Highly Diastereoselective Catalytic MPV Reductions

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Supporting Information

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General Comments: An HPLC fitted with an Ace C-8 column, auto-injector and diode array detector provided information on reaction progress and assay yield. Relevant HPLC parameters include 0.1% H_3PO_4 in H_2O/MeCN mobile phase, 35 ^oC column temperature, and monitoring at 210 nm. A ChiralPak AD-H (4.6 x 150 mm) column was used for measuring the ee's of compound **3a,e** with 0.1/10/90 of TFA/*i*PrOH/heptane as the mobile phase and a flow rate of 1.5 mL/min at 30 °C. A 400 MHz NMR system captured all ^1H, ^{13}C and ^{19}F spectral data associated with all compounds. All columns were packed with 40-63 μm silica gel. Ketones **2a–h** were prepared according to the slightly modified literature procedure from aryl Gringards.[1] Other ketones are commercially available.

General Procedure for MPV reduction in Tables 2 and 3: A mixture of ketone (0.637 mmol, 1.0 equiv), $Al(O\textit{i}Pr)_3$ (0.2 to 0.6 equiv), and *i*PrOH (0.536 mL, 11 equiv) in toluene (0.80 mL, 1.3 mL/mmol) was heated at 50 °C under N_2 until LC revealed complete conversion. Unless specified otherwise, the reaction was quenched with 4 mL of 1 N HCl and 4 mL of EtOAc. The organic layer was washed with 4 mL of water and concentrated. Crude ^1H NMR was taken to determine the diastereoselectivity. The product was further purified to >95% pure by LC with a d.r. of >50/1 by SiO_2 column chromatography or a hexane tituration if necessary.

General Procedure for $NaBH_4$ reduction in Tables 2 and 3: A solution of ketone (60mg) in MeOH (0.5mL) (0.5mL THF was added to help dissolve the ketone in some cases) at rt was treated with 2 equiv of solid $NaBH_4$. After 5-30 min when LC reveals complete conversion, the reaction was quenched with 4 mL 1N HCl and 4 mL EtOAc.

The organic layer was washed with 4 mL water and concentrated. NMR was taken of the crude material, which was always pure with only two product isomers.

(1*R*,2*S*)-1-(3',5'-Bistrifluoromethylphenyl)-2-benzyloxycarbonylamino-1-propanol (3a) The general procedure provided **3a**, 260 mg at 97% isolated yield as a white solid with >99% ee (retention times: desired *1R,2S*-enantiomer, 2.6 min; undesired, 4.7 min). M.p. 141–142 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 9.6 Hz, 3 H), 7.33-7.40 (m, 5 H), 5.14 (s, 2 H), 5.05 (br s, 1 H), 4.95 (br d, *J* = 4.4 Hz, 1 H), 4.06 (br s, 1 H), 3.40 (br s, 1 H), 1.01 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 143.5, 136.0, 131.5 (q, *J* = 33.3 Hz), 128.6, 128.4, 128.1, 126.5 (m), 123.3 (q, *J* = 273 Hz), 121.5 (m), 75.3, 67.3, 52.5, 13.9. Anal. Calcd. for $C_{19}H_{17}F_6NO_3$: C, 54.16; H, 4.07; N, 3.32. Found: C, 54.15; H, 3.84; N, 3.29.

Characteristic ^{1}H NMR signals for the minor isomer: 1.21 (d, *J* = 6.9 Hz, 3 H).

(1*R*,2*S*)-1-Phenyl-2-benzyloxycarbonylamino-1-propanol (3b)[2] The general procedure provided **3b**, 174 mg at 95% isolated yield as a white solid. M.p. 115–116 °C (lit. m.p.[2] 111–113 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15-7.55 (m, 10 H), 5.12 (s, 2 H), 5.08 (br d, *J* = 8.0 Hz, 1 H), 4.88 (br s, 1 H), 4.06 (br s, 1 H), 3.0 (br s, 1 H), 1.00 (d, *J* =- 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.5, 140.7, 136.4, 128.5, 128.24, 128.17, 128.12, 127.5, 126.2, 76.2, 66.9, 52.4, 14.4; Anal. Calcd. for $C_{17}H_{19}NO_3$: C, 71.56; H, 6.71; N, 4.91 Found: C, 71.26; H, 6.70; N, 4.82.

