Supplementary Materials for

**Enantioselective Hydrogenation of Quinolines Catalyzed by
Ir(BINAP)-Cored Dendrimers: Dramatic Enhancement of
Catalytic Activity**

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1. General Information

Unless otherwise noted, all experiments were carried out under an inert atmosphere of dry nitrogen by using standard Schlenk-type techniques, or performed in a nitrogen-filled glovebox. ^1H NMR, ^{31}P NMR and ^{13}C NMR spectra were recorded on a Bruker Model Avance DMX 300 Spectrometer (^1H 300 MHz, ^{31}P 121 MHz and ^{13}C 75 MHz respectively). Chemical shifts (δ) are given in ppm and are referenced to residual solvent peaks (^1H and ^{13}C NMR) or to an external standard (85% H_3PO_4 , ^{31}P NMR). MALDI-TOF mass spectra were obtained on a BIFLEX III instrument with α -cyano-4-hydroxycinnamic acid (CCA) as the matrix. Elemental analyses were performed on a Flash EA 1112 Elemental Analyzer. Melting points were uncorrected. 5,5'-Diamino BINAP (*S*)-**1** was synthesized according to our previously reported method.¹ All solvents were dried using standard, published methods and were distilled under a nitrogen atmosphere before use. All other chemicals were used as received from Aldrich or Acros without further purification.

2. General procedure for the preparation of dendritic BINAP ligands

(*S*)-**G₁DenBINAP**: A 10 mL flask was charged with polyether dendritic acid ($\text{G}_1\text{-COOH}$) (200 mg, 0.6 mmol), (*S*)-5, 5'-diamino BINAP (*S*)-**1** (178 mg, 0.27 mmol) and anhydrous calcium chloride (200 mg). This was added triphenylphosphite (0.15 mL), pyridine (0.3 mL) and N-methyl-2-pyrrolidone (NMP, 1 mL) under nitrogen atmosphere. The reaction mixture was then stirred at 120 °C for 8-16h. After cooled to room temperature, the mixture was poured into cold methanol (20 mL). The precipitate was collected by centrifugation, and dried in vacuo. Pure **G₁DenBINAP**

was obtained via flash chromatography on silica gel (287 mg, 80% yield) as a white powder; m.p. 187–189 °C; $[\alpha]_D^{30} +140.7$ (*c* 0.3, toluene); ^1H NMR (300 MHz, CDCl_3): δ 8.15 (s, 2H), 7.91–7.88 (m, 4H), 7.51–7.34 (m, 22H), 7.22–7.06 (m, 24H), 6.96 (t, *J* = 8.09 Hz, 2H), 6.84 (s, 2H), 6.71 (d, *J* = 8.48 Hz, 2H), 5.14 (s, 8H); ^{13}C NMR (75 MHz, CDCl_3): δ 165.8, 160.3, 145.9, 145.6, 145.3, 137.7, 137.6, 137.6, 137.5, 137.1, 136.8, 136.7, 136.7, 136.6, 136.4, 136.4, 136.2, 134.4, 134.4, 134.2, 134.1, 134.0, 133.9, 133.9, 133.0, 132.9, 132.8, 132.0, 131.2, 128.7, 128.3, 128.2, 127.8, 127.6, 127.0, 125.8, 125.6, 121.7, 120.8, 106.2, 105.8, 70.4; ^{31}P NMR (121 MHz, CDCl_3): δ -14.77; MALDI-TOF MS for $\text{C}_{86}\text{H}_{66}\text{N}_2\text{O}_6\text{P}_2$ $[\text{M}]^+$ calcd: 1285.4; found 1285.4; HRMS (FAB) for $\text{C}_{86}\text{H}_{66}\text{N}_2\text{O}_6\text{P}_2$ $[\text{M}+\text{H}]^+$ calcd: 1285.4474; found 1285.4433.

