Transfer Hydrogenation of Activated C=C Bonds Catalyzed by Ruthenium Amido-Complexes: Reaction Scope, Limitation and Enantioselectivity

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General Methods. Melting points were determined in open capillaries and were uncorrected. NMR spectra were recorded with tetramethylsilane as the internal standard. Column chromatography was performed using silica gel (200-300 mesh) eluting with ethyl acetate and petroleum ether or menthol and Methylene chloride. Optical rotations were measured at 589 nm. TLC was performed on glass-backed silica plates. Enantiomeric excess was determined by HPLC analysis on Chiralpak OD, AD and OJ columns and GC analysis on a CP CHIPASIL-DEX column. Commercial grade solvents were dried and purified by standard procedures as specified in Purification of Laboratory Chemicals, 4th Ed (Armarego, W. L.F.; Perrin, D. D. Butterworth Heinemann: 1997). Methylene chloride was distilled from CaH₂. Methanol was distilled from Mg. All catalytic reactions and manipulations were performed under argon.

General procedure for monosulfonylation of chiral Ligands, 2a-2h

Chiral 1,2-diphenylenediamine was prepared in our laboratory according to Corey procedure,¹ $[\alpha]_D^{20} +106.7^\circ$ (c 1.0, CH₃OH). To a stirred solution of (*R,R*)-Diamine (1.0 mmol) and DIPEA (0.19 mL, 1.1 mmol) in DCM (10 mL) was added a solution of arylsulfonyl chloride (1.1 mmol) in DCM (5 mL) dropwise at 0 °C. The solution was stirred overnight at room temperature. After washed with water, the solution was dried, concentrated and flash chromatography (DCM/methanol) gave the monosulfonylated ligand.

(2c)² Yield: 74%; White solid. Mp: 174.3-176.1°C; $[\alpha]_D^{28} +39.3^\circ$ (c 0.16, CHCl₃). ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.44-7.32 (m, 10H), 4.70 (d, $J = 2.7$ Hz, 1H), 4.40 (d, $J = 2.9$ Hz, 1H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 140.4, 139.2, 128.9, 128.8, 128.2, 128.1, 126.3, 125.9, 121.2, 116.9, 64.1, 60.1.

(2d)³ Yield: 85%; Solid. Mp: 121.2 -123.4°C; $[\alpha]_D^{28} +89.3^\circ$ (c 0.58, CHCl₃). ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 8.61 (d, $J = 8.0$ Hz, 1H), 7.85 (d, $J = 9.8$ Hz, 1H), 7.77 (dd, $J = 7.38$ Hz, 1.1Hz) 7.63 (dt, $J = 6.7, 3.0$ Hz, 1H), 7.55 (dt, $J = 8.1, 1.2$ Hz, 1H), 7.18 (t, $J = 7.6$ Hz, 1H), 6.93 (m, 10H), 4.39 (d, $J = 6.0$ Hz, 1H), 4.01(d, $J = 6.0$ Hz, 1H), 1.28(m, 3H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 141.1, 138.5, 134.9, 133.9, 133.5, 129.2, 128.7, 128.0, 127.8, 127.7, 127.29, 127.2, 126.7, 126.3, 126, 124.7, 123.7, 63.6, 60.3; IR (KBr) ν 3379, 3300, 3060, 1595, 1500, 1454, 1320, 1055, 981, 804, 769, 592 cm⁻¹.

(2h)⁴ Yield: 73%; Glassy solid; $[\alpha]_D^{28} +49.4^\circ$ (c 0.36, CHCl₃). ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.17-6.92 (m, 10H), 6.82 (s, 1H), 6.79 (s, 1H), 4.47 (d, $J = 7.9$ Hz, 1H), 4.01-3.91 (m, 3H), 2.87-2.78 (m, 1H), 1.21-1.15 (m, 12H), 1.04 (d, $J = 6.9$ Hz, 6H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 152.2, 149.6, 141.8, 138.6, 133.9, 128.2, 127.7, 127.4, 127.3, 127.2, 126.8, 123.2, 63.6, 61.1, 34.0, 24.8, 24.7, 23.6, 23.5, 19.7; IR (KBr) 3289, 2959, 1601, 1457, 1317, 1151 cm⁻¹; HRMS (ESI) calcd for C₂₉H₃₈N₂O₂S+H 479.2732, obsd 479.2727.

Procedure for preparation of ligand 2k and 2l

To a stirred solution of (*R,R*)-1,2-bis(2-nitrophenyl)ethane-1,2-diamine⁵ (303 mg, 1.0 mmol) and DIPEA (0.19 mL, 1.1 mmol) in DCM (10 mL) was added a solution of the arylsulfonyl chloride (1.1 mmol) in DCM (5 mL) dropwise at 0 °C. The solution was stirred overnight at room temperature. After washed with water, the solution was dried, concentrated and flash chromatography (DCM/methanol) gave the ligand **2k** or **2l**.

Procedure for preparation of the ligand 2m

To a suspension of (*R,R*)-*N*-Boc-*N*-Boc-1,2-bis(2-acetoamido-phenyl)ethane-1,2-diamine⁵ (263 mg, 0.5 mmol) in EtOAc was added HCl/EtOAc (2 mL) in an ice bath. The mixture was stirred and the solid was dissolved rapidly. After 3h, the solvent was removed in vacuum. The mixture was neutralized with ammonia and stirred at room temperature for 1h and water was removed in vacuum. The resulting solid was dissolved in CH₂Cl₂ (10 mL) and DIPEA (0.1 mL, 0.6 mmol) in DCM (5 mL) and a solution of 4-methylbenzene-1-sulfonyl chloride (105 mg, 0.55 mmol) in DCM (5 mL) was added dropwise at 0 °C. The solution was stirred

overnight at room temperature. After washed with water, the solution was dried, concentrated and flash chromatography (DCM/methanol) gave the ligand **2m**.

Procedure for preparation of the ligand **2n**

To a suspension of (*R,R*)-*N*-Boc-*N*-Boc-1,2-bis(2-acetoamido-phenyl) ethane-1,2-diamine⁵ (305 mg, 0.5 mmol) in EtOAc was added HCl/EtOAc (2 mL) in an ice bath. The mixture was stirred and the solid was dissolved rapidly. After 3h, the solvent was removed in vacuum. The mixture was neutralized with ammonia and stirred at room temperature for 1h and water was removed in vacuum. The resulting solid was dissolved in CH₂Cl₂ (10 mL) and DIPEA (0.1 mL, 0.6 mmol) in DCM (5 mL) and a solution of 4-methylbenzene-1-sulfonyl chloride (105 mg, 0.55 mmol) in DCM (5 mL) was added dropwise at 0 °C. The mixture was stirred overnight at room temperature. After washed with water, the solution was dried, concentrated and flash chromatography (DCM/methanol) gave the ligand **2n**.

