Enantioselective Strecker Reaction of Phosphinoyl Ketoimines Catalyzed by *in situ* Prepared Chiral *N,N'*- Dioxides

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SUPPORTING INFORMATION

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1 General

^1H NMR spectra were recorded on a 400 MHz, 300 MHz or 600 MHz spectrometer. Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (CDCl_3 , $\delta = 7.26$). Data 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 data were collected on a 100 MHz or 75 MHz spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from the tetramethylsilane with the solvent resonance as internal standard (CDCl_3 , $\delta = 77.0$). ^{29}Si NMR spectra were recorded on 60 MHz spectrometer. The enantiomeric excesses were determined by HPLC analysis on chiral DAICEL CHIRALCEL OJ, OJ-H, OD, OD-H or CHIRALPAK AD-H, AS-H column at 210 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, chlorodiphenylphosphine and amines were commercially purchased.

2 General procedure for the preparation of *N*-diphenylphosphinoyl ketoimine¹

General procedure for the preparation of oxime: To a stirred solution of $\text{NH}_2\text{OH}\cdot\text{HCl}$ (30 mmol) and NaOAc (30 mmol) in $\text{EtOH} / \text{H}_2\text{O}$ (1/1, 16 mL), ketone (20 mmol) was added and then heated to reflux. The reaction was monitored by TLC. When it was completed, the mixture was cooled down to ambient temperature and allowed to lay icebox for 24 h at $-20\text{ }^\circ\text{C}$. Then the mixture was filtered and washed by water (5×20 mL). The product was dried under infrared lamp and used direct next process.

General procedure for the preparation of ketoimine: To a stirred solution of an oxime (5 mmol) and triethylamine (5 mmol) in petroleum ether / CH_2Cl_2 (1/1, 15 mL), a solution of chlorodiphenylphosphine (5 mol) in CH_2Cl_2 (5 mL) was added from a dropping funnel over 30 min at -45 to $-40\text{ }^\circ\text{C}$. After the reaction was finished, the cooling bath was removed and the reaction temperature was gradually increased. The mixture was then allowed to stir for 1 h at ambient temperature before evaporating the solvent. The residue was dissolved in CH_2Cl_2 , washed by 1M KHSO_4 , sat. NaHCO_3 , brine, dried over MgSO_4 and concentrated. The residue was purified by silica gel flash column chromatography using AcOEt /petroleum ether (1/1) as eluent to obtain almost pure ketoimines. The product was further purified by recrystallization from CH_2Cl_2 /hexane.

(1) Krzyzanowska, B.; Stec, W. J. *Synthesis* **1982**, 270 - 273.

3 Typical procedure for catalyst preparation²

To a solution of (*S*)-1-*N*-Boc-piperidine-2-carboxylic acid (917 mg, 4 mmol) in CH₂Cl₂ (40 mL) was added Et₃N (0.62 mL, 4.4 mmol), isobutyl carbonochloridate (576 mg, 4.4 mmol) at 0 °C under stirring. After 15 min, amine (666 mg, 4.4 mmol) was added. The reaction was allowed to warm to ambient temperature and detected by TLC. The mixture was washed with 1 M KHSO₄, saturated NaHCO₃, brine, dried over anhydrous MgSO₄ and concentrated. To the residue in CH₂Cl₂ (4 mL) was added TFA (4 mL) and stirred until the reaction was finished. Then, the solvent was evaporated, and H₂O (10 mL) was added. The pH value of the mixture was brought into the range of 8-10 by the addition of 1M NaOH. The aqueous phase was extracted with CH₂Cl₂ (5×20 mL). The combined organic phase was washed with brine, dried over anhydrous MgSO₄ and evaporated in vacuo. The residue was directly used for next step. To a solution of (*S*)-1-*N*-Boc-piperidine-2-carbonamide in CH₃CN (4 mL) was added K₂CO₃ (608 mg, 4.4 mmol) and 1, 3-dibromopropane (204 uL, 2 mmol) under stirring. It was kept at 80 °C, and monitored by TLC. Then, K₂CO₃ was removed by filtration. The residue was concentrated and purified by silica gel column chromatography (EtOAc) to give a white product **3f** (1.060 g, 94% yield).

To a solution of **3f** (564 mg, 1 mmol) in CH₂Cl₂ (20 mL) was added *m*-CPBA (383 mg, 2.2 mmol) at 0 °C under stirring. After the reaction was completed, the mixture was concentrated and purified by the basic aluminum oxide column chromatography (EtOAc / MeOH = 3:1) to give a white powder **9** (548 mg, 92% yield).

catalyst **1**: white solid; $[\alpha]_D^{25} = -31.80$ ($c = 0.50$ in CHCl₃); ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): $\delta = 10.59$ (d, $J = 6.8$ Hz, 2H; NH), 3.77 (m, 2H), 3.62 (m, 2H), 3.32-3.60 (m, 8H), 2.39-2.64 (m, 8H), 1.57-2.03 (m, 12H), 1.27-1.35 ppm (m, 10H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): $\delta = 166.3, 76.5, 67.6, 64.7, 47.3, 32.7, 32.3, 27.4, 25.3, 24.4, 19.7$ ppm; EI-HRMS Calcd for C₂₅H₄₄N₄O₄ (M⁺): 464.3363, Found: 464.3428.

(2) Wen, Y. H.; Huang, X.; Huang, J. L.; Xiong, Y.; Qin, B.; Feng, X. M. *Synlett* **2005**, 2445 – 2448.

catalyst **2**: white powder; m.p. 110-112 °C; $[\alpha]_D^{25} = -114.80$ ($c = 0.23$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 7.21$ (d, $J = 8.8$ Hz, 2H, NH), 3.67-3.74 (m, 2H), 3.14 (t, $J = 6.8$ Hz, 2H), 2.92-2.96 (m, 2H), 2.50 (t, $J = 7.2$ Hz, 4H), 2.23-2.29 (m, 2H), 2.08-2.18 (m, 4H), 1.57-1.84 (m, 16H), 1.31-1.40 (m, 4H), 1.07-1.21 ppm (m, 6H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.6, 67.7, 54.1, 53.8, 47.0, 33.0, 30.5, 28.4, 25.4, 24.6, 24.1$ ppm; EI-HRMS Calcd for $\text{C}_{25}\text{H}_{44}\text{N}_4\text{O}_2$ (M^+): 432.3464, Found: 432.3955.

catalyst **3a**: white powder; m.p. 168-170 °C; $[\alpha]_D^{25} = -133.20$ ($c = 0.50$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 6.49$ (d, $J = 8.4$ Hz, 2H, NH), 3.73-3.78 (m, 2H), 3.04-3.07 (m, 2H), 2.60-2.62 (m, 2H), 2.41-2.47 (m, 2H), 2.12-2.18 (m, 2H), 1.85-1.97 (m, 8H), 1.60-1.72 (m, 12H), 1.35-1.50 (m, 8H), 1.11-1.25 ppm (m, 8H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.5, 68.3, 54.6, 51.4, 47.1, 33.1, 30.8, 25.4, 25.0, 24.8, 24.5, 23.4$ ppm; EI-HRMS Calcd for $\text{C}_{27}\text{H}_{48}\text{N}_4\text{O}_2$ (M^+): 460.3777, Found: 460.4456.

catalyst **3b**: 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, NH), 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.

catalyst **3c**: white powder; m.p. 130-132 °C; $[\alpha]_D^{25} = -140.4$ ($c = 0.50$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 6.53$ (s, 2H, NH), 4.18 (m, 2H), 3.04 (m, 2H), 2.61 (m, 2H), 2.40 (m, 2H), 2.16-2.20 (m, 4H), 1.94 (m, 8H), 1.67 (m, 10H), 1.24-1.36 ppm (m, 12H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.8, 68.1, 54.6, 51.3, 50.1, 32.8, 30.5, 24.7, 23.6, 23.5, 23.3$ ppm; EI-HRMS Calcd for $\text{C}_{25}\text{H}_{44}\text{N}_4\text{O}_2$ (M^+): 432.3464, Found: 432.4338.

catalyst **3d**: white powder; m.p. 108-110 °C; $[\alpha]_D^{25} = -161.00$ ($c = 0.50$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 6.42$ (d, $J = 8.0$ Hz, 2H, NH), 4.05 (m, 2H), 3.05 (d, $J = 10.4$ Hz, 2H), 2.61 (d, $J = 10.4$ Hz, 2H), 2.41-2.43 (m, 2H), 2.17-2.18 (m, 4H), 1.94 (d, $J = 11.2$ Hz, 4H), 1.68 (m, 6H), 1.34-1.47 (m, 4H), 1.22-1.28 (m, 2H), 1.13-1.46 ppm (m, 10H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.5$, 68.2, 54.7, 51.4, 40.4, 30.6, 24.9, 24.6, 23.4, 22.7 ppm; EI-HRMS Calcd for $\text{C}_{21}\text{H}_{40}\text{N}_4\text{O}_2$ (M^+): 380.3151, Found: 380.3652.

catalyst **3e**: white oil ; $[\alpha]_D^{25} = -137.80$ ($c = 0.50$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 6.52$ (s, 2H), 3.05 (d, $J = 10.8$ Hz, 2H), 2.42-2.53 (m, 4H), 2.16-2.22 (m, 2H), 1.93-1.99 (m, 4H), 1.64-1.71 (m, 6H), 1.19-1.51 ppm (m, 24H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.6$, 68.8, 54.5, 51.2, 50.0, 30.4, 28.5, 24.7, 24.3, 23.2 ppm; EI-HRMS Calcd for $\text{C}_{23}\text{H}_{44}\text{N}_4\text{O}_2$ (M^+): 408.3464, Found: 408.4117.