(*S*)-**G₂DenBINAP**: Yield 85%; m.p. 96–98 °C; $[\alpha]_D^{30} +98.1$ (*c* 0.3, toluene). ^1H NMR (300 MHz, CDCl_3): δ 8.14 (s, 2H), 7.93 (d, *J* = 8.34 Hz, 4H), 7.52 (d, *J* = 8.32 Hz, 2H), 7.43–7.29 (m, 40H), 7.18–7.05 (m, 24H), 6.94 (t, *J* = 8.05 Hz, 2H), 6.79–6.58 (m, 16H), 5.06 (s, 8H), 5.04 (s, 16H); ^{13}C NMR (75 MHz, CDCl_3): δ 165.8, 160.3, 160.2, 145.9, 145.3, 138.8, 137.6, 137.1, 136.7, 136.6, 136.4, 134.5, 134.4, 134.3, 134.1, 134.0, 134.0, 133.0, 132.9, 132.7, 132.0, 131.2, 128.6, 128.5, 128.2, 128.0, 127.8, 127.6, 127.2, 127.1, 125.8, 125.7, 121.8, 120.9, 106.4, 106.3, 101.7, 70.3, 70.2; ^{31}P NMR (121 MHz, CDCl_3): δ -14.26; MALDI-TOF MS for $\text{C}_{142}\text{H}_{114}\text{N}_2\text{O}_{14}\text{P}_2$ $[\text{M}]^+$ calcd: 2134.4; found 2133.1. Elemental analysis: calcd. C 79.91, H 5.38, N 1.31; found C 79.52, H 5.06, N 1.57.

(*S*)-**G₃DenBINAP**: Yield 90%; m.p. 88–90 °C; $[\alpha]_D^{30} +59.2$ (*c* 0.3, toluene); ^1H

NMR (300 MHz, CDCl₃): δ 8.09 (s, 2H), 7.87 (d, J = 8.71 Hz, 2H), 7.81 (d, J = 7.12 Hz, 2H), 7.43 (d, J = 8.68 Hz, 2H), 7.34-7.18 (m, 80H), 7.16-6.97 (m, 24H), 6.85 (t, J = 7.91 Hz, 2H), 6.74-6.51 (m, 40 H), 4.97-4.50 (m, 56H); ¹³C NMR (75 MHz, CDCl₃): δ 165.8, 160.2, 160.2, 145.9, 145.6, 145.3, 139.2, 138.8, 137.7, 137.2, 136.9, 136.8, 136.6, 136.4, 134.4, 134.3, 134.1, 134.0, 133.9, 133.00, 132.9, 132.7, 132.1, 131.2, 128.6, 128.4, 128.4, 128.3, 128.2, 128.2, 128.0, 127.8, 127.6, 127.6, 127.3, 127.2, 125.8, 122.1, 121.0, 106.6, 106.5, 101.8, 101.7, 70.3, 70.2, 70.1; ³¹P NMR (121 MHz, CDCl₃): δ -14.72; MALDI-TOF MS for C₂₅₄H₂₁₀N₂O₃₀P₂ [M]⁺ calcd: 3832.3; found 3832.5. Elemental analysis: calcd. C 79.60, H 5.52, N 0.73; found C 79.36, H 5.61, N 0.62.

(*S*)-**G₄DenBINAP**: Yield 90%; m.p. 80-82 °C; [α]_D²⁰ +33.3 (c 0.3, toluene); ¹H NMR (300 MHz, CDCl₃): δ 8.10 (s, 2H), 7.91 (d, J = 8.72 Hz, 2H), 7.84 (d, J = 7.28 Hz, 2H), 7.48 (d, J = 8.11 Hz, 2H), 7.40-7.27 (m, 160H), 7.22-7.06 (m, 24H), 6.91 (t, J = 7.62 Hz, 2H), 6.79-6.56 (m, 88H), 4.98 (m, 120H); ¹³C NMR (75 MHz, CDCl₃): δ 165.8, 160.2, 160.1, 139.2, 138.8, 137.2, 137.1, 136.9, 136.8, 136.4, 134.4, 134.2, 134.1, 132.8, 132.7, 132.1, 131.2, 129.7, 129.1, 128.6, 128.5, 128.4, 128.3, 128.2, 128.0, 127.8, 127.6, 127.4, 127.2, 125.8, 122.2, 121.2, 106.5, 106.4, 101.6, 70.1, 70.0; ³¹P NMR (121 MHz, CDCl₃) δ -14.40; Elemental analysis for C₄₇₈H₄₀₂N₂O₆₂P₂: calcd. C 79.43, H 5.61, N 0.39; found: C 79.41, H 5.65, N 0.41.

