Supporting Information

Synthesis and Physical Properties of π-Extended Molecules having *p*- Methylenequinone Unit

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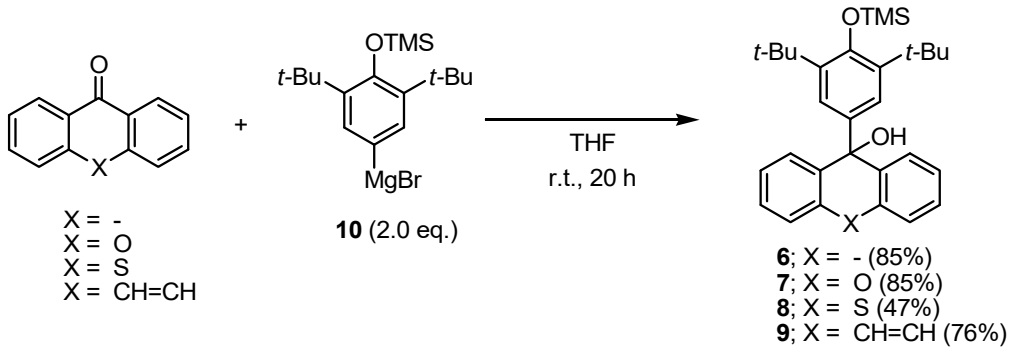
CONTENTS

1. General

FT-IR spectra were recorded on a JASCO FT/IR-4100 instrument. ^{1}H NMR spectra were recorded at 400 MHz and ^{13}C NMR spectra at 100 MHz on a JEOL AL400 or ECS400. Chemical shifts were reported in ppm relative to tetramethylsilane or residual solvent as the internal standard. Mass spectral analyses were performed on a JEOL JMS-700 spectrometer for EI and FAB ionization. Preparative HPLC separation was undertaken with a JAI LC-908 chromatograph using 600 mm x 20 mm JAIGEL-1H and 2H GPC columns with $CHCl_3$ as an eluent. All reagents were obtained from commercial suppliers and used without purification.

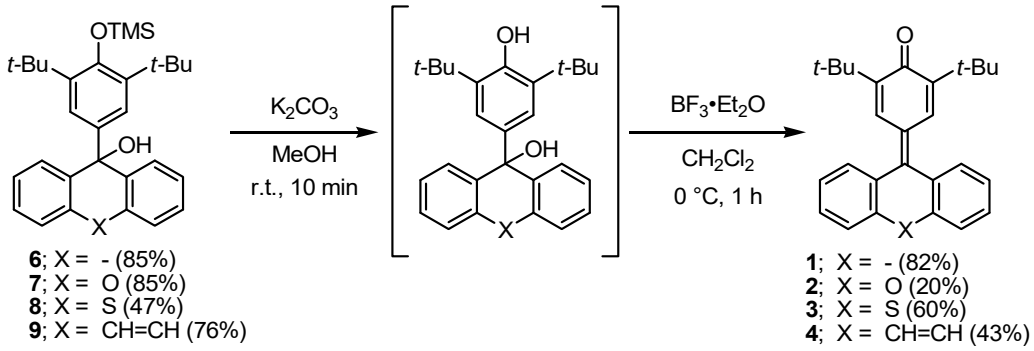
2. Synthesis of 1-9 and 11

2-1. General Synthesis of **6**-**9**



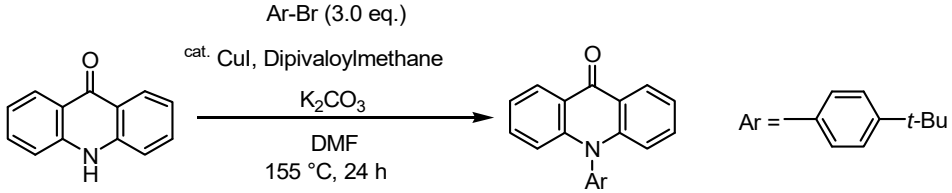
A solution of aryl magnesium bromide **10** (2.0 mmol), which was prepared from Mg turnings (486 mg, 20 mmol) and (4-bromo-2,6-di*tert*-butylphenoxy)trimethylsilane (2.0 mmol) in THF (10 mL), was added to a solution of the corresponding aromatic ketone (1.0 mmol) in THF (8.0 mL) at room temperature. After being stirred for 20 h at room temperature, to the reaction mixture was added water, then the resulting mixture was extracted several times with $CHCl_3$ and the organic fraction was washed with brine and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by chromatography on SiO_2 to give the compound **6**-**9**. Further purification was carried out a recyclable preparative HPLC, if necessary.

2-2. General Synthesis of **1**-**4**



To a solution of **6**-**9** (0.3 mmol) in CH_3OH (5.0 mL) was slowly added to K_2CO_3 (1.2 mmol, 0.166 g) at room temperature for 10 min. After removal of the solvent, the residue was diluted with $CHCl_3$ and washed with NH_4Cl aq. and brine. The organic layer was dried over $MgSO_4$. After removal of drying agent, the organic solution was concentrated under reduced pressure to afford the crude diol derivatives. The crude products were used without further purification in the next step. To the solution of crude diol in CH_2Cl_2 (10 mL) added $BF_3 \cdot Et_2O$ (0.3 mmol, 0.042 g) at 0 ºC. After being stirred for 1 h at 0 ºC, to the reaction mixture was added water, then the resulting mixture was extracted several times with $CHCl_3$ and the organic fraction was washed with brine and dried over $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by chromatography on SiO_2 to give the compound **1**-**4**. Further purification was carried out a recyclable preparative HPLC, if necessary. In the case of the purification of **2** was carried out the chromatography on SiO_2 and recyclable preparative HPLC followed by the recrystallization with hexane.

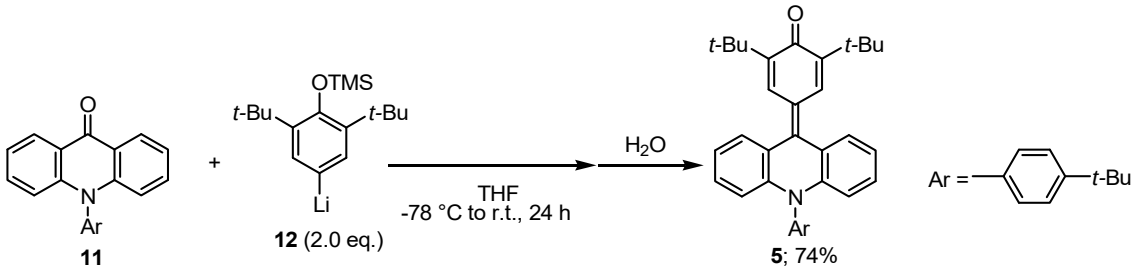
2-3. Synthesis of **11**



11; 81%

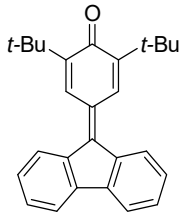
A solution of 9(10*H*)-acridone (0.50 mmol, 0.098 g), 1-bromo-4-*tert*-butylbenzene (0.50 mmol, 0.106 g), CuI (0.052 mmol, 0.010 g), dipivaloylmethane (0.11 mmol, 0.020 g), and K_2CO_3 (1.5 mmol, 0.103 g) in DMF (4.0 mL) was stirred at 155 ºC under an argon atmosphere. After being stirred at 155 ºC for 16 and 20 h, 1-bromo-4-*tert*-butylbenzene (0.50 mmol, 0.106 g) was added each time. After being stirred at 155 ºC for 24 h, the reaction mixture was added with water and the resulting precipitate was collected by suction filtration and washed with CH_3OH to give **11** (81%, 0.41 mmol, 0.144 g).

2-4. Synthesis of **5**



A solution of *N*-aryl acridone **11** (0.5 mmol, 0.164 g) in THF (20 mL) was added to a solution of the lithium agent **12**, which was prepared from *n*-BuLi (1.6 mmol, 1.0 mL; 1.6 M in hexane

solution) and (4-bromo-2,6-di*tert*-butylphenoxy)trimethylsilane (1.5 mmol, 0.536 g) in THF (4.0 mL) at -78 ºC for 1 h. The reaction was conducted at -78 ºC and gradually warmed to room temperature for 24 h, to the reaction mixture was added water, then the resulting mixture was extracted several times with $CHCl_3$. The organic fraction was washed with brine and dried over $MgSO_4$. After removal of the drying agent and solvent, the residue was purified by chromatography on SiO_2 ($CHCl_3$/ethyl acetate/hexane＝1/1/2 as an eluent) to give the compound **5** (74%, 0.37 mmol, 0.178 g).



1

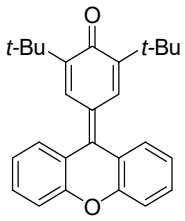
^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 2H), 7.91 (d, *J* = 7.6 Hz, 2H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.37 (td, *J* = 7.6, 1.2 Hz, 2H), 7.03 (td, *J* = 7.6, 1.2 Hz, 2H), 1.41 (s, 18H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 186.7, 149.0, 146.5, 141.9, 137.8, 132.9, 129.9, 129.4, 127.8, 127.6, 120.3, 35.8, 29.8.

IR (KBr) ν_{max} 3170, 3053, 3012, 2979, 2952, 2915, 2861, 1639, 1591, 1518, 1479, 1467, 1445, 1388, 1354, 1337, 1303, 1281, 1251, 1198, 1169, 1158, 1102, 1085, 1022, 972, 946, 930, 911, 876, 852, 820, 783, 744, 729, cm^{-1}.

MS (EI): *m/z* 368 (M^+). HRMS (EI): calcd for $C_{27}H_{28}O$: 368.2140. found 368.2168.

m.p. = 225-229 °C



2

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.77 (s, 2H), 7.66 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.18 (td, *J* = 8.4, 1.6 Hz, 2H), 7.36 (dd, *J* = 8.0, 1.0 Hz, 2H), 7.29 (td, *J* = 7.6, 1.2 Hz, 2H), 1.32 (s, 18H).

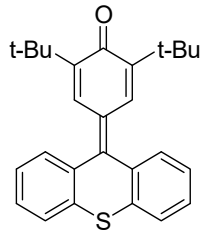
^{13}C-NMR (100 MHz, $CDCl_3$) δ 186.7, 154.1, 148.0, 137.5, 130.0, 129.9, 129.1, 125.1, 123.8, 123.3, 116.9, 35.6, 29.6.

IR (KBr) ν_{max} 3060, 2992, 2959, 2905, 2891, 1645, 1632, 1602, 1584, 1516, 1481, 1450, 1386, 1362, 1345, 1303, 1255, 1208, 1177, 1156, 1118, 1099, 1090, 1025, 966, 927, 916,

884, 858, 822, 804, 768, 759 cm^{-1}.

MS (EI): *m/z* 384 (M^+). HRMS (EI): calcd for $C_{27}H_{28}O_2$: 384.2089. found 384.2080.

m.p. = 227-231 °C



3

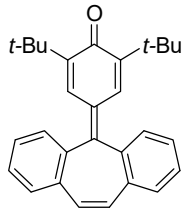
^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.61 (dd, *J* = 7.2, 1.2 Hz, 2H), 7.55-7.53 (m, 4H), 7.39 (td, *J* = 7.8, 1.6 Hz, 2H), 7.34 (td, *J* = 7.8, 1.6 Hz, 2H), 1.29 (s, 18H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 186.6, 148.4, 145.3, 135.1, 134.3, 130.14, 130.11, 127.9, 127.1, 126.9, 125.9, 35.6, 29.5.

IR (KBr) ν_{max} 2957, 2859, 1631, 1608, 1579, 1565, 1515, 1455, 1431, 1386, 1361, 1340, 1257, 1088, 1072, 1024, 963, 927, 881, 821, 771, 755, 743 cm^{-1}.

MS (EI): *m/z* 400 (M^+). HRMS (EI): calcd for $C_{27}H_{28}OS$: 400.1861. found 400.1860.

m.p. = 238-239 °C



4

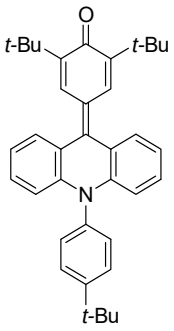
^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.46-7.35 (m, 8H), 7.11 (s, 2H), 7.00 (s, 2H), 1.22 (s, 18H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 186.18, 151.7, 147.8, 136.5, 134.2, 131.0, 129.9, 129.1, 128.9, 128.4, 127.9, 127.6, 35.2, 29.4.