Procedure for preparation of the ligand **2p**¹

To a stirred solution of (*R,R*)-1,2-bis(4-methoxyphenyl)ethane-1,2-diamine¹ (272 mg, 1.0 mmol) and DIPEA (0.19 mL, 1.1 mmol) in DCM (10 mL) was added a solution of 2,4,6-triethylbenzene-1-sulfonyl chloride (282 mg, 1.1 mmol) in DCM (5 mL) dropwise at 0 °C. The solution was stirred overnight at room temperature. After washed with water, the solution was dried, concentrated and flash chromatography (DCM/methanol) gave **2p**.

Procedure of the transfer hydrogenation of α,β -unsaturated ketones and olefins

Diamine ligand (0.0028 mmol), [RuCl₂(cymene)]₂ (0.76 mg, 0.00125 mmol) and triethylamine (0.69 μ L, 0.005 mmol) were heated in methanol (0.5 mL) for 0.5h. Methanol was then removed under vacuum. Olefin substrate (0.5 mmol) in DCM (0.5 mL) and azeotrope of formic acid and triethylamine (0.2 mL) were added in turn. The mixture was stirred at 30°C. After completion, the solution was diluted with EtOAc, washed with water, and dried. Flash chromatography gave the pure products.

(*E*)-4-Phenylbut-3-en-2-ol (4a) Colorless oil; $[\alpha]_D^{25} +0.9^\circ$ (c 0.24, CHCl₃). ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.40-7.23 (m, 5H), 6.57 (d, *J* = 16.7 Hz, 1H), 6.26 (dd, *J* = 16.7, 6.5 Hz, 1H), 4.51-4.47 (m, 1H), 1.62 (s, OH), 1.37 (d, *J* = 6.4 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 136.7, 133.5, 129.4, 128.4, 127.6, 126.4, 68.9, 23.4. 39% ee was determined by HPLC on OD column, 15% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, *t*_{major} = 6.78 min, *t*_{minor} = 9.67 min.

(E)-3-Methyl-4-phenylbut-3-en-2-ol (4b) Colorless oil; $[\alpha]_D^{25} -7.0^\circ$ (c

0.27, CHCl_3). ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.38-7.23 (m, 5H),

6.54 (s, 1H), 4.41 (q, $J = 6.6$ Hz, 1H), 1.91 (s, 3H), 1.62 (s, OH), 1.39 (d, $J = 6.6$ Hz, 3H); ^{13}C

NMR (CDCl_3 , 75 MHz), δ (ppm) 141.6, 137.6, 128.9, 128.1, 126.3, 124.3, 73.5, 21.7, 13.4.

76% ee was determined by HPLC on OD column, 2.5% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, $t_{\text{major}} = 13.62$ min, $t_{\text{minor}} = 15.96$ min.

(E)-3-Methyl-4-(4-nitrophenyl)but-3-en-2-ol (4c) Yellow oil;

$[\alpha]_D^{25} -1.8^\circ$ (c 0.22, CHCl_3). ^1H NMR (CDCl_3 , 300 MHz), δ (ppm)

8.18 (2H, d, $J = 8.8$ Hz), 7.40 (2H, d, $J = 8.8$ Hz), 6.59 (1H, s, CH),

4.39 (1H, q, $J = 6.4$ Hz), 1.90 (s, 3H), 1.38 (d, $J = 6.4$ Hz, 3H); ^{13}C NMR (CDCl_3 , 75 MHz), δ

(ppm) 145.9, 144.6, 129.5, 123.4, 122.3, 73.0, 21.9, 14.0. 38% ee was determined by HPLC

on OD column, 2.5% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, $t_{\text{major}} = 27.13$ min, $t_{\text{minor}} = 30.40$ min.

(E)-4-(4-Methoxyphenyl)-3-methylbut-3-en-2-ol (4d)

Colorless oil; $[\alpha]_D^{25} -10.6^\circ$ (c 0.32, CHCl_3). ^1H NMR (CDCl_3 ,

300 MHz), δ (ppm) 7.20 (d, $J = 8.8$ Hz, 2H), 6.88 (d, $J = 8.8$ Hz,

2H), 6.44 (s, 1H), 4.35 (q, $J = 6.0$ Hz, 1H), 1.90 (s, OH), 3.80 (s, 3H), 1.87 (s, 3H), 1.35 (d, J

= 6.4 Hz, 3H); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 158.0, 139.8, 130.2, 130.1, 123.8, 113.8,

113.5, 73.6, 55.1, 21.6, 13.2. 69% ee was determined by HPLC on AD column, 2.5%

2-propanol/hexane, 1.0 mL/min, UV 254 nm, $t_{\text{major}} = 20.97$ min, $t_{\text{minor}} = 19.35$ min.

1,3-Diphenylpropan-1-one (5e) White solid. Mp: 51.6-52.9°C; ^1H

NMR (Aceton- d_6 , 300 MHz), δ (ppm) 7.98 (2H, d, $J = 7.5$ Hz, Ph-H),

7.58 (1H, t, $J = 7.2$ Hz, Ph-H), 7.47 (2H, t, $J = 7.5$ Hz, Ph-H), 7.38-7.03 (5H, m, Ph-H), 3.33 (2H, t, $J = 8.1$ Hz, CH₂), 3.09 (2H, t, $J = 7.8$ Hz, CH₂); ¹³C NMR (Aceton-d₆, 75 MHz), δ (ppm) 199.1, 141.3, 136.8, 133.0, 128.5, 128.4, 128.2, 128.0, 126.1, 40.4, 30.1.

1,3-Diphenylpropan-1-ol (6e) Colorless oil. $[\alpha]_D^{25} +24.1^\circ$ (c 0.22, EtOAc) ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.37-7.18 (m, 10H), 4.71-4.67 (m, 1H), 2.82-2.67 (m, 2H), 2.17-2.14 (m, 2H), 1.63 (s, 1H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 144.5, 141.7, 128.5, 128.4, 128.3, 128.2, 127.6, 125.9, 73.8, 40.4, 32.0. 93% ee was determined by HPLC on OD column, 10% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, $t_{\text{major}} = 9.05$ min, $t_{\text{minor}} = 10.38$ min.

