Supplementary Material (ESI) for Chemical Communications

Asymmetric *meso*-Aziridine Ring-Opening Reactions Using A Chiral Zr Catalyst

Kazutaka Seki, Rongmin Yu, Yumi Yamazaki, Yasuhiro Yamashita, and Shū Kobayashi*

Department of Chemistry, School of Science and Graduate School of Pharmaceutical Sciences, The University of Tokyo, and the HERE Division, ERATO, Japan Science Technology Agency (JST), Hongo, bunkyo-ku, Tokyo 113-0033, Japan

Supporting Information

Experimental Section

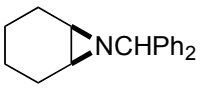
General:

^{1}H and ^{13}C NMR spectra were recorded on a JEOL ECX-400, ECX-500, ECA-500 and ECX-600 spectrometer in $CDCl_3$ unless otherwise noted. Tetramethylsilane (TMS) served as internal standard ($\delta = 0$) for ^{1}H NMR, and $CDCl_3$ was used as internal standard ($\delta = 77.0$) for ^{13}C NMR. IR spectra were measured with JASCO FT/IR-610 spectrometers. High-performance liquid chromatography was carried out using following apparatuses; SHIMAZU LC-8A, LC-10ATvp, LC-20AB (liquid chromatograph), SHIMAZU SPD-10A (UV detector), SHIMADZU SPD-20A (UV/VIS detector), SHIMAZUSPD-M20A (photodiode array detector), and SHIMADZU C-R8A (Chromatopac). High resolution mass spectrometry was carried out using BRUKER DALTONICS BioTOF Ⅱ and JEOL JMS-T100TD. Preparative thin layer chromatography was carried out using glass plates with Wakogel B-5F. Commercially available chemicals purchased from Aldrich, Kanto Chemical, Tokyo Chemical Industry and Wako Pure Chemical Industry, were purified according to standard procedures. Zirconium *tert*-butoxide ($Zr(O^tBu)_4$) and Hafnium *tert*-butoxide ($Hf(O^tBu)_4$) were purchased from Tri Chemical Laboratory Inc. Aziridines were prepared in accordance with literature protocol[1]. Tridentate BINOL ligands were synthesized according to our literature procedure[2]. Absolute configurations of the products have not been determined yet. All reactions were carried out under argon atmosphere in well-dried glassware.

Typical experimental procedure for asymmetric *meso*-aziridine ring-opening reaction:

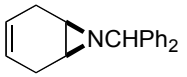
$Zr(O^tBu)_4$ (0.015 mmol) and a ligand (0.0165 mmol) were added into a frame-dried 10mL reaction tube inside an argon glove box system, and the tube was capped with a sleeve stopper. After toluene (0.2 ml) was added, the mixture was stirred at 60 °C for 2 h. The mixture was cooled to rt , and then ^{n}pentanol (0.075 mmol) was added. After the mixture was stirring for 1 h at rt, the aziridine (0.15 mmol) in toluene (0.15 ml) and aniline (0.18 mmol) in toluene (0.15 ml) were successively added at 0 °C. After the mixture was stirred for 24 h, water was added to quench the reaction. After addition of dichloromethane (CH_2Cl_2, 10 mL), the organic layer was separated and the aqueous layer was extracted three times with CH_2Cl_2 (15 mL x 3). The organic layers were combined and dried over anhydrous Na_2SO_4. After filtration and concentration under reduced pressure, the crude product was purified by preparative thin layer chromatography (hexane-ethyl acetate = 4:1 or 3:1) to afford the desired product.

7-Benzhydryl-7-azabicyclo[4.1.0]heptane (4a)



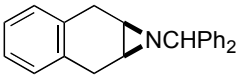
^{1}H NMR ($CDCl_3$) δ 7.44 (d, 4H, *J* = 7.6 Hz), 7.25-7.29 (m, 4H), 7.17-7.20 (m, 2H), 3.52 (s, 1H), 1.76-1.80 (m, 2H), 1.65-1.68 (m, 4H), 1.47-1.51 (m, 2H), 1.18-1.21 (m, 2H); ^{13}C NMR ($CDCl_3$) δ, 144.3, 128.1, 127.4, 126.7, 78.1, 38.3, 24.6, 20.6; FT-IR (KBr) 3065, 3026, 2882, 1491, 1422, 1301, 1191, 1117, 1030, 861, 756, 705 cm^{-1}; HRMS: calcd. for $C_{19}H_{22}N$ [M+H$^+$]: 264.1752, found: 264.1759.

7-Benzhydryl-7-azabicyclo[4.1.0]hept-3-ene (4b)



^{1}H NMR ($CDCl_3$) δ 7.44 (d, 4H, *J* = 8.9 Hz), 7.26-7.30 (m, 4H), 7.19-7.22 (m, 2H), 5.52 (s, 2H), 3.66 (s, 1H), 2.26-2.39 (m, 4H), 1.87 (s, 2H); ^{13}C NMR ($CDCl_3$) δ 143.8, 128.2, 127.5, 126.8, 122.9, 78.1, 37.5, 24.7; FT-IR (KBr) 3065, 3026, 2882, 1491, 1422, 1301, 1191, 1117, 1030, 861, 756, 705 cm^{-1}; HRMS : calcd for $C_{19}H_{20}N$ [M+H$^+$]: 262.1596, found 262.1590.

1-Benzhydryl-1a, 2,7,7a-tetrahydro-1*H*-naphtho[2,3-*b*]azirine (4c)

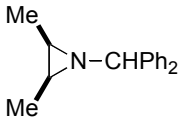


^{1}H NMR ($CDCl_3$) δ 7.38 (d, 4H, *J* = 7.7 Hz), 7.25-7.26 (m, 4H), 7.12-7.18 (m, 4H), 7.03-7.05 (m, 2H), 3.74 (s, 1H), 3.09 (d, 2H, *J* = 16.5 Hz), 2.99 (d, 2H, *J* = 16.4 Hz), 2.07 (s, 2H); ^{13}C NMR ($CDCl_3$) δ 144.0, 133.8, 129.1, 128.2, 127.3, 126.8, 125.9, 77.2, 38.3, 29.7; FT-IR (KBr) 3063, 3023, 2985, 2898, 2828, 1492, 1452, 1304, 1236, 1186, 1071, 829, 744, 702 cm^{-1}; HRMS : calcd for $C_{23}H_{22}N$ [M+H$^+$]: 312.1752, found 312.1747.

6-Benzhydryl-6-azabicyclo[3, 1, 0]hexane (4d)

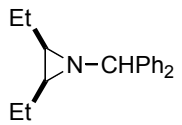
^{1}H NMR ($CDCl_3$) δ 7.40-7.41 (m, 4H), 7.24-7.29 (m, 4H), 7.18-7.20 (m, 2H), 3.56 (s, 1H), 2.11 (s, 2H), 1.85-1.89 (m, 2H), 1.45-1.61 (m, 4H); ^{13}C NMR ($CDCl_3$) δ 144.2, 128.1, 127.3, 126.7, 75.0, 45.2, 27.7, 21.2; FT-IR (KBr) 3024, 2923, 1492, 1450, 1070, 852, 743, 700 cm^{-1}; HRMS : calcd for $C_{18}H_{20}N$ [M+H$^+$]: 250.1596, found 250.1586.

***cis*-1-Benzhydryl-2, 3-dimethylaziridine (4e)**



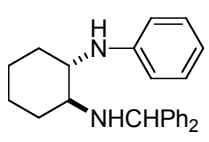
^{1}HNMR ($CDCl_3$) δ 7.40 (d, 4H, *J* = 7.9 Hz), 7.28-7.31 (m, 4H), 7.19-7.25 (m, 2H), 3.61 (s, 1H), 1.63 (m, 2H), 1.13 (d, 6H, *J* = 4.5 Hz); ^{13}C NMR ($CDCl_3$) δ 143.8, 128.2, 127.5, 126. 8, 78.4, 39.1, 13.0; FT-IR (neat) 2958, 2360, 1492, 1452, 1098, 742, 700 cm^{-1}; HRMS: calcd. for $C_{17}H_{20}N$ [M+H$^+$]: 238.1590; found: 238.1599.

***cis*-1-Benzhydryl-2,3-diethylaziridine (4f)**



^{1}HNMR ($CDCl_3$) δ 7.39-7.41 (m, 4H), 7.25-7.29 (m, 4H), 7.19-7.21 (m, 2H), 3.53 (s, 1H) , 1.38-1.52 (m, 6H), 0.73 (t, 6H, *J*=7.2 Hz); ^{13}C NMR ($CDCl_3$) δ 143.8, 128.1, 127.8, 126.8, 79.0, 46.2, 21.4, 11.9; FT-IR (neat) 2965, 1600, 1493, 1453, 1303, 1069, 743, 700 cm^{-1}; HRMS : calcd. for $C_{19}H_{24}N$ [M+H$^+$]: 266.1909; found: 266.1919.

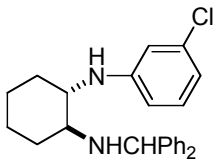
***trans*-*N*- Benzhydryl -*N*'-phenylcyclohexan-1,2-diamine (6aa)**



^{1}HNMR ($CDCl_3$) δ 7.23-7.26 (m, 6H), 7.13-7.18 (m, 3H), 7.07-7.10 (m, 3H), 6.62 (t, 1H, *J* = 7.2 Hz), 6.56 (d, 2H, *J* = 7.6 Hz), 4.89 (s, 1H), 3.46 (br, 1H), 3.06 (m. 1H), 2.06-2.22 (m, 4H), 1.56-1.64 (m 2H), 1.08-1.14 (m, 3H), 0.90-0.92 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 148.3, 144.7, 144.1,

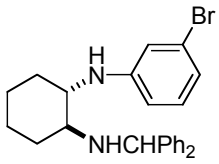
129.2, 128.6, 128.3, 127.6, 127.1, 127.0, 126.7, 117.4, 113.8, 63.5, 58.7, 57.6, 32.2, 31.6, 24.7, 24.5; HPLC: Daicel Chiralcel OD-H, hexane / ^{i}PrOH = 100 /1, flow rate = 1.0 mL /min, 254 nm: *tR* = 7.8 min (*major*), *tR* = 8.6 min (*minor*); FT-IR (neat) 1600, 1500, 1097, 695 cm^{-1}; HRMS: calcd. for $C_{25}H_{29}N_2$ [M+H$^+$]: 357.2331; found: 357.2330; $[\alpha]_D^{21}$ - 5.57 (c 1.35, $CHCl_3$) for 73% ee product.

***trans-N*- Benzhydryl -*N'*-3-chlorophenylcyclohexan-1,2-diamine (6ab)**



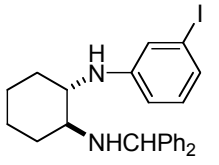
^{1}HNMR ($CDCl_3$) δ 7.31-7.36 (m, 6H), 7.23-7.27 (m, 3H), 7.15-7.17 (m, 1H), 7.04-7.07 (m, 1H), 6.64-6.65 (m, 1H), 6.61 (t, 1H, *J* = 2.1 Hz), 6.47-6.49 (m, 1H), 4.96 (s, 1H), 3.69 (br, 1H), 3.07 (s, 1H), 2.21-2.29 (m, 2H), 2.11-2.14 (m, 1H), 1.8-2.0 (br, 1H); 1.64-1.71 (m, 2H), 1.28-1.34 (m, 1H), 1.16-1.20 (m, 2H), 0.95-1.02 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 149.5, 144.6, 144.0, 135.0, 130.2, 128.7, 128.4, 127.6, 127.2, 127.1, 126.8, 117.1, 113.2, 112.0, 63.6, 58.7, 57.5, 32.2, 31.6, 24.6, 24.6; HPLC: Daicel Chiralpak AD-H, hexane /^{i}PrOH = 100 /1, flow rate = 1.0 mL /min, 254 nm : *tR* = 8.6 min (*major*), *tR* = 13.9 min (*minor*); FT-IR (neat) 2929, 1596, 1492, 1090, 700 cm^{-1}; HRMS : calcd. for $C_{25}H_{28}ClN_2$ [M+H$^+$]: 391.1936; found: 391.1925. $[\alpha]_D^{20}$ -12.0 (c 1.0, $CHCl_3$) for 86% ee product.

***trans-N*- Benzhydryl -*N'*-3-bromophenylcyclohexan-1,2-diamine (6ac)**



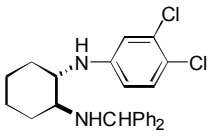
^{1}HNMR ($CDCl_3$) δ 7.25-7.28 (m, 6H), 7.16-7.19 (m, 3H), 7.08-7.10 (m, 1H), 6.91-6.94 (m, 1H), 6.70-6.73 (m, 2H), 6.44-6.46 (m, 1H), 4.89 (s, 1H), 3.69 (s, 1H), 2.99 (m, 1H), 2.14-2.22 (m, 2H), 2.03-2.06 (m, 1H), 1.8-2.0 (1H, br), 1.57-1.65 (m, 2H), 1.18-1.23 (m, 1H), 1.07-1.12 (m, 2H), 0.88-0.95 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 149.6, 144.6, 144.0, 130.5, 128.6, 128.3, 127.5, 127.1, 127.0, 126.8, 123.2, 120.0, 116.1, 112.3, 63.6, 58.7, 57.5, 32.1, 31.6, 24.6, 24.5; HPLC: Daicel Chiralpak AD-H, hexane /^{i}PrOH = 100 /1, flow rate = 1.0 mL /min, 254 nm : *tR* = 10.4 min (*major*), *tR* = 15.1 min (*minor*); FT-IR [cm^{-1}] (neat) 1594, 1070, 586; HRMS (m/z) calcd. for $C_{25}H_{28}BrN_2$: 435.1430; found: 435.1420 [M+H$^+$]; $[\alpha]_D^{22}$ +13.3 (c 0.95, $CHCl_3$) for 83% ee product.

***trans-N*- Benzhydryl -*N'*-(3-iodophenyl)cyclohexan-1,2-diamine (6ad)**



^{1}HNMR ($CDCl_3$) δ 7.24-7.27 (m, 6H), 7.16-7.20 (m, 3H), 7.08-7.11 (m, 1H), 6.91-6.94 (m, 2H), 6.77-6.80 (m, 1H), 6.48-6.50 (m, 1H), 4.89 (s, 1H), 3.54 (br, 1H), 2.99 (m, 1H), 2.14-2.21 (m, 2H), 2.02-2.10 (m, 1H), 1.8-2.0 (br, 1H), 1.58-1.65 (m, 2H), 1.21-1.27 (m, 1H), 1.08-1.15 (m, 2H), 0.88-0.94 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 149.6, 144.6, 144.0, 130.7, 128.6, 128.4, 127.6, 127.1, 127.0, 126.8, 126.1, 122.1, 112.9, 95.3, 63.6, 58.7, 57.5, 32.2, 31.6, 24.6, 24.5; HPLC: Daicel Chiralpak AD-H, hexane /^{i}PrOH = 100 /1, flow rate = 1.0 mL /min, 254 nm : *tR* = 10.8 min (*major*), *tR* = 16.8 min (*minor*); FT-IR (neat) 2928, 1589, 1493, 1101, 760 cm^{-1}; HRMS : calcd. for $C_{25}H_{28}IN_2$ [M+H$^+$]: 483.1292; found: 483.1290. $[\alpha]_D^{20}$ +16.2 (c 1.00, $CHCl_3$) for 83% ee product.

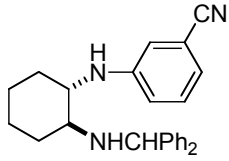
***trans-N*- Benzhydryl -*N'*- (3,4-dichlorophenyl)cyclohexan-1,2-diamine (6ae)**



^{1}H NMR ($CDCl_3$) δ 7.31-7.33 (m, 6H), 7.22-7.25 (m, 3H), 7.14-7.17 (m, 2H), 6.69 (d, 1H, *J* = 2.7 Hz), 6.42 (dd, 1H, *J* = 8.9 Hz, 2.8 Hz), 4.96 (s, 1H,), 3.71 (br, 1H), 3.01 (br, 1H), 2.20-2.29 (m, 2H), 2.08-2.10 (m, 1H), 1.85 (br, 1H), 1.64-1.72 (m, 2H), 1.18-1.29 (m, 3H), 0.95-1.02 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 147.9, 144.5, 144.0, 132.7, 130.5, 128.6, 128.4, 127.5, 127.2, 127.0, 126.8, 119.5, 114.5, 113.3, 63.7, 58.7, 57.7, 32.0, 31.6, 24.5, 24.5; IR (KBr) 3063, 3024, 2929, 2855, 1596, 1492, 1316, 1238, 1131, 1028, 745, 701 cm^{-1}; HPLC: Daicel Chiralpak AD-H, hexane / ^{i}PrOH = 100/1, flow rate = 1.0 ml /min: *t*R = 18.0 min

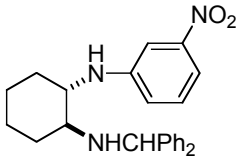
(major), *t*R = 20.7 min (minor); HRMS : Calcd for $C_{25}H_{27}Cl_2N_2$ [M+H$^+$]: 425.1551, found 425.1557; $[\alpha]_D^{25}$ +31.5 (c 0.725, $CHCl_3$) for 85% ee product.

***trans*-3-(2'-(Benzhydrylamino)cyclohexylamino)benzonitrile (6af)**



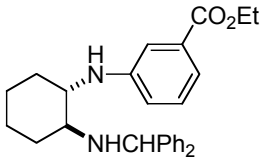
^{1}HNMR ($CDCl_3$) δ 7.15-7.35 (m, 11H), 6.93 (d, 1H, *J* = 6.8 Hz), 6.78-6.81 (m, 2H), 4.98 (s, 1H), 3.94 (br, 1H), 3.07 (br, 1H), 2.23-2.32 (m, 2H), 2.10-2.13 (m, 1H), 2.00-1.74(m, 3H), 1.18-1.37 (m, 3H), 0.98-1.06 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 148.6, 144.4, 143.9, 129.9, 128.7, 128.4, 127.6, 127.3, 127.1, 127.0, 120.6, 119.5, 118.0, 115.7, 112.9, 63.8, 58.7, 57.4, 31.9, 31.6, 24.6, 24.4; HPLC: Daicel Chiralcel OD-H, hexane /^{i}PrOH = 100 /1, flow rate = 1.0 mL /min, 254 nm : *tR* = 31.0 min (*minor*), *tR* = 40.0 min (*major*); FT-IR (neat) 3370, 3026, 2928, 2226, 1600, 1452, 1335, 1098, 848, 701 cm^{-1}; HRMS : calcd. for $C_{26}H_{28}N_3$ [M+H$^+$]: 382.2283; found: 382.2273; $[\alpha]_D^{24}$ +10.9 (c 0.605, $CHCl_3$) for 80% ee product.

***trans*-*N*- Benzhydryl-*N'*-(3-nitrophenyl)cyclohexan-1, 2-diamine (6ag)**



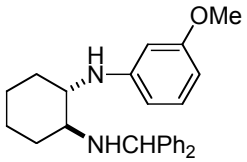
^{1}HNMR ($CDCl_3$) δ 7.49-7.51(m, 1H), 7.41-7.42(m, 1H), 7.31-7.36 (m, 6H), 7.22-7.29 (m, 4H), 7.15-7.18 (m, 1H), 6.87 (d, *J* = 8.5 Hz, 1H), 4.99 (s, 1H), 4.06 (br, 1H), 3.15 (m, 1H), 2.35 (m, 1H), 2.24-2.26 (m, 1H),2,13-2.16 (m, 1H), 1.60-1.90 (m, 3H), 1.31-1.39 (m, 1H), 1.18-1.27 (m, 2H), 1.00-1.09 (m, 1H). ^{13}C NMR ($CDCl_3$) δ 149.4, 149.1, 144.4, 144.1, 129.7, 128.7, 128.4, 127.6, 127.3, 127.0, 127.0, 119.4, 111.8, 107.1, 63.8, 58.8, 57.4, 32.0, 31.6, 24.6, 24.5; HPLC: Daicel Chiralpak AD-H, hexane /^{i}PrOH = 9/1, flow rate = 1.0 mL /min, 254 nm : *tR* = 7.7 min (*major*), *tR* = 10.9 min (*minor*); FT-IR (neat) 3396, 2927, 1717, 1620, 1526, 1348, 1093, 701 cm^{-1}; HRMS: calcd. for $C_{25}H_{28}N_3O_2$ [M+H$^+$]: 402.2182; found: 402.2187. $[\alpha]_D^{25}$ +12.1 (c 0.333, $CHCl_3$) for 84% ee product.

***trans*-Ethyl 3-(2'-(benzhydrylamino)cyclohexylamino)benzoate (6ah)**



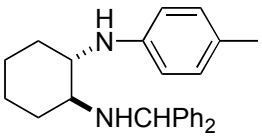
^{1}HNMR ($CDCl_3$) δ 7.31-7.38(m, 8H), 7.19-7.27(m, 4H), 7.13-7.17 (m, 1H), 6.80 (dd, 1H, *J* = 8.2, 2.0 Hz), 4.98 (s, 1H), 4.36 (q, 2H, *J* = 7.2 Hz), 3.70 (br, 1H), 3.18 (m, 1H), 2.13-2.32 (m, 3H), 2.0 (br, 1H), 1.64-1.73 (m, 2H), 1.29-1.40 (m, 4H), 1.16-1.26 (m, 2H), 0.96-1.04 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 167.1, 148.3, 144.6, 144.0, 131.4, 129.2, 128.6, 128.3, 127.6, 127.1, 127.1, 126.8, 118.5, 117.9, 114.6, 63.7, 60.8, 58.9, 57.6, 32.2, 31.7, 24.7, 24.6, 14.4; HPLC: Daicel Chiralpak AS-H, hexane /^{i}PrOH = 100 /1, flow rate = 0.5 mL /min, 254 nm : *tR* = 25.8 min (*minor*), *tR* = 29.1 min (*major*); FT-IR (neat) 3378, 2927, 1714, 1604, 1102, 753, 701 cm^{-1}; HRMS : calcd. for $C_{28}H_{33}N_2O_2$ [M+H$^+$]: 429.2542; found: 429.2550; $[\alpha]_D^{24}$ +5.4 (c 0.80, $CHCl_3$) for 80% ee product.

***trans*-*N*- Benzhydryl -*N'*-(3-methoxyphenyl)cyclohexan-1,2-diamine (6ai)**



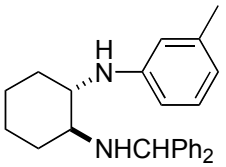
^{1}HNMR ($CDCl_3$) δ 7.31-7.34(m, 6H), 7.22-7.27 (m, 3H), 7.14-7.17 (m, 1H), 7.07(t, 1H, *J* = 7.9 Hz), 6.25-6.28 (m, 2H), 6.21 (t, *J* = 2.3 Hz, 1H), 4.96 (s, 1H), 3.77 (s, 3H), 3.5 (br, 1H), 3.12(td, 1H , *J* = 10.2, 3.6 Hz,), 2.28 (td, 1H, *J* = 9.6, 3.8 Hz), 2.14-2.22 (m, 2H), 1.9 (br, 1H), 1.63-1.72 (m, 2H), 1.15-1.34 (m, 3H), 0.94-1.00 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 160.9, 149.7, 144.7, 144.1, 130.0, 128.6, 128.3, 127.6, 127.1, 127.1, 126.8, 107.0, 102.5, 99.9, 63.6, 58.8, 57.7, 55.1, 32.4, 31.7, 24.7, 24.6; HPLC: Daicel Chiralpak AD-H, hexane /^{i}PrOH = 9 /1, flow rate = 1.0 mL /min, 254 nm : *tR* = 6.3 min (*major*), *tR* = 10.3 min (*minor*); FT-IR (neat) 3388, 2929, 1720, 1613, 1492, 1454, 1161, 1093, 1049, 757, 701 cm^{-1}; HRMS : calcd. for $C_{26}H_{31}N_2O$ [M+H$^+$]: 387.2436; found: 387.2440; $[\alpha]_D^{25}$ +3.49 (c 0.833, $CHCl_3$) for 80% ee product.

***trans-N-* Benzhydryl -*N'*-(4-methylphenyl)cyclohexan-1,2-diamine (6aj)**



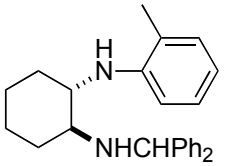
^{1}HNMR ($CDCl_3$) δ 7.35-7.30 (m, 6H), 7.20-7.25 (m, 3H), 7.15 (m, 1H), 6.99 (d, 2H, *J* = 8.2 Hz), 6.58 (d, 2H, *J* = 8.2 Hz), 4.97 (s, 1H), 3.4 (br, 1H), 3.10 (m, 1H), 2.24 (s, 3H), 2.10-2.30 (m, 4H), 1.60-1.71 (m, 2H), 1.23-1.34 (m, 1H), 1.12-1.23 (m, 2H), 0.93-1.0 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 145.9, 144.6, 144.0, 129.7, 128.6, 128.3, 127.5, 127.0, 127.0, 126.8, 126.7, 114.1, 63.4, 58.7, 58.0, 32.3, 31.5, 24.7, 24.5, 20.4; HPLC: Daicel Chiralcel OD-H, hexane /^{i}PrOH = 100 /1, flow rate = 0.8 mL /min, 254 nm : *tR* = 7.5 min (*major*), *tR* = 8.4 min (*minor*)

***trans-N-* Benzhydryl -*N'*-(3-methylphenyl)cyclohexan-1,2-diamine (6ak)**



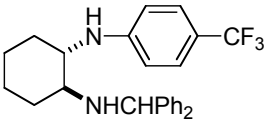
^{1}HNMR ($CDCl_3$) δ 7.30-7.35 (m, 6H), 7.22-7.26 (m, 3H), 7.15 (m, 1H), 7.06 (t, 1H, *J* = 7.6 Hz), 6.53 (d, 1H, *J* = 7.6 Hz), 6.44-6.55 (m, 2H), 4.97 (s, 1H), 3.45 (br, 1H), 3.14 (m, 1H), 2.28 (s, 3H), 2.12-2.31 (m, 4H), 1.63-1.72 (m, 2H), 1.15-1.35 (m, 3H), 0.98 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 148.3, 144.7, 144.0, 139.0, 129.1, 128.6, 128.3, 127.5, 127.1, 127.0, 126.7, 118.4, 114.6, 111.0, 63.4, 58.7, 57.6, 32.3, 31.5, 24.7, 24.5, 21.6; HPLC: Daicel Chiralpak AD-H, hexane /^{i}PrOH = 100 /1, flow rate = 1.0 mL /min, 254 nm : *tR* = 7.5 min (*major*), *tR* = 10.7 min (*minor*).

***trans-N-* Benzhydryl -*N'*-(2-methylphenyl)cyclohexan-1,2-diamine (6al)**



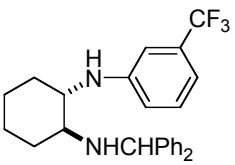
^{1}HNMR ($CDCl_3$) δ 7.32-7.37 (m, 6H), 7.23-7.27 (m, 3H), 7.16 (m, 1H), 7.11 (m, 1H), 7.08 (d, 1H, *J* = 6.8 Hz), 6.68 (d, 1H, *J* = 7.6 Hz), 6.66 (t, 1H, *J* = 7.6 Hz), 5.01 (s, 1H), 3.70 (br, 1H), 3.19 (m, 1H), 2.21-2.30 (m, 3H), 2.17 (s, 3H), 2.1 (br, 1H), 1.75 (m, 1H), 1.67 (m, 1H), 1.34 (m, 1H), 1.21 (m, 2H), 0.98 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 146.1, 144.6, 143.9, 130.2, 128.6, 128.3, 127.5, 127.0, 127.0, 126.7, 122.7, 116.8, 110.6, 63.2, 58.3, 57.2, 32.2, 31.4, 24.7, 24.6, 17.8; HPLC: Daicel Chiralcel OD-H, hexane /^{i}PrOH = 100 /1, flow rate = 0.8 mL /min, 254 nm : *tR* = 8.9 min (*major*), *tR* = 9.9 min (*minor*).

