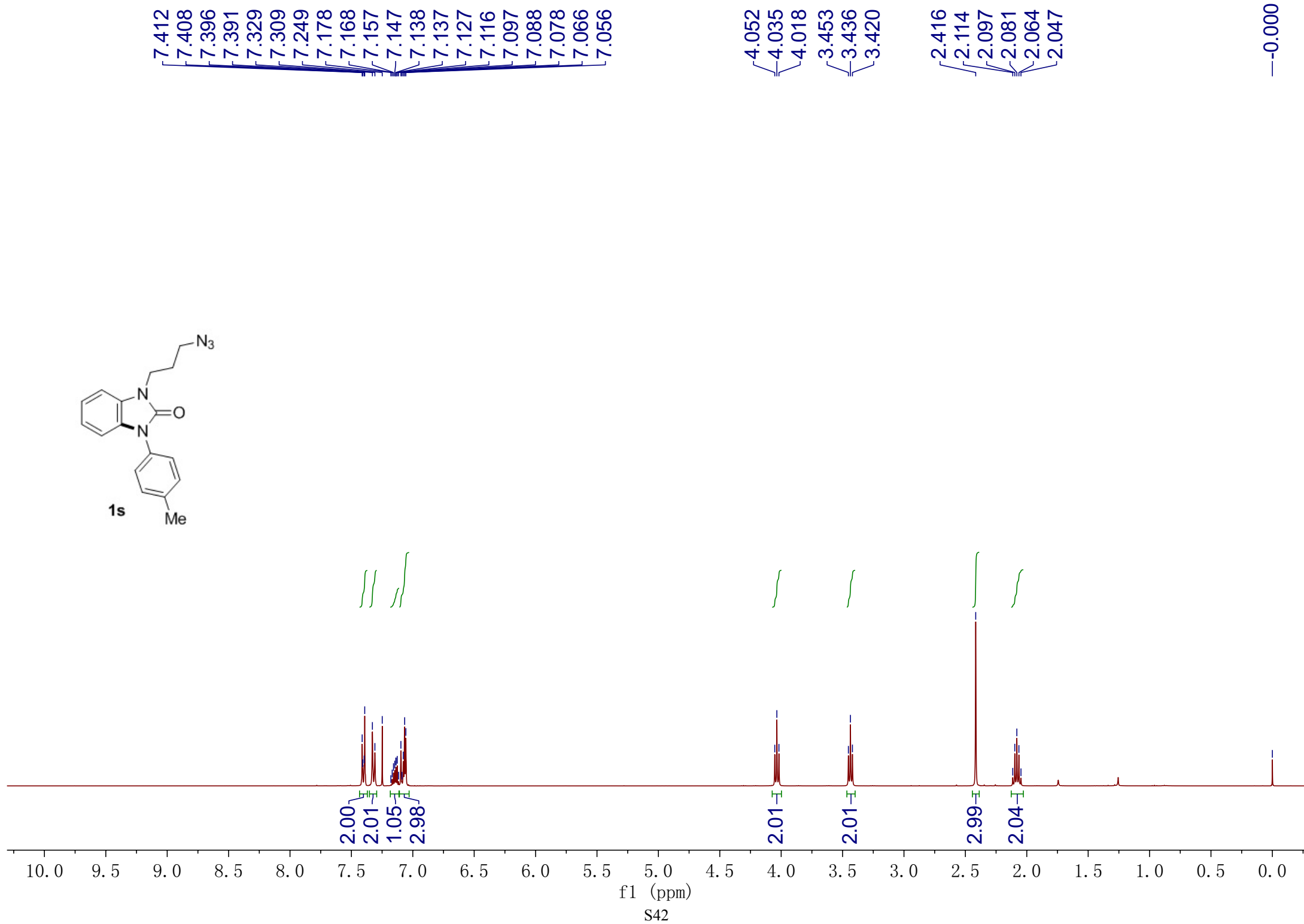
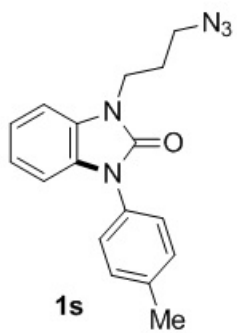


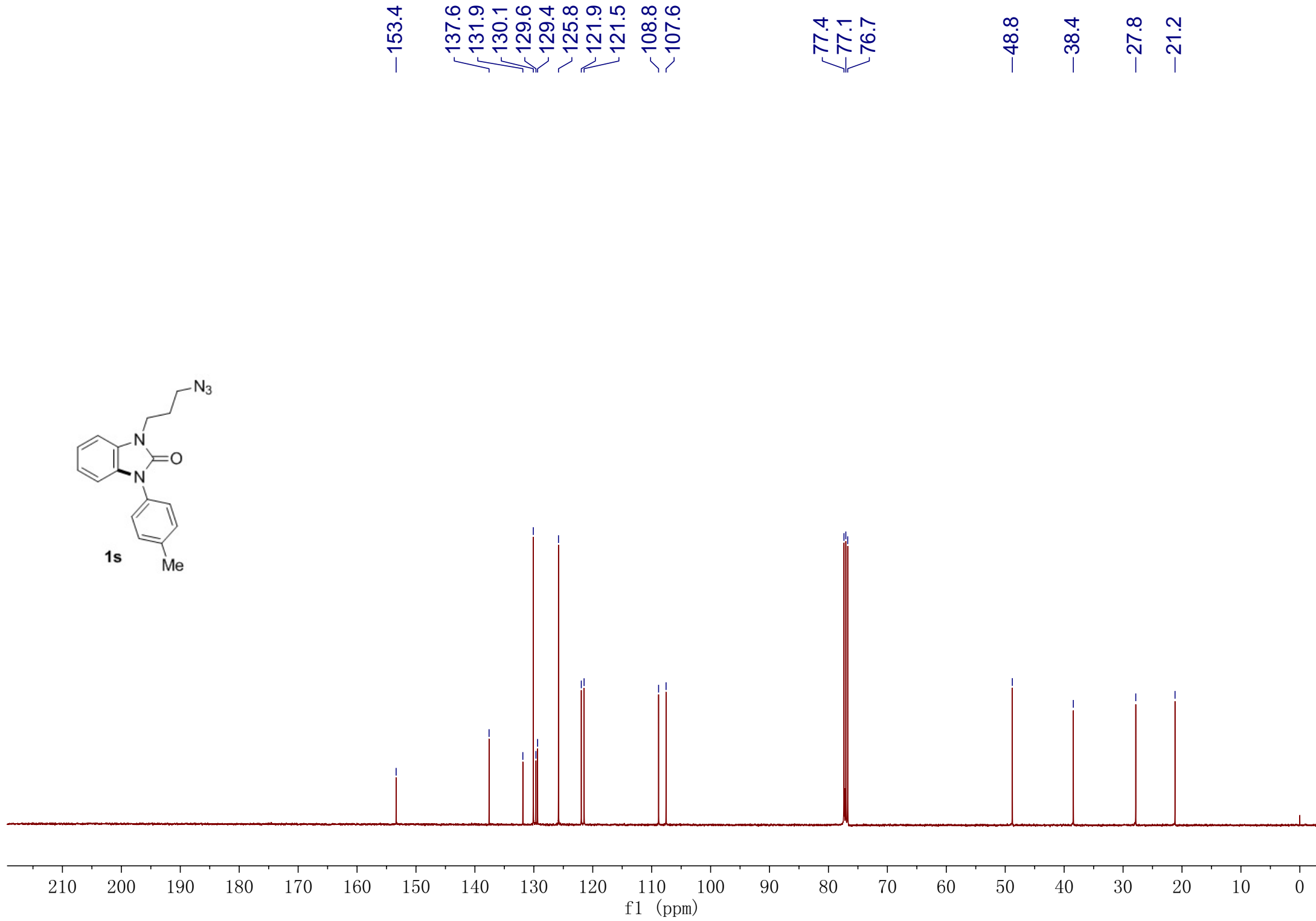
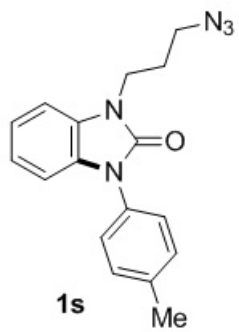


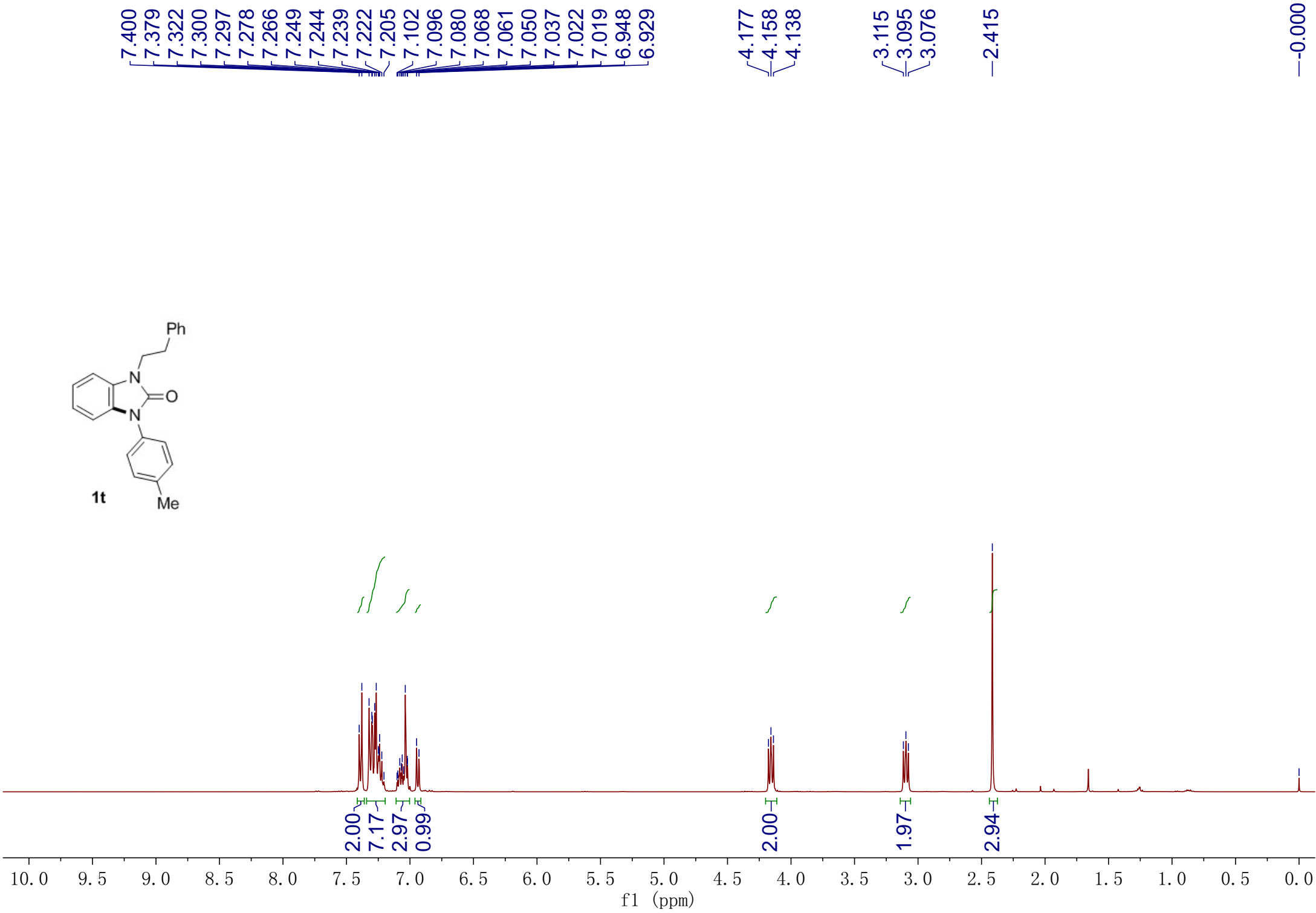
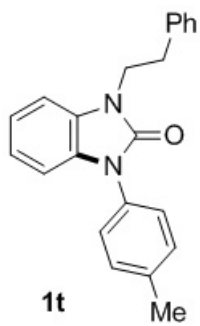




