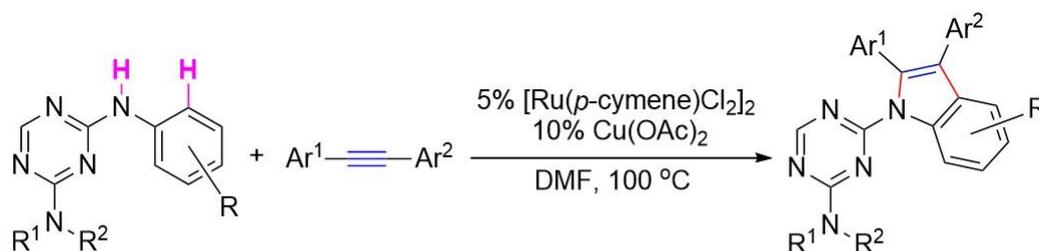


# Ruthenium Catalyzed Oxidative Synthesis of *N*-(2-triazine)indoles by C-H Activation

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- 17 examples yields up to 76%
- Triazine ring as directing group
- Lower loading of oxidant

1,3,5 triazines, especially indole functionalized triazine derivatives, exhibit excellent activities, such as anti-tumor, antibacterial, and anti-inflammatory activities. Traditional methods for the synthesis of *N*-(2-triazine) indoles suffer from unstable materials and tedious operations. Transition-metal-catalyzed C-C/C-N coupling provides a powerful protocol for the synthesis of indoles by the C-H activation strategy. Here, we report the efficient ruthenium-catalyzed oxidative synthesis of *N*-(2-triazine) indoles by C-H activation from alkynes and various substituted triazine derivatives in a moderate to good yield, and all of the *N*-(2-triazine) indoles were characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, and HRMS. This protocol can apply to the gram-scale synthesis of the *N*-(2-triazine) indole in a moderate yield. Moreover, the reaction is proposed to be performed via a six-membered ruthenacycle (II) intermediate, which suggests that the triazine ring could offer chelation assistance for the formation of *N*-(2-triazine) indoles.

## The $^1\text{H}$ and $^{13}\text{C}$ spectra of compounds

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Figure S35	$^1\text{H}$ spectra of <b>1a</b>	S38
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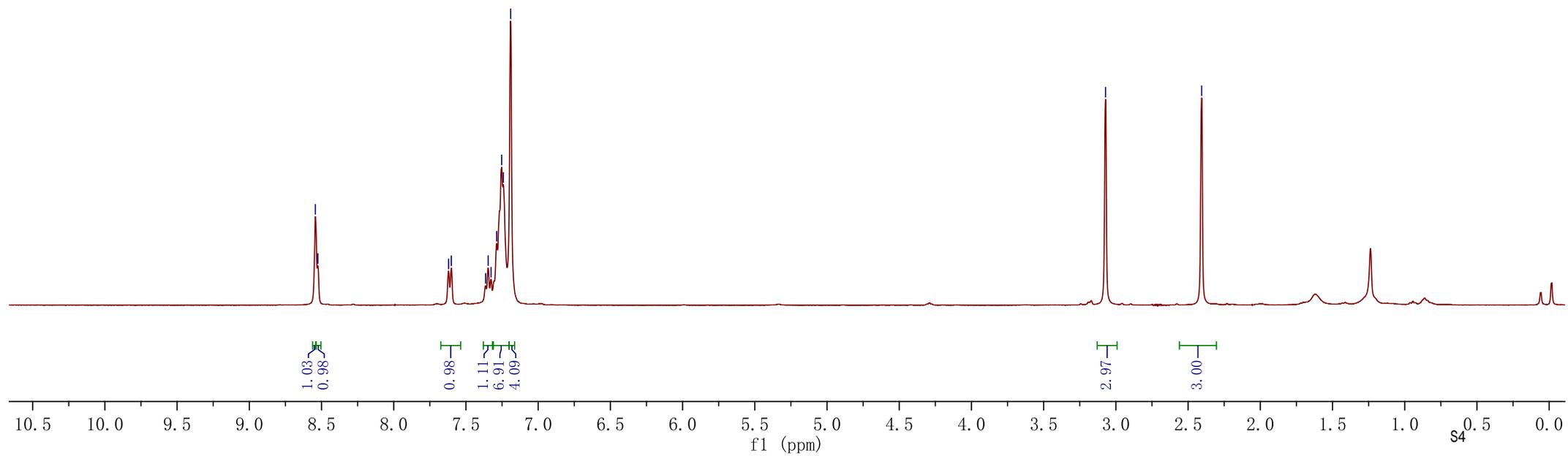
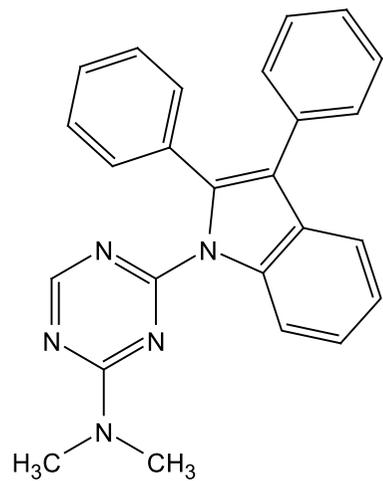
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7.6199  
7.6013  
7.3637  
7.3460  
7.3259  
7.2870  
7.2526  
7.2408  
7.1902

3.0716

2.4062

**Figure S1**, <sup>1</sup>H NMR spectrum of 4-(2,3-diphenyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3a**) in CDCl<sub>3</sub>



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20201221-C13-WHF-HT201120  
CDC13

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164.1273  
162.9550

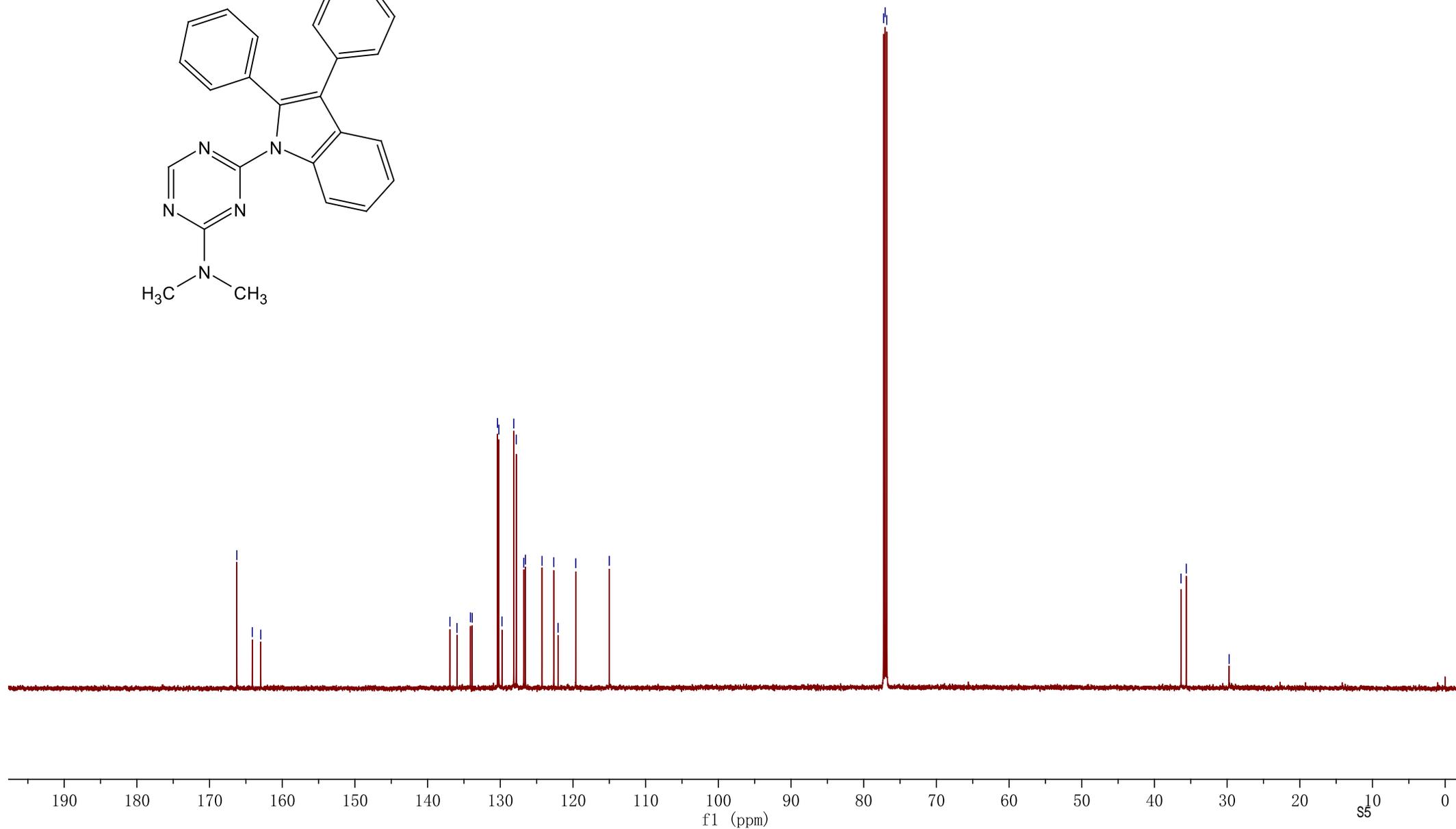
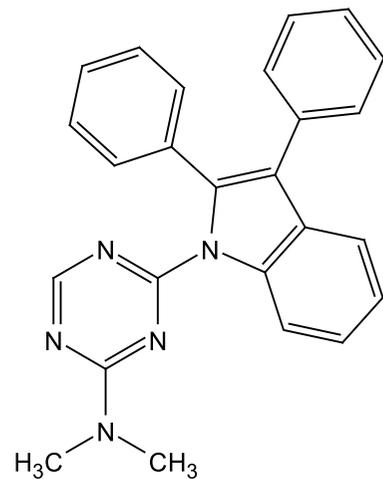
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133.8647  
130.3848  
130.2008  
129.7703  
128.1488  
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126.7782  
126.5456  
124.2590  
122.6470  
122.0544  
119.6210  
115.0074

77.2571  
77.0455  
76.8338

36.3460  
35.6192

29.7229

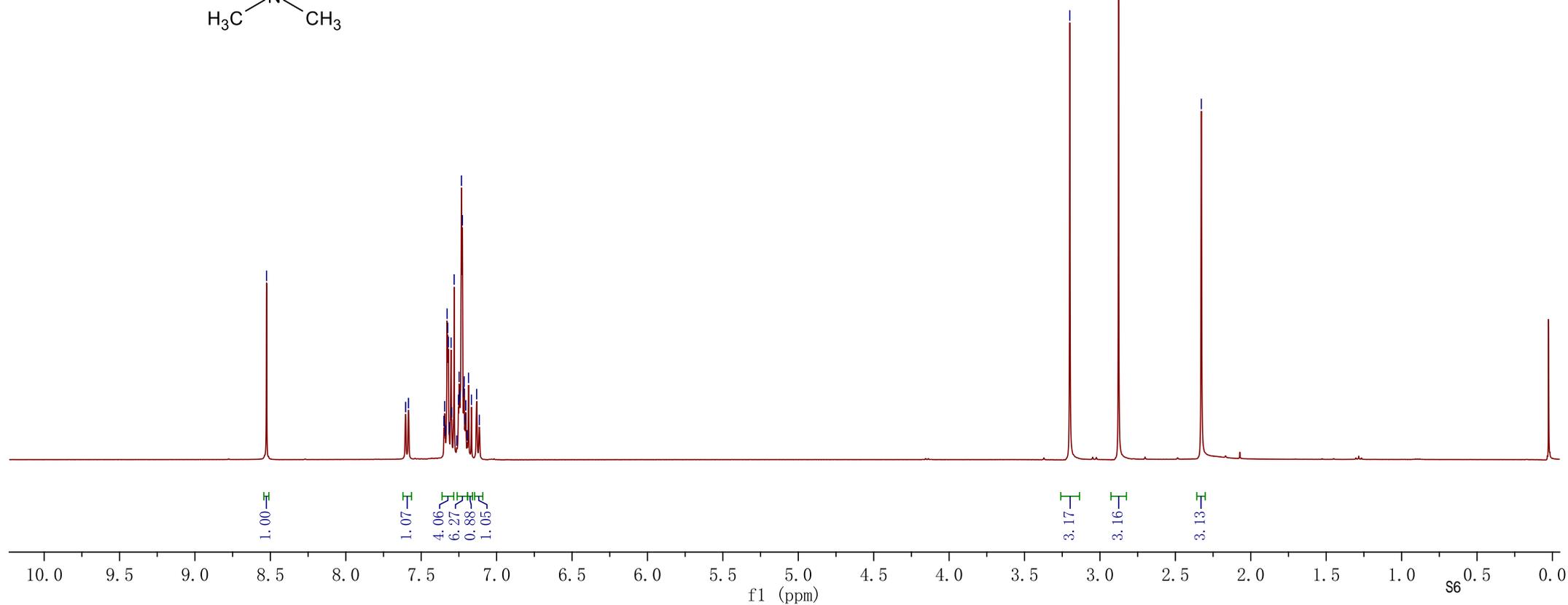
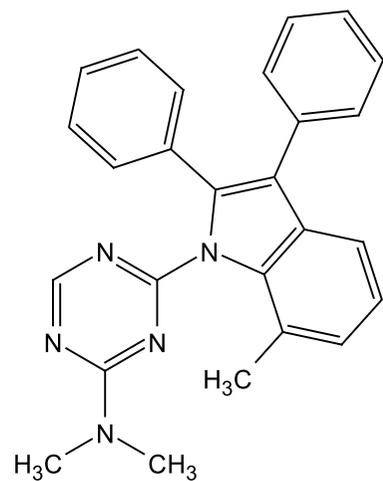
**Figure S2**,  $^{13}\text{C}$  NMR spectrum of 4-(2,3-diphenyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3a**) in  $\text{CDCl}_3$



8.5254  
7.6032  
7.5843  
7.5493  
7.3447  
7.3394  
7.3281  
7.3241  
7.3197  
7.3142  
7.3018  
7.2976  
7.2813  
7.2640  
7.2529  
7.2484  
7.2443  
7.2330  
7.2269  
7.2182  
7.2149  
7.2094  
7.2043  
7.1953  
7.1861  
7.1669  
7.1322  
7.1144

3.2000  
2.8767  
2.3277

**Figure S3**, <sup>1</sup>H NMR spectrum of 4--4-(7-methyl-2,3-diphenyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3b**) in CDCl<sub>3</sub>



20220117zm  
F210904

165.8925  
164.5306  
164.4068

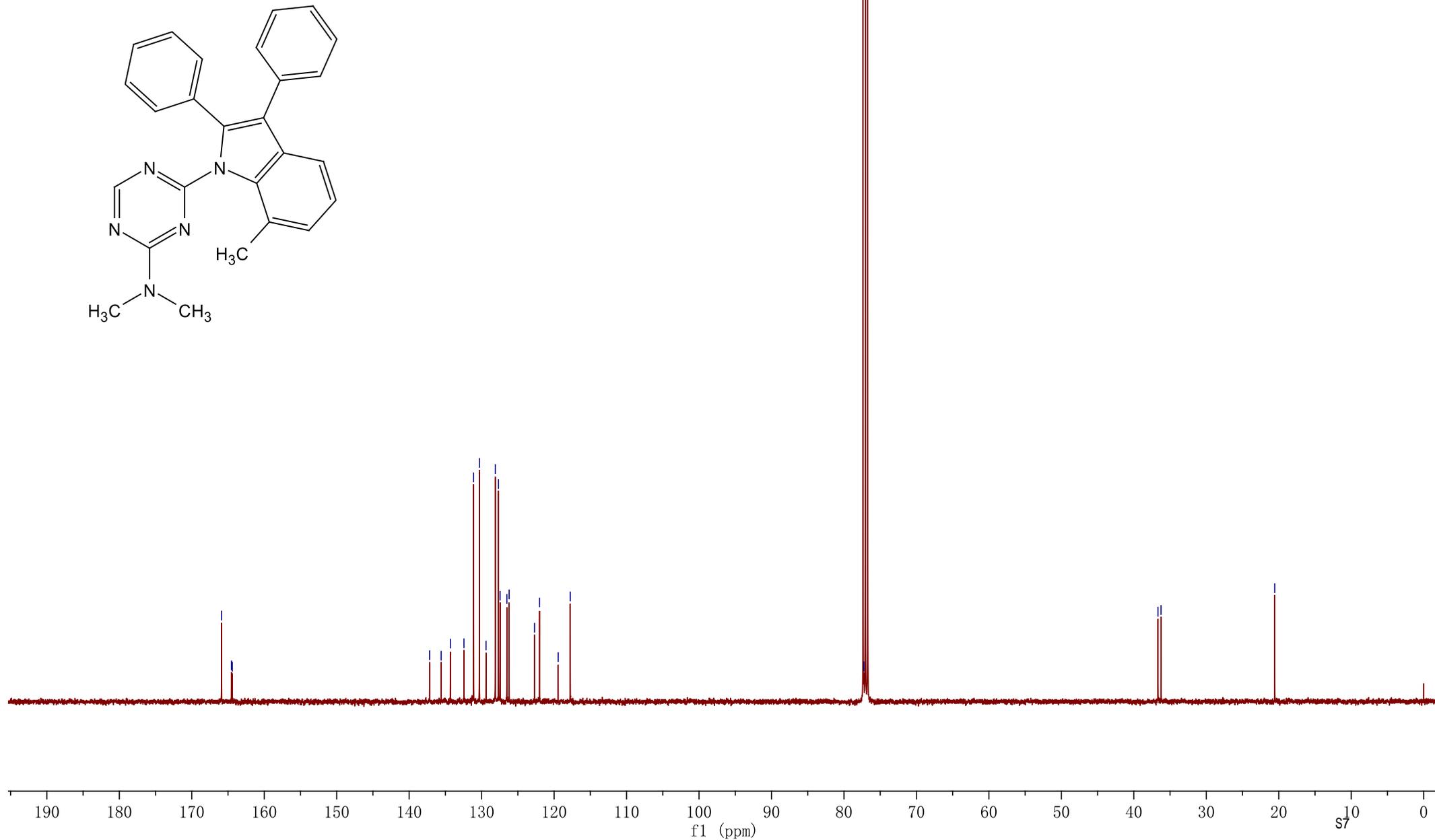
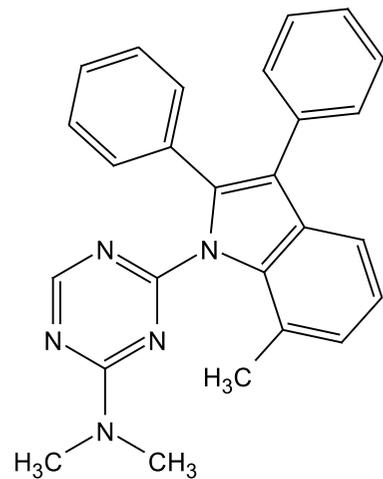
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127.4557  
126.5162  
126.2096  
122.6984  
122.0107  
119.4366  
117.7681

77.3593  
77.2458  
77.0417  
76.7241

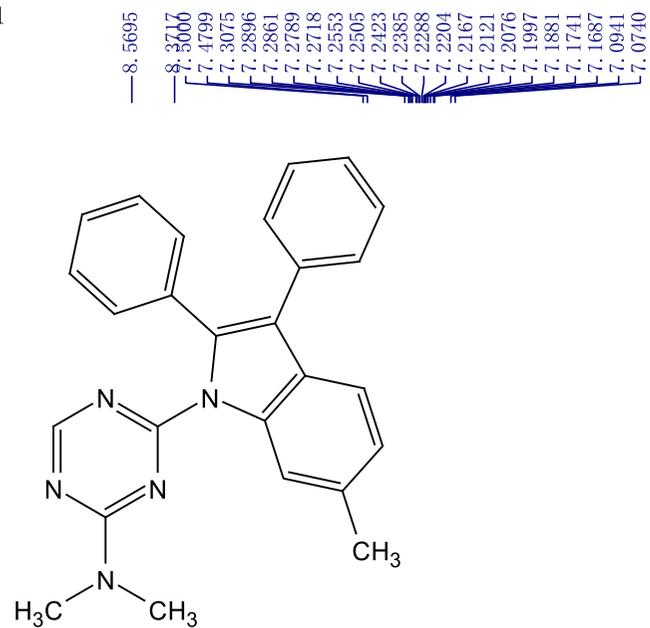
36.6652  
36.2457

20.5575

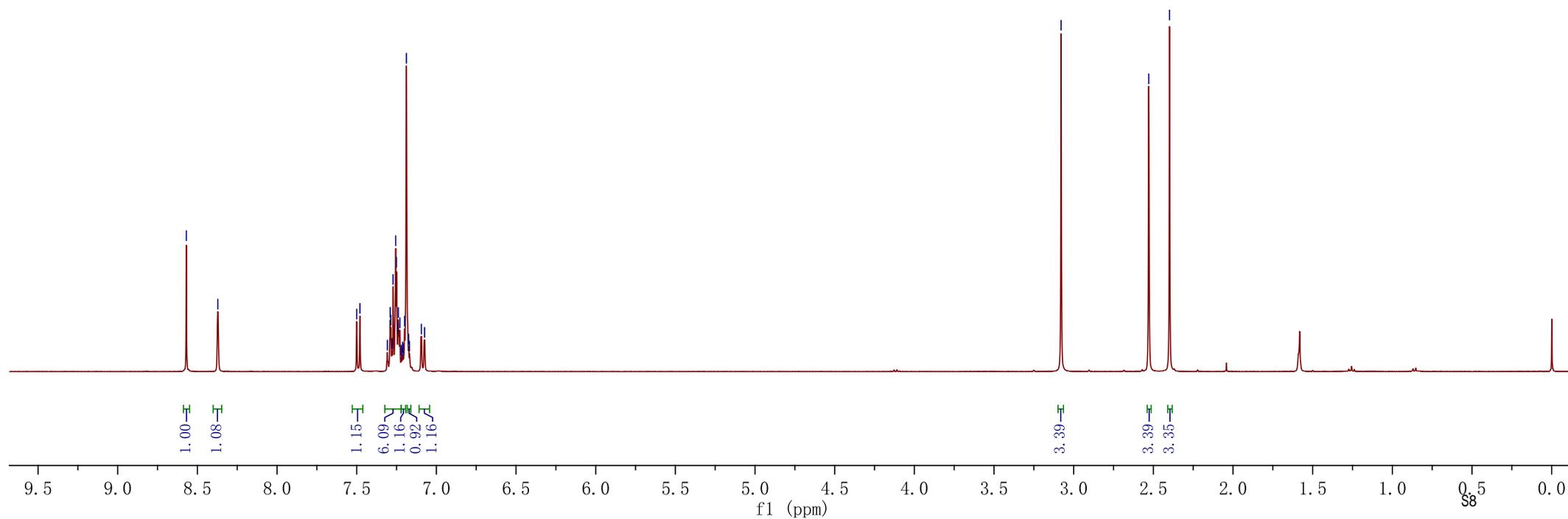
**Figure S4**,  $^{13}\text{C}$  NMR spectrum of 4--4-(7-methyl-2,3-diphenyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3b**) in  $\text{CDCl}_3$