3-Benzylpentane-2,4-dione (5f) Colorless oil. ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.31-7.14 (5H, m, Ph-H), 4.01 (t, $J = 7.6$ Hz, CH), 3.66 (s, CH₂), 3.15 (d, $J = 7.5$ Hz, CH₂), 2.12 (s, CH₃), 2.07 (s, CH₃); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 203.5, 191.9, 139.6, 137.9, 128.7, 128.6, 128.5, 127.4, 126.7, 126.3, 108.2, 69.9, 34.2, 32.8, 29.7, 23.3. *Enolization product was observed.*

Ethyl 2-benzyl-3-oxo-3-phenylpropanoate (5g) Colorless oil. ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.96 (dd, $J = 7.2, 0.71$ Hz, 2H), 7.54 (t, $J = 7.3$ Hz, 1H), 7.44 (t, $J = 7.2$ Hz, 2H), 7.27-7.21 (m, 5H), 4.62 (t, $J = 7.3$ Hz, 1H), 4.11 (q, $J = 7.1$ Hz, 2H), 3.32 (d, $J = 7.3$ Hz, 2H), 1.10 (t, $J = 7.1$ Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 194.5, 169.2, 138.4, 136.2, 133.5, 128.9, 128.7, 128.6, 128.5, 126.6, 61.5, 56.1, 34.7, 13.9.

3-Acetyl-3, 4-dihydrochromen-2-one (5h) White solid. ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 13.4 (s, 1H), 7.26-7.00 (4H, m, Ar-H), 3.69 (s,

2H), 2.12 (s, 3H); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 177.3, 168.9, 150.2, 128.4, 128.3, 127.9, 124.9, 124.5, 119.9, 116.8, 116.7, 90.5, 52.4, 25.9, 25.7, 19.2. *Enolization product was observed.*

1-(2-Nitroethyl) benzene (8b) Yellow oil. ^1H NMR (CDCl_3 , 200 MHz), δ (ppm) 7.33-7.18 (5H, m, Ph-H), 4.61 (2H, t, $J = 7.4$ Hz, CH_2), 3.32 (2H, t, $J = 7.4$ Hz, CH_2); ^{13}C NMR (CDCl_3 , 50 MHz), δ (ppm) 135.6, 128.8, 128.5, 127.3, 76.1, 33.3.

1-Nitro-1,2-diphenylethane (8c) Colorless oil. ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.53-7.40 (5H, m, Ph-H), 7.29-7.15 (m, 5H), 5.69 (1H, dd, $J = 5.8, 9.4$ Hz, CH), 3.80 (1H, dd, $J = 9.4, 14.3$ Hz, CH_2), 3.35 (1H, dd, $J = 5.8, 14.3$ Hz, CH_2); ^{13}C NMR (CDCl_3 , 50 MHz), δ (ppm) 135.5, 134.3, 130.0, 129.1, 129.0, 128.8, 127.7, 127.4, 92.6, 40.4. Ee: determined by HPLC on AD column, 1% 2-propanol/hexane, 1.0 mL/min, $t_1 = 9.75$ min, $t_2 = 10.99$ min.

2-(4-Chlorophenyl)-3-phenylpropanenitrile (8d) ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.33-7.27 (5H, m, Ar-H), 7.18-7.09 (m, 4H), 3.99 (1H, t, $J = 7.2$ Hz, CH), 3.22-3.07 (2H, m, CH_2); ^{13}C NMR (CDCl_3 , 50 MHz), δ (ppm) 135.8, 134.2, 133.6, 129.2, 129.1, 128.9, 128.7, 127.5, 119.9, 42.0, 39.1. Ee: determined by HPLC on OD column, 10% 2-propanol/hexane, 1.0 mL/min, $t_1 = 10.98$ min, $t_2 = 12.59$ min.

Dimethyl 2-benzylmalonate (8e) Colorless oil. ^1H NMR (CDCl_3 , 200 MHz), δ (ppm) 7.27-7.16 (5H, m, Ph-H), 3.6-3.7 (4H, m, CH,

CH₃), 3.21 (2H, d, J = 7.9 Hz, CH₂); ¹³C NMR (CDCl₃, 50 MHz), δ (ppm) 169.1, 137.6, 128.6, 128.5, 126.7, 53.5, 32.4, 34.6.

Ethyl 2-cyano-3-phenylpropanoate (8f) Colorless oil. ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.37-7.26 (5H, m, Ph-H), 4.23 (2H, q, J =

7.2 Hz, CH₂), 3.74-3.67 (1H, m, CH), 3.32-3.15 (2H, m, CH₂), 1.27 (3H, t, J = 7.2 Hz, CH₃);

¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 165.5, 135.2, 128.9, 128.8, 127.7, 116.1, 62.9, 39.6, 35.7, 13.9.

Ethyl 2-nitro-3-phenylpropanoate (8g) Colorless oil. ¹H NMR (CDCl₃, 200 MHz), δ (ppm) 7.32-7.18 (5H, m, Ph-H), 5.37-5.29 (1H,

m, CH), 4.27 (2H, q, J = 7.1 Hz, CH₂), 3.55-3.48 (2H, m, CH₂), 1.27 (3H, t, J = 7.1 Hz, CH₃);

¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 164.0, 134.0, 129.7, 129.5, 128.9, 127.9, 127.7, 89.1, 56.9, 36.1, 13.8.

Ethyl 2-cyano-3-(4-nitrophenyl)propanoate (8h) Colorless oil. ¹H NMR (CDCl₃, 200 MHz), δ (ppm) 8.22 (2H, d, J = 8.6 Hz,

Ar-H), 7.47 (2H, d, J = 8.6 Hz, Ar-H), 4.26 (2H, q, J = 7.1 Hz,

CH₂), 3.82-3.75 (1H, m, CH), 3.36-3.24 (2H, m, CH₂), 1.28 (3H, t, J = 7.1 Hz, CH₃); ¹³C

NMR (CDCl₃, 75 MHz), δ (ppm) 164.8, 147.4, 142.6, 130.2, 123.9, 115.5, 63.3, 38.7, 34.9,

13.9.

