Asymmetric Rearrangement of Racemic Epoxides Catalyzed by Chiral Brønsted Acids

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Supporting Information

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N-triflylphosphoramide **5e** were synthesized according to the reported method.[1]

(*S*)-6,6'-Bis(2,4,6-triisopropylphenyl)-1,1'-spirobiindanyl-7,7'-diylhydrogen *N*-triflylphosphoramide (5e). Yellow solid, m.p. 105-108 ºC; $[\alpha]_D^{20}$ -75.4 (*c* 0.4, $CHCl_3$); IR (film) 3450, 2961, 1461, 1212, 1180, 1125 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.26-7.06 (m, 6H), 7.02 (s, 1H), 6.93 (s, 1H), 3.19-3.12 (m, 2H), 2.97-2.60 (m, 8H), 2.36-2.27 (m, 2H), 2.21-1.95 (m, 2H), 1.29-1.08 (m, 30H), 0.93-0.82 (m, 6H); ^{31}P NMR (122 MHz, $CDCl_3$) δ -17.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -75.3; HRMS (FT-ICRMS) calcd for $C_{48}H_{59}F_3NO_5PSNa$ (M+Na): 872.3701, found: 872.3702.

Representative Procedure for the Rearrangement of Epoxide (Table 1, entry 1). A dried Schlenk flask charged with chiral spirobiindane *N*-triflyl phosphoramide **5e** (0.0170 g, 0.02 mmol) and CH_2Cl_2/THF (1.0 mL, 1/1 volume ratio) was cooled to -78 ºC and stirred at this temperature for 10 min before α-methylstyrene oxide (**1a**) (0.0536 g, 0.40 mmol) was added. The reaction mixture was stirred at -78 ºC until the TLC indicating the reaction was complete. $NaBH_4$ (0.0296 g, 0.80 mmol) and MeOH (2 mL) were then added sequentially, and the mixture was stirred at 0 ºC for 1 h. After being quenched with diluted HCl (2 N, 10 mL), the resulting mixture was extracted diethyl ether (10 mL x 3). The combined organic phase was washed with aq NaOH (2 N) and brine, dried over Na_2SO_4, filtered, concentrated, and the residue was purified by flash chromatography on silica gel (petroleum ether/diethyl ether = 3:1, v/v) to afford the desired product **4a** as a colorless oil.

Procedure for One Pot Synthesis of Chiral Alcohol from Alkene (Scheme 3). To a dried Schlenk flask was added *m*-CPBA (85%, 0.0757 g, 0.44 mmol), CH_2Cl_2 (1.0 mL), and α-methylstyrene (**6**) (0.0472 g, 0.40 mmol). The reaction mixture was stirred at room temperature for 1 h. Then THF (1.0 mL) was added, and the mixture was cooled -78 ºC and stirred at this temperature for 10 min before addition of chiral spirobiindane *N*-triflyl phosphoramide **5e** (0.0170 g, 0.02 mmol). The reaction mixture was stirred at -78 ºC until TLC indicating the reaction was complete. $NaBH_4$

(0.0296 g, 0.80 mmol) and MeOH (2 mL) were added, and the mixture was stirred at 0 ºC for 1 h. After being quenched with diluted HCl (2 N, 10 mL), and extracted with diethyl ether (10 mL x 3), the combined organic phase was washed with aq NaOH (2 N, 15 mL) and brine (15 mL), dried, filtered, and concentrated. The residue was purified by flash chromatography on silica gel (petroleum ether/diethyl ether = 3:1, v/v) to afford the desired product **4a** as a colorless oil.

Table S1 Optimization of Solvents for the Asymmetric Rearrangement of Epoxide **1a**[a]

entry	catalyst	solvent	conv (%)[b]	time (h)	ee (%)[c]
1	**5d**	toluene	>99	0.25	26
2	**5d**	THF	>99	0.5	24
3	**5d**	Et_2O	>99	3	0
4	**5d**	acetone	>99	0.25	10
5	**5e**	toluene	>99	3.5	6
6	**5e**	CH_2Cl_2	>99	0.3	14
7	**5e**	THF	>99	21	32
8	**5e**	Et_2O	NR[d]	4	-
9	**5e**	*n*-hexane	trace	4	ND[e]
10	**5e**	EtOAc	>99	5.5	0
11	**5e**	CH_2Cl_2/THF (1/1)[f]	>99	4	54
12	**5e**	CH_2Cl_2/THF (1/5)[f]	>99	10	44
13[g]	**5e**	CH_2Cl_2/THF (1/1)[f]	>99	3	48

[a]All reactions were carried out with epoxide **1a** (0.10 mmol), phosphoramide **5e** (0.01 mmol), and solvent (1.5 mL) at -78 ºC unless other noted. [b] The conversion was determined by crude ^{1}H NMR. [c] The ee was determined by chiral GC. [d] No reaction. [e] Not determined. [f] The ratio was in volume. [g]5 mol % catalyst was used.

(*R*)-2-Phenylpropan-1-ol (4a) (Table 1, entry 1). Colorless oil, 68% yield; $[\alpha]_D^{20}$ +4.1 (*c* 0.8, $CHCl_3$) (48% ee) ($[\alpha]_D$ +14.3 (*c* 1.65, $CHCl_3$), 99% ee for *R*)[2]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.30 (m, 2H), 7.26-7.20 (m, 3H), 3.71 (d, *J* = 5.6 Hz, 1H), 3.69 (d, *J* = 5.2 Hz, 1H), 3.00-2.88 (m, 1H), 1.36 (br, 1H), 1.28(d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.9, 128.9, 127.7, 126.9, 68.9, 42.7, 17.8.

2-(4-Fluorophenyl)propan-1-ol (4b) (Table 1, entry 2). Colorless oil, 65% yield; $[\alpha]_D^{20}$ +0.9 (*c* 0.5, $CHCl_3$) (33% ee); IR (film) 3354, 1604, 1511, 1223, 833 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.19 (dd, *J* = 8.8, 5.2 Hz, 2H), 7.02 (dd, *J* = 8.8, 8.8 Hz, 2H), 3.73-3.63 (m, 2H), 2.98-2.90 (m, 1H), 1.43 (br, 1H), 1.26 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9 (d, J_{C-F} = 242.8 Hz), 139.6 (d, J_{C-F} = 3.3 Hz), 129.1 (d, J_{C-F} = 7.8 Hz), 115.6 (d, J_{C-F} = 20.9 Hz), 68.9, 41.9, 17.9; HRMS (TOF-EI) calcd for $C_9H_{11}FO$ (M): 154.0794, found: 154.0796.

(*R*)-2-(4-Chlorophenyl)propan-1-ol (4c) (Table 1, entry 3). Colorless oil, 61% yield; $[\alpha]_D$ +1.4 (*c* 0.6, $CHCl_3$) (41% ee) ($[\alpha]_D^{20}$ +13.3 (*c* 1.1, $CHCl_3$), 90% ee for *R*)[3]; ^1H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 7.6 Hz, 2H), 7.17 (d, *J* = 7.6 Hz, 2H), 3.67 (d, *J* = 7.2 Hz, 1H), 3.65 (d, *J* = 7.2 Hz, 1H), 2.97-2.85 (m, 1H), 1.46 (br, 1H), 1.25 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.5, 132.5, 129.0, 128.9, 68.7, 42.1, 17.7.

2-(4-Bromophenyl)propan-1-ol (4d) (Table 1, entry 4).[4] Colorless oil, 59% yield; $[\alpha]_D^{20}$ +2.8 (*c* 0.9, $CHCl_3$) (33% ee); ^1H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.4 Hz, 2H), 3.74-3.61 (m, 2H), 2.96-2.86 (m, 1H), 1.47 (br, 1H), 1.26 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.0, 131.9, 129.5, 120.6, 68.7, 42.2, 17.7.

(*R*)-2-*p*-Tolylpropan-1-ol 4e (Table 1, entry 5). Colorless oil, 62% yield; $[\alpha]_D^{20}$ +1.8 (*c* 0.4, $CHCl_3$) (33% ee) ($[\alpha]_D^{20}$ +8.7 (*c* 2.75, $CHCl_3$), 74% ee for *R*)[5]; ^1H NMR (400 MHz, $CDCl_3$) δ 7.20-7.10 (m, 4H), 3.74-3.64 (m, 2H), 2.97-2.88 (m, 1H), 2.34 (s, 3H), 1.41 (br, 1H), 1.27 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.8, 136.4, 129.5, 127.5, 69.0, 42.2, 21.2, 17.9.

2-(4-Butylphenyl)propan-1-ol (4f) (Table 1, entry 6). Colorless oil, 48% yield; $[\alpha]_D^{20}$ +2.4 (*c* 0.8, $CHCl_3$) (33% ee); IR (film) 3353, 1513, 1458, 1379, 1038, 1013 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.19-7.10 (m, 4H), 3.69 (d, *J* = 6.8 Hz, 2H), 2.98-2.86 (m, 1H), 2.59 (t, *J* = 8.0 Hz, 2H), 1.64-1.53 (m, 2H), 1.43 (br, 1H), 1.41-1.31 (m, 2H), 1.27 (d, *J* = 7.2 Hz, 3H) , 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 140.9, 128.9, 127.5, 69.0, 42.3, 35.5, 33.9, 22.6, 17.8, 14.2;

HRMS (TOF-EI) calcd for $C_{13}H_{20}O$ (M): 192.1514, found: 192.1516.

2-(4-Isopropylphenyl)propan-1-ol (4g) (Table 1, entry 7). Colorless oil, 59% yield; $[\alpha]_D^{20}$ +2.6 (*c* 0.8, $CHCl_3$) (35% ee); IR (film) 3354, 1510, 1460, 1038, 1012, 828 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.23-7.14 (m, 4H), 3.69 (d, *J* = 6.8 Hz, 2H), 2.99-2.83 (m, 2H), 1.43 (br, 1H), 1.27 (d, *J* = 8.4 Hz, 3H), 1.25 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 141.1, 127.6, 126.9, 69.0, 42.2, 33.9, 24.2, 17.8; HRMS (TOF-EI) calcd for $C_{12}H_{18}O$ (M): 178.1358, found: 178.1361.

2-(Biphenyl-4-yl)propan-1-ol (4h) (Table 1, entry 8).[6] Colorless oil, 53% yield; $[\alpha]^{20}_D$ +1.7 (*c* 0.6, $CHCl_3$) (33% ee); ^1H NMR (400 MHz, $CDCl_3$) δ 7.60-7.52 (m, 4H), 7.43 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.38-7.28 (m, 3H), 3.75 (d, *J* = 6.8 Hz, 2H), 3.05-2.95 (m, 1H), 1.44 (br, 1H), 1.31 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.0, 141.2, 139.9, 129.0, 128.1, 127.6, 127.4, 127.3, 68.9, 42.4, 17.8.

2-(3-Fluorophenyl)propan-1-ol (4i) (Table 1, entry 9). Colorless oil, 67% yield; $[\alpha]_D^{20}$ +2.8 (*c* 1.0, $CHCl_3$) (38% ee); IR (film) 3356, 1614, 1590, 1488, 1448, 1249, 1151, 1028, 922 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.32-7.24 (m, 1H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.97-6.88 (m, 2H), 3.69 (d, *J* = 6.8 Hz, 2H), 3.03-2.90 (m, 1H), 1.43 (br, 1H), 1.27 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3 (d, $J_{C\text{-}F}$ = 244.1 Hz), 146.7 (d, $J_{C\text{-}F}$ = 7.0 Hz), 130.2 (d, $J_{C\text{-}F}$ = 8.1 Hz), 123.4 (d, $J_{C\text{-}F}$ = 2.6 Hz), 114.5 (d, $J_{C\text{-}F}$ = 21.1 Hz), 113.7 (d, $J_{C\text{-}F}$ = 20.9 Hz), 68.7, 42.5 (d, $J_{C\text{-}F}$ = 1.3 Hz), 17.7; HRMS (TOF-EI) calcd for $C_{15}H_{16}O$ (M): 154.0794, found: 154.0796.

2-*m*-Tolylpropan-1-ol (4j) (Table 1, entry 10).[7] Colorless oil, 67% yield; $[\alpha]_D^{20}$ +7.3 (*c* 1.2, $CHCl_3$) (35% ee); ^1H NMR (400 MHz, $CDCl_3$) δ 7.26-7.18 (m, 1H), 7.07-7.01 (m, 3H), 3.69 (d, *J* = 6.8 Hz, 2H), 2.95-2.88 (m, 1H), 2.35 (s, 3H), 1.27 (br, 1H), 1.26 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 138.5, 128.8, 128.5, 127.7, 124.7, 68.9, 42.6, 21.7, 17.8.

2-(3-Methoxyphenyl)propan-1-ol (4k) (Table 1, entry 11).[8] Colorless oil, 61% yield; $[\alpha]_D^{20}$ +2.8 (*c* 1.0, $CHCl_3$) (37% ee); ^1H NMR (400 MHz, $CDCl_3$) δ 7.28-7.21 (m, 1H), 6.86-6.75 (m, 3H), 3.80

(s, 3H), 3.69 (d, *J* = 6.8 Hz, 2H), 2.96-2.88 (m, 1H), 1.45 (br, 1H), 1.26 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 145.6, 129.8, 120.0, 113.7, 111.9, 68.8, 55.4, 42.7, 17.8.

2-(Biphenyl-3-yl)propan-1-ol (4l) (Table 1, entry 12). Colorless oil, 65% yield; $[\alpha]_D^{20}$ +0.3 (*c* 1.0, $CHCl_3$) (42% ee); IR (film) 3355, 1598, 1479, 1029, 758 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.6 Hz, 2H), 7.49-7.30 (m, 6H), 7.26-7.20 (m, 1H), 3.75 (d, *J* = 6.8 Hz, 2H), 3.08-2.95 (m, 1H), 1.43 (br, 1H), 1.32 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 141.9, 141.5, 129.3, 129.0, 127.5, 127.4, 126.7, 126.6, 125.8, 68.9, 42.8, 17.9; HRMS (TOF-EI) calcd for $C_9H_{11}FO$ (M): 212.1201, found: 212.1204.

2-(Biphenyl-2-yl)propan-1-ol (4m) (Table 1, entry 13). Colorless oil, 74% yield; $[\alpha]_D^{20}$ −4.8 (*c* 1.5, $CHCl_3$) (19% ee); IR (film) 3354, 1597, 1480, 1032 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.20 (m, 9H), 3.68 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.59 (dd, *J* = 10.8, 6.8 Hz, 1H), 3.22-3.10 (m, 1H), 1.34 (br, 1H), 1.18 (d, *J* = 6.8Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 141.8, 141.4, 130.5, 129.6, 128.3, 128.0, 127.1, 126.2, 126.1, 68.6, 37.6, 18.7; HRMS (TOF-EI) calcd for $C_{15}H_{16}O$ (M): 212.1201, found: 212.1204.

2-Phenylbutan-1-ol (4n) (Table 1, entry 14).[9] Colorless oil, 68% yield; $[\alpha]_D^{20}$ -3.2 (*c* 0.7, $CHCl_3$) (20% ee); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (t, *J* = 7.2 Hz, 2H), 7.26-7.18 (m, 3H), 3.81-3.71 (m, 2H), 2.75-2.64 (m, 1H), 1.81-1.70 (m, 1H), 1.65-1.53 (m, 1H), 1.32 (br, 1H), 0.84 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$): δ 142.5, 128.8, 128.3, 126.9, 67.6, 50.7, 25.2, 12.2.

2-Phenylbutan-1-ol (7). Colorless oil, 84% yield; IR (film) 3374, 1494, 1076 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.37 (m, 2H), 7.36-7.27 (m, 3H), 5.35 (s, 1H), 5.30 (s, 1H), 4.62 (dd, *J* = 7.6, 4.0 Hz, 1H), 1.77 (br, 1H), 1.63-1.23 (m, 6H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$): δ 152.3, 140.2, 128.5, 127.8, 127.1, 112.7, 74.1, 35.9, 28.0, 22.7, 14.2; HRMS (TOF-EI) calcd for $C_{15}H_{16}O$ (M): 190.1358, found: 190.1361.