3. General procedure for the asymmetric hydrogenation of quinolines and catalyst recycling

A mixture of [Ir(COD)Cl]₂ (0.85 mg, 0.00125 mmol) and (*S*)-**G₂DenBINAP** (5.8

mg, 0.00275 mmol) in THF (1.25 mL) was stirred at room temperature for 3 h in glovebox, the mixture was then transferred by a syringe to a stainless steel autoclave, in which I₂ (3.2 mg, 0.0125 mmol) and quinaldine **2a** (36 mg, 0.25 mmol) were charged beforehand. The hydrogenation was performed at room temperature under H₂ (45 atm) for 1.5 h. After carefully releasing of the hydrogen, the reaction mixture was diluted with dichloromethane (5 mL) and saturated sodium carbonate aqueous solution (2 mL), then stirred for 15 min and separated. The aqueous layer was extracted with dichloromethane (3 x 5 mL), and the combined organic layer was dried over sodium sulfate and concentrated to afford the crude product. Purification was performed by a silica gel column eluted with petroleum ether / dichloromethane to give pure product. The enantiomeric excesses were determined by chiral HPLC with chiral columns (OJ-H, AS-H and OD-H).

Catalyst recycling: A mixture of [Ir(COD)Cl]₂ (0.85 mg, 0.00125 mmol) and (*S*)-**G₃DenBINAP** (10.5 mg, 0.00275 mmol) in THF (1.25 mL) was stirred at room temperature for 3 h in glovebox, the mixture was then transferred by a syringe to a stainless steel autoclave, in which I₂ (4.0 mg, 0.0156 mmol) and quinaldine **2a** (358 mg, 2.5 mmol) were charged beforehand. The hydrogenation was performed at room temperature under H₂ (45 atm) for 8 h. The reaction mixture was added n-hexane (10 mL) to precipitate the dendritic catalyst, which was filtered, washed with n-hexane, dried under reduced pressure, and then used directly in the next run. The reduced product in the n-hexane phase was used for the determination of conversion and enantioselectivity.

4. ^1H and ^{13}C NMR and MS spectra data of the reduced products ²

2-Methyl-1,2,3,4-tetrahydroquinoline (**3a**): ^1H NMR (300 MHz, CDCl_3): δ 6.98-6.95 (m, 2H), 6.61 (t, $J = 8.49$ Hz, 1H), 6.48 (d, $J = 8.49$ Hz, 1H), 3.44-3.38 (m, 1H), 2.85-2.74 (m, 2H), 1.94-1.91 (m, 1H), 1.64-1.55 (m, 1H), 1.22 (d, $J = 6.27$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 144.8, 129.3, 126.7, 121.1, 117.0, 114.0, 47.2, 30.2, 26.6, 22.6; EI-MS for $\text{C}_{10}\text{H}_{13}\text{N}$ $[\text{M}+1]^+$ calcd: 148.2; found 148.1. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-OJ-H (hexanes: *i*-PrOH 95: 5 at 0.5 mL / min): $t_S = 25.4$ min, $t_R = 28.2$ min.

2-Ethyl-1,2,3,4-tetrahydroquinoline (**3b**): ^1H NMR (300 MHz, CDCl_3): δ 7.05-7.00 (m, 2H), 6.66 (t, $J = 7.52$ Hz, 1H), 6.52 (d, $J = 8.37$ Hz, 1H), 3.24-3.20 (m, 1H), 2.88-2.80 (m, 2H), 2.05-2.00 (m, 1H), 1.67-1.54 (m, 3H), 1.05 (t, $J = 7.46$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 144.8, 129.3, 126.8, 121.4, 116.9, 114.1, 53.1, 29.5, 27.7, 26.5, 10.1; EI-MS for $\text{C}_{11}\text{H}_{15}\text{N}$ $[\text{M}+1]^+$ calcd: 162.3; found 162.1. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-OJ-H (hexanes: *i*-PrOH 95: 5 at 0.5 mL / min): $t_S = 22.1$ min, $t_R = 24.7$ min.