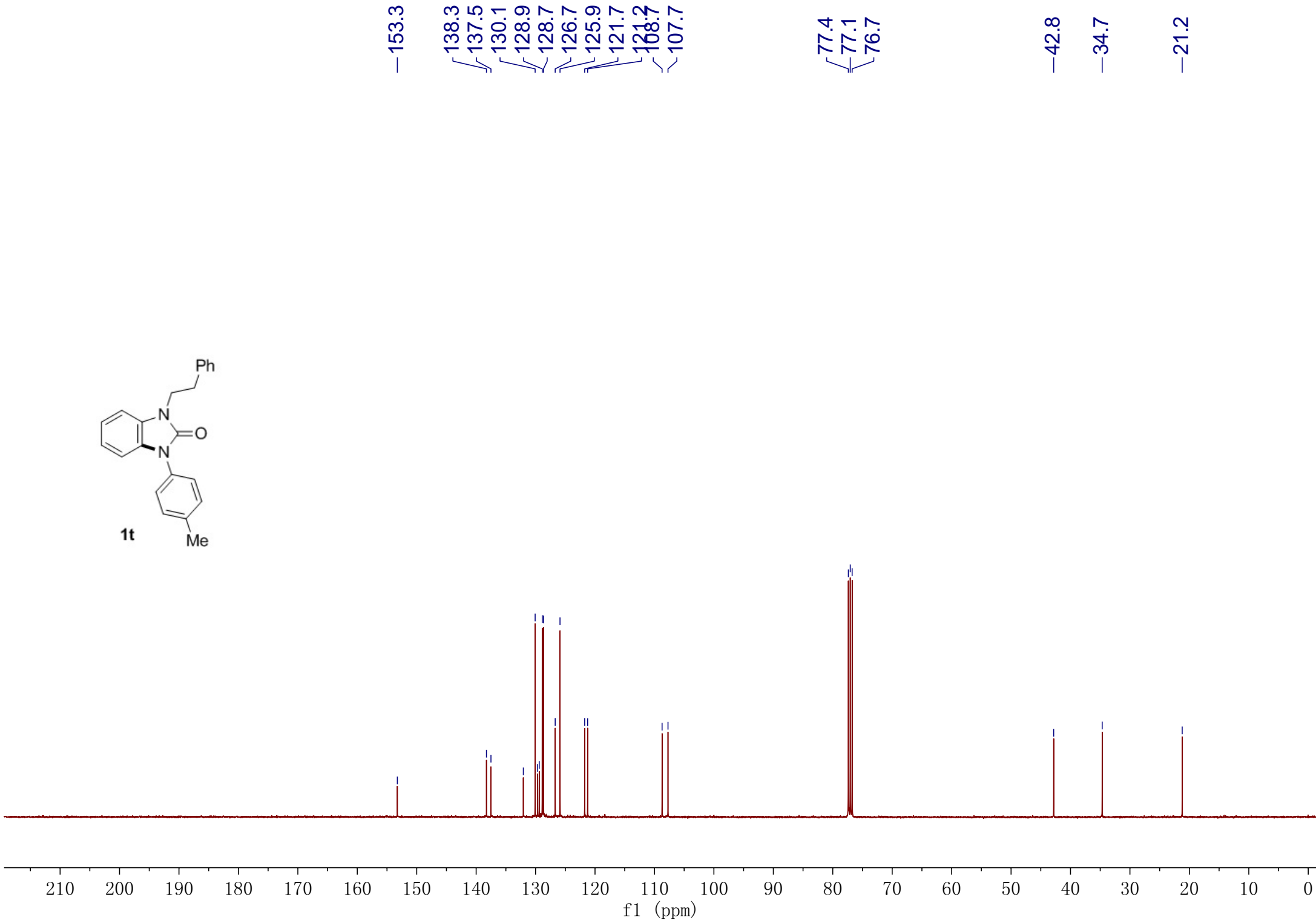
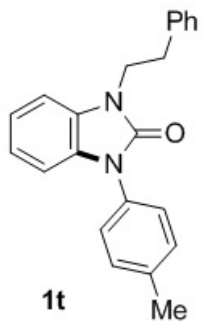


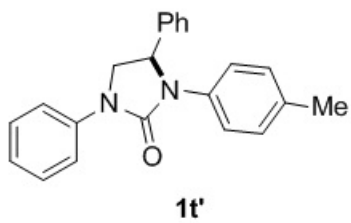












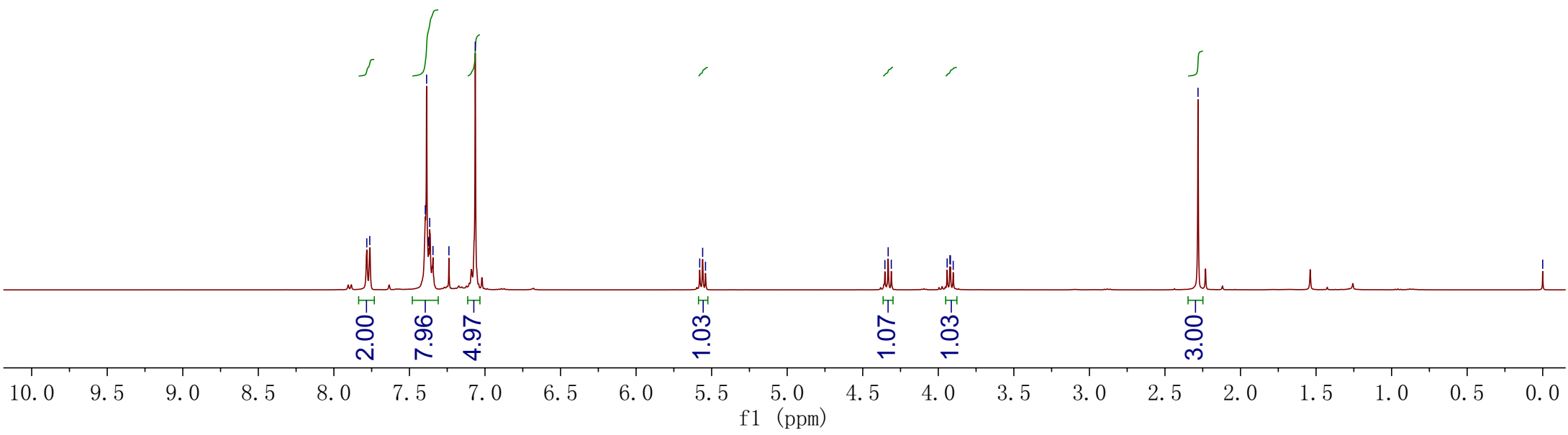
7.782  
7.763  
7.395  
7.386  
7.373  
7.366  
7.344  
7.239  
7.064