PROTON\_01  
zm-55



**Figure S5**,  $^1\text{H}$  NMR spectrum of *N,N*-dimethyl-4-(6-methyl-2,3-diphenyl-1H-indol-1-yl)-1,3,5-triazin-2-amine (**3c**) in  $\text{CDCl}_3$



20210924-C13-WHF-55  
20210924-C13-WHF-55  
CDC13

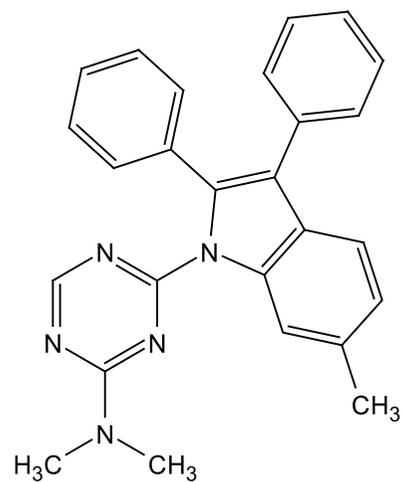
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164.5135  
162.9462

137.3060  
135.3162  
134.2918  
134.2553  
134.0445  
130.3374  
130.1711  
128.0990  
127.7556  
127.6401  
126.6182  
126.4585  
124.1321  
122.0097  
119.2526  
115.0464

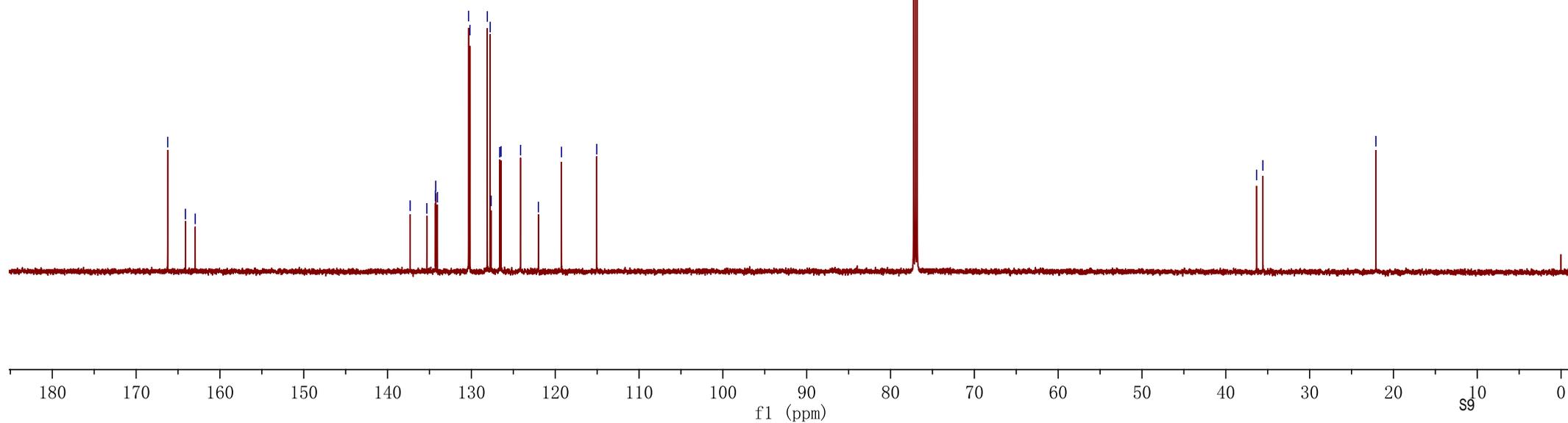
77.2483  
77.0318  
76.8200

36.3241  
35.5770

22.0939



**Figure S6**, <sup>13</sup>C NMR spectrum of *N,N*-dimethyl-4-(6-methyl-2,3-diphenyl-1*H*-indol-1-yl)-1,3,5-triazin-2-amine (**3c**) in CDCl<sub>3</sub>



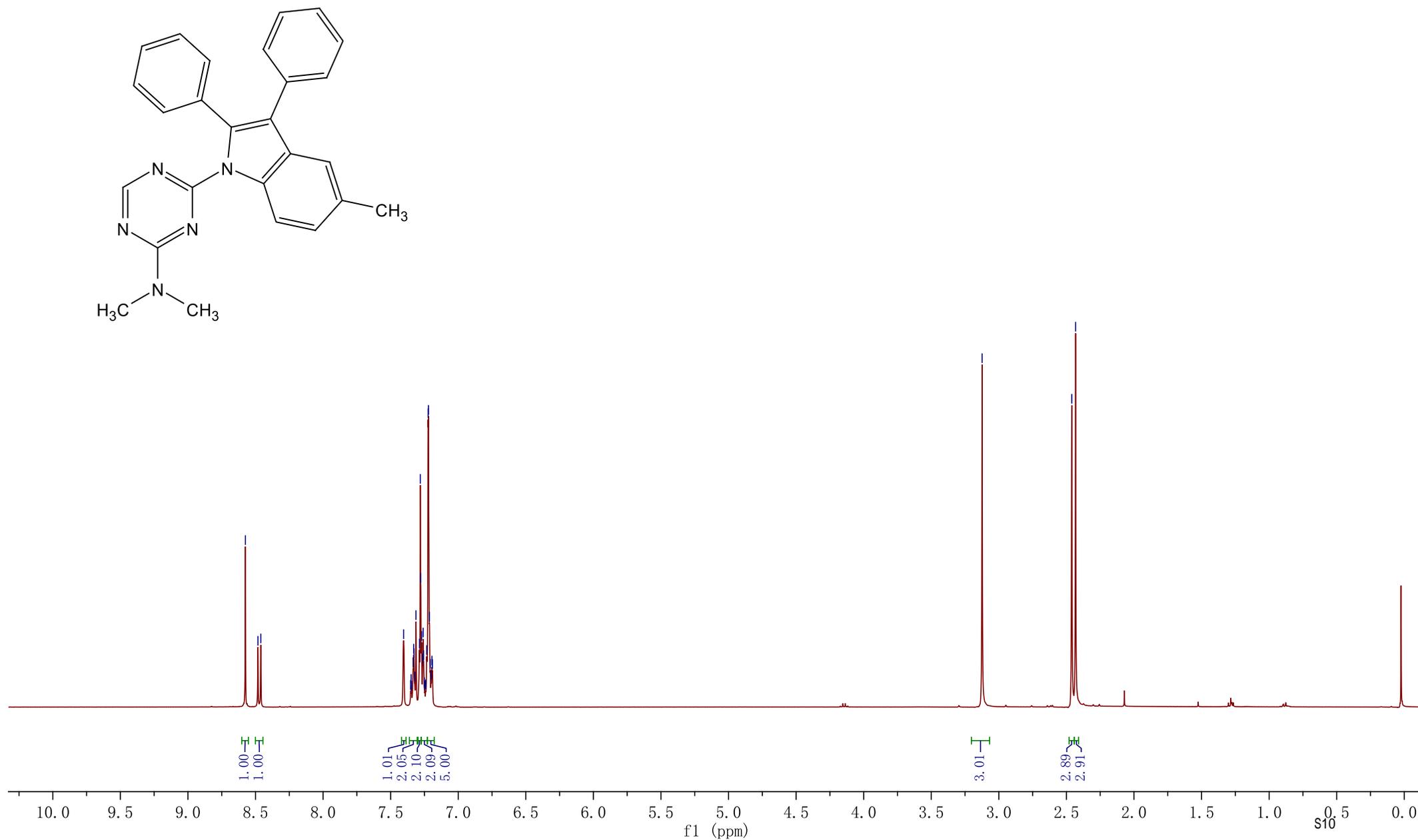
20220112zm  
F210607

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8.4821  
8.4608  
7.4040  
7.3518  
7.3485  
7.3446  
7.3335  
7.3298  
7.3272  
7.3226  
7.3129  
7.2867  
7.2806  
7.2771  
7.2707  
7.2634  
7.2596  
7.2561  
7.2503  
7.2466  
7.2407  
7.2331  
7.2226  
7.2203  
7.2129  
7.2065  
7.2001  
7.1945  
7.1910

— 3.1237

2.4604  
2.4321

**Figure S7**,  $^1\text{H}$  NMR spectrum of *N,N*-dimethyl-4-(5-methyl-2,3-diphenyl-1*H*-indol-1-yl)-1,3,5-triazin-2-amine (**3d**) in  $\text{CDCl}_3$



20220117zm  
F210607

165.8063  
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162.7801

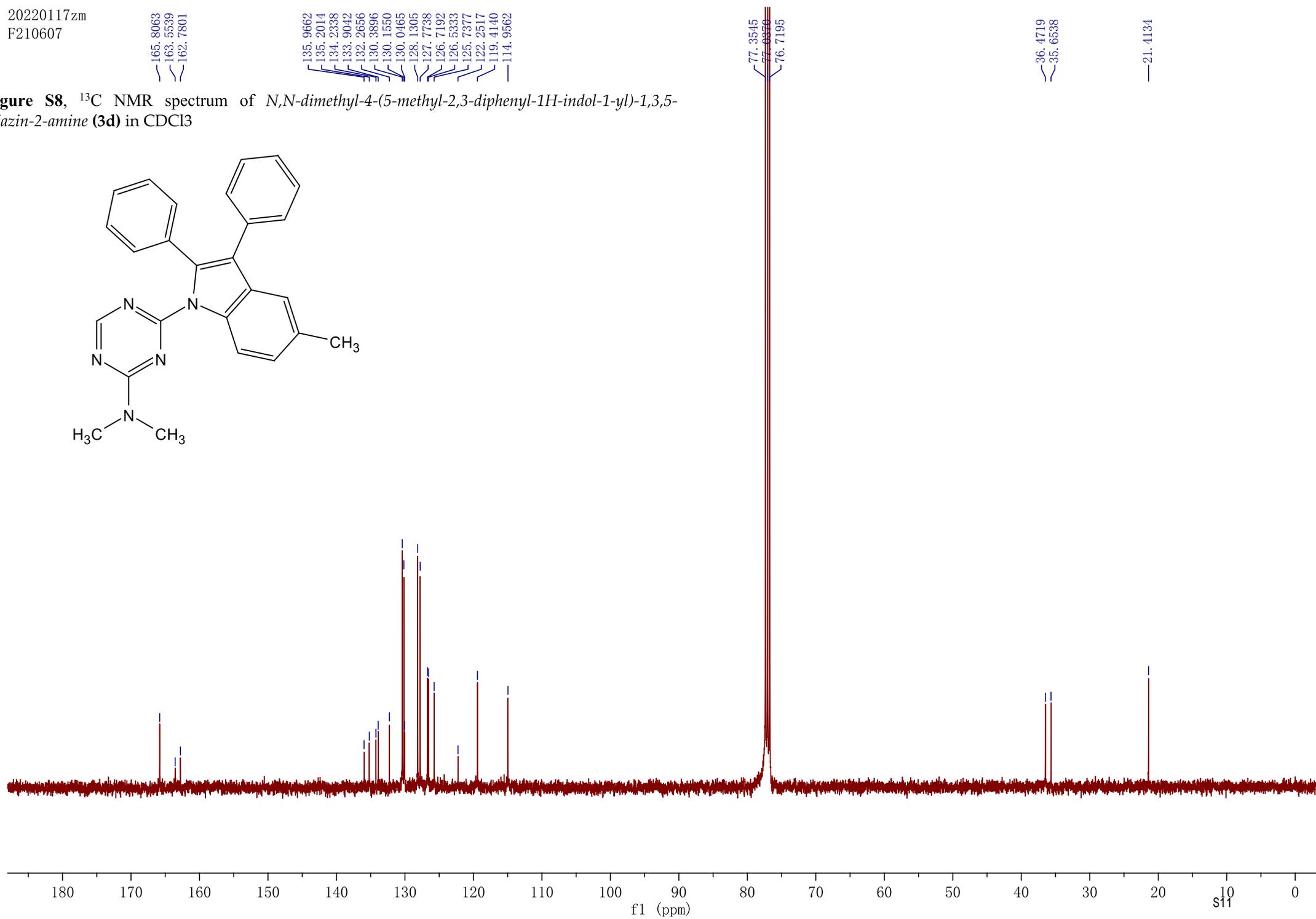
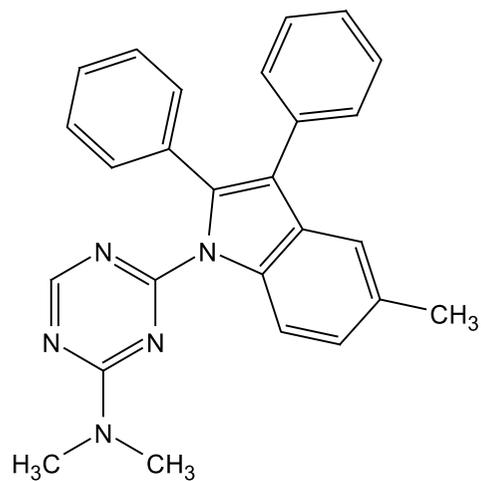
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134.2338  
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132.2656  
130.3896  
130.1550  
130.0465  
128.1305  
127.7738  
126.7192  
126.5333  
125.7377  
122.2517  
119.4140  
114.9662

77.3545  
77.0376  
76.7195

36.4719  
35.6538

21.4134

**Figure S8**,  $^{13}\text{C}$  NMR spectrum of *N,N*-dimethyl-4-(5-methyl-2,3-diphenyl-1*H*-indol-1-yl)-1,3,5-triazin-2-amine (**3d**) in  $\text{CDCl}_3$



F-20220222  
F20220222

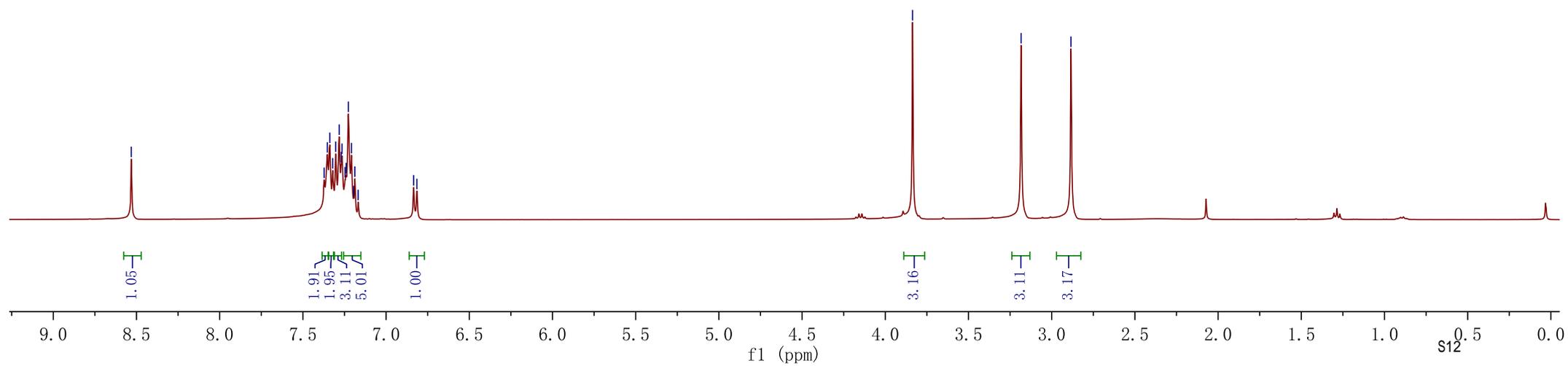
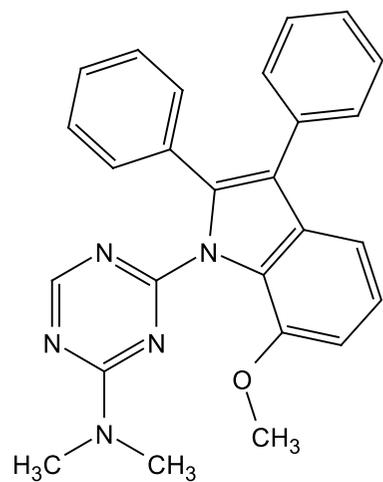
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7.3531  
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7.3210  
7.3030  
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7.2700  
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7.2468  
7.2400  
7.2266  
7.2081  
7.1949  
7.1878  
7.1680  
6.8343  
6.8148

3.8361

3.1839

2.8843

**Figure S9**,  $^1\text{H}$  NMR spectrum of 4-(7-methoxy-2,3-diphenyl-1H-indol-1-yl)-*N,N*-dimethyl-1,3,5-triazin-2-amine (**3e**) in  $\text{CDCl}_3$



20220406zm  
F220222

165.4022  
164.6150  
164.1040

147.3147

137.1958  
134.3227  
132.0595  
131.1781  
130.7233  
130.2138  
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127.6723  
127.5065  
126.3411  
126.1944  
122.4463  
119.2994

112.6496

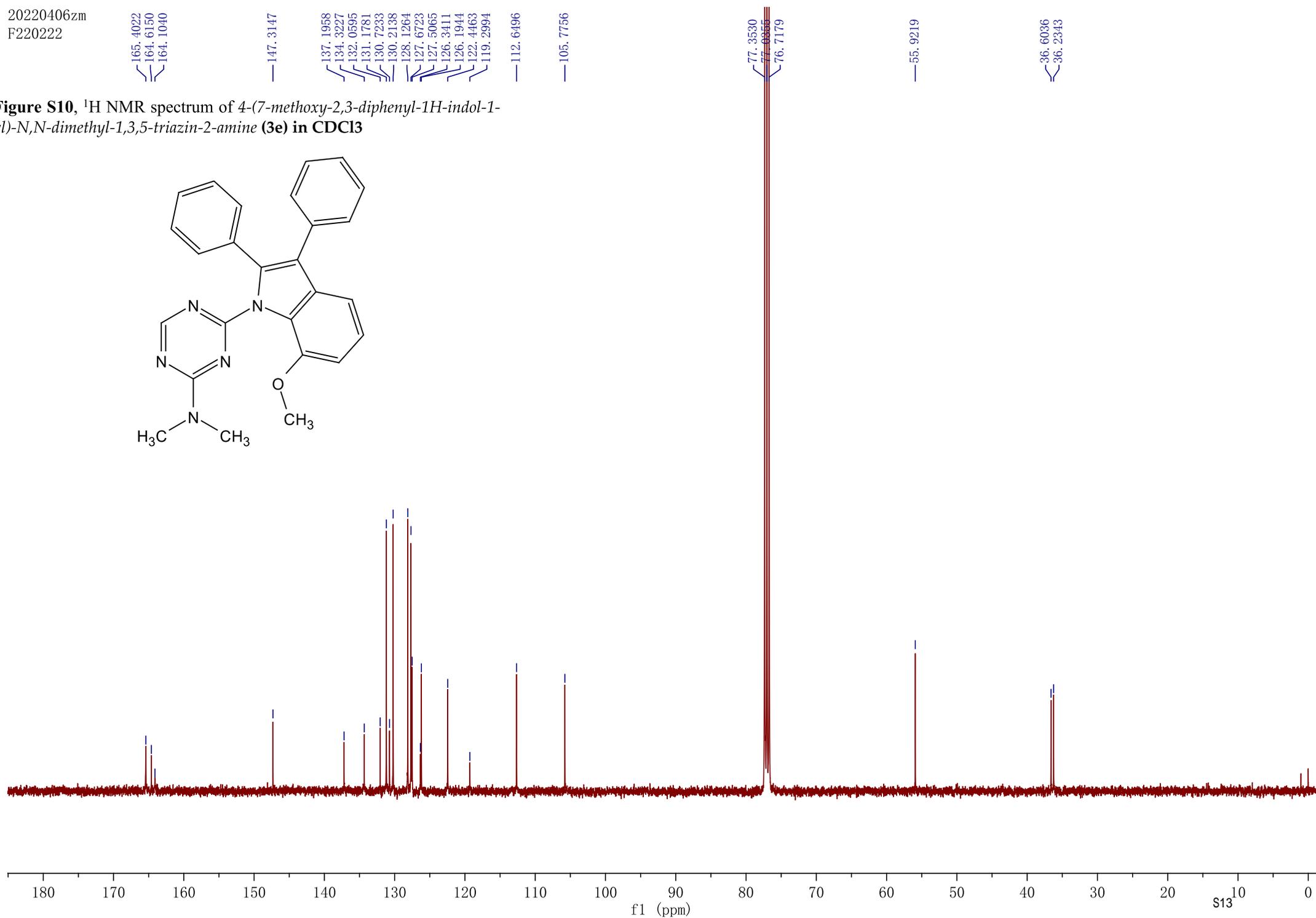
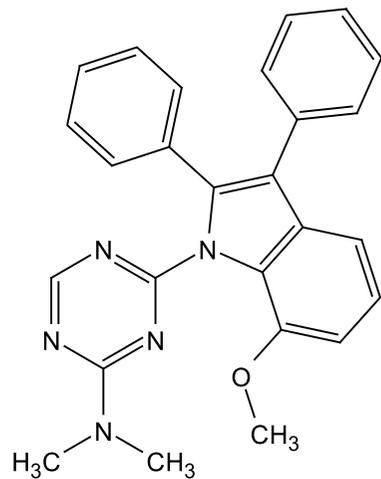
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77.3530  
77.0356  
76.7179