2-Propyl-1,2,3,4-tetrahydroquinoline (**3c**): ^1H NMR (300 MHz, CDCl_3): δ 7.02-6.97 (m, 2H), 6.64 (t, $J = 7.36$ Hz, 1H), 6.51 (d, $J = 8.21$ Hz, 1H), 3.33-3.26 (m, 1H), 2.88-2.73 (m, 2H), 2.04-1.97 (m, 1H), 1.67-1.44 (m, 5H), 1.01 (t, $J = 7.11$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 144.8, 129.3, 126.7, 121.4, 116.9,

114.1, 51.4, 38.9, 28.2, 26.5, 18.9, 14.2; EI-MS for C₁₂H₁₇N [M+1]⁺ calcd: 176.3; found 176.2. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-OJ-H (hexanes: *i*-PrOH 95: 5 at 0.5 mL / min): t_S = 20.5 min, t_R = 26.4 min.

2-Phenethyl-1,2,3,4-tetrahydroquinoline (**3d**): ¹H NMR (300 MHz, CDCl₃): δ 7.31-7.16 (m, 5H), 6.95-6.92 (m, 2H), 6.60 (t, *J* = 7.55 Hz, 1H), 6.43 (d, *J* = 8.16 Hz, 1H), 3.32-3.23 (m, 1H), 2.80-2.69 (m, 4H), 1.98-1.94 (m, 1H), 1.85-1.78 (m, 2H), 1.69-1.64 (m, 1H); ¹³C NMR (75 MHz, CDCl₃): δ 144.6, 141.9, 129.3, 128.6, 128.4, 126.8, 126.0, 121.3, 117.1, 114.2, 51.2, 38.3, 32.2, 28.0, 26.3; EI-MS for C₁₇H₁₉N [M+1]⁺ calcd: 238.4; found 238.2. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-AS-H (hexanes: *i*-PrOH 95: 5 at 0.5 mL / min): t_S = 5.7 min, t_R = 6.3 min.

2-(3',4'-Dimethoxyphenethyl)-1,2,3,4-tetrahydroquinoline (**3e**): ¹H NMR (300 MHz, CDCl₃): 7.01-6.96 (m, 2H), 6.85-6.76 (m, 3H), 6.63 (t, *J* = 7.55 Hz, 1H), 6.46 (d, *J* = 8.17 Hz, 1H), 3.90 (s, 3H), 3.88 (s, 3H), 3.35-3.31 (m, 1H), 2.84-2.69 (m, 4H), 2.05-2.00 (m, 1H), 1.88-1.69 (m, 3H); ¹³C NMR (75 MHz, CDCl₃): δ 149.2, 147.6, 144.7, 134.7, 129.5, 126.9, 121.5, 120.4, 117.3, 114.4, 112.0, 111.7, 56.2, 56.1, 51.5, 38.6, 32.0, 28.2, 26.4; EI-MS for C₁₉H₂₃NO₂ [M+1]⁺ calcd: 298.4; found 298.2. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-AS-H (hexanes: *i*-PrOH 95: 5 at 1 mL

/ min): $t_S = 14.4$ min, $t_R = 15.2$ min.

2-Methyl-1-(1,2,3,4-tetrahydroquinolin-2-yl)-propan-2-ol (**3f**): ^1H NMR (300 MHz, CDCl_3): 6.98-6.93 (m, 2H), 6.59 (t, $J = 7.39$ Hz, 1H), 6.49 (d, $J = 7.86$ Hz, 1H), 3.62-3.53 (m, 1H), 2.94-2.69 (m, 2H), 1.88-1.57 (m, 4H), 1.33 (s, 3H), 1.32 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 144.6, 129.2, 126.7, 120.9, 116.7, 114.4, 72.0, 48.8, 48.5, 32.8, 29.8, 27.9, 26.6; EI-MS for $\text{C}_{13}\text{H}_{19}\text{NO}$ $[\text{M}+1]^+$ calcd: 206.3; found 206.2. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-OD-H (hexanes: *i*-PrOH 95: 5 at 1 mL / min): $t_S = 9.8$ min, $t_R = 11.7$ min.