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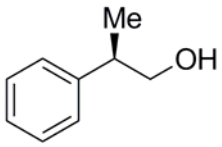
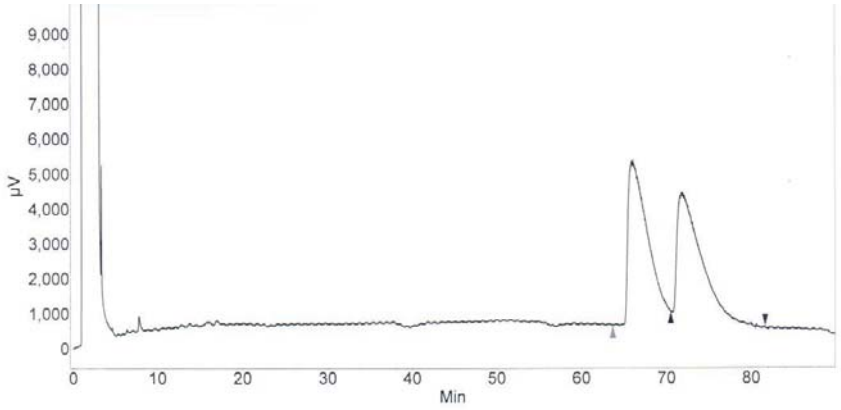
The chromatograms for determination of the enantiomeric excess

Table 1, entry 1



GC Conditions: Column: capillary B-DM, **T:** 70 ^{o}C**; P:** 30 psi**;**

Racemic



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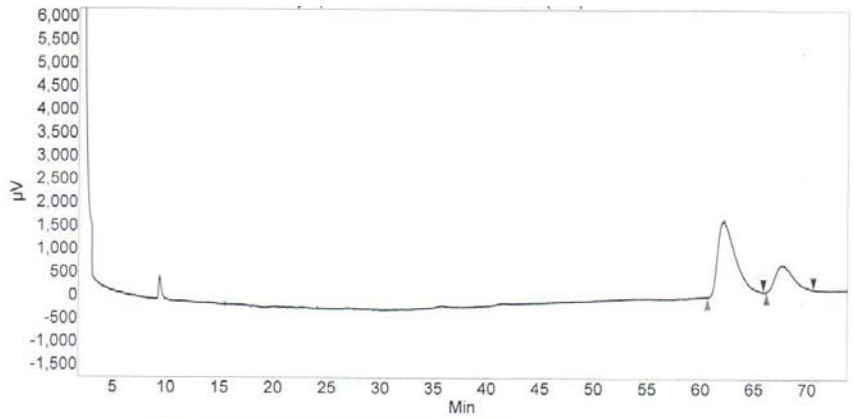
Total		100.000		

Chiral



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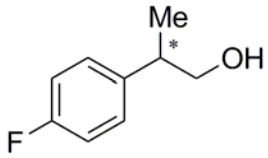
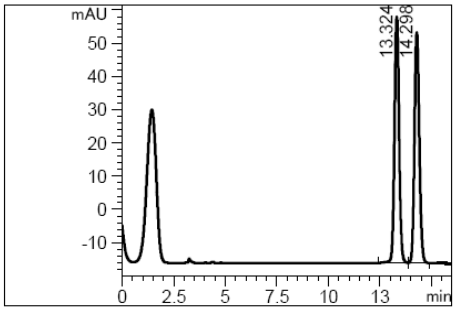
2	67.60	26.046	66.15	70.54
Total		100.000		

Table 1, entry 2



HPLC Conditions: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98⁄2); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



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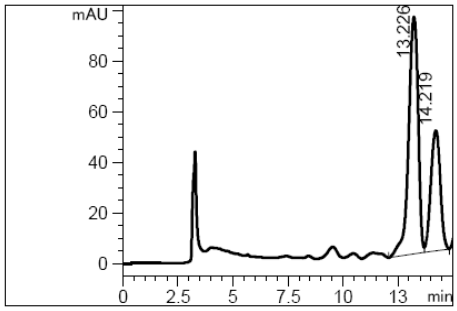
Chiral



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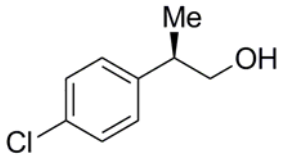
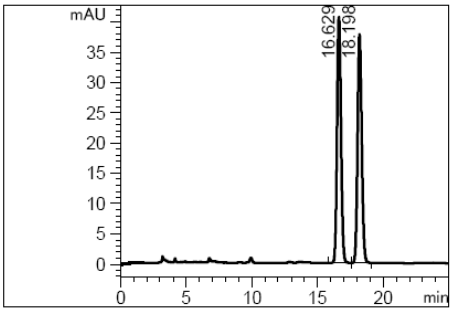


HPLC Conditions: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98⁄2); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



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Chiral

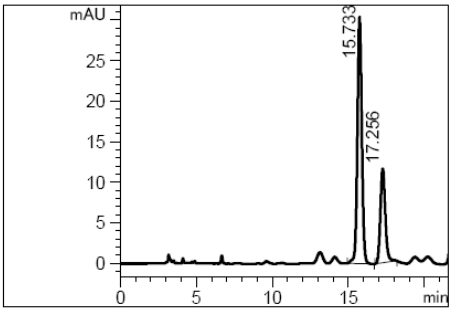

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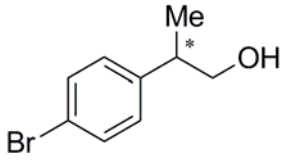
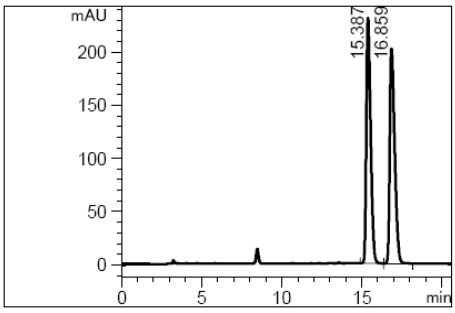
Table 1, entry 4



HPLC Conditions: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98⁄2); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



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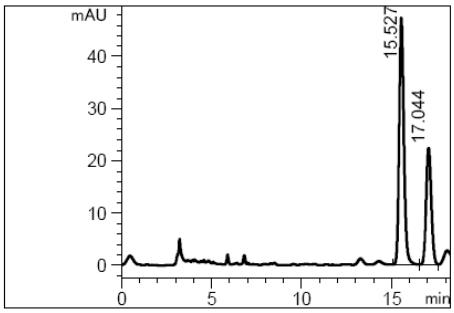
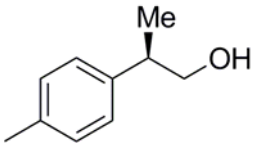
2	16.859	49.959	4.248e3

Chiral



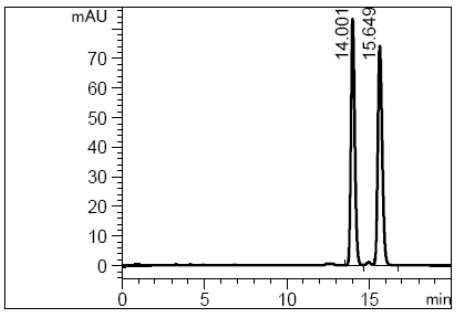
Peak #	RT [min]	Area %	Area
1	15.527	66.651	874.469
2	17.044	33.349	437.536

Table 1, entry 5



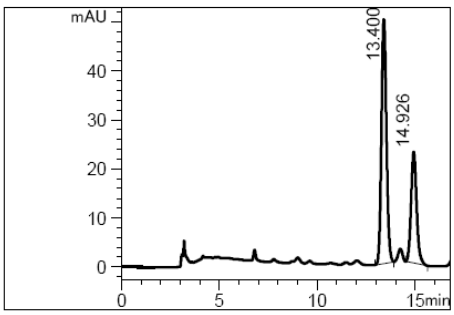
HPLC Conditions: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98⁄2); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



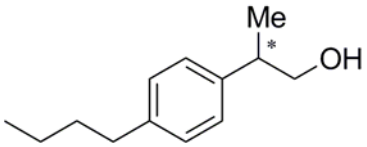
Peak #	RT [min]	Area %	Area
1	14.001	50.170	1.363e3
2	15.649	49.830	1.354e3

Chiral



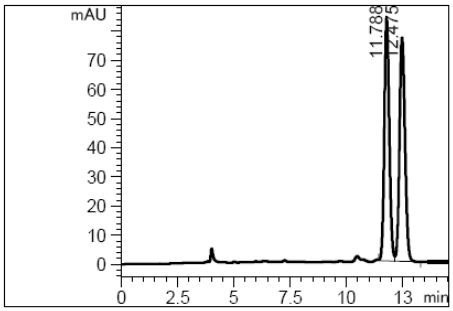
Peak #	RT [min]	Area %	Area
1	13.400	66.245	878.138
2	14.926	33.755	447.449

Table 1, entry 6



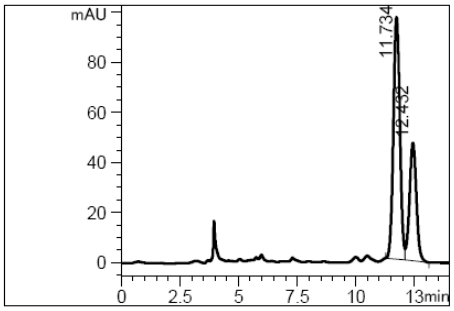
HPLC Conditions: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (99/1); **Flow rate:** 0.8 mL/min; **Detection:** UV 254 nm

Racemic



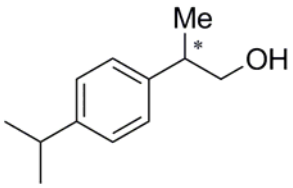
Peak #	RT [min]	Area %	Area
1	11.788	49.778	1.281e3
2	12.475	50.222	1.292e3

Chiral



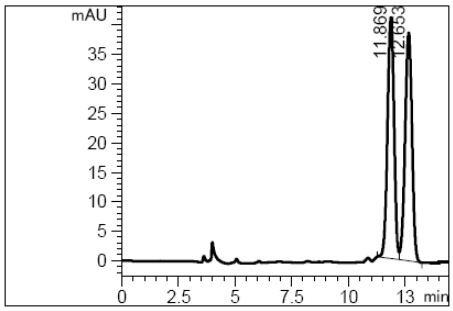
Peak #	RT [min]	Area %	Area
1	11.734	66.359	1.888e3
2	12.432	33.641	957.184

Table 1, entry 7



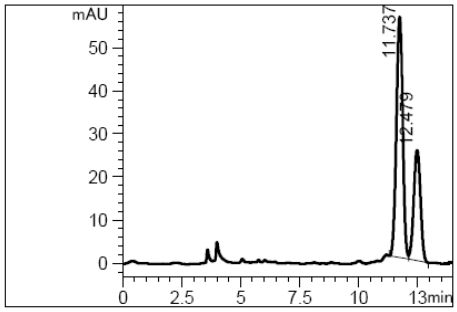
HPLC Conditions: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (99/1); **Flow rate:** 0.8 mL/min; **Detection:** UV 254 nm

Racemic



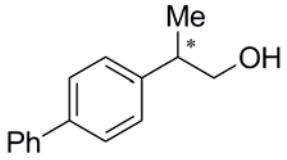
Peak #	RT [min]	Area %	Area
1	11.869	49.631	809.328
2	12.653	50.369	821.349

Chiral



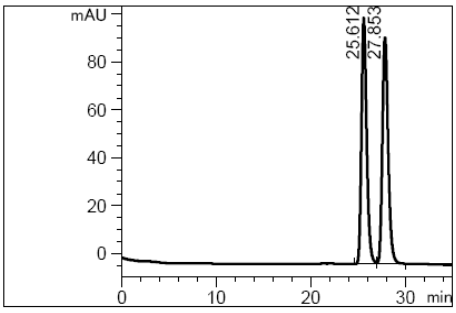
Peak #	RT [min]	Area %	Area
1	11.737	67.435	1.057e3
2	12.479	32.565	510.382

Table 1, entry 8



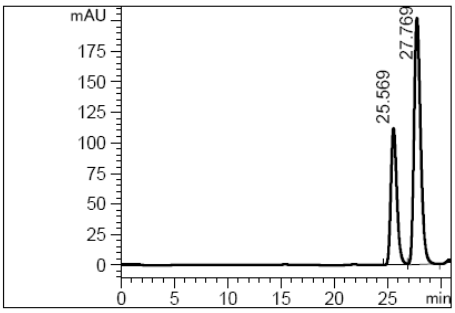
HPLC Conditions: Column: Chiralcel AS-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98⁄2); **Flow rate:** 0.8 mL/min; **Detection:** UV 254 nm

Racemic



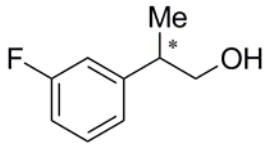
Peak #	RT [min]	Area %	Area
1	25.612	49.961	3.975e3
2	27.853	50.039	3.981e3

Chiral



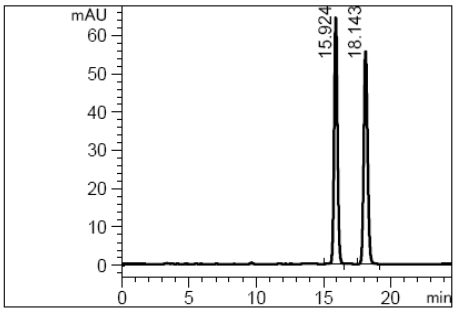
Peak #	RT [min]	Area %	Area
1	25.569	33.457	4.296e3
2	27.769	66.543	8.543e3

Table 1, entry 9



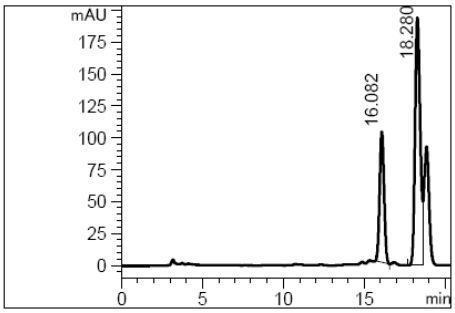
HPLC Conditions: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98⁄2); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic



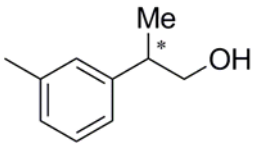
Peak #	RT [min]	Area %	Area
1	15.924	50.075	1.114e3
2	18.143	49.925	1.111e3

Chiral



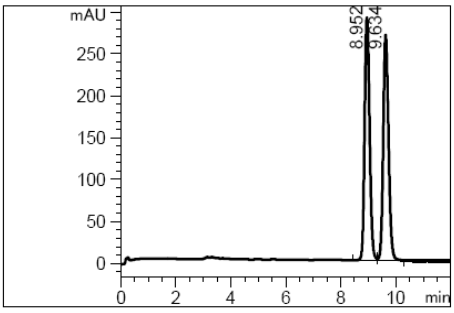
Peak #	RT [min]	Area %	Area
1	16.082	31.028	1.910e3
2	18.280	68.972	4.246e3

Table 1, entry 10



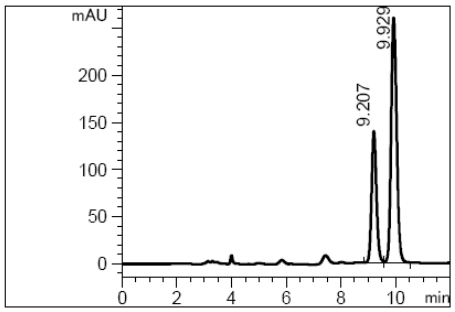
HPLC Conditions: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98⁄2); **Flow rate:** 1 mL/min; **Detection:** UV 220 nm

Racemic



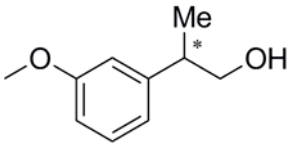
Peak #	RT [min]	Area %	Area
1	8.952	49.692	3.594e3
2	9.634	50.308	3.639e3

