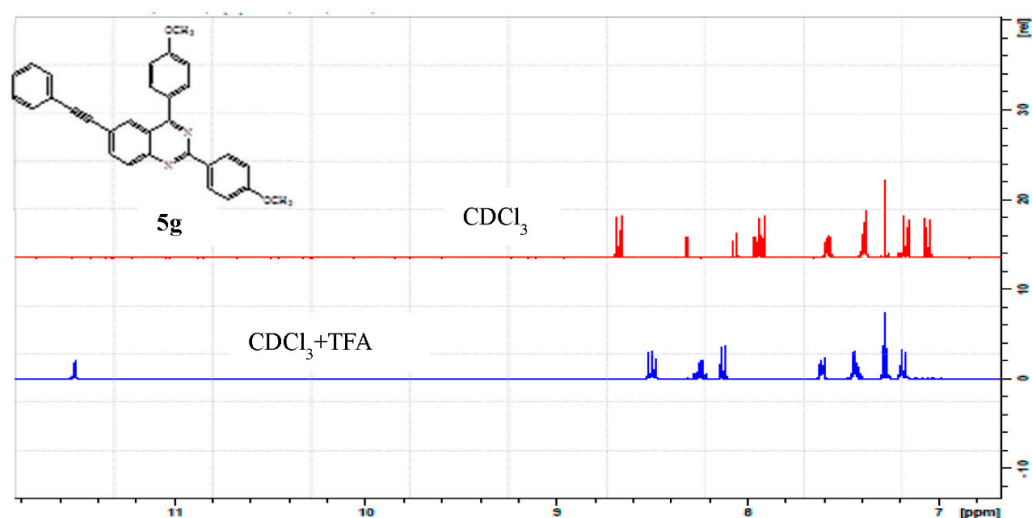
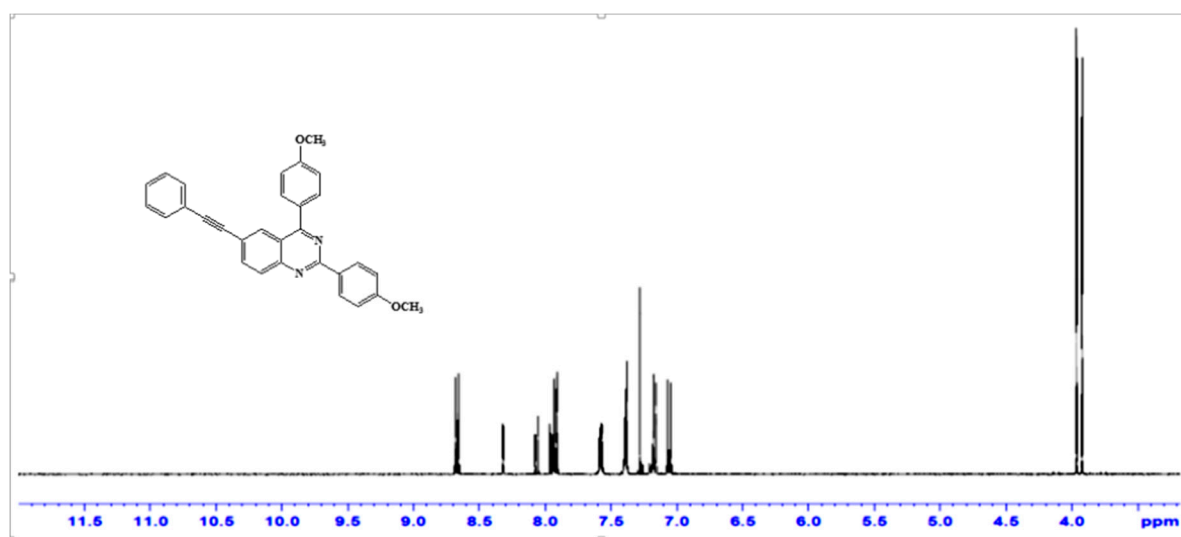


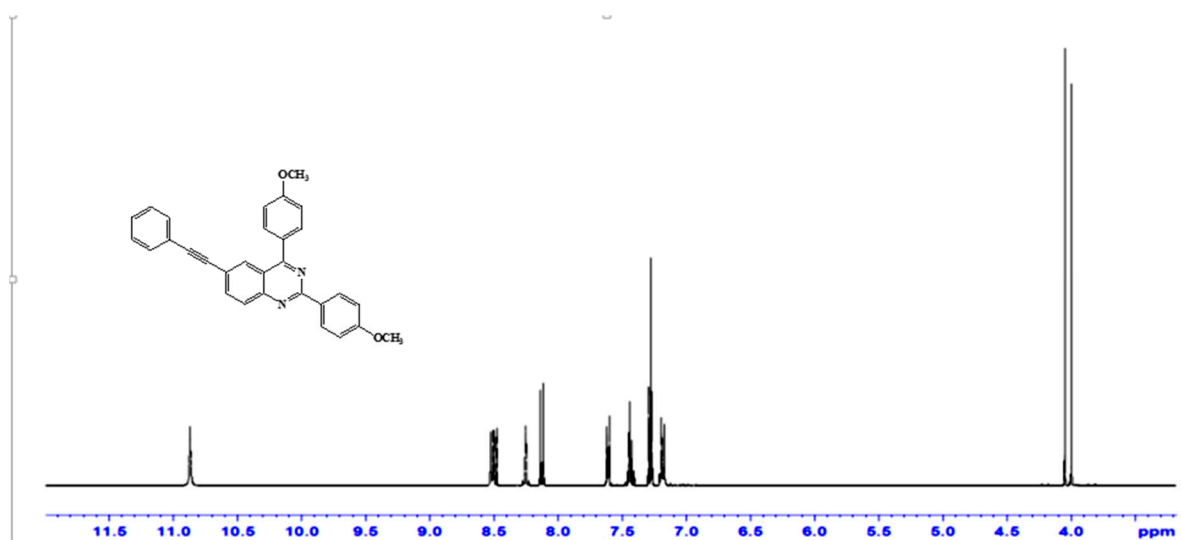
## Supporting Information



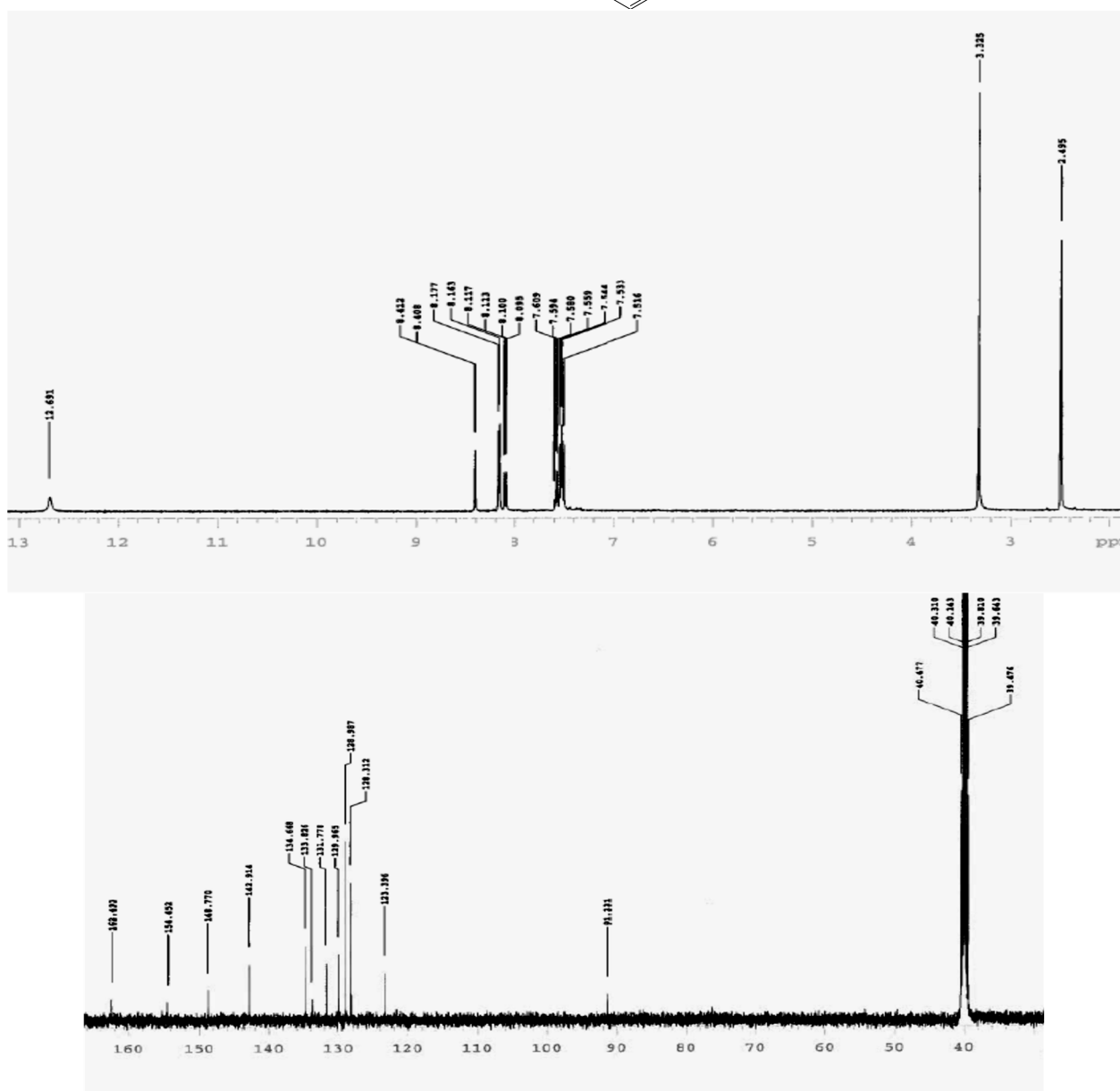
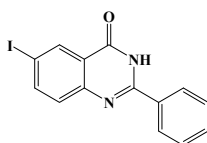
**Figure S1.** Portion of  $^1\text{H}$ -NMR spectra of **5g** in  $\text{CDCl}_3$  (red) and in  $\text{CDCl}_3 + \text{TFA}$  (blue).



**Figure S2.**  $^1\text{H}$ -NMR spectrum of **5g** in  $\text{CDCl}_3$ .

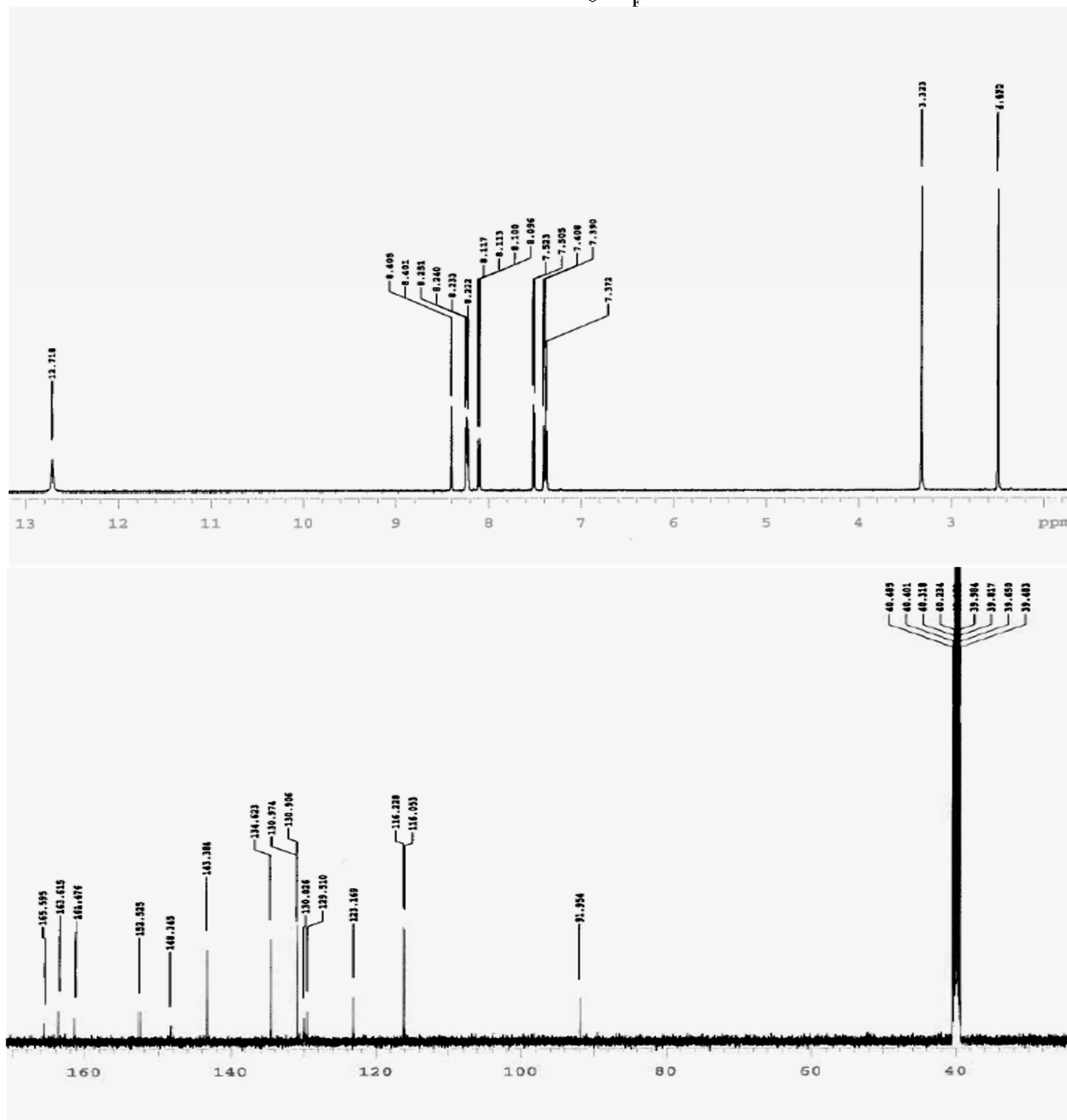
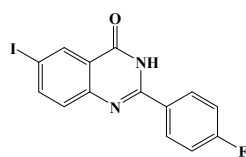


**Figure S3.**  $^1\text{H}$ -NMR spectrum of **5g** in  $\text{CDCl}_3$ -TFA mixture.



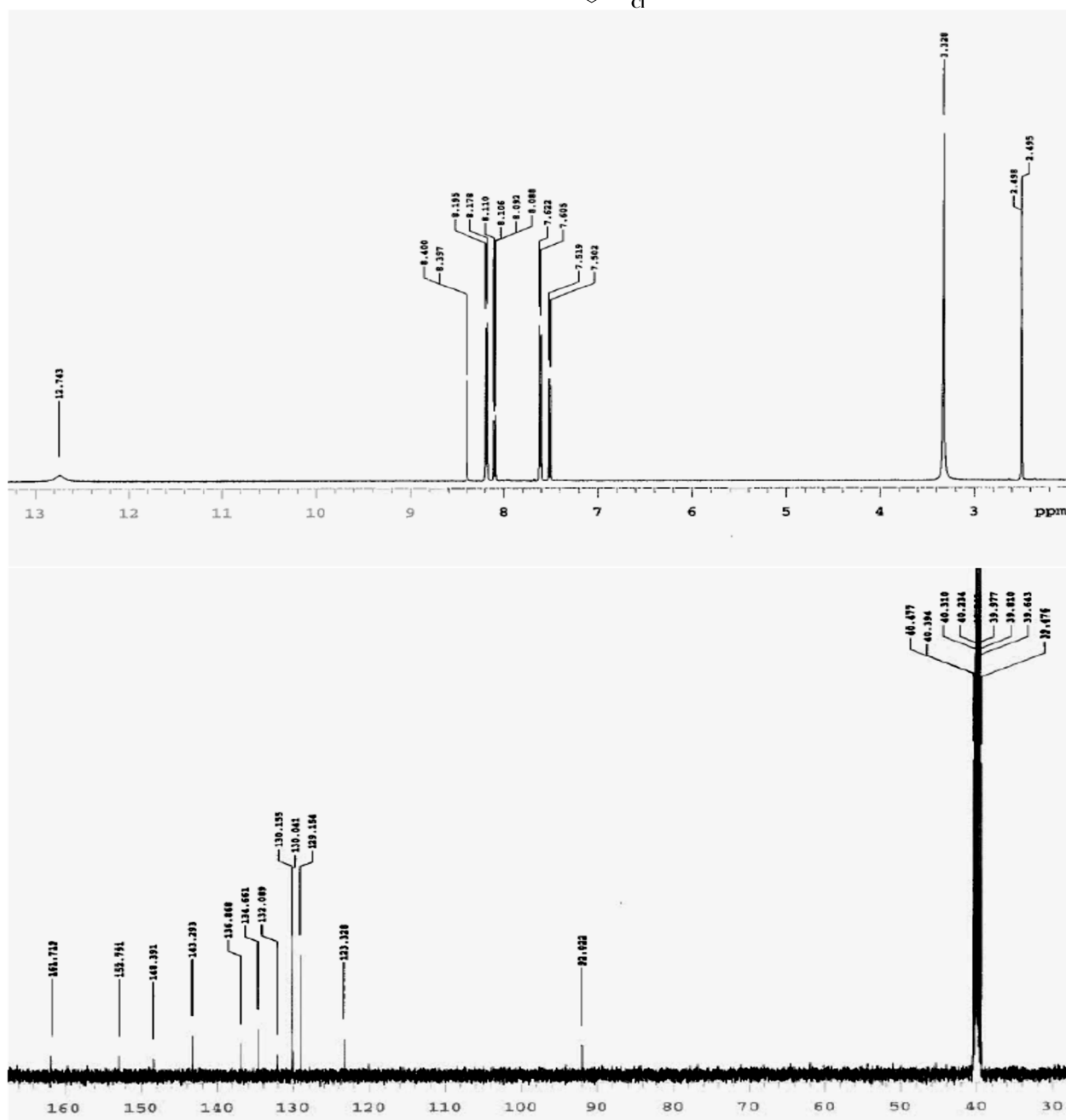
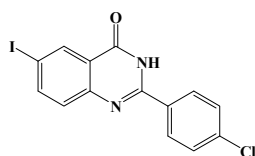
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **2a** (DMSO-*d*<sub>6</sub>).

**Figure S4.** *Cont.*



<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **2b** (DMSO-*d*<sub>6</sub>).

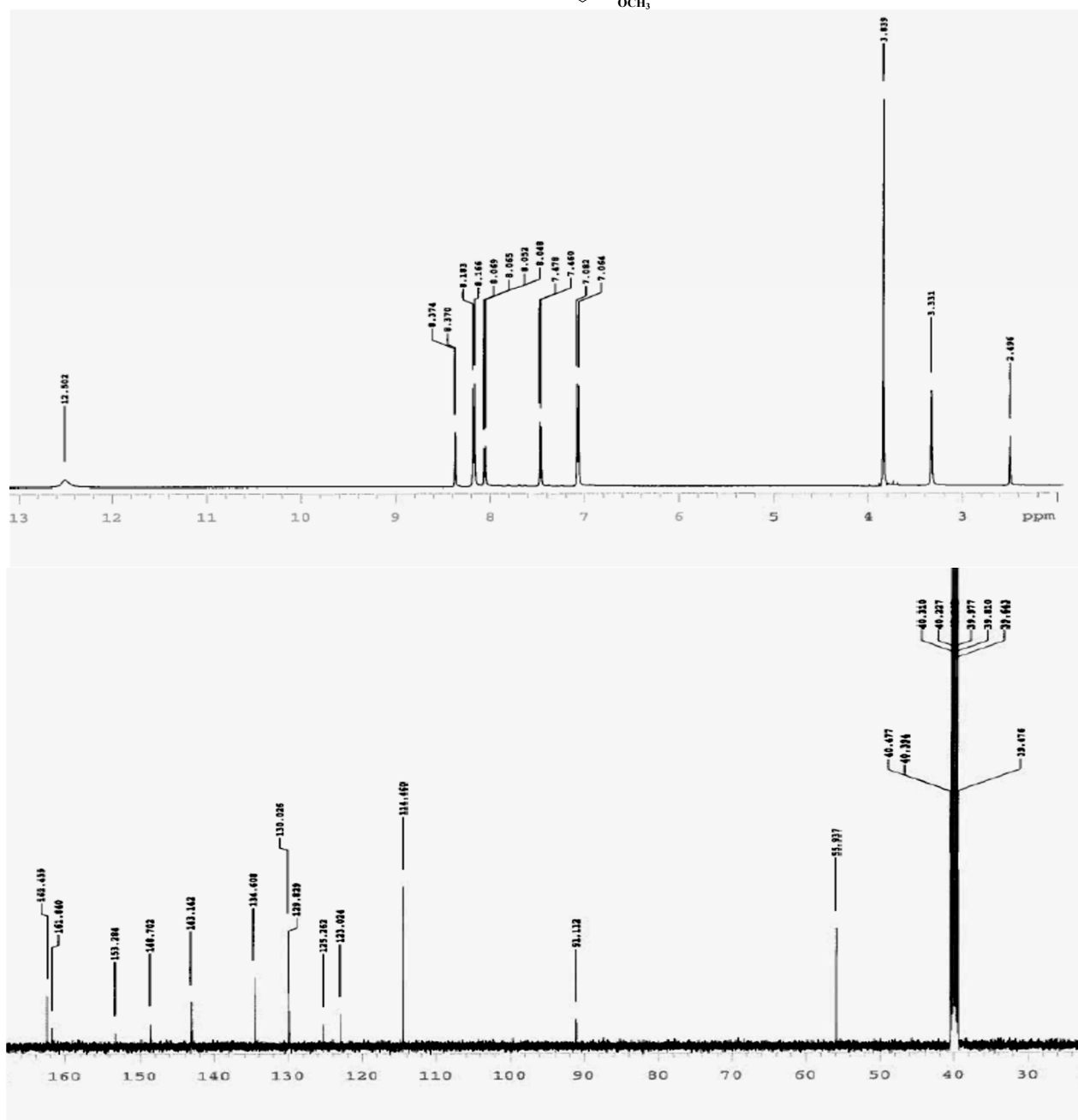
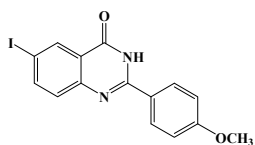
Figure S4. *Cont.*



<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **2c** (DMSO-*d*<sub>6</sub>).