1-(1,2,3,4-tetrahydroquinolin-2-ylmethyl)-cyclohexanol (**3g**): ^1H NMR (300 MHz, CDCl_3): 6.98-6.93 (m, 2H), 6.59 (t, $J = 7.12$ Hz, 1H), 6.49 (d, $J = 7.67$ Hz, 1H), 3.62-3.55 (m, 1H), 2.92-2.69 (m, 2H), 1.88-1.28 (m, 14H); ^{13}C NMR (75 MHz, CDCl_3): δ 144.6, 129.2, 126.7, 121.0, 116.7, 114.5, 72.6, 47.8, 47.3, 40.6, 35.8, 30.0, 26.6, 25.8, 22.2, 22.2; EI-MS for $\text{C}_{16}\text{H}_{23}\text{NO}$ $[\text{M}+1]^+$ calcd: 246.4; found 246.2. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-OD-H (hexanes: *i*-PrOH 95: 5 at 1 mL / min): $t_S = 14.9$ min, $t_R = 17.3$ min.

1,1-Diphenyl-2-(1,2,3,4-tetrahydroquinolin-2-yl)-ethanol (**3h**): ^1H NMR (300 MHz, CDCl_3): 7.44-7.20 (m, 10H), 6.92-6.88 (m, 2H), 6.59 (t, $J = 7.21$ Hz,

1H), 6.38 (d, $J = 7.89$ Hz, 1H), 3.33-3.27 (m, 1H), 2.72-2.68 (m, 2H), 2.47-2.43 (m, 2H), 1.78-1.69 (m, 2H); ^{13}C NMR (75 MHz, CDCl_3): δ 147.8, 146.1, 143.9, 129.3, 128.4, 128.3, 127.3, 126.9, 126.7, 126.1, 125.9, 121.5, 117.5, 115.4, 79.0, 48.3, 47.1, 29.4, 25.7; EI-MS for $\text{C}_{23}\text{H}_{23}\text{NO}$ $[\text{M}+1]^+$ calcd: 330.4; found 330.3. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-OD-H (hexanes: *i*-PrOH 95: 5 at 1 mL / min): $t_S = 12.6$ min, $t_R = 14.7$ min.

6-Methoxy-2-methyl-1,2,3,4-tetrahydroquinoline (**3i**): ^1H NMR (300 MHz, CDCl_3): 6.54 (m, 2H), 6.38 (d, $J = 8.12$ Hz, 1H), 3.65 (s, 3H), 3.29-3.23 (m, 1H), 2.78-2.60 (m, 2H), 1.88-1.80 (m, 1H), 1.53-1.48 (m, 1H), 1.13 (d, $J = 6.23$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 151.9, 138.9, 122.5, 115.3, 114.7, 112.9, 55.8, 47.5, 30.3, 26.9, 22.6; EI-MS for $\text{C}_{11}\text{H}_{15}\text{NO}$ $[\text{M}+1]^+$ calcd: 178.3; found 178.2. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-OJ-H (hexanes: *i*-PrOH 95: 5 at 0.5 mL / min): $t_S = 38.5$ min, $t_R = 46.9$ min.

2,6-Dimethyl-1,2,3,4-tetrahydroquinoline (**3j**): ^1H NMR (300 MHz, CDCl_3): δ 6.81-6.78 (m, 2H), 6.42 (d, $J = 8.41$ Hz, 1H), 3.42-3.35 (m, 1H), 2.83-2.68 (m, 2H), 2.22 (s, 3H), 1.96-1.89 (m, 1H), 1.64-1.57 (m, 1H), 1.22 (d, $J = 6.26$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 142.4, 129.8, 127.2, 126.3, 121.3, 114.3, 47.3, 30.4, 26.6, 22.6, 20.4; EI-MS for $\text{C}_{11}\text{H}_{15}\text{N}$ $[\text{M}+1]^+$ calcd: 162.3; found 178.2. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-OJ-H (hexanes: *i*-PrOH 90: 10 at 0.5 mL / min): $t_S = 22.6$ min, $t_R = 27.4$ min.

6-Fluoro-2-methyl-1,2,3,4-tetrahydroquinoline (**3j**): ^1H NMR (300 MHz, CDCl_3): δ 6.71-6.66 (m, 2H), 6.43-6.38 (m, 1H), 3.369-3.32 (m, 1H), 2.83-2.72 (m, 2H), 1.95-1.89 (m, 1H), 1.60-1.54 (m, 1H), 1.21 (d, $J = 6.26$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3): δ 157.1, 154.0, 141.0, 122.5, 122.4, 115.4, 115.2, 114.8, 114.7, 113.3, 113.0, 47.3, 29.9, 26.7, 22.5; EI-MS for $\text{C}_{10}\text{H}_{12}\text{FN}$ $[\text{M}+1]^+$ calcd: 166.2; found 166.1. Enantiomeric excess of the product was measured by chiral stationary phase HPLC analysis using Chiracel-OD-H (hexanes: *i*-PrOH 95: 5 at 0.5 mL / min): $t_{\text{S}} = 13.5$ min, $t_{\text{R}} = 15.6$ min.