Chiral



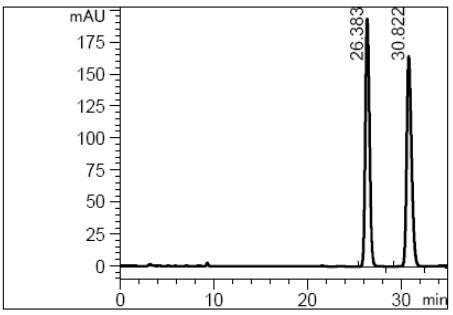
Peak #	RT [min]	Area %	Area
1	9.207	32.729	1.756e3
2	9.929	67.271	3.610e3

Table 1, entry 11



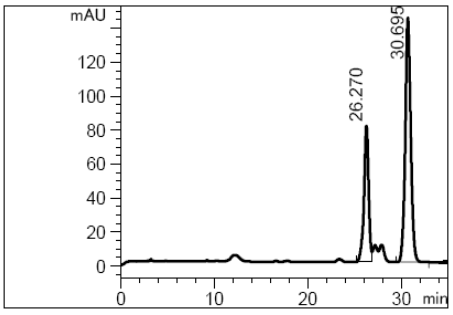
HPLC Conditions: Column: Chiralcel AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98⁄2); **Flow rate:** 1 mL/min; **Detection:** UV 254 nm

Racemic



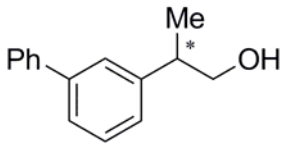
Peak #	RT [min]	Area %	Area
1	26.383	49.712	5.929e3
2	30.822	50.288	5.998e3

Chiral



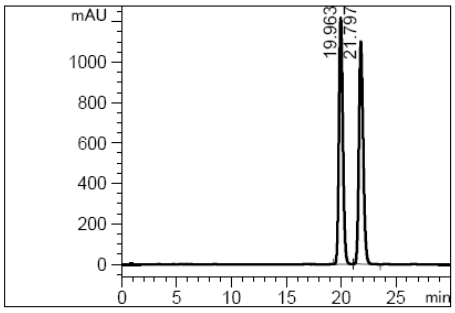
Peak #	RT [min]	Area %	Area
1	26.270	31.561	2.722e3
2	30.695	68.439	5.902e3

Table 1, entry 12



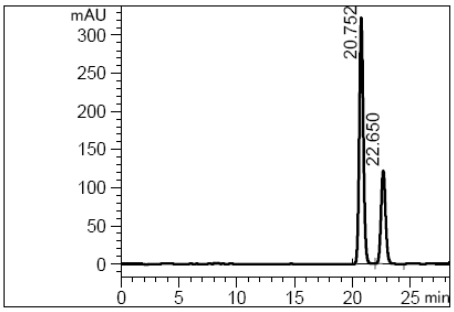
HPLC Conditions: Column: Chiralcel AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1 mL/min; **Detection:** UV 254 nm

Racemic



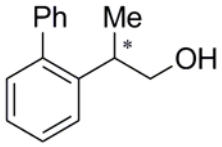
Peak #	RT [min]	Area %	Area
1	19.963	49.987	3.008e4
2	21.797	50.013	3.010e4

Chiral



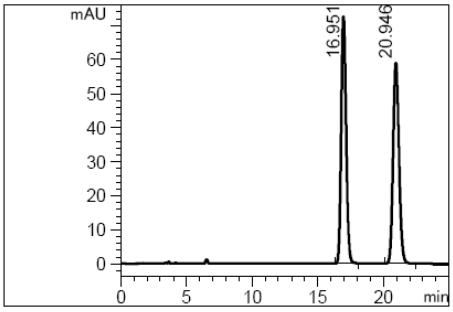
Peak #	RT [min]	Area %	Area
1	20.752	70.783	7.946e3
2	22.650	29.217	3.280e3

Table 1, entry 13



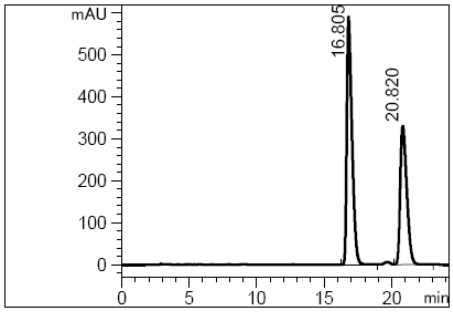
HPLC Conditions: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (99/1); **Flow rate:** 1 mL/min; **Detection:** UV 254 nm

Racemic



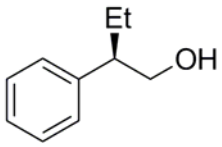
Peak #	RT [min]	Area %	Area
1	16.951	50.006	1.867e3
2	20.946	49.994	1.866e3

Chiral



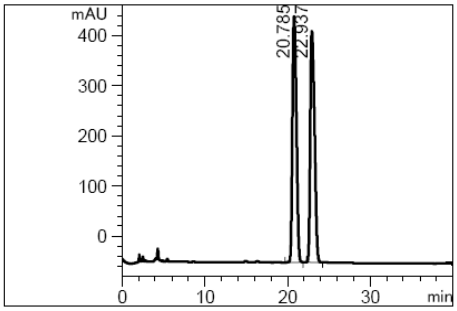
Peak #	RT [min]	Area %	Area
1	16.805	59.656	1.632e4
2	20.820	40.344	1.104e4

Table 1, entry 14



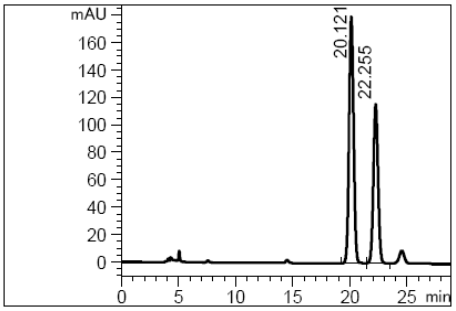
HPLC Conditions: Column: Chiralcel AD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.75 mL/min; **Detection:** UV 220 nm

Racemic



Peak #	RT [min]	Area %	Area
1	20.785	49.119	1.617e4
2	22.937	50.881	1.675e4

Chiral



Peak #	RT [min]	Area %	Area
1	20.121	60.055	5.086e3
2	22.255	39.945	3.383e3

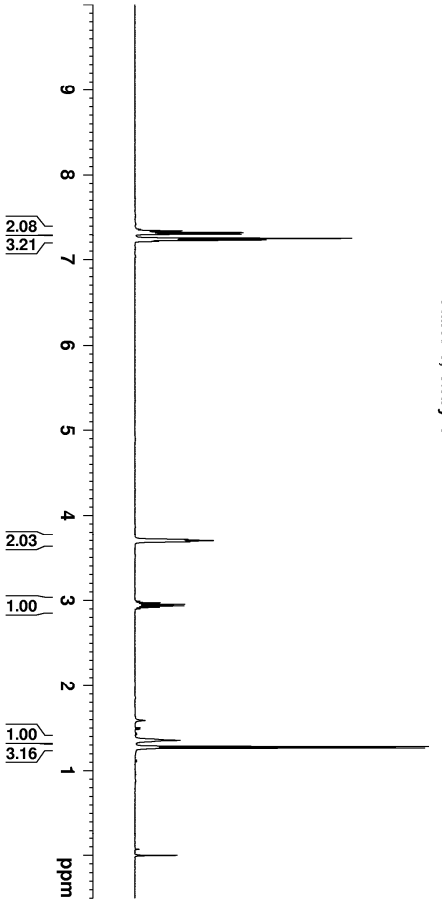
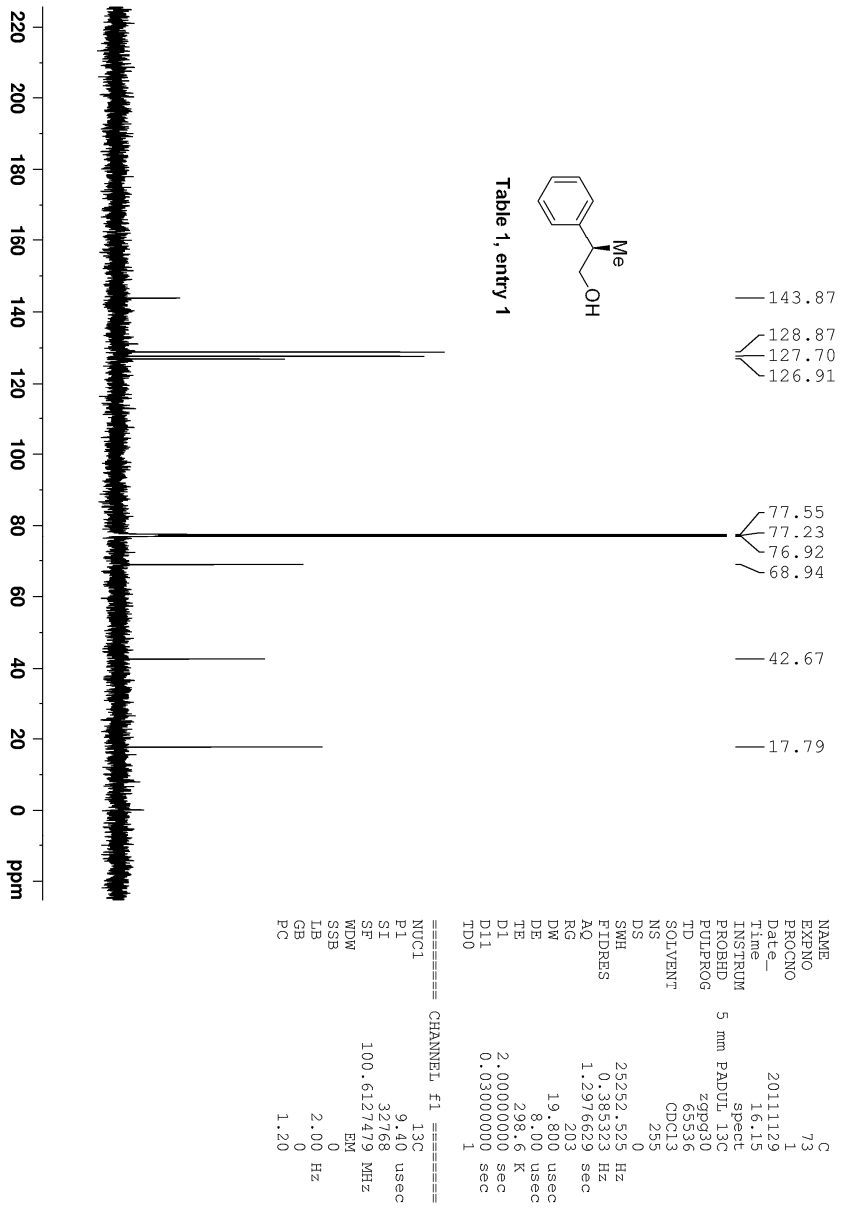
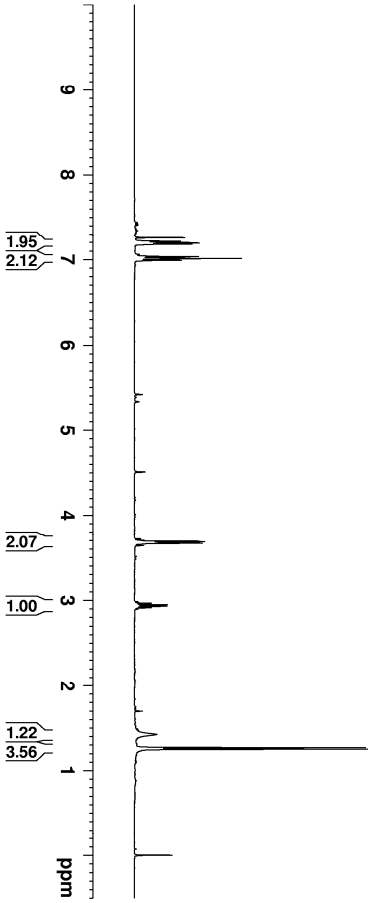


Table 1, entry 1

NAME	H
EXPNO	75
PROCNO	14
Date_	20101224
Time	12.35
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	203
DW	41.600 usec
DE	6.00 usec
TE	297.8 K
D1	5.00000000 sec
TD0	1
========	CHANNEL f1 ========
NUC1	1H
P1	12.60 usec
PL1	-1.00 dB
SFO1	400.1332010 MHz
SI	32768
SF	400.1300152 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00





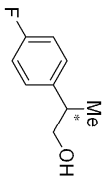
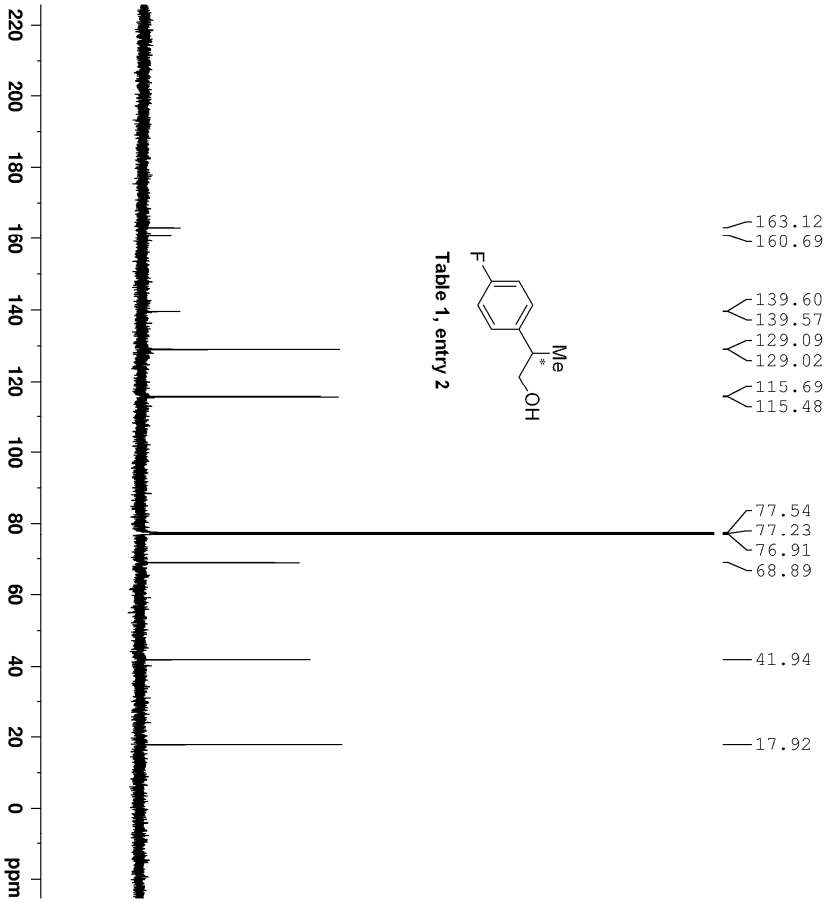
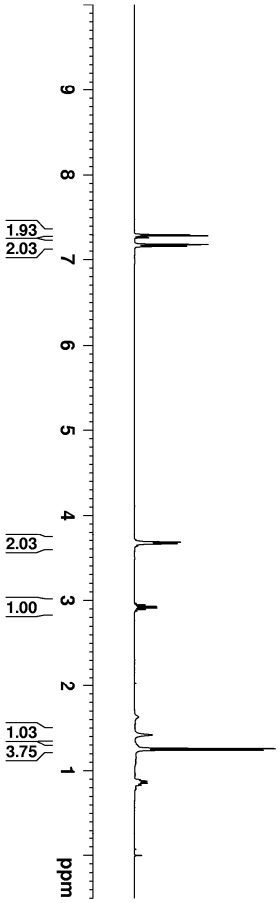