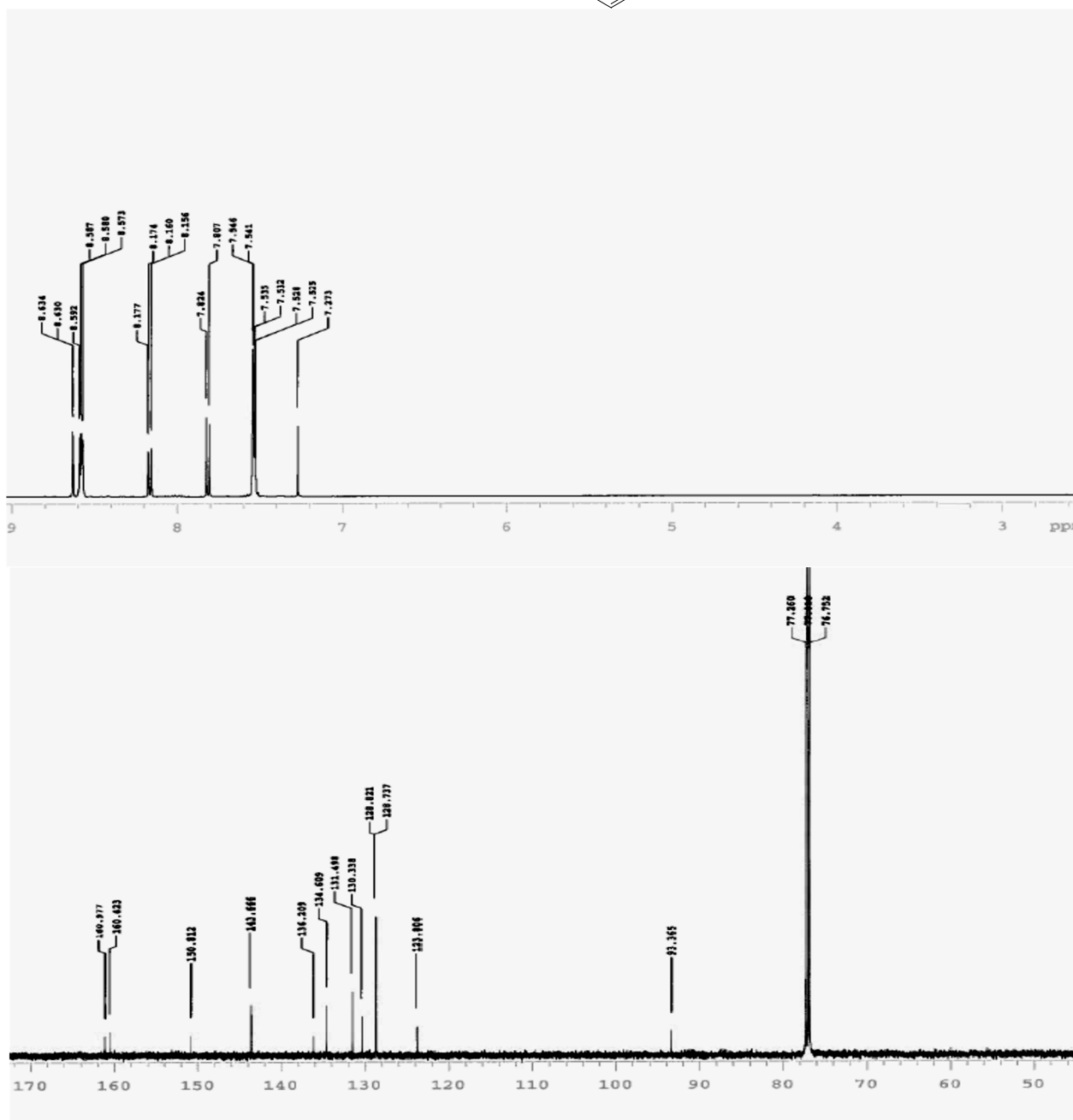
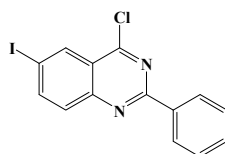
Figure S4. *Cont.*





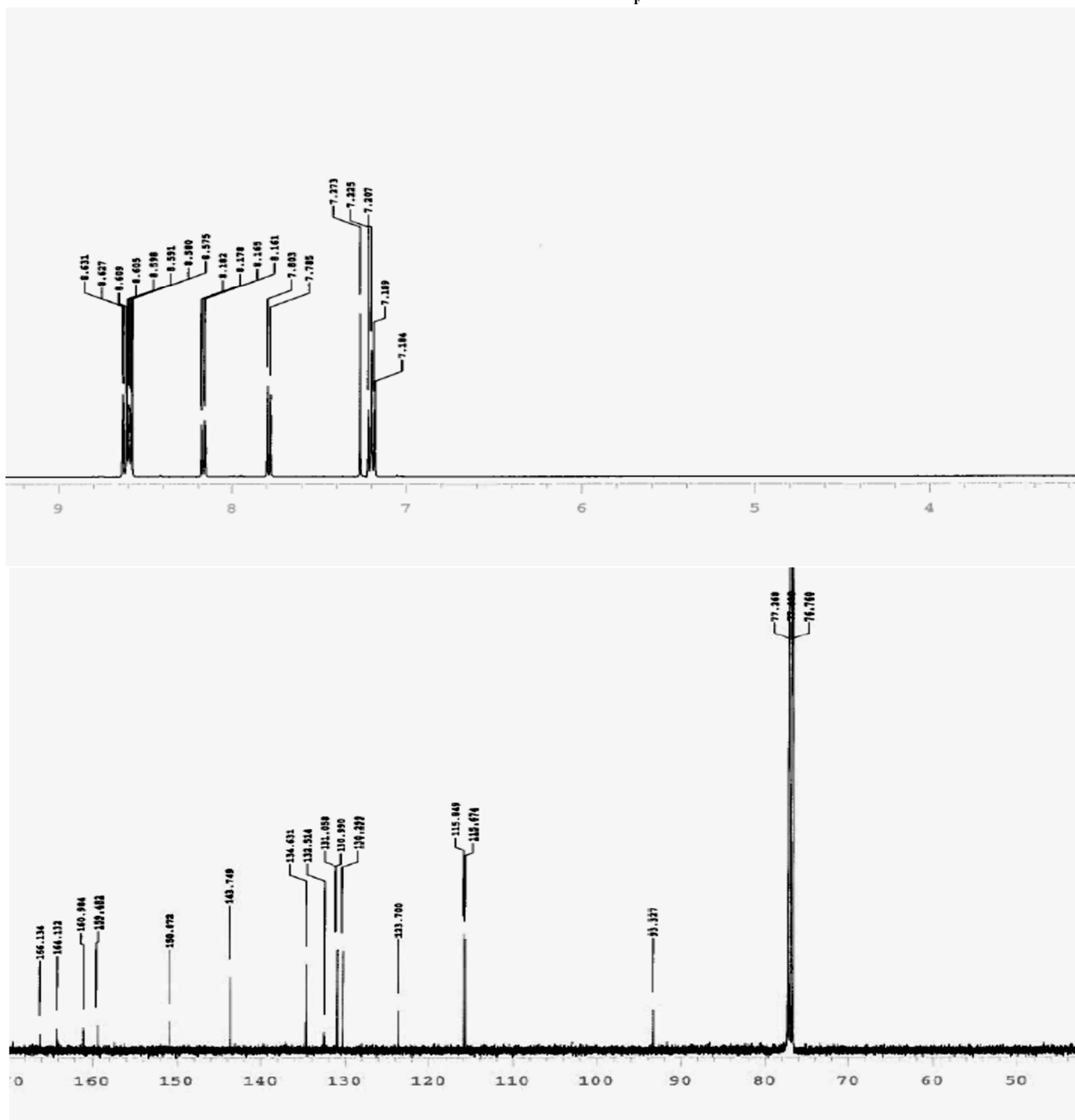
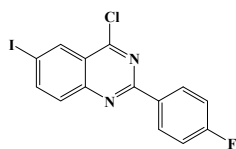
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **2d** (DMSO-*d*<sub>6</sub>).

Figure S4. *Cont.*



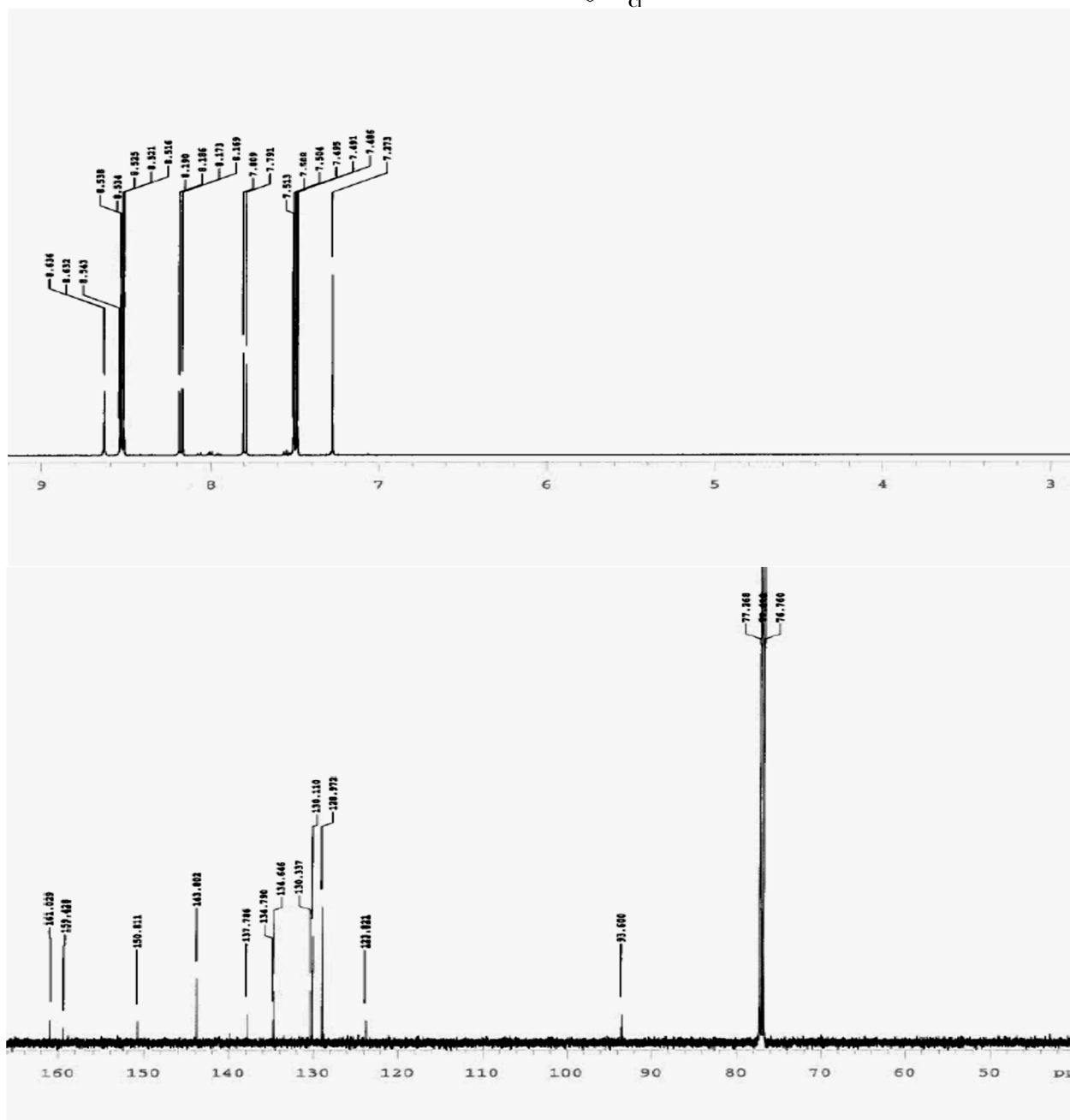
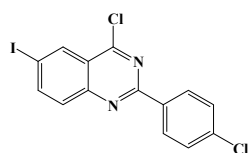
$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **3a** ( $\text{CDCl}_3$ ).

**Figure S4.** *Cont.*



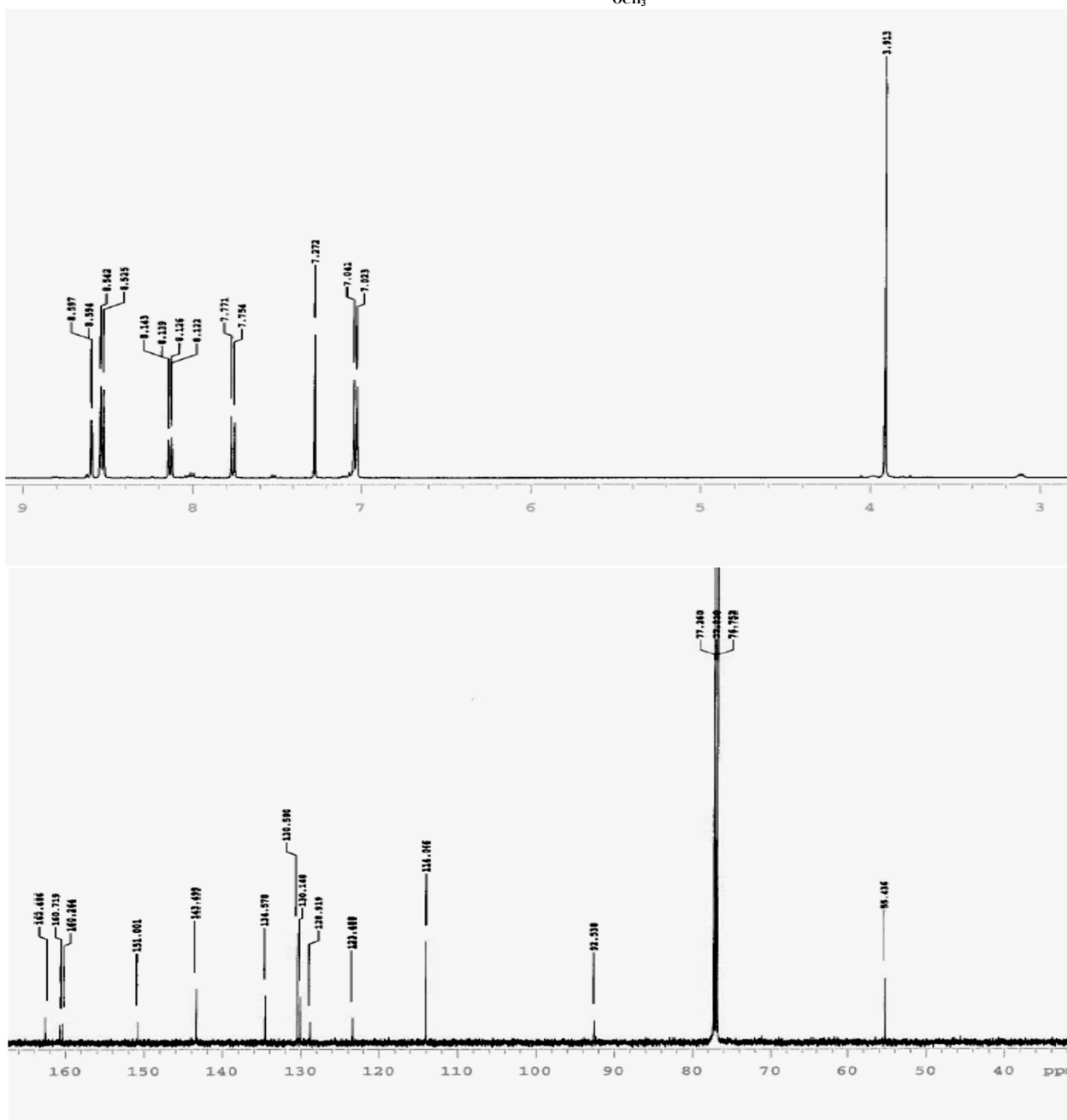
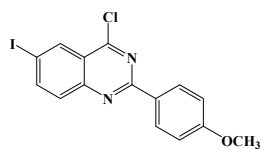
$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **3b** ( $\text{CDCl}_3$ ).

Figure S4. *Cont.*



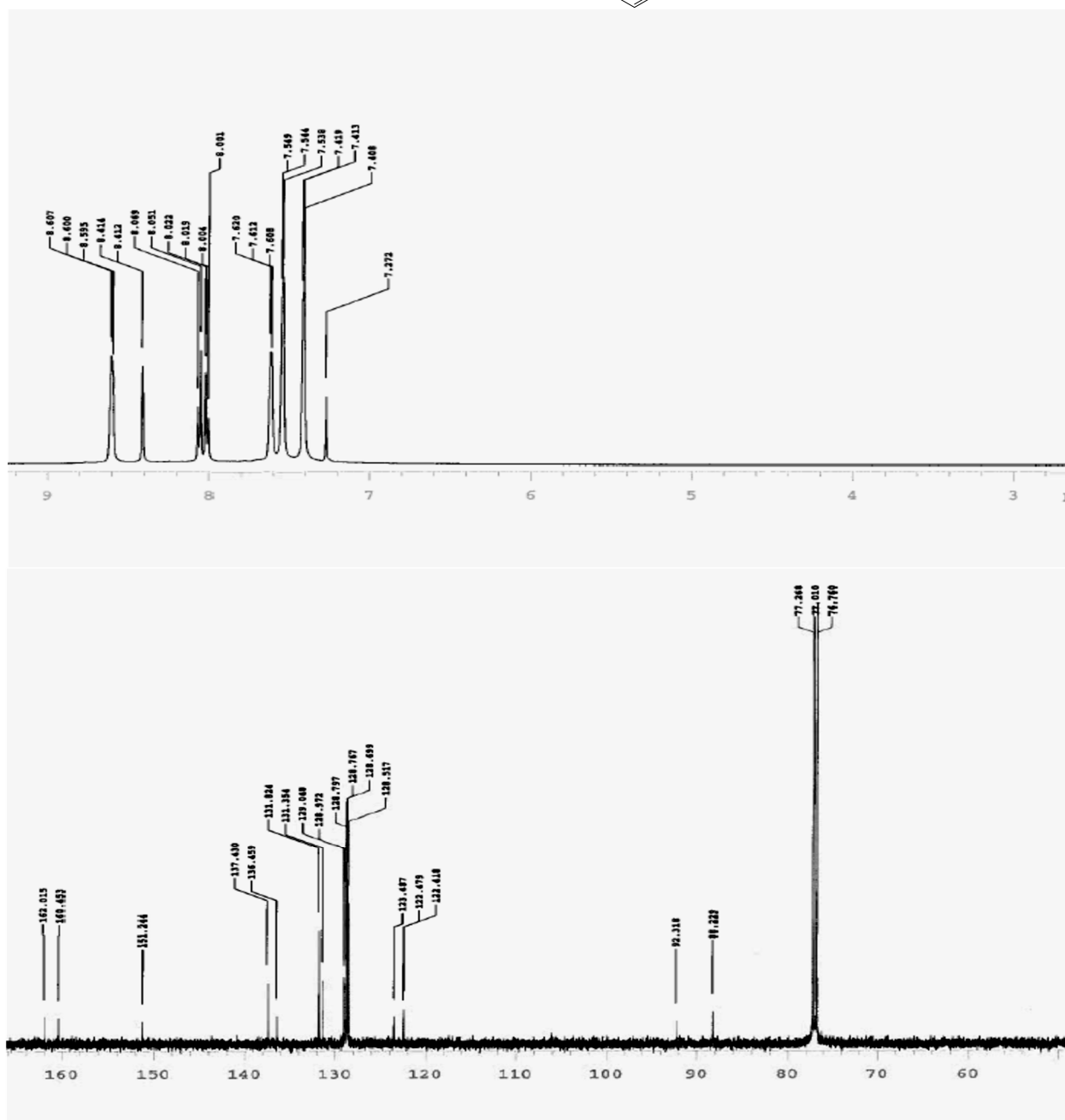
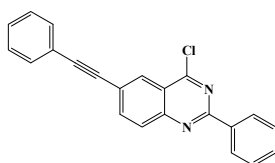
$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **3c** ( $\text{CDCl}_3$ ).

**Figure S4.** *Cont.*



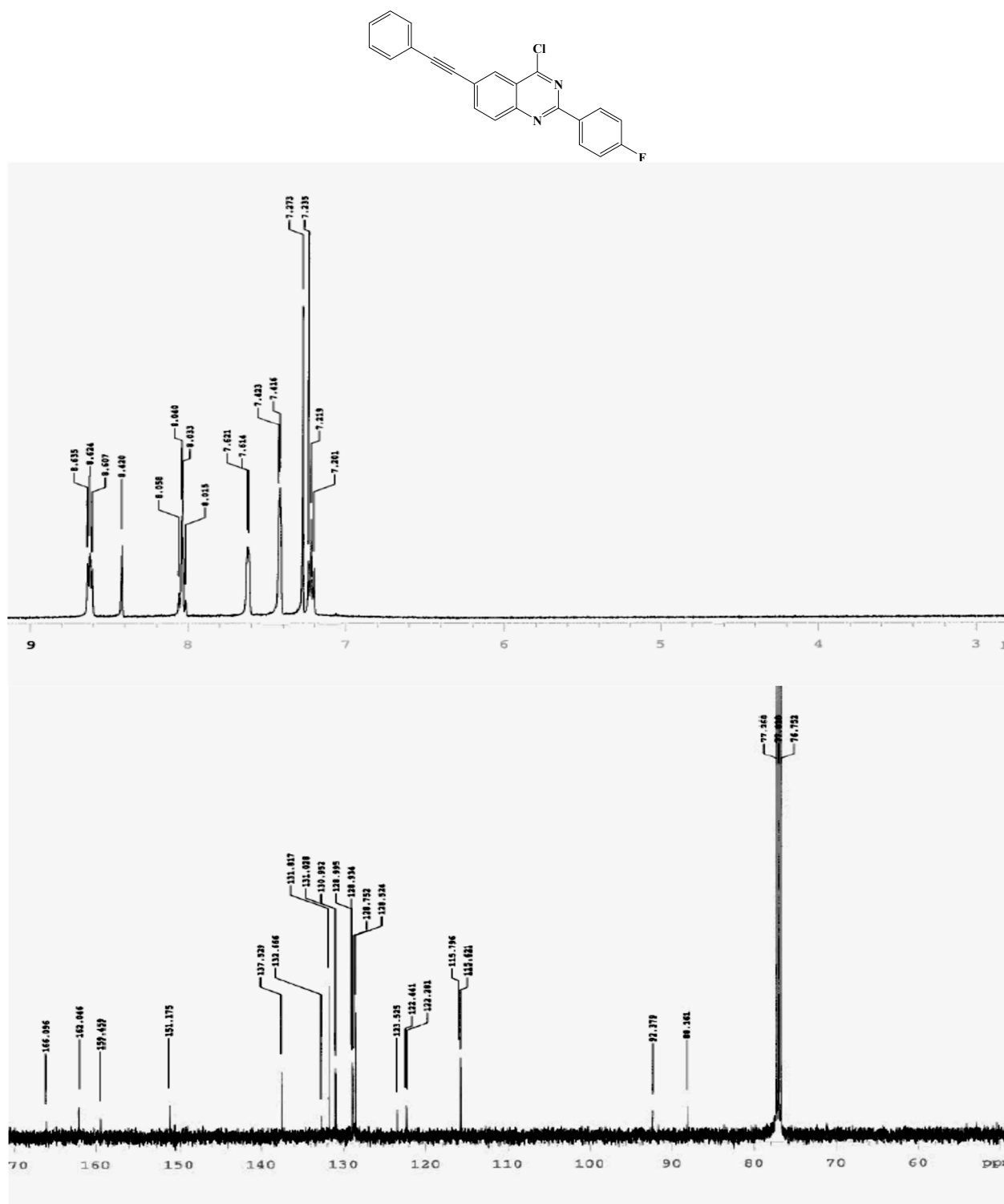
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **3d** (CDCl<sub>3</sub>).

**Figure S4.** *Cont.*



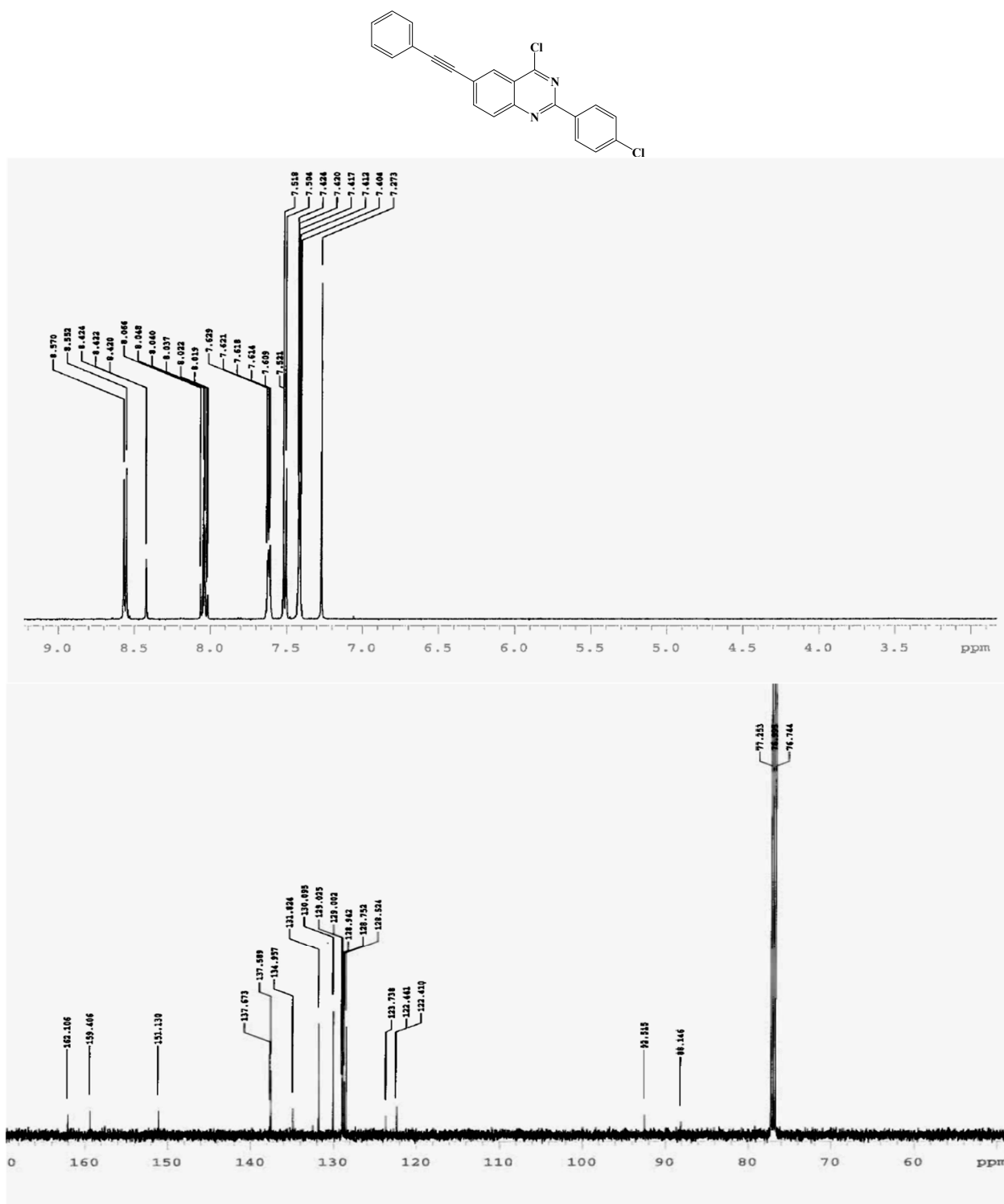
$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **4a** ( $\text{CDCl}_3$ ).

Figure S4. *Cont.*



$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **4b** ( $\text{CDCl}_3$ ).

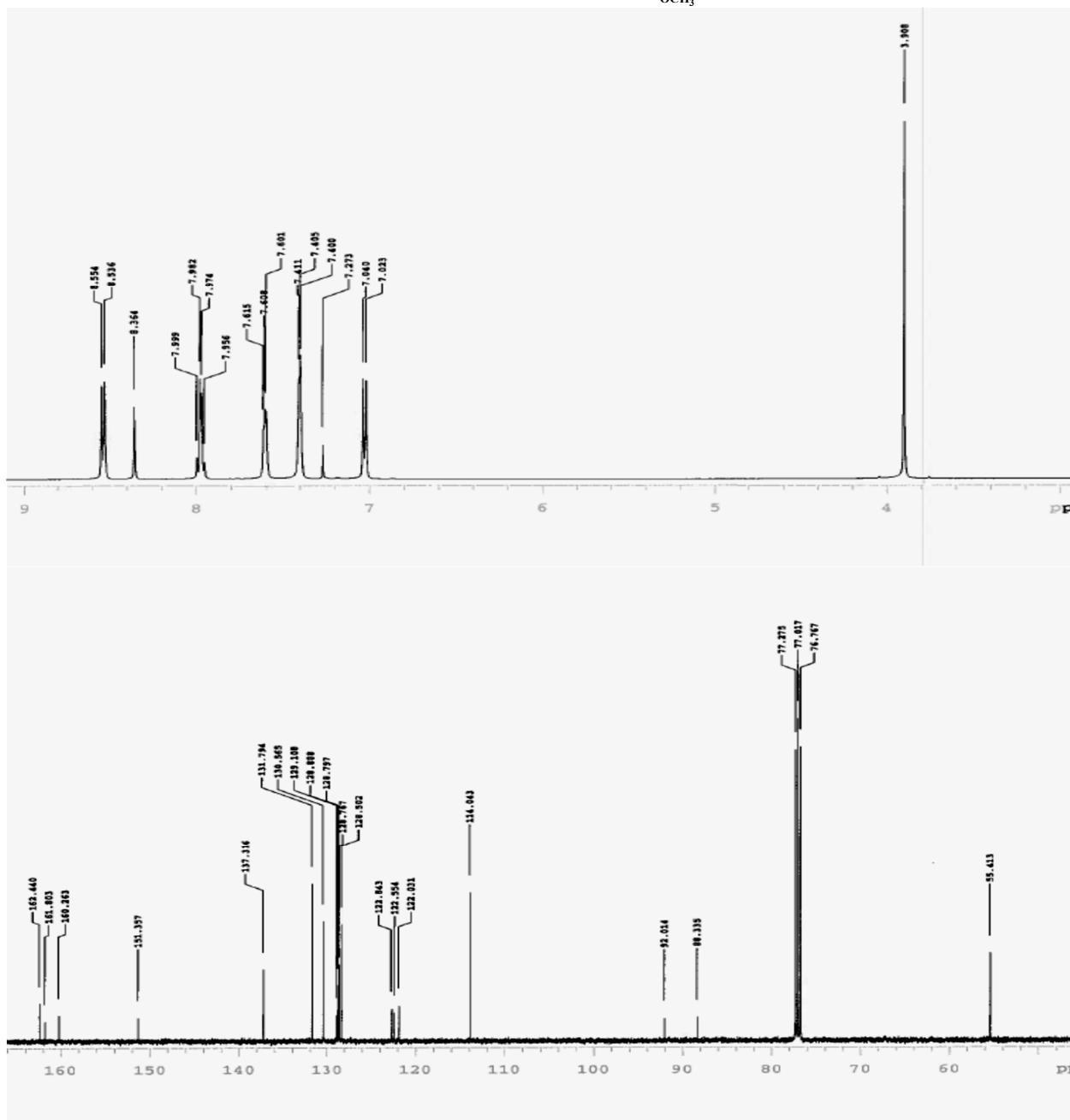
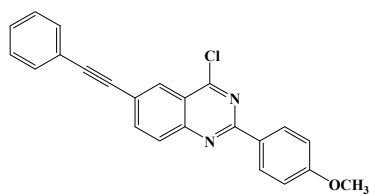
Figure S4. *Cont.*



<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **4c** (CDCl<sub>3</sub>).