55.9219

36.6086  
36.2343

**Figure S10**,  $^1\text{H}$  NMR spectrum of 4-(7-methoxy-2,3-diphenyl-1H-indol-1-yl)-*N,N*-dimethyl-1,3,5-triazin-2-amine (**3e**) in  $\text{CDCl}_3$



20190419-H1-WHF-327  
20190419-H1-WHF-327  
CDC13

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8.4804  
7.3178  
7.3153  
7.3046  
7.2978  
7.2927  
7.2512  
7.2482  
7.2388  
7.2152  
7.2129  
7.2079  
7.2002  
7.1972  
7.1930  
7.1851  
7.1830  
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7.0531  
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6.9760  
6.9717

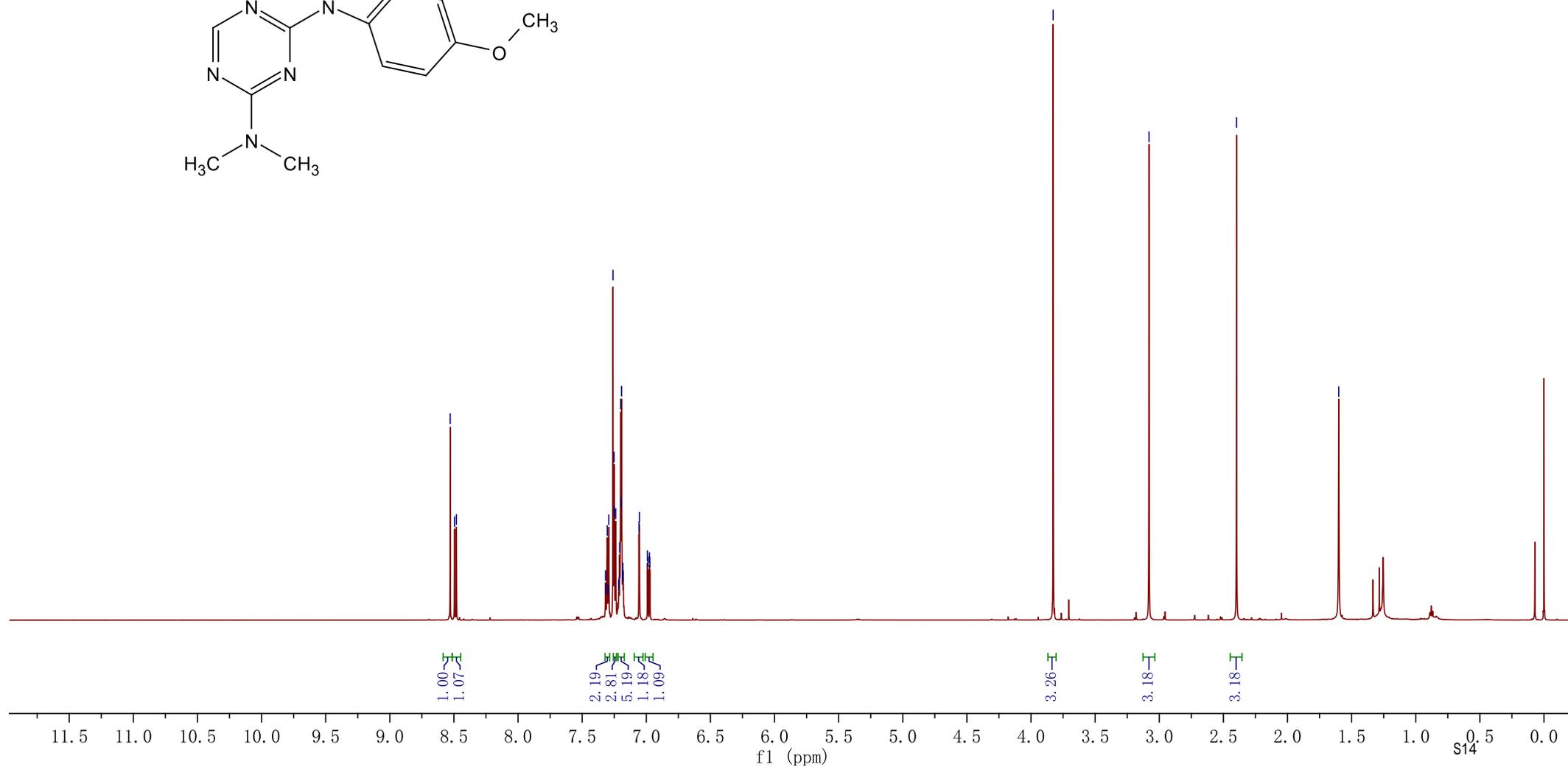
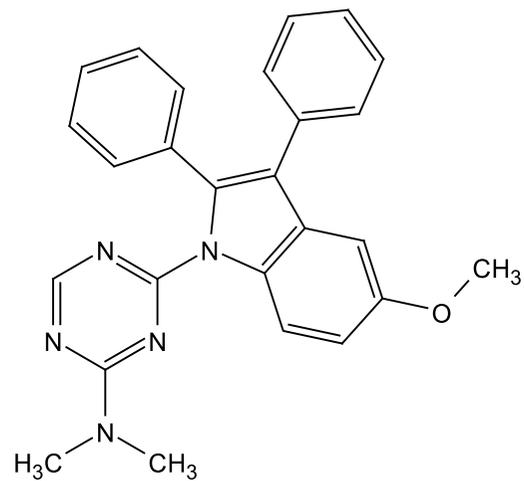
3.8273

3.0802

2.3973

1.6003

**Figure S11**,  $^1\text{H}$  NMR spectrum of 4-(5-methoxy-2,3-diphenyl-1H-indol-1-yl)-*N,N*-dimethyl-1,3,5-triazin-2-amine (**3f**) in  $\text{CDCl}_3$



13C  
F-1016

166.0213  
163.8460  
162.7520

156.1021

136.6085  
134.2326  
133.8760  
131.7571  
130.5632  
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126.7526  
126.5496  
122.2180

116.2150  
113.2545

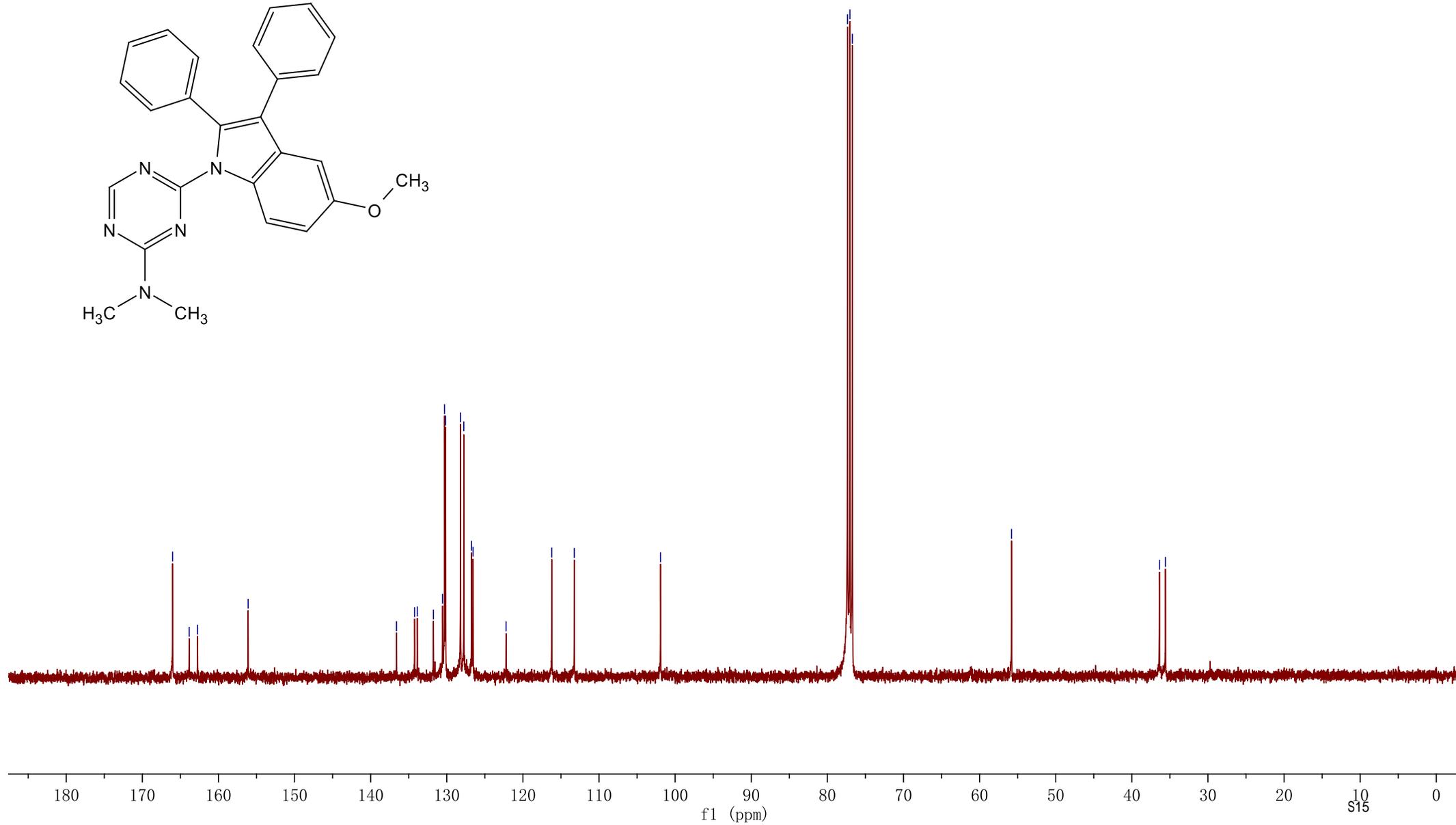
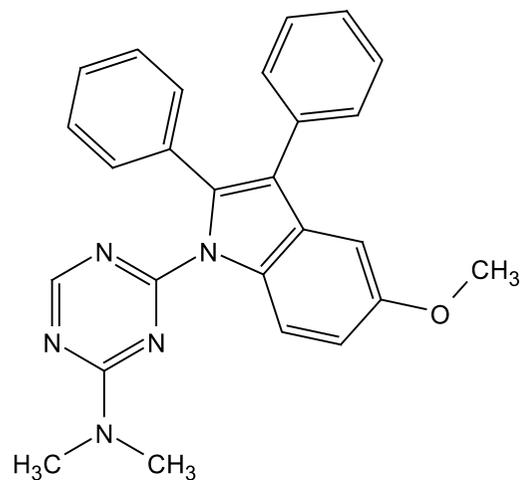
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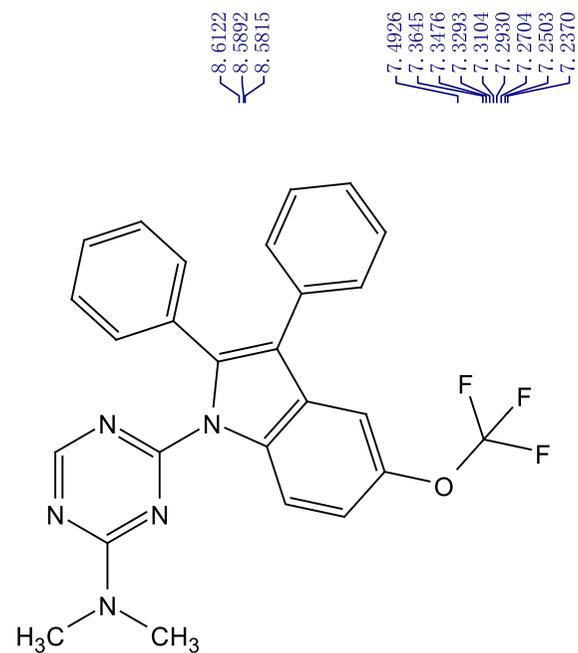
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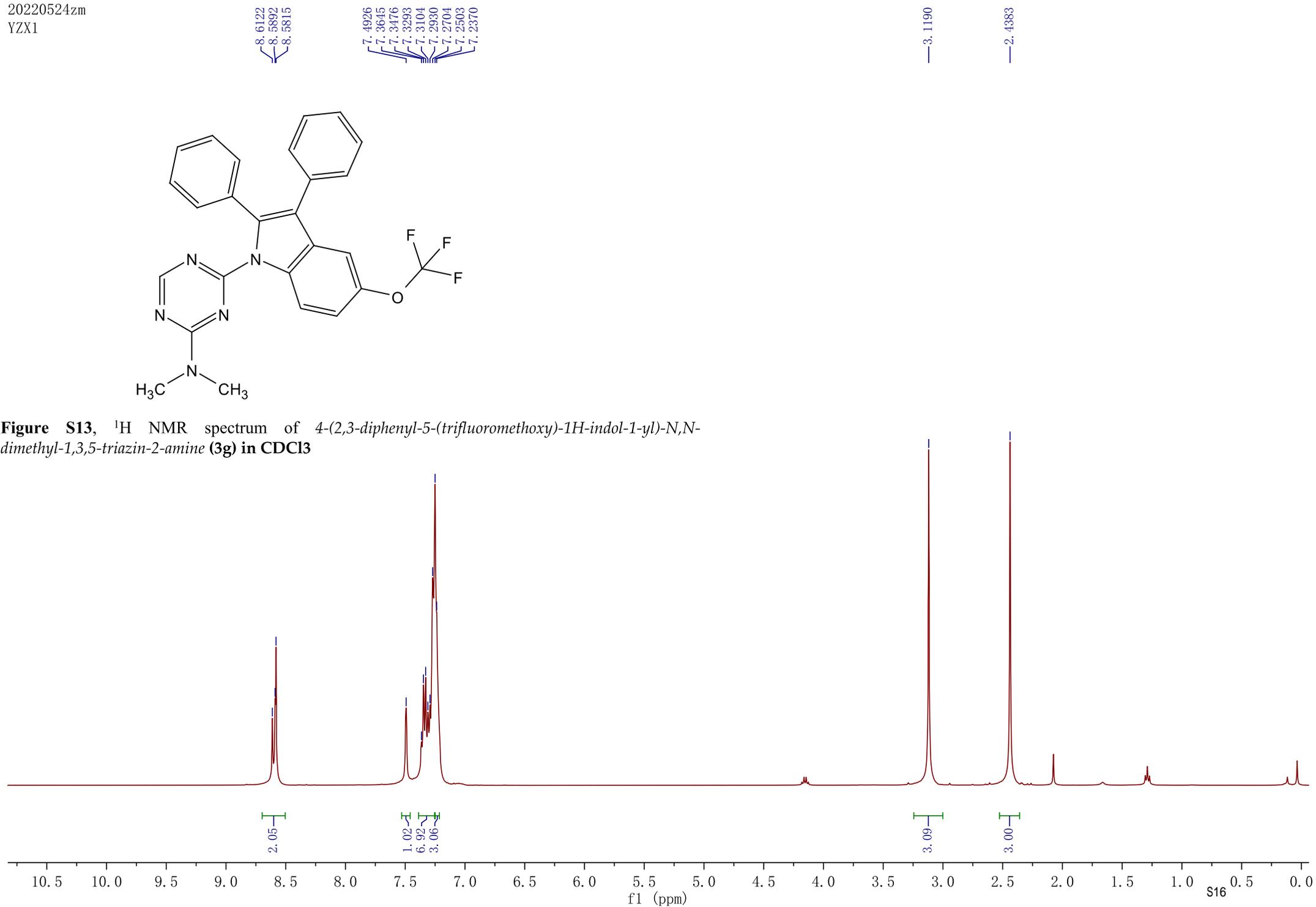
36.3747  
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**Figure S12**, <sup>1</sup>H NMR spectrum of 4-(5-methoxy-2,3-diphenyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3f**) in CDCl<sub>3</sub>

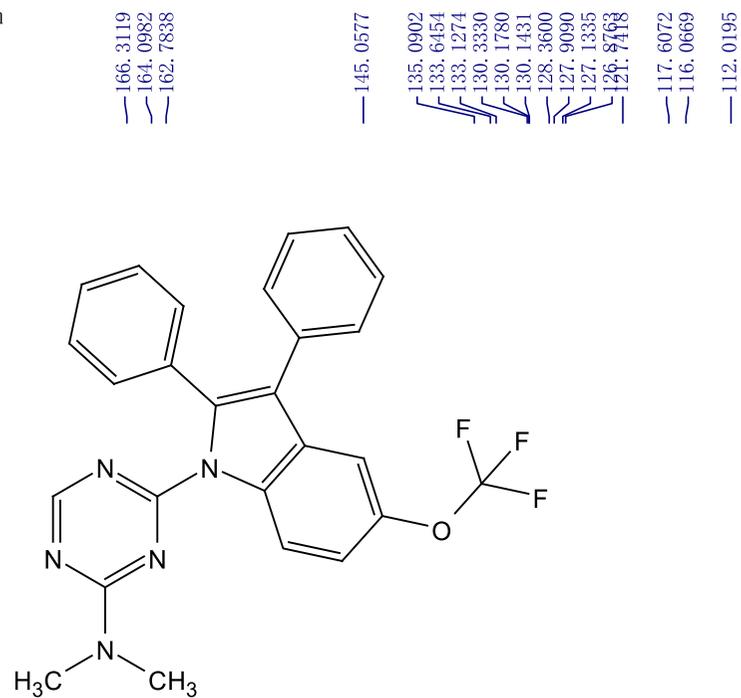




**Figure S13**, <sup>1</sup>H NMR spectrum of 4-(2,3-diphenyl-5-(trifluoromethoxy)-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3g**) in CDCl<sub>3</sub>



20220526zm  
YZX1



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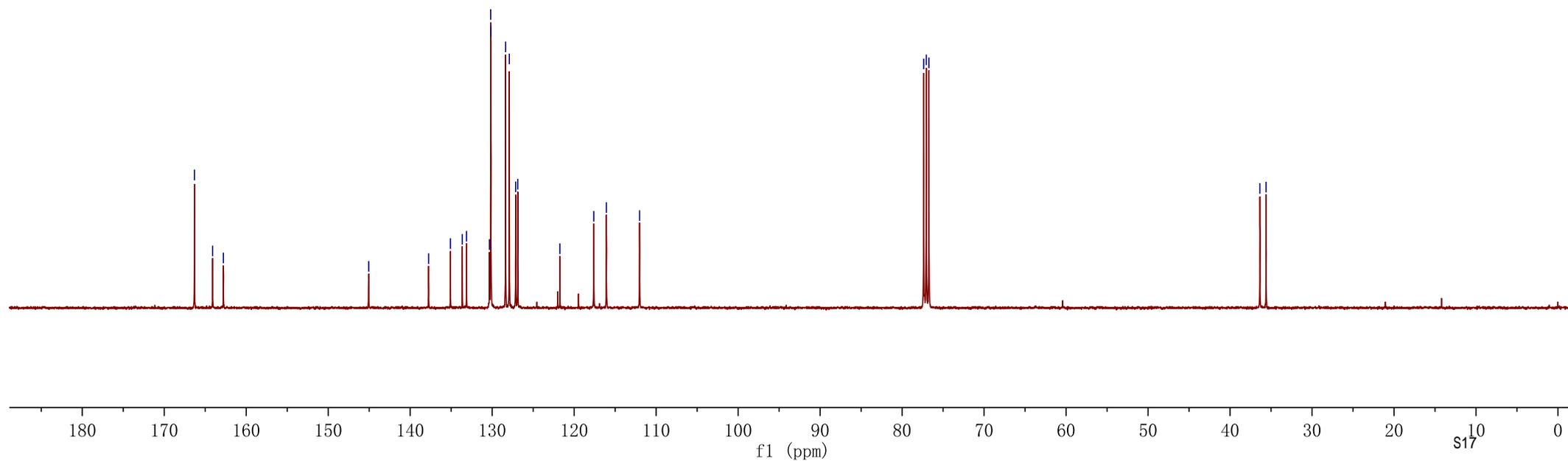
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126.8463  
121.7418