5. Spectra of the dendritic BINAP ligands

^1H NMR ($\text{G}_1\text{DenBINAP}$):

¹³C NMR (G₁DenBINAP):

³¹P NMR (G₁DenBINAP):

MALDI-TOF (**G₁DenBINAP**):

HRMS (FAB) (**G₁DenBINAP**):

¹H NMR (G₂DenBINAP):

¹³C NMR (G₂DenBINAP):

^{31}P NMR ($\text{G}_2\text{DenBINAP}$):

MALDI-TOF ($\text{G}_2\text{DenBINAP}$):

¹H NMR (G₃DenBINAP):

¹³C NMR (G₃DenBINAP):

³¹P NMR (G₃DenBINAP):

MALDI-TOF (G₃DenBINAP):

¹H NMR (G₄DenBINAP):

¹³C NMR (G₄DenBINAP):

³¹P NMR (G₄DenBINAP):

6. Spectra of the reduced products

Current Data Parameters
NAME wzj4Hquinoline
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061013
Time 21:26
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 5172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084880 sec
RG 64
DM 81.000 uSBC
DE 8.00 uSBC
TE 300.2 K
D1 2.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.30 uSBC
PL1 -1.00 dB
SFO1 300.1318634 MHz

F2 - Processing parameters
SI 32768
SF 300.1300658 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.500 ppm
F1 3151.36 Hz
F2P -0.500 ppm
F2 -160.06 Hz
PPMCH 0.55000 ppm/cm
HZCH 180.07150 Hz/cm

Current Data Parameters
NAME wzj4Hquinoline
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061013
Time 21:31
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 17380.011 Hz
FIDRES 0.274439 Hz
AQ 1.6219958 sec
RG 4096
DM 27.800 uSBC
DE 8.00 uSBC
TE 300.2 K
D1 2.0000000 sec
S11 0.03000000 sec
S12 0.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 uSBC
PL1 -1.00 dB
SFO1 75.4753293 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 uSBC
PL2 -1.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 300.1312006 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 200.000 ppm
F1 10063.06 Hz
F2P -4.000 ppm
F2 -377.34 Hz
PPMCH 9.31818 ppm/cm
HZCH 763.22217 Hz/cm

2-phenethyl-4H-quinoline-E

Current Data Parameters
NAME wzj4Hquinolin-
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060823
Time 21:51
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 13
DS 4
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3094860 sec
RG 101.6
DM 81.000 usec
DE 8.00 usec
TE 300.2 K
D1 2.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 -1.00 dB
SFO1 300.1318634 MHz

F2 - Processing parameters
SI 32768
SF 300.1300266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.500 ppm
F1 3151.37 Hz
F2P -0.500 ppm
F2 -160.06 Hz
PPMCH 0.66000 ppm/cm
HZCH 180.07152 Hz/cm

Current Data Parameters
NAME wzj4Hquinolin-
EXPNO 61
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060823
Time 21:56
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 61
DS 4
SWH 17380.011 Hz
FIDRES 0.274439 Hz
AQ 1.6219908 sec
RG 724.1
DM 27.800 usec
DE 8.00 usec
TE 300.2 K
D1 2.0000000 sec
d11 0.0300000 sec
d12 0.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 75.4753193 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -1.00 dB
PL12 16.00 dB
PL13 16.00 dB
SFO2 300.1312006 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 200.000 ppm
F1 10063.06 Hz
F2P -4.000 ppm
F2 -377.34 Hz
PPMCH 9.31818 ppm/cm
HZCH 763.22217 Hz/cm

Current Data Parameters
NAME wj-628-THF-J-1
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060913
Time 16 05
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084860 sec
RG 90.5
DM 81.000 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 9.30 usec
PL1 -1.00 dB
SFO1 300.1318634 MHz

F2 - Processing parameters
SI 32768
SF 300.1300560 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 10.600 ppm
F1 3101.36 Hz
F2P 0.500 ppm
F2 -150.07 Hz
APPCN 0.68000 ppm/cm
HZCN 150.08500 Hz/cm