IR (KBr) ν_{max} 3057, 2998, 2949, 2923, 2858, 1737, 1645, 1610, 1561, 1534, 1482, 1455, 1431, 1408, 1387, 1362, 1338, 1306, 1254, 1219, 1198, 1178, 1160, 1102, 1083, 1040, 1024, 965, 927, 916, 878, 850, 821, 803, 767, 741, 721, 693, 662, 645, 626, 601 cm^{-1}.

MS (EI): *m/z* 394 (M^+). HRMS (EI): calcd for $C_{29}H_{30}O$: 394.2297. found 394.2316.

m.p. = 218-220 °C



5

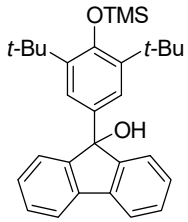
^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.0 Hz, 2H), 7.78 (s, 2H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.29-7.25 (m, 4H), 7.19 (t, *J* = 8.0 Hz, 2H), 6.70 (d, *J* = 8.0 Hz, 2H), 1.45 (s, 9H), 1.35 (s, 18H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 185.7, 152.4, 146.3, 143.2, 142.5, 136.3, 131.0, 129.81, 129.77, 129.56, 127.8, 123.5, 121.1, 121.0, 114.8, 35.6, 35.0, 31.4, 29.7.

IR (KBr) ν_{max} 3081, 2954, 2905, 2876, 1595, 1573, 1576, 1505, 1481, 1451, 1424, 1383, 1356, 1283, 1252, 1207, 1170, 1139, 1107, 1093, 1052, 1018, 972, 923, 882, 845, 835, 814, 778, 752 cm^{-1}.

MS (EI): *m/z* 515 (M^+). HRMS (EI): calcd for $C_{37}H_{41}NO$: 515.3188. found 515.3171.

m.p. >250 °C



6

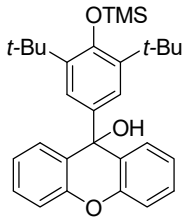
^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 6.8 Hz, 2H), 7.46 (dd, *J* = 7.0, 0.4 Hz, 2H), 7.37 (td, *J* = 7.4, 1.2 Hz, 2H), 7.31 (s, 2H), 7.30-7.26 (m, 2H), 2.44 (s, 1H), 1.33 (s, 18H), 0.39 (s, 9H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 152.5, 150.2, 140.1, 139.5, 134.1, 128.8, 128.1, 124.9, 123.2, 119.9, 83.9, 35.2, 31.1, 3.9.

IR (KBr) ν_{max} 3545, 3447, 3038, 2956, 1749, 1605, 1558, 1508, 1489, 1472, 1449, 1420, 1392, 1361, 1338, 1257, 1233, 1209, 1180, 1122, 1037, 987, 921, 889, 867, 845, 769, 757, 740 cm^{-1}.

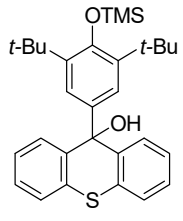
MS (EI): *m/z* 458 (M^+). HRMS (EI): calcd for $C_{30}H_{38}O_2Si$: 458.2641. found 458.2616.

m.p. = 54-55 °C



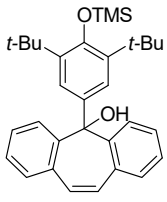
7

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.29 (td, *J* = 8.0, 2.0 Hz, 2H), 7.19-7.17 (m, 4H), 7.10 (td, *J* = 7.6, 1.2 Hz, 2H), 2.60 (s, 1H), 1.30 (s, 18H), 0.37 (s, 9H).
^{13}C-NMR (100 MHz, $CDCl_3$) δ 151.8, 150.0, 140.0, 138.5, 128.7, 128.3, 127.9, 123.9, 123.3, 116.2, 70.9, 35.1, 3.8.
IR (KBr) ν_{max} 3544, 3030, 2958, 1600, 1572, 1473, 1446, 1418, 1391, 1362, 1308, 1237, 1205, 1178, 1151, 1124, 1094, 1050, 970, 944, 924, 882, 843, 751 cm^{-1}.
MS (EI): *m/z* 474 (M^+). HRMS (EI): calcd for $C_{30}H_{37}O_2Si$: 457.2563. found 457.2568.
m.p. = 121-122 °C



8

^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.02 (dd, *J* = 7.8, 0.8 Hz, 2H), 7.38 (dd, *J* = 7.8, 0.8 Hz, 2H), 7.34 (td, *J* = 7.6, 1.6 Hz, 2H), 7.25-7.21 (m, 2H), 6.80 (s, 2H) 2.79 (br, 1H), 1.19 (s, 18H), 0.33 (s, 9H)
^{13}C-NMR (100 MHz, $CDCl_3$) δ 152.4, 140.4, 139.7, 133.9, 131.6, 127.0, 126.33, 126.29, 125.7, 124.9, 77.2, 35.0, 30.9, 3.9.
IR (KBr) ν_{max} 3586, 3059, 2954, 1457, 1441, 1421, 1391, 1362, 1257, 1205, 1178, 1124, 1032, 924, 886, 842, 754 cm^{-1}.
MS (EI): *m/z* 490 (M^+). HRMS (EI): calcd for $C_{30}H_{38}O_2SSi$: 490.2362. found 490.2362.
m.p. = 205-206 °C



9

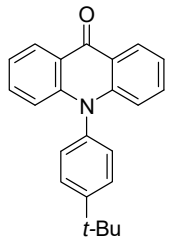
^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.0 Hz, 2H), 7.49-7.45 (m, 2H), 7.31-7.26 (m, 4H), 6.60 (s, 2H), 6.46 (s, 2H), 2.27 (br, 1H), 1.14 (s, 18H), 0.31 (s, 9H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 152.1, 143.1, 139.4, 136.9, 133.4, 131.0, 128.3, 127.8, 126.4, 124.8, 124.4, 78.6, 34.9, 31.1, 3.5.

IR (KBr) ν_{max} 3573, 3019, 2956, 1483, 1422, 1392, 1361, 1321, 1258, 1241, 1208, 1171, 1159, 1125, 1047, 1018, 970, 950, 921, 881, 842, 803, 773, 733 cm^{-1}.

MS (EI): *m/z* 484 (M^+). HRMS (EI): calcd for $C_{32}H_4O_2Si$: 484.2798 found 484.2810.

m.p. = 248-249 °C



11

^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.29-7.26 (m, 4H), 6.79 (d, *J* = 8.8 Hz, 2H), 1.46 (s, 9H).

^{13}C-NMR (100 MHz, $CDCl_3$) δ 178.2, 152.8, 143.2, 136.0, 133.2, 129.3, 127.9, 127.2, 121.7, 121.4, 116.9, 35.0, 31.4.

IR (KBr) ν_{max} 3068, 2962, 1680, 1636, 1599, 1525, 1508, 1483, 1459, 1359, 1345, 1302, 1270, 1200, 1171, 1159, 1118, 1102, 1040, 1022, 935, 867, 840, 830 757 cm^{-1}.

MS (EI): *m/z* 327 (M^+). HRMS (EI): calcd for $C_{23}H_{21}NO$: 327.1623. found 327.1633.

m.p. >250 °C

3. UV/vis Absorption Spectra of 5 in Various Solvents

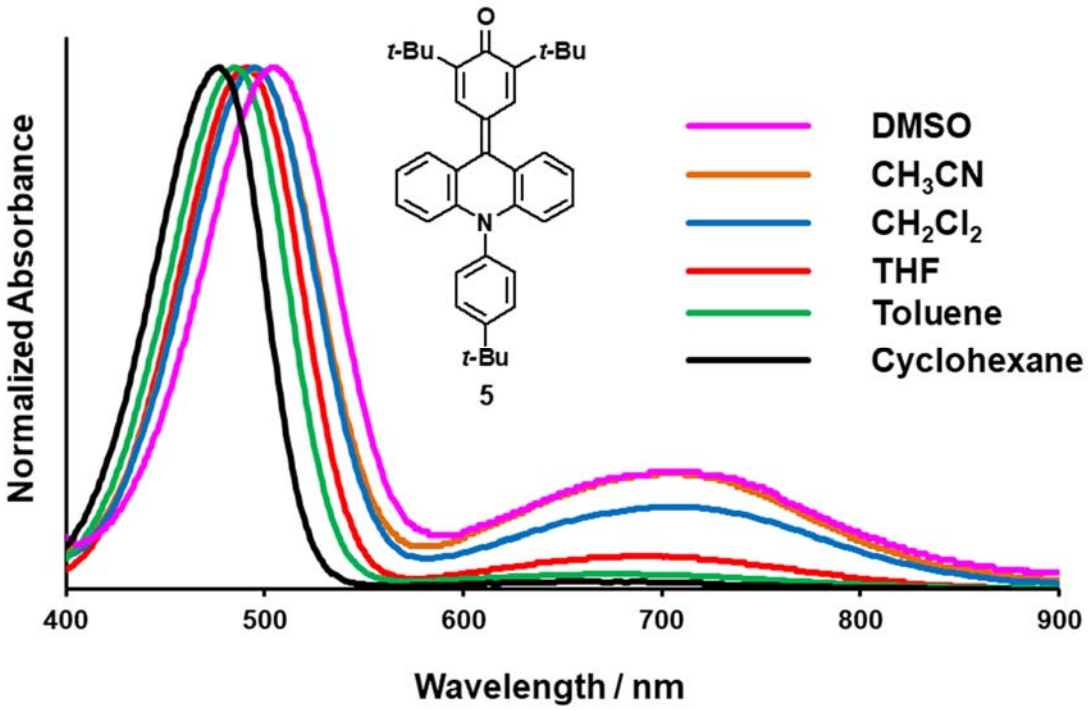


Figure S1. UV/vis Absorption Spectra of **5** in Various Solvents

Figure S2. Color Changes of **5** in Different Solvent

4. Cyclic Voltammogram of Fuchsone and 1-5

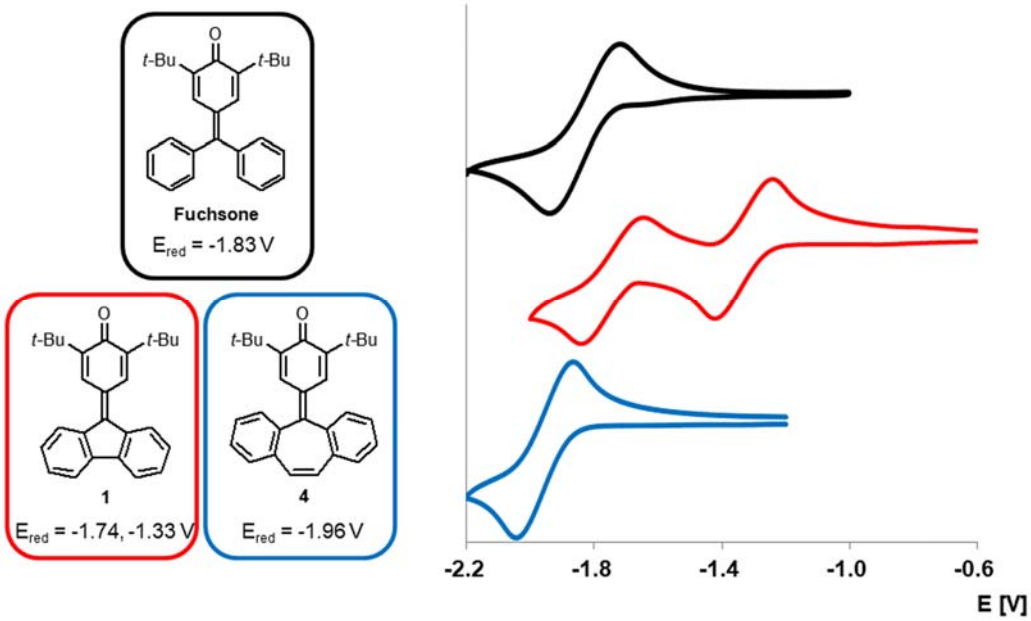


Figure S3. Cyclic voltammogram of Fuchsone, **1**, and **4** in THF; V versus (Ag/Ag^{+}) in 0.1 M with $n$$Bu_4NPF_6$ in THF scan rate: 100 mV/S, working electrode: glassy carbon, ferrocene / ferrocenium (Fc/Fc^{+}) = 0 V

