Enantioselective Allylation of Ketones Catalyzed by *N,N'*-Dioxide and Indium (III) Complex

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General Information.

^1H NMR spectra were recorded on commercial instruments (400 or 300 MHz). Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (CDCl_3 , $\delta = 7.26$). Spectra are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz), integration, and assignment. ^{13}C NMR spectra were collected on commercial instruments (100 or 75 MHz) with complete proton decoupling. Chemical shifts are reported in ppm from the tetramethylsilane with the solvent resonance as internal standard (CDCl_3 , $\delta = 77.0$). The enantiomeric excesses were determined by HPLC analysis on chiral DAICEL CHIRALCEL OJ-H or CHIRALCEL OD-H column at 254 nm. Optical rotations were reported as follows: $[\alpha]^{25}_{\text{D}}$ (c g/100 mL, in solvent). HRMS was recorded on a commercial apparatus (ESI Source). All ketones, *L*-proline, (*S*)-1-*N*-Boc-piperidine-2-carboxylic acid, and tetraallyltin were commercially purchased and used without further purification. CH_2Cl_2 and CH_3CN were distilled over CaH_2 before use. DMF was distilled under pressure over K_2CO_3 before use. The other solvents were distilled over metal sodium before use.

General procedure for the preparation of chiral ligands.

- i) The precursor of *N,N'*-dioxides were prepared according to the methods reported in the literature.¹⁻³
- ii) The *N,N'*-dioxdes were synthesized by the same procedure in the literature.^{2, 3}

Characterization of *N,N'*-dioxides.

N,N'-dioxide **L1**: white solid; m.p. 93-95°C; $[\alpha]_D^{25} = -87.5$ ($c = 0.352$ in CHCl_3); ^1H NMR (300 MHz, CDCl_3 , 25 °C, TMS): $\delta = 12.78$ (s, 2H), 7.47-7.50 (m, 4H), 7.23-7.28 (m, 4H), 7.03-7.07 (m, 2H), 3.35-3.51 (m, 8H), 2.85-2.94 (m, 2H), 2.47-2.61 (m, 2H), 2.28-2.43 (m, 6H), 1.99-2.04 (d, 2H), 1.84-1.88 (d, 2H), 1.62-1.67 (d, 2H), 1.32-1.46 (m, 2H) ppm; ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, TMS): $\delta = 166.3$, 137.5, 128.9, 124.1, 119.9, 76.5, 66.8, 64.6, 26.2, 22.2, 20.1, 16.3 ppm; EI-HRMS Calcd for $\text{C}_{27}\text{H}_{36}\text{N}_4\text{O}_4$ ($\text{M}+\text{H}^+$): 481.2815, Found: 481.2816.

N,N'-dioxide **L2**: white solid; m.p. 91-93 °C; $[\alpha]_D^{25} = -74.6$ ($c = 0.122$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 12.66$ (s, 2H), 7.97-7.99 (m, 2H), 7.10-7.16 (m, 4H), 7.00-7.01 (m, 2H), 3.45-3.55 (m, 8H), 2.89-2.96 (m, 2H), 2.62-2.66 (m, 2H), 2.44-2.51 (m, 2H), 2.36-2.40 (m, 2H), 2.25-2.28 (m, 6H), 2.06-2.09 (m, 2H), 1.87-1.90 (m, 2H), 1.67-1.87 (m, 2H), 1.41-1.46 (m, 2H) ppm; ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 166.4$, 136.2, 130.4, 128.2, 126.6, 124.4, 121.2, 66.8, 64.6, 31.6, 26.6, 22.7, 20.2, 18.4 ppm; EI-HRMS Calcd for $\text{C}_{29}\text{H}_{40}\text{N}_4\text{O}_4$ ($\text{M}+\text{H}^+$): 509.3128, Found: 509.3147.

N,N'-dioxide **L3**: white solid; m.p. 96-98 °C; $[\alpha]^{25}_D = -93.9$ ($c = 0.266$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 12.63$ (s, 2H), 7.37-7.39 (m, 4H), 7.05-7.07 (m, 4H), 3.39-3.50 (m, 8H), 2.87-2.90 (m, 2H), 2.30-2.61 (m, 12H), 1.86-2.05 (m, 4H), 1.19-1.42 (m, 4H), ppm; ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 166.2, 135.0, 129.5, 120.0, 68.1, 64.7, 31.6, 22.7, 20.9, 20.2, 14.1$ ppm; EI-HRMS Calcd for $\text{C}_{29}\text{H}_{40}\text{N}_4\text{O}_4$ ($\text{M}+\text{H}^+$): 509.3128, Found: 509.3147

N,N'-dioxide **L4**: white solid; m.p. 108-109 °C; $[\alpha]^{25}_D = -80.4$ ($c = 0.204$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 10.82$ -10.84 (d, $J = 8.8$ Hz; 2H), 7.27 (m, 10H), 5.06-5.10 (m, 2H), 3.22-3.25 (m, 4H), 2.13-2.63 (m, 14H), 1.94-1.97 (d, 2H), 1.81-1.84 (d, 2H), 1.55-1.59 (d, 2H), 1.44-1.46 (m, 6H), 1.34-1.37 (m, 2H) ppm; ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 167.5, 143.6, 128.7, 127.4, 126.4, 75.7, 65.0, 64.6, 48.2, 26.1, 22.2, 21.9, 20.1, 15.4$ ppm; EI-HRMS Calcd for $\text{C}_{31}\text{H}_{44}\text{N}_4\text{O}_4$ ($\text{M}+\text{Na}^+$): 559.3260, Found: 559.3065.