Characteristic ^{1}H NMR signals for the minor isomer: 1.12 (d, *J* = 6.8 Hz, 3 H).

(1*R*,2*S*)-1-*p*-Tolyl-2-benzyloxycarbonylamino-1-propanol (3c) The general procedure provided **3c**, 172 mg at 90% isolated yield as a white solid. M.p. 120–121 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.38 (m, 5 H), 7.14-7.24 (m, 4 H), 5.12 (s, 2 H), 5.03 (br d, *J*

= 7.6 Hz, 1 H), 4.85 (br s, 1 H), 4.04 (br s, 1 H), 2.67 (br s, 1 H), 2.35 (s, 3 H), 1.01 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.5, 137.8, 137.3, 136.6, 129.0, 128.6, 128.21, 128.17, 126.2, 76.3, 66.9, 52.5, 21.2, 14.6; Anal. Calcd. for $C_{18}H_{21}NO_3$: C, 72.22; H, 7.07; N, 4.68; Found: C, 71.83; H, 7.04; N, 4.57.

Characteristic ^{1}H NMR signals for the minor isomer: 2.37 (s, 3 H), 1.12 (d, *J* = 6.8 Hz, 3 H).

(1*R*,2*S*)-1-*o*-Tolyl-2-benzyloxycarbonylamino-1-propanol (3d) The general procedure provided **3d**, 164 mg at 86% isolated yield as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.53 (m, 1 H), 7.36-7.37 (m, 5 H), 7.16-7.24 (m, 3 H), 5.44 (br d, *J* = 7.6 Hz, 1 H), 5.08-5.16 (m, 3 H), 3.99 (br s, 1 H), 2.98 (br s, 1 H), 2.40 (br s, 2.4 H) + 2.14 (br s, 0.6 H), 1.02 (d, *J* = 6.7 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.1, 139.3, 136.5, 124.7, 130.4, 128.6, 128.4, 128.16, 128.14, 127.3, 126.1, 125.8, 72.6, 66.7, 50.5, 19.0, 13.2. HRMS $C_{18}H_{21}NO_3$ calcd for [M+Na]: 322.14136, found 322.14234.

Characteristic ^{1}H NMR signals for the minor isomer: 1.20 (d, *J* = 6.8 Hz, 3 H).

(1*R*,2*S*)-1-(2'-Methoxyphenyl)-2-benzyloxycarbonylamino-1-propanol (3e) The general procedure provided **3e**, 193 mg at 96% isolated yield as a colorless oil with >99% ee (retention times: desired *1R,2S*-enantiomer, 9.9 min; undesired, 11.3 min). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.39 (m, 7 H), 6.96 (t, *J* = 7.4 Hz, 1 H), 6.86 (d, *J* = 8.0 Hz, 1 H), 5.21 (br m, 1 H), 5.08 (br s, 3 H), 4.13 (br s, 1 H), 3.83 (br s, 2.4 H) + 3.67 (br s, 0.6 H), 2.96 (br s, 1 H), 1.05 (d, *J* = 6.8 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.5, 156.2, 136.7, 129.1, 128.60, 128.55, 128.1, 127.7, 120.7, 110.5, 72.8, 66.6, 55.4, 51.2, 15.2; Anal. Calcd. for $C_{18}H_{21}NO_4$: C, 68.55; H, 6.71; N, 4.44; Found: C, 68.28; H, 6.74; N, 4.36.

Characteristic ^{1}H NMR signals for the minor isomer: 1.19 (d, J = 6.7 Hz, 3 H).