catalyst **3f**: white powder; m.p. 74-76 °C, $[\alpha]_D^{25} = -103.60$ ($c = 0.50$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 6.38$ (s, 2H), 3.05 (d, $J = 11.2$ Hz, 2H), 2.46-2.52 (m, 4H), 2.16-2.22 (m, 2H), 2.07-2.10 (m, 8H), 1.92-1.98 (m, 14H), 1.65-1.68 (m, 18H), 1.34-1.45 (m, 4H), 1.22-1.28 ppm (m, 2H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.7$, 69.2, 54.7, 51.4, 50.9, 41.6, 36.2, 30.8, 29.3, 25.0, 24.5, 23.5 ppm; EI-HRMS Calcd for $\text{C}_{35}\text{H}_{56}\text{N}_4\text{O}_2$ (M^+): 564.4403, Found: 564.5426.

catalyst **3g**: white powder; m.p. 122-124 °C; $[\alpha]_D^{25} = -138.20$ ($c = 0.50$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 7.22$ -7.32 (m, 10H), 6.81 (d, $J = 8.8$ Hz, 2H, NH), 5.08-5.16 (m, 2H), 2.79 (d, $J = 11.2$ Hz, 2H), 2.53-2.56 (m, 2H), 2.18 (m, 4H), 1.94-2.07 (m, 4H), 1.58-1.76 (m, 6H), 1.19-1.48 ppm (m, 12H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.5$, 148.2, 128.7, 127.4, 126.1, 68.1, 54.5, 51.5, 47.7, 30.5, 25.8, 24.8, 23.4, 21.3 ppm; EI-HRMS Calcd for $\text{C}_{31}\text{H}_{44}\text{N}_4\text{O}_2$ (M^+): 504.3464, Found: 504.4309.

catalyst **3h**: white powder; m.p. 64-66 °C; $[\alpha]_D^{25} = -95.6$ ($c = 0.50$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 7.19$ (s, 2H), 4.50-4.54 (m, 2H), 3.71-3.72 (d, 6H), 3.16 (m, 2H), 2.65-2.68 (m, 2H), 2.532 (m, 2H), 2.11-2.18 (m, 6H), 1.95 (m, 4H), 1.80-1.82 (m, 2H), 1.69 (m, 4H), 1.45-1.47 (m, 4H), 1.25 (m, 2H), 0.89-0.95 ppm (m, 10H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 174.8, 172.2, 68.5, 56.0, 54.8, 52.0, 51.4, 31.2, 25.2, 25.0, 23.5, 19.1, 17.6$ ppm; EI-HRMS Calcd for $\text{C}_{27}\text{H}_{48}\text{N}_4\text{O}_6$ (M^+): 524.3574, Found: 524.4366.

catalyst **4**: white powder; m.p. 70-72 °C; $[\alpha]_D^{25} = -103.2$ ($c = 0.50$ in CHCl_3); ^1H NMR (300 MHz, CDCl_3 , 25 °C, TMS): $\delta = 7.01$ (s, 2H, NH), 3.06-3.10 (t, 2H), 2.74-2.79 (m, 2H), 2.44-2.49 (t, 4H), 2.16-2.23 (m, 2H), 1.99-2.11 (m, 8), 1.89 (m, 12H), 1.64-1.75 (m, 6H), 1.60 ppm (s, 14H); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.6, 68.4, 53.9, 53.5, 50.5, 41.5, 36.1, 30.4, 29.2, 28.2, 23.9$ ppm; EI-HRMS Calcd for $\text{C}_{33}\text{H}_{52}\text{N}_4\text{O}_2$ (M^+): 536.4090, Found: 536.4157.

catalyst **5**: white powder; m.p. 133-135 °C; $[\alpha]_D^{25} = -94.2$ ($c = 0.50$ in CHCl_3); ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): $\delta = 6.94$ (s, 2H, NH), 2.95-3.01 (m, 4H), 2.36-2.59 (m, 8H), 1.97-2.07 (m, 18H), 1.60-1.68 (m, 22H), 1.32-1.45 (m, 6H) ppm; ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.2, 71.4, 70.7, 54.3, 50.4, 42.0, 41.6, 38.1, 36.2, 35.0, 32.3, 29.2, 27.8, 24.2$ ppm; EI-HRMS Calcd for $\text{C}_{39}\text{H}_{60}\text{N}_4\text{O}_2$ (M^+): 616.4716, Found: 616.5887.

catalyst **6a**: white powder; m.p. 88-90 °C; $[\alpha]_D^{25} = -88.2$ ($c = 0.50$ in CHCl_3); ^1H NMR (300 MHz, CDCl_3 , 25 °C, TMS): $\delta = 6.43$ (s, 2H, NH), 3.00-3.04 (m, 2H), 2.72-2.76 (m, 2H), 2.53-2.56 (m, 2H), 2.21-2.22 (m, 2H), 2.01-2.04 (m, 8H), 1.97 (s, 12H), 1.86-1.91 (m, 2H), 1.65 (s, 16H), 1.37-1.45 (m, 4H), 1.20-1.31 ppm (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.2, 68.6, 53.6, 51.7, 50.9, 41.5, 36.3, 29.7, 29.3, 24.5, 23.3$ ppm; EI-HRMS Calcd for $\text{C}_{34}\text{H}_{54}\text{N}_4\text{O}_2$ (M^+): 550.4247, Found: 550.4318.

catalyst **6b**: white powder; m.p. 60-62 °C; $[\alpha]_D^{25} = -93.2$ ($c = 0.50$ in CHCl_3); ^1H NMR (300 MHz, CDCl_3 , 25 °C, TMS): $\delta = 6.42$ (s, 2H, NH), 2.99-3.03 (d, 2H), 2.42-2.56 (m, 4H), 2.31 (s, 1H), 2.00-2.15 (m, 9H), 1.84-2.00 (m, 16H), 1.65 (s, 20H), 1.33-1.50 (m, 6H), 1.17- 1.28 ppm (m, 6H); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.8$, 69.1, 56.6, 51.3, 50.8, 41.6, 36.3, 30.7, 29.3, 27.4, 25.3, 25.0, 23.5 ppm; EI-HRMS Calcd for $\text{C}_{37}\text{H}_{60}\text{N}_4\text{O}_2$ (M^+): 592.4716, Found: 592.4796.

catalyst **9**: white powder; m.p. 88-90 °C, $[\alpha]_D^{25} = -88.20$ ($c = 0.50$ in CHCl_3); ^1H NMR (300 MHz, CDCl_3 , 25 °C, TMS): $\delta = 9.90$ (s, 2H, NH), 3.20-3.40 (m, 10H), 2.78-2.86 (m, 2H), 2.31-2.40 (m, 2H), 2.18-2.16 (m, 4H), 1.83-1.96 (m, 22H), 1.70-1.74 (m, 2H), 1.50-1.64 (m, 10H), 1.26-1.35 ppm (m, 2H); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, TMS): $\delta = 167.1$, 76.2, 66.3, 64.5, 51.2, 41.3, 36.1, 29.2, 26.1, 22.1, 20.0, 16.6 ppm; EI-HRMS Calcd for $\text{C}_{35}\text{H}_{56}\text{N}_4\text{O}_4$ (M^+) 596.4302, Found: 596.4370.

catalyst **10**: white powder; m.p. 70-72 °C, $[\alpha]_D^{25} = -53.80$ ($c = 0.50$ in CHCl_3); ^1H NMR (300 MHz, CDCl_3 , 25 °C, TMS): $\delta = 10.11$ (s, 1H, NH), 6.21 (s, 1H, NH), 3.30-3.41 (m, 1H), 3.16-3.28 (m, 4H), 2.99-3.02 (m, 2H), 2.31-2.53 (m, 5H), 2.03-2.19 (m, 1H), 1.88-1.98 (m, 23H), 1.75-1.80 (m, 1H), 1.61-1.71 (m, 10H), 1.22-1.45 (m, 6H), 1.08-1.13 ppm (m, 1H); ^{13}C NMR (75 MHz, CDCl_3 , 25 °C, TMS): $\delta = 173.2$, 167.2, 74.4, 69.2, 68.2, 64.6, 53.7, 51.3, 51.2, 51.1, 41.6, 41.5, 36.3, 36.2, 30.6, 29.3, 26.1, 24.5, 23.3, 22.2, 21.0, 20.2, 14.8 ppm. EI-HRMS Calcd for $\text{C}_{35}\text{H}_{56}\text{N}_4\text{O}_3$ (M^+) 580.4352, Found: 580.4363.

4 Typical procedure for the preparation of racemate

To a stirred solution of ketimine (0.2 mmol) in DMF (1 mL) was added TMSCN (54.6 μL , 0.4 mmol) and K_2CO_3 (0.2 mmol) at ambient temperature. After the reaction was completed, water (8 mL) was added. The aqueous

phase was extracted with CH₂Cl₂ (5×10 mL). The combined organic phase was washed with brine, dried over anhydrous MgSO₄ and evaporated in vacuo. The residue was purified by silica gel column chromatography (EtOAc/petroleum ether = 1:1) to give a white powder.

5 Confirmation of the absolute configurations

The configuration of **8a** (*R*) was compared with literature data.³ In order to determine the absolute configurations of the other products, the CD (Circular Dichroism) spectra of **8** were measured in ethanol. The other compounds exhibited a similar (+) Cotton effect in their CD spectra. It can be deduced that these compounds possess the same (*R*) configuration as **8a**.