***trans-N-* Benzhydryl -*N'*-(4-trifluoromethylphenyl)cyclohexan-1,2-diamine (6am)**



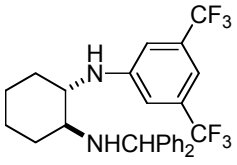
^{1}HNMR ($CDCl_3$) δ 7.22-7.39 (m, 11H), 7.15 (m, 1H), 6.60 (d, 2H, *J* = 8.2 Hz), 4.96 (s, 1H), 3.94 (m, 1H), 3.15 (m, 1H), 2.12-2.32 (m, 3H), 1.89 (br, 1H), 1.66-1.74 (m, 2H), 1.30-1.36 (m, 1H), 1.19-1.22 (m, 2H), 0.99 -1.06 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 150.8, 144.4, 144.0, 128.7, 128.4, 127.6, 127.2, 127.0, 126.9, 126.6, 125.0 (q, J_F = 269 Hz), 118.6 (q, J_F = 33.2 Hz), 112.5, 63.7, 58.6, 57.1, 32.0, 31.6, 24.5, 24.5; HPLC: Daicel Chiralpak AD-H, hexane /^{i}PrOH = 100 /1, flow rate = 1.0 mL /min, 254 nm : *tR* = 9.4 min (*minor*), *tR* = 14.6 min (*major*); FT-IR (neat) 2930, 1616, 1323, 1107, 700 cm^{-1}; HRMS : calcd. for $C_{26}H_{28}F_3N_2$ [M+H]:425.2199; found: 425.2200; $[\alpha]_D^{25}$ +8.0 (c 0.72, $CHCl_3$) for 83% ee product.

***trans-N-* Benzhydryl-*N'*-(3-trifluoromethylphenyl)cyclohexan-1,2-diamine (6an)**



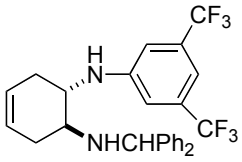
^{1}HNMR ($CDCl_3$) δ 7.31-7.35 (m, 6H), 7.22-7.27 (m, 4H). 7.15-7.17 (m, 1H), 6.91 (d, 1H, *J* = 7.6 Hz), 6.83 (s, 1H), 6.75 (d, 1H, *J* = 8.2 Hz), 4.97 (s, 1H), 3.80 (br, 1H), 3.13 (m, 1H), 2.12-2.32 (m, 3H), 1.90 (br, 1H), 1.66-1.74 (m, 2H), 1.11-1.40 (m, 3H), 0.99-1.05 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 148.5, 144.6, 144.0, 131.5 (q, J_F = 31.0 Hz), 129.6, 128.6, 128.4, 127.6, 127.2, 127.0 126.8, 124.3 (q, J_F = 273 Hz), 116.5, 113.6 (q, J_F = 4.8 Hz), 109.7 (q, J_F = 3.6 Hz), 63.7, 58.9, 57.5, 32.2, 31.6, 24.6, 24.6; HPLC: Daicel Chiralpak AD-H, hexane /^{i}PrOH = 100 /1, flow rate = 1.0 mL /min, 254 nm : *tR* = 8.2 min (*major*), *tR* = 9.0 min (*minor*); FT-IR (neat) 2930, 1613, 1491, 1340, 1121, 698 cm^{-1}; HRMS : calcd. for $C_{26}H_{28}F_3N_2$ [M+H$^+$]: 425.2199; found: 425.2215; $[\alpha]_D^{25}$ -3.2 (c 1.6, $CHCl_3$) for 86% ee product

***trans*-*N*- Benzhydryl -*N'*-[3,5-bis(trifluoromethyl)phenyl]cyclohexan-1,2-diamine (6ao)**



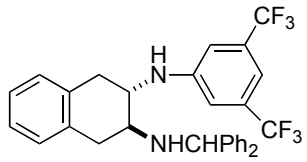
^{1}HNMR ($CDCl_3$) δ 7.31-7.36 (m, 6H), 7.23-7.30 (m, 3H), 7.15-7.18 (m, 1H), 7.13 (s, 1H), 6.94 (s, 2H), 4.89 (s, 1H), 4.07 (d, 1H, *J* = 6.9 Hz), 3.10-3.14 (m, 1H), 2.26-2.33 (m, 2H), 2.10-2.16 (m, 1H), 1.69-1.77 (m, 3H), 1.33-1.37 (m, 1H), 1.20-1.26 (m, 2H), 1.03-1.07 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 149.0, 144.4, 144.0, 132.3 (q, J_F = 32.3 Hz), 128.7, 128.4, 128.4, 127.6, 127.3, 127.0, 123.6 (q, J_F = 272 Hz), 112.5, 109.9, 63.9, 59.2, 57.5, 32.1, 31.8, 24.6, 24.5; HPLC: Daicel Chiralcel OD-H, hexane /iPrOH = 100 /1, flow rate = 1.0 mL /min, 254 nm : *tR* = 7.5 min (*minor*), *tR* = 10.4 min (*major*); FT-IR (neat) 1619, 1395, 1129, 700 cm^{-1}; HRMS : calcd. for $C_{27}H_{27}F_6N_2$ [M+H$^+$]: 493.2073; found: 493.2062; $[\alpha]_D^{25}$ +0.65 (c 1.4, $CHCl_3$) for 92% ee product.

***trans*-*N*- Benzhydryl -*N'*- [3,5-bis(trifluoromethyl)phenyl]cyclohex-4-en-1,2-diamine (6bo)**



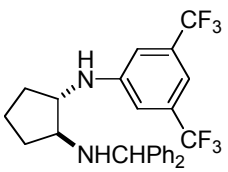
^{1}H NMR ($CDCl_3$) δ 7.40 (d, 2H, *J* = 6.8 Hz), 7.32-7.36 (m, 4H), 7.22-7.27 (m, 3H), 7.18 (t, 1H, *J* = 7.6 Hz), 7.10 (s, 1H), 6.90 (s, 2H), 5.63 (m, 2H), 5.01 (s, 1H), 4.31 (d, 1H, *J* = 7.6 Hz), 3.57 (m, 1H), 2.83(q, 1H, *J* = 6.9 Hz), 2.68 (d, 1H, *J* = 17.8 Hz), 2.49 (d, 1H, *J* = 17.9 Hz), 2.08-2.11 (m, 1H), 1.89-1.93 (m, 1H), 1.68 (br, 1H); ^{13}C NMR ($CDCl_3$) δ 148.6, 144.4, 143.6, 132.3 (q, J_F = 33.2Hz), 128.8, 128.6, 127.4, 127.4, 127.2, 127.1, 125.2, 124.2, 123.6 (q, J_F = 272 Hz), 112.4, 110.0, 64.4, 52.7, 52.3, 30.3, 29.9; FT-IR (KBr): 3409, 3030, 2917, 2843, 1620, 1522, 1493, 1474, 1396, 1278, 1176, 1130, 996, 861, 746, 701 cm^{-1}; HPLC: Daicel Chiralcel OD-H, hexane / ^{i}PrOH = 100/1, flow rate = 1.0 ml /min: *t*R = 8.1 min (minor), *t*R = 10.3 min (major); HRMS : Calcd for $C_{27}H_{25}F_6N_2$ [M+H$^+$]: 491.1922, found 491.1910; $[\alpha]_D^{25}$ -25.9 (c 0.620, $CHCl_3$) for 93% ee product.

***trans*-*N*- Benzhydryl -*N'*- [3,5-bis(trifluoromethyl)phenyl]-1,2,3,4-tetrahydronaphthalen-2,3-diamine (6co)**



^{1}H NMR ($CDCl_3$) δ 7.42 (d, 2H, *J* = 6.9 Hz), 7.37 (d, 2H, *J* = 6.8 Hz), 7.33 (t, 2H, *J* = 7.6 Hz), 7.23-7.28 (m, 3H), 7.11-7.20 (m, 5H), 7.08 (d, 1H, *J* = 6.8 Hz), 6.92 (s, 2H), 5.09 (s, 1H), 4.32 (d, 1H, *J* = 6.9 Hz), 3.71-3.75 (m, 1H), 3.38 (dd, 1H, *J* = 16.5, 5.5 Hz), 3.22 (dd, 1H, *J* = 16.5, 4.8 Hz), 3.00-3.03 (m, 1H), 2.82 (dd, 1H, *J* = 16.5, 6.8 Hz), 2.65 (dd, 1H, *J* = 16.5, 6.8 Hz), 1.71 (br, 1H); ^{13}C NMR ($CDCl_3$) δ 148.3, 144.2, 143.4, 133.8, 133.1, 132.4 (q, J_F = 34.7 Hz), 129.3, 129.2, 128.8, 128.6, 127.5, 127.4, 127.2, 127.0, 126.6, 126.4, 123.5 (q, J_F = 271 Hz), 112.4, 110.2, 64.5, 53.6, 53.1, 34.0, 33.6; FT-IR (KBr): 2925, 2362, 1620, 1523, 1493, 1475, 1394, 1278, 1177, 1129, 950, 862, 745, 701 cm^{-1}; HPLC: Daicel Chiralcel OD-H, hexane / ^{i}PrOH = 100/1, flow rate = 1.0 ml /min: *t*R = 19.9 min (minor), *t*R = 24.3 min (major); HRMS : Calcd for $C_{31}H_{27}F_6N_2$ (M+H)$^+$: 541.2078, found 541.2062. $[\alpha]_D^{25}$ -55.9 (c 0.99, $CHCl_3$) for 92% ee product.

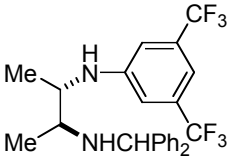
***trans*-*N*- Benzhydryl -*N'*-[3,5-bis(trifluoromethyl)phenyl]cyclopentan-1,2-diamine (6do)**



^{1}H NMR ($CDCl_3$) δ 7.37 (t, 4H, *J* = 6.2 Hz), 7.28 (t, 4H, *J* = 7.6 Hz), 7.19-7.22 (m, 2H), 7.13 (s, 1H), 6.94 (s, 2H), 4.92 (s, 1H), 4.02 (d, 1H, *J* = 6.2 Hz), 3.54 (quint, 1H, *J* = 6.8 Hz), 2.85 (q, 1H, *J* = 6.8 Hz), 2.18-2.24 (m, 1H), 2.01-2.06 (m, 1H), 1.74-1.81 (m, 1H), 1.61-1.67 (m, 2H), 1.47-1.53(m, 1H), 1.34-1.39 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 148.7, 144.2, 143.7, 132.4 (q, J_F = 33.2 Hz), 128.6, 128.6, 127.3, 127.2, 127.2, 127.1, 123.6 (q, J_F = 271 Hz), 112.3, 109.9, 65.7, 63.7, 60.8, 31.3, 31.0, 21.3; FT-IR (KBr): 3415, 2944, 1624, 1523, 1476, 1395, 1277, 1164, 1123, 864, 749, 708 cm^{-1}; HPLC: Daicel Chiralpak AD-H, hexane / ^{i}PrOH = 100/1, flow rate = 1.0 ml /min: *t*R = 5.7 min (minor), *t*R = 6.3 min

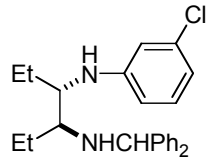
(major); HRMS : Calcd for $C_{26}H_{25}F_6N_2$ [M+H$^+$]: 479.1922, found 479.1903; $[\alpha]_D^{25}$ -23.0 (c 0.738, $CHCl_3$) for 86% ee product.

(2S*,3S*)-*N*- Benzhydryl -*N'*-[3,5-bis(trifluoromethyl)phenyl]butan-2,3-diamine (6eo)



^{1}H NMR ($CDCl_3$) δ 7.2-7.4 (m, 10H), 7.08 (s, 1H), 6.85 (s, 2H), 4.97 (s, 1H), 4.31 (dbr, 1H, *J* = 8.2 Hz), 3.42 (m, 1H), 2.71 (dq, 1H, *J* = 6.2, 5.5 Hz), 1.52 (br, 1H), 1.17 (d, 3H, *J* = 6.2 Hz), 1.13 (d, 3H, *J* = 6.2 Hz); ^{13}C NMR ($CDCl_3$) δ 148.5, 144.3, 143.5, 132.4 (q, J_F = 33.2 Hz), 128.6, 128.6, 127.5, 127.3, 127.1, 123.6 (q, J_F = 273 Hz), 112.1, 109.7, 64.7, 54.1, 53.1, 16.9, 16.7; FT-IR (KBr): 3029, 2974, 2931, 1620, 1520, 1493, 1475, 1395, 1278, 1172, 1129, 1027, 861, 746, 701 cm^{-1}; HPLC: The title compound was converted to 1-(3,5-bis(trifluoromethyl)phenyl)-3-benzhydryl -4,5-dimethylimidazolidin-2-one after being reacted by triphosgen in CH_2Cl_2. Daicel Chiralpak AD-H, hexane / ^{i}PrOH = 100/1, flow rate = 1.0 ml /min: *t*R = 5.7 min (major), *t*R = 7.9 min (minor). HRMS : Calcd for $C_{25}H_{25}F_6N_2$ [M+H$^+$]: 467.1922, found: 467.1903. $[\alpha]_D^{25}$ -13.5 (c 1.93, $CHCl_3$) for 93% ee product.

(3S*,4S*)-*N*- Benzhydryl -*N'*-(3-Chlorophenyl)hexan-3,4-diamine (6fb)

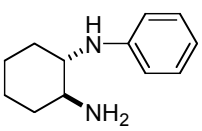


^{1}HNMR ($CDCl_3$) δ 7.20-7.43 (m, 10H), 6.95 (t, 1H, *J* = 8.0), 6.55 (dd, 1H, *J* = 7.8, 1.4), 6.46 (t, 1H, *J* = 2.1 Hz), 6.27(dd, 1H, *J* = 8.0, 2.1), 4.96 (s, 1H), 3.86 (br, 1H), 3.22 (br, 1H), 2.53-2.57 (m, 1H), 1.35-1.70 (m, 5H), 0.88 (t, 3H, *J* = 7.6 Hz), 0.80 (t, 3H, *J* = 7.3 Hz); ^{13}C NMR ($CDCl_3$) δ 149.7, 144.4, 144.0, 134.9, 130.1, 128.5, 128.4, 127.7, 127.3, 127.1, 127.1, 116.2, 112.2, 110.9, 65.3, 58.0, 56.3, 24.5, 23.7, 11.0, 10.9; HPLC: The title compound was converted to 1-(3,5-bis(trifluoromethyl)phenyl)-3-benzhydryl-4,5-diethylimidazolidin-2-one after being reacted by triphosgen in CH_2Cl_2. Daicel Chiralpak AD-H, hexane /^{i}PrOH = 9/1, flow rate = 1.0 mL /min, 254 nm : *tR* = 8.3 min (*major*), *tR* = 19.0 min (*minor*); FT-IR (neat) 3410, 3025, 2961, 1597, 1494, 1325, 1092, 904, 838, 760, 702 cm^{-1}; HRMS : calcd. For $C_{25}H_{30}ClN_2$ [M+H$^+$]: 393.2098; found: 393.2090; $[\alpha]_D^{22}$ +10.1 (c 0.830, $CHCl_3$) for 80% ee product..

The typical procedure for deprotection of N- Benzhydryl group

The Polymer-incarcerated Pd (PI Pd, 5 mol%)[3] was added to a solution of the amine adduct in EtOH. The mixture was stirred for 36 h at 70 ^{o}C under hydrogen atmosphere (1 atm). The catalyst was filtered and washed with dichloromethane, and the solvents of filtrate were combined and evaporated under reduced pressure. Et_2O and 1M-HCl were added to the residue, and the mixture was stirred for 10 min. The organic layer was separated, and the aqueous layer was washed with Et_2O (3 times). The aqueous layer was basicified with saturated $NaHCO_3$. The aqueous layer was extracted with CH_2Cl_2 (3 times). The organic layers were combined and dried over anhydrous Na_2SO_4. After filtration and concentration under reduced pressure, the pale yellow solid was obtained (quantitative yield).

***trans*-*N*-Phenylcyclohexane-1, 3-diamine**



^{1}HNMR ($CDCl_3$) δ 7.15-7.17 (m, 2H), 6.67-6.70(m, 3H), 3.44 (br, 1H), 2.94-2.98 (m, 1H), 2.49-2.53 (m, 1H), 2.12-2.14 (m, 1H), 1.98-2.00 (m, 1H), 1.70-1.74 (m, 4H), 1.21-1.33 (m, 3H), 1.04-1.09 (m, 1H). ^{13}C NMR ($CDCl_3$) δ 148.1, 129.2, 117.4, 113.6, 60.1, 56.1, 35.1, 32.4, 25.3, 25.0. FT-IR (KBr) 3357, 2927, 2855, 1604, 1498, 1318, 1153, 745, 693 cm^{-1}. HRMS : calcd. for $C_{12}H_{19}N_2$[M+H$^+$]: 191.1548; found: 191.1540. $[\alpha]_D^{21}$ –34.7 (c 0.850, $CHCl_3$).

The experiment of non-linear effect

(a) Low ee ligand catalyst

Preparation of low ee BINOL derivatives is following; Optically pure (*R*)- and (*S*)- BINOL derivatives were mixed in dichloromethane in proper ratio, and stirred for 5 h at room temperature, and then, solvent was removed under reduced pressure for 2 h at same temperature. The optical purity was determined by HPLC analysis using a chiral column. The asymmetric reactions using these low ee ligands were performed according to the typical experimental procedure.

(b) Mixed catalyst

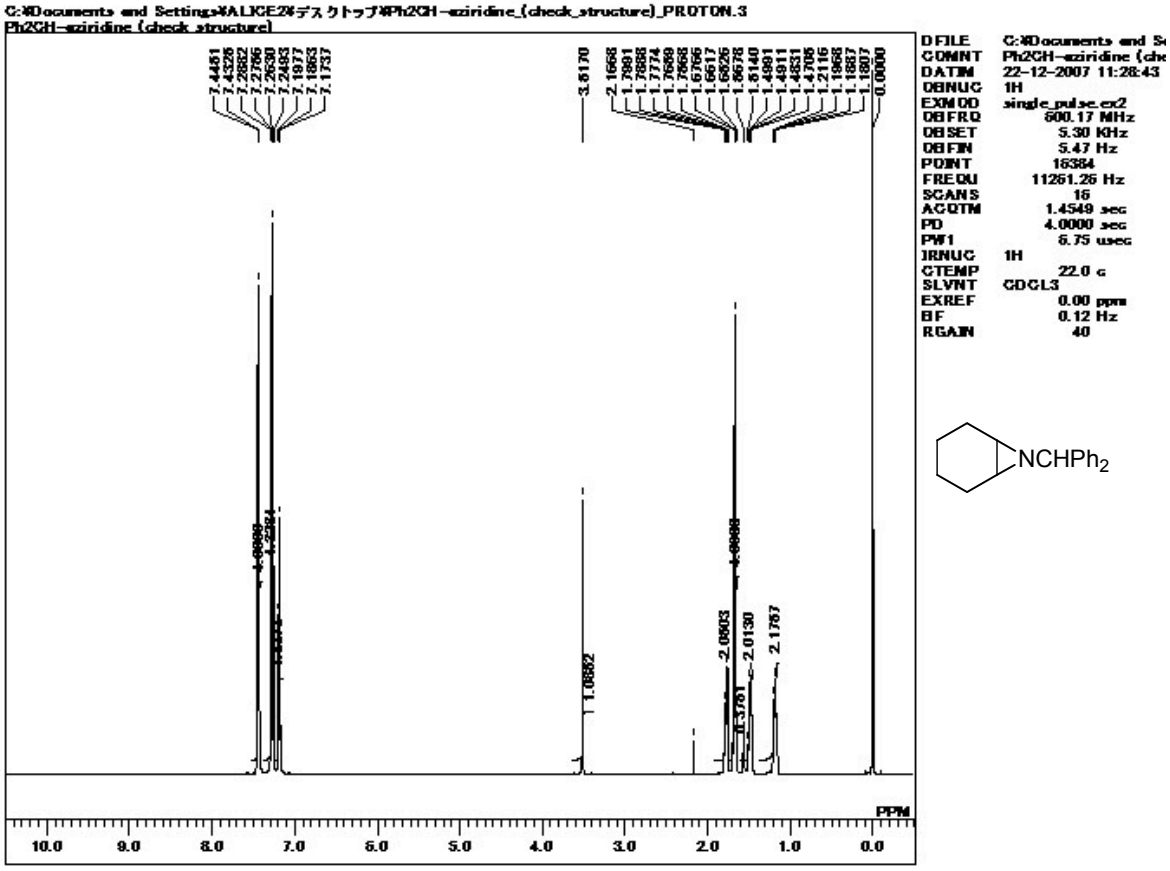
Optically pure (*R*)- and (*S*)- zirconium catalysts were prepared respectively according to the typical experimental procedure (0.03M in toluene). The catalyst solutions were mixed in appreciate ratios (total 1ml) and stirred for 30 min or 3 h at room temperature, and then aziridine **4a** (0.15 mmol) was added at same temperature. After Cooled to 0 ^{o}C, aniline **5a** (0.18 mmol) was added. The mixture was stirred for 24 h, and treatment after reaction was conducted according to the typical experimental procedure.

Reference

(1) (a) Watson, D. G. Iain; Yudin, K. A. *J. Org. Chem*. **2003**, *68*, 5160; (b) Pujala, S. B.; Chakraborti, A. K. *J. Org. Chem*. **2007**, *72*, 3713.

(2) Kobayashi, S.; Arai, K.; Shimizu, H.; Ihori, Y.; Ishitani, H.; Yamashita, Y. *Angew. Chem. Int. Ed*. **2005**, *44*, 761.