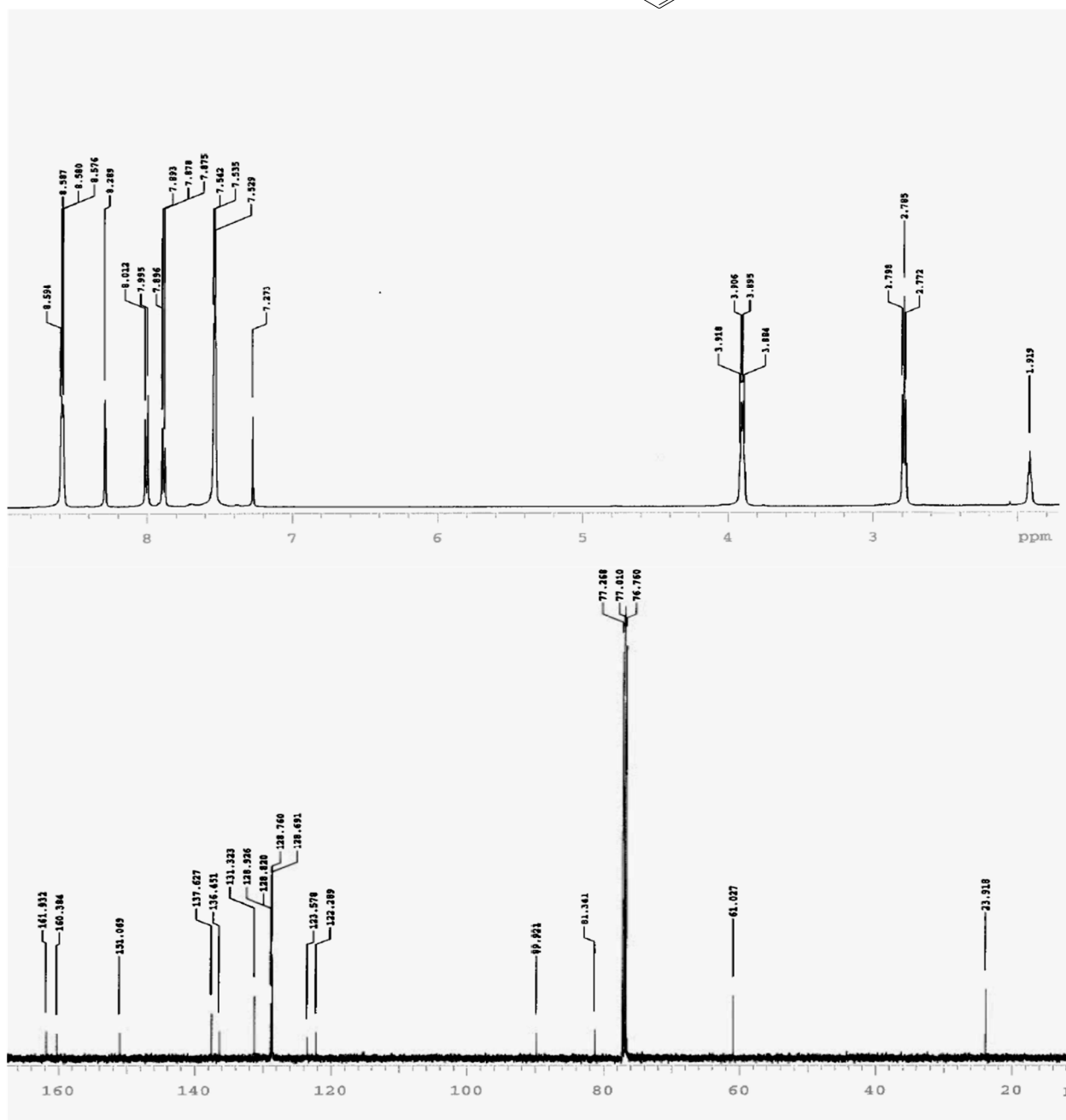
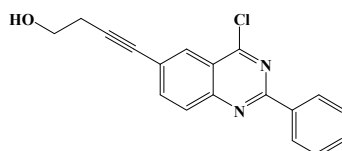
Figure S4. *Cont.*





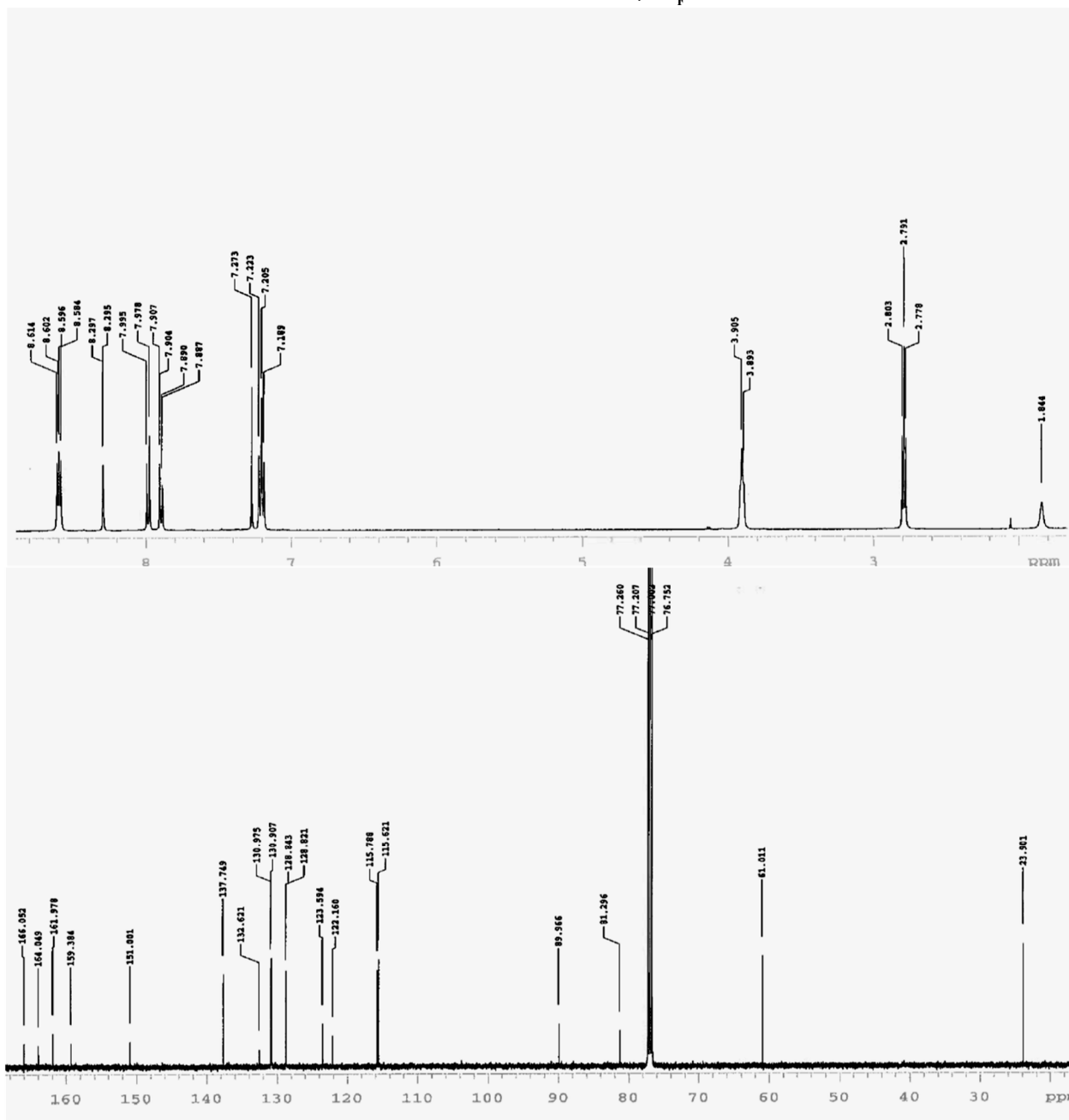
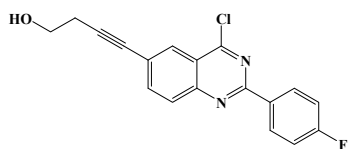
$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **4d** ( $\text{CDCl}_3$ ).

Figure S4. *Cont.*



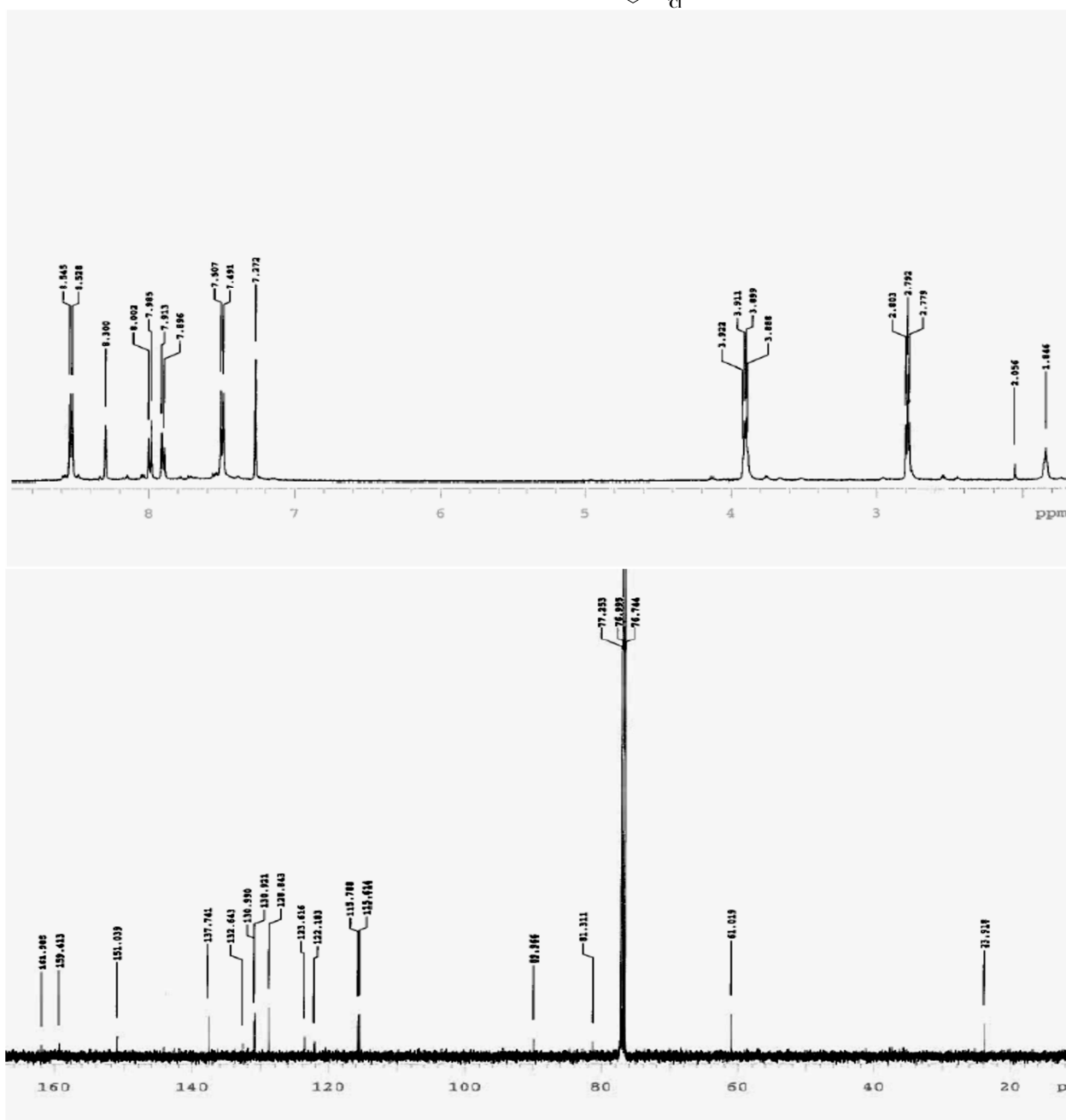
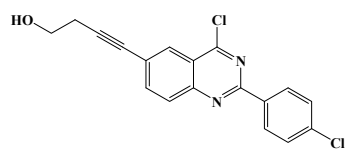
$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **4e** ( $\text{CDCl}_3$ ).

Figure S4. Cont.



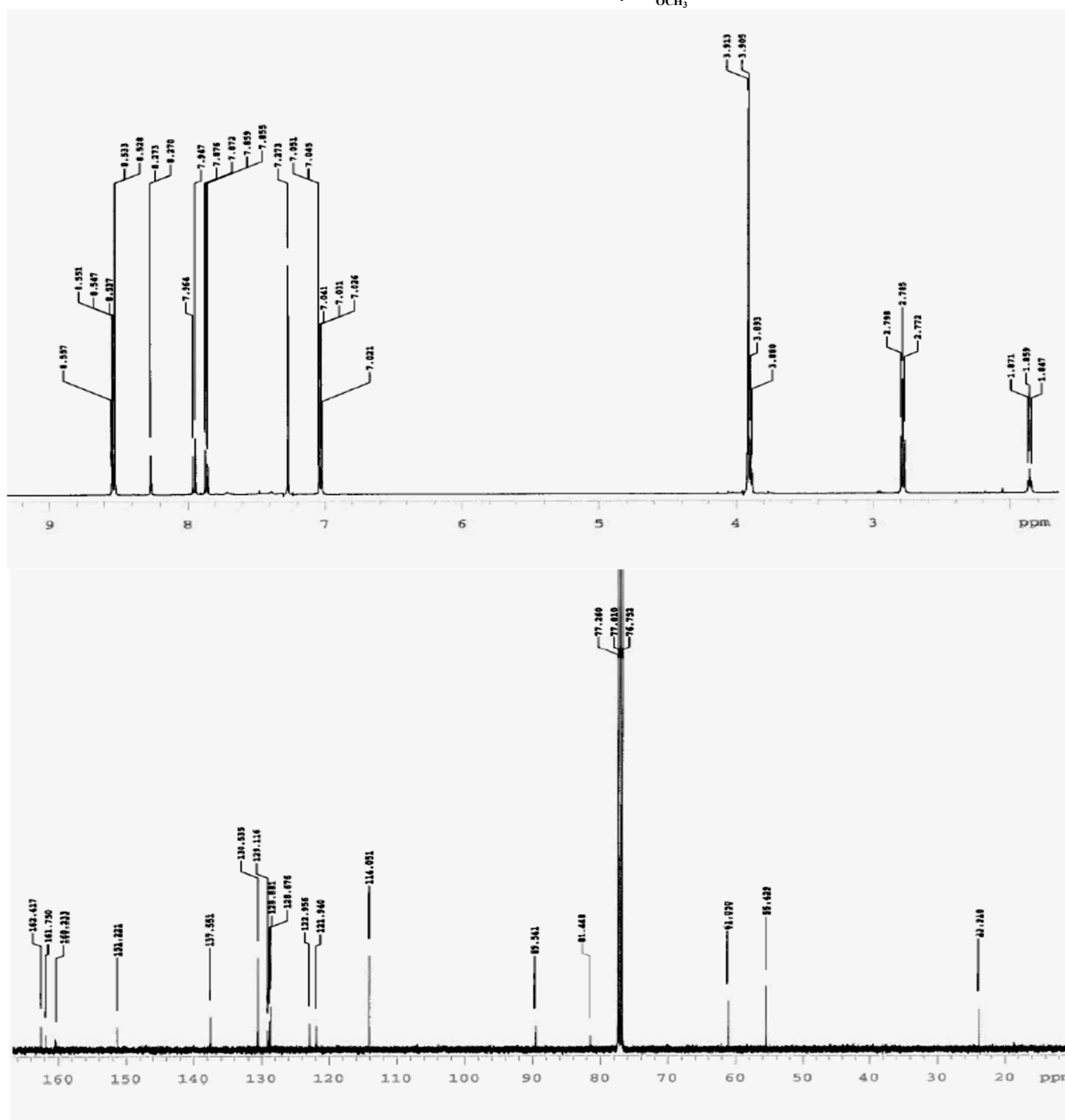
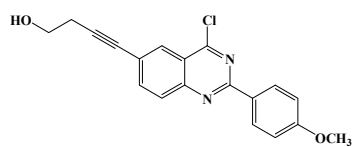
$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **4f** ( $\text{CDCl}_3$ ).

Figure S4. *Cont.*



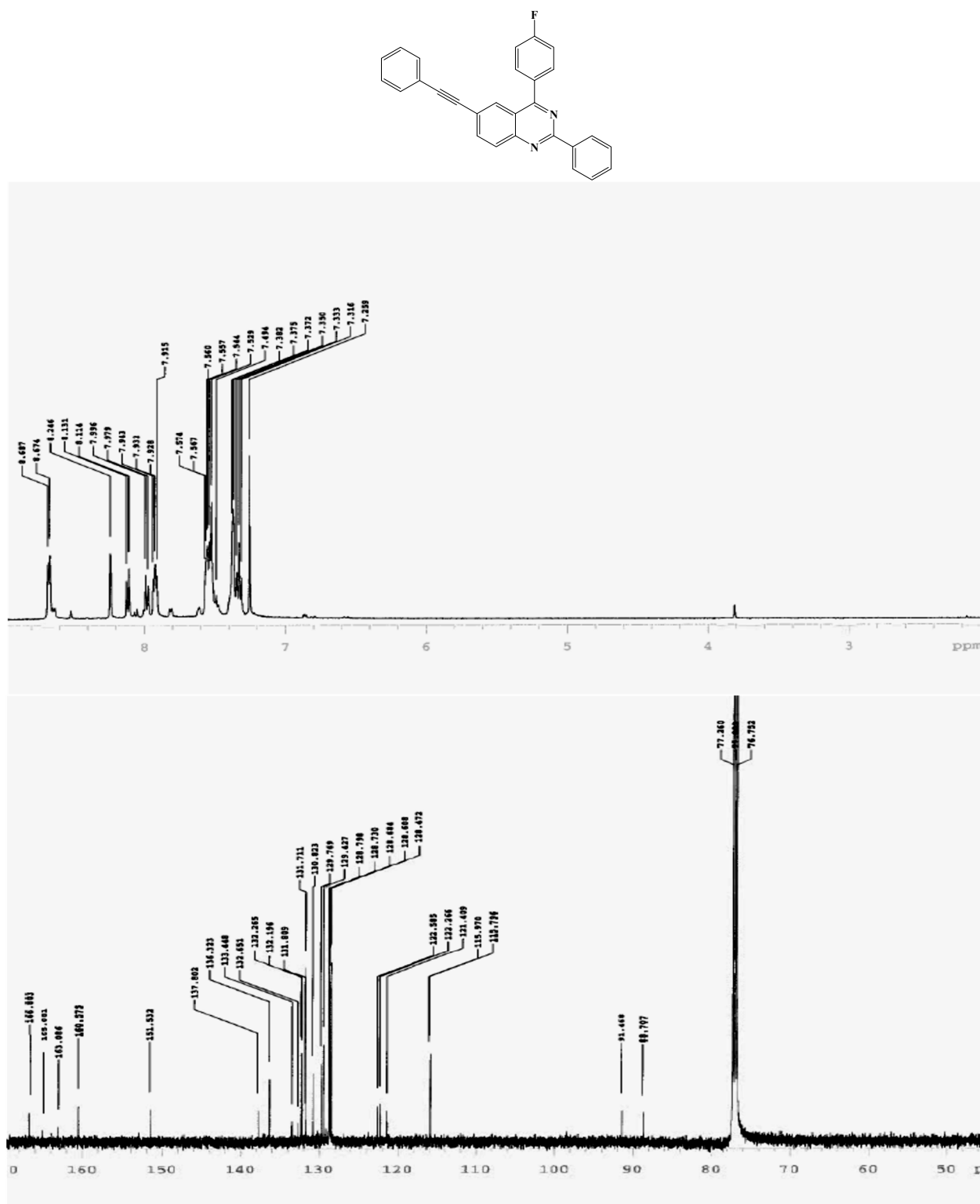
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **4g** (CDCl<sub>3</sub>).

Figure S4. *Cont.*



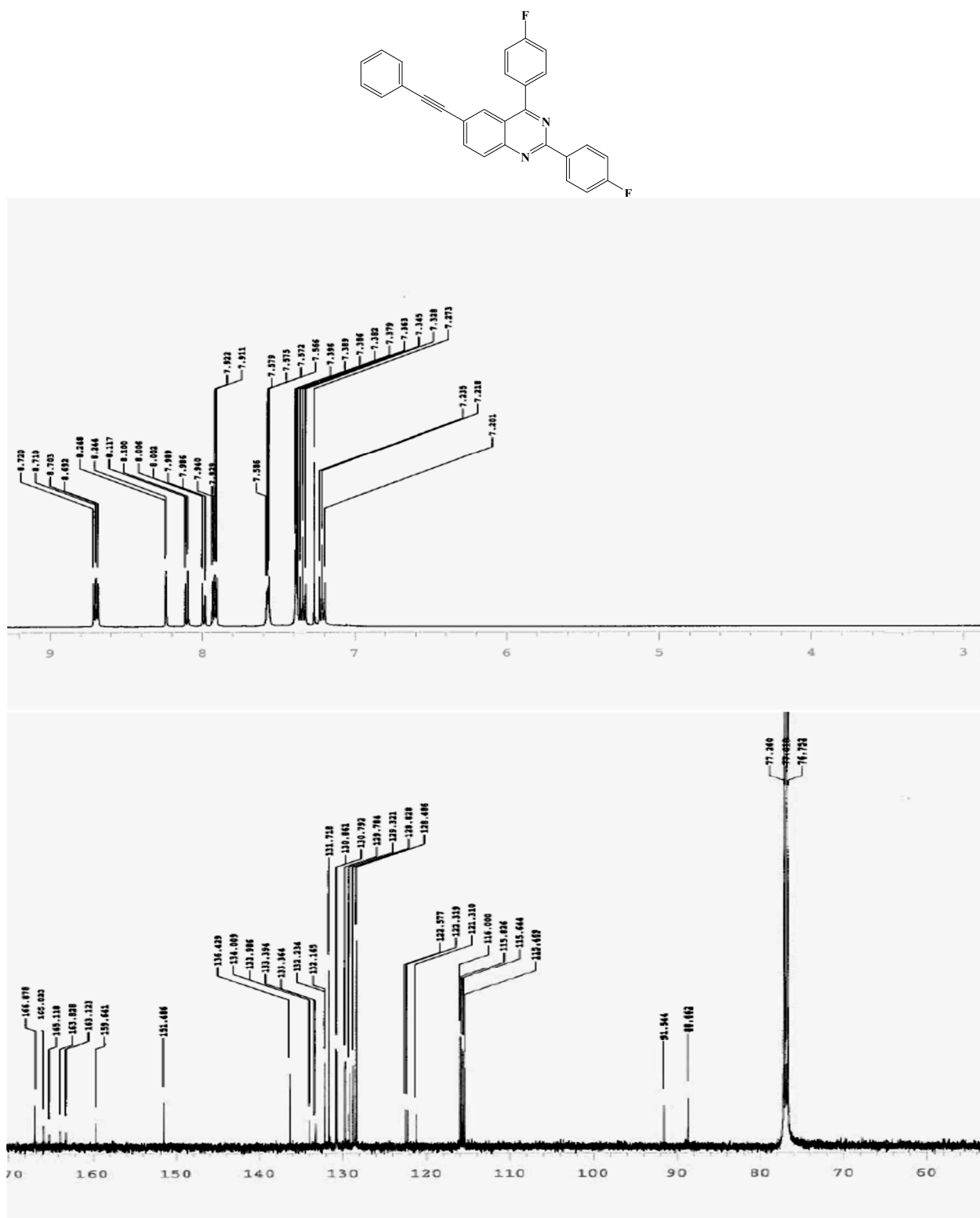
$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **4h** ( $\text{CDCl}_3$ ).