Ethyl 2-cyano-3-(4-methoxyphenyl)propanoate (8i)

Colorless oil. ¹H NMR (CDCl₃, 200 MHz), δ (ppm) 7.19 (2H, d,

J = 8.6 Hz, Ar-H), 6.86 (2H, d, J = 8.6 Hz, Ar-H), 4.23 (q, J = 7.1 Hz, 2H, CH₂), 3.79 (3H, s,

CH₃), 3.71-3.64 (1H, m, CH), 3.20-3.14 (2H, m, CH₂), 1.27 (3H, t, J = 7.1 Hz, CH₃); ¹³C

NMR (CDCl₃, 75 MHz), δ (ppm) 165.5, 159.0, 130.1, 127.2, 116.2, 114.1, 62.8, 55.2, 39.9, 34.9, 13.9.

Ethyl 2-cyano-octanoate (8j) Colorless oil. ¹H NMR (CDCl₃, 200 MHz), δ (ppm) 4.26 (2H, q, J = 7.1 Hz, CH₂), 3.47 (1H, t, J = 7.1 Hz, CH), 1.99-1.88 (2H, m, CH₂), 1.55-1.28 (11H, m, CH₃, (CH₂)₄), 0.88 (3H, t, J = 6.6 Hz, CH₃); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 166.2, 116.6, 62.6, 37.5, 31.3, 29.8, 28.3, 26.6, 22.4, 13.9.

2-Benzylmalononitrile (8k) ¹H NMR (CDCl₃, 200 MHz), δ (ppm) 7.46-7.28 (5H, m, Ph-H), 3.90 (1H, t, J = 7.0 Hz, CH), 3.28 (2H, d, J = 7.0 Hz, CH₂); ¹³C NMR (CDCl₃, 50 MHz), δ (ppm) 132.9, 129.1, 128.8, 128.6, 112.2, 36.4, 24.8.

2-Phenylpropanoic acid (8m) Colorless oil; $[\alpha]_D^{25}$ -3.6° (c 0.33, CHCl₃). ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.34-7.27 (m, 5H), 3.74 (q, J = 7.1 Hz), 1.52 (d, J = 7.1 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 180.6, 139.7, 128.6, 127.5, 127.3, 45.3, 18.0. 7% ee was determined by GC on CP-Cyclodex-236M column, T_c = 150 °C, H₂ = 10 psi, t_{major} = 10.03 min, t_{minor} = 9.62 min.

Ethyl 2-Phenylpropanoate (8n) Colorless oil; $[\alpha]_D^{25}$ -10.9° (c 0.45, CHCl₃). ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.33-7.25 (m, 5H, ArH), 4.10 (q, J = 7.1 Hz, 2H, CH₂), 3.70 (q, J = 7.1 Hz, 1H, CH₂), 1.50 (d, J = 7.1 Hz, 3H, CH₃), 1.21 (t, J = 7.1 Hz, 3H, CH₃); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 174.5, 140.6, 128.5, 128.0, 127.4, 127.0, 60.6, 45.5, 18.5, 14.1. 20% ee was determined by HPLC on OJ column, 5% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, t₁ = 9.25 min, t₂ = 8.30 min.

2-(1-Phenylethyl)malononitrile (8r) Colorless oil; $[\alpha]_D^{28} -17.2^\circ$ (c 1.20, CHCl_3). ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.41-7.31 (m, 5H), 3.85 (d, $J = 6.2$ Hz, 1H), 3.50-3.41 (m, 1H), 1.66 (d, $J = 7.1$ Hz, 3H); ^{13}C NMR (CDCl_3 , 50 MHz), δ (ppm) 138.2, 129.2, 128.8, 127.2, 111.9, 111.7, 41.1, 31.2, 17.7. 73% ee was determined by HPLC on OD column, 20% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, $t_S = 10.89$ min, $t_R = 12.74$ min.

General procedures for the preparation of olefins 7r and 10a-i⁶

Malononitrile (32 mmol) and the ketone (28 mmol) were dissolved in 20 mL of toluene containing ammonium acetate (500 mg, 6.5 mmol) and glacial acetic acid (2 mL) in a 50 mL flask. By refluxing vigorously, the water formed in the reaction was removed by a Dean and Stark trap placed under the reflux condenser. Evaporation of the toluene left a residue that was recrystallized from alcohol or distilled under vacuum to give pure products.

2-(2,3-Dihydronaphthalen-4(1H)-ylidene) malononitrile (10a) Yield: 88%; White solid. Mp: 115.3-117.8°C; ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 8.20 (dd, $J = 7.9, 0.6$ Hz, 1H), 7.48 (dd, $J = 7.5, 1.2$ Hz, 1H), 7.36-7.27 (m, 2H), 3.02 (t, $J = 6.3$ Hz, 2H), 2.89 (t, $J = 6.2$ Hz, 2H), 1.97 (t, $J = 6.5$ Hz, 2H); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 172.4, 141.9, 133.6, 133.2, 129.9, 129.4, 127.8, 126.7, 113.9, 113.3, 79.6, 32.9, 29.6, 22.0; MS (EI) m/z 50, 65, 82, 114, 126, 130, 139, 252, 165, 179, 194 (M^+).

2-(1,2-Dihydroinden-3-ylidene) malononitrile (10b) Yield: 40%; solid. Mp: 157.2-159.3 °C; ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 8.39 (d, $J =$

8.1Hz, 1H, ArH), 7.63-7.58 (m, 1H, ArH) 7.50-7.40 (m, 2H, ArH), 3.28 (t, $J = 6.2$ Hz, 2H, CH₂), 3.19 (t, $J = 6.2$ Hz, 2H, CH₂); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 179.2, 154.0, 135.6, 135.1, 128.0, 126.2, 126.0, 113.4, 112.8, 34.5, 29.6.

2-(1-Phenylethylidene) malononitrile (7r) Yield: 61%. ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.56-7.50 (m, 5H, ArH), 2.63 (s, 3H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 175.4, 135.7, 132.1, 128.9, 127.2, 112.7, 112.6, 84.5, 24.1.

2-(2,3-Dihydrochromen-4-ylidene) malononitrile (10c) Yield: 60%; Solid. Mp: 155.7- 158.4 °C; ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 8.36 (d, $J = 6.9$ Hz, 1H, ArH), 7.50-7.46 (m, 1H, ArH), 7.06-6.96 (m, 2H, ArH), 4.38 (t, $J =$

6.2 Hz, 2H, CH₂), 3.13 (t, $J = 6.2$ Hz, 2H, CH₂); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 163.3, 157.3, 136.7, 127.2, 121.5, 118.6, 117.1, 113.6, 113.1, 64.6, 30.8; MS (EI) m/z 38, 64, 90, 113, 170, 196 (M⁺).