6 The results of asymmetric Strecker reaction

(*R*)-N-(1-cyano-1-phenylethyl)-N,N-diphenylphosphinamide (8a): Reaction time: 196 h, White powder; m.p. 122-124 °C; [α]_D²⁵ = +14.02 (c = 0.214 in CHCl₃); ¹H NMR (400 Hz, CDCl₃, 25 °C, TMS): δ = 8.01-8.07 (m, 2H), 7.81-7.86 (m, 2H), 7.73-7.76 (m, 2H), 7.33-7.60 (m, 9H), 3.68 (d, *J* = 7.6 Hz, 1H, NH), 2.29 ppm (s, 3H); HPLC (DAICEL CHIRALCEL OD, hexane/2-propanol 95/5, 0.6 mL/min), *t*_R (minor) = 40.63 min, *t*_R (major) = 45.66 min, 91% yield, 90% ee. [lit.³ [α]_D²³ = -19.1 (c = 1.00 in CHCl₃) (>99% ee)].

(*R*)-N-(1-cyano-1-(4-fluorophenyl)ethyl)-N,N-diphenylphosphinamide (8b): Reaction time: 144 h, white powder; m.p. 116-118 °C; [α]_D²⁵ = +2.00 (c = 0.150 in CH₂Cl₂); ¹H NMR (300 Hz, CDCl₃, 25 °C, TMS): δ = 7.96-8.03 (m, 2H), 7.78-7.82 (m, 2H), 7.68-7.76 (m, 2H), 7.51-7.55 (m, 4H), 7.40-7.48 (m, 2H), 7.01-7.07 (m, 2H), 3.76 (d, *J* = 7.80 Hz, 1H, NH), 1.92 ppm (s, 3H); ¹³C NMR (75 Hz, CDCl₃, 25 °C, TMS): δ = 164.4, 161.2, 136.7, 132.3 (t, *J* = 8.0 Hz), 131.3 (d, *J* = 9.5 Hz), 128.8 (t, *J* = 13.1 Hz), 127.6 (d, *J* = 8.4 Hz), 121.3 (d, *J* = 3.4 Hz), 115.9 (d, *J* = 21.8 Hz), 56.4, 29.7 ppm; EI-HRMS Calcd for C₂₁H₁₈FN₂OP (M⁺): 364.1141, Found: 364.0658; HPLC (DAICEL CHIRALCEL OD-H, hexane/2-propanol 95/5, 1.0 mL/min), *t*_R (minor) = 25.22 min, *t*_R (major) = 28.64 min, 95% yield, 90% ee.

(3) Masumoto, S.; Usuda, H.; Suzuki, M.; Kanai, M.; Shibasaki, M. *J. Am. Chem. Soc.*, **2003**, *125*, 5634 - 5635.

(R)-N-(1-(4-chlorophenyl)-1-cyanoethyl)-N,N-diphenylphosphinamide (8c):

Reaction time: 68 h, white powder; m.p. 103-105 °C; $[\alpha]_D^{25} = +8.05$ ($c = 0.174$ in CH_2Cl_2); ^1H NMR (600 Hz, CDCl_3 , 25 °C, TMS): $\delta = 8.00$ -8.03 (m, 2H), 7.79-7.82 (m, 2H), 7.69 (d, $J = 8.58$ Hz, 2H), 7.58-7.61 (m, 1H), 7.51-7.56 (m, 3H), 7.43-7.46 (m, 2H), 7.35 (d, $J = 8.58$ Hz, 2H), 3.67 (d, $J = 7.86$ Hz, 1H, NH), 1.93 ppm (s, 3H); HPLC (DAICEL CHIRALCEL OJ, hexane/2-propanol 95/5, 1.0 mL/min), t_R (minor) = 10.93 min, t_R (major) = 15.83 min, 98% yield, 89% ee.

(R)-N-(1-(4-bromophenyl)-1-cyanoethyl)-N,N-diphenylphosphinamide (8d):

Reaction time: 196 h, White powder; m.p. 113-116 °C; $[\alpha]_D^{25} = +10.23$ ($c = 0.088$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.92$ -7.98 (m, 2H), 7.72-7.79 (m, 2H), 7.36-7.59 (m, 10H), 4.00 (d, $J = 7.64$ Hz, 1H, NH), 1.89 ppm (s, 3H); ^{13}C NMR (75 Hz, CDCl_3 , 25 °C, TMS): $\delta = 140.0$, 132.3, 132.1, 131.7, 131.3 (d, $J = 10.2$ Hz), 128.7 (t, $J = 13.4$ Hz), 127.3, 123.0, 120.9 (d, $J = 4.1$ Hz), 55.4, 29.7 ppm (d, $J = 3.8$ Hz); EI-HRMS Calcd for $\text{C}_{21}\text{H}_{18}\text{BrN}_2\text{OP}$ (M^+): 424.0340, Found: 424.0248; HPLC (DAICEL CHIRALCEL OD-H, hexane/2-propanol 95/5, 1.0 mL/min), t_R (minor) = 24.43 min, t_R (major) = 28.04 min, 92% yield, 91% ee.

(R)-N-(1-cyano-1-(4-methoxyphenyl)ethyl)-N,N-diphenylphosphinamide (8e):

Reaction time: 144 h, white powder; m.p. 122-124 °C; $[\alpha]_D^{25} = +5.00$ (c = 0.56 in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.99$ -8.05 (m, 2H), 7.99-7.86 (m, 2H), 7.71 (m, $J = 8.79$ Hz, 2H), 7.41-7.57 (m, 6H), 6.88 (d, $J = 8.78$ Hz, 2H), 3.80 (s, 3H), 3.62 (d, $J = 7.87$ Hz, 1H), 1.93 ppm (s, 3H); ^{13}C NMR (75 Hz, CDCl_3 , 25 °C, TMS): $\delta = 160.0$, 133.1, 133.0, 132.1-132.3 (m), 131.3 (d, $J = 9.7$ Hz), 128.7 (t, $J = 13.5$ Hz), 126.8, 121.5 (d, $J = 4.1$ Hz), 114.2, 56.3, 55.4, 29.6 ppm (d, $J = 3.5$ Hz); EI-HRMS Calcd for $\text{C}_{22}\text{H}_{21}\text{N}_2\text{O}_2\text{P}$ (M^+): 376.1341, Found: 376.1139; HPLC (DAICEL CHIRALCEL OJ-H, hexane/2-propanol 90/10, 1.0 mL/min), t_R (minor) = 14.73 min, t_R (major) = 26.23 min, 93% yield, 89% ee.

(R)-N-(1-cyano-1-p-tolyethyl)-N,N-diphenylphosphinamide (8f): Reaction time:

196 h, white powder; m.p. 112-114 °C; $[\alpha]_D^{25} = +6.50$ (c = 0.400 in CH_2Cl_2); ^1H NMR (600 Hz, CDCl_3 , 25 °C, TMS): $\delta = 8.03$ -8.06 (m, 2H), 7.82-7.85 (m, 2H), 7.63 (d, $J = 8.22$ Hz, 2H), 7.49-7.59 (m, 4H), 7.42-7.45 (m, 2H), 7.21 (d, $J = 8.22$ Hz, 2H), 3.62 (d, $J = 7.98$ Hz, 1H, NH), 2.36 (s, 3H), 1.93 ppm (s, 3H); HPLC (DAICEL CHIRALCEL OD, hexane/2-propanol 95/5, 0.4 mL/min), t_R (minor) = 62.41 min, t_R (major) = 67.69 min, 97% yield, 92% ee.

(R)-N-(1-(3-chlorophenyl)-1-cyanoethyl)-N,N-diphenylphosphinamide (8g):

Reaction time: 72 h, white powder; m.p. 119-121 °C, $[\alpha]_D^{25} = +4.44$ ($c = 0.180$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.91$ -7.98 (m, 2H), 7.74-7.81 (m, 2H), 7.61-7.65 (m, 2H), δ 7.48-7.56 (m, 4H), 7.38-7.43 (m, 2H), 7.29-7.31 (m, 2H), 4.02 (d, $J = 7.4$ Hz, 1H, NH), 1.91 ppm (s, 3H); ^{13}C NMR (75 Hz, CDCl_3 , 25 °C, TMS): $\delta = 142.9$, 134.9, 132.1-132.4 (m), 131.4 (d, $J = 9.8$ Hz), 130.3, 129.1, 128.7 (t, $J = 12.0$ Hz), 125.8, 123.8, 120.9 (d, $J = 3.8$ Hz), 56.3, 29.7 ppm; EI-HRMS Calcd for $\text{C}_{21}\text{H}_{18}\text{ClN}_2\text{OP}$ (M^+): 380.0845, Found: 380.0833; HPLC (DAICEL CHIRALPAK AS-H, hexane/2-propanol 85/15, 1.0 mL/min), t_R (major) = 21.63 min, t_R (minor) = 27.33 min, 95% yield, 88% ee.

(R)-N-(1-cyano-1-(3-nitrophenyl)ethyl)-N,N-diphenylphosphinamide (8h):

Reaction time: 60 h, white powder; m.p. 110-112 °C; $[\alpha]_D^{25} = +8.89$ ($c = 0.540$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 8.47$ (s, 1H), 8.16 (d, $J = 7.98$ Hz, 2H), 7.90-7.94 (m, 2H), 7.77-7.81 (m, 2H), 7.44-7.61 (m, 7H), 3.76 (d, $J = 6.83$ Hz, 1H), 2.01 ppm (s, 3H); ^{13}C NMR (75 Hz, CDCl_3 , 25 °C, TMS): $\delta = 148.2$, 142.4, 132.1, 132.4 (m), 131.4 (d, $J = 8.5$ Hz), 130.0, 128.7 (d, $J = 8.9$ Hz), 123.7, 121.0, 120.5, 55.9, 30.3 ppm; EI-HRMS Calcd for $\text{C}_{21}\text{H}_{18}\text{N}_3\text{O}_3\text{P}$ (M^+): 391.1086, Found: 391.1023; HPLC (DAICEL CHIRALPAK AS-H, hexane/2-propanol 90/10, 1.0 mL/min), t_R (major) = 65.08 min, t_R (minor) = 89.97 min, 94% yield, 88% ee.