Figure S4. *Cont.*



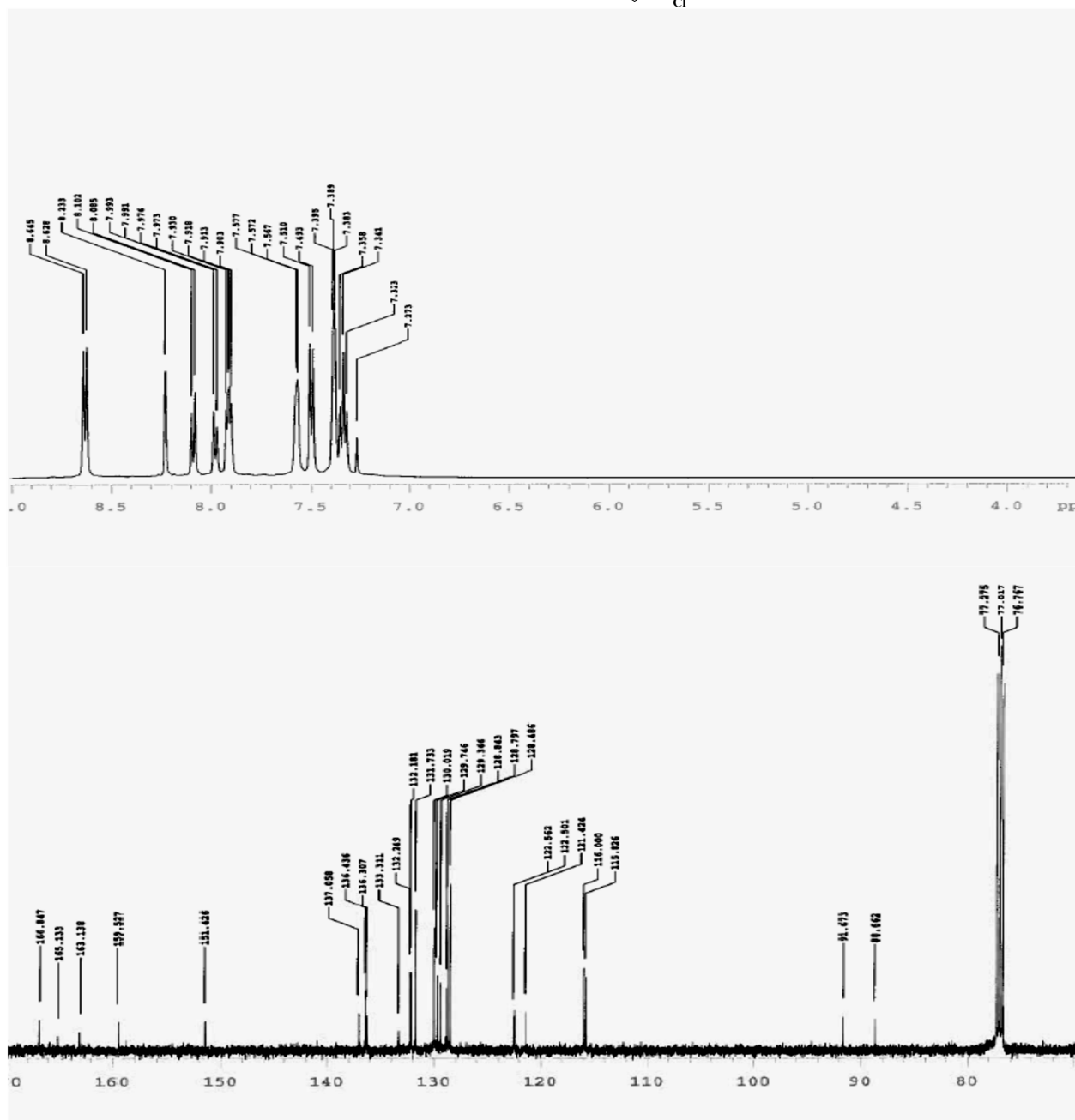
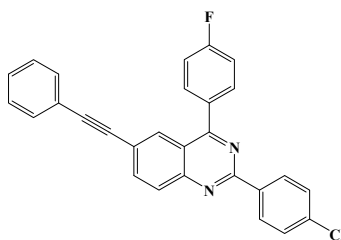
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **5a** (CDCl<sub>3</sub>).

**Figure S4.** *Cont.*



<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **5b** (CDCl<sub>3</sub>).

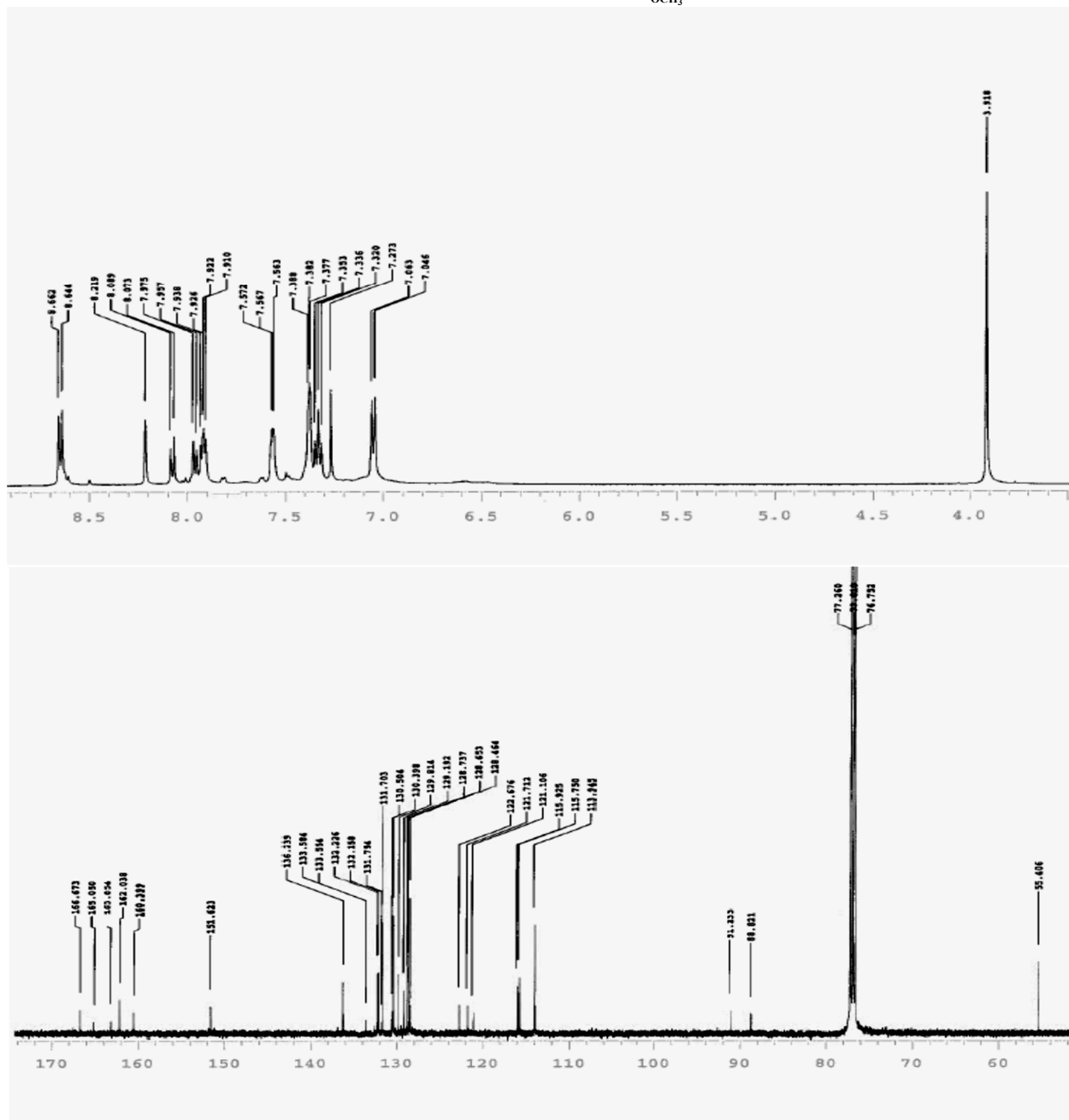
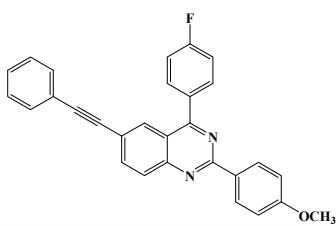
Figure S4. *Cont.*



$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **5c** ( $\text{CDCl}_3$ ).

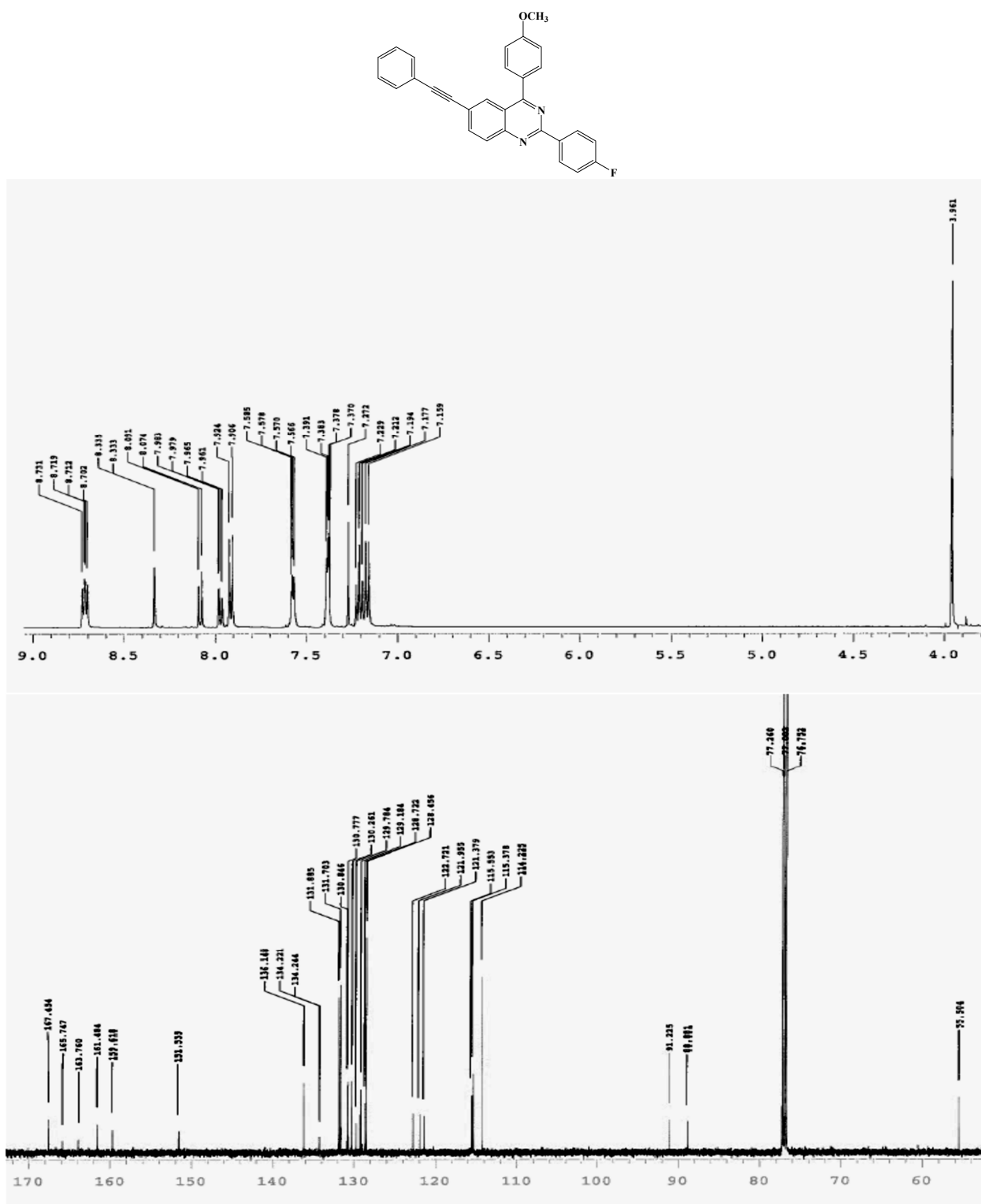
Figure S4. *Cont.*





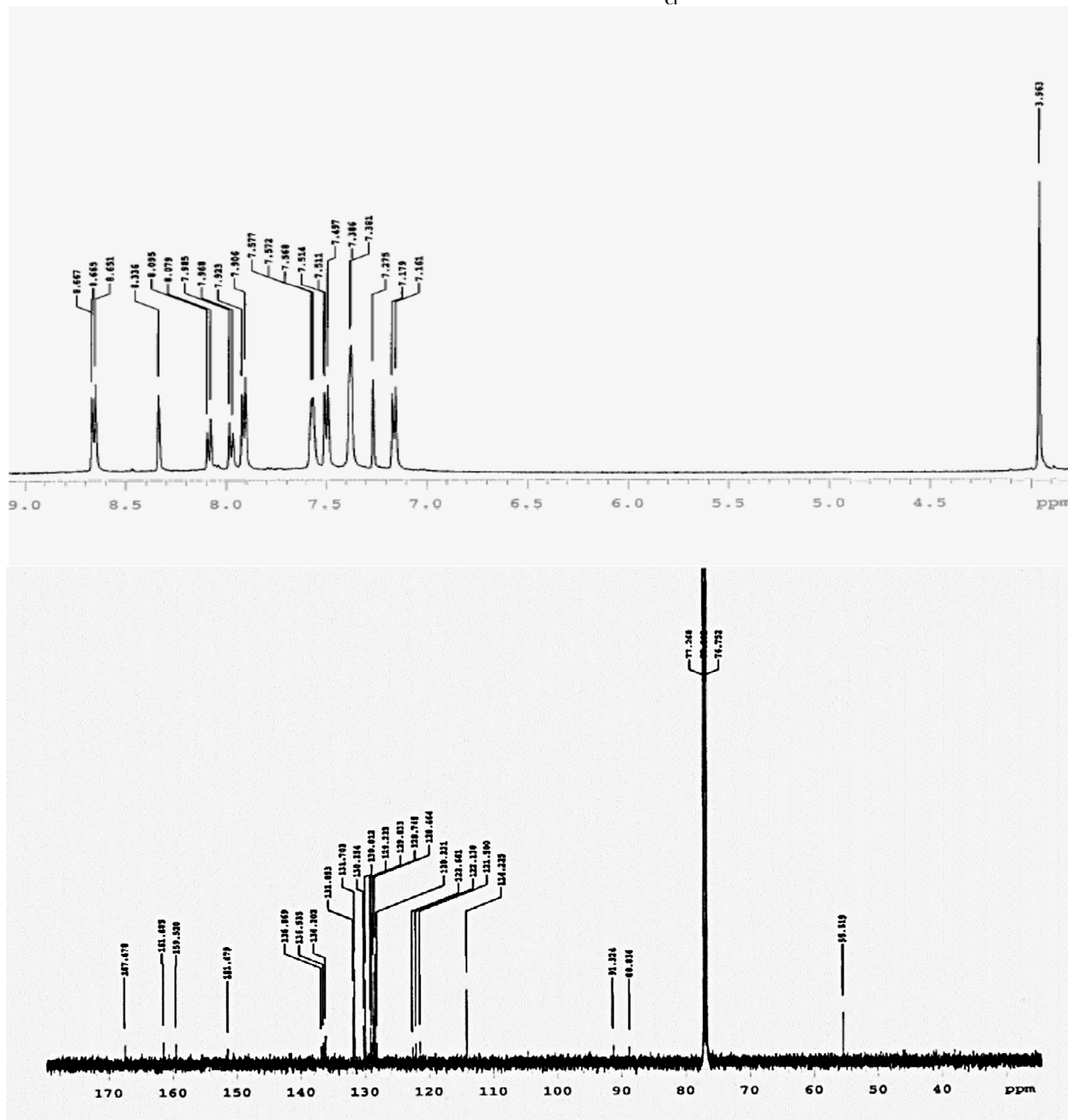
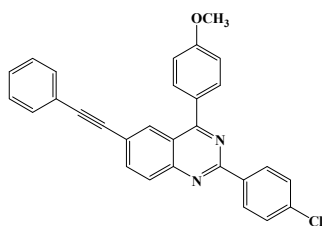
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **5d** (CDCl<sub>3</sub>).

Figure S4. *Cont.*



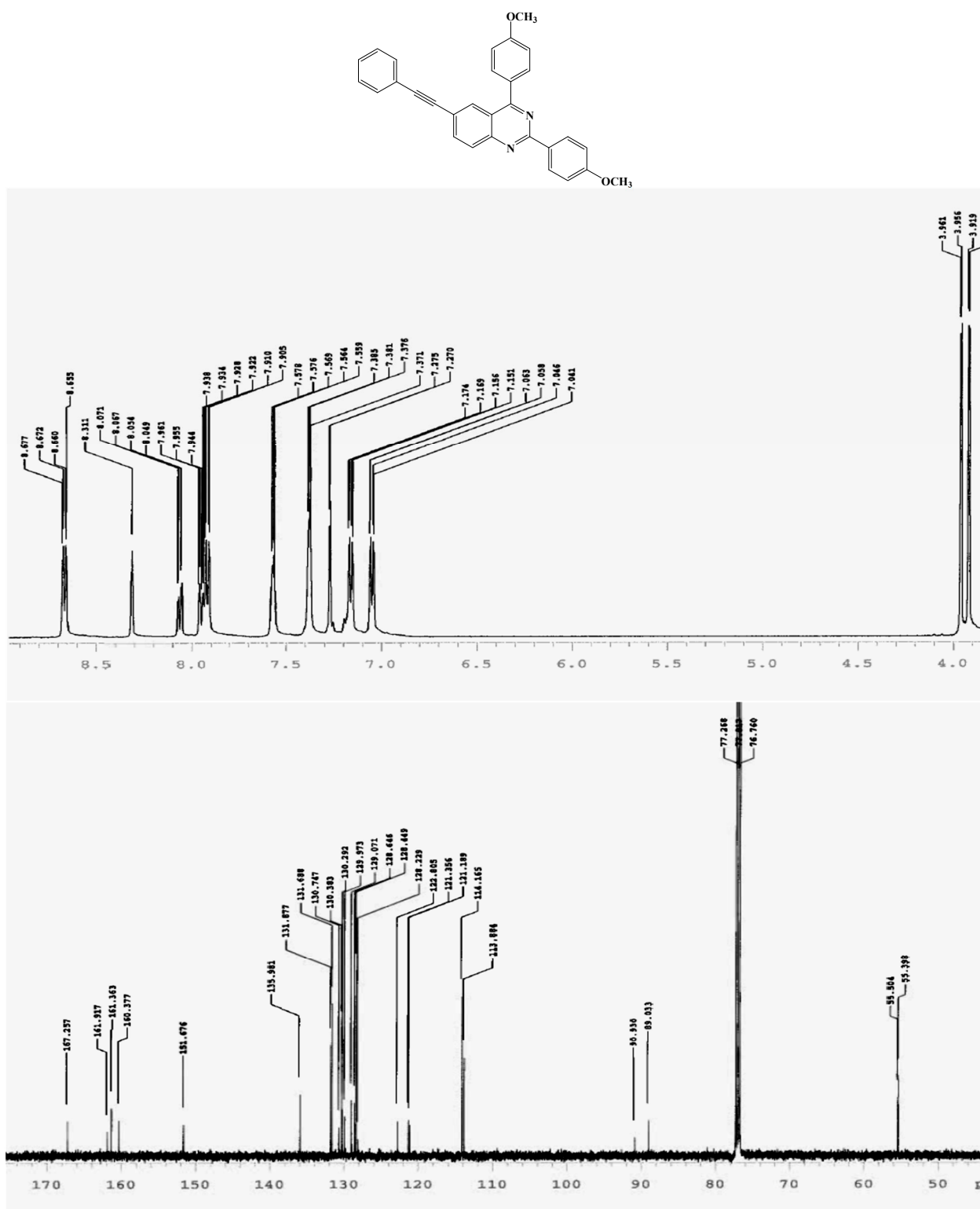
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **5e** (CDCl<sub>3</sub>).

Figure S4. *Cont.*



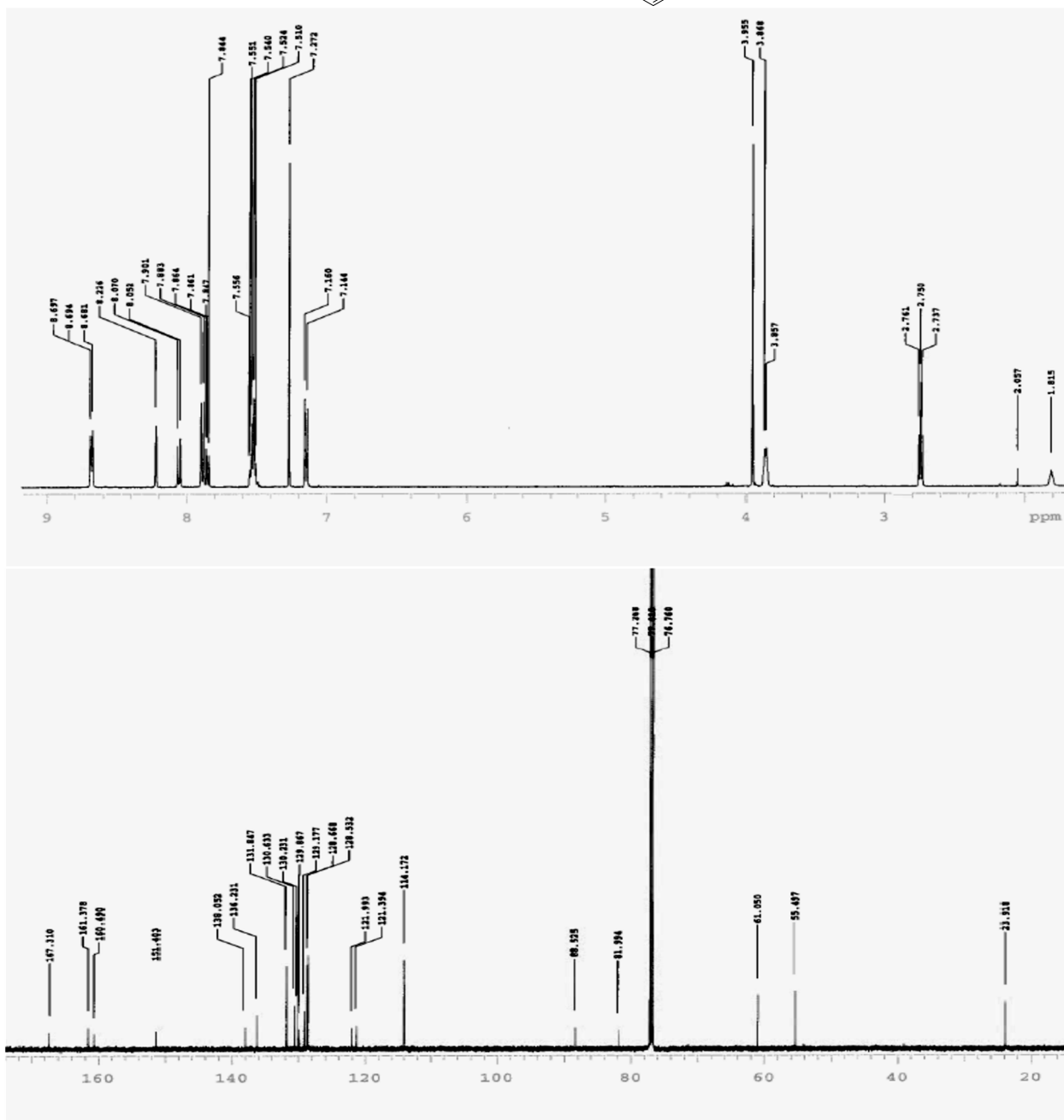
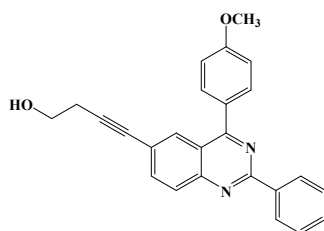
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **5f** (CDCl<sub>3</sub>).

Figure S4. *Cont.*



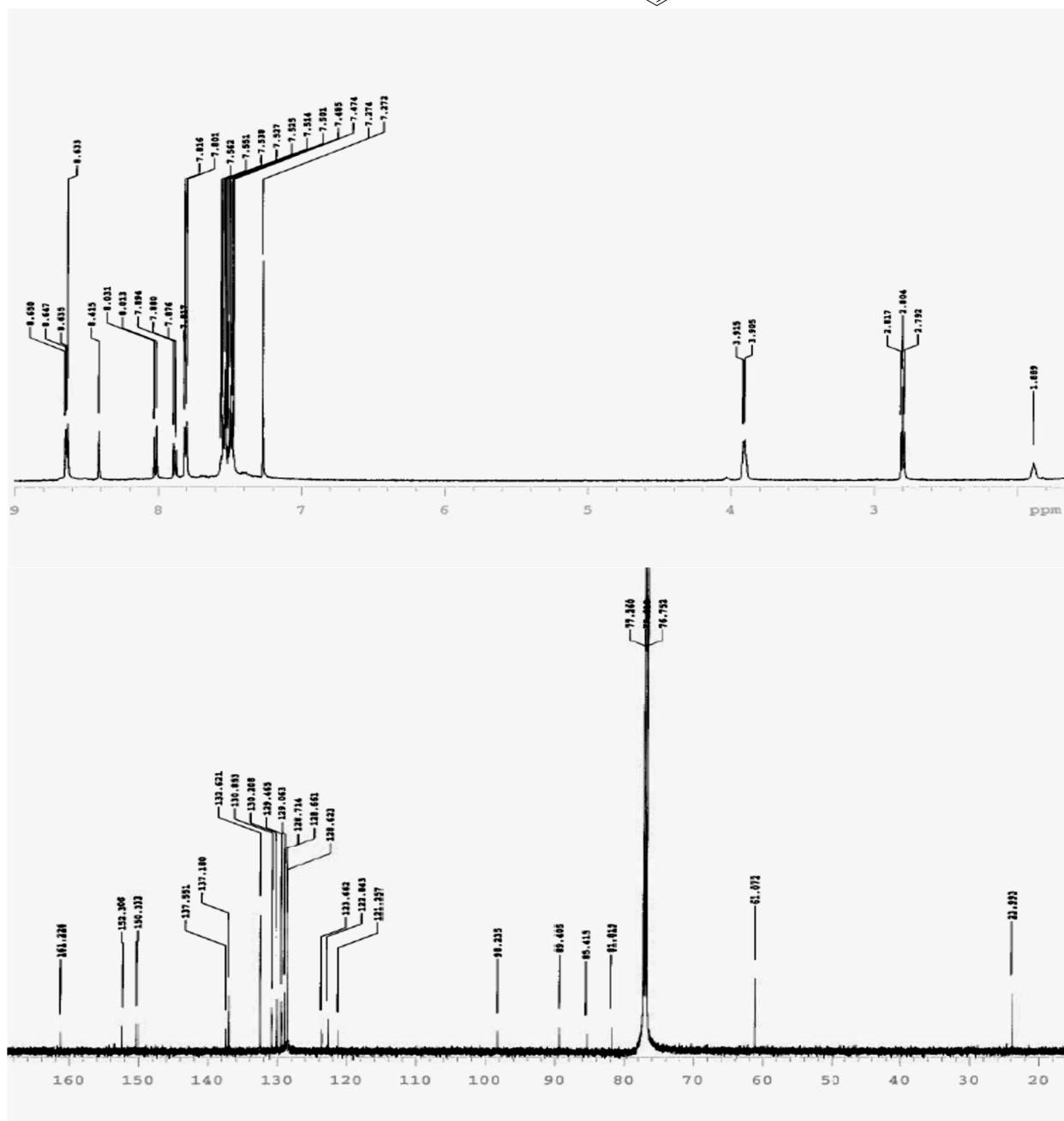
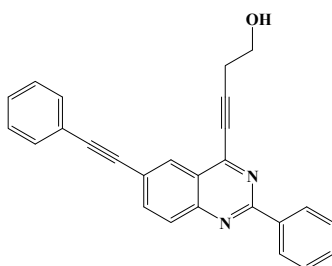
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **5g** (CDCl<sub>3</sub>).