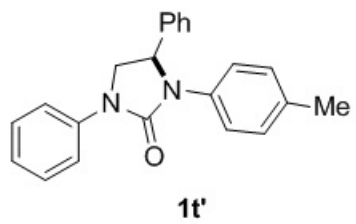
5.579  
5.559  
5.541

4.353  
4.332  
4.311  
3.942  
3.923  
3.920  
3.901

-2.281

-0.000



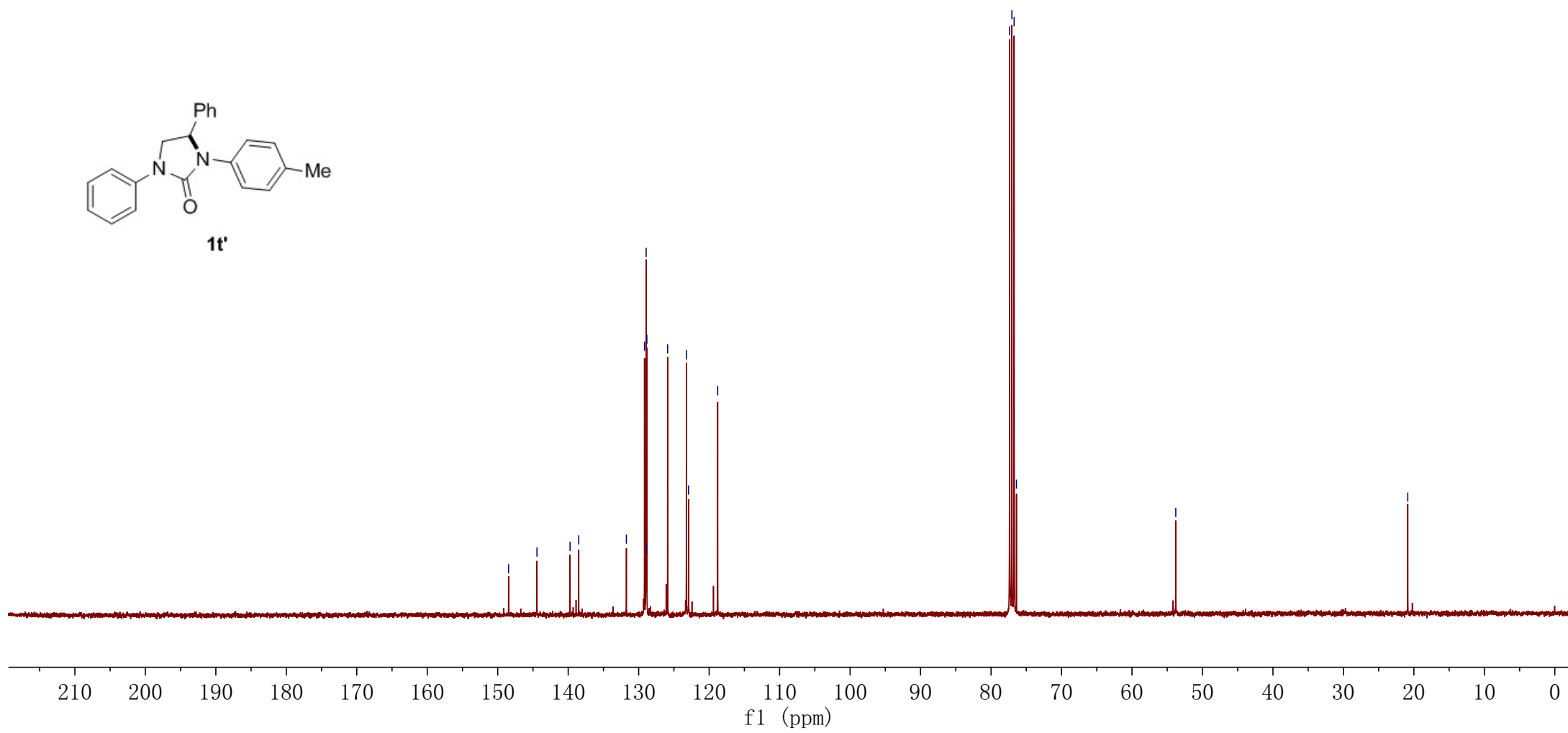


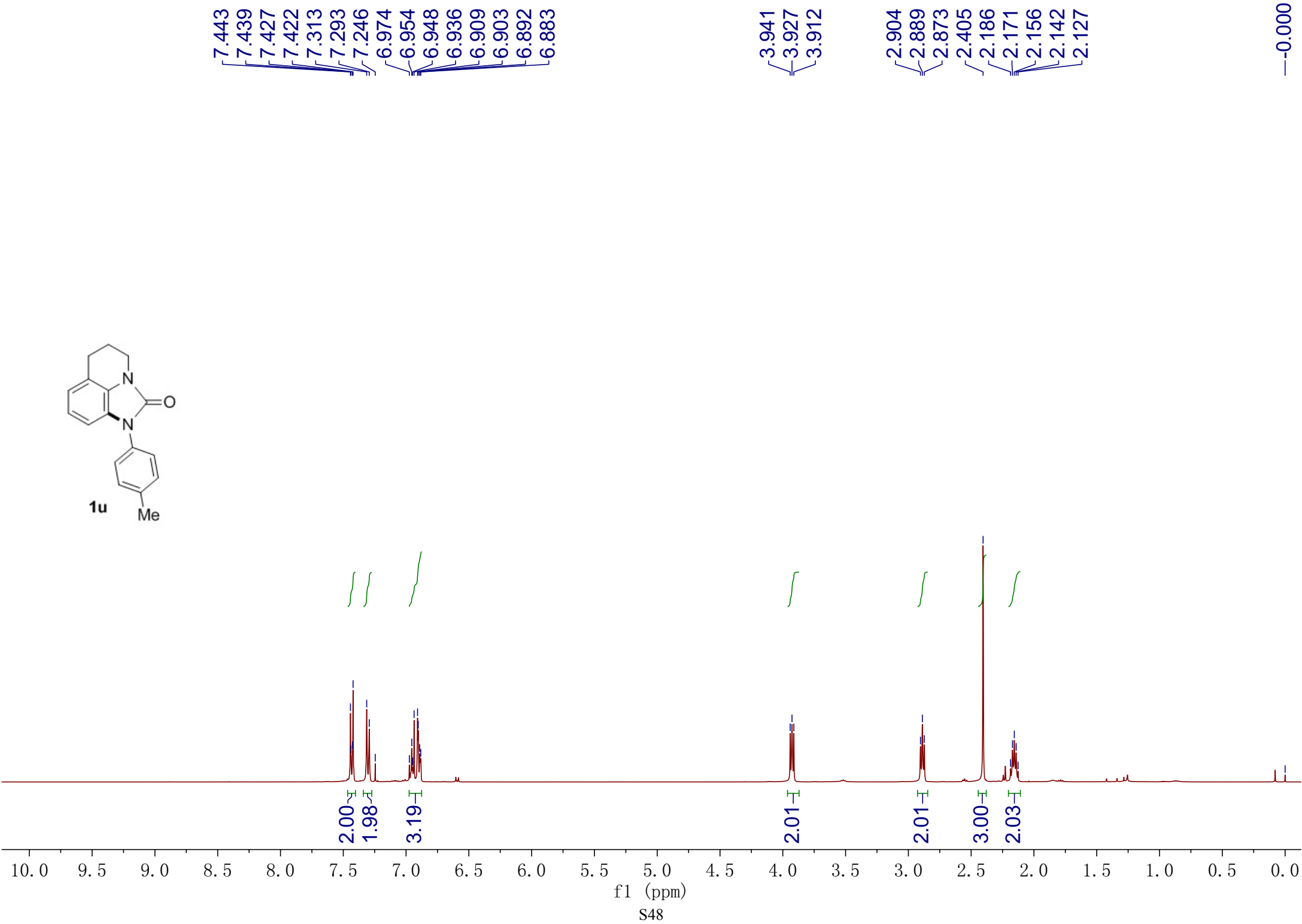
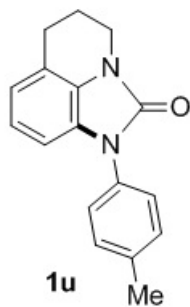
148.5  
144.4  
139.7  
138.5  
131.7  
129.2  
128.9  
128.9  
128.8  
125.9  
123.2  
122.9  
118.8

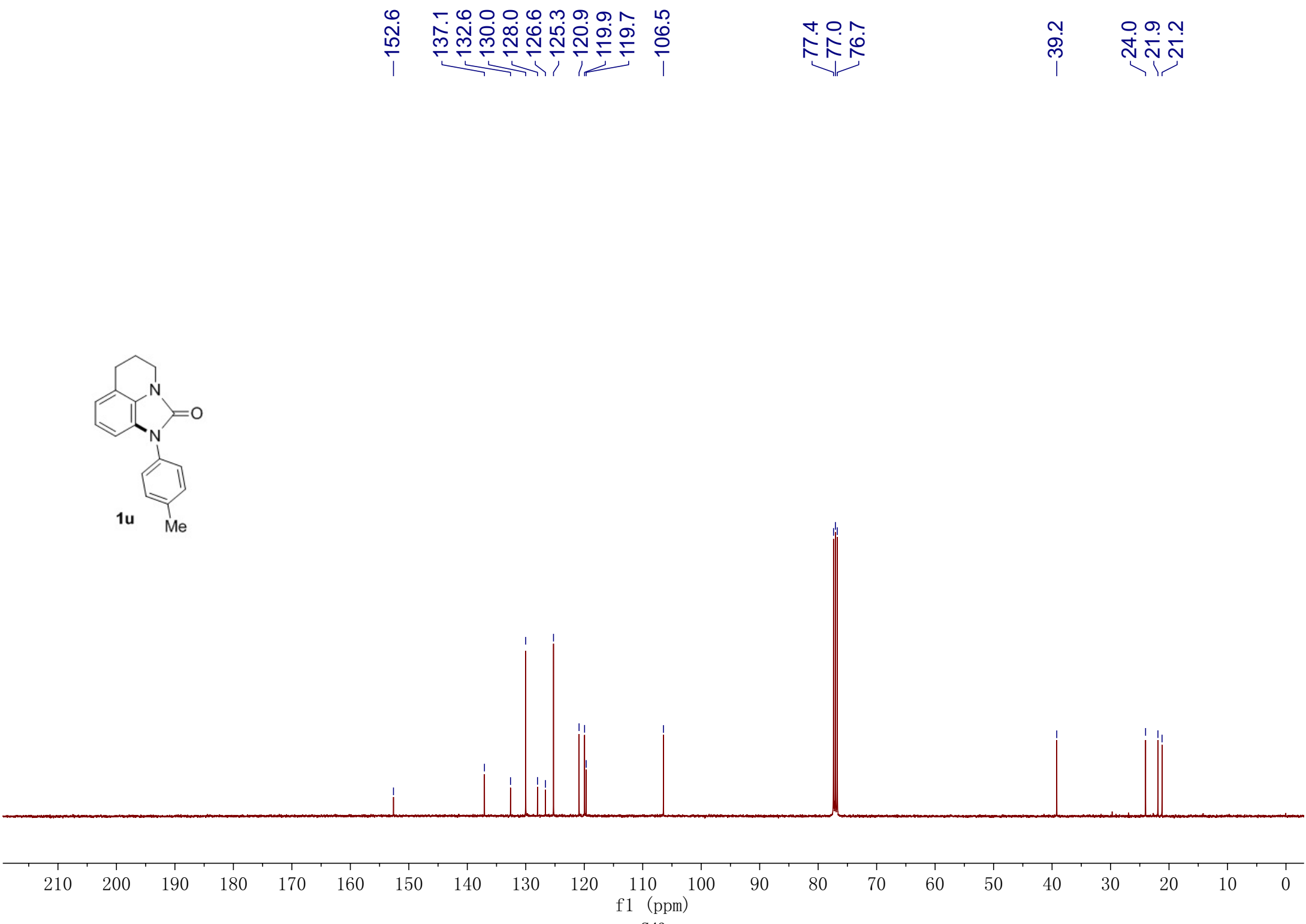
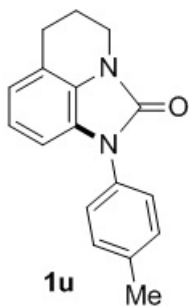
77.4  
77.0  
76.7  
76.4

