Supporting Information

Synthesis of Substituted Dihydrobenzofurans and Bis-dihydrobenzofurans

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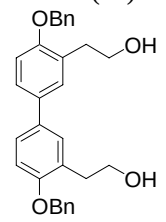
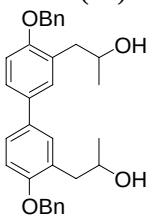
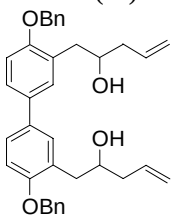
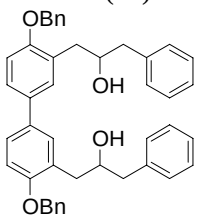
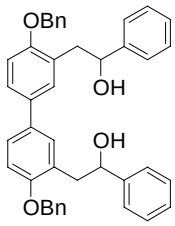
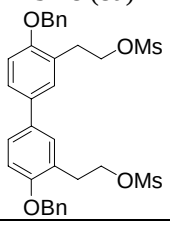
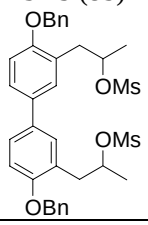
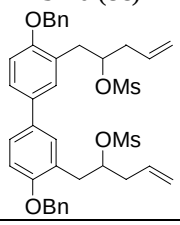
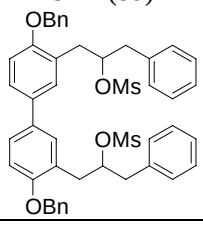
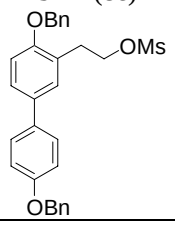
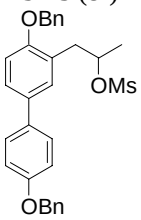
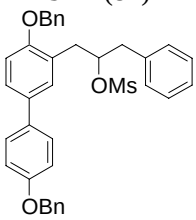
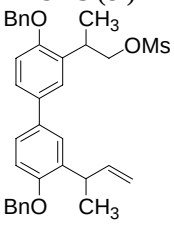
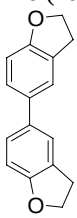
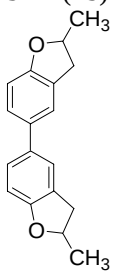
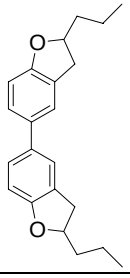
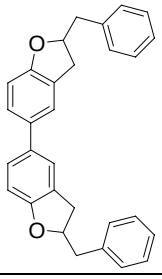
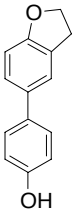
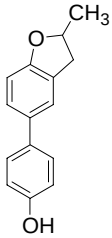
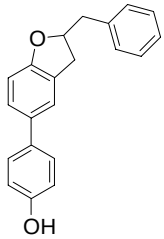
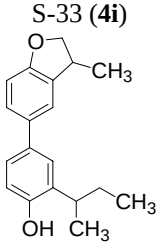
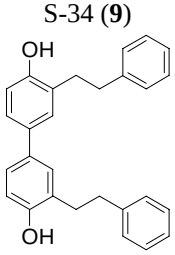
S-13 (**7a**) 	S-14 (**7b**) 	S-15 (**7c**) 	S-16 (**7d**) 	S-17 (**7e**) 
S-18 (**8a**) 	S-19 (**8b**) 	S-20 (**8c**) 	S-21 (**8d**) 	S-22 (**8e**) 
S-23 (**8f**) 	S-24 (**8h**) 	S-25 (**8i**) 	S-26 (**4a**) 	S-27 (**4b**) 
S-28 (**4c**) 	S-29 (**4d**) 	S-30 (**4e**) 	S-31 (**4f**) 	S-32 (**4h**) 
S-33 (**4i**) 	S-34 (**9**) 			

Experimental section

1. General. All other reagents and solvents were obtained from commercial sources and used without further purification. Reactions were routinely carried out under an atmosphere of dry nitrogen with magnetic stirring. Products in organic solvents were dried with anhydrous magnesium sulfate before concentration in vacuo. Melting points were determined with a SMP3 melting apparatus. ^{1}H and ^{13}C NMR spectra were recorded on a Varian INOVA-400 spectrometer operating at 200/400 and at 50/100 MHz, respectively. Chemical shifts (δ) are reported in parts per million (ppm) and the coupling constants (*J*) are given in Hertz. High resolution mass spectra (HRMS) were measured with a mass spectrometer Finnigan/Thermo Quest MAT 95XL. X-ray crystal structures were obtained with an Enraf-Nonius FR-590 diffractometer (CAD4, Kappa CCD). Elemental analyses were carried out with Heraeus Vario III-NCSH, Heraeus CHN-OS-Rapid Analyzer or Elementar Vario EL III.

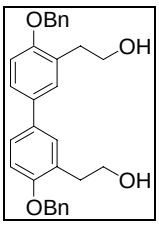
3. A representative procedure of skeleton (6) is as follows: K_2CO_3 (4.14 g, 30.0 mmol) was added to a stirred solution of compound (**3**) (1.86 g, 10.0 mmol) in acetone (50 mL) at rt. The reaction mixture was stirred at reflux for 10 min. Benzyl bromide (3.54 g, 20.5 mmol) was added to the reaction mixture at reflux. The reaction mixture was stirred at reflux for 10 h. The solvent was concentrated under reduced pressure and water (20 mL) was added to the reaction mixture. The residue was extracted with EtOAc (3 x 30 mL). The combined organic layers were washed with brine, dried, filtered and evaporated to afford crude product under reduced pressure in quantitative yield. Without further purification, $AlCl_3$ (2.67 g, 20.0 mmol) was added to a solution of the resulting dibenzyl compound in DCM (50 mL) at rt. After being stirred at rt for 10 min, a solution of chloroacetaldehyde (1.57 g, 20.0 mmol for compound (**6a**); 0.78 g, 10.0 mmol for compound (**6b**) or 2-chloropropanaldehyde (1.85 g, 20.0 mmol, for compound (**6c**)) in DCM (5 mL) was added to the reaction mixture at -30 ^{o}C. The reaction mixture was stirred at -30 ^{o}C for 10 h. After being stirred at rt for 5 h, The solvent was concentrated under reduced pressure and water (20 mL) was added to the reaction mixture. The residue was extracted with EtOAc (3 x 30 mL). The combined organic layers were washed with brine, dried, filtered and evaporated to afford crude product under reduced pressure. Purification on silica gel (hexanes/EtOAc = 8/1~5/1) afforded compounds (**6a**)~(**6c**).

3.1. [4,4'-Bis-benzyloxy-3'-(2-oxo-ethyl)-biphenyl-3-yl]-acetaldehyde (6a). Yield = 51% (2.29 g); Colorless oil; HRMS (ESI, M^{+}+1) calcd for $C_{30}H_{27}O_4$ 451.1909, found 451.1912; ^{1}H NMR (200 MHz, $CDCl_3$): δ 9.77 (br s, 2H), 7.42-7.27 (m, 14H), 7.02 (d, *J* = 8.4 Hz, 2H), 5.13 (s, 4H), 3.77 (s, 4H).

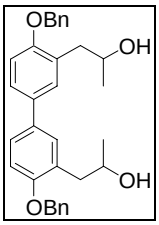
3.2. [(4,4'-Bis-benzyloxy-biphenyl-3-yl)-acetaldehyde (6b). Yield = 60% (2.45 g); Colorless oil; HRMS (ESI, M^{+}+1) calcd for $C_{28}H_{25}O_3$ 409.1804, found 409.1809; ^{1}H NMR (200 MHz, $CDCl_3$): δ 9.78 (br s, 2H), 7.49-7.35 (m, 14H), 7.05-7.01 (m, 2H), 5.13 (s, 2H), 5.11 (s, 2H), 3.76 (s, 2H).

3.3. 2-[4,4'-Bis-benzyloxy-3'-(1-methyl-2-oxo-ethyl)-biphenyl-3-yl]-propionaldehyde (6c). Yield = 21% (1.0 g); Colorless oil; HRMS (ESI, M^{+}+1) calcd for $C_{32}H_{31}O_4$ 479.2222, found 479.2231; ^{1}H NMR (200 MHz, $CDCl_3$): δ 9.21 (br s, 2H), 7.48-7.30 (m, 14H), 6.99 (d, *J* = 8.4 Hz, 2H), 5.12 (s, 4H), 3.89 (q, *J* = 7.0 Hz, 2H), 1.44 (d, *J* = 7.0 Hz, 6H).

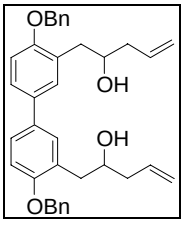
4. A representative procedure of compounds (7a)~(7d) is as follows: $NaBH_4$ (103 mg, 3.0 mmol; for compound (**7a**)) or Grignard reagent (1.0 M, 3.0 mL, 3.0 mmol, R = Me, allyl, Bn, Ph; for compounds (**7b**)~(**7e**)) was added to a solution of compound (**6a**) (450 mg, 1.0 mmol) in THF (10 mL) at rt. The reaction mixture was stirred at rt for 5 h. $HCl_{(aq)}$ (6 N, 4 mL) was added to the reaction mixture and the solvent was concentrated under reduced pressure. The residue was extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine, dried, filtered and evaporated to afford crude product under reduced pressure. Purification on silica gel (hexanes/EtOAc = 4/1~1/1) afforded compounds (**7a**)~(**7d**).



4.1. 2-[4,4'-Bis-benzyloxy-3'-(2-hydroxy-ethyl)-biphenyl-3-yl]-ethanol (7a). Yield = 88% (400 mg); Colorless solid; M.p. = 128-129 ^oC (recrystallized from hexanes and EtOAc); HRMS (ESI, M^++1) calcd for $C_{30}H_{31}O_4$ 452.2222, found 452.2228; ^1H NMR (400 MHz, $CDCl_3$): δ 7.46-7.33 (m, 14H), 6.98 (d,*J* = 8.4 Hz, 2H), 5.12 (s, 4H), 3.90 (t, *J* = 6.8 Hz, 4H), 3.01 (t, *J* = 6.4 Hz, 4H), 1.81 (br s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.92 (2x), 136.95 (2x), 133.48 (2x), 129.48 (2x), 128.61 (4x), 127.95 (2x), 127.59 (2x), 127.23 (4x), 125.89 (2x), 112.04 (2x), 70.14 (2x), 62.78 (2x), 34.34 (2x).

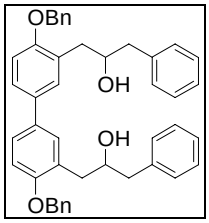


4.2. 1-[4,4'-Bis-benzyloxy-3'-(2-hydroxy-propyl)-biphenyl-3-yl]-propan-2-ol (7b). Yield = 76% (366 mg); Colorless solid; M.p. = 105-106 ^oC (recrystallized from hexanes and EtOAc); HRMS (ESI, M^++1) calcd for $C_{32}H_{35}O_4$ 483.2535, found 483.2541; ^1H NMR (400 MHz, $CDCl_3$): δ 7.46-7.32 (m, 14H), 6.98 (d, *J* = 9.2 Hz, 2H), 5.13 (s, 4H), 4.19-4.11 (m, 2H), 2.98 (dd, *J* = 4.4, 13.2 Hz, 2H), 2.81 (dd, *J* = 8.0, 13.2 Hz, 2H), 1.26 (d, *J* = 6.0 Hz, 6H), 2.00 (br s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.93 (2x), 136.94 (2x), 133.47, 133.45, 129.89 (2x), 128.64 (4x), 127.95 (2x), 127.65 (2x), 127.17 (4x), 125.95 (2x), 112.12 (2x), 70.19 (2x), 68.05 (2x), 40.68 (2x), 23.08 (2x); Anal. Calcd for $C_{32}H_{34}O_4$: C, 79.64; H, 7.10. Found: C,79.87; H, 7.32.

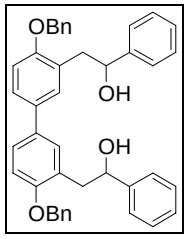


4.3. 1-[4,4'-Bis-benzyloxy-3'-(2-hydroxy-pent-4-enyl)-biphenyl-3-yl]-pent-4-en-2-ol (7c). Yield =

89% (475 mg); Colorless solid; M.p. = 117-118 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{36}H_{39}O_4$ 535.2848, found 535.2850; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44-7.31 (m, 14H), 6.96 (d, *J* = 9.2 Hz, 2H), 5.91-5.81 (m, 2H), 5.16-5.09 (m, 4H), 5.11 (s, 4H), 4.03-3.97 (m, 2H), 3.01 (dd, *J* = 4.0, 13.6 Hz, 2H), 2.80 (dd, *J* = 4.0, 13.6 Hz, 2H), 2.37-2.23 (m, 4H), 2.11 (br s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.92 (2x), 136.92 (2x), 135.04 (2x), 133.47 (2x), 129.90 (2x), 128.58 (4x), 127.93 (2x), 127.58 (2x), 127.20 (4x), 125.93 (2x), 117.63 (2x), 112.13 (2x), 70.94 (2x), 70.21 (2x), 41.53 (2x), 38.28 (2x); Anal. Calcd for $C_{36}H_{38}O_4$: C, 80.87; H, 7.16. Found: C, 80.54; H, 7.32.



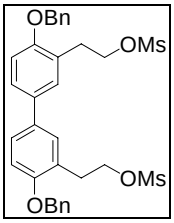
4.4. 1-[4,4'-Bis-benzyloxy-3'-(2-hydroxy-3-phenyl-propyl)-biphenyl-3-yl]-3-phenyl-propan-2-ol (7d). Yield = 80% (507 mg); Colorless solid; M.p. = 164-165 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{44}H_{43}O_4$ 635.3161, found 635.3170; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42-7.33 (m, 14H), 7.30-7.17 (m, 10H), 6.98 (d, *J* = 9.2 Hz, 2H), 5.11 (s, 4H), 4.25-4.20 (m, 2H), 3.06 (dd, *J* = 4.0, 13.6 Hz, 2H), 2.89-2.79 (m, 6H), 2.01 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.96 (2x), 138.76 (2x), 136.95 (2x), 133.50 (2x), 129.95 (2x), 129.42 (4x), 128.64 (4x), 128.40 (4x), 127.95 (2x), 127.57 (2x), 127.25 (4x), 126.28 (2x), 125.98 (2x), 112.12 (2x), 72.53 (2x), 70.24 (2x), 43.73 (2x), 38.52 (2x).



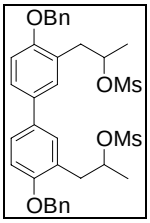
4.5. 2-[4,4'-Bis-benzyloxy-3'-(2-hydroxy-2-phenyl-ethyl)-biphenyl-3-yl]-1-phenyl-ethanol (7e). Yield = 80% (485 mg); Colorless solid; M.p. = 146-147 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{42}H_{39}O_4$ 607.2848, found 607.2855; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50-7.27 (m, 22H), 7.21 (d, *J* = 2.0 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 5.15 (s, 4H), 5.07-5.03 (m, 2H), 3.24 (dt, *J* = 4.0, 13.6 Hz, 2H), 3.03 (ddd, *J* = 3.2, 8.8, 13.6 Hz, 2H), 2.05 (br s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.96 (2x), 144.47 (2x), 136.92 (2x), 133.47 (2x), 130.16 (2x), 128.65 (4x), 128.26 (4x), 128.05 (2x), 127.38 (4x), 127.27 (2x), 127.15 (2x), 126.13 (2x), 125.75 (4x), 112.04 (2x), 74.16 (2x), 70.32 (2x), 41.56 (2x).

5. A representative procedure of compounds (8a)~(8d) is as follows: Et_3N (304 mg, 3.0 mmol) was added to a solution of compounds (**7a**)~(**7d**) (1.0 mmol) in DCM (40 mL) at rt. MsCl (275 mg, 2.4 mmol) was added to a reaction mixture at rt. The reaction mixture was stirred at rt for 5h. Saturated $NaHCO_{3\,(aq)}$ solution (5 mL) was added to the reaction mixture and the solvent was concentrated under

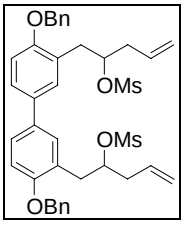
reduced pressure. The residue was extracted with EtOAc (3 x 30 mL). The combined organic layers were washed with brine, dried, filtered and evaporated to afford crude product under reduced pressure. Purification on silica gel (hexanes/EtOAc = 4/1~2/1) afforded compounds (**8a**)~(**8d**).



5.1. Methanesulfonic acid 2-[4,4'-bis-benzyloxy-3'-(2-methanesulfonyloxy-ethyl)-biphenyl-3-yl] -ethyl ester (8a). Yield = 89% (543 mg); Colorless solid; M.p. = 121-122 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{32}H_{35}O_8S_2$ 611.1773, found 611.1778; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48-7.34 (m, 14H), 7.00 (d, *J* = 8.4 Hz, 2H), 5.13 (s, 4H), 4.49 (t, *J* = 7.2 Hz, 4H), 3.18 (t, *J* = 7.2 Hz, 4H), 2.79 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.88 (2x), 136.72 (2x), 133.18 (2x), 129.48 (2x), 128.64 (4x), 128.05 (2x), 127.34 (4x), 126.48 (2x), 124.95 (2x), 112.02 (2x), 70.14 (2x), 69.27 (2x), 37.04 (2x), 31.00 (2x); Anal. Calcd for $C_{32}H_{34}O_8S_2$: C, 62.93; H, 5.61. Found: C, 63.21; H, 5.86.

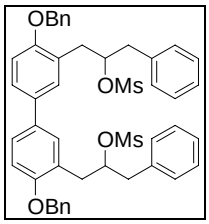


5.2. Methanesulfonic acid 2-[4,4'-bis-benzyloxy-3'-(2-methanesulfonyloxy-propyl)-biphenyl-3-yl] -1-methyl-ethyl ester (8b). Yield = 77% (491 mg); Colorless solid; M.p. = 102-103 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{34}H_{39}O_8S_2$ 639.2086, found 639.2091; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49-7.34 (m, 14H), 7.00 (d, *J* = 8.8 Hz, 2H), 5.14 (s, 4H), 5.06-5.02 (m, 2H), 3.10-3.01 (m, 4H), 2.43 (s, 3H), 2.42 (s, 3H), 1.48 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.85 (2x), 136.58 (2x), 132.98 (2x), 129.94, 129.91, 128.68 (4x), 128.15 (2x), 127.57 (4x), 126.42 (2x), 125.64 (2x), 112.03 (2x), 80.07 (2x), 70.26 (2x), 38.09, 38.07, 37.21, 37.18, 21.54 (2x); Anal. Calcd for $C_{34}H_{38}O_8S_2$: C, 63.93; H, 6.00. Found: C, 63.88; H, 6.29.



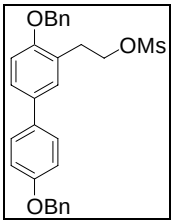
5.3. Methanesulfonic acid 1-[4,4'-bis-benzyloxy-3'-(2-methanesulfonyloxy-pent-4-enyl)-biphenyl-3-ylmethyl]-but-3-enyl ester (8c). Yield = 90% (621 mg); Colorless gum; HRMS (ESI, M^{+}+1) calcd for $C_{38}H_{43}O_8S_2$ 691.2399, found 691.2402; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47-7.33 (m, 14H), 6.99 (d, *J* = 8.4 Hz, 2H), 5.87-5.76 (m, 2H), 5.17-5.12 (m, 4H), 5.12 (s, 4H), 5.02-4.96 (m, 2H), 3.16 (dd, *J*

= 4.8, 14.0 Hz, 2H), 2.95 (ddd, *J* = 2.8, 4.0, 14.0 Hz, 2H), 2.37-2.23 (t, *J* = 6.8 Hz, 4H), 2.38 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.97 (2x), 136.58 (2x), 132.98 (2x), 130.12 (2x), 130.10 (2x), 128.67 (4x), 128.18 (2x), 127.66 (4x), 126.42 (2x), 125.76 (2x), 119.01 (2x), 112.10 (2x), 82.56 (2x), 70.37 (2x), 39.58 (2x), 37.47, 37.42, 35.79, 35.75.

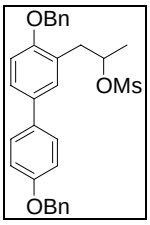


5.4. Methanesulfonic acid 1-benzyl-2-[4,4'-bis-benzyloxy-3'-(2-methanesulfonyloxy-3-phenyl -propyl)-biphenyl-3-yl]-ethyl ester (8d). Yield = 82% (648 mg); Colorless solid; M.p. = 119-120 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{46}H_{47}O_8S_2$ 791.2712, found 791.2710; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42-7.34 (m, 14H), 7.29-7.17 (m, 10H), 6.98 (d, *J* = 8.0 Hz, 2H), 5.19-5.12 (m, 2H), 5.11 (d, *J* = 12.0 Hz, 2H), 5.08 (d, *J* = 12.0 Hz, 2H), 3.18 (dd, *J* = 5.2, 14.0 Hz, 2H), 3.09-2.97 (m, 6H), 2.11 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.97 (2x), 136.70 (2x), 136.65 (2x), 133.06 (2x), 130.31 (2x), 130.28 (2x), 129.73 (4x), 128.68 (4x), 128.49 (4x), 128.08 (2x), 127.60 (2x), 126.88 (2x), 126.45 (2x), 125.64 (2x), 112.10 (2x), 84.41 (2x), 70.32 (2x), 41.58, 41.55, 37.04, 37.01, 36.34, 36.29.

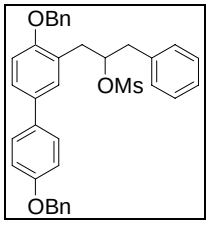
6. A representative procedure of compounds (8e)~(8h) is as follows: $NaBH_4$ (52 mg, 1.5 mmol, for compound (**8e**); 39 mg, 1.0 mmol, for compound (**8i**)) or Grignard reagent (1.0 M, 1.5 mL, 1.5 mmol, R = Me, allyl, Bn, Ph; for compounds (**8f**)~(**8h**)) was added to a solution of compound (**6b**) (405 mg, 1.0 mmol) or alkenyl aldehyde (143 mg, 0.3 mmol, for compound (**8i**)) in THF (10 mL) at rt. The reaction mixture was stirred at rt for 5 h. $HCl_{(aq)}$ solution (6 N, 4 mL) was added to the reaction mixture and the solvent was concentrated under reduced pressure. The residue was extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine, dried, filtered and evaporated to afford crude product under reduced pressure. Without further purification, Et_3N (152 mg, 1.5 mmol, for compounds (**8e**)~(**8h**); 51 mg, 0.5 mmol, for compound (**8i**)) was added to a solution of the resulting alcohol in DCM (40 mL) at rt. MsCl (140 mg, 1.2 mmol, for compounds (**8e**)~(**8h**); 58 mg, 0.5 mmol, for compound (**8i**)) was added to a reaction mixture at rt. The reaction mixture was stirred at rt for 5 h. Saturated $NaHCO_{3\,(aq)}$ solution (5 mL) was added to the reaction mixture and the solvent was concentrated under reduced pressure. The residue was extracted with EtOAc (3 x 30 mL). The combined organic layers were washed with brine, dried, filtered and evaporated to afford crude product under reduced pressure. Purification on silica gel (hexanes/EtOAc = 4/1~2/1) afforded compounds (**8e**)~(**8i**).



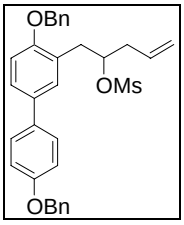
6.5. Methanesulfonic acid 2-(4,4'-bis-benzyloxy-biphenyl-3-yl)-ethyl ester (8e). Yield = 72% (351 mg); Colorless solid; M.p. = 107-108 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{29}H_{29}O_5S$ 489.1736, found 489.1742; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49-7.35 (m, 14H), 7.06-6.99 (m, 3H), 5.13 (s, 2H), 5.11 (s, 2H), 4.48 (t, *J* = 7.2 Hz, 2H), 3.17 (t, *J* = 7.2 Hz, 2H), 2.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.04, 155.81, 136.96, 136.79, 133.66, 133.22, 129.56, 128.68 (2x), 128.58 (2x), 128.08, 127.95, 127.71 (2x), 127.44 (2x), 127.38 (2x), 126.55, 124.90, 115.17 (2x), 112.01, 70.19, 70.07, 69.31, 37.08, 31.12; Anal. Calcd for $C_{29}H_{28}O_5S$: C, 71.29; H, 5.78. Found: C, 71.56; H, 5.90.



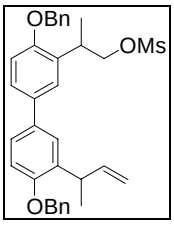
6.6. Methanesulfonic acid 2-(4,4'-bis-benzyloxy-biphenyl-3-yl)-1-methyl-ethyl ester (8f). Yield = 80% (402 mg); Colorless solid; M.p. = 110-111 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{30}H_{31}O_5S$ 503.1892, found 503.1899; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48-7.33 (m, 14H), 7.06-6.99 (m, 3H), 5.13 (s, 2H), 5.11 (s, 2H), 5.05-5.00 (m, 1H), 3.09-2.99 (m, 2H), 2.39 (s, 3H), 1.47 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.09, 155.77, 136.95, 136.70, 133.60, 133.12, 130.08, 128.74 (2x), 128.60 (2x), 128.20, 127.98, 127.67 (2x), 127.64 (2x), 127.45 (2x), 126.52, 125.61, 115.22 (2x), 112.00, 80.21, 70.34, 70.09, 38.25, 37.21, 21.65; Anal. Calcd for $C_{30}H_{30}O_5S$: C, 71.69; H, 6.02. Found: C, 71.87; H, 6.34.



6.7. Methanesulfonic acid 1-(4,4'-bis-benzyloxy-biphenyl-3-ylmethyl)-but-3-enyl ester (8g). Yield = 85% (449 mg); M.p. = 89-90 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{32}H_{33}O_5S$ 529.2049, found 529.2050; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48-7.31 (m, 14H), 7.03-6.96 (m, 3H), 5.87-5.74 (m, 1H), 5.17-4.94 (m, 3H), 5.11 (s, 2H), 5.09 (s, 2H), 3.17-2.78 (m, 2H), 2.34 (s, 3H), 2.09-2.04 (m, 2H).

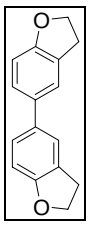


6.8. Methanesulfonic acid 1-benzyl-2-(4,4'-bis-benzyloxy-biphenyl-3-yl)-ethyl ester (8h). Yield = 79% (457 mg); Colorless solid; M.p. = 108-109 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{36}H_{35}O_5S$ 579.2205, found 579.2210; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48-7.32 (m, 14H), 2.76-7.15 (m, 5H), 7.04-6.97 (m, 3H), 5.18-5.05 (m, 5H), 3.17 (dd, *J* = 4.8, 13.6 Hz, 1H), 3.10-2.95 (m, 3H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.04, 155.82, 136.95, 136.71, 136.60, 133.52, 133.12, 130.32, 129.72 (2x), 128.68 (2x), 128.59 (2x), 128.48 (2x), 128.07, 127.97, 127.66 (2x), 127.60 (2x), 127.45 (2x), 126.87, 126.47, 125.57, 115.18 (2x), 112.03, 84.45, 70.30, 70.07, 41.58, 36.96, 36.30.



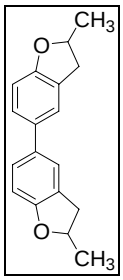
4.9. Methanesulfonic acid 2-[4,4'-bis-benzyloxy-3'-(1-methyl-allyl)-biphenyl-3-yl]-propyl ester (8i). Yield = 76% (127 mg); Colorless gum; HRMS (ESI, M^{+}+1) calcd for $C_{34}H_{37}O_5S$ 557.2362, found 557.2366; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51-7.30 (m, 14H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 6.16-6.07 (m, 1H), 5.15-5.05 (m, 6H), 4.46 (dd, *J* = 5.6, 8.0 Hz, 1H), 4.26 (dd, *J* = 8.0, 9.2 Hz, 1H), 4.07-4.03 (m, 1H), 3.80-3.65 (m, 1H), 2.74 (s, 3H), 1.41 (d, *J* = 7.2 Hz, 3H), 1.39 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.30, 155.16, 142.56, 137.30, 136.80, 134.69, 134.22, 133.48, 129.80, 128.69 (2x), 128.53 (2x), 128.10, 127.79, 127.49 (2x), 127.13 (2x), 126.48, 126.38, 126.15, 125.28, 113.18, 112.22, 112.15, 73.84, 70.35, 70.21, 36.97, 35.97, 33.41, 19.39, 16.30.

7. A representative procedure of compounds (4a)~(4i) is as follows: Palladium on activated carbon (10%, 20 mg) was added to a solution of compounds (**8a**)~(**8i**) (0.5 mmol) in EtOAc (30 mL) at rt. Then hydrogen was bubbled into the mixture for 10 min, and stirring occurred at rt for 20 h. The reaction mixture was filtered and evaporated to yield crude product. Purification on silica gel (hexanes/EtOAc = 6/1) afforded compounds (**4a**)~(**4i**).