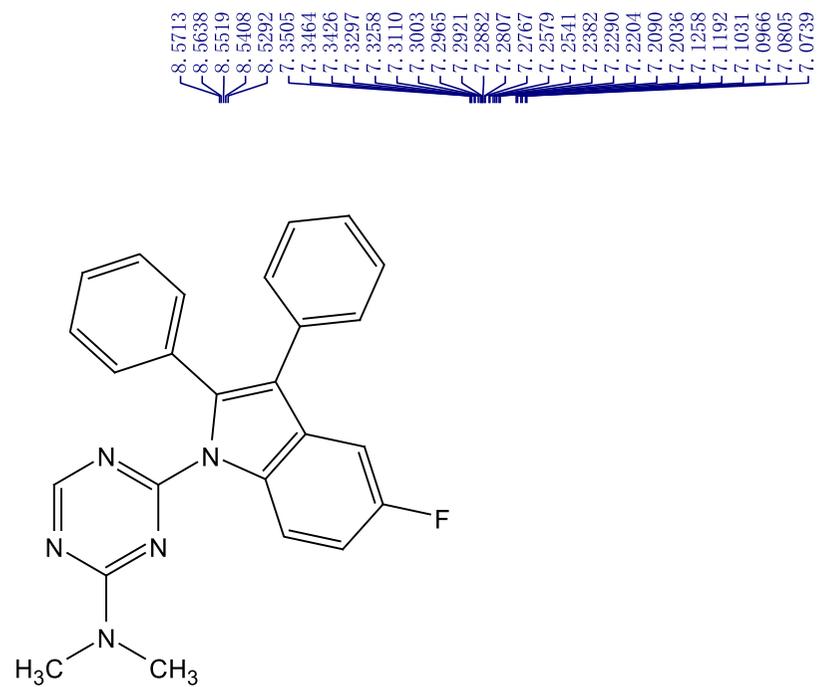
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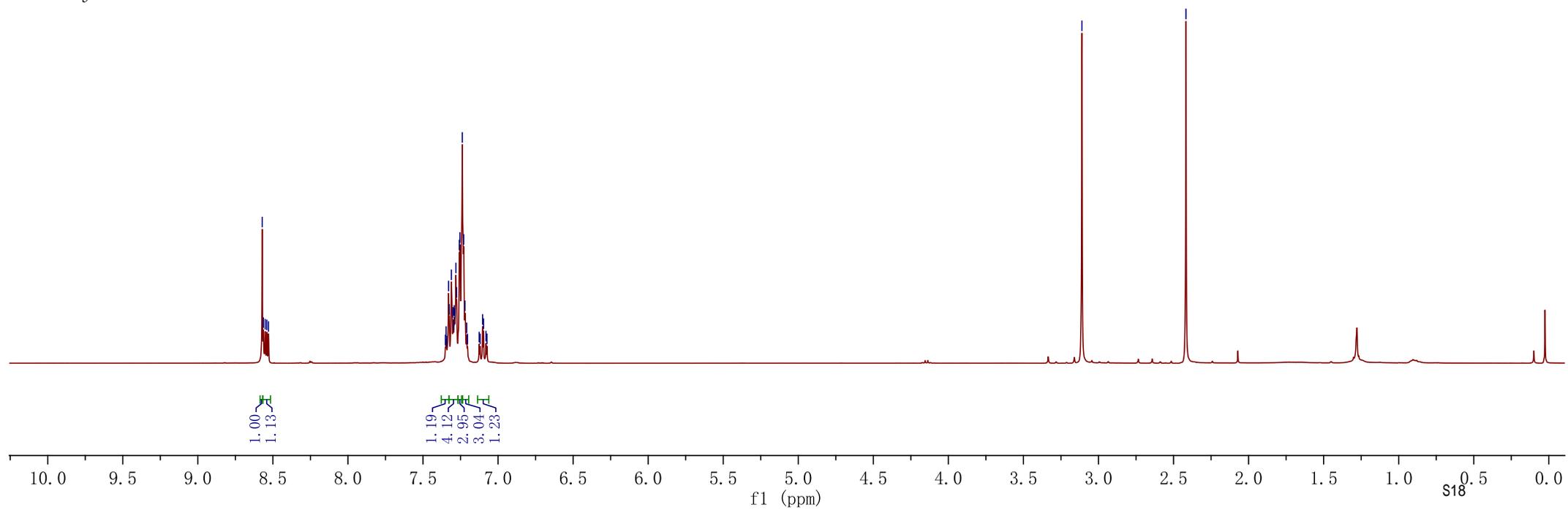
36.3607  
35.6037



LFY211015  
F-1015



**Figure S15**, <sup>1</sup>H NMR spectrum of 4-(5-fluoro-2,3-diphenyl-1H-indol-1-yl)-*N,N*-dimethyl-1,3,5-triazin-2-amine (**3h**) in CDCl<sub>3</sub>



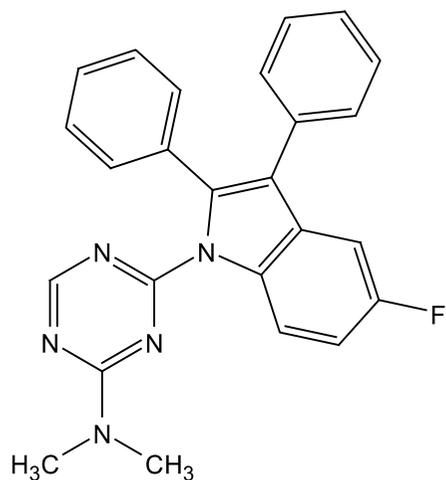
<sup>13</sup>C  
F-1015

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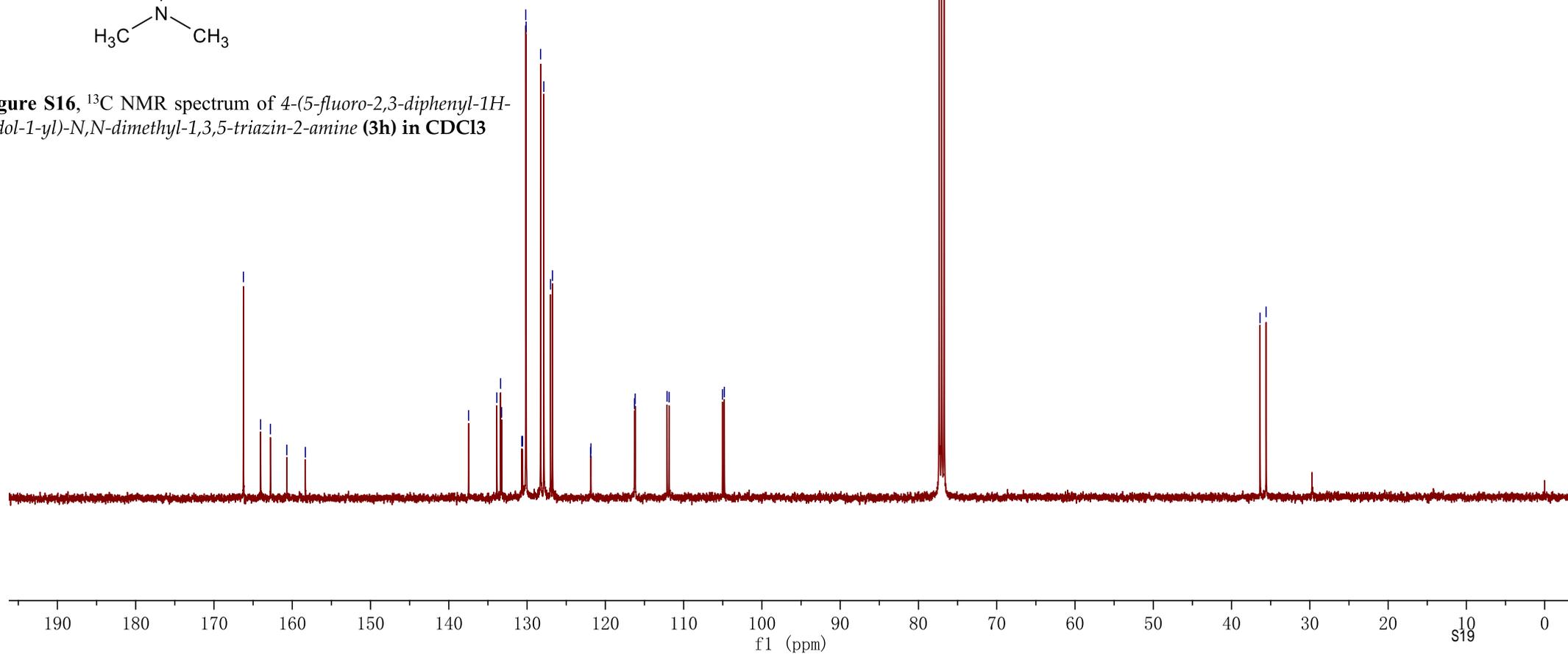
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127.0009  
126.7548  
121.8803  
121.8405  
116.2823  
116.1943  
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111.8614  
105.0377  
104.7973

77.3619  
77.0444  
76.7267

36.3619  
35.5868

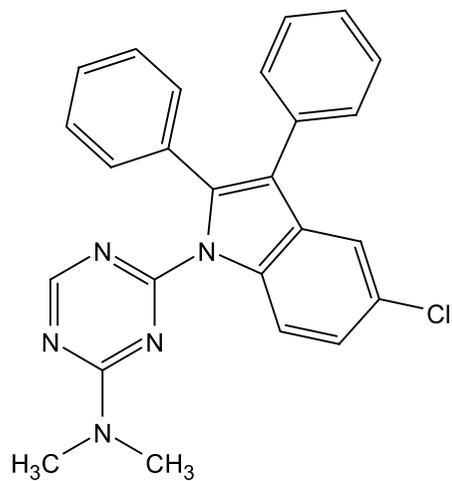


**Figure S16,** <sup>13</sup>C NMR spectrum of 4-(5-fluoro-2,3-diphenyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3h**) in CDCl<sub>3</sub>

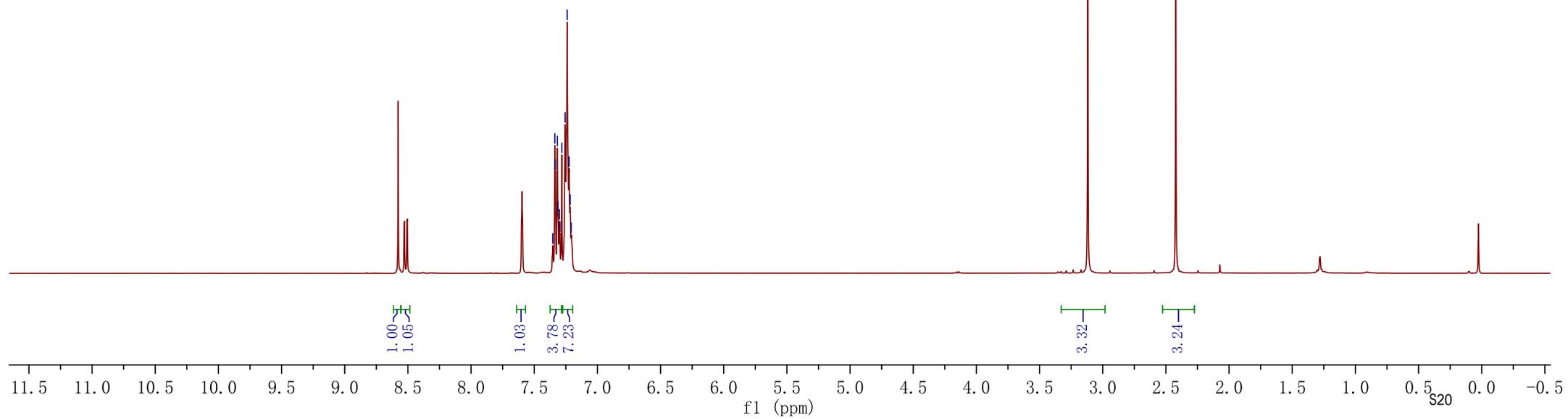


<sup>1</sup>H  
F-1017

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7.3115  
7.3010  
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7.2818  
7.2559  
7.2396  
7.2241  
7.2158  
7.2074



**Figure S17**, <sup>1</sup>H NMR spectrum of 4-(5-chloro-2,3-diphenyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3i**) in CDCl<sub>3</sub>



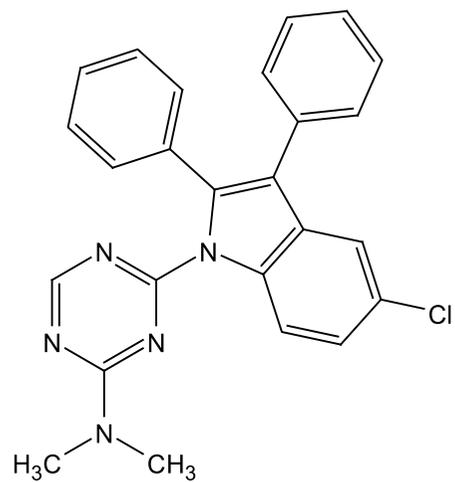
<sup>13</sup>C  
F-1017

166.1768  
163.9146  
162.7343

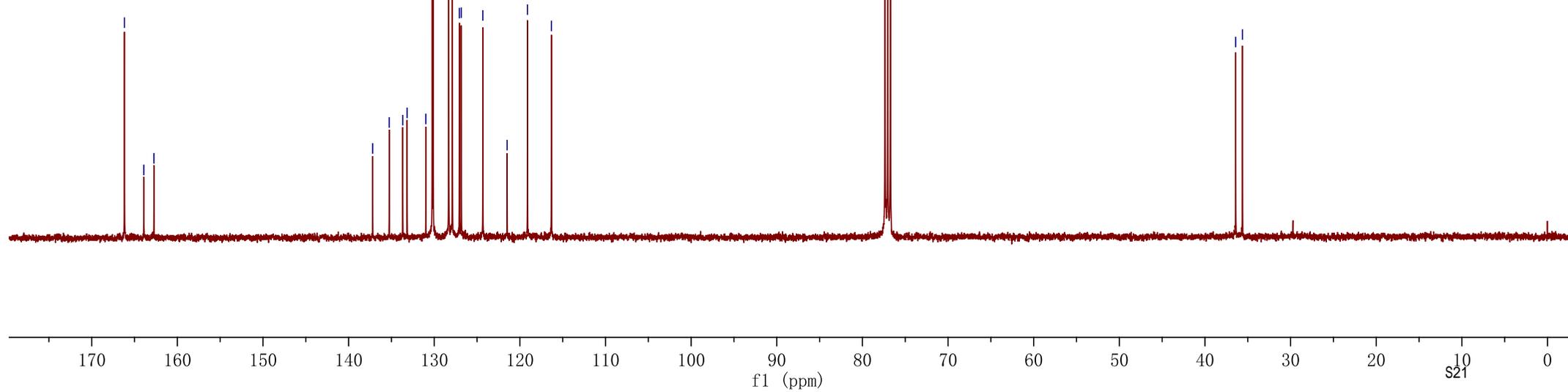
137.1919  
135.2610  
133.6750  
133.1681  
130.9850  
130.2400  
130.1249  
128.3094  
127.8865  
127.0700  
126.8412  
124.3258  
121.4922  
119.1165  
116.3226

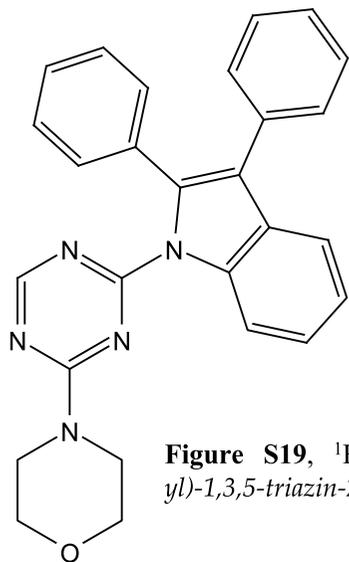
77.3664  
77.0488  
76.7312

36.4143  
35.6196

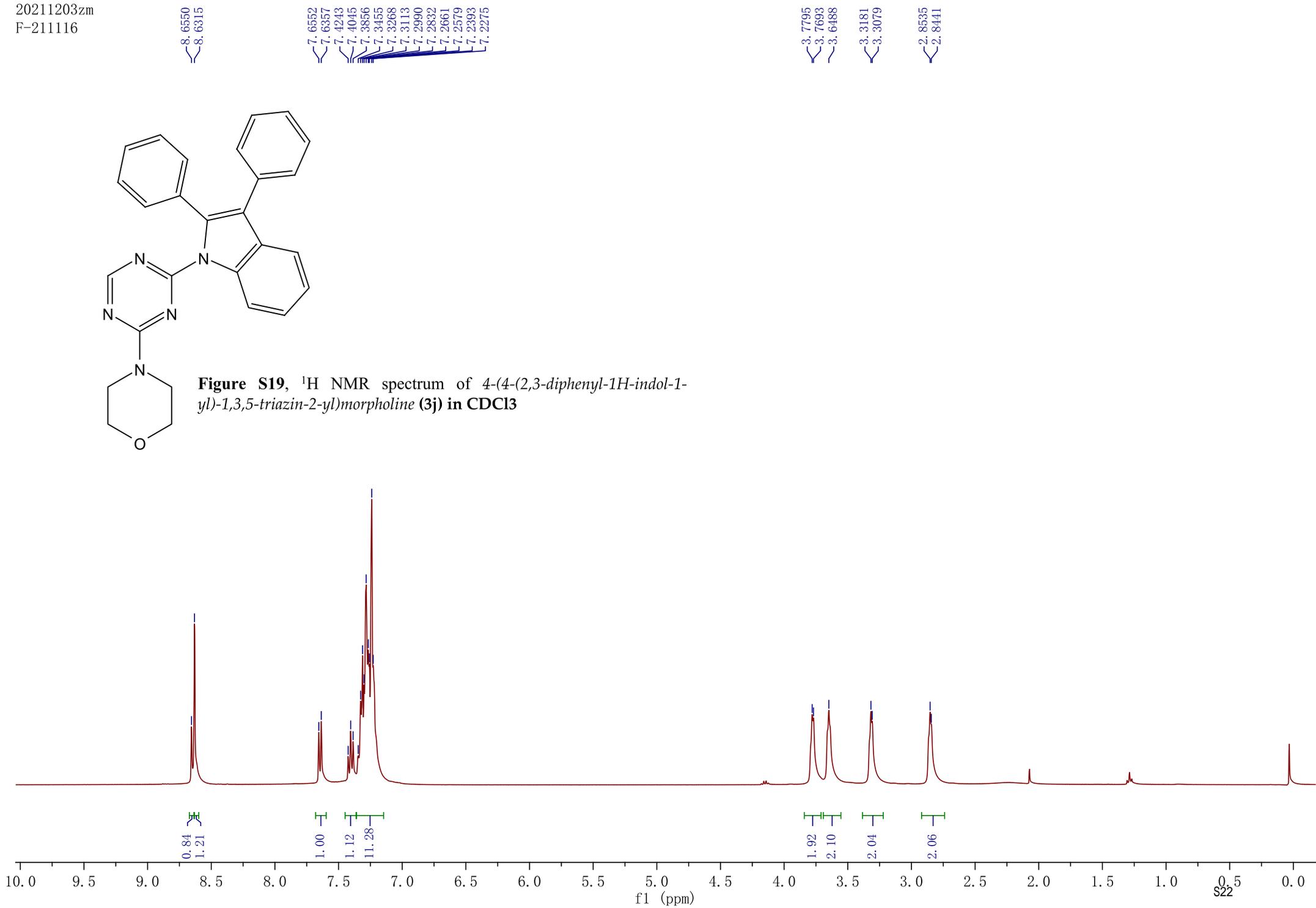


**Figure S18,** <sup>13</sup>C NMR spectrum of 4-(5-chloro-2,3-diphenyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3i**) in CDCl<sub>3</sub>





**Figure S19**,  $^1\text{H}$  NMR spectrum of 4-(4-(2,3-diphenyl-1H-indol-1-yl)-1,3,5-triazin-2-yl)morpholine (**3j**) in  $\text{CDCl}_3$



20211208zm  
f2111116

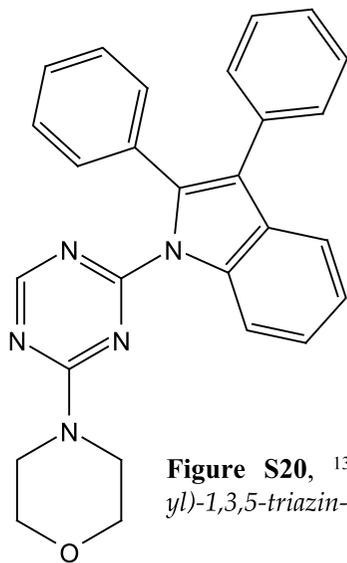
166.3939  
163.0566  
162.9570

136.9068  
135.7344  
134.3674  
133.5844  
130.3428  
130.1969  
129.8748  
128.1776  
127.8280  
126.7536  
126.6792  
124.5148  
122.9354  
122.7516  
119.7056  
115.4352

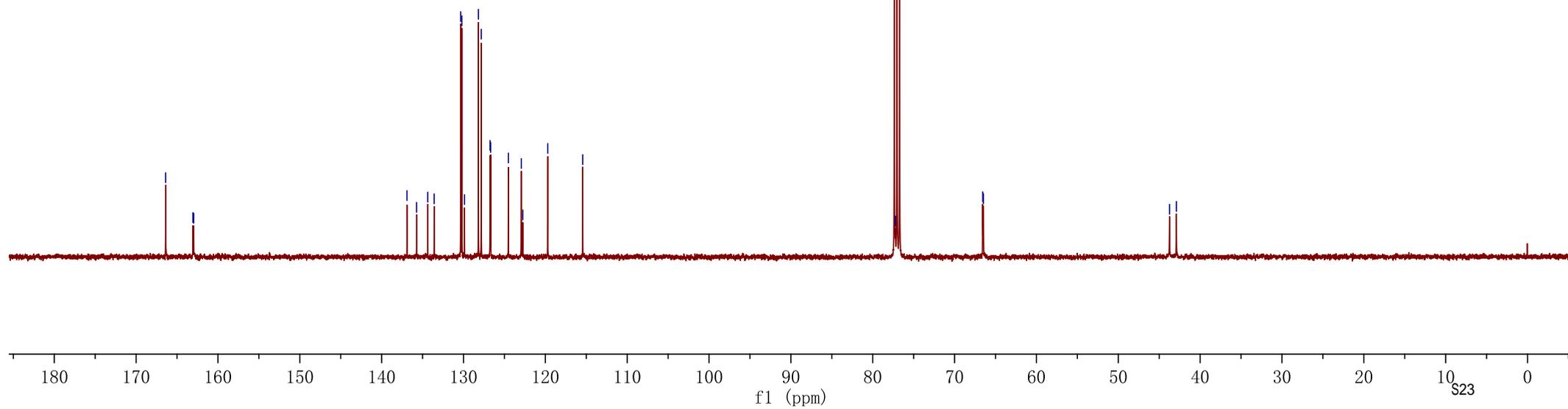
77.3593  
77.2450  
77.0417  
76.7241

66.5612  
66.4730

43.7372  
42.8995



**Figure S20**,  $^{13}\text{C}$  NMR spectrum of 4-(4-(2,3-diphenyl-1H-indol-1-yl)-1,3,5-triazin-2-yl)morpholine (**3j**) in  $\text{CDCl}_3$



20211203zm  
1118

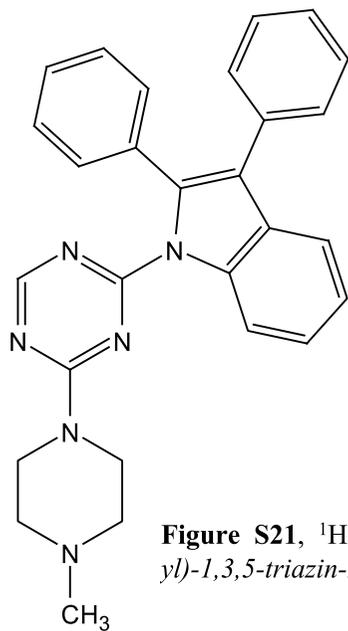
8.6400  
8.6191  
8.6011

7.6529  
7.6338  
7.4151  
7.4120  
7.3971  
7.3942  
7.3913  
7.3763  
7.3732  
7.3459  
7.3427  
7.3383  
7.3359  
7.3247  
7.3212  
7.3145  
7.3071  
7.2881  
7.2807  
7.2740  
7.2701  
7.2574  
7.2557  
7.2451  
7.2402  
7.2318  
7.2301  
7.2246  
7.2224