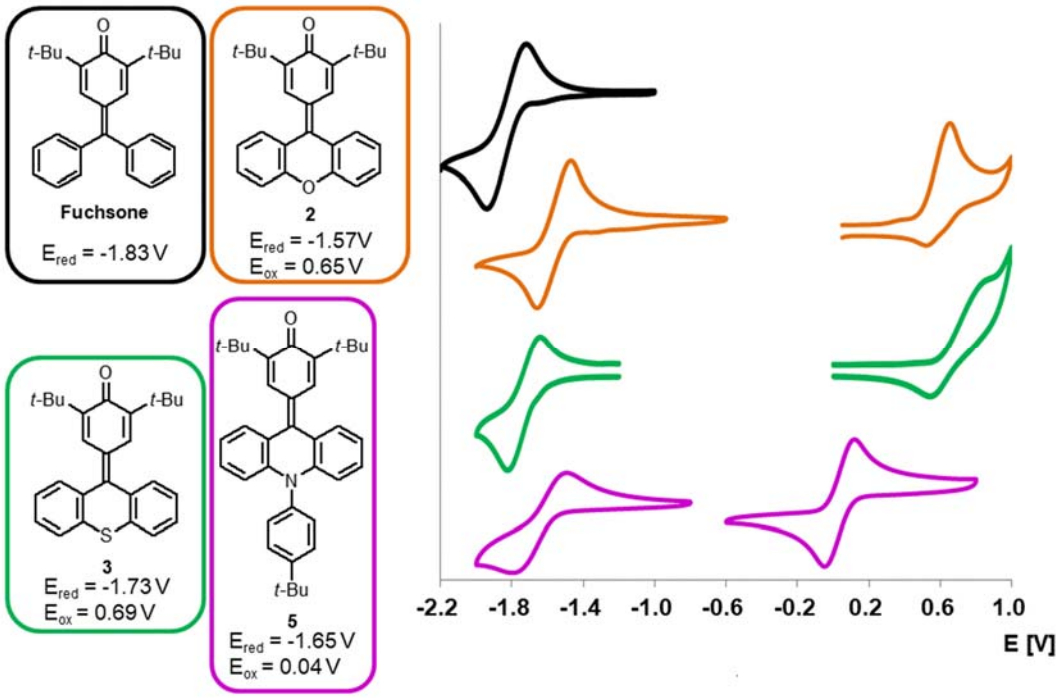
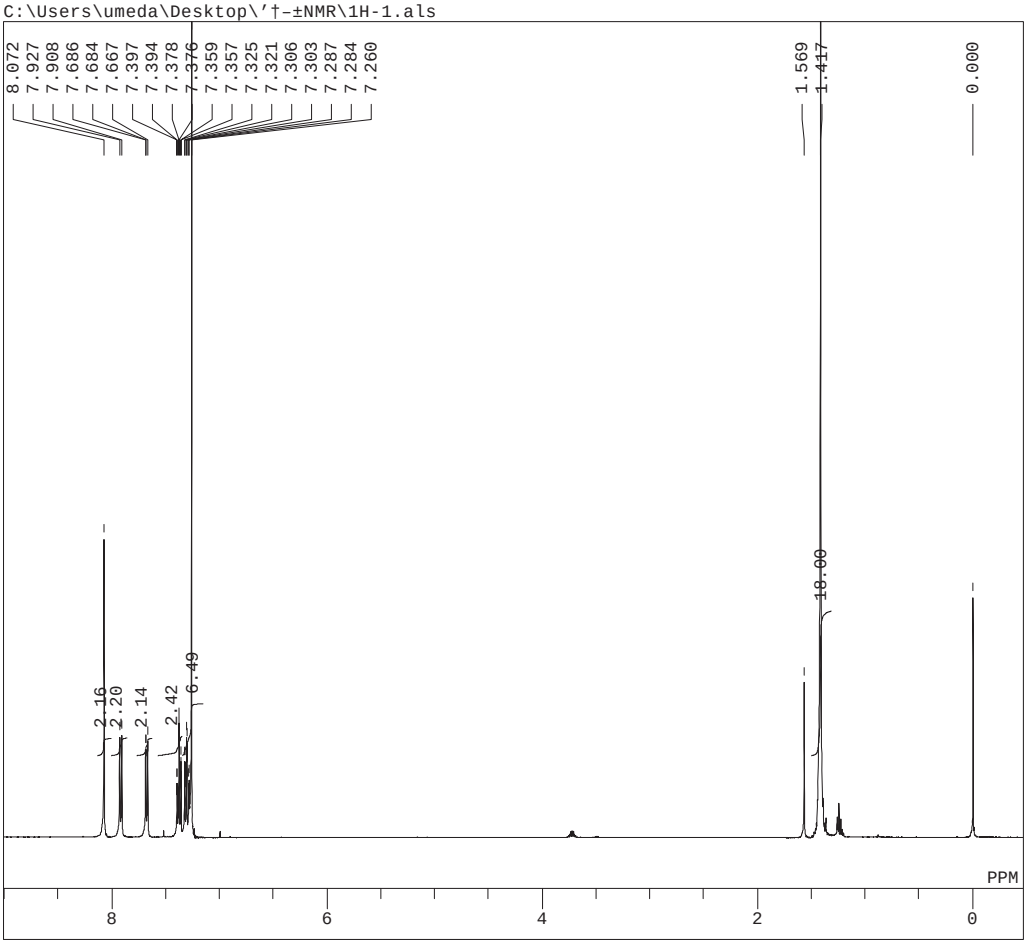


Figure S4. Cyclic voltammogram of Fuchsone, **2**, **3**, and **5** in THF; V versus (Ag/Ag^{+}) in 0.1 M with $n$$Bu_4NPF_6$ in THF scan rate: 100 mV/S, working electrode: glassy carbon, ferrocene / ferrocenium (Fc/Fc^{+}) = 0 V

5. ^{1}H and ^{13}C NMR Spectra of 1-9 and 11

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EXMOD   NON
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OBSET         124.00 KHz
OBFIN       10500.00 Hz
POINT          32768
FREQU         7992.01 Hz
SCANS             32
ACQTM          4.1001 sec
PD             2.9000 sec
PW1              6.50 usec
IRNUC   1H
CTEMP           19.1 c
SLVNT   CDCL3
EXREF            0.00 ppm
BF               0.12 Hz
RGAIN              15
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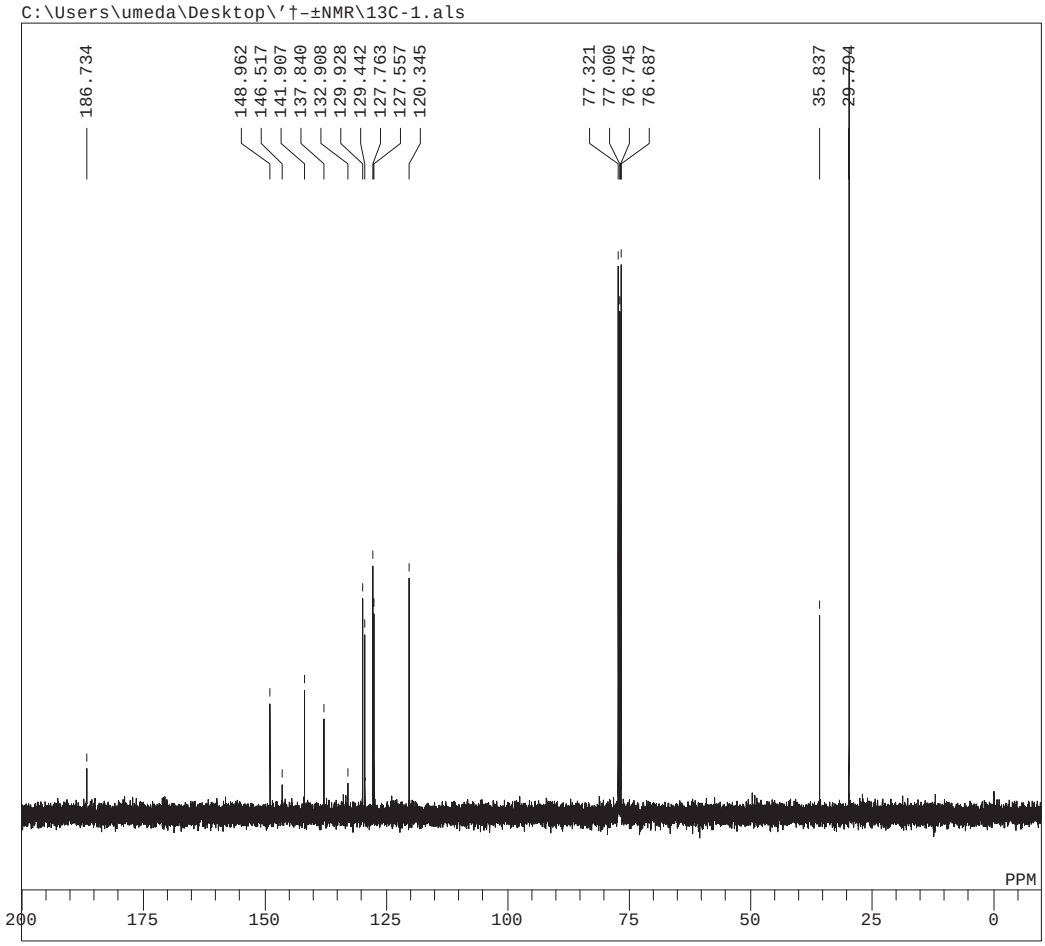


