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Asymmetric SN2'-Type C-H Functionalization of Arenes with Propargylic Alcohols

Shangze Wu, Xin Huang, Chunling Fu and Shengming Ma*

Laboratory of Molecular Recognition and Synthesis, Department of Chemistry, Zhejiang University, Hangzhou 310027, Zhejiang, P. R. China

Fax: (+86)21-64167510

E-mail: masm@sioc.ac.cn

Supporting Information

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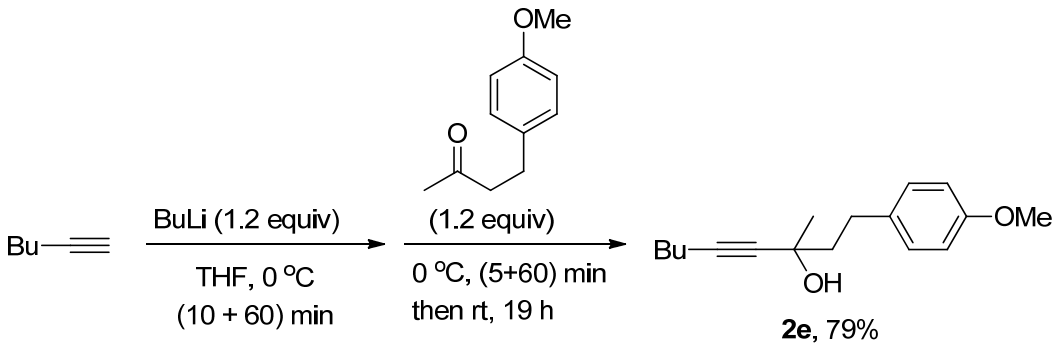
General Experimental Methods

$[Cp^*RhCl_2]_2$ was purchased from Strem. *N*-Methoxybenzamides,[1] propargylic alcohols,[2] and optically active propargylic alcohols (*S*-**2f** and *S*-**2i)**[3-4] were prepared according to the literature procedures. $H_2{}^{18}O$ was purchased from Dr. Mao chemicals. Other commercially available chemicals were purchased and used without additional purification unless noted otherwise. ^1H NMR spectra were recorded on a Bruker-300 MHz spectromete and ^{13}C NMR spectra were recorded at 75 MHz. All ^1H NMR experiments were measured with tetramethylsilane (0 ppm) or the signal of residual $CHCl_3$ (7.26 ppm) in $CDCl_3$ as the internal reference, ^{13}C NMR experiments were measured in relative to the signal of $CDCl_3$ (77.0 ppm). Infrared spectra were recorded from the film of pure samples on sodium chloride plates for liquid or in the form of KBr discs for the solid samples. Mass and HRMS spectra were carried out in EI mode. Elemental analyses were carried out by Elementar Vario MICRO cube. Thin layer chromatography was performed on pre-coated glassback plates and visualized with UV light at 254 nm. Flash column chromatography was performed on silica gel.