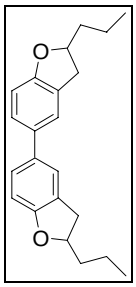


7.1. 2,3,2',3'-Tetrahydro-[5,5']bibenzofuranyl (4a). Yield = 90% (107 mg); Colorless solid; M.p. = 141-142 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{16}H_{15}O_2$

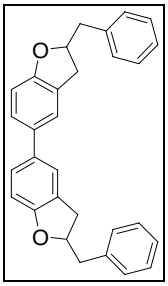
239.1072, found 239.1076; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (br s, 2H), 7.27 (dd, *J* = 1.2, 8.4 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 4.60 (t, *J* = 8.8 Hz, 4H), 3.25 (t, *J* = 8.8 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.13 (2x), 134.19 (2x), 127.45 (2x), 126.62 (2x), 123.46 (2x), 109.31 (2x), 71.35 (2x), 29.79 (2x); Anal. Calcd for $C_{16}H_{314}O_2$: C, 80.65; H, 5.92. Found: C, 80.33; H, 6.13. Single-crystal X-ray diagram: crystal of compound (**4a**) was grown by slow diffusion of EtOAc into a solution of compound (**4a**) in DCM to yield colorless prism. The compound crystallizes in the triclinic crystal system, space group P 1 21/c 1, *a*=5.8246(2) Å, *b*=12.8801(4) Å, *c*=7.7281(3) Å, *V*=572.71(3) Å^3, *Z*=2, d_{calcd}=1.382 g/cm^3, *F*(000)=252, 2θ range 3.88~26.37^o, R indices (all data) R1 = 0.0724, wR2 = 0.1211.



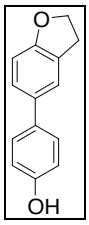
7.2. 2,2'-Dimethyl-2,3,2',3'-tetrahydro-[5,5']bibenzofuranyl (4b). Yield = 88% (117 mg); Colorless solid; M.p. = 89-90 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^++1) calcd for $C_{18}H_{19}O_2$ 267.1385, found 267.1388; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 (s, 2H), 7.26 (dd, *J* = 2.0, 8.0 Hz, 2H), 6.79 (d, *J* = 8.0 Hz, 2H), 5.01-4.92 (m, 2H), 3.35 (dd, *J* = 8.0, 15.6 Hz, 2H), 2.86 (dd, *J* = 8.0, 15.6 Hz, 2H), 1.50 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.58 (2x), 134.10 (2x), 127.56 (2x), 126.61 (2x), 123.50 (2x), 109.25 (2x), 79.84 (2x), 37.17 (2x), 21.76 (2x); Anal. Calcd for $C_{18}H_{18}O_2$: C, 81.17; H, 6.81. Found: C, 81.45; H, 6.68.



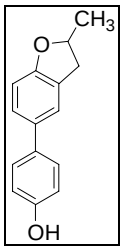
7.3. 2,2'-Dipropyl-2,3,2',3'-tetrahydro-[5,5']bibenzofuranyl (4c). Yield = 91% (147 mg); Colorless solid; M.p. = 78-79 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^++1) calcd for $C_{22}H_{27}O_2$ 323.2011, found 323.2018; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29 (s, 2H), 7.24 (dd, *J* = 2.0, 8.4 Hz, 2H), 6.77 (d, *J* = 8.4 Hz, 2H), 4.85-4.77 (m, 2H), 3.29 (dd, *J* = 9.2, 15.6 Hz, 2H), 2.88 (dd, *J* = 8.0, 15.6 Hz, 2H), 1.89-1.80 (m, 2H), 1.71-1.43 (m, 6H), 0.99 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.66 (2x), 134.00 (2x), 127.51 (2x), 126.56 (2x), 123.45 (2x), 109.18 (2x), 83.49 (2x), 38.24 (2x), 35.52 (2x), 18.71 (2x), 13.99 (2x); Anal. Calcd for $C_{22}H_{26}O_2$: C, 81.95; H, 8.13. Found: C, 82.23; H, 8.38.



7.4. 2,2'-Dibenzyl-2,3,2',3'-tetrahydro-[5,5']bibenzofuranyl (4d). Yield = 85% (178 mg); Colorless solid; M.p. = 127-128 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{30}H_{27}O_2$ 419.2011, found 419.2019; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.24 (m, 14H), 6.81 (d, *J* = 8.0 Hz, 2H), 5.09-5.01 (m, 2H), 3.24 (ddd, *J* = 8.8, 12.0, 15.6 Hz, 4H), 2.98 (dt, *J* = 7.2, 15.6 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.51 (2x), 137.42 (2x), 134.19 (2x), 129.38 (4x), 128.53 (4x), 127.19 (2x), 126.70 (2x), 126.61 (2x), 123.54 (2x), 109.43 (2x), 83.88 (2x), 43.02 (2x), 35.00 (2x); Anal. Calcd for $C_{30}H_{26}O_2$: C, 86.09; H, 6.26. Found: C, 86.27; H, 6.52.

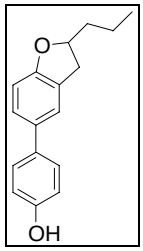


7.5. 4-(2,3-Dihydro-benzofuran-5-yl)-phenol (4e). Yield = 80% (85 mg); Colorless solid; M.p. = 172-173 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{14}H_{13}O_2$ 213.0916, found 213.0922; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42-7.36 (m, 3H), 7.29-7.26 (m, 1H), 6.89-6.86 (m, 2H), 6.83 (d, *J* = 8.4 Hz, 1H), 4.83 (br s, 1H), 4.61 (t, *J* = 8.8 Hz, 2H), 3.26 (t, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.25, 154.49, 134.24, 133.63, 128.00 (2x), 127.52, 126.59, 123.40, 115.54 (2x), 109.38, 71.39, 29.78; Anal. Calcd for $C_{14}H_{12}O_2$: C, 79.22; H, 5.70. Found: C, 79.47; H, 5.89. Single-crystal X-ray diagram: crystal of compound (**4e**) was grown by slow diffusion of EtOAc into a solution of compound (**4e**) in DCM to yield colorless prism. The compound crystallizes in the monoclinic crystal system, space group P 1 21/c 1, *a*=8.4518(13) Å, *b*=6.1787(9) Å, *c*=21.735(3) Å, *V*=1063.0(3) Å^3, *Z*=4, d_{calcd}=1.326 g/cm^3, *F*(000)=448, 2θ range 2.00~26.63^{o}, R indices (all data) R1 = 0.0920, wR2 = 0.1328.

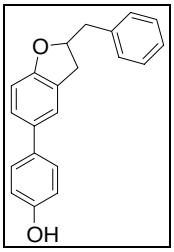


7.6. 4-(2-Methyl-2,3-dihydro-benzofuran-5-yl)-phenol (4f). Yield = 82% (93 mg); Colorless solid; M.p. = 135-137 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{15}H_{15}O_2$ 227.1072, found 227.1079; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41-7.37 (m, 2H), 7.32 (s, 1H), 7.27 (dd, *J*

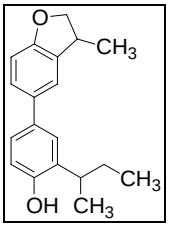
= 1.6, 8.0 Hz, 1H), 6.89-6.85 (m, 2H), 6.79 (d, *J* = 8.0 Hz, 1H), 4.99-4.92 (m, 1H), 4.87 (br s, 1H), 3.36 (dd, *J* = 8.8, 15.6 Hz, 1H), 2.86 (dd, *J* = 7.6, 15.6 Hz, 1H), 1.49 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.73, 154.46, 134.27, 133.44, 127.97 (2x), 126.60 (2x), 123.45, 115.51 (2x), 109.33, 79.91, 37.14, 21.77.



7.7. 4-(2-Propyl-2,3-dihydro-benzofuran-5-yl)-phenol (4g). Yield = 85% (108 mg); Colorless solid; M.p. = 86-88 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{17}H_{19}O_2$ 255.1385, found 255.1388; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41-7.37 (m, 2H), 7.32 (d, *J* = 1.6 Hz, 1H), 7.27-7.25 (m, 1H), 6.89-6.85 (m, 2H), 6.79 (d, *J* = 8.4 Hz, 1H), 4.97 (br s, 1H), 4.86-4.79 (m, 1H), 3.31 (dd, *J* = 8.4, 15.2 Hz, 1H), 2.90 (dd, *J* = 8.0, 15.2 Hz, 1H), 1.90-1.83 (m, 2H), 1.70-1.42 (m, 2H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.81, 154.48, 134.24, 133.33, 127.95 (2x), 127.61, 126.54, 123.40, 115.50 (2x), 109.26, 83.56, 38.23, 35.48, 18.70, 14.01.

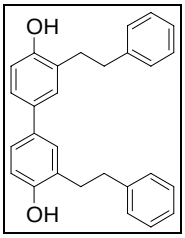


7.8. 4-(2-Benzyl-2,3-dihydro-benzofuran-5-yl)-phenol (4h). Yield = 84% (127 mg); Colorless solid; M.p. = 79-80 ^{o}C (recrystallized from hexanes and EtOAc); HRMS (ESI, M^{+}+1) calcd for $C_{21}H_{19}O_2$ 303.1385, found 303.1390; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.26 (m, 9H), 6.88-6.85 (m, 2H), 6.82 (d, *J* = 8.4 Hz, 1H), 5.08-5.04 (m, 1H), 4.87 (br s, 1H), 3.29-3.19 (m, 2H), 3.03-2.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.65, 154.49, 137.39, 134.23, 133.60, 129.39 (2x), 128.54 (2x), 127.99 (2x), 127.27, 126.66, 126.63, 123.48, 115.53 (2x), 109.49, 83.92, 42.01, 34.98.



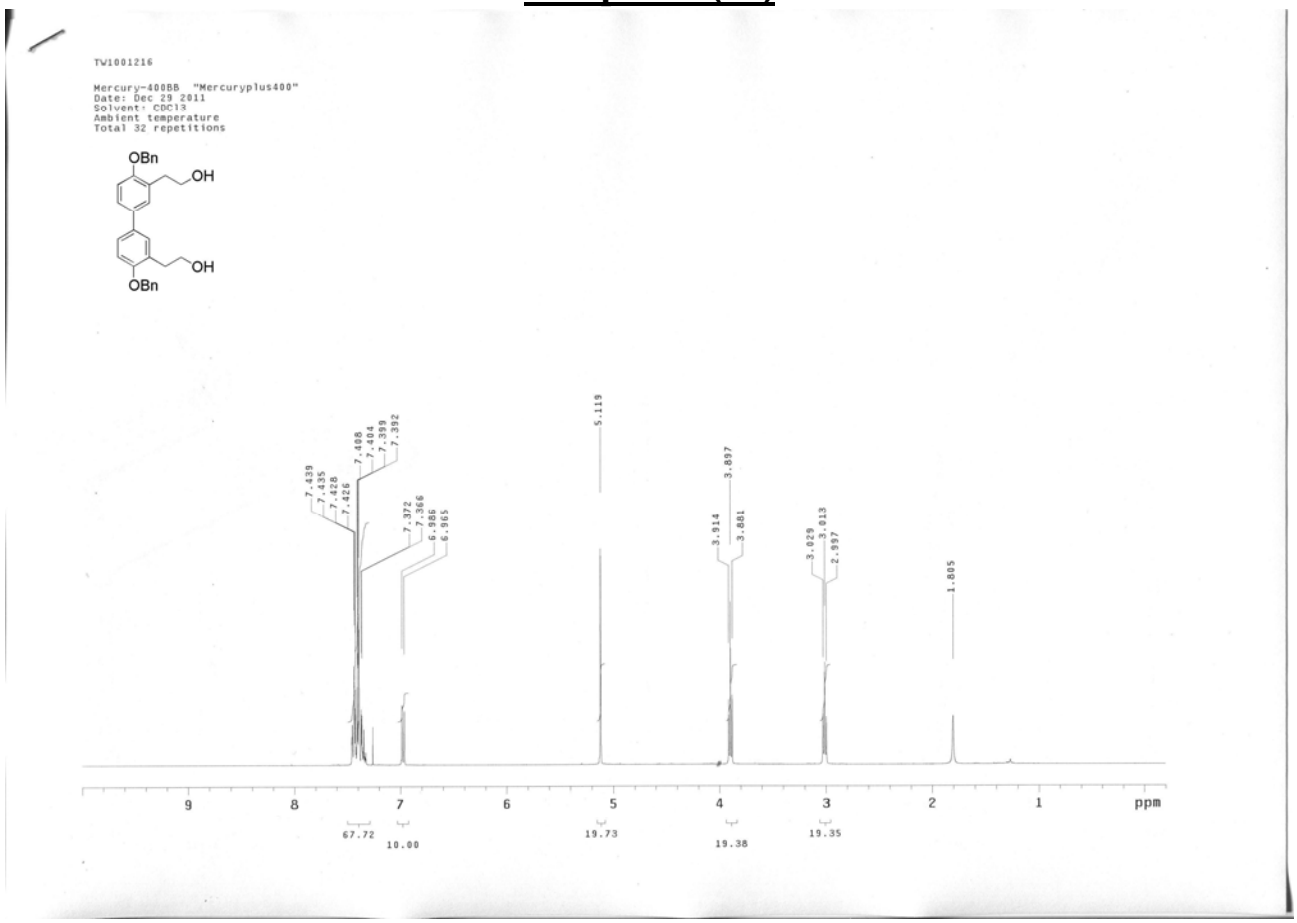
7.9. 2-sec-Butyl-4-(3-methyl-2,3-dihydro-benzofuran-5-yl)-phenol (4i). Yield = 78% (110 mg); Colorless gum; HRMS (ESI, M^{+}+1) calcd for $C_{19}H_{23}O_2$ 283.1698, found 283.1696; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.27 (m, 3H), 7.22 (dd, *J* = 2.0, 8.0 Hz, 1H), 6.82 (d, *J* = 8.4 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 4.78 (br s, 1H), 4.72 (t, *J* = 8.8 Hz, 1H), 4.12 (dd, *J* = 7.6, 8.8 Hz, 1H), 3.63-3.53 (m,

1H), 3.04-2.95 (m, 1H), 1.77-1.62 (m, 2H), 1.37 (d, *J* = 6.8 Hz, 3H), 1.28 (dd, *J* = 3.2, 6.8 Hz, 3H), 0.92 (dt, *J* = 3.2, 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.88, 152.11, 134.37, 134.32, 133.40, 132.80, 126.73, 125.75, 124.97, 122.35, 115.56, 109.44, 78.84, 36.56, 34.19, 29.85, 20.48, 19.33, 12.23.



6. 3,3'-Diphenethyl-biphenyl-4,4'-diol (9). Et_3N (61 mg, 0.6 mmol) was added to a solution of compound (**7e**) (120 mg, 0.2 mmol) in DCM (10 mL) at rt. MsCl (58 mg, 0.5 mmol) was added to a reaction mixture at rt. The reaction mixture was stirred at rt for 5 h. Saturated $NaHCO_{3\,(aq)}$ solution (5 mL) was added to the reaction mixture and the solvent was concentrated under reduced pressure. The residue was extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine, dried, filtered and evaporated to afford crude product under reduced pressure. Without further purification, palladium on activated carbon (10%, 10 mg) was added to a solution of the resulting compound in EtOAc (15 mL) at rt. Then hydrogen was bubbled into the mixture for 10 min, and stirring occurred at rt for 20 h. The reaction mixture was filtered and evaporated to yield crude product. Purification on silica gel (hexanes/EtOAc = 6/1) afforded compound (**9**). Yield = 69% (54 mg); Colorless gum; HRMS (ESI, M^++1) calcd for $C_{28}H_{27}O_2$ 395.2011, found 395.2019; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32-7.16 (m, 14H), 6.77 (d, *J* = 8.4 Hz, 2H), 4.68 (br s, 2H), 2.95 (s, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.57 (2x), 141.93 (2x), 133.83 (2x), 128.86 (2x), 128.54 (4x), 128.43 (4x), 127.97 (2x), 126.01 (2x), 125.52 (2x), 115.64 (2x), 36.31 (2x), 32.48 (2x).

Compound (7a)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Date: Dec 29 2011
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
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OH
OBn
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7.435
7.428
7.426
7.406
7.404
7.399
7.392
7.372
7.366
6.986
6.965
5.119
3.897
3.914
3.881
3.029
3.013
2.997
1.805
9
8
7
6
5
4
3
2
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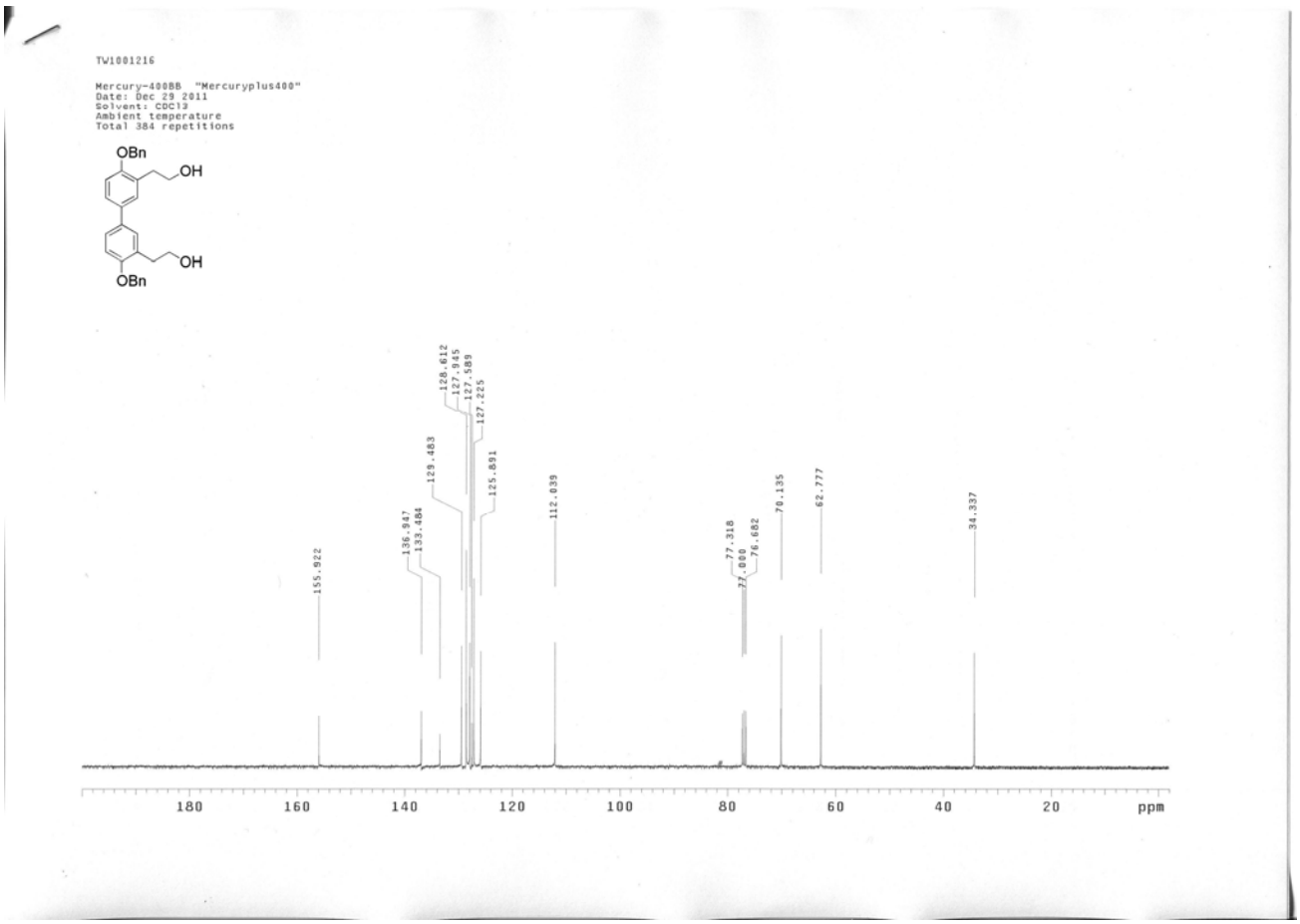
ppm
67.72
10.00
19.73
19.38
19.35


TW1001216
Mercury-400BB "Mercuryplus400"
Date: Dec 29 2011
Solvent: CDCl3
Ambient temperature
Total 384 repetitions
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OH
OBn
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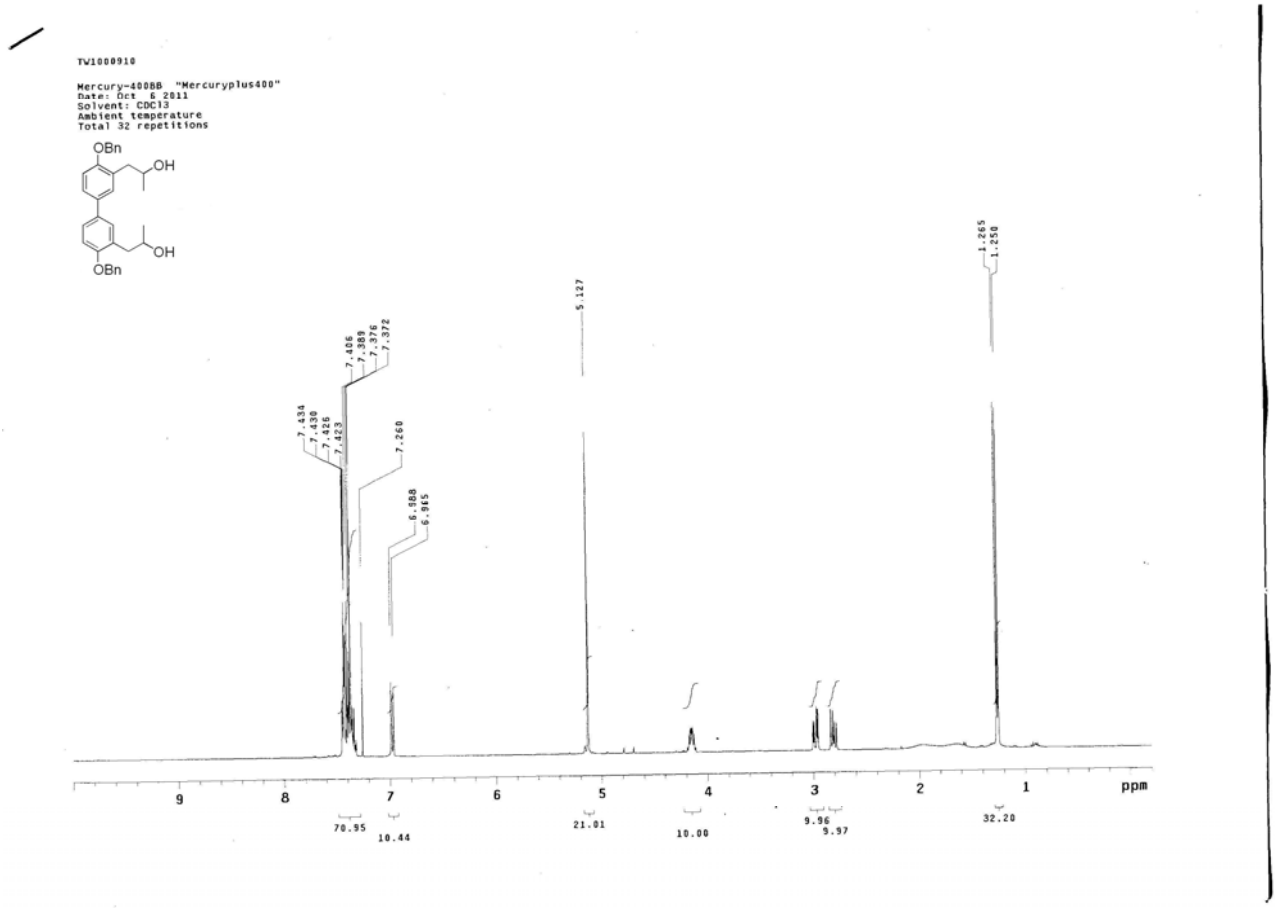
136.947
133.484
129.483
128.612
127.945
127.589
127.225
125.891
112.039
77.318
77.000
76.682
70.135
62.777
34.337
180
160
140
120
100
80
60
40
20
ppm

Compound (7b)


TW1000910
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Date: Oct 6 2011
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
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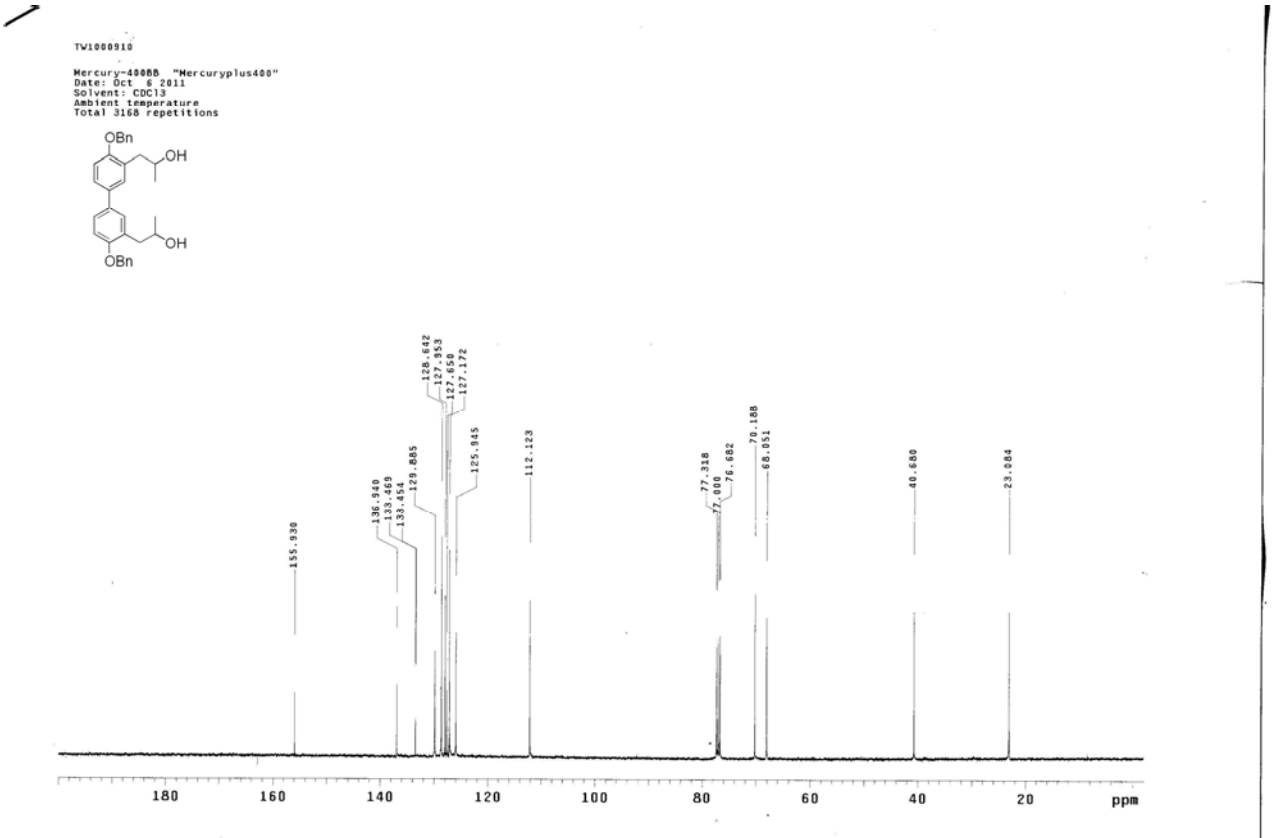
OH
OBn
7.434
7.430
7.425
7.423
7.406
7.389
7.376
7.372
7.260
6.988
6.965
5.127
1.265
1.250
ppm
70.95
10.44
21.01
10.00
9.96
9.97
32.20