(1*R*,2*S*)-1-(5'-Methoxy-3'-pyridyl)-2-benzyloxycarbonylamino-1-propanol (3f) The general procedure provided a reaction mixture of **3f**. It was filtered with 1 mL toluene rinse to give the first crop of product (106 mg). The filtrate was passed through a pad of silica gel (2 x 2 cm) with EtOAc (130 mL), concentrated, and crystallized from 3 mL toluene to give the second crop of product (58 mg, combined 164 mg, 82% yield) as an off-white solid. M.p. 141–143 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (br s, 2 H), 7.19-7.39 (m, 6 H), (5.12-5.15 (m, 3 H), 4.93 (br s, 1 H), 4.06 (br s, 1 H), 3.83 (s, 3 H), 1.04 (d, J = 6.8 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 155.8, 140.0, 137.5, 136.6, 136.3, 128.7, 128.3, 128.2, 118.7, 74.2, 67.1, 55.6, 52.5, 14.5. HRMS $C_{17}H_{20}N_2O_4$ calcd for [M+Na]: 339.13153, found 339.13251.

Characteristic ^{1}H NMR signals for the minor isomer: 1.15 (d, J = 6.8 Hz, 3 H).

(1*R*,2*S*)-1-(2',4'-Difluorophenyl)-2-benzyloxycarbonylamino-1-propanol (3g) The general procedure provided **3g**, 190 mg at 93% isolated yield as a white solid. M.p. 68–69 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.37 (m, 4 H), 7.19-7.24 (m, 2 H), 6.91-6.96 (m, 2 H), 5.09-5.13 (br m, 4 H), 4.10 (br s, 1 H), 3.48 (br s, 1 H), 1.02 (d, J = 6.8 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5 (dd, J = 242, 1.7 Hz), 156.7, 155.4 (d, J = 245 Hz), 136.2, 130.0 (m, 1 C), 128.5, 128.2, 128.1, 116.2 (dd, J = 25, 8.6 Hz), 115.3 (dd, J = 24, 8.6 Hz), 114.8 (dd, J = 25, 1.7 Hz),70.3, 67.0, 51.3, 14.6 ; ^{19}F NMR (377 MHz, $CDCl_3$) δ -118.6, -123.7. Anal. Calcd. for $C_{17}H_{17}F_2NO_3$: C, 63.55; H, 5.33; N, 4.36. Found: C, 63.51; H, 5.30; N, 4.31.

Characteristic ^{1}H NMR signals for the minor isomer: 1.23 (d, J = 6.8 Hz, 3 H).

(1*R*,2*S*)-1-(4'-Cyanophenyl)-2-benzyloxycarbonylamino-1-propanol (3h) The general procedure provided **3h**, 180 mg at 91% isolated yield as a white solid. M.p. 93–95 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2 H), 7.45 (d, *J* = 8.0 Hz, 2 H), 7.34-7.37 (m, 5 H), 5.11 (s, 2 H), 4.93 (s, 1 H), 4.02 (br s, 1 H), 3.52 (br s, 1 H), 0.98 (d, *J* = 6.8 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.5, 146.4, 136.1, 132.0, 128.6, 128.3, 128.1, 127.0, 118.7, 111.2, 75.6, 67.1, 52.4, 14.1; Anal. Calcd. for $C_{18}H_{18}N_2O_3$: C, 69.66; H, 5.85; N, 9.03. Found: C, 69.43; H, 5.82; N, 8.78.

Characteristic ^{1}H NMR signals for the minor isomer: 1.18 (d, *J* = 6.8 Hz, 3 H).

(2*S*,3*S*)-1-Chloro-3-benzyloxycarbonylamino-3-benzyl-2-propanol (3i)[3] The general procedure provided **3i**, 201 mg at 94% isolated yield as a white solid. M.p. 152–153 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19-7.36 (m, 10 H), 5.05 (s, 2 H), 4.86 (d, *J* = 7.2 Hz, 1 H), 3.97-4.04 (m, 1 H), 3.87 (br s, 1 H), 3.67 (dd, *J*= 11.2, 3.8 Hz, 1 H, 3.59 (dd, *J* = 11.2, 7.6 Hz, 1 H), 2.91-3.03 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.3, 137.1, 136.3, 129.5, 128.7, 128.6, 128.3, 128.0, 126.8, 73.3, 67.0, 54.8, 47.7, 35.8.