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EXMOD   BCM
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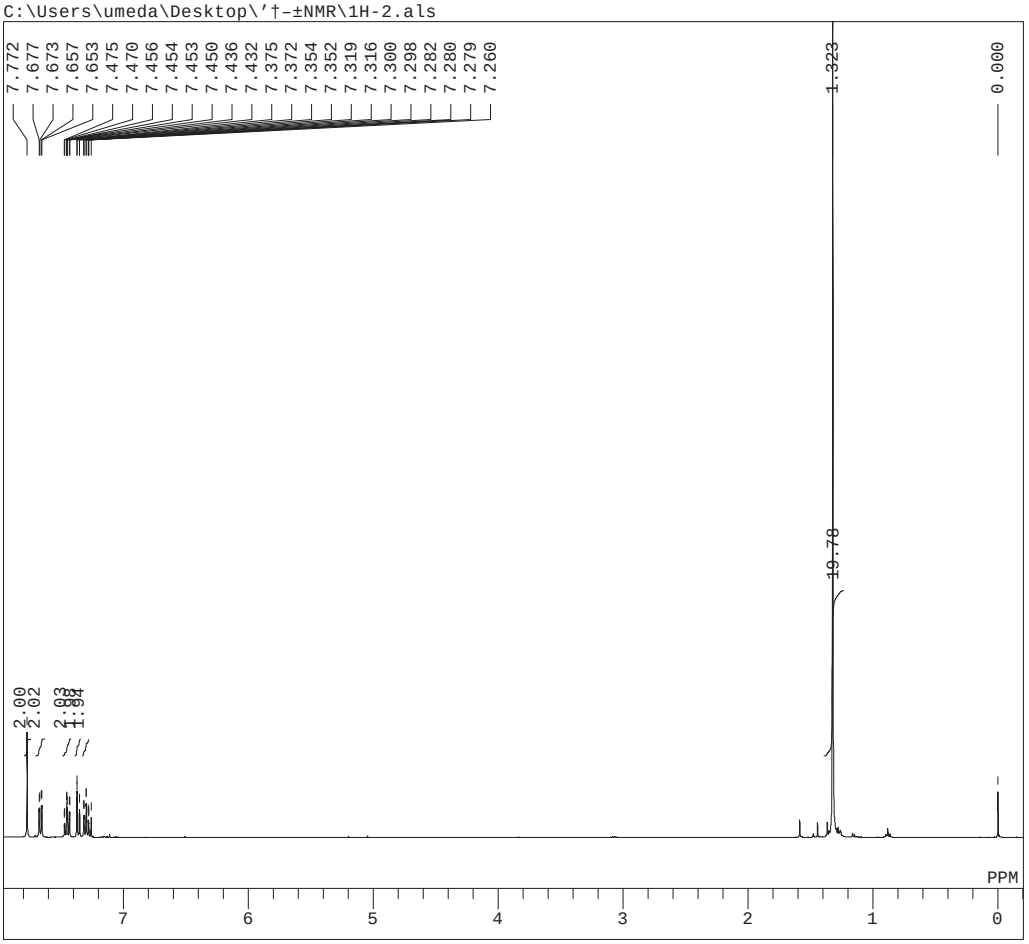
OBSET         125.00 KHz
OBFIN       10500.00 Hz
POINT          32768
FREQU       27118.64 Hz
SCANS            256
ACQTM          1.2083 sec
PD             1.7920 sec
PW1              5.70 usec
IRNUC   1H
CTEMP           19.4 c
SLVNT   CDCL3
EXREF           77.00 ppm
BF               0.12 Hz
RGAIN              24
```

Fig. S5. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **1** in $CDCl_3$

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EXMOD   NON
OBFRQ         399.65 MHz
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OBFIN       10500.00 Hz
POINT          32768
FREQU         7992.01 Hz
SCANS             32
ACQTM          4.1001 sec
PD             2.9000 sec
PW1              6.50 usec
IRNUC   1H
CTEMP           18.1 c
SLVNT   CDCL3
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             13
```
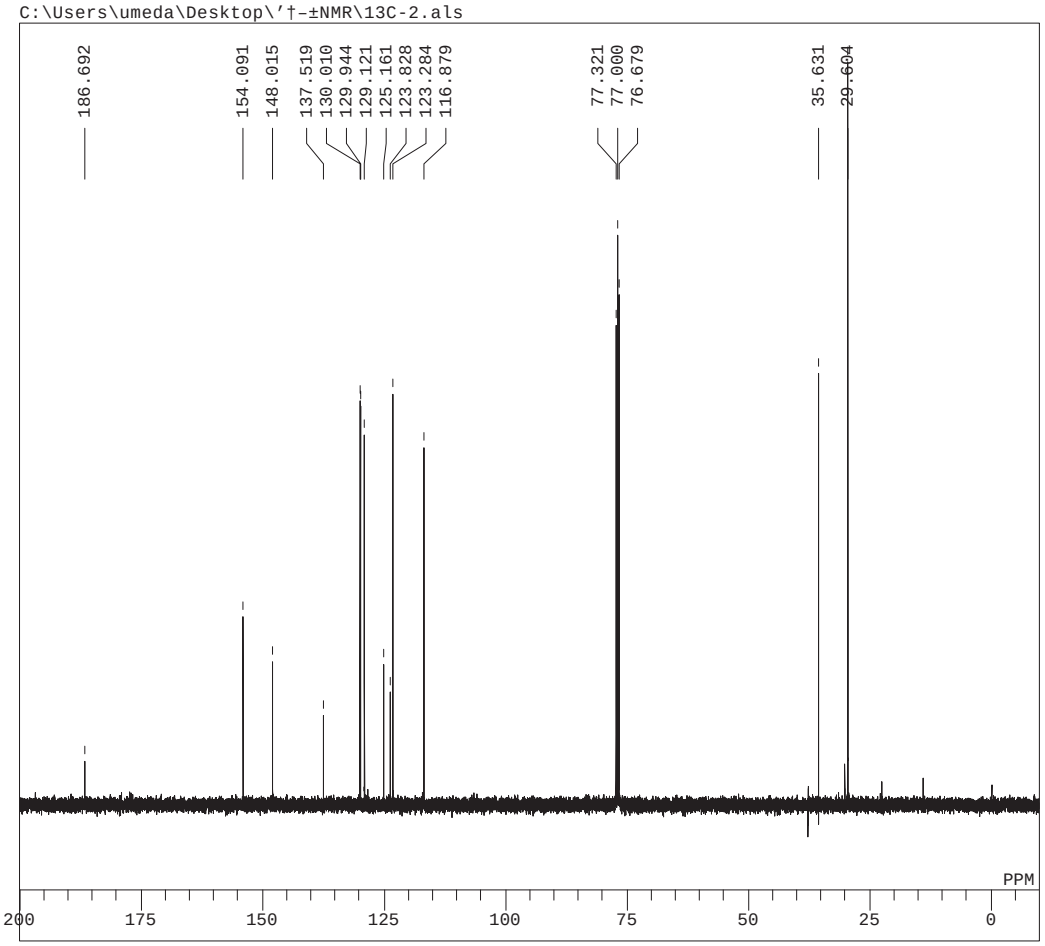
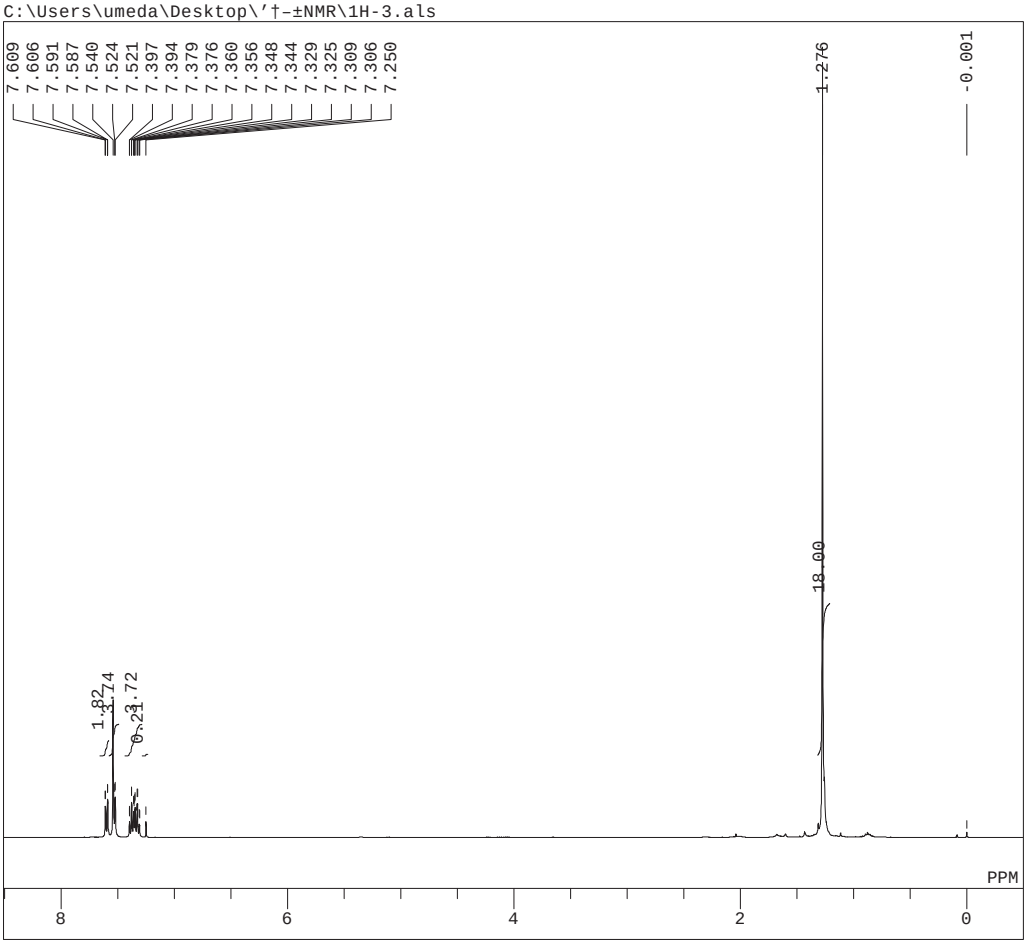
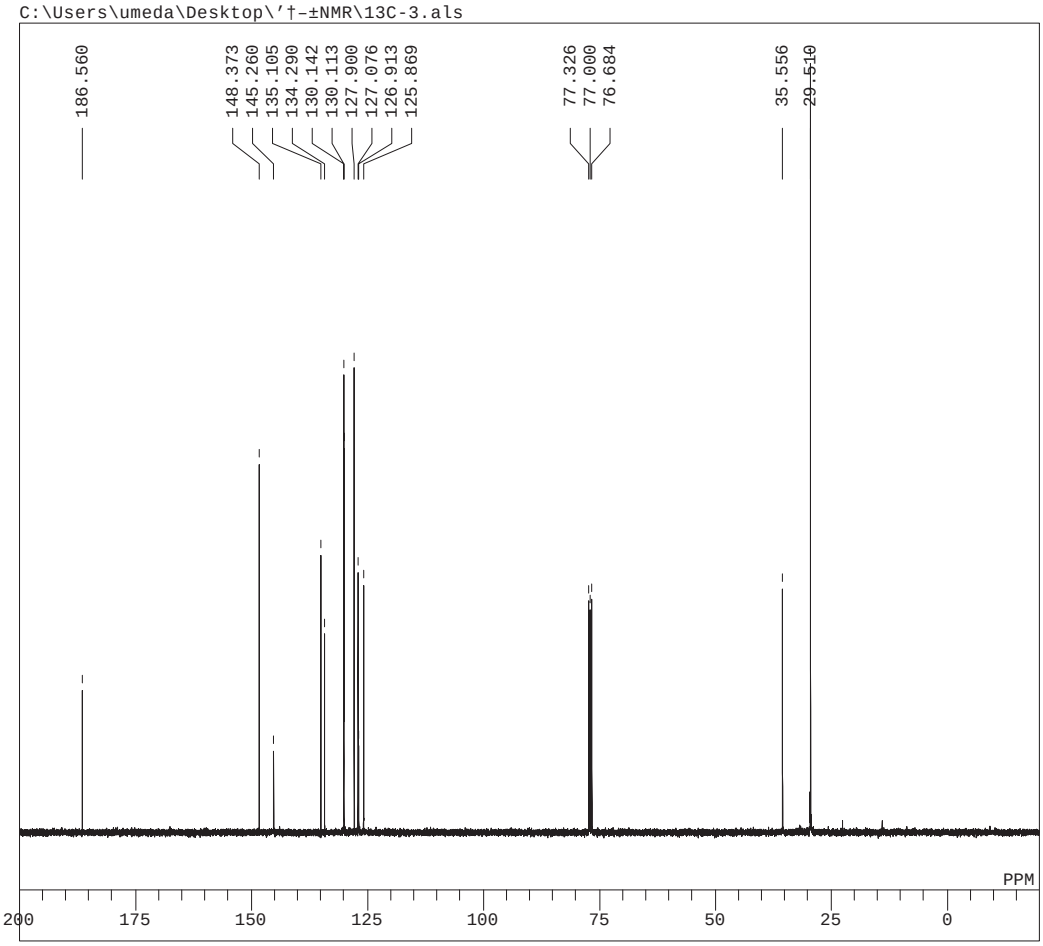




```
DFILE   13C-2.als
COMNT   auto
DATIM   Sun Dec 05 16:34:55 2010
OBNUC   13C
EXMOD   BCM
OBFRQ         100.40 MHz
OBSET         125.00 KHz
OBFIN       10500.00 Hz
POINT          32768
FREQU       27118.64 Hz
SCANS            512
ACQTM          1.2083 sec
PD             1.7920 sec
PW1              5.70 usec
IRNUC   1H
CTEMP           18.6 c
SLVNT   CDCL3
EXREF          77.00 ppm
BF              0.12 Hz
RGAIN             24
```

Fig. S6. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **2** in $CDCl_3$

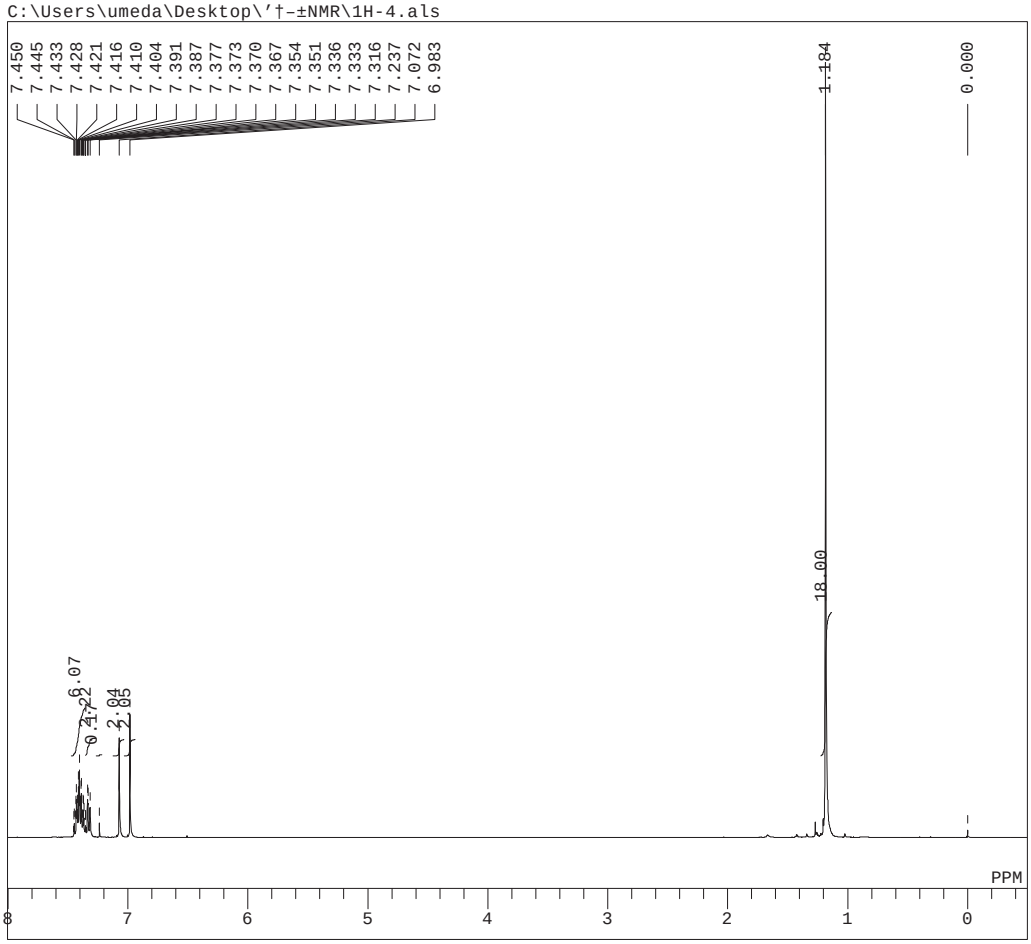



```
DFILE   1H-3.als
COMNT   single_pulse
DATIM   2012-09-09 22:37:44
OBNUC   1H
EXMOD   proton.jxp
OBFRQ         395.88 MHz
OBSET           6.28 KHz
OBFIN           0.87 Hz
POINT          16384
FREQU        7422.80 Hz
SCANS             32
ACQTM         2.2073 sec
PD            5.0000 sec
PW1             5.85 usec
IRNUC   1H
CTEMP           23.7 c
SLVNT   CDCL3
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             24
```