Figure S4. *Cont.*



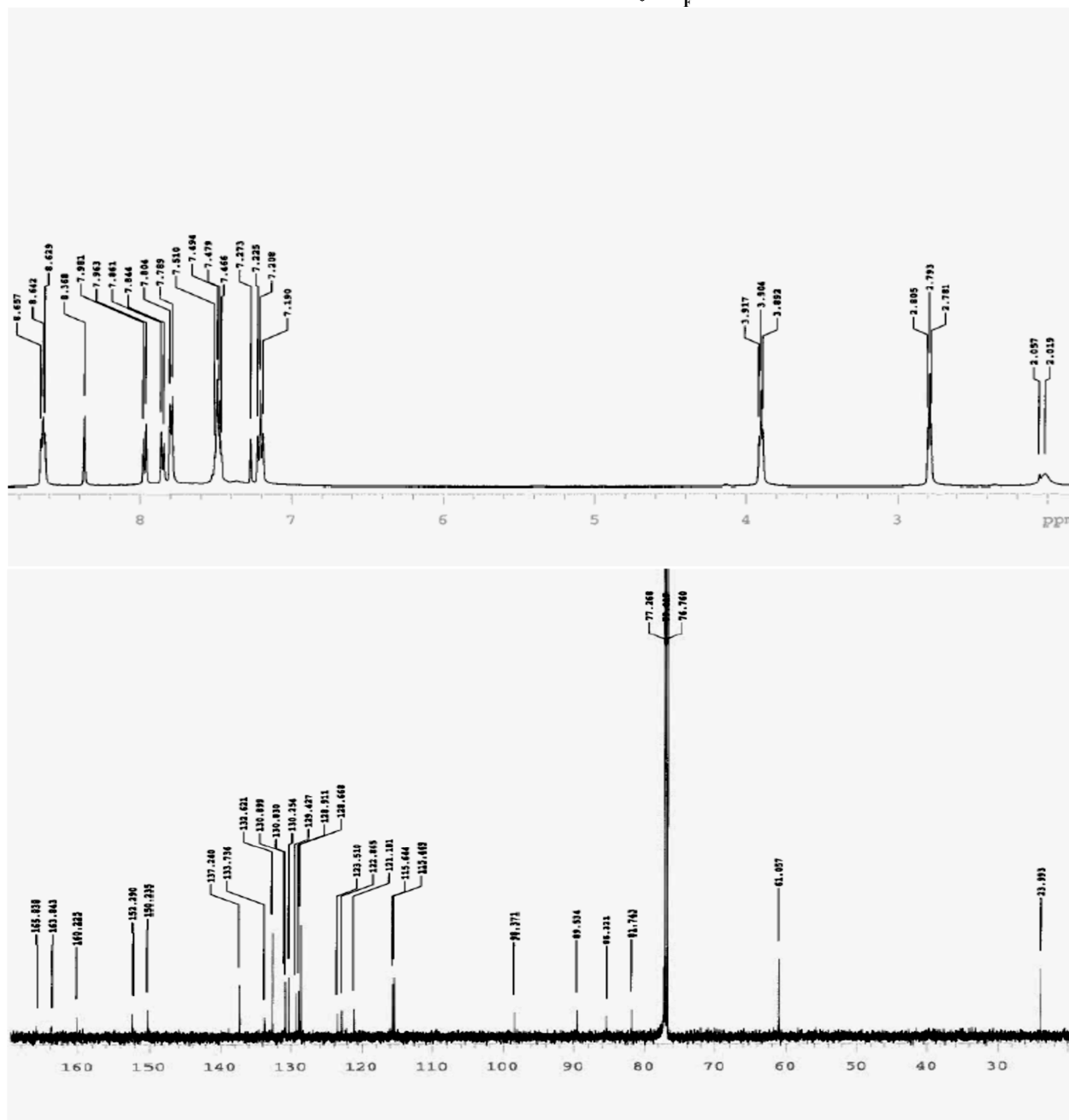
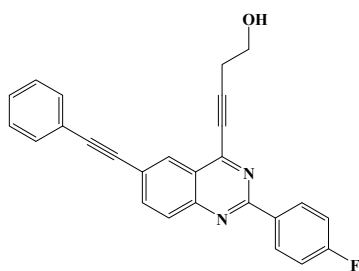
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **5h** (CDCl<sub>3</sub>).

Figure S4. *Cont.*



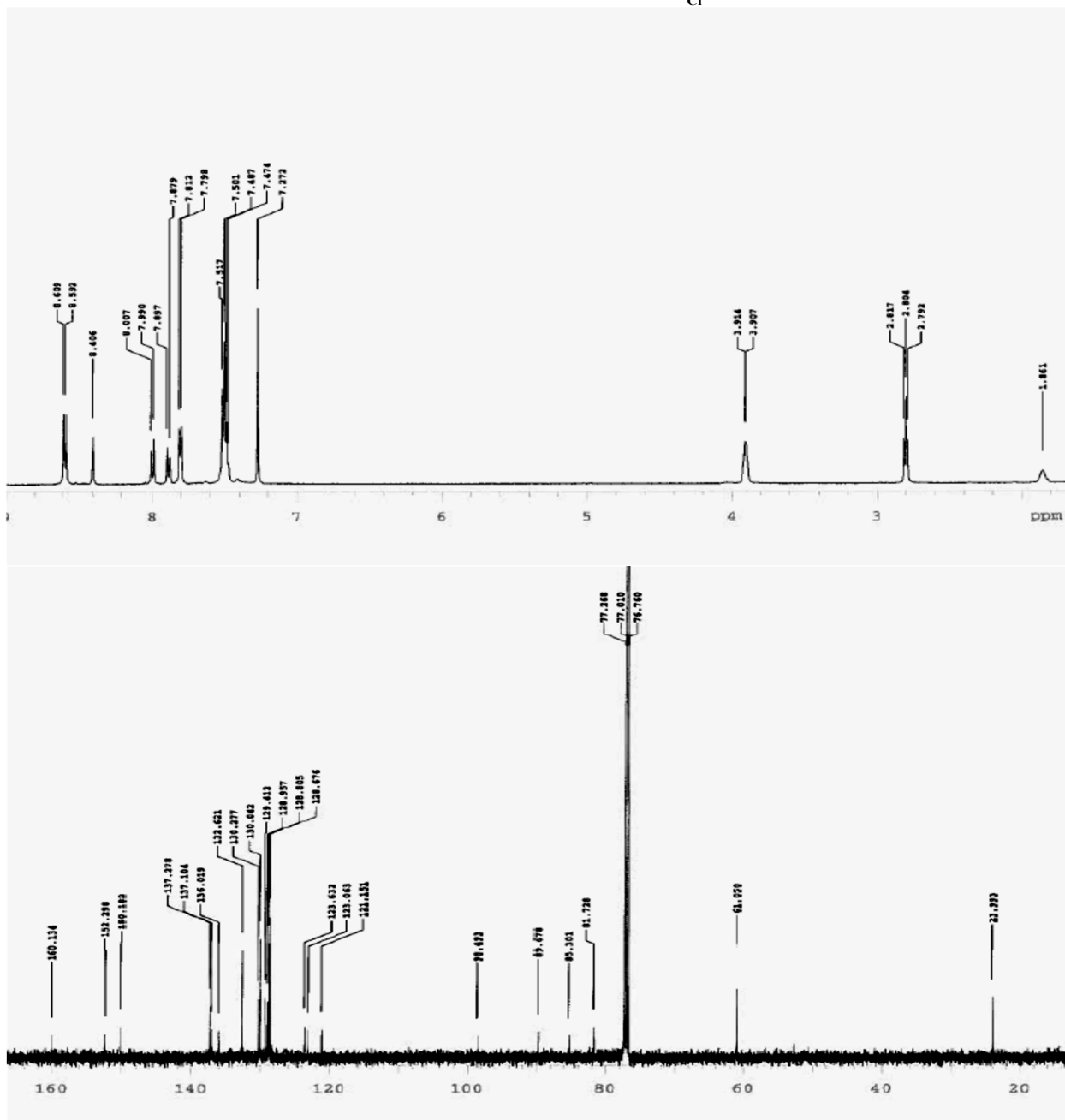
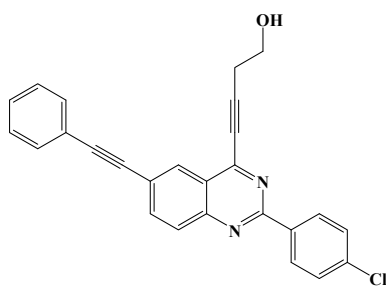
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **6a** (CDCl<sub>3</sub>).

**Figure S4.** *Cont.*



<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **6b** (CDCl<sub>3</sub>).

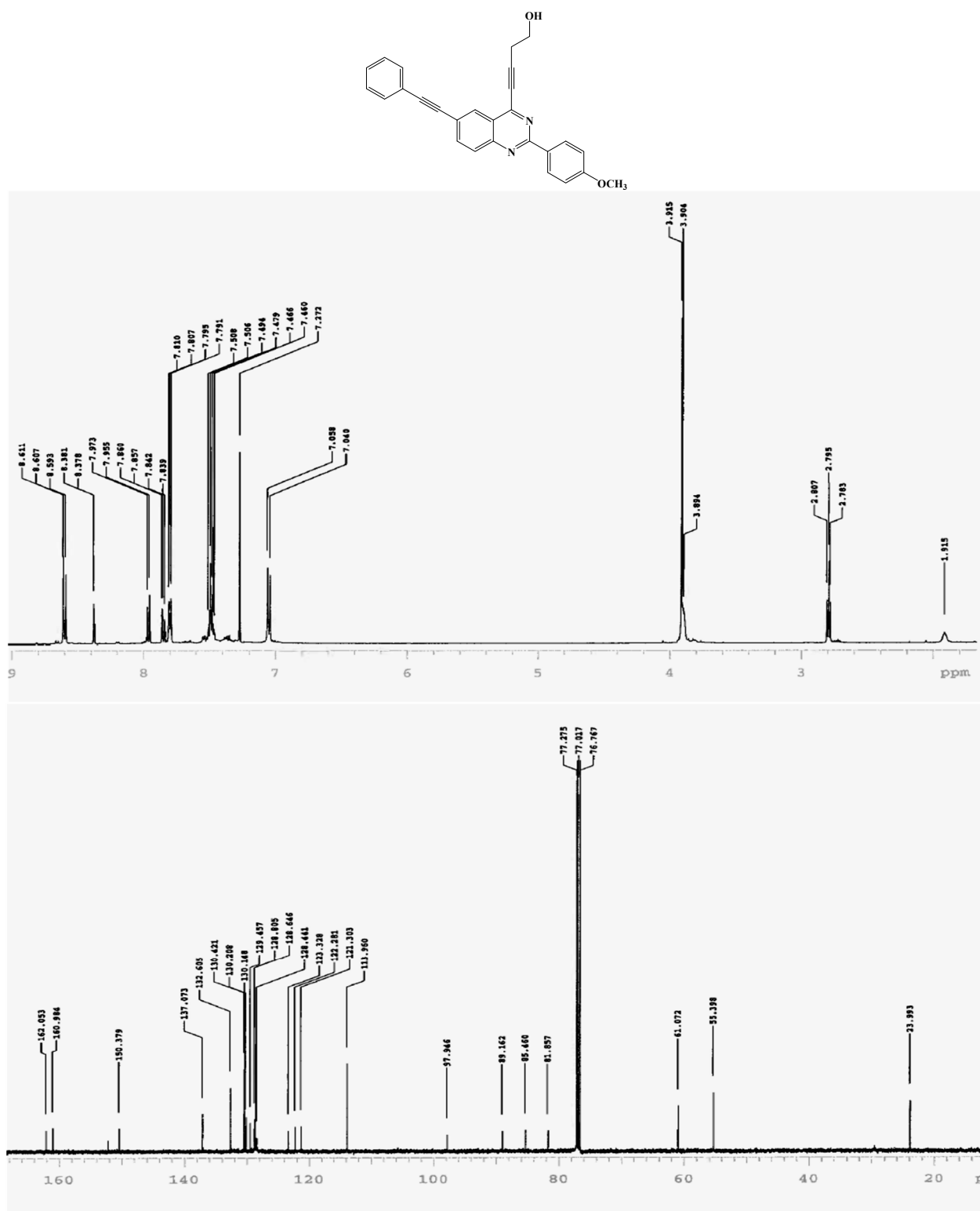
Figure S4. *Cont.*



<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **6c** (CDCl<sub>3</sub>).

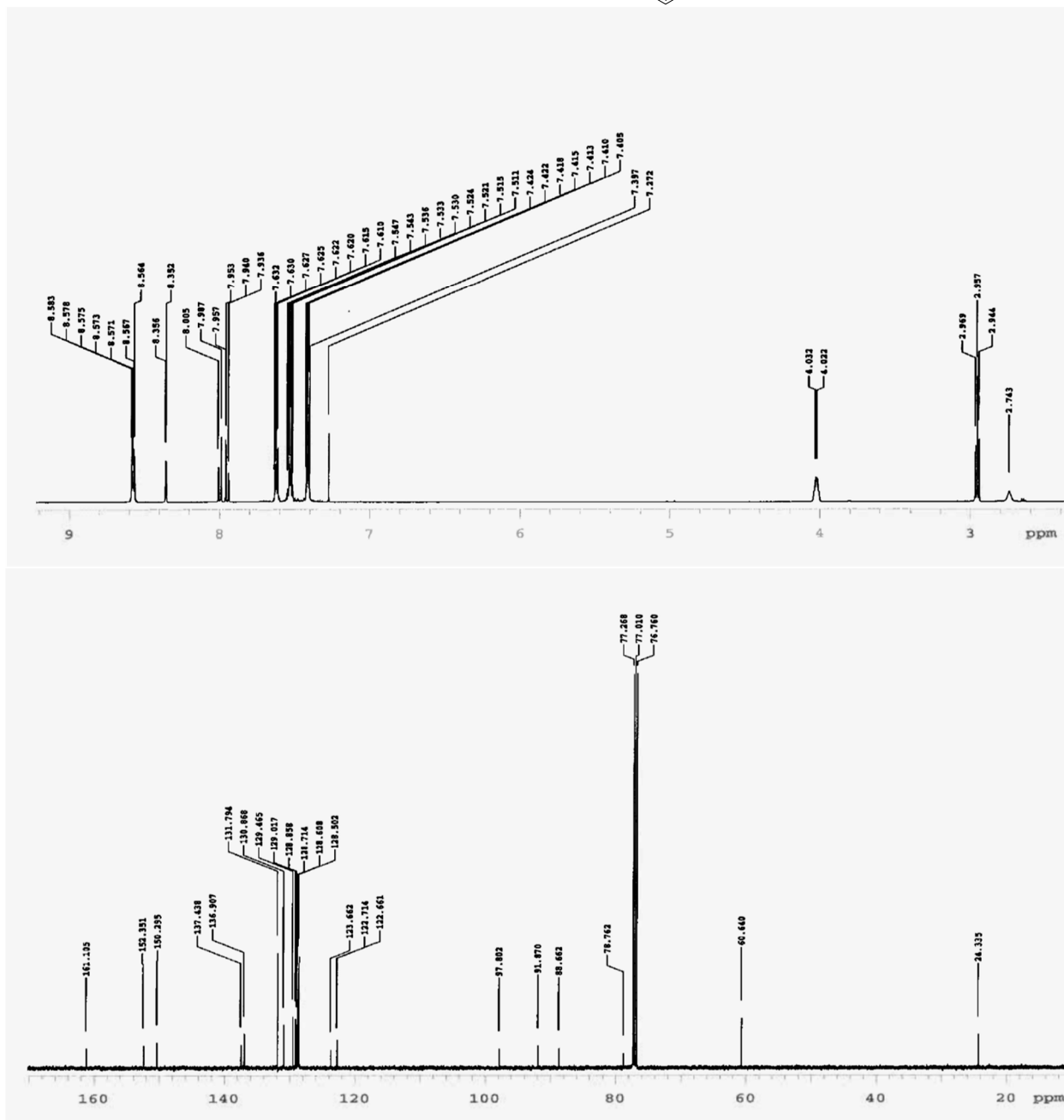
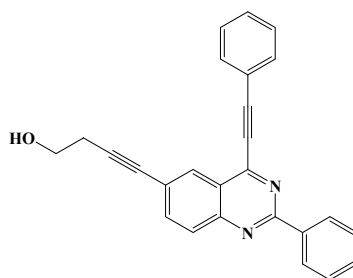
**Figure S4.** *Cont.*





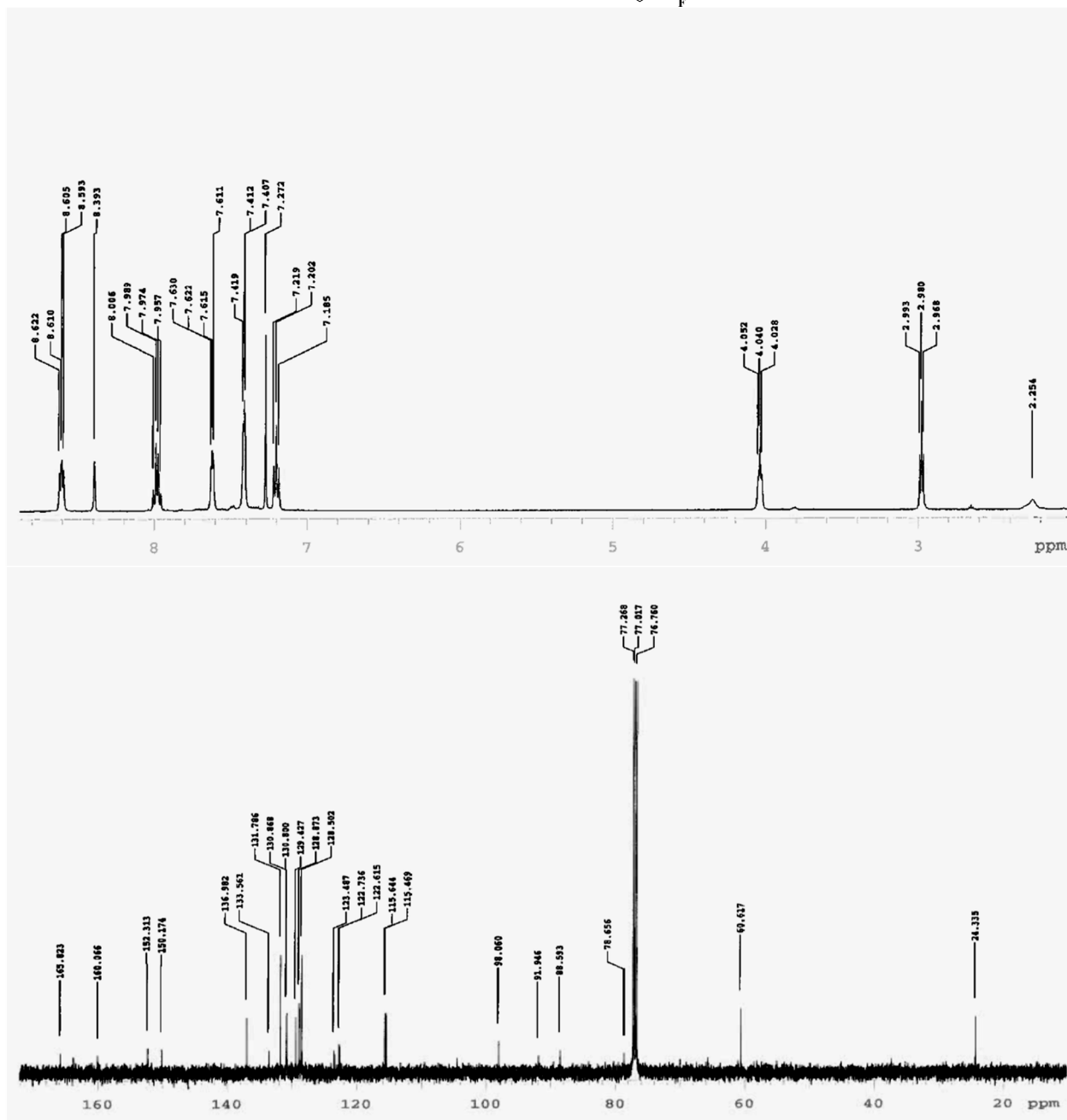
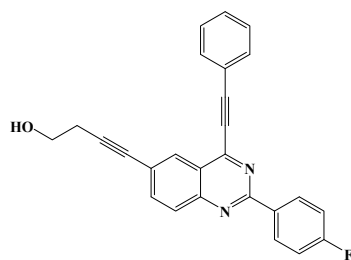
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **6d** (CDCl<sub>3</sub>).

Figure S4. *Cont.*



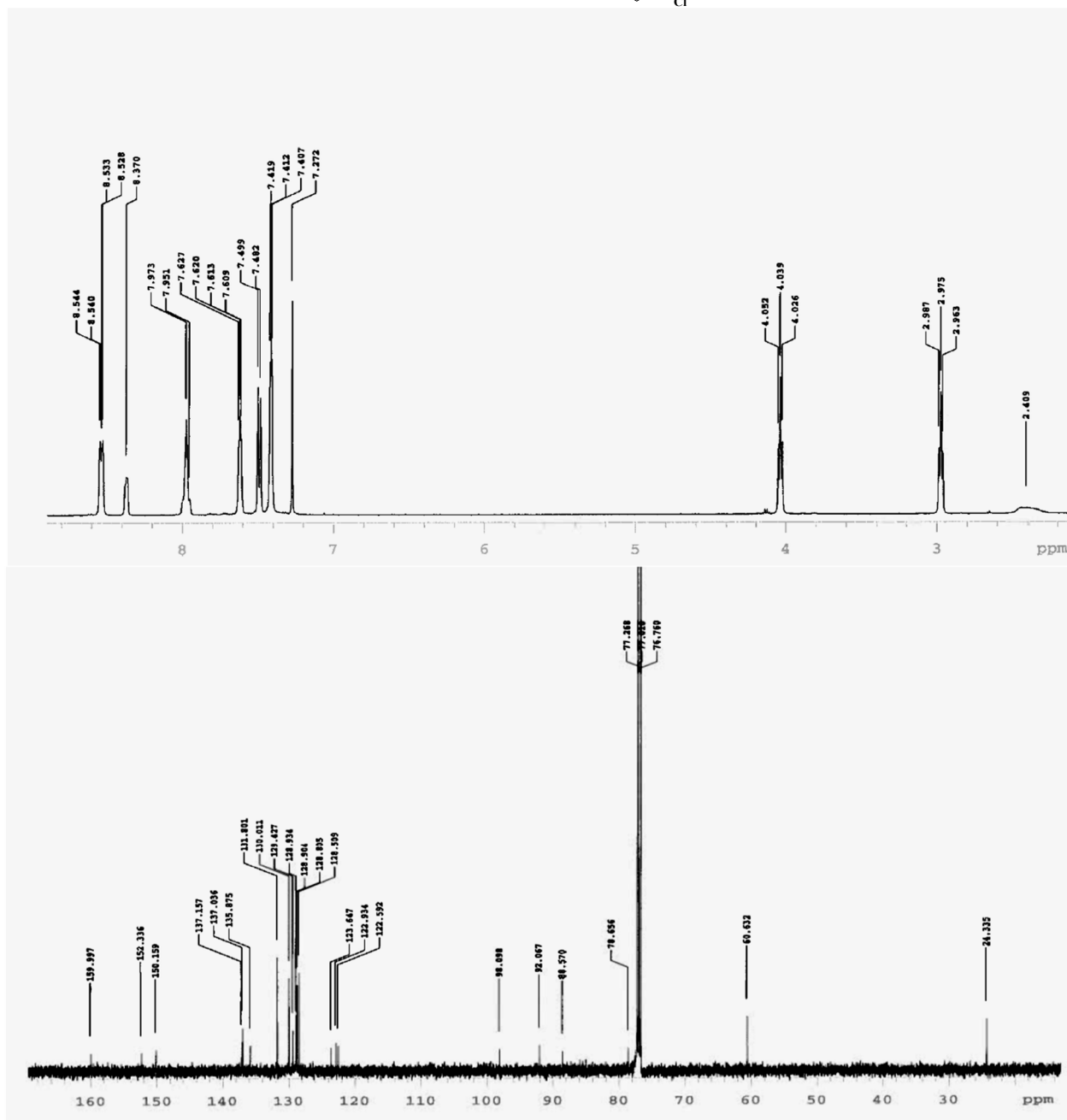
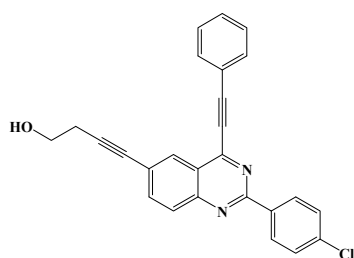
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **6e** (CDCl<sub>3</sub>).