Characteristic ^{1}H NMR signals for the minor isomer: 5.18 (d, *J* = 8.8 Hz, 1 H), 5.09 (s, 2 H).

(2*S*,3*S*)-1-Chloro-3-*p*-tosylamino-3-benzyl-2-propanol (3j) The general procedure provided 225 mg of an oil at 100% isolated yield for the combined isomers. Flash silica gel column gave 187 mg of the main isomer **3j** (83% yield) as a solid and 38 mg of the minor isomer that was contaminated with some main isomer. Main isomer: M.p. 77–78 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.2 Hz, 2 H), 7.16-7.20 (m, 5 H), 6.96 (d, *J* = 7.2 Hz, 2 H), 4.76 (d, *J* = 8.4 Hz, 1 H), 3.85-3.90 (m, 1 H), 3.71 (dd, *J* = 11.4, 4.6 Hz, 1 H), 3.58-3.66 (m, 2 H), 2.82 (dd, *J* = 14.0, 7.6 Hz, 1 H), 2.69 (dd, *J* = 14.0, 5.2 Hz, 1

H), 2.42 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 136.6, 136.0, 129.7, 129.5, 128.6, 126.9, 126.7, 72.6, 56.9, 46.6, 35.1, 21.5; Anal. Calcd. for $C_{17}H_{20}ClNO_3S$: C, 57.70; H, 5.70; N, 3.96. Found: C, 57.73; H, 5.70; N, 3.91.

Minor isomer **(2*R*,3*S*)-1-Chloro-3-*p*-tosylamino-3-benzyl-2-propanol**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 2 H), 7.17-7.25 (m, 5 H), 7.01-7.04 (m, 2 H), 5.19 (d, *J* = 9.2 Hz, 1 H), 3.67-3.71 (m, 1 H), 3.56-3.63 (m, 2 H), 3.47 (dd, *J* = 11.2, 4.0 Hz, 1 H), 2.87 (dd, *J* = 13.1, 9.3 Hz, 1 H), 2.62 (dd, *J* = 13.1, 5.6 Hz, 1 H), 2.43 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 137.7, 126.8, 129.8, 129.2, 128.7, 126.9, 126.8, 70.7, 56.7, 47.6, 38.8, 21.5.

***syn*-2-Methoxy-1,2-diphenylethanol (8)**[4] The general procedure carried out in 5.0 mmol scale provided syn-product **8** and its anti-isomer **9** in a ratio of 93.7/6.3, 1.15 g at 100% isolated yield as a white solid. M.p. 52–53.5 °C (lit.[5] syn- mp 53 °C; anti- mp 100 °C); $NaBH_4$ reduction gave a syn/anti ratio of 8.3/91.7. ^{1}H NMR data for both isomers are in accord with the literature.[4] GC-MS, *m/e* 228 (M^+), 210 (M^+–H_2O).

***syn*-2-Ethoxy-1,2-diphenylethanol (11)**[6] The general procedure carried out in 2.55 mmol scale provided a mixture of syn-product **11** and its anti-isomer in a ratio of 95.5/4.5, 584 mg at 95% isolated yield as an oil. $NaBH_4$ reduction gave a syn/anti ratio of 12/88. ^{1}H NMR data for both isomers are in accord with the literature.[6] GC-MS, *m/e* 242 (M^+), 224 (M^+–H_2O).

***syn*-2-Isopropoxy-1,2-diphenylethanol (12)**[4] The general procedure carried out in 2.55 mmol scale provided syn-product **12** and its anti-isomer in a ratio of 96.1/3.9, 640 mg at 98% isolated yield as a colorless oil. $NaBH_4$ reduction gave a syn/anti ratio of 21/79. ^{1}H

NMR data for both isomers are in accord with the literature.[4] GC-MS, *m/e* 256 (M^+), 238 (M^+–H_2O).