53.8

20.9

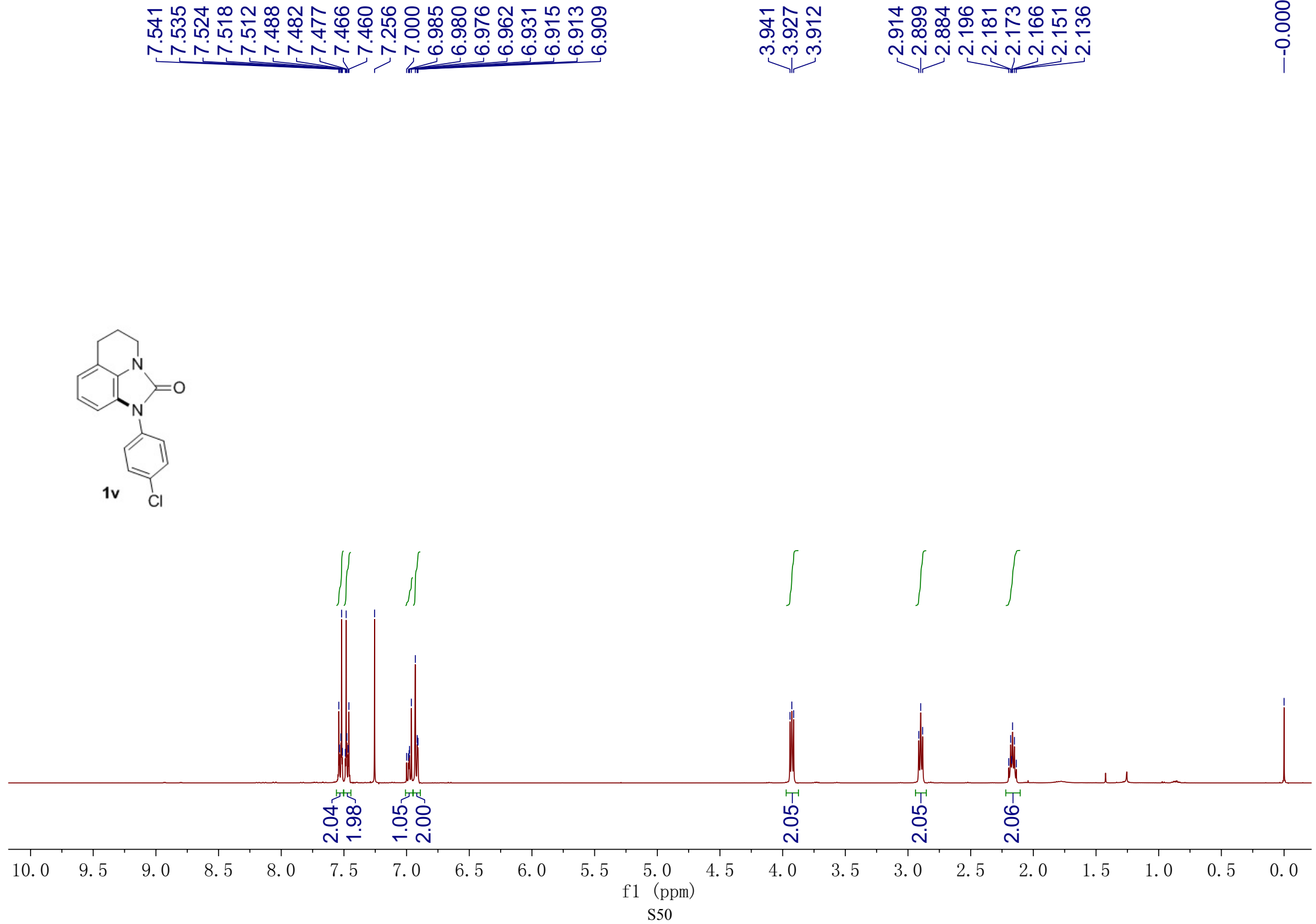
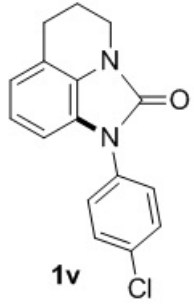


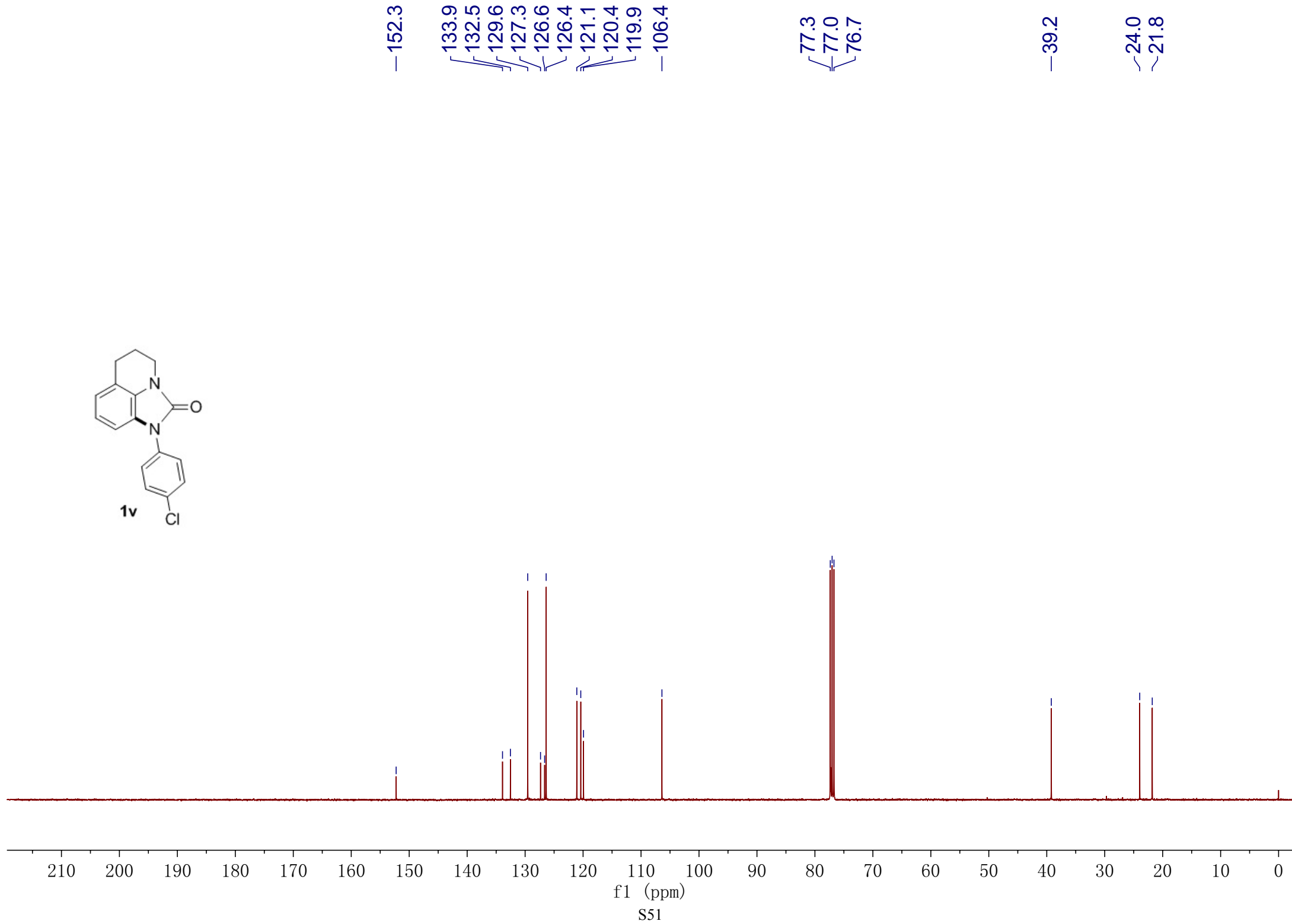
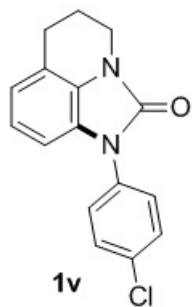


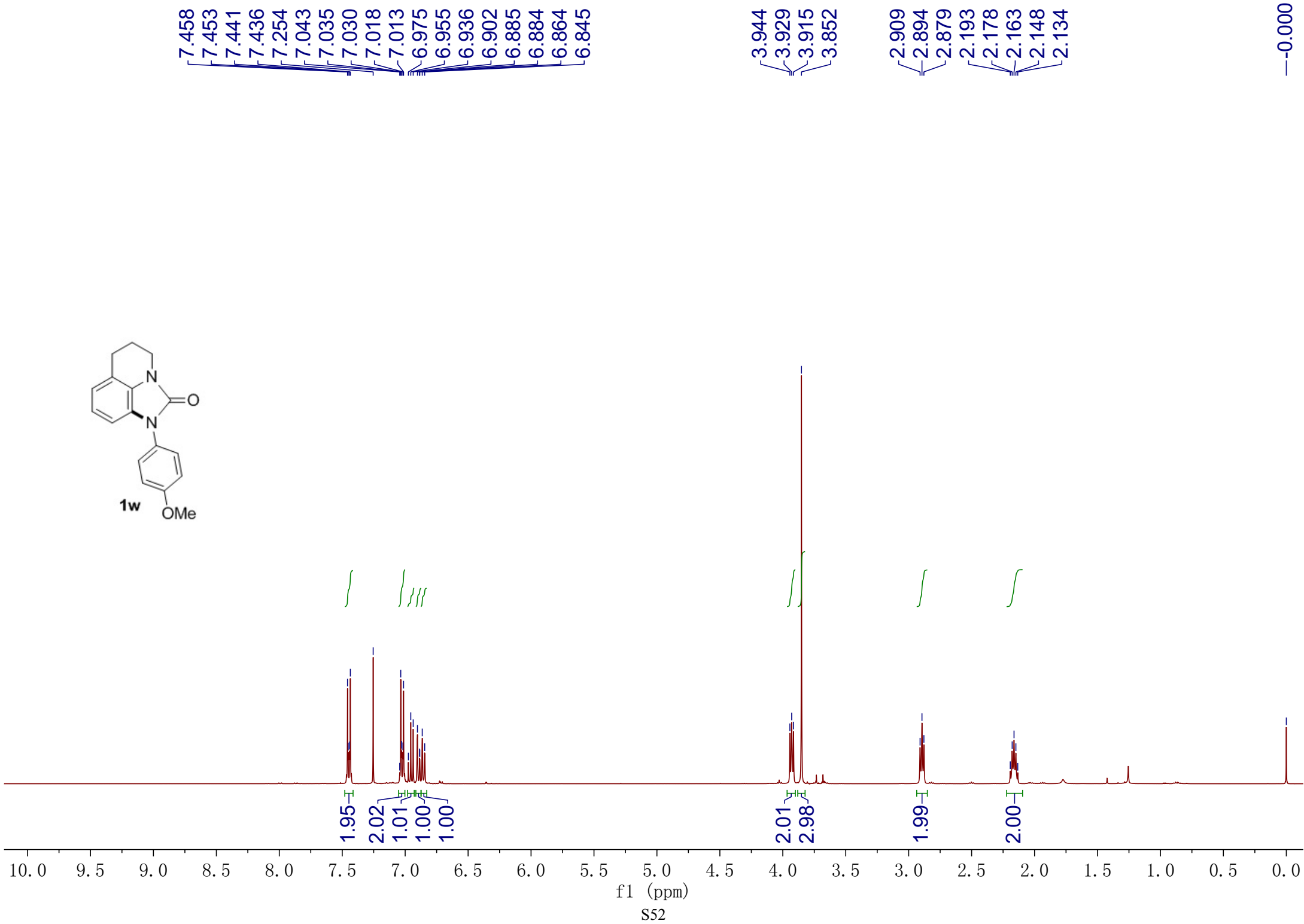
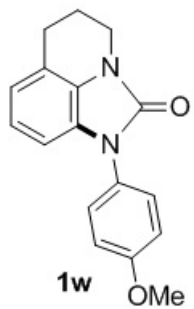


f1 (ppm)