(3) Akiyama, R.; Kobayashi, S. *J. Am. Chem. Soc.* **2003**, *125*, 3412.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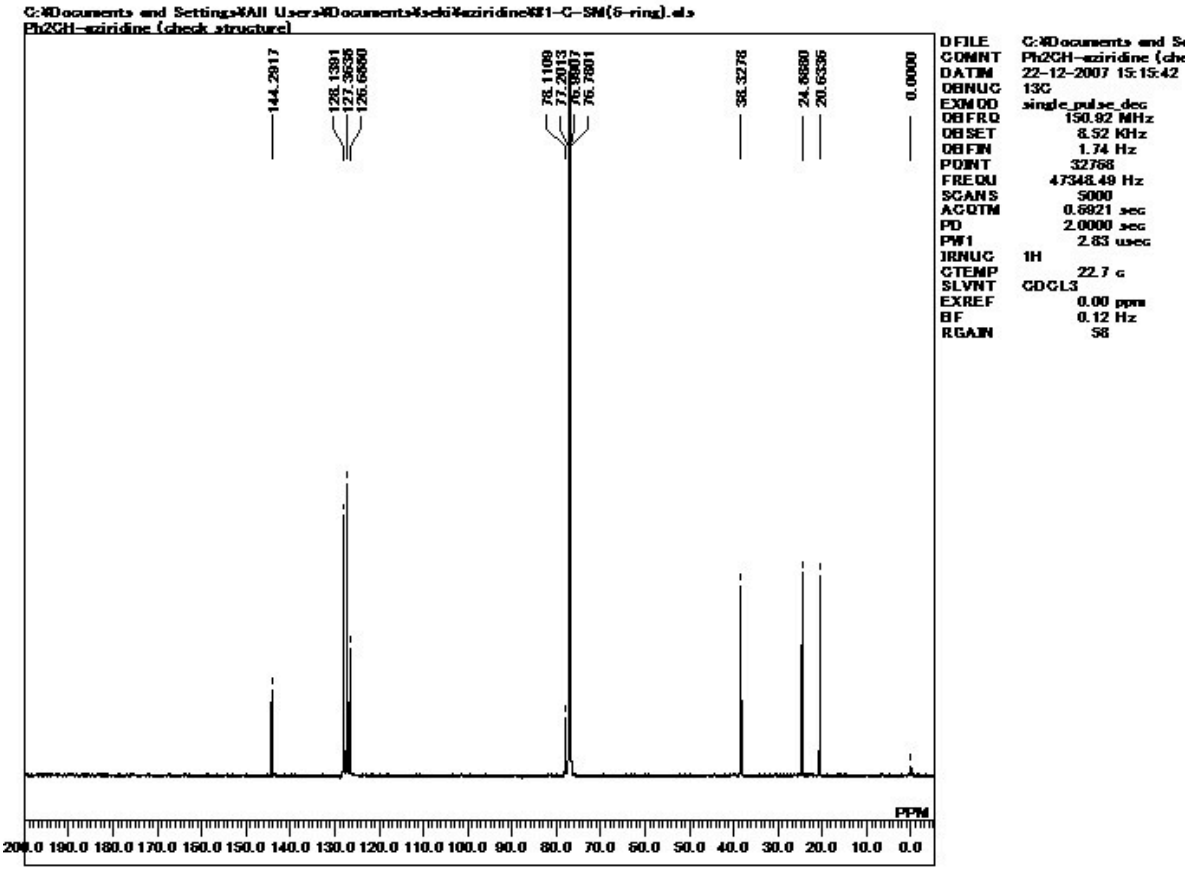
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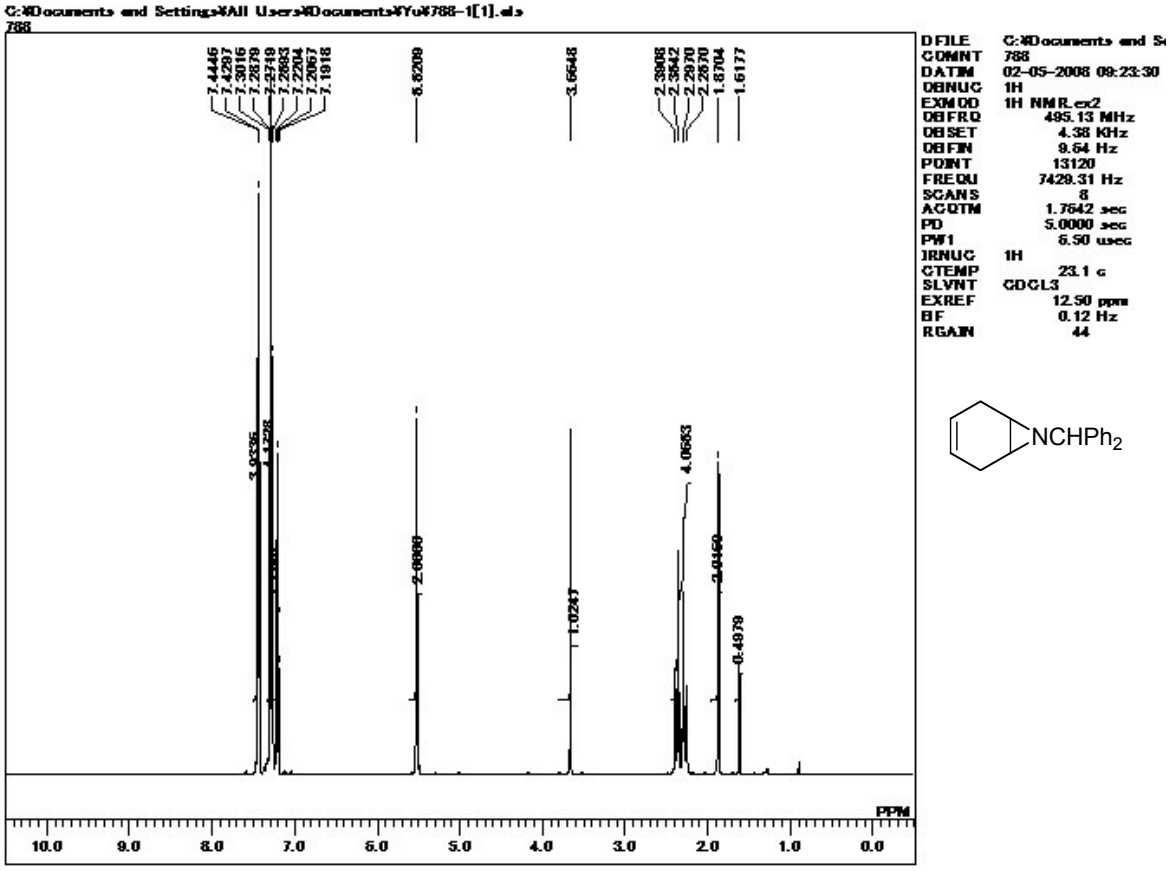
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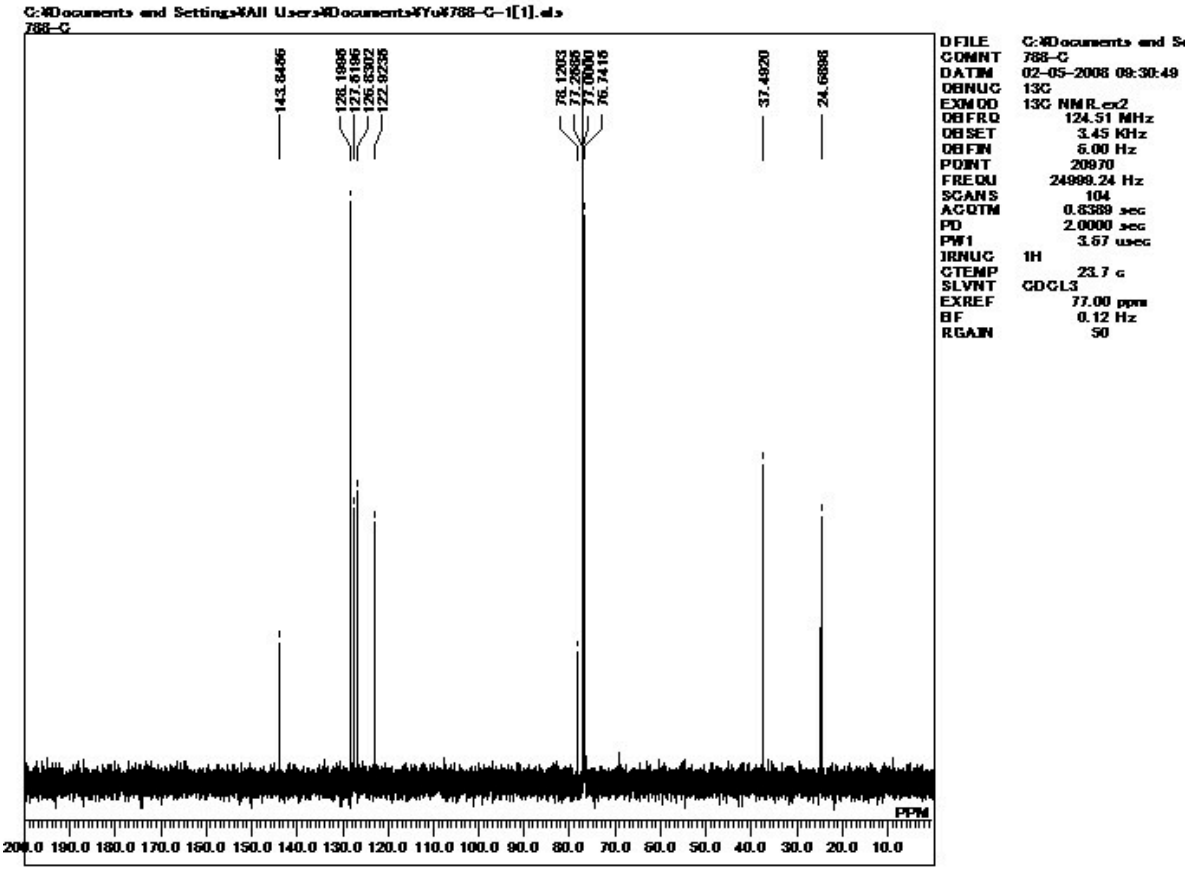
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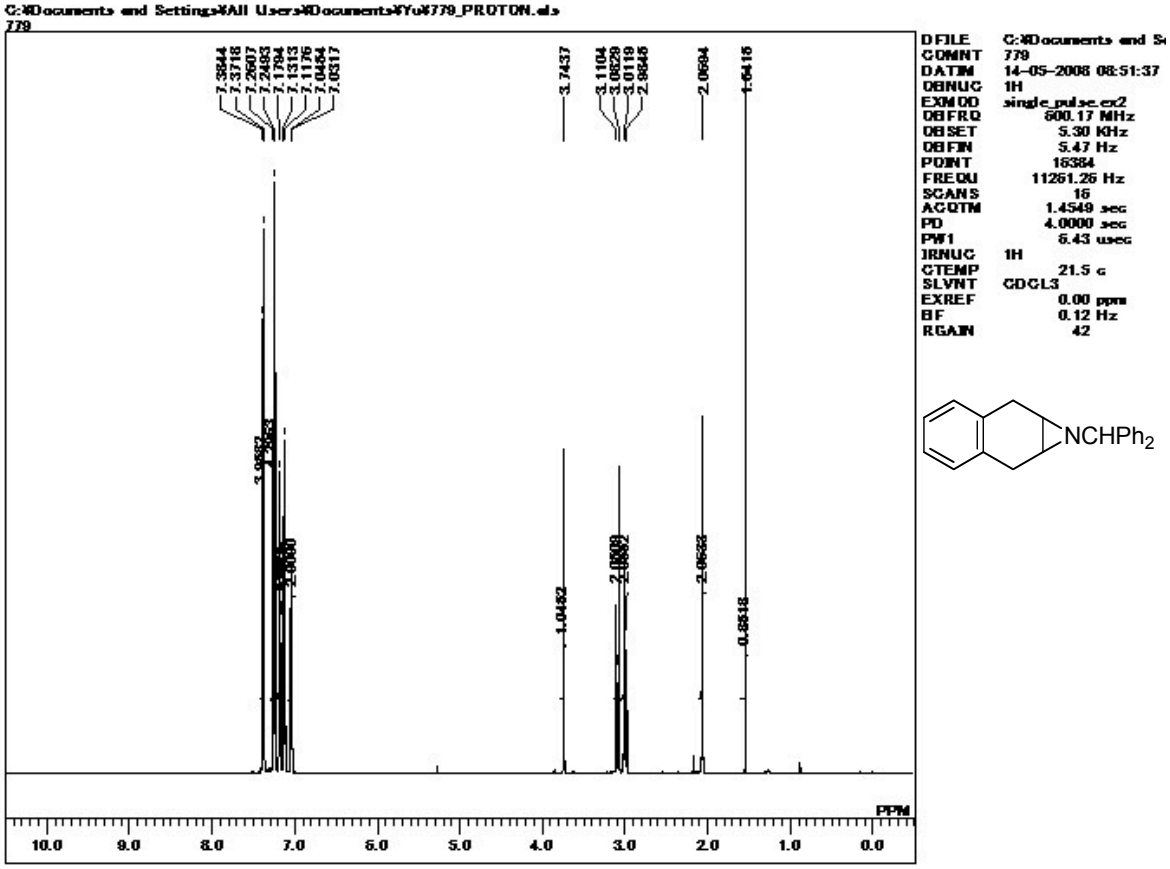
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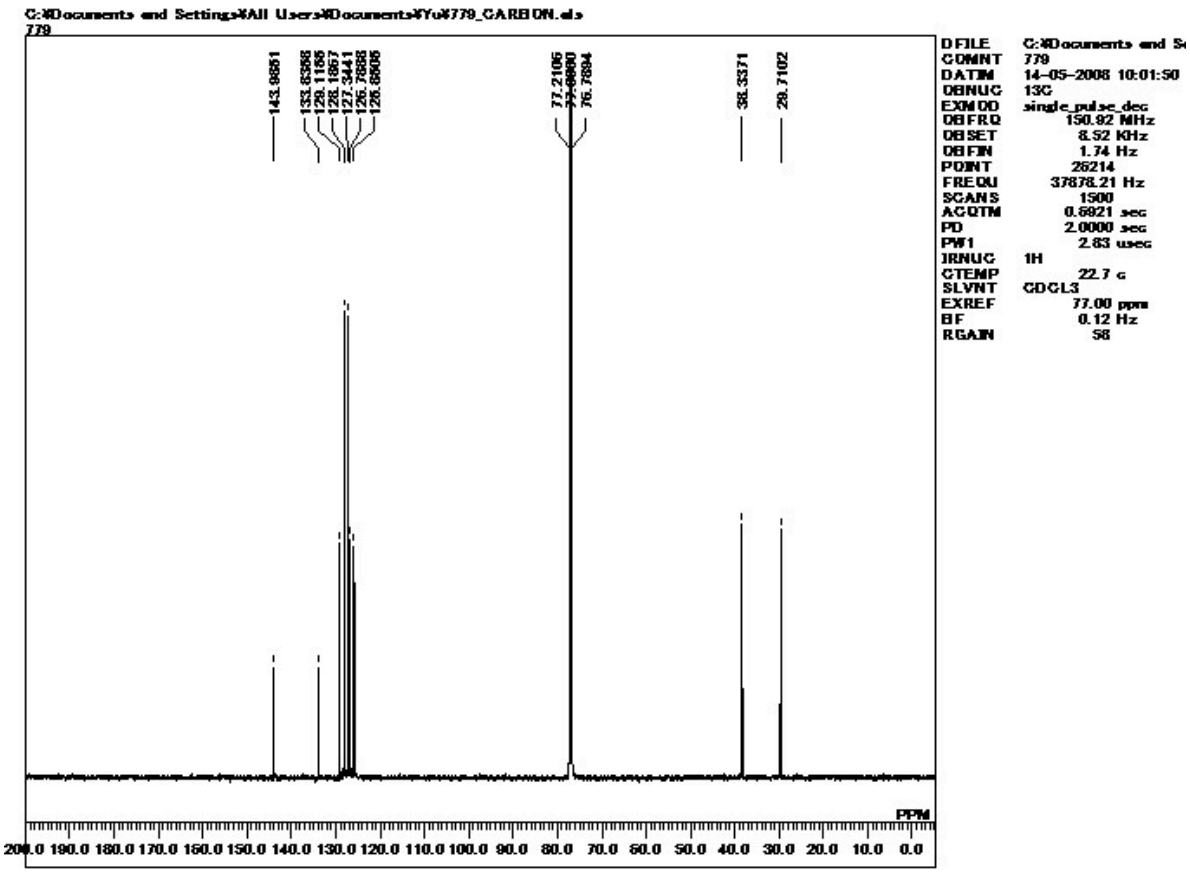
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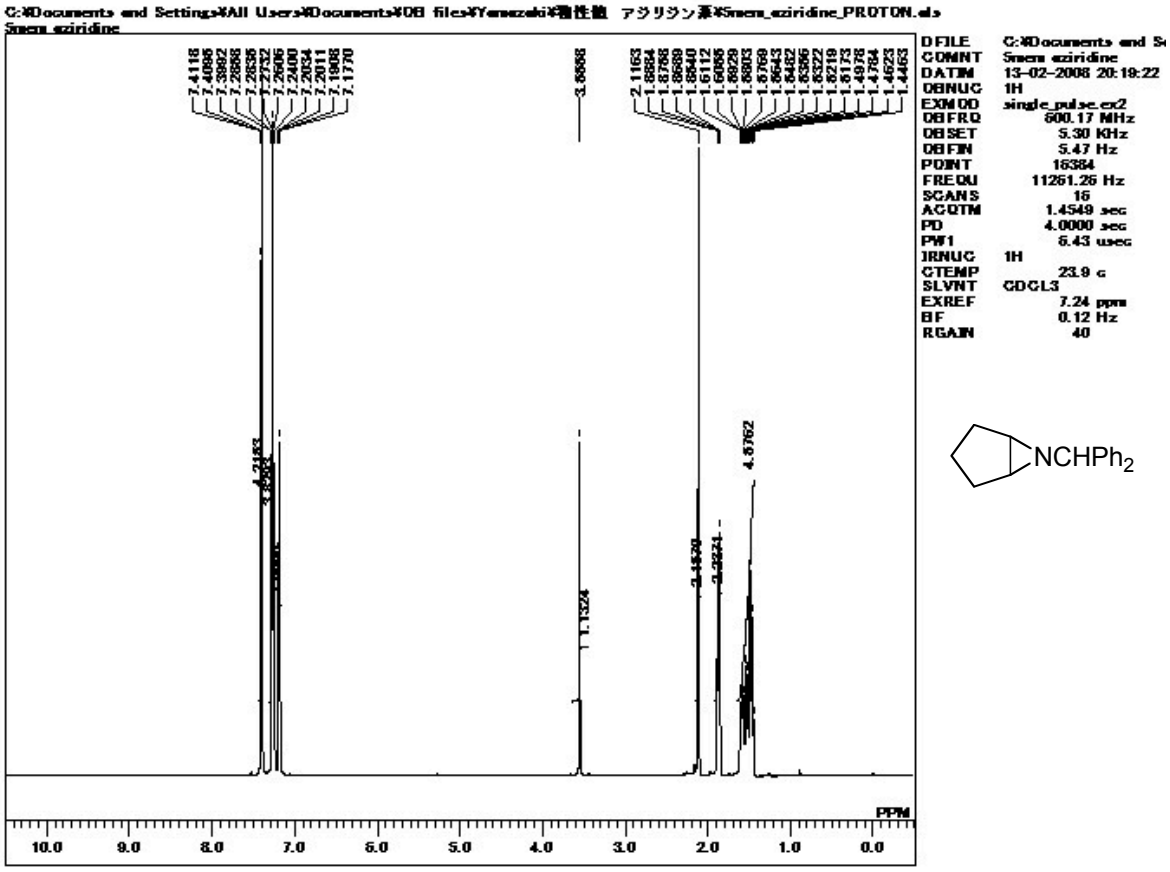
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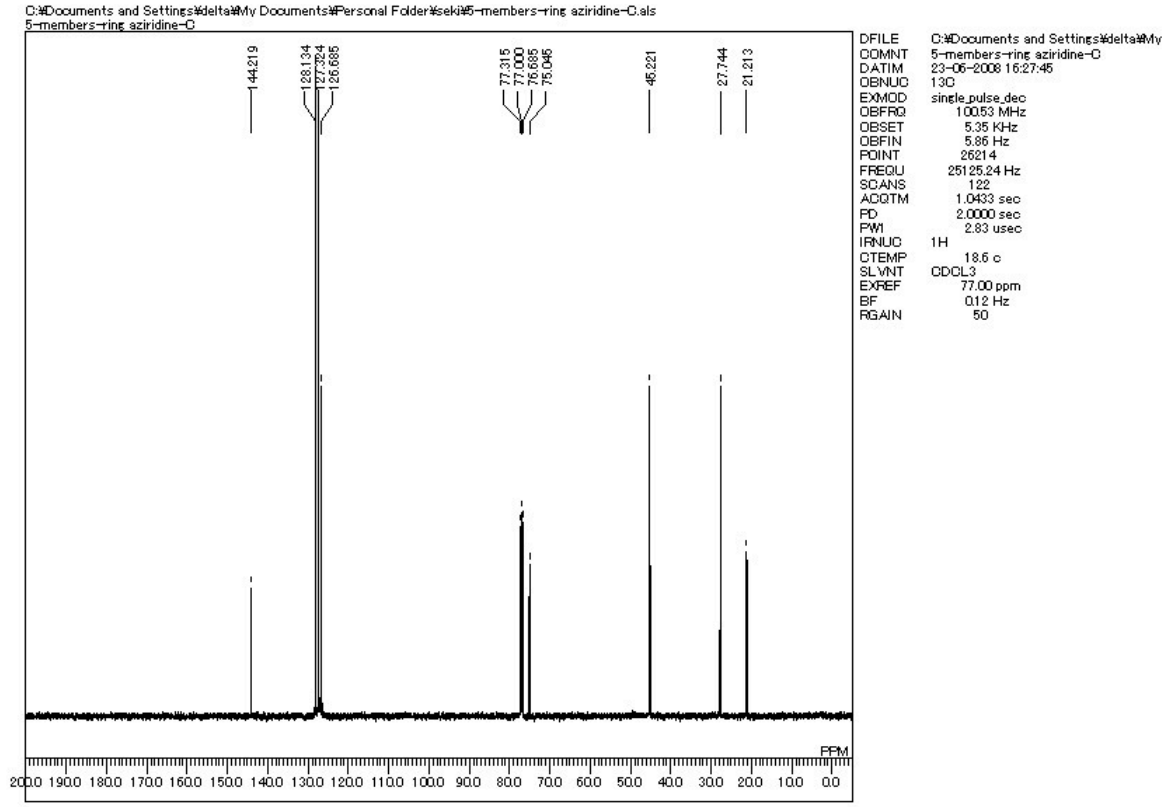
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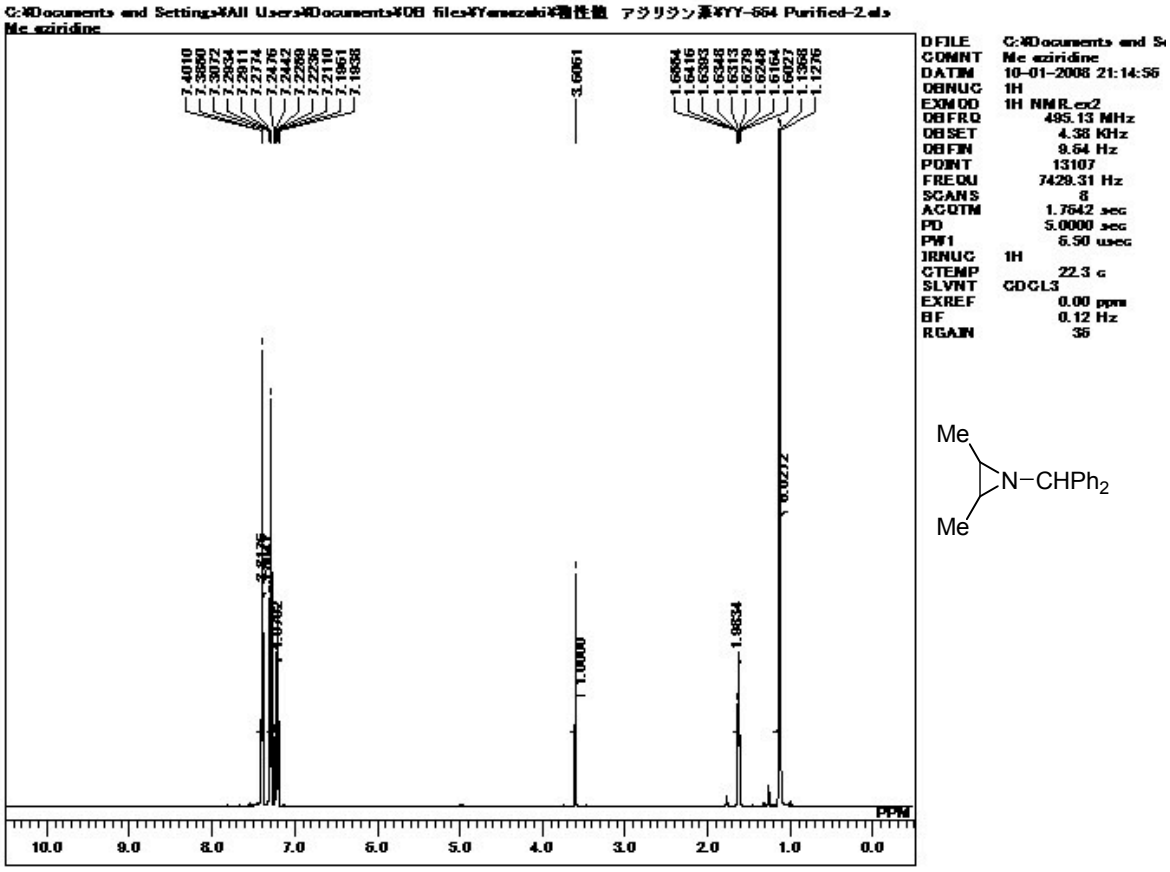
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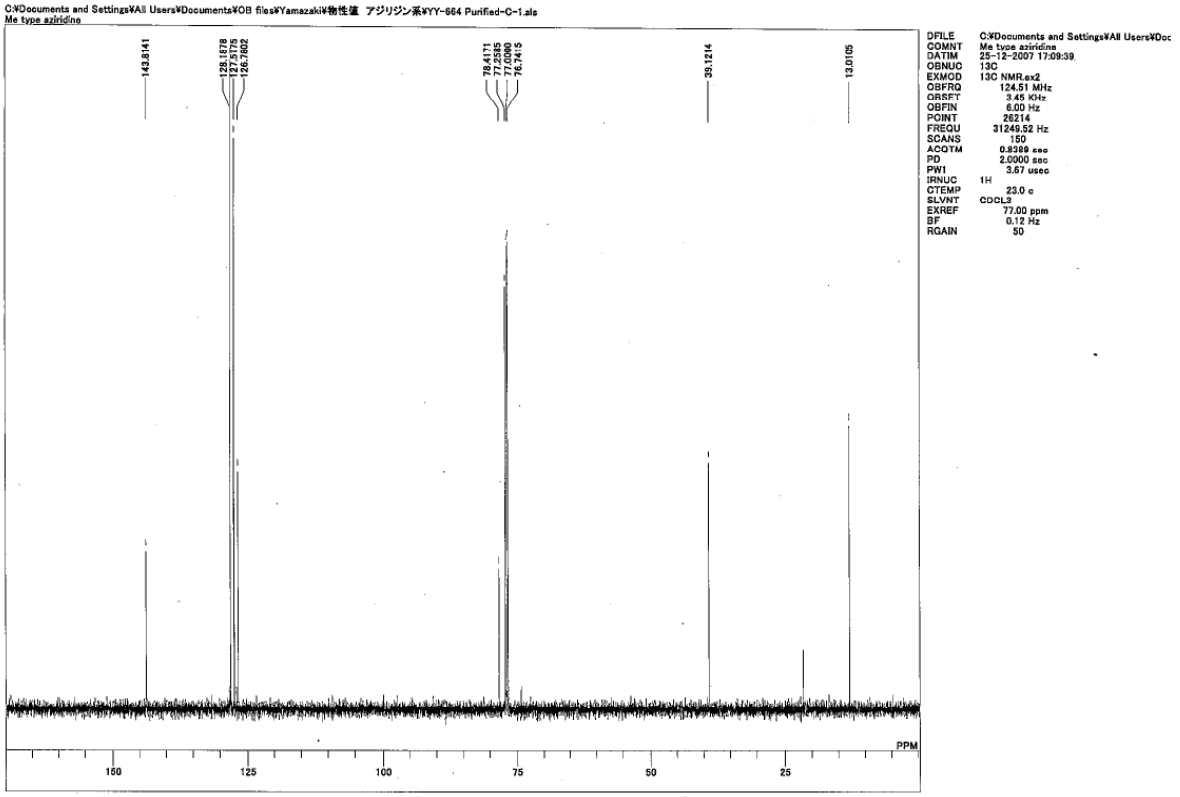
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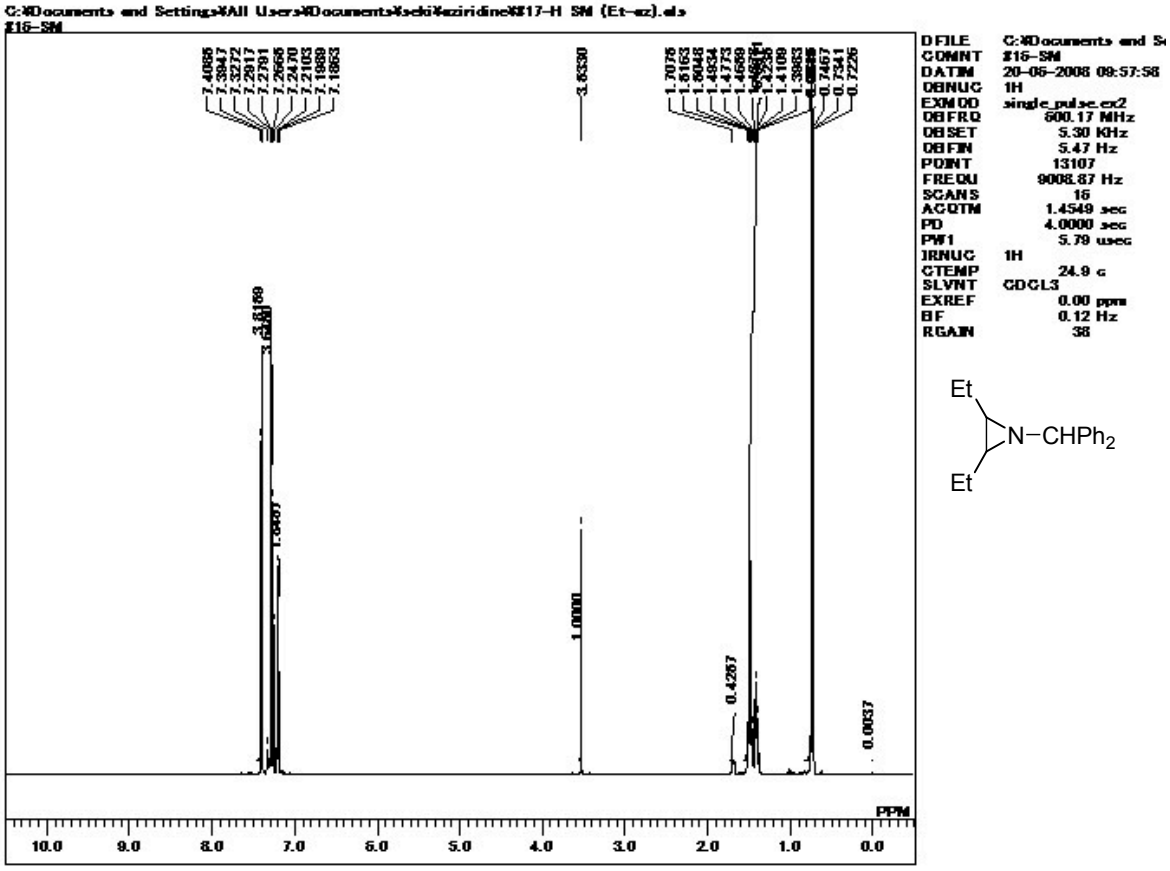
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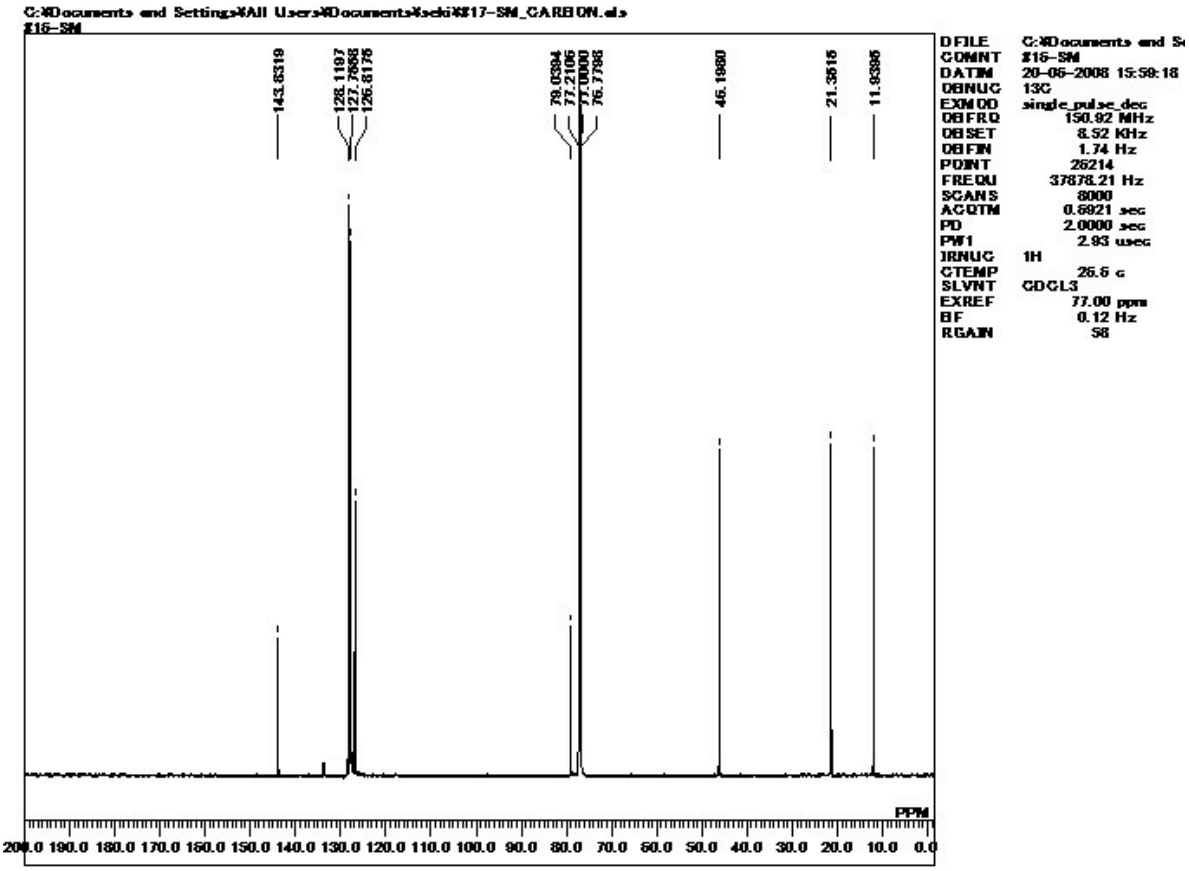
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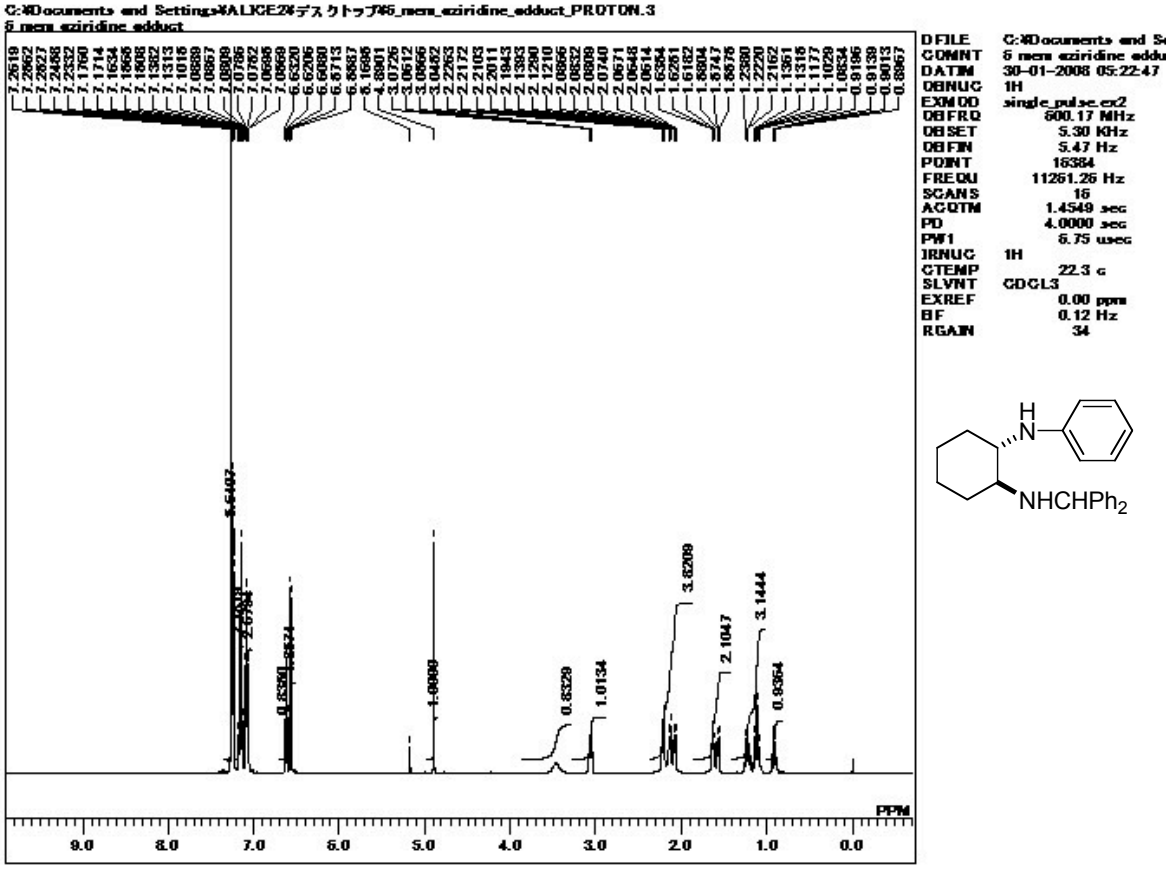
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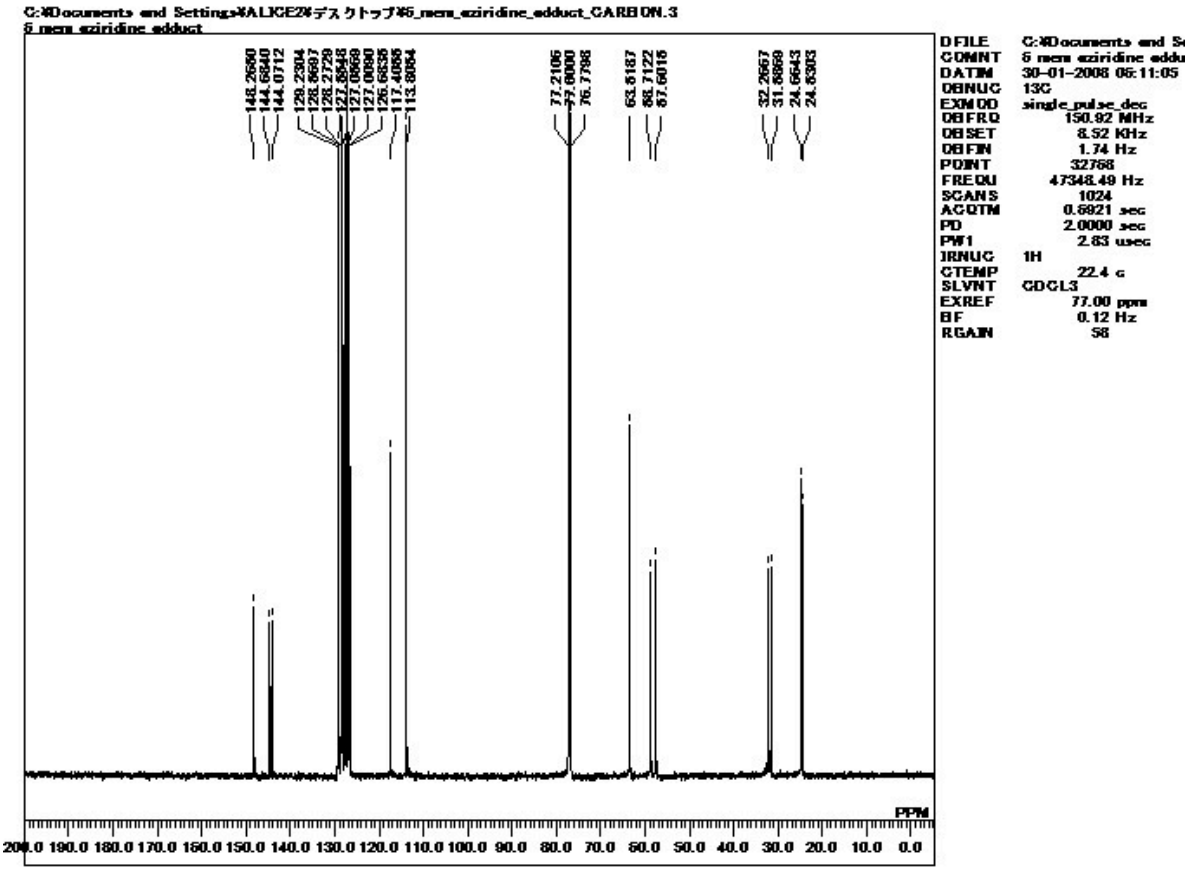
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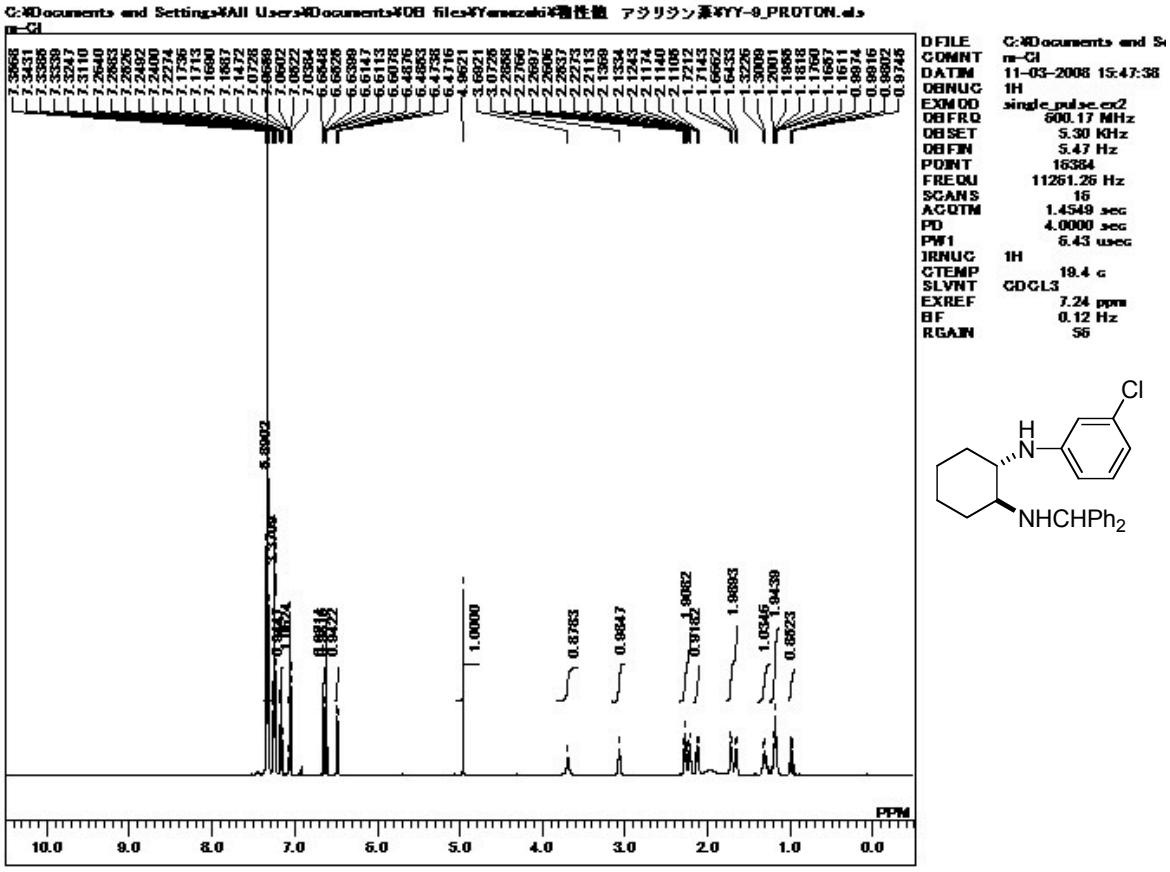
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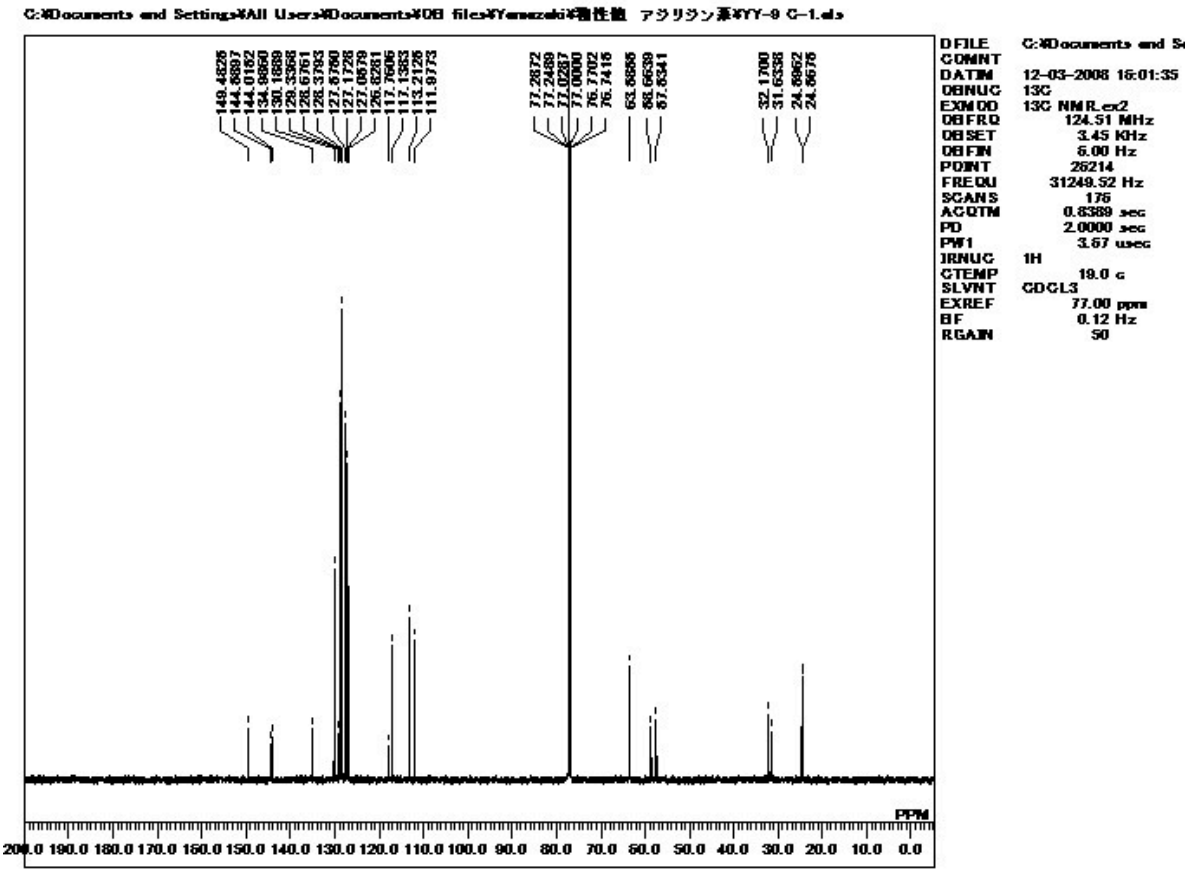
NHCHPh2
PPM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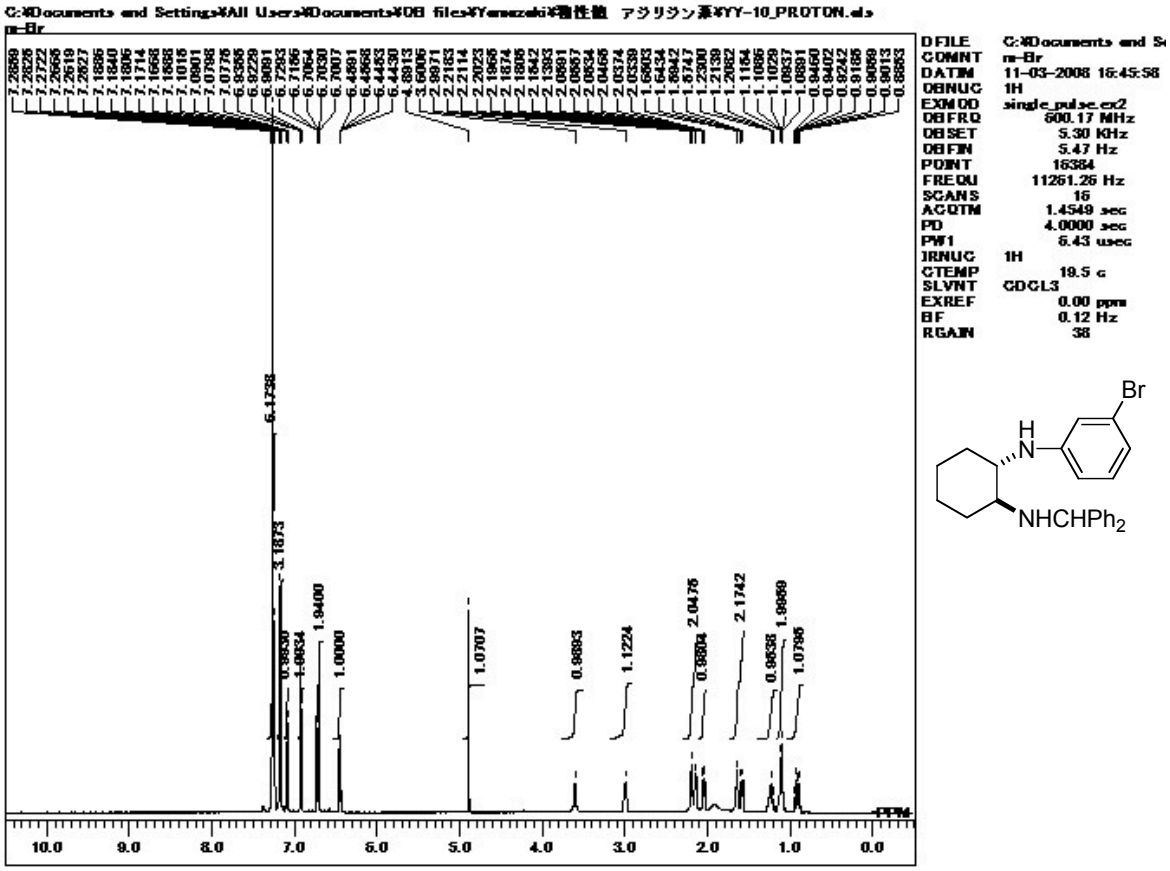
RGAIN 50
PPM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m-Br
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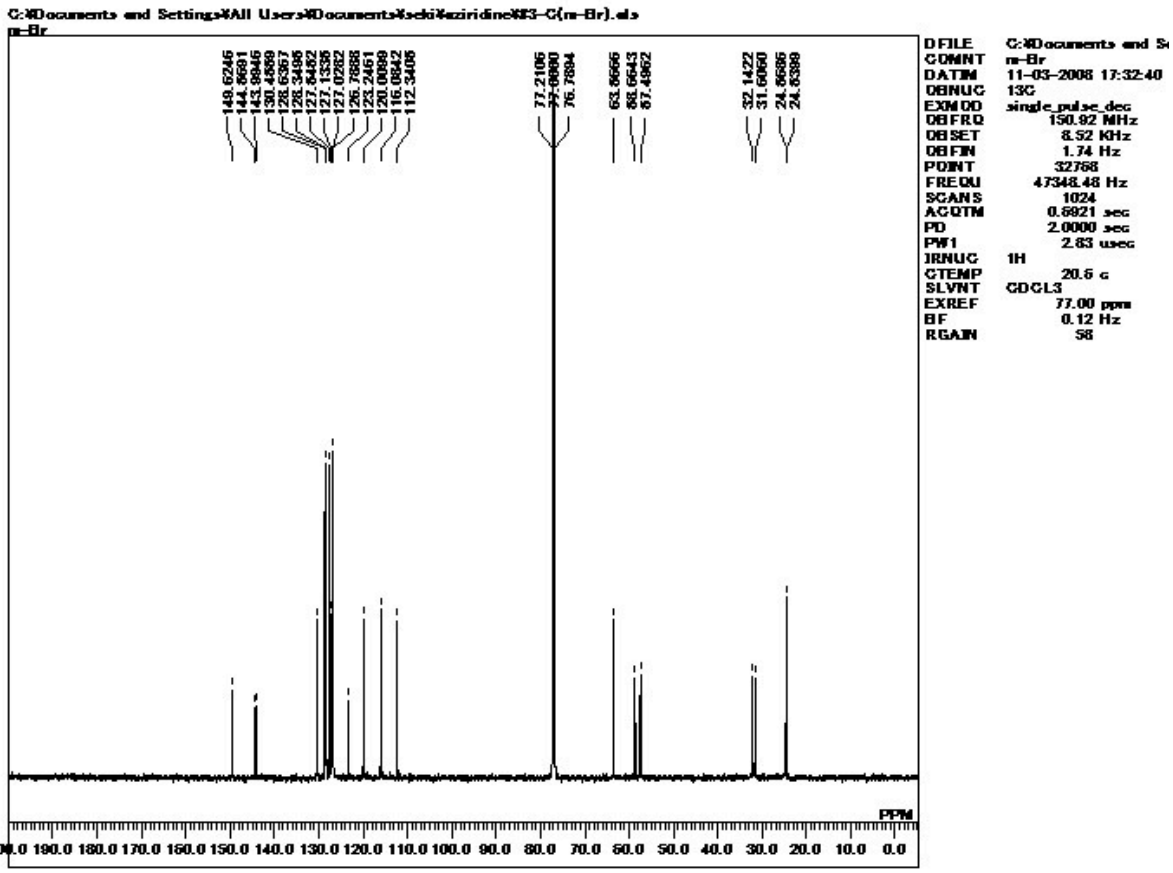
DATIM 11-03-2008 16:45:58
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 19.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 38
Br
H
N
NHCHPh2
PPM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m-Br
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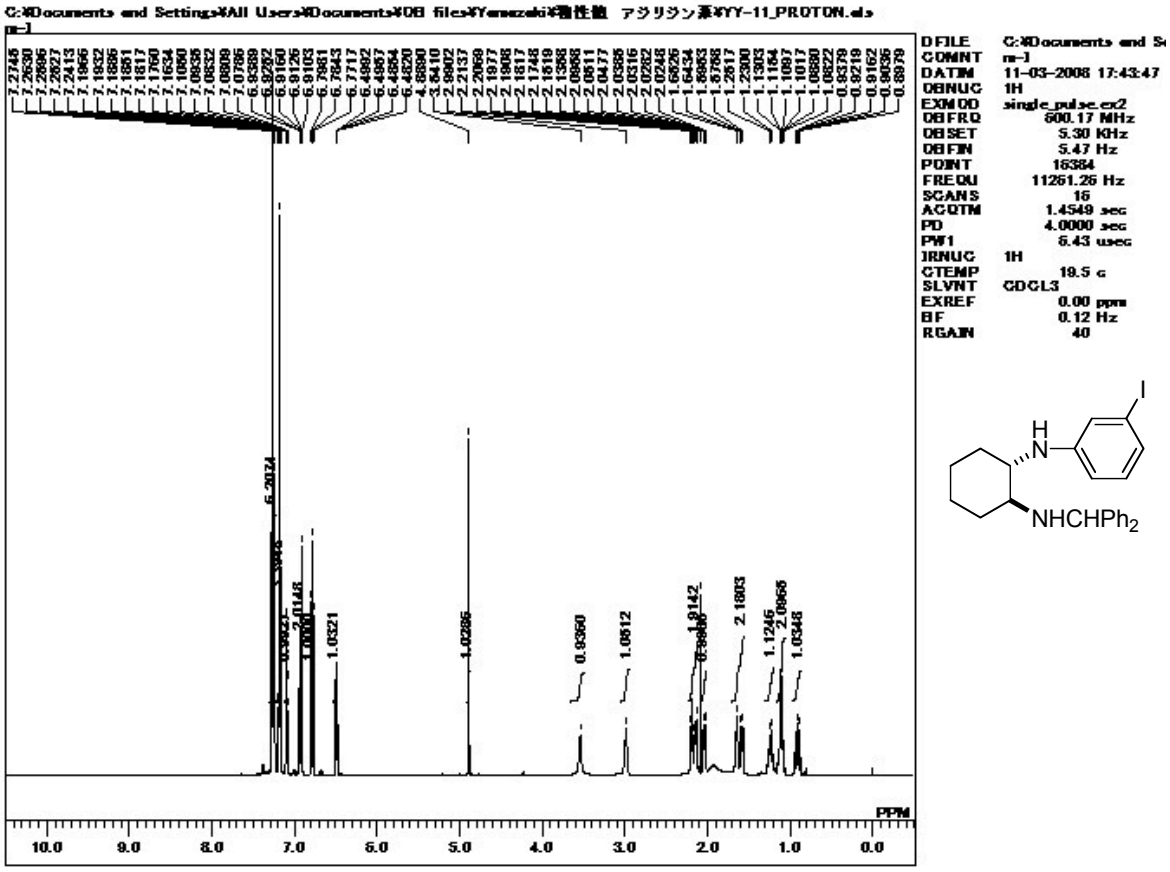
DATIM 11-03-2008 17:32:40
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32768
FREQU 47348.48 Hz
SCANS 1024
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 20.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 58
PPM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COMNT
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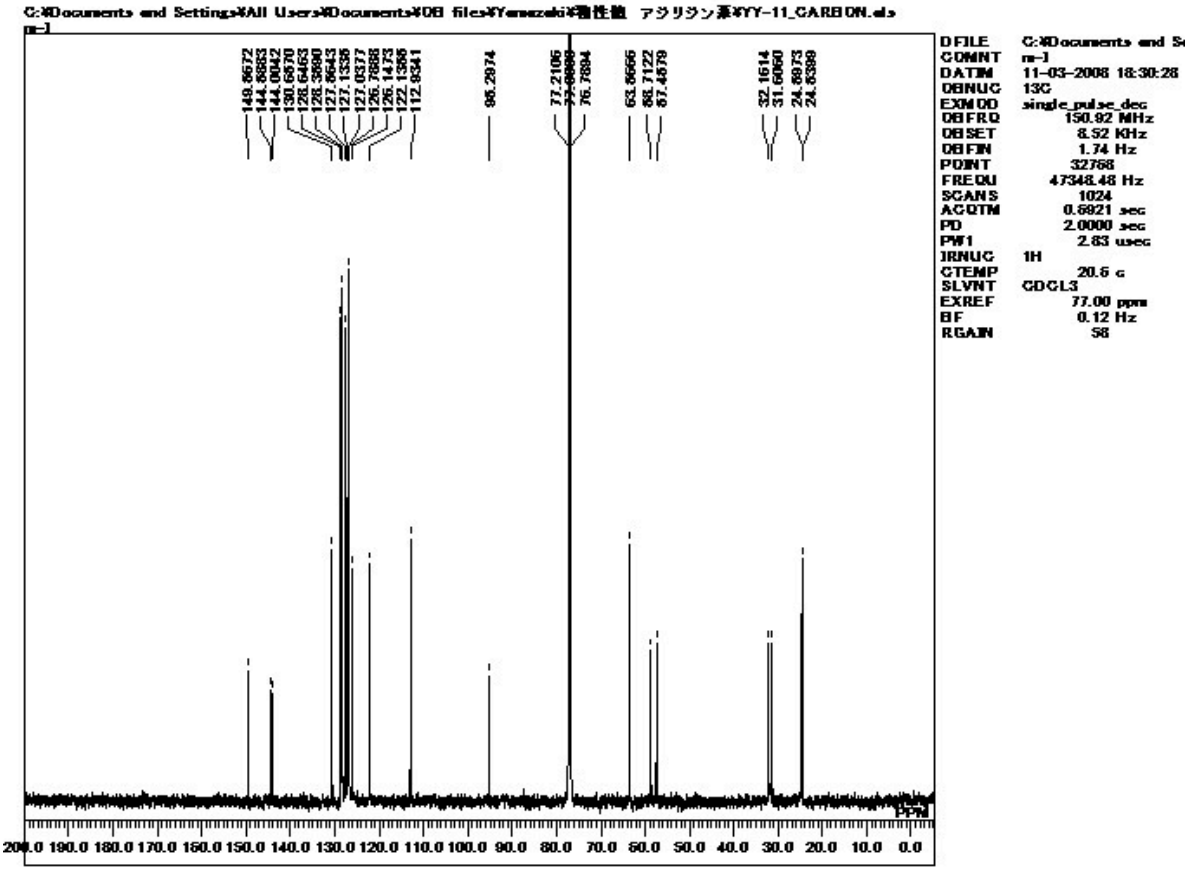
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 19.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 40
I
H
N
NHCHPh2
PPM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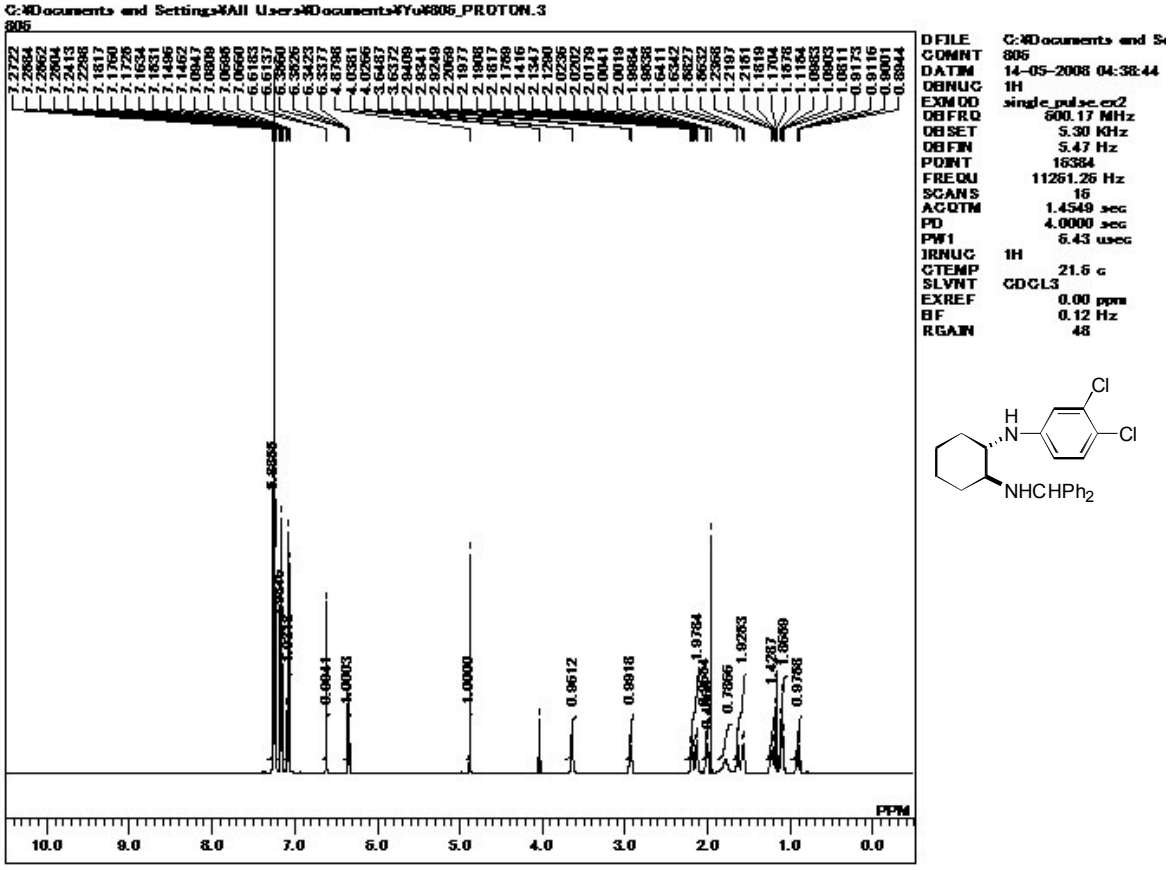
COMNT
DATIM 11-03-2008 18:30:28
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32768
FREQU 47348.48 Hz
SCANS 1024
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 58
PPM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DATIM 14-05-2008 04:38:44
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 21.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 48
Cl
H
N
Cl
NHCHPh2
PPM
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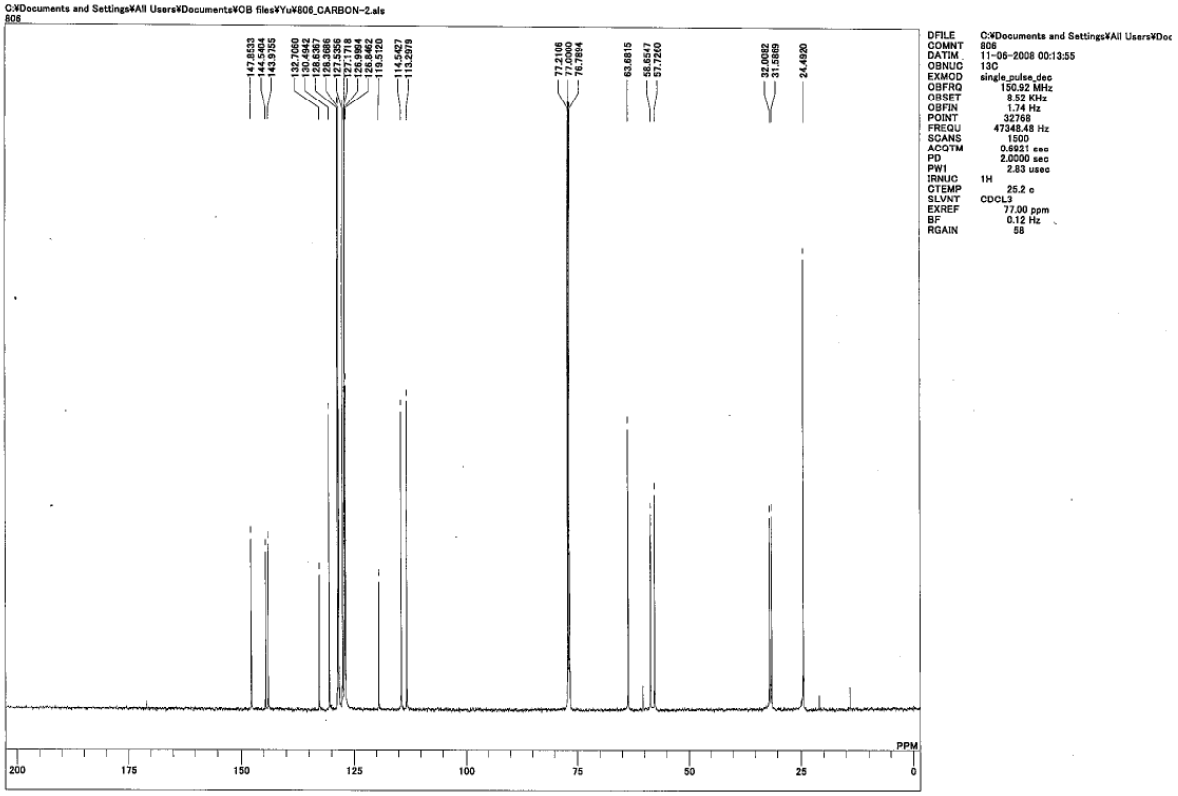
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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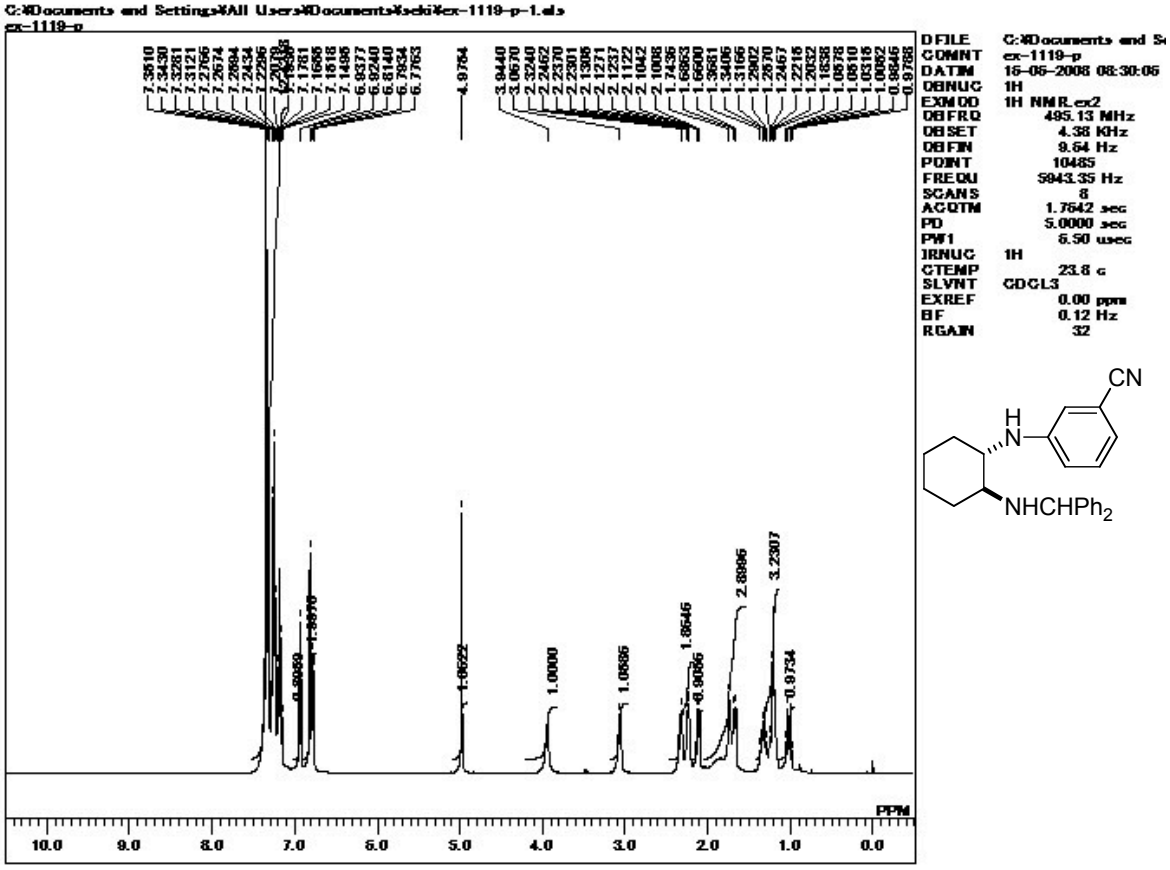
DATIM 11-06-2008 00:13:55