Synthesis of new starting materials

1. Preparation of 1-(4-methoxyphenyl)-3-methylnon-4-yn-3-ol **2e**.[2] (Wsz-9-71)

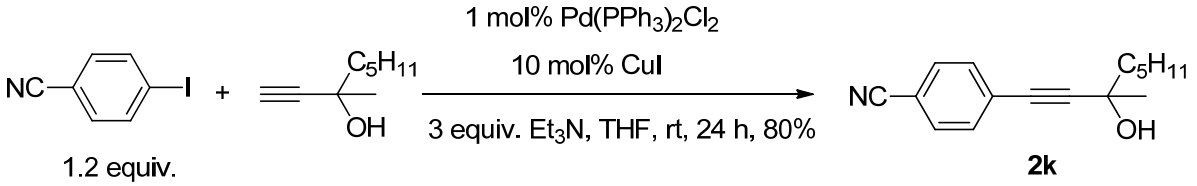


2e, 79%

To a solution of hex-1-yne (2.9 mL, d = 0.72 g/mL, 2.0880 g, 25 mmol) in THF (80 mL) was added dropwise *n*-BuLi (2.5 M in hexane, 12 mL, 30 mmol) at 0 °C within 10 minutes. After lithiation for 1 h at 0 °C, 4-(4-methoxyphenyl)butan-2-one (5.1 mL, d = 1.042 g/mL, 5.3142 g, 30 mmol) was added dropwise at this temperature within 5 minutes. After being stirred for another 1 h, the resulting mixture was warmed up to room temperature and stirred for 19 h as monitored by TLC (eluent: petroleum ether/ethyl acetate = 5/1). Then the resulting mixture was warmed up to room temperature and quenched with a saturated aqueous solution of NH_4Cl. The organic phase was separated and the acqueous phase was extracted with ether (30 mL × 3). The combined organic phase was washed with brine and dried over anhydrous Na_2SO_4. After filtration, evaporation of the solvent and chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1) afforded **2e** (5.2009 g, 79%) as an oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.17-7.08 (m, 2 H, Ar-H), 6.87-6.78 (m, 2 H, Ar-H), 3.78 (s, 3 H, OCH_3), 2.87-2.72 (m, 2 H, CH_2), 2.22 (t, J = 6.9 Hz, 2 H, CH_2), 2.10 (brs, 1 H, OH), 1.98-1.83 (m, 2 H, CH_2), 1.57-1.36 (m, 7 H, CH_3 + CH_2 × 2), 0.92 (t, J = 7.2 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.6, 134.1, 129.2, 113.7, 84.1, 83.7, 68.1, 55.2, 45.9, 30.7, 30.33, 30.29, 21.9, 18.2, 13.5; IR ν (neat, cm^{-1}) 3435, 2955, 2932, 2870, 2862, 2835, 2237, 1612, 1584,

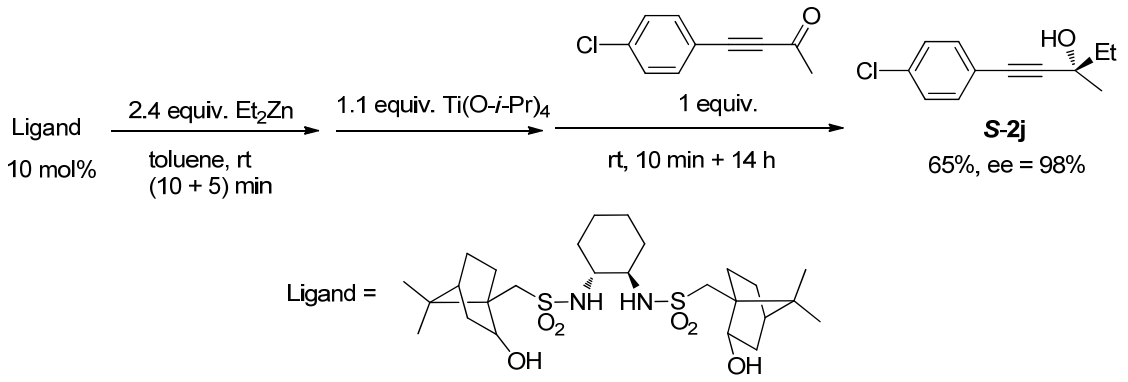
1513, 1464, 1455, 1443, 1368, 1300, 1246, 1177, 1109, 1083, 1037; MS (EI, 70 eV) *m*/z (%) 260 (M^+, 6.21), 121 (100); HRMS calcd. for $C_{17}H_{24}O_2$ (M^+): 260.1776; Found: 260.1776.