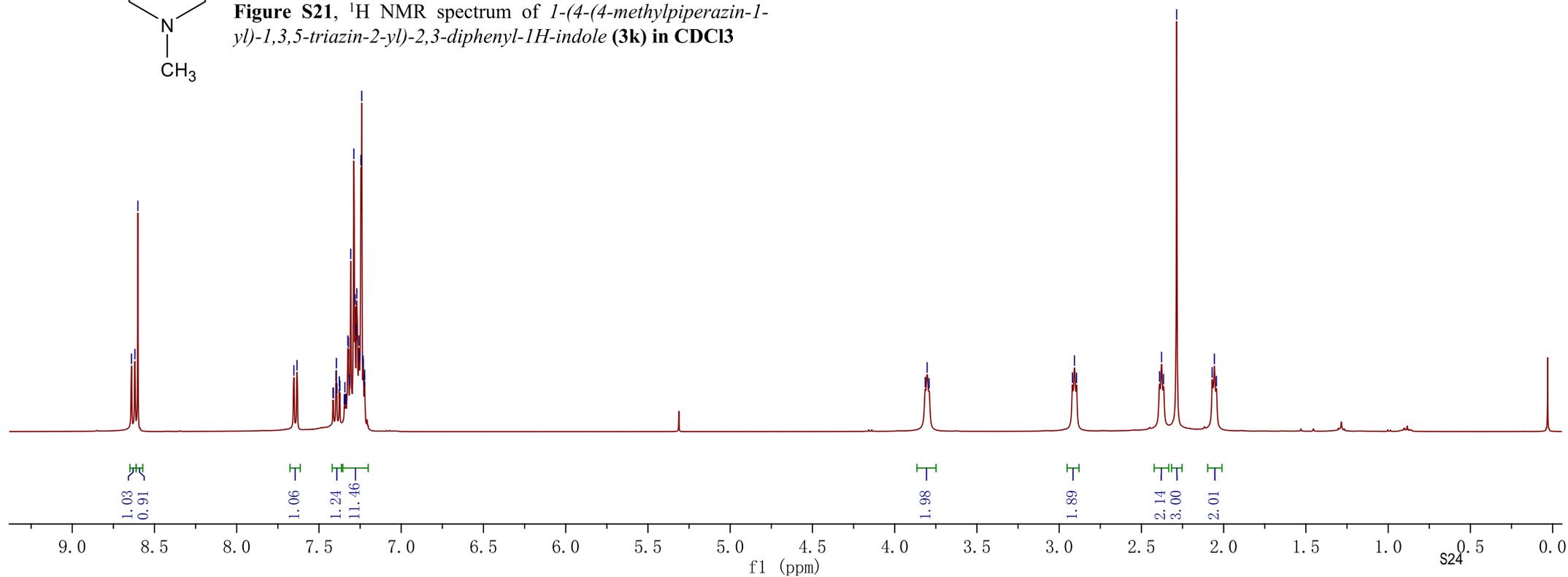
3.8142  
3.8029  
3.7908

2.9192  
2.9072  
2.8946

2.3899  
2.3777  
2.3655  
2.2857  
2.0698  
2.0564  
2.0442



**Figure S21**, <sup>1</sup>H NMR spectrum of *1-(4-(4-methylpiperazin-1-yl)-1,3,5-triazin-2-yl)-2,3-diphenyl-1H-indole (3k)* in CDCl<sub>3</sub>



20211208zm  
f211118

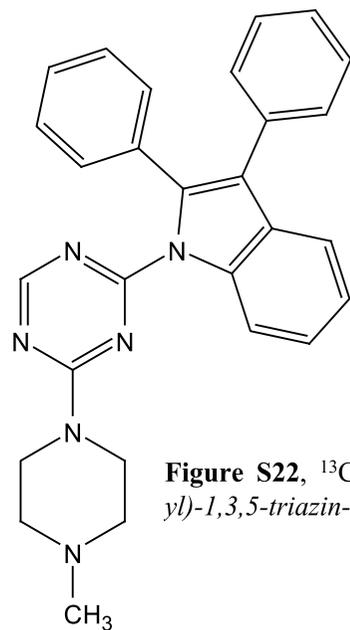
166.5801  
163.1975  
163.1454

136.9187  
135.8370  
134.2987  
133.7254  
130.3664  
130.1923  
129.8109  
128.1522  
127.8107  
126.7819  
126.5986  
124.3845  
122.7779  
122.4091  
119.6369  
115.3383

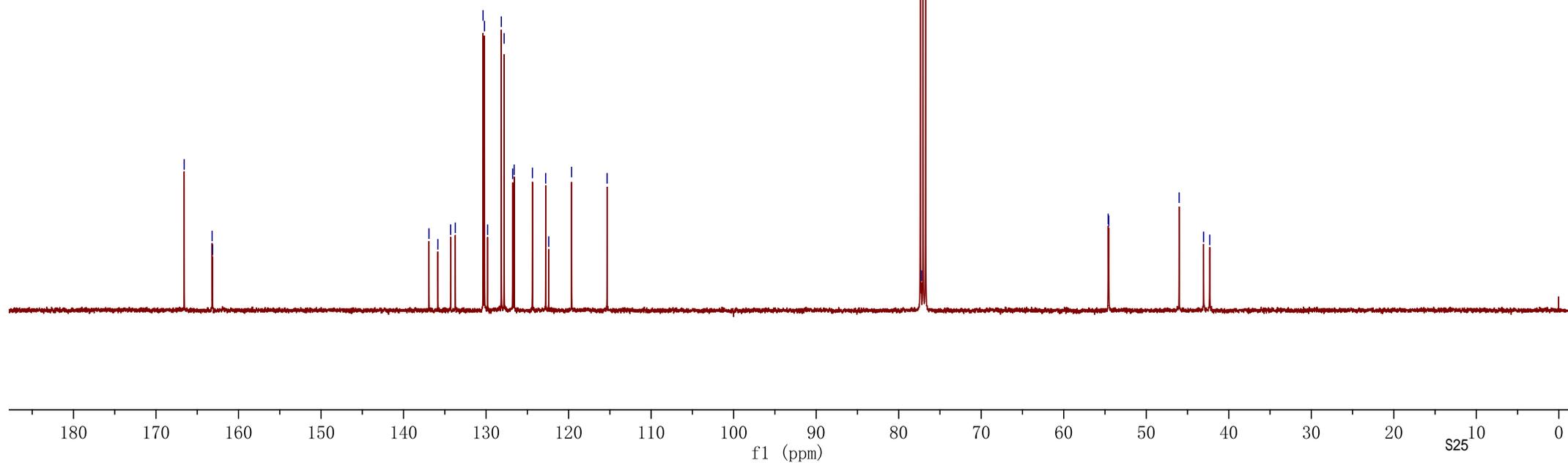
77.3690  
77.2546  
77.0515  
76.7338

54.6191  
54.5432

46.0174  
43.0515  
42.3092



**Figure S22**,  $^{13}\text{C}$  NMR spectrum of 1-(4-(4-methylpiperazin-1-yl)-1,3,5-triazin-2-yl)-2,3-diphenyl-1H-indole (**3k**) in  $\text{CDCl}_3$



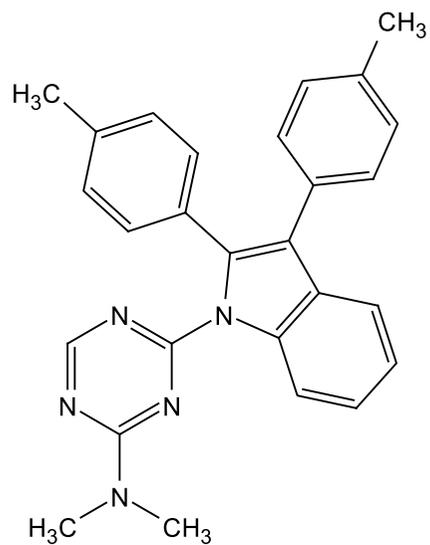
20211223zm  
f211204

8.5720  
8.5529  
8.5321

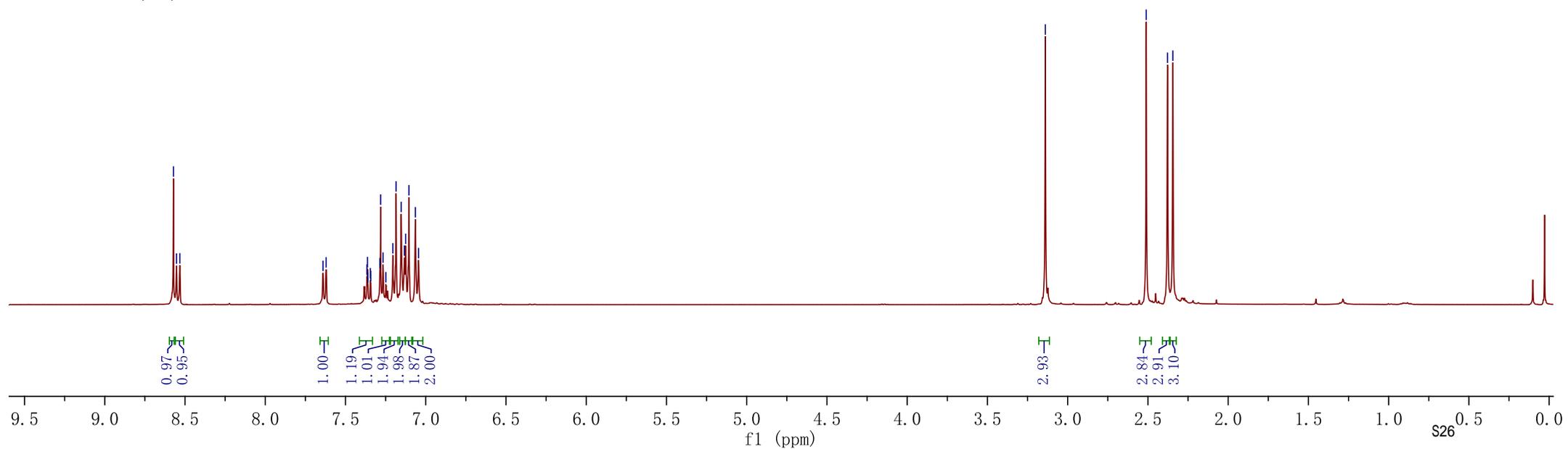
7.6402  
7.6209  
7.3661  
7.3632  
7.3603  
7.3454  
7.3422  
7.2857  
7.2811  
7.2662  
7.2486  
7.2051  
7.1848  
7.1529  
7.1327  
7.1231  
7.1047  
7.0646  
7.0446

3.1392

2.5106  
2.3780  
2.3447



**Figure S23**,  $^1\text{H}$  NMR spectrum of 4-(2,3-di-p-tolyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3m**) in  $\text{CDCl}_3$



20220406zm  
F211204

165.9234  
163.8258  
162.9190

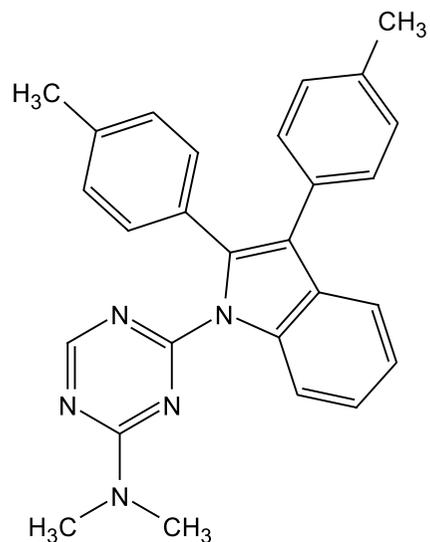
136.8942  
136.3947  
136.0465  
135.8652

130.1727  
130.0296  
128.8994  
122.5799  
121.8298  
119.6228  
114.8960

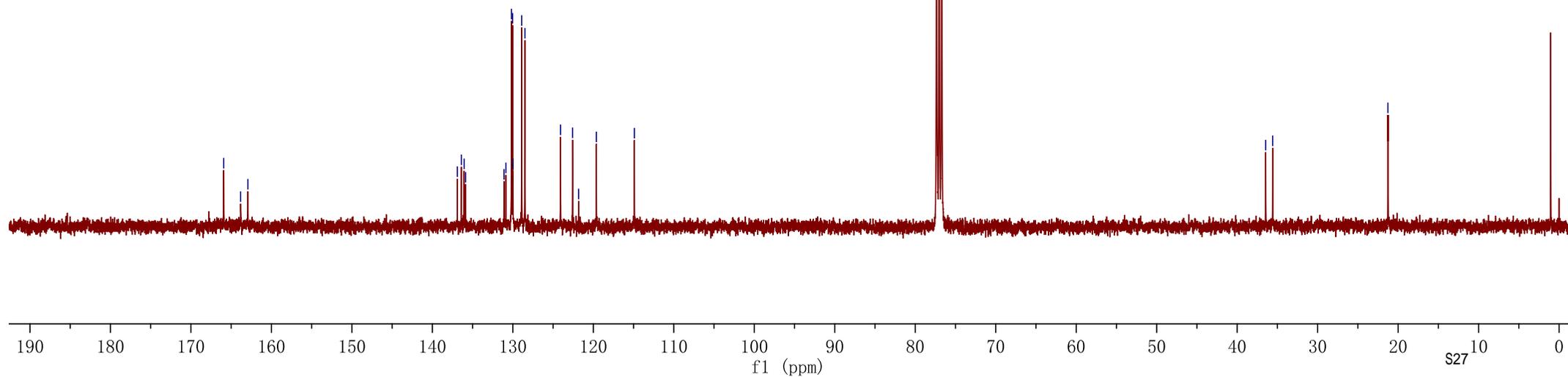
77.3444  
77.0269  
76.7094

36.4547  
35.5879

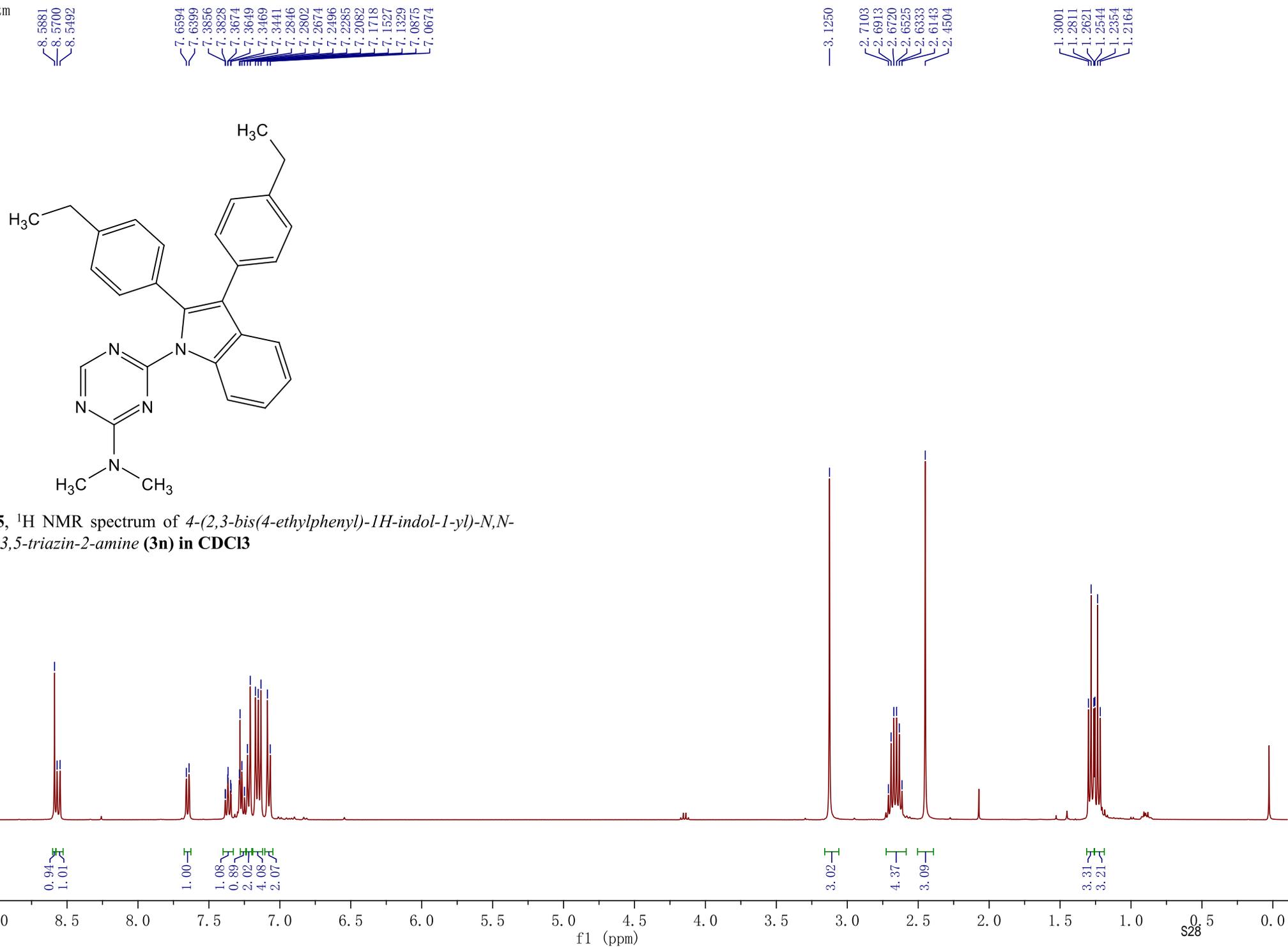
21.2698



**Figure S24**, <sup>13</sup>C NMR spectrum of 4-(2,3-di-p-tolyl-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3m**) in CDCl<sub>3</sub>



20220112zm  
F211209



**Figure S25**, <sup>1</sup>H NMR spectrum of 4-(2,3-bis(4-ethylphenyl)-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3n**) in CDCl<sub>3</sub>

20220117zm  
F211209

165.9791  
163.8273  
162.9218

142.8310  
142.2831

136.9093  
135.8797

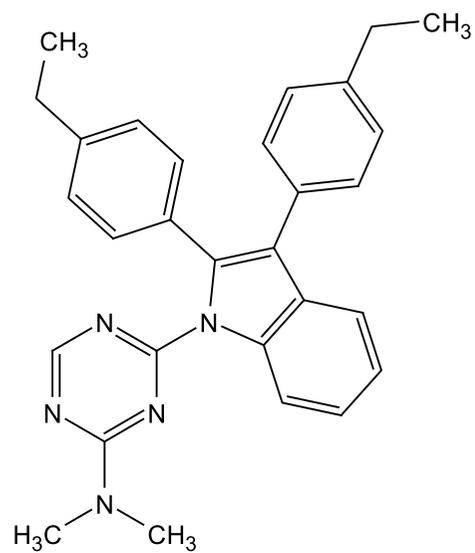
131.0688  
130.2161  
130.1092  
130.0094  
127.6159  
127.3232  
124.0782  
122.5692  
119.6865

77.3635  
77.0460  
76.7285

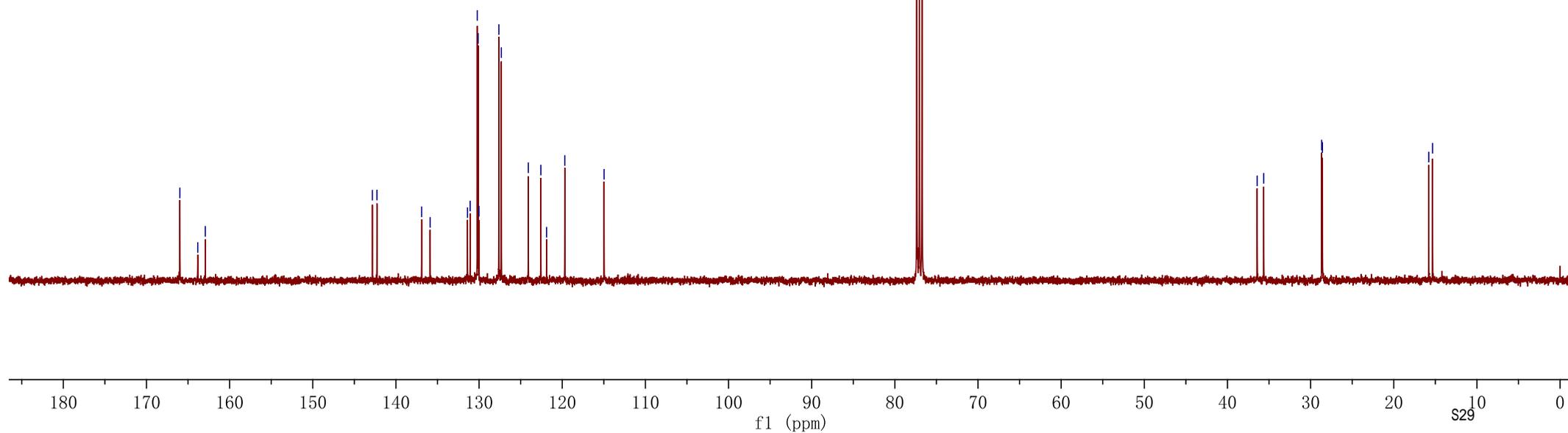
36.4228  
35.6374

28.6689  
28.5767

15.7903  
15.3317



**Figure S26,**  $^{13}\text{C}$  NMR spectrum of 4-(2,3-bis(4-ethylphenyl)-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3n**) in  $\text{CDCl}_3$