***trans*-2-Methoxy-cyclohexanol (15)**[4] The general procedure carried out in 2.55 mmol scale with 0.10 equiv of biphenyl as internal standard provided a mixture of the trans-product **15** and its cis-isomer in a ratio of 86/14 in a combined 97% NMR yield. ^{1}H NMR data for both isomers are in accord with the literature.[4] GC-MS, *m/e* 130 (M^+).

***cis*-2-Phenyl-cyclohexanol (17)**[7] The general procedure carried out in 2.55 mmol scale provided a mixture of the cis-product **17** and its trans-isomer[8] in a ratio of 83/17 in a combined 100% yield. ^{1}H NMR data for both isomers are in accord with the literature.[7,8] GC-MS, *m/e* 176 (M^+).

***N*-Cbz-phenylalanyl epoxide (6)**[3] Chlorohydrin **3i** (47 mg, 0.14 mmol) was suspended in EtOH (2 mL), and KOH solid (89%, 11 mg, 0.17 mmol) was added at rt. After aging at rt for 60 min when LC revealed complete conversion, the reaction mixture was concentrated and partitioned between EtOAc (8 mL) and water (6 mL). The organic layer was washed with water (6 mL) and concentrated to give **6** as a white solid (41 mg, 99%). ^{1}H NMR data are in accord with the literature.[3] LC-MS, *m/e* 320.1 ($M+Na^+$), 298.1 ($M+H^+$).

2-(*N*-Ethyl-*N*-benzyloxycarbonyl-amino)-1-phenyl-1-prapanone (18) To a mixture of 2-(*N*-Ethylamino)-1-phenyl-1-prapanone hydrochloride (741 mg, 3.47 mmol) in THF (4 mL) and water (4 mL) at 0 °C was added K_2CO_3 (1.20 g, 8.68 mmol) as a solid. CbzCl (0.521 mL, 3.47 mmol) was then added over 5 min while keeping temp < 5 °C. After 10 min, LC revealed ~95% conversion. More CbzCl (0.026 mL, 0.17 mmol) was added for complete conversion. The reaction mixture was concentrated and partitioned between

EtOAc (20 mL) and water (20 mL). The organic layer was washed with water (20 mL) and concentrated to a colorless oil, which was vacuum pumped at 35 °C to remove any residual BnCl (carried over from CbzCl) to give 1.08 g of the title compound (100% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.6 Hz, 1.4 H, major conformer), 7.80 (d, *J* = 6.6 Hz, 0.6 H, minor conformer), 7.54 (q, *J* = 7.2 Hz, 1 H), 7.43 (t, *J* = 7.6 Hz, 1 H), 7.32-7.39 (m, 6 H), 5.75 (q, *J* = 6.8 Hz, 0.7 H), 5.43 (q, *J* = 6.1 Hz, 0.3 H), 5.07-5.8 (m, 2 H), 3.11-3.25 (m, 2 H), 1.43 (d, *J* = 7.0 Hz, 3 H), 1.08 (t, *J* = 7.0 Hz, 0.9 H), 1.01 (t, *J*= 7.0 Hz, 2.1 H); ^{13}C NMR (100 MHz, $CDCl_3$) of the major conformer δ 199.2, 156.2, 136.7, 135.6, 133.2, 128.6, 128.47, 128.43, 127.9, 127.6, 67.4, 55.4, 38.7, 15.4, 14.6; Anal. Calcd. for $C_{19}H_{21}NO_3$: C, 73.29; H, 6.80; N, 4.50. Found: C, 73.61; H, 6.66; N, 4.48.