Table 1, entry 2

```
NAME                 zhuangminyang
EXPNO                          76
PROCNO                          1
Date_                    20120512
Time                        16.00
INSTRUM                      spect
PROBHD     5 mm PADUL 13C
PULPROG                    zg30
TD                         32768
SOLVENT                    CDCl3
NS                             11
DS                              0
SWH                    12019.230 Hz
FIDRES                 0.366798 Hz
AQ                     1.3631988 sec
RG                           161
DW                        41.600 usec
DE                         6.50 usec
TE                        300.0 K
D1                     2.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         1H
P1                        12.60 usec
SI                         65536
SF                400.1300175 MHz
WDW                           EM
SSB                            0
LB                          0.50 Hz
GB                             0
PC                          1.00
```




```
NAME                 zhuangminyang-C1
EXPNO                              37
PROCNO                              1
Date_                        20120517
Time                             9.53
INSTRUM                          spect
PROBHD     5 mm PADUL 13C
PULPROG                       zgpg30
TD                             32768
SOLVENT                       CDCl3
NS                               401
DS                                 0
SWH                        25252.525 Hz
FIDRES                      0.770646 Hz
AQ                          0.648856 sec
RG                               203
DW                          19.800 usec
DE                           6.50 usec
TE                           300.0 K
D1                         2.00000000 sec
D11                        0.03000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                            13C
P1                           9.40 usec
SI                             32768
SF                    100.6127479 MHz
WDW                               EM
SSB                                0
LB                          1.00 Hz
GB                                 0
PC                           1.40
```



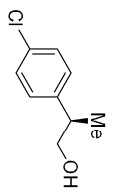
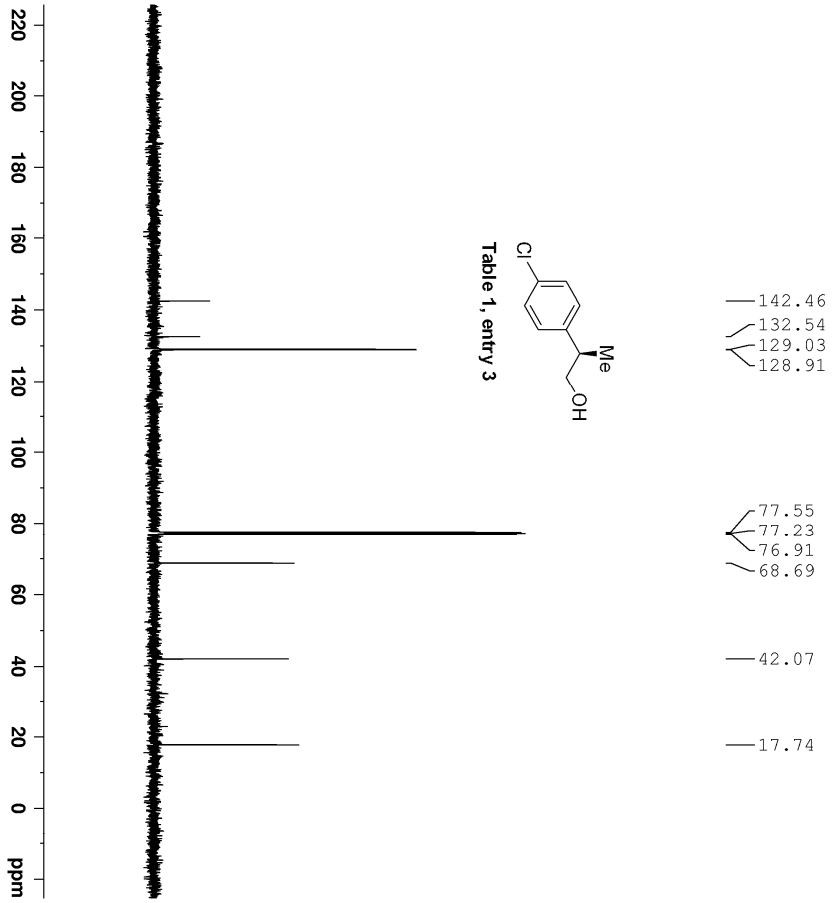


Table 1, entry 3

```
NAME                                   H
EXPNO                                 78
PROCNO                                23
Date_                       20110629
Time                           19.44
INSTRUM                         spect
PROBHD     5 mm PADUL 13C
PULPROG                        zg30
TD                            65536
SOLVENT                       CDCl3
NS                                8
DS                                0
SWH                       12019.230 Hz
FIDRES                    0.183399 Hz
AQ                        2.7263477 sec
RG                              144
DW                         41.600 usec
DE                          6.00 usec
TE                         300.4 K
D1                        5.00000000 sec
TD0                               1

======== CHANNEL f1 ========
NUC1                             1H
P1                          12.60 usec
SI                             32768
SF                    400.1300130 MHz
WDW                              EM
SSB                               0
LB                         0.00 Hz
GB                                0
PC                             1.00
```




```
NAME                                    C
EXPNO                                  44
PROCNO                                  1
Date_                            20110616
Time                                11.41
INSTRUM                              spect
PROBHD                5 mm PADUL 13C
PULPROG                           zgpg30
TD                                 65536
SOLVENT                           CDCl3
NS                                    52
DS                                     0
SWH                          25252.525 Hz
FIDRES                        0.385323 Hz
AQ                            1.2976629 sec
RG                                   203
DW                            19.800 usec
DE                             8.00 usec
TE                               300.9 K
D1                           2.00000000 sec
D11                          0.03000000 sec
TD0                                    1

======== CHANNEL f1 ========
NUC1                                 13C
P1                              9.40 usec
SI                                 32768
SF                       100.6127487 MHz
WDW                                   EM
SSB                                    0
LB                              2.00 Hz
GB                                     0
PC                              1.20
```

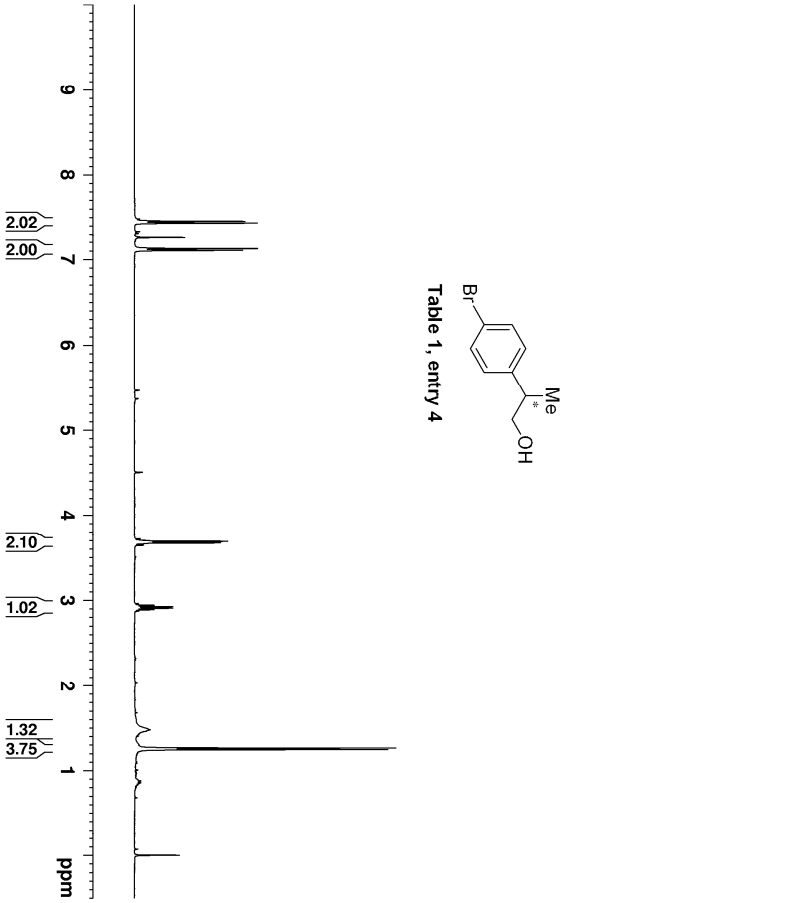
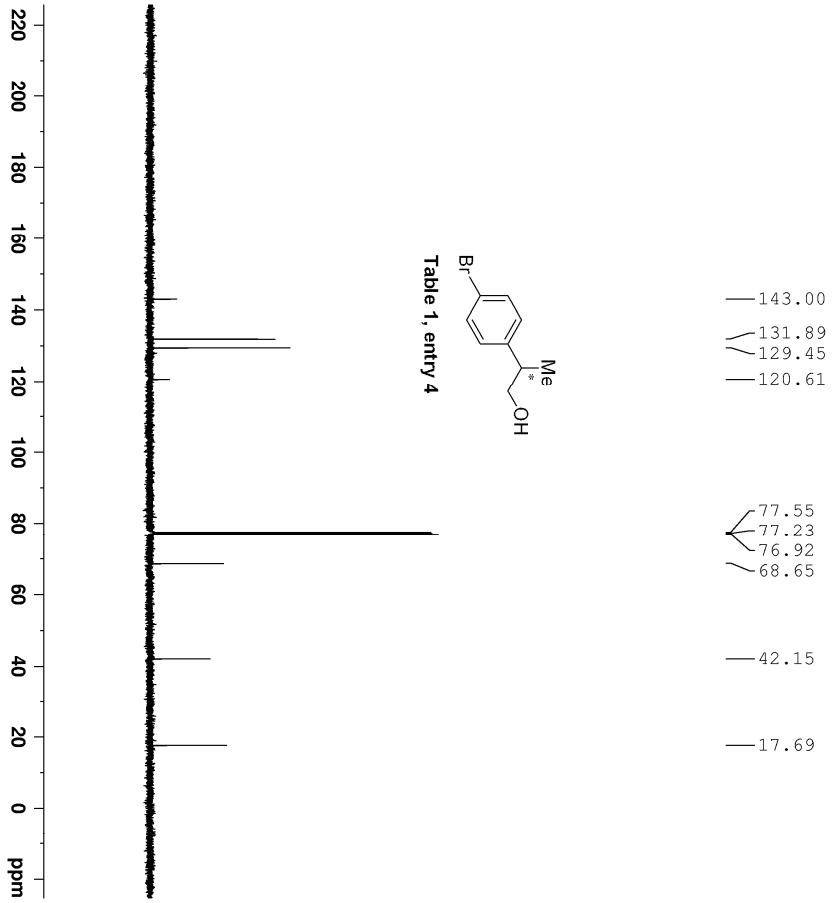
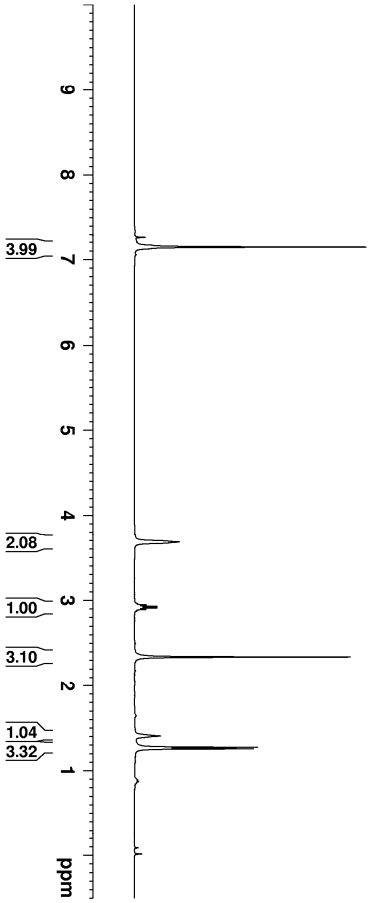


Table 1, entry 4

```
NAME                 zhuangminyang
EXPNO                         121
PROCNO                          1
Date_               20120615
Time_                    5.39
INSTRUM                  spect
PROBHD     5 mm PADUL 13C
PULPROG              zg30
TD                  32768
SOLVENT               CDCl3
NS                       14
DS                        0
SWH                12019.230 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                       203
DW                      41.600 usec
DE                       6.50 usec
TE                     300.0 K
D1                     2.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
SI                      65536
SF                400.1300177 MHz
WDW                        EM
SSB                         0
LB                       0.50 Hz
GB                          0
PC                       1.00
```




```
NAME                 zhuangminyang-C1
EXPNO                              68
PROCNO                              1
Date_                        20120615
Time                             5.41
INSTRUM                          spect
PROBHD     5 mm PADUL 13C
PULPROG                       zgpg30
TD                             32768
SOLVENT                        CDCl3
NS                               149
DS                                 0
SWH                        25252.525 Hz
FIDRES                      0.770646 Hz
AQ                          0.6488564 sec
RG                               203
DW                          19.800 usec
DE                           6.50 usec
TE                              300.0 K
D1                          2.00000000 sec
D11                         0.03000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                             13C
P1                          9.40 usec
SI                             32768
SF                    100.6127487 MHz
WDW                               EM
SSB                                0
LB                          1.00 Hz
GB                                 0
PC                          1.40
```



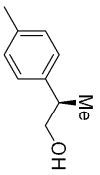
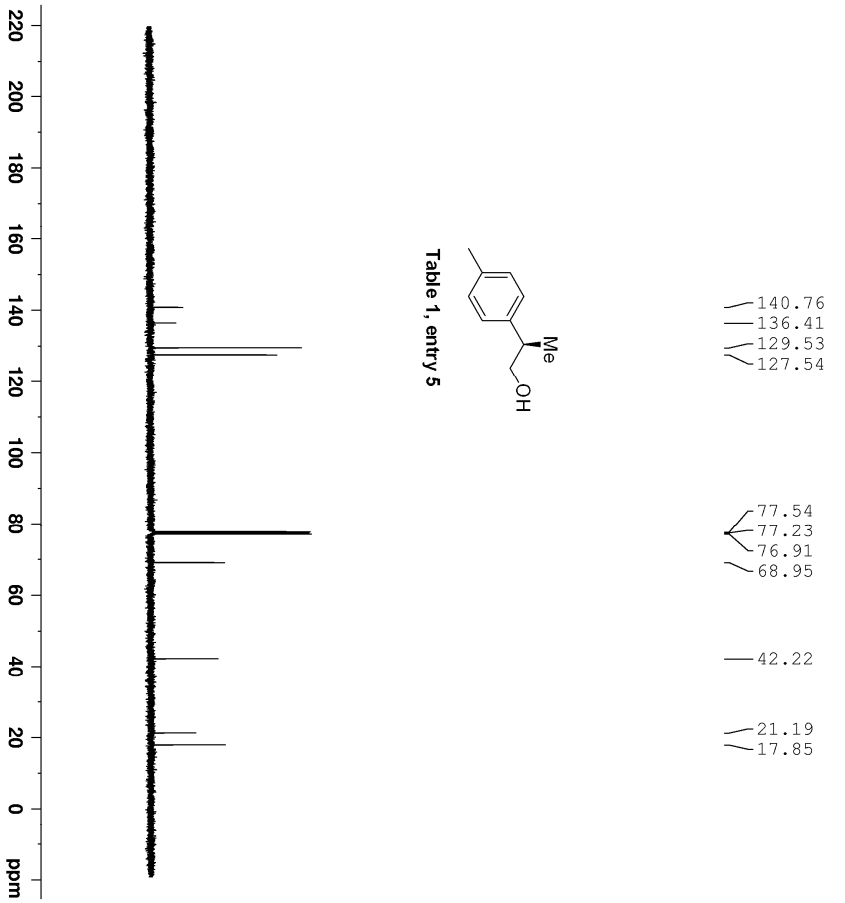


Table 1, entry 5

```
NAME                 zhuangminyang
EXPNO                          16
PROCNO                          1
Date_                20120228
Time_                    11.08
INSTRUM                   spect
PROBHD     5 mm PADUL 13C
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                           4
DS                           0
SWH                  12019.230 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         114
DW                      41.600 usec
DE                       6.50 usec
TE                      300.0 K
D1                    2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
SI                       65536
SF                400.1300176 MHz
WDW                         EM
SSB                          0
LB                        0.50 Hz
GB                           0
PC                        1.00
```




```
NAME                 zhuangminyang-C1
EXPNO                               7
PROCNO                              1
Date_                        20120228
Time                            11.09
INSTRUM                          spect
PROBHD     5 mm PADUL 13C
PULPROG                       zgpg30
TD                             65536
SOLVENT                        CDCl3
NS                                 38
DS                                  4
SWH                        24038.461 Hz
FIDRES                      0.366798 Hz
AQ                          1.3631988 sec
RG                                203
DW                           20.800 usec
DE                            6.50 usec
TE                             300.0 K
D1                         2.00000000 sec
D11                        0.03000000 sec
TD0                                 1

======== CHANNEL f1 ========
NUC1                              13C
P1                           9.40 usec
SI                             32768
SF                     100.6127530 MHz
WDW                               EM
SSB                                0
LB                          1.00 Hz
GB                                 0
PC                          1.40
```