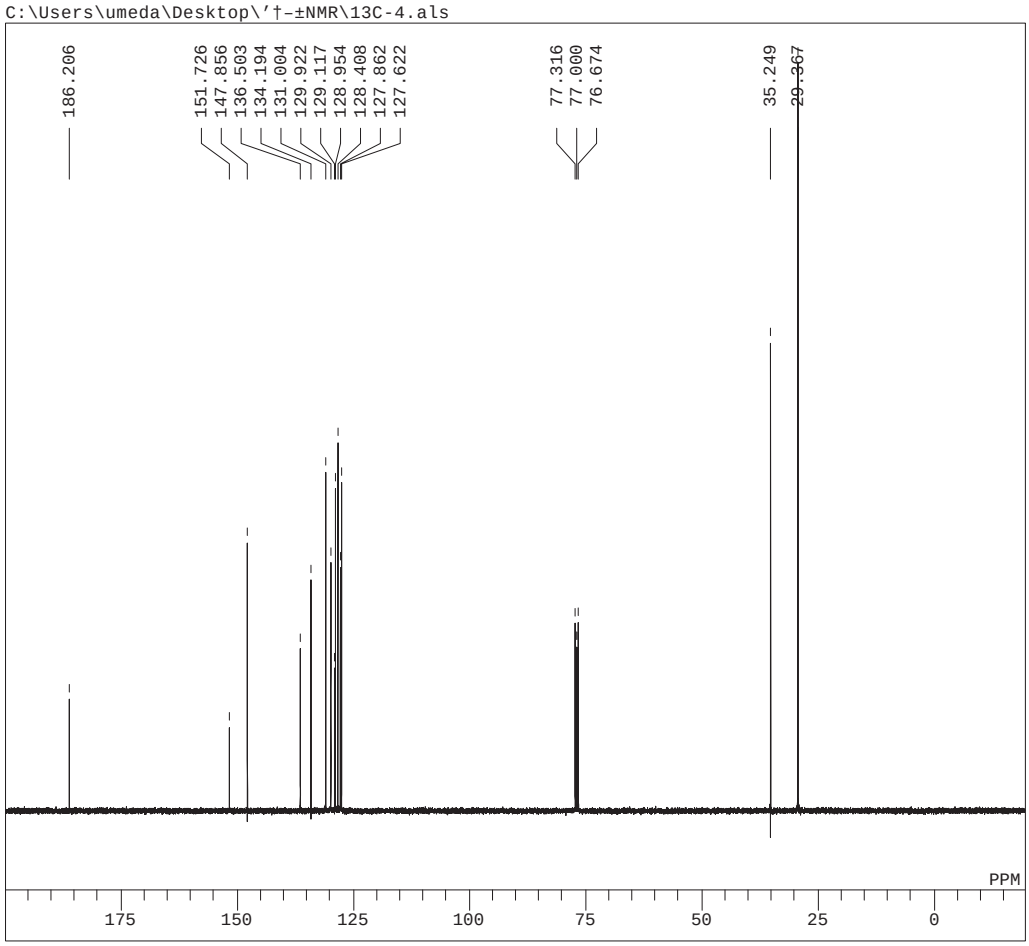



```
DFILE   13C-3.als
COMNT   single pulse decoupled gated N
DATIM   2012-09-09 22:42:04
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ          99.55 MHz
OBSET           5.13 KHz
OBFIN           0.98 Hz
POINT          32767
FREQU       31250.00 Hz
SCANS            256
ACQTM         1.0486 sec
PD            2.0000 sec
PW1             3.15 usec
IRNUC   1H
CTEMP           23.9 c
SLVNT   CDCL3
EXREF          77.00 ppm
BF              0.12 Hz
RGAIN             60
```

Fig. S7. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **3** in $CDCl_3$

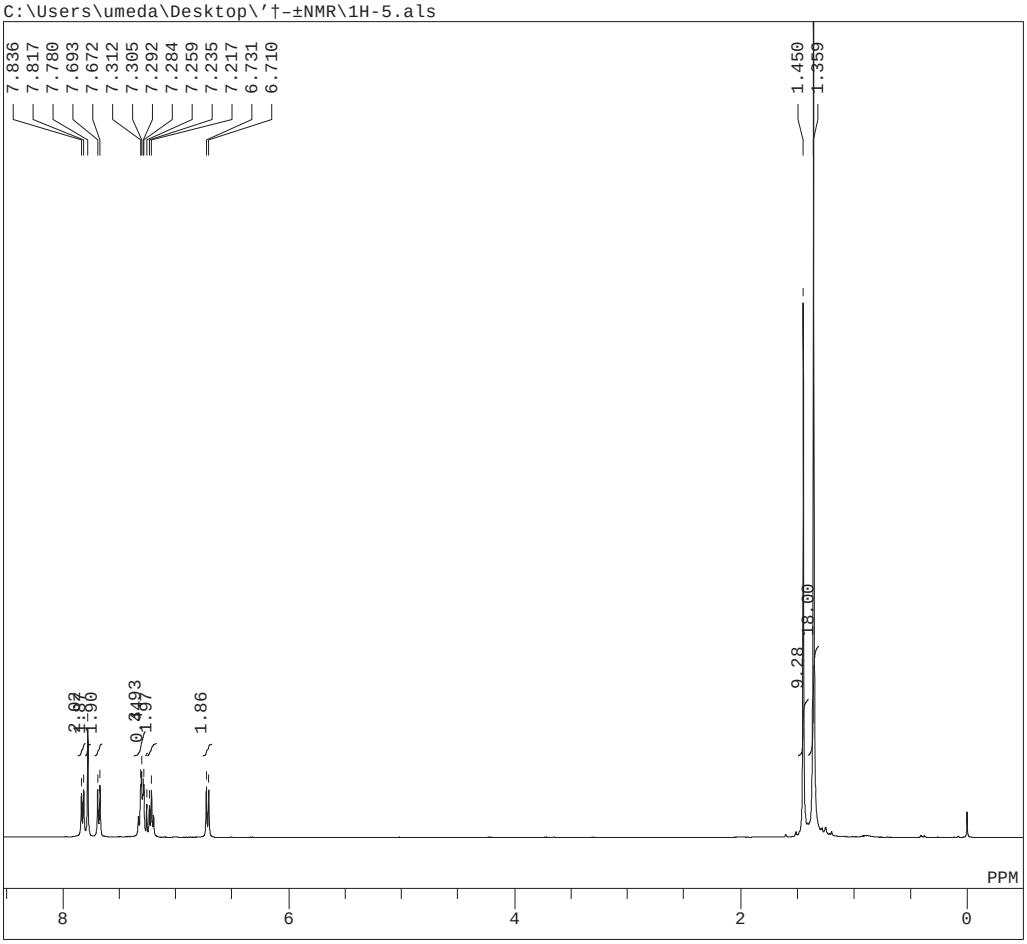



```
DFILE   1H-4.als
COMNT   single_pulse
DATIM   2012-07-19 15:35:52
OBNUC   1H
EXMOD   proton.jxp
OBFRQ         395.88 MHz
OBSET           6.28 KHz
OBFIN           0.87 Hz
POINT          16384
FREQU        7422.80 Hz
SCANS             16
ACQTM         2.2073 sec
PD            5.0000 sec
PW1             5.85 usec
IRNUC   1H
CTEMP           22.9 c
SLVNT   CDCL3
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             22
```

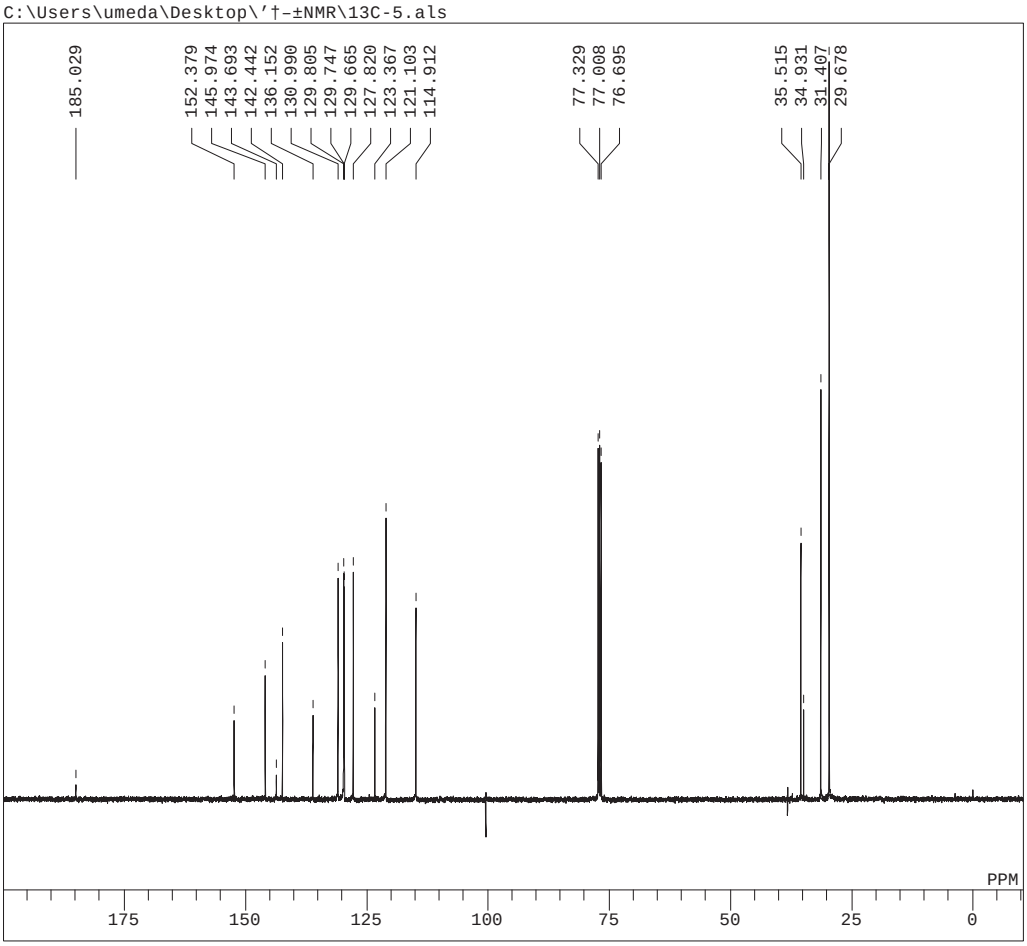



```
DFILE   13C-4.als
COMNT   single pulse decoupled gated N
DATIM   2012-07-19 15:38:17
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ          99.55 MHz
OBSET           5.13 KHz
OBFIN           0.98 Hz
POINT          32767
FREQU       31250.00 Hz
SCANS            256
ACQTM         1.0486 sec
PD            2.0000 sec
PW1             3.15 usec
IRNUC   1H
CTEMP           23.4 c
SLVNT   CDCL3
EXREF          77.00 ppm
BF              0.12 Hz
RGAIN             60
```