2-(Ethylamino)-1-phenyl-1-propanol (*anti*- 19;[9] *syn*- 20[10]) A mixture of compound **18** (198 mg, 0.673 mmol), Al(O*i*Pr)$_3$ (40 mg, 0.30 equiv), and *i*PrOH (0.536 mL, 11 equiv) in toluene (0.80 mL) was heated at 50 °C under N_2 for 64 h. The reaction was quenched with 4 mL 1 N HCl and 4 mL EtOAc. The organic layer was washed with 4 mL water and concentrated to an oil. The residue was treated with MeOH (0.5 mL) and 50%wt/wt KOH aq (1.0 mL) at 50 °C for 16 h. The mixture was extracted with *i*PrOAc (4 mL + 1 mL). The combined organic layers were extracted with 3 mL 1 N HCl. The resulting aq HCl layer was treated with 1.2 mL 50%wt/wt aq KOH and extracted with MTBE (5 + 2 mL). The combined MTBE layers were dried and concentrated to a solid (102 mg, 89%). ^{1}H NMR revealed an *anti/syn* (**19**/**20**) ratio of 30/70. Characteristic signals: *anti*-isomer **19**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.83 (d, *J* = 6.5 Hz, 3 H), 4.71 (d, *J* = 4.0 Hz, 1 H);

LC-MS, 162.1 (MH^+–OH); *syn*-isomer **20**: 0.88 (d, J = 6.4 Hz, 3 H), 4.14 (d, J = 8.4 Hz, 1 H). LC-MS, 162.1 (MH^+–OH).

***syn*-1-Phenyl-2-phthalimido-1-propanol (22)**[11] The general procedure carried out in 2.55 mmol scale using 0.90 equiv of $Al(OiPr)_3$ provided a mixture of the *syn*-product **22** and its *anti*-isomer[12] in a ratio of 78/22 in a combined 98% yield. ^1H NMR data for both isomers are in accord with the literature.[11,12] Characteristic signals: *syn*-isomer **22**: ^1H NMR (400 MHz, $CDCl_3$) δ 1.42 (d, J = 7.2 Hz, 3 H), 3.35 (d, J = 7.2 Hz, 1 H), 4.72 (pent, J = 7.2 Hz, 1 H), 5.16 (d, J = 7.6 Hz, 1 H). LC-MS, 264.1 (MH^+–OH); *anti*-isomer **23**: ^1H NMR (400 MHz, $CDCl_3$) δ 1.49 (d, J = 7.0 Hz, 3 H), 3.66 (d, J = 6.4 Hz, 1 H), 4.59-4.63 (m, 1 H), 5.19 (d, J = 5.2 Hz, 1 H). LC-MS, 304.1 ($M+Na^+$).

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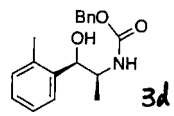

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156.1 139.3 136.5 134.7 130.4 128.6 128.4 128.2 127.3 126.1 125.8 77.5 77.1 76.8 72.6 66.7 50.5 19.0 13.2