Current Data Parameters
NAME wj-628-THF-J-1
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060913
Time 16 11
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 17986.011 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1280.2
DM 27.800 usec
DE 6.00 usec
TE 301.2 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.0002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 75.476363 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 300.1312006 MHz

F2 - Processing parameters
SI 32768
SF 75.467354 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 200.000 ppm
F1 10063.06 Hz
F2P -5.000 ppm
F2 -371.12 Hz
APPCN 9.31818 ppm/cm
HZCN 703.22206 Hz/cm

Chemical structure: C1=CC=C2C(=C1)N(C2)CC3CCCCC3O

¹H NMR spectrum (400 MHz, CDCl₃) data:

Chemical Shift (ppm)	Integration
~10.2	0.991
7.2 - 7.5	1.994
6.5 - 6.8	1.000
3.3 - 3.5	1.182
2.2 - 2.5	2.245
1.5 - 1.8	1.082
1.2 - 1.4	12.843
1.0 - 1.2	1.431

```

Current Data Parameters
NAME      w1-528-THF-f-1
EXPNO     20
PROCNO    1

D2 - Acquisition Parameters
Date_      20061024
Time       20 40
INSTRUM    ag
PROBHD      5 mm NMR D5-13
PULPROG     zgpg30
TD          65536
SOLVENT     DMSO
NS          16
DS          2
SWH         6172.933 Hz
FIDRES      0.094190 Hz
AQ          5.3048680 sec
RG          101.0
DE          81.810000 MHz
TE          299.4 K
D1          2.00000000 sec

----- CHANNEL f1 -----
NUC1        13
P1          9.30 usec
PL1         -1.00 dB
SFO1        300.115584 MHz

D2 - Processing parameters
F1          32768
SF          300.1300923 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

ID NMR job parameters
C1          12 80.00 cm
C2          12 80.00 cm
CP          20 20.00 cm
P1          3101.35 usec
F2P         -0.500 MHz
F2          -169.07 Hz
NUC2        0 500.000000 ppm/Hz
FQ2         150.000000 Hz/cm

```

13C NMR spectrum of compound 1. The x-axis is labeled 'ppm' and ranges from 0 to 180. The spectrum shows several sharp peaks. Key peaks are labeled with their chemical shifts: 144.968, 129.233, 126.702, 120.952, 116.703, 114.461, 77.501, 77.078, 76.854, 72.571, 47.848, 40.617, 35.838, 29.950, 26.631, 25.766, 22.245, and 22.483. The peak at 77.078 ppm is the most intense, indicating the solvent (CDCl₃).

```

Current Data Parameters
NAME          m31-G08-Tr-F-1
PCPWR0        21
FXFREQ0       1

F2 - Acquisition Parameters
Data_         20061024
Time          17:00
INSTRUM       mw300
PWR0          5 MW @ 130-1
FREQ0         1.6510000 MHz
T0            65526
DELTA0        0.0213
DELTA0        5.7
DELTA0        4
SM1           17880 MHz
FIDRES        0.274433 Hz
AQ            1.6510000 sec
PCPWR1        1280.2
SM0           27.980 uBBB
AQ            1.6510000 sec
TC            2300 s
OL            2.0000000 sec
OL1           0.3300000 BNC
OL2           0.0005000 BNC

***** CHANNEL f1 *****
PL1           9.4 dB
PL2           -1.00 dB
SF02          75.478293 MHz

***** CHANNEL f2 *****
OCPWR02       141216
PCPWR0        89.00 uBBB
PL2           -1.00 dB
PL3           18.00 dB
PL4           18.00 dB
SF02          300.1392005 MHz

F2 - Processing parameters
SI            37.768
SF            75.467490 MHz
ADW           1.00
SGB0          1.00 Hz
SGB1          1.00 Hz
PC            1.00 Hz

10 MHz plot parameters
F2            27.98 MHz
CY            5.00 dB
F1P           200.000 BPP
F1F           200.000 BPP
F2P           -5.00 dB
F2F           -37.374 dB
PVCEN         5.31810 dBp/Hz
PVCN          768.00 dB/Hz