***N*-(1-cyano-1-(2-fluorophenyl)ethyl)-*N,N*-diphenylphosphinamide (8i):** Reaction time:

144 h, white powder; m.p. 110-112 °C; $[\alpha]_D^{25} = +19.60$ ($c = 0.712$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.76$ -7.90 (m, 4H), 7.37-7.60 (m, 7H), 7.26-7.32 (m, 1H), 7.00-7.11 (m, 2H), 4.01 (d, $J = 7.12$ Hz, 1H, NH), 2.08 ppm (s, 3H); ^{13}C NMR (75 Hz, CDCl_3 , 25 °C, TMS): $\delta = 161.7$, 158.4, 132.2 (d, $J = 1.8$ Hz), 132.0 (d, $J = 10.0$ Hz), 131.6

(d, $J = 9.8$ Hz), 131.1 (d, $J = 8.8$ Hz), 128.6 (d, $J = 13.0$ Hz), 127.5, 124.5 (d, $J = 3.08$ Hz), 120.3 (d, $J = 3.90$ Hz), 116.8 (d, $J = 21.7$ Hz), 53.1, 27.4 ppm; EI-HRMS Calcd for $\text{C}_{21}\text{H}_{18}\text{FN}_2\text{OP}$ (M^+): 364.1141, Found: 364.1033; HPLC (DAICEL CHIRALPAK AS-H, hexane/2-propanol 90/10, 1.0 mL/min), t_R (major) = 41.10 min, t_R (minor) = 50.51 min, 98% yield, 81% ee.

***N*-(1-cyano-1-(naphthalen-2-yl)ethyl)-*N,N*-diphenylphosphinamide (8j):** Reaction

time: 168 h, white powder; m.p. = 108-110 °C; $[\alpha]_D^{25} = +4.55$ ($c = 0.088$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 8.12$ (s, 1H), 8.00-8.07 (m, 2H), 7.78-7.88 (m, 6H), 7.44-7.55 (m, 6H), 7.38-7.41 (m, 2H), 3.85 (d, $J = 8.03$ Hz, 1H, NH), 2.01 ppm (s, 3H); HPLC (DAICEL CHIRALPAK AD-H, hexane/2-propanol 95/5, 0.6 mL/min), t_R

(major) = 117.41 min, t_R (minor) = 128.44 min, 90 % yield, 92% ee.

***N*-(1-(benzo[d][1,3]dioxol-5-yl)-1-cyanoethyl)-*N,N*-diphenylphosphinamide (8k):**

Reaction time: 168 h, white powder; m.p. 117-119°C; $[\alpha]_D^{25} = +16.25$ ($c = 0.560$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.94$ -8.00 (m, 2H), 7.76-7.83 (m, 2H), 7.40-7.55 (m, 6H), 7.17-7.19 (m, 2H), 6.73 (d, $J = 8.68$ Hz, 1H), 5.95 (s, 2H), 3.84 (d, $J = 7.82$ Hz, 1H, NH), 1.89 ppm (s, 3H); ^{13}C NMR (75 Hz, CDCl_3 , 25 °C, TMS): $\delta = 148.1$, 148.0, 134.8, 133.7, 132.2 (d, $J = 9.98$ Hz), 131.3 (d, $J = 9.75$ Hz), 128.7 (t, $J =$

12.23 Hz), 121.4 (d, $J = 4.05$ Hz), 119.1, 108.0, 106.2, 101.5, 56.5, 29.7 ppm; EI-HRMS Calcd for $\text{C}_{22}\text{H}_{19}\text{N}_2\text{O}_3\text{P}$ (M^+): 390.1133, Found: 390.1207; HPLC (DAICEL CHIRALCEL OD-H, hexane/2-propanol 95/5, 0.5 mL/min), t_R (major) = 67.313 min, t_R (minor) = 79.717 min, 91% yield, 89% ee.

***(R)*-*N*-(1-cyano-1-(3,4-dimethoxyphenyl)ethyl)-*N,N*-diphenylphosphinamide (8l):**

Reaction time: 96 h, white powder; m.p. 114-116 °C; $[\alpha]_D^{25} = +14.00$ ($c = 0.200$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.97$ -8.03 (m, 2H), 7.74-7.81 (m, 2H), 7.48-7.55 (m, 4H), 7.39-7.45 (m, 2H), 7.26-7.31 (d, 1H), 7.22-7.25 (m, 1H), 6.78-6.81 (d, 1H), 3.92 (s, 3H), 3.86 (s, 3H), 3.74 (d, $J = 7.64$ Hz, 1H, NH), 1.93 ppm (s, 3H); ^{13}C NMR (75 Hz, CDCl_3 , 25 °C, TMS): $\delta = 149.4$, 149.2, 133.6, 132.3, 132.2, 131.3 (d, $J = 9.8\text{Hz}$), 128.5-129.0 (m), 121.5 (d, $J = 4.9\text{Hz}$), 117.7, 110.8, 109.0, 56.8, 56.01, 55.97, 29.7 ppm; EI-HRMS Calcd for $\text{C}_{23}\text{H}_{23}\text{N}_2\text{O}_3\text{P}$ (M^+): 406.1446, Found : 406.1142; HPLC (DAICEL CHIRALPAK AD-H, hexane/2-propanol 85/15, 1.0 mL/min), t_R (major) = 16.85 min, t_R (minor) = 21.41 min, 99% yield, 88% ee.

8m

(R)-N-(1-cyano-2,3-dihydro-1H-inden-1-yl)-N,N-diphenylphosphinamide (8m):

Reaction time: 144 h, white powder; m.p. 106-108 °C; $[\alpha]_D^{25} = +17.33$ ($c = 0.65$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.82$ -7.96 (m, 4H), 7.42-7.56 (m, 7H), 7.25-7.26 (m, 3H), 3.51 (d, $J = 6.82$ Hz, 1H, NH), 3.20-3.23 (m, 1H), 2.86-2.92 (m, 2H), 2.54-2.59 (m, 1H); HPLC (DAICEL CHIRALCEL OJ-H, hexane/2-propanol 90/10, 1.0 mL/min), t_R (major) = 12.29 min, t_R (minor) = 18.92 min, 91% yield, 90% ee.

8n

N-(1-cyano-1-phenylbutyl)-N,N-diphenylphosphinamide (8n): Reaction time: 196 h, white

powder; m.p. 142-144 °C; $[\alpha]_D^{25} = +4.65$ ($c = 0.710$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.94$ -8.01 (m, 2H), 7.73-7.81 (m, 2H), 7.62-7.66 (m, 2H), 7.45-7.53 (m, 4H), 7.32-7.42 (m, 5H), 3.63 (d, $J = 6.82$ Hz, 1H, NH), 2.17-2.25 (m, 2H), 0.77-0.89 (m, 2H), 0.73-0.77 ppm (t, 3H); HPLC (DAICEL CHIRALCEL OD, hexane/2-propanol 90/10, 1.0 mL/min), t_R (major) = 8.39 min, t_R (minor) = 9.85 min, 91% yield, 78% ee.

(R)-N-(1-(4-chlorophenyl)-1-cyanopropyl)-N,N-diphenylphosphinamide (8o):

Reaction time: 72 h, white powder; m.p. 118-120 °C; $[\alpha]_D^{25} = +9.25$ ($c = 0.162$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.87$ -7.94 (m, 2H), 7.68-7.75 (m, 2H), 7.37-7.54 (m, 8H), 7.25-7.428 (t, 2H), 3.97 (d, $J = 6.46$ Hz, 1H, NH), 2.26-2.33 (q, 2H), 0.745-0.794 ppm (t, 3H); ^{13}C NMR (75 Hz, CDCl_3 , 25 °C, TMS): $\delta = 136.6$, 134.9, 132.2 (d, $J = 9.6$ Hz), 131.5 (d, $J = 9.8$ Hz), 128.8, 128.6, 128.4, 127.8, 119.9 (d, $J = 3.5$ Hz), 61.8, 35.2, 9.2 ppm; EI-HRMS Calcd for $\text{C}_{22}\text{H}_{20}\text{ClN}_2\text{OP}$ (M^+): 394.1002, Found: 394.0757; HPLC (DAICEL CHIRALCEL OJ, hexane/2-propanol 95/5, 1.0 mL/min), t_R (minor) = 12.79 min, t_R (major) = 17.95 min, 97% yield, 76% ee.

N-(2-cyano-3,3-dimethylbutan-2-yl)-N,N-diphenylphosphinamide (8p):

Reaction time: 108 h, white powder; m.p. 108-110 °C; $[\alpha]_D^{25} = +9.90$ ($c = 0.313$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.95$ -8.02 (m, 2H), 7.74-7.81 (m, 2H), 7.41-7.55 (m, 6H), 3.33 (d, $J = 8.29$ Hz, 1H, NH), 1.58 (s, 3H), 1.14 ppm (s, 9H); ^{13}C NMR (75 Hz, CDCl_3 , 25 °C, TMS): $\delta = 132.2$, (d, $J = 10.0$ Hz), 131.0 (d, $J = 9.8$ Hz), 128.8 (d, $J = 5.70$ Hz), 128.7 (d, $J = 5.33$ Hz), 121.6 (d, $J = 3.4$ Hz), 60.4, 38.6, 24.7, 19.9 ppm (d, $J = 3.3$ Hz); EI-HRMS Calcd for $\text{C}_{19}\text{H}_{23}\text{N}_2\text{OP}$ (M^+): 326.1548, Found: 326.1322; HPLC (DAICEL CHIRALCEL OD, hexane/2-propanol 97/3, 1.0 mL/min), t_R (minor) = 22.78 min, t_R (major) = 25.50 min, 98% yield, 80% ee.

