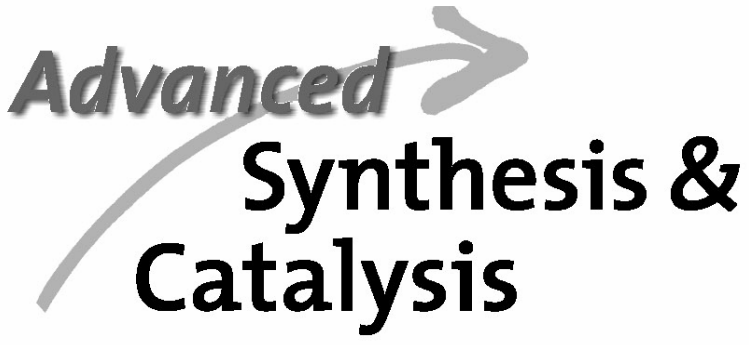


Supporting Information

Asymmetric Ring Opening of *meso*-Epoxides with Aromatic Amines Catalyzed by a New Proline-based *N*,*N*'-dioxide-In(OTf)$_3$ Complex

Bo Gao,[a] **Yuehong Wen**,[a] **Zhigang Yang**,[a] **Xiao Huang**,[a] **Xiaohua Liu**,[a] **Xiaoming Feng**[a,b *]

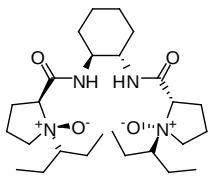
[a] *Key Laboratory of Green Chemistry & Technology (Sichuan University), Ministry of Education, College of Chemistry, Sichuan University, Chengdu 610064, China*
[b] *State Key Laboratory of Biotherapy, Sichuan University, Chengdu 610041, China*

Fax: (+86)28-8541-8249; e-mail: xmfeng@scu.edu.cn

Supporting Information

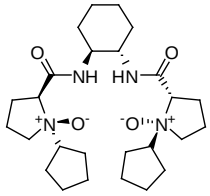
Materials. THF, Toluene and Et_2O were distilled freshly from sodium/benzophenone ketyl. CH_2Cl_2 was distilled freshly from CaH_2. Epoxides **2a**, **2b**, **2c** were prepared according to the reported procedure.[1] All other compounds were commercially available and used as received except aromatic amines, which were distilled prior to use. Racemic products of **3a-r** were prepared with achiral *N*-oxide-In(OTf)$_3$ complex as the catalyst.

Analytical data for 1a, 1b, 1d-h.

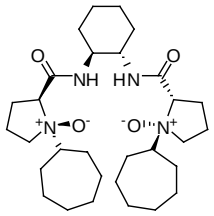


(1*R*,1'*R*,2*S*,2'*S*)-2,2'-(1*S*,2*S*)-cyclohexane-1,2-diylbis(azanediyl)bis(oxomethylene)bis(1-(pentan-3-yl)pyrrolidine 1-oxide) (1a). hygrometric yellow solid. $[\alpha]^{25}_D$ = -8.0° (c = 0.388, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 1.04-1.09 (m, 12H), 1.59-1.72 (m, 7H), 1.76-1.83 (m, 4H), 1.89-1.93 (m, 4H), 2.33-2.45 (m, 9H), 3.18-3.21 (m, 2H), 3.22-3.32 (m, 2H), 3.36-3.41 (m, 2H), 3.78 (m, 2H), 3.98 (m, 2H), 11.73 (br, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 12.0, 12.2, 20.0, 21.6, 22.6, 22.9, 27.5, 28.1, 48.4, 63.9, 72.0, 78.5,

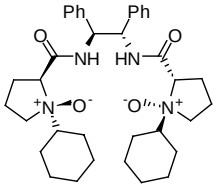
167.4. ESI-HRMS Calcd for ($C_{26}H_{48}N_4O_4$+H^+) 481.3754, Found: 481.3754.



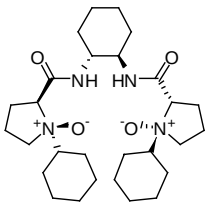
(1*R*,1'*R*,2*S*,2'*S*)-2,2'-(1*S*,2*S*)-cyclohexane-1,2-diylbis(azanediyl)bis(oxomethylene)bis(1-cyclopentylpyrrolidine 1-oxide) (1b). hygrometric white foam. $[\alpha]^{25}_D$ = -20.2° (c = 0.362, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 1.41-1.61 (m, 10H), 1.76-1.81 (m, 7H), 1.87-2.03 (m, 7H), 2.12-2.17 (m, 2H), 2.39-2.46 (m, 6H), 3.30-3.34 (m, 2H), 3.41-3.46 (m, 2H), 3.57-3.61 (m, 2H), 3.73-3.77 (m, 2H), 3.97 (m, 2H), 11.60 (d, *J* = 6.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 20.2, 22.1, 24.0, 24.3, 27.3, 27.5, 28.3, 28.9, 49.1, 66.8, 74.6, 77.3, 167.8. ESI-HRMS Calcd for ($C_{26}H_{44}N_4O_4$+H^+) 477.3441, Found: 477.3441.



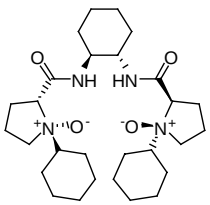
(1*R*,1'*R*,2*S*,2'*S*)-2,2'-(1*S*,2*S*)-cyclohexane-1,2-diylbis(azanediyl)bis(oxomethylene)bis(1-cycloheptylpyrrolidine 1-oxide) (1d). hygrometric white solid. $[\alpha]^{25}_D$ = -6.5° (c = 0.248, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 1.56-1.59 (m, 2H), 1.67-1.71 (m, 8H), 1.81-1.95 (m, 20 H), 2.08-2.10 (m, 2H), 2.32-2.46 (m, 6H), 2.60-2.63 (m, 2H), 3.27-3.31 (m, 4H), 3.58-3.61 (m, 2H), 3.71-3.76 (m, 2H), 3.93 (m, 2H), 11.58 (br, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 20.0, 22.1, 24.6, 25.3, 27.5, 27.8, 28.3, 28.6, 29.6, 49.0, 63.0, 71.6, 76.3, 167.3. ESI-HRMS Calcd for ($C_{30}H_{52}N_4O_4$+H^+) 533.4067, Found: 533.4067.



(1*R*,1'*R*,2*S*,2'*S*)-2,2'-((1*S*,2*S*)-1,2-diphenylethane-1,2-diyl)bis(azanediyl)bis(oxomethylene)bis(1-cyclohexylpyrrolidine 1-oxide) (1e). white solid; m. p. 134-136 °C. $[\alpha]^{25}_D$ = -48.7° (c = 1.412, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 0.96-1.01 (m, 4H), 1.31-1.40 (m, 2H), 1.54-1.55 (m, 2H), 1.61-1.67 (m, 2H), 1.71-1.73 (m, 2H), 1.79-1.82 (m, 3H), 1.90-1.92 (m, 2H), 2.14-2.17 (m, 2H), 2.38-2.40 (m, 3H), 2.50 (m, 2H), 2.66-2.73 (m, 4H), 3.11-3.22 (m, 3H), 3.42-3.47 (m, 2H), 3.55-3.60 (m, 2H), 5.42-5.44 (m, 2H), 7.22-7.33 (m, 2H), 7.34-7.38 (m, 5H), 7.44-7.46 (m, 4H), 11.81 (d, *J* = 5.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 19.8, 24.7, 24.9, 25.1, 26.6, 27.4, 28.4, 58.0, 65.3, 72.3, 75.2, 126.5, 127.2, 128.5, 139.7, 168.8. ESI-HRMS Calcd for ($C_{36}H_{50}N_4O_4$+H^+) 603.3910, Found: 603.3910.

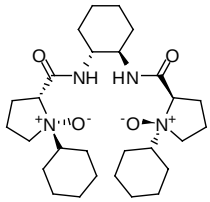


(1*R*,1'*R*,2*S*,2'*S*)-2,2'-(1*R*,2*R*)-cyclohexane-1,2-diylbis(azanediyl)bis(oxomethylene)bis(1-cyclohexylpyrrolidine 1-oxide) (1f). hygrometric white foam. $[\alpha]^{25}_D$ = -30.5° (c = 0.436, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 1.11-1.15 (m, 2H), 1.31-1.36 (m, 4H), 1.52-1.59 (m, 3H), 1.62-1.71 (m, 6H), 1.87-1.90 (m, 8H), 1.96-1.99 (m, 2H), 2.08-2.17 (m, 2H), 2.35-2.40 (m, 9H), 3.04-3.10 (m, 2H), 3.21-3.26 (m, 2H), 3.40-3.44 (m, 2H), 3.59-3.64 (m, 2H), 3.78 (m, 2H), 10.91 (d, *J* = 7.2 Hz, 2H).



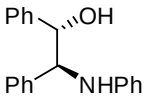
(1*S*,1'*S*,2*R*,2'*R*)-2,2'-(1*S*,2*S*)-cyclohexane-1,2-diylbis(azanediyl)bis(oxomethylene)bis(1-cyclohexylpyrrolidine 1-oxide) (1g). hygrometric white foam. $[\alpha]^{25}_D$ = 24.6° (c = 0.398, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 1.11-1.18 (m, 2H), 1.21-1.31 (m, 6H), 1.34-1.42 (m, 6H), 1.52-1.58 (m, 4H), 1.87-1.90 (m, 6H), 1.96 (m, 2H), 2.05-2.17 (m, 2H), 2.35-2.40 (m, 8H), 3.05-3.11 (m, 2H), 3.19-3.26 (m,

2H), 3.40-3.45 (m, 2H), 3.60-3.64 (m, 2H), 3.78 (m, 2H), 10.89 (d, *J* = 4.8 Hz, 2H).

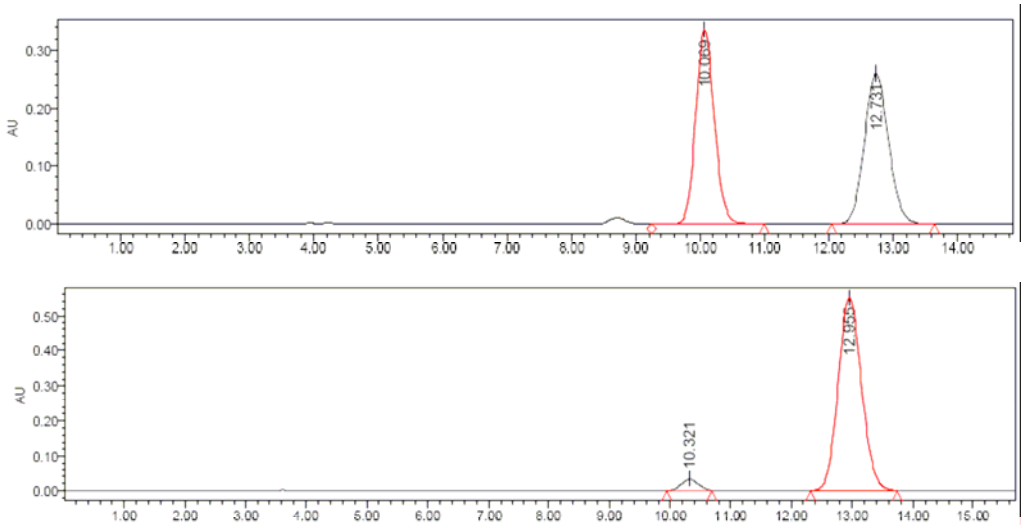


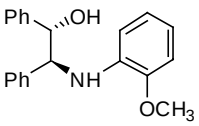
(1*S*,1'*S*,2*R*,2'*R*)-2,2'-(1*R*,2*R*)-cyclohexane-1,2-diylbis(azanediyl)bis(oxomethylene)bis(1-cyclohexylpyrrolidine 1-oxide) (1h). hygrometric white foam. $[\alpha]^{25}_{D}$ = 14.9° (c = 0.396, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 1.11-1.15 (m, 1H), 1.18 (m, 1H), 1.25-1.49 (m, 11H), 1.52-1.58 (m, 4H), 1.80-1.94 (m, 9H), 2.01-2.04 (m, 2H), 2.34-2.46 (m, 6H), 2.54-2.57 (m, 2H), 3.24-3.33 (m, 4H), 3.35-3.40 (m, 2H), 3.64-3.68 (m, 2H), 3.92 (m, 2H), 11.53 (d, *J* = 4.4 Hz, 2H).

Analytical data for 3a-r.

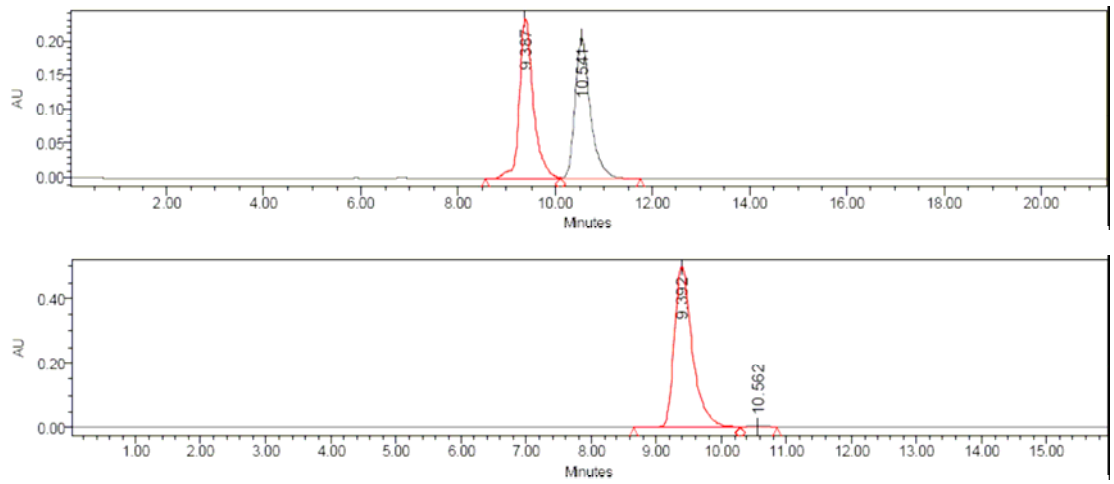


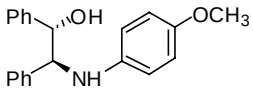
(1*S*,2*S*)-1,2-diphenyl-2-(phenylamino)ethanol (3a). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a white solid; m. p. 84-86 °C. The ee was determined by HPLC using a Chiralcel OD-H column (*i*-PrOH/hexane = 15/85, flow rate = 1 mL/min; t_R = 10.3 min (1*R*, 2*R*) and 13.0 min (1*S*, 2*S*)). 91% ee: $[\alpha]^{25}_{D}$ = -49.1° (c = 0.468, CH_2Cl_2). [lit. $[\alpha]^{24}_{D}$ = -45.2° (c = 0.520, CH_2Cl_2), 91% ee].[2] ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.57 (br, 1H), 4.53 (d, *J* = 6.0 Hz, 1H), 4.87 (d, *J* = 6.0 Hz, 1H), 6.52-6.54 (m, 2H), 6.63-6.69 (m, 1H), 7.04-7.08 (m, 2H), 7.19-7.30 (m, 10H).



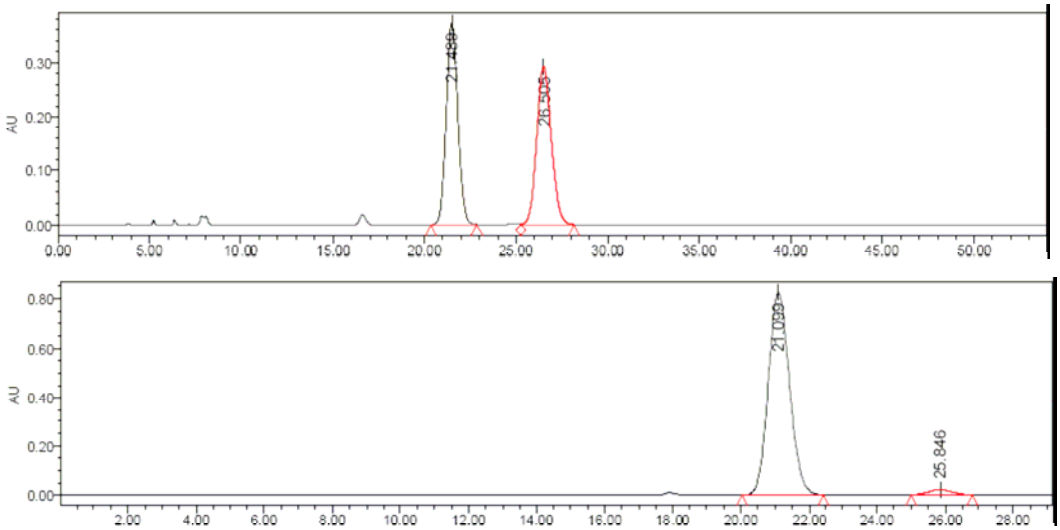


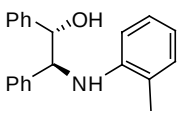
(1*S*,2*S*)-2-(2-methoxyphenylamino)-1,2-diphenylethanol (3b). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a white solid; m. p. 92-93 °C. The ee was determined by HPLC using a Chiralpak AS-H column (*i*-PrOH/hexane = 10/90, flow rate = 1 mL/min, t_R = 9.4 min (1*S*, 2*S*) and 10.6 min (1*R*, 2*R*)). 98% ee: $[\alpha]^{25}_{D}$ = -59.5° (c = 0.560, CH_2Cl_2). [lit. $[\alpha]^{24}_{D}$ = -48.0° (c = 0.540, CH_2Cl_2), 93% ee].[2] ^{1}H NMR (600 MHz, $CDCl_3$): δ = 2.73 (br, 1H), 3.86 (s, 3H), 4.51 (d, *J* = 6.3 Hz, 1H), 4.88 (d, *J* = 6.3 Hz, 1H), 5.26 (br, 1H), 6.38 (dd, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 6.62 (dd, *J* = 7.8 Hz, *J* = 1.8 Hz, 1H), 6.66 (dd, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 6.74 (dd, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 7.16-7.22 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 55.6, 65.0, 78.4, 109.6, 111.8, 117.2, 121.1, 126.8, 127.3, 127.4, 127.8, 128.1, 128.4, 137.2, 140.2, 140.7, 147.4.



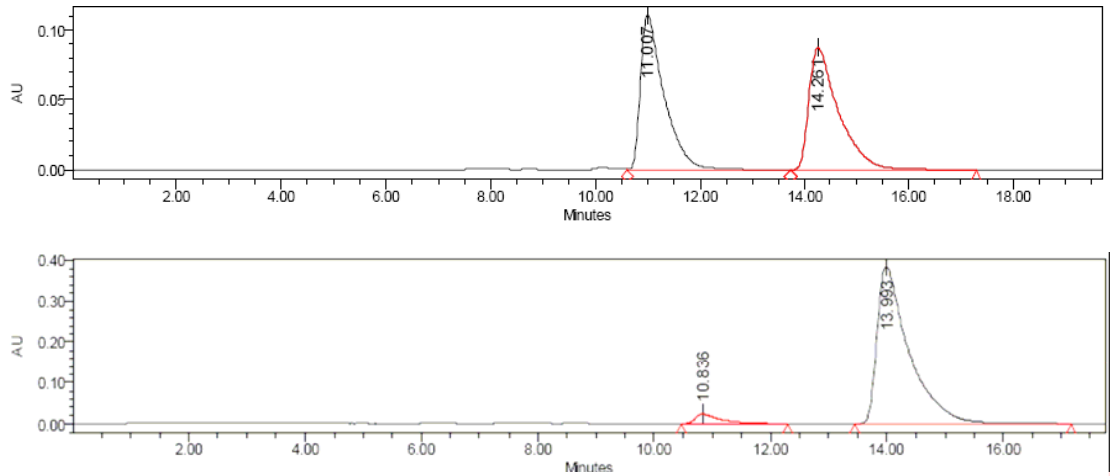


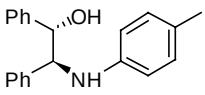
(1*S*,2*S*)-2-(4-methoxyphenylamino)-1,2-diphenylethanol (3c). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a yellow solid; m. p. 98-100 °C. The ee was determined by HPLC using a Chiralcel OD-H column (*i*-PrOH/hexane = 10/90, flow rate = 0.8 mL/min, t_R = 21.1 min (1*S*, 2*S*) and 25.8 min (1*R*, 2*R*)). 94% ee: $[\alpha]^{25}_D$ = -28.4° (c = 0.402, CH_2Cl_2). [lit. $[\alpha]^{23}_D$ = +25.1° (c = 0.61, CH_2Cl_2), 82% ee].[3] ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.67 (s, 3H), 4.41 (d, J = 6.4 Hz, 1H), 4.83 (d, J = 6.4 Hz, 1H), 6.52 (d, J = 8.8 Hz, 2H), 6.66 (d, J = 8.8, 2H) 7.15-7.24 (m, 10H).