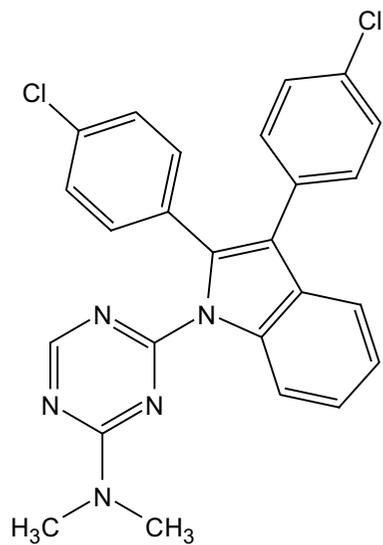


20220112zm  
F211210

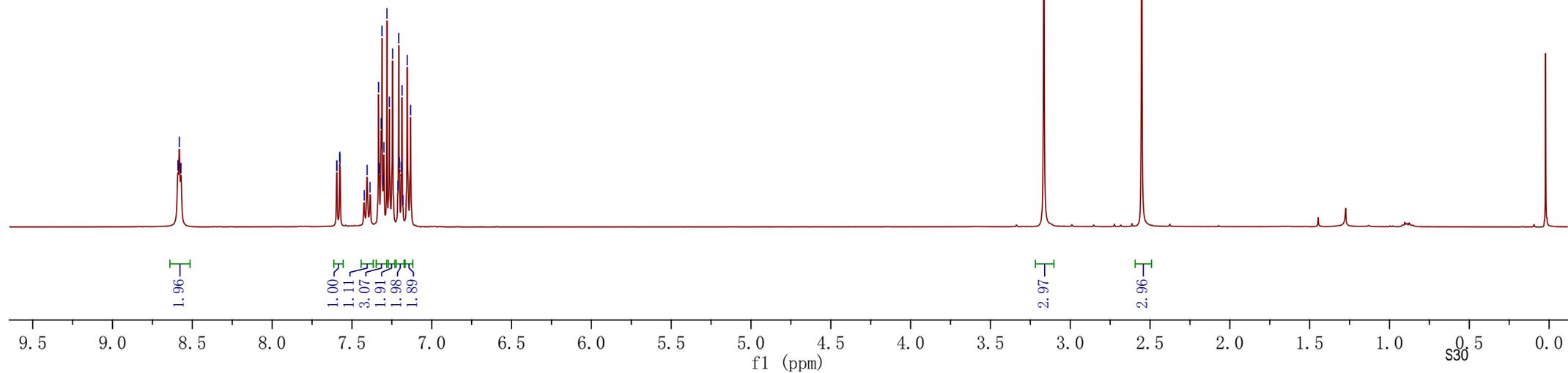
8.5903  
8.5814  
8.5709  
7.5957  
7.5938  
7.5761  
7.5744  
7.4229  
7.4049  
7.3866  
7.3332  
7.3286  
7.3173  
7.3120  
7.3059  
7.2999  
7.2808  
7.2661  
7.2450  
7.2125  
7.2069  
7.2021  
7.1902  
7.1857  
7.1798  
7.1533  
7.1322

3.1653

2.5525



**Figure S27**,  $^1\text{H}$  NMR spectrum of 4-(2,3-bis(4-chlorophenyl)-1H-indol-1-yl)-*N,N*-dimethyl-1,3,5-triazin-2-amine (**3o**) in  $\text{CDCl}_3$

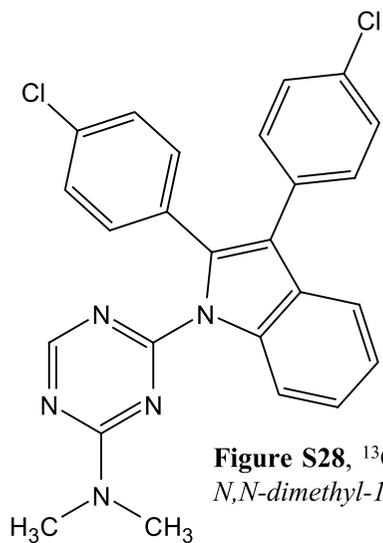


165.9031  
163.6416  
162.7415

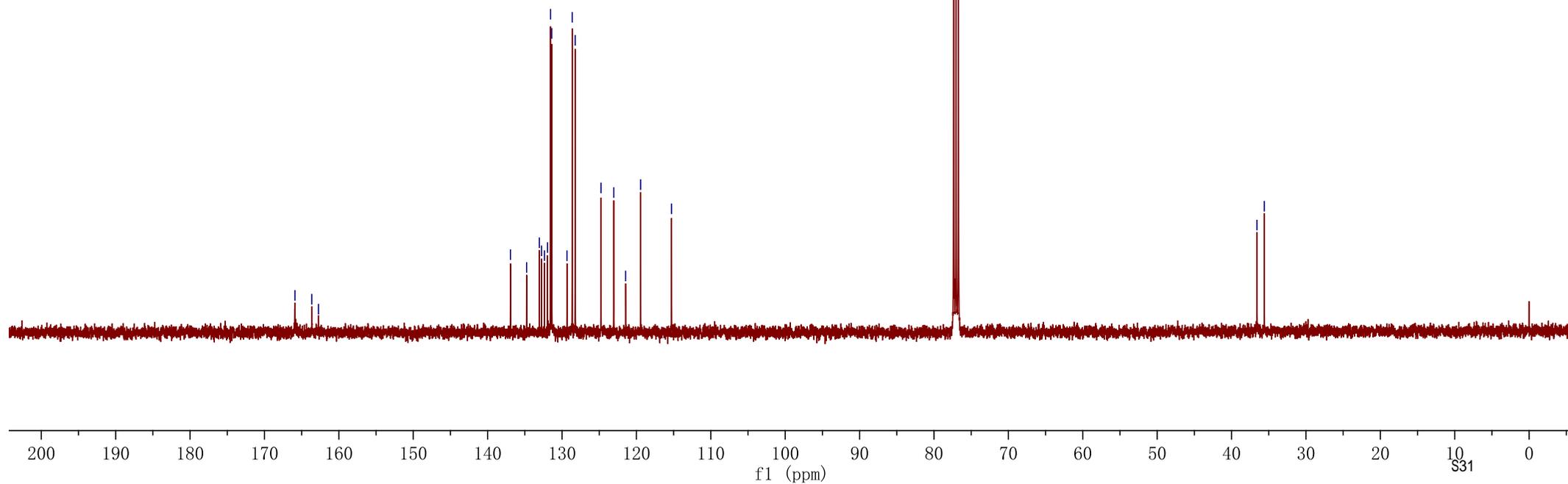
136.9326  
134.7584  
133.0519  
132.7572  
132.3628  
131.9512  
131.5409  
131.3864  
129.3373  
128.6839  
128.2311  
124.7626  
123.0449  
121.4573  
119.4343  
115.2807

77.3551  
77.0375  
76.7200

36.5844  
35.5963



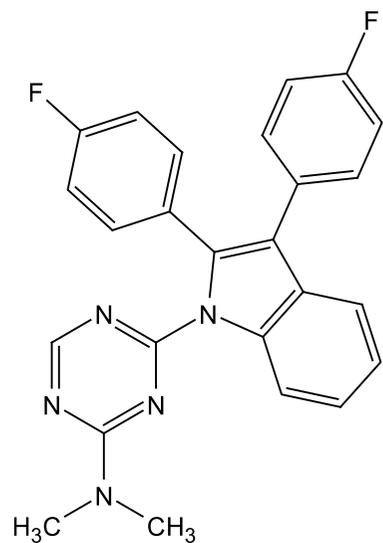
**Figure S28**,  $^{13}\text{C}$  NMR spectrum of 4-(2,3-bis(4-chlorophenyl)-1H-indol-1-yl)-*N,N*-dimethyl-1,3,5-triazin-2-amine (**3o**) in  $\text{CDCl}_3$



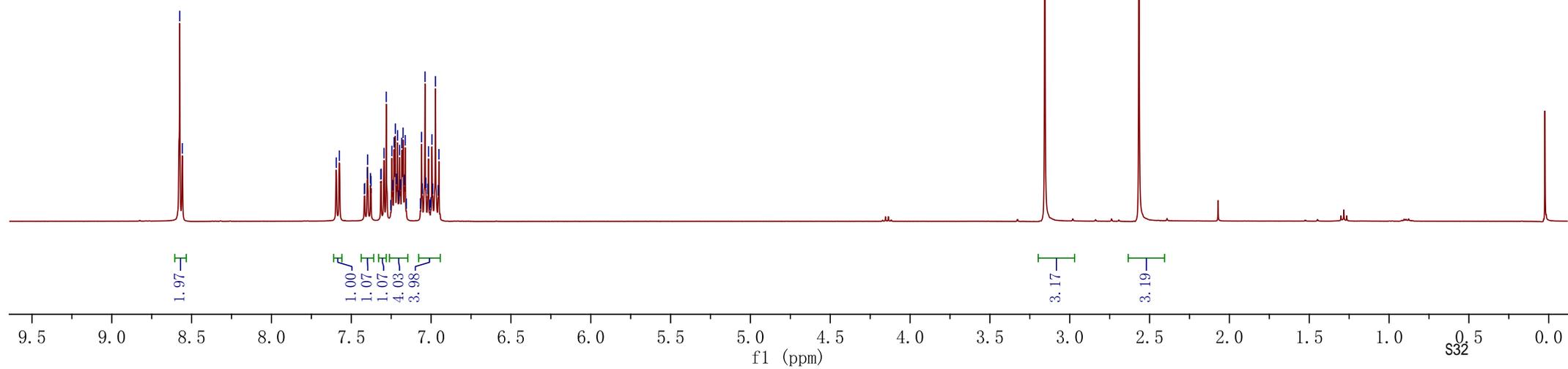
8.5743  
8.5582  
7.5940  
7.5747  
7.4184  
7.4155  
7.4004  
7.3976  
7.3796  
7.3148  
7.3128  
7.2951  
7.2810  
7.2526  
7.2456  
7.2402  
7.2318  
7.2237  
7.2155  
7.2100  
7.2026  
7.1975  
7.1922  
7.1839  
7.1757  
7.1675  
7.1622  
7.1550  
7.0669  
7.0599  
7.0547  
7.0380  
7.0330  
7.0211  
7.0161  
7.0088  
7.0015  
6.9946  
6.9895  
6.9728  
6.9558  
6.9509

—3.1560

—2.5665



**Figure S29**, <sup>1</sup>H NMR spectrum of 4-(2,3-bis(4-fluorophenyl)-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3p**) in CDCl<sub>3</sub>



20220117zm  
F220101

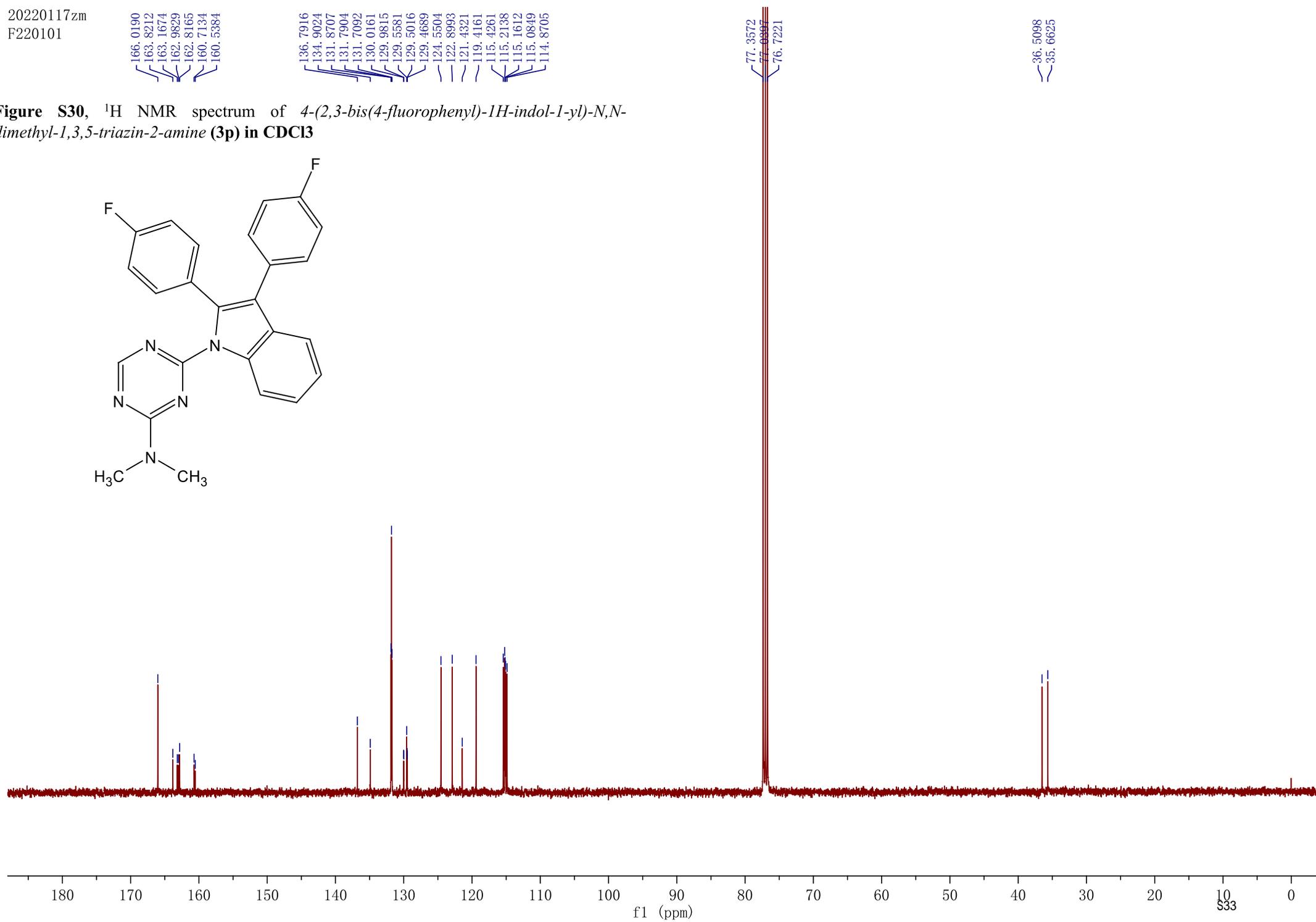
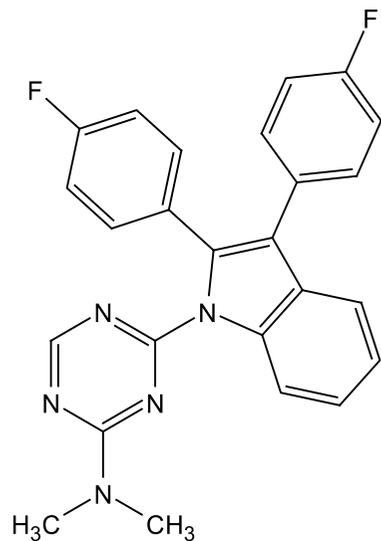
166.0190  
163.8212  
163.1674  
162.9829  
162.8165  
160.7134  
160.5384

136.7916  
134.9024  
131.8707  
131.7904  
131.7092  
130.0161  
129.9815  
129.5581  
129.5016  
129.4689  
124.5504  
122.8993  
121.4321  
119.4161  
115.4261  
115.2138  
115.1612  
115.0849  
114.8705

77.3572  
77.0887  
76.7221

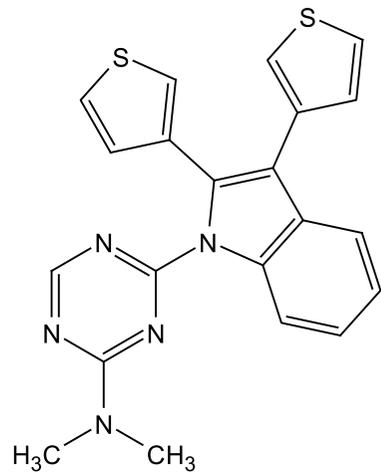
36.5098  
35.6625

**Figure S30,**  $^1\text{H}$  NMR spectrum of 4-(2,3-bis(4-fluorophenyl)-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3p**) in  $\text{CDCl}_3$

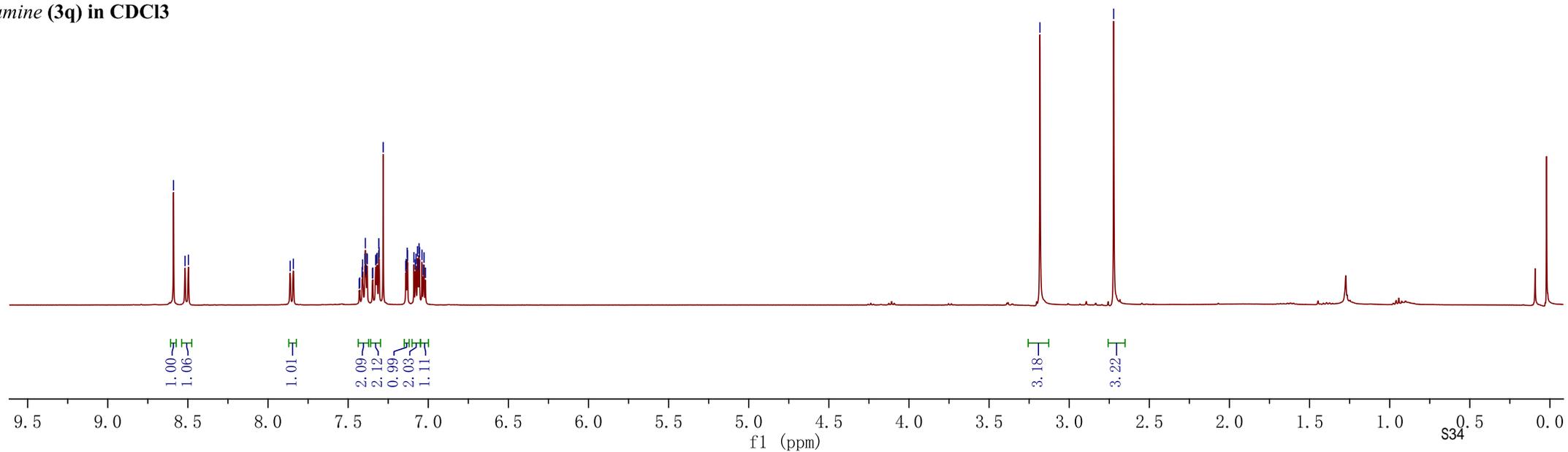


20220112zm  
F220105

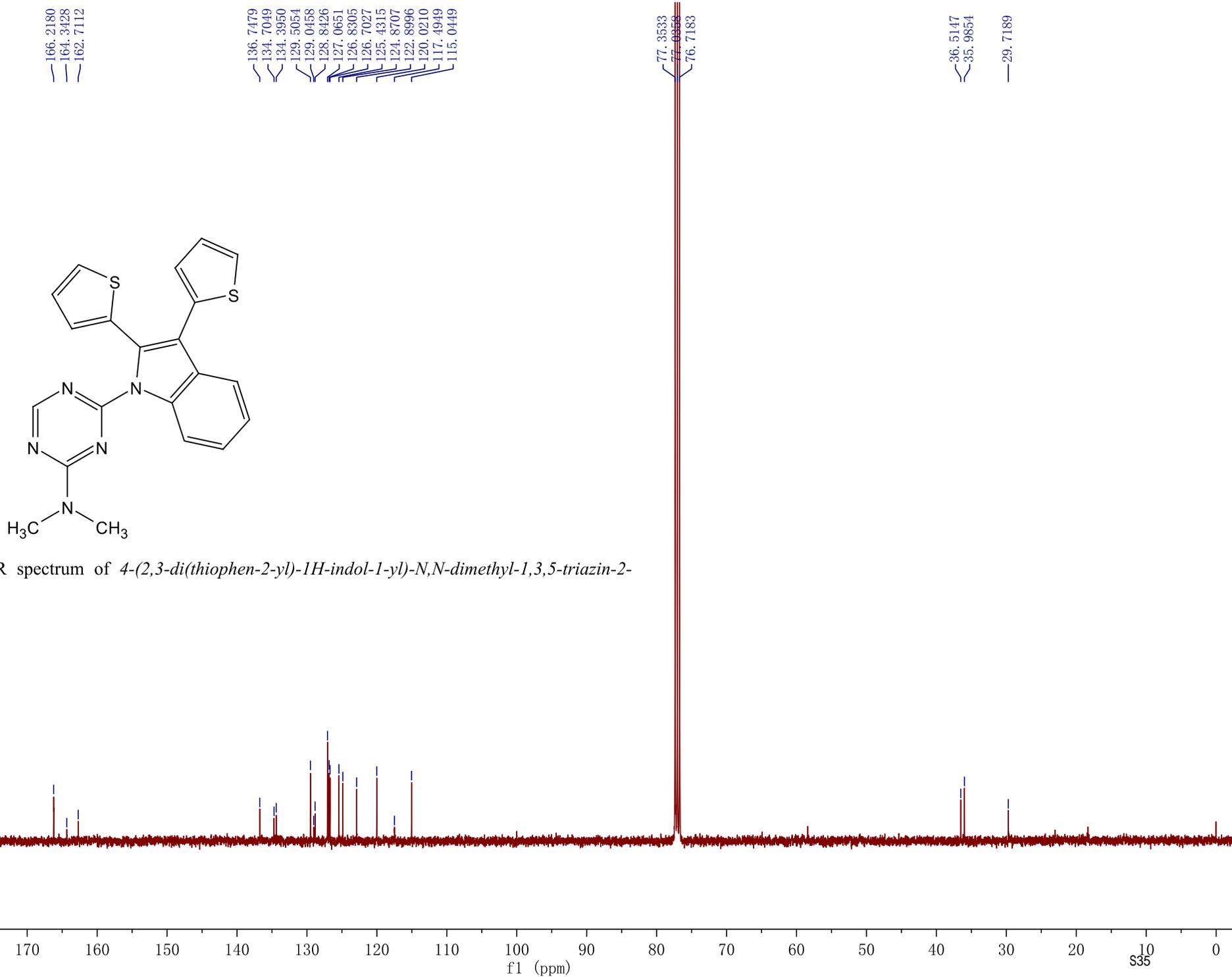
8.5895  
8.5176  
8.4967  
7.8616  
7.8420  
7.4304  
7.4275  
7.4122  
7.4096  
7.3955  
7.3924  
7.3889  
7.3831  
7.3803  
7.3479  
7.3461  
7.3281  
7.3212  
7.3187  
7.3085  
7.3062  
7.2811  
7.1400  
7.1375  
7.1312  
7.1287  
7.0891  
7.0801  
7.0764  
7.0668  
7.0632  
7.0572  
7.0544  
7.0387  
7.0297  
7.0262  
7.0173  
3.1825  
2.7224