***N*-(1-cyano-1-(furan-2-yl)ethyl)-*N,N*-diphenylphosphinamide(**8q**):** Reaction time: 120 h, white powder; m.p. 165-167 °C; $[\alpha]_D^{25} = +5.50$ ($c = 0.200$ in CH_2Cl_2); ^1H NMR (300Hz, CDCl_3 , 25 °C, TMS): $\delta = 7.79\text{--}7.91$ (m, 4H), 7.43-7.52 (m, 6H), 7.31-7.32 (q, 1H), 6.42-6.44 (q, 1H), 6.25-6.27 (q, 1H), 3.79 (d, $J = 6.79$ Hz, 1H, NH), 2.04-2.05 ppm (d, 3H); HPLC (DAICEL CHIRALCEL OJ-H, hexane/2-propanol 95/5, 1.0 mL/min), t_R (major) =

22.58 min, t_R (minor) = 30.17 min, 92% yield, 77% ee.

***N*-(1-cyano-1-(pyridin-2-yl)ethyl)-*N,N*-diphenylphosphinamide (**8r**):** Reaction time: 196 h, white powder; m.p. 119–121 °C; $[\alpha]_D^{25} = +2.35$ ($c = 0.638$ in CH_2Cl_2); ^1H NMR (300 Hz, CDCl_3 , 25 °C, TMS): $\delta = 8.55$ (d, $J = 4.67$ Hz, 1H), 7.96-8.02 (m, 2H), 7.86-7.92 (m, 2H), 7.78-7.83 (m, 1H), 7.65-7.68 (d, 1H), 7.43-7.55 (m, 6H), 7.30-7.34 (m, 1H), 5.54 (d, $J = 8.67$ Hz, 1H, NH), 2.05 ppm. (s, 3H); HPLC (DAICEL

CHIRALCEL OJ-H, hexane/2-propanol 90/10, 1.0 mL/min), t_R (minor) = 15.572 min, t_R (major) = 21.286 min, 91% yield, 72% ee.

7 Mechanism investigation

No reaction was observed with only piperidinamide **3f** or *m*-CPBA as the catalyst (Table 1, entries 1-2). In addition, the results of the additive MeOH proved that it is the addition of TMSCN to ketoimine in the catalytic system (Table 1, entry 3). Furthermore, we isolated the *N,N'*-dioxide **9** and *N*-oxide **10**. As the table 1 shown, the *in situ* generated **9** and isolated **9** gave the same ee's and conversions (Table 1, entries 4-5). No reaction was observed with isolated *N*-oxide **10** (Table 1, entry 6), suggesting that TMSCN was likely to be activated by the two donors (N-O) of catalyst **9**. So, we thought that the chiral *N,N'*-dioxide **9** coordinated the silicon to form the possible hexavalent silicate, enhancing the nucleophilicity of TMSCN. Furthermore, there was no reaction in the presence of Ph₃P(O) (Table 1, entry 7). And there was no background reaction (Table 1, entry 8).

TABLE 1 Study of Mechanism ^a

entry	catalyst	Addition (mol%)	conversion (%) ^b	ee (%) ^c
1	3f (20 mol%)	-	N. R. ^d	-
2	<i>m</i> -CPBA (20 mol%)	-	N. R. ^d	-
3	3f (20 mol%) + <i>m</i> -CPBA (40 mol%)	MeOH (2.0 equiv.)	N. R. ^d	-
4	3f (20 mol%) + <i>m</i> -CPBA (40 mol%)	-	64	80
5	9 (20 mol%)	-	66	79
6	10 (20 mol%)	-	N. R. ^d	-
7	Ph ₃ P(O) (100 mol%)	-	N. R. ^d	-
8	-	-	N. R. ^d	-

^a All reaction were carried out in the air at 0 °C for 24 h, concentration of ketoimine **7a**: 0.1 M in toluene. ^b Conversion were determined by chiral HPLC. ^c All ee values were determined by chiral HPLC (Chiralcel OD). ^d No reaction.

8 Copy of ²⁹Si NMR spectra of TMSCN

When a 1:1 mixture of TMSCN and catalyst **9** (*N*-oxide of **3f**) in CDCl₃ at 25 °C was monitored by ²⁹Si NMR, another strong TMS signal was found at δ = 0.51 ppm as compared to -17.9 ppm for TMSCN.

N-0 29Si NMR BBI

F2 - Acquisition Parameters
Date_ 20060427
Time 17.25
INSTRUM dpX300
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4896
DS 2
SWH 11990.407 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 1000
DM 41.700 usec
DE 6.00 usec
TE 300.0 K
D1 10.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 29Si
P1 15.00 usec
PL1 2.00 dB
SFO1 59.6261805 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 27.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 59.6277894 MHz
WDW EN
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FIP 31.986 ppm
F1 1907.23 Hz
F2P -124.557 ppm
F2 -7427.07 Hz
PPMCH 7.82714 ppm/cm
HZCH 466.71521 Hz/cm

17.933

Current Data Parameters
NAME: 51.001
EXPNO: 21
PROCNO: 1

F2 - Acquisition Parameters

Date_: 20090408
Time: 14.05
INSTRUM: 60x300
PROBHD: 5 mm Duj 13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 1490
DS: 2
SWH: 11090.407 Hz
FIDRES: 0.182959 Hz
AQ: 2.7325011 sec
RG: 1000
DM: 41.700 usec
DE: 6.00 usec
TE: 300.0 K
D1: 10.00000000 sec
d11: 0.03000000 sec

***** CHANNEL f1 *****
NUC1: 29Si
P1: 15.00 usec
PL1: 2.00 dB
SFO1: 59.6261805 MHz

***** CHANNEL f2 *****
DPRP02: waltz16
NUC2: 1H
PCPD2: 80.00 usec
PL2: 120.00 dB
PL12: 27.00 dB
SFO2: 300.1312005 MHz

F2 - Processing parameters

SI: 32768
SF: 59.6277894 MHz
MOM: EM
SSB: 0
LB: 0.50 Hz
GB: 0
PC: 1.00

1D 1H plot parameters
CX: 20.00 cm
FLP: 39.512 00
FL: 2379.85 Hz
FAP: -66.877 dB
F2: -3975.79 Hz
PCWCH: 5.32943 dB/cn
HZCN: 317.78183 Hz/cn

9 Copy of the CD spectra of the products

10 Copy of ^1H NMR and ^{13}C NMR spectra of the catalyst

Pulse Sequence: zgpg30

9

77.31
77.01
76.61
76.41

67.51
64.71

47.25

32.71
32.21
27.41
25.31
24.41
24.36
19.91
19.71

L8

Pulse Sequence: zgpg30

Solvent: CDCl₃

Ambient temperature

INOVA-400 "INOVAA400"

PULSE SEQUENCE

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.363 sec

Width 25141.4 Hz

220 repetitions

OBSERVE C13, 100.552858 MHz

DECOUPLE H1, 399.8941107 MHz

Power 32 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 11 hr, 58 min, 41 sec

7.270
7.219
7.197

08-C05

Pulse Sequence: szpu1
Solvent: CDCl3
Ambient Temperature
INNOVA-400 "INNOVA400"

PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 3.181 sec
Width 4101.7 Hz
4 repetitions
OBSERVE N1 389.8921036 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 20 sec

3.740
3.715
3.703
3.692
3.666
3.159
3.142
3.122
2.960
2.948
2.936
2.924
2.521
2.502
2.484
2.281
2.268
2.251
2.228
2.181
2.147
2.132
2.125
2.104
2.080
1.841
1.831
1.811
1.766
1.731
1.705
1.682
1.669
1.659
1.648
1.637
1.610
1.592
1.571
1.566
1.366
1.339
1.312
1.305
1.208
1.178
1.170
1.156
1.129
1.101
1.073
0.933

08-C05

Pulse Sequence: zgpg30

Solvent: CDCl₃

Acquisition Temperature

INOVA-400 100V4000

PULSE SEQUENCE

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.383 sec

NUC1 13C101.4 Hz

SIEMENS

DECOUPLE 13C100.558574 MHz

DECOUPLE 1H1 399.894107 MHz

Power 32 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 85 hr, 56 min, 5 sec

173.649

77.320

77.000

76.687

67.729

54.078

53.811

47.012

33.048

33.071

30.537

28.408

25.432

24.647

24.578

24.074

MUL-L9

Pulse Sequence: szpul
 Solvent: CDCl3
 Ambient Temperature
 INOVA-400 "INOVA400"
 PULSE SEQUENCE
 Relax delay 2.000 sec
 Pulse delay 2.000 sec
 Acq. time 9.187 sec
 Width 4174.5 Hz
 4 repetitions
 OBSERVE H1, 399.892090 MHz
 DATA PROCESSING
 FT size 32768
 Total time 9 min, 20 sec

HOL-L9

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

INNOVA-400 "INNOVA400"

PULSE SEQUENCE

Relax. delay 8.000 sec

Pulse 45.0 degrees

Acq. time 1.383 sec

Width 2514.2 Hz

148 repetitions

Observed C13, 100.5529374 MHz

Decouple M1, 399.8941107 MHz

Power 32 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 35 hr, 56 min, 5 sec

— 173.466

77.320
77.000
76.687

— 68.309

— 54.627

— 51.376

— 47.119

33.086
33.025
30.835
25.371
24.982
24.781
24.730
24.509
23.433

Pulse Sequence: s2pu1

HJL-L

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
INOVA-100 "INOVA400"