Figure S4. Cont.



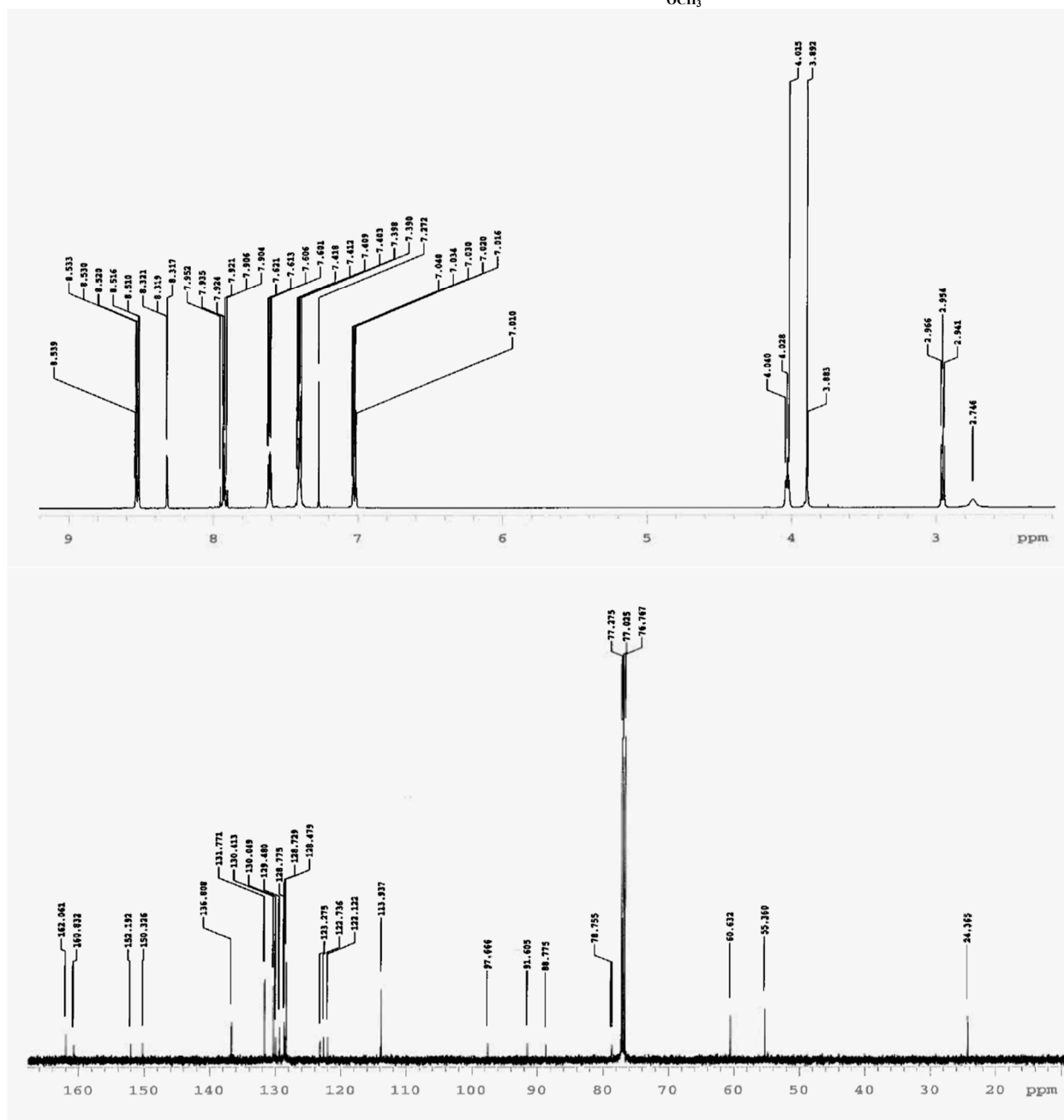
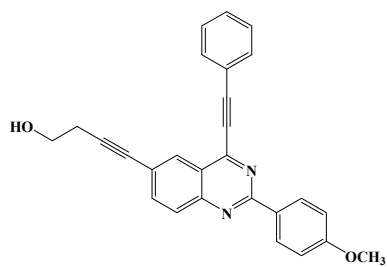
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **6f** (CDCl<sub>3</sub>).

Figure S4. *Cont.*



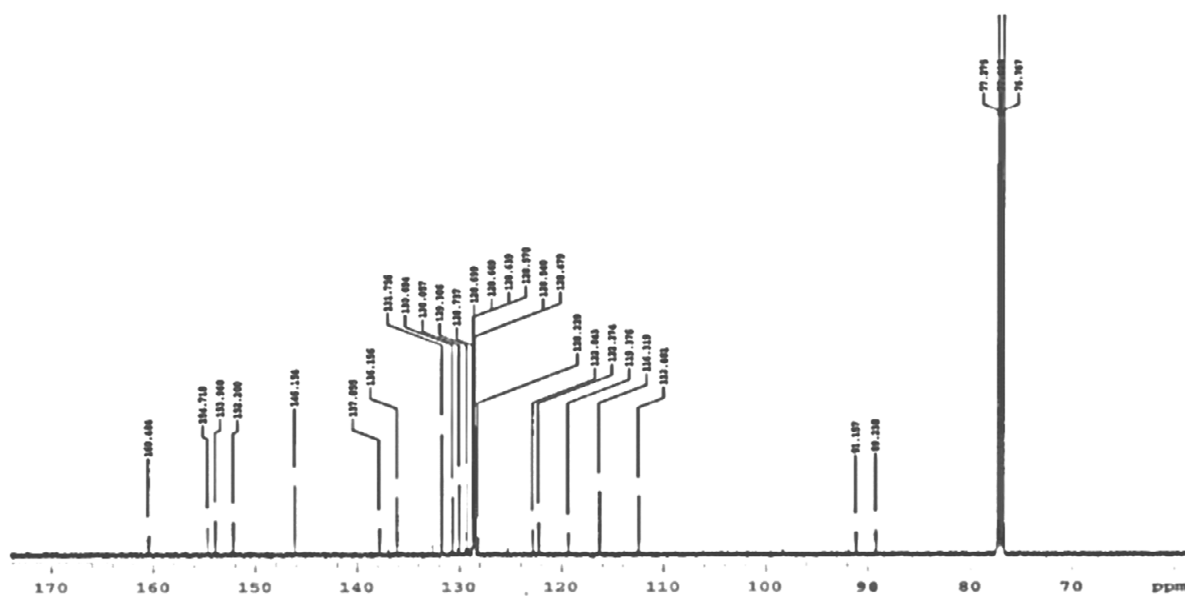
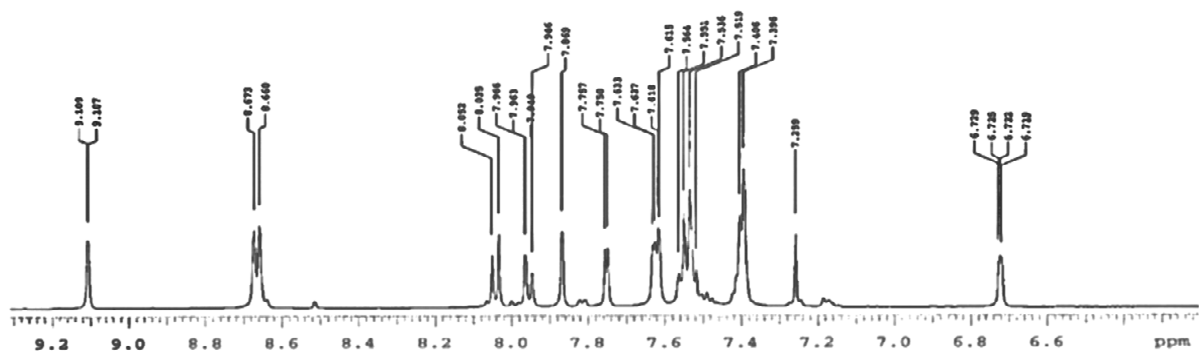
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **6g** (CDCl<sub>3</sub>).

Figure S4. *Cont.*

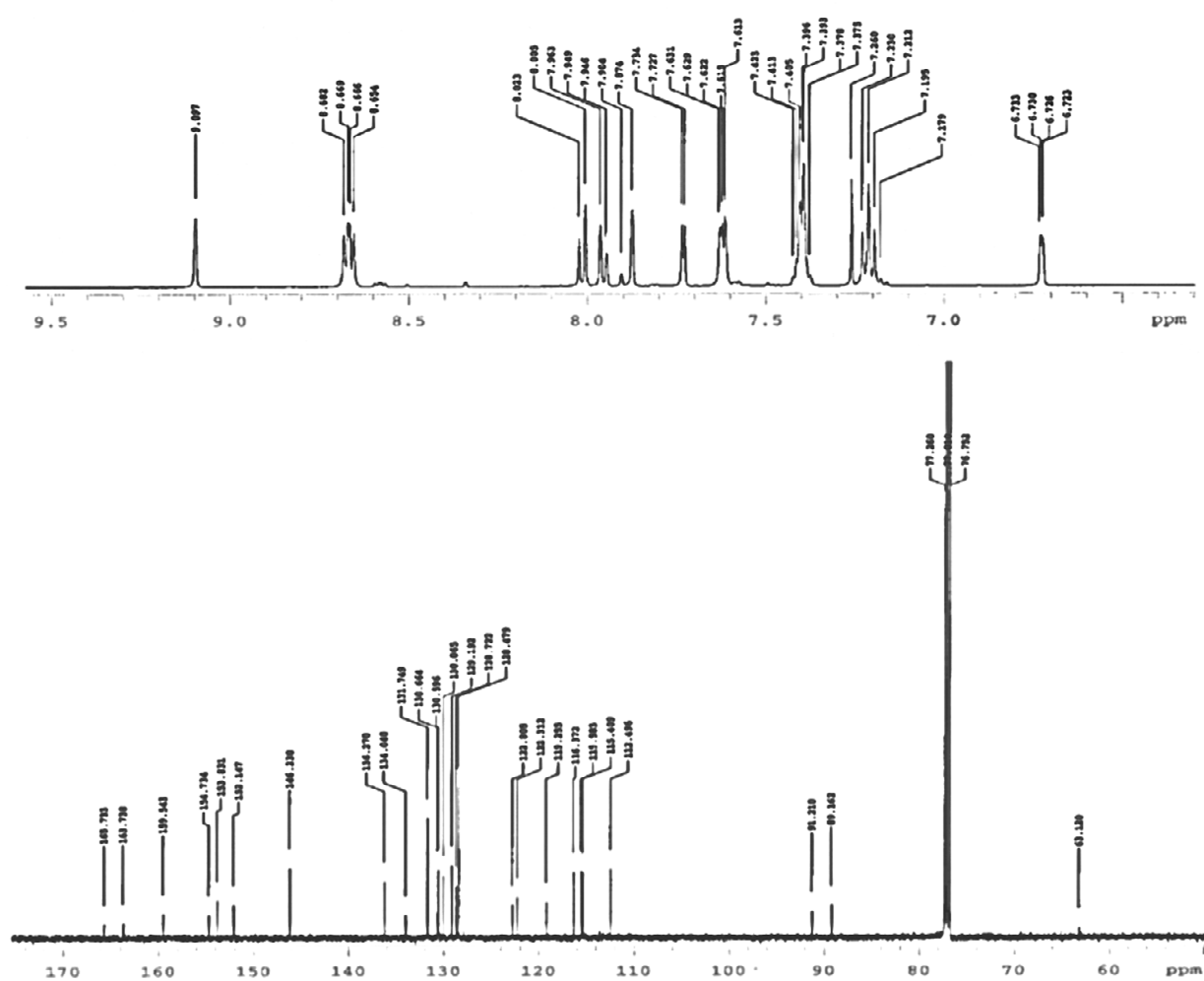
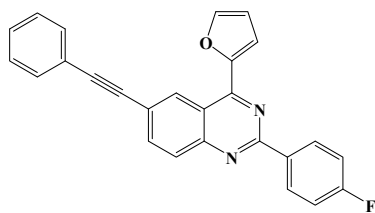


<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **6h** (CDCl<sub>3</sub>).

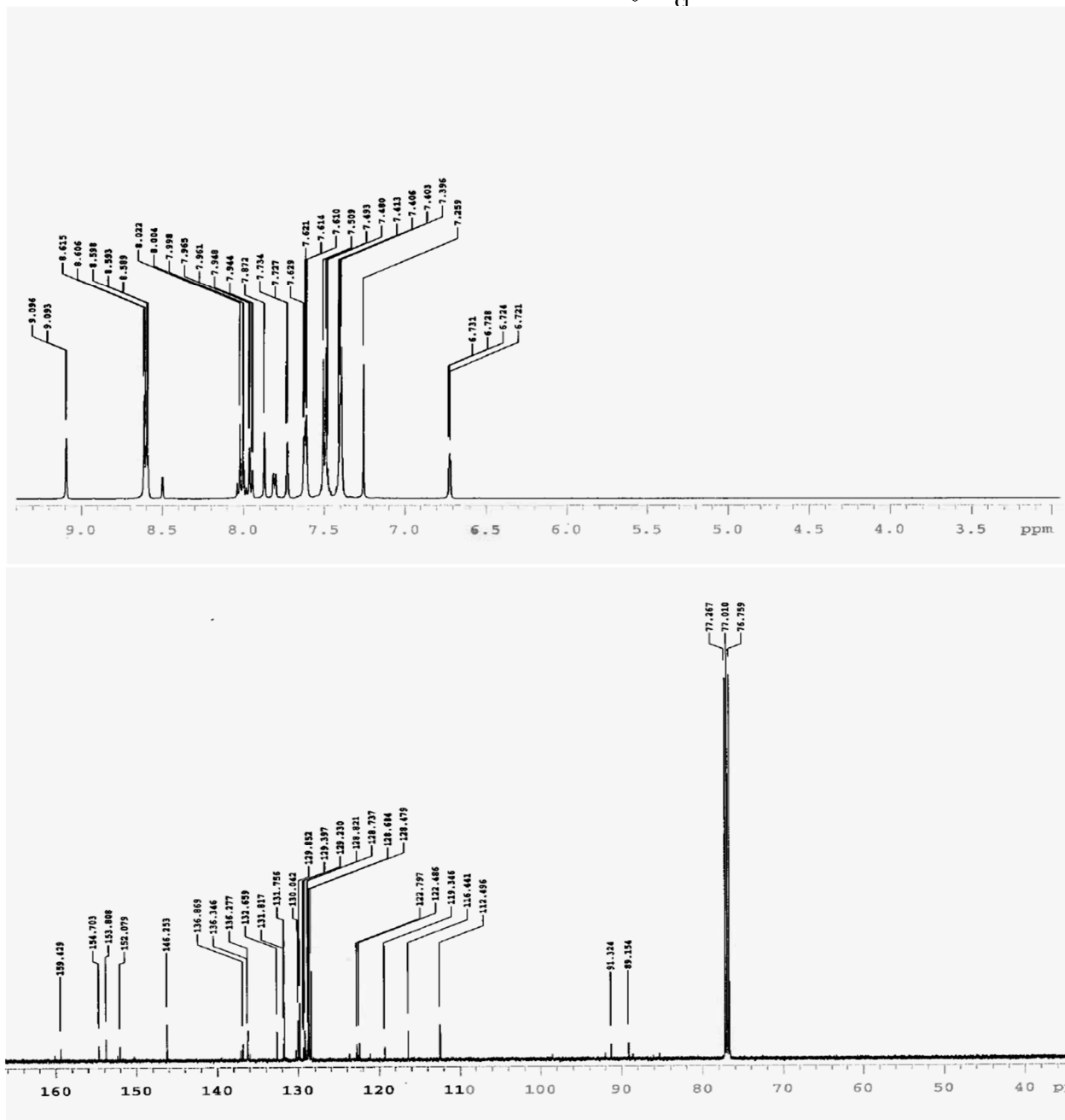
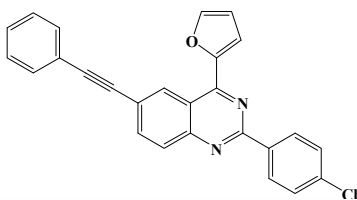
Figure S4. *Cont.*



**Figure S4. Cont.**



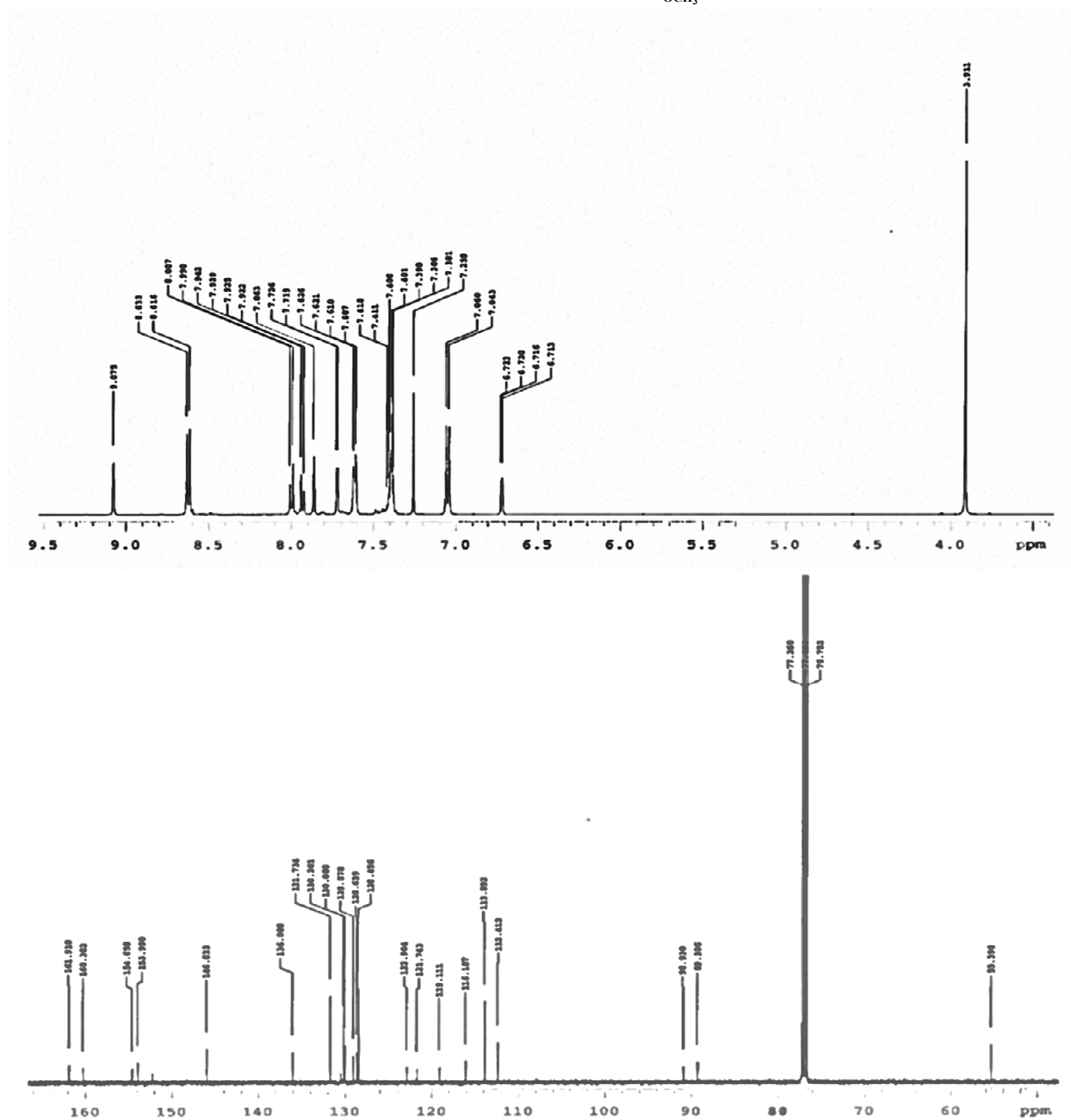
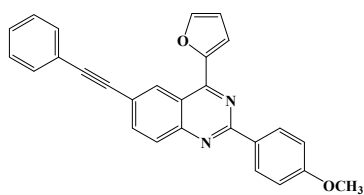
<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **7b** (CDCl<sub>3</sub>).



$^1\text{H}$ -NMR and  $^{13}\text{C}$ -NMR Spectra of **7c** ( $\text{CDCl}_3$ ).

Figure S4. *Cont.*





<sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of **7d** (CDCl<sub>3</sub>).

**Figure S4.** <sup>1</sup>H-NMR and <sup>13</sup>C-NMR Spectra of new compounds.

**Table S1.** Cartesian coordinates of optimized structures in the gas phase of compounds **5a–h**.

| <b>5a</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | -1.7090130 | -1.4105190 | 0.1102520  |
| C         | -0.8525360 | -0.3299510 | 0.0440680  |
| C         | 0.5461400  | -0.5126530 | 0.1118310  |
| C         | 1.0716860  | -1.8264390 | 0.1940300  |
| C         | 0.1789240  | -2.9238820 | 0.2802880  |
| C         | -1.1698210 | -2.7218260 | 0.2457900  |
| H         | -1.2638970 | 0.6626960  | -0.0826520 |
| C         | 1.5208000  | 0.5354230  | 0.0622110  |
| H         | 0.6076620  | -3.9161460 | 0.3579620  |
| H         | -1.8546160 | -3.5604860 | 0.3037650  |
| C         | 3.2037510  | -1.0370400 | 0.0421320  |
| N         | 2.8034270  | 0.2623160  | -0.0019700 |
| N         | 2.4036060  | -2.0706180 | 0.1714870  |
| C         | 1.1620860  | 1.9767110  | 0.0699070  |
| C         | 1.8460580  | 2.8490450  | -0.7814830 |
| C         | 0.2110930  | 2.4993210  | 0.9500420  |
| C         | 1.5679080  | 4.2065480  | -0.7829050 |
| H         | 2.6031730  | 2.4452600  | -1.4433510 |
| C         | -0.0688760 | 3.8591870  | 0.9696360  |
| H         | -0.2964290 | 1.8448530  | 1.6496030  |
| C         | 0.6103510  | 4.6883480  | 0.0947950  |
| H         | 2.0802420  | 4.8942970  | -1.4452410 |
| H         | -0.7938940 | 4.2821360  | 1.6547500  |
| C         | -3.1224800 | -1.2292270 | 0.0350950  |
| C         | -4.3211570 | -1.0871310 | -0.0276240 |
| C         | -5.7375520 | -0.9156570 | -0.1036830 |
| C         | -6.5928960 | -2.0184820 | 0.0164230  |
| C         | -6.2885260 | 0.3571740  | -0.3000620 |
| C         | -7.9671920 | -1.8481940 | -0.0585970 |
| H         | -6.1673930 | -3.0041640 | 0.1682910  |
| C         | -7.6638990 | 0.5192060  | -0.3742500 |
| H         | -5.6272380 | 1.2113100  | -0.3940170 |
| C         | -8.5065050 | -0.5809610 | -0.2538820 |
| H         | -8.6211000 | -2.7088780 | 0.0356450  |
| H         | -8.0807170 | 1.5092400  | -0.5270680 |
| H         | -9.5820930 | -0.4509550 | -0.3123360 |
| F         | 0.3388580  | 6.0015640  | 0.1020220  |
| C         | 4.6637120  | -1.2836370 | -0.0433970 |
| C         | 5.1536490  | -2.5918450 | -0.0490600 |
| C         | 5.5613800  | -0.2171780 | -0.1208500 |
| C         | 6.5177470  | -2.8274560 | -0.1323500 |
| H         | 4.4474150  | -3.4109000 | 0.0127260  |
| C         | 6.9262730  | -0.4567540 | -0.2040330 |
| H         | 5.1728600  | 0.7936530  | -0.1111190 |
| C         | 7.4081420  | -1.7608870 | -0.2104850 |
| H         | 6.8891830  | -3.8471400 | -0.1368650 |
| H         | 7.6168450  | 0.3783930  | -0.2624110 |
| H         | 8.4755640  | -1.9466040 | -0.2755340 |

**Table S1. Cont.**

| <b>5b</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | -1.9775040 | -1.4181700 | 0.1172610  |
| C         | -1.1635150 | -0.3051880 | 0.0516420  |
| C         | 0.2409240  | -0.4329290 | 0.1246210  |
| C         | 0.8170850  | -1.7250730 | 0.2120900  |
| C         | -0.0323780 | -2.8562340 | 0.2977410  |
| C         | -1.3879180 | -2.7070110 | 0.2578020  |
| H         | -1.6129610 | 0.6703170  | -0.0788050 |
| C         | 1.1732910  | 0.6529210  | 0.0751270  |
| H         | 0.4341280  | -3.8309660 | 0.3795950  |
| H         | -2.0395450 | -3.5717120 | 0.3153820  |
| C         | 2.9162220  | -0.8519590 | 0.0666360  |
| N         | 2.4661640  | 0.4306510  | 0.0166230  |
| N         | 2.1578760  | -1.9165490 | 0.1954740  |
| C         | 0.7575040  | 2.0786280  | 0.0764800  |
| C         | 1.4062400  | 2.9742930  | -0.7781800 |
| C         | -0.2142420 | 2.5661360  | 0.9541960  |
| C         | 1.0739410  | 4.3195730  | -0.7850590 |
| H         | 2.1787550  | 2.5989340  | -1.4390090 |
| C         | -0.5483080 | 3.9137080  | 0.9684200  |
| H         | -0.6957120 | 1.8946110  | 1.6560120  |
| C         | 0.0975660  | 4.7661070  | 0.0905460  |
| H         | 1.5584770  | 5.0245180  | -1.4502140 |
| H         | -1.2899950 | 4.3099900  | 1.6516160  |
| C         | -3.3965510 | -1.2917810 | 0.0363490  |
| C         | -4.5994080 | -1.1946120 | -0.0316510 |
| C         | -6.0207590 | -1.0749080 | -0.1139070 |
| C         | -6.8358120 | -2.2089550 | -0.0052310 |
| C         | -6.6167220 | 0.1783250  | -0.3049450 |
| C         | -8.2150400 | -2.0883180 | -0.0861270 |
| H         | -6.3754310 | -3.1794840 | 0.1424530  |
| C         | -7.9966900 | 0.2906500  | -0.3849880 |
| H         | -5.9865460 | 1.0565630  | -0.3901200 |
| C         | -8.7991730 | -0.8402760 | -0.2759160 |
| H         | -8.8375990 | -2.9728310 | -0.0007630 |
| H         | -8.4486230 | 1.2658030  | -0.5335780 |
| H         | -9.8784860 | -0.7491190 | -0.3389510 |
| F         | -0.2262890 | 6.0671720  | 0.0926690  |
| C         | 4.3834640  | -1.0400390 | -0.0113110 |
| C         | 4.9269490  | -2.3277410 | -0.0093560 |
| C         | 5.2394610  | 0.0609870  | -0.0890970 |
| C         | 6.2973490  | -2.5174470 | -0.0851580 |
| H         | 4.2545030  | -3.1745180 | 0.0527220  |
| C         | 6.6131120  | -0.1148720 | -0.1654960 |
| H         | 4.8114020  | 1.0555610  | -0.0853340 |
| C         | 7.1182210  | -1.4038410 | -0.1625710 |
| H         | 6.7384620  | -3.5072700 | -0.0859270 |
| H         | 7.2943550  | 0.7257920  | -0.2248360 |
| F         | 8.4465870  | -1.5812550 | -0.2364960 |