**Figure S31,**  $^1\text{H}$  NMR spectrum of 4-(2,3-di(thiophen-2-yl)-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3q**) in  $\text{CDCl}_3$



20220117zm  
F220101



**Figure S32,** <sup>13</sup>C NMR spectrum of 4-(2,3-di(thiophen-2-yl)-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3q**) in CDCl<sub>3</sub>

20211112zm  
f211104

8.5926  
8.5770  
8.5561

7.6283  
7.6088  
7.3888  
7.3687  
7.3504  
7.2927  
7.2811  
7.2739  
7.2555  
7.2193  
7.2146  
7.1978  
7.1317  
7.1141  
7.0669  
7.0469  
7.8817  
6.8606

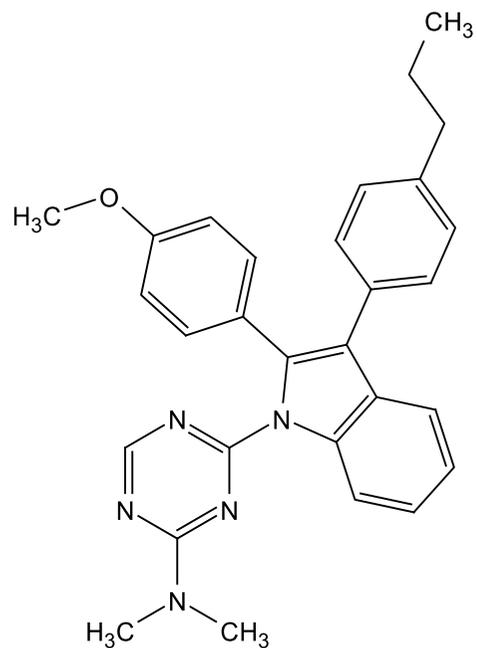
3.8351

3.1455  
3.1337

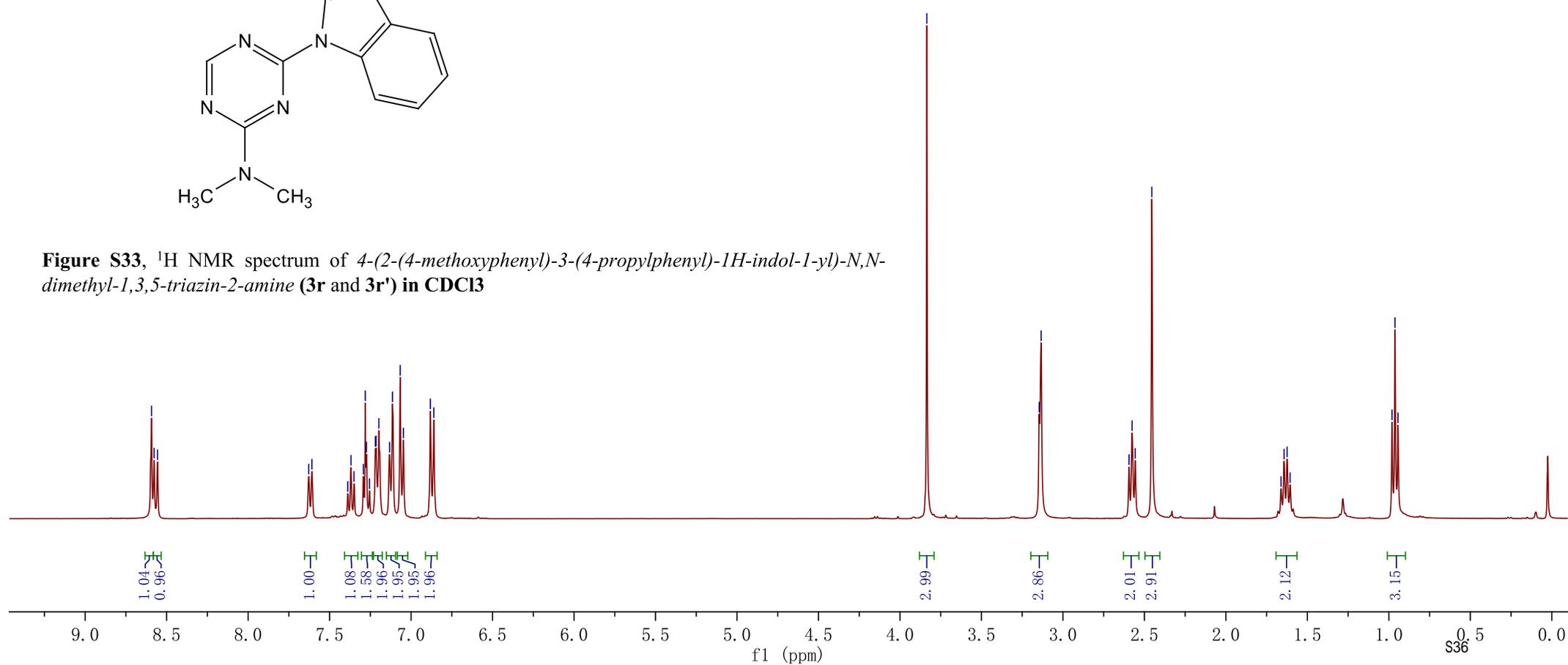
2.5945  
2.5757  
2.5566  
2.4545

1.6614  
1.6428  
1.6243  
1.6060

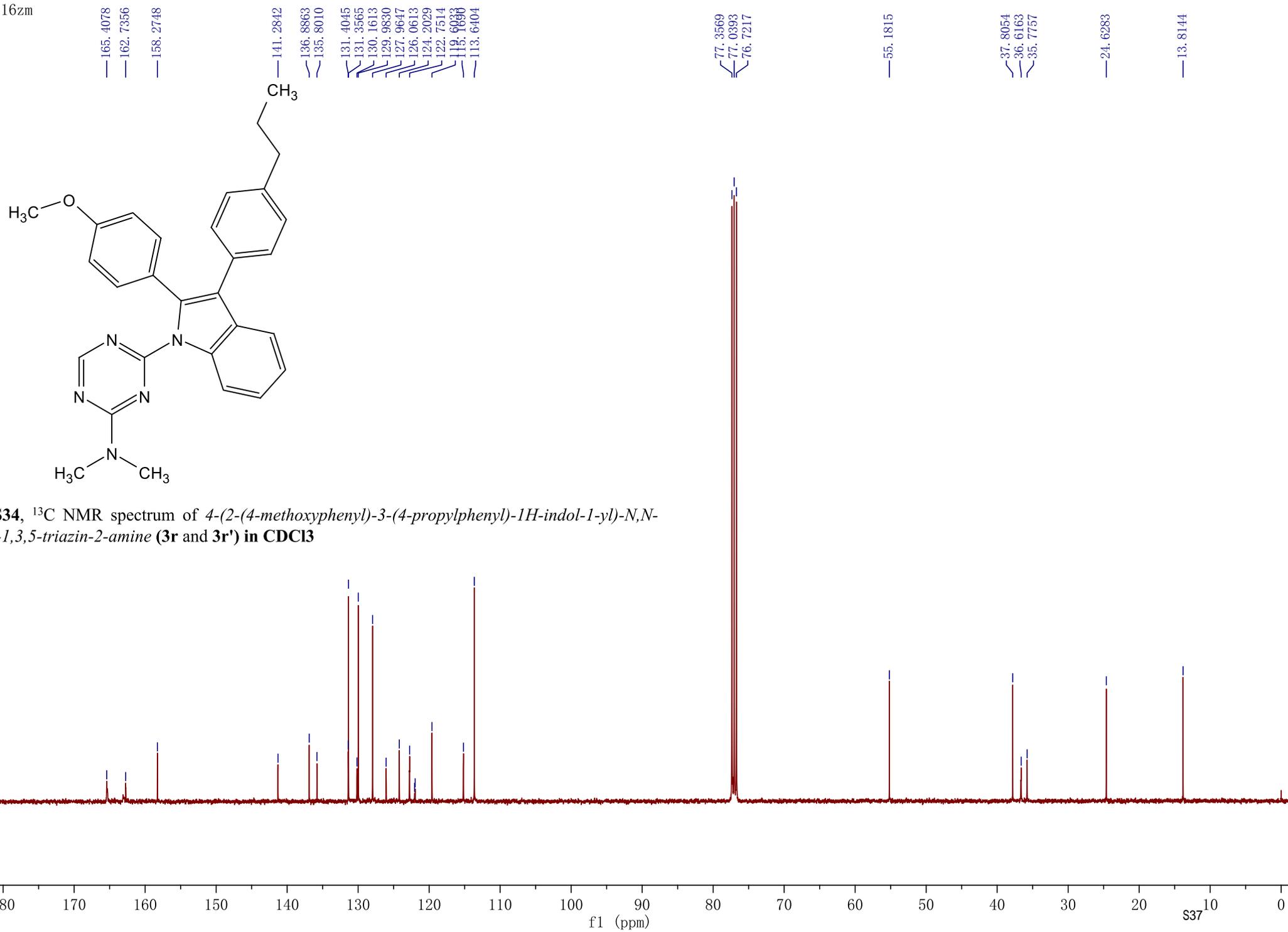
0.9807  
0.9625  
0.9442



**Figure S33**,  $^1\text{H}$  NMR spectrum of 4-(2-(4-methoxyphenyl)-3-(4-propylphenyl)-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3r** and **3r'**) in  $\text{CDCl}_3$



20211116zm  
1104

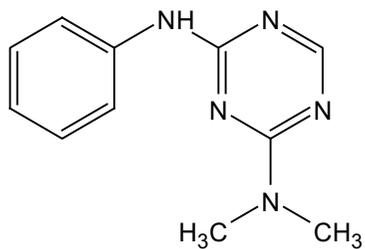


**Figure S34**, <sup>13</sup>C NMR spectrum of 4-(2-(4-methoxyphenyl)-3-(4-propylphenyl)-1H-indol-1-yl)-N,N-dimethyl-1,3,5-triazin-2-amine (**3r** and **3r'**) in CDCl<sub>3</sub>

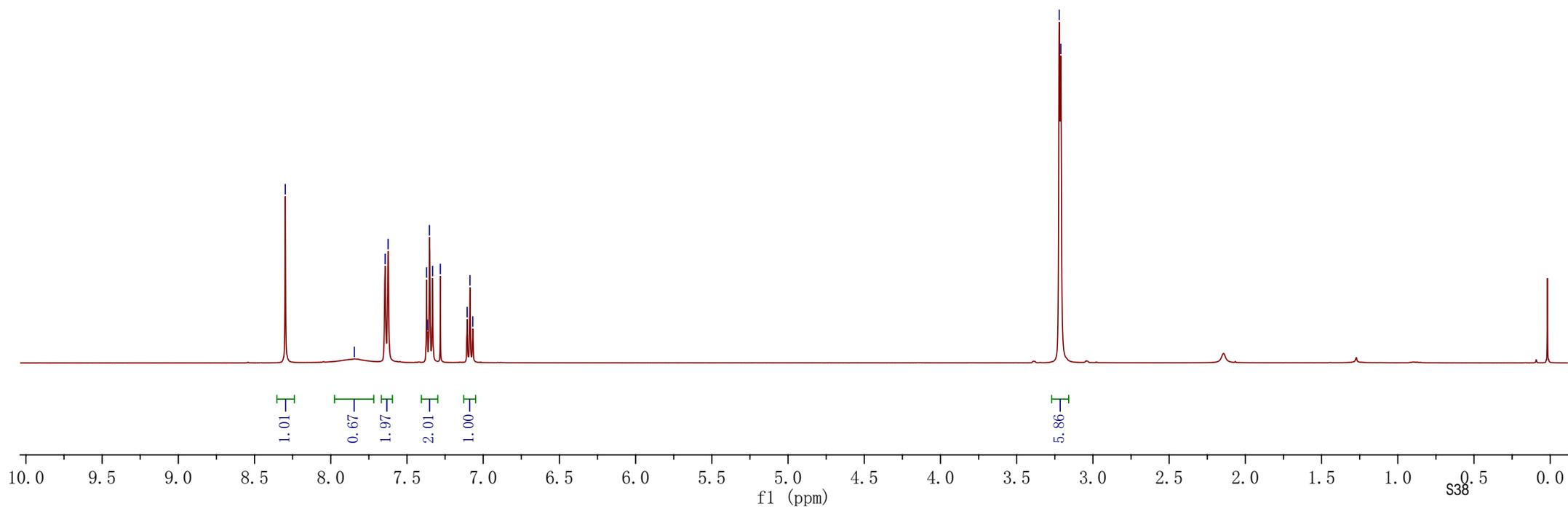
8.2984

7.8451  
7.6433  
7.6239  
7.3715  
7.3667  
7.3527  
7.3316  
7.2811  
7.1052  
7.0867  
7.0682

3.2213  
3.2106



**Figure S35,** <sup>1</sup>H NMR spectrum of *N*<sup>2</sup>,*N*<sup>2</sup>-dimethyl-*N*<sup>4</sup>-phenyl-1,3,5-triazine-2,4-diamine (1a) in CDCl<sub>3</sub>



20220117zm  
20211128

165.3911  
164.5384  
163.1780

138.7478

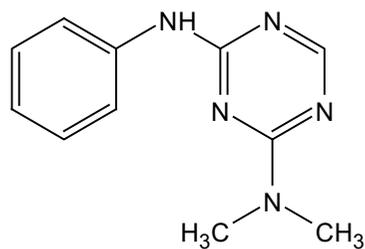
128.8372

123.1583

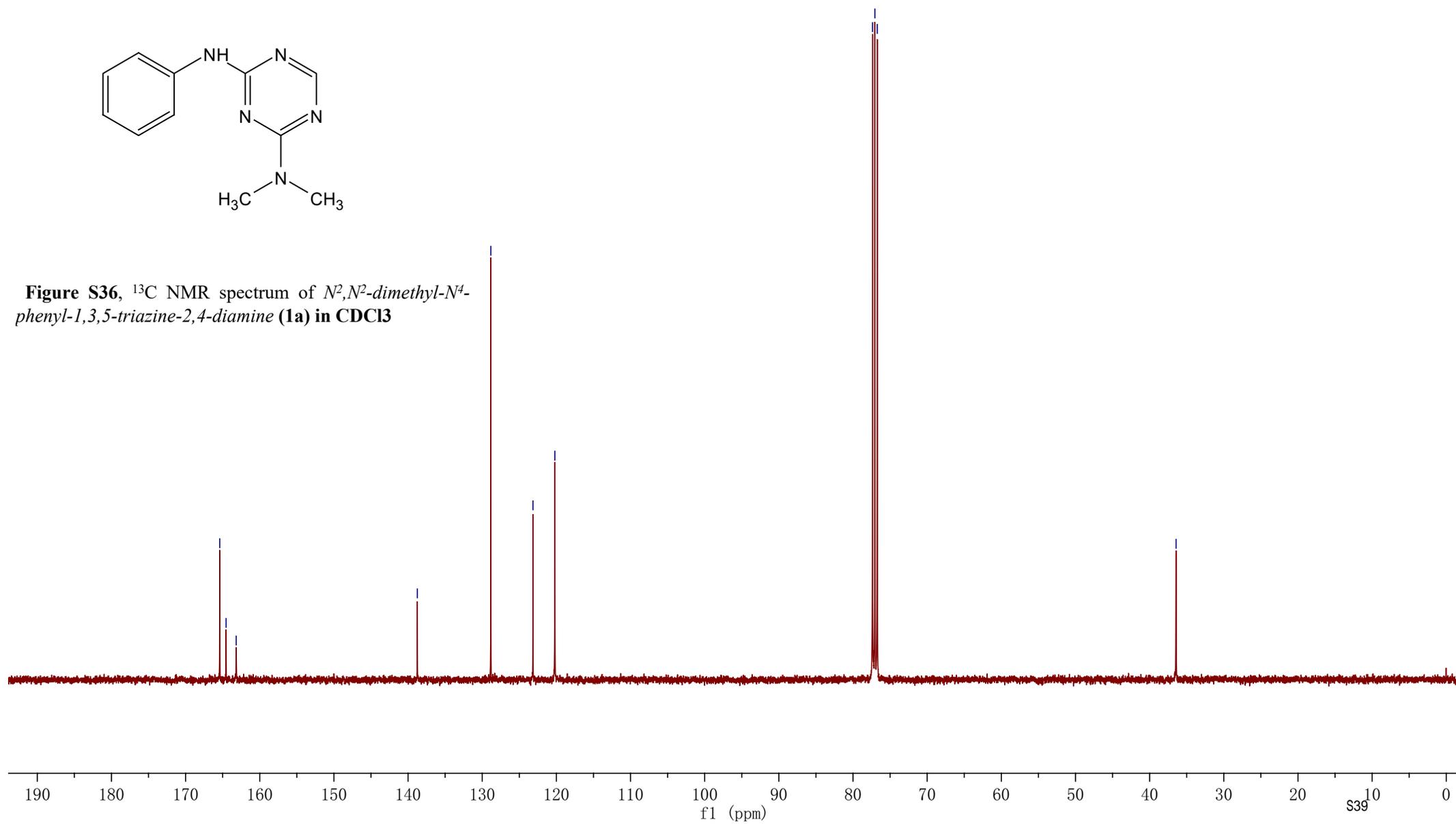
120.2078

77.3639  
77.0463  
76.7287

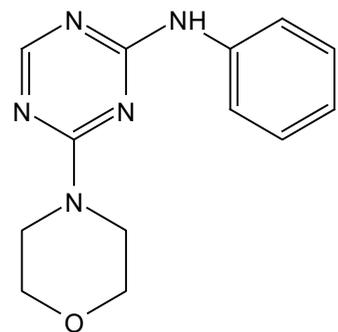
36.4359



**Figure S36**,  $^{13}\text{C}$  NMR spectrum of  $N^2,N^2$ -dimethyl- $N^4$ -phenyl-1,3,5-triazine-2,4-diamine (**1a**) in  $\text{CDCl}_3$



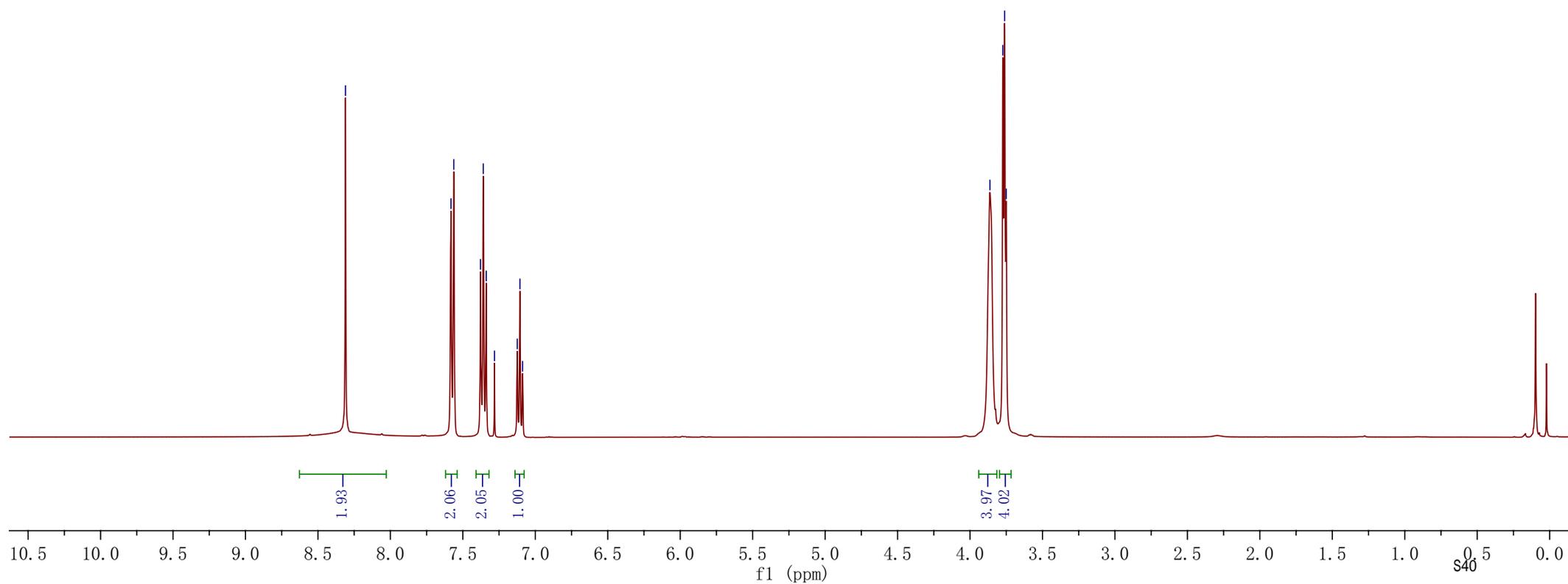
20230412zm  
1j CDC13



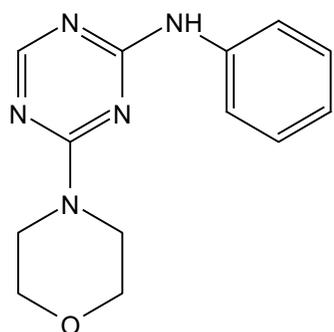
8.3099  
7.5816  
7.5625  
7.3781  
7.3592  
7.3385  
7.2815  
7.1245  
7.1060  
7.0875