2-(6-Bromo-2,3-dihydronaphthalen-4(1H)-ylidene) malononitrile (10d) Yield: 71%; Solid. Mp: 120.9-123.2°C. ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 8.45 (d, $J = 1.8$ Hz, 1H, ArH), 7.56 (dd, $J = 8.9, 1.8$ Hz,

1H, ArH), 6.88 (d, $J = 8.9$ Hz, 1H, ArH), 4.38 (t, $J = 6.2$ Hz, 2H, CH₂), 3.12 (t, $J = 6.2$ Hz, CH₂); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 161.5, 156.2, 139.2, 129.2, 120.4, 118.4, 113.7, 113.0, 112.6, 78.5, 64.7, 30.4; MS (EI) m/z 39, 88, 87, 113, 139, 261, 274 (M⁺).

2-(2,3-Dihydro-6,7-dimethylchromen-4-ylidene) malononitrile (10e) Yield: 63%; Solid. Mp: 166.6-169.1°C. ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 8.15 (s, 1H, ArH), 6.76 (s, 1H, ArH), 4.31 (t, $J = 6.2$ Hz, 2H, CH₂),

3.09 (t, $J = 6.3$ Hz, 2H, CH₂), 2.27 (s, 3H, CH₃), 2.23 (s, 3H, CH₃); ¹³C NMR (CDCl₃, 75

MHz), δ (ppm) 162.9, 155.9, 148.0, 130.5, 127.1, 119.1, 114.9, 114.1, 113.6, 64.6, 31.0, 20.5, 18.9; MS (EI) m/z 50, 63, 76, 89, 112, 140, 152, 166, 181, 195, 224 (M^+).

2-(2,3-Dihydrothiophene-4-ylidene) malononitrile (10f) Yield: 43%;

Solid. Mp: 122.2-125.6°C; ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.94 (d, J = 8.1 Hz, 1H, ArH), 7.39-7.19 (m, 3H, ArH), 3.29 (t, J = 6.4 Hz, 2H, CH_2), 3.15

(t, J = 6.4 Hz, CH_2); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 169.7, 138.8, 133.4, 129.3, 128.2, 127.9, 124.9, 113.2, 112.7, 81.8, 32.6, 25.6; MS (EI) m/z 50, 69, 77, 113, 125, 133, 147, 172, 186, 212 (M^+).

2-(1-Phenylpropylidene)malononitrile (10g) Yield: 65%; Solid. Mp:

72.5-75.8°C; ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.53-7.40 (m, 5H, ArH), 2.98 (q, J = 7.5 Hz, 2H, CH_2), 1.11 (t, J = 7.5 Hz, 3H, CH_3); ^{13}C NMR

(CDCl_3 , 75 MHz), δ (ppm) 181.5, 134.5, 131.9, 129.1, 127.4, 112.6, 112.3, 31.0, 12.7; MS (EI) m/z 65, 78, 91, 104, 140, 155, 182 (M^+).

2-(1,2-Diphenylethylidene) malononitrile (10h) Yield: 80%; Solid.

Mp: 85.4-88.9°C; ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.51-7.40 (m, 5H), 7.26-7.23 (m, 3H), 7.08-7.06 (m, 2H), 4.26 (s, 2H); ^{13}C NMR (CDCl_3 , 75

MHz), δ (ppm) 177.6, 134.8, 134.32, 132.0, 129.1, 128.8, 127.9, 127.8, 112.9, 112.7, 43.3; MS (EI) m/z 51, 63, 78, 91, 140, 179, 217, 244 (M^+).

2-(1-(Naphthalen-6-yl)ethylidene) malononitrile (10i) Yield: 60%;

Solid. Mp: 114.1-116.1°C. ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 8.08 (d, J = 0.7 Hz, 1H, ArH), 7.96-7.92 (m, 3H, ArH), 7.63-7.56 (m, 3H,

ArH), 2.73 (s, 3H); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 175.2, 134.6, 133.0, 132.4, 129.04,

129.01, 128.6, 128.3, 127.7, 127.3, 123.3, 112.9, 112.8, 84.5, 24.2; MS (EI) m/z 76, 98, 127, 153, 177, 199, 204, 218 (M^+).

2-(3-Methylbutan-2-ylidene) malononitrile (10j) Yield: 50%; Colorless oil.

^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 3.24 (m, 1H, CH), 2.18 (s, 3H, CH_3), 1.15 (d, $J = 6.8$ Hz, 6H, CH_3); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 187.0, 111.9, 111.3, 84.6, 35.5, 20.0, 17.5; MS (EI) m/z 40, 66, 78, 94, 106, 134 (M^+).

General procedures for asymmetric transfer hydrogenation of olefins

Monosulfonylated chiral ligand (0.0044 mmol), $[\text{RuCl}_2(\text{cymene})]_2$ (1.2 mg, 0.002 mmol) and triethylamine (1.1 μL , 0.008 mmol) were heated in 2-propanol (0.5 mL) for 2 h. Then 2-propanol was removed under vacuum. Olefin substrate (0.4 mmol) in THF (0.4 mL) and the azeotrope of formic acid and triethylamine (0.25 mL) were added in turn. The mixture was stirred at 30°C. After completion, the solution was diluted with EtOAc, washed with water, and dried. Flash chromatography on silica gel gave the pure products.

2-(1,2,3,4-Tetrahydronaphthalen-4-yl) malononitrile (11a) Colorless

oil; $[\alpha]_{\text{D}}^{28} -57.6^\circ$ (c 1.54, CHCl_3). ^1H NMR (CDCl_3 , 300 MHz), δ (ppm)

7.27-7.17 (m, 4H), 4.13 (d, $J = 6.3$ Hz, 1H), 3.53 (q, $J = 6.3$ Hz, 1H),

2.92-2.83 (m, 2H), 2.30-2.25 (m, 1H), 2.14-1.99 (m, 2H), 1.87-1.85 (m, 1H); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 138.0, 131.9, 130.0, 128.1, 127.9, 126.4, 112.6, 112.1, 39.2, 29.4, 28.8, 26.7, 19.6. 84% ee was determined by HPLC on OD column, 20% 2-propanol/ hexane, 1.0 mL/min, UV 254 nm, $t_{\text{major}} = 12.97$ min, $t_{\text{minor}} = 20.04$ min.