TW1000910
Mercury-400BB "Mercuryplus400"
Date: Oct 6 2011
Solvent: CDCl3
Ambient temperature
Total 3168 repetitions
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OH
OH
OBn
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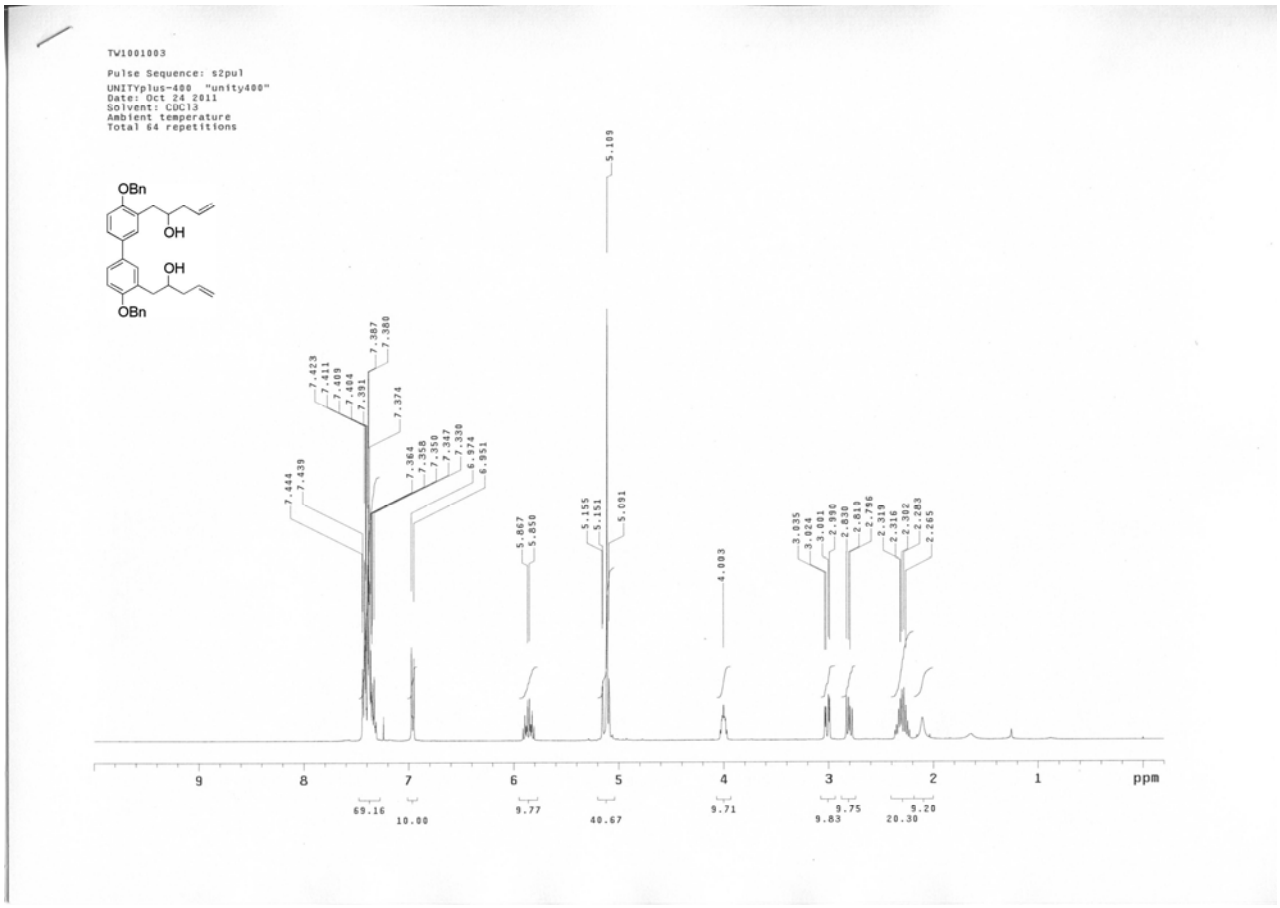
136.940
133.469
133.454
129.885
128.642
127.953
127.650
127.172
125.945
112.123
77.318
77.000
76.682
70.188
68.051
40.680
23.084
ppm

Compound (7c)


TV1001003
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
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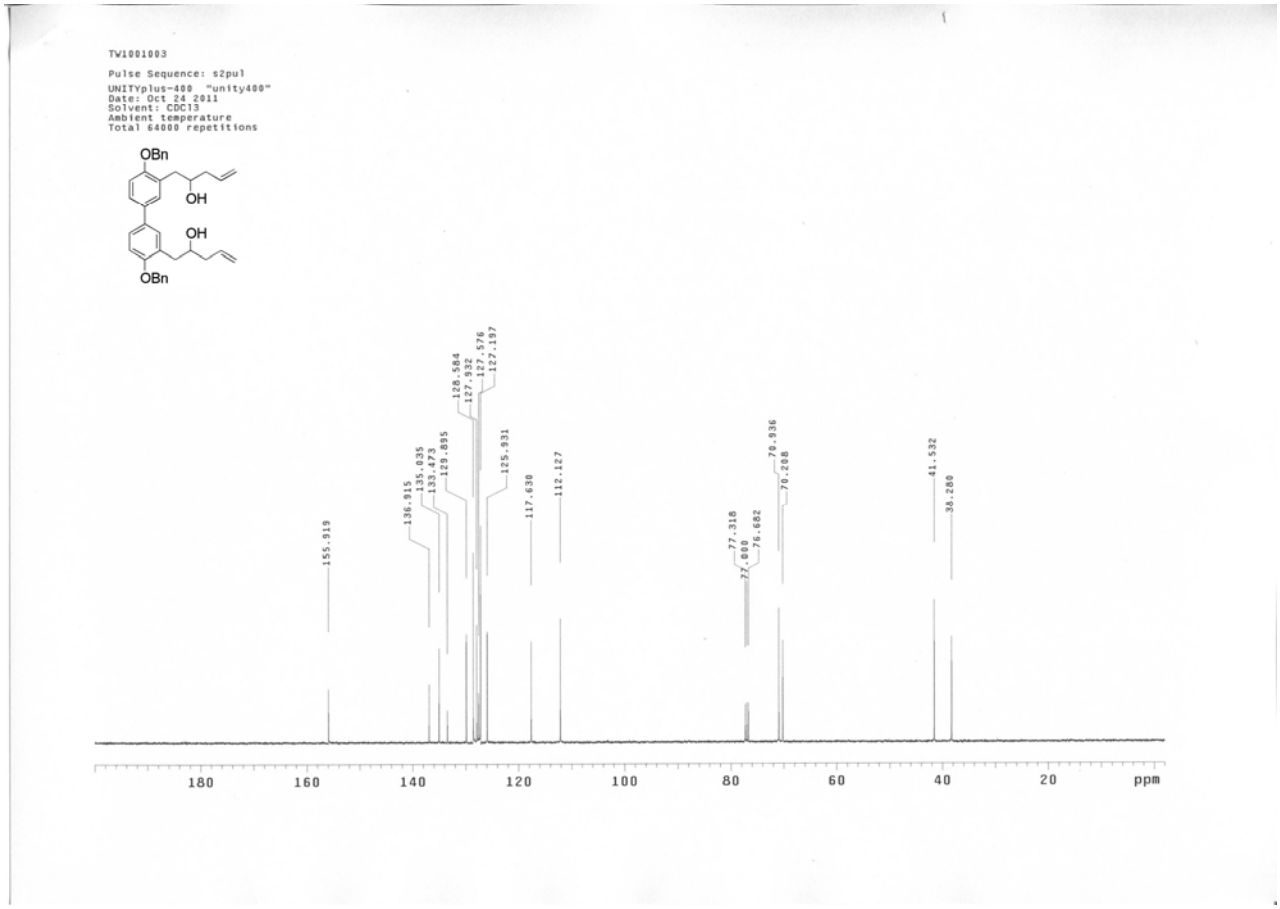
OH
OH
OBn
7.444
7.439
7.423
7.411
7.409
7.404
7.391
7.387
7.380
7.374
7.364
7.358
7.350
7.347
7.330
6.974
6.951
5.867
5.850
5.169
5.155
5.151
5.091
4.003
3.035
3.024
3.011
2.991
2.830
2.813
2.756
2.319
2.316
2.302
2.283
2.265
9
8
7
6
5
4
3
2
1
ppm
69.16
10.00
9.77
40.67
9.71
9.83
9.75
20.30
9.20


TV1001003
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 64000 repetitions
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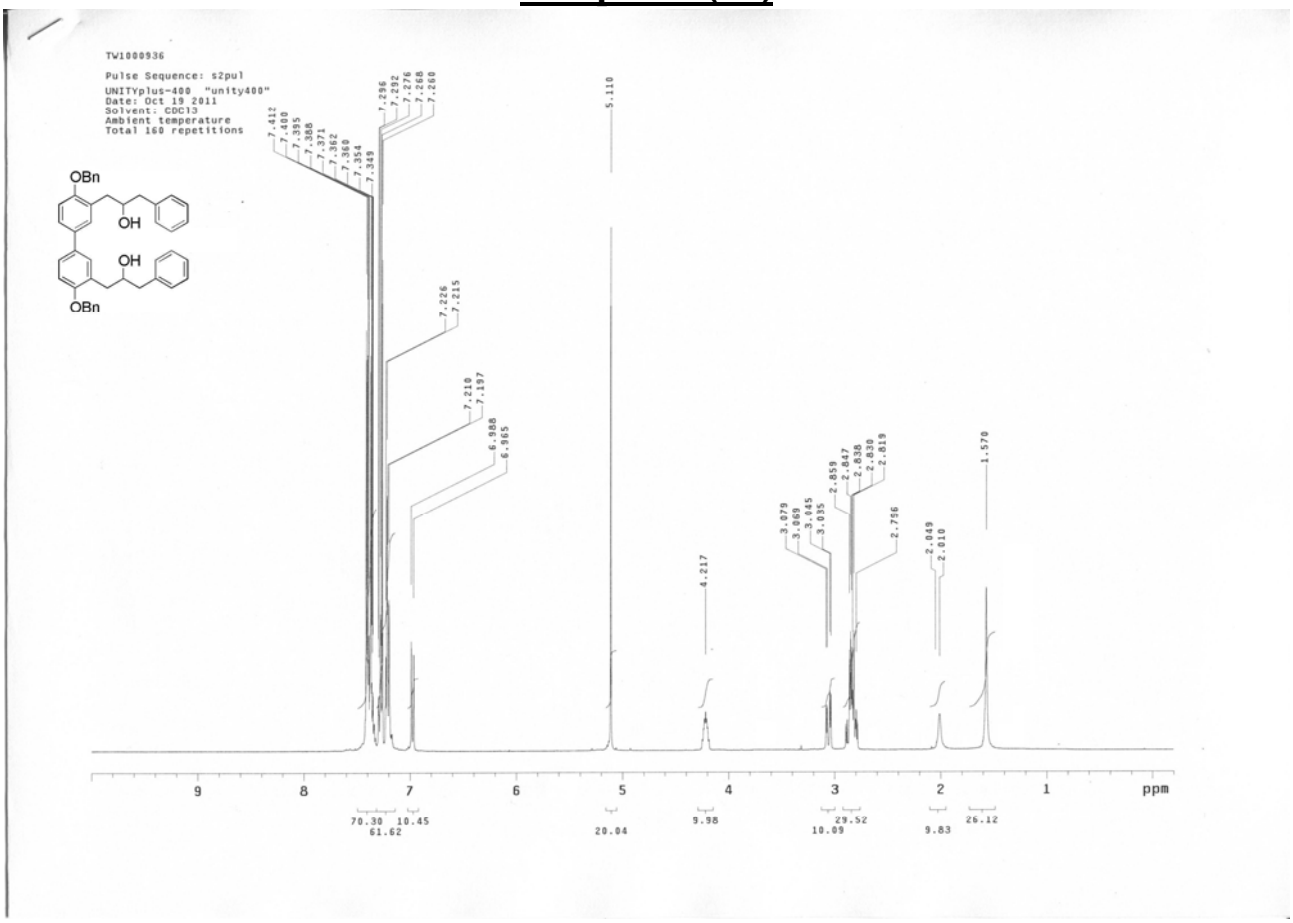
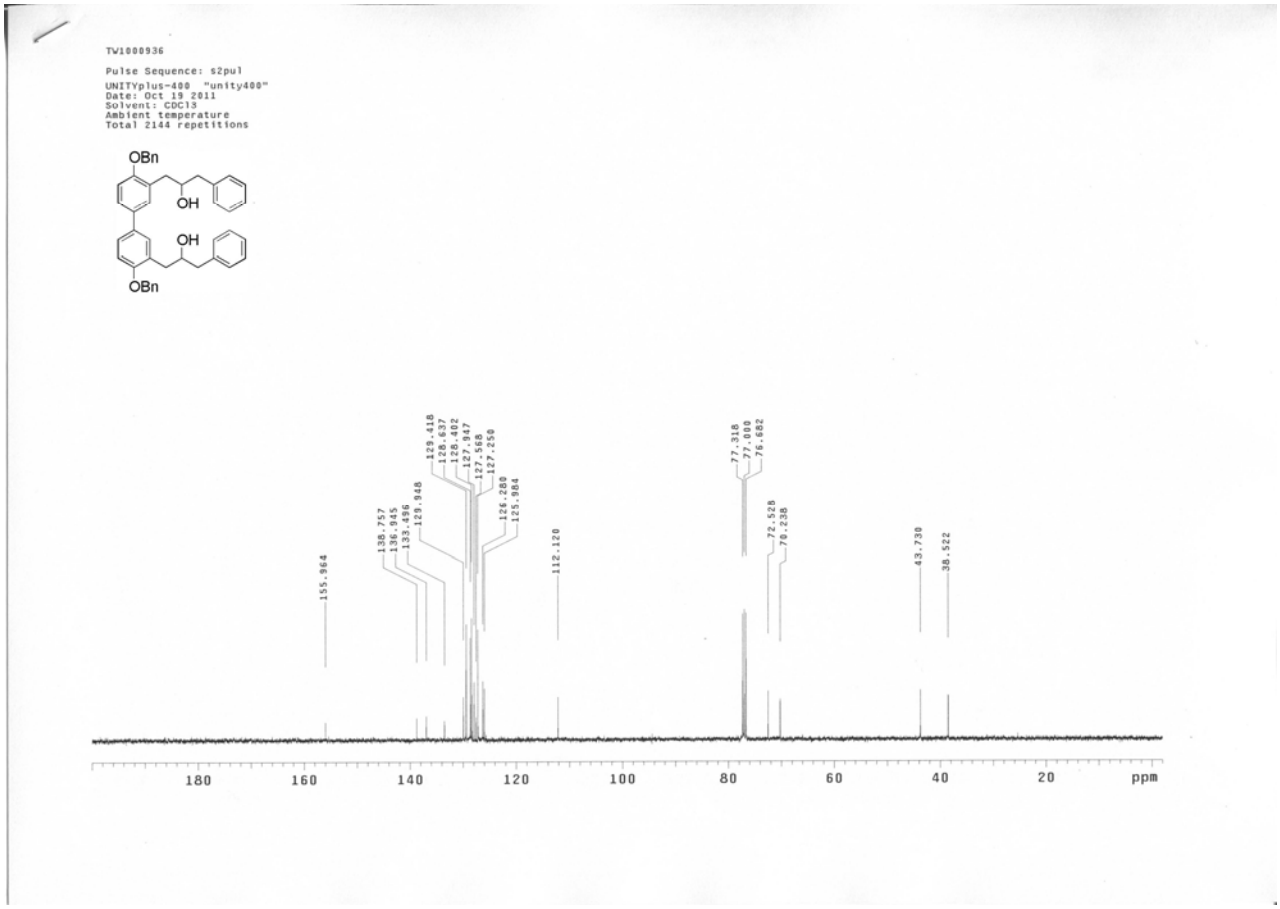
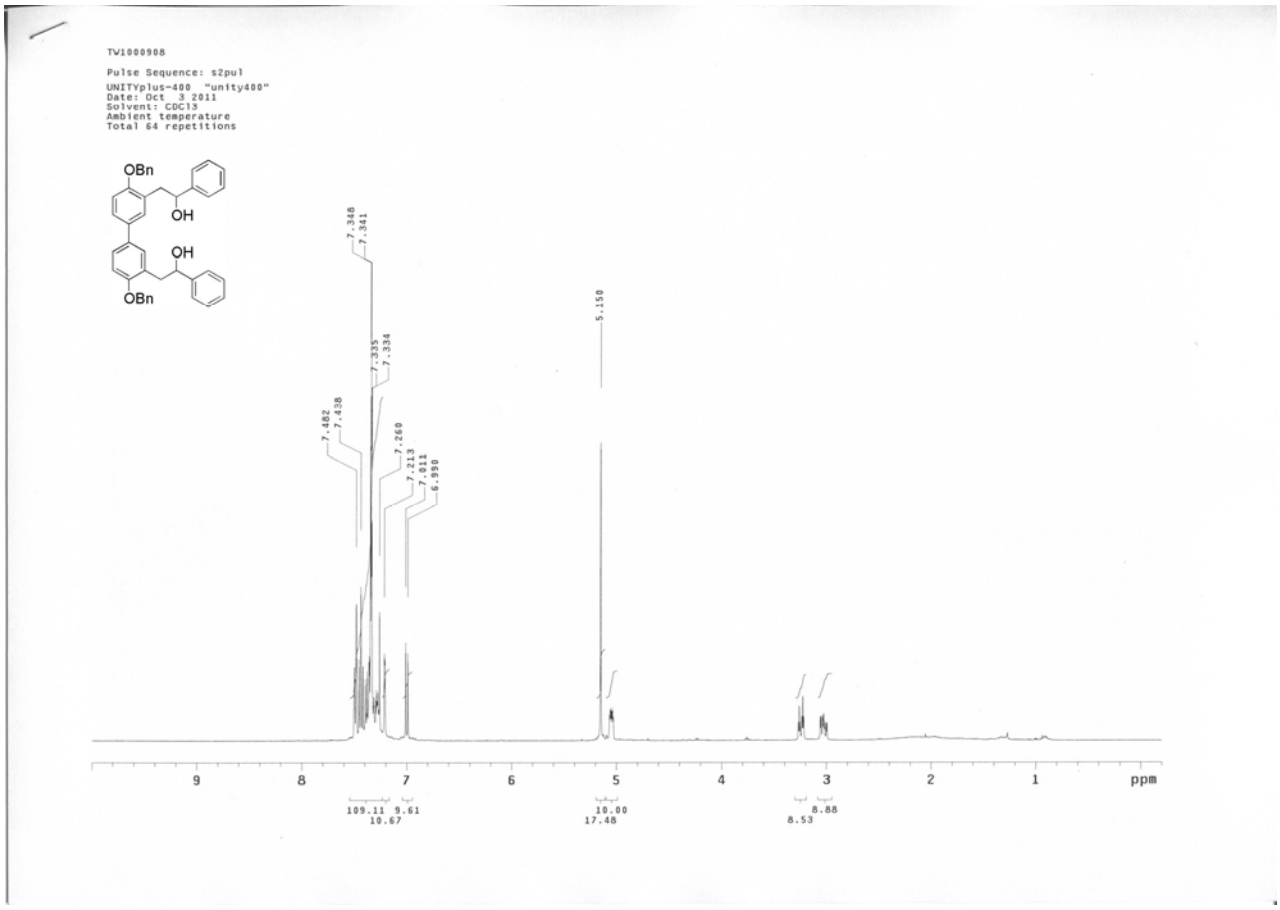
OH
OH
OBn
155.919
136.915
135.035
133.473
129.895
128.584
127.932
127.576
127.197
125.931
117.630
112.127
77.318
77.000
76.682
70.936
70.208
41.532
38.280
180
160
140
120
100
80
60
40
20
ppm

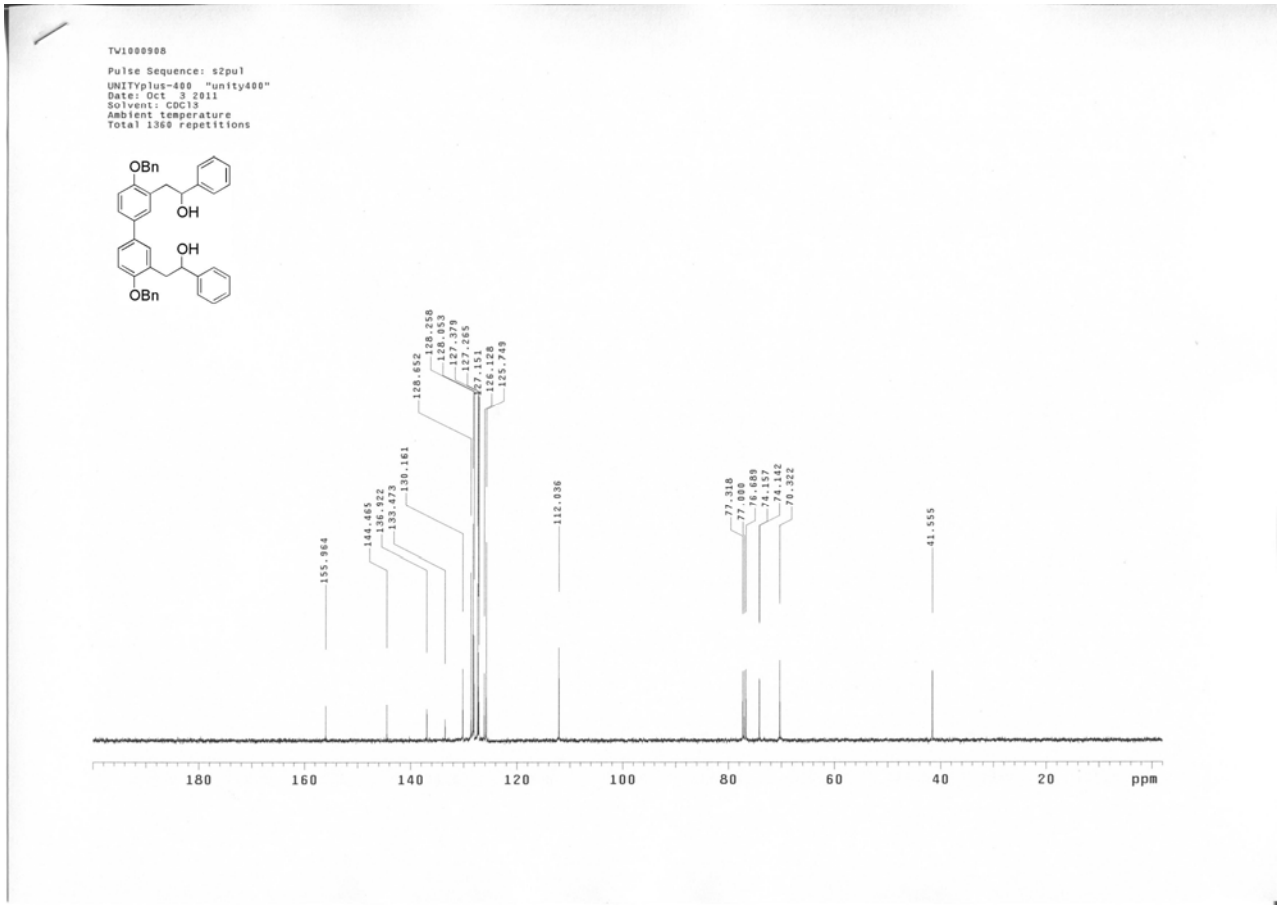
Compound (7d)


TW1000936
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 19 2011
Solvent: CDCl3
Ambient temperature
Total 160 repetitions
OBn
OH
OH
OBn
7.412
7.400
7.395
7.388
7.371
7.362
7.360
7.354
7.349
7.296
7.292
7.276
7.268
7.260
5.110
7.226
7.215
7.210
7.197
6.988
6.965
4.217
3.079
3.069
3.045
3.035
2.859
2.847
2.838
2.830
2.819
2.756
2.049
2.010
1.570
9
8
7
6
5
4
3
2
1
ppm
70.30
10.45
61.62
20.04
9.98
29.52
10.09
9.83
26.12

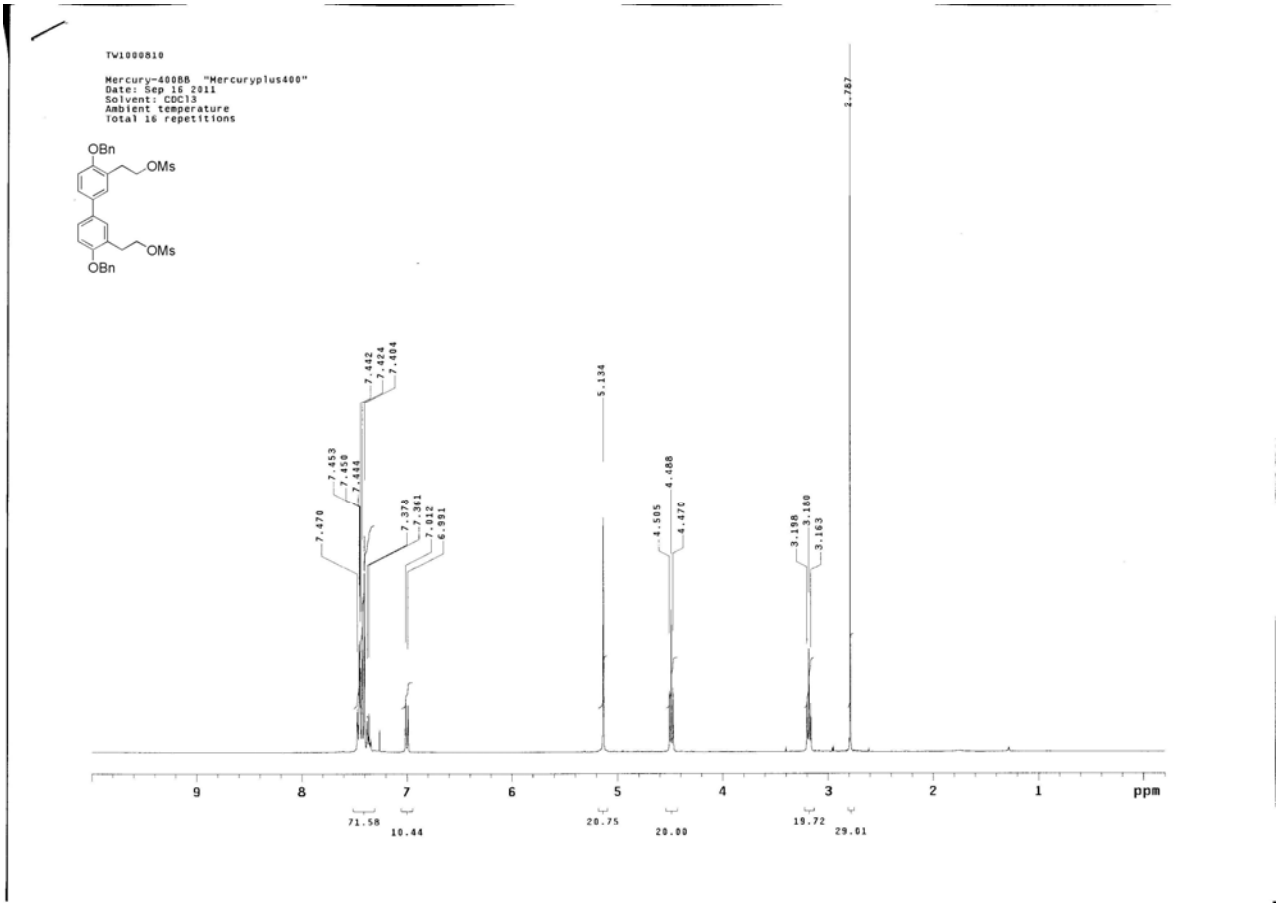

TW1000936
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 19 2011
Solvent: CDCl3
Ambient temperature
Total 2144 repetitions
OBn
OH
OH
OBn
155.964
138.757
136.945
133.496
129.948
129.418
128.637
128.402
127.947
127.568
127.250
126.280
125.984
112.120
77.318
77.000
76.682
72.528
70.238
43.730
38.522
180
160
140
120
100
80
60
40
20
ppm