N,N'-dioxide **L5**: white solid; m.p. 102-104 °C; $[\alpha]^{25}_D = -72.4$ ($c = 0.170$ in CHCl_3); ^1H NMR (300 MHz, CDCl_3 , 25 °C, TMS): $\delta = 13.32$ (s, 2H), 7.55-7.59 (m, 4H), 7.26-7.31 (m, 4H), 7.08 (m, 2H), 3.63-3.69 (m, 4H), 3.47-3.56 (m, 4H), 3.29-3.37 (m, 2H), 2.44-2.76 (m, 8H), 2.06-2.09 (m, 2H) ppm; ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 165.2, 137.7, 128.9, 124.2, 120.1, 68.1, 64.7, 27.6, 22.6, 20.3, 14.1$ ppm; EI-HRMS Calcd for $\text{C}_{25}\text{H}_{33}\text{N}_4\text{O}_4$ ($\text{M}+\text{H}^+$): 453.2502, Found: 453.2498

N,N'-dioxide **L6**: white solid; m.p. 100-101 °C; $[\alpha]^{25}_{\text{D}} = -55.6$ ($c = 0.660$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 13.13$ (s, 2H), 8.05-8.07 (m, 2H), 6.99-7.02 (m, 2H), 3.57-3.75 (m, 8H), 3.31-3.34 (m, 2H), 2.70-2.76 (m, 2H), 2.40-2.60 (m, 6H), 2.25-2.30 (m, 8H), 2.04-2.09 (m, 2H), ppm; ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 165.2$, 136.3, 130.4, 128.3, 126.5, 124.4, 121.4, 67.9, 64.9, 27.8, 20.3, 20.1, 18.4 ppm; EI-HRMS Calcd for $\text{C}_{27}\text{H}_{36}\text{N}_4\text{O}_4$ ($\text{M}+\text{Na}^+$): 503.2634, Found: 503.2519.

N,N'-dioxide **L7**: white solid; m.p. 106-108 °C; $[\alpha]^{25}_{\text{D}} = -73.4$ ($c = 0.218$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 13.06$ (s, 2H), 7.43-7.52 (m, 4H), 7.07-7.13 (m, 4H), 3.63-3.71 (m, 4H), 3.44-3.58 (m, 4H), 3.28-3.35 (m, 2H), 2.48-2.73 (m, 6H), 2.30-2.40 (m, 8H), 2.01-2.17 (m, 2H), ppm; ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 165.0$, 135.1, 133.9, 129.5, 129.4, 120.1, 68.1, 64.7, 27.6, 20.9, 20.2 ppm; EI-HRMS Calcd for $\text{C}_{27}\text{H}_{36}\text{N}_4\text{O}_4$ ($\text{M}+\text{Na}^+$): 503.2634, Found: 503.2684.

N,N'-dioxide **L8**: white solid; m.p. 117-118 °C; $[\alpha]^{25}_{\text{D}} = -31.8$ ($c = 0.550$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 12.77$ (s, 2H), 7.38-7.53 (m, 4H), 7.14-7.17 (m, 4H), 3.80-3.85 (m, 2H), 3.62-3.69 (m, 6H), 3.33-3.36 (m, 2H), 2.55-2.77 (m, 18H), 1.34-1.41 (m, 10H) ppm; ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 165.3$, 143.2, 134.5, 127.1, 126.7, 126.5, 125.9, 67.7, 64.9, 34.6, 31.7, 30.8, 26.8, 20.2, 19.9 ppm; EI-HRMS Calcd for $\text{C}_{33}\text{H}_{48}\text{N}_4\text{O}_4$ ($\text{M}+\text{H}^+$): 565.3748, Found: 565.3745.

N,N'-dioxide **L9**: white solid; m.p. 111-112 °C; $[\alpha]_D^{25} = -50.4$ ($c = 0.274$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 12.47$ (s, 2H), 7.17-7.29 (m, 6H), 3.37-3.87 (m, 10H), 3.02-3.09 (m, 4H), 2.46-2.87 (m, 8H), 2.07-2.13 (m, 2H), 1.12-1.24 (m, 24H) ppm; ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 166.3, 144.8, 130.8, 127.8, 123.2, 67.9, 63.9, 28.9, 27.5, 23.7, 23.1, 20.2, 19.8$ ppm; EI-HRMS Calcd for $\text{C}_{37}\text{H}_{56}\text{N}_4\text{O}_4$ ($\text{M}+\text{H}^+$): 621.4380, Found: 621.4403.

Ligand **L10**: white powder; m.p. 94-96 °C; $[\alpha]_D^{25} = -133.4$ ($c = 0.50$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 8.57$ (s, 2H), 7.48-7.50 (m, 4H), 7.27-7.31 (m, 4H), 7.05-7.09 (m, 2H), 5.29 (s, 2H), 3.07-3.10 (m, 2H), 2.80-2.83 (m, 2H), 2.53-2.60 (m, 2H), 2.30-2.37 (m, 2H), 1.97-2.10 (m, 4H), 1.42-1.82 (m, 10H), 1.26-1.35 ppm (m, 2H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 172.4, 137.7, 129.0, 123.9, 119.2, 68.2, 54.5, 53.0, 51.0, 29.5, 24.4, 23.2$ ppm; EI-HRMS Calcd for $\text{C}_{27}\text{H}_{36}\text{N}_4\text{O}_2$ (M^+): 448.2838, Found: 448.3444.

Typical experimental procedure for the enantioselective allylation of ketones.