PULSE SEQUENCE

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.198 sec

Width 5354.0 Hz

4 repetitions

OBSERVE H1, 399.8921060 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 20 sec

8.565

7.496
7.476
7.307
7.287
7.267
7.089
7.070
7.052

5.290
3.099
3.070
2.830
2.821
2.804
2.795
2.601
2.581
2.570
2.560
2.549
2.529
2.368
2.351
2.335
2.319
2.302
2.110
2.104
2.081
2.075
2.052
2.047
2.001
1.973
1.822
1.803
1.785
1.766
1.744
1.734
1.721
1.711
1.702
1.652
1.622
1.613
1.588
1.558
1.533
1.524
1.504
1.476
1.444
1.415
1.346
1.338
1.316
1.293
1.285
0.000

3b

3b

— 172.443

— 137.686

— 128.987

— 123.921

— 119.235

77.320
77.000
76.687

— 68.232

— 54.497

— 50.957

— 29.500

— 24.395

— 23.159

HJL-L

Pulse Sequence: szpul

Solvent: CDCl₃

Ambient temperature

INOVA-400 "INOVA400"

PULSE SEQUENCE

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 2341.303 Hz

32 Spectra

ASPECT 13, 100.552974 MHz

DECOUPLE H1, 399.894107 MHz

Power 32 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 35 hr, 56 min, 5 sec

Pulse Sequence: s2pul

HJL-L8

Pulse Sequence: s2pul

Solvent: CDCl₃
Ambient temperature
INOVA-400 "INOVA400"

PULSE SEQUENCE

Relax: delay 2.000 sec

Pulse: 45.0 degrees

Acq. time: 3.187 sec

Width: 3835.5 Hz

4 repetitions

ORSEKPR11; 399.8920812 MHz

DATA PROCESSING

File: 52768

Total time 0 min, 20 sec

3c

HJL-111
 Pulse Sequence: s2pu1
 Solvent: CMC13
 Ambient Temperature
 INOVA-400 "INOVA400"
 PULSE SEQUENCE
 Relax delay 2.000 sec
 Pulse 45.0 degrees
 Acq. time 3.197 sec
 Width 3649.0 Hz
 4 repetitions
 OBSERVE H1 399.8820592 MHz
 DATA PROCESSING
 FI size 32768
 Total time 0 min, 20 sec

— 6.520

HJL-L11

Pulse Sequence: szpu1

Solvent: CDCl3

Ambient temperature

INOVA-400 "INOVA400"

PULSE SEQUENCE

Relax. delay 3.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 25141.4 Hz

64 repetitions

OBSERVE C13, 100.552867 MHz

DECOUPLE H1, 399.894167 MHz

Power 32 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 35 hr, 56 min, 5 sec

— 173.626

77.320
77.000
76.680

— 68.767

— 54.482
— 51.163
— 50.011

— 30.385
— 28.485
— 24.730
— 24.341
— 23.242

3h

H)13

Current Data Parameters
NAME fam-2006-65
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060703
Time 11.17
INSTRUM sv300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 80
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.445188 sec
RG 8192
DM 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 5.50 usec
PL1 -6.00 dB
SF01 75.4775588 MHz

***** CHANNEL f2 *****
COPPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.70 dB
PL13 17.71 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677637 MHz
WDW EM
SSB 0
B 3.00 Hz
GB 0
PC 1.40

10 NMR plot parameters
CX 20.00 cm
CY 10.00 cm
ZP 200.005 ppm
Z1 15093.93 Hz
Z2 -0.005 ppm
Z3 -0.38 Hz
ZPMCM 10.00050 ppm/cm
ZTCM 754.71545 Hz/cm

HJL-L2

Pulse Sequence: szpu1

HJL-L2

Pulse Sequence: szpu1

Solvent: CDCl3
Acquisition Temperature: 300.2 K
Pulse Sequence: INOVA-400 "INOVA400"

PULSE SEQUENCE
Relax: delay 2.000 sec
Pulse: 45.0 degrees
Acq: 1280.0 Hz
Width: 3731.3 Hz
4 repetitions
OBSERVE: H1, 399.8920902 MHz
DATA PROCESSING
F1 size 32768
Total time 0 min, 20 sec

6.940

HLL-12

Pulse Sequence: szpu1

Solvent: CDCl₃

Ambient temperature

INNOVA-400 "INNOVA400"

PULSE SEQUENCE

Relax, delay 3.000 sec

Pulse 135.0 degrees

Acq time 1.383 sec

NUC1 25141.4 Hz

204 repetitions

OBSERVE C13, 100.552805 MHz

DECOUPLE H1, 399.894107 MHz

Power 32 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 35 hr, 56 min, 5 sec

173.184

77.320
77.000
76.680
71.430
70.728

54.284
50.423

42.044
41.579
38.092
36.199
35.039
32.262
29.240
27.783
24.173

Current Data Parameters
NAME fxm-2006-62
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060630
Time 15.46
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 512
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
O1 1.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 3.00 usec
PL1 -2.00 dB
SFO1 300.1320882 MHz

F2 - Processing parameters
SI 32768
SF 300.1300126 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.562900 ppm/cm
HZCM 157.56825 Hz/cm

H₁ 11

Current Data Parameters
NAME f1m-2006-62
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060630
Time 15.49
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 4
SMH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.445188 sec
RG 8192
DM 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 5.50 usec
PL1 -6.00 dB
SFO1 75.4775598 MHz

***** CHANNEL f2 *****
CPOPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.70 dB
PL13 17.71 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.467569 MHz
WDW EM
SSB 0
-B 3.00 Hz
GB 0
-C 1.40

10 NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 200.005 ppm
F1 15093.93 Hz
ZP -0.005 ppm
-2p -0.38 Hz
-2 10.00050 ppm/cm
-2CM 754.71533 Hz/cm

Current Data Parameters

NAME fkm-2006-64

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20060630

Time 18.10

INSTRUM av300

PROBHD 5 mm QNP 1H/13

PULPROG zg30

TD 32768

SOLVENT CDCl₃

NS 8

DS 0

SWH 5995.204 Hz

FIDRES 0.182959 Hz

AQ 2.7329011 sec

RG 256

DM 83.400 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

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

NUC1 1H

P1 3.00 usec

PL1 -2.00 dB

SFO1 300.1320882 MHz

F2 - Processing parameters

SI 32768

SF 300.1300126 MHz

WDW EM

SSB 0

LB 0.10 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

CY 10.00 cm

F1P 10.000 ppm

F1 3001.30 Hz

F2P -0.500 ppm

F2 -150.06 Hz

PPMCM 0.52500 ppm/cm

HZCM 157.56825 Hz/cm

H) 12

ppm

173.849

77.424
77.000
76.576
69.066
56.616
51.308
50.801
41.581
36.277
30.695
29.306
27.440
25.370
24.951
23.499

Current Data Parameters
NAME f4m-2006-64
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060630
Time 18.14
INSTRUM 5 mm QNP 1H/13
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TO 65536
SOLVENT CDCl3
NS 72
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.445188 sec
RG 8192
DM 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.0002000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 5.50 usec
PL1 -6.00 dB
SF01 75.4775598 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD02 80.00 usec
PL2 -2.00 dB
PL12 17.70 dB
PL13 17.71 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677572 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

10 NMR plot parameters
CY 20.00 cm
F1P 10.00 cm
F1 200.005 ppm
F1 15093.93 Hz
F2P -0.005 ppm
F2 -0.38 Hz
SFOCN 10.00050 ppm/cm
HZCN 754.71533 Hz/cm

Current Data Parameters
NAME IAR-2006-06
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 2006/03
Time 11:26
INSTRUM qv300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5995.204 Hz
FIDRES 0.162559 Hz
AQ 2.7369011 sec
RG 256
DM 63.400 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 3.00 usec
PL1 -2.00 dB
SFO1 300.136082 MHz

F2 - Processing parameters
SI 32768
SF 300.1360126 MHz
MCH EH
SSB 0
-B 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
FIP 12.000 dBm
F1 3601.56 Hz
F2 0.500 dBm
C2 -150.06 Hz
PPOW 0.62500 dBm/cm
H2O 187.58125 Hz/cm

Current Data Parameters
NAME 1m-2006-66
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060703
Time 11.30
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 54
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451189 sec
RG 8192
CH 22.050 usec
DE 6.00 usec
TE 300.0 K
C1 2.00000000 sec
C11 0.03000000 sec
C12 0.00000000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 9.50 usec
PL1 -6.00 dB
SF01 75.475998 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
P2 120.00 usec
PCPD2 -2.00 dB
PL2 17.70 dB
PL12 17.71 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677505 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

1D NMR D101 parameters
C1 20.00 cm
C11 10.00 cm
C12 200.005 ppm
F1 10093.93 Hz
F2 -0.005 ppm
F2 -0.38 Hz
ZPGM 10.00050 ppm/cm
WZCM 754.71533 Hz/cm

Current Data Parameters
NAME fxm-2006-159
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060704
Time 11.53
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 256
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 3.00 usec
PL1 -2.00 dB
SFO1 300.1320884 MHz

F2 - Processing parameters
SI 32768
SF 300.1300124 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.560 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm

Current Data Parameters
NAME: 17m-2006-159
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20060707
Time: 18.46
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg
TD: 65536
SOLVENT: CDCl3
NS: 917
DS: 4
SWH: 22675.736 Hz
FIDRES: 0.346004 Hz
AQ: 1.445188 sec
RG: 8192
DM: 22.050 usec
DE: 6.00 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
SFO1: 75.475558 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 80.00 usec
PL2: -2.00 dB
PL12: 17.70 dB
PL13: 17.71 dB
SFO2: 300.1312005 MHz