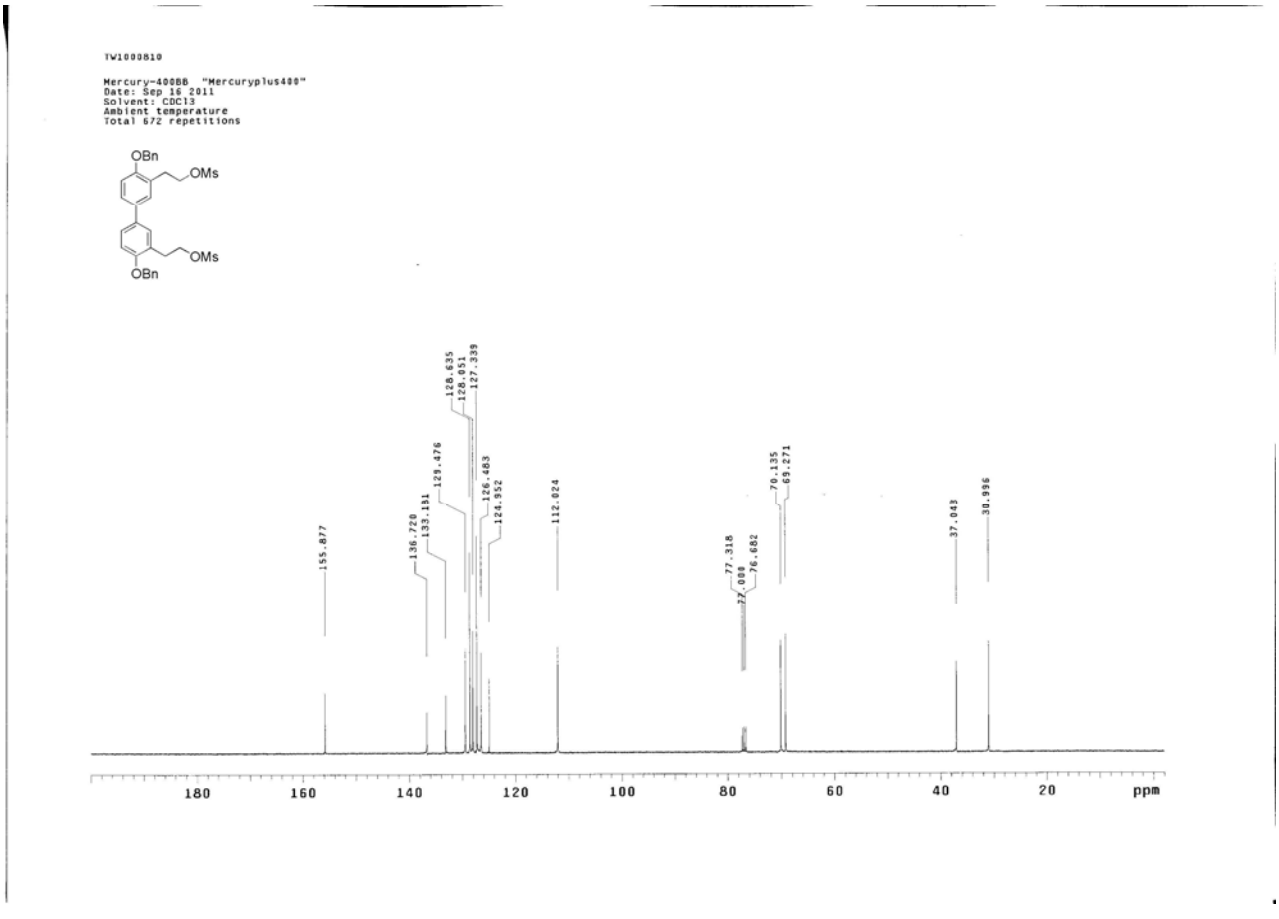
Compound (7e)


TW1000908
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 3 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
OBn
OH
OH
OBn
7.348
7.341
7.335
7.334
7.482
7.438
7.260
7.213
7.011
6.990
5.150
9
8
7
6
5
4
3
2
1
ppm
109.11 9.61
10.67
10.00
17.48
8.88
8.53

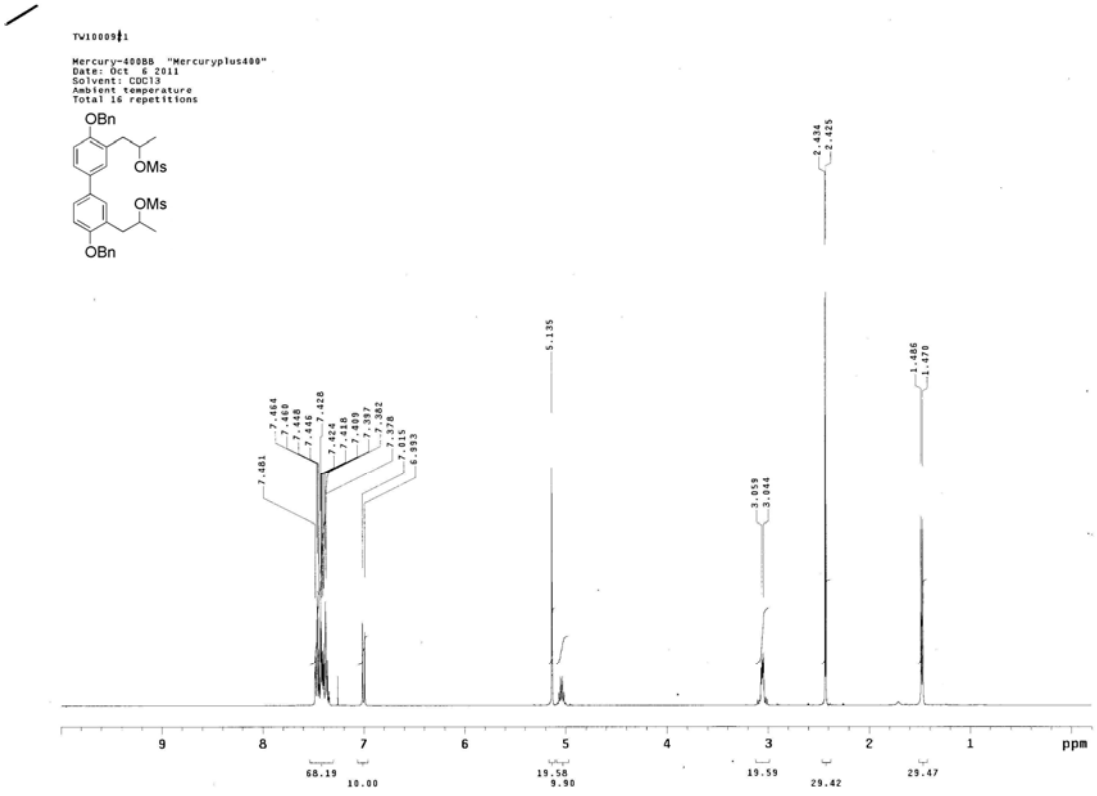

TW1000908
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 3 2011
Solvent: CDCl3
Ambient temperature
Total 1360 repetitions
OBn
OH
OH
OBn
155.964
144.465
136.922
133.473
130.161
128.652
128.258
128.053
127.379
127.265
127.151
126.128
125.749
112.036
77.318
77.000
76.689
74.157
74.142
70.322
41.555
180
160
140
120
100
80
60
40
20
ppm

Compound (8a)


TW1000810
Mercury-400BB "Mercuryplus400"
Date: Sep 16 2011
Solvent: CDCl3
Ambient temperature
Total 16 repetitions
OBn
OMs
OMs
OBn
7.470
7.453
7.450
7.444
7.442
7.424
7.404
7.378
7.361
7.012
6.991
5.134
4.505
4.488
4.472
3.198
3.180
3.163
2.787
9
8
7
6
5
4
3
2
1
ppm
71.58
10.44
20.75
20.00
19.72
29.01


TW1000810
Mercury-400BB "Mercuryplus400"
Date: Sep 16 2011
Solvent: CDCl3
Ambient temperature
Total 672 repetitions
OBn
OMs
OMs
OBn
155.877
136.720
133.181
129.476
128.635
128.051
127.339
126.483
124.952
112.024
77.318
77.000
76.682
70.135
69.271
37.043
30.996
180
160
140
120
100
80
60
40
20
ppm

Compound (8b)


TW10009#1
Mercury-400BB "Mercuryplus400"
Date: Oct 6 2011
Solvent: CDCl3
Ambient temperature
Total 16 repetitions
OBn
OMs
OMs
OBn
7.464
7.460
7.446
7.428
7.424
7.418
7.409
7.397
7.382
7.378
7.015
6.993
7.461
5.135
3.059
3.044
2.434
2.425
1.486
1.478
9
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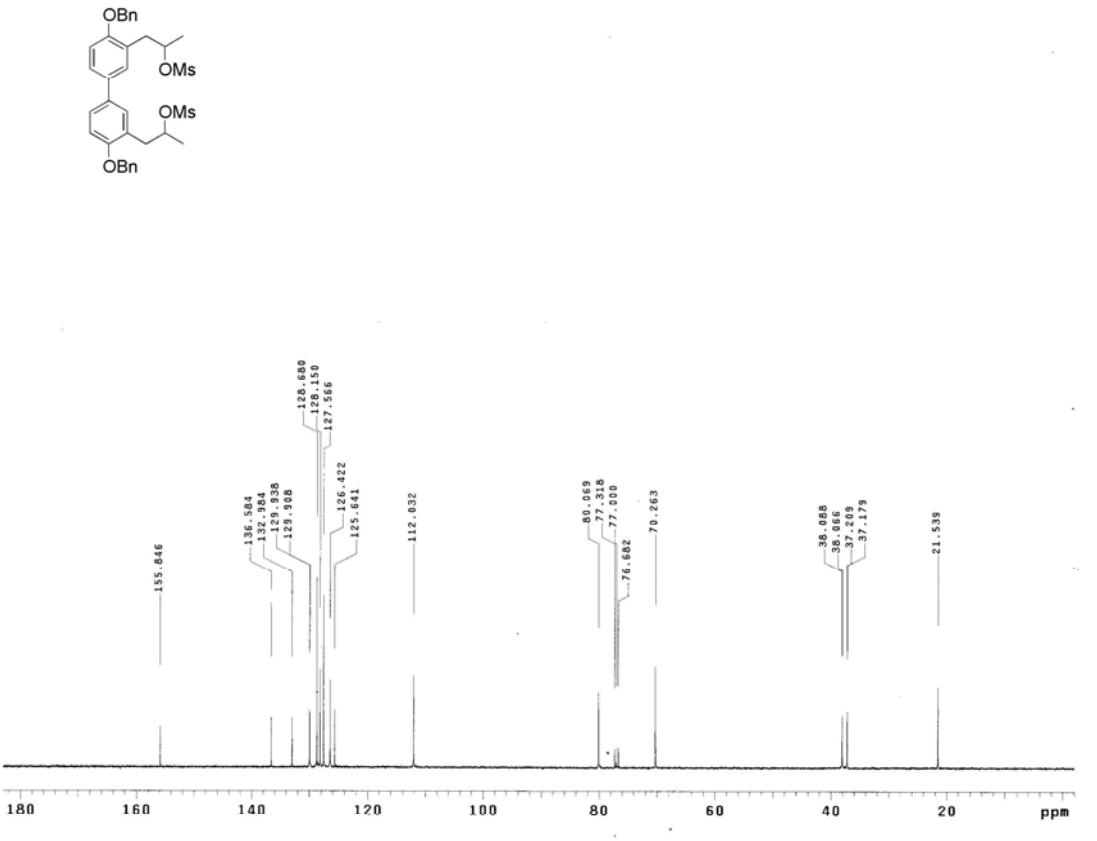
10.00
19.58
9.90
19.59
29.42
29.47


OBn
OMs
OMs
OBn
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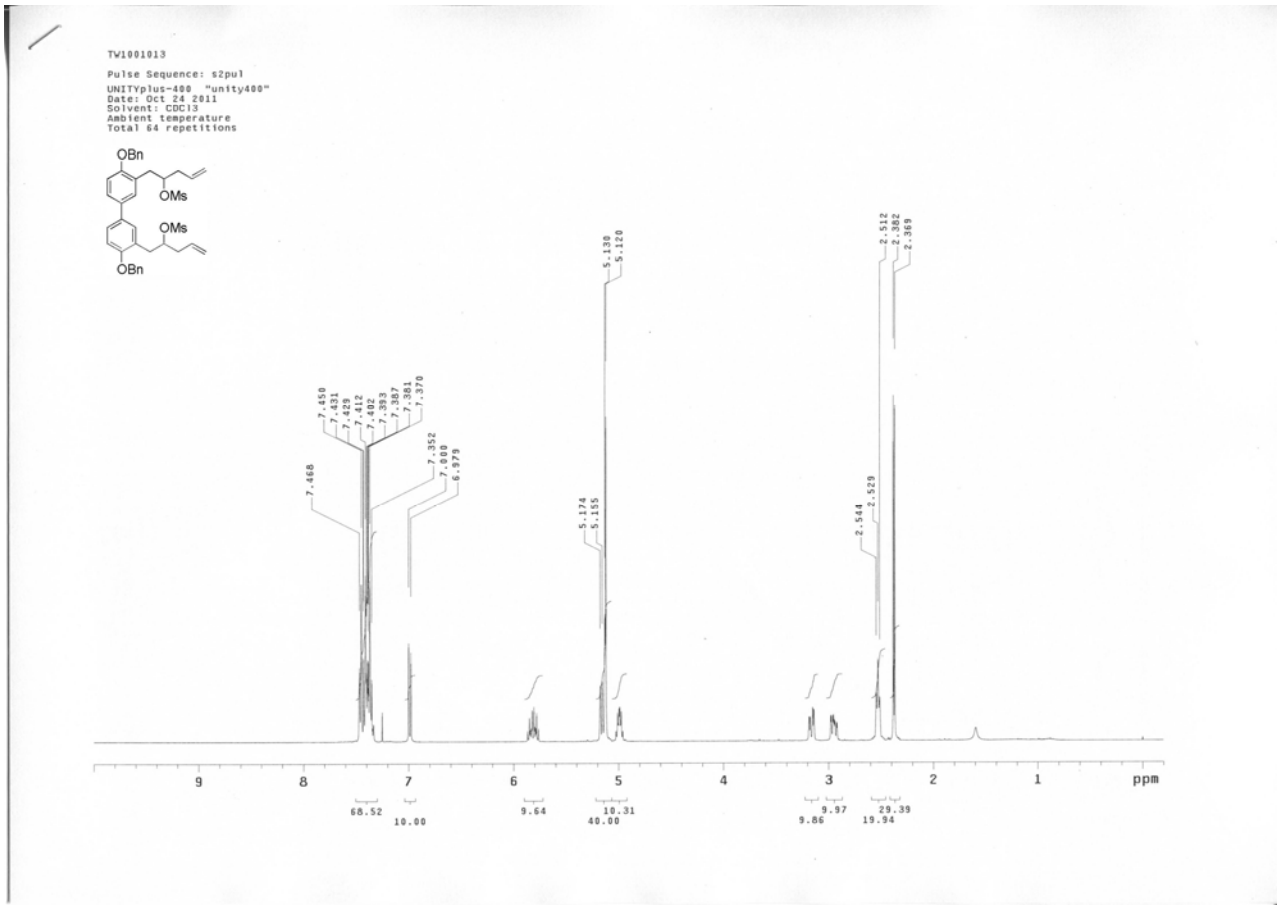
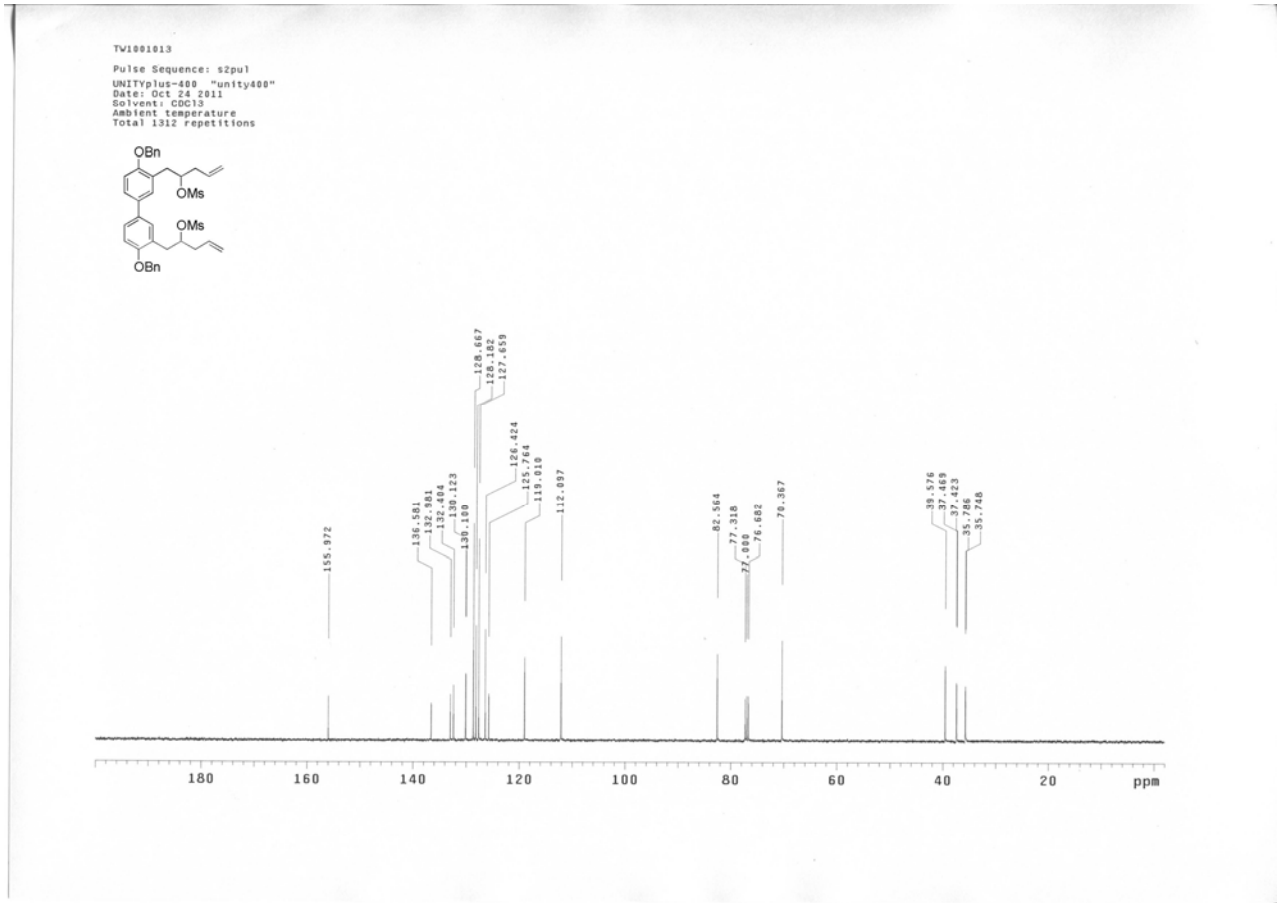
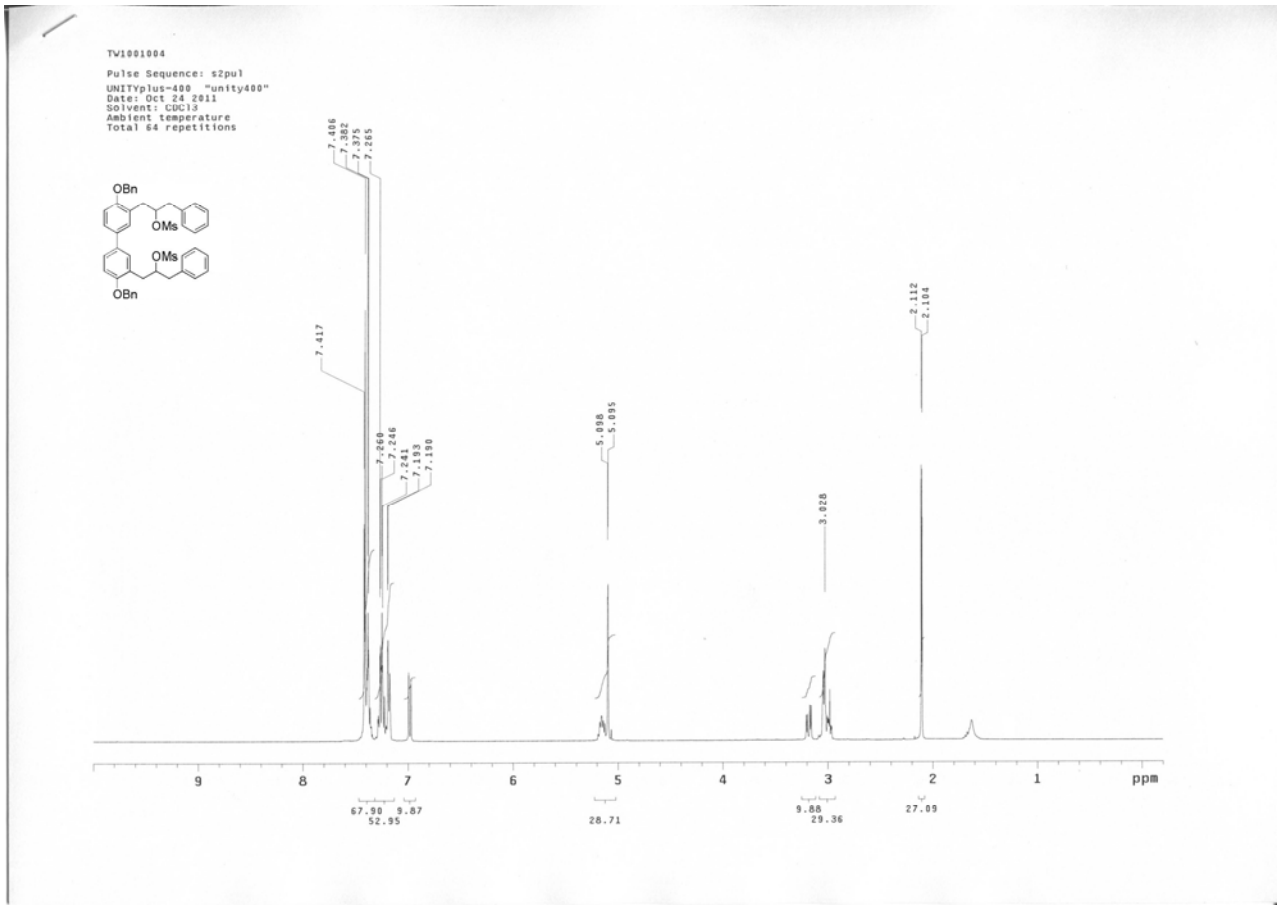
132.984
129.938
129.908
128.680
128.150
127.566
126.422
125.641
112.032
80.069
77.318
77.000
76.682
70.263
38.088
38.066
37.209
37.179
21.539
180
160
140
120
100
80
60
40
20
ppm

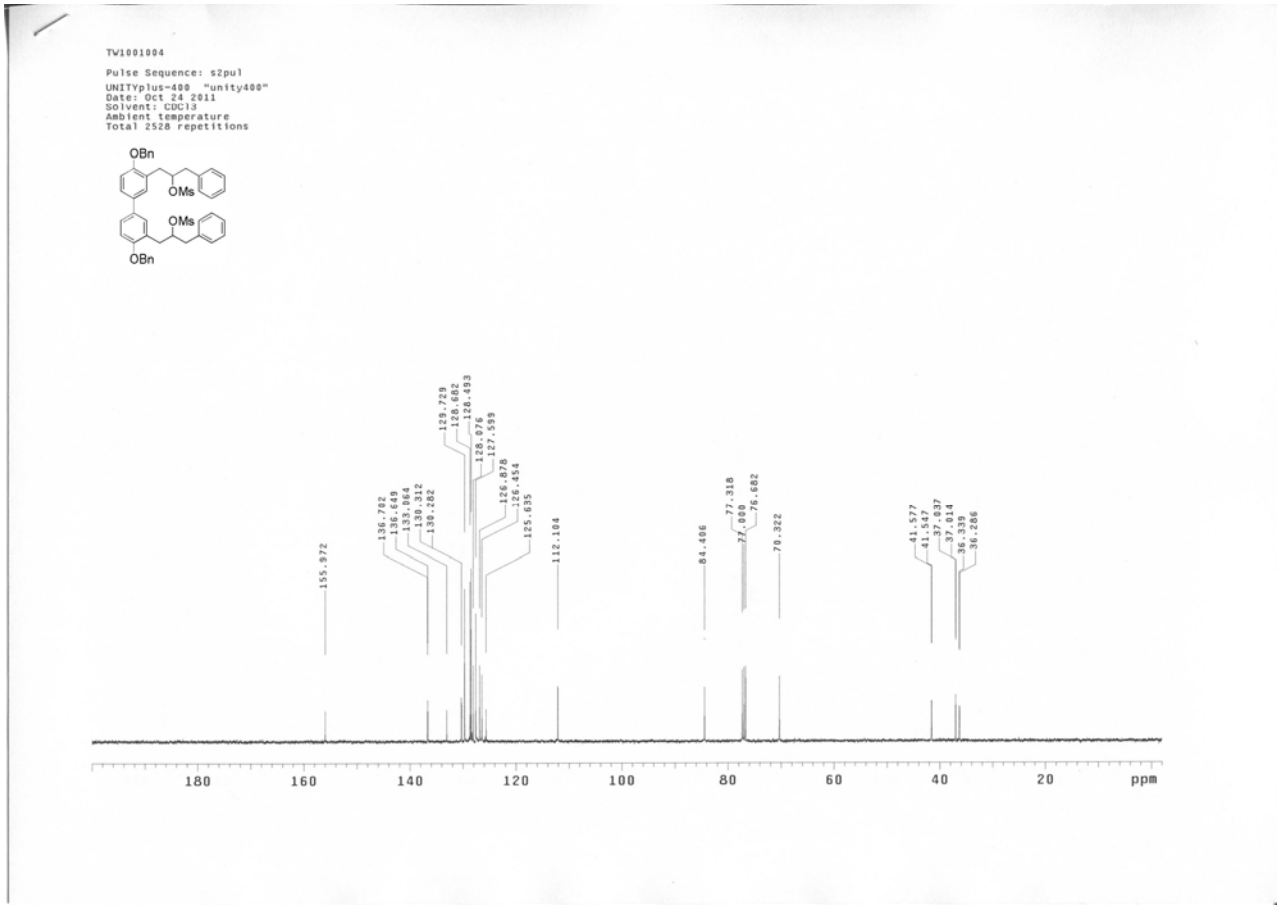
Compound (8c)


TW1001013
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
OBn
OMs
OMs
OBn
7.468
7.450
7.431
7.429
7.412
7.402
7.393
7.387
7.381
7.370
7.352
7.000
6.979
5.174
5.165
5.130
5.120
2.544
2.529
2.512
2.382
2.369
9
8
7
6
5
4
3
2
1
ppm
68.52
10.00
9.64
10.31
40.00
9.97
9.86
29.39
19.94

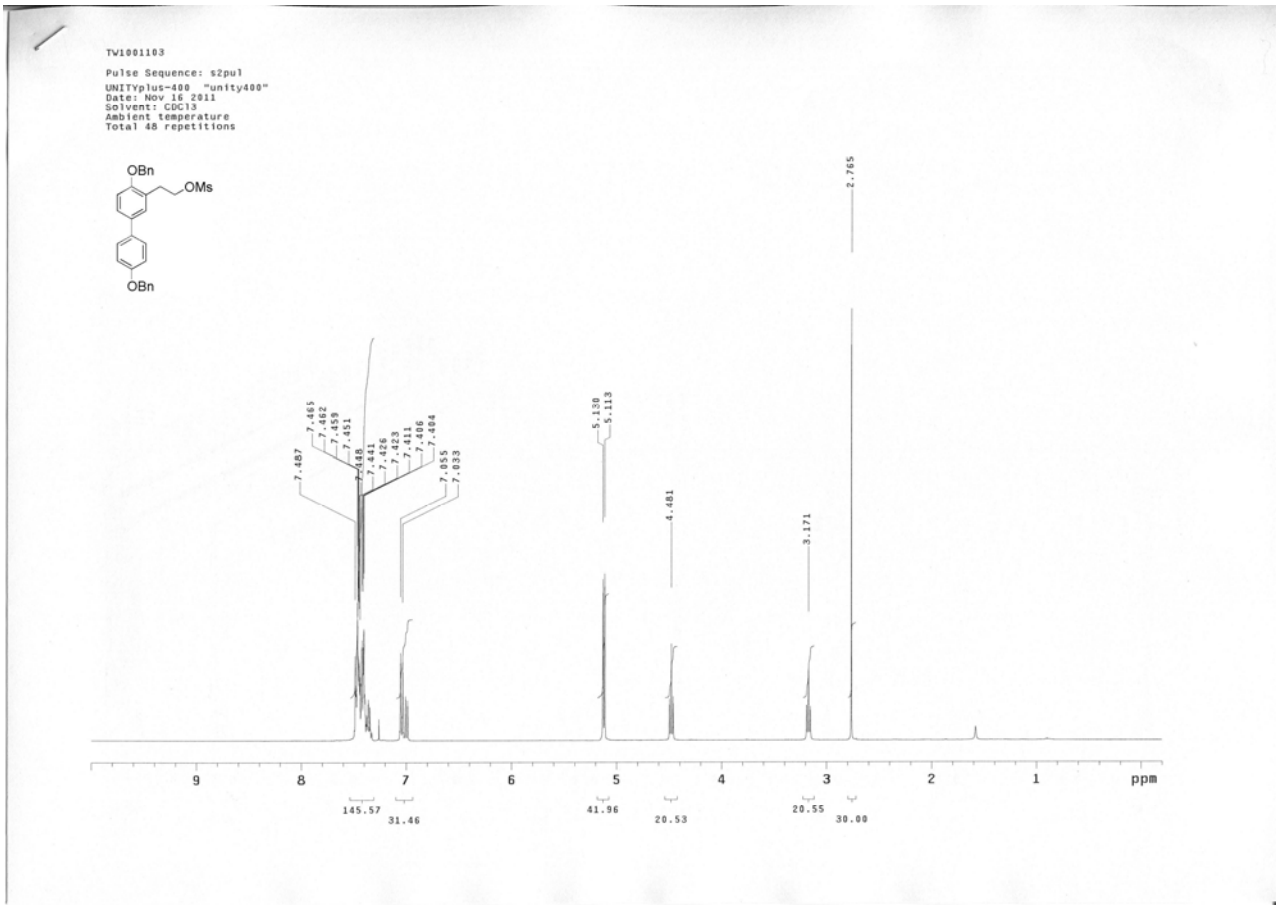

TW1001013
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 1312 repetitions
OBn
OMs
OMs
OBn
155.972
136.581
132.811
132.404
130.123
130.100
128.667
128.182
127.659
126.424
125.764
119.016
112.097
82.564
77.318
77.000
76.682
70.367
39.576
37.469
37.423
35.786
35.748
180
160
140
120
100
80
60
40
20
ppm