To an oven dried tube equipped with a magnetic stirring bar were added InBr_3 (21.3 mg, 0.06 mmol) and **L1** (57.6 mg, 0.12 mmol) in anhydrous DMF (0.4 ml), which was allowed to stir at ambient temperature for 2 h under N_2 atmosphere. The tetraallyltin (144 μL , 0.6 mmol) was added at -20 °C, in sequence, acetophenone (24 μL , 0.2 mmol). The reaction mixture was stirred at -20 °C for 72 h and directly purified by column chromatography on silica gel eluted with diethyl ether/petroleum ether (1:10 v/v) to afford product **3a** as colorless oil in 72% isolated yield with 80% ee [determined with chiral HPLC,

DAICEL CHIRALCEL OJ-H, isopropanol:hexane = 2:98, 1.0 mL/min, λ = 254 nm, t_R (major) = 12.019 min, t_R (minor) = 15.512 min]; $[\alpha]_D^{25} = +42.6$ (c = 0.108, CHCl_3).

Characterization of products.

(*R*)-2-phenylpent-4-en-2-ol (**3a**): was obtained as a colorless oil in 72% isolated yield and 80% ee [determined with chiral HPLC, DAICEL CHIRALCEL OJ-H, isopropanol:hexane = 2:98, 1.0 mL/min, λ = 254 nm, t_R (major) = 12.019 min, t_R (minor) = 15.512 min]; $[\alpha]_D^{25} = +42.6$ (c = 0.108, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.43-7.46 (m, 2H), 7.33-7.37 (m, 2H), 7.24-7.26 (m, 1H), 5.58-5.63 (m, 1H), 5.11-5.17 (m, 2H), 2.69 (dd, J = 13.6 Hz, 6.4 Hz, 1H), 2.50 (dd, J = 13.6 Hz, 8.4 Hz, 1H), 2.05 (s, 1H), 1.55 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 146.6, 132.6, 127.2, 125.6, 123.7, 118.5, 72.6, 47.4, 28.9 ppm. ESI-HRMS Calcd for ($\text{C}_{11}\text{H}_{14}\text{O}-\text{H}_2\text{O}$) 144.0939, Found: 144.0943.⁴

2-(2-methoxyphenyl)pent-4-en-2-ol (**3b**): was obtained as a colorless oil in 69% isolated yield and 83% ee [determined with chiral HPLC, Daicel Chiralcel OD-H, isopropanol:hexane = 1:99, 1.0 mL/min, λ = 254 nm, t_R (major) = 7.817 min, t_R (minor) = 10.196 min]; $[\alpha]_D^{25} = +2.9$ (c = 0.140, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.22-7.32 (m, 2H), 6.90-6.97 (m, 2H), 5.60-5.65 (m, 1H), 5.00-5.15 (m, 1H), 3.90 (s, 1H), 3.89 (s, 3H), 2.80 (dd, J = 13.6 Hz, 6.8 Hz, 1H), 2.60 (dd, J = 13.6 Hz, 7.6 Hz, 1H), 1.56 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ =

155.6, 133.8, 133.4, 127.2, 125.8, 119.8, 116.7, 110.2, 73.2, 54.2, 45.6, 25.9 ppm; ESI-HRMS Calcd for (C₁₂H₁₆O₂ + Na⁺) 215.1048, Found: 215.1048.

(*R*)-2-(4-methoxyphenyl)pent-4-en-2-ol (**3c**): was obtained as a colorless oil in 48% isolated yield and 80% ee [determined with chiral HPLC, Daicel Chiralcel OD-H, isopropanol:hexane = 1:99, 1.0 mL/min, λ = 254 nm, t_R (major) = 13.752 min, t_R (minor) = 14.981 min; $[\alpha]_D^{25}$ = +43.0 (c = 0.200, CHCl₃); ¹H NMR (400 MHz, CDCl₃): δ = 7.34-7.36 (m, 2H), 6.89-6.86 (m, 2H), 5.57-5.68 (m, 1H), 5.10-5.15 (m, 2H), 3.81 (s, 3H), 2.65 (dd, J = 13.6 Hz, 6.4 Hz, 1H), 2.47 (dd, J = 13.6 Hz, 8.4 Hz, 1H), 2.01 (s, 1H), 1.52 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ = 158.3, 139.9, 133.8, 125.9, 119.3, 73.4, 55.2, 48.6, 29.9 ppm; ESI-HRMS Calcd for (C₁₂H₁₆O₂ + Na⁺) 215.1048, Found: 215.1046.

2-(3-methoxyphenyl)pent-4-en-2-ol (**3d**): was obtained as a colorless oil in 85% isolated yield and 74% ee [determined with chiral HPLC, Daicel Chiralcel OD-H, isopropanol:hexane = 1:99, 1.0 mL/min, λ = 254 nm, t_R (minor) = 18.790 min, t_R (major) = 19.997 min]; $[\alpha]_D^{25} = +40.8$ (c = 0.404, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.24-7.28 (m, 1H), 6.98-7.03 (m, 2H), 6.76-6.79 (m, 1H), 5.62-5.64 (m, 1H), 5.10-5.16 (m, 2H), 3.81 (s, 3H), 2.66 (dd, J = 14.0 Hz, 6.4 Hz, 1H), 2.49 (dd, J = 14.0 Hz, 7.6 Hz, 1H), 2.08 (s, 1H), 1.53 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 159.5, 149.5, 133.6, 129.2, 119.5, 117.2, 111.71, 111.0, 73.6, 55.2, 48.4, 29.9 ppm; ESI-HRMS Calcd for $(\text{C}_{12}\text{H}_{16}\text{O}_2 + \text{Na}^+)$ 215.1048, Found: 215.1048.