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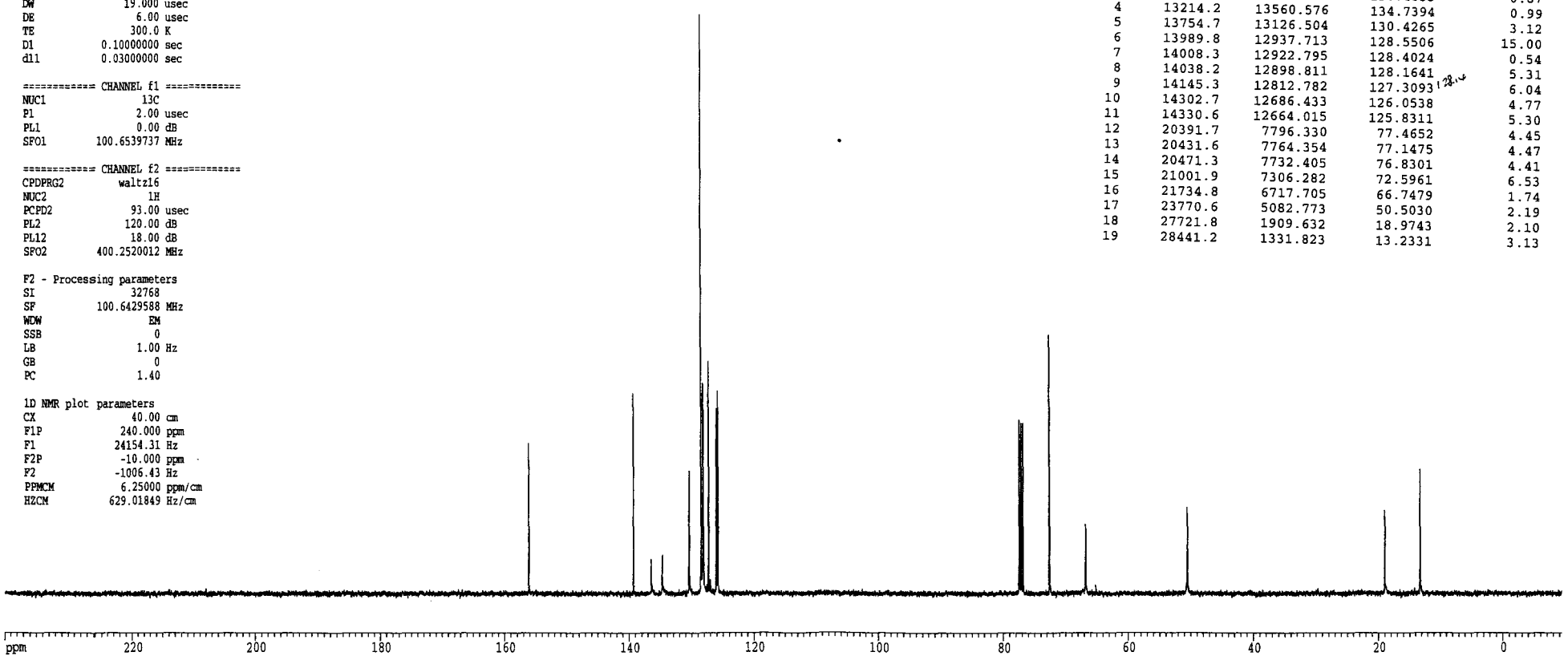
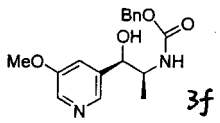
DU=/w, USER=yin, NAME=179818-134B-C, EXPNO=1, PROCNO=1
F1=240.000ppm, F2=-10.000ppm, MI=0.50cm, MAXI=10000.00cm,

#	ADDRESS	FREQUENCY [Hz]	[PPM]	INTENSITY
1	10531.9	15714.694	156.1430	3.77
2	12643.1	14019.227	139.2966	5.06
3	12997.9	13734.269	136.4653	0.87
4	13214.2	13560.576	134.7394	0.99
5	13754.7	13126.504	130.4265	3.12
6	13989.8	12937.713	128.5506	15.00
7	14008.3	12922.795	128.4024	0.54
8	14038.2	12898.811	128.1641	5.31
9	14145.3	12812.782	127.3093	6.04
10	14302.7	12686.433	126.0538	4.77
11	14330.6	12664.015	125.8311	5.30
12	20391.7	7796.330	77.4652	4.45
13	20431.6	7764.354	77.1475	4.47
14	20471.3	7732.405	76.8301	4.41
15	21001.9	7306.282	72.5961	6.53
16	21734.8	6717.705	66.7479	1.74
17	23770.6	5082.773	50.5030	2.19
18	27721.8	1909.632	18.9743	2.10
19	28441.2	1331.823	13.2331	3.13





Current Data Parameters
NAME 179818-124Br-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050404
Time 17.49
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 1804
DS 4
SWH 26315.789 Hz
FIDRES 0.401547 Hz
AQ 1.2452340 sec
RG 8192
DW 19.000 usec
DE 6.00 usec
TE 300.0 K
D1 0.10000000 sec
d11 0.03000000 sec

========== CHANNEL f1 ==========
NUC1 13C
P1 2.60 usec
PL1 5.00 dB
SFO1 100.5584112 MHz

========== CHANNEL f2 ==========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 22.00 dB
SFO2 399.8719994 MHz

F2 - Processing parameters
SI 32768
SF 100.5473900 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 40.00 cm
F1P 240.000 ppm
F1 24131.38 Hz
F2P -10.000 ppm
F2 -1005.47 Hz
PPMCM 6.25000 ppm/cm
HZCM 628.42120 Hz/cm