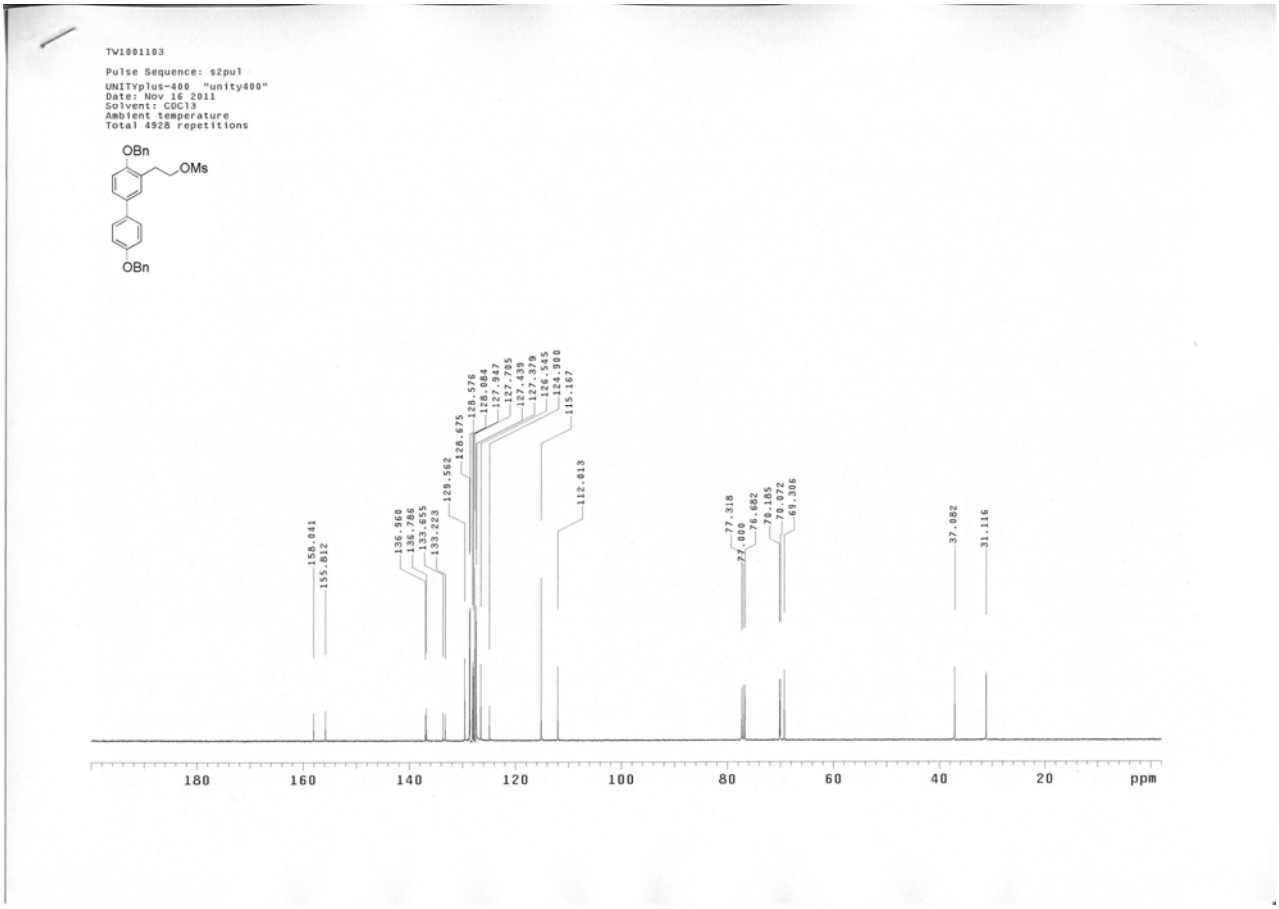
Compound (8d)


TW1001004
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
OBn
OMs
OMs
OBn
7.406
7.382
7.375
7.265
7.417
7.260
7.246
7.241
7.193
7.190
5.098
5.095
3.028
2.112
2.104
9
8
7
6
5
4
3
2
1
ppm
67.90
9.87
52.95
28.71
9.88
29.36
27.09

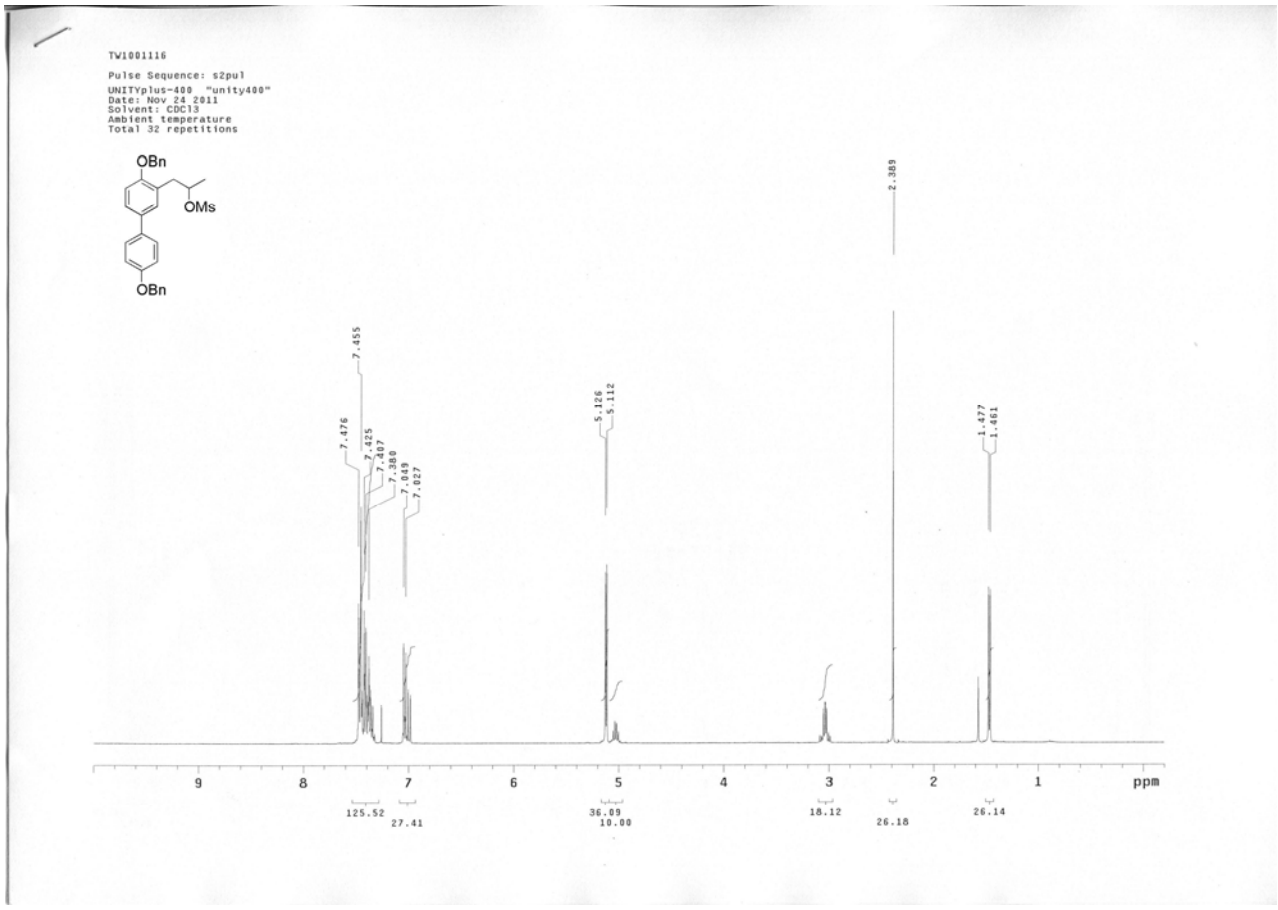

TW1001004
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 2528 repetitions
OBn
OMs
OMs
OBn
155.972
136.702
136.649
133.064
130.312
130.282
129.729
128.682
128.493
128.076
127.599
126.878
126.454
125.855
112.104
84.406
77.318
77.000
76.682
70.322
41.577
41.547
37.037
37.014
36.339
36.086
180
160
140
120
100
80
60
40
20
ppm

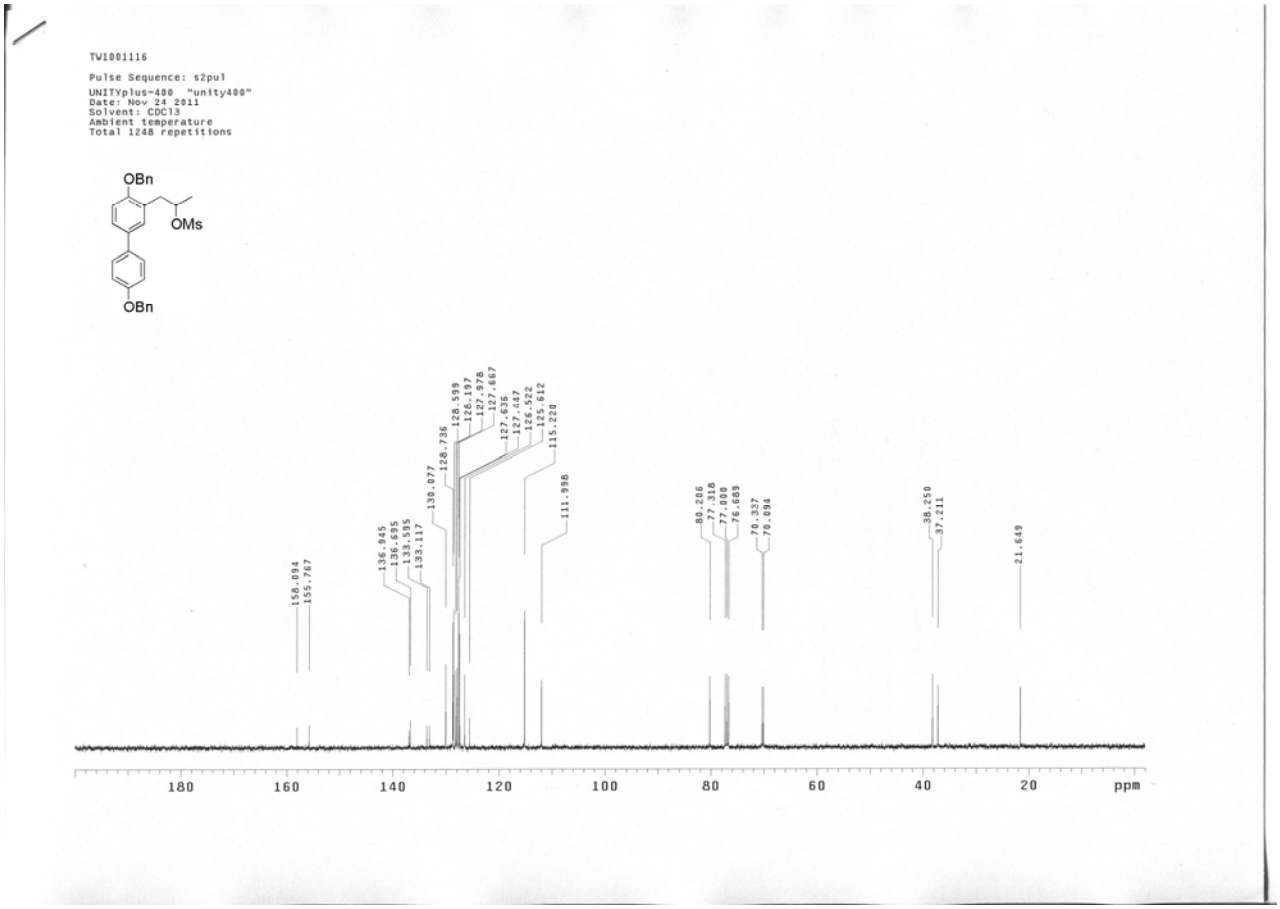
Compound (8e)


TW1001103
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 16 2011
Solvent: CDCl3
Ambient temperature
Total 48 repetitions
OBn
OMs
OBn
7.487
7.465
7.462
7.459
7.451
7.441
7.426
7.423
7.411
7.406
7.404
7.055
7.053
5.130
5.113
4.481
3.171
2.765
ppm
145.57
31.46
41.96
20.53
20.55
30.00

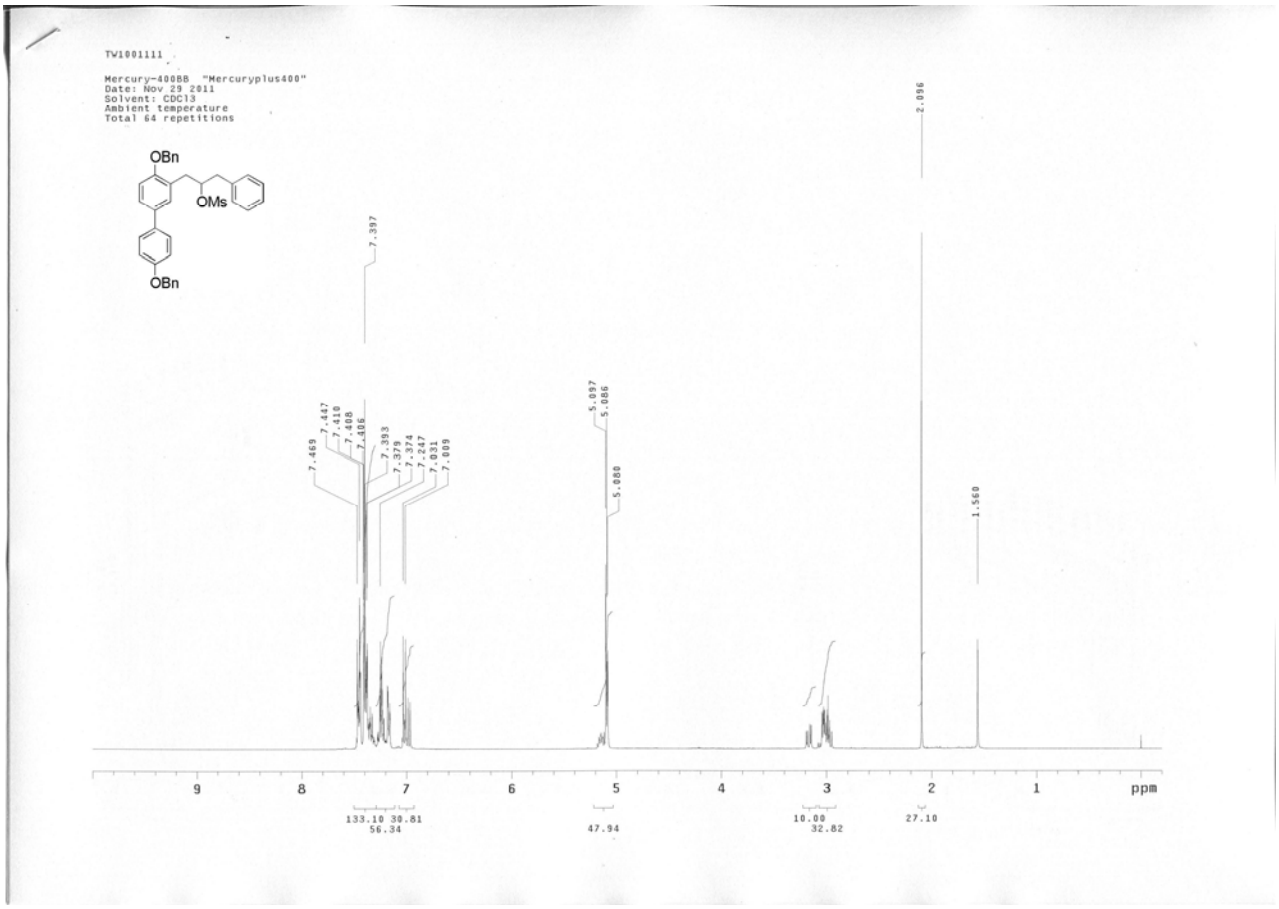

TW1001103
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 16 2011
Solvent: CDCl3
Ambient temperature
Total 4928 repetitions
OBn
OMs
OBn
158.041
155.812
136.960
136.786
133.655
133.223
129.562
128.675
128.576
128.384
128.087
127.705
127.439
127.379
126.545
124.900
115.167
112.013
77.318
77.000
76.682
70.185
70.072
69.306
37.082
31.116
ppm

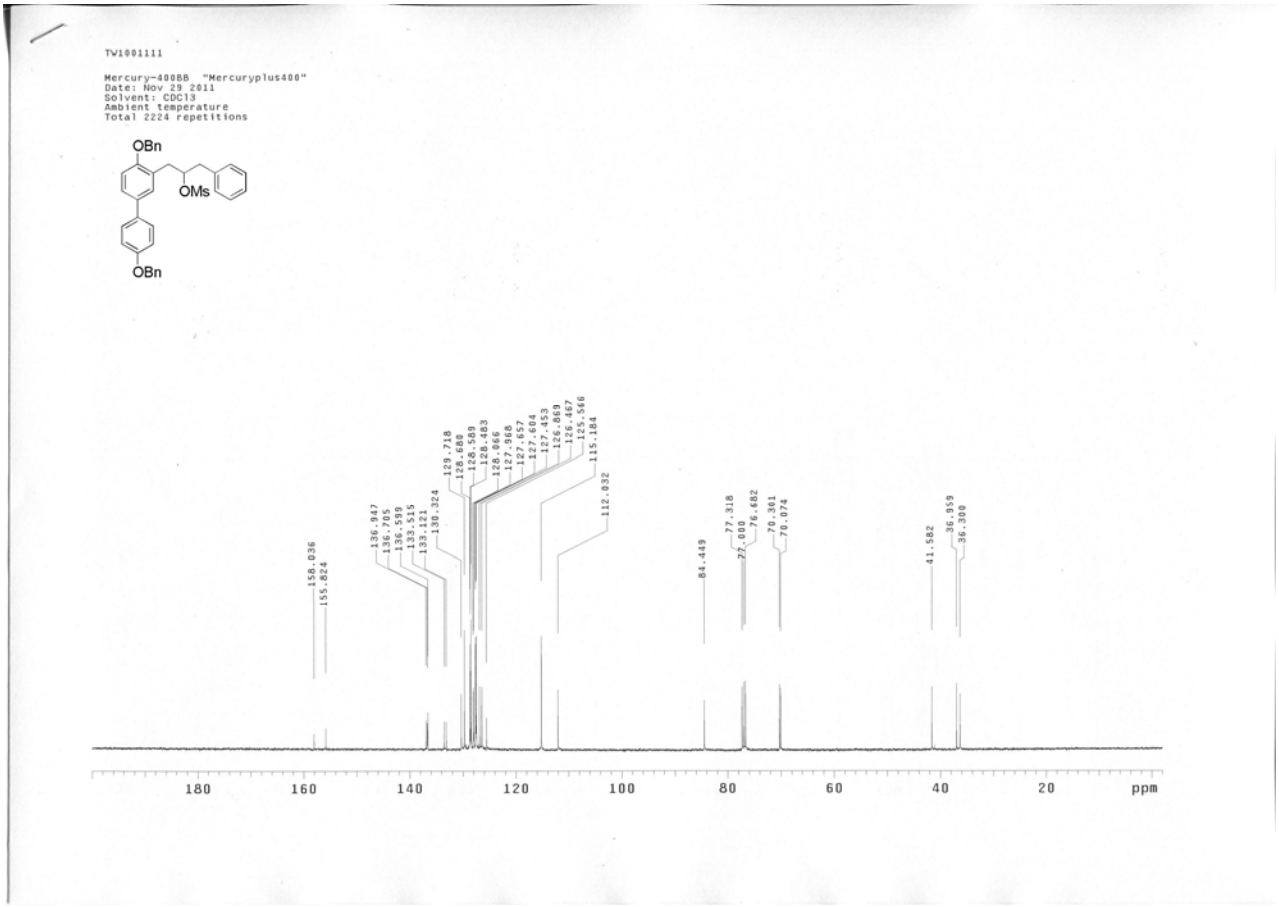
Compound (8f)


TW1001116
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 24 2011
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
OBn
OMs
OBn
7.476
7.455
7.425
7.407
7.380
7.049
7.027
5.126
5.112
2.389
1.477
1.461
9
8
7
6
5
4
3
2
1
ppm
125.52
27.41
36.09
10.00
18.12
26.18
26.14

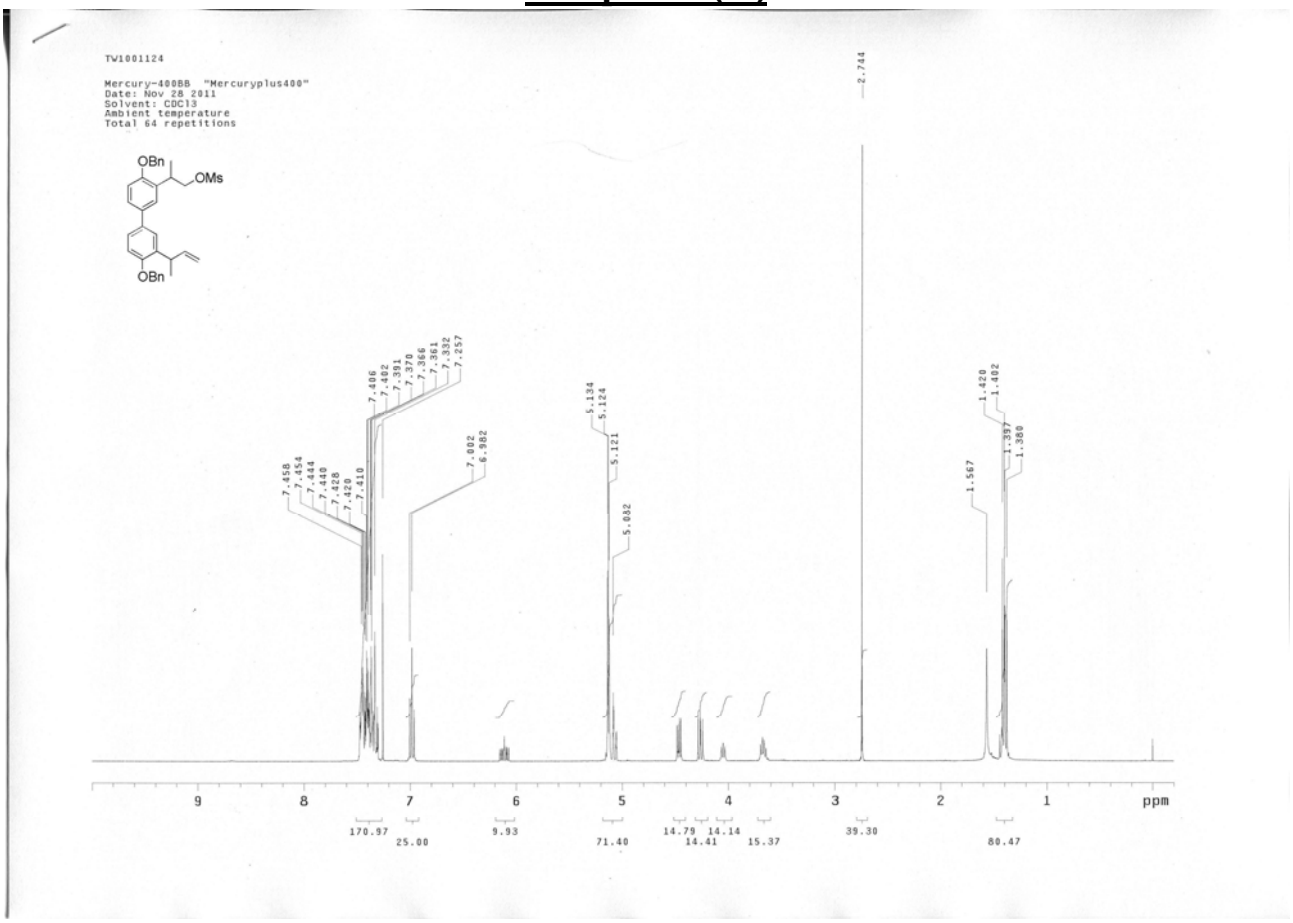

TW1001116
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 24 2011
Solvent: CDCl3
Ambient temperature
Total 1248 repetitions
OBn
OMs
OBn
158.094
155.767
136.945
136.695
133.595
133.117
130.077
128.736
128.599
128.197
127.978
127.667
127.636
127.447
126.522
125.612
115.220
111.998
80.206
77.318
77.000
76.689
70.337
70.094
38.250
37.211
21.649
180
160
140
120
100
80
60
40
20
ppm

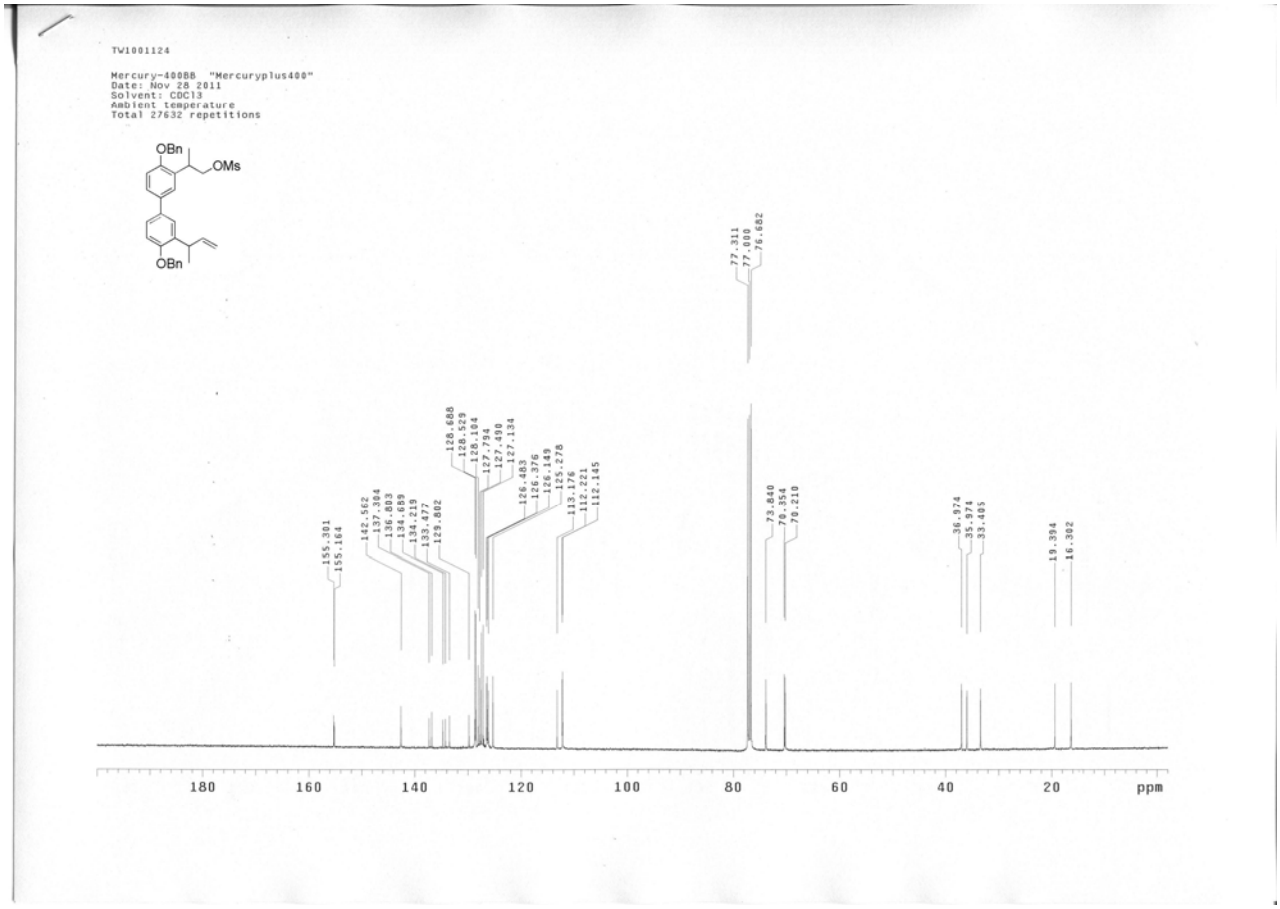
Compound (8h)


TW1001111
Mercury-400BB "Mercuryplus400"
Date: Nov 29 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
OBn
OMs
OBn
7.397
7.469
7.447
7.410
7.408
7.406
7.393
7.379
7.374
7.247
7.031
7.009
5.097
5.086
5.080
2.096
1.560
9
8
7
6
5
4
3
2
1
ppm
133.10 30.81
56.34
47.94
10.00
32.82
27.10