3.8624  
3.7737  
3.7611  
3.7500

**Figure S37**,  $^1\text{H}$  NMR spectrum of *4-morpholino-N-phenyl-1,3,5-triazin-2-amine (1j)* in  $\text{CDCl}_3$



20230412zm  
1j CDC13



165.7942  
164.0647  
163.5188

138.5026

128.8647

123.4780

120.5691

77.3777

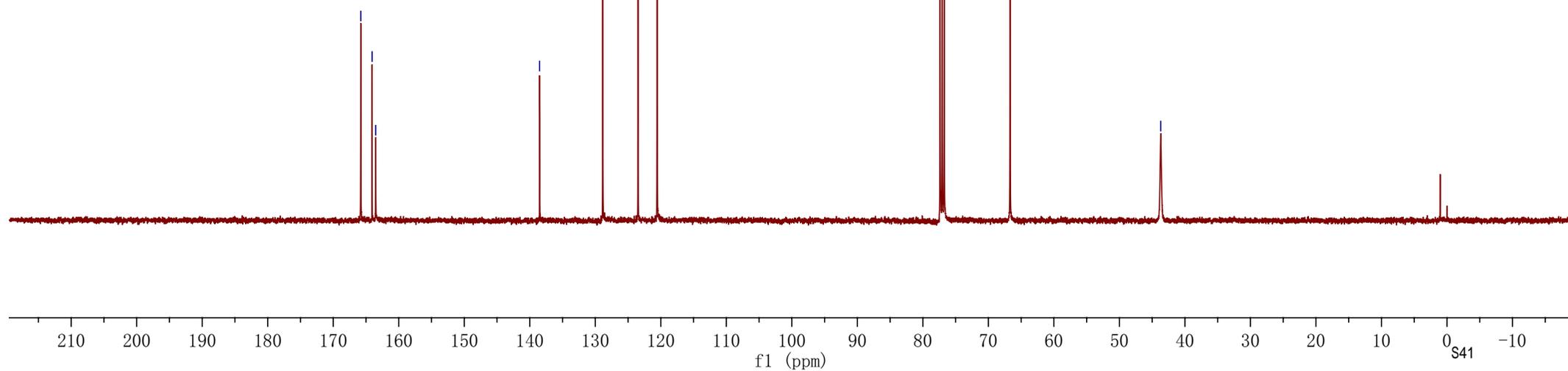
77.0599

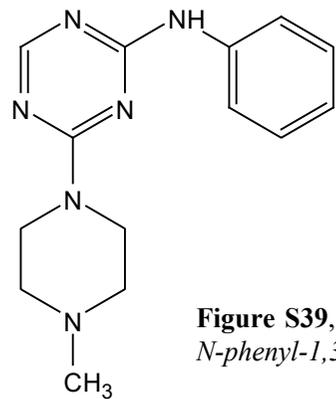
76.7422

66.6841

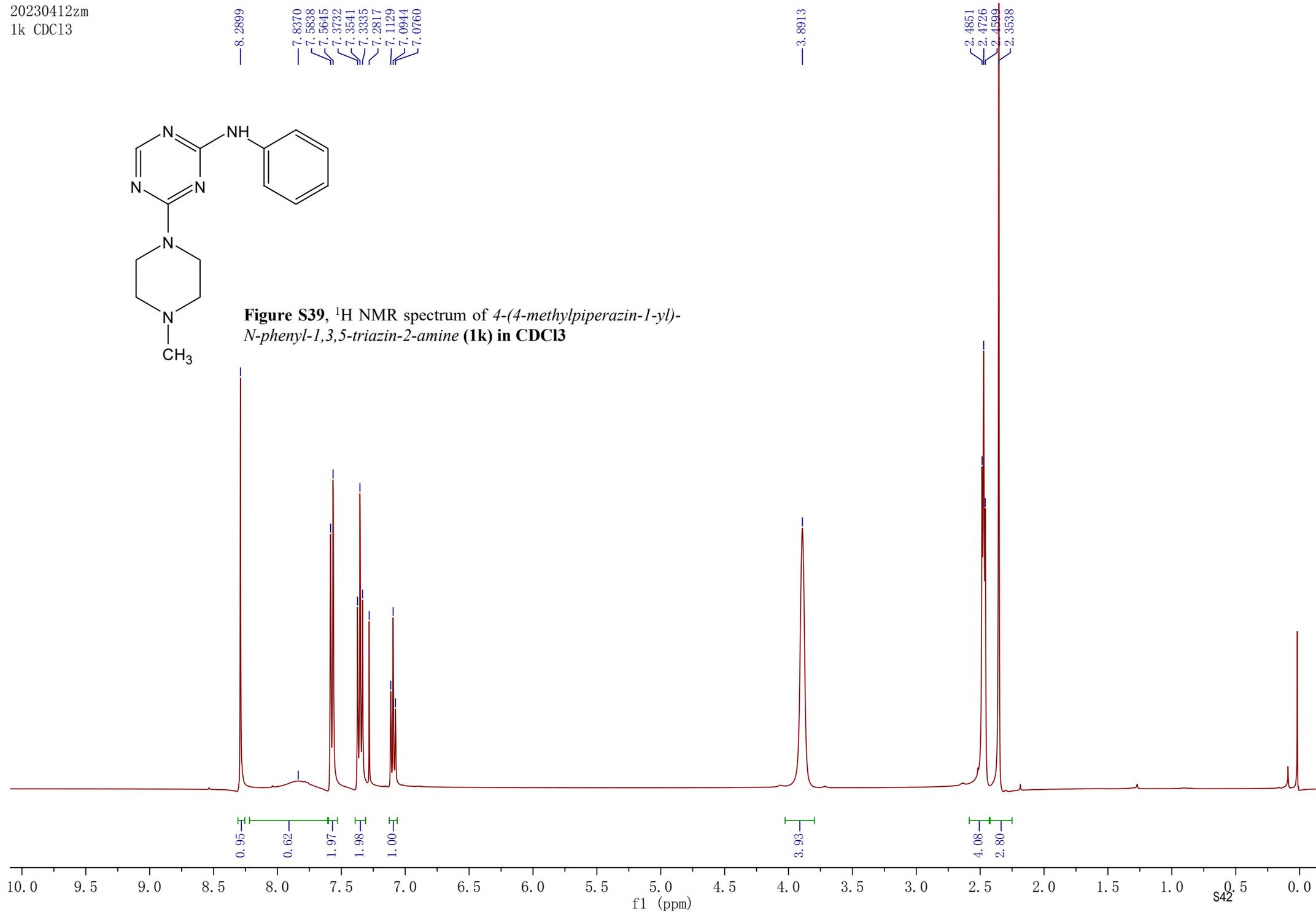
43.6969

**Figure S38,**  $^{13}\text{C}$  NMR spectrum of *4-morpholino-N-phenyl-1,3,5-triazin-2-amine (1j)* in  $\text{CDCl}_3$





**Figure S39**, <sup>1</sup>H NMR spectrum of 4-(4-methylpiperazin-1-yl)-N-phenyl-1,3,5-triazin-2-amine (**1k**) in CDCl<sub>3</sub>



20230412zm  
1k CDC13

165.8184  
163.8658  
163.5359

138.5601

128.8527

123.3341

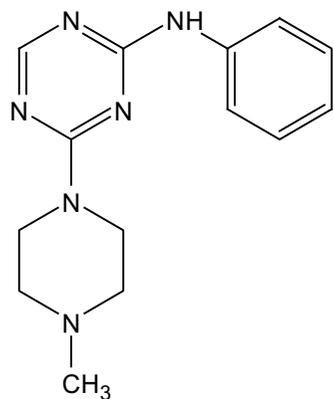
120.4190

77.3552  
77.2389  
77.0376  
76.7201

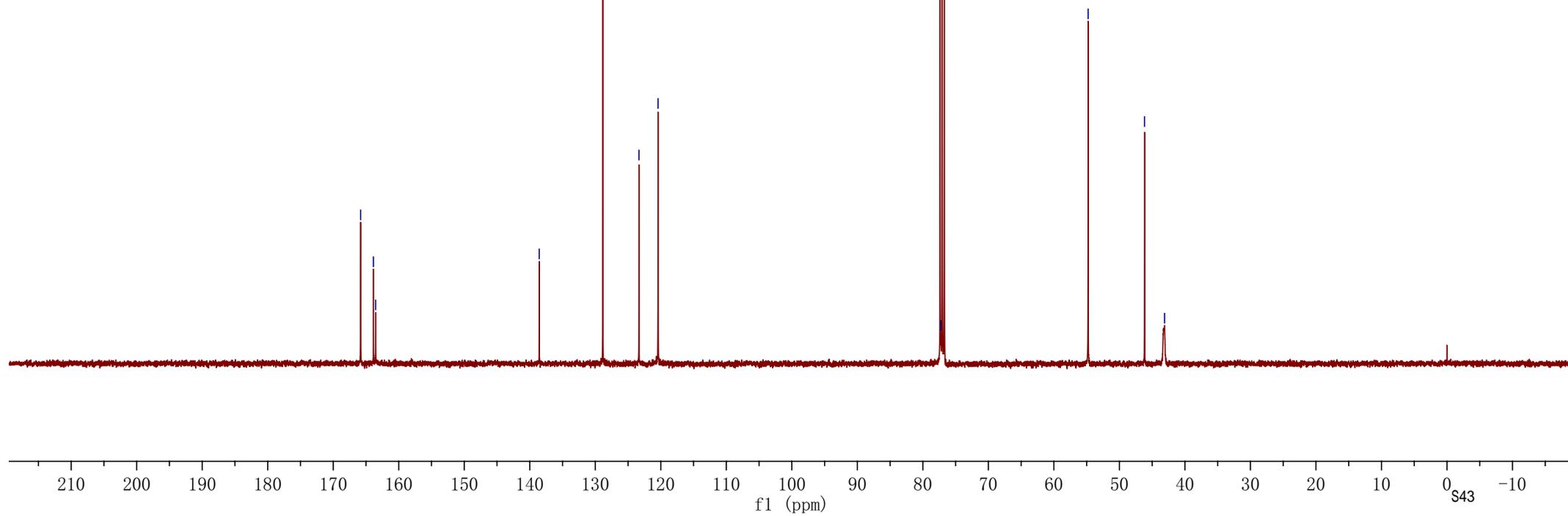
54.7750

46.1673

43.1069

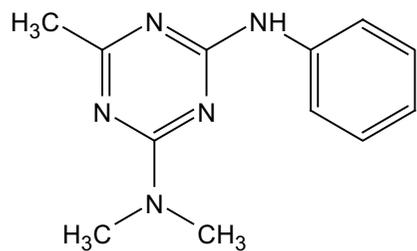


**Figure S40**,  $^{13}\text{C}$  NMR spectrum of 4-(4-methylpiperazin-1-yl)-*N*-phenyl-1,3,5-triazin-2-amine (**1k**) in  $\text{CDCl}_3$

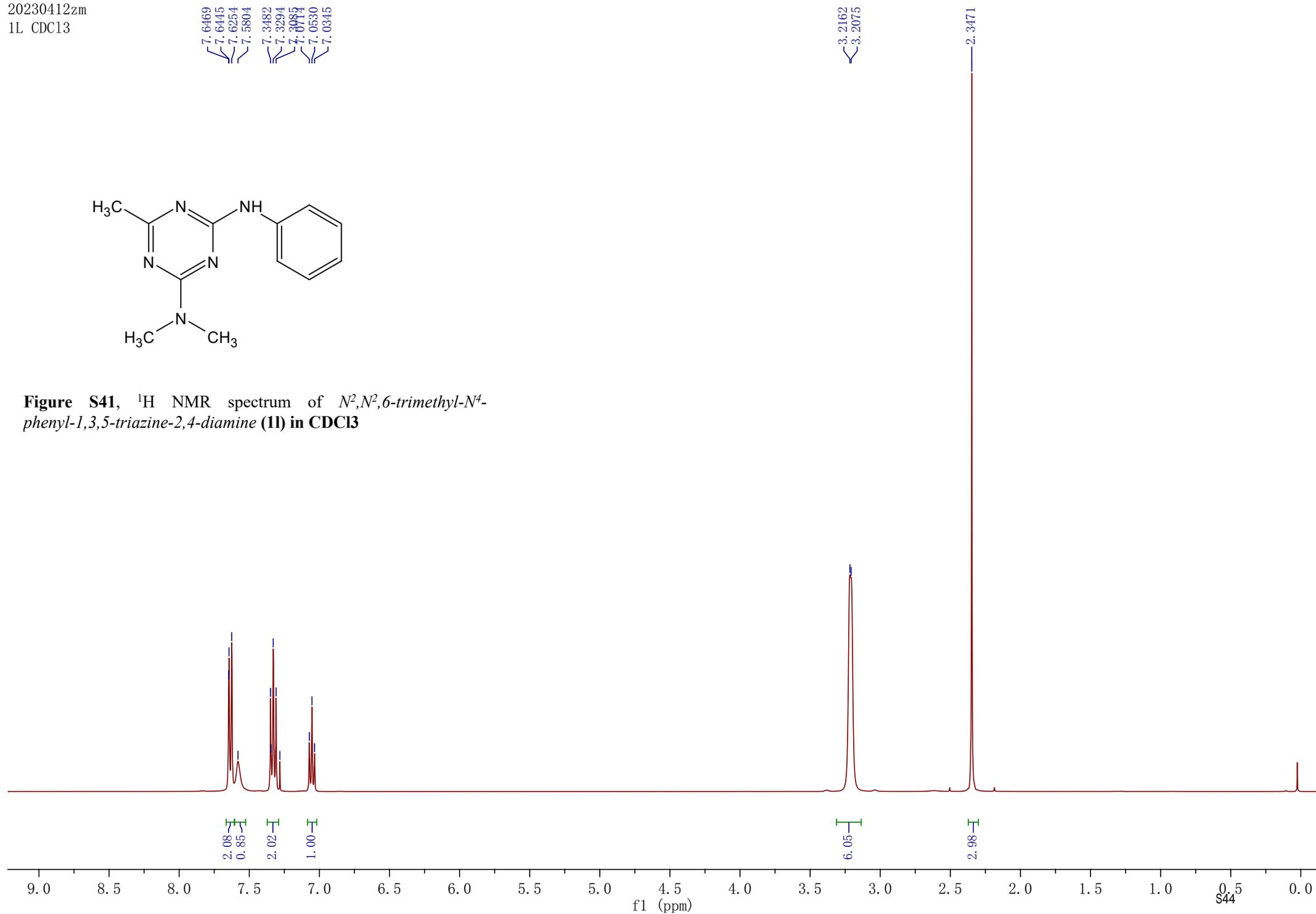


20230412zm  
1L CDC13

7.6469  
7.6445  
7.6254  
7.5804  
7.3482  
7.3294  
7.3085  
7.0714  
7.0530  
7.0345



**Figure S41,**  $^1\text{H}$  NMR spectrum of  $N^2,N^2,6$ -trimethyl- $N^4$ -phenyl-1,3,5-triazine-2,4-diamine (**1**) in  $\text{CDCl}_3$



20230412zm  
1L CDC13

175.0900

165.3097  
163.7453

139.1333

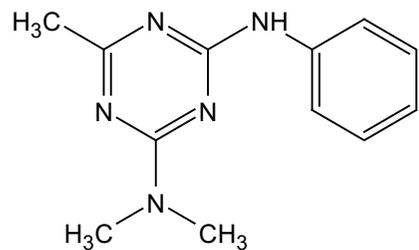
128.7543

122.7231  
119.8718  
119.8587

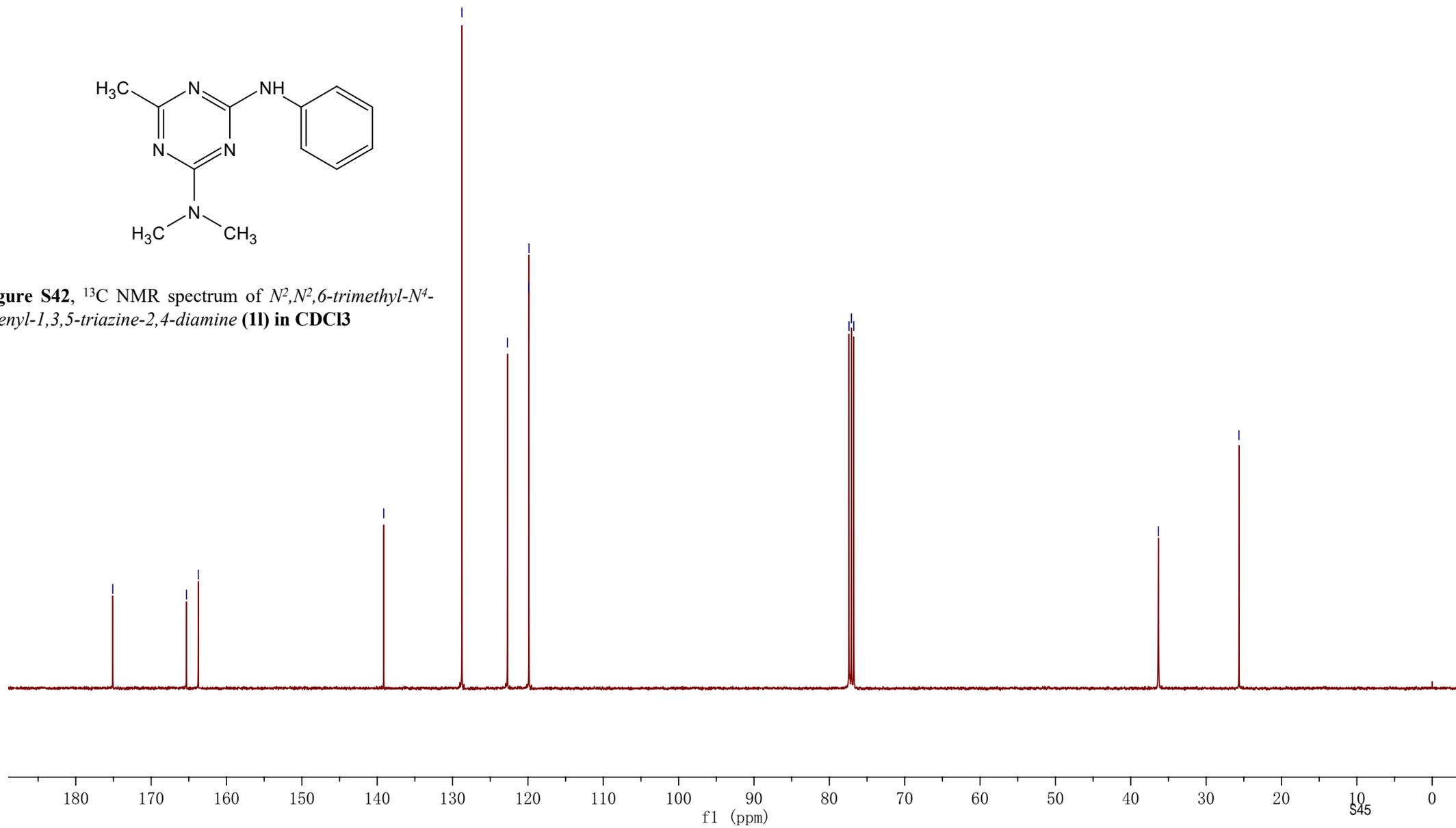
77.3986  
77.0759  
76.7582

36.3332

25.6442



**Figure S42**, <sup>13</sup>C NMR spectrum of *N*<sup>2</sup>,*N*<sup>2</sup>,6-trimethyl-*N*<sup>4</sup>-phenyl-1,3,5-triazine-2,4-diamine (**1**) in CDCl<sub>3</sub>



20211112zm  
f211104

8.5926  
8.5770  
8.5561

7.6283  
7.6088  
7.3888  
7.3687  
7.3504  
7.2927  
7.2811  
7.2739  
7.2555  
7.2193  
7.2146  
7.1978  
7.1317  
7.1141  
7.0669  
7.0469  
6.8817  
6.8606

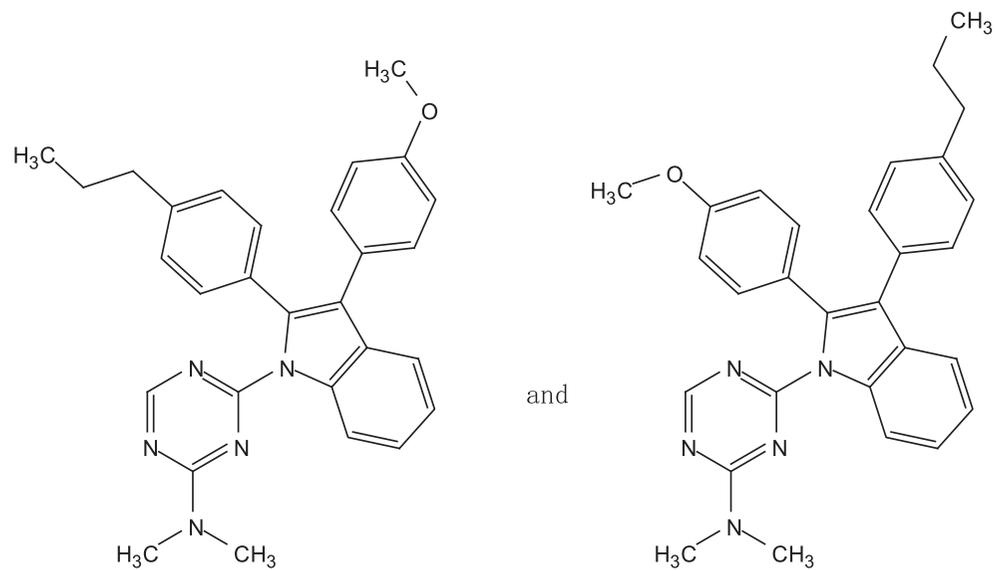
3.8351

3.1455  
3.1337

2.5945  
2.5757  
2.5566  
2.4545

1.6793  
1.6614  
1.6428  
1.6243  
1.6060  
1.5880

0.9807  
0.9625  
0.9442



and

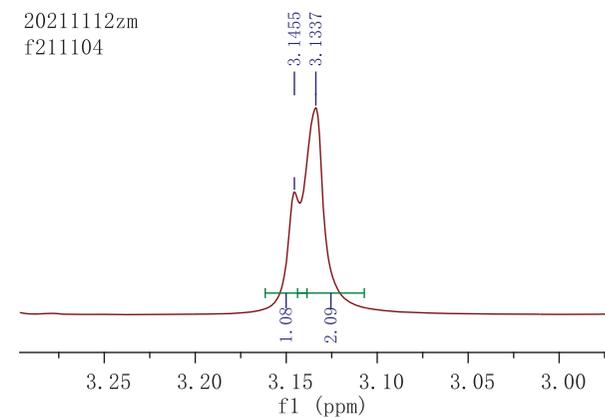


Figure S43. The isomers **3r** and **3r'**.