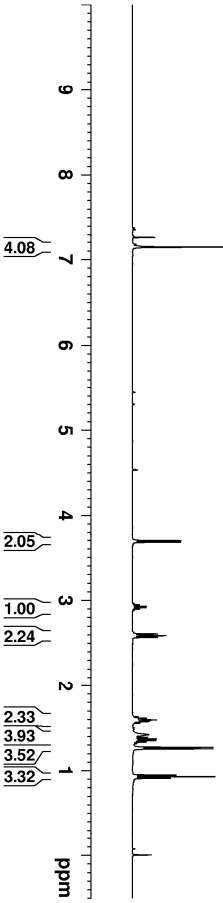
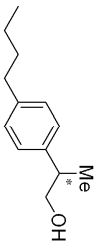
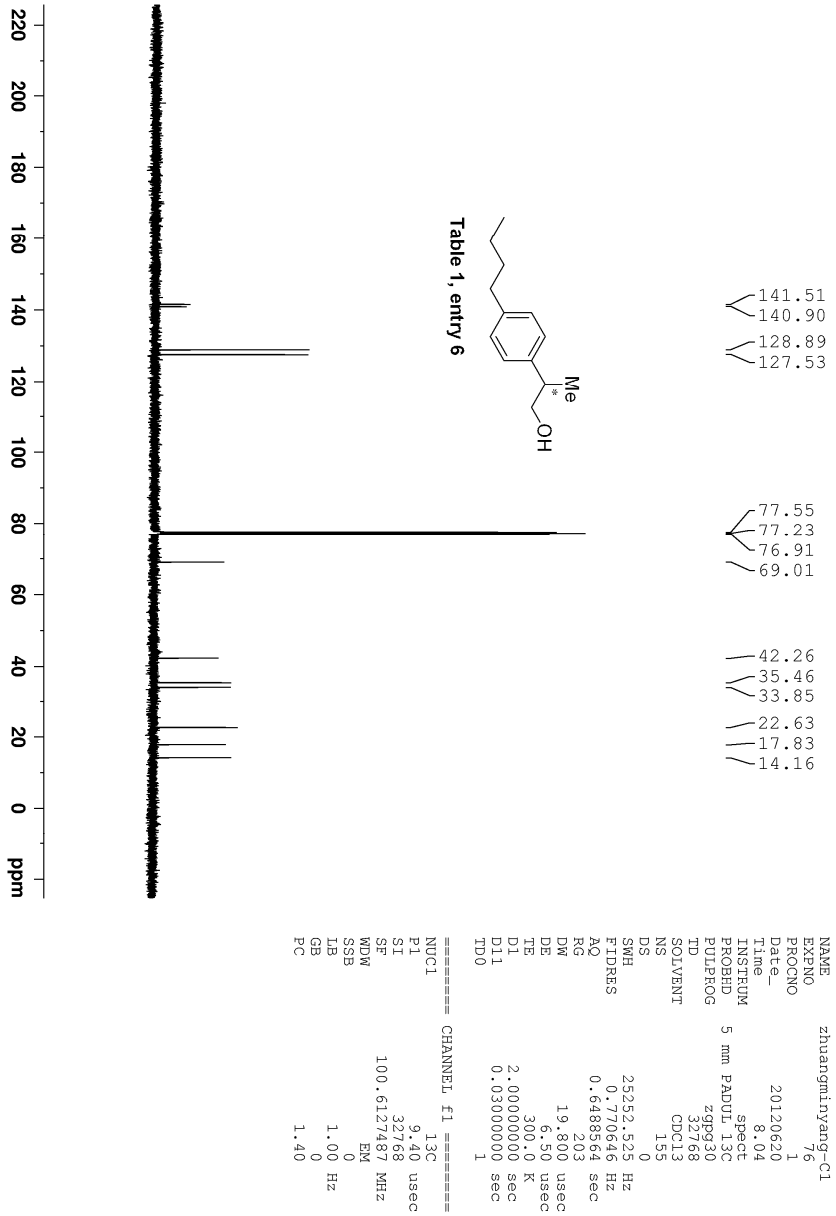
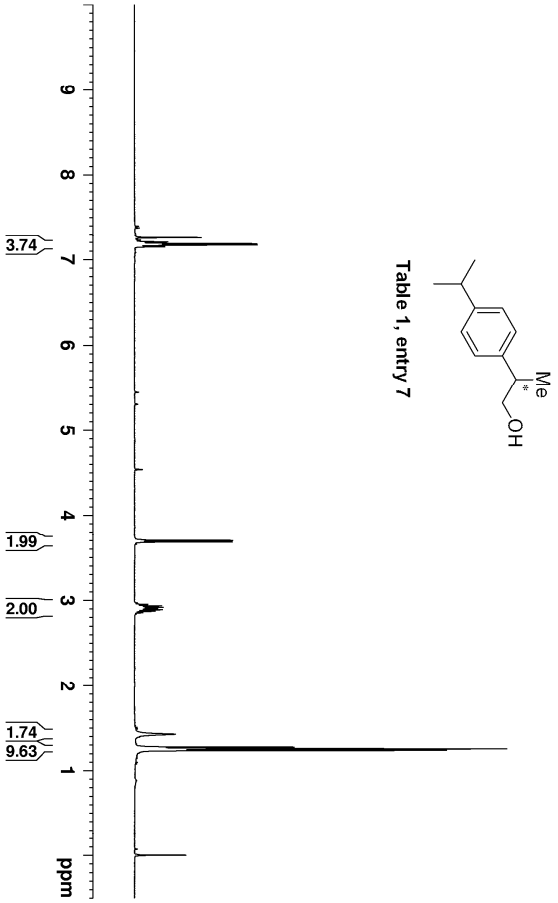


Table 1, entry 6

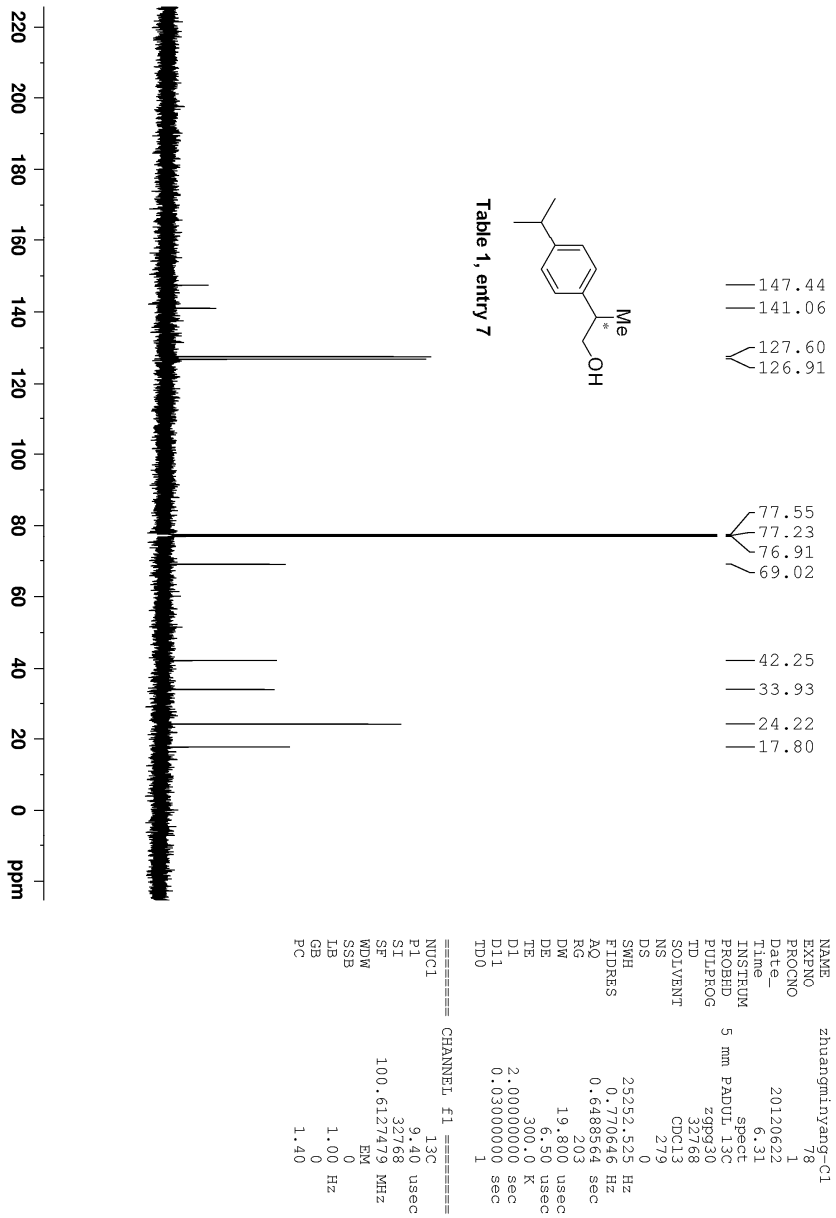



```
NAME                 zhuangminyang
EXPNO                         131
PROCNO                          1
Date_                    20120620
Time_                        7.55
INSTRUM                      spect
PROBHD     5 mm PADUL 13C
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                           8
DS                           0
SWH                  12019.230 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         203
DW                      41.600 usec
DE                       6.50 usec
TE                      300.0 K
D1                    2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
SI                       65536
SF                400.1300176 MHz
WDW                         EM
SSB                          0
LB                        0.50 Hz
GB                           0
PC                        1.00
```

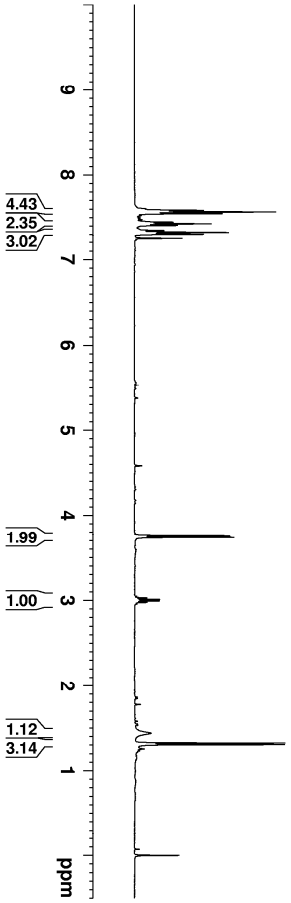

220
200
180
160
140
120
100
80
60
40
20
0
ppm
Table 1, entry 6
Me
OH
141.51
140.90
128.89
127.53
77.55
77.23
76.91
69.01
42.26
35.46
33.85
22.63
17.83
14.16
NAME zhuangminyang-C1
EXPNO 76
PROCNO 1
Date_ 20120620
Time 8.04
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 155
DS 0
SWH 25252.525 Hz
FIDRES 0.770646 Hz
AQ 0.6488564 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
SI 32768
SF 100.6127487 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
NAME                 zhuangminyang
EXPNO                         133
PROCNO                          1
Date_                    20120622
Time_                        6.29
INSTRUM                      spect
PROBHD     5 mm PADUL 13C
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                           8
DS                           0
SWH                  12019.230 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         203
DW                      41.600 usec
DE                       6.50 usec
TE                      300.0 K
D1                    2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
SI                       65536
SF                400.1300177 MHz
WDW                         EM
SSB                          0
LB                        0.50 Hz
GB                           0
PC                        1.00
```




```
NAME                 zhuangminyang-C1
EXPNO                              78
PROCNO                              1
Date_                        20120622
Time                             6.31
INSTRUM                          spect
PROBHD     5 mm PADUL 13C
PULPROG                       zgpg30
TD                             32768
SOLVENT                       CDCl3
NS                               279
DS                                 0
SWH                        25252.525 Hz
FIDRES                      0.770646 Hz
AQ                          0.6488564 sec
RG                               203
DW                          19.800 usec
DE                           6.50 usec
TE                           300.0 K
D1                         2.00000000 sec
D11                        0.03000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                            13C
P1                           9.40 usec
SI                             32768
SF                    100.6127479 MHz
WDW                               EM
SSB                                0
LB                          1.00 Hz
GB                                 0
PC                           1.40
```



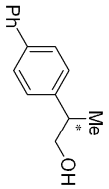
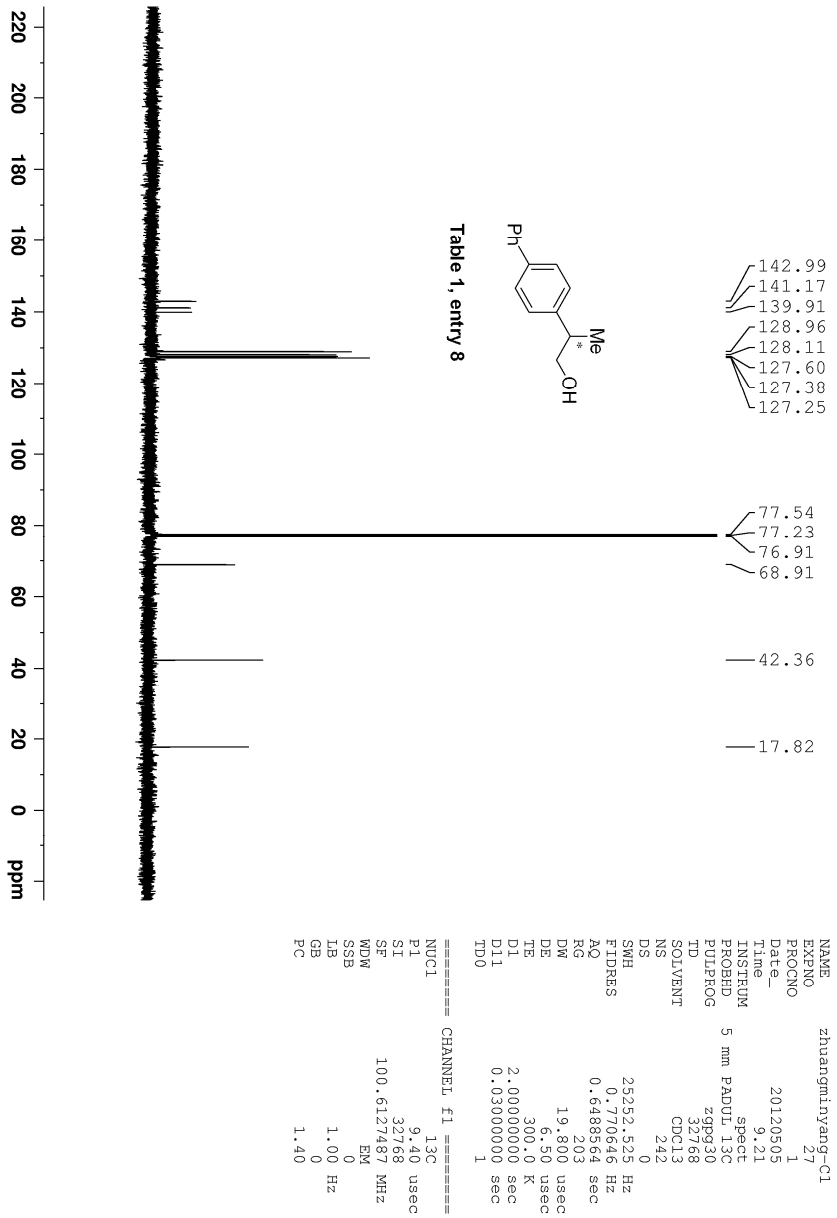
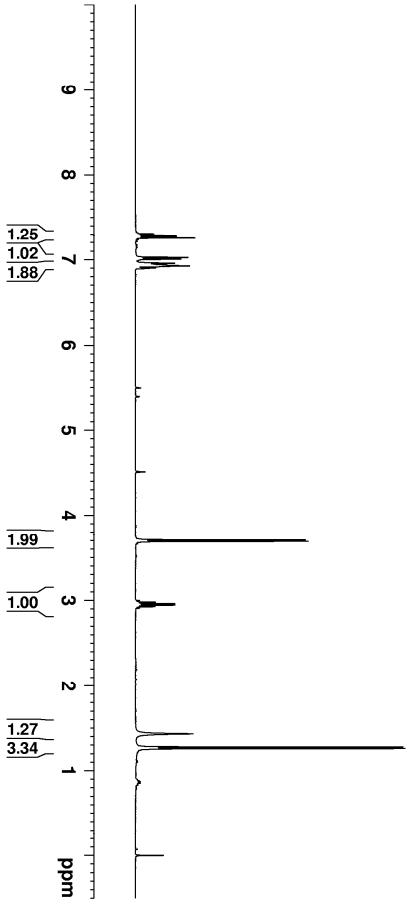


Table 1, entry 8