2-(2,3-Dihydro-1H-inden-3-yl) malononitrile (11b) Colorless oil; $[\alpha]_D^{28}$

-13.2° (c 0.44, CHCl_3). ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.45 (d, $J = 6.9$

Hz, 1H), 7.34-7.27 (m, 3H), 3.93 (d, $J = 6.3$ Hz, 1H), 3.83 (q, $J = 5.7$ Hz, 1H), 3.18-3.13 (m,

1H), 3.03-3.00 (m, 1H), 2.63-2.56 (m, 1H), 2.23-2.16 (m, 1H); ^{13}C NMR (CDCl_3 , 75 MHz), δ

(ppm) 143.9, 138.7, 129.0, 127.1, 125.3, 124.1, 112.2, 112.0, 45.9, 30.5, 29.7, 27.9. 58% ee

was determined by HPLC on OD column, 20% 2-propanol/hexane, 1.0 mL/min, UV 254 nm,

$t_{\text{major}} = 11.20$ min, $t_{\text{minor}} = 16.91$ min.

2-(3,4-Dihydro-2H-chromen-4-yl) malononitrile (11c) Colorless oil;

$[\alpha]_D^{28} -30.1^\circ$ (c 1.08, CHCl_3). ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.29-7.21

(m, 2H), 7.01-6.90 (m, 2H), 4.37-4.24 (m, 2H), 4.15 (d, $J = 6.9$ Hz, 1H), 3.56

(q, $J = 6.6$ Hz, 1H), 2.43-2.29 (m, 2H); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 154.9, 130.1,

128.2, 121.1, 117.9, 117.5, 112.1, 111.5, 62.5, 35.2, 28.6, 25.6. 84.8% ee was determined by

HPLC on OD column, 20% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, $t_{\text{major}} = 20.54$ min,

$t_{\text{minor}} = 23.52$ min.

2-(6-Bromo-3,4-dihydro-2H-chromen-4-yl) malononitrile (11d)

Colorless oil; $[\alpha]_D^{28} -81.3^\circ$ (c 1.18, CHCl_3). ^1H NMR (CDCl_3 , 300 MHz),

δ (ppm) 7.38-7.32 (m, 2), 6.82 (d, $J = 8.7$ Hz, 1H), 4.37-4.33 (m, 1H),

4.29-4.26 (m, 1H), 4.14 (d, $J = 6.3$ Hz, 1H), 3.53 (q, $J = 6.3$ Hz, 1H), 2.42-2.31 (m, 2H); ^{13}C

NMR (CDCl_3 , 75 MHz), δ (ppm) 154.2, 133.0, 130.7, 119.9, 119.4, 112.9, 111.8, 111.2, 62.7,

34.9, 28.6, 25.2. 83% ee was determined by HPLC on OD column, 20% 2-propanol/hexane,

1.0 mL/min, UV 254 nm, $t_{\text{major}} = 18.17$ min, $t_{\text{minor}} = 21.48$ min.

2-(3,4-Dihydro-6,7-dimethyl-2H-chromen-4-yl) malononitrile (11e)

White solid. Mp: 152.9-154.7°C; $[\alpha]_D^{28}$ -65.3° (c 1.10, CHCl₃). ¹H NMR

(CDCl₃, 300 MHz), δ 6.93 (s, 1H), 6.70 (s, 1H), 4.30-4.26 (m, 1H),

4.23-4.20 (m, 1H), 4.14 (d, *J* = 6.6 Hz, 1H), 3.49 (q, *J* = 6.3 Hz, 1H), 2.39-2.34 (m, 1H),

2.32-2.25 (m, 1H), 2.22 (s, 3H), 2.20 (s, 3H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 15 2.8,

138.9, 129.4, 128.6, 118.6, 114.5, 112.2, 111.6, 62.5, 34.9, 28.8, 25.9, 19.5, 18.8. 88% ee was

determined by HPLC on OD column, 20% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, *t*_{major}

= 9.15 min, *t*_{minor} = 16.02 min.

2-(3,4-Dihydro-2H-thiophene-4-yl) malononitrile (11f) Colorless oil;

$[\alpha]_D^{28}$ +13.7° (c 1.00, CHCl₃). ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.26-7.13

(m, 4H), 4.17 (d, *J* = 6.0 Hz, 1H), 3.60-3.54 (m, 1H), 3.15-3.07 (m, 2H),

2.72-2.65 (m, 1H), 2.29-2.22 (m, 1H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 132.9, 130.5,

129.4, 127.6, 124.9, 111.9, 111.7, 39.8, 26.2, 24.9, 22.0. 82% ee was determined by HPLC on

OD column, 20% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, *t*_{major} = 12.76 min, *t*_{minor} =

37.07 min.

2-(1-Phenylpropyl) malononitrile (11g) Colorless oil; $[\alpha]_D^{20}$ -18° (c 0.1,

EtOAc). ¹H NMR (CDCl₃, 300 MHz), δ (ppm) 7.45-7.38 (m, 3H), 7.31-7.29

(m, 2H), 3.89 (d, *J* = 6.3 Hz, 1H), 3.12 (m, 1H), 2.05 (m, 1H), 0.91 (t, *J* =

7.3 Hz, 3H); ¹³C NMR (CDCl₃, 75 MHz), δ (ppm) 136.6, 129.4, 129.0, 128.0, 112.0, 48.3,

30.2, 25.5, 11.8. 43% ee was determined by HPLC on OJ-H column, 5% 2-propanol/hexane,

1.0 mL/min, UV 254 nm, *t*_{major} = 37.00 min, *t*_{minor} = 41.00 min.

2-(1,2-Diphenylethyl) malononitrile (11h) Colorless oil; $[\alpha]_D^{20} -1.5^\circ$ (c 1.0, EtOAc). ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.42-7.40 (m, 5H), 7.33-7.25 (m, 3H), 7.21-7.18 (m, 2H), 3.84 (d, $J = 5.1$ Hz, 1H), 3.45 (m, 1H), 3.26 (d, $J = 6.7$ Hz); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 136.7, 136.5, 129.3, 129.2, 129.1, 129.0, 128.1, 127.7, 112.1, 111.6, 48.4, 38.6, 28.6. 15% ee was determined by HPLC on OD column, 30% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, $t_{\text{major}} = 12.09$ min, $t_{\text{minor}} = 27.10$ min.