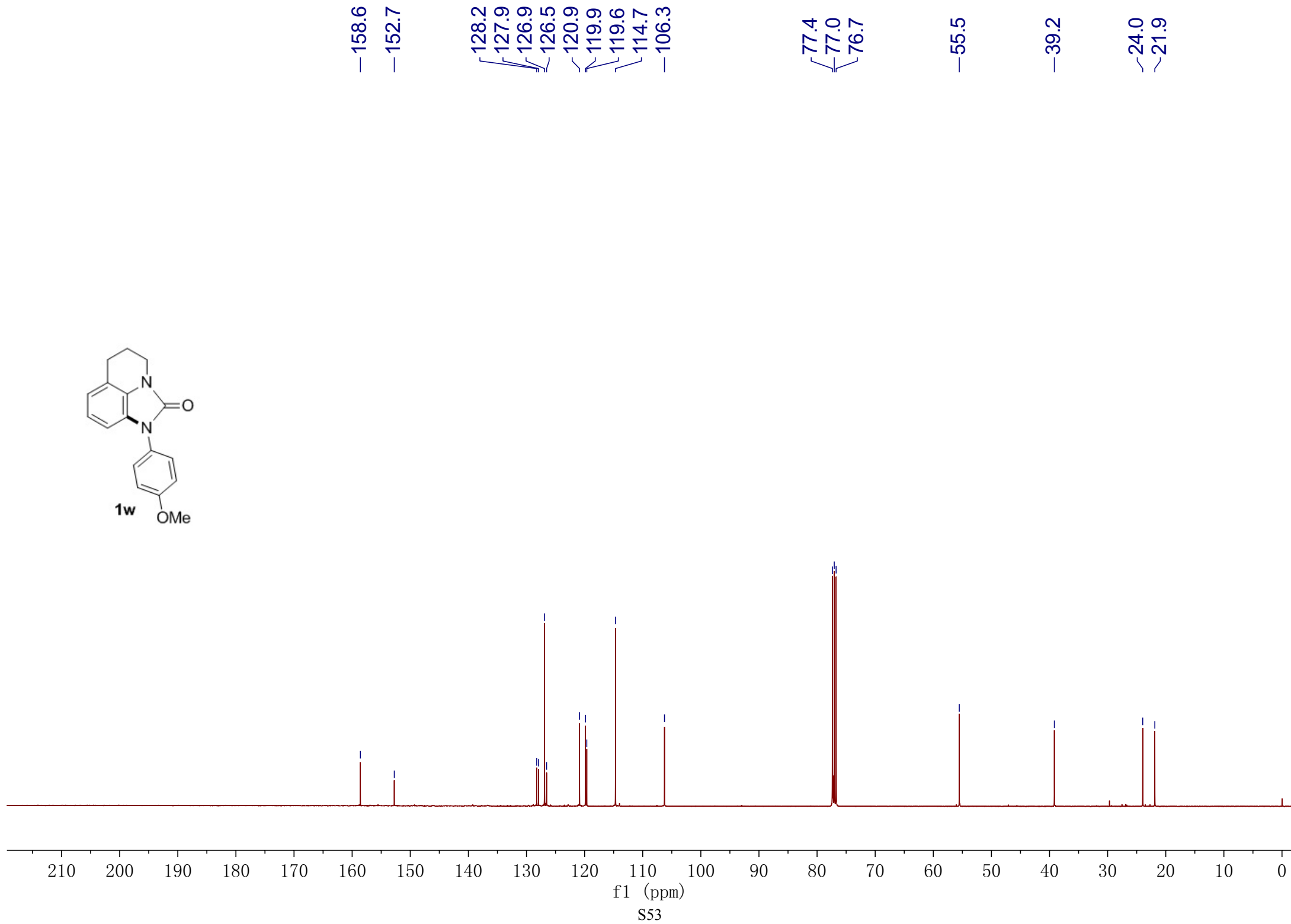
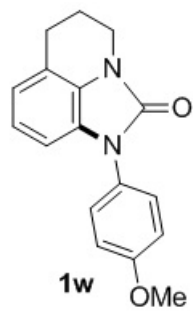
S49

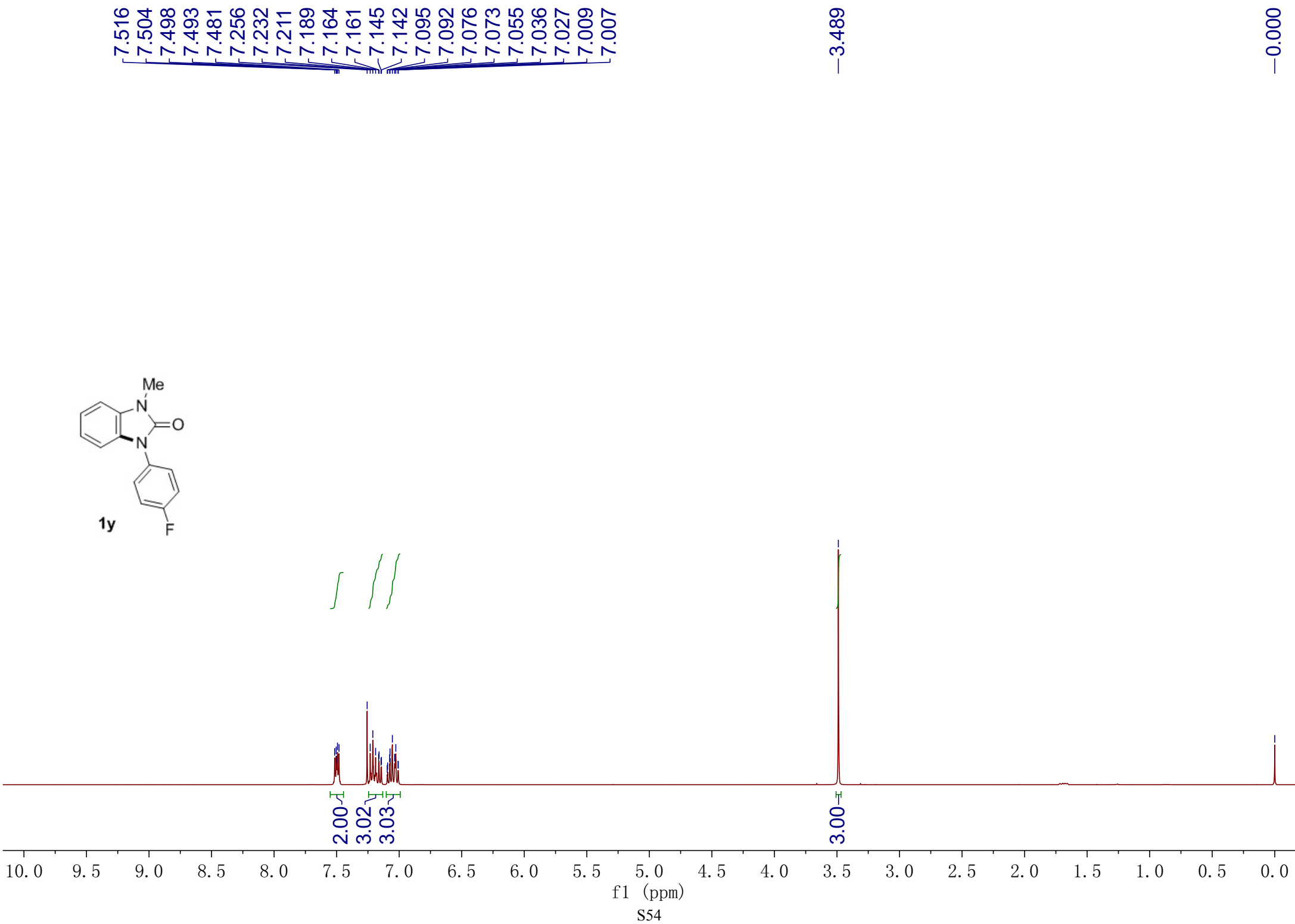
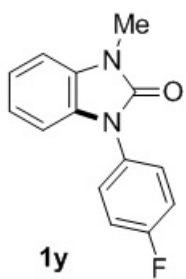


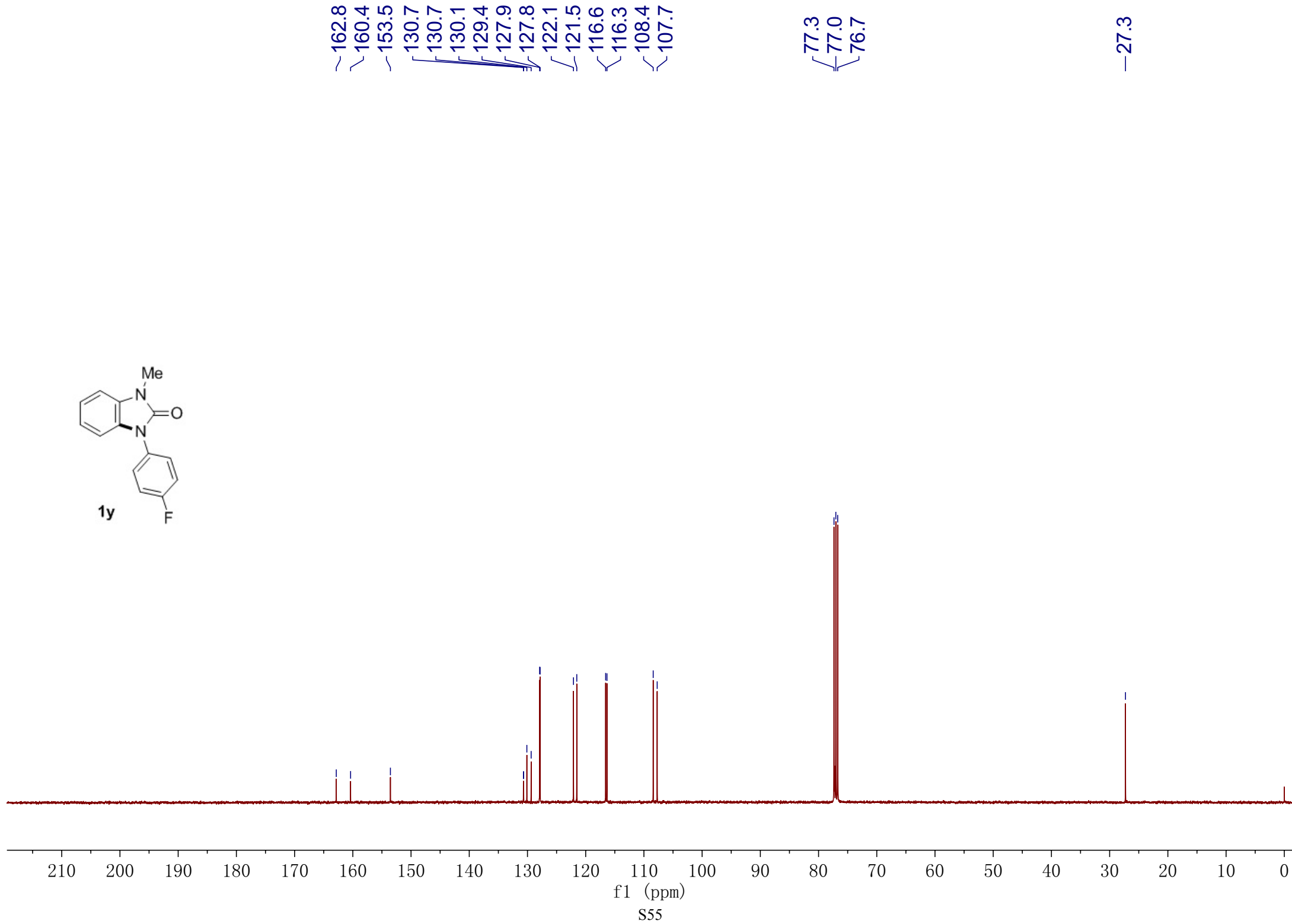
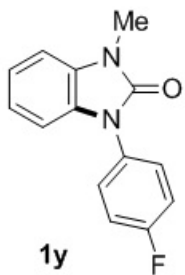