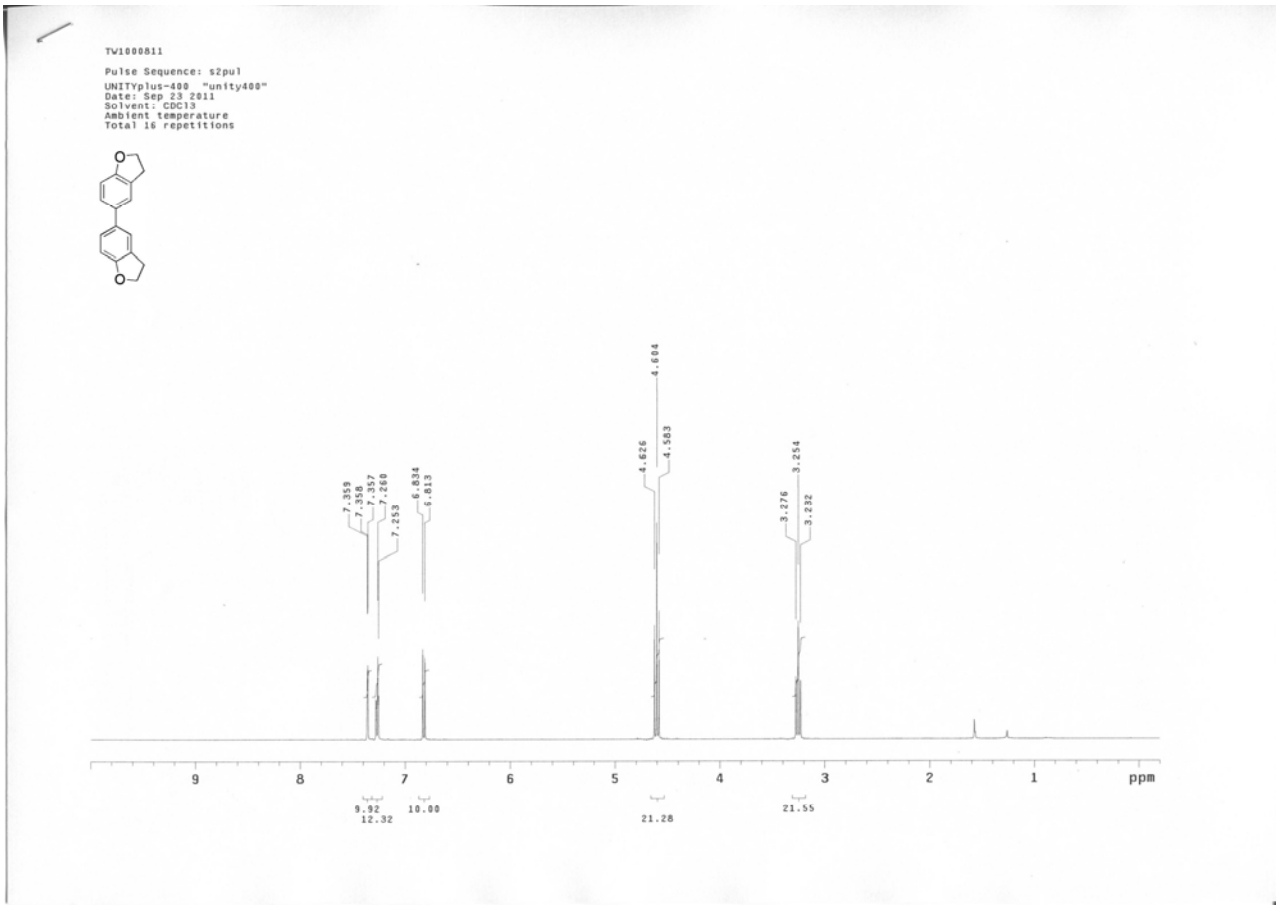

TW1001111
Mercury-400BB "Mercuryplus400"
Date: Nov 29 2011
Solvent: CDCl3
Ambient temperature
Total 2224 repetitions
OBn
OMs
OBn
158.036
155.824
136.947
136.765
136.558
133.515
133.121
130.324
129.718
128.680
128.569
128.483
128.066
127.968
127.657
127.604
127.453
126.869
126.467
115.566
115.184
112.032
84.449
77.318
77.000
76.682
70.361
70.074
41.582
36.959
36.300
180
160
140
120
100
80
60
40
20
ppm

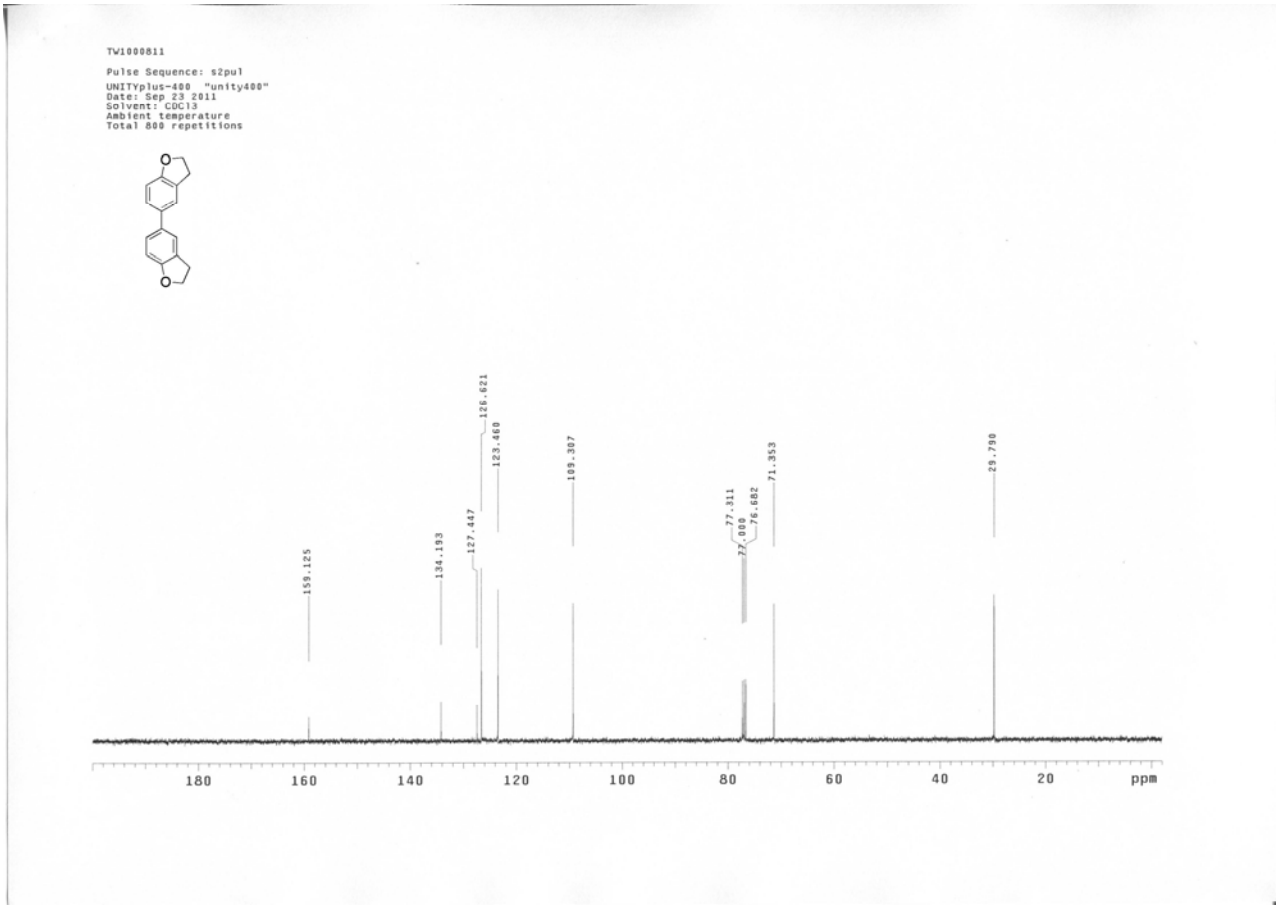
Compound (8i)


TW1001124
Mercury-400BB "Mercuryplus400"
Date: Nov 28 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
OBn
OMs
OBn
2.744
7.458
7.454
7.444
7.440
7.438
7.420
7.410
7.406
7.402
7.391
7.370
7.366
7.361
7.332
7.257
7.002
6.982
5.134
5.124
5.121
5.082
1.567
1.420
1.402
1.397
1.380
9
8
7
6
5
4
3
2
1
ppm
170.97
25.00
9.93
71.40
14.79
14.14
14.41
15.37
39.30
80.47

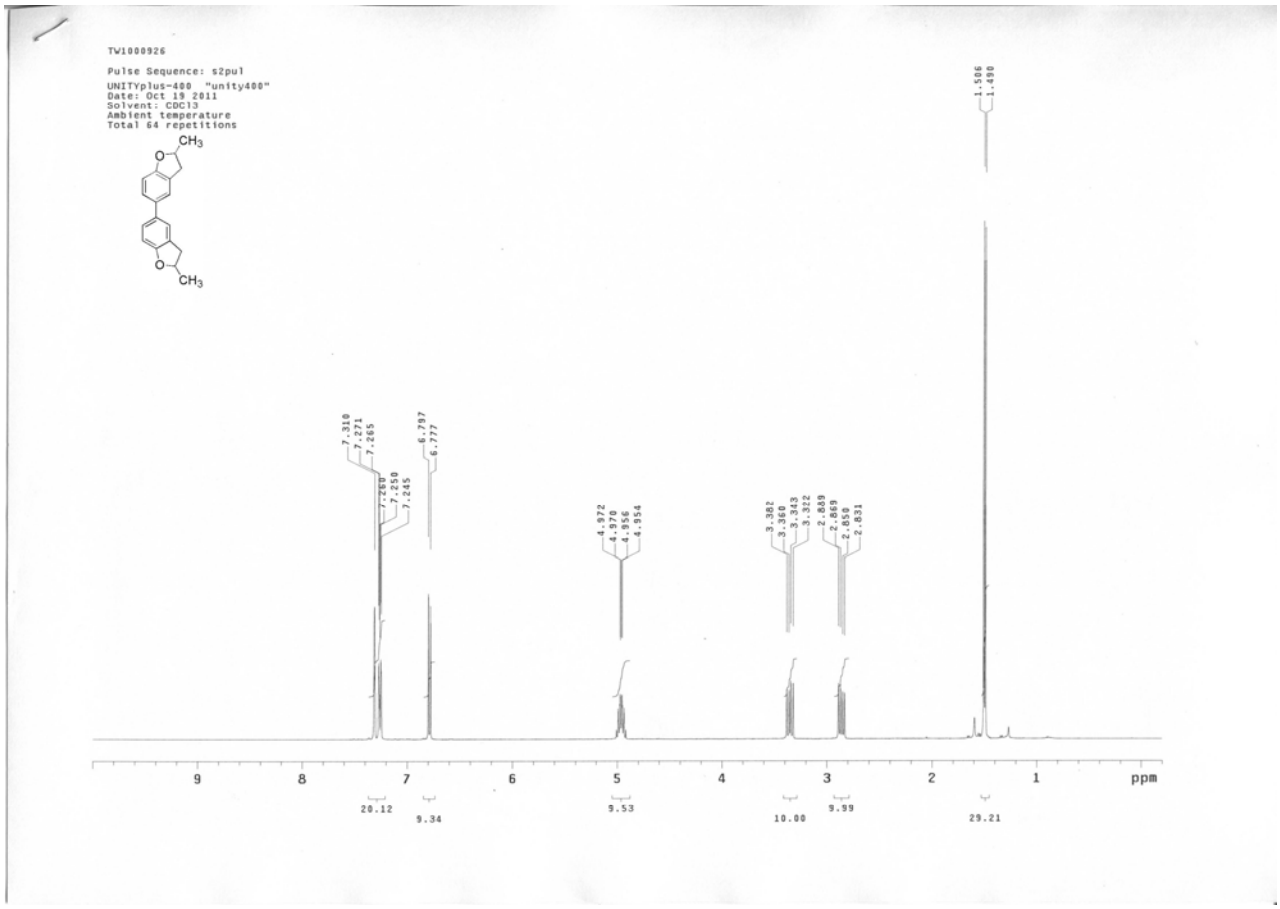

TW1001124
Mercury-400BB "Mercuryplus400"
Date: Nov 28 2011
Solvent: CDCl3
Ambient temperature
Total 27632 repetitions
OBn
OMs
OBn
77.311
77.000
76.682
155.301
155.164
142.562
137.384
136.803
134.169
134.139
133.477
129.802
128.688
128.529
128.184
127.794
127.498
127.184
126.483
126.376
126.149
125.278
113.176
112.221
112.145
73.840
70.354
70.210
36.974
35.974
33.405
19.394
16.302
180
160
140
120
100
80
60
40
20
ppm

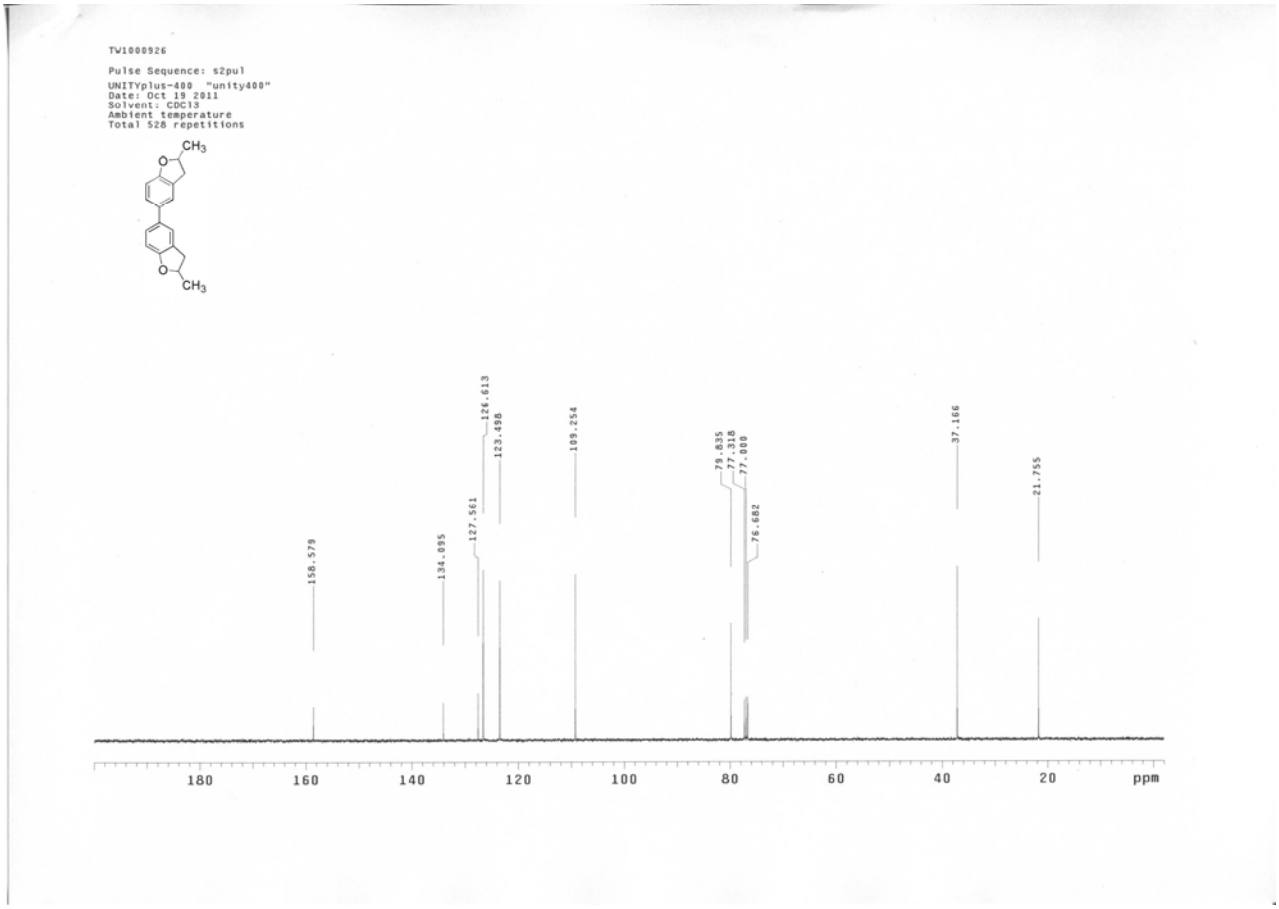
Compound (4a)


TW1000811
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Sep 23 2011
Solvent: CDCl3
Ambient temperature
Total 16 repetitions
7.359
7.358
7.357
7.260
7.253
6.834
6.613
4.604
4.626
4.583
3.276
3.254
3.232
9
8
7
6
5
4
3
2
1
ppm
9.92
12.32
10.00
21.28
21.55

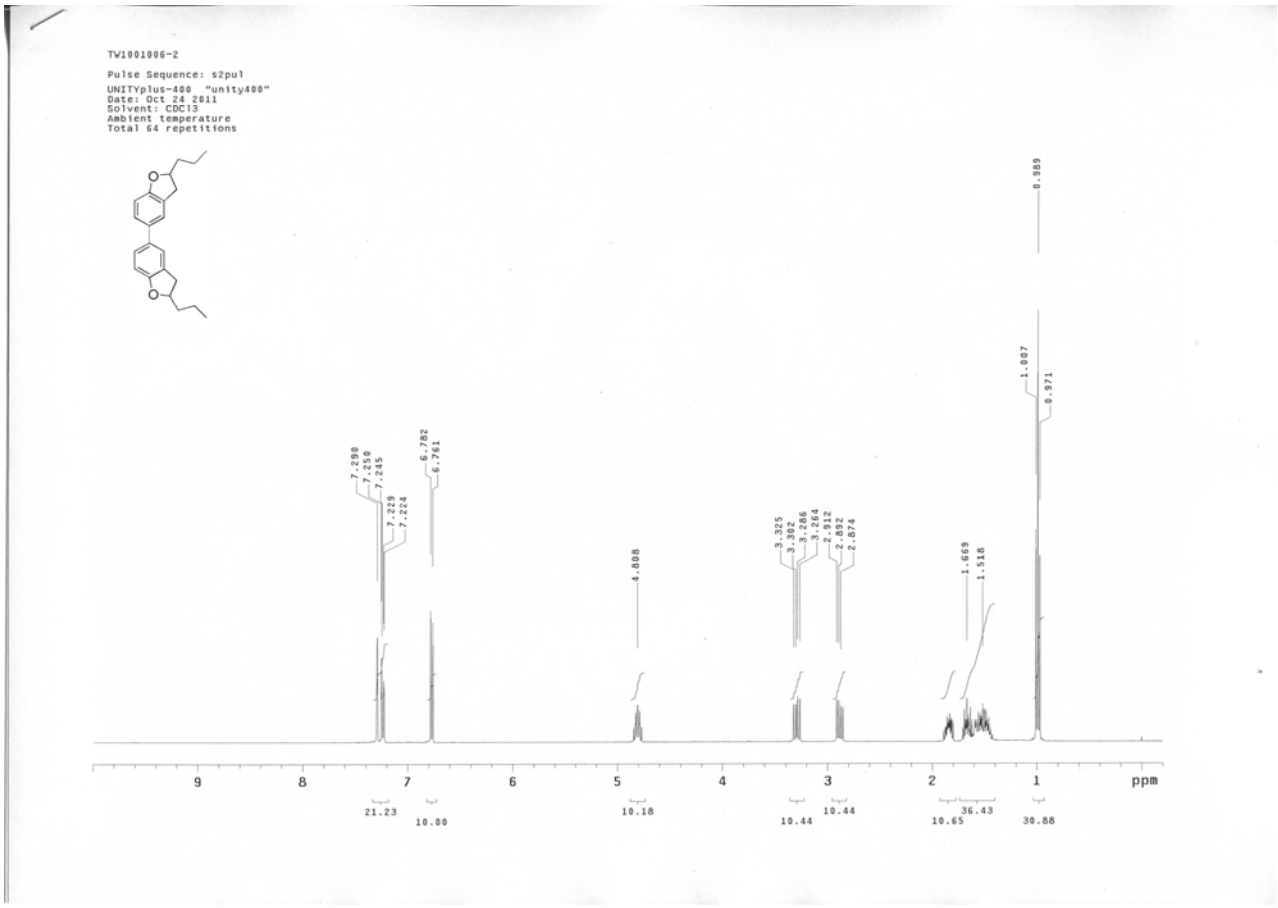

TW1000811
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Sep 23 2011
Solvent: CDCl3
Ambient temperature
Total 800 repetitions
159.125
134.193
127.447
126.621
123.460
109.307
77.311
77.000
76.682
71.353
29.790
180
160
140
120
100
80
60
40
20
ppm

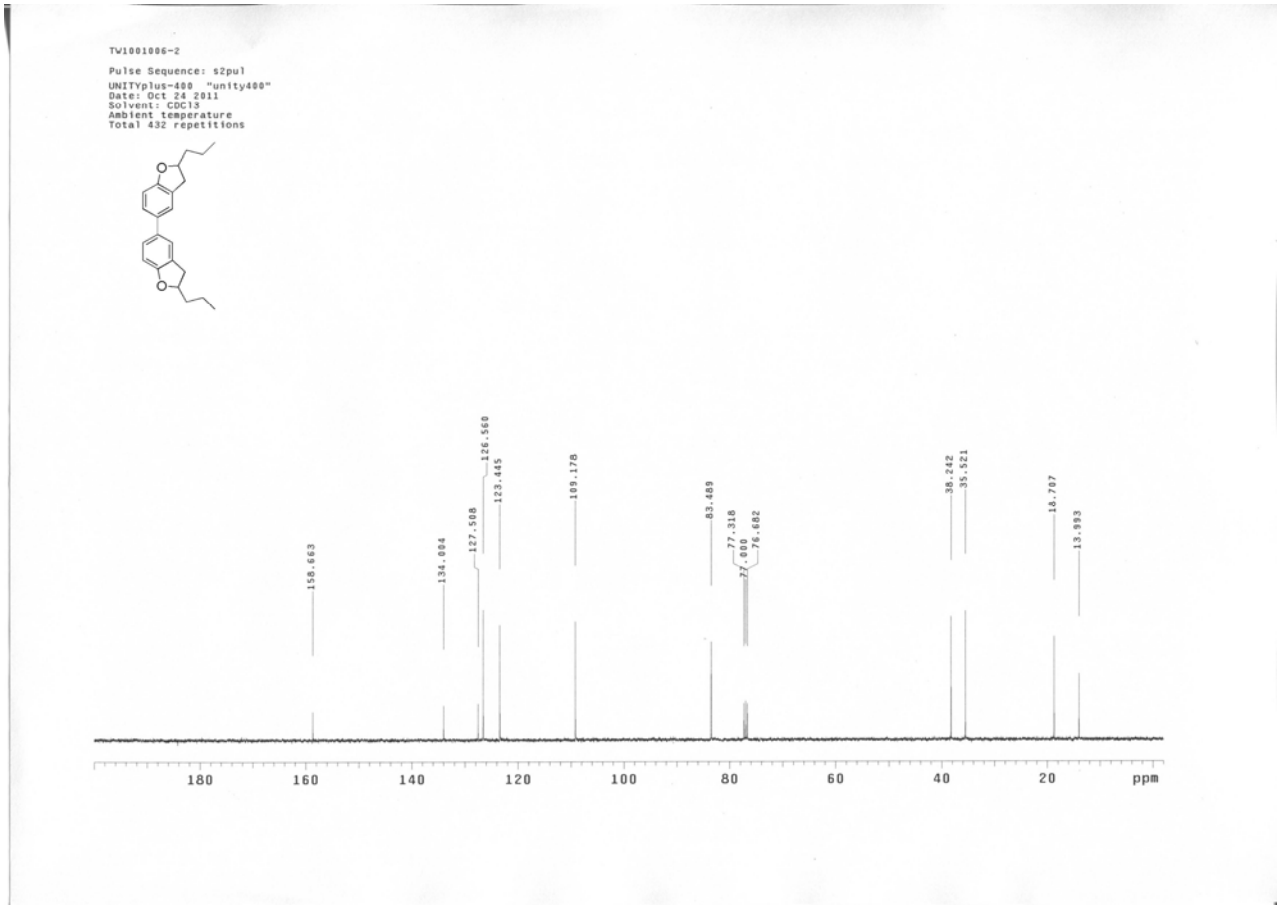
Compound (4b)


TW1000926
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 19 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
CH3
O
O
CH3
7.310
7.271
7.265
7.260
7.250
7.245
6.797
6.777
4.972
4.970
4.956
4.954
3.382
3.360
3.343
3.322
2.869
2.849
2.850
2.831
1.506
1.490
9
8
7
6
5
4
3
2
1
ppm
20.12
9.34
9.53
10.00
9.99
29.21

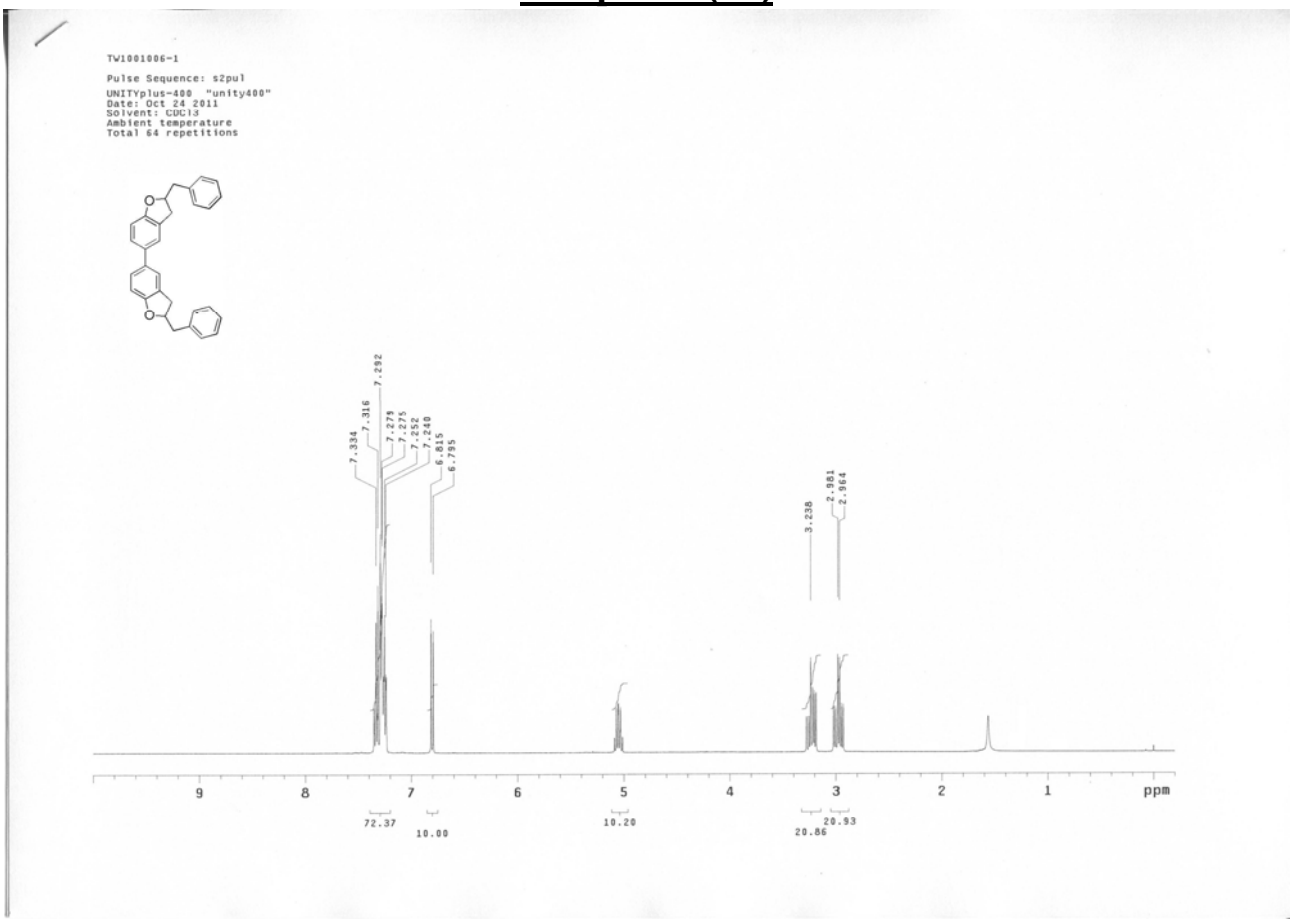

TW1000926
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 19 2011
Solvent: CDCl3
Ambient temperature
Total 528 repetitions
CH3
O
O
CH3
158.579
134.095
127.561
126.613
123.498
109.254
79.835
77.318
77.000
76.682
37.166
21.755
180
160
140
120
100
80
60
40
20
ppm