Fig. S8. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **4** in $CDCl_3$

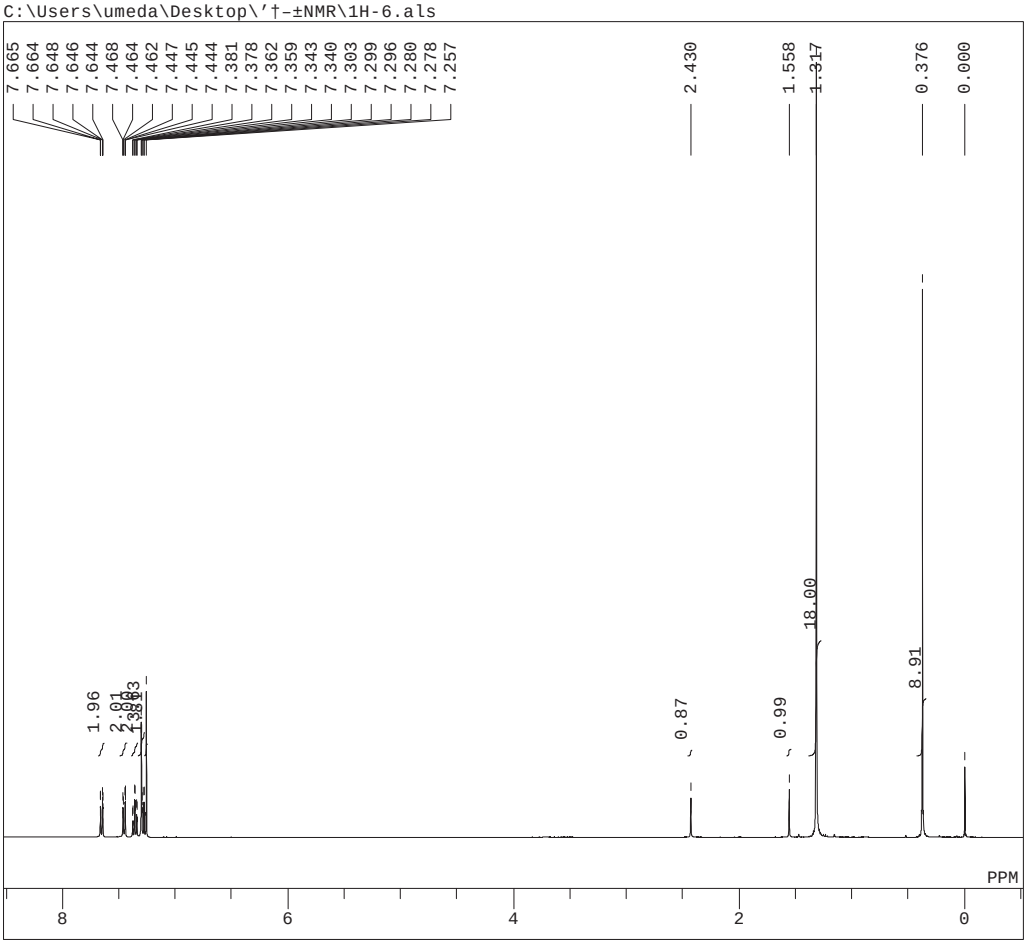


DFILE 1H-5.als
COMNT auto
DATIM Sun Jan 23 03:45:33 2011
OBNUC 1H
EXMOD NON
OBFRQ 399.65 MHz
OBSET 124.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 7992.01 Hz
SCANS 32
ACQTM 4.1001 sec
PD 2.9000 sec
PW1 6.50 usec
IRNUC 1H
CTEMP 11.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 11

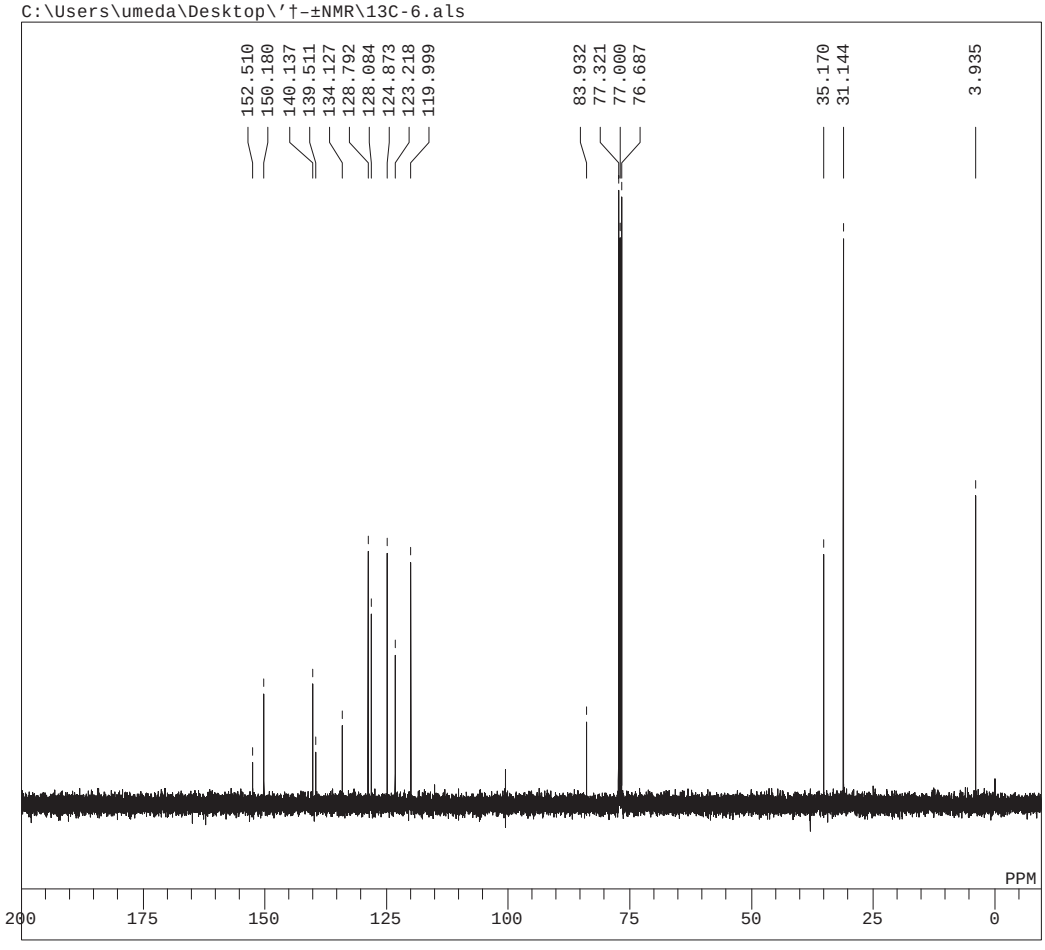


DFILE 13C-5.als
COMNT auto
DATIM Sun Jan 23 04:44:35 2011
OBNUC 13C
EXMOD BCM
OBFRQ 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.00 Hz
POINT 32768
FREQU 27118.64 Hz
SCANS 512
ACQTM 1.2083 sec
PD 1.7920 sec
PW1 5.70 usec
IRNUC 1H
CTEMP 11.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

Fig. S9. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **5** in $CDCl_3$

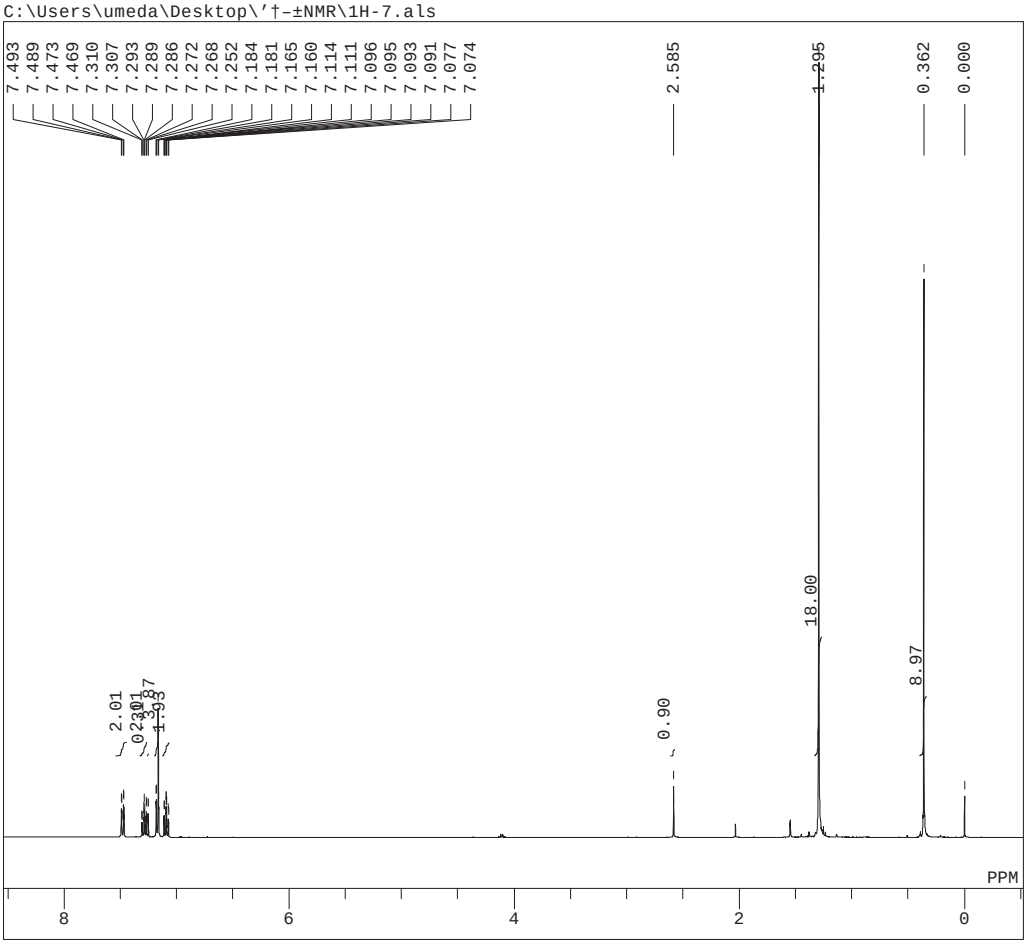



```
DFILE   1H-6.als
COMNT   auto
DATIM   Sat Dec 11 22:52:37 2010
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN      10500.00 Hz
POINT         32768
FREQU        7992.01 Hz
SCANS             32
ACQTM         4.1001 sec
PD            2.9000 sec
PW1             6.50 usec
IRNUC   1H
CTEMP           17.0 c
SLVNT   CDCL3
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             15
```

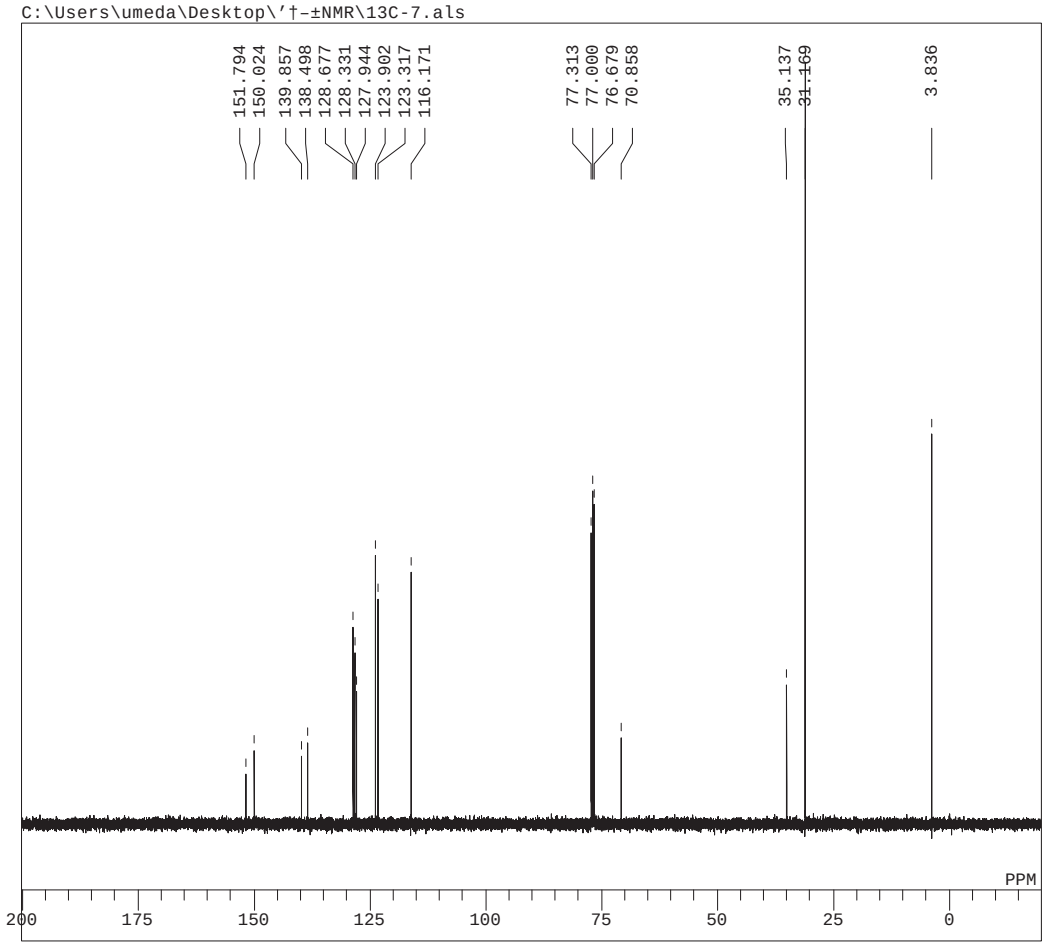



```
DFILE   13C-6.als
COMNT   auto
DATIM   Sat Dec 11 23:06:57 2010
OBNUC   13C
EXMOD   BCM
OBFRQ        100.40 MHz
OBSET        125.00 KHz
OBFIN      10500.00 Hz
POINT         32768
FREQU      27118.64 Hz
SCANS           256
ACQTM         1.2083 sec
PD            1.7920 sec
PW1             5.70 usec
IRNUC   1H
CTEMP           17.7 c
SLVNT   CDCL3
EXREF          77.00 ppm
BF              0.12 Hz
RGAIN             24
```