```
NAME                 zhuangminyang
EXPNO                          63
PROCNO                          1
Date_                    20120505
Time_                        9.18
INSTRUM                      spect
PROBHD     5 mm PADUL 13C
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                  12019.230 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                          203
DW                       41.600 usec
DE                        6.50 usec
TE                       300.0 K
D1                    2.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         1H
P1                        12.60 usec
SI                        65536
SF                400.1300217 MHz
WDW                         EM
SSB                          0
LB                        0.50 Hz
GB                           0
PC                        1.00
```


220
200
180
160
140
120
100
80
60
40
20
0
ppm
Table 1, entry 8
Ph
Me
*
OH
142.99
141.17
139.91
128.96
128.11
127.60
127.38
127.25
77.54
77.23
76.91
68.91
42.36
17.82
NAME zhuangminyang-C1
EXPNO 27
PROCNO 1
Date_ 20120505
Time 9.21
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 242
DS 0
SWH 25252.525 Hz
FIDRES 0.770646 Hz
AQ 0.6488564 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
SI 32768
SF 100.6127487 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



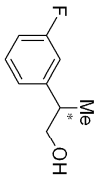
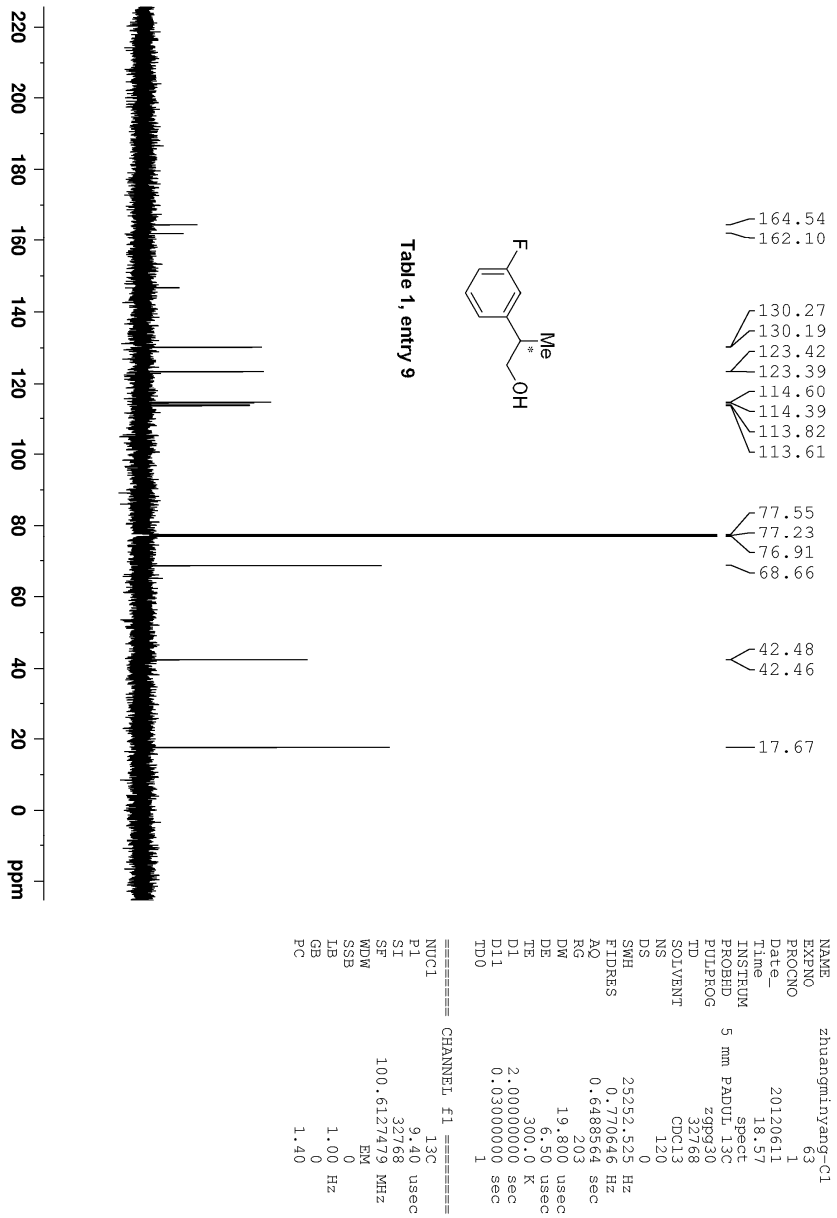
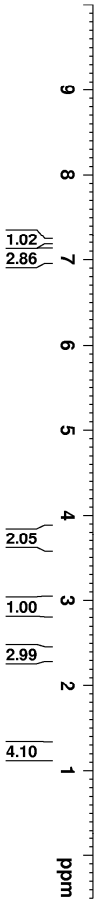


Table 1, entry 9

```
NAME                 zhuangminyang
EXPNO                         116
PROCNO                          1
Date_                    20120611
Time_                       18.55
INSTRUM                      spect
PROBHD     5 mm PADUL 13C
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                           3
DS                           0
SWH                  12019.230 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         114
DW                      41.600 usec
DE                       6.50 usec
TE                      300.0 K
D1                    2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
SI                       65536
SF                400.1300189 MHz
WDW                         EM
SSB                          0
LB                        0.50 Hz
GB                           0
PC                        1.00
```




```
NAME                 zhuangminyang-C1
EXPNO                              63
PROCNO                              1
Date_                        20120611
Time                            18.57
INSTRUM                          spect
PROBHD                5 mm PADUL 13C
PULPROG                       zgpg30
TD                             32768
SOLVENT                       CDCl3
NS                               120
DS                                 0
SWH                        25252.525 Hz
FIDRES                      0.770646 Hz
AQ                          0.6488564 sec
RG                               203
DW                          19.800 usec
DE                           6.50 usec
TE                           300.0 K
D1                         2.00000000 sec
D11                        0.03000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                             13C
P1                          9.40 usec
SI                             32768
SF                     100.6127479 MHz
WDW                               EM
SSB                                0
LB                          1.00 Hz
GB                                 0
PC                          1.40
```



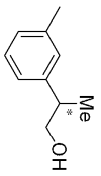
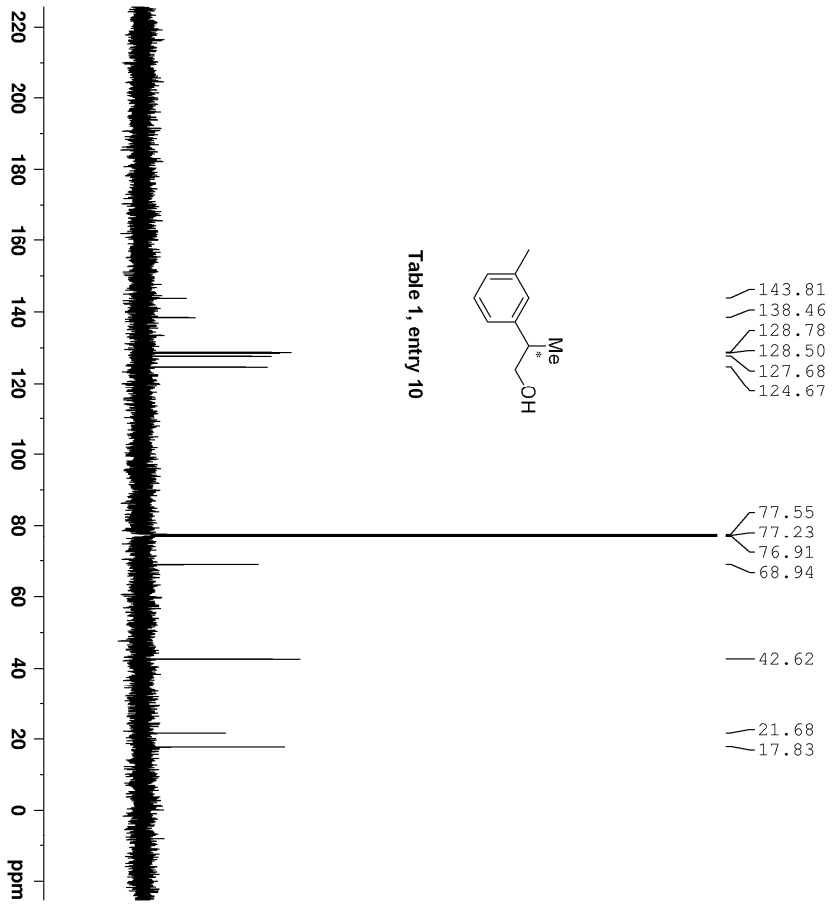
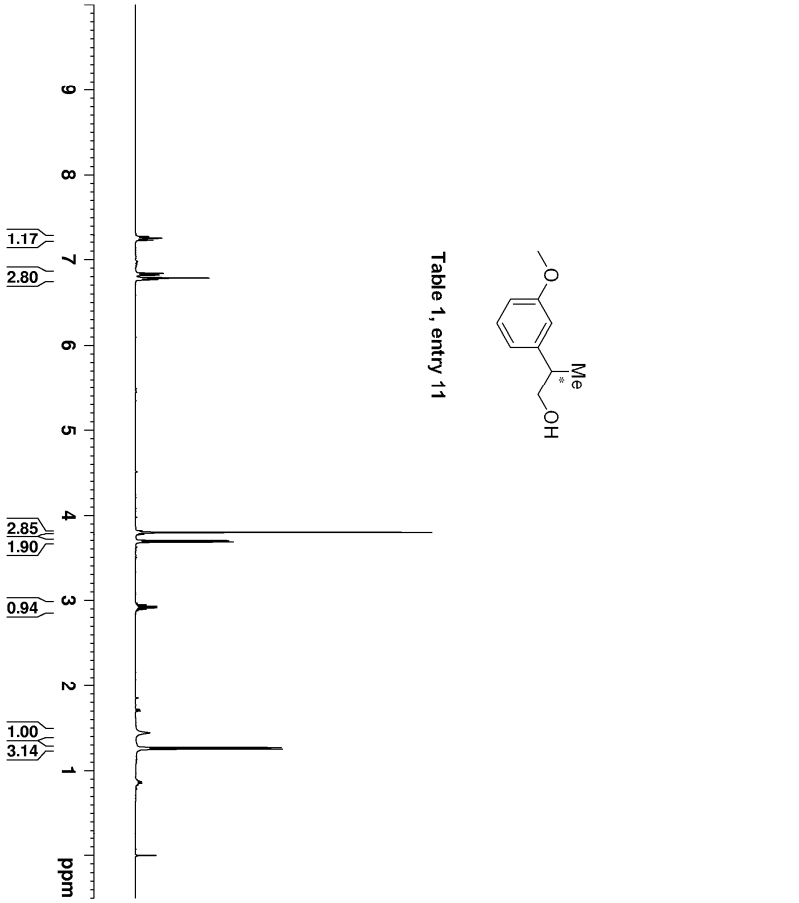


Table 1, entry 10

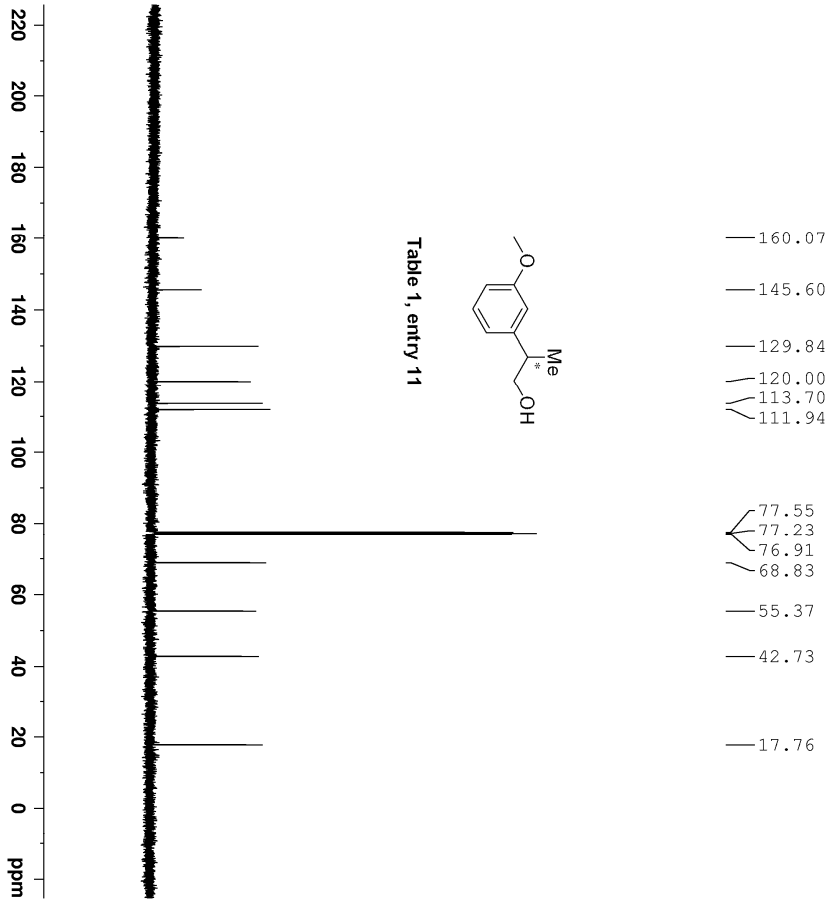
```
NAME                 zhuangminyang
EXPNO                          87
PROCNO                          1
Date_                    20120521
Time_                       16.23
INSTRUM                      spect
PROBHD     5 mm PADUL 13C
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                  12019.230 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                          203
DW                       41.600 usec
DE                        6.50 usec
TE                       300.0 K
D1                    2.00000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         1H
P1                        12.60 usec
SI                        65536
SF                400.1300199 MHz
WDW                         EM
SSB                          0
LB                        0.50 Hz
GB                           0
PC                        1.00
```



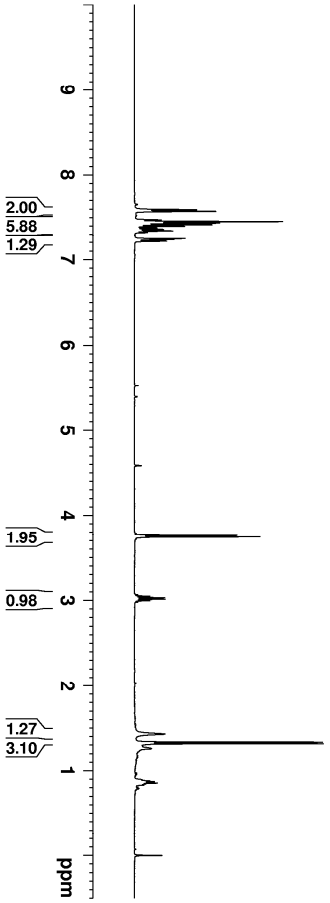