(*R*)-2-(4-tolyl)pent-4-en-2-ol (**3e**): was obtained as a colorless oil in 70% isolated yield and 81% ee [determined with chiral HPLC, Daicel Chiralcel OJ-H, isopropanol:hexane = 2:98, 1.0 mL/min, λ = 254 nm, t_R (major) = 10.041 min, t_R (minor) = 14.403 min]; $[\alpha]_D^{25}$ = +54.4 (c = 0.206, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.32-7.33 (m, 2H), 7.14-7.15 (m, 2H), 5.59-5.66 (m, 1H), 5.10-5.15 (m, 2H), 2.66 (dd, J = 13.6 Hz, 6.4 Hz, 1H), 2.49 (dd, J = 13.6 Hz, 8.4 Hz, 1H), 2.34 (s, 3H), 2.01 (s, 1H), 1.53 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 144.7, 136.1, 133.8, 128.8, 124.7, 119.3, 73.5, 48.4, 29.9, 20.9 ppm; ESI-HRMS Calcd for ($\text{C}_{12}\text{H}_{16}\text{O} + \text{Na}^+$) 199.1099, Found: 199.1091.

2-(4-fluorophenyl)pent-4-en-2-ol (**3f**): was obtained as a colorless oil in 61% isolated yield and 81% ee [determined with chiral HPLC, Daicel Chiralcel OJ-H, isopropanol:hexane = 2:98, 1.0 mL/min, λ = 254 nm, t_R (major) = 10.868 min, t_R (minor) = 13.287 min]; $[\alpha]_D^{25}$ = +36.8 (c = 0.076, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.39-7.42 (m, 2H), 6.99-7.04 (m, 2H), 5.56-5.66 (m, 1H), 5.11-5.16 (m, 2H), 2.64 (dd, J = 14.0 Hz, 6.4 Hz, 1H), 2.49 (dd, J = 13.6 Hz, 8.4 Hz, 1H), 2.03 (s, 1H), 1.54 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 162.8, 143.4, 136.1, 133.8, 126.5, 119.7, 114.9, 73.4, 48.6, 30.0 ppm; ESI-HRMS Calcd for ($\text{C}_{11}\text{H}_{13}\text{FO} - \text{H}_2\text{O}$) 163.0923, Found: 163.0930.

2-(4-chlorophenyl)pent-4-en-2-ol (**3g**): was obtained as a colorless oil in 86% isolated yield and 80% ee [determined with chiral HPLC, Daicel Chiralcel OJ-H, isopropanol:hexane = 2:98, 0.4 mL/min, λ = 254 nm, t_R (major) = 26.951 min, t_R (minor) = 31.913 min]; $[\alpha]_D^{25}$ = +47.5 (c = 0.598, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.31-7.36 (m, 2H), 7.26-7.29 (m, 2H), 5.56-5.62 (m, 1H), 5.12-5.15 (m, 2H), 2.65 (dd, J = 9.2 Hz, 4.0 Hz, 1H), 2.50 (dd, J = 9.2 Hz, 5.6 Hz, 1H), 2.04 (s, 1H), 1.53 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 146.2, 132.4, 128.2, 126.3, 119.8, 73.4, 48.3, 30.9, 29.9 ppm; ESI-HRMS Calcd for ($\text{C}_{11}\text{H}_{13}\text{ClO} + \text{K}^+$) 235.0292, Found: 235.0287.

2-(4-bromophenyl)pent-4-en-2-ol (**3h**): was obtained as a colorless oil in 94% isolated yield and 79% ee [determined with chiral HPLC, Daicel Chiralcel OD-

H, isopropanol:hexane = 1:99, 1.0 mL/min, λ = 254 nm, t_R (minor) = 9.877 min, t_R (major) = 10.533 min]; $[\alpha]_D^{25} = +10.2$ (c = 0.498, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.42-7.48 (m, 2H), 7.26-7.33 (m, 2H), 5.54-5.65 (m, 1H), 5.12-5.15 (m, 2H), 2.65 (dd, J = 13.6 Hz, 6.4 Hz, 1H), 2.48 (dd, J = 13.6 Hz, 8.4 Hz, 1H), 2.09 (s, 1H), 1.52 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 146.7, 133.2, 131.2, 126.8, 119.9, 73.4, 48.3, 29.9 ppm; ESI-HRMS Calcd for $(\text{C}_{11}\text{H}_{13}\text{BrO} + \text{H}^+)$ 241.0228, Found: 241.0229.

2-(3-chlorophenyl)pent-4-en-2-ol (**3i**): was obtained as a colorless oil in 77% isolated yield and 70% ee [determined with chiral HPLC, Daicel Chiralcel OJ-

H, isopropanol:hexane = 1:99, 1.0 mL/min, λ = 254 nm, t_R (minor) = 8.801 min, t_R (major) = 9.209 min]; $[\alpha]_D^{25} = +34.8$ (c = 0.428, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.48 (s, 1H), 7.20-7.30 (m, 3H), 5.55-5.65 (m, 1H), 5.13-5.17 (m, 2H), 2.66 (dd, J = 13.6 Hz, 6.4 Hz, 1H), 2.48 (dd, J = 13.6 Hz, 8.4 Hz, 1H), 2.07 (s, 1H), 1.53 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 148.8, 133.2, 132.0, 128.4, 125.7, 124.24, 122.0, 119.0, 72.4, 47.3, 28.8 ppm; ESI-HRMS Calcd for $(\text{C}_{11}\text{H}_{13}\text{ClO} + \text{K}^+)$ 235.0292, Found: 235.0285.