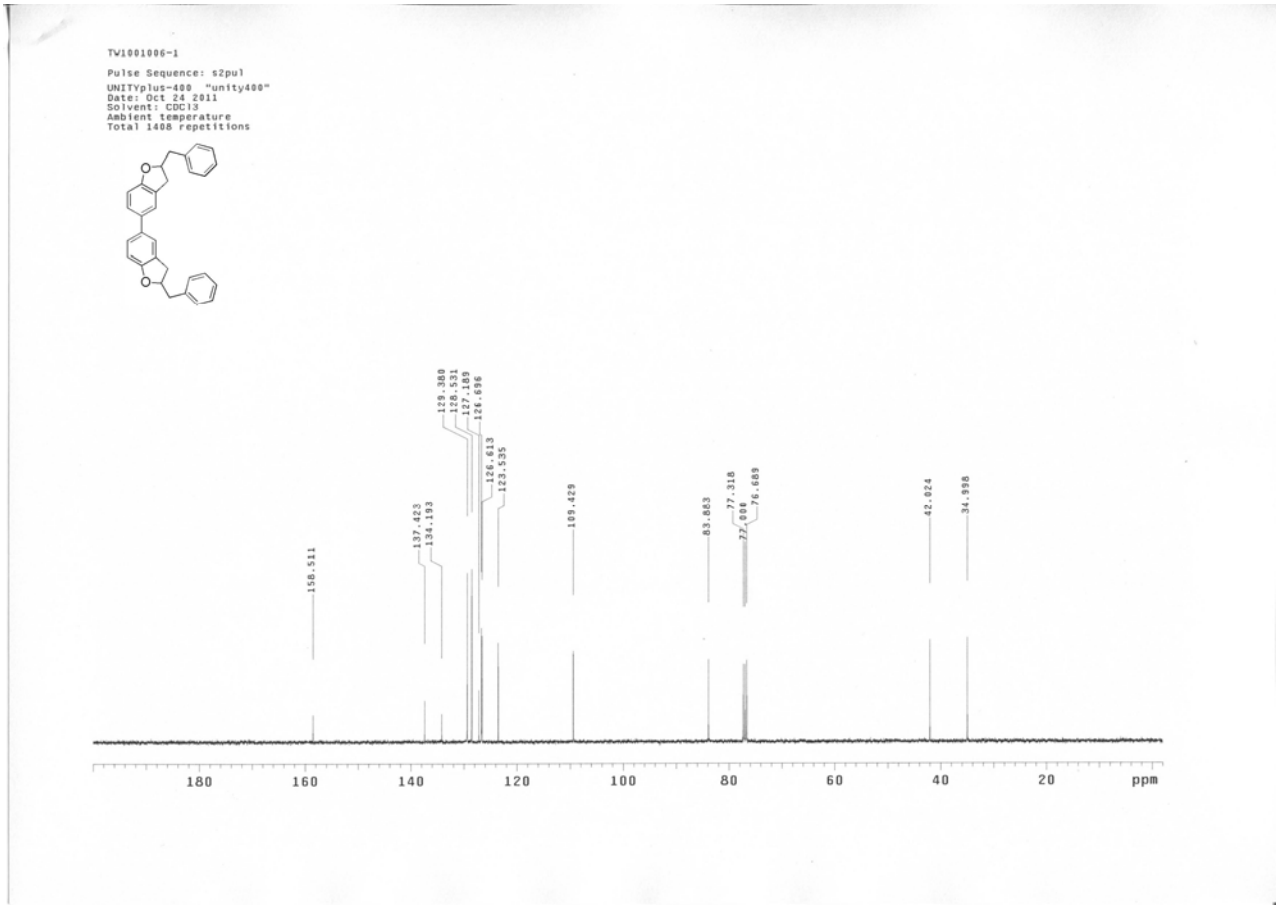
Compound (4c)


TW1001006-2
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
7.290
7.250
7.245
7.229
7.224
6.782
6.761
4.808
3.325
3.302
3.286
3.264
2.912
2.892
2.674
1.669
1.518
0.989
1.007
0.971
ppm
21.23
10.00
10.18
10.44
10.44
10.65
36.43
30.88

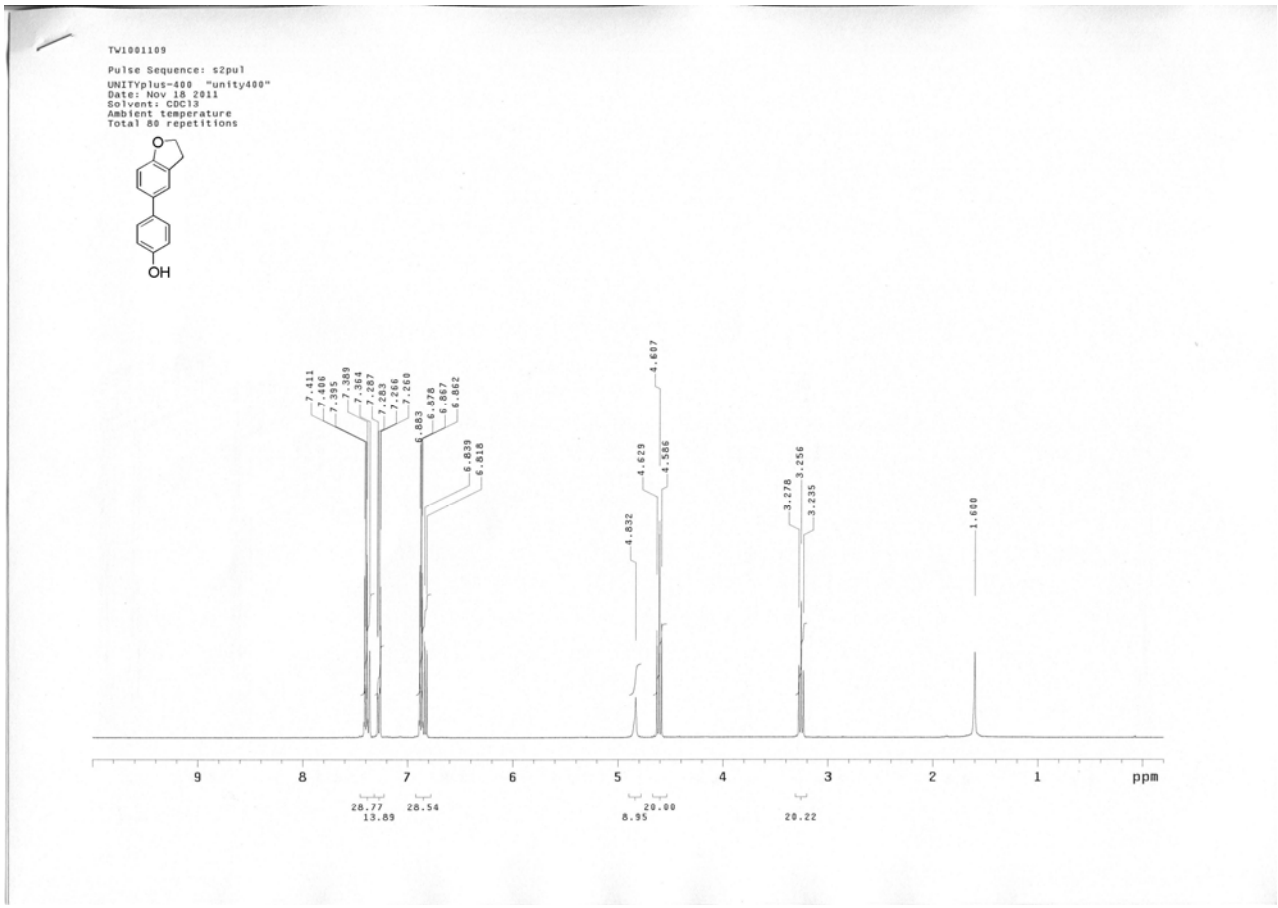

TW1001006-2
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 432 repetitions
158.663
134.004
127.568
126.560
123.445
109.178
83.489
77.318
77.000
76.682
38.242
35.521
18.707
13.993
ppm

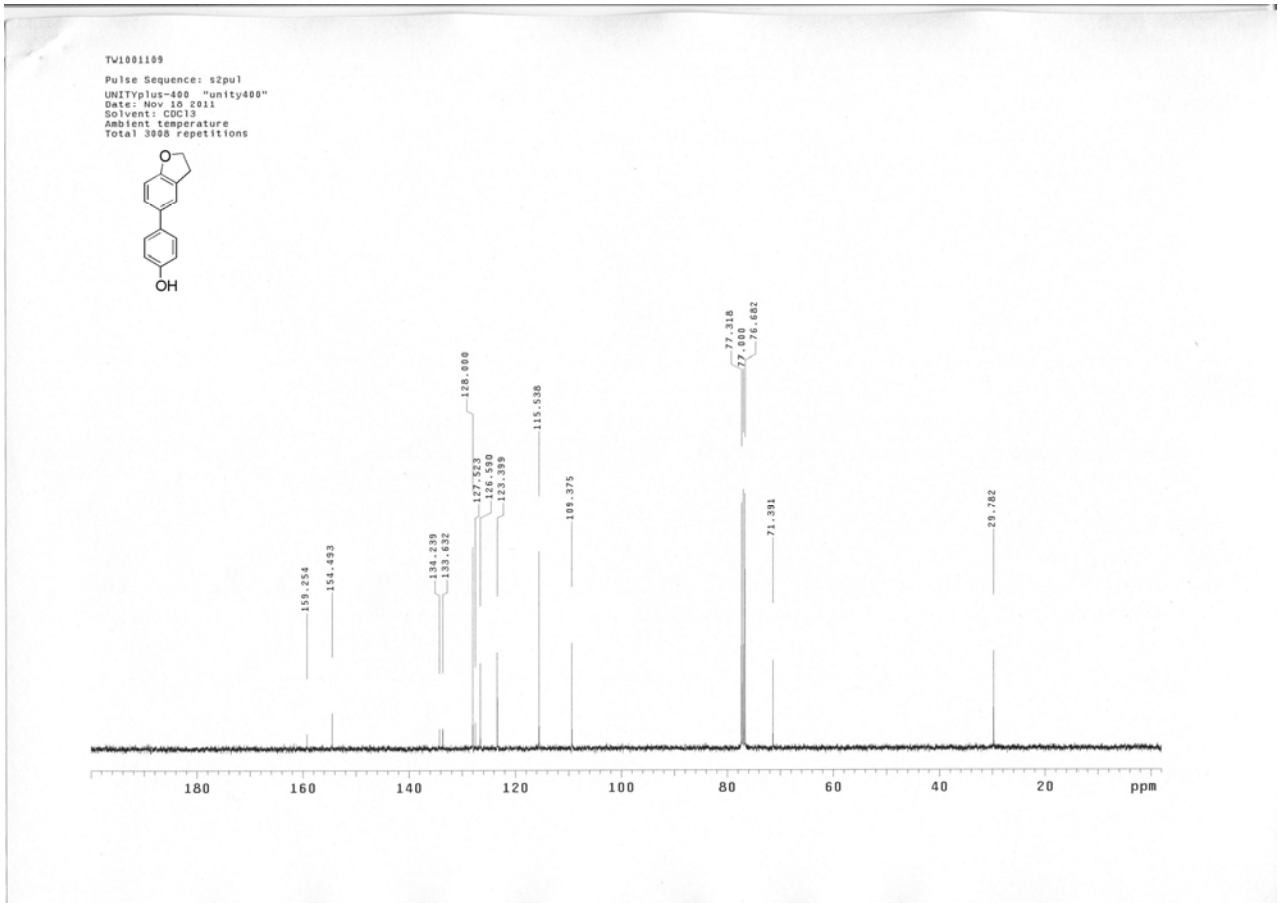
Compound (4d)


TW1001006-1
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
7.334
7.316
7.292
7.279
7.275
7.252
7.240
6.815
6.795
3.238
2.981
2.964
9
8
7
6
5
4
3
2
1
ppm
72.37
10.00
10.20
20.86
20.93

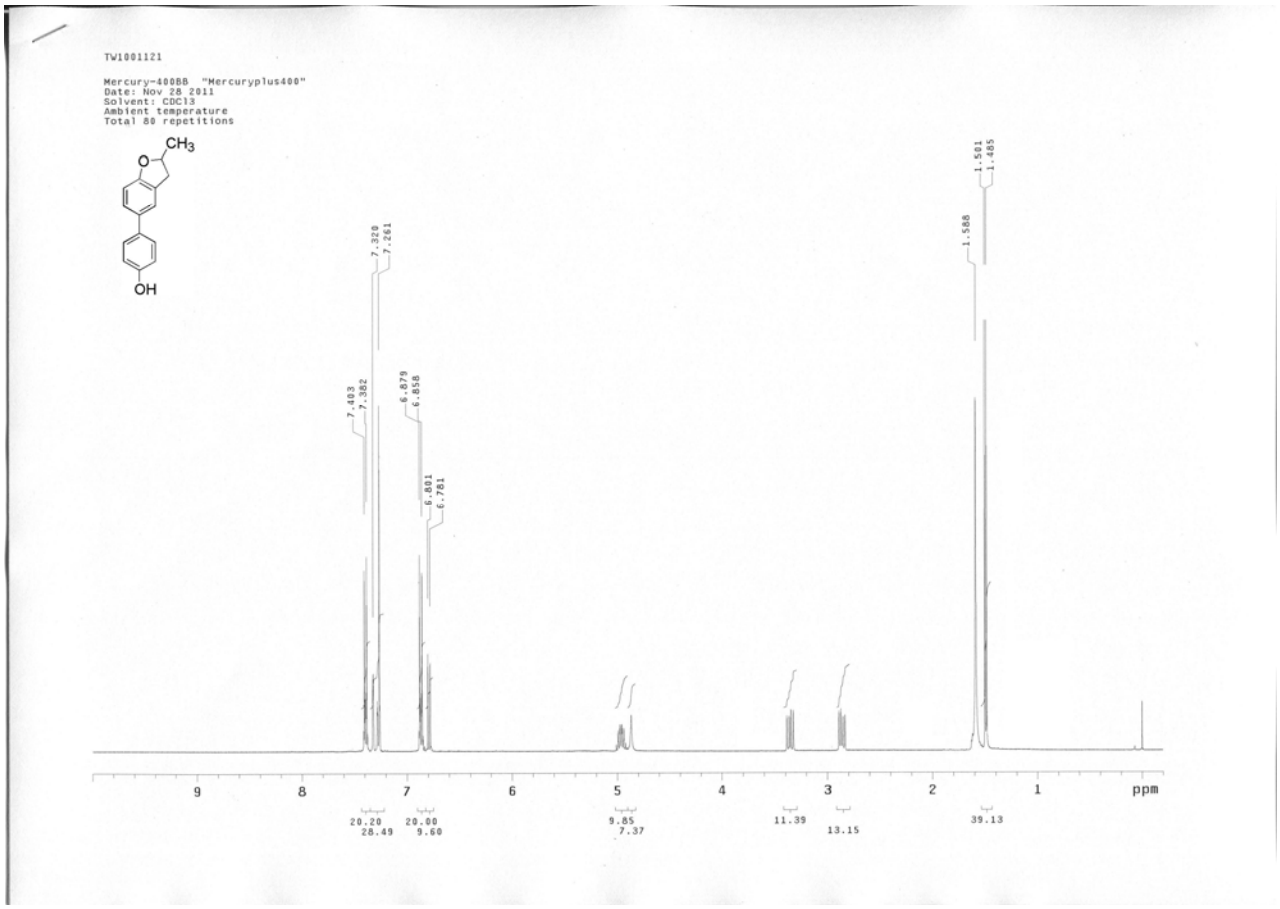

TW1001006-1
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Oct 24 2011
Solvent: CDCl3
Ambient temperature
Total 1408 repetitions
158.511
137.423
134.193
129.380
128.531
127.185
126.696
126.613
123.535
109.429
83.863
77.318
77.000
76.689
42.024
34.998
180
160
140
120
100
80
60
40
20
ppm

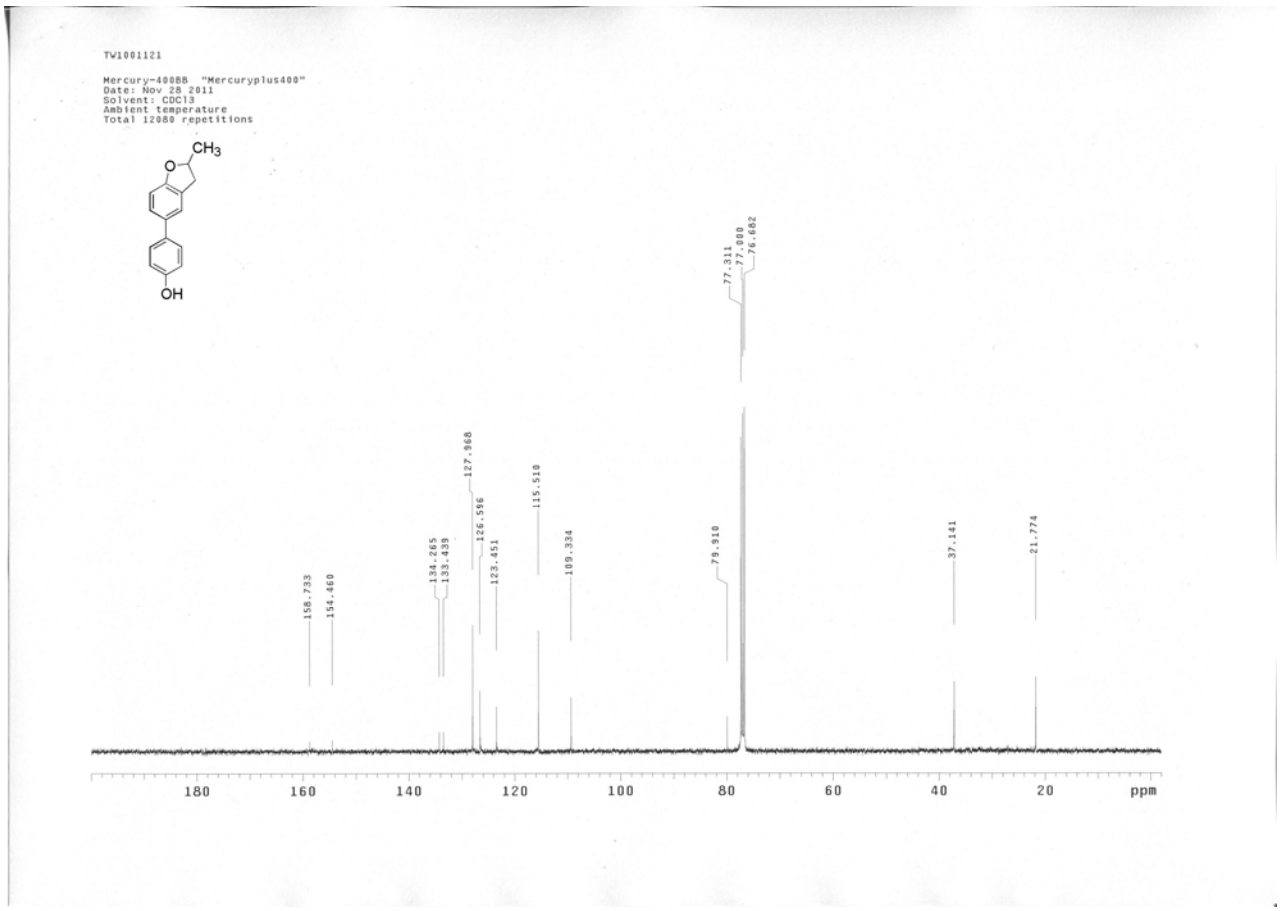
Compound (4e)


TW1001109
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 18 2011
Solvent: CDCl3
Ambient temperature
Total 80 repetitions
OH
7.411
7.406
7.395
7.389
7.384
7.267
7.283
7.266
7.260
6.883
6.878
6.867
6.862
6.839
6.818
4.607
4.629
4.566
4.832
3.278
3.256
3.235
1.660
9
8
7
6
5
4
3
2
1
ppm
28.77
13.89
28.54
20.00
8.95
20.22

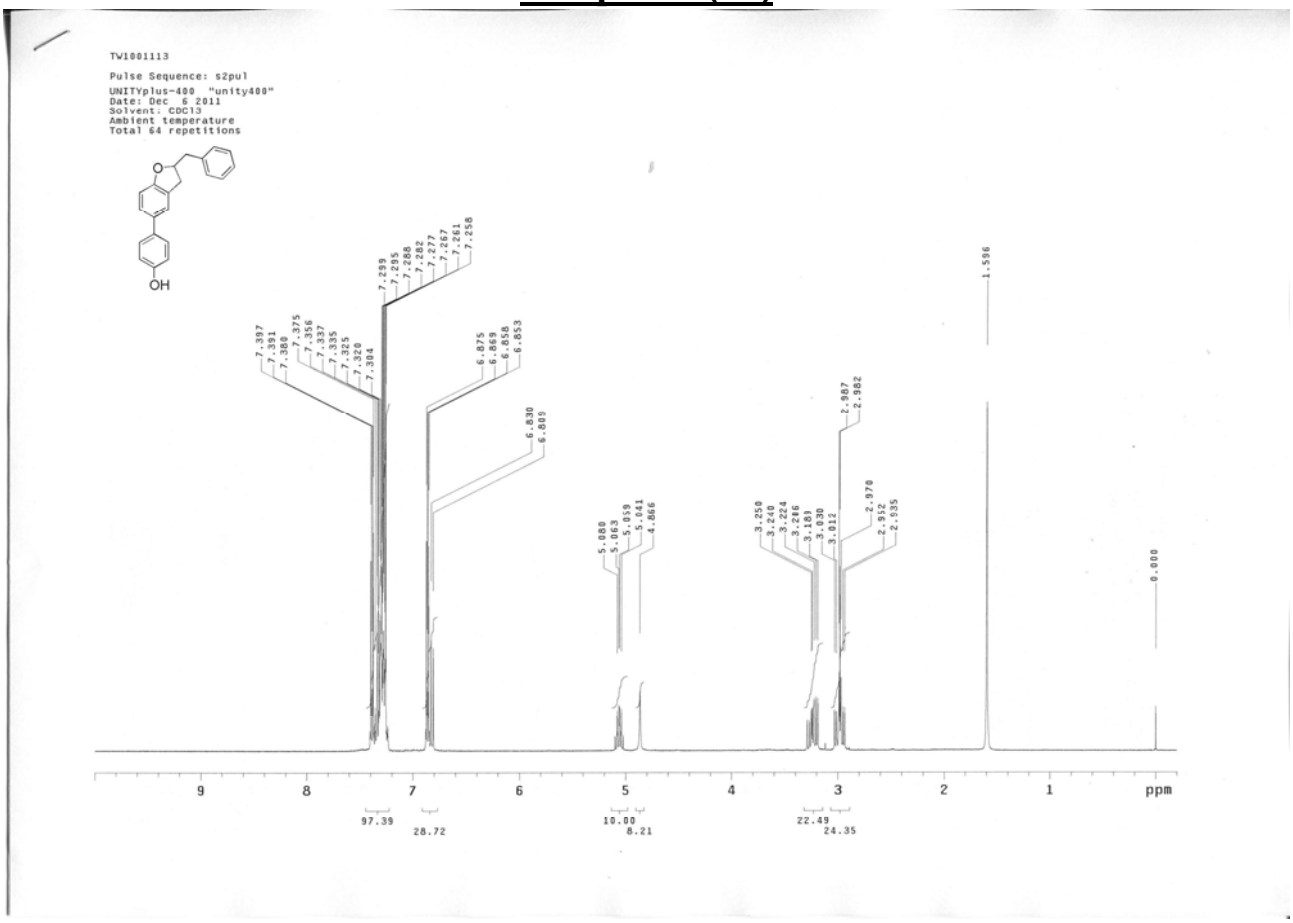

TW1001109
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 10 2011
Solvent: CDCl3
Ambient temperature
Total 3008 repetitions
OH
159.254
154.493
134.239
133.632
128.000
127.523
126.590
123.399
115.538
109.375
77.318
77.000
76.682
71.391
29.782
180
160
140
120
100
80
60
40
20
ppm

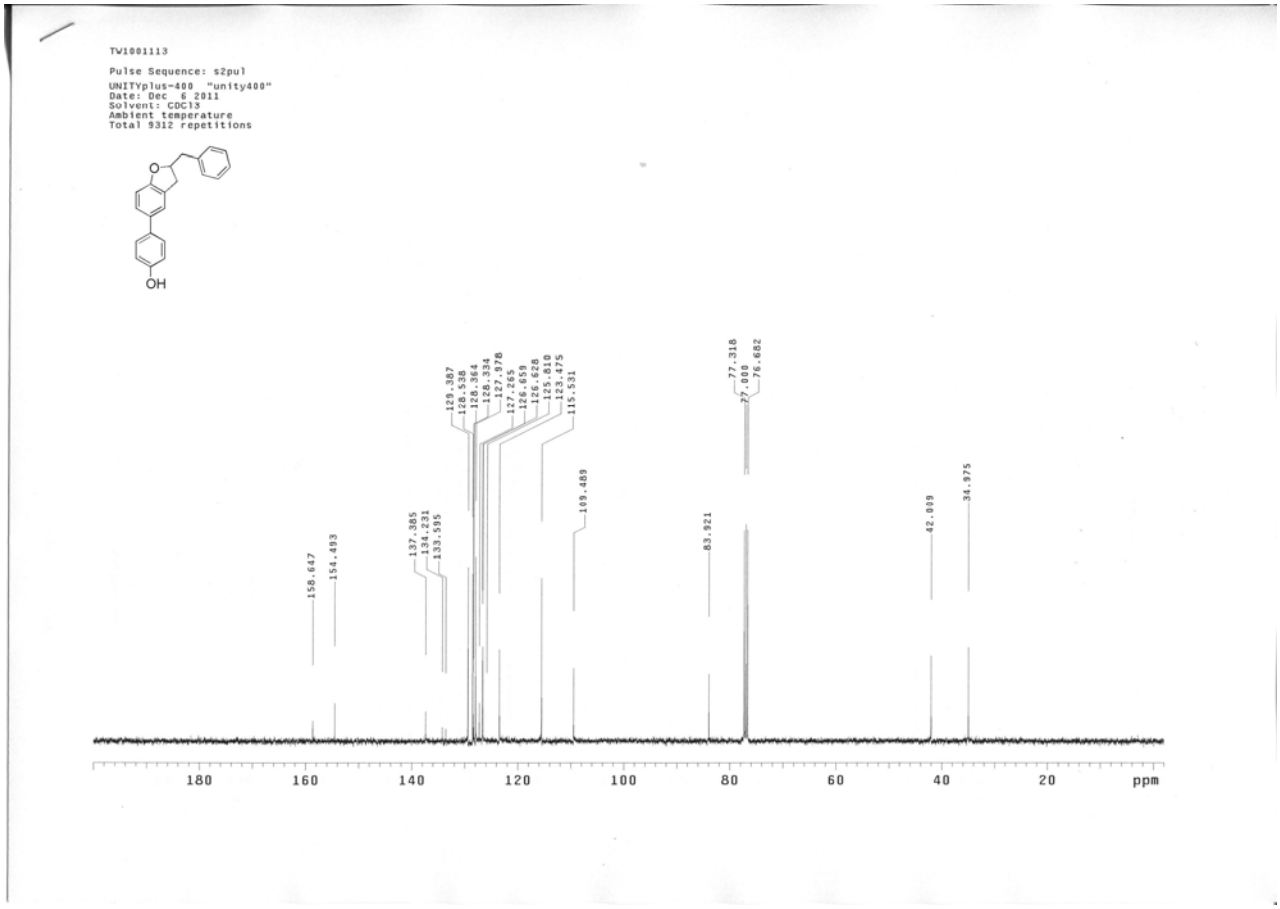
Compound (4f)


TW1001121
Mercury-400BB "Mercuryplus400"
Date: Nov 28 2011
Solvent: CDCl3
Ambient temperature
Total 80 repetitions
CH3
O
OH
7.403
7.382
7.329
7.261
6.879
6.858
6.801
6.781
1.588
1.501
1.485
9
8
7
6
5
4
3
2
1
ppm
20.20
28.49
20.00
9.60
9.85
7.37
11.39
13.15
39.13