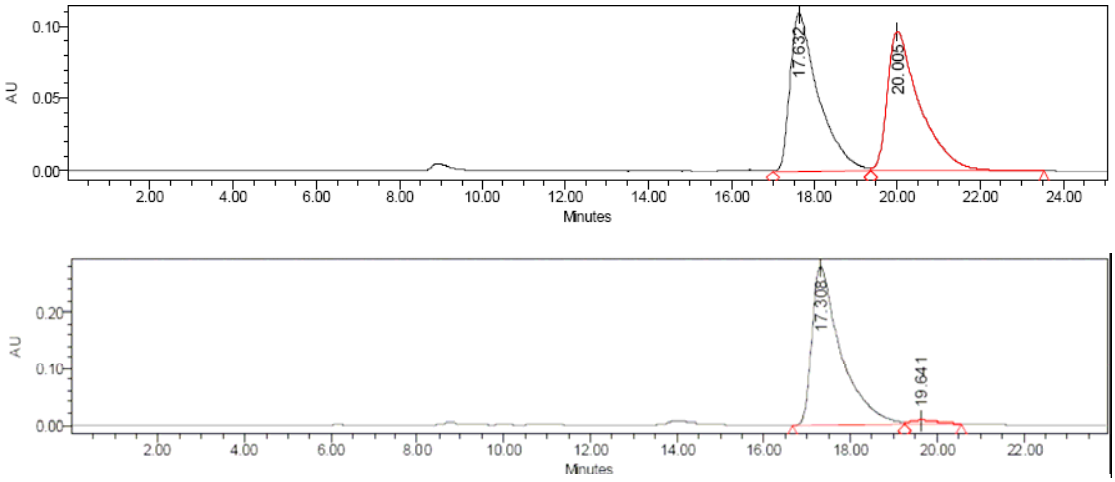


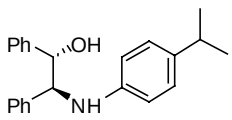
(1*S*,2*S*)-1,2-diphenyl-2-(*o*-tolylamino)ethanol (3d). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a hygrometric white solid. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 20/80, flow rate = 0.5 mL/min, t_R = 10.8 min (1*R*, 2*R*) and 14.0 min (1*S*, 2*S*)). 91% ee: $[\alpha]^{25}_D$ = -79.2° (c = 0.614, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.19 (s, 3H), 4.56 (d, J = 5.2 Hz, 1H), 4.96 (d, J = 5.2 Hz, 1H), 6.28 (d, J = 8.0 Hz, 1H), 6.56-6.59 (m, 1H), 6.87-6.90 (m, 1H), 7.01 (d, J = 7.2 Hz, 1H), 7.22-7.29 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 17.6, 64.6, 78.1, 111.6, 117.4, 122.8, 126.5, 126.9, 127.2, 127.6, 128.0, 128.4, 128.7, 130.0, 140.4, 140.7, 145.2. ESI-HRMS Calcd for ($C_{21}H_{21}NO$+Na^+) 326.1521, Found: 326.1521.



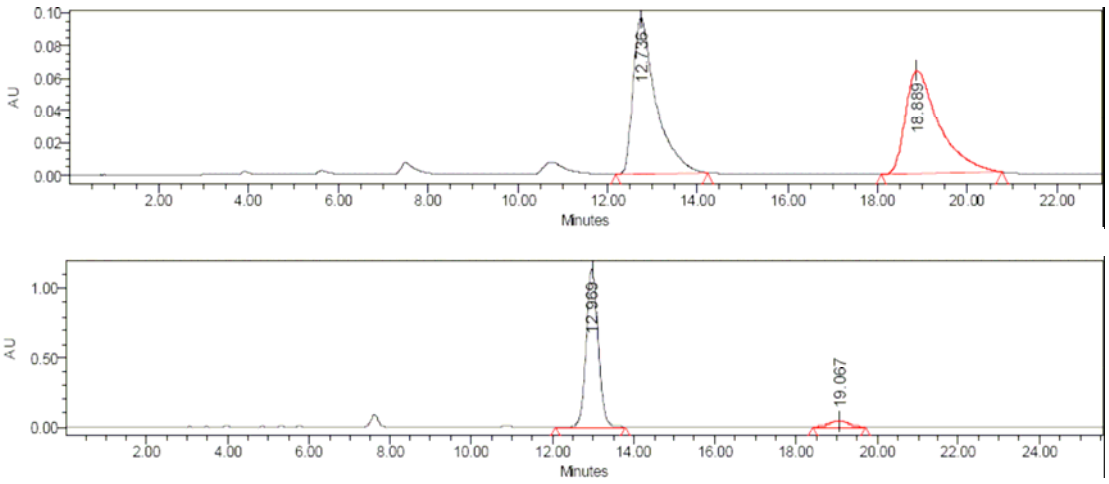


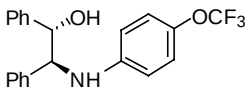
(1*S*,2*S*)-1,2-diphenyl-2-(*p*-tolylamino)ethanol (3e). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a white solid; m. p. 102-104 °C. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 20/80, flow rate = 0.5 mL/min, t_R = 17.3 min (1*S*, 2*S*) and 19.6 min (1*R*, 2*R*)). 96% ee: $[\alpha]^{25}_D$ = -34.7° (c = 0.412, CH_2Cl_2). [lit. $[\alpha]^{27}_D$ = +22.6° (c = 1, $CHCl_3$), 77% ee].[4] ^{1}H NMR (400 MHz, $CDCl_3$): 2.16 (s, 3H), 2.67 (br, 1H), 4.48 (d, *J* = 6.0 Hz, 1H), 4.86 (d, *J* = 6.0 Hz, 1H), 6.46 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 2H), 7.19-7.26 (m, 10H).



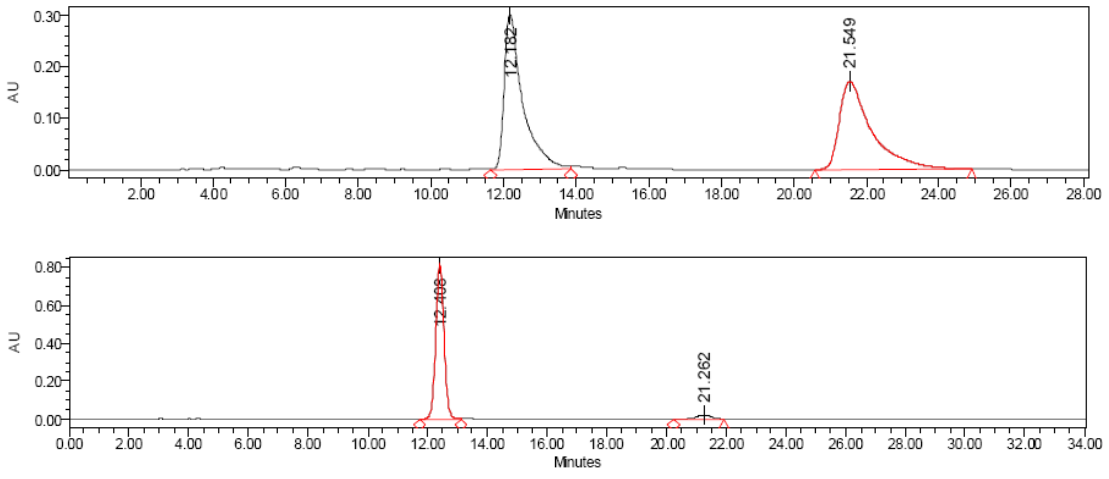


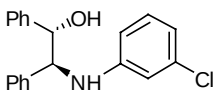
(1*S*,2*S*)-2-(4-isopropylphenylamino)-1,2-diphenylethanol (3f). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a white solid; m. p. 79-81 °C. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 10/90, flow rate = 1 mL/min, t_R = 13.0 min (1*S*, 2*S*) and 19.1 min (1*R*, 2*R*)). 91% ee: $[\alpha]^{25}_D$ = -24.7° (c = 0.660, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 1.14 (d, *J* = 7.2 Hz, 6H), 2.70 (br, 1H), 2.71-2.75 (m, 1H), 4.47 (d, *J* = 6.0 Hz, 1H), 4.84 (d, *J* = 6.4 Hz, 1H), 6.48-6.50 (m, 2H), 6.92-6.94 (m, 2H), 7.20-7.26 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$): 24.3, 33.2, 65.3, 78.2, 114.4, 126.8, 127.0, 127.4, 127.5, 127.9, 128.3, 128.6, 138.5, 140.5, 140.7, 145.4. ESI-HRMS Calcd for ($C_{23}H_{25}NO$+Na^+) 354.1834, Found: 354.1834.



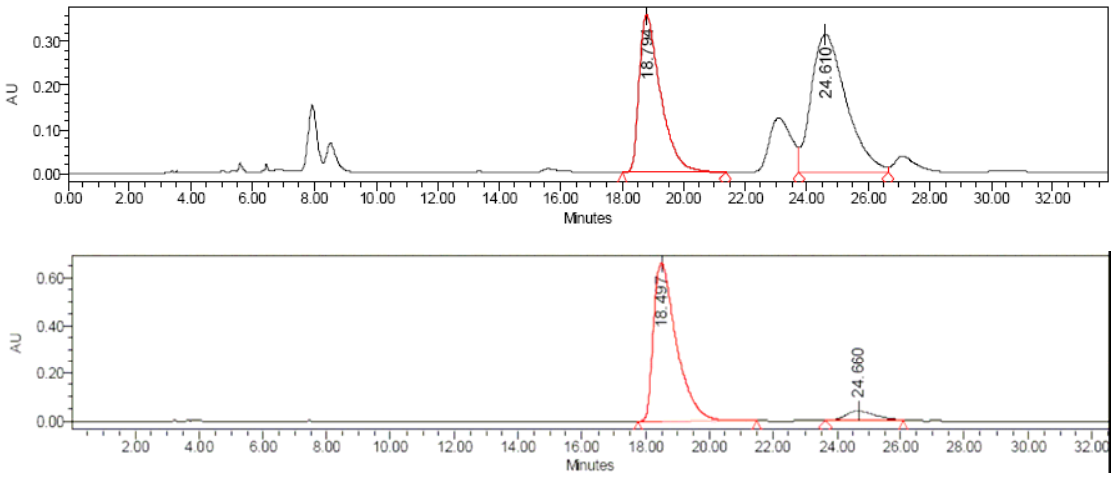


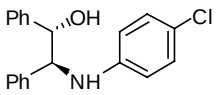
(1*S*,2*S*)-1,2-diphenyl-2-(4-(trifluoromethoxy)phenylamino)ethanol (3g). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a white solid; m. p. 75-77 °C. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 10/90, flow rate = 1 mL/min, t_R = 12.4 min (1*S*, 2*S*) and 21.3 min (1*R*, 2*R*)). 92% ee: $[\alpha]^{25}_D$ = -43.1° (c = 0.518, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 2.37 (br, 1H), 4.48 (d, *J* = 5.6 Hz, 1H), 4.88 (d, *J* = 5.6 Hz, 1H), 6.43-6.47 (m, 2H), 6.88-6.91(m, 2H), 7.20-7.25 (m, 2H), 7.28-7.32 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): 64.9, 78.1, 114.4, 119.4, 122.0, 122.2, 126.5, 127.3, 127.7, 128.1, 128.4, 128.7, 139.9, 140.5, 140.8, 146.2. ESI-HRMS Calcd for ($C_{21}H_{18}F_3NO_2$+Na^+) 396.1187, Found: 396.1188.



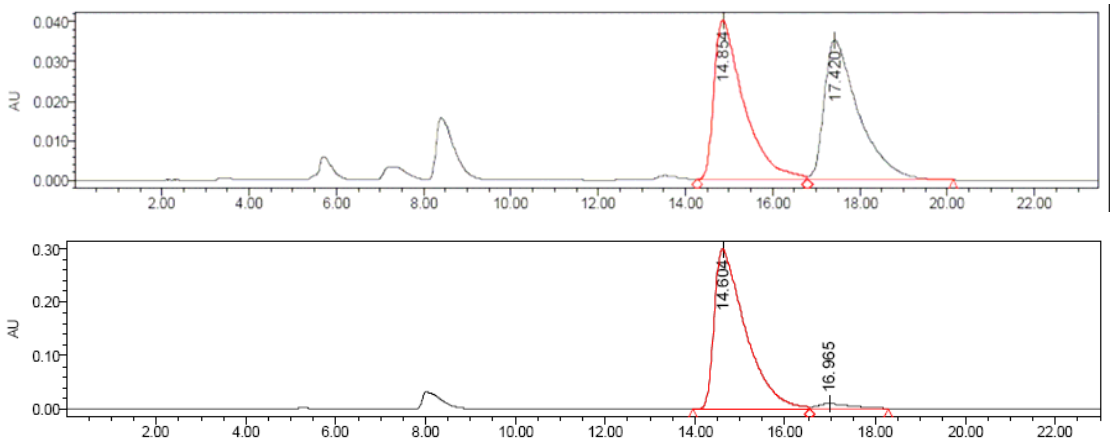


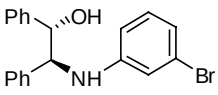
(1*S*,2*S*)-2-(3-chlorophenylamino)-1,2-diphenylethanol (3h).[5] The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a liquid. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 10/90, flow rate = 1 mL/min, t_R = 18.5 min (1*S*, 2*S*) and 24.7 min (1*R*, 2*R*)). 86% ee: $[\alpha]^{25}_D$ = -35.5° (c = 0.588, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 2.33 (d, *J* = 2.8 Hz, 1H), 4.52-4.53 (m, 1H), 4.83 (br, 1H), 4.89-4.91 (m, 1H), 6.35-6.37 (m, 1H), 6.48 (s, 1H), 6.59 (d, *J* = 9.6 Hz, 1H), 6.92-6.96 (m, 1H), 7.23-7.32 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$): 64.3, 77.9, 112.1, 113.8, 117.7, 126.5, 127.2, 127.7, 128.1, 128.4, 128.7, 130.1, 134.8, 139.8, 140.5, 148.5. ESI-HRMS Calcd for ($C_{20}H_{18}ClNO$+Na^+) 346.0975, Found: 346.0975.



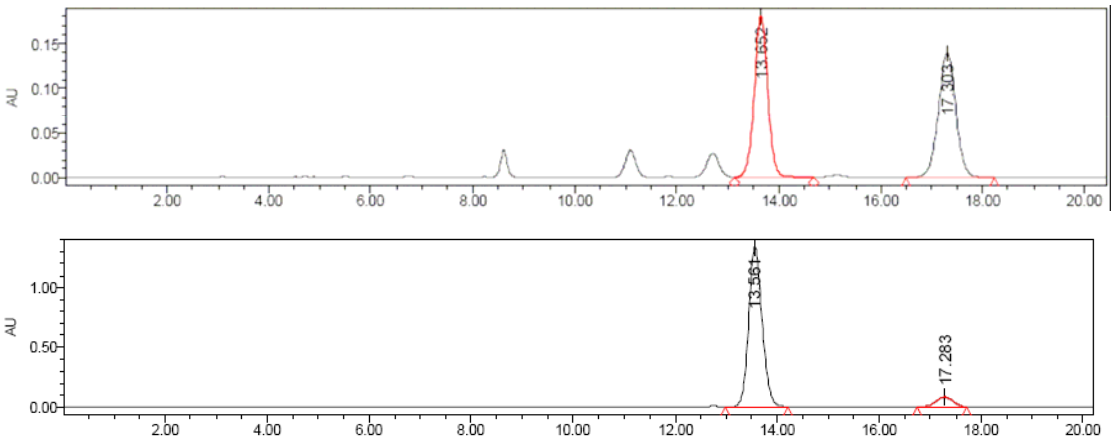


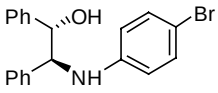
(1*S*,2*S*)-2-(4-chlorophenylamino)-1,2-diphenylethanol (3i). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a liquid. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 10/90, flow rate = 1 mL/min, t_R = 14.6 min (1*S*, 2*S*) and 17.0 min (1*R*, 2*R*)). 94% ee: $[\alpha]^{25}_D$ = -33.1° (c = 0.559, CH_2Cl_2). [lit. $[\alpha]^{27}_D$ = +40.6° (c = 1.2, $CHCl_3$), 77% ee].[4] ^{1}H NMR (400 MHz, $CDCl_3$): 2.37 (br, 1H), 4.48 (d, *J* = 5.6 Hz, 1H), 4.72 (br, 1H), 4.89 (d, *J* = 5.6 Hz, 1H), 6.42 (d, *J* = 8.8 Hz, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 7.20-7.23 (m, 5H), 7.27-7.29 (m, 5H).



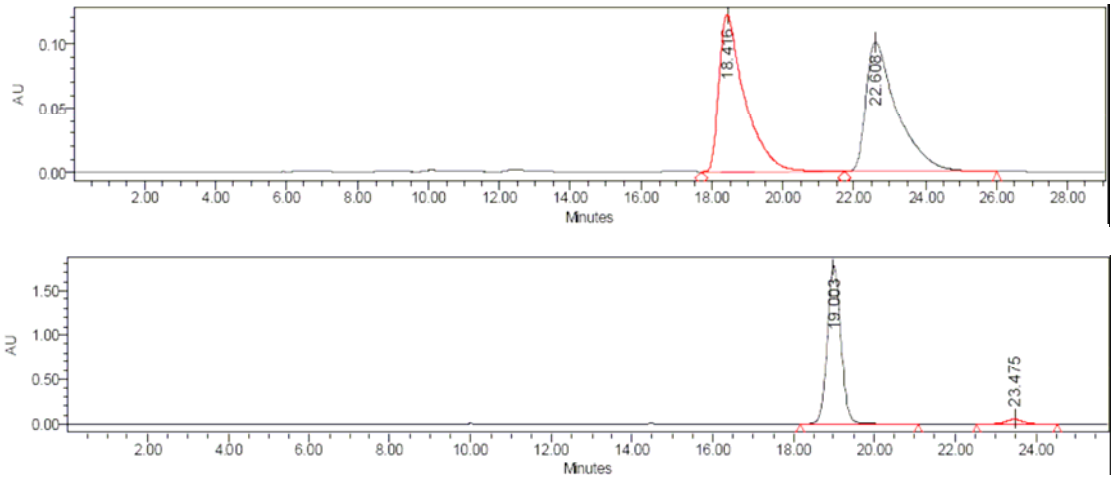


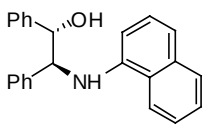
(1*S*,2*S*)-2-(3-bromophenylamino)-1,2-diphenylethanol (3j). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a hygrometric white solid. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 10/90, flow rate = 1 mL/min, t_R = 13.6 min (1*S*, 2*S*) and 17.3 min (1*R*, 2*R*)). 86% ee: $[\alpha]^{25}_D$ = -31.7° (c = 0.561, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 2.30 (d, *J* = 2.8 Hz, 1H), 4.50-4.52 (m, 1H), 4.81 (d, *J* = 4.4 Hz, 1H), 4.90 (dd, *J* = 5.2 Hz, *J* = 3.2 Hz, 1H), 6.38-6.40 (m, 1H), 6.65 (s, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 6.86-6.90 (m, 1H), 7.23-7.25 (m, 3H), 7.29-7.32 (m, 7H). ^{13}C NMR (100 MHz, $CDCl_3$): 64.2, 77.9, 112.5, 116.8, 120.6, 123.0, 126.5, 127.2, 127.8, 128.1, 128.4, 128.7, 130.4, 139.8, 140.4, 148.7. ESI-HRMS Calcd for ($C_{20}H_{18}BrNO$+Na^+) 390.0469, Found: 390.0470.