(*R*)-2-(naphthalen-2-yl)pent-4-en-2-ol (**3j**): was obtained as a colorless oil in 89% isolated yield and 73% ee [determined with chiral HPLC, Daicel Chiralcel OD-H, isopropanol:hexane = 1:99, 1.0 mL/min, λ = 254 nm, t_R

(minor) = 20.653 min, t_R (major) = 25.643 min]; $[\alpha]_D^{25} = +50.7$ ($c = 0.270$, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.90-7.91 (m, 1H), 7.81-7.85 (m, 3H), 7.45-7.55 (m, 3H) 5.56-5.63 (m, 1H), 5.10-5.18 (m, 2H), 2.79 (dd, $J = 13.6\text{Hz}$, 6.4 Hz, 1H), 2.57 (dd, $J = 13.6\text{Hz}$, 8.4 Hz, 1H), 2.20 (s, 1H), 1.63 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 144.0, 133.6, 132.2, 131.2, 127.1, 126.9, 126.5, 125.0, 124.7, 122.5, 122.2, 118.6, 72.8, 47.3, 28.9 ppm; ESI-HRMS Calcd for $(\text{C}_{15}\text{H}_{16}\text{O} + \text{Na}^+)$ 235.1099, Found: 235.1099.

(*R*)-1-allyl-1,2,3,4-tetrahydronaphthalen-1-ol (**3k**): was obtained as a colorless oil in 36% isolated yield and 75% ee [determined with chiral HPLC, Daicel Chiralcel OD-H, isopropanol:hexane = 1:99, 1.0 mL/min, λ = 254 nm, t_R (major) = 11.655 min, t_R (minor) = 13.431 min]; $[\alpha]_D^{25} = +23.6$ (c = 0.208, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.54-7.57 (m, 1H), 7.18-7.26 (m, 2H), 7.07-7.09 (m, 1H), 5.77 (m, 1H), 5.11-5.16 (m, 2H), 2.79 (dd, J = 15.6 Hz, 9.6Hz, 1H), 2.57 (dd, J = 16.8 Hz, 10.8Hz, 1H), 2.60-2.62 (m, 2H), 2.02 (s, 1H), 1.79-1.92 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3): δ = 141.9, 136.8, 134.0, 128.9, 127.1, 126.4, 126.3, 118.6, 72.0, 47.0, 36.1, 29.8, 19.7 ppm; ESI-HRMS Calcd for ($\text{C}_{13}\text{H}_{16}\text{O} + \text{Na}^+$) 211.1099, Found: 211.1099.

1,1,1-trifluoro-2-phenylpent-4-en-2-ol (**3l**): was obtained as a colorless oil in 70% isolated yield and 73% ee [determined with chiral HPLC, Daicel Chiralcel OD-H, isopropanol:hexane = 1:99, 1.0 mL/min, λ = 254 nm, t_R (minor) = 8.439 min, t_R (major) = 8.780 min]; $[\alpha]_D^{25} = +46.0$ (c = 0.126, CHCl_3); ^1H NMR (400 MHz, CDCl_3): δ = 7.56-7.59 (m, 2H), 7.36-7.43 (m, 3H), 5.50-5.62 (m, 1H), 5.20-5.28 (m, 2H), 2.95 (dd, J = 14.4 Hz, 6.4 Hz, 1H), 2.85 (dd, J = 14.0 Hz, 8.0 Hz, 1H), 2.61 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ = 136.6, 130.2, 128.3, 128.1, 126.5, 126.2, 123.7, 121.8, 40.1 ppm; ESI-HRMS Calcd for ($\text{C}_{11}\text{H}_{11}\text{F}_3\text{O} + \text{Na}^+$) 239.0660, Found: 239.0660.

(*S*)-3-methyl-1-phenylhex-5-en-3-ol (**3m**): was obtained as a colorless oil in

49% isolated yield and 53% ee [determined with chiral HPLC, Daicel

Chiralcel OD-H, isopropanol:hexane = 1:99, 1.0 mL/min, λ = 254 nm, t_R

(major) = 20.419 min, t_R (minor) = 24.234 min; $[\alpha]_D^{25} = +33.7$ (c = 0.190, CHCl_3); ^1H NMR (400 MHz,

CDCl_3): δ = 7.30-7.19 (m, 5H), 5.94-5.84 (m, 1H), 5.18-5.13 (m, 2H), 2.73-2.68(m, 2H), 2.30-2.29 (d,

2H), 1.80-1.76 (m, 2H), 1.50 (s, 1H), 1.25(s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ = 141.5, 132.8, 127.4,

127.3, 124.7, 117.9, 71.0, 45.5, 42.7, 29.3, 25.8 ppm.

Reference

- (1) Krzyzanowska, B.; Stec, W. J. *Synthesis* **1982**, 270 – 273.
- (2) Wen, Y. H.; Huang, X.; Huang, J. L.; Xiong, Y.; Qin, B.; Feng, X. M. *Synlett* **2005**, 2445 – 2448.
- (3) Huang, J. L. ; Liu, X. H.; Wen, Y. H.; Qin, B.; Feng, X. M. *J. Org. Chem.* **2007**, 72, 204-208.
- (4) Loh, T. P.; Teo, Y. C.; Goh, J. D. *Org. Lett.* **2005**, 7, 2743-2745.