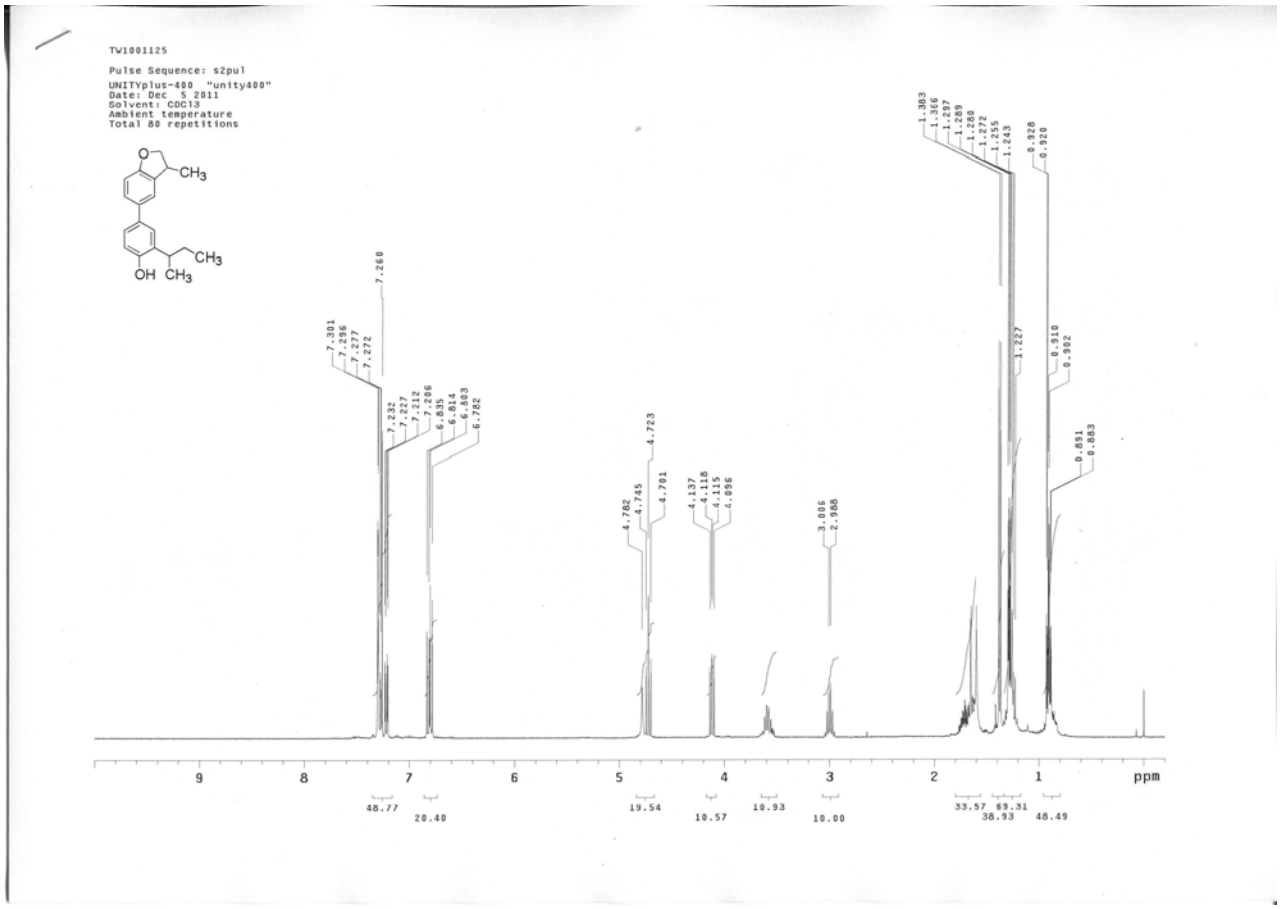

TW1001121
Mercury-400BB "Mercuryplus400"
Date: Nov 28 2011
Solvent: CDCl3
Ambient temperature
Total 12080 repetitions
CH3
O
OH
77.311
77.000
76.682
158.733
154.460
134.265
133.439
127.968
126.596
123.451
115.510
109.334
79.910
37.141
21.774
180
160
140
120
100
80
60
40
20
ppm

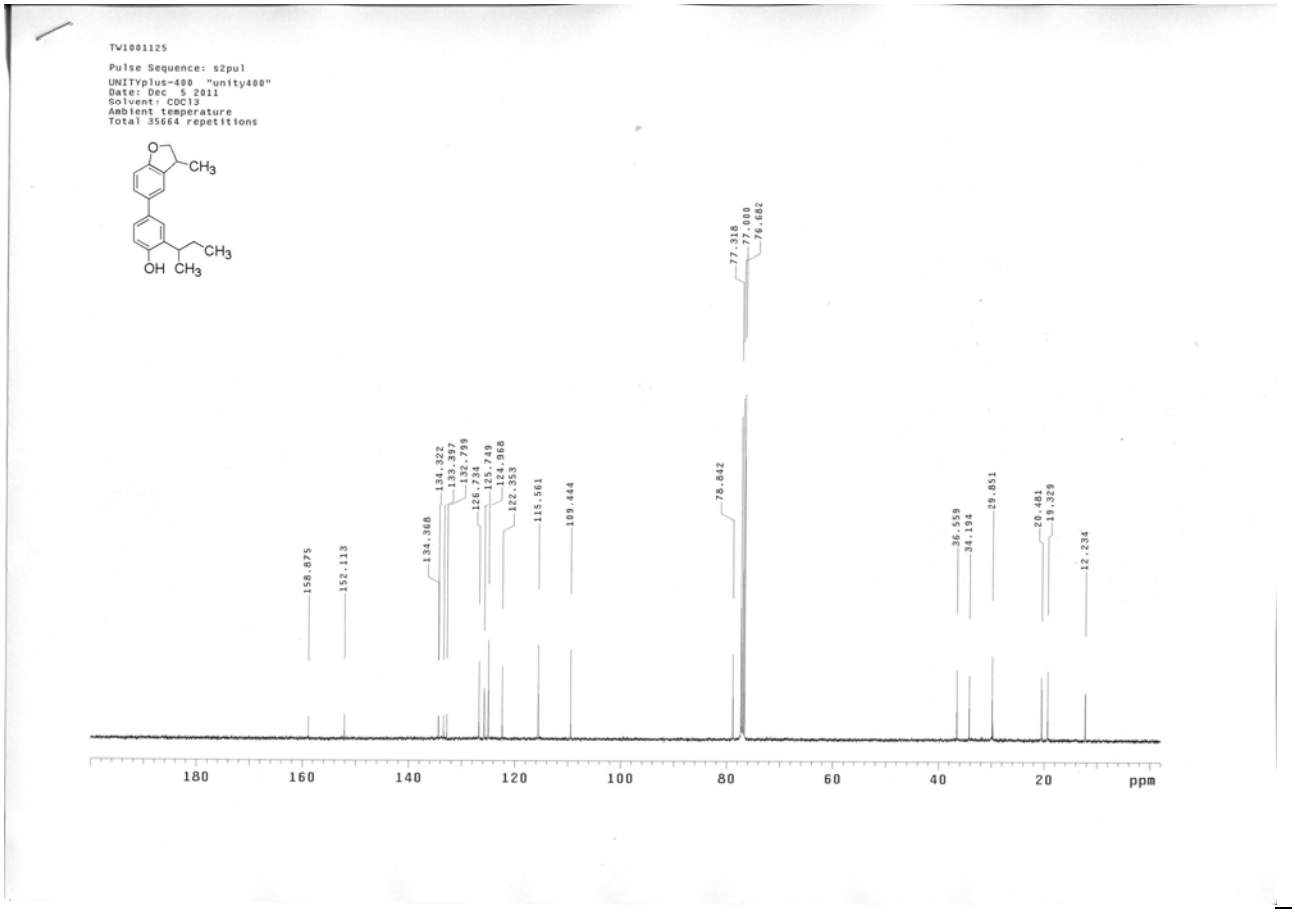
Compound (4h)


TW1001113
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 6 2011
Solvent: CDCl3
Ambient temperature
Total 64 repetitions
OH
7.397
7.391
7.380
7.375
7.356
7.337
7.335
7.325
7.320
7.304
7.299
7.295
7.288
7.282
7.277
7.267
7.261
7.258
6.875
6.869
6.856
6.853
6.830
6.809
5.080
5.063
5.059
5.041
4.866
3.258
3.240
3.224
3.246
3.189
3.030
3.012
2.987
2.982
2.970
2.912
2.735
1.596
0.000
9
8
7
6
5
4
3
2
1
ppm
97.39
28.72
10.00
8.21
22.49
24.35

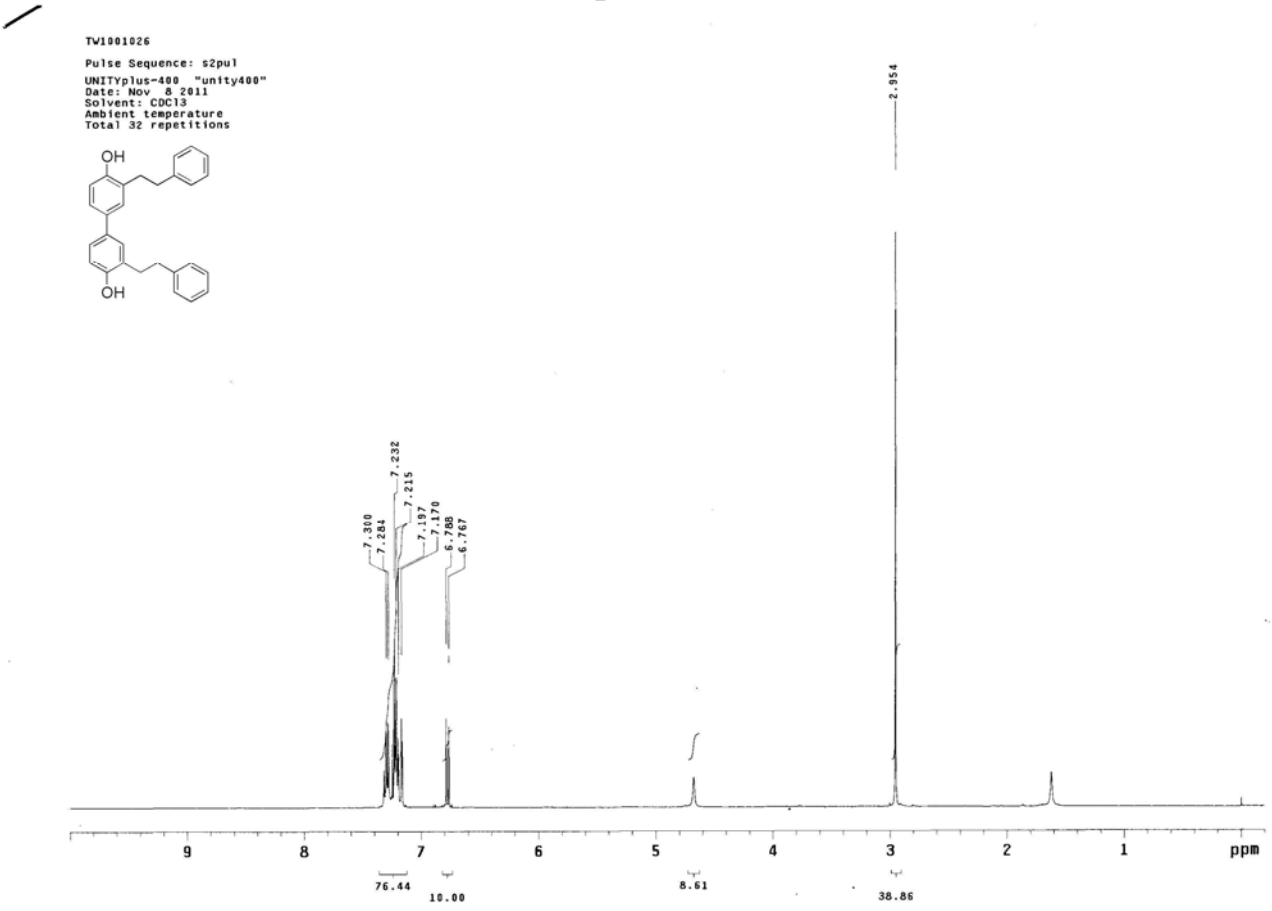

TW1001113
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 6 2011
Solvent: CDCl3
Ambient temperature
Total 9312 repetitions
OH
158.647
154.493
137.385
134.231
133.595
129.387
128.538
128.364
128.334
127.978
127.265
126.659
126.628
125.810
123.475
115.531
109.489
83.921
77.318
77.000
76.682
42.009
34.975
180
160
140
120
100
80
60
40
20
ppm

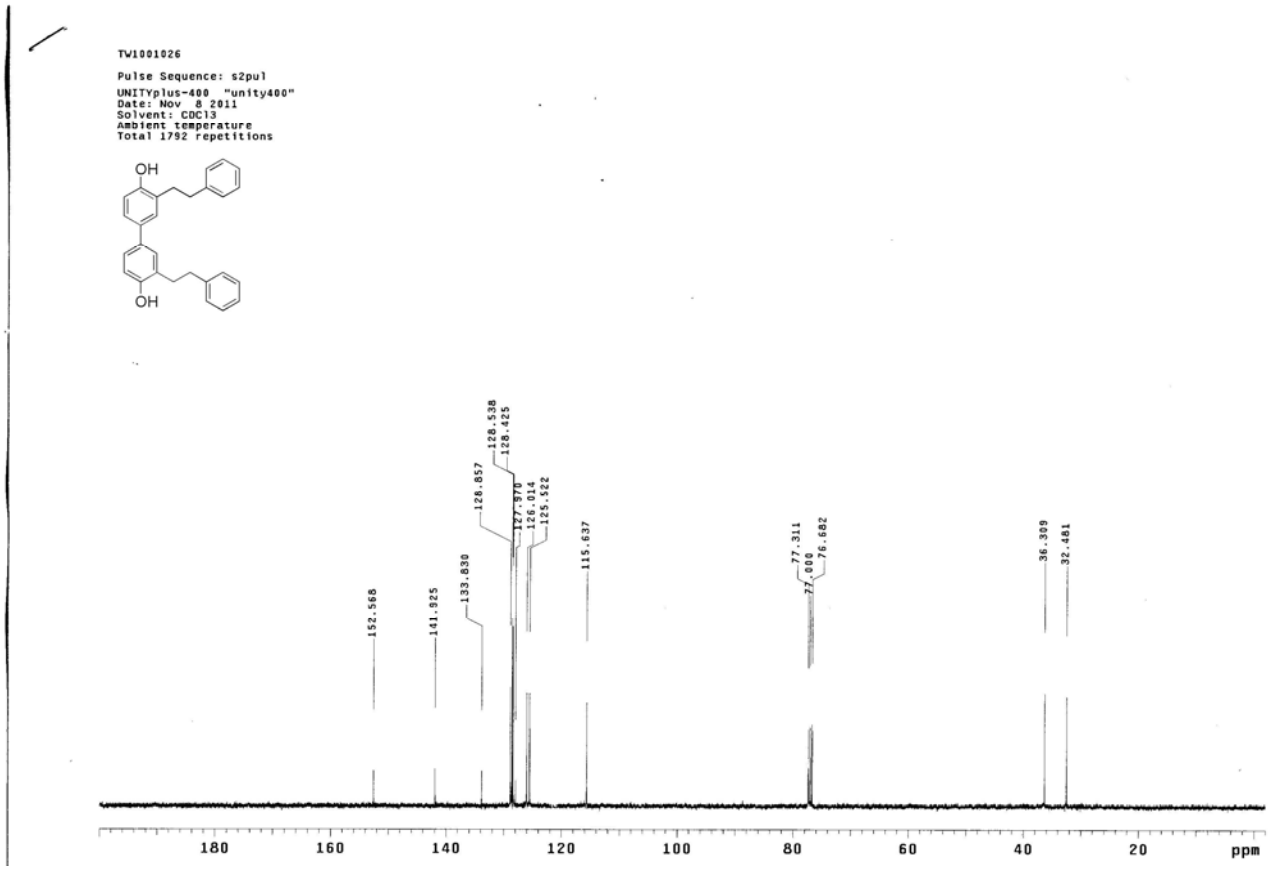
Compound (4i)


TW1001125
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 5 2011
Solvent: CDCl3
Ambient temperature
Total 80 repetitions
CH3
CH3
OH CH3
7.260
7.301
7.296
7.277
7.272
7.232
7.227
7.212
7.206
6.835
6.814
6.803
6.782
4.782
4.745
4.723
4.701
4.137
4.118
4.115
4.096
3.006
2.988
1.383
1.366
1.297
1.288
1.280
1.272
1.255
1.243
1.227
0.928
0.920
0.910
0.902
0.891
0.883
9
8
7
6
5
4
3
2
1
ppm
48.77
20.40
19.54
10.57
10.93
10.00
33.57
69.31
38.93
48.49


TW1001125
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Dec 5 2011
Solvent: CDCl3
Ambient temperature
Total 35664 repetitions
CH3
CH3
OH CH3
77.318
77.000
76.682
158.875
152.113
134.368
134.322
133.397
132.799
126.734
125.749
124.968
122.353
115.561
109.444
78.842
36.559
34.194
29.851
20.481
19.329
12.234
180
160
140
120
100
80
60
40
20
ppm

Compound (9)


TW1001026
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 8 2011
Solvent: CDCl3
Ambient temperature
Total 32 repetitions
OH
OH
2.954
7.300
7.284
7.232
7.215
7.197
7.170
6.788
6.767
9
8
7
6
5
4
3
2
1
ppm
76.44
10.00
8.61
38.86


TW1001026
Pulse Sequence: s2pul
UNITYplus-400 "unity400"
Date: Nov 8 2011
Solvent: CDCl3
Ambient temperature
Total 1792 repetitions
OH
OH
152.568
141.925
133.830
128.857
128.538
128.425
127.970
126.014
125.522
115.637
77.311
77.000
76.682
36.309
32.481
180
160
140
120
100
80
60
40
20
ppm

For X-ray crystal data of compound (4a)

Table 1. Crystal data and structure refinement for 111204_0m.

Identification code	111204_0m	
Empirical formula	C16 H14 O2	
Formula weight	238.27	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 5.8246(2) Å	α= 90°.
	b = 12.8801(4) Å	β= 98.953(2)°.
	c = 7.7281(3) Å	γ = 90°.
Volume	572.71(3) $Å^3$	
Z	2	
Density (calculated)	1.382 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
F(000)	252	
Crystal size	0.15 x 0.15 x 0.03 mm^3	
Theta range for data collection	3.88 to 26.37°.	
Index ranges	-7<=h<=7, -16<=k<=16, -9<=l<=9	
Reflections collected	4701	
Independent reflections	1166 [R(int) = 0.0326]	
Completeness to theta = 26.37°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.8723	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1166 / 0 / 82	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0426, wR2 = 0.1059	
R indices (all data)	R1 = 0.0724, wR2 = 0.1211	
Largest diff. peak and hole	0.145 and -0.226 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 111204_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	855(2)	1752(1)	8365(2)	60(1)
C(1)	1883(3)	2702(1)	8739(2)	44(1)
C(2)	4125(3)	2637(1)	9626(2)	40(1)
C(3)	5353(3)	3528(1)	10118(2)	40(1)
C(4)	4363(2)	4510(1)	9722(2)	36(1)
C(5)	2099(3)	4532(1)	8803(2)	45(1)
C(6)	843(3)	3639(1)	8308(2)	50(1)
C(7)	2566(3)	963(1)	8977(2)	52(1)
C(8)	4757(3)	1509(1)	9887(2)	49(1)

Table 3. Bond lengths [Å] and angles [°] for 111204_0m.

O(1)-C(1)	1.3728(18)
O(1)-C(7)	1.4501(19)
C(1)-C(6)	1.368(2)
C(1)-C(2)	1.380(2)
C(2)-C(3)	1.375(2)
C(2)-C(8)	1.504(2)
C(3)-C(4)	1.403(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.397(2)
C(4)-C(4)#1	1.494(3)
C(5)-C(6)	1.384(2)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.529(2)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700

C(1)-O(1)-C(7)	107.53(12)
C(6)-C(1)-O(1)	124.96(15)
C(6)-C(1)-C(2)	121.59(15)
O(1)-C(1)-C(2)	113.45(14)
C(3)-C(2)-C(1)	119.84(14)
C(3)-C(2)-C(8)	131.59(14)
C(1)-C(2)-C(8)	108.57(14)
C(2)-C(3)-C(4)	120.92(14)
C(2)-C(3)-H(3)	119.5
C(4)-C(3)-H(3)	119.5
C(5)-C(4)-C(3)	116.89(14)
C(5)-C(4)-C(4)#1	121.11(16)
C(3)-C(4)-C(4)#1	121.99(16)
C(6)-C(5)-C(4)	122.68(14)
C(6)-C(5)-H(5)	118.7
C(4)-C(5)-H(5)	118.7
C(1)-C(6)-C(5)	118.07(14)
C(1)-C(6)-H(6)	121.0
C(5)-C(6)-H(6)	121.0

O(1)-C(7)-C(8)	108.01(14)
O(1)-C(7)-H(7A)	110.1
C(8)-C(7)-H(7A)	110.1
O(1)-C(7)-H(7B)	110.1
C(8)-C(7)-H(7B)	110.1
H(7A)-C(7)-H(7B)	108.4
C(2)-C(8)-C(7)	102.33(13)
C(2)-C(8)-H(8A)	111.3
C(7)-C(8)-H(8A)	111.3
C(2)-C(8)-H(8B)	111.3
C(7)-C(8)-H(8B)	111.3
H(8A)-C(8)-H(8B)	109.2

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 111204_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	51(1)	42(1)	81(1)	-2(1)	-10(1)	-8(1)
C(1)	41(1)	41(1)	46(1)	-2(1)	0(1)	-5(1)
C(2)	39(1)	38(1)	40(1)	2(1)	3(1)	1(1)
C(3)	34(1)	40(1)	43(1)	0(1)	-3(1)	1(1)
C(4)	34(1)	39(1)	34(1)	-1(1)	2(1)	1(1)
C(5)	39(1)	38(1)	54(1)	0(1)	-5(1)	5(1)
C(6)	35(1)	49(1)	62(1)	-1(1)	-11(1)	1(1)
C(7)	59(1)	39(1)	56(1)	-1(1)	3(1)	0(1)
C(8)	51(1)	36(1)	57(1)	0(1)	-1(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 111204_0m.

	x	y	z	U(eq)
H(3)	6860	3480	10721	48
H(5)	1408	5172	8512	54
H(6)	-664	3675	7700	61
H(7A)	2921	556	7996	62
H(7B)	1966	500	9790	62
H(8A)	5076	1333	11121	59
H(8B)	6097	1334	9341	59

For X-ray crystal data of compound (4e)

Table 1. Crystal data and structure refinement for mo_111203_0m.

Identification code	mo_111203_0m	
Empirical formula	C14 H12 O2	
Formula weight	212.24	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 8.4518(13) Å	α= 90°.
	b = 6.1787(9) Å	β= 110.525(6)°.
	c = 21.735(3) Å	γ = 90°.
Volume	1063.0(3) $Å^3$	
Z	4	
Density (calculated)	1.326 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	448	
Crystal size	0.15 x 0.12 x 0.03 mm^3	
Theta range for data collection	2.00 to 26.63°.	
Index ranges	-10<=h<=10, -5<=k<=7, -27<=l<=27	
Reflections collected	8374	
Independent reflections	2201 [R(int) = 0.0314]	
Completeness to theta = 26.63°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.8874	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2201 / 0 / 145	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0459, wR2 = 0.1117	
R indices (all data)	R1 = 0.0920, wR2 = 0.1328	
Largest diff. peak and hole	0.178 and -0.189 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_111203_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2106(2)	621(2)	222(1)	48(1)
O(2)	11859(2)	1025(2)	4338(1)	54(1)
C(1)	3435(2)	870(3)	810(1)	38(1)
C(2)	3583(3)	2541(3)	1242(1)	49(1)
C(3)	4987(3)	2552(3)	1811(1)	48(1)
C(4)	6226(2)	947(3)	1959(1)	34(1)
C(5)	7708(2)	999(3)	2584(1)	35(1)
C(6)	8973(3)	-557(4)	2733(1)	50(1)
C(7)	10341(3)	-524(4)	3312(1)	51(1)
C(8)	10483(2)	1070(3)	3768(1)	39(1)
C(9)	7905(2)	2601(4)	3052(1)	48(1)
C(10)	9273(2)	2645(4)	3634(1)	47(1)
C(11)	2336(3)	-1462(4)	-47(1)	58(1)
C(12)	4059(3)	-2328(4)	363(1)	56(1)
C(13)	4609(2)	-755(3)	930(1)	38(1)
C(14)	6003(2)	-727(3)	1502(1)	40(1)

Table 3. Bond lengths [Å] and angles [°] for mo_111203_0m.

O(1)-C(1)	1.382(2)
O(1)-C(11)	1.454(3)
O(2)-C(8)	1.370(2)
O(2)-H(2)	0.8176
C(1)-C(13)	1.371(3)
C(1)-C(2)	1.373(3)
C(2)-C(3)	1.381(2)
C(2)-H(2A)	0.9300
C(3)-C(4)	1.395(3)
C(3)-H(3A)	0.9300
C(4)-C(14)	1.399(3)
C(4)-C(5)	1.492(2)
C(5)-C(9)	1.387(3)
C(5)-C(6)	1.389(3)
C(6)-C(7)	1.379(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.372(3)
C(7)-H(7)	0.9300
C(8)-C(10)	1.367(3)
C(9)-C(10)	1.383(2)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(12)	1.513(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.510(3)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.381(2)
C(14)-H(14)	0.9300

C(1)-O(1)-C(11)	106.88(14)
C(8)-O(2)-H(2)	109.5
C(13)-C(1)-C(2)	122.30(17)
C(13)-C(1)-O(1)	113.21(16)
C(2)-C(1)-O(1)	124.48(17)
C(1)-C(2)-C(3)	117.37(18)
C(1)-C(2)-H(2A)	121.3

C(3)-C(2)-H(2A)	121.3
C(2)-C(3)-C(4)	122.90(18)
C(2)-C(3)-H(3A)	118.6
C(4)-C(3)-H(3A)	118.6
C(3)-C(4)-C(14)	117.26(16)
C(3)-C(4)-C(5)	121.18(16)
C(14)-C(4)-C(5)	121.55(17)
C(9)-C(5)-C(6)	116.03(17)
C(9)-C(5)-C(4)	122.01(17)
C(6)-C(5)-C(4)	121.96(16)
C(7)-C(6)-C(5)	122.17(18)
C(7)-C(6)-H(6)	118.9
C(5)-C(6)-H(6)	118.9
C(8)-C(7)-C(6)	120.21(19)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(10)-C(8)-O(2)	122.78(17)
C(10)-C(8)-C(7)	119.20(17)
O(2)-C(8)-C(7)	118.01(17)
C(10)-C(9)-C(5)	122.13(19)
C(10)-C(9)-H(9)	118.9
C(5)-C(9)-H(9)	118.9
C(8)-C(10)-C(9)	120.24(18)
C(8)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
O(1)-C(11)-C(12)	108.24(16)
O(1)-C(11)-H(11A)	110.0
C(12)-C(11)-H(11A)	110.0
O(1)-C(11)-H(11B)	110.0
C(12)-C(11)-H(11B)	110.0
H(11A)-C(11)-H(11B)	108.4
C(13)-C(12)-C(11)	102.11(17)
C(13)-C(12)-H(12A)	111.3
C(11)-C(12)-H(12A)	111.3
C(13)-C(12)-H(12B)	111.3
C(11)-C(12)-H(12B)	111.3
H(12A)-C(12)-H(12B)	109.2
C(1)-C(13)-C(14)	119.63(17)
C(1)-C(13)-C(12)	108.70(16)
C(14)-C(13)-C(12)	131.67(19)

C(13)-C(14)-C(4)	120.54(18)
C(13)-C(14)-H(14)	119.7
C(4)-C(14)-H(14)	119.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_111203_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	44(1)	53(1)	34(1)	-1(1)	-2(1)	2(1)
O(2)	50(1)	56(1)	38(1)	-4(1)	-6(1)	3(1)
C(1)	36(1)	46(1)	29(1)	6(1)	7(1)	-2(1)
C(2)	46(1)	51(1)	40(1)	0(1)	3(1)	16(1)
C(3)	50(1)	48(1)	39(1)	-9(1)	7(1)	9(1)
C(4)	31(1)	43(1)	28(1)	-1(1)	10(1)	-1(1)
C(5)	31(1)	44(1)	30(1)	-2(1)	11(1)	0(1)
C(6)	52(1)	54(1)	35(1)	-11(1)	5(1)	10(1)
C(7)	47(1)	56(1)	40(1)	-3(1)	2(1)	16(1)
C(8)	34(1)	48(1)	31(1)	2(1)	6(1)	-3(1)
C(9)	38(1)	55(1)	45(1)	-11(1)	8(1)	9(1)
C(10)	42(1)	55(1)	40(1)	-16(1)	7(1)	0(1)
C(11)	55(1)	61(2)	45(1)	-13(1)	2(1)	0(1)
C(12)	54(1)	58(2)	43(1)	-13(1)	-1(1)	2(1)
C(13)	38(1)	42(1)	32(1)	-3(1)	9(1)	-3(1)
C(14)	36(1)	44(1)	37(1)	-4(1)	9(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for mo_111203_0m.

	x	y	z	U(eq)
H(2)	11851	2095	4558	81
H(2A)	2769	3624	1156	59
H(3A)	5113	3679	2108	58
H(6)	8895	-1658	2432	60
H(7)	11170	-1584	3394	61
H(9)	7091	3681	2972	57
H(10)	9370	3750	3936	57
H(11A)	2260	-1293	-500	69
H(11B)	1463	-2462	-35	69
H(12A)	3983	-3791	512	68
H(12B)	4826	-2309	119	68
H(14)	6799	-1830	1585	48