2. Preparation of 1-(4-cyanophenyl)-3-methyloct-1-yn-3-ol **2k**.[5] (Wsz-8-154)



A dried three-necked flask equipped with a Teflon-coated magnetic stirring bar was evacuated and backfilled with nitrogen for three times. Then 4-iodobenzonitrile (6. 8710 g, 30 mmol), $Pd(PPh_3)_2Cl_2$ (0.1751 g, 0.25 mmol), CuI (0.4770 mg, 2.5 mmol), Et_3N (10.4 mL, d = 0.726 g/mL, 7.5504 g, 75 mmol), 3-methyloct-1-yn-3-ol (3.5043 g, 25 mmol), and THF (50 mL) were added sequentially. The resulting mixture was stirred at rt and the reaction was complete after 24 h as monitored by TLC (eluent: petroleum ether/ethyl acetate = 5/1). Filtration through a short column of silica gel (eluent: ethyl acetate 40 mL × 3) and evaporation afforded the crude product, which was purified by flash column chromatography on silica gel (eluent: petroleum/ethyl acetate = 15/1 (800 mL) to 5/1) to afford **2k** (4.8112 g, 80%): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62-7.55 (m, 2 H, Ar-H), 7.52-7.45 (m, 2 H, Ar-H), 2.57 (s, 1 H, OH), 1.82-1.71 (m, 2 H, CH_2), 1.64-1.48 (m, 5 H, CH_3 + CH_2), 1.43-1.27 (m, 4 H, CH_2 × 2), 0.91 (t, *J* = 6.9 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 132.0, 131.8, 127.8, 118.3, 111.3, 97.6, 81.5, 68.5, 43.4, 31.7, 29.5, 24.3, 22.4, 13.9; IR (neat, cm^{-1}) 3439, 2956, 2933, 2861, 2228, 1604, 1501, 1466, 1406, 1371, 1308, 1271, 1257, 1207, 1179, 1150, 1130, 1093, 1056, 1040, 1018; MS (EI): *m/z* (%) 242 (M^++1, 4.45), 241 (M^+, 0.45), 170 (100); Anal. Calcd for $C_{16}H_{19}NO$: C 79.63, H 7.94, N 5.80. Found: C 79.28, H 7.92, N 5.55.

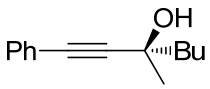
3. Preparation of *S*-1-(4-chlorophenyl)-3-methylpent-1-yn-3-ol ***S*-2j**.[3-4] (Wsz-8-38)



A dried three-necked flask equipped with a Teflon-coated magnetic stirring bar was evacuated and backfilled with nitrogen for three times. Then the ligand (0.6563 g, 30 mmol) and toluene (40 mL) were added. To the resulting mixture was added dropwise Et_2Zn (2 M in toluene, 14.4 mL, 28.8 mmol) at rt within 10 minutes. After being stirred at rt for 5 minutes, $Ti(O\text{-}i\text{-}Pr)_4$ (3.9 mL, d = 0.96 g/mL, 3.7440 g, 13.2 mmol) was added within 3 minutes. Then a solution of 4-(4-chlorophenyl)but-3-yn-2-one (2.1428 g, 12 mmol) in toluene (15 mL) was added dropwise at rt within 10 minutes. The resulting mixture was stirred for another 14 h and MeOH (10 mL) was added dropwise at 0 ^oC. After being stirred for a few minutes, a saturated aqueous solution of NH_4Cl (40 mL) was added at 0 ^oC to quench the reaction. After filtration through a short column of silica gel (eluent: ethyl acetate 40 mL × 3), the organic phase of the filtrate was separated and the acqueous phase was extracted with ethyl acetate (40 mL × 3), and the combined organic phase was washed with brine and dried over anhydrous Na_2SO_4. After filtration, evaporation of the solvent and chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1) afforded ***S*-2j** (1624.6 g, 65%): oil, 98% ee (HPLC conditions: Chiralcel OD-H column, hexane/*i*-PrOH = 100/1, 0.5 mL/min, λ = 207

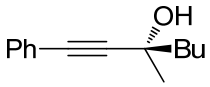
nm, t_R(major) = 64.290 min, t_R(minor) = 59.320 min); $[\alpha]_D^{20}$ = -1.2 (*c* = 1.14, $CHCl_3$); ^1H NMR (300 MHz, $CDCl_3$) δ 7.38-7.32 (m, 2 H, Ar-H), 7.32-7.23 (m, 2 H, Ar-H), 2.04 (s, 1 H, OH), 1.84-1.71 (m, 2 H, CH_2), 1.56 (s, 3 H, CH_3), 1.10 (t, *J* = 7.5 Hz, 3 H, Me); ^{13}C NMR (75 MHz, $CDCl_3$) δ 134.2, 132.9, 128.6, 121.3, 93.6, 82.3, 69.1, 36.6, 29.2, 9.0; IR (neat, cm^{-1}) 3373, 2973, 2935, 2879, 2224, 1489, 1462, 1398, 1370, 1324, 1298, 1155, 1125, 1090, 1052, 1034, 1015; MS (EI, 70 eV) *m/z* (%) 210 ($M(^{37}Cl)^+$, 2.10), 208 ($M(^{35}Cl)^+$, 6.67), 43 (100); HRMS calcd. for $C_{12}H_{13}O^{35}Cl$ (M^+): 208.0655; Found: 208.0659.