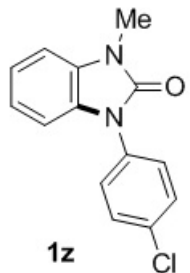








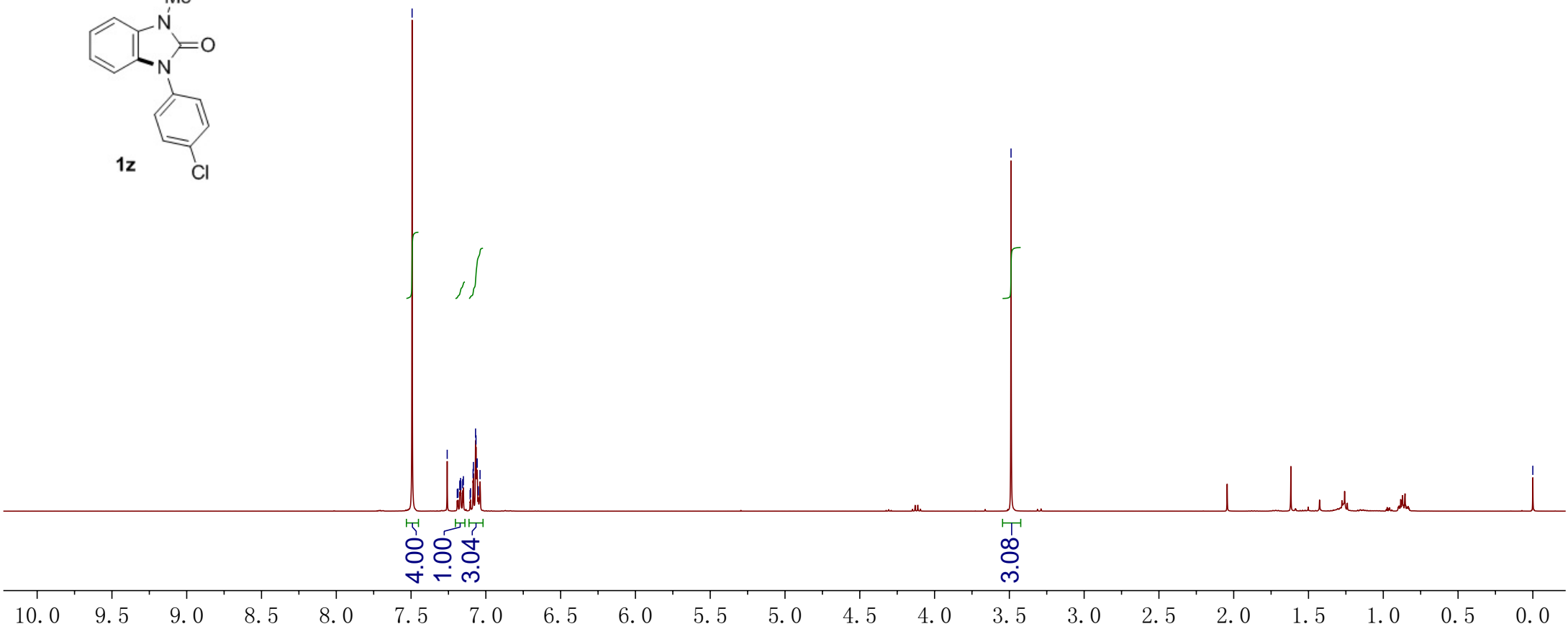




7.493  
7.258  
7.191  
7.186  
7.174  
7.172  
7.169  
7.167  
7.155  
7.150  
7.105  
7.103  
7.085  
7.083  
7.069  
7.066  
7.060  
7.058  
7.051  
7.039

—3.489

—0.000

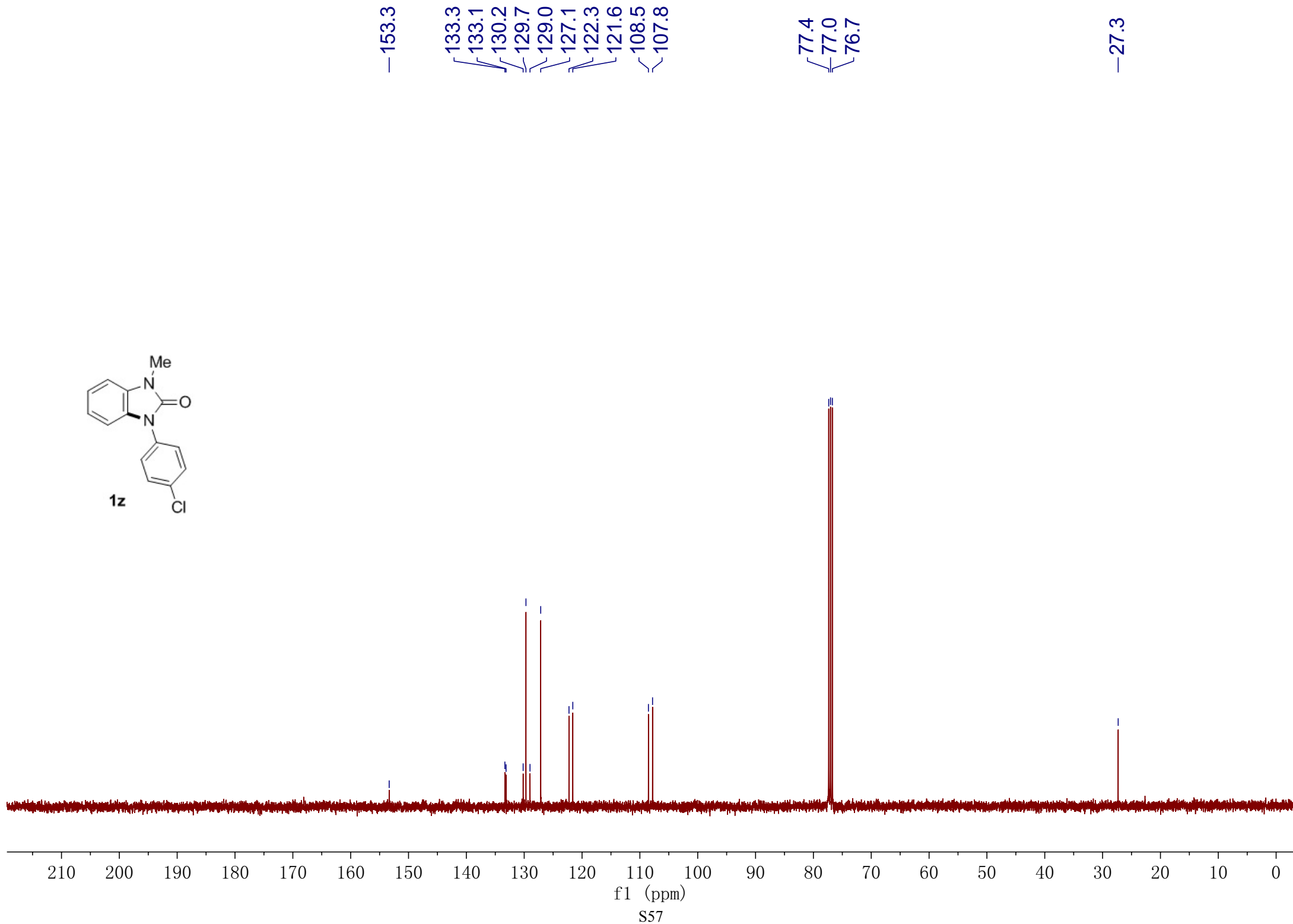
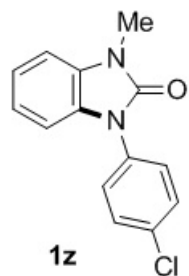


4.00  
1.00  
3.04

3.08

f1 (ppm)

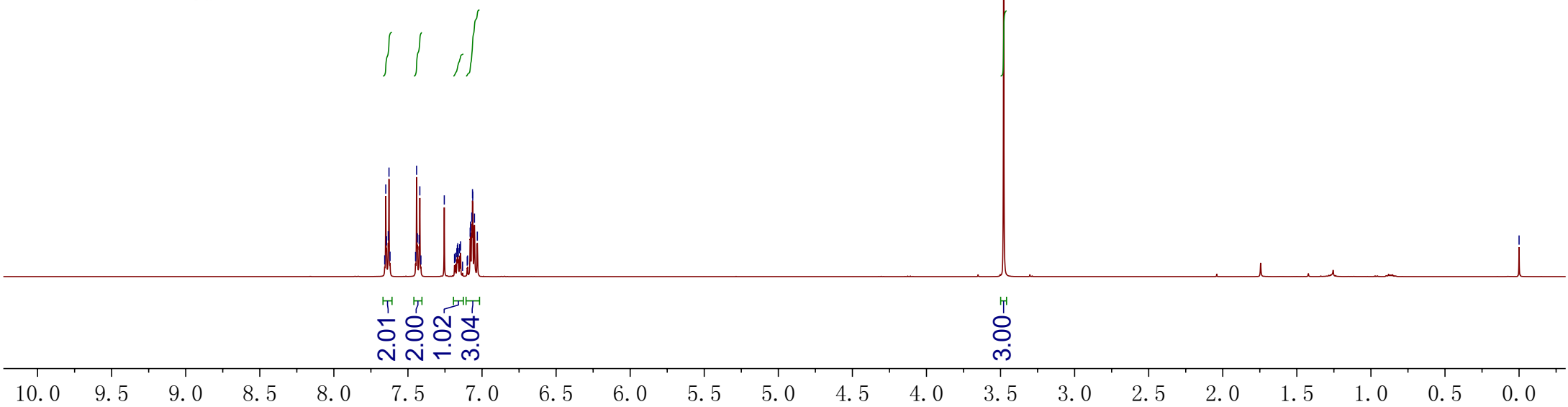
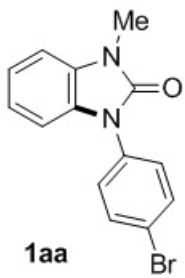
S56



7.657  
7.650  
7.645  
7.633  
7.628  
7.621  
7.448  
7.442  
7.436  
7.425  
7.420  
7.413  
7.255  
7.186  
7.179  
7.170  
7.166  
7.164  
7.160  
7.151  
7.144  
7.131  
7.100  
7.098  
7.080  
7.078  
7.069  
7.064  
7.063  
7.051  
7.032