```
NAME                 zhuangminyang-C1
EXPNO                              43
PROCNO                              1
Date_                        20120521
Time                            16.25
INSTRUM                          spect
PROBHD     5 mm PADUL 13C
PULPROG                       zgpg30
TD                             32768
SOLVENT                       CDCl3
NS                               108
DS                                 0
SWH                        25252.525 Hz
FIDRES                      0.770646 Hz
AQ                          0.6488564 sec
RG                               203
DW                          19.800 usec
DE                           6.50 usec
TE                            300.0 K
D1                         2.00000000 sec
D11                        0.03000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                             13C
P1                          9.40 usec
SI                             32768
SF                     100.6127479 MHz
WDW                               EM
SSB                                0
LB                          1.00 Hz
GB                                 0
PC                          1.40
```




```
NAME                 zhuangminyang
EXPNO                          37
PROCNO                          1
Date_                    20120411
Time_                        9.56
INSTRUM                      spect
PROBHD     5 mm PADUL 13C
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                  12019.230 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         128
DW                        41.600 usec
DE                         6.50 usec
TE                        300.0 K
D1                    2.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
SI                       65536
SF                400.1300200 MHz
WDW                        EM
SSB                         0
LB                       0.50 Hz
GB                          0
PC                       1.00
```




```
NAME                 zhuangminyang-C1
EXPNO                              11
PROCNO                              1
Date_                        20120411
Time                            10.00
INSTRUM                          spect
PROBHD     5 mm PADUL 13C
PULPROG                       zgpg30
TD                             32768
SOLVENT                       CDCl3
NS                                 73
DS                                  0
SWH                         25252.525 Hz
FIDRES                       0.770646 Hz
AQ                           0.6488564 sec
RG                                203
DW                           19.800 usec
DE                            6.50 usec
TE                            300.0 K
D1                           2.00000000 sec
D11                          0.03000000 sec
TD0                                 1

======== CHANNEL f1 ========
NUC1                              13C
P1                            9.40 usec
SI                               32768
SF                    100.6127503 MHz
WDW                                EM
SSB                                 0
LB                             1.00 Hz
GB                                  0
PC                             1.40
```



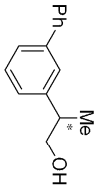


Table 1, entry 12

```
NAME                  zhuangminyang
EXPNO                           125
PROCNO                            1
Date_                      20120616
Time_                          7.08
INSTRUM                        spect
PROBHD     5 mm PADUL 13C
PULPROG                    zg30
TD                            32768
SOLVENT                       CDCl3
NS                                5
DS                                0
SWH                       12019.230 Hz
FIDRES                        0.366798 Hz
AQ                        1.3631988 sec
RG                              181
DW                           41.600 usec
DE                            6.50 usec
TE                           300.0 K
D1                        2.00000000 sec
TD0                               1

======== CHANNEL f1 ========
NUC1                           1H
P1                          12.60 usec
SI                            65536
SF                    400.1300224 MHz
WDW                              EM
SSB                               0
LB                             0.50 Hz
GB                                0
PC                             1.00
```

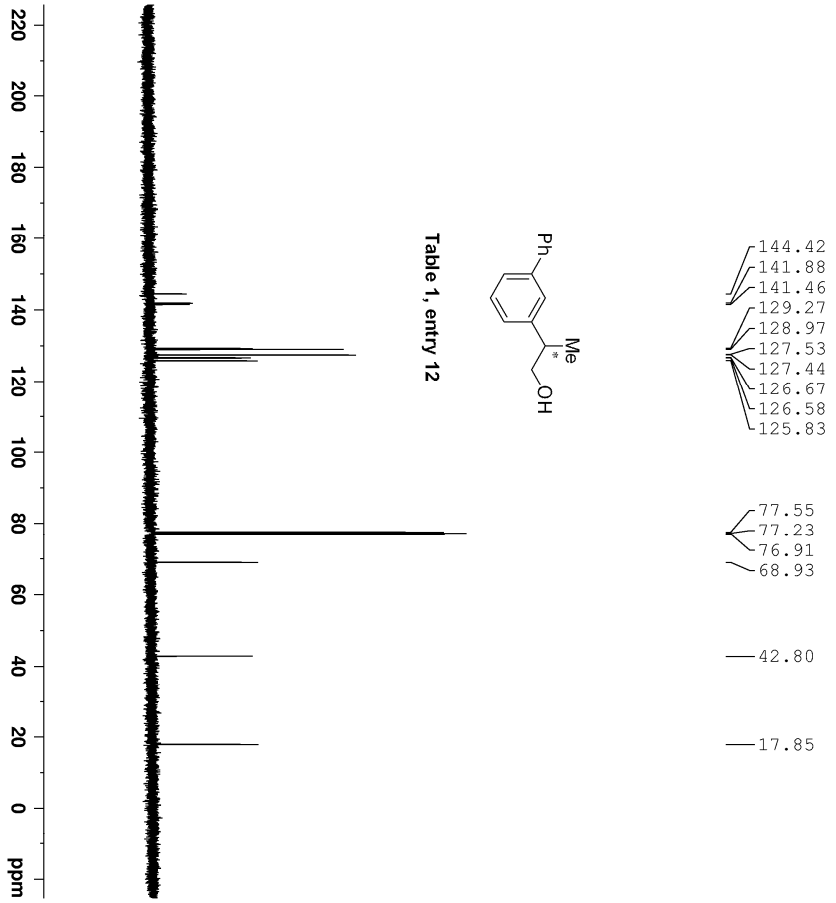
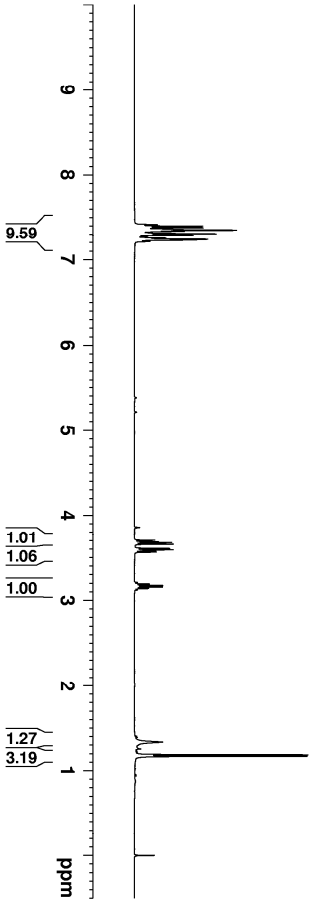


Table 1, entry 12

```
NAME                 zhuangminyang-C1
EXPNO                              71
PROCNO                              1
Date_                        20120616
Time                             7.09
INSTRUM                          spect
PROBHD     5 mm PADUL 13C
PULPROG                       zgpg30
TD                             32768
SOLVENT                       CDCl3
NS                               152
DS                                 0
SWH                        25252.525 Hz
FIDRES                     0.770646 Hz
AQ                         0.6488564 sec
RG                               203
DW                          19.800 usec
DE                           6.50 usec
TE                            300.0 K
D1                       2.00000000 sec
D11                      0.03000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                            13C
P1                           9.40 usec
SI                             32768
SF                     100.6127495 MHz
WDW                               EM
SSB                                0
LB                          1.00 Hz
GB                                 0
PC                              1.40
```



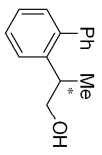


Table 1, entry 13

```
NAME                 zhuangminyang
EXPNO                          42
PROCNO                          1
Date_                20120418
Time_                    16.36
INSTRUM                    spect
PROBHD     5 mm PADUL 13C
PULPROG                    zg30
TD                        32768
SOLVENT                   CDCl3
NS                            3
DS                            0
SWH                 12019.230 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                          101
DW                       41.600 usec
DE                        6.50 usec
TE                       300.0 K
D1                    2.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        1H
P1                       12.60 usec
SI                        65536
SF                400.1300246 MHz
WDW                        EM
SSB                         0
LB                       0.50 Hz
GB                          0
PC                       1.00
```

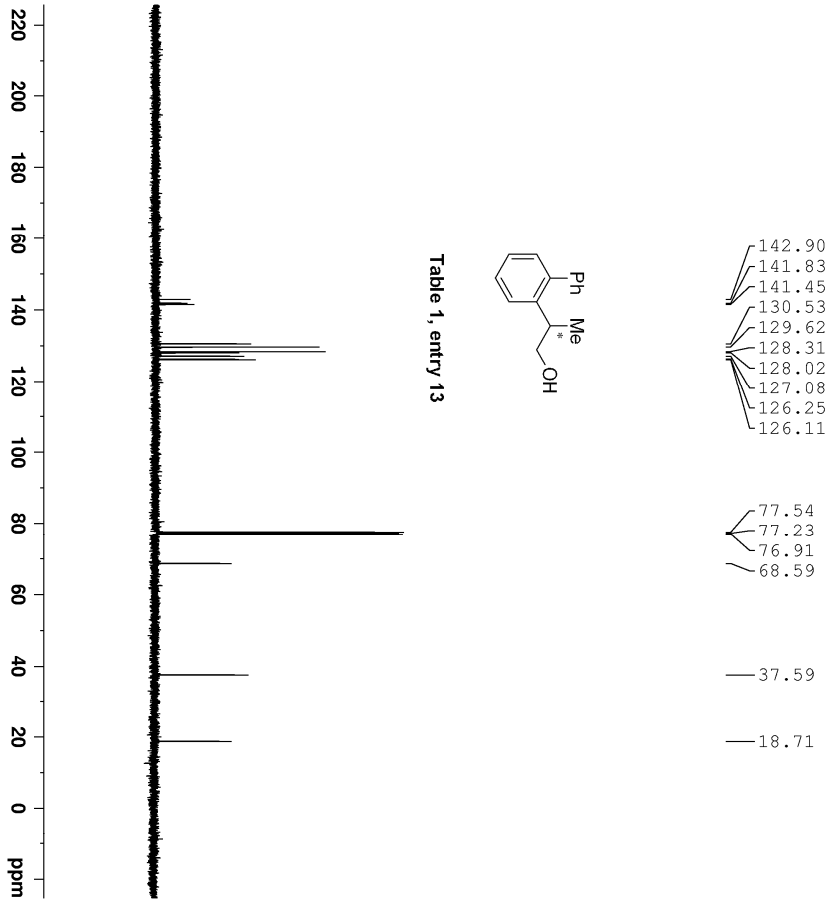
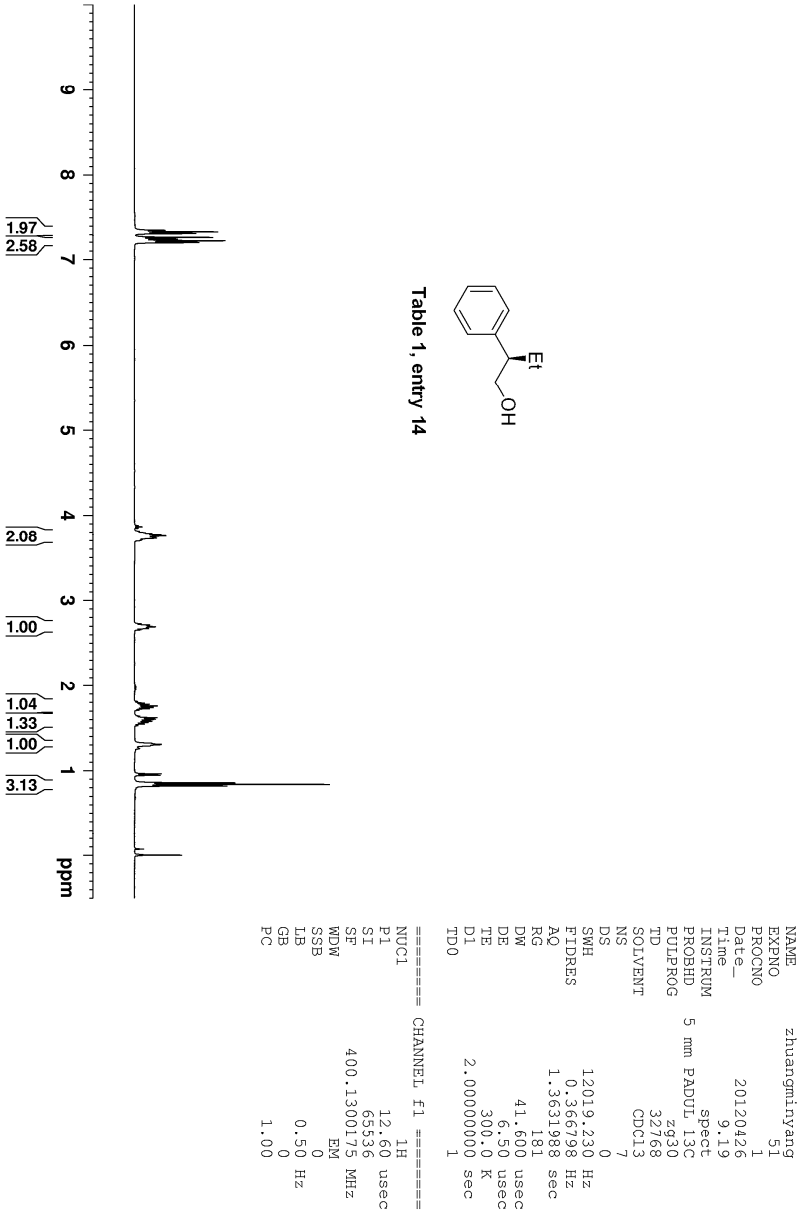
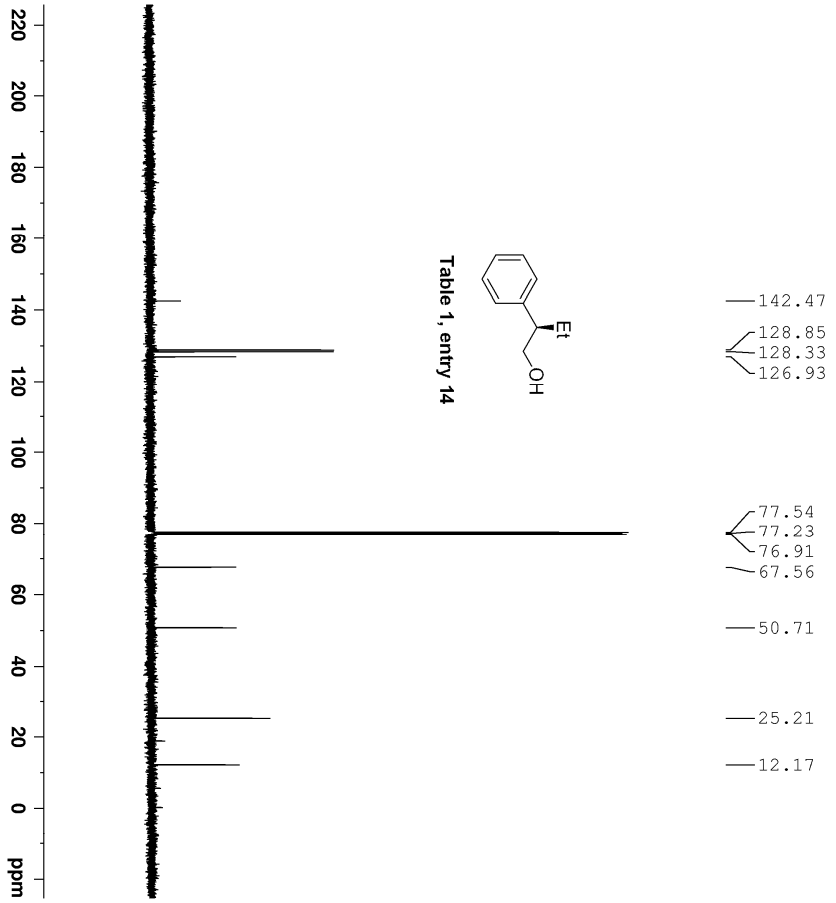


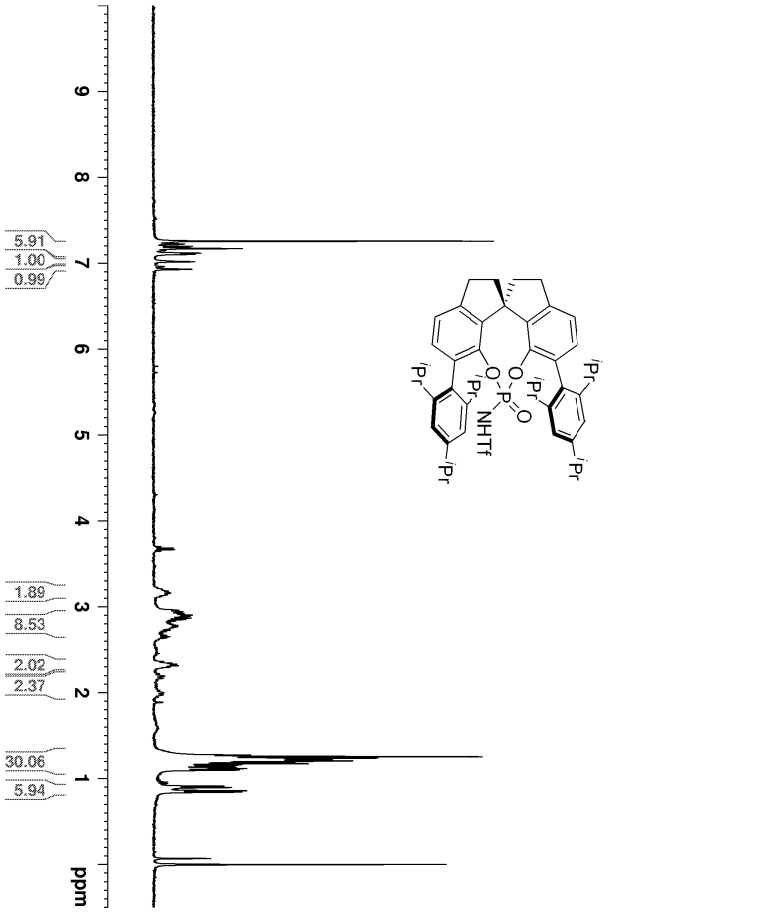
Table 1, entry 13