4. The characterization of *R*- and *S*-3-methyl-1-phenylhept-1-yn-3-ols ***R*-2h** and ***S*-2h** (Wsz-6-132).



***R*-2h**

Compound ***R*-2h** was prepared by preparative HPLC separation of racemic 3-methyl-1-phenylhept-1-yn-3-ol[2]: oil, >99% ee (HPLC conditions: Chiralcel OD-H column, hexane/*i*-PrOH = 100/1, 1.5 mL/min, λ = 207 nm, t_R(major) = 22.408 min); $[\alpha]_D^{20}$ = +1.6 (*c* = 1.12, $CHCl_3$); ^1H NMR (300 MHz, $CDCl_3$) δ 7.47-7.37 (m, 2 H, Ar-H), 7.36-7.26 (m, 3 H, Ar-H), 2.05 (s, 1 H, OH), 1.82-1.71 (m, 2 H, CH_2), 1.63-1.48 (m, 5 H, CH_3 + CH_2), 1.47-1.33 (m, 2 H, CH_2), 0.95 (t, *J* = 7.2 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 131.6, 128.22, 128.19, 122.8, 93.0, 83.2, 68.7, 43.5, 29.8, 27.0, 22.8, 14.1; IR (neat, cm^{-1}) 3371, 2956, 2934, 2862, 2227, 1596, 1489, 1471, 1438, 1370, 1310, 1260, 1221, 1156, 1130, 1090, 1046, 1025; MS (EI): *m/z* (%) 202 (M^+, 2.11), 145 (100); HRMS calcd. for $C_{14}H_{18}O$ (M^+): 202.1358; Found: 202.1359.

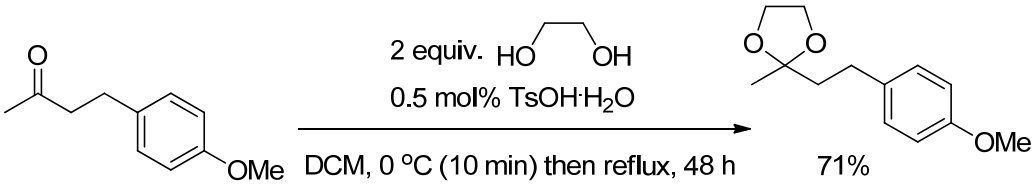


***S*-2h**

Compound ***S*-2h** was prepared by preparative HPLC separation of racemic 3-methyl-1-phenylhept-1-yn-3-ol[2]: oil, 95% ee (HPLC conditions: Chiralcel OD-H column, hexane/*i*-PrOH = 100/1, 1.5 mL/min, λ = 207 nm, t_R(major) = 37.828 min, t_R(minor) = 22.343 min); $[\alpha]_D^{20}$ = -1.7 (*c* = 0.92, $CHCl_3$); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46-7.38 (m, 2 H, Ar-H), 7.34-7.27 (m, 3 H, Ar-H), 2.05 (s, 1 H, OH), 1.81-1.72 (m, 2 H, CH_2), 1.64-1.47 (m, 5 H, CH_3 + CH_2), 1.46-1.33 (m, 2 H, CH_2), 0.95 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 131.6, 128.22, 128.19, 122.8, 93.0, 83.2, 68.6, 43.5, 29.8, 26.9, 22.8, 14.1; IR (neat, cm^{-1}) 3388, 2957, 2934, 2862, 2230, 1598, 1489, 1466, 1443, 1267, 1212, 1156, 1130, 1086, 1048, 1028; MS (EI): *m/z* (%) 202 (M^+, 1.95), 145 (100); HRMS calcd. for $C_{14}H_{18}O$ (M^+): 202.1358; Found: 202.1359.