Fig. S10. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **6** in $CDCl_3$

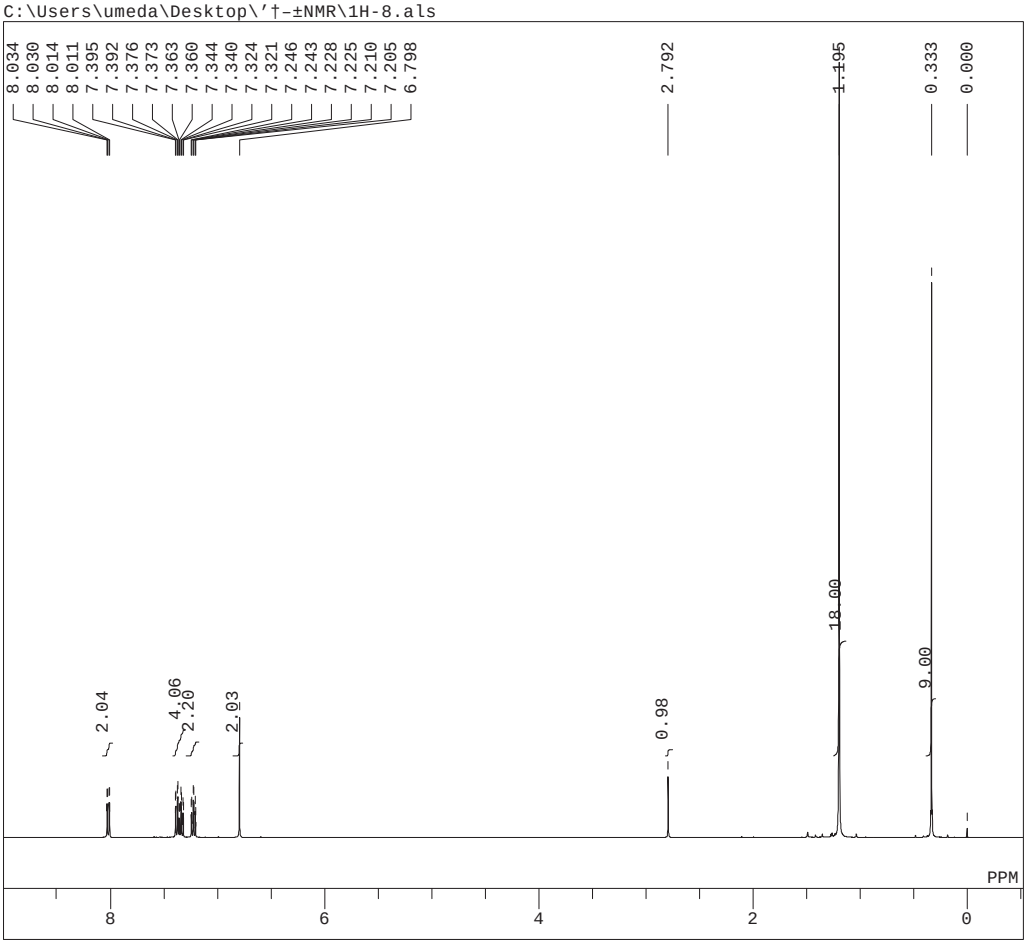



```
DFILE   1H-7.als
COMNT
DATIM   Thu Nov 25 20:38:57 2010
OBNUC   1H
EXMOD   NON
OBFRQ         399.65 MHz
OBSET         124.00 KHz
OBFIN       10500.00 Hz
POINT          32768
FREQU         7992.01 Hz
SCANS             32
ACQTM          4.1001 sec
PD             2.9000 sec
PW1              6.50 usec
IRNUC   1H
CTEMP           19.5 c
SLVNT   CDCL3
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             13
```

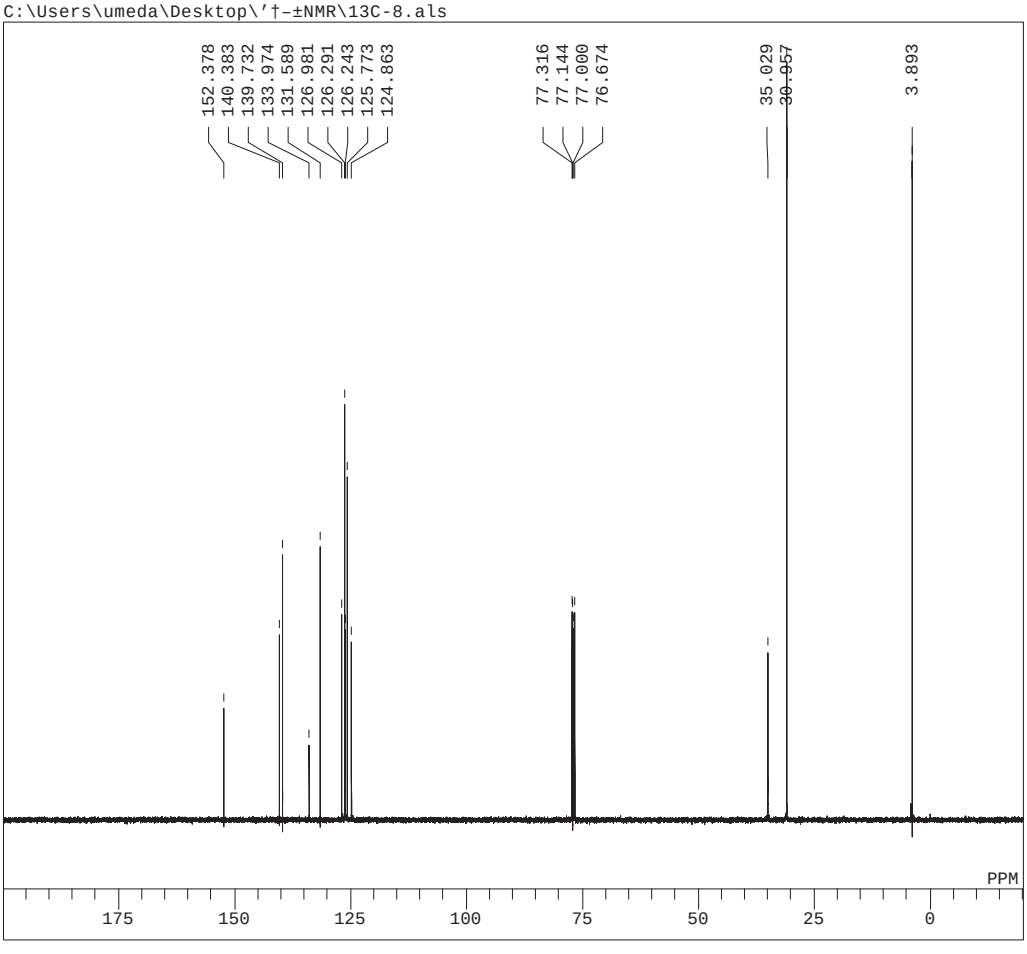



```
DFILE   13C-7.als
COMNT   auto
DATIM   Thu Nov 25 20:53:12 2010
OBNUC   13C
EXMOD   BCM
OBFRQ         100.40 MHz
OBSET         125.00 KHz
OBFIN       10500.00 Hz
POINT          32768
FREQU        27118.64 Hz
SCANS            256
ACQTM          1.2083 sec
PD             1.7920 sec
PW1              5.70 usec
IRNUC   1H
CTEMP           20.3 c
SLVNT   CDCL3
EXREF           77.00 ppm
BF              0.12 Hz
RGAIN             24
```

Fig. S11. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **7** in $CDCl_3$

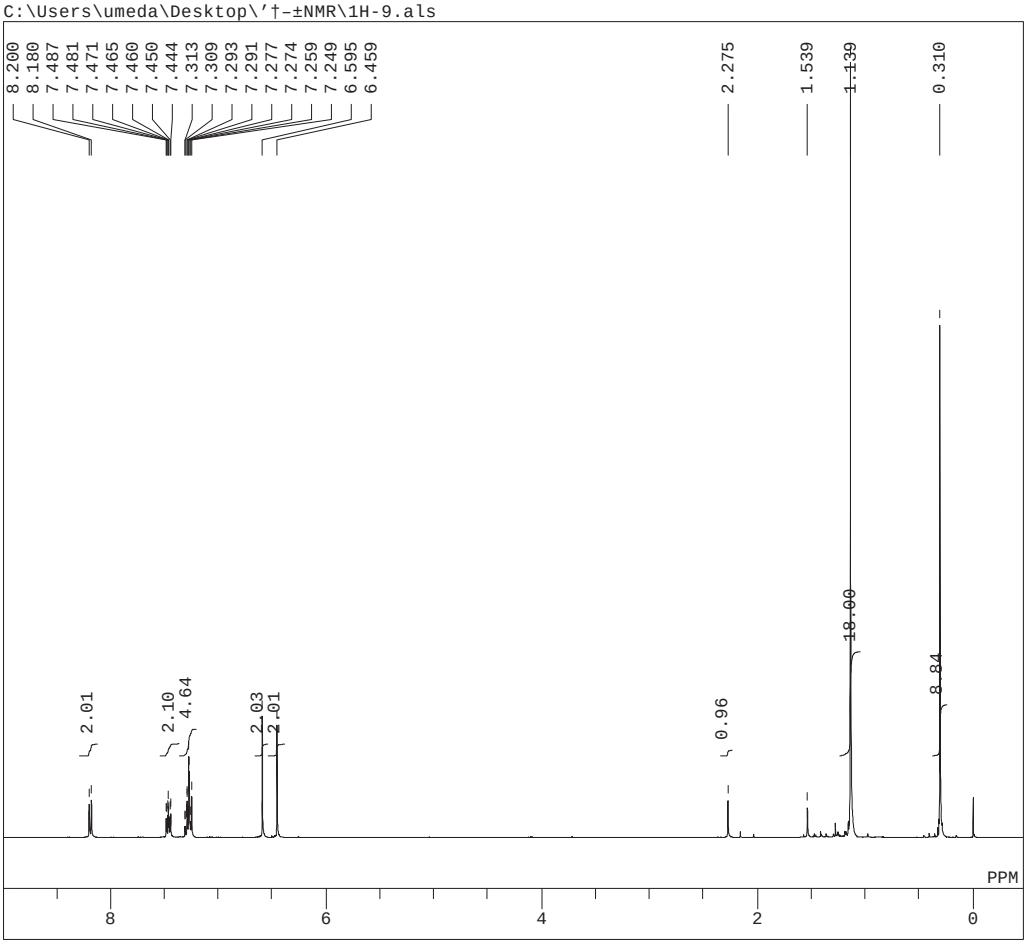



```
DFILE   1H-8.als
COMNT   single_pulse
DATIM   2012-09-18 17:06:48
OBNUC   1H
EXMOD   proton.jxp
OBFRQ         395.88 MHz
OBSET           6.28 KHz
OBFIN           0.87 Hz
POINT          16384
FREQU        7422.80 Hz
SCANS             32
ACQTM          2.2073 sec
PD             5.0000 sec
PW1              5.85 usec
IRNUC   1H
CTEMP           23.9 c
SLVNT   CDCL3
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             20
```