3.479

0.000

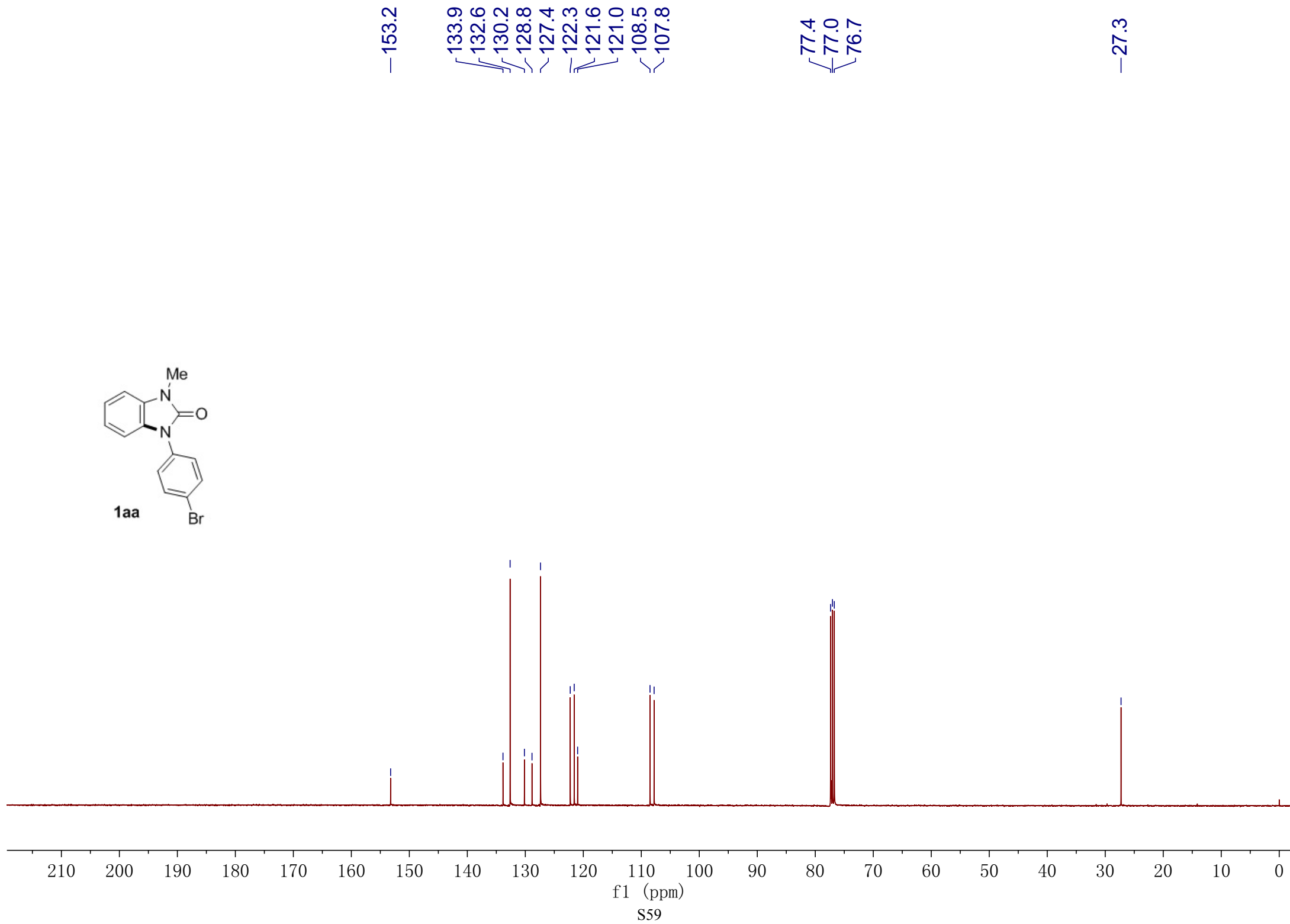
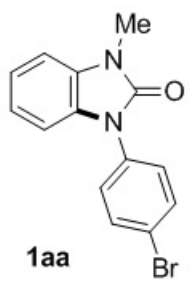


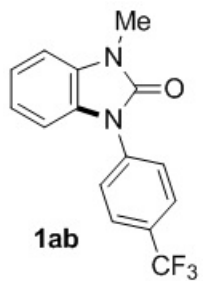
2.01  
2.00  
1.02  
3.04

3.00

f1 (ppm)

S58

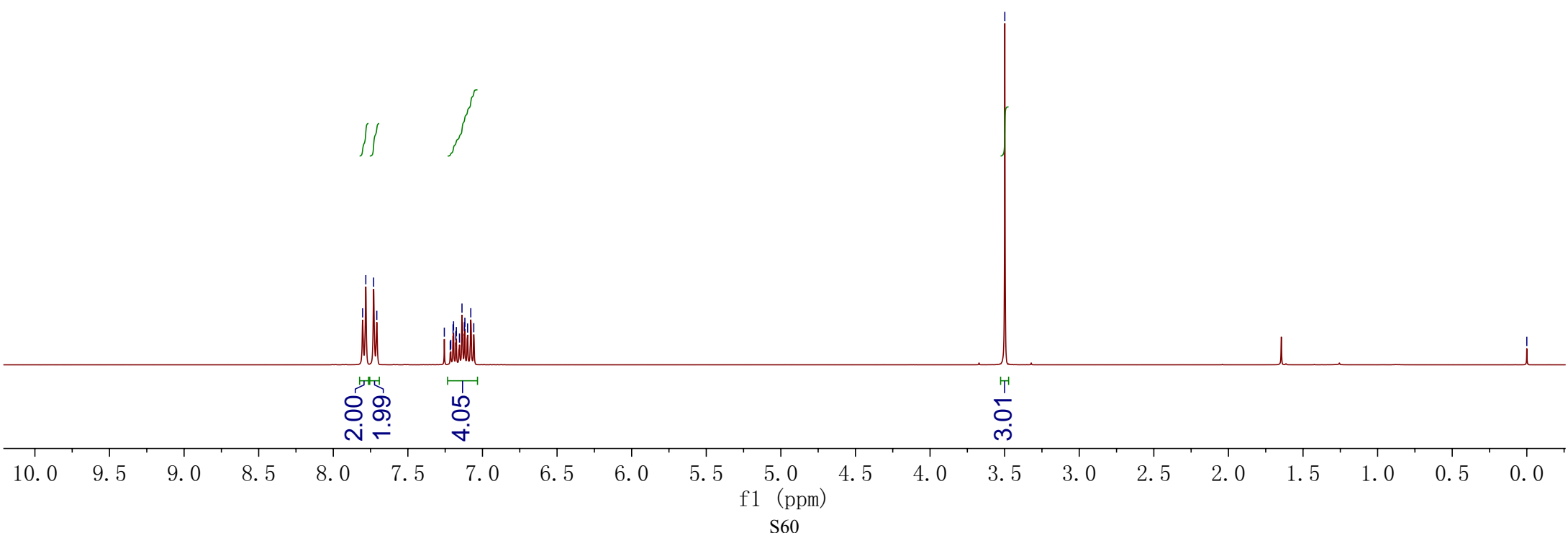




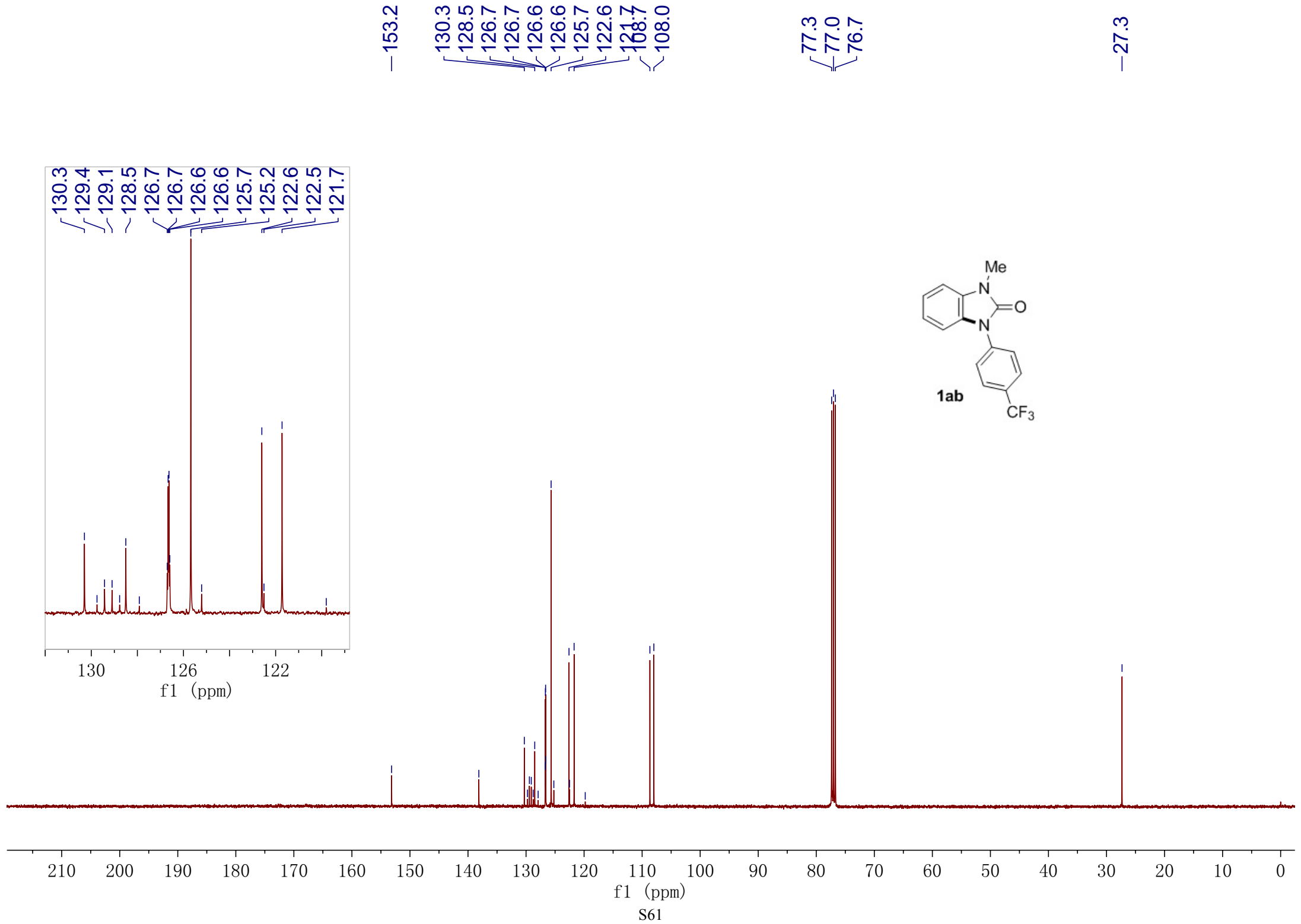
7.803  
7.782  
7.729  
7.708  
7.256  
7.216  
7.213  
7.197  
7.194  
7.179  
7.175  
7.154  
7.137  
7.121  
7.118  
7.100  
7.078  
7.058