2-(1-(Naphthalen-6-yl)ethyl) malononitrile (11i) Colorless oil; $[\alpha]_D^{28} -9.0^\circ$ (c 1.40, EtOAc). ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.93-7.82 (m, 4H), 7.56-7.44 (m, 3H), 3.96 (d, $J = 6.3$ Hz, 1H), 3.69-3.60 (m, 1H), 1.76 (d, $J = 7.2$ Hz, 3H); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 135.6, 133.3, 133.2, 129.1, 128.1, 127.8, 126.8, 126.7, 126.6, 124.6, 112.2, 112.0, 41.1, 31.0, 17.8. 59% ee was determined by HPLC on OD column, 20% 2-propanol/hexane, 1.0 mL/min, UV 254 nm, $t_{\text{minor}} = 116.12$ min, $t_{\text{major}} = 19.05$ min.

2-(3-Methylbutan-2-yl) malononitrile (11j) Colorless oil; $[\alpha]_D^{25} -2.3^\circ$ (c 0.4, CHCl_3). ^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 3.76 (1H, d, $J = 6.0$ Hz, CH), 2.02-1.87 (2H, m, CH, CH), 1.25 (3H, d, $J = 6.6$ Hz, CH_3), 1.03 (3H, d, $J = 6.6$ Hz, CH_3), 0.99 (3H, d, $J = 6.6$ Hz, CH_3); ^{13}C NMR (CDCl_3 , 75 MHz), δ (ppm) 112.9, 112.0, 41.3, 30.4, 27.5, 20.5, 17.9, 13.4. 27% ee was determined by GC on CP-Cyclodex-236M column, $T_c = 100^\circ\text{C}$, $H_2 = 10$ psi, $t_{\text{major}} = 15.257$ min, $t_{\text{minor}} = 15.598$ min.

General procedure for deuterium labeling experiments

TsDPEN-RuCl(cymene) (2.6 mg, 0.004 mmol) was dissolved in 0.5 mL of DCM. Activated olefin **7k** (62 mg, 0.4 mmol), triethylamine (112 μ L, 0.8 mmol) and deuterium labeled formic acid (78 μ L, 2.0 mmol) were added in turn. Then the solution was stirred at 30 °C. After completion, the mixture was concentrated and flash chromatography directly on silica gel gave the reduced product.

^1H NMR (CDCl_3 , 200 MHz), δ (ppm) 7.46-7.28 (5H, m, Ph-H), 3.90 (t, J = 7.0 Hz, 1H), 3.28 (d, J = 7.0 Hz, 2H); ^{13}C NMR (CDCl_3 , 50 MHz), δ (ppm) 132.9, 129.1, 128.8, 128.6, 112.2, 36.4, 24.8.

^1H NMR (CDCl_3 , 300 MHz), δ (ppm) 7.44-7.33 (m, 5H), 3.92 (d, J = 6.9 Hz, 1H), 3.29 (d, J = 6.9 Hz, 1H).

References

- (1) For the synthesis of (*R,R*)-1,2-diphenylenediamine and (*R,R*)-1,2-bis(4-methoxyphenyl)-ethane-1,2-diamine, see: Corey, E. J.; Kuhnle, F. N. K. *Tetrahedron Lett.* **1997**, 38, 8631.
- (2) For ligand **2c**, also see: Mohar, B.; Vallex, A.; Desmurs, J. R.; Felemez, M.; Wagner, A.; Mioskowski, C. *Chem. Commun.* **2001**, 2572.
- (3) For ligand **2d**, also see: Uematsu, N.; Fuji, A.; Hashiguchi, S.; Ikariya, T.; Noyori, R. *J. Am. Chem. Soc.* **1996**, 118, 4916.
- (4) For ligand **2h**, also see: (a) Meuzelaar, G. J.; Van Vliet, M. C. A.; Maat, L.; Sheldon, R. A. *Eur. J. Org. Chem.* **1999**, 9, 2315; (b) Sterk, D.; Stephan, M. S.; Mohar, B. *Tetrahedron Lett.* **2004**, 45, 535.

(5) The details of the synthesis will be published elsewhere.

(6) For the synthesis of substrate **7s** and **10a-i**, see: Mowry, D. T., *J. Am. Chem. Soc.* **1945**, 67, 1050.

NMR and MS spectra of lignads and reduced products

Current Data Parameters
NAME 1397-xd-137
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030717
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INSTRUM av300
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TD 32768
SOLVENT CDCl3
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DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
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DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

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F2 - Processing parameters
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LB 0.10 Hz
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1D NMR plot parameters
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F2P -0.500 ppm
F2 -150.06 Hz
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Current Data Parameters
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PROCNO 1

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DE 6.00 usec
TE 300.0 K
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d12 0.00002000 sec

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SFO1 75.4775526 MHz

***** CHANNEL f2 *****
COPROG2 waltz16
NUC2 1H
PCNCH2 80.00 usec
PL2 -2.00 dB
PL12 17.70 dB
PL13 17.70 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677524 MHz
WDW EM
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GB 0
PC 1.40

1D NMR plot parameters
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F2P -20.295 ppm
F2 -1533.88 Hz
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Current Data Parameters
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PROCNO 1

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RG 1024
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
DS 1.00000000 sec

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HZCH 157.56825 Hz/cm

\\stock02\SP-EE_X\NMR\SIMS_Bruker\Berg\10\data\471_xsp1r Mon Jun 28 10:26:47 2004

7disk2b/SPICS_XIN/P-SIMS-DengJi+Geng/16/pdata/1/ xspec: Mon Jun 28 10:44:51 2024

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PROCNO 1

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FIDRES 0.182959 Hz
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RG 1024
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DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

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PL1 -2.00 dB
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F2 - Processing parameters
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SSB 0
LB 0.10 Hz
GB 0
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1D NMR plot parameters
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CY 12.00 cm
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F2P -0.500 ppm
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HZCM 157.56825 Hz/cm

Current Data Parameters
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EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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SOLVENT CDCl3
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SWH 22675.736 Hz
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RG 8192
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DE 6.00 usec
TE 300.0 K
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d11 0.03000000 sec
d12 0.00020000 sec

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PL1 -5.00 dB
SFO1 75.4752588 MHz