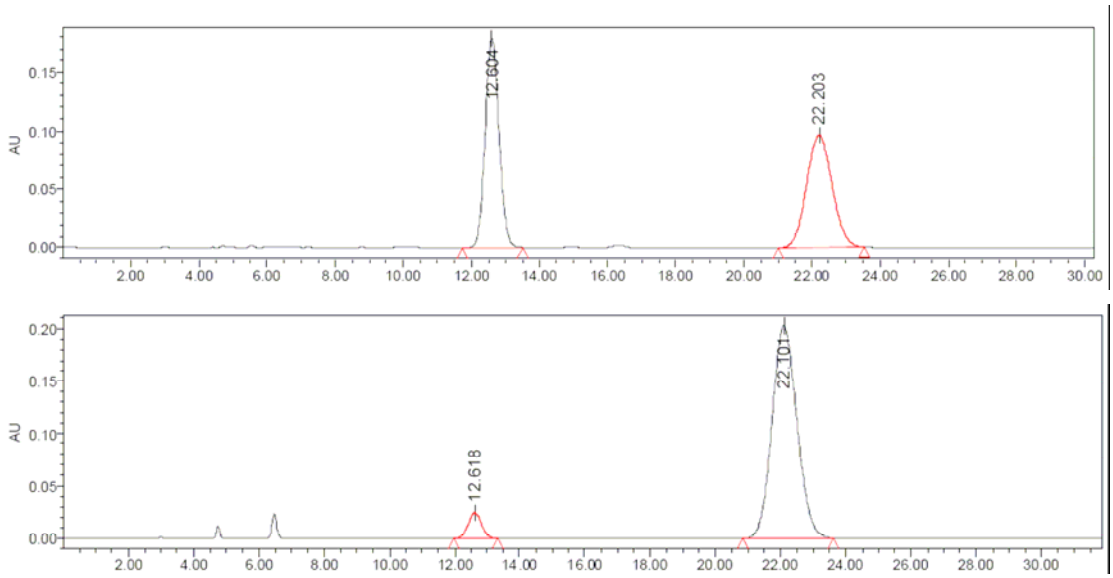


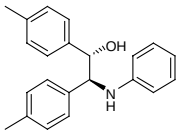
(1*S*,2*S*)-2-(4-bromophenylamino)-1,2-diphenylethanol (3k).[6] The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a hygrometric white solid. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 20/80, flow rate = 0.5 mL/min, t_R = 19.0 min (1*S*, 2*S*) and 23.5 min (1*R*, 2*R*)). 93% ee: $[\alpha]^{25}_D$ = -50.0° (c = 0.612, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 2.39 (br, 1H), 4.48 (d, *J* = 5.6 Hz, 1H), 4.89 (d, *J* = 5.6 Hz, 1H), 6.35-6.39 (m, 2H), 7.09-7.13 (m, 2H), 7.20-7.28 (m, 10H).



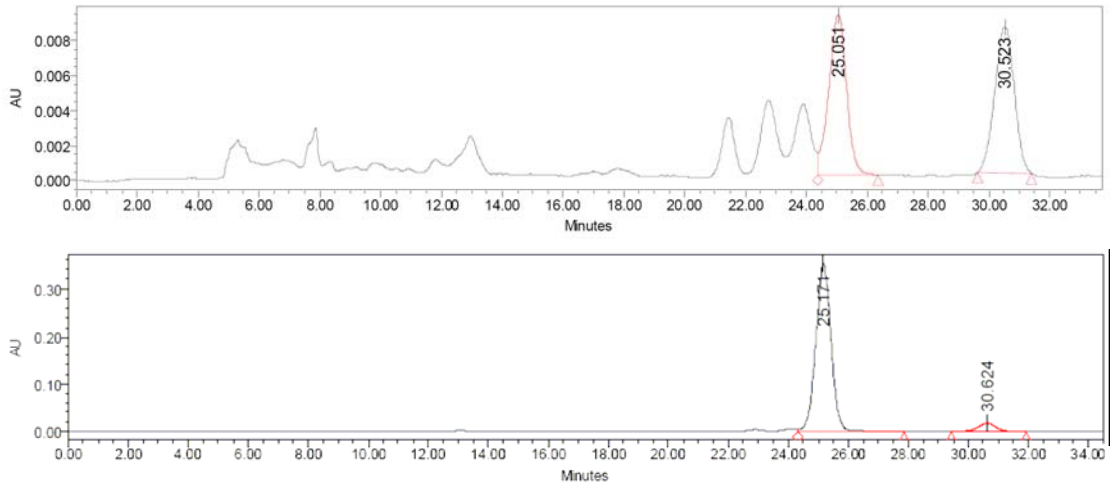


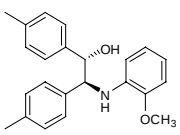
(1*S*,2*S*)-2-(naphthalen-1-ylamino)-1,2-diphenylethanol (3l). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a white solid; m. p. 52-55 °C. The ee was determined by HPLC using a Chiralcel OD-H column (*i*-PrOH/hexane = 10/90, flow rate = 1 mL/min, t_R = 12.6 min (1*R*, 2*R*) and 22.1 min (1*S*, 2*S*)). 88% ee: $[\alpha]^{25}_D$ = -131.0° (c = 0.306, CH_2Cl_2). [lit. $[\alpha]^{22}_D$ = -144.9° (c = 0.390, CH_2Cl_2), 91% ee].[2] ^{1}H NMR (400 MHz, $CDCl_3$): 2.55 (br, 1H), 4.73 (d, *J* = 5.6 Hz, 1H), 5.20 (d, *J* = 5.2 Hz, 1H), 5.60 (br, 1H), 6.29-6.33 (m, 1H), 7.11-7.18 (m, 2H), 7.25-7.37 (m, 10H), 7.45-7.51 (m, 2H), 7.76-7.79 (m, 1H), 8.00 (m, 1H).





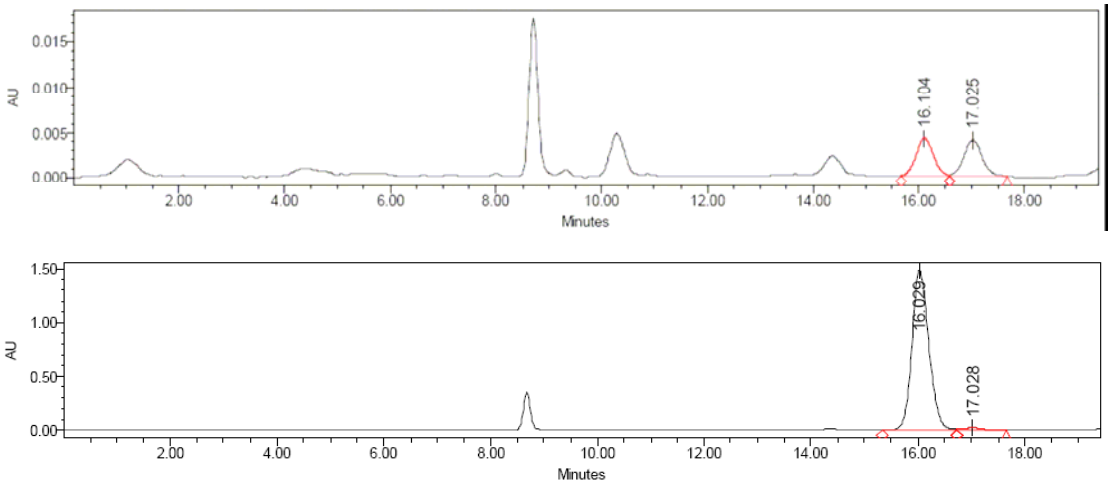
(1*S*,2*S*)-2-(phenylamino)-1,2-di*p*-tolylethanol (3m). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a hygrometric white solid. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 5/95, flow rate = 1 mL/min, t_R = 25.2 min (1*S*, 2*S*) and 30.6 min (1*R*, 2*R*)). 89% ee: $[\alpha]^{25}_D$ = -47.0° (c = 0.434, CH_2Cl_2). [lit. $[\alpha]^{24}_D$ = -47.3° (c = 0.54, CH_2Cl_2), 90% ee].[2] ^{1}H NMR (400 MHz, $CDCl_3$): 2.32 (s, 3H), 2.34 (s, 3H), 2.52 (br, 1H), 4.51 (d, *J* = 5.6 Hz, 1H), 4.65 (br, 1H), 4.84 (d, *J* = 5.6 Hz, 1H), 6.53-6.55 (m, 2H), 6.64-6.68 (m, 1H), 7.06-7.15 (m, 8H), 7.18-7.20 (m, 2H).

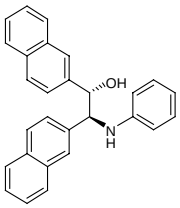




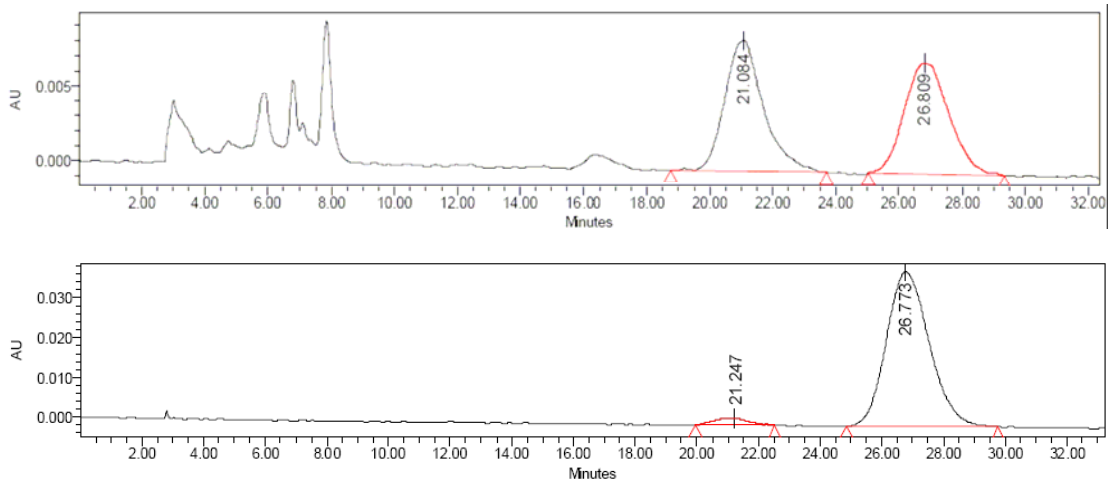
(1*S*,2*S*)-2-(2-methoxyphenylamino)-1,2-di*p*-tolylethanol (3n). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 10 : 1) as a hygrometric white solid. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 10/90, flow rate = 1 mL/min, t_R = 16.0 min (1*S*, 2*S*) and 17.0 min (1*R*, 2*R*)). 97% ee: $[\alpha]^{25}_D$ = -49.5° (c = 1.048, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 2.28 (s, 3H), 2.31 (s, 3H), 2.62 (d, *J* = 2.4 Hz, 1H), 3.86 (s, 3H), 4.47 (d, *J* = 6.0 Hz, 1H), 4.84 (dd, *J* = 6.0 Hz, *J* = 1.6 Hz, 1H), 5.21 (br, 1H), 6.38 (dd, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 6.58-6.62 (m, 1H), 6.64-6.68 (m, 1H),

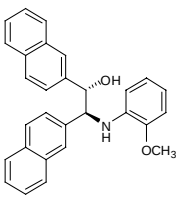
6.72-6.74 (m, 1H), 7.02-7.08 (m, 6H), 7.14-7.16 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 21.1, 21.2, 55.6, 64.4, 78.1, 109.6, 111.7, 117.0, 121.1, 126.7, 127.2, 128.8, 129.2, 136.9, 137.2, 137.3, 137.4, 137.8, 147.4. ESI-HRMS Calcd for ($C_{23}H_{25}NO_2$+Na^+)370.1783, Found:370.1778.





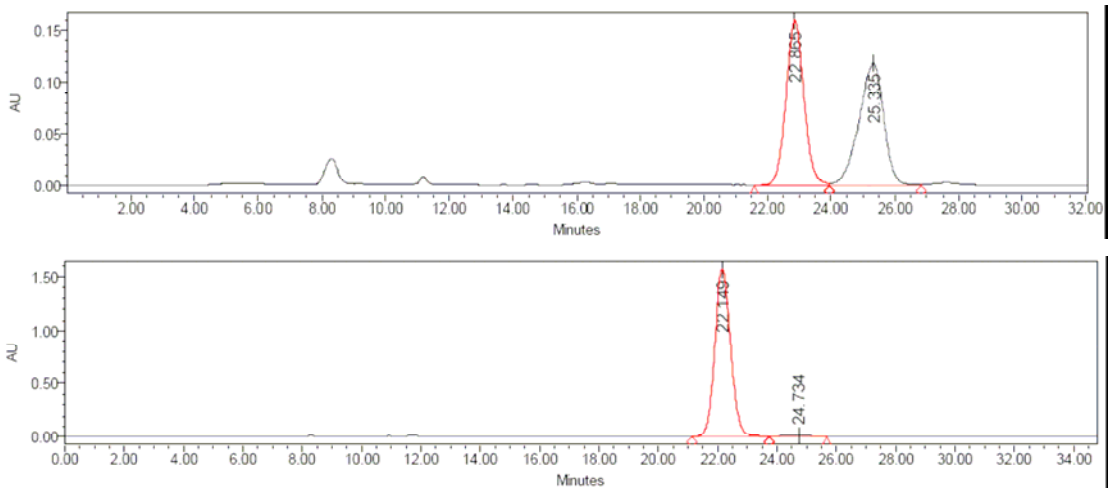
(1*S*,2*S*)-2-(phenylamino)-1,2-di(naphthalen-2-yl)ethanol (3o). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 9 : 1) as a white solid; m. p. 153-155 °C. The ee was determined by HPLC using a Chiralcel OD-H (*i*-PrOH/hexane = 20/80, flow rate = 1 mL/min, t_R = 21.2 min (1*R*, 2*R*) and 26.8 min (1*S*, 2*S*)). 93% ee: $[\alpha]^{25}_D$ = -122.4° (c = 0.637, CH_2Cl_2). [lit. $[\alpha]^{22}_D$ = -133.8° (c = 0.410, CH_2Cl_2), 91% ee].[2] ^{1}H NMR (400 MHz, $CDCl_3$): 2.58 (br, 1H), 4.82 (d, *J* = 5.2 Hz, 1H), 5.17 (d, *J* = 5.2 Hz, 1H) 6.54-6.56 (m, 2H), 6.60-6.63 (m, 1H), 7.00-7.04 (m, 2H), 7.36-7.48 (m, 6H), 7.72-7.82 (m, 8H).

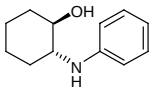




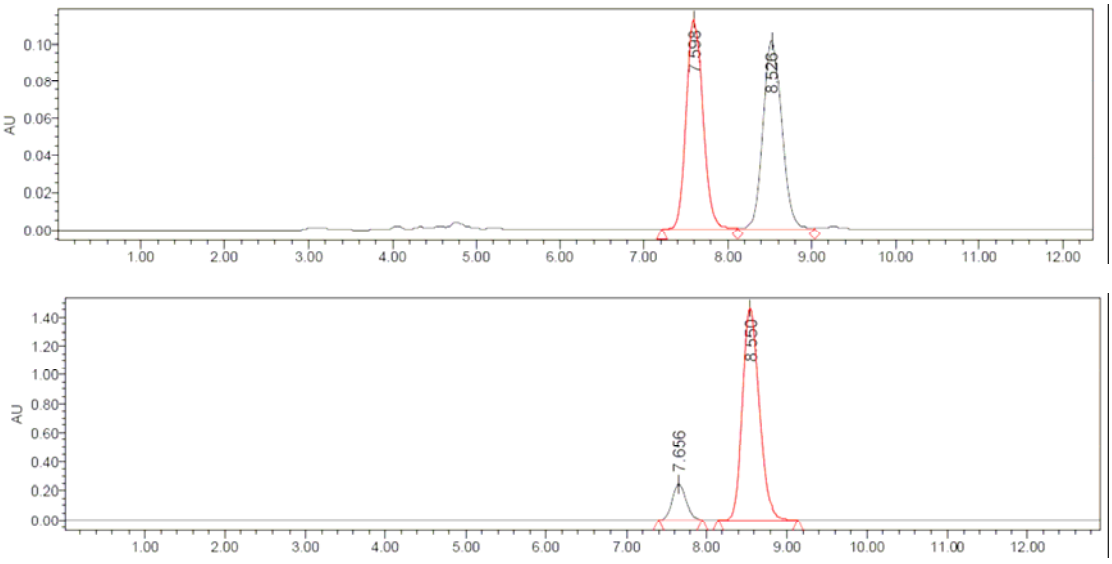
(1*S*,2*S*)-2-(2-methoxyphenylamino)-1,2-di(naphthalen-2-yl)ethanol (3p). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 9 : 1) as a white solid; m. p. 65-67 °C. The ee was determined by HPLC using a Chiralpak AD-H column (*i*-PrOH/hexane = 15/85, flow rate = 1 mL/min, t_R = 22.1 min (1*S*, 2*S*) and 24.7 min (1*R*, 2*R*)). 98% ee: $[\alpha]^{25}_D$ = -126.2° (c = 0.806, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$): 2.82 (br, 1H), 3.84 (s, 3H), 4.77 (d, *J* = 6.0 Hz, 1H), 5.16 (d, *J* = 6.0 Hz, 1H), 5.27 (br, 1H), 6.39-6.41 (m, 1H), 6.58-6.63 (m, 2H), 6.71-6.73 (m, 1H), 7.30-7.36 (m,

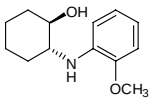
2H), 7.39-7.45 (m, 4H), 7.69-7.79 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$): 55.7, 65.0, 78.2, 109.6, 111.9, 117.3, 121.1, 124.6, 125.4, 125.8, 125.9, 126.0, 126.3, 127.6, 127.9, 128.0, 128.1, 128.3, 133.0, 133.1, 133.1, 133.4, 137.2, 137.8, 138.1, 147.4. ESI-HRMS Calcd for ($C_{29}H_{25}NO_2$+Na^+)442.1783, Found: 442.1778.





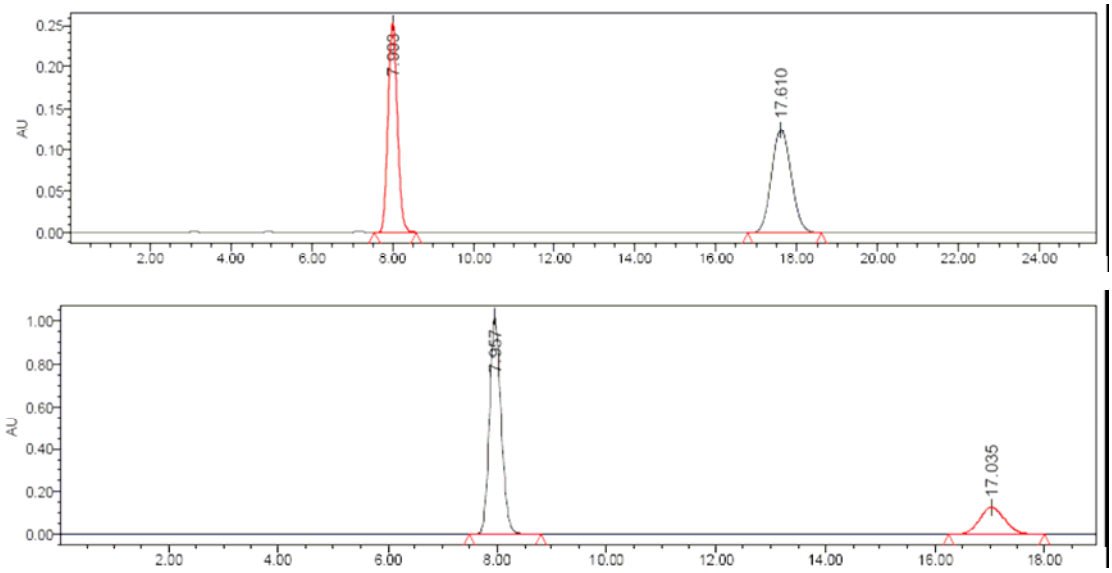
(1*R*,2*R*)-2-(phenylamino)cyclohexanol (3q). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 6 : 1) as a white solid; m. p. 66-68 °C. The ee was determined by HPLC using a Chiralcel OD-H column (*i*-PrOH/hexane = 15/85, flow rate = 1 mL/min, t_R = 7.6 min (1*S*, 2*S*) and 8.6 min (1*R*, 2*R*)). 76% ee: $[\alpha]^{25}_D$ = -72.7° (c = 0.384, CH_2Cl_2). [lit. $[\alpha]^{23}_D$ = -37.7° (c = 0.535, CH_2Cl_2), 54% ee].[3] ^{1}H NMR (400 MHz, $CDCl_3$): 1.05-1.09 (m, 1H), 1.27-1.44 (m, 3H), 1.73-1.81 (m, 2H), 2.12-2.16 (m, 2H), 2.78 (br, 1H), 3.14-3.20 (m, 1H), 3.34-3.39 (m, 1H), 6.73-6.79 (m, 3H), 7.18-7.28 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 24.3, 25.0, 31.6, 33.2, 60.2, 74.5, 114.4, 118.4, 129.4, 147.9.