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32768
FREQU 47348.48 Hz
SCANS 1500
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 25.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 58
PPM
200
175
150
125
100
75
50
25
0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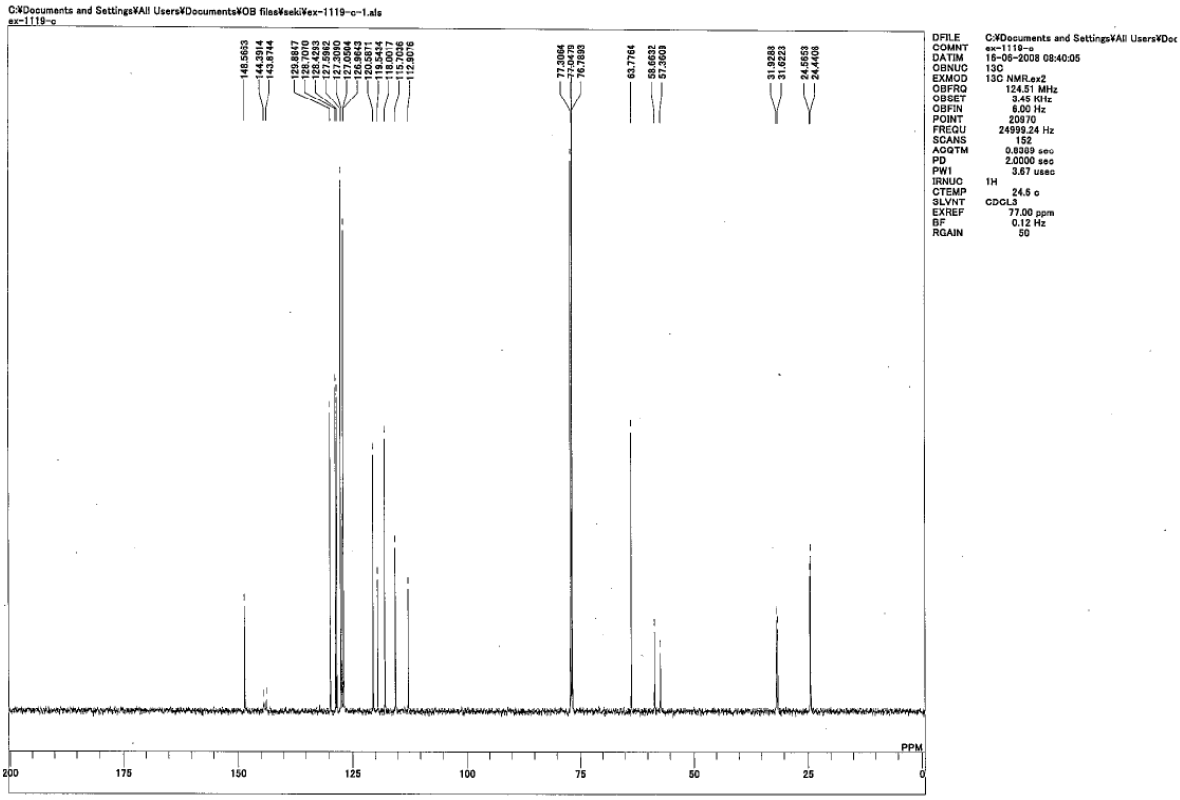
DFILE C:¥Documents and Se
COMNT ex-1119-p
DATIM 16-06-2008 08:30:05
OBNUC 1H
EXMOD 1H NMR.ex2
OBFRQ 495.13 MHz
OBSET 4.38 KHz
OBFIN 9.54 Hz
POINT 10485
FREQU 5943.35 Hz
SCANS 8
ACQTM 1.7642 sec
PD 5.0000 sec
PW1 6.50 usec
IRNUC 1H
CTEMP 23.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 32
CN
H
N
NHCHPh2
PPM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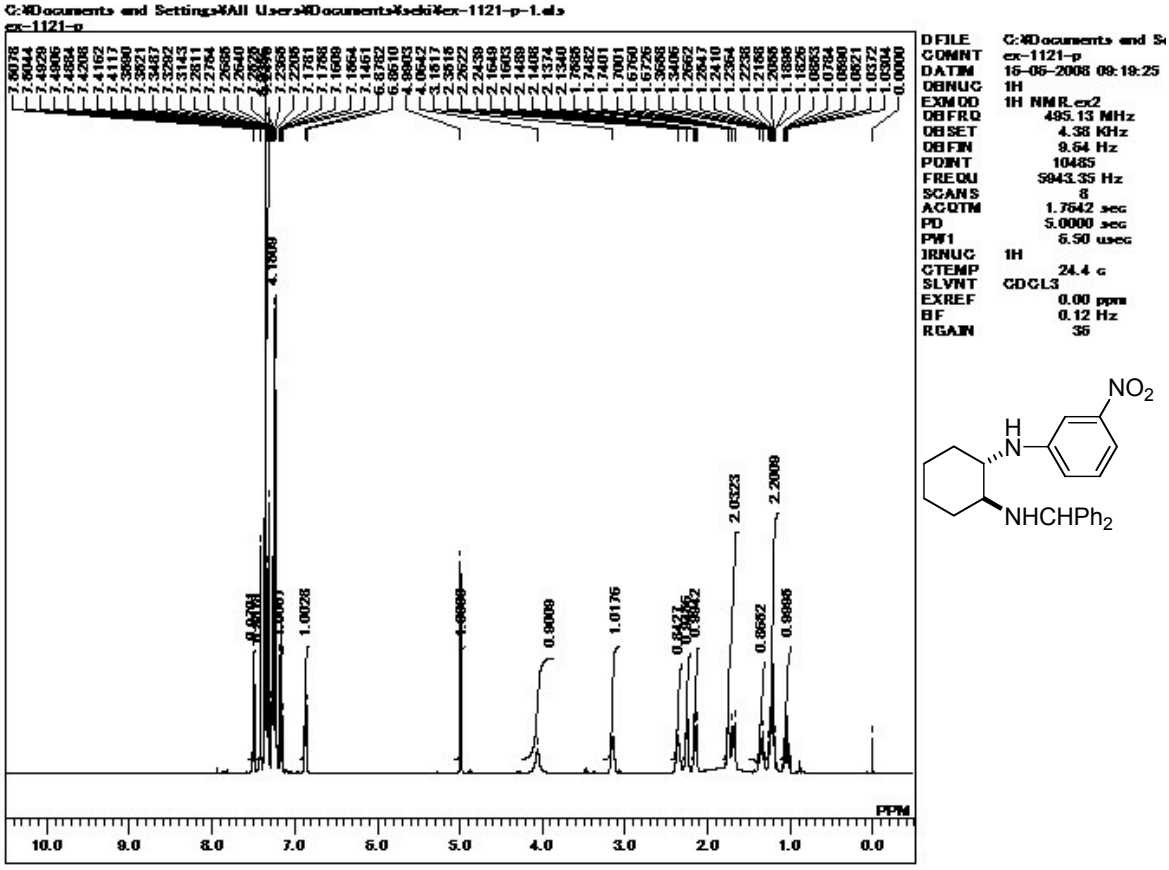
ex-1119-c
DFILE C:¥Documents and Settings¥All Users¥Doc
COMNT ex-1119-c
DATIM 16-06-2008 08:40:05
OBNUC 13C
EXMOD 13C NMR.ex2
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 20970
FREQU 24999.24 Hz
SCANS 152
ACQTM 0.8389 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 24.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
PPM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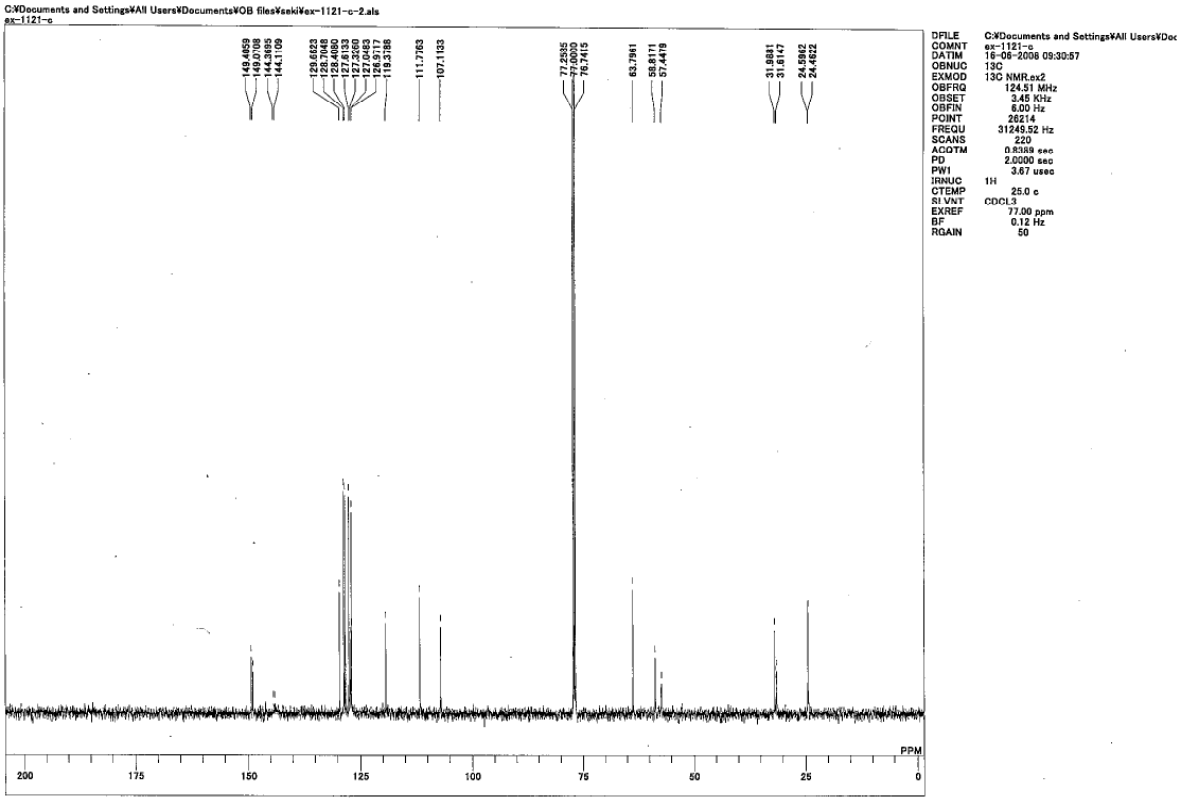
DATIM 16-06-2008 09:19:25
OBNUC 1H
EXMOD 1H NMR.ex2
OBFRQ 495.13 MHz
OBSET 4.38 KHz
OBFIN 9.54 Hz
POINT 10485
FREQU 5943.35 Hz
SCANS 8
ACQTM 1.7642 sec
PD 5.0000 sec
PW1 6.50 usec
IRNUC 1H
CTEMP 24.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 35
NO2
H
N
NHCHPh2
PPM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ex-1121-c
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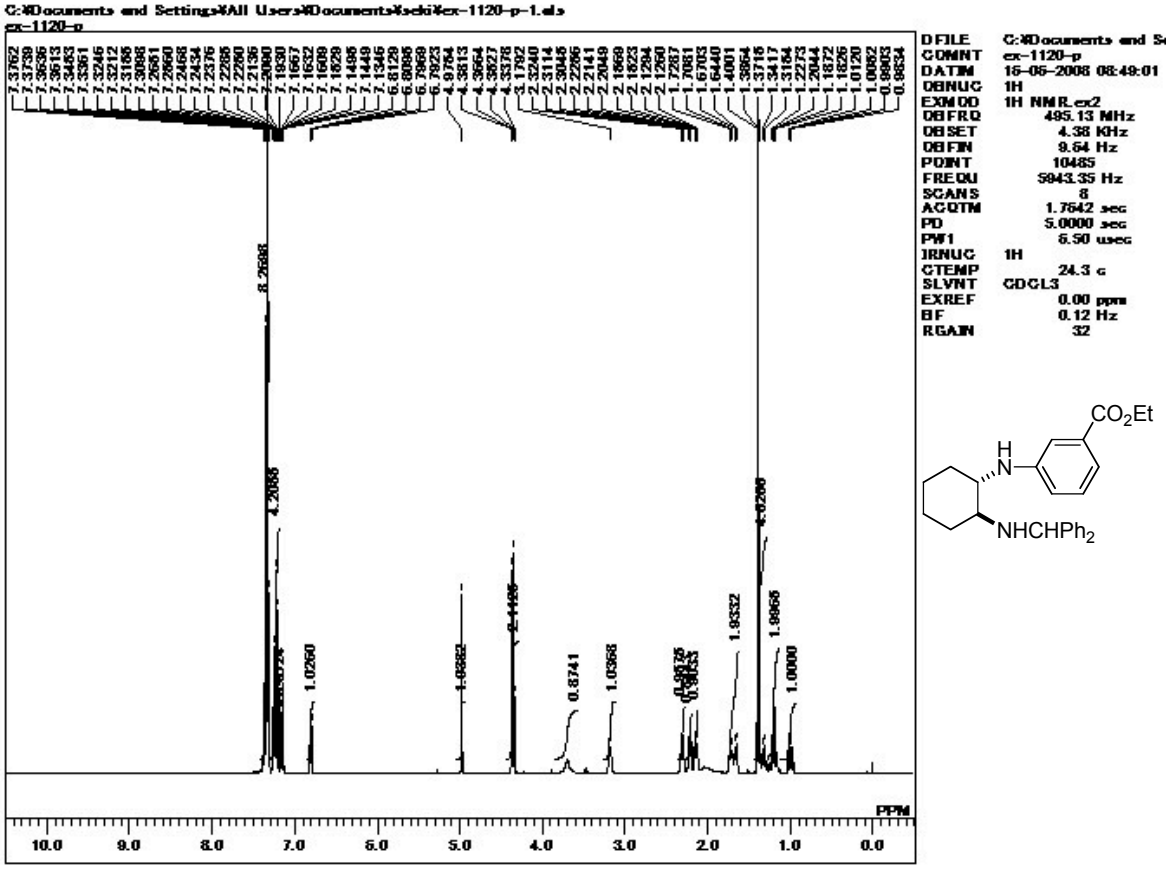
DATIM 16-06-2008 09:30:57
OBNUC 13C
EXMOD 13C NMR.ex2
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 26214
FREQU 31249.52 Hz
SCANS 220
ACQTM 0.8389 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 25.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
PPM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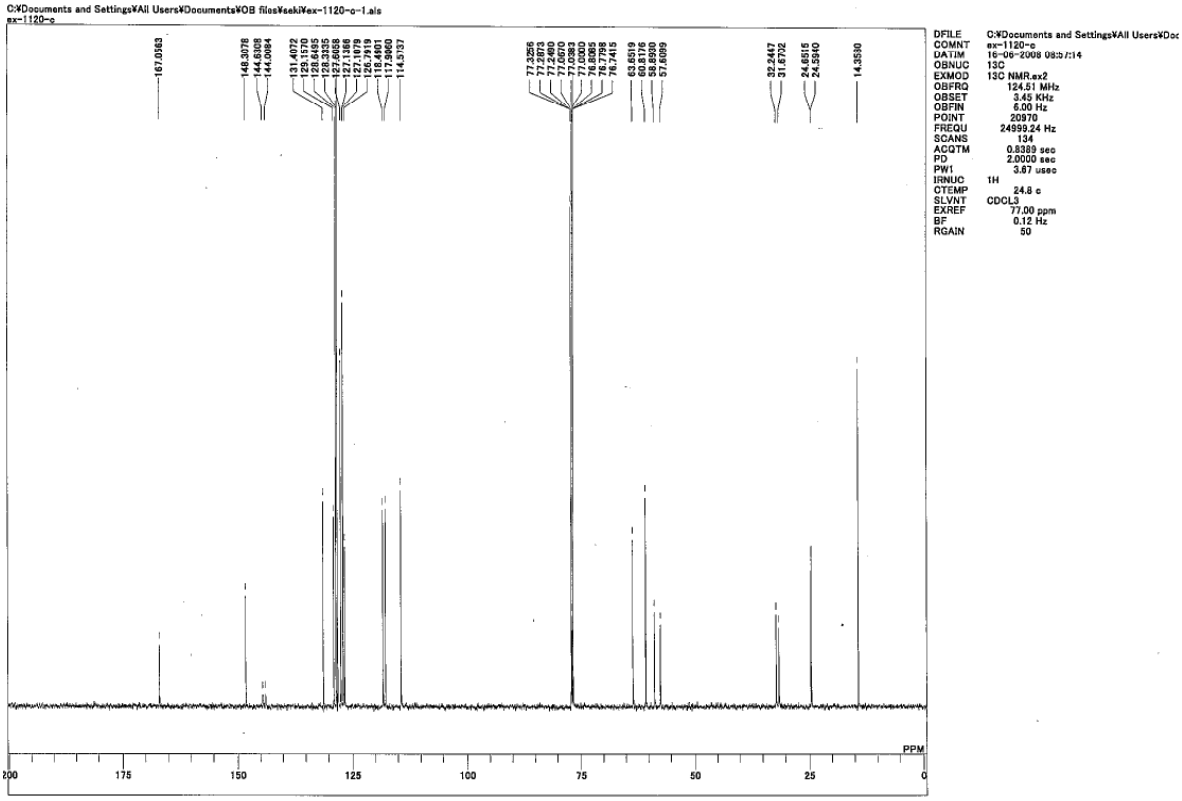
ex-1120-p
DFILE C:¥Documents and Se
COMNT ex-1120-p
DATIM 16-06-2008 08:49:01
OBNUC 1H
EXMOD 1H NMR.ex2
OBFRQ 495.13 MHz
OBSET 4.38 KHz
OBFIN 9.54 Hz
POINT 10485
FREQU 5943.35 Hz
SCANS 8
ACQTM 1.7642 sec
PD 5.0000 sec
PW1 6.50 usec
IRNUC 1H
CTEMP 24.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 32
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
CO2Et
H
N
NHCHPh2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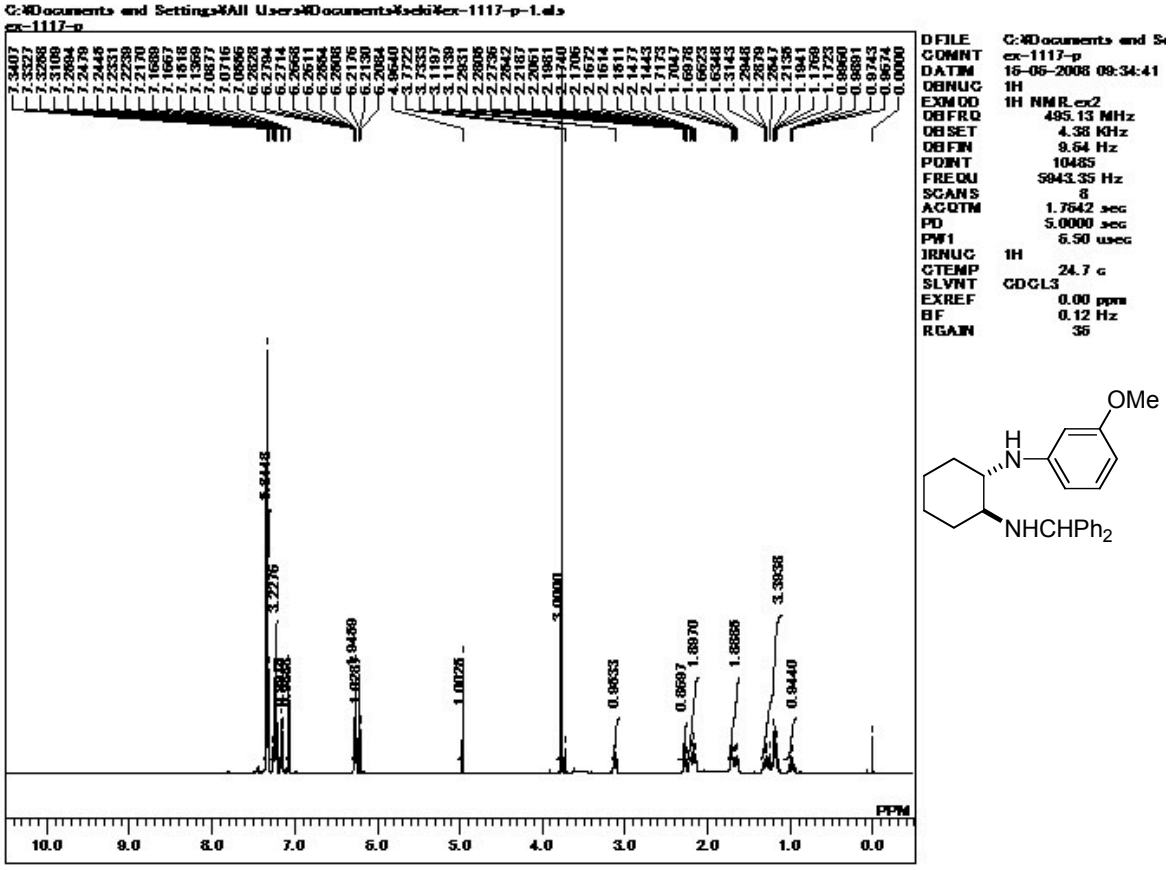
DATIM 16-06-2008 08:57:14
OBNUC 13C
EXMOD 13C NMR.ex2
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 20970
FREQU 24999.24 Hz
SCANS 134
ACQTM 0.8389 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 24.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
PPM
200
175
150
125
100
75
50
25
0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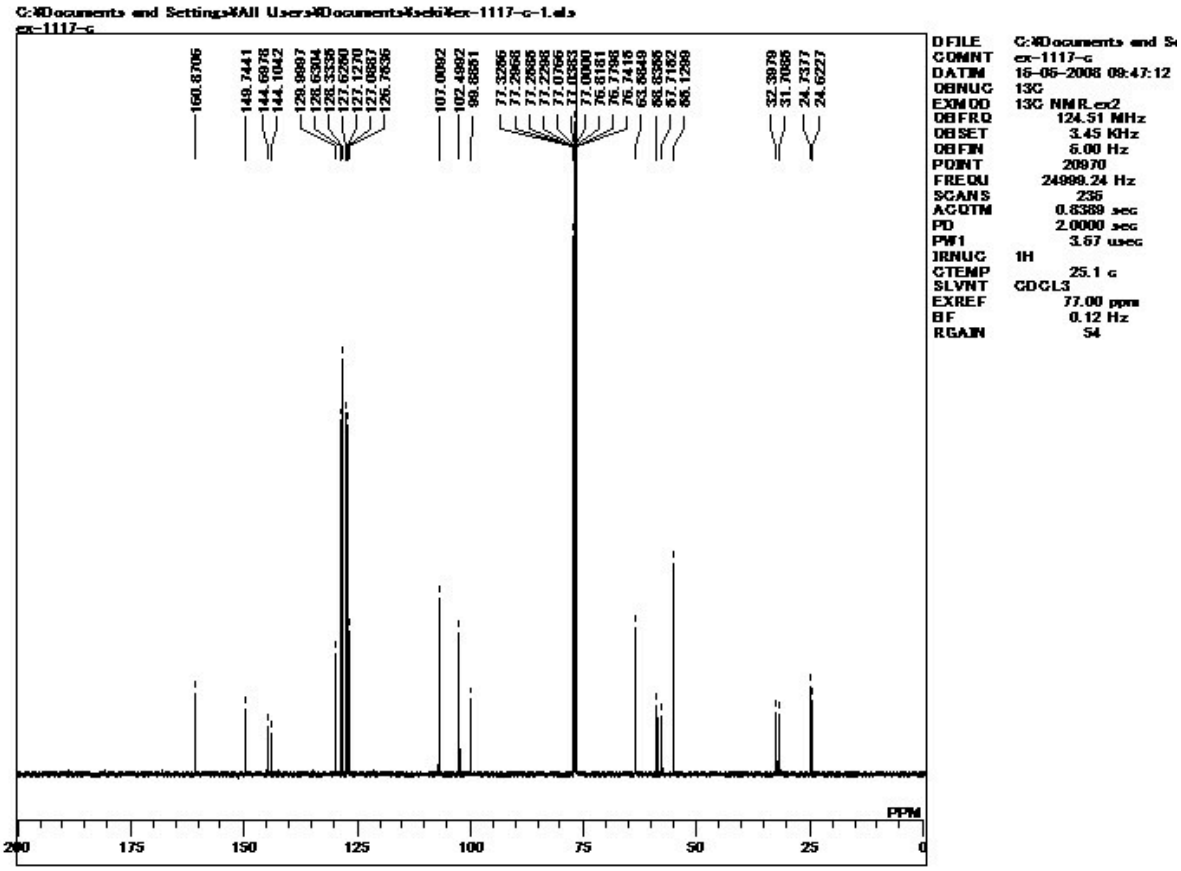
ex-1117-p
DFILE C:¥Documents and S
COMNT ex-1117-p
DATIM 16-05-2008 09:34:41
OBNUC 1H
EXMOD 1H NMR.ex2
OBFRQ 495.13 MHz
OBSET 4.38 KHz
OBFIN 9.54 Hz
POINT 10485
FREQU 5943.35 Hz
SCANS 8
ACQTM 1.7642 sec
PD 5.0000 sec
PW1 6.50 usec
IRNUC 1H
CTEMP 24.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 35
OMe
H
N
NHCHPh2
PPM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ex-1117-c
DFILE C:¥Documents and S
COMNT ex-1117-c
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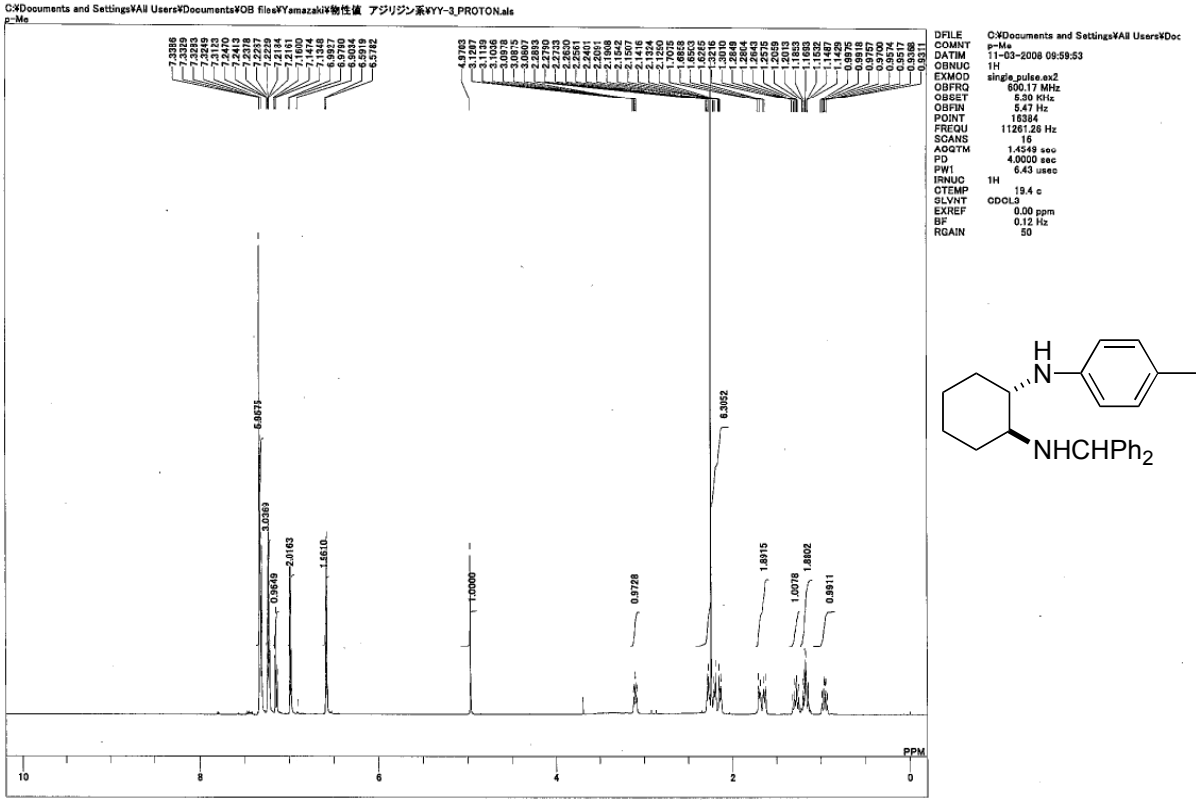