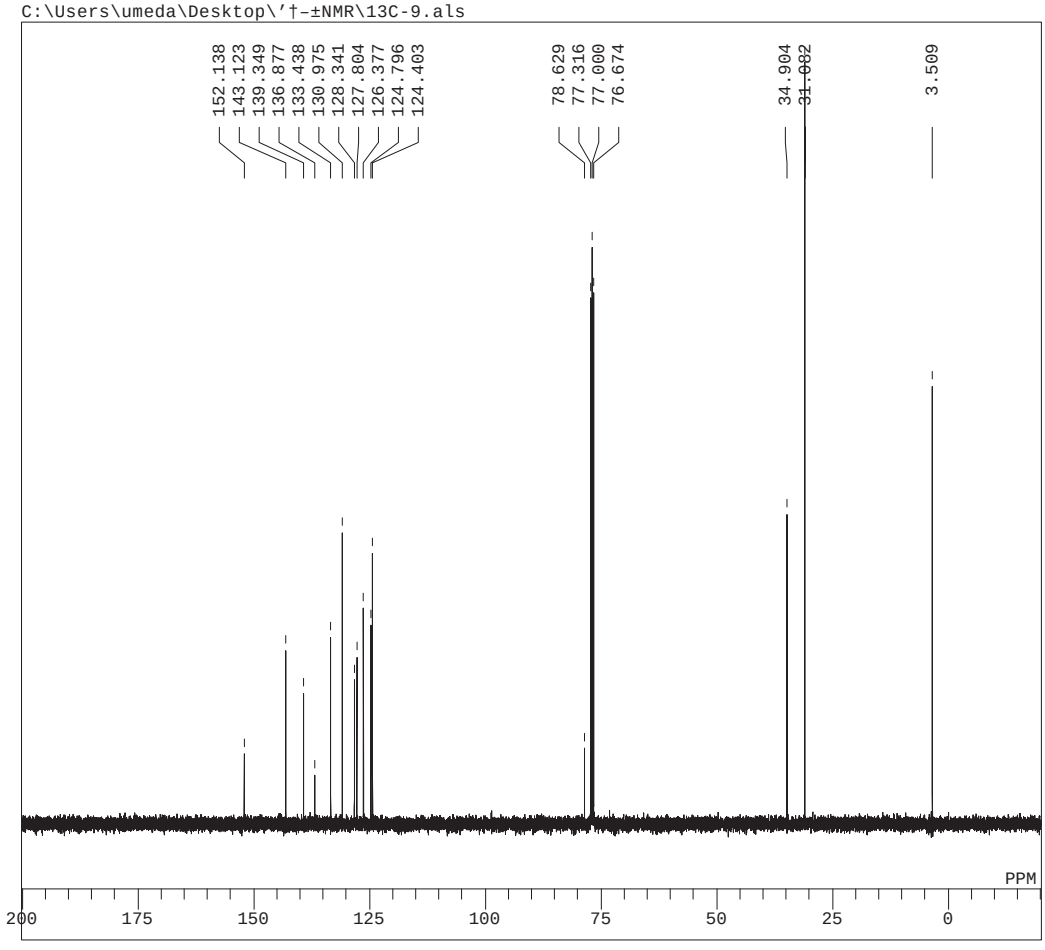



```
DFILE   13C-8.als
COMNT   single pulse decoupled gated N
DATIM   2012-09-18 17:11:08
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ          99.55 MHz
OBSET           5.13 KHz
OBFIN           0.98 Hz
POINT          32767
FREQU       31250.00 Hz
SCANS            256
ACQTM          1.0486 sec
PD             2.0000 sec
PW1              3.15 usec
IRNUC   1H
CTEMP           24.2 c
SLVNT   CDCL3
EXREF          77.00 ppm
BF              0.12 Hz
RGAIN             60
```

Fig. S12. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **8** in $CDCl_3$

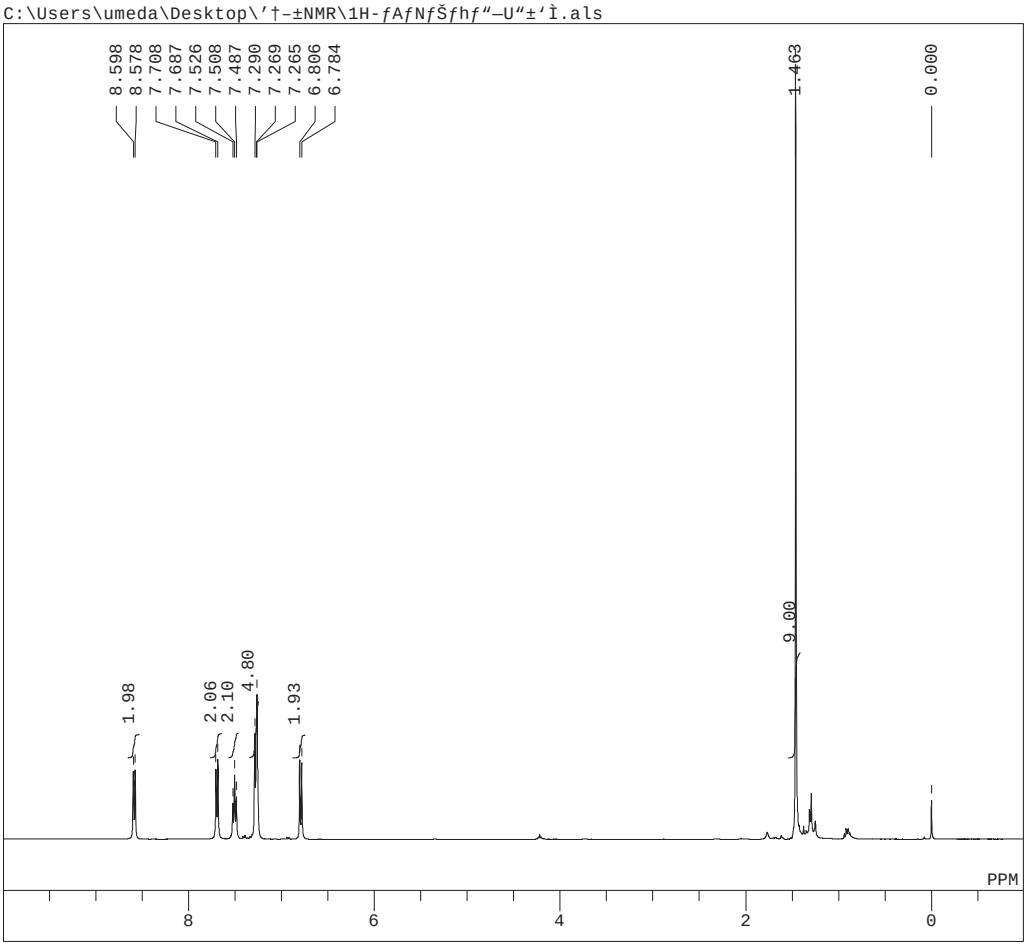



```
DFILE   1H-9.als
COMNT   single_pulse
DATIM   2012-07-19 15:56:34
OBNUC   1H
EXMOD   proton.jxp
OBFRQ         395.88 MHz
OBSET           6.28 KHz
OBFIN           0.87 Hz
POINT          16384
FREQU        7422.80 Hz
SCANS             16
ACQTM         2.2073 sec
PD            5.0000 sec
PW1             5.85 usec
IRNUC   1H
CTEMP           23.0 c
SLVNT   CDCL3
EXREF           0.00 ppm
BF              0.12 Hz
RGAIN             32
```

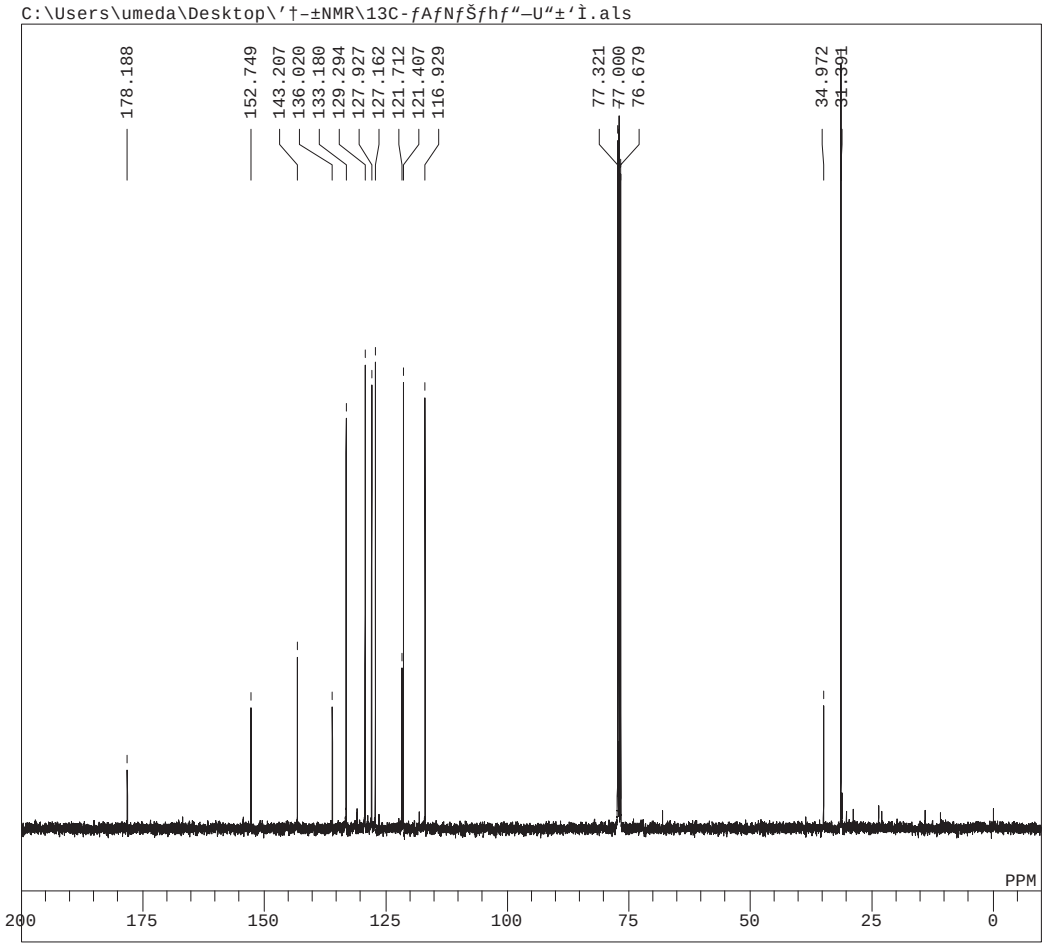



```
DFILE   13C-9.als
COMNT   single pulse decoupled gated N
DATIM   2012-07-19 15:58:59
OBNUC   13C
EXMOD   carbon.jxp
OBFRQ          99.55 MHz
OBSET           5.13 KHz
OBFIN           0.98 Hz
POINT          32767
FREQU       31250.00 Hz
SCANS            256
ACQTM         1.0486 sec
PD            2.0000 sec
PW1             3.15 usec
IRNUC   1H
CTEMP           23.5 c
SLVNT   CDCL3
EXREF          77.00 ppm
BF              0.12 Hz
RGAIN             60
```

Fig. S13. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **9** in $CDCl_3$




```
DFILE   1H-ƒAƒNƒŠƒhƒ"—U"±'Ì.als
COMNT   auto
DATIM   Tue Feb 15 14:36:37 2011
OBNUC   1H
EXMOD   NON
OBFRQ         399.65 MHz
OBSET         124.00 KHz
OBFIN       10500.00 Hz
POINT          32768
FREQU        7992.01 Hz
SCANS             32
ACQTM         4.1001 sec
PD            2.9000 sec
PW1             6.50 usec
IRNUC   1H
CTEMP           12.4 c
SLVNT   CDCL3
EXREF           0.00 ppm
BF              1.20 Hz
RGAIN             13
```




```
DFILE   13C-ƒAƒNƒŠƒhƒ"—U"±'Ì.als
COMNT   auto
DATIM   Tue Feb 15 15:03:39 2011
OBNUC   13C
EXMOD   BCM
OBFRQ         100.40 MHz
OBSET         125.00 KHz
OBFIN       10500.00 Hz
POINT          32768
FREQU       27118.64 Hz
SCANS            512
ACQTM         1.2083 sec
PD            1.7920 sec
PW1             5.70 usec
IRNUC   1H
CTEMP           12.4 c
SLVNT   CDCL3
EXREF          77.00 ppm
BF              1.20 Hz
RGAIN             25
```

Fig. S14. ^{1}H (400 MHz) and ^{13}C NMR (100 MHz) Spectra of **11** in $CDCl_3$