```

2-benzophenone-subed-4H-quinaldine-1

Current Data Parameters
NAME wzj4quinalin-
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060924
Time 9.43
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084860 sec
RG 181
DM 81.000 usec
DE 8.00 usec
TE 301.4 K
D1 2.0000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 9.30 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1306177 MHz
WF 64
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 5.00 cm
F1P 10.600 ppm
F1 3151.36 Hz
F2P -0.500 ppm
F2 -160.07 Hz
PPHM 0.50000 ppm/cm
HZCN 150.08500 Hz/cm

2-benzophenone-subed-4H-quinaldine-1

Current Data Parameters
NAME wzj4quinalin-
EXPNO 121
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060924
Time 9.48
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 93
DS 4
SWH 17888.011 Hz
FIDRES 0.274439 Hz
AQ 1.6019008 sec
RG 1024
DM 27.800 usec
DE 8.00 usec
TE 301.5 K
D1 2.0000000 sec
d11 0.0300000 sec
d12 0.0000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 8.40 usec
PL1 -1.00 dB
SFO1 75.4752993 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.00 dB
PL13 16.00 dB
SFO2 300.1312000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677480 MHz
WF 64
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 10.00 cm
F1P 200.000 ppm
F1 10062.08 Hz
F2P -5.000 ppm
F2 -371.34 Hz
PPHM 5.31818 ppm/cm
HZCN 763.23217 Hz/cm

6-MeO-4Hquinolindine

Current Data Parameters
NAME wj4Hquinolindin-
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060623
Time 21:39
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3094860 sec
RG 143.7
DM 81.000 uSBC
DE 8.00 uSBC
TE 300.2 K
D1 2.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.30 uSBC
PL1 -1.00 dB
SFO1 300.1318634 MHz

F2 - Processing parameters
SI 32768
SF 300.1300266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.500 ppm
F1 3151.37 Hz
F2P -0.500 ppm
F2 -160.06 Hz
PPMCH 0.65000 ppm/cm
HZCM 180.07152 Hz/cm

Current Data Parameters
NAME wj4Hquinolindin-
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060623
Time 21:42
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 60
DS 4
SWH 17380.011 Hz
FIDRES 0.274439 Hz
AQ 1.6219908 sec
RG 645.1
DM 27.800 uSBC
DE 8.00 uSBC
TE 300.2 K
D1 2.0000000 sec
d11 0.0300000 sec
d12 0.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 uSBC
PL1 -1.00 dB
SFO1 75.4753193 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 uSBC
PL2 -1.00 dB
PL12 16.00 dB
PL13 16.00 dB
SFO2 300.1312006 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 200.000 ppm
F1 10063.06 Hz
F1P -4.000 ppm
F2 -377.34 Hz
PPMCH 9.31818 ppm/cm
HZCM 763.22217 Hz/cm

Current Data Parameters
NAME wj44quinolin-
EXPNO 119
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060524
Time 9 27
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084860 sec
RG 181.3
DM 81.000 usec
DE 6.00 usec
TE 301.4 K
D1 2.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 9.30 usec
PL1 -1.00 dB
SFO1 300.1318634 MHz

F2 - Processing parameters
SI 32768
SF 300.1300650 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 10.600 ppm
F1 3101.36 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PRCM 0.58000 ppm/cm
HZCM 150.08500 Hz/cm

Current Data Parameters
NAME wj44quinolin-
EXPNO 111
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060524
Time 3.30
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 116
DS 4
SWH 17986.011 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1140.4
DM 27.800 usec
DE 6.00 usec
TE 301.7 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.40 usec
PL1 -1.00 dB
SFO1 75.4763293 MHz

===== CHANNEL f2 =====
CPDPRG2 wj4216
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 300.1312008 MHz

F2 - Processing parameters
SI 32768
SF 75.4671480 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 280.000 ppm
F1 10993.08 Hz
F2P -5.000 ppm
F2 -371.13 Hz
PRCM 9.31818 ppm/cm
HZCM 703.22217 Hz/cm

References

1. Huang, Y. Y.; Deng, G. J.; Wang, X. Y.; Fan, Q. H. *Chinese J. Chem.* **2004**, 22, 891.
2. Wang, W.; Lu, S.; Yang, P.; Han, X.; Zhou, Y. *J. Am. Chem. Soc.* **2003**, 125, 10536.