Copy of ^1H NMR and ^{13}C NMR spectra of L1

N-25

Current Data Parameters
 NAME km-2005-256
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061013
 Time 9.18
 INSTRUM av300
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TO 65536
 SOLVENT CDCl3
 NS 180
 DS 4
 SMH 22675.736 Hz
 FIDRES 0.346004 Hz
 AQ 1.465188 sec
 RG 8192
 CM 22.050 usec
 DE 5.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.00000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 5.50 usec
 PL1 -6.00 dB
 SF01 75.477558 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 -2.00 dB
 PL12 17.70 dB
 PL13 17.71 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 65536
 SF 75.4677544 MHz
 NCH 4
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 FIP 200.500 ppm
 F1 15131.29 Hz
 F2 -0.500 ppm
 F2 -37.73 Hz
 PPM04 10.05000 ppm/cm
 HZCM 758.45089 Hz/cm

26.201
22.174
20.119
16.930

77.423
77.000
76.576
76.198
66.828
64.612

137.495
128.931
124.139
119.955

166.383

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
 Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air

Current Data Parameters
 NAME 2007-01-12 zhangxin-N55
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070112
 Time_ 17.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.135483 Hz
 AQ 3.9846387 sec
 RG 287
 DW 60.800 usec
 DE 6.00 usec
 TE 293.1 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300074 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
 Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air

Current Data Parameters
 NAME 2007-01-12 zhangxin-N35
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070113
 Time 5.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 12288
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 297.8 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.628298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127671 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 EC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

ZH089905 Customer: SICHUAN UNI CHINA
 I/D Z-GRD Z104450/0077 Sample depth: 20 Gas: air

Current Data Parameters
 NAME 2007-01-12 zhangxin-N34
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070112
 Time_ 17.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 456
 CW 60.800 usec
 DE 6.00 usec
 TE 292.6 K
 D1 1.90000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300675 MHz
 WDW DO
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
 Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air

Current Data Parameters
 NAME 2007-01-12 zhangxin-N34
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070113
 Time 8.49
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 55536
 SOLVENT CDCl3
 NS 4096
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 295.3 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127698 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air

F2 - Acquisition Parameters
Date_ 20061229
Time_ 10.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 228
DW 62.400 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SF01 400.1325009 MHz

F2 - Processing parameters
SI 32768
SF 400.1300949 MHz
WDW nc
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
 Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air

Current Data Parameters
 NAME 2006-12-29 zhangxin-M13
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061229
 Time_ 10.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 735
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 295.8 K
 DI 2.0000000 sec
 d11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.6228296 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1315005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
 Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air

Current Data Parameters
 NAME 2007-01-12 zhangxin-l1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070112
 Time 15.46
 INSTRUM spect
 PROBU 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 456
 DW 62.400 usec
 DE 6.00 usec
 TE 292.5 K
 DL 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1328009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300076 MHz
 WDW 00
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
 Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air

Current Data Parameters
 NAME 2007-01-12 zhangxin-L1
 EXNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070113
 Time_ 12:39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CUC13
 NS 2689
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.363198 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 293.5 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SF01 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 PL13 14.00 dB
 SF02 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127700 MHz
 WDW no
 SSF 0
 LB 0.00 Hz
 GB 0
 PC 1.40

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z10450/0077 Sample depth: 20 Gas: air

Current Data Parameters
 NAME 2006-12-16 zhangxin-Na
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061216
 Time 17.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 161
 DW 60.800 usec
 DE 6.00 usec
 TE 295.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 PL 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300049 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 EC 1.00

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas: air

Current Data Parameters
 NAME 2006-12-16 zhangxin-N4
 EXNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061216
 Time_ 17.56
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 297.6 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

F2 - Acquisition Parameters

Date_	20061217	Retention time
time	12.42	spec
INSTRUM	5 mm PABBO BS	
PROBD	2930	
PULPROG	65536	
TD	UDC13	
SOLVENT	NS	
NS	64	
DS	Q	
SWH	5393.862 Hz	
FTDRES	0.1937563 Hz	
AQ	5.1249652 sec	
RG	322	
DW	78.200 usec	
DE	6.00 usec	
TE	295.1 K	
DI	1.00000000 sec	
TD0	1	

```
===== CHANNEL f1 =====
NUC1      1H
PL        12.00 usec
PL1       -2.00 dB
SF01      400.1328009 MHz
```

F2 - Processing parameters	
SI	32768
SE	400.130065 MHz
WDW	EQ
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

System: AV400 OrderNo.: ZH08905 Customer: SICHUAN UNI CHINA
Probe: 5 mm PAB0 BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas: air

[illegible]

Current Data Parameters	
NAME	2006-12-17 zhangxin-N32
EXENO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20061217
time	12.51
INSTRUM	SPECT
PROBHD	5 mm PABBO HB-
PULPROG	ZQC30
TD	65536
SOLVENT	CDC13
NS	1024
DS	4
SSM	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
GC	20.800 usec
DE	6.00 usec
TE	295.7 K
D1	2.00000000 sec
dil1	0.03000000 sec
TD0	1

```

===== CHANNEL F1 =====
NUC1      13C
P1         9.60 usec
PL1        -1.00 dB
SF01      100.628300 MHz

```

```
===== CHANNEL F2 =====
CPDRG2      waltz16
NUC2        1H
PCPD2       80.00 usec
PL2         -2.00 dB
PLI2        14.00 dB
SFO2        400.131600 MHz
```

F2 - Processing parameters	
SI	32768
SF	100.612768 MHz
WDW	NO
SSB	0
LB	0.00 Hz
GB	0
FC	1.40

L6

Pulse Sequence: s2pul

12.473
7.294
7.278
7.255
7.187
7.168
3.867
3.847
3.838
3.818
3.759
3.654
3.561
3.421
3.396
3.069
3.052
3.035
2.846
2.736
2.635
1.242
1.225
1.172
-0.000

L6

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
INOVA-400 "INOVA400"

PULSE SEQUENCE
Pulse delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 7840.9 Hz
Single scan
OBSERVE H1, 399.892082 MHz
DATA PROCESSING
FT size 85536
Total time 0 min, 4 sec

14 12 10 8 6 4 2 0 -2 ppm
1.00
3.63
5.67 2.22 6.29 1.29 13.36

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA Gas: air
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth: 20