**Table S1. Cont.**

| <b>5c</b> |             |            |            |
|-----------|-------------|------------|------------|
| C         | -2.2691240  | -1.4282850 | 0.1217220  |
| C         | -1.4888970  | -0.2913540 | 0.0562870  |
| C         | -0.0815110  | -0.3764790 | 0.1343750  |
| C         | 0.5325690   | -1.6507130 | 0.2269900  |
| C         | -0.2823510  | -2.8068590 | 0.3120350  |
| C         | -1.6416530  | -2.6985680 | 0.2670900  |
| H         | -1.9671630  | 0.6697570  | -0.0782320 |
| C         | 0.8172920   | 0.7372990  | 0.0853040  |
| H         | 0.2130200   | -3.7668980 | 0.3976780  |
| H         | -2.2671760  | -3.5823250 | 0.3243810  |
| C         | 2.6037890   | -0.7143000 | 0.0873820  |
| N         | 2.1167600   | 0.5537090  | 0.0320790  |
| N         | 1.8788910   | -1.8013580 | 0.2155950  |
| C         | 0.3587420   | 2.1496030  | 0.0811180  |
| C         | 0.9837490   | 3.0621200  | -0.7734940 |
| C         | -0.6307660  | 2.6099220  | 0.9536870  |
| C         | 0.6111050   | 4.3966880  | -0.7854440 |
| H         | 1.7697380   | 2.7086460  | -1.4305020 |
| C         | -1.0051850  | 3.9468490  | 0.9628570  |
| H         | -1.0946020  | 1.9262770  | 1.6556740  |
| C         | -0.3817580  | 4.8159840  | 0.0851340  |
| H         | 1.0767750   | 5.1141330  | -1.4506960 |
| H         | -1.7610840  | 4.3224150  | 1.6421490  |
| C         | -3.6909410  | -1.3443170 | 0.0357410  |
| C         | -4.8958260  | -1.2816990 | -0.0364530 |
| C         | -6.3196850  | -1.2017810 | -0.1235520 |
| C         | -6.9500430  | 0.0360450  | -0.3042150 |
| C         | -7.1025650  | -2.3595600 | -0.0298680 |
| C         | -8.3323270  | 0.1101370  | -0.3887110 |
| H         | -6.3446940  | 0.9326030  | -0.3777920 |
| C         | -8.4843250  | -2.2771070 | -0.1152190 |
| H         | -6.6154680  | -3.3181610 | 0.1097630  |
| C         | -9.1027910  | -1.0441390 | -0.2945300 |
| H         | -8.8111390  | 1.0735910  | -0.5291150 |
| H         | -9.0819450  | -3.1796720 | -0.0415270 |
| H         | -10.1840000 | -0.9829210 | -0.3610360 |
| F         | -0.7446300  | 6.1065070  | 0.0822940  |
| C         | 4.0776490   | -0.8587500 | 0.0164110  |
| C         | 4.6601150   | -2.1278500 | 0.0252230  |
| C         | 4.9002280   | 0.2658090  | -0.0614220 |
| C         | 6.0362330   | -2.2752610 | -0.0440310 |
| H         | 4.0156590   | -2.9961880 | 0.0872660  |
| C         | 6.2789790   | 0.1305140  | -0.1311740 |
| H         | 4.4446710   | 1.2481400  | -0.0630980 |
| C         | 6.8355980   | -1.1412960 | -0.1223290 |
| H         | 6.4907340   | -3.2588150 | -0.0382940 |
| H         | 6.9200660   | 1.0019770  | -0.1902440 |
| Cl        | 8.5712310   | -1.3196170 | -0.2103650 |

**Table S1. Cont.**

| <b>5d</b> |             |            |            |
|-----------|-------------|------------|------------|
| C         | -2.2417810  | -1.4332100 | 0.1249080  |
| C         | -1.4854530  | -0.2803500 | 0.0575670  |
| C         | -0.0767320  | -0.3351150 | 0.1363240  |
| C         | 0.5657670   | -1.5951350 | 0.2312450  |
| C         | -0.2257780  | -2.7680500 | 0.3185160  |
| C         | -1.5870080  | -2.6892870 | 0.2728870  |
| H         | -1.9839600  | 0.6702070  | -0.0790720 |
| C         | 0.7992320   | 0.7967250  | 0.0853490  |
| H         | 0.2900550   | -3.7171030 | 0.4063010  |
| H         | -2.1933040  | -3.5863300 | 0.3318580  |
| C         | 2.6195530   | -0.6162880 | 0.0891550  |
| N         | 2.1013890   | 0.6418240  | 0.0324520  |
| N         | 1.9138690   | -1.7180060 | 0.2205940  |
| C         | 0.3105260   | 2.1996310  | 0.0786290  |
| C         | 0.9176370   | 3.1238240  | -0.7762250 |
| C         | -0.6898380  | 2.6408490  | 0.9484750  |
| C         | 0.5171390   | 4.4503740  | -0.7912100 |
| H         | 1.7128720   | 2.7854970  | -1.4300610 |
| C         | -1.0925950  | 3.9697200  | 0.9545170  |
| H         | -1.1405200  | 1.9487450  | 1.6507430  |
| C         | -0.4860530  | 4.8502330  | 0.0765230  |
| H         | 0.9692740   | 5.1763530  | -1.4565890 |
| H         | -1.8576610  | 4.3303340  | 1.6316870  |
| C         | -3.6652090  | -1.3793620 | 0.0383950  |
| C         | -4.8711940  | -1.3422610 | -0.0340350 |
| C         | -6.2963870  | -1.2924890 | -0.1214950 |
| C         | -6.9537760  | -0.0675280 | -0.2937740 |
| C         | -7.0545390  | -2.4673380 | -0.0365570 |
| C         | -8.3373360  | -0.0227120 | -0.3785560 |
| H         | -6.3679480  | 0.8424370  | -0.3605990 |
| C         | -8.4377570  | -2.4142390 | -0.1221890 |
| H         | -6.5469020  | -3.4161680 | 0.0965730  |
| C         | -9.0829470  | -1.1938520 | -0.2931040 |
| H         | -8.8366610  | 0.9312660  | -0.5123670 |
| H         | -9.0156190  | -3.3301540 | -0.0552580 |
| H         | -10.1652160 | -1.1555660 | -0.3598290 |
| F         | -0.8762580  | 6.1333910  | 0.0706430  |
| C         | 4.0910570   | -0.7265510 | 0.0156300  |
| C         | 4.7070480   | -1.9765260 | 0.0276440  |
| C         | 4.8963440   | 0.4159460  | -0.0694370 |
| C         | 6.0879110   | -2.0996410 | -0.0442930 |
| H         | 4.0839500   | -2.8603780 | 0.0945950  |
| C         | 6.2704400   | 0.3072470  | -0.1417570 |
| H         | 4.4217050   | 1.3893780  | -0.0740120 |
| C         | 6.8767420   | -0.9521140 | -0.1301420 |
| H         | 6.5352770   | -3.0852630 | -0.0335990 |
| H         | 6.9049890   | 1.1838310  | -0.2063240 |
| O         | 8.2312210   | -0.9556270 | -0.2056090 |
| C         | 8.8987060   | -2.1994510 | -0.1943220 |
| H         | 9.9626950   | -1.9737430 | -0.2617610 |
| H         | 8.7062950   | -2.7524380 | 0.7322670  |
| H         | 8.6081200   | -2.8214330 | -1.0488040 |

**Table S1. Cont.**

| <b>5e</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | 1.9982260  | -1.6717670 | 0.1102090  |
| C         | 1.1773060  | -0.5624050 | 0.0689140  |
| C         | -0.2259440 | -0.6989200 | 0.1445400  |
| C         | -0.7938610 | -1.9960340 | 0.2051790  |
| C         | 0.0622180  | -3.1236320 | 0.2671640  |
| C         | 1.4169760  | -2.9662530 | 0.2274840  |
| H         | 1.6202330  | 0.4180740  | -0.0447220 |
| C         | -1.1636010 | 0.3853030  | 0.1209180  |
| H         | -0.3987780 | -4.1024250 | 0.3299900  |
| H         | 2.0735680  | -3.8282790 | 0.2666350  |
| C         | -2.8964250 | -1.1323750 | 0.0729360  |
| N         | -2.4557460 | 0.1532600  | 0.0541000  |
| N         | -2.1337040 | -2.1960620 | 0.1826100  |
| C         | -0.7554080 | 1.8094400  | 0.1576580  |
| C         | -1.4227840 | 2.7302840  | -0.6476590 |
| C         | 0.2361790  | 2.2850380  | 1.0256590  |
| C         | -1.0986010 | 4.0801970  | -0.6278620 |
| H         | -2.2101170 | 2.3745370  | -1.3023810 |
| C         | 0.5590860  | 3.6278560  | 1.0671420  |
| H         | 0.7383270  | 1.6010600  | 1.7007840  |
| C         | -0.0992900 | 4.5344290  | 0.2327130  |
| H         | -1.6286010 | 4.7637710  | -1.2785420 |
| H         | 1.3146040  | 4.0058220  | 1.7461960  |
| C         | 3.4163430  | -1.5350170 | 0.0267870  |
| C         | 4.6183470  | -1.4288650 | -0.0431060 |
| C         | 6.0385740  | -1.2980980 | -0.1275940 |
| C         | 6.6266350  | -0.0358350 | -0.2800130 |
| C         | 6.8609770  | -2.4300550 | -0.0597740 |
| C         | 8.0055770  | 0.0872550  | -0.3625040 |
| H         | 5.9909150  | 0.8409370  | -0.3331310 |
| C         | 8.2391070  | -2.2986810 | -0.1428530 |
| H         | 6.4069130  | -3.4076140 | 0.0581310  |
| C         | 8.8152710  | -1.0417210 | -0.2942790 |
| H         | 8.4510470  | 1.0695360  | -0.4808230 |
| H         | 8.8671170  | -3.1818770 | -0.0892400 |
| H         | 9.8937560  | -0.9421430 | -0.3590500 |
| C         | -4.3627570 | -1.3282010 | -0.0158680 |
| C         | -4.8980120 | -2.6188230 | -0.0484470 |
| C         | -5.2255720 | -0.2312570 | -0.0701720 |
| C         | -6.2669180 | -2.8154290 | -0.1354160 |
| H         | -4.2199800 | -3.4622760 | -0.0041790 |
| C         | -6.5978290 | -0.4138750 | -0.1574040 |
| H         | -4.8030100 | 0.7652160  | -0.0393900 |
| C         | -7.0946180 | -1.7056030 | -0.1890180 |
| H         | -6.7015920 | -3.8077500 | -0.1628180 |
| H         | -7.2843330 | 0.4236220  | -0.1988610 |
| F         | -8.4219570 | -1.8895850 | -0.2737050 |
| O         | 0.2963500  | 5.8263120  | 0.3370020  |
| C         | -0.3450820 | 6.7911660  | -0.4712420 |
| H         | 0.1191470  | 7.7465250  | -0.2285770 |
| H         | -0.2027260 | 6.5824020  | -1.5376750 |
| H         | -1.4182530 | 6.8475160  | -0.2565310 |

**Table S1. Cont.**

| <b>5f</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | 2.2553140  | -1.6940530 | -0.1144020 |
| C         | 1.4784810  | -0.5533570 | -0.0741280 |
| C         | 0.0712770  | -0.6343770 | -0.1560010 |
| C         | -0.5463990 | -1.9083210 | -0.2220490 |
| C         | 0.2646670  | -3.0686320 | -0.2825200 |
| C         | 1.6243940  | -2.9646060 | -0.2367220 |
| H         | 1.9591560  | 0.4086270  | 0.0436550  |
| C         | -0.8225490 | 0.4862170  | -0.1335530 |
| H         | -0.2341250 | -4.0284250 | -0.3494080 |
| H         | 2.2468340  | -3.8516170 | -0.2749000 |
| C         | -2.6128160 | -0.9623480 | -0.0974790 |
| N         | -2.1234110 | 0.3045740  | -0.0730530 |
| N         | -1.8934380 | -2.0553380 | -0.2057930 |
| C         | -0.3590380 | 1.8931970  | -0.1641070 |
| C         | -0.9955620 | 2.8370830  | 0.6396510  |
| C         | 0.6556770  | 2.3323770  | -1.0246510 |
| C         | -0.6195100 | 4.1734490  | 0.6256590  |
| H         | -1.8000050 | 2.5104780  | 1.2887340  |
| C         | 1.0302520  | 3.6618180  | -1.0603330 |
| H         | 1.1352940  | 1.6314720  | -1.6987920 |
| C         | 0.4020170  | 4.5910370  | -0.2274540 |
| H         | -1.1268820 | 4.8752820  | 1.2749200  |
| H         | 1.8039310  | 4.0121200  | -1.7337350 |
| C         | 3.6772510  | -1.6126720 | -0.0250890 |
| C         | 4.8821100  | -1.5520840 | 0.0494730  |
| C         | 6.3059150  | -1.4742430 | 0.1389940  |
| C         | 6.9406800  | -0.2329260 | 0.2751780  |
| C         | 7.0849440  | -2.6374710 | 0.0919940  |
| C         | 8.3229520  | -0.1608930 | 0.3620060  |
| H         | 6.3384760  | 0.6680010  | 0.3122080  |
| C         | 8.4667210  | -2.5570970 | 0.1794060  |
| H         | 6.5946310  | -3.5988230 | -0.0132950 |
| C         | 9.0894640  | -1.3206490 | 0.3144250  |
| H         | 8.8049170  | 0.8054760  | 0.4675340  |
| H         | 9.0610160  | -3.4641190 | 0.1419950  |
| H         | 10.1706790 | -1.2609820 | 0.3825510  |
| C         | -4.0874030 | -1.1011110 | -0.0166880 |
| C         | -4.6735490 | -2.3681710 | 0.0096530  |
| C         | -4.9065680 | 0.0272740  | 0.0360530  |
| C         | -6.0498360 | -2.5099150 | 0.0891980  |
| H         | -4.0314310 | -3.2394090 | -0.0332730 |
| C         | -6.2854320 | -0.1021000 | 0.1157250  |
| H         | -4.4473200 | 1.0075620  | 0.0101700  |
| C         | -6.8455430 | -1.3720510 | 0.1422360  |
| H         | -6.5070890 | -3.4920000 | 0.1108400  |
| H         | -6.9239210 | 0.7724090  | 0.1552480  |
| O         | 0.8475630  | 5.8667670  | -0.3256030 |
| C         | 0.2374190  | 6.8538770  | 0.4802900  |
| H         | 0.7396560  | 7.7912310  | 0.2432880  |
| H         | -0.8311440 | 6.9514990  | 0.2576740  |
| H         | 0.3637760  | 6.6374410  | 1.5471760  |
| Cl        | -8.5818240 | -1.5429730 | 0.2432680  |

**Table S1. Cont.**

| <b>5g</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | 2.2187300  | -1.7048410 | 0.1168700  |
| C         | 1.4685600  | -0.5464600 | 0.0750700  |
| C         | 0.0600350  | -0.5939120 | 0.1579180  |
| C         | -0.5889450 | -1.8521270 | 0.2264190  |
| C         | 0.1958890  | -3.0310290 | 0.2886090  |
| C         | 1.5576000  | -2.9596670 | 0.2416840  |
| H         | 1.9716760  | 0.4038160  | -0.0447460 |
| C         | -0.8082210 | 0.5466180  | 0.1339670  |
| H         | -0.3255250 | -3.9786170 | 0.3576610  |
| H         | 2.1586710  | -3.8613330 | 0.2811940  |
| C         | -2.6355080 | -0.8589950 | 0.1004840  |
| N         | -2.1120640 | 0.3967760  | 0.0744430  |
| N         | -1.9379750 | -1.9681600 | 0.2115950  |
| C         | -0.3113660 | 1.9431830  | 0.1618640  |
| C         | -0.9265530 | 2.9001070  | -0.6428590 |
| C         | 0.7139370  | 2.3605590  | 1.0203770  |
| C         | -0.5199030 | 4.2276700  | -0.6315360 |
| H         | -1.7397370 | 2.5906460  | -1.2894270 |
| C         | 1.1194360  | 3.6812420  | 1.0531850  |
| H         | 1.1781560  | 1.6497930  | 1.6949970  |
| C         | 0.5118440  | 4.6230640  | 0.2195790  |
| H         | -1.0121460 | 4.9399070  | -1.2811710 |
| H         | 1.9019540  | 4.0146360  | 1.7250130  |
| C         | 3.6422910  | -1.6570300 | 0.0269180  |
| C         | 4.8483070  | -1.6251800 | -0.0478430 |
| C         | 6.2735140  | -1.5813200 | -0.1373330 |
| C         | 6.9389080  | -0.3549380 | -0.2628570 |
| C         | 7.0243440  | -2.7633970 | -0.1007760 |
| C         | 8.3225640  | -0.3159220 | -0.3493740 |
| H         | 6.3589440  | 0.5607630  | -0.2917960 |
| C         | 8.4076990  | -2.7161050 | -0.1878550 |
| H         | 6.5107060  | -3.7133860 | -0.0037800 |
| C         | 9.0607530  | -1.4942680 | -0.3121630 |
| H         | 8.8278510  | 0.6393920  | -0.4465140 |
| H         | 8.9795230  | -3.6378040 | -0.1585460 |
| H         | 10.1431190 | -1.4604590 | -0.3800180 |
| C         | -4.1080470 | -0.9603020 | 0.0181780  |
| C         | -4.7304170 | -2.2068260 | -0.0017400 |
| C         | -4.9072340 | 0.1877520  | -0.0437000 |
| C         | -6.1117330 | -2.3212280 | -0.0826490 |
| H         | -4.1117570 | -3.0949670 | 0.0473770  |
| C         | -6.2817010 | 0.0878490  | -0.1247470 |
| H         | -4.4268260 | 1.1581560  | -0.0230250 |
| C         | -6.8943260 | -1.1681600 | -0.1452200 |
| H         | -6.5639910 | -3.3046070 | -0.0969910 |
| H         | -6.9116140 | 0.9689560  | -0.1714270 |
| O         | 0.9867840  | 5.8892650  | 0.3150460  |
| C         | 0.3971020  | 6.8877830  | -0.4912790 |
| H         | 0.9204380  | 7.8144340  | -0.2574800 |
| H         | 0.5159150  | 6.6667050  | -1.5581630 |
| H         | -0.6686720 | 7.0096970  | -0.2668600 |
| O         | -8.2491270 | -1.1630980 | -0.2267890 |
| C         | -8.9219620 | -2.4036380 | -0.2446630 |
| H         | -8.7348240 | -2.9778050 | 0.6700980  |
| H         | -9.9848570 | -2.1720340 | -0.3103450 |
| H         | -8.6315650 | -3.0084310 | -1.1115450 |



**Table S1. Cont.**

| <b>5h</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | -2.5501110 | -1.4254260 | -0.2404200 |
| C         | -1.6101510 | -0.4167120 | -0.1949620 |
| C         | -0.2375550 | -0.7130140 | -0.0388180 |
| C         | 0.1767970  | -2.0670560 | 0.0143870  |
| C         | -0.8018750 | -3.0912630 | -0.0147050 |
| C         | -2.1254950 | -2.7797990 | -0.1320470 |
| H         | -1.9329050 | 0.6101950  | -0.3031250 |
| C         | 0.8150310  | 0.2567960  | 0.0309230  |
| H         | -0.4577390 | -4.1173600 | 0.0429560  |
| H         | -2.8769640 | -3.5608870 | -0.1627090 |
| C         | 2.3678710  | -1.4455020 | 0.0445110  |
| N         | 2.0748830  | -0.1181170 | 0.0390170  |
| N         | 1.4849160  | -2.4172060 | 0.0698740  |
| C         | 0.5688310  | 1.7178360  | 0.0868540  |
| C         | 1.3904780  | 2.5744580  | -0.6430900 |
| C         | -0.4183460 | 2.2841310  | 0.9035990  |
| C         | 1.2231580  | 3.9522080  | -0.5998630 |
| H         | 2.1748580  | 2.1452880  | -1.2560060 |
| C         | -0.5868760 | 3.6542130  | 0.9683100  |
| H         | -1.0407710 | 1.6464950  | 1.5214100  |
| C         | 0.2270520  | 4.4982430  | 0.2092820  |
| H         | 1.8711240  | 4.5852790  | -1.1922300 |
| H         | -1.3384910 | 4.1007420  | 1.6090310  |
| C         | -3.9404320 | -1.1302120 | -0.4041190 |
| C         | -5.1171200 | -0.9072360 | -0.5435430 |
| C         | 3.8077500  | -1.8054880 | 0.0450800  |
| C         | 4.1944360  | -3.1472470 | 0.0084100  |
| C         | 4.7886410  | -0.8128950 | 0.0810240  |
| C         | 5.5388130  | -3.4881790 | 0.0064640  |
| H         | 3.4240410  | -3.9083690 | -0.0179270 |
| C         | 6.1335430  | -1.1575690 | 0.0788060  |
| H         | 4.4786160  | 0.2242300  | 0.1144720  |
| C         | 6.5125720  | -2.4946910 | 0.0412700  |
| H         | 5.8296210  | -4.5334060 | -0.0227900 |
| H         | 6.8890110  | -0.3788880 | 0.1083950  |
| O         | -0.0225220 | 5.8253650  | 0.3316100  |
| C         | 0.7830560  | 6.7278430  | -0.3972280 |
| H         | 0.4202370  | 7.7252660  | -0.1506990 |
| H         | 1.8380410  | 6.6476600  | -0.1114410 |
| H         | 0.6910770  | 6.5685330  | -1.4777050 |
| H         | 7.5643690  | -2.7629860 | 0.0398400  |
| C         | -6.5416020 | -0.6226890 | -0.6988960 |
| H         | -6.6955580 | 0.4601770  | -0.7647680 |
| H         | -6.9047900 | -1.0545560 | -1.6380250 |
| C         | -7.3966990 | -1.1724290 | 0.4376830  |
| H         | -7.0237860 | -0.7839080 | 1.3952580  |
| H         | -8.4275410 | -0.8112350 | 0.3055490  |
| O         | -7.3325990 | -2.5813580 | 0.3857060  |
| H         | -7.7706740 | -2.9369940 | 1.1662800  |

**Table S2.** Cartesian coordinates of optimized structures in DCM of compounds **5a–h**.

| <b>5a</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | -1.7053770 | -1.4095080 | -0.1097670 |
| C         | -0.8493610 | -0.3279980 | -0.0462040 |
| C         | 0.5489710  | -0.5127180 | -0.1114370 |
| C         | 1.0736750  | -1.8266760 | -0.1917300 |
| C         | 0.1816560  | -2.9244070 | -0.2752550 |
| C         | -1.1676760 | -2.7218270 | -0.2409960 |
| H         | -1.2595090 | 0.6659580  | 0.0737790  |
| C         | 1.5217420  | 0.5368240  | -0.0632150 |
| H         | 0.6048830  | -3.9192600 | -0.3509970 |
| H         | -1.8506860 | -3.5619420 | -0.2970630 |
| C         | 3.2066880  | -1.0340730 | -0.0435760 |
| N         | 2.8059480  | 0.2648980  | -0.0025540 |
| N         | 2.4077840  | -2.0690460 | -0.1692180 |
| C         | 1.1588390  | 1.9766190  | -0.0692890 |
| C         | 1.8212360  | 2.8466810  | 0.8018370  |
| C         | 0.2218280  | 2.4978260  | -0.9658250 |
| C         | 1.5372490  | 4.2035020  | 0.8041710  |
| H         | 2.5628980  | 2.4461670  | 1.4829480  |
| C         | -0.0633190 | 3.8568000  | -0.9848120 |
| H         | -0.2709950 | 1.8457700  | -1.6778290 |
| C         | 0.5959650  | 4.6828850  | -0.0920330 |
| H         | 2.0326000  | 4.8883300  | 1.4821960  |
| H         | -0.7778100 | 4.2775280  | -1.6821410 |
| C         | -3.1195900 | -1.2277130 | -0.0358310 |
| C         | -4.3188480 | -1.0862090 | 0.0266110  |
| C         | -5.7364960 | -0.9176830 | 0.1022000  |
| C         | -6.5870430 | -2.0278850 | 0.0116840  |
| C         | -6.2910110 | 0.3585920  | 0.2685100  |
| C         | -7.9623860 | -1.8608460 | 0.0863880  |
| H         | -6.1595210 | -3.0160950 | -0.1168930 |
| C         | -7.6675180 | 0.5166610  | 0.3425430  |
| H         | -5.6343540 | 1.2186460  | 0.3390200  |
| C         | -8.5059950 | -0.5904040 | 0.2518800  |
| H         | -8.6130170 | -2.7260410 | 0.0153600  |
| H         | -8.0879820 | 1.5083570  | 0.4716860  |
| H         | -9.5818280 | -0.4632560 | 0.3100940  |
| F         | 0.3189490  | 5.9974980  | -0.0989990 |
| C         | 4.6686770  | -1.2792100 | 0.0415650  |
| C         | 5.1645750  | -2.5859550 | 0.0317440  |
| C         | 5.5647800  | -0.2118240 | 0.1354720  |
| C         | 6.5298970  | -2.8191600 | 0.1135540  |
| H         | 4.4650220  | -3.4098390 | -0.0401820 |
| C         | 6.9310450  | -0.4478910 | 0.2176850  |
| H         | 5.1767080  | 0.7990970  | 0.1415680  |
| C         | 7.4177120  | -1.7508630 | 0.2068390  |
| H         | 6.9037990  | -3.8377950 | 0.1052580  |
| H         | 7.6182190  | 0.3888530  | 0.2895000  |
| H         | 8.4854210  | -1.9341820 | 0.2708210  |