5. Synthesis of 3-^{18}O-1-(4-methoxyphenyl)-3-methylnon-4-yn-3-ol **2e-^{18}O**

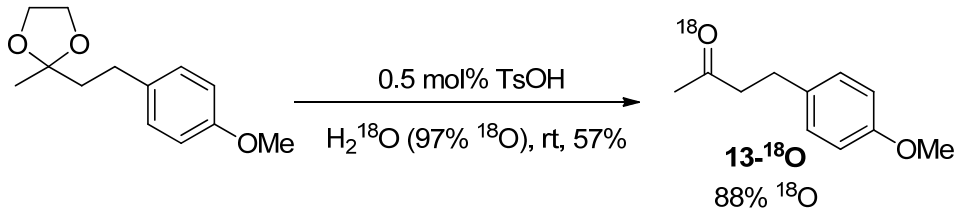
(1) The preparation of 2-(4-methoxyphenethyl)-2-methyl-1,3-dioxolane.[6] (Wsz-9-90)



To a solution of 4-(4-methoxyphenyl)butan-2-one (5.1 mL, d = 1.042 g/mL, 5.3142 g, 30 mmol) and $TsOH{\cdot}H_2O$ (0.0279 g, 0.15 mmol) in DCM (40 mL) was added dropwise ethan-1,2-diol (3.3 mL, d = 1.120 g/mL, 3.6960 g, 60 mmol) at 0 °C within 10 minutes. Then the resulting mixture was warmed to rt and then refluxed with a condenser. After being stirred

for 48 h, the reaction was complete as monitored by TLC (eluent: petroleum ether/ethyl acetate = 10/1) and quenched with a saturated aqueous solution of $NaHCO_3$ (30 mL). The organic phase was separated and the acqueous phase was extracted with diethyl ether (30 mL × 3). The combined organic phase was washed with brine and dried over anhydrous Na_2SO_4. After filtration, evaporation of the solvent and column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1 (500 mL) to 5/1) afforded 2-(4-methoxyphenethyl)-2-methyl-1,3-dioxolane (4.6829 g, 71%) as an oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.16-7.08 (m, 2 H, Ar-H), 6.87-6.78 (m, 2 H, Ar-H), 4.03-3.94 (m, 4 H, OCH_2 × 2), 3.78 (s, 3 H, OCH_3), 2.71-2.61 (m, 2 H, CH_2), 1.98-1.88 (m, 2 H, CH_2), 1.37 (s, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.6, 134.2, 129.1, 113.7, 109.6, 64.7, 55.2 41.2, 29.3, 23.9; IR ν (neat, cm^{-1}) 2981, 2952, 2932, 2880, 2835, 1612, 1584, 1513, 1464, 1455, 1376, 1300, 1246, 1178, 1135, 1110, 1087, 1055, 1038; MS (EI, 70 eV) *m*/*z* (%) 222 (M^+, 8.31), 87 (100); HRMS calcd. for $C_{13}H_{18}O_3$ (M^+): 222.1256; Found: 222.1259.

(2) The preparation of 2-^{18}O-4-(4-methoxyphenyl)butan-2-one **13-^{18}O**. (Wsz-9-147)



A dried Schlenk tube equipped with a Teflon-coated magnetic stirring bar was evacuated and backfilled with nitrogen for three times. Then TsOH (0.0089 g, 0.05 mmol), 2-(4-methoxyphenethyl)-2-methyl-1,3-dioxolane (2.2235 g, 10 mmol), and $H_2{}^{18}O$ (1 mL, d = 1.109 g/mL, 0.9017 g, 45 mmol, 97% ^{18}O) were added sequentially at rt in the glovebox.