Current Data Parameters
 NAME 2006-11-18 zhangxin-801
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061118
 Time 16.37
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.5631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 295.3 K
 DL 2.0000000 sec
 CL1 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.6226300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1315000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6128729 MHz
 WDW KC
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D 2-GRD Z104450/0077

Current Data Parameters
 NAME 2008-11-18 zhangxin-803
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061119
 Time 10.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9046387 sec
 RG 256
 DW 60.800 usec
 DE 6.00 usec
 TE 295.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300092 MHz
 WDW HC
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077
 Sample depth:20 Gas: air, Operator: Deng

Current Data Parameters
 NAME 2006-11-18 zhangxin-803
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061119
 Time 12.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT GDC13
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 297.9 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SF01 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SF02 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6128721 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth: 20 Gas: air

Current Data Parameters
 NAME 2006-11-18 zhangxin-802
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061118
 Time 17.46
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 256
 DW 60.800 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300094 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth: 20 Gas: air

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077
 Sample depth: 20 Gas: air, Operator: Deng

Current Data Parameters
 NAME 2006-11-18 zhangxin-804
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061119
 Time_ 12.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 64
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 144
 DW 60.800 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDC 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300108 MHz
 WDW GO
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077
 Sample depth:20 Gas: air, Operator: Deng

Current Data Parameters
 NAME 2006-11-18 zhangxin-804
 EXPMO 2
 PROCNE 1

F2 - Acquisition Parameters
 Date_ 20061119
 Time_ 14.12
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.600 usec
 DE 6.00 usec
 TE 297.9 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.622600 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.131600 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW 0
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

-Acceptance-System:AV600 OrderNo.:ZH089805 Customer:Sichuan University
P/N Console:H03128/2528 Probe:5 mm PATXI 1H/D 2-GRD Z104450/0077 Sample depth:20 Gas:air

7.332
7.319
7.259
7.159
7.146
5.663
5.652
5.651
5.650
5.648
5.646
5.635
5.624
5.622
5.618
5.610
5.609
5.607
5.606
5.604
5.593
5.297
5.295
5.145
5.144
5.117
5.104
5.103
5.101
2.691
2.680
2.668
2.657
2.507
2.494
2.484
2.471
2.339
2.170
1.009
1.530

Current Data Parameters
NAME 812
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20061026
Time_ 15.35
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 144
LW 40.533 usec
DE 6.00 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 7.40 usec
PL1 -1.00 dB
SFO1 600.1337060 MHz

F2 - Processing parameters
SI 32768
SF 600.1300118 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

-Acceptance-System:AV600 OrderNo.:ZH089805 Customer:Sichuan University
P/N Console:H03128/2528 Probe:5 mm PATXI 1H/D Z-GRD Z10450/0077 Sample depth:20 Gas:air

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077
 Sample depth: 20 Gas: air, Operator: Deng

Current Data Parameters
 NAME 2006-11-18 zhangxin-805
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061119
 Time 14.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CUC13
 NS 64
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 256
 DW 60.800 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.50000000 sec
 TDG 1

----- CHANNEL f1 -----

NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters

SI 32768
 SF 400.1300090 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D 2-GRD Z104450/0077
 Sample depth:20 Gas: air, Operator: Deng

Current Data Parameters
 NAME 2006-11-18 zhangkin-805
 EXPNO 2
 F2PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061119
 Time_ 15.41
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWE 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 297.9 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127650 MHz
 WDW NO
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

-Acceptance-System:AV600 OrderNo.:ZH089805 Customer:Sichuan University
P/N Console:H03128/2528 Probe:5 mm PATXI 1H/D Z-GRD Z104450/0077 Sample dept

Current Data Parameters
NAME 808
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061026
Time_ 13.30
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 144
DW 40.533 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 7.40 usec
PL1 -1.00 dB
SFO1 600.1337060 MHz

F2 - Processing parameters
SI 32768
SF 600.1300098 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

-Acceptance-System:AV600 P/N Console:H03128/2528 OrderNo.:ZH089805 Customer:Sichuan University Probe:5 mm PATXI 1H/D Z-GRD Z104450/0077 Sample dept

Current Data Parameters
NAME 808
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061026
Time_ 13.59
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 2050
DW 13.867 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 -3.00 dB
SFO1 150.9178990 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 19.50 dB
PL13 19.50 dB
SFO2 600.1324000 MHz

F2 - Processing parameters
SI 32768
SF 150.9028090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 nmm

System: AV400 OrderNo.: 2H089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-LH/D Z-GRD Z104450/0077 Sample depth: 20 Gas: air

Current Data Parameters
 NAME 2006-12-16 zhongxin-899
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061216
 Time 16.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 161
 DW 60.800 usec
 DE 6.00 usec
 TE 295.8 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300103 MHz
 XQ 0
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

0.072
 -0.000

Current Data Parameters	
NAME	2006-12-16 zhengxin-809
EXPNO	2
PROCNO	1

E2 - Acquisition Parameters

	time	20061218
	16.33	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPRPG	95C30	
g5536	25536	
ID	DOLCI	
SOLVENT	DCL13	
NS	1024	
DS	0	
SWH	24038.461 Hz	
FIDRES	0.365798 Hz	
AQ	1.3651988 sec	
RG	2050	
CW	20.800 us/c	
DE	6.00 us/c	
TE	296.7 K	
DI	2.00000000 sec	
Hill	0.03600000 sec	
TDO	1	

```
===== CHANNEL f1 =====
NUC1      13C
pl        9.60 usec
PL1       -1.00 dB
SFO1      100.6229300 MHz
```

```
===== CHANNEL f2 =====
CPDRG2      waltz16
NUC2        1H
ECPD2       80.00 usec
PL2         -2.00 dB
PL12        14.00 dB
SFO2        400.131600 MHz
```