***** CHANNEL f2 *****
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PL2 -2.00 dB
PL12 17.70 dB
PL13 17.71 dB
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F2 - Processing parameters
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GB 0
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1D NMR plot parameters
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F2 -0.38 Hz
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HZCM 754.71527 Hz/cm

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Current Data Parameters
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EXPNO 1
PROCNO 1

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DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 1024
OW 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 300.130126 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
PUNCH 0.55500 ppm/cm
HZCM 157.56825 Hz/cm

Current Data Parameters
NAME 1397-xd-580
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041123
Time 8.52
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TO 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 22675.736 Hz
FIDRES 0.346604 Hz
AQ 1.445186 sec
RG 8192
OW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 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 75.4775598 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 222.147 ppm
F1 16780.00 Hz
F2P -5.263 ppm
F2 -397.21 Hz
PUNCH 11.38050 ppm/cm
HZCM 858.86050 Hz/cm

Current Data Parameters
NAME 1397-xd-583
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041123
Time 15.43
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 1024
OW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 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 12.00 cm
FIP 15.000 ppm
F1 4501.95 Hz
F2 -150.06 Hz
PPMCH 0.77500 ppm/cm
HZCM 232.60075 Hz/cm

Current Data Parameters
NAME 1397-xd-581
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041123
Time 13.12
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 22675.736 Hz
FIDRES 0.346004 Hz
AQ 1.4451188 sec
RG 8192
OW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
d12 0.0000200 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.50 usec
PL1 -8.00 dB
SFO1 75.4775988 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 75.4677552 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
FIP 202.777 ppm
F1 15303.12 Hz
F2 -1.345 ppm
PPMCH 10.20632 ppm/cm
HZCM 770.24805 Hz/cm

Current Data Parameters
NAME 1397-xd-618
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041208
Time 15.22
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 1024
OW 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 300.1300128 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

Current Data Parameters
NAME 1397-xd-617
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041208
Time 15.28
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 1024
OW 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 300.1300128 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

Current Data Parameters
 NAME 1397-xd-618
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041208
 Time 15.46
 INSTRUM av300
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 1024
 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 300.1320862 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300128 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
 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

Current Data Parameters
 NAME 1397-xd-612
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041207
 Time 10.55
 INSTRUM av300
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 32768
 SOLVENT CDCl3
 NS 24
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 1024
 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 300.1320862 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 7.00 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

Current Data Parameters
NAME 1397-xd-614
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041207
Time 11:17
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 17
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 1024
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 300.1300124 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 7.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCH 0.52500 ppm/cm
HZCM 157.56825 Hz/cm

Current Data Parameters
NAME 1397-xd-615
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041207
Time 11:39
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 1024
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 300.1307370 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 7.00 cm
F1P 10.000 ppm
F1 3001.31 Hz
F2P -0.500 ppm
F2 -150.07 Hz
PPMCH 0.52500 ppm/cm
HZCM 157.56863 Hz/cm

Current Data Parameters
NAME 1397-x0-584
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041122
Time 17:02
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 1024
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 3.00 usec
PL1 -2.00 dB
SF01 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 12.00 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

Current Data Parameters
NAME 1397-x0-588
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041123
Time 11:11
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT D2O
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 1024
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 3.00 usec
PL1 -2.00 dB
SF01 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 12.00 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

Current Data Parameters
 NAME 1397-xd-592
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041123
 Time 15.54
 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 1024
 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 300.1320882 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300128 MHz
 WDW EN
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 15.00 cm
 FIP 10.000 ppm
 F1 3001.30 Hz
 F2 -0.500 ppm
 F2 -150.06 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 157.56825 Hz/cm

Current Data Parameters
NAME scien
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020508
Time 16.27
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 24
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SF01 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
FIP 8.160 ppm
F1 2449.15 Hz
F2P -0.938 ppm
F2 -281.43 Hz
PPMCM 0.45490 ppm/cm
HZCM 136.52951 Hz/cm

Current Data Parameters
NAME first-13c
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030521
Time 10.06
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 73336
SOLVENT CDCl3
NS 12000
DS 2
SWH 20964.361 Hz
FIDRES 0.278315 Hz
AQ 1.7960751 sec
RG 4096
DM 23.850 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec
D11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.30 usec
PL1 2.00 dB
SFO1 75.475564 MHz

===== CHANNEL f2 =====
CPROG2 waltz16
NUC2 1H
PCPG2 80.00 usec
PL2 120.00 dB
PL12 27.00 dB
SFO2 300.1315007 MHz

F2 - Processing parameters
SI 65536
SF 75.4677570 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 154.401 ppm
F1 11637.20 Hz
F2P -11.185 ppm
F2 -644.11 Hz
PPMCH 8.26330 ppm/cm
HZCM 624.06525 Hz/cm

Current Data Parameters
NAME scien
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020606
Time 17.20
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 24
DM 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 4.50 usec
PL1 2.00 dB
SFO1 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 300.1300010 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.340 ppm
F1 2503.22 Hz
F2P -0.670 ppm
F2 -200.97 Hz
PPMCH 0.45050 ppm/cm
HZCM 135.20572 Hz/cm

Current Data Parameters
 NAME 1307-12-370
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040330
 Time 11.50
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 65536
 SOLVENT CDCl3
 NS 1990
 DS 4
 SWH 22675.736 Hz
 FIDRES 0.346004 Hz
 AQ 1.445188 sec
 RG 8192
 DW 22.050 usec
 DE 6.00 usec
 TE 300.0 K
 D1 3.0000000 sec
 d11 0.0300000 sec
 d12 0.0002000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 6.00 usec
 PL1 -6.00 dB
 SFO1 75.475098 MHz

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

F2 - Processing parameters
 SI 65536
 SF 75.467745 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 FIP 250.000 ppm
 F1 18866.94 Hz
 F2P -15.000 ppm
 F2 -754.68 Hz
 PPMCH 13.00000 ppm/cm
 HZCH 981.08053 Hz/cm

Current Data Parameters
 NAME scien
 EXPNO 15
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020305
 Time 15.18
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 40
 DW 111.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 50 usec
 PL1 00 dB
 SFO1 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300010 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 FIP 9.235 ppm
 F1 2771.67 Hz
 F2P -0.123 ppm
 F2 -36.88 Hz
 PPMCH 0.46789 ppm/cm
 HZCH 140.42755 Hz/cm