F2 - Processing parameters
SI: 32768
SF: 75.4677550 MHz
WDW: EM
SSB: 0
LB: 3.00 Hz
GB: 0
PC: 1.40

10 NMR plot parameters
CX: 20.00 cm
CY: 8.00 cm
F1P: 200.005 60m
F1: 15093.93 Hz
F2P: -0.005 60m
F2: -0.38 Hz
PPMCM: 10.00050 60m/cm
HZCM: 754.71533 Hz/cm

11 Copy of NMR spectra of the product

Current Data Parameters
 NAME: 1m-2005-136
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20051026
 Time: 16.34
 INSTRUM: g300
 PNUCNO: 5 m DNP 14/13
 PULPROG: zg30
 TD: 32768
 SOLVENT: CDCl3
 NS: 32
 DS: 0
 SWH: 5999.204 Hz
 FIDRES: 0.182959 Hz
 AQ: 2.7329011 sec
 RG: 128
 DW: 83.400 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 3.00 usec
 PL1: -2.00 dB
 SFO1: 300.1326882 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1300124 MHz
 WDW: EM
 SSB: 0
 GB: 0.10 Hz
 GR: 0
 PC: 1.00

10 MHz plot parameters
 CX: 20.00 cm
 CY: 10.00 cm
 ZP: 10.000 ppm
 F1: 3001.30 Hz
 F2: -0.500 ppm
 F2: -150.05 Hz
 SFO1: 0.56200 ppm/cm
 FIDRES: 157.56825 Hz/cm

Current Data Parameters
NAME fme-2006-97
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060420
Time 11:13
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5095.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 512
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 3.00 usec
PL1 -2.00 dB
SFO1 300.1320864 MHz

F2 - Processing parameters
SI 32768
SF 300.1300124 MHz
RG 1
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCH 0.52000 ppm/ci
HZCH 157.56825 Hz/cm

Current Data Parameters
 NAME 7a-2005-120
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20050927
 Time 14.34
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 SFO 300.136082
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.108559 Hz
 AQ 2.7329011 sec
 RG 256
 CW 63.400 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.00000000 sec
 ----- CHANNEL f1 -----
 NUC1 1H
 P1 3.00 usec
 PL 2.1
 SFO1 300.136082 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.136082 MHz
 WDM CM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00
 ID NMR plot parameters
 CX 20.00 cm
 CY 15.00 cm
 FID 10.000 ppm
 FI 3001.36 Hz
 F2 -150.96 Hz
 F2 0.52500 ppm/cm
 SPC 157.56825 Hz/cm

Current Data Parameters
 NAME: fva-2006-98
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20060420
 Time: 11.20
 INSTRUM: av300
 PULPROG: 5 mm QNP 1H/13
 RQCPRG: zg30
 TO: 32768
 SOLVENT: CDCl3
 NS: 16
 DS: 0
 SWH: 5995.204 Hz
 FIDRES: 0.182959 Hz
 AQ: 2.7329011 sec
 RG: 512
 DM: 83.400 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 3.00 usec
 PL1: -2.00 dB
 SFO1: 300.1300884 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1300124 MHz
 WDM: EM
 SSB: 0
 RB: 0.10 Hz
 GB: 0
 PC: 1.00

10 NMR plot parameters
 CX: 20.00 cm
 CY: 12.00 cm
 FIDP: 10.000 ppm
 FI: 3001.30 Hz
 F2P: -0.500 ppm
 F2: -150.06 Hz
 PPMCH: 0.52500 ppm/
 HZCM: 157.56825 Hz/c

Current Data Parameters
 NAME 1m-2005-58
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050722
 Time 11.06
 INSTRUM av300
 PPGNO 5 mm QNP 1H/13
 F1 101.625 MHz
 F2 125.761 MHz
 PULPROG zgpg30
 TO 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 512
 DN 83.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 3.00 usec
 PL1 -2.00 dB
 SFO1 300.1320882 MHz

F2 - Processing parameters
 SI 32768
 SF 300.130124 MHz
 WDW EM
 SSB 0
 AB 0.10 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 CY 20.00 cm
 FIP 10.000 cm
 F1 3001.30 Hz
 F2 -0.500 cm
 T2 -150.06 Hz
 ZPGPC 0.52550 cm
 ZPGW 15.56825 Hz

Current Data Parameters
NAME: 1m-2005-152
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20060621
Time: 14.59
INSTRUM: svt300
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 0
SWH: 5995.204 Hz
FIDRES: 0.182959 Hz
AQ: 2.732011 sec
RG: 512
DN: 93.400 usec
DE: 6.00 usec
TE: 300.0 K
D1: 1.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 3.00 usec
PL1: -2.00 dB
SFO1: 300.1320882 MHz

F2 - Processing parameters
SI: 32768
SF: 300.1300124 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 15.00 cm
C1P: 10.000 ppm
Z1: 3001.30 Hz
F2P: -0.500 ppm
F2: -150.06 Hz
PPhCH: 0.52500 ppm/cm
WCH: 157.55825 Hz/cm

Current Data Parameters
 NAME: JAR-2006-151
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20060621
 Time: 14.53
 INSTRUM: av300
 PROBHD: 5 mm QNP 1H/13
 PULPROG: zgpg30
 TO: 32768
 SOLVENT: CDCl3
 NS: 16
 DS: 0
 SWH: 5995.204 Hz
 FIDRES: 0.162959 Hz
 AQ: 2.7329011 sec
 RG: 512
 DM: 83.400 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 3.00 usec
 PL1: -2.00 dB
 SF01: 300.1360882 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1360124 MHz
 WDM: FM
 SSB: 0
 LB: 0.10 Hz
 GB: 0
 PC: 1.00

10 NMR plot parameters
 CX: 20.00 cm
 CY: 12.00 cm
 ZP: 10.000 ppm
 F1: 300.130 Hz
 F2: -0.500 ppm
 F2: -150.06 Hz
 JPICM: 0.52500 ppm/cm
 HZCM: 157.56825 Hz/cm

Current Data Parameters
NAME: 2006-153
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20060621
Time: 15.08
INSTRUM: av300
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl₃
NS: 8
DS: 0
SWH: 5995.204 Hz
FIDRES: 0.182059 Hz
AQ: 2.7329011 sec
RG: 512
RM: 0.1460 usec
DE: 6.00 usec
TE: 300.2 K
D1: 1.00000000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 3.00 usec
PL1: -2.00 dB
SFO1: 300.136082 MHz

F2 - Processing parameters
SI: 32768
SF: 300.1300124 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 10.00 cm
F1P: 10.000 ppm
F1: 300.130 Hz
F2P: -0.500 ppm
F2: -150.06 Hz
SFOCM: 0.52500 ppm/cm
F2CM: 157.56825 Hz/cm

Current Data Parameters
NAME f-m-2006-100
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060420
Time 17:22
INSTRUM hν300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TO 2030
SOLVENT CDCl₃
NS 16
DS 0
SWH 5565.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 512
CM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 3.00 usec
PL1 -2.00 dB
SFO1 300.1320884 MHz

F2 - Processing parameters
SI 32768
SF 300.1300124 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCH 0.52500 ppm/
HZCM 157.55825 Hz/c

Current Data Parameters
NAME fm-2005-115
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050915
Time 16.04
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 512
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 3.00 usec
PL1 -2.00 dB
SFO1 300.1320862 MHz

F2 - Processing parameters
SI 32768
SF 300.130128 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 20.00 cm
CY 50.00 cm
F1 10.000 ppm
F2 300.130 Hz
F2P -0.500 ppm
F2 -150.05 Hz
OPNCK 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

Current Data Parameters
NAME: fmr-2006-103
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20060426
Time: 14.41
INSTRUM: mv300
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 0
SWH: 5995.204 Hz
FIDRES: 0.122959 Hz
AQ: 2.7329011 sec
RG: 128
DM: 83.400 usec
DE: 6.00 usec
TE: 300.0 K
D1: 1.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 3.00 usec
PL1: -2.00 dB
SF01: 300.1320864 MHz

F2 - Processing parameters
SI: 32768
SF: 300.1300121 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
CY: 5.00 cm
F1P: 10.000 ppm
F1: 300.130 MHz
F2P: -0.500 ppm
F2: -150.06 Hz
FREQCH: 0.50500 ppm/cm
HZCH: 157.55825 Hz/cm

Current Data Parameters
 NAME Jan-2006-99
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060420
 Time 11:30
 INSTRUM av300
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 512
 DM R3.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 3.00 usec
 PL1 -2.00 dB
 SF01 300.1300584 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300124 MHz
 MDN EN
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 CY 35.00 cm
 F1 10.000 ppm
 F2 300.130 Hz
 ZF2 -0.500 ppm
 F2 -150.06 Hz
 RFPCMH 0.52500 ppm/c
 HZCM 157.56825 Hz/cm

Current Data Parameters
NAME: 1m-2006-106
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20060427
Time: 10.32
INSTRUM: 0V300
PROBHD: 5 mm QNP 1H/13
PULPROG: zg30
TO: 32768
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 5995.204 Hz
FIDRES: 0.162959 Hz
AQ: 2.7329011 sec
RG: 256
DM: 0.3400 usec
DE: 6.00 usec
TE: 300.0 K
D1: 1.00000000 sec

***** CHANNEL f1 *****
NUC1: 1H
P1: 3.00 usec
PL1: -2.00 dB
SFO1: 300.1320884 MHz

F2 - Processing parameters
SI: 32768
SF: 300.130121 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00

10 NMR plot parameters
CX: 20.00 cm
CY: 10.00 cm
FIP: 10.000 ppm
F1: 300.130 Hz
F2P: -0.500 ppm
F2: -150.05 Hz
PPHCH: 0.52500 ppm/c
H2O: 157.56825 Hz/cm