**Table S2.** *Cont.*

| <b>5b</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | -1.9739920 | -1.4181330 | -0.1103250 |
| C         | -1.1605850 | -0.3040620 | -0.0492590 |
| C         | 0.2435980  | -0.4339240 | -0.1192380 |
| C         | 0.8189320  | -1.7264300 | -0.2024090 |
| C         | -0.0297220 | -2.8581500 | -0.2822360 |
| C         | -1.3858750 | -2.7084210 | -0.2430340 |
| H         | -1.6090110 | 0.6731110  | 0.0719060  |
| C         | 1.1741240  | 0.6533600  | -0.0734560 |
| H         | 0.4317280  | -3.8357020 | -0.3598300 |
| H         | -2.0357100 | -3.5746000 | -0.2967320 |
| C         | 2.9189440  | -0.8497950 | -0.0658220 |
| N         | 2.4684970  | 0.4324550  | -0.0201280 |
| N         | 2.1617570  | -1.9159940 | -0.1871610 |
| C         | 0.7541740  | 2.0775320  | -0.0732800 |
| C         | 1.3811990  | 2.9697290  | 0.8016060  |
| C         | -0.2032790 | 2.5644920  | -0.9674820 |
| C         | 1.0431350  | 4.3140870  | 0.8095690  |
| H         | 2.1379430  | 2.5966240  | 1.4817010  |
| C         | -0.5424780 | 3.9110280  | -0.9808630 |
| H         | -0.6700880 | 1.8961720  | -1.6819550 |
| C         | 0.0834060  | 4.7591960  | -0.0847350 |
| H         | 1.5106230  | 5.0153030  | 1.4906180  |
| H         | -1.2734100 | 4.3056890  | -1.6763890 |
| C         | -3.3939360 | -1.2908500 | -0.0328920 |
| C         | -4.5974710 | -1.1937880 | 0.0318900  |
| C         | -6.0201010 | -1.0760930 | 0.1099450  |
| C         | -6.6193470 | 0.1804140  | 0.2717000  |
| C         | -6.8307680 | -2.2162270 | 0.0260860  |
| C         | -8.0004590 | 0.2898000  | 0.3476540  |
| H         | -5.9935520 | 1.0635690  | 0.3371020  |
| C         | -8.2110640 | -2.0978290 | 0.1027280  |
| H         | -6.3686580 | -3.1891990 | -0.0990040 |
| C         | -8.7992010 | -0.8467730 | 0.2635080  |
| H         | -8.4556550 | 1.2665120  | 0.4732000  |
| H         | -8.8306780 | -2.9858910 | 0.0368050  |
| H         | -9.8787720 | -0.7576810 | 0.3232030  |
| F         | -0.2459400 | 6.0616020  | -0.0863170 |
| C         | 4.3883690  | -1.0363560 | 0.0086690  |
| C         | 4.9358050  | -2.3229830 | 0.0043870  |
| C         | 5.2435290  | 0.0659860  | 0.0865320  |
| C         | 6.3072460  | -2.5108400 | 0.0760780  |
| H         | 4.2695080  | -3.1745830 | -0.0554850 |
| C         | 6.6183820  | -0.1064440 | 0.1590580  |
| H         | 4.8177210  | 1.0613060  | 0.0878060  |
| C         | 7.1245610  | -1.3947570 | 0.1523960  |
| H         | 6.7479580  | -3.5008470 | 0.0745470  |
| H         | 7.2957520  | 0.7373210  | 0.2187900  |
| F         | 8.4559120  | -1.5699300 | 0.2223270  |

**Table S2.** *Cont.*

| <b>5c</b> |             |            |            |
|-----------|-------------|------------|------------|
| C         | -2.2654150  | -1.4300690 | -0.1161390 |
| C         | -1.4861030  | -0.2918560 | -0.0557500 |
| C         | -0.0789090  | -0.3788570 | -0.1306490 |
| C         | 0.5346320   | -1.6534250 | -0.2182910 |
| C         | -0.2791600  | -2.8103120 | -0.2973330 |
| C         | -1.6391030  | -2.7018070 | -0.2532270 |
| H         | -1.9636550  | 0.6709160  | 0.0689650  |
| C         | 0.8176210   | 0.7364760  | -0.0853400 |
| H         | 0.2116010   | -3.7731560 | -0.3784240 |
| H         | -2.2625920  | -3.5871370 | -0.3063240 |
| C         | 2.6059960   | -0.7127660 | -0.0869630 |
| N         | 2.1185790   | 0.5547770  | -0.0367610 |
| N         | 1.8828960   | -1.8017300 | -0.2076230 |
| C         | 0.3545670   | 2.1469290  | -0.0795190 |
| C         | 0.9571820   | 3.0547860  | 0.7964190  |
| C         | -0.6201140  | 2.6074540  | -0.9691520 |
| C         | 0.5786290   | 4.3882440  | 0.8099160  |
| H         | 1.7268160   | 2.7025730  | 1.4731790  |
| C         | -0.9997860  | 3.9431260  | -0.9769810 |
| H         | -1.0686730  | 1.9277510  | -1.6845740 |
| C         | -0.3969500  | 4.8069770  | -0.0799730 |
| H         | 1.0268110   | 5.1010520  | 1.4918960  |
| H         | -1.7444280  | 4.3178140  | -1.6689870 |
| C         | -3.6881510  | -1.3452140 | -0.0333730 |
| C         | -4.8936450  | -1.2821120 | 0.0363680  |
| C         | -6.3185830  | -1.2025690 | 0.1200310  |
| C         | -7.0987030  | -2.3646140 | 0.0484390  |
| C         | -6.9505160  | 0.0387170  | 0.2748470  |
| C         | -8.4813440  | -2.2825180 | 0.1302970  |
| H         | -6.6113030  | -3.3258510 | -0.0712720 |
| C         | -8.3337130  | 0.1117520  | 0.3559940  |
| H         | -6.3483290  | 0.9387670  | 0.3307750  |
| C         | -9.1020530  | -1.0464030 | 0.2840180  |
| H         | -9.0772730  | -3.1872790 | 0.0739100  |
| H         | -8.8143470  | 1.0768940  | 0.4760640  |
| H         | -10.1833640 | -0.9857360 | 0.3477250  |
| F         | -0.7655610  | 6.0986930  | -0.0762800 |
| C         | 4.0819890   | -0.8553880 | -0.0180020 |
| C         | 4.6682050   | -2.1232510 | -0.0294200 |
| C         | 4.9031930   | 0.2706150  | 0.0617980  |
| C         | 6.0452370   | -2.2689880 | 0.0372750  |
| H         | 4.0300480   | -2.9960500 | -0.0906960 |
| C         | 6.2830050   | 0.1390910  | 0.1293730  |
| H         | 4.4497330   | 1.2536420  | 0.0688300  |
| C         | 6.8401550   | -1.1322250 | 0.1163570  |
| H         | 6.4989540   | -3.2528430 | 0.0289480  |
| H         | 6.9195960   | 1.0136550  | 0.1903870  |
| Cl        | 8.5800670   | -1.3073720 | 0.2012170  |

**Table S2.** *Cont.*

| <b>5d</b> |             |            |            |
|-----------|-------------|------------|------------|
| C         | -2.2380430  | -1.4350860 | -0.1218500 |
| C         | -1.4826950  | -0.2808790 | -0.0592010 |
| C         | -0.0741250  | -0.3373300 | -0.1350460 |
| C         | 0.5681900   | -1.5973690 | -0.2258200 |
| C         | -0.2220330  | -2.7710420 | -0.3077890 |
| C         | -1.5839840  | -2.6923420 | -0.2625670 |
| H         | -1.9805270  | 0.6713060  | 0.0681850  |
| C         | 0.7992760   | 0.7962870  | -0.0874870 |
| H         | 0.2891230   | -3.7230310 | -0.3918140 |
| H         | -2.1879210  | -3.5910950 | -0.3177370 |
| C         | 2.6224780   | -0.6138970 | -0.0913760 |
| N         | 2.1029720   | 0.6437630  | -0.0396600 |
| N         | 1.9184170   | -1.7175510 | -0.2158640 |
| C         | 0.3051760   | 2.1968680  | -0.0781280 |
| C         | 0.8872520   | 3.1153100  | 0.8005620  |
| C         | -0.6788920  | 2.6388540  | -0.9666900 |
| C         | 0.4798440   | 4.4403040  | 0.8177020  |
| H         | 1.6645290   | 2.7778540  | 1.4761190  |
| C         | -1.0878400  | 3.9660180  | -0.9708510 |
| H         | -1.1124430  | 1.9514310  | -1.6840090 |
| C         | -0.5043390  | 4.8402830  | -0.0712610 |
| H         | 0.9123290   | 5.1607810  | 1.5017990  |
| H         | -1.8403520  | 4.3262700  | -1.6620460 |
| C         | -3.6623450  | -1.3808720 | -0.0376460 |
| C         | -4.8688900  | -1.3437080 | 0.0337860  |
| C         | -6.2951360  | -1.2944990 | 0.1192460  |
| C         | -6.9536220  | -0.0665920 | 0.2704180  |
| C         | -7.0505870  | -2.4730830 | 0.0530450  |
| C         | -8.3379830  | -0.0228330 | 0.3532130  |
| H         | -6.3708400  | 0.8464040  | 0.3221930  |
| C         | -8.4345940  | -2.4203070 | 0.1365650  |
| H         | -6.5430050  | -3.4241820 | -0.0638470 |
| C         | -9.0816100  | -1.1973090 | 0.2865790  |
| H         | -8.8388950  | 0.9323220  | 0.4703890  |
| H         | -9.0110010  | -3.3379000 | 0.0843350  |
| H         | -10.1638910 | -1.1595820 | 0.3515570  |
| F         | -0.9011980  | 6.1239380  | -0.0640080 |
| C         | 4.0957240   | -0.7215180 | -0.0189920 |
| C         | 4.7175790   | -1.9698770 | -0.0288610 |
| C         | 4.8998400   | 0.4224920  | 0.0648920  |
| C         | 6.0988040   | -2.0906740 | 0.0421260  |
| H         | 4.1015350   | -2.8588090 | -0.0924800 |
| C         | 6.2749580   | 0.3173060  | 0.1363490  |
| H         | 4.4270720   | 1.3967650  | 0.0714870  |
| C         | 6.8860670   | -0.9408880 | 0.1256940  |
| H         | 6.5480160   | -3.0752410 | 0.0329530  |
| H         | 6.9037960   | 1.1983390  | 0.2004550  |
| O         | 8.2387550   | -0.9422730 | 0.2000890  |
| C         | 8.9116220   | -2.1904380 | 0.1931200  |
| H         | 9.9742850   | -1.9614240 | 0.2606650  |
| H         | 8.6195030   | -2.8067980 | 1.0495900  |
| H         | 8.7191480   | -2.7432150 | -0.7321590 |

**Table S2.** *Cont.*

| <b>5e</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | 1.9948780  | -1.6712720 | 0.1039230  |
| C         | 1.1743470  | -0.5610280 | 0.0667680  |
| C         | -0.2286580 | -0.6990730 | 0.1409540  |
| C         | -0.7957500 | -1.9964700 | 0.1981920  |
| C         | 0.0596270  | -3.1244800 | 0.2550650  |
| C         | 1.4150020  | -2.9668580 | 0.2152910  |
| H         | 1.6165240  | 0.4205760  | -0.0394190 |
| C         | -1.1647090 | 0.3866750  | 0.1215080  |
| H         | -0.3962640 | -4.1059520 | 0.3145620  |
| H         | 2.0696780  | -3.8303650 | 0.2509310  |
| C         | -2.8995310 | -1.1300920 | 0.0733510  |
| N         | -2.4584580 | 0.1550340  | 0.0592760  |
| N         | -2.1375620 | -2.1949980 | 0.1768570  |
| C         | -0.7538070 | 1.8092290  | 0.1583340  |
| C         | -1.4076750 | 2.7306540  | -0.6592080 |
| C         | 0.2296930  | 2.2829800  | 1.0371780  |
| C         | -1.0798120 | 4.0796740  | -0.6392000 |
| H         | -2.1846270 | 2.3789950  | -1.3285750 |
| C         | 0.5554460  | 3.6254390  | 1.0791840  |
| H         | 0.7233220  | 1.6005170  | 1.7199620  |
| C         | -0.0898360 | 4.5331280  | 0.2339910  |
| H         | -1.5979870 | 4.7627160  | -1.2995330 |
| H         | 1.3051540  | 3.9988670  | 1.7673880  |
| C         | 3.4137850  | -1.5337960 | 0.0227120  |
| C         | 4.6164670  | -1.4280440 | -0.0449160 |
| C         | 6.0380960  | -1.3003990 | -0.1259690 |
| C         | 6.6299440  | -0.0369850 | -0.2587280 |
| C         | 6.8554740  | -2.4376600 | -0.0739590 |
| C         | 8.0101240  | 0.0819210  | -0.3376280 |
| H         | 5.9990860  | 0.8440640  | -0.2992970 |
| C         | 8.2347780  | -2.3097700 | -0.1533410 |
| H         | 6.3992320  | -3.4160170 | 0.0287120  |
| C         | 8.8154870  | -1.0518820 | -0.2852450 |
| H         | 8.4593990  | 1.0640260  | -0.4404950 |
| H         | 8.8594450  | -3.1958020 | -0.1121650 |
| H         | 9.8943000  | -0.9553230 | -0.3470990 |
| C         | -4.3678150 | -1.3248580 | -0.0137520 |
| C         | -4.9066010 | -2.6147120 | -0.0445380 |
| C         | -5.2301860 | -0.2268880 | -0.0695040 |
| C         | -6.2763550 | -2.8100460 | -0.1292610 |
| H         | -4.2346470 | -3.4629050 | -0.0016550 |
| C         | -6.6034580 | -0.4066300 | -0.1547030 |
| H         | -4.8106890 | 0.7707820  | -0.0434250 |
| C         | -7.1008690 | -1.6980210 | -0.1830580 |
| H         | -6.7102420 | -3.8027580 | -0.1549100 |
| H         | -7.2862630 | 0.4338020  | -0.1976050 |
| F         | -8.4307830 | -1.8803500 | -0.2655290 |
| O         | 0.3069140  | 5.8229840  | 0.3392560  |
| C         | -0.3210470 | 6.7904200  | -0.4866800 |
| H         | 0.1437530  | 7.7441740  | -0.2410890 |
| H         | -0.1618710 | 6.5731510  | -1.5478290 |
| H         | -1.3956660 | 6.8495430  | -0.2862280 |

**Table S2.** *Cont.*

| <b>5f</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | 2.2508630  | -1.6963270 | 0.1098240  |
| C         | 1.4751450  | -0.5543090 | 0.0728510  |
| C         | 0.0681330  | -0.6360030 | 0.1533460  |
| C         | -0.5494660 | -1.9099020 | 0.2165670  |
| C         | 0.2601310  | -3.0709980 | 0.2730180  |
| C         | 1.6205570  | -2.9675860 | 0.2272770  |
| H         | 1.9557130  | 0.4084370  | -0.0385710 |
| C         | -0.8232340 | 0.4865790  | 0.1347200  |
| H         | -0.2344360 | -4.0332120 | 0.3371830  |
| H         | 2.2404990  | -3.8563290 | 0.2626910  |
| C         | -2.6160210 | -0.9597980 | 0.0978660  |
| N         | -2.1257660 | 0.3063460  | 0.0781230  |
| N         | -1.8984580 | -2.0544770 | 0.2010040  |
| C         | -0.3558020 | 1.8914230  | 0.1658780  |
| C         | -0.9774780 | 2.8361120  | -0.6503410 |
| C         | 0.6508420  | 2.3278490  | 1.0378920  |
| C         | -0.5967180 | 4.1711440  | -0.6354340 |
| H         | -1.7712570 | 2.5138860  | -1.3147420 |
| C         | 1.0293730  | 3.6564920  | 1.0747480  |
| H         | 1.1211620  | 1.6280190  | 1.7195480  |
| C         | 0.4153270  | 4.5871440  | 0.2311700  |
| H         | -1.0913950 | 4.8725830  | -1.2945140 |
| H         | 1.7970920  | 4.0015920  | 1.7578490  |
| C         | 3.6736290  | -1.6147100 | 0.0221240  |
| C         | 4.8790750  | -1.5541770 | -0.0512140 |
| C         | 6.3039800  | -1.4775210 | -0.1385710 |
| C         | 7.0805430  | -2.6434130 | -0.0968440 |
| C         | 6.9397480  | -0.2351510 | -0.2669420 |
| C         | 8.4631650  | -2.5640940 | -0.1819400 |
| H         | 6.5903400  | -3.6055580 | 0.0024450  |
| C         | 8.3229050  | -0.1648750 | -0.3515240 |
| H         | 6.3404500  | 0.6679750  | -0.2996030 |
| C         | 9.0876310  | -1.3268770 | -0.3092760 |
| H         | 9.0561530  | -3.4719490 | -0.1487140 |
| H         | 8.8063410  | 0.8012340  | -0.4509040 |
| H         | 10.1689160 | -1.2683660 | -0.3755280 |
| C         | -4.0925600 | -1.0967450 | 0.0175290  |
| C         | -4.6825060 | -2.3627210 | -0.0027520 |
| C         | -4.9103340 | 0.0329320  | -0.0421860 |
| C         | -6.0595520 | -2.5030900 | -0.0812030 |
| H         | -4.0469100 | -3.2383280 | 0.0432200  |
| C         | -6.2901140 | -0.0929740 | -0.1212750 |
| H         | -4.4536220 | 1.0143130  | -0.0242810 |
| C         | -6.8508280 | -1.3626220 | -0.1400470 |
| H         | -6.5160000 | -3.4856050 | -0.0975250 |
| H         | -6.9239420 | 0.7845710  | -0.1666830 |
| O         | 0.8629230  | 5.8604970  | 0.3312660  |
| C         | 0.2664670  | 6.8508390  | -0.4910080 |
| H         | 0.7699690  | 7.7860120  | -0.2503630 |
| H         | 0.4085730  | 6.6264170  | -1.5530470 |
| H         | -0.8033730 | 6.9517230  | -0.2819780 |
| Cl        | -8.5909110 | -1.5308350 | -0.2397660 |

**Table S2. Cont.**

| <b>5g</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | 2.2147030  | -1.7070300 | 0.1166490  |
| C         | 1.4656180  | -0.5474020 | 0.0765150  |
| C         | 0.0572420  | -0.5953940 | 0.1581340  |
| C         | -0.5918790 | -1.8533020 | 0.2256370  |
| C         | 0.1914810  | -3.0328350 | 0.2862260  |
| C         | 1.5539380  | -2.9622450 | 0.2391410  |
| H         | 1.9686730  | 0.4034610  | -0.0386180 |
| C         | -0.8083890 | 0.5471760  | 0.1365700  |
| H         | -0.3255810 | -3.9829480 | 0.3544280  |
| H         | 2.1523230  | -3.8656190 | 0.2775390  |
| C         | -2.6389710 | -0.8560700 | 0.1028170  |
| N         | -2.1139080 | 0.3989160  | 0.0806470  |
| N         | -1.9429670 | -1.9667890 | 0.2109300  |
| C         | -0.3073260 | 1.9412930  | 0.1644280  |
| C         | -0.9066270 | 2.8985070  | -0.6536890 |
| C         | 0.7091320  | 2.3561700  | 1.0353500  |
| C         | -0.4951640 | 4.2245870  | -0.6413820 |
| H         | -1.7080710 | 2.5931440  | -1.3168360 |
| C         | 1.1185470  | 3.6758860  | 1.0696140  |
| H         | 1.1634260  | 1.6465670  | 1.7177970  |
| C         | 0.5260390  | 4.6188170  | 0.2244820  |
| H         | -0.9735850 | 4.9360300  | -1.3017730 |
| H         | 1.8941810  | 4.0043860  | 1.7520000  |
| C         | 3.6390120  | -1.6593980 | 0.0270340  |
| C         | 4.8455060  | -1.6279470 | -0.0485260 |
| C         | 6.2717140  | -1.5853670 | -0.1383920 |
| C         | 6.9372220  | -0.3583730 | -0.2644360 |
| C         | 7.0204260  | -2.7695270 | -0.1014510 |
| C         | 8.3215300  | -0.3210270 | -0.3513660 |
| H         | 6.3597860  | 0.5590260  | -0.2934100 |
| C         | 8.4044400  | -2.7231780 | -0.1889130 |
| H         | 6.5075690  | -3.7199920 | -0.0039640 |
| C         | 9.0583810  | -1.5010570 | -0.3138600 |
| H         | 8.8277320  | 0.6335640  | -0.4488730 |
| H         | 8.9754180  | -3.6451840 | -0.1593730 |
| H         | 10.1406410 | -1.4683310 | -0.3819450 |
| C         | -4.1129410 | -0.9548920 | 0.0194780  |
| C         | -4.7412970 | -2.1998160 | 0.0035980  |
| C         | -4.9108520 | 0.1943400  | -0.0494210 |
| C         | -6.1227620 | -2.3123240 | -0.0781720 |
| H         | -4.1299420 | -3.0927240 | 0.0558330  |
| C         | -6.2861030 | 0.0975730  | -0.1316770 |
| H         | -4.4327300 | 1.1659290  | -0.0354850 |
| C         | -6.9036650 | -1.1573370 | -0.1468150 |
| H         | -6.5769460 | -3.2946180 | -0.0887360 |
| H         | -6.9100430 | 0.9828760  | -0.1842860 |
| O         | 1.0027160  | 5.8822710  | 0.3223930  |
| C         | 0.4272450  | 6.8843140  | -0.5003220 |
| H         | 0.9508560  | 7.8087720  | -0.2610390 |
| H         | 0.5636050  | 6.6560100  | -1.5623200 |
| H         | -0.6401090 | 7.0084140  | -0.2908560 |
| O         | -8.2561660 | -1.1504330 | -0.2297340 |
| C         | -8.9351050 | -2.3950820 | -0.2465430 |
| H         | -8.7508900 | -2.9633780 | 0.6710110  |
| H         | -9.9962510 | -2.1598590 | -0.3168490 |
| H         | -8.6408900 | -2.9994860 | -1.1108140 |



Table S2. *Cont.*

| <b>5h</b> |            |            |            |
|-----------|------------|------------|------------|
| C         | -2.3889690 | -1.7570480 | -0.4424550 |
| C         | -1.5641530 | -0.6579150 | -0.3141280 |
| C         | -0.1595510 | -0.8063220 | -0.3002830 |
| C         | 0.4009160  | -2.1058550 | -0.3656200 |
| C         | -0.4571470 | -3.2226470 | -0.5171640 |
| C         | -1.8113970 | -3.0527310 | -0.5598300 |
| H         | -2.0048430 | 0.3238500  | -0.2030510 |
| C         | 0.7811040  | 0.2683040  | -0.1808480 |
| H         | -0.0057390 | -4.2060280 | -0.5802680 |
| H         | -2.4688420 | -3.9082780 | -0.6665640 |
| C         | 2.4991900  | -1.2648280 | -0.0724570 |
| N         | 2.0664220  | 0.0231870  | -0.0422830 |
| N         | 1.7373870  | -2.3175010 | -0.2631190 |
| C         | 0.3829240  | 1.6954490  | -0.1933390 |
| C         | 0.9829090  | 2.5803710  | 0.7018980  |
| C         | -0.5335700 | 2.2095390  | -1.1204160 |
| C         | 0.6656550  | 3.9322100  | 0.7091020  |
| H         | 1.7085210  | 2.1973690  | 1.4105430  |
| C         | -0.8471450 | 3.5555830  | -1.1354510 |
| H         | -0.9832750 | 1.5559750  | -1.8595750 |
| C         | -0.2571660 | 4.4259990  | -0.2141490 |
| H         | 1.1402160  | 4.5860150  | 1.4291560  |
| H         | -1.5444590 | 3.9605760  | -1.8599750 |
| C         | -3.8129600 | -1.6095300 | -0.4483380 |
| C         | -5.0147280 | -1.5003600 | -0.4560270 |
| C         | 3.9588760  | -1.4776340 | 0.1047610  |
| C         | 4.4840590  | -2.7727630 | 0.1218530  |
| C         | 4.8229570  | -0.3913370 | 0.2601910  |
| C         | 5.8462320  | -2.9759930 | 0.2912330  |
| H         | 3.8089100  | -3.6113300 | 0.0016280  |
| C         | 6.1861230  | -0.5971350 | 0.4297670  |
| H         | 4.4122030  | 0.6104680  | 0.2447940  |
| C         | 6.7019490  | -1.8887990 | 0.4458600  |
| H         | 6.2427320  | -3.9860500 | 0.3034480  |
| H         | 6.8481310  | 0.2544430  | 0.5487850  |
| O         | -0.6374700 | 5.7226480  | -0.2993330 |
| C         | -0.0617900 | 6.6538680  | 0.6025870  |
| H         | -0.5014230 | 7.6202790  | 0.3600290  |
| H         | -0.2960700 | 6.4007880  | 1.6416870  |
| H         | 1.0246250  | 6.7098010  | 0.4797090  |
| H         | 7.7671540  | -2.0486370 | 0.5783360  |
| C         | -6.4693020 | -1.3502240 | -0.4597330 |
| H         | -6.7447530 | -0.4581680 | -1.0325080 |
| H         | -6.9251120 | -2.2070380 | -0.9672950 |
| C         | -7.0712640 | -1.2378570 | 0.9368770  |
| H         | -6.6192900 | -0.3883460 | 1.4650810  |
| H         | -8.1467880 | -1.0381880 | 0.8365280  |
| O         | -6.8336040 | -2.4553270 | 1.6170570  |
| H         | -7.1524900 | -2.3599560 | 2.5221840  |