OBNUC 13C
EXMOD 13C NMR.ex2
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 20970
FREQU 24999.24 Hz
SCANS 235
ACQTM 0.8389 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 25.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 54
PPM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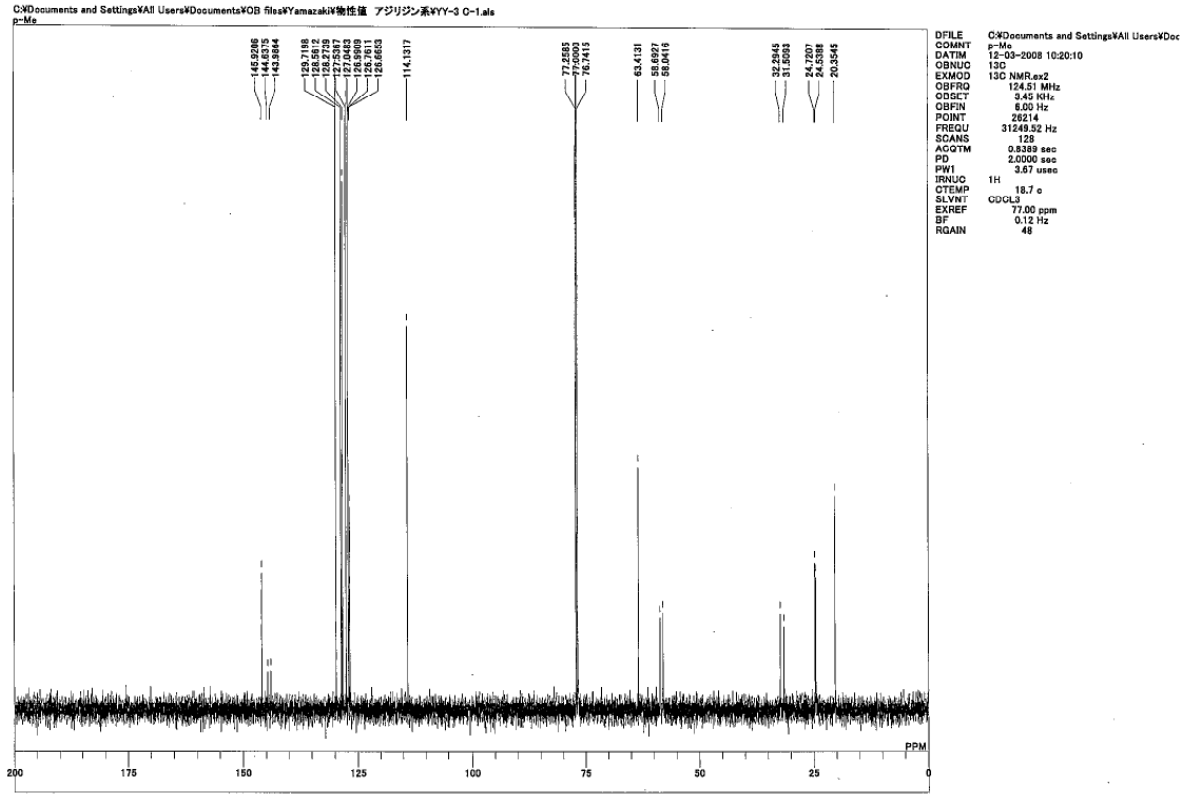
DATIM 11-03-2008 09:59:53
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 19.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 50
6.9075
3.0369
0.9549
2.0163
1.5610
1.0000
0.5728
6.3052
1.8915
1.0078
1.8802
0.9911
PPM
H
N
NHCHPh2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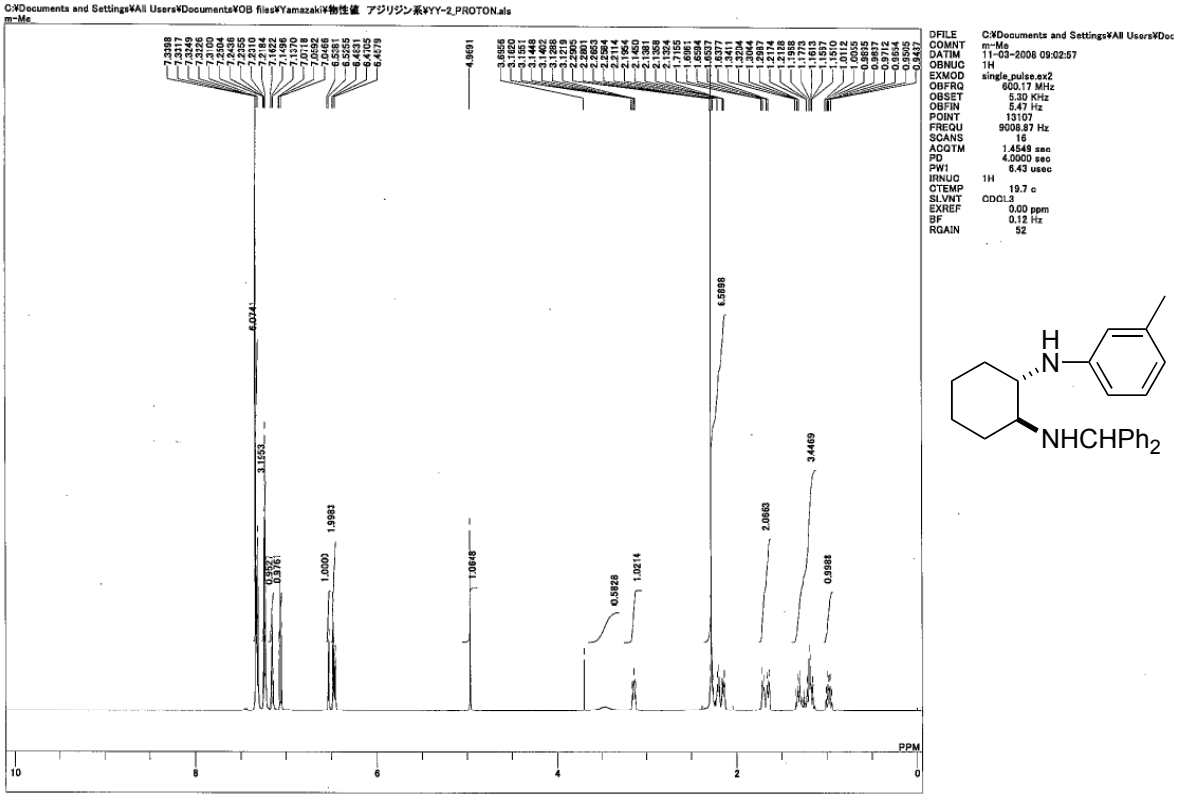
DATIM 12-03-2008 10:20:10
OBNUC 13C
EXMOD 13C NMR.ex2
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 29214
FREQU 31249.52 Hz
SCANS 128
ACQTM 0.9389 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 18.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 48
PPM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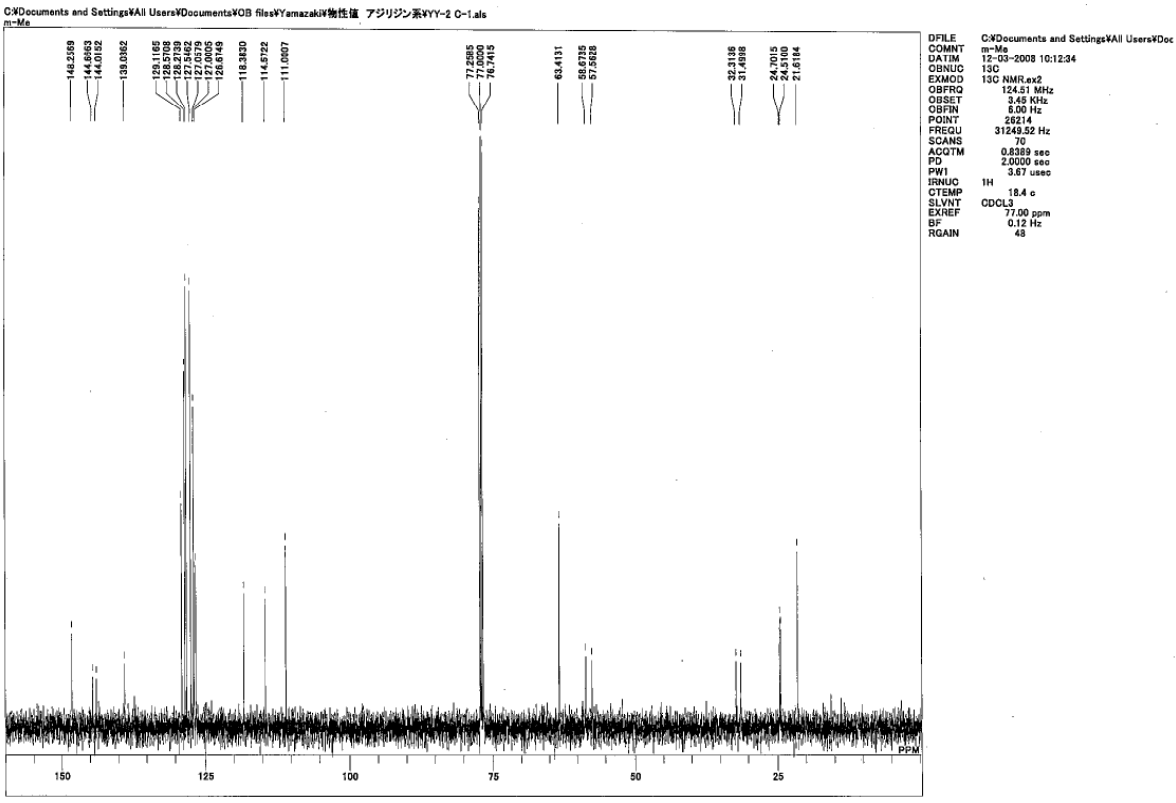
COMNT m-Me
DATIM 11-03-2008 09:02:57
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 13107
FREQU 9008.87 Hz
SCANS 16
ACQTM 1.4548 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 52
6.0741
3.1653
0.9921
0.9761
1.0000
1.9983
1.0646
0.5828
1.0214
6.5898
2.0663
3.4469
0.9988
PPM
10
8
6
4
2
0
H
N
NHCHPh2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COMNT m-Me
DATIM 12-03-2008 10:12:34
OBNUC 13C
EXMOD 13C NMR.ex2
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 26214
FREQU 31249.52 Hz
SCANS 70
ACQTM 0.8389 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 18.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 48
148.2389
144.6563
144.0152
139.0362
129.1165
128.5708
128.2393
127.5462
127.0579
127.0005
126.6748
118.3830
114.5722
111.0607
77.2585
77.0000
76.7415
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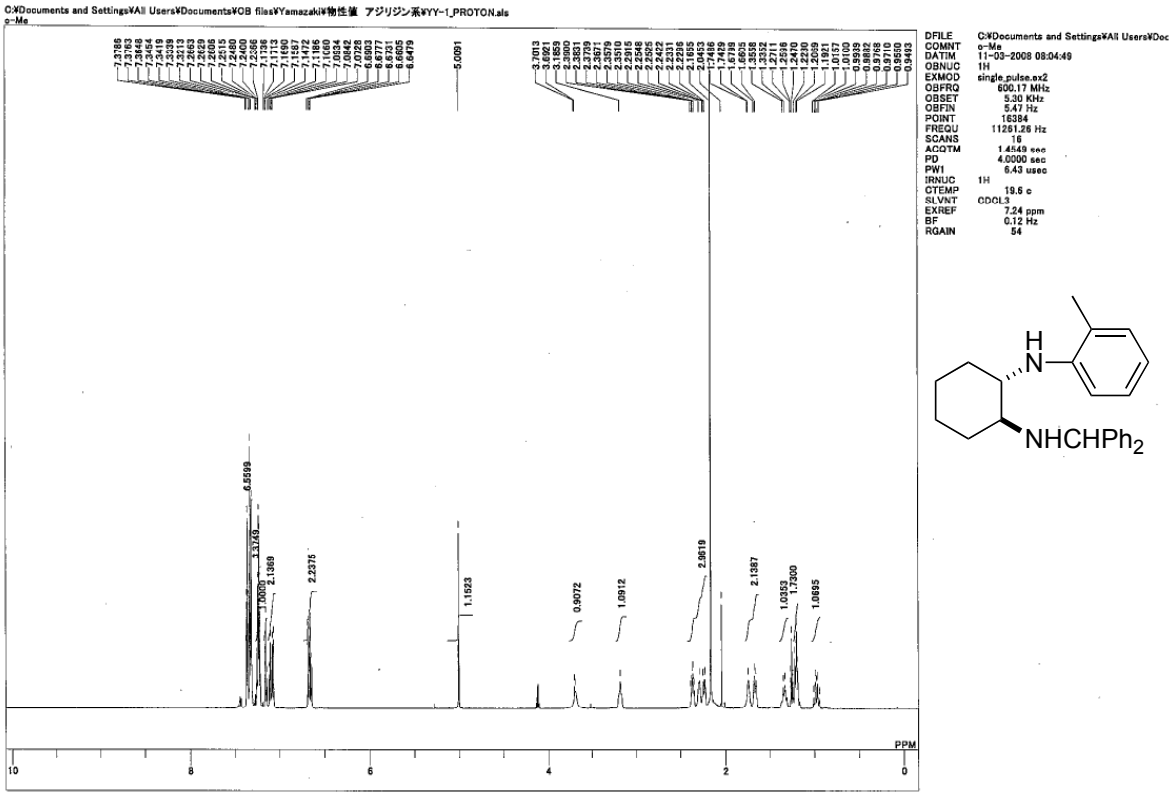
21.6184
PPM
150
125
100
75
50
25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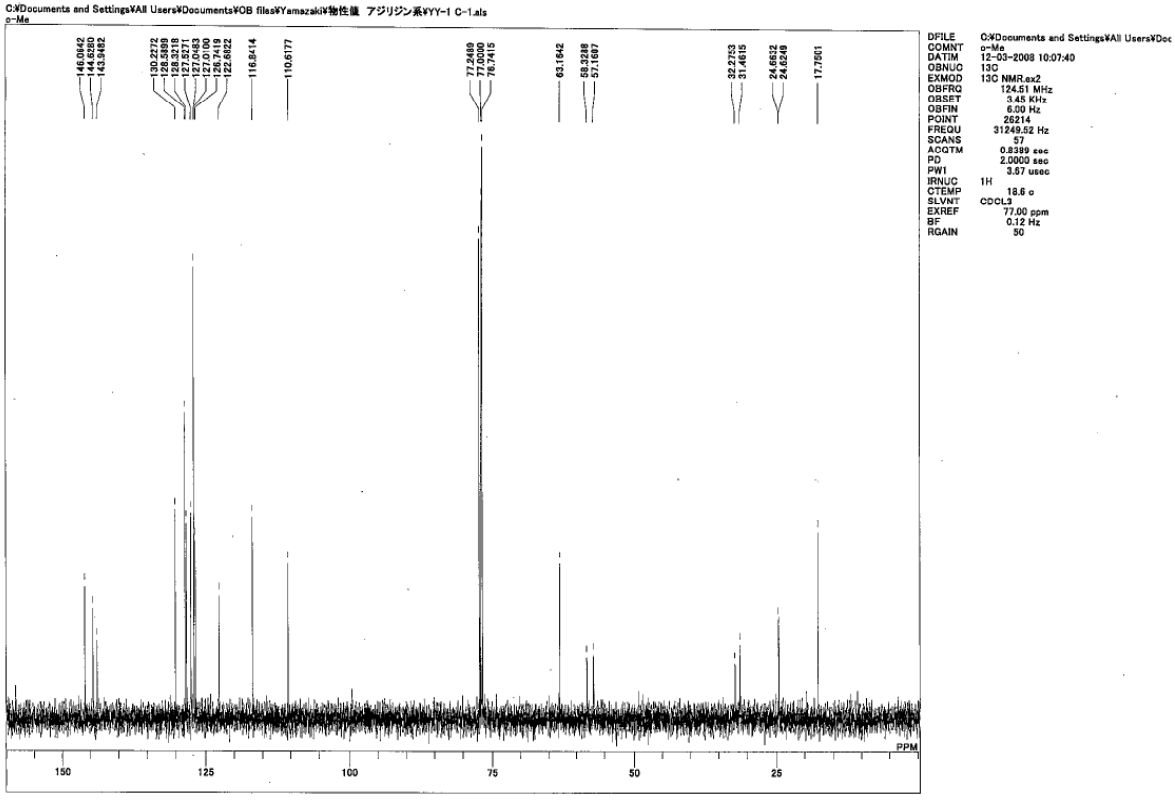
o-Me
DFILE C:¥Documents and Settings¥All Users¥Doc
COMNT o-Me
DATIM 11-03-2008 08:04:49
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 19.6 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 54
NHCHPh2
PPM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o-Me
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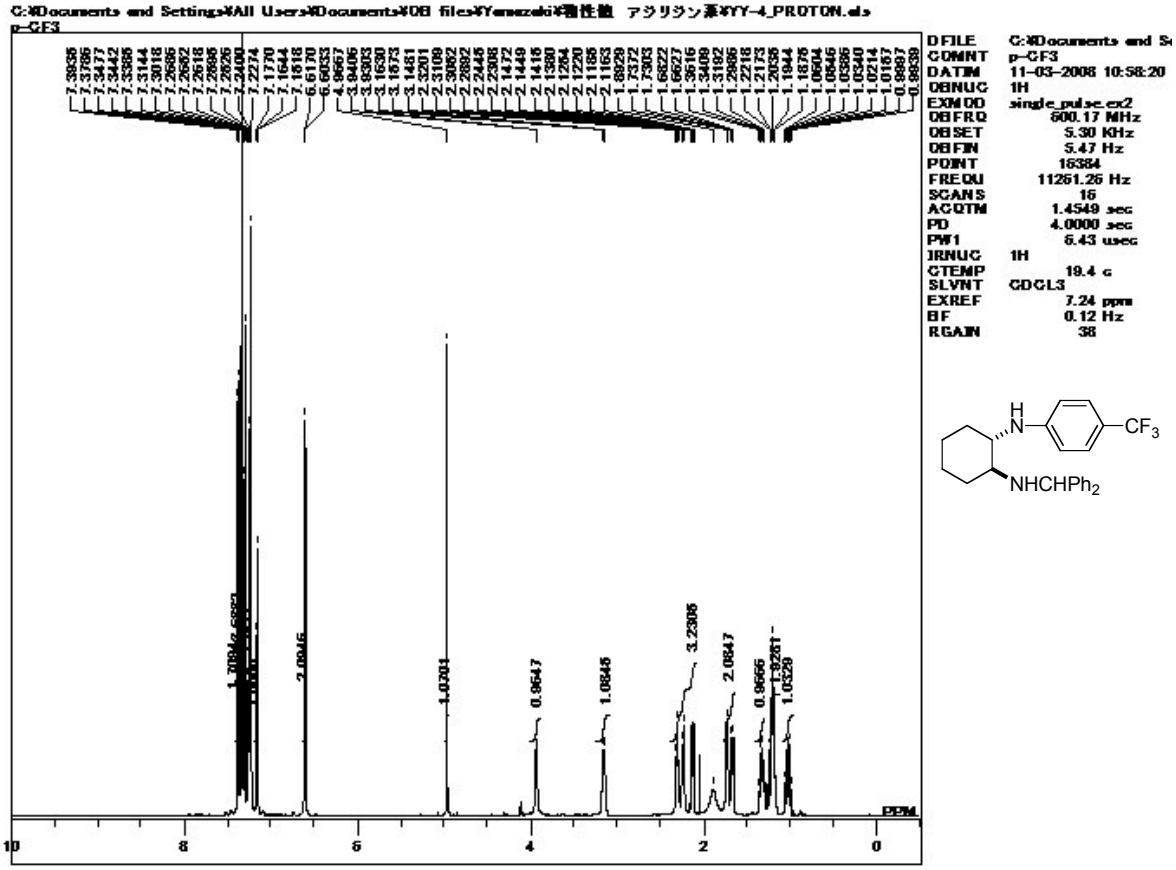
COMNT o-Me
DATIM 12-03-2008 10:07:40
OBNUC 13C
EXMOD 13C NMR.ex2
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 26214
FREQU 31249.52 Hz
SCANS 57
ACQTM 0.8389 sec
PD 2.0000 sec
PW1 3.57 usec
IRNUC 1H
CTEMP 18.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
PPM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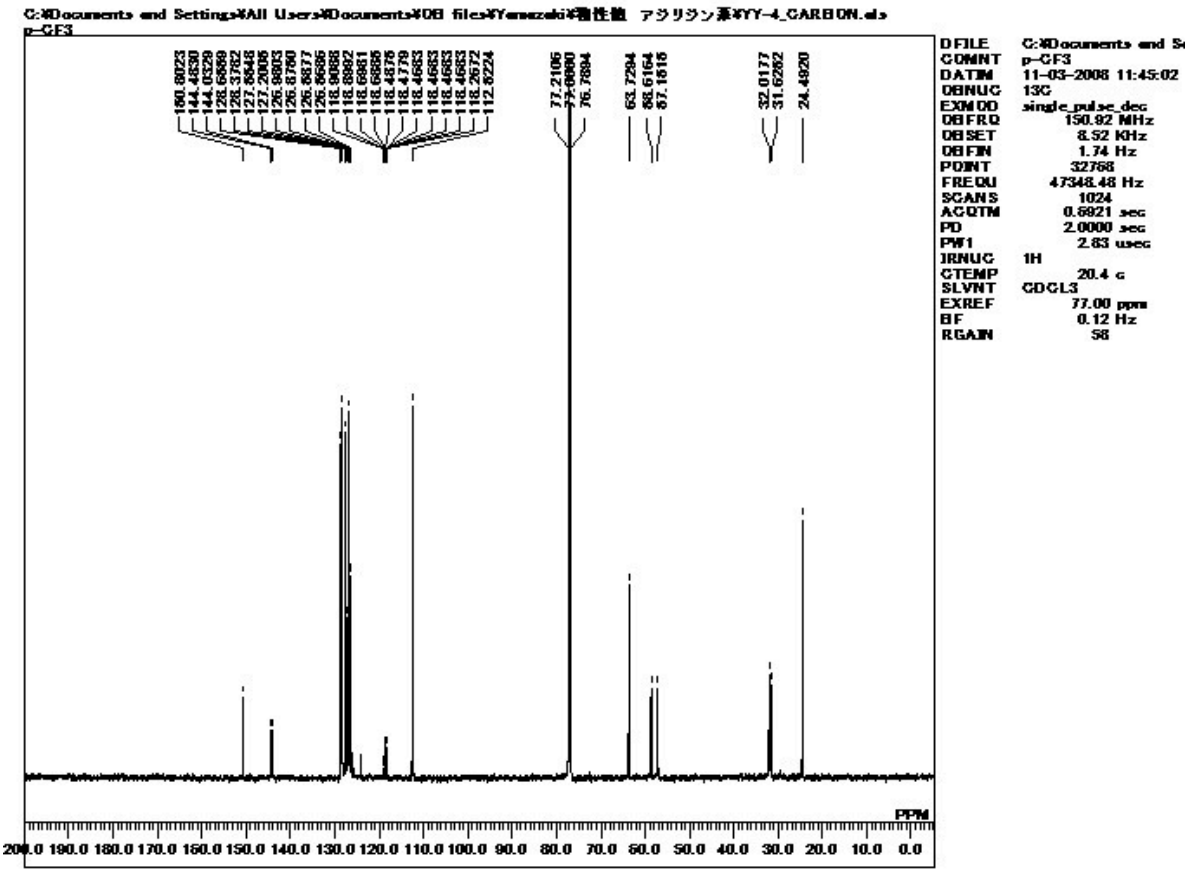
DATIM 11-03-2008 10:58:20
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 19.4 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 38
H
N
CF3
NHCHPh2
PPM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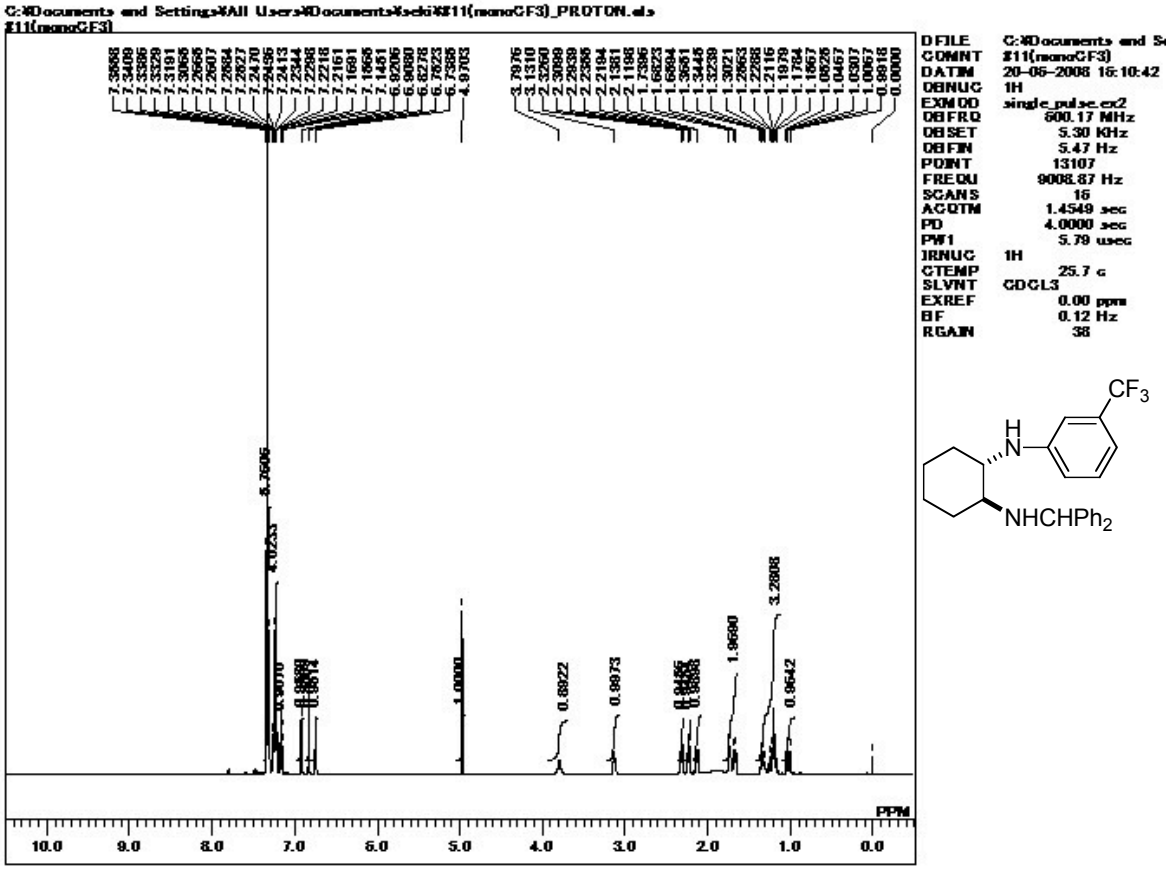
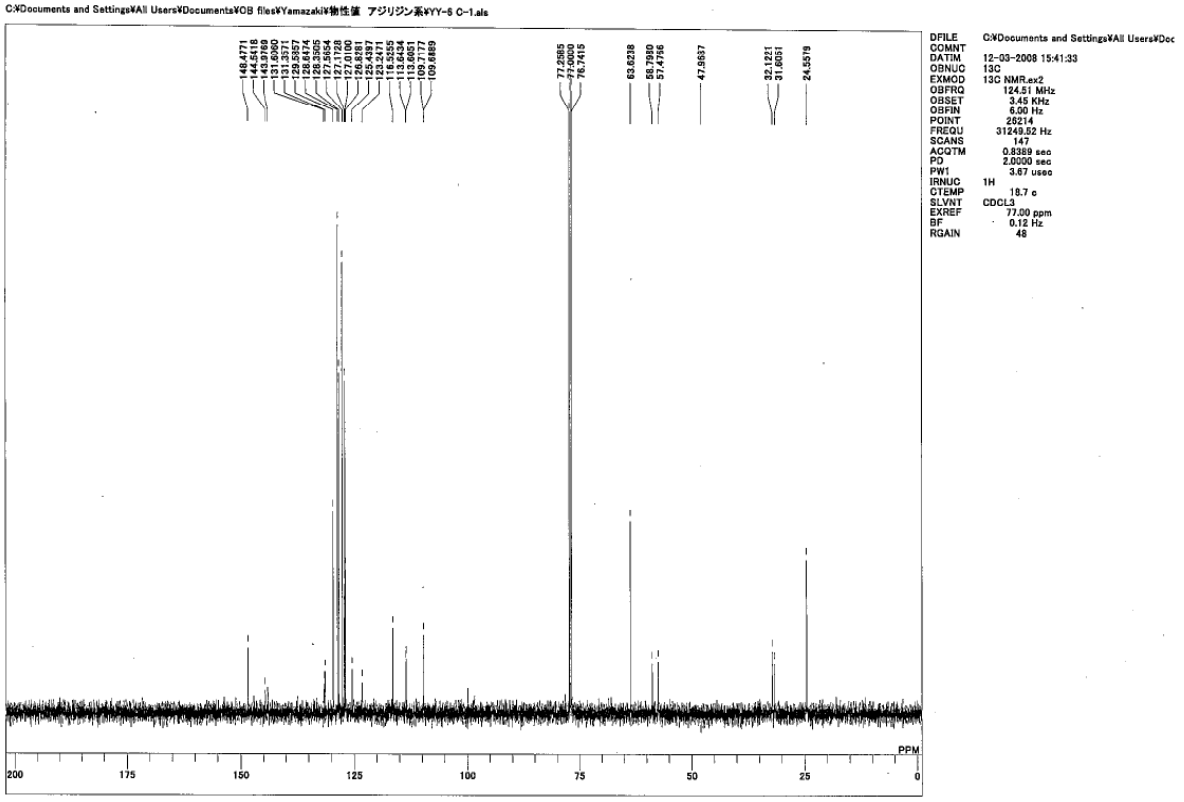
DATIM 11-03-2008 11:45:02
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32768
FREQU 47348.48 Hz
SCANS 1024
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 20.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 58
PPM