```
NAME                 zhuangminyang-C1
EXPNO                              14
PROCNO                              1
Date_                        20120418
Time                            15.42
INSTRUM                          spect
PROBHD     5 mm PADUL 13C
PULPROG                       zgpg30
TD                             32768
SOLVENT                       CDCl3
NS                                 45
DS                                  0
SWH                        25252.525 Hz
FIDRES                      0.770646 Hz
AQ                          0.6488564 sec
RG                                203
DW                           19.800 usec
DE                            6.50 usec
TE                             300.0 K
D1                         2.00000000 sec
D11                        0.03000000 sec
TD0                                 1

======== CHANNEL f1 ========
NUC1                              13C
P1                             9.40 usec
SI                             32768
SF                    100.6127526 MHz
WDW                               EM
SSB                                0
LB                              1.00 Hz
GB                                 0
PC                              1.40
```


1.97
2.58
2.08
1.00
1.04
1.33
1.00
3.13
ppm
Et
OH
Table 1, entry 14
NAME zhuangminyang
EXPNO 51
PROCNO 1
Date_ 20120426
Time_ 9.19
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 41.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
SI 65536
SF 400.1300175 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

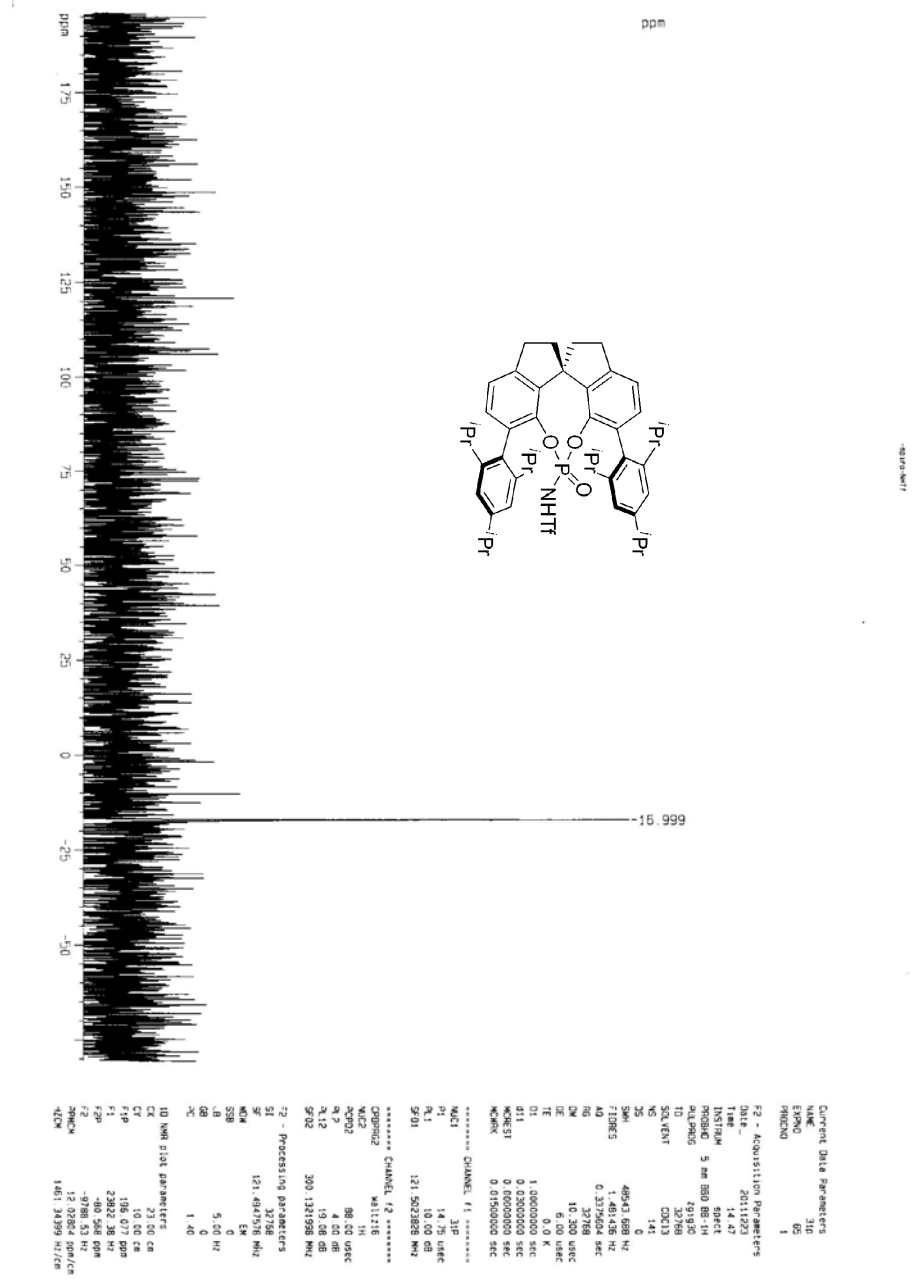


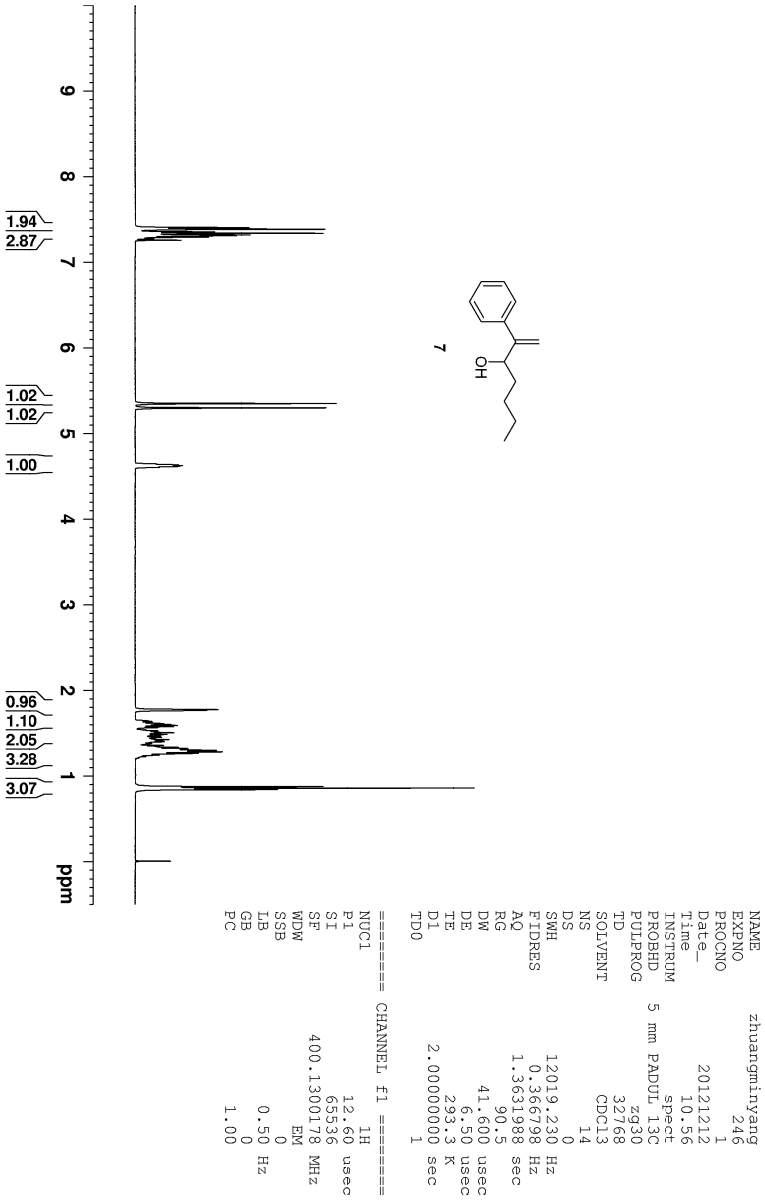

```
NAME                 zhuangminyang-C1
EXPNO                              20
PROCNO                              1
Date_                        20120426
Time                             9.24
INSTRUM                          spect
PROBHD     5 mm PADUL 13C
PULPROG                       zgpg30
TD                             32768
SOLVENT                       CDCl3
NS                               217
DS                                 0
SWH                        25252.525 Hz
FIDRES                     0.770646 Hz
AQ                         0.6488564 sec
RG                               203
DW                        19.800 usec
DE                         6.50 usec
TE                             300.0 K
D1                        2.00000000 sec
D11                       0.03000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                             13C
P1                            9.40 usec
SI                             32768
SF                    100.6127495 MHz
WDW                               EM
SSB                                0
LB                              1.00 Hz
GB                                 0
PC                              1.40
```

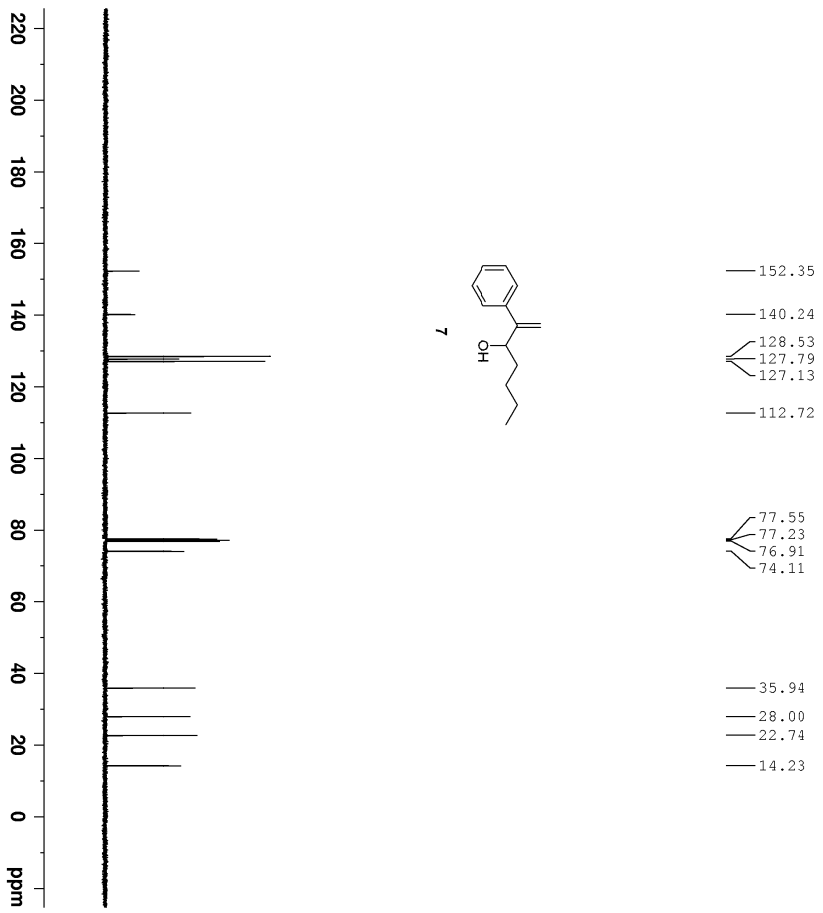



```
NAME                                   H
EXPNO                                 80
PROCNO                                16
Date_                           20120105
Time                               20.58
INSTRUM                             spect
PROBHD     5 mm PADUL 13C
PULPROG                         zg30
TD                                65536
SOLVENT                         CDCl3
NS                                    9
DS                                    0
SWH                           12019.230 Hz
FIDRES                        0.183399 Hz
AQ                            2.7263477 sec
RG                                  203
DW                             41.600 usec
DE                              6.00 usec
TE                                298.4 K
D1                             5.00000000 sec
TD0                                   1

======== CHANNEL f1 ========
NUC1                                1H
P1                             12.60 usec
SI                                32768
SF                    400.1300120 MHz
WDW                                 EM
SSB                                  0
LB                              0.00 Hz
GB                                   0
PC                                1.00
```

```
NAME                                    19F
EXPNO                                     3
PROCNO                                    1
Date_                              20111223
Time_                                 12.50
INSTRUM                               spect
PROBHD     5 mm BBO BB-1H
PULPROG                            zgflqn
TD                                    32768
SOLVENT                             CD3CN
NS                                       16
DS                                        0
SWH                              75187.969 Hz
FIDRES                           2.294555 Hz
AQ                               0.2179572 sec
RG                                     45.3
DW                                    6.650 usec
DE                                    6.00 usec
TE                                   673.2 K
D1                               1.00000000 sec

========== CHANNEL f1 ==========
NUC1                                    19F
P1                                    12.50 usec
PL1                                    0.00 dB
SFO1                          376.4418792 MHz
SI                                    65536
SF                            376.4983540 MHz
WDW                                      EM
SSB                                       0
LB                                    10.00 Hz
GB                                        0
PC                                     0.10
```


ppm
175
150
125
100
75
50
25
0
-25
-50
-16.999
ppm
NHTf
iPr


1.94
2.87
1.02
1.02
1.00
0.96
1.10
2.05
3.28
3.07
ppm
OH
7
NAME zhuangminyang
EXPNO 246
PROCNO 1
Date_ 20121212
Time 10.56
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 14
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 90.5
DW 41.600 usec
DE 6.50 usec
TE 293.3 K
D1 2.00000000 sec
TD0 1
========== CHANNEL f1 ==========
NUC1 1H
P1 12.60 usec
SI 65536
SF 400.1300178 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00




```
NAME                 zhuangminyang-C1
EXPNO                              91
PROCNO                              1
Date_                        20121212
Time                            10.59
INSTRUM                         spect
PROBHD     5 mm PADUL 13C
PULPROG                      zgpg30
TD                               32768
SOLVENT                      CDC13
NS                                  85
DS                                   0
SWH                      25252.525 Hz
FIDRES                       0.770646 Hz
AQ                           0.6488564 sec
RG                                 203
DW                              19.800 usec
DE                               6.50 usec
TE                             293.9 K
D1                           2.00000000 sec
D11                          0.03000000 sec
TD0                                  1

======== CHANNEL f1 ========
NUC1                              13C
P1                               9.40 usec
SI                               32768
SF                    100.6127533 MHz
WDW                                EM
SSB                                 0
LB                               1.00 Hz
GB                                  0
PC                               1.40
```