Current Data Parameters
 NAME fra-2005-168
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060714
 Time 16.02
 INSTRUM av300
 PROBRW 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 9995.204 Hz
 FIDRES 0.162769 Hz
 AQ 2.7329011 sec
 RG 256
 CW 83.400 usec
 DE 6.00 usec
 TE 300.2 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 a1 3.00 usec
 PL1 -2.00 dB
 SF01 300.1360882 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300126 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.00 cm
 F1P 10.000.000
 F1 3601.30 Hz
 F2P -0.500.000
 F2 -150.06 Hz
 PPMCN 0.52350 ppm/cm
 HzCM 137.56825 Hz/cm

Current Data Parameters
NAME: 140-2005-118
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters

Date_: 2005-02-25
Time: 23.11
INSTRUM: AV300
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg
TD: 65536
SOLVENT: CDCl3
NS: 1026
DS: 4
SWH: 22675.736 Hz
FIDRES: 0.34604 Hz
AQ: 1.445188 sec
RG: 8192
DM: 22.659 usec
DE: 6.00 usec
TE: 300.0 K
B1: 2.00000000 sec
C11: 0.03000000 sec
C12: 0.00020000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 5.50 usec
PL1: -6.00 dB
SFO1: 75.475598 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 80.00 usec
PL2: -2.00 dB
PL12: 17.70 dB
PL13: 17.71 dB
SFO2: 200.1312005 MHz

F2 - Processing parameters
SI: 32768
SF: 75.467581 MHz
WDW: EM
SSB: 0
GB: 3.00 Hz
CB: 0
PC: 1.40

===== NMR plot parameters =====
CX: 20.00 cm
CY: 7.00 cm
CZ: 180.005 ppm
F1: 12594.57 Hz
F2: -0.005 ppm
F3: -0.36 Hz
GPMCH: 9.00050 ppm/cm
A2CH: 679.2424 Hz/cm

Current Data Parameters

NAME	EXPNO	PROCNO
74m-2006-97	2	1

2 - Acquisition Parameters

Date_	Time
20060428	23:15

INSTRUM 3000
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 766
DS 4
SWH 22675.736 Hz
FIDRES 0.34604 Hz
AQ 1.4461188 sec
RG 8192
DM 22.050 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.50 usec
PL1 -6.00 dB
SFO1 75.475598 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.70 dB
PL13 17.71 dB
SFO2 300.1312005 MHz

2 - Processing parameters

SF	22762
WDM 75.4677556 MHz	FW
SSB 0	0
GB 0	0
PC 1.40	1.40

10 NMR plot parameters

EX	20.00 cm
EV 8.00 cm	8.00 cm
F1P 180.050 ppm	180.050 ppm
F1 135.8797 Hz	135.8797 Hz
F2P -0.005 ppm	-0.005 ppm
F2 -0.38 Hz	-0.38 Hz
PPM/CM 9.00275 ppm/cm	9.00275 ppm/cm
HZ/CM 679.41736 Hz/cm	679.41736 Hz/cm

Current Data Parameters

NAME	lab-2016-56
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20160419
Time	20.59
INSTRUM	AV300
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	3790
DS	4
SWH	22675.736 Hz
FIDRES	0.346004 Hz
AQ	1.4451188 sec
RG	8192
DM	22.050 uSFC
DE	5.00 uSFC
TE	300.2 K
DE	2.0000000 sec
DE	0.0300000 sec
DE	0.0002000 sec

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

NUC1	13C
PT	5.50 uSFC
PL1	-6.00 dB
PR01	75.477598 MHz

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

CPDPRG2	zgpg30
NUC2	1H
PCPD2	80.00 uSFC
PL2	-2.00 dB
PL12	17.70 dB
PL13	17.71 dB
PR02	300.1312005 MHz

F2 - Processing parameters

SI	32768
SF	75.4677538 MHz
KON	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

13 NMR FID parameters

EX	20.00 cm
FX	10.00 cm
FIDP	180.005 ppm
F1	12584.57 Hz
F2	-0.005 ppm
F2	-0.38 Hz
290CM	9.00550 ppm/cm

Current Data Parameters
NAME: Jan-2006-113
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20050428
Time: 23.08
INSTRUM: sxt300
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg
TD: 65536
SOLVENT: CDCl3
NS: 2446
DS: 4
SWH: 22675.736 Hz
FIDRES: 0.346004 Hz
AQ: 1.445188 sec
RG: 8192
DM: 22.000 usec
DE: 6.00 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: -0.00 dB
SFO1: 75.4775980 MHz

===== CHANNEL f2 =====
OPPRG2: waltz16
NUC2: 1H
PCPD2: 60.00 usec
PL2: -2.00 dB
PL12: 17.70 dB
PL13: 17.71 dB
SFO2: 300.1312905 MHz

F2 - Processing parameters
SI: 32768
SF: 75.4677544 MHz
WDW: EM
SSB: 0
LB: 3.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CX: 22.00 cm
CY: 10.00 cm
F1: 180.005 MHz
F1: 135.0457 Hz
F2: -9.005 MHz
F2: -0.38 Hz
SFOCN: 9.00500 ppm/cm
WFA: 670.24256 MHz

Current Data Parameters
NAME 7A-2005-152
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050622
Time 14.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2148
DS 4
SWH 22679.736 Hz
FIDRES 0.146004 Hz
AQ 1.4451189 sec
RG 8192
DM 22.050 usec
DE 6.00 usec
TE 300.0 K
SI 2.00000000 sec
S1 0.03000000 sec
S12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 -6.00 dB
SFO1 75.475598 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 90.00 usec
PL2 -2.00 dB
PL12 17.70 dB
PL13 17.71 dB
SFO2 300.132005 MHz

F2 - Processing parameters
SI 32768
SF 75.467549 MHz
WDW EM
SSB 0
CB 3.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 200.0005 DM
F1 15053.93 Hz
F2P -0.005 DM
F2 -0.38 Hz
SFOCM 754.71533 MHz
F2CM

Current Data Parameters

NAME	7a-200h-1c3
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20050522
Time	22.35
INSTRUM	av300
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg
TD	65536
SOLVENT	CDCl3
NS	256
DS	4
SWH	20675.736 Hz
FIDRES	0.346304 Hz
AQ	1.445188 sec
RG	8192
CM	22.050 usec
DE	6.00 usec
TE	300.0 K
D1	2.0000000 sec
d11	0.0300000 sec
d12	0.0000000 sec

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

NUC1	13C
P1	5.00 usec
PL1	-6.00 dB
SFO1	75.477598 MHz

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

CROSS2	wa1215
NUC2	1H
PCPD2	80.00 usec
PL2	-2.00 dB
PL12	17.70 dB
PL13	17.71 dB
SFO2	300.1312005 MHz

F2 - Processing parameters

SI	32768
SF	75.4677553 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

CK	20.00 cm
CV	6.00 cm
F1P	180.00500 MHz
F1	125.04 57 MHz
F2P	-0.00500 MHz
F2	-0.38 MHz
PPMCH	5.00050 ppm/Hz
ACQ	575.24756 MHz

Current Data Parameters
NAME 1m-2005-100
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050429
Time 21:39
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1512
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 6192
DM 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.50 usec
PL1 -5.00 dB
SFO1 75.475598 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -2.00 dB
PL12 17.70 dB
PL13 17.71 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677529 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.00 cm
F1P 100.005 GHz
F1 135.94 GHz
F2P -0.005 GHz
F2 -0.38 Hz
SFOCM 9.00050 GHz/cm
HZCM 679.24744 kHz/cm

Current Data Parameters
 NAME 1m-2006-103
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060423
 Time 21.16
 INSTRUM mv300
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TO 655.36
 SOLVENT CDCl3
 NS 316
 DS 4
 SWH 22675.736 Hz
 FIDRES 0.346004 Hz
 AQ 1.4461188 sec
 RG 6152
 DM 22.650 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 d12 0.0002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.50 usec
 PL1 -6.00 dB
 SF01 75.4775998 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 17.70 dB
 PL13 17.71 dB
 SF02 300.1312093 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677541 MHz
 KW EN
 SSF 0
 LB 3.00 Hz
 GB 0
 PC 1.40

10 NMR pilot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 180.005 ppm
 F1 13584.57 Hz
 F2P -0.005 ppm
 F2 -0.38 Hz
 PPM2H 9.00650 ppm/cm
 HZ2H 679.24744 Hz/cm

Current Data Parameters
NAME: Jan-2006-99
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20060420
Time: 20.39
INSTRUM: av300
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 65536
FIDRES: 0.0000000
SOLVENT: CDCl3
NS: 370
DS: 4
SWH: 22675.736 Hz
FIDRES: 0.346004 Hz
AQ: 1.443198 sec
RG: 8192
DM: 22.000 usec
DE: 6.00 usec
TE: 300.0 K
D1: 2.00000000 sec
d11: 0.03000000 sec
d12: 0.00000000 sec

***** CHANNEL f1 *****
NUC1: 13C
a1: 5.50 usec
PL1: -6.00 dB
SF01: 75.475598 MHz

***** CHANNEL f2 *****
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 80.00 usec
PL2: -2.00 dB
PL12: 17.70 dB
PL13: 17.71 dB
SF02: 300.1312005 MHz

F2 - Processing parameters
SI: 32768
SF: 75.4617562 MHz
WDW: EM
SSB: 0
LB: 3.00 Hz
GB: 0
PC: 1.40

10 MHz plot parameters
CX: 20.00 cm
CY: 12.00 cm
F1P: 180.005 ppm
F1: 13584.57 Hz
F2P: -5.000 ppm
F2: -377.34 Hz
ppb/cn: 9.25025 ppm/cn
Hz/cm: 500.09564 Hz/cm