C:¥Documents and Settings¥All Users¥Documents¥seki¥#11(monoCF3)_PROTON.als
#11(monoCF3)
DFILE C:¥Documents and Se
COMNT #11(monoCF3)
DATIM 20-06-2008 16:10:42
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 13107
FREQU 9008.87 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 5.79 usec
IRNUC 1H
CTEMP 25.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 38
CF3
H
N
NHCHPh2
PPM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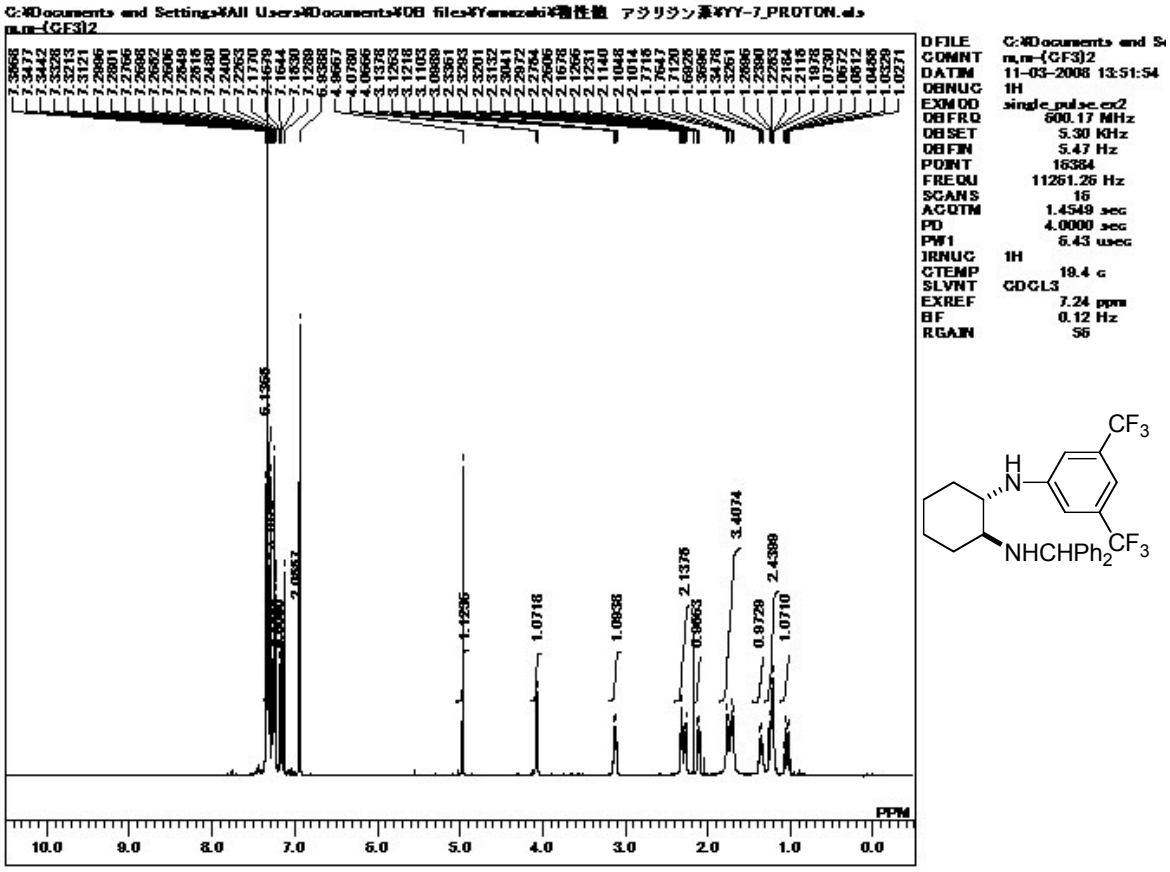
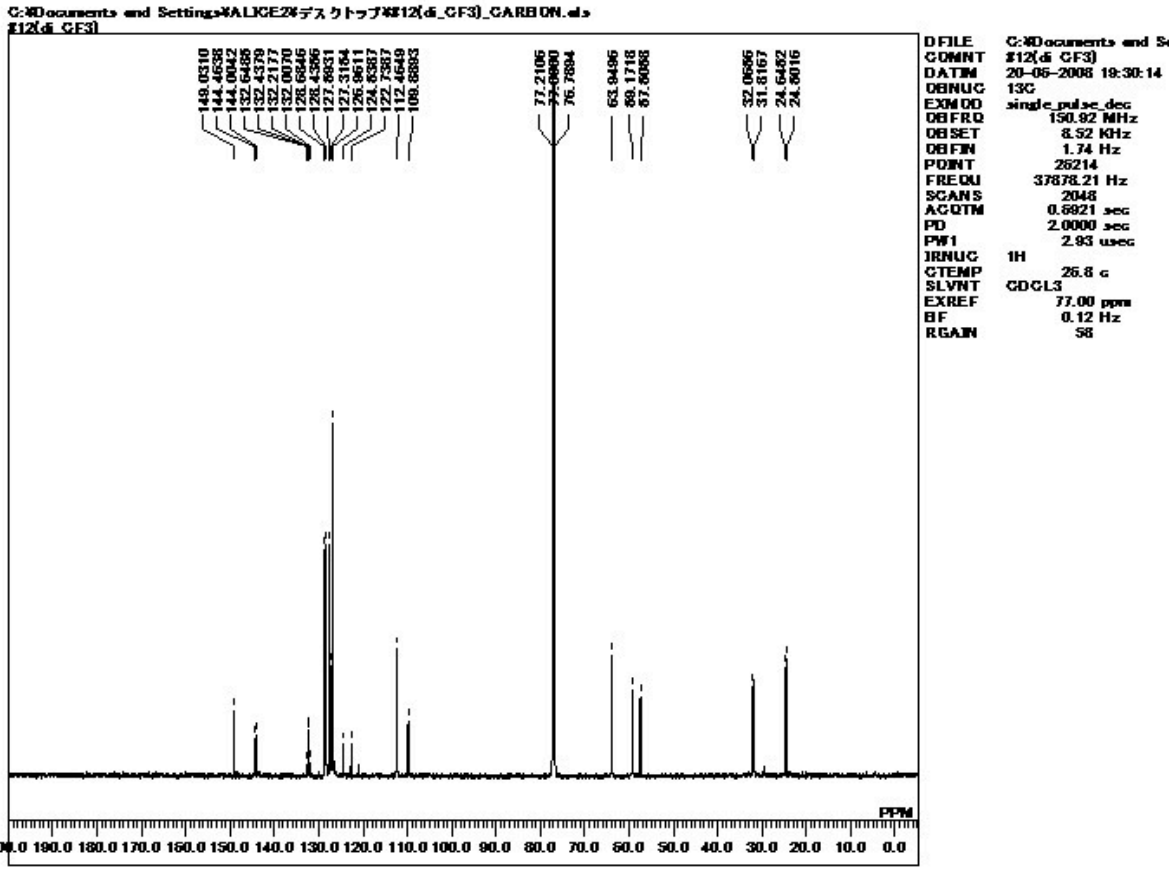
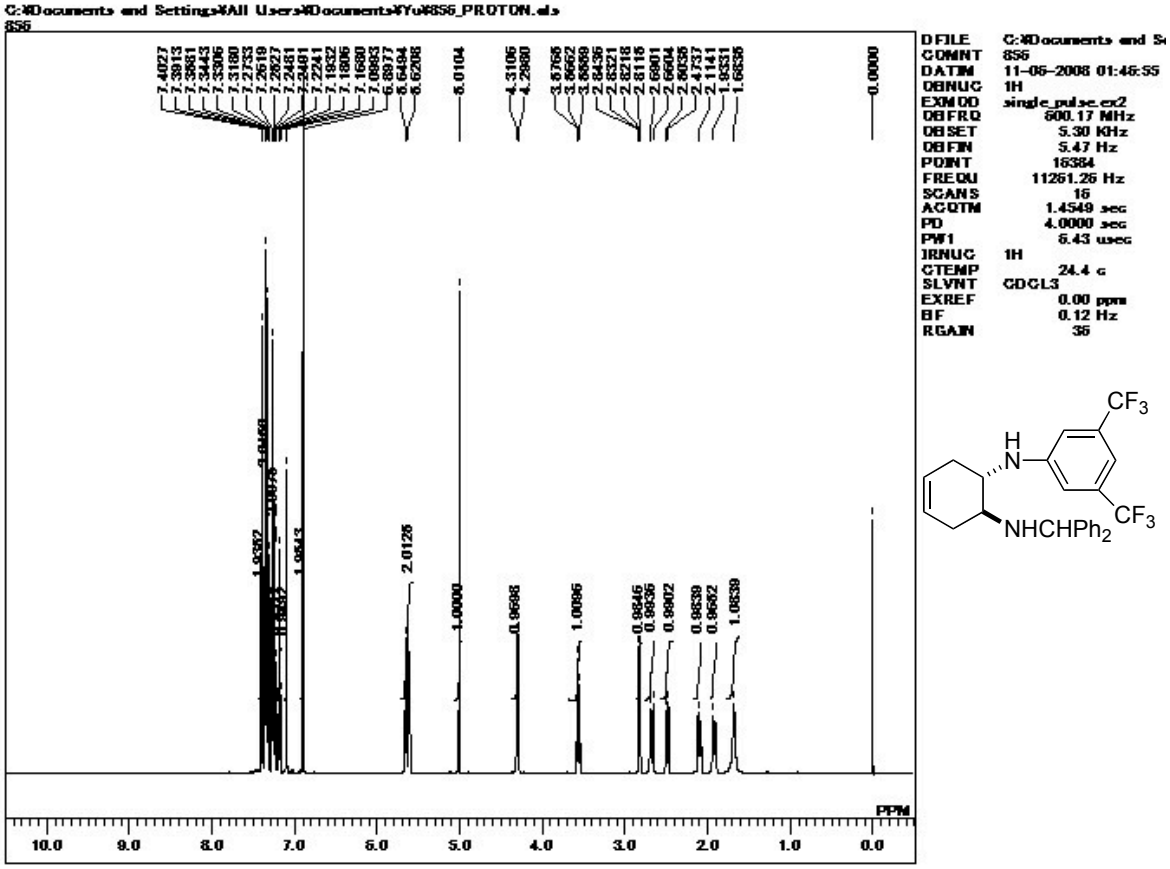
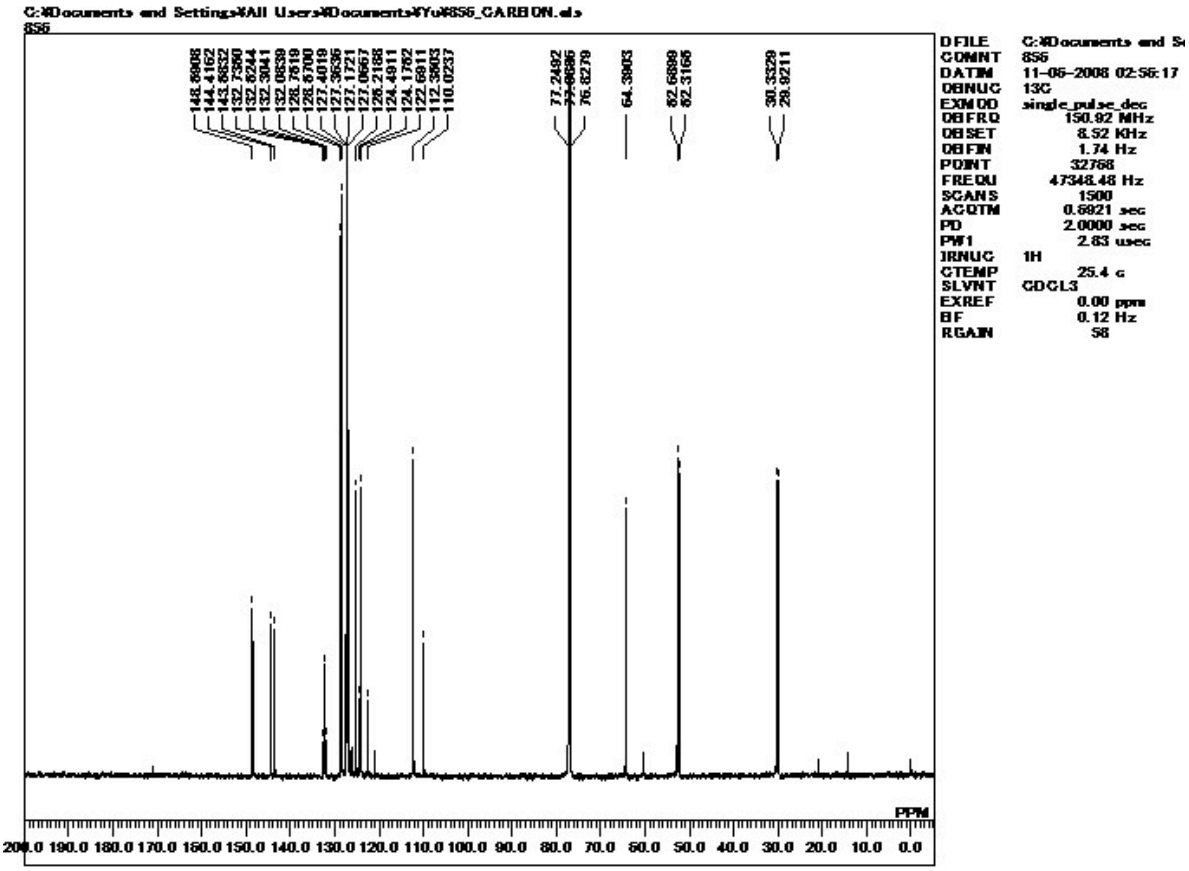
DFILE C:¥Documents and Settings¥All Users¥Doc
COMNT
DATIM 12-03-2008 15:41:33
OBNUC 13C
EXMOD 13C NMR.ex2
OBFRQ 124.51 MHz
OBSET 3.45 KHz
OBFIN 6.00 Hz
POINT 26214
FREQU 31249.92 Hz
SCANS 147
ACQTM 0.8389 sec
PD 2.0000 sec
PW1 3.67 usec
IRNUC 1H
CTEMP 18.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 48
PPM