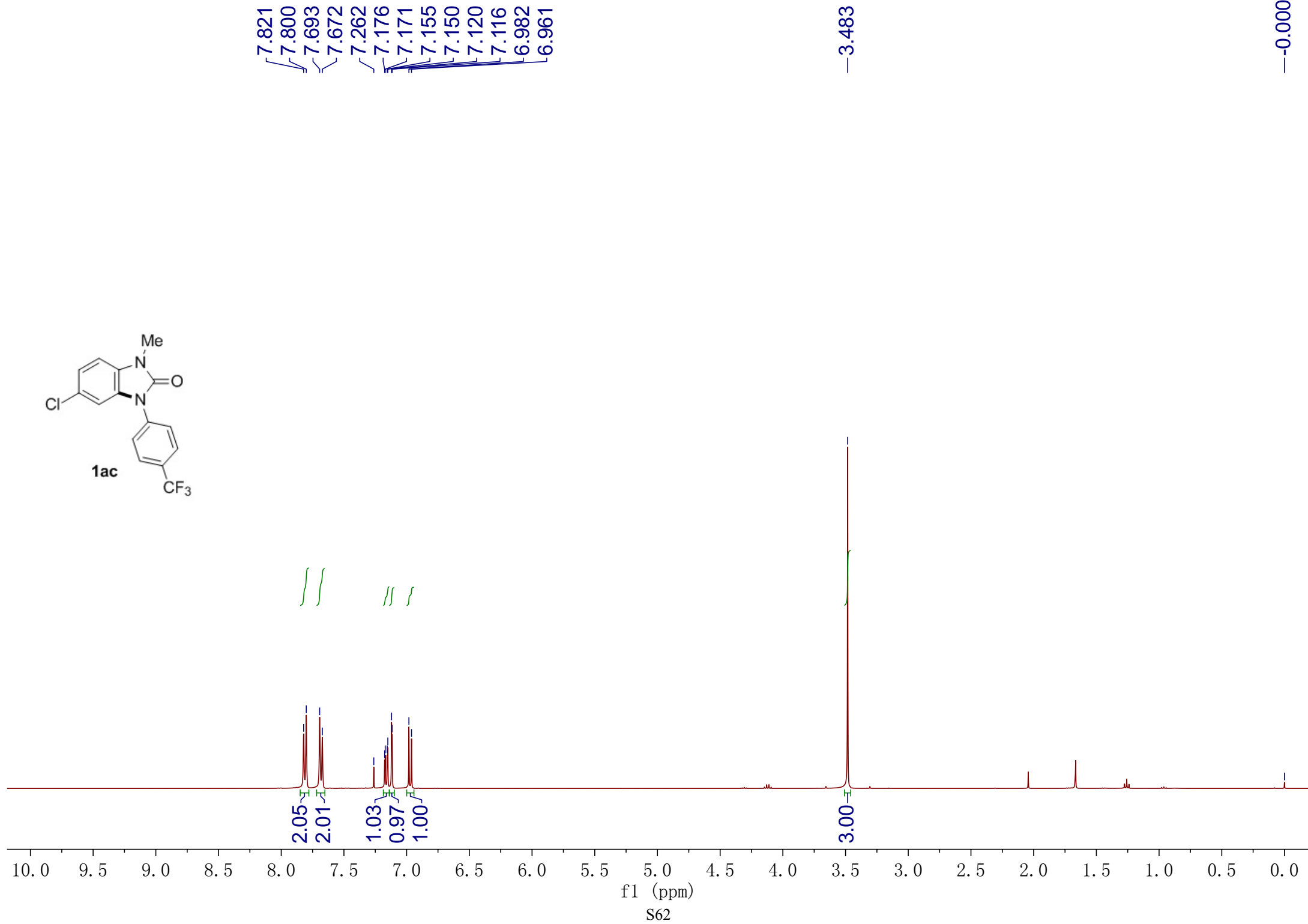
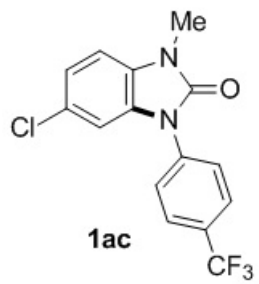
3.499

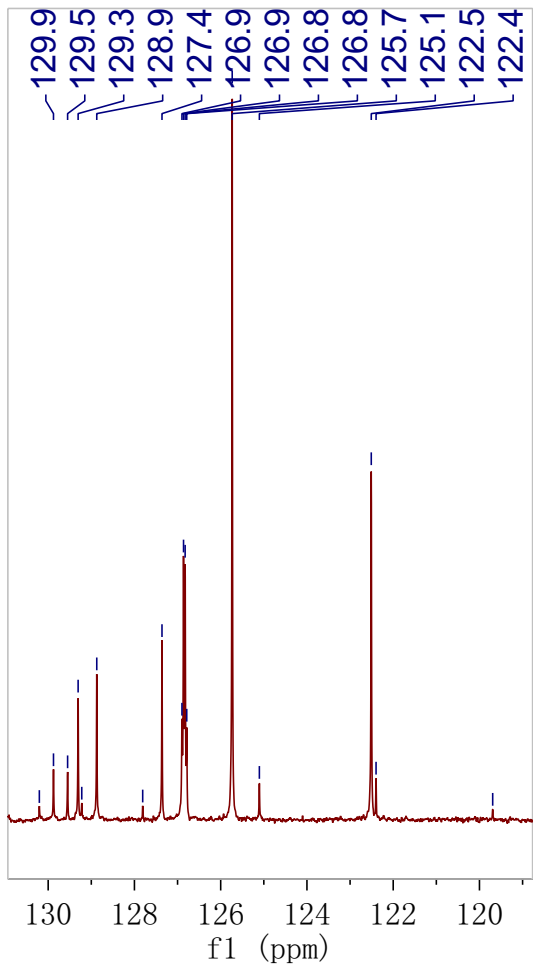
0.000







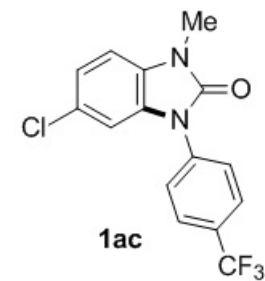




153.1  
129.3  
128.9  
127.4  
126.9  
126.9  
126.8  
126.8  
125.7  
122.5  
108.7

77.4  
77.0  
76.7

27.5



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

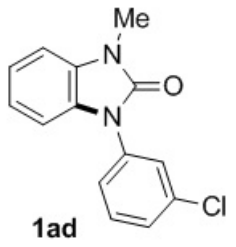
f1 (ppm)

S63

7.578  
7.575  
7.572  
7.569  
7.568  
7.463  
7.460  
7.455  
7.449  
7.447  
7.380  
7.375  
7.372  
7.366  
7.363  
7.358  
7.352  
7.256  
7.192  
7.185  
7.177  
7.172  
7.170  
7.166  
7.157  
7.151  
7.110  
7.098  
7.097  
7.091  
7.083  
7.080  
7.055  
7.036

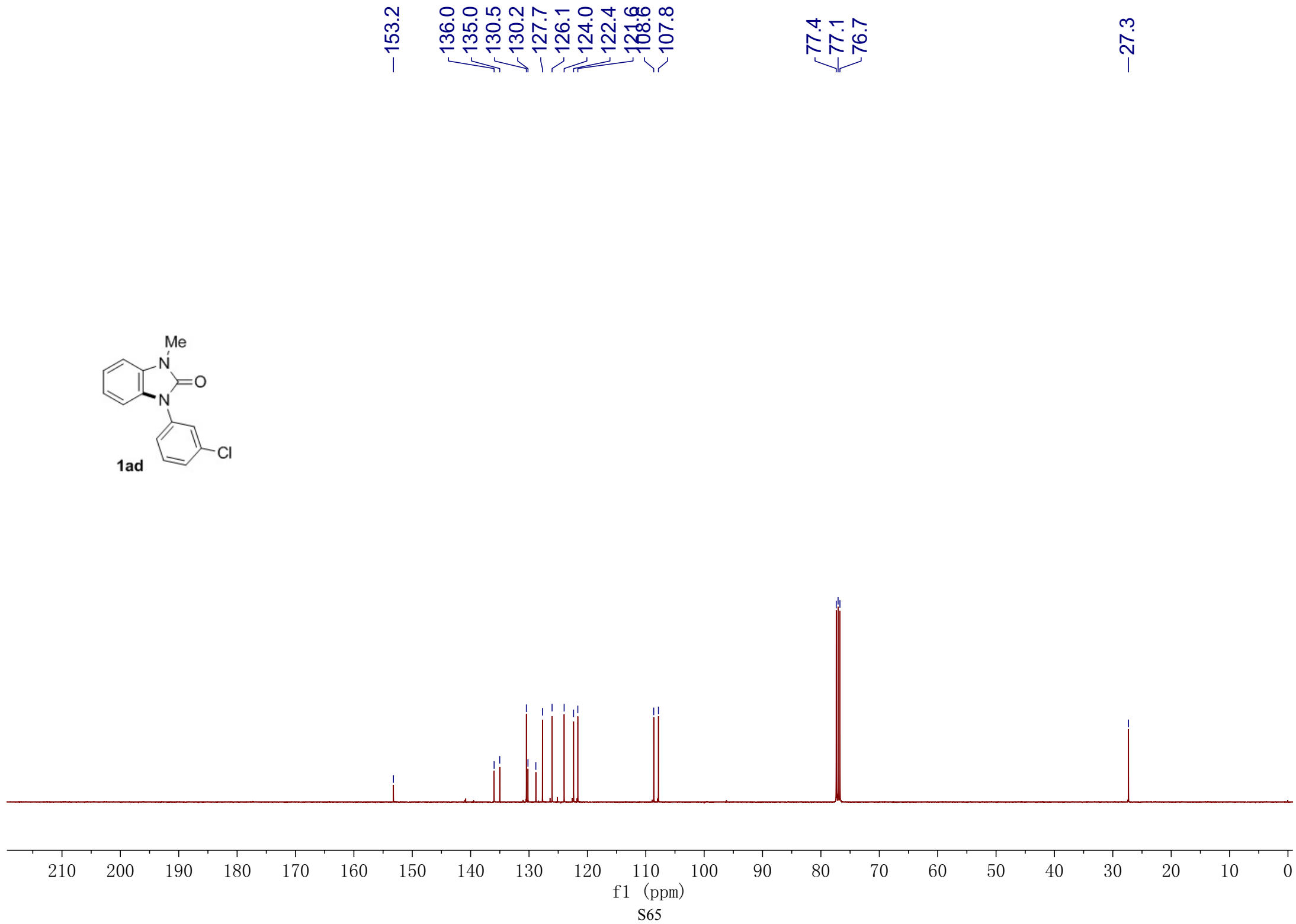
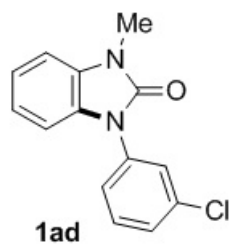
3.486

0.000



f1 (ppm)

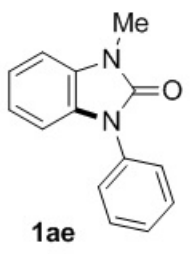
S64



7.545  
7.543  
7.532  
7.524  
7.518  
7.502  
7.496  
7.410  
7.403  
7.395  
7.389  
7.382  
7.375  
7.367  
7.252  
7.173  
7.167  
7.157  
7.154  
7.151  
7.148  
7.138  
7.132  
7.091  
7.077  
7.074  
7.061  
7.058  
7.050  
7.041  
7.039  
7.031

—3.491

—0.000



f1 (ppm)

S66