F2 - Processing parameters	
SI	32768
SF	100.6127690 MHz
NDW	NC
SSB	0
LB	0.00 HZ
GB	0
EC	1.40

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth: 20 Gas: air

Current Data Parameters
 NAME 2006-12-16 zhangxin-807
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061216
 Time_ 15.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 161
 DM 60.800 usec
 DE 6.00 usec
 TE 295.7 K
 D1 1.00000000 sec
 T00 1

===== CHANNEL F1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1306098 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

0.000
0.073

2.680
2.664
2.646
2.630
2.508
2.487
2.474
2.453
2.071
1.528

7.293
7.292
7.287
7.286
7.269
7.259
7.246
7.227
7.222
7.218
7.208
7.204
7.199
5.633
5.636
5.638
5.632
5.616
5.613
5.608
5.592
5.585
5.586
5.569
5.564
5.548
5.165
5.160
5.130

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA Gas: air
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth: 20

Current Data Parameters
 NAME 2006-12-16 zhangxin-807
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061216
 Time 15.36
 INSTRUM spect
 FROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 808
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.365798 Hz
 AQ 1.5631988 sec
 RG 2050
 DM 20.800 usec
 DE 6.00 usec
 TE 296.8 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.628300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.618735 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D 2-GRD Z104450/0077
 Sample depth: 20 Gas: air, Operator: Deng

Current Data Parameters
 NAME 2006-11-18 zhangxin-806
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061119
 Time_ 15:55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 64
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 181
 DW 60.800 usec
 DE 6.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300149 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077
 Sample depth: 20 Gas: air, Operator: Deng

Current Data Parameters
 NAME 2006-11-18 zhangxin-806
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061119
 Time 17.07
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366793 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 297.9 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.628300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 ECPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1316000 MHz

F2 - Processing Parameters
 SI 32768
 SF 100.618740 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077
 Sample depth: 20 Gas: air, Operator: Deng

Current Data Parameters
 NAME 2006-11-21 zhangxin-913
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20061121
 Time 15.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 181
 DW 60.800 usec
 DE 6.00 usec
 TE 298.0 K
 O1 1.00000000 sec
 TDO 1
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL -2.00 dB
 SFO1 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300114 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077
 Sample depth: 20 mm Gas flow: 1.0 L/min, Operator: Deng

Current Data Parameters
 NAME 2006-11-21 zhangxin-813
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061121
 Time 15:09
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 551
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====

NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters

SI 32768
 SF 100.6127690 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

47.05
 36.14
 29.76
 19.73

77.85
 77.03
 76.71
 71.97

141.8
 136.81
 134.0
 128.9
 127.1
 126.3
 126.2
 126.0
 118.0

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077
 Sample depth: 20 Gas: air, Operator: Deng

System: AV400 OrderNo.: ZH089905 Customer: SICHUAN UNI CHINA
 Probe: 5 mm PABBO BB-1H/D Z-GRD Z104450/0077
 Sample depth:20 Gas: air, Operator: Deng

Current Data Parameters
 NAME 2006-11-21 zhangxin-815
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061121
 Time_ 16.36
 INSTRUM Spect
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.00 usec
 TE 297.9 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SFO1 100.6228300 MHz

===== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SFO2 400.1316000 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6121907 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GE 0
 PC 1.40

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
 Probe:5 mm PABBO BB-1H/D 2-GRD Z104450/0077 Sample depth:20 Gas:air

Current Data Parameters
 NAME 2007-3-14 13:37:17-821
 EXPNO 1
 PROCNO 1

22 - Acquisition Parameters

Date_ 20070314
 Time_ 11:30
 INSTRUM spect
 PROBE1 5 mm PABBO BB-
 PULPROG zg30
 TO 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DB 6.00 usec
 TS 298.0 K
 D1 1.00000000 sec
 TD 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1328009 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300125 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

7.300
7.281
7.262
7.253
7.205
7.186
5.940
5.921
5.915
5.897
5.878
5.859
5.854
5.835
5.181
5.176
5.173
5.157
5.130
2.726
2.711
2.697
2.682
2.308
2.289
1.798
1.781
1.771
1.755
1.618
1.490
1.254
0.072
0.001

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
 Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air

Current Data Parameters
 NAME 2007-3-14 zhangxin-8.
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070314
 Time_ 17.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 15000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DM 20.800 usec
 DE 6.00 usec
 TE 295.9 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 CDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.60 usec
 PL1 -1.00 dB
 SF01 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 SF02 400.1315005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6128712 MHz
 WDW 0
 SSB 0
 LB 0
 GB 0
 PC 1.40

160 140 120 100 80 60 40 20 0 ppm

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
 Probe:5 mm PABBO BB-1H/D 2-GRD Z104450/0077 Sample depth:20 Gas:air

Current Data Parameters
 NAME 2007-4-28 Zhangxin-azhx
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070428
 Time 16.29
 INSTRUM spect
 PROBE 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9546387 sec
 RG 144
 DW 60.900 usec
 DE 6.00 usec
 TE 296.4 K
 D1 1.00000000 sec
 TDD 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1299996 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

(A) Part of the ^1H NMR of **L1** in CDCl_3 ;

(B) Part of the ^1H NMR of In(III)-L1 complex in d_6 -DMSO.

As we known, in one molecule **L1**, there are two NH and ten Ar-H atoms (A). When **L1** and InBr_3 (1:2) were mixed, there might be show four NH and twenty Ar-H atoms in ^1H NMR spectra, but the ^1H NMR data of In(III)-L1 complex in d_6 -DMSO indicates only one NH group and twenty Ar-H atoms (B). So we speculate that three H atoms combine three Br from InBr_3 to form three molecules HBr.