m,m-(CF3)2
DFILE C:¥Documents and Se
COMNT m,m-(CF3)2
DATIM 11-03-2008 13:51:54
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 19.4 c
SLVNT CDCL3
EXREF 7.24 ppm
BF 0.12 Hz
RGAIN 56
6.1365
1.0716
1.0838
2.1376
0.9663
3.4074
0.9729
2.4389
1.0710
PPM
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

CF3
H
N
NHCHPh2
CF3


#12(di_CF3)
DFILE C:¥Documents and Se
COMNT #12(di CF3)
DATIM 20-05-2008 19:30:14
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 26214
FREQU 37878.21 Hz
SCANS 2048
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.93 usec
IRNUC 1H
CTEMP 26.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 58
149.0310
144.4638
144.0042
132.6486
132.4379
132.2177
132.0070
128.6846
128.4366
127.8631
127.3184
126.9611
124.8387
122.7387
112.4649
109.8893
77.2106
77.0000
76.7894
63.9496
60.1718
57.6668
32.0666
31.6167
24.6482
24.5016
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0


C:\Documents and Settings\All Users\Documents\Yu\856_PROTON.als
856
DFILE C:\Documents and S
COMNT 856
DATIM 11-05-2008 01:45:55
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 24.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 35
CF3
H
N
NHCHPh2
CF3
PPM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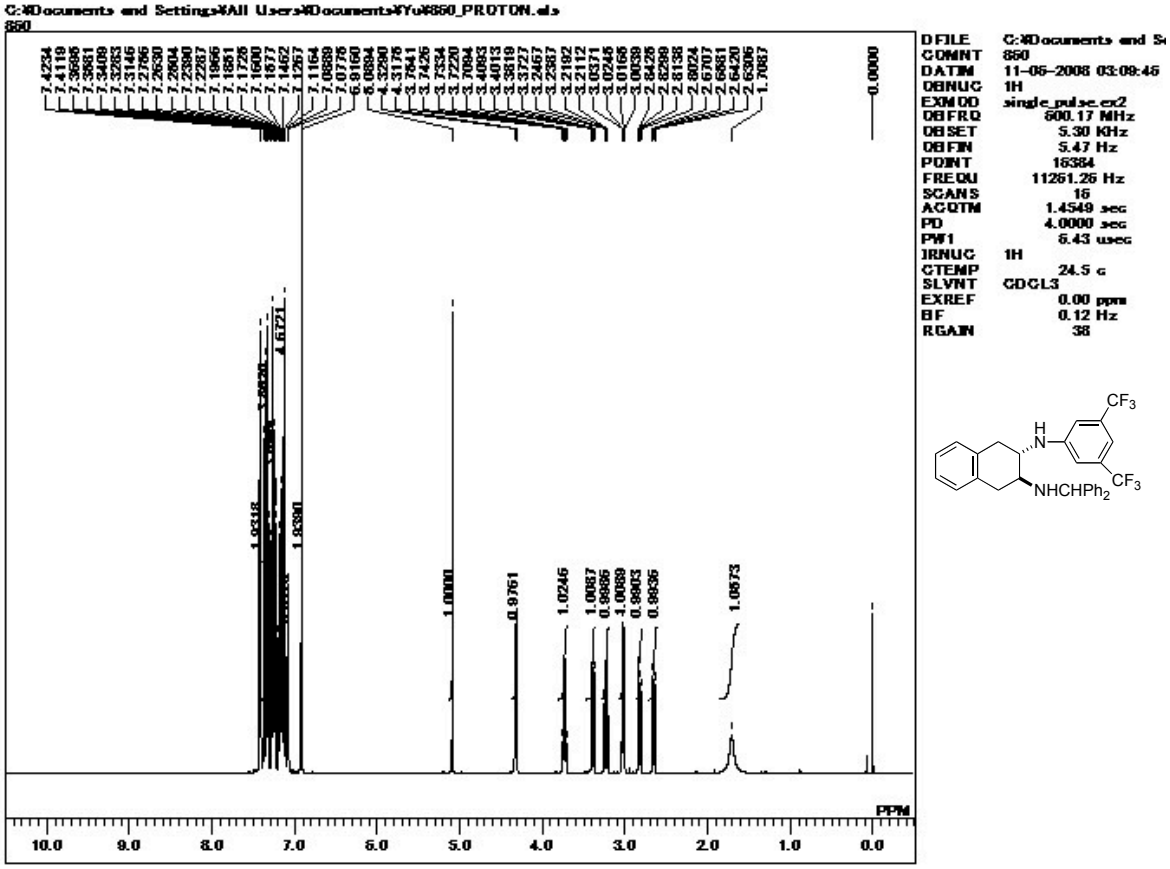
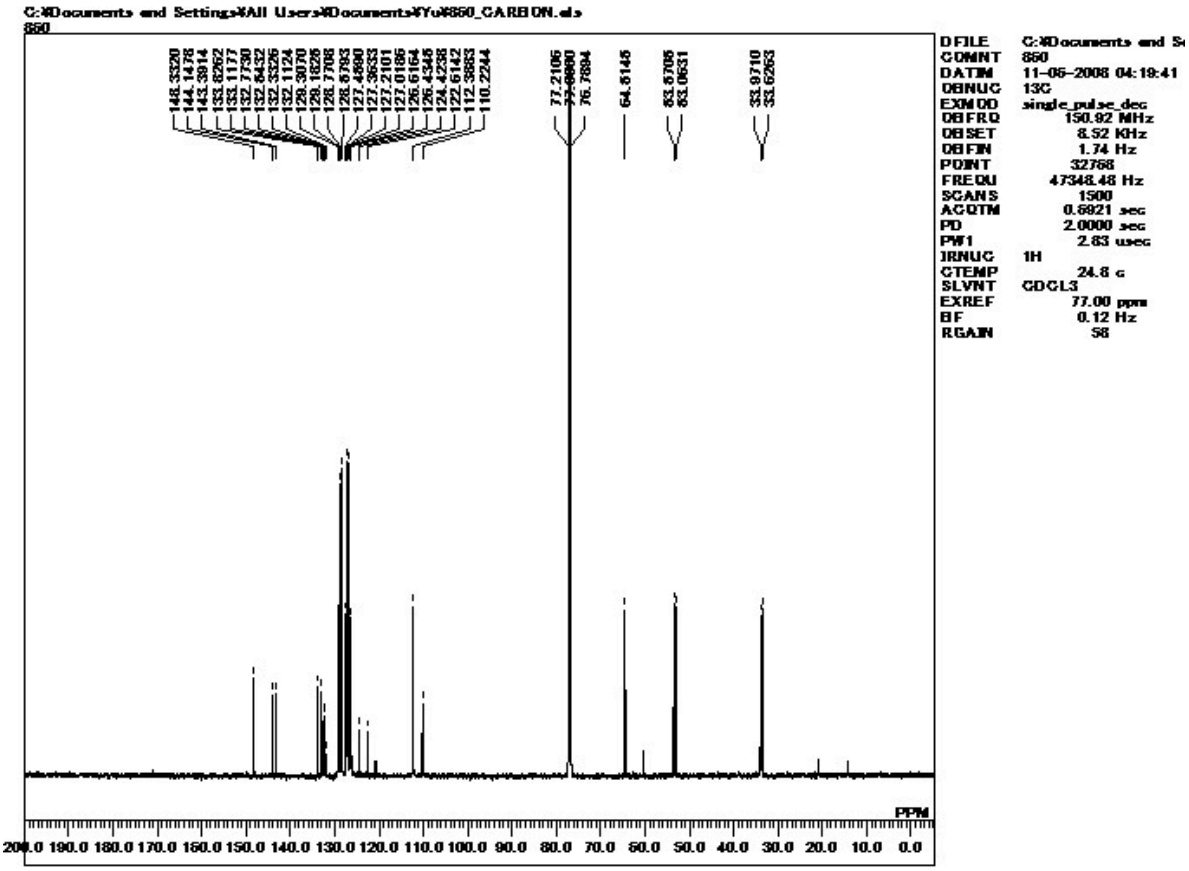
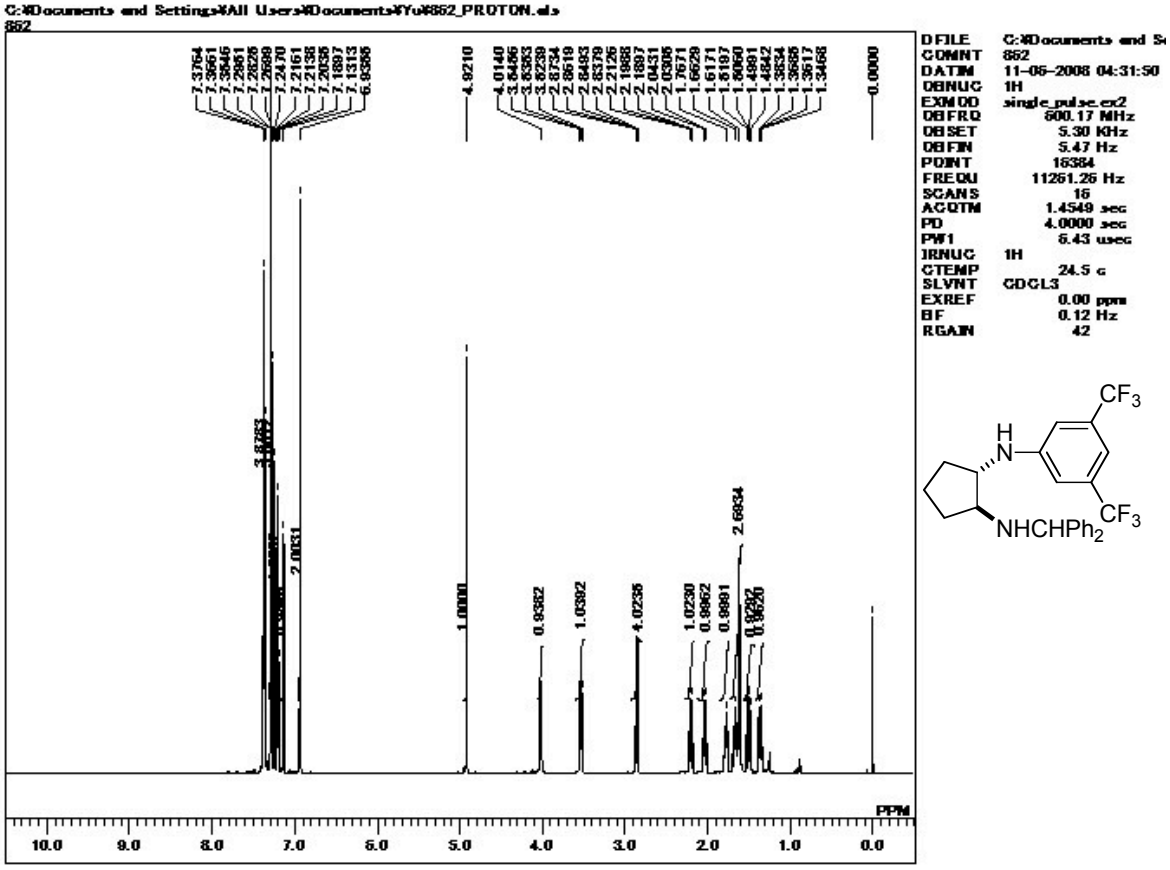
856
DFILE C:\Documents and S
COMNT 856
DATIM 11-05-2008 02:55:17
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32768
FREQU 47348.48 Hz
SCANS 1500
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 25.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 58
PPM