(1*R*,2*R*)-2-(2-methoxyphenylamino)cyclohexanol (3r). The title compound was purified by silica gel chromatography (petroleum ether : ethyl acetate = 6 : 1) as a white solid; m. p. 62-63 °C. The ee was determined by HPLC using a Chiralcel OD-H column (*i*-PrOH/hexane = 15/85, flow rate = 1 mL/min, t_R = 8.0 min (1*R*, 2*R*) and 17.0 min (1*S*, 2*S*)).

57% ee: $[\alpha]^{25}_D$ = -62.1° (c = 0.314, CH_2Cl_2). [lit. $[\alpha]^{20}_D$ = -40.8° (c = 0.6, $CHCl_3$), 82% ee].[7] ^{1}H NMR (400 MHz, $CDCl_3$): 1.05-1.09 (m, 1H), 1.29-1.43 (m, 3H), 1.70-1.80 (m, 2H), 2.06-2.15 (m, 2H), 2.80 (br, 1H), 3.15-3.18 (m, 1H), 3.39-3.43 (m, 1H), 3.85 (s, 3H), 3.99 (br, 1H), 6.68-6.72 (m, 1H), 6.77-6.80 (m, 2H), 6.84-6.88 (m, 1H).



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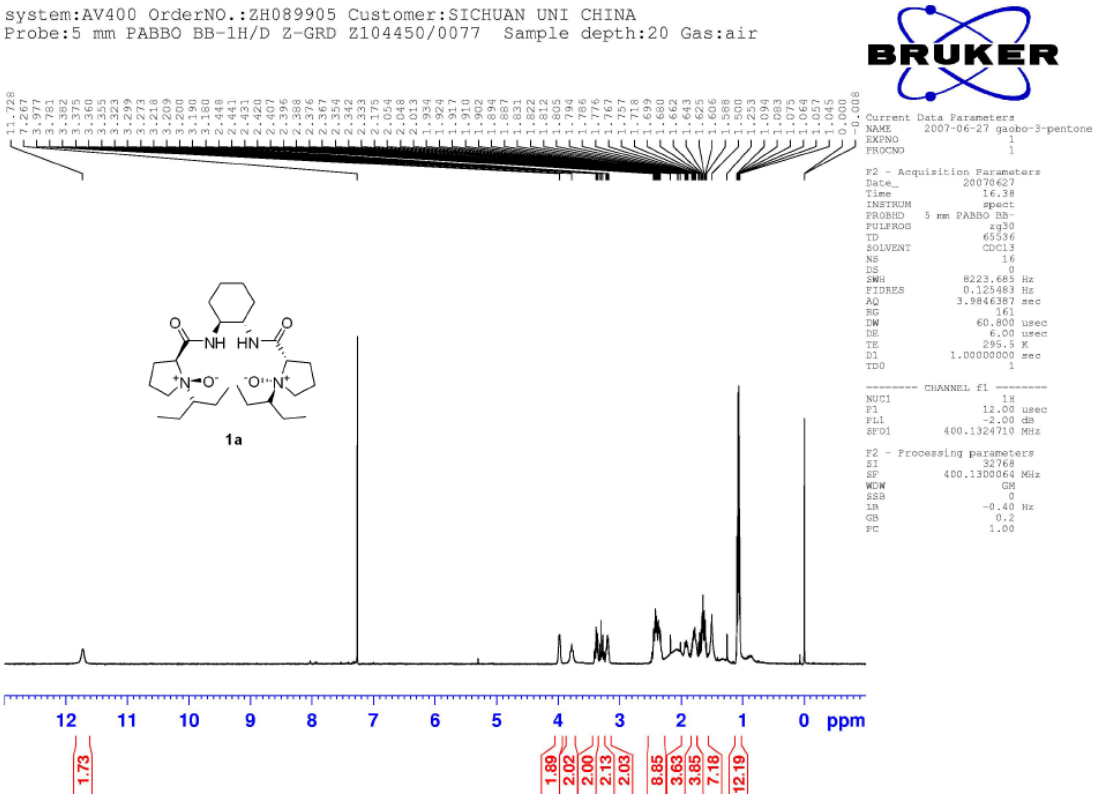
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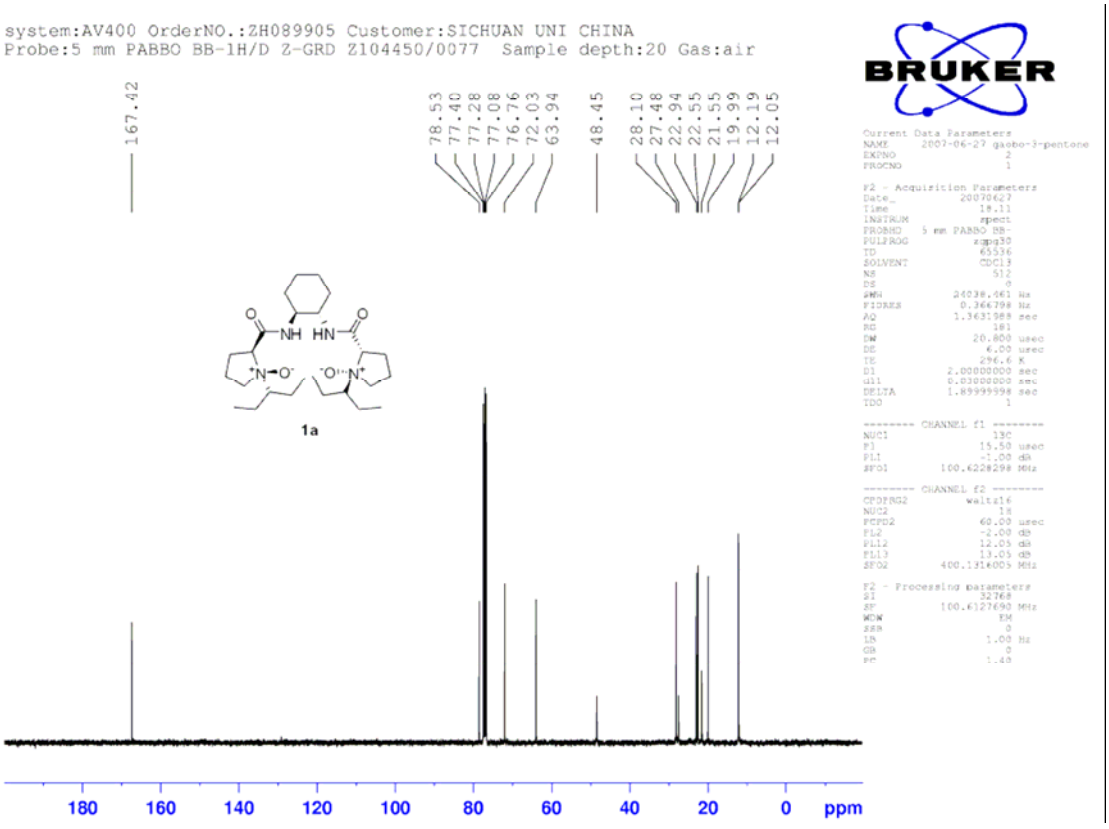
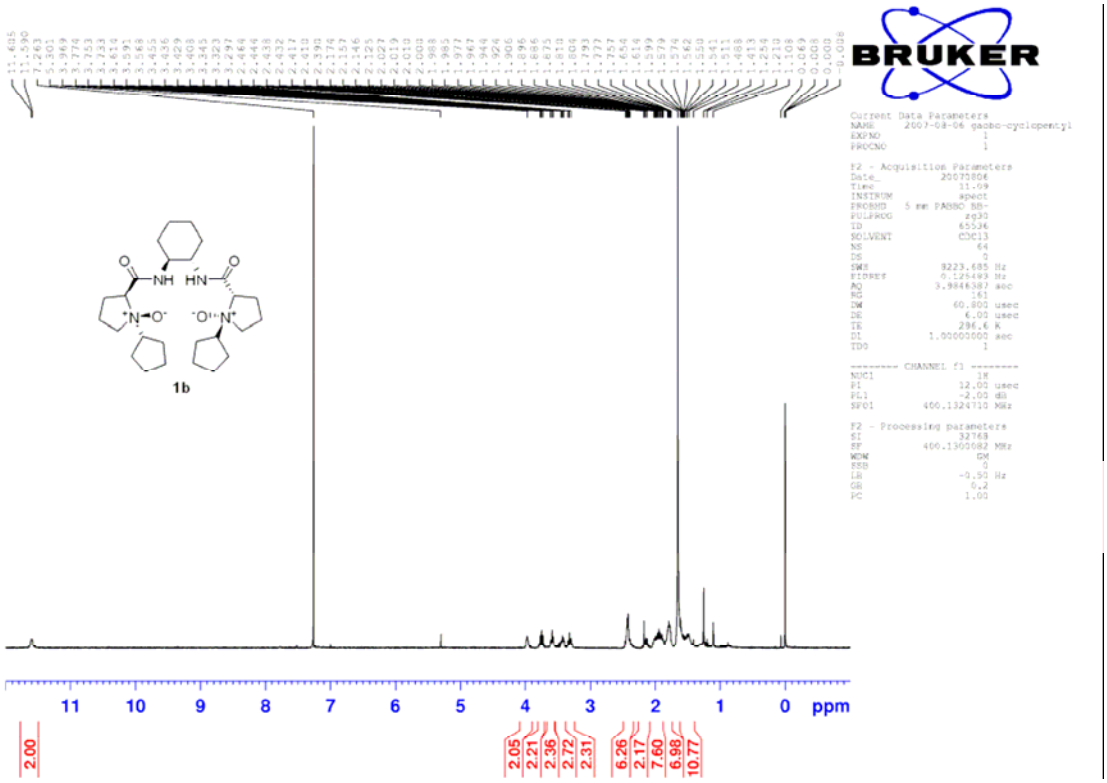
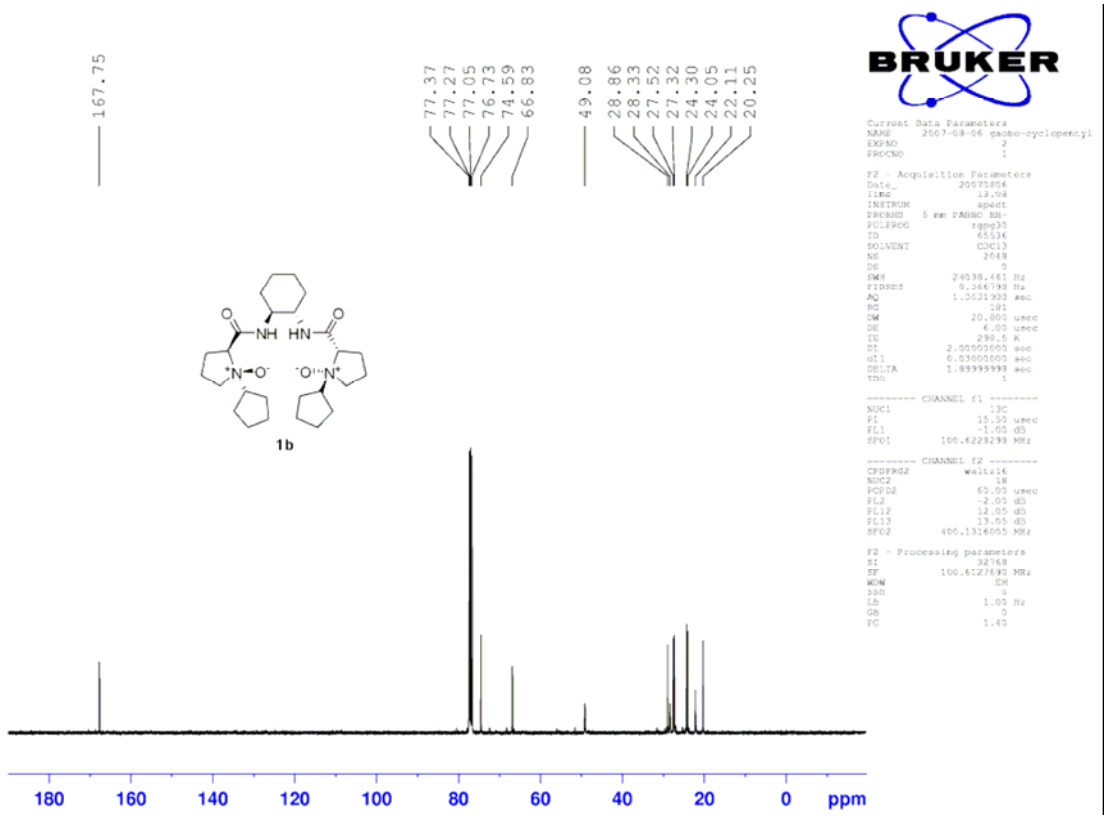
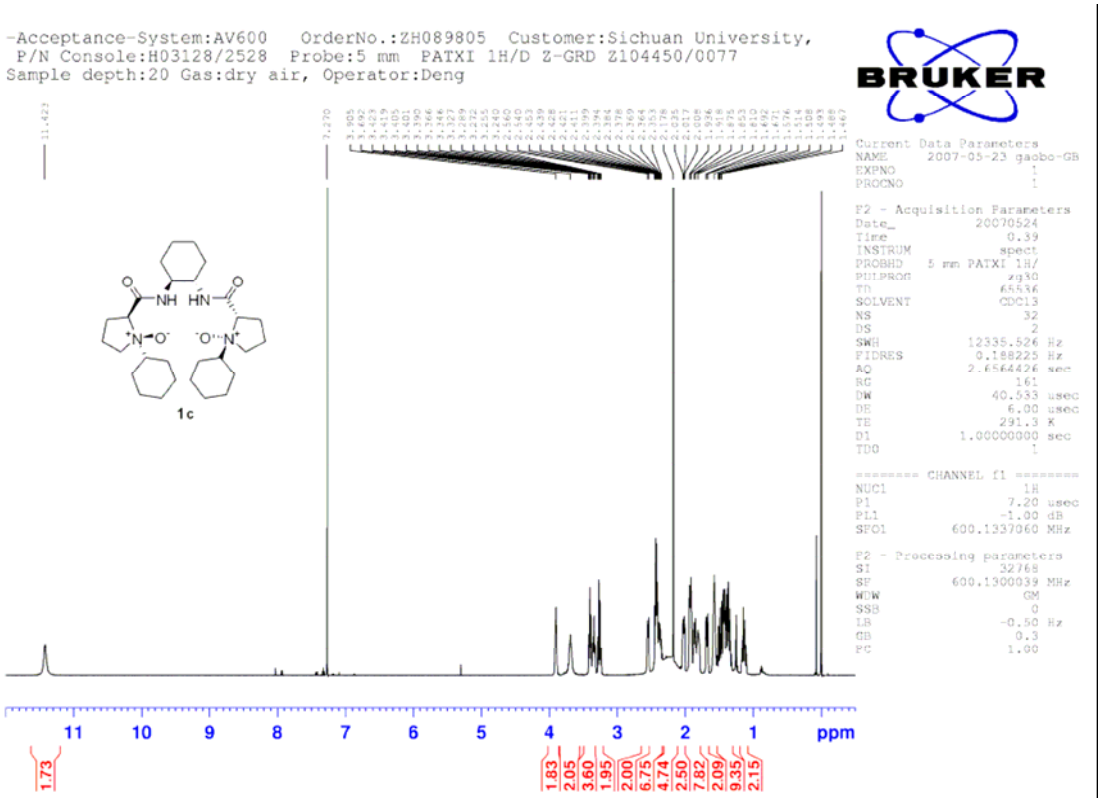
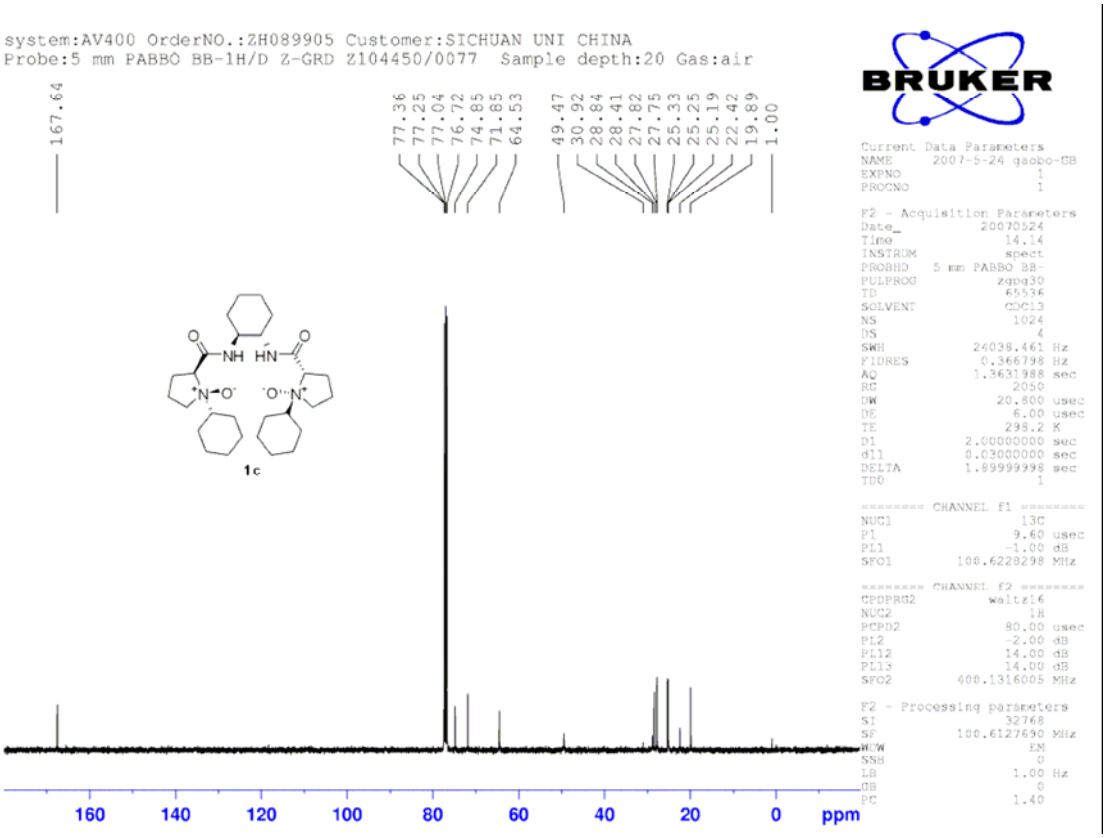
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
BRUKER
Current Data Parameters
NAME 2007-06-27 gaobo-3-pentone
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070627
Time 16.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300064 MHz
WDW GM
SSB 0
LB -0.40 Hz
GB 0.2
PC 1.00
1a
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.73 1.89 2.02 2.00 2.13 2.03 8.85 3.63 3.85 7.18 12.19

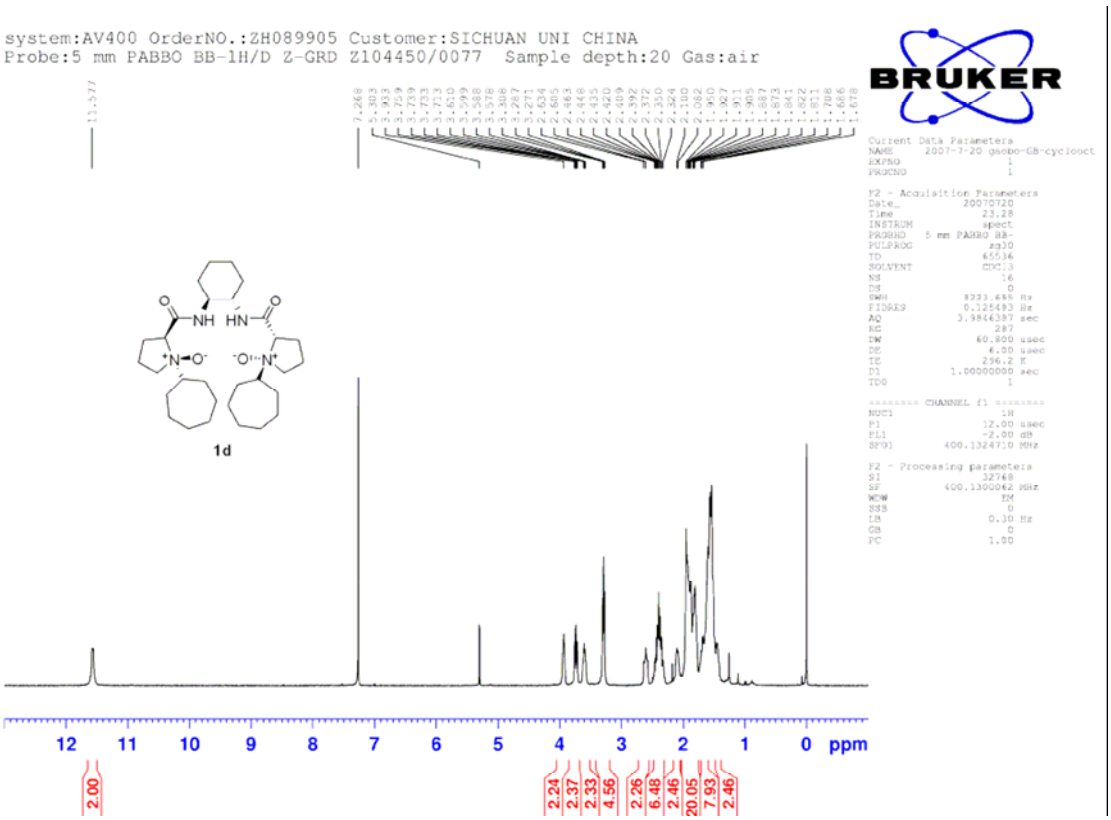

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
BRUKER
Current Data Parameters
NAME 2007-06-27 gaobo-3-pentone
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070627
Time 18.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631589 sec
RG 181
DW 20.800 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 15.50 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -2.00 dB
PL12 12.05 dB
PL13 13.05 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
167.42 78.53 77.40 77.28 77.08 76.76 72.03 63.94 48.45 28.10 27.48 22.94 22.55 21.55 19.99 12.19 12.05
1a
180 160 140 120 100 80 60 40 20 0 ppm

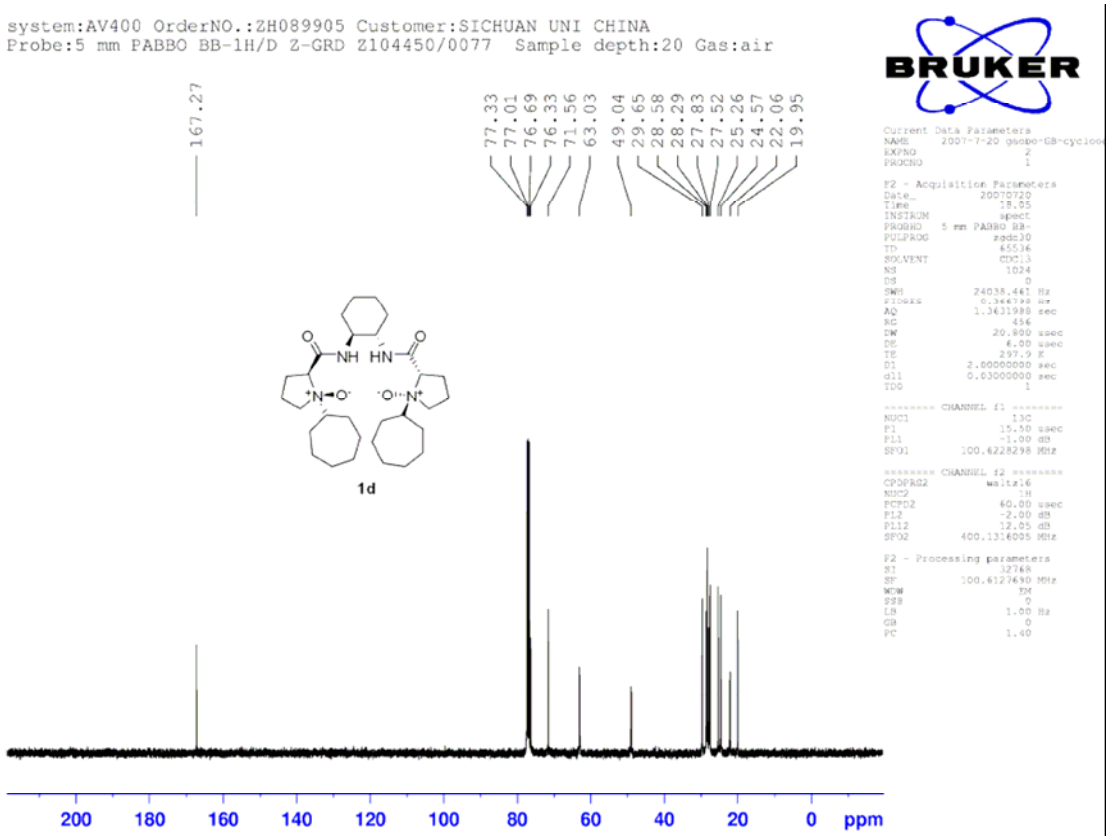

BRUKER
NH HN
1b
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.05 2.21 2.36 2.72 2.31
6.26 2.17 7.60 6.98 10.77

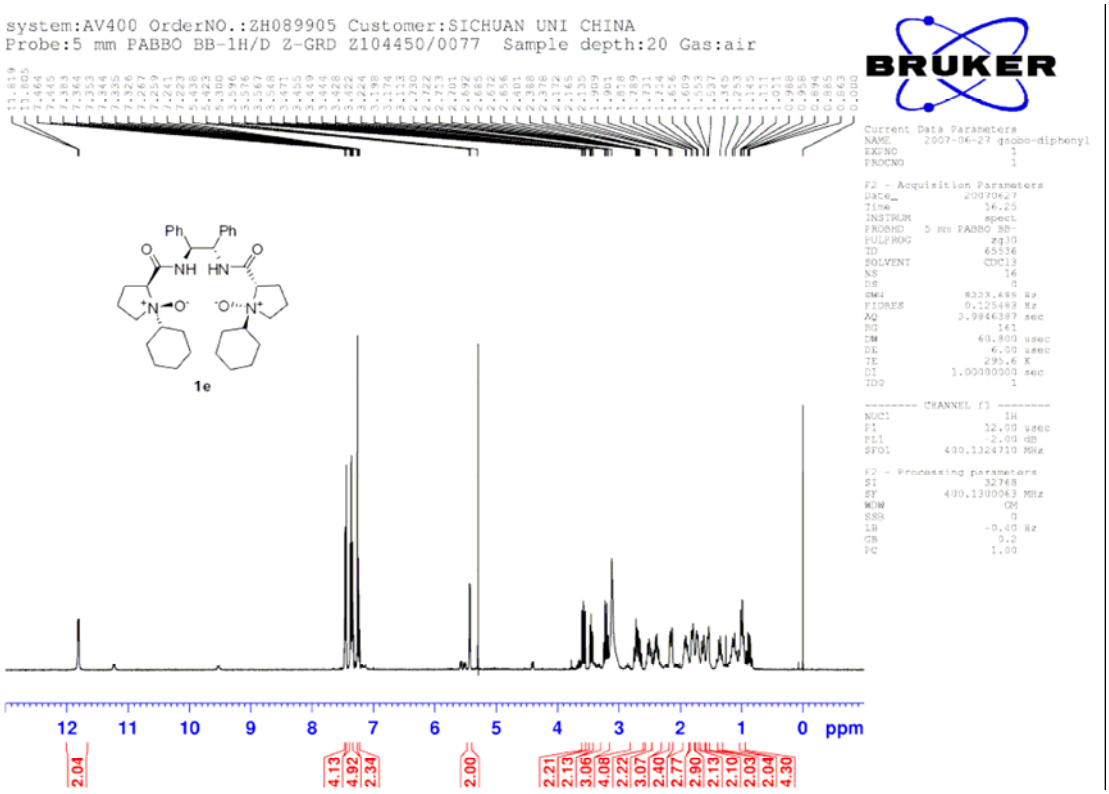

BRUKER
167.75
77.37 77.27 77.05 76.73 74.59 66.83
49.08
28.86 28.33 27.52 27.32 24.30 24.05 22.11 20.25
NH HN
1b
180 160 140 120 100 80 60 40 20 0 ppm


-Acceptance-System:AV600 OrderNo.:ZH089805 Customer:Sichuan University,
P/N Console:H03128/2528 Probe:5 mm PATXI 1H/D Z-GRD Z104450/0077
Sample depth:20 Gas:dry air, Operator:Deng
BRUKER
1c
11 10 9 8 7 6 5 4 3 2 1 ppm
1.73
1.83 2.05 3.60 1.95 2.00 6.75 4.74 2.50 7.82 2.09 9.35 2.15
Current Data Parameters
NAME 2007-05-23 gaobo-GB
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070524
Time 0.39
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6564426 sec
RG 161
DW 40.533 usec
DE 6.00 usec
TE 291.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 7.20 usec
PL1 -1.00 dB
SFO1 600.1337060 MHz
F2 - Processing parameters
SI 32768
SF 600.1300039 MHz
WDW GM
SSB 0
LB -0.50 Hz
GB 0.3
PC 1.00


system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
BRUKER
1c
160 140 120 100 80 60 40 20 0 ppm
Current Data Parameters
NAME 2007-5-24 gaobo-GB
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070524
Time 14.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
BRUKER
1d
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00 2.24 2.37 2.33 4.56 2.26 6.48 2.46 20.05 7.93 2.46


system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
BRUKER
1d
167.27
77.33 77.01 76.69 76.33 71.56 63.03 49.04 29.65 28.58 28.29 27.83 27.52 25.26 24.57 22.06 19.95
200 180 160 140 120 100 80 60 40 20 0 ppm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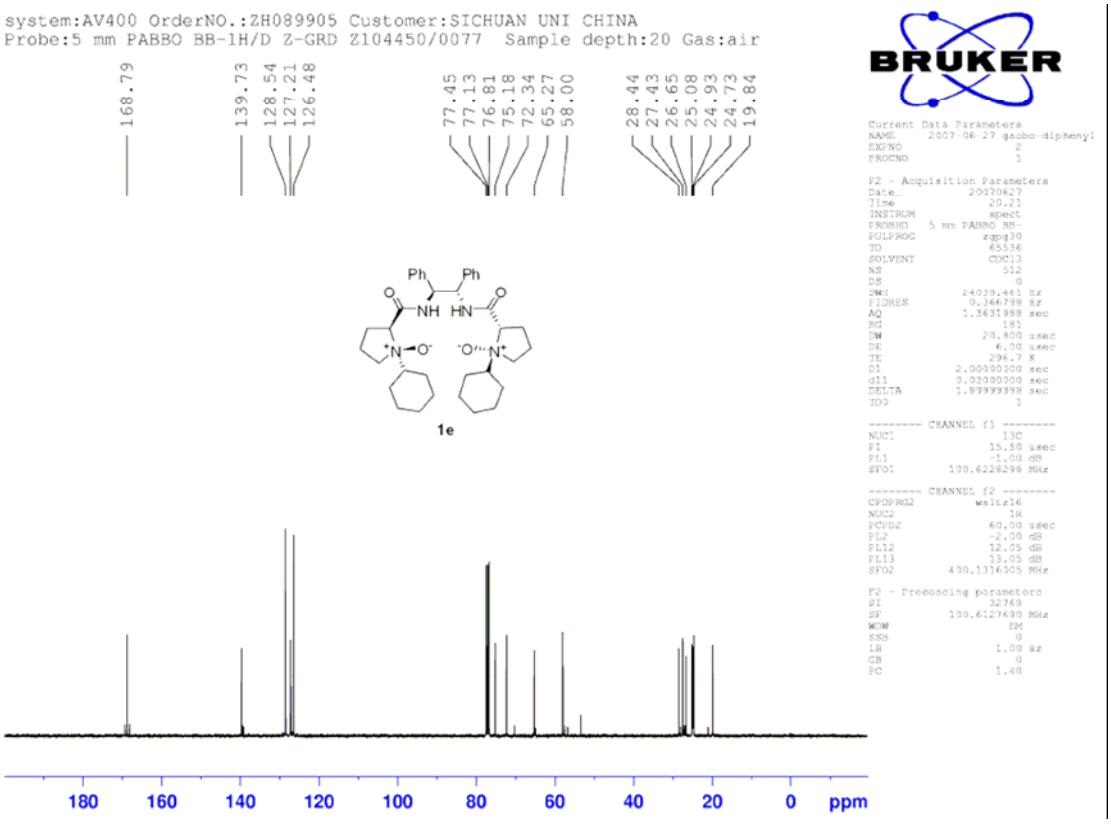
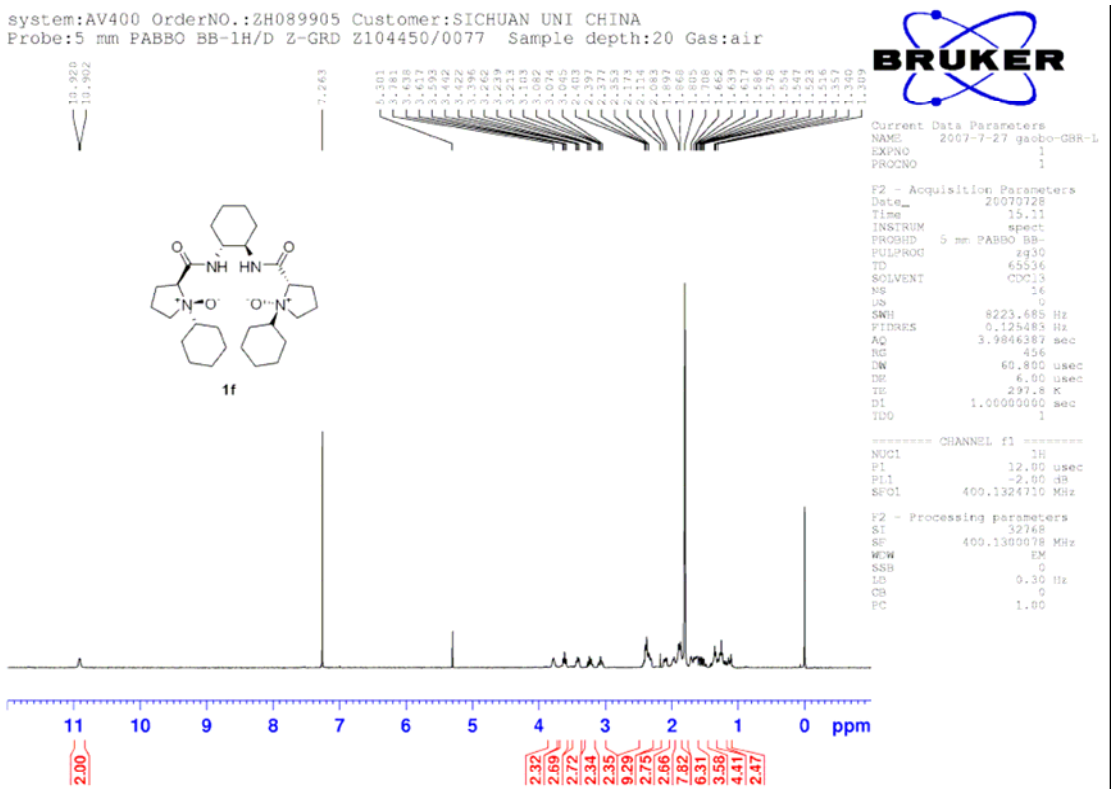
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
Ph
Ph
NH
HN
1e
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.04
4.13
4.92
2.34
2.00
2.21
2.13
3.06
4.08
2.22
3.07
2.40
2.77
2.90
2.13
2.10
2.03
2.04
4.30


system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
168.79
139.73
128.54
127.21
126.48
77.45
77.13
76.81
75.18
72.34
65.27
58.00
28.44
27.43
26.65
25.08
24.93
24.73
19.84
Ph
Ph
NH
HN
1e
180
160
140
120
100
80
60
40
20
0
ppm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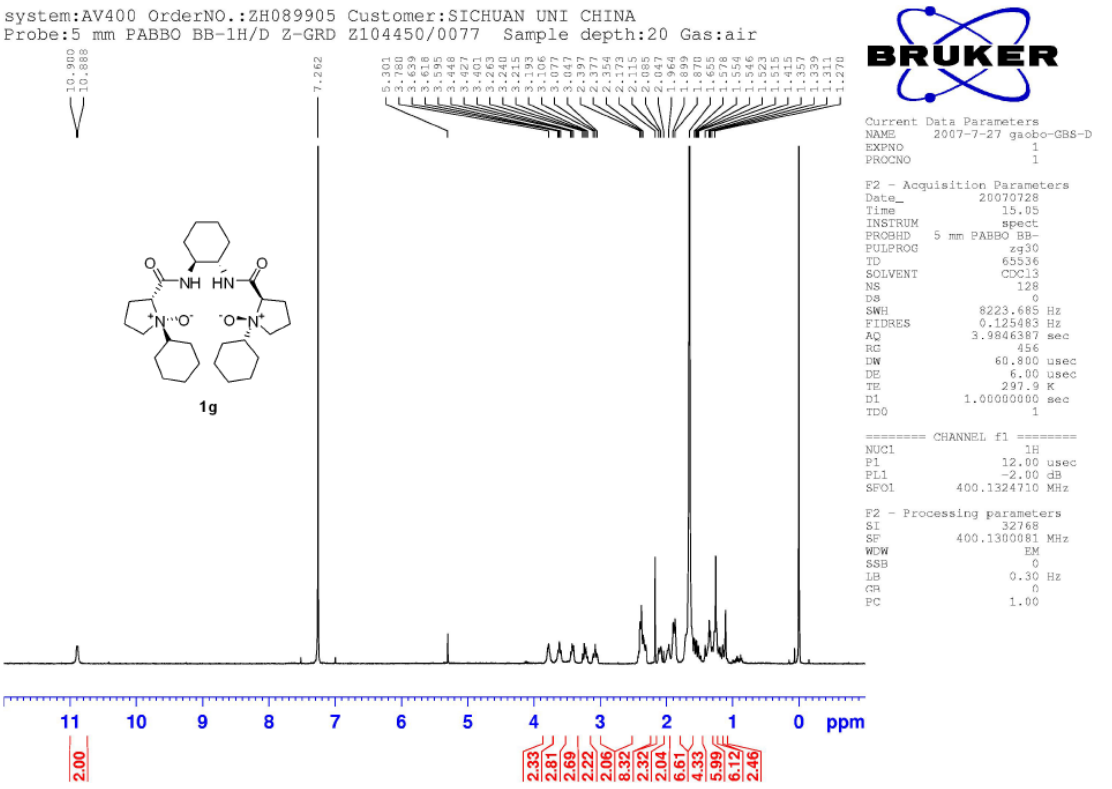
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
BRUKER
Current Data Parameters
NAME 2007-7-27 gaobo-GBR-L
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070728
Time 15.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 456
DW 60.800 usec
DE 6.00 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.80
1f
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.32 2.69 2.72 2.34 2.35 9.29 2.75 2.66 7.82 6.31 3.58 4.41 2.47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Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
BRUKER
Current Data Parameters
NAME 2007-7-27 gaobo-GBS-D
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070728
Time 15.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 456
DW 60.800 usec
DE 6.00 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1g
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
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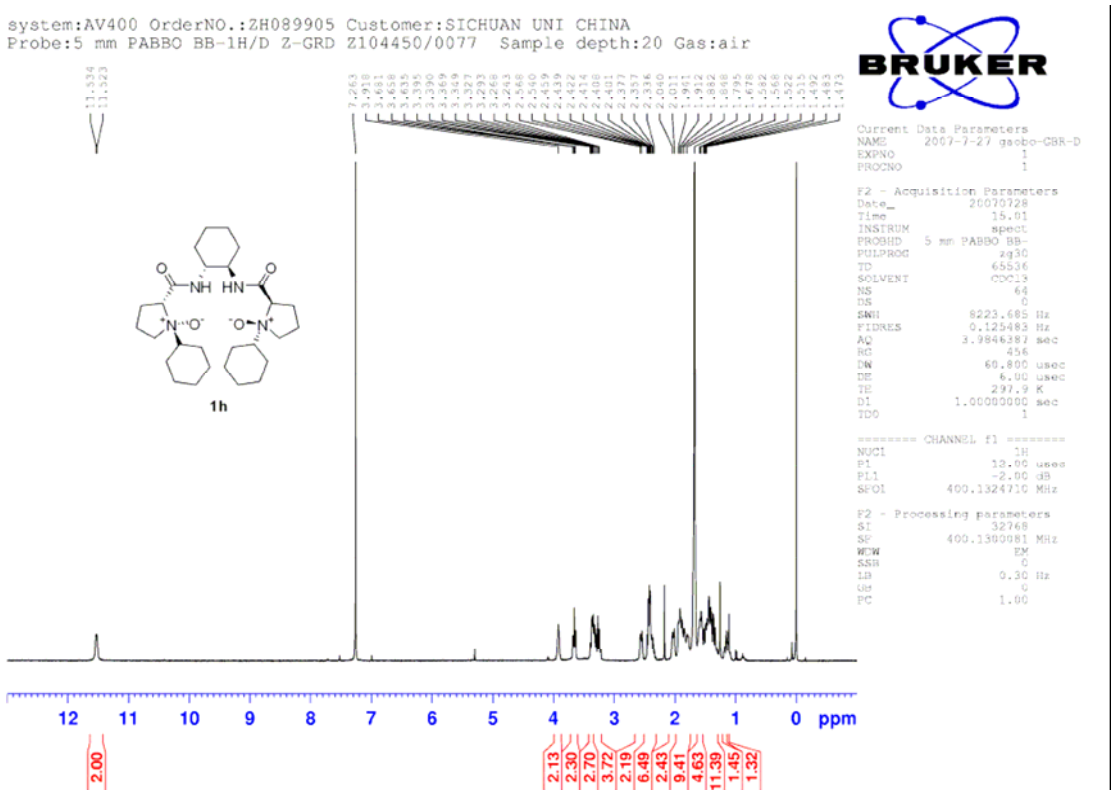
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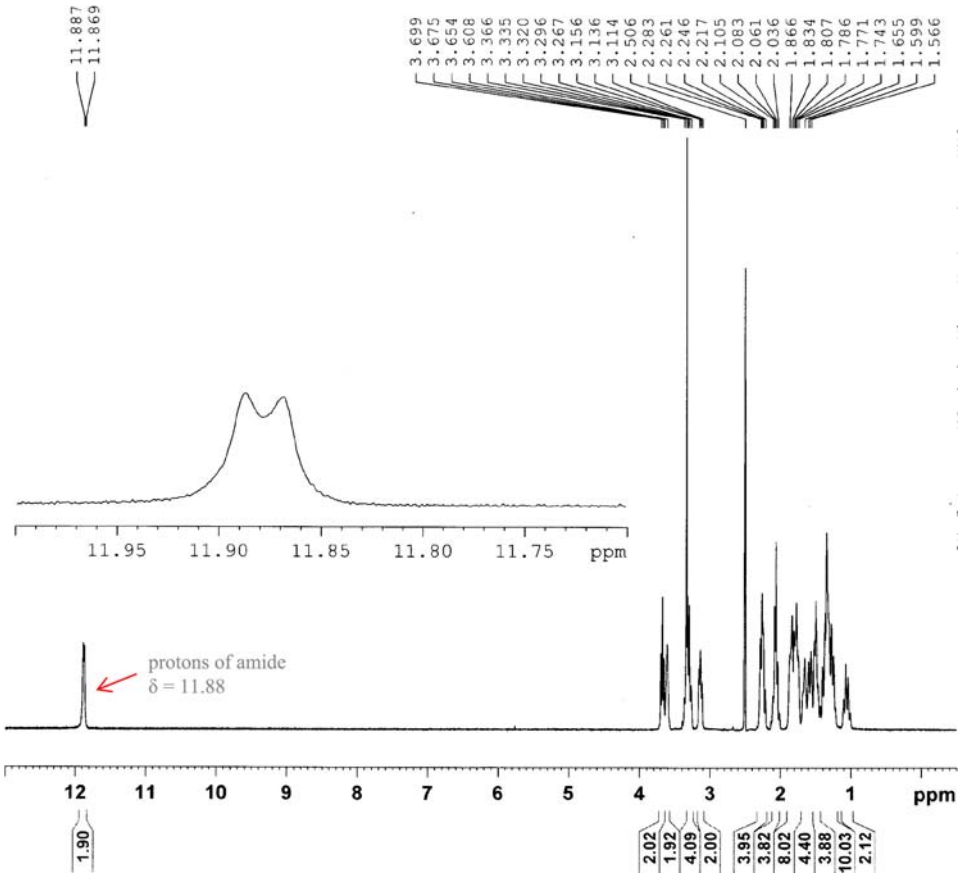
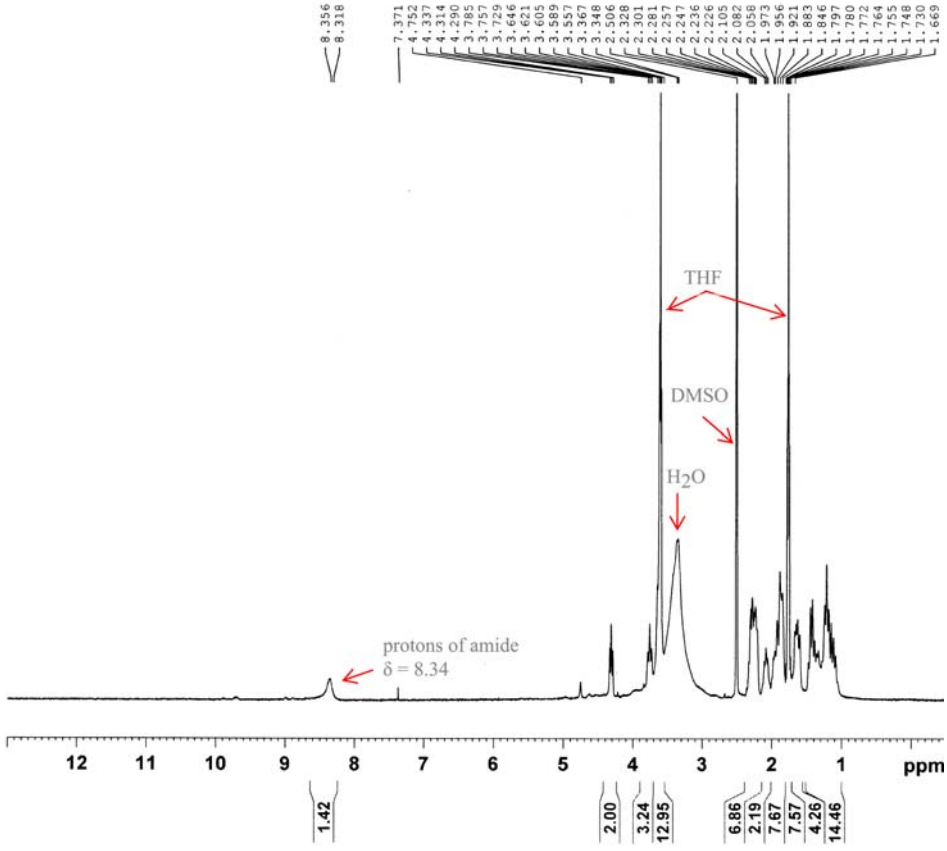
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
BRUKER
Current Data Parameters
NAME 2007-7-27 gaobo-CBR-D
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070728
Time 15.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 0
SWH 8223.685 Hz
FIDRES 0.125485 Hz
AQ 3.9846287 sec
RG 456
DW 60.800 usec
DE 6.00 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
NH HN
1h
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.13 2.30 2.70 3.72 2.19 6.49 2.43 9.41 4.63 11.39 1.45 1.32

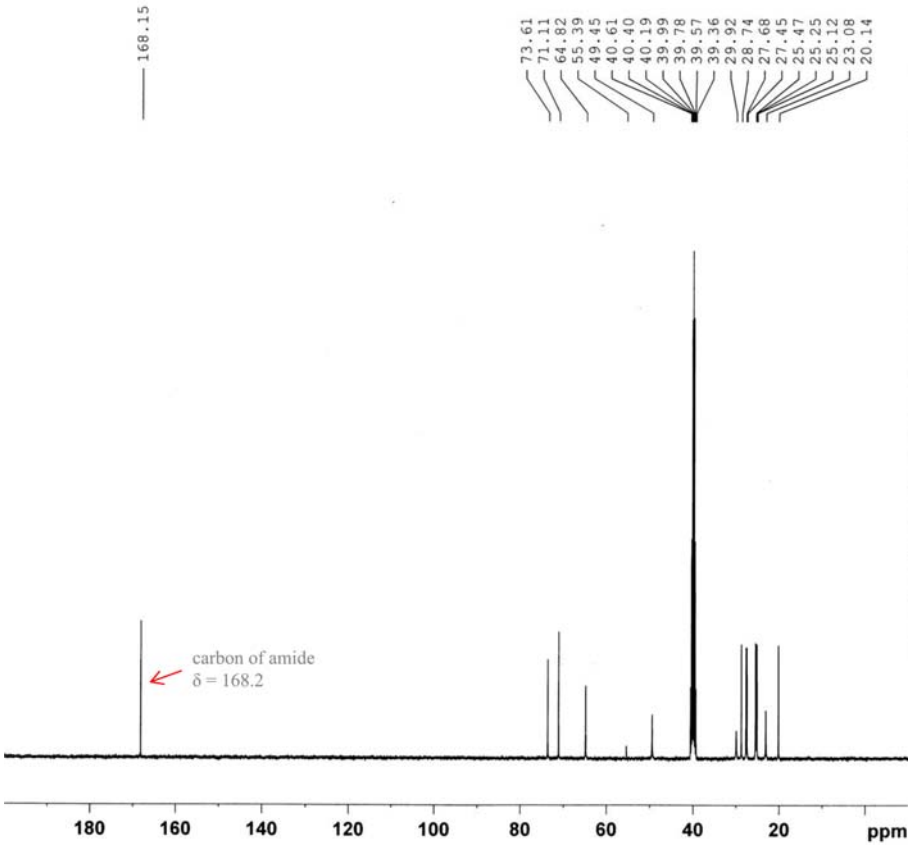
^{1}H NMR of **1C** in DMSO-d_6 (400 MHz)



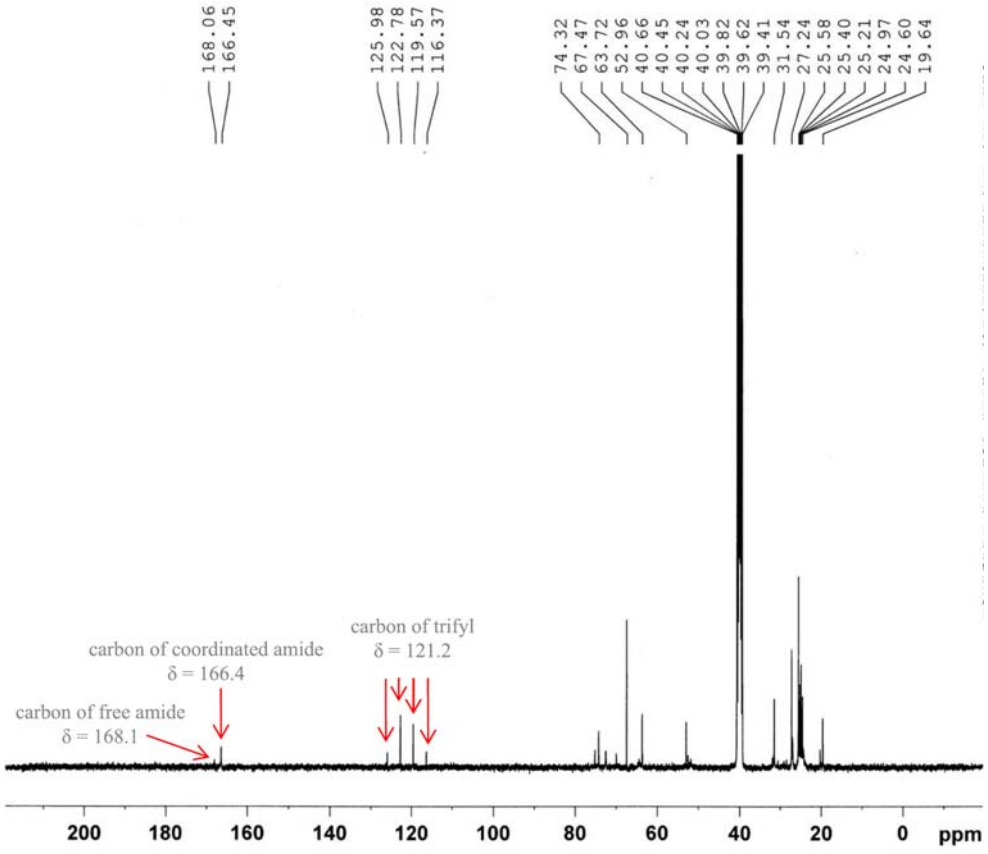
^{1}H NMR of **1C**+In(OTf)$_3$ in DMSO-d_6 (400 MHz)

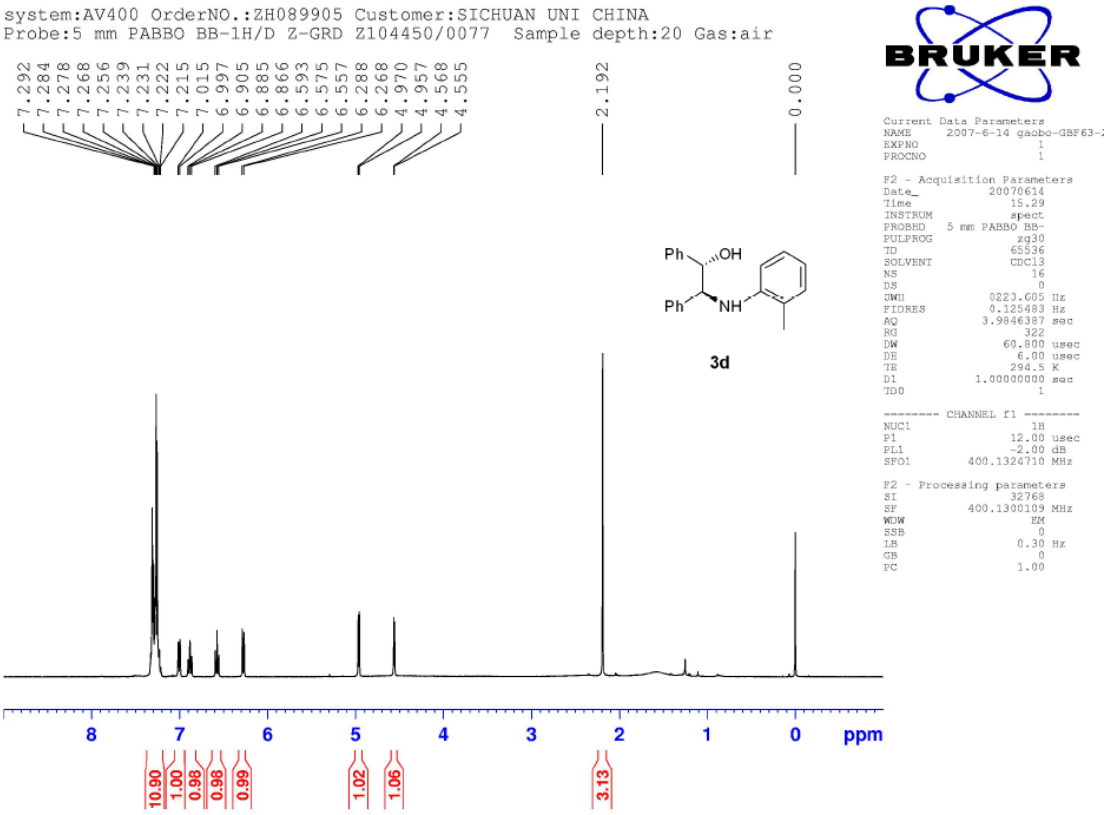


^{13}C NMR of **1C** in DMSO-d_6 (100 MHz)



^{13}C NMR of **1C**+In(OTf)$_3$ in DMSO-d_6 (100 MHz)




system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
7.292
7.284
7.278
7.268
7.256
7.239
7.231
7.222
7.215
7.015
6.997
6.905
6.885
6.866
6.593
6.575
6.557
6.288
6.268
4.970
4.957
4.568
4.555
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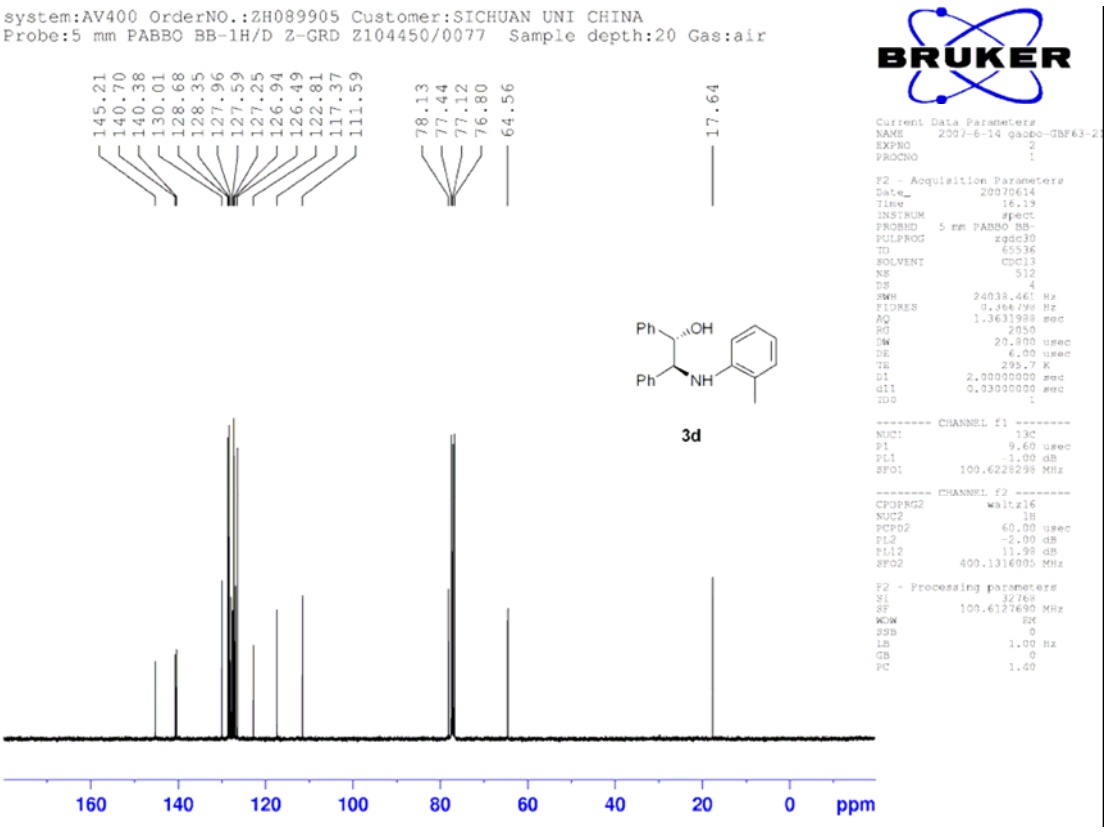
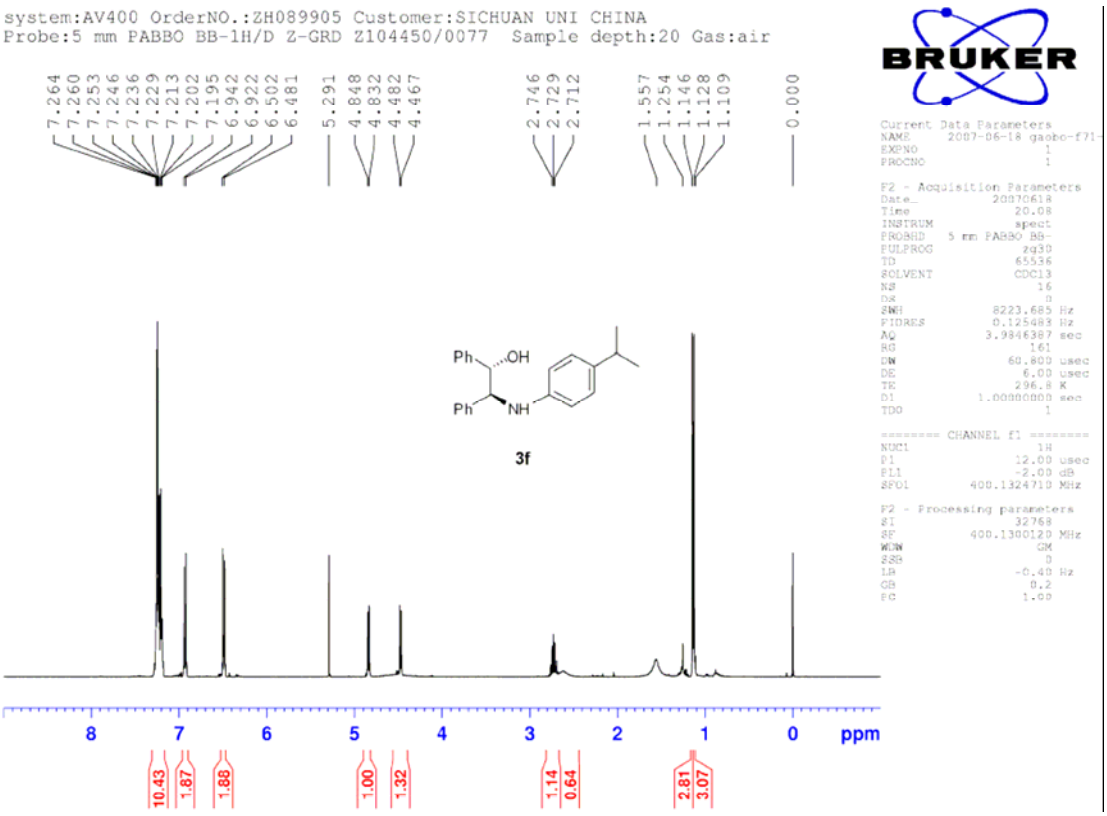
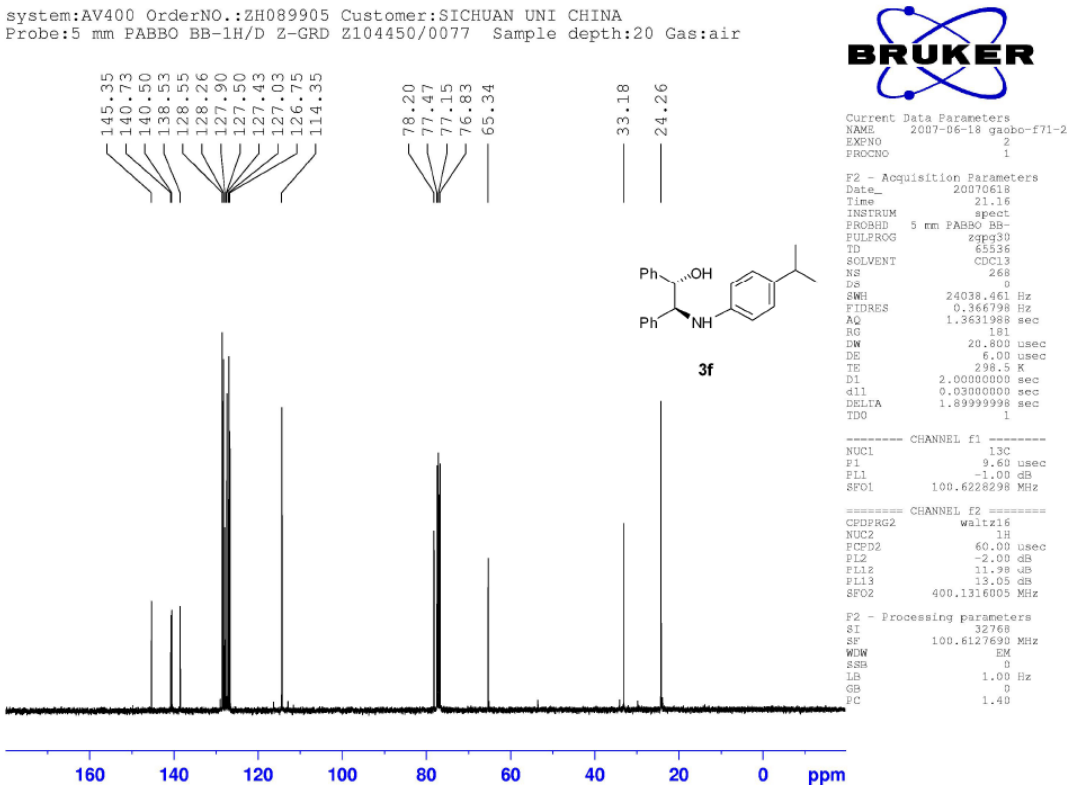
0.000
Ph
OH
Ph
NH
3d
8
7
6
5
4
3
2
1
0
ppm
10.90
1.00
0.98
0.98
0.99
1.02
1.06
3.13

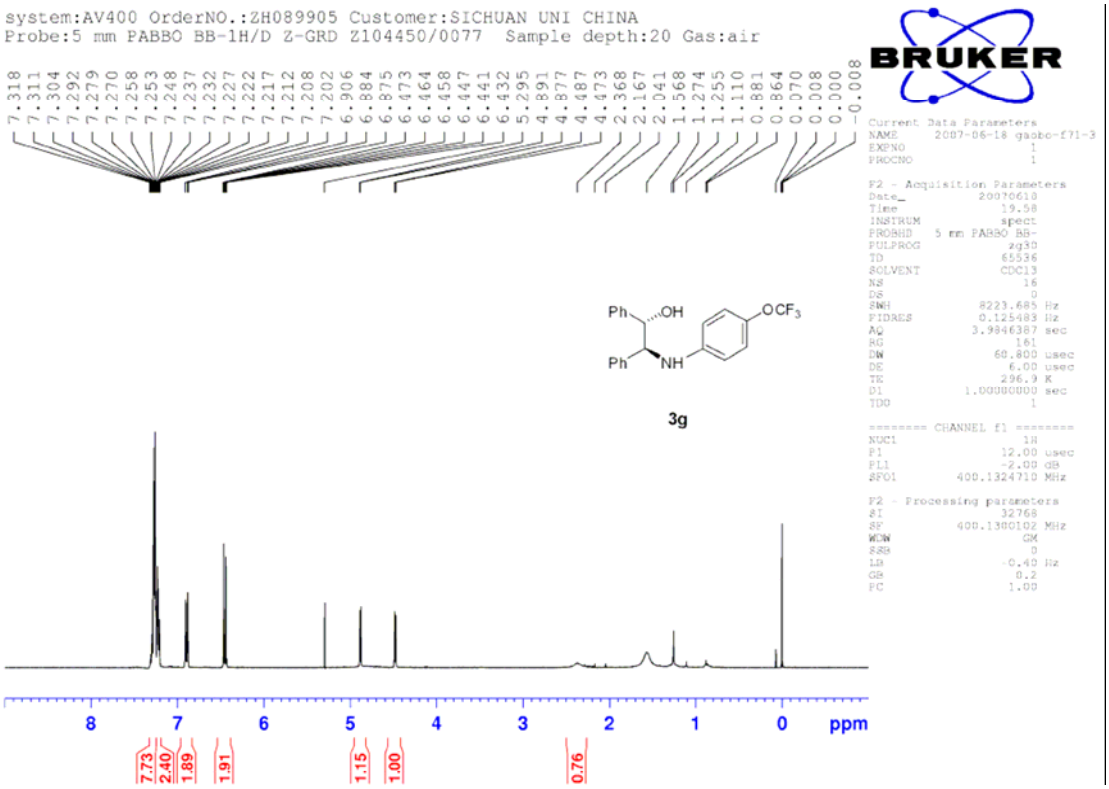
BRUKER
Current Data Parameters
NAME 2007-6-14 gaobo-GBF63-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070614
Time 15.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.605 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 322
DW 60.800 usec
DE 6.00 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

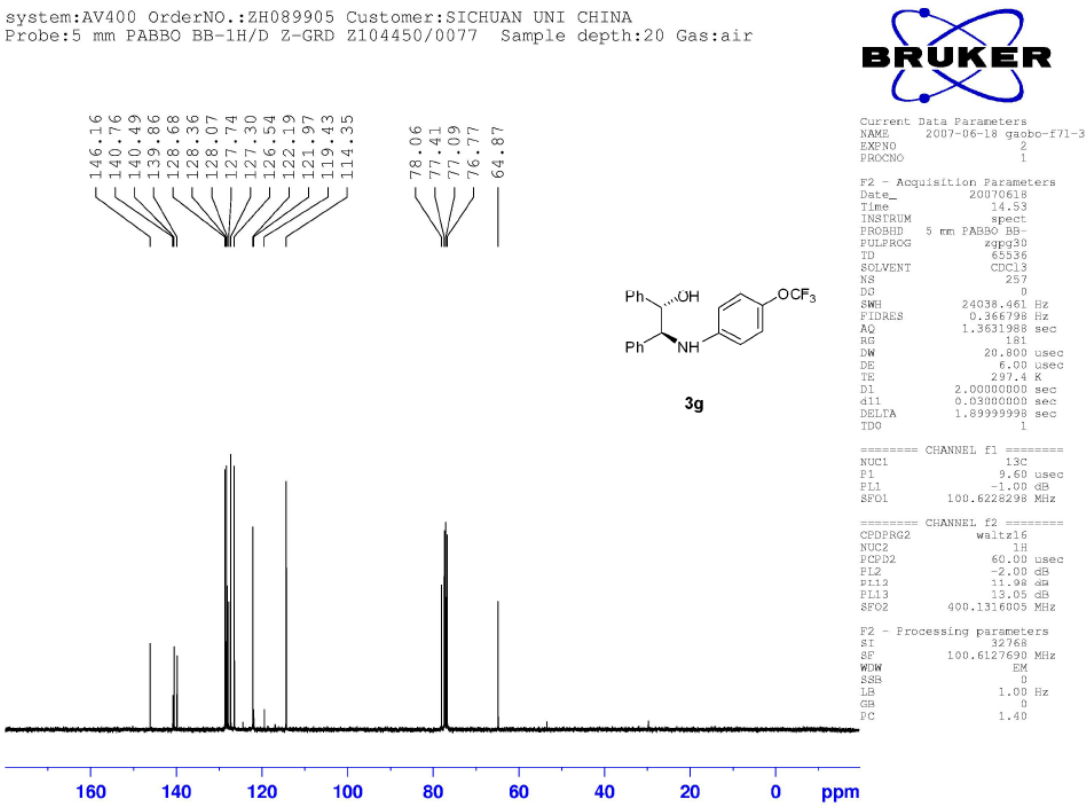

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
145.21
140.70
140.38
130.01
128.68
128.35
127.96
127.59
127.25
126.94
126.49
122.81
117.37
111.59
78.13
77.44
77.12
76.80
64.56
17.64
Ph
OH
Ph
NH
3d
160
140
120
100
80
60
40
20
0
ppm

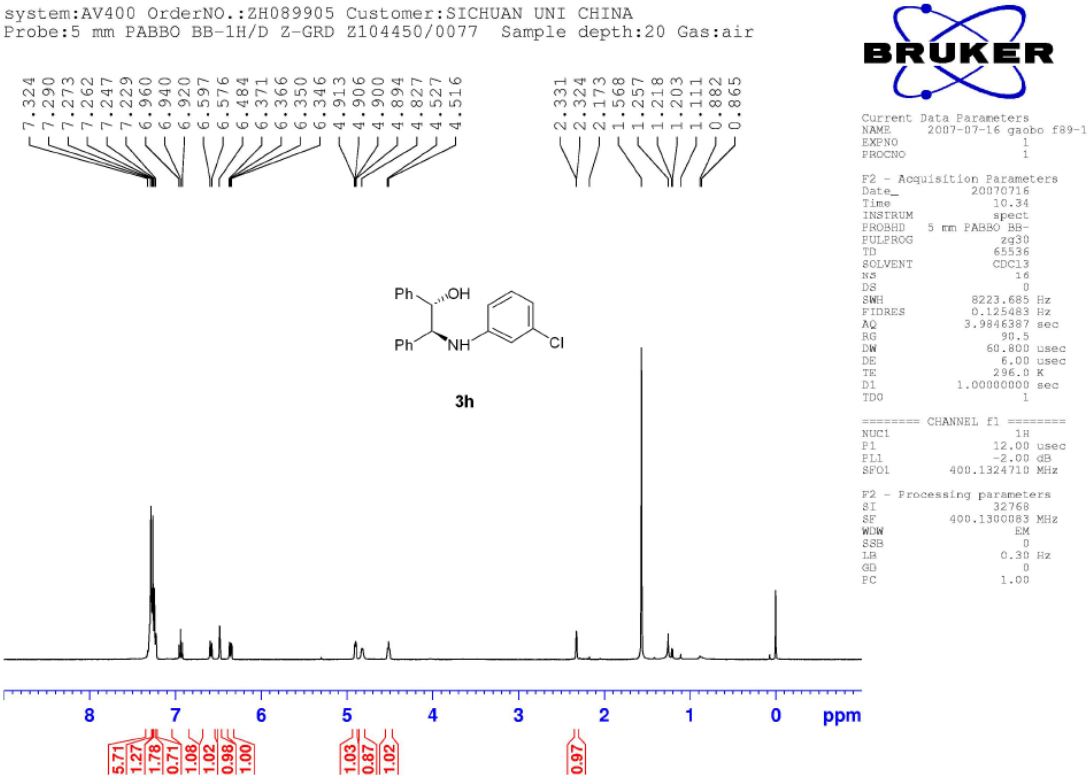
BRUKER
Current Data Parameters
NAME 2007-6-14 gaobo-GBF63-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070614
Time 16.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366796 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 295.7 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 9.60 usec
PL1 1.00 dB
SFO1 100.6228298 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -2.00 dB
PL12 11.98 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

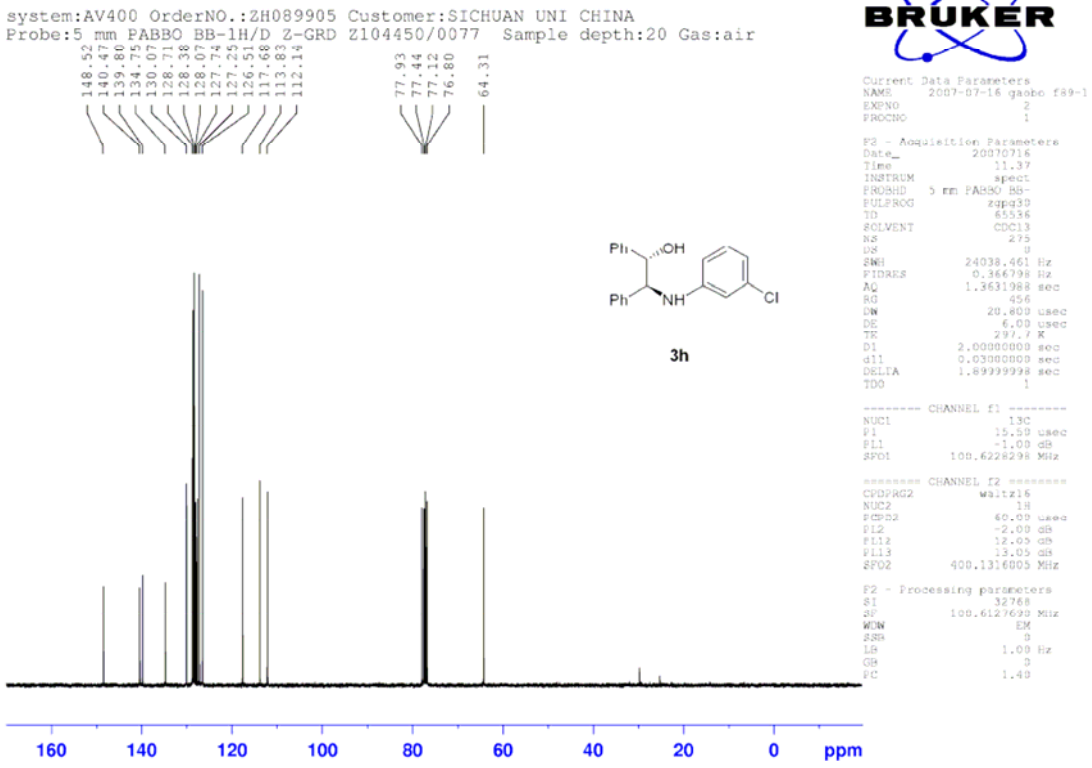

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
7.264
7.260
7.253
7.246
7.236
7.229
7.213
7.202
7.195
6.942
6.922
6.502
6.481
5.291
4.848
4.832
4.482
4.467
2.746
2.729
2.712
1.557
1.254
1.146
1.128
1.109
0.000
Ph
OH
Ph
NH
3f
8
7
6
5
4
3
2
1
0
ppm
10.43
1.87
1.86
1.00
1.32
1.14
0.64
2.81
3.07
BRUKER
Current Data Parameters
NAME 2007-06-18 gaobo-f71-
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070618
Time 20.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300120 MHz
WDW EM
SSB 0
LB -0.40 Hz
GB 0.2
PC 1.00

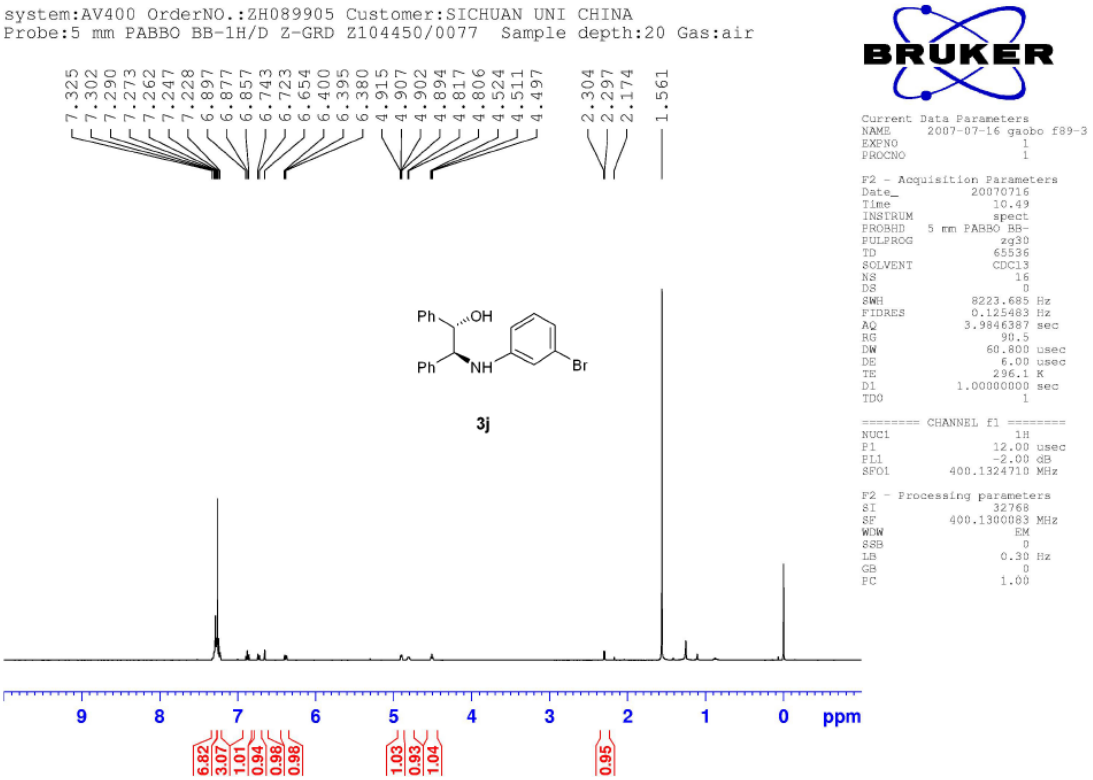

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
145.35
140.73
140.50
138.53
128.55
128.26
127.90
127.50
127.43
127.03
126.75
114.35
78.20
77.47
77.15
76.83
65.34
33.18
24.26
Ph
OH
Ph
NH
3f
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME 2007-06-18 gaobo-f71-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070618
Time 21.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 268
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.00 usec
TE 298.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -2.00 dB
PL12 11.98 dB
PL13 13.05 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

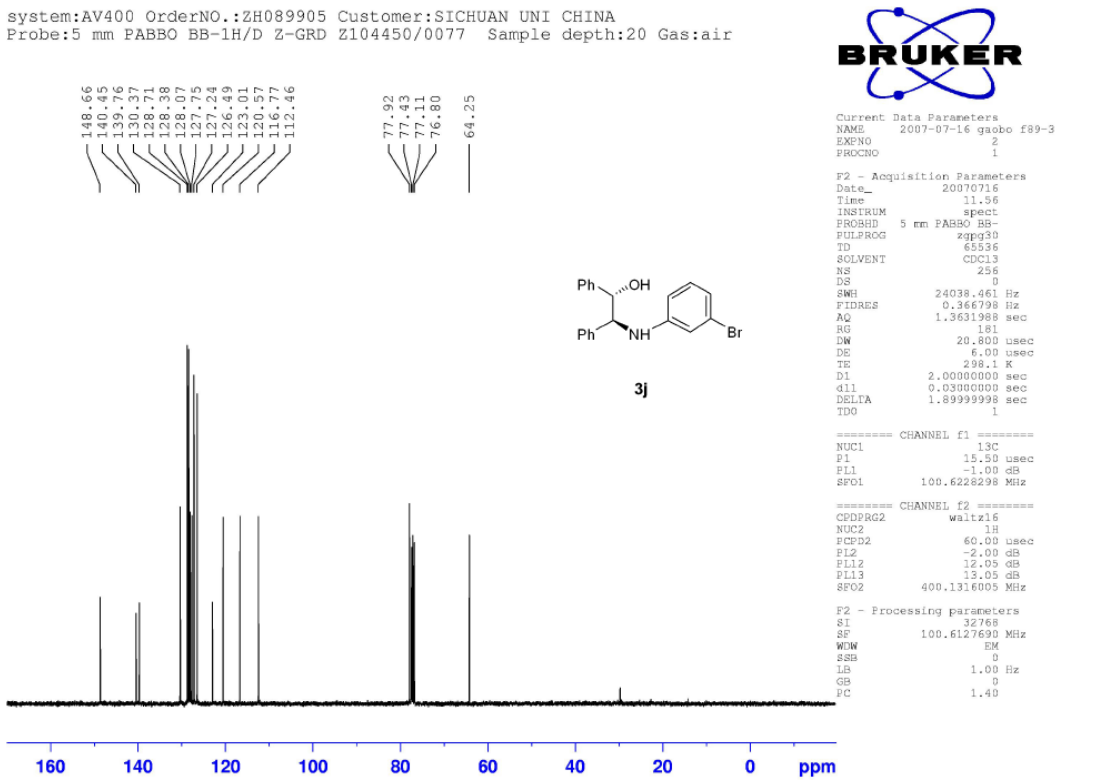

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
7.318 7.311 7.304 7.292 7.279 7.270 7.258 7.253 7.248 7.237 7.232 7.227 7.222 7.217 7.212 7.208 7.202 6.906 6.884 6.875 6.473 6.464 6.458 6.447 6.441 6.432 5.295 4.891 4.877 4.487 4.473 2.368 2.167 2.041 1.568 1.274 1.255 1.110 0.881 0.864 0.070 0.008 0.000 -0.008
BRUKER
Current Data Parameters
NAME 2007-06-18 gaobo-f71-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070610
Time 19.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300102 MHz
WDW GM
SSB 0
LB -0.40 Hz
GB 0.2
PC 1.00
Ph OH OCF3 Ph NH
3g
8 7 6 5 4 3 2 1 0 ppm
7.73 2.40 1.89 1.91 1.15 1.00 0.76

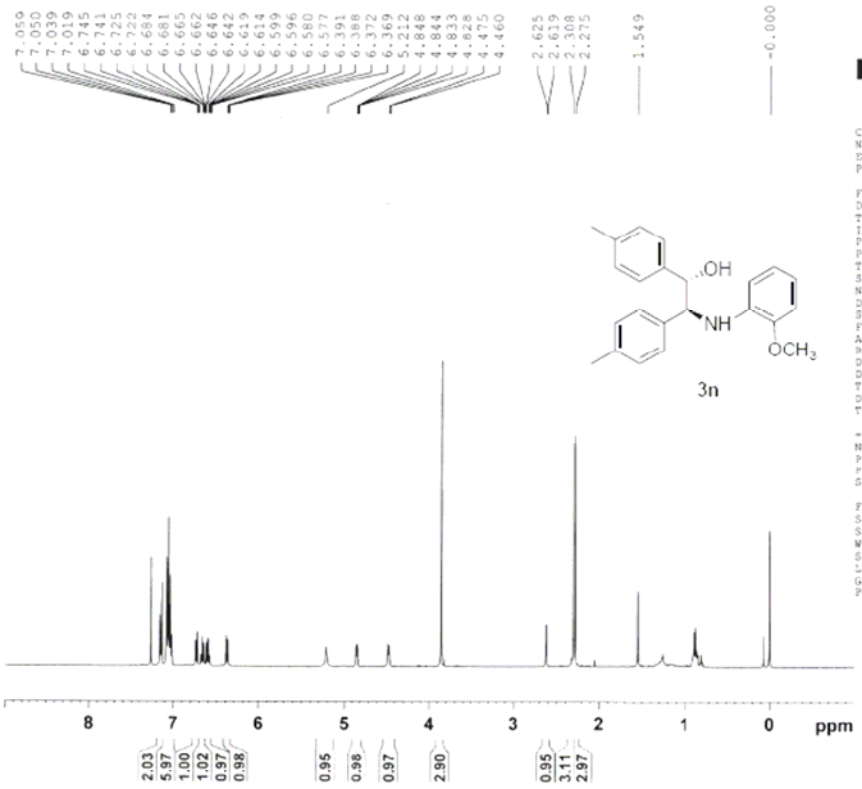

system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
146.16 140.76 140.49 139.86 128.68 128.36 128.07 127.74 127.30 126.54 122.19 121.97 119.43 114.35
78.06 77.41 77.09 76.77 64.87
BRUKER
Current Data Parameters
NAME 2007-06-18 gaobo-f71-3
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070618
Time 14.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 257
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.00 usec
TE 297.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -2.00 dB
PL12 11.98 dB
PL13 13.05 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Ph OH OCF3 Ph NH
3g
160 140 120 100 80 60 40 20 0 ppm


system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
7.324
7.290
7.273
7.262
7.247
7.229
6.960
6.940
6.920
6.597
6.576
6.484
6.371
6.366
6.350
6.346
4.913
4.906
4.900
4.894
4.827
4.527
4.516
2.331
2.324
2.173
1.568
1.257
1.218
1.203
1.111
0.882
0.865
Ph
OH
Ph
NH
Cl
3h
8
7
6
5
4
3
2
1
0
ppm
5.71
1.27
1.78
0.71
1.08
1.02
0.98
1.00
1.03
0.87
1.02
0.97
BRUKER
Current Data Parameters
NAME 2007-07-16 gaobo f89-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070716
Time 10.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 90.5
DW 60.800 usec
DE 6.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
148.52
140.47
139.80
134.75
130.07
128.71
128.38
128.07
127.74
127.25
126.51
117.68
113.83
112.14
77.93
77.44
77.12
76.80
64.31
Ph
OH
Ph
NH
Cl
3h
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME 2007-07-16 gaobo f89-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070716
Time 11.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 275
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 456
DW 20.800 usec
DE 6.00 usec
TE 297.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -2.00 dB
PL12 12.05 dB
PL13 13.05 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
7.325
7.302
7.290
7.273
7.262
7.247
7.228
6.897
6.877
6.857
6.743
6.723
6.654
6.400
6.395
6.380
4.915
4.907
4.902
4.894
4.817
4.806
4.524
4.511
4.497
2.304
2.297
2.174
1.561
Ph
OH
Ph
NH
Br
3j
9
8
7
6
5
4
3
2
1
0
ppm
6.82
3.07
1.01
0.94
0.96
0.98
1.03
0.93
1.04
0.95
BRUKER
Current Data Parameters
NAME 2007-07-16 gaobo f89-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070716
Time 10.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 90.5
DW 60.800 usec
DE 6.00 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


system:AV400 OrderNO.:ZH089905 Customer:SICHUAN UNI CHINA
Probe:5 mm PABBO BB-1H/D Z-GRD Z104450/0077 Sample depth:20 Gas:air
148.66
140.45
139.76
130.37
128.71
128.38
128.07
127.75
127.24
126.49
123.01
120.57
116.77
112.46
77.92
77.43
77.11
76.80
64.25
Ph
OH
Ph
NH
Br
3j
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME 2007-07-16 gaobo f89-3
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070716
Time 11.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 -2.00 dB
PL12 12.05 dB
PL13 13.05 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

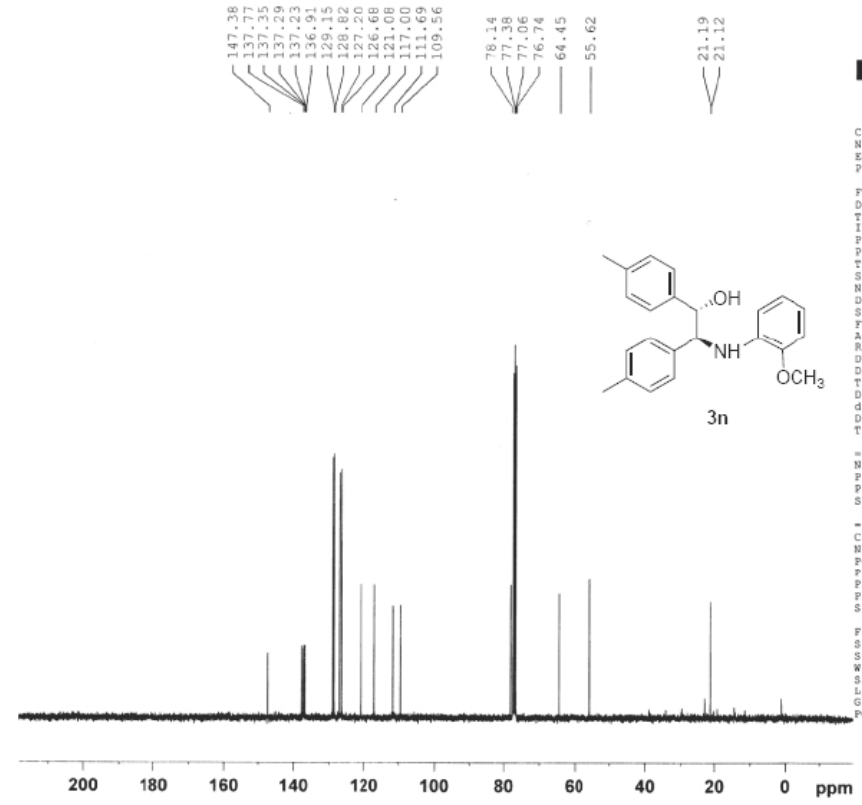



```
Current Data Parameters
NAME      2007-12-21 gaobo-G13-2
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_              20071221
Time                 17.01
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              CDCl3
NS                      16
DS                       0
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894966 sec
RG                     362
DW                62.400 usec
DE                 6.50 usec
TE                293.4 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.00 usec
PL1                  -2.00 dB
SFO1          400.1326008 MHz

F2 - Processing parameters
SI                   32768
SF            400.1300106 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



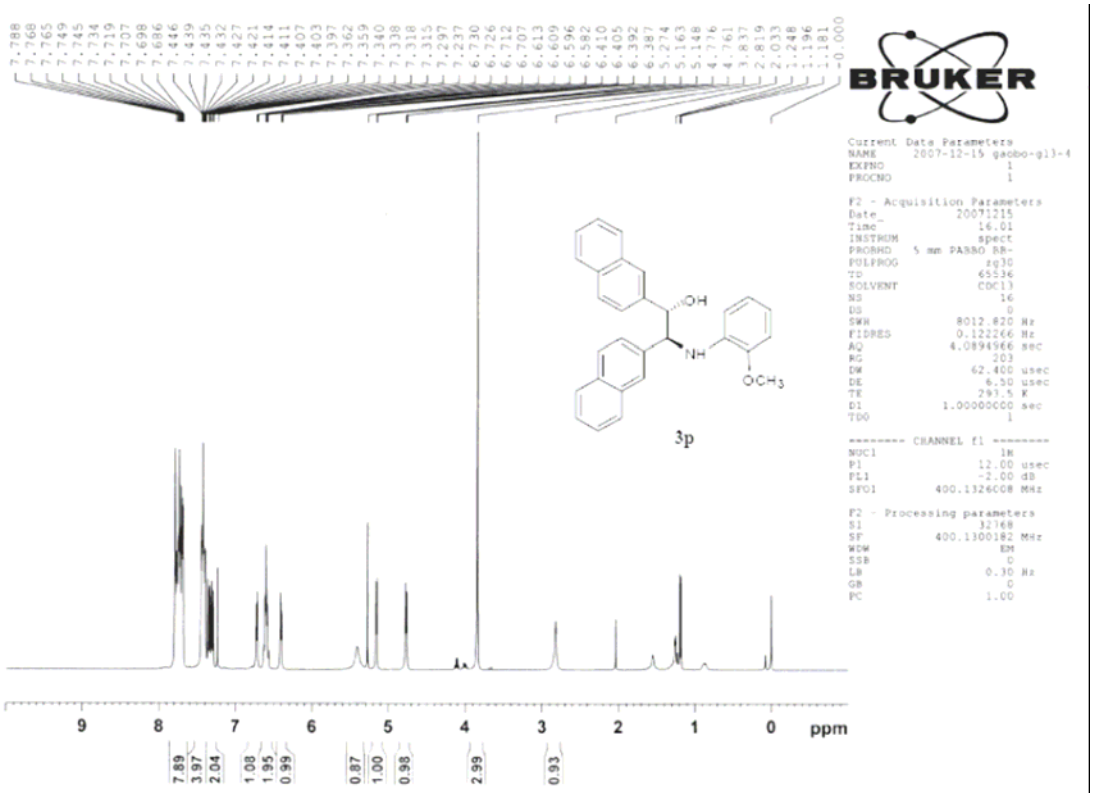

```
Current Data Parameters
NAME      2007-12-21 gaobo-G13-2
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_              20071221
Time                 18.02
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT              CDCl3
NS                     256
DS                       0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    2050
DW                20.800 usec
DE                 6.50 usec
TE                295.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                   15.50 usec
PL1                  -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                60.00 usec
PL12                 12.05 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```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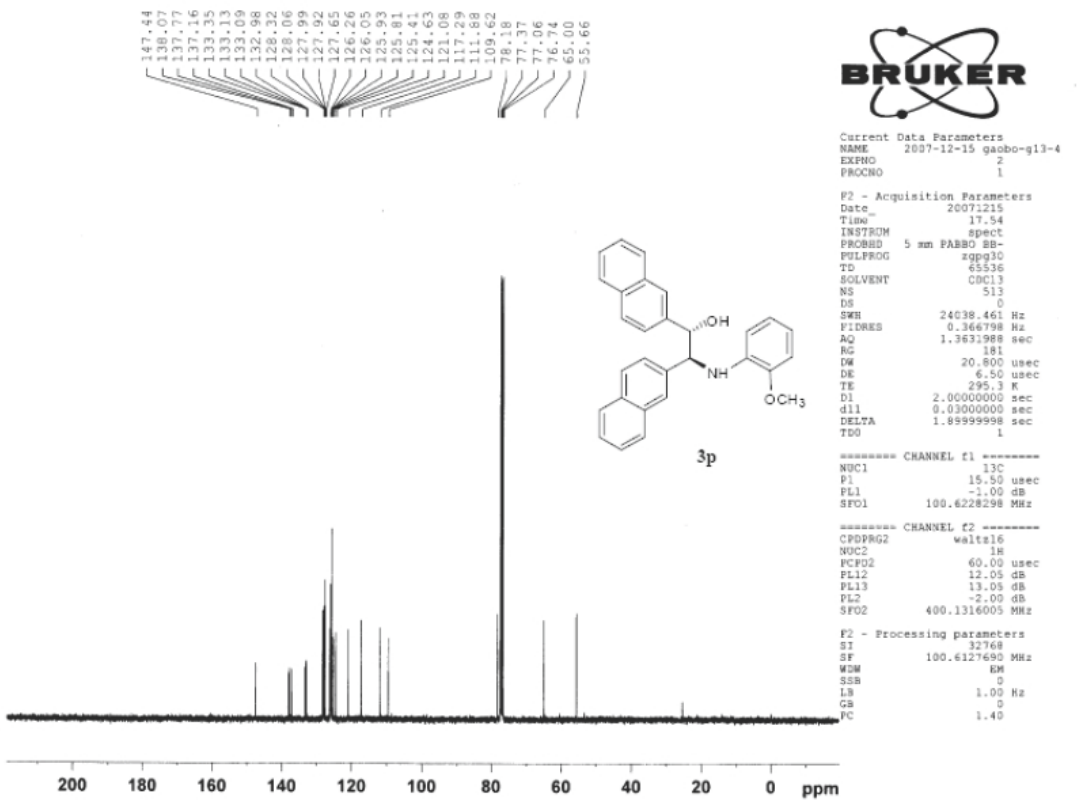
7.765
7.749
7.745
7.734
7.719
7.707
7.698
7.686
7.446
7.439
7.435
7.432
7.427
7.421
7.414
7.411
7.407
7.403
7.397
7.362
7.359
7.340
7.338
7.318
7.315
7.297
7.237
6.730
6.726
6.712
6.707
6.613
6.609
6.596
6.582
6.410
6.405
6.392
6.387
5.274
5.163
5.148
4.776
4.761
3.837
2.819
2.033
1.248
1.196
1.181
-0.000
OH
NH
OCH3
3p
9
8
7
6
5
4
3
2
1
0
ppm
7.89
3.97
2.04
1.08
1.95
0.99
0.87
1.00
0.98
2.99
0.93
BRUKER
Current Data Parameters
NAME 2007-12-15 gaobo-g13-4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071215
Time_ 16.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -2.00 dB
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300182 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00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137.77
137.16
133.35
133.13
133.09
132.98
128.32
128.06
127.99
127.92
127.65
126.26
126.05
125.93
125.81
125.41
124.63
121.08
117.29
111.88
109.62
78.18
77.37
77.06
76.74
65.00
55.66
OH
NH
OCH3
3p
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME 2007-12-15 gaobo-g13-4
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071215
Time_ 17.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 513
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL12 12.05 dB
PL13 13.05 dB
PL2 -2.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40