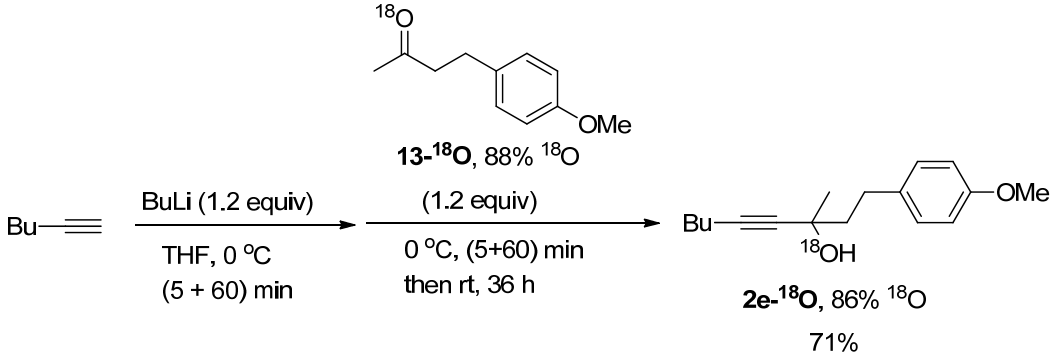
After being stirred for 108 h in the glovebox at rt as monitored by TLC, the reaction was stopped. Evaporation and purification by flash column chromatography on silica gel (eluent: petroleum/ethyl acetate = 10/1) afforded **13-^{18}O** (1.0311 g, 57%, 88% ^{18}O): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.13-7.05 (m, 2 H, Ar-H), 6.86-6.78 (m, 2 H, Ar-H), 3.77 (s, 3 H, OCH_3), 2.87-2.78 (m, 2 H, CH_2), 2.76-2.68 (m, 2 H, CH_2), 2.13 (s, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 208.1, 157.9, 132.9, 129.1, 113.8, 55.2, 45.4, 30.0, 28.8; IR ν (neat, cm^{-1}) 3031, 3000, 2955, 2935, 2914, 2836, 1715, 1612, 1583, 1513, 1465, 1443, 1366, 1301, 1247, 1179, 1160, 1109, 1035; MS (EI, 70 eV) *m*/*z* (%) 180 (M (^{18}O)$^+$, 21.23), 178 (M (^{16}O)$^+$, 2.77), 121 (100); HRMS Calcd for $C_{11}H_{14}{}^{16}O_2$ (M^+): 178.0994. Found: 178.0996. HRMS Calcd for $C_{11}H_{14}{}^{16}O^{18}O$ (M^+): 180.1036. Found: 180.1036.

The ^{18}O% incorporation of **13-^{18}O** was determined via the analysis of MS spectrum. The natural abundances of the stable isotopes of C, H, and O are known. The naturally occurring isotopic ^{18}O will also produce [M(^{18}O)]$^+$ peak. According to the natural abundance of ^{18}O, the ratio $C_{11}H_{14}{}^{16}O_2$: $C_{11}H_{14}{}^{16}O^{18}O$ is 99.76:0.2. Thus, the intensity of [M(^{18}O)$^+$] ($C_{11}H_{14}{}^{16}O^{18}O)^+$ peak will be 0.2% of the intensity of the molecular peak [M(^{16}O)$^+$] ($C_{11}H_{14}{}^{16}O_2$). According to the MS spectrum of **13-^{18}O**, the relative abundances of **13-^{16}O** 178 [M(^{16}O)$^+$] and **13-^{18}O** 180 [M(^{18}O)$^+$] are 2.77, 21.23, respectively. The ^{18}O% of **13-^{18}O** can be calculated as follows: ([M(^{18}O)$^+$] - [M(^{16}O)$^+$] × 0.2%)/([M(^{18}O)$^+$] - [M(^{16}O)$^+$] × 0.2% + [M(^{16}O)$^+$]) = 21.23-21.23×0.002/(21.23-21.23×0.002 + 2.77) ≈ 88.43%.

In addition, the contributions to the isotope peak intensities from background peaks or from impurities in the sample must be considered. According to the MS spectrum of **13**, such contribution of **13** to [M(^{16}O)+2]$^+$ is (0.34-30.78×0.002)% (≈ 0.28%).

So the ^{18}O% of **13-^{18}O** is 88.43% - 0.28% ≈ 88%.

(3) The preparation of 3-^{18}O-1-(4-methoxyphenyl)-3-methylnon-4-yn-3-ol **2e-^{18}O**. (Wsz-9-151)



To a solution of hex-1-yne (0.3285 g, 4 mmol) in THF (3 mL) was added