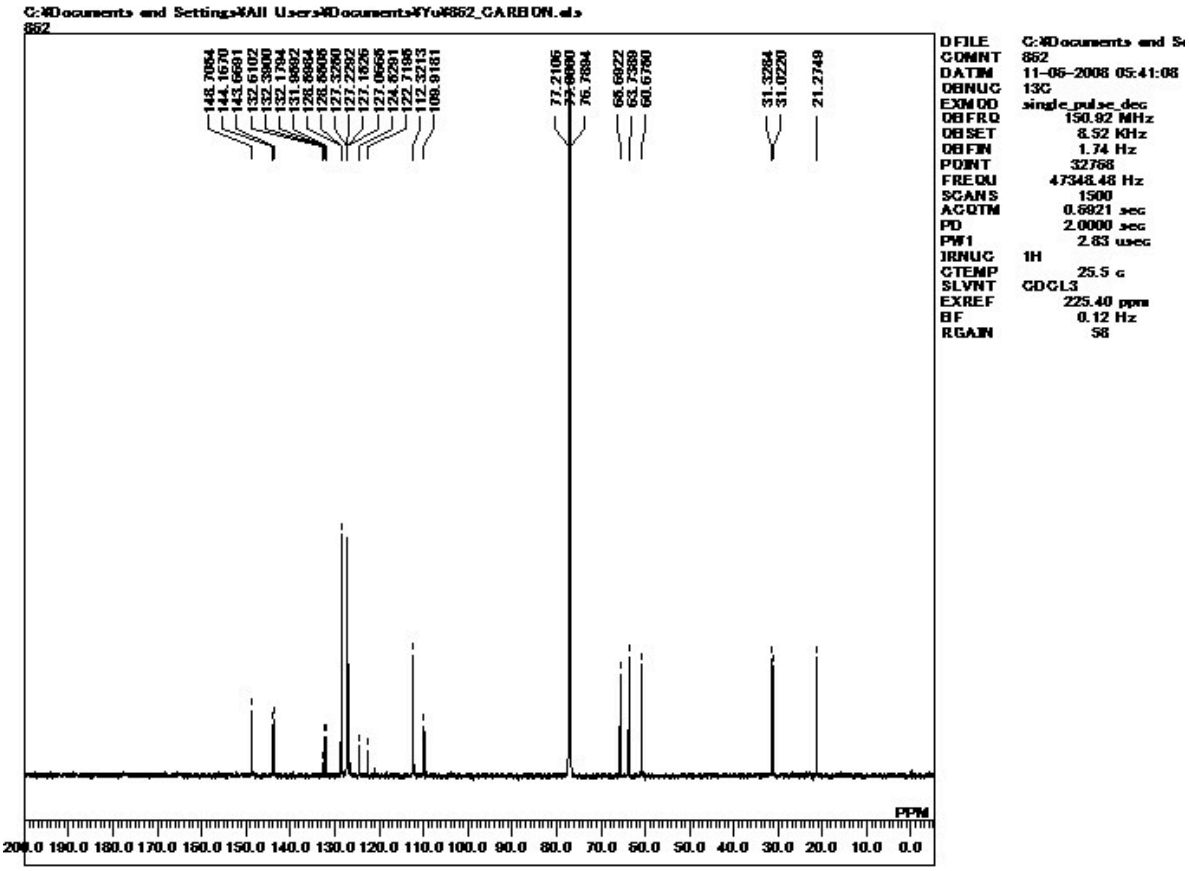

C:\Documents and Settings\All Users\Documents\Yu\860_PROTON.als
860
DFILE C:\Documents and S
COMNT 860
DATIM 11-05-2008 03:09:45
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 24.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 38
PPM
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

CF3
H
N
CF3
NHCHPh2


C:\Documents and Settings\All Users\Documents\Yu\860_CARBON.als
860
DFILE C:\Documents and S
COMNT 860
DATIM 11-05-2008 04:19:41
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32768
FREQU 47348.48 Hz
SCANS 1500
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 24.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 58
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0


C:\Documents and Settings\All Users\Documents\Yu\862_PROTON.als
862
DFILE C:\Documents and S
COMNT 862
DATIM 11-05-2008 04:31:50
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 500.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 24.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 42
PPM
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0

CF3
H
N
NHCHPh2
CF3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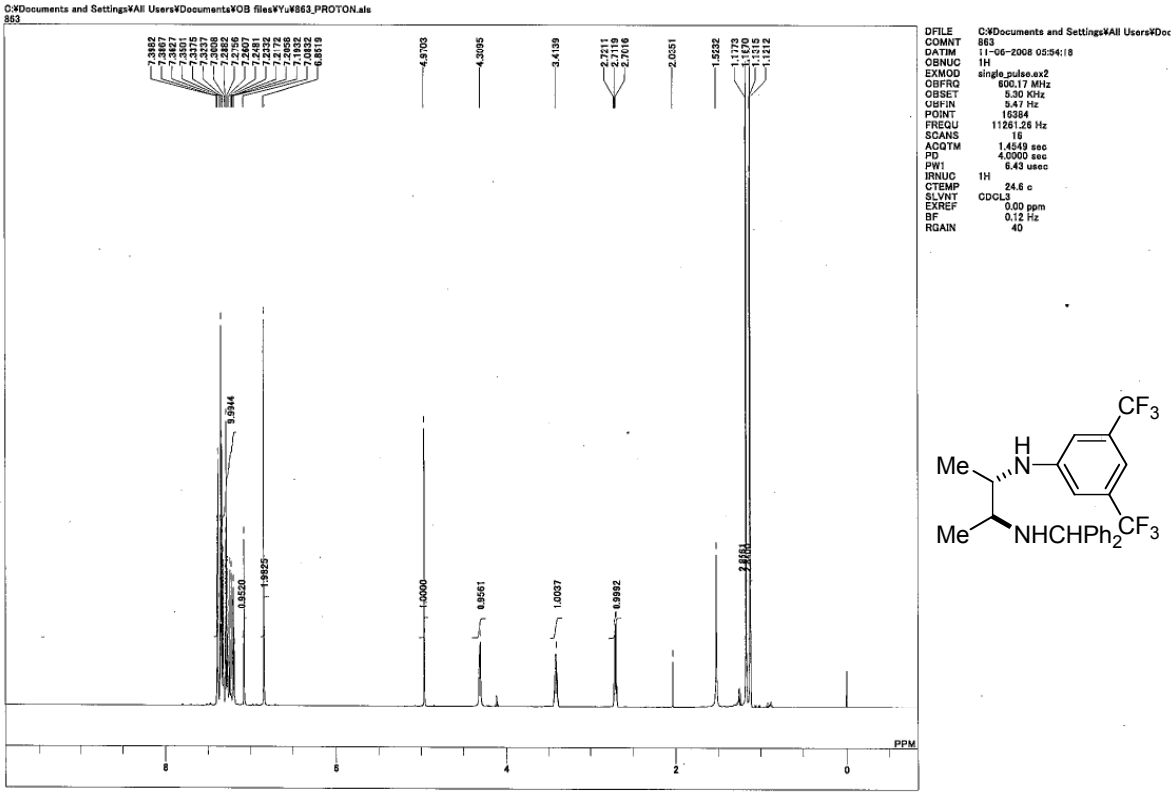
862
DFILE C:\Documents and S
COMNT 862
DATIM 11-05-2008 05:41:08
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32768
FREQU 47348.48 Hz
SCANS 1500
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 25.5 c
SLVNT CDCL3
EXREF 225.40 ppm
BF 0.12 Hz
RGAIN 58
PPM
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0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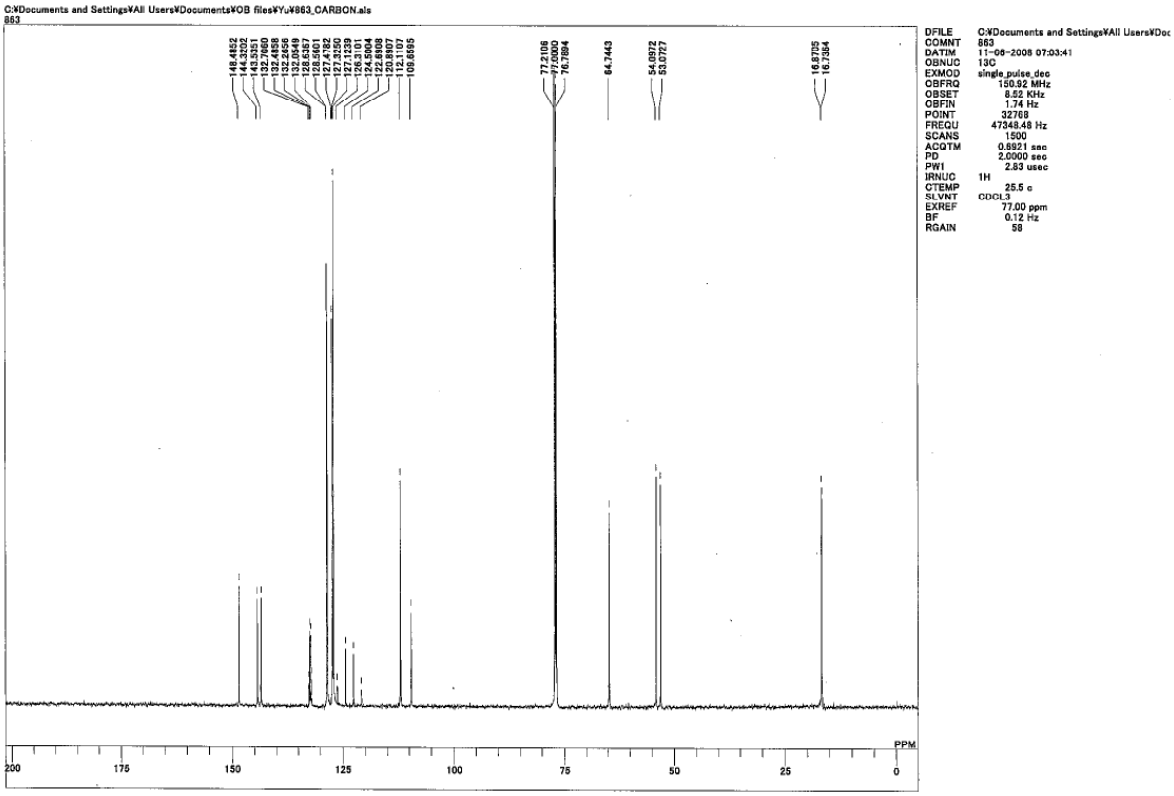
863
DFILE C:¥Documents and Settings¥All Users¥Doc
COMNT 863
DATIM 11-06-2008 05:54:18
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 16
ACQTM 1.4549 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 24.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 40
PPM

CF3
H
N
Me
Me
NHCHPh2
CF3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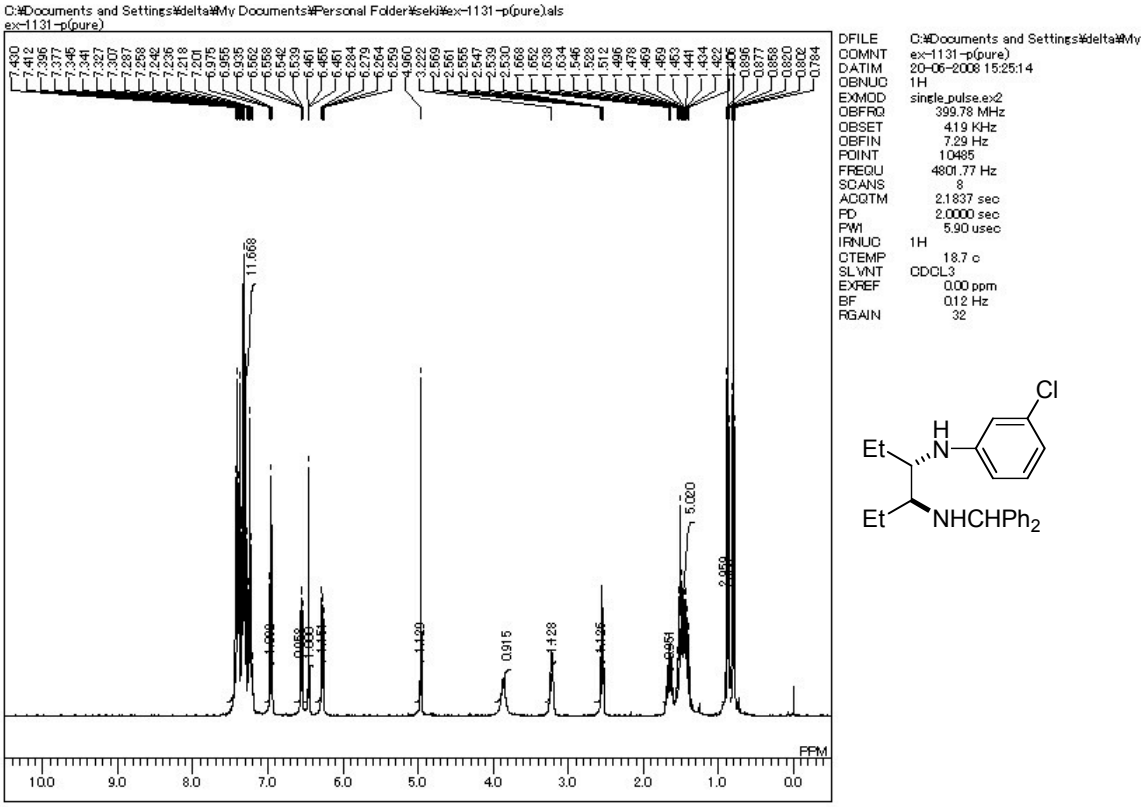
863
DFILE C:¥Documents and Settings¥All Users¥Doc
COMNT 863
DATIM 11-06-2008 07:03:41
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32768
FREQU 47348.48 Hz
SCANS 1500
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 25.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 58
PPM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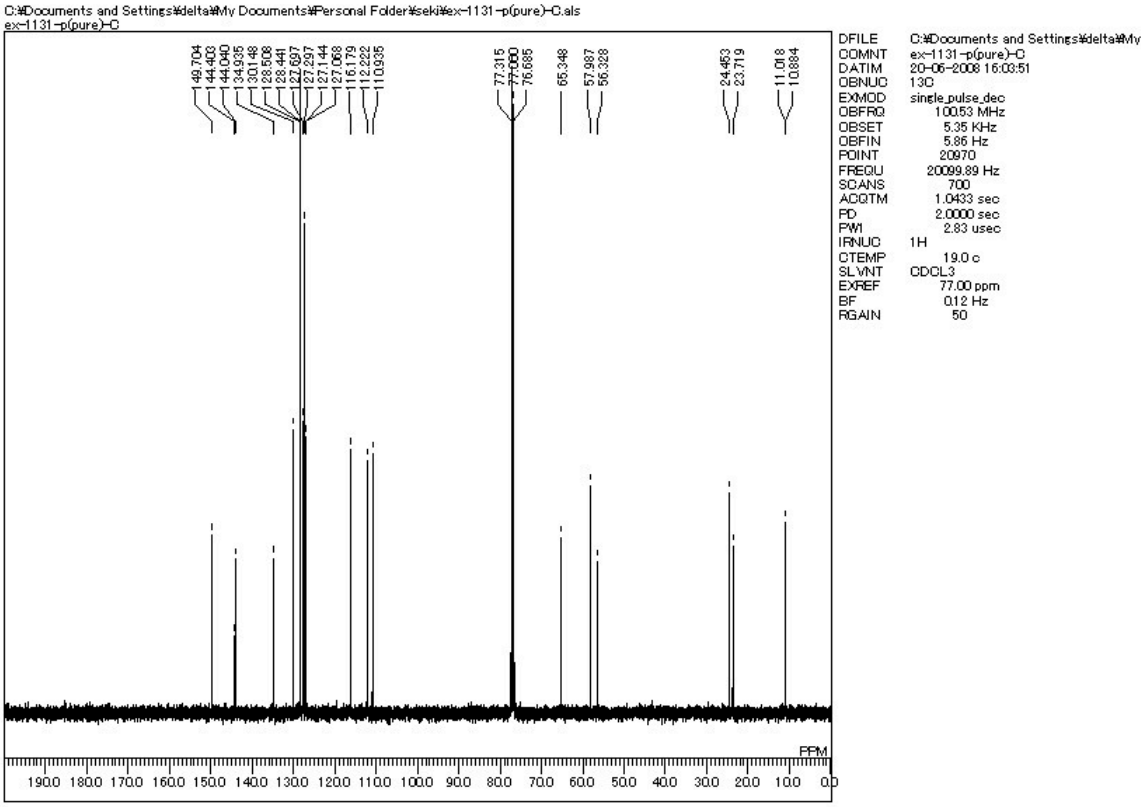
ex-1131-p(pure)
DFILE C:¥Documents and Settings¥delta¥My
COMNT ex-1131-p(pure)
DATIM 20-06-2008 15:25:14
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 10485
FREQU 4801.77 Hz
SCANS 8
ACQTM 2.1837 sec
PD 2.0000 sec
PW1 5.90 usec
IRNUC 1H
CTEMP 18.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 32
11.668
5.020
2.059
1.429
0.915
1.428
1.196
0.951
PPM
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
Cl
H
N
Et
Et
NHCHPh2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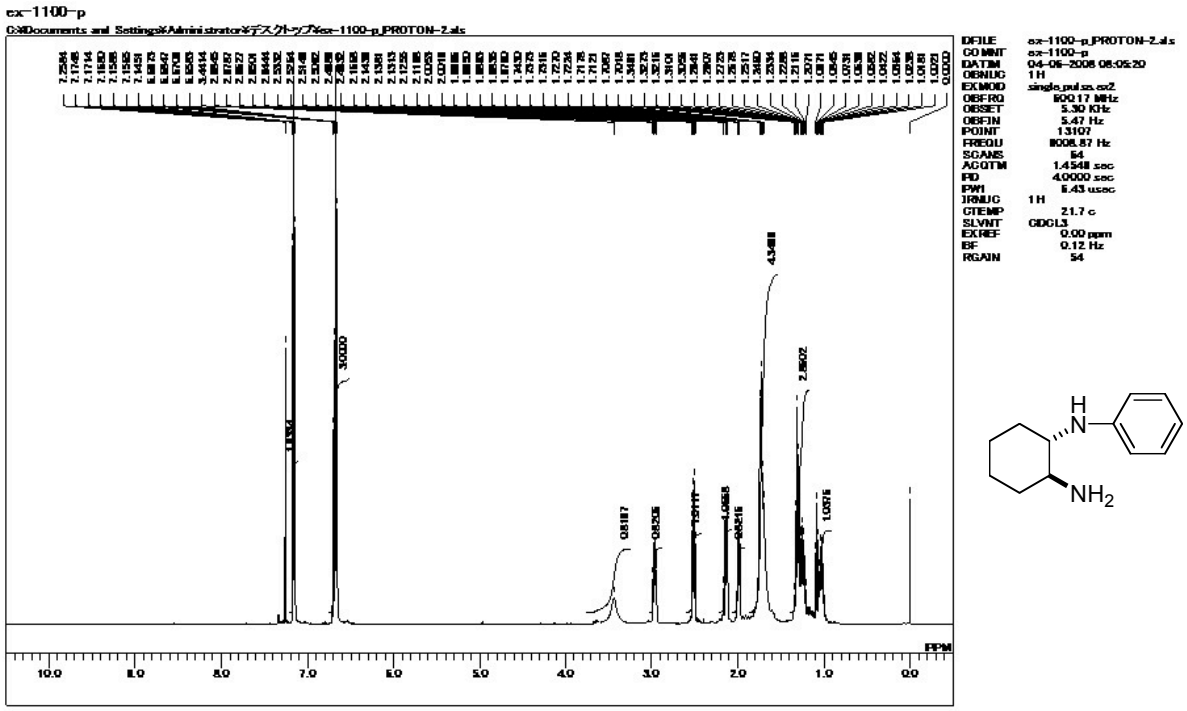
ex-1131-p(pure)-C
DFILE C:¥Documents and Settings¥delta¥My
COMNT ex-1131-p(pure)-C
DATIM 20-06-2008 16:03:51
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 20970
FREQU 20099.89 Hz
SCANS 700
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 19.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
149.704
144.403
144.040
134.935
130.148
128.508
128.441
127.697
127.297
127.144
127.068
116.179
112.222
110.935
77.315
77.000
76.685
65.348
57.987
56.328
24.463
23.719
11.018
10.884
PPM
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0


ex-1100-p
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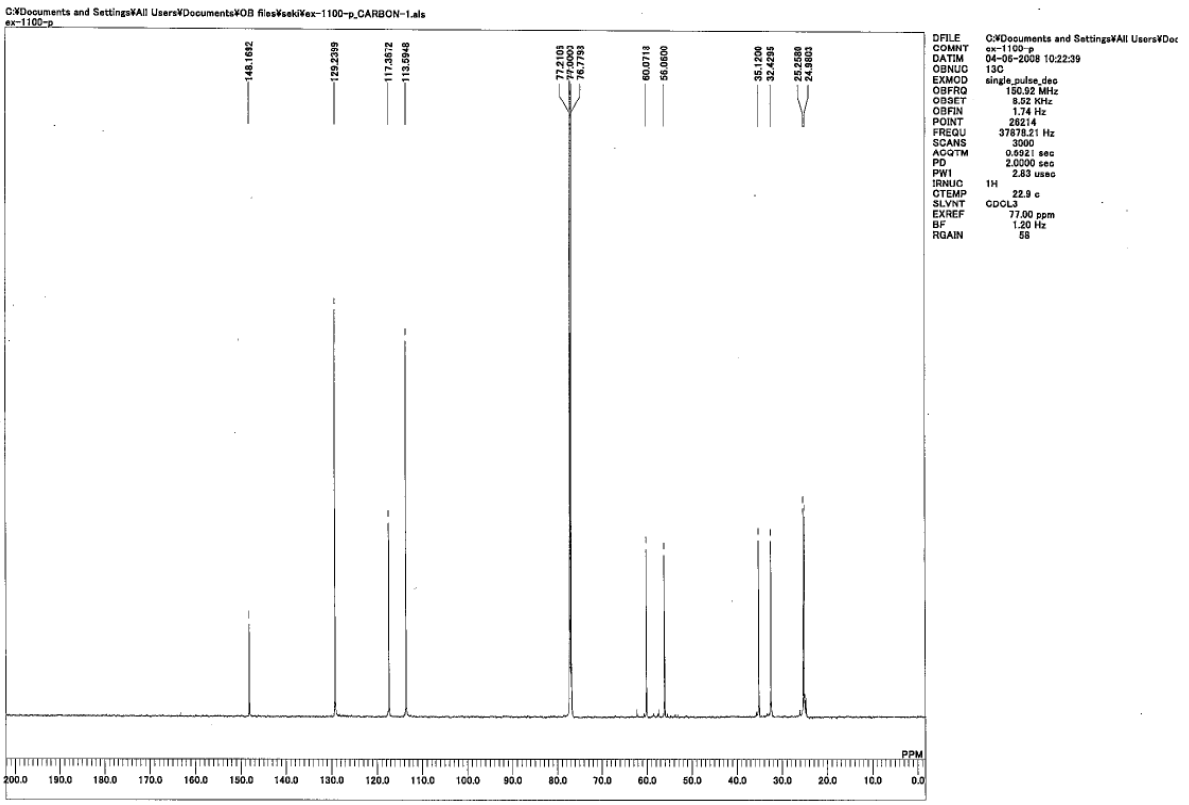
COMNT ex-1100-p
DATIM 04-06-2008 08:05:20
OBNUC 1H
EXMOD single_pulse_co2
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 13107
FREQU 8008.87 Hz
SCANS 64
ACQTM 1.4548 sec
PD 4.0000 sec
PW1 6.43 usec
IRNUC 1H
CTEMP 21.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 54
PPM
H
N
NH2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ex-1100-p
DFILE C:¥Documents and Settings¥All Users¥Doc
COMNT ex-1100-p
DATIM 04-06-2008 10:22:39
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 26214
FREQU 37878.21 Hz
SCANS 3000
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 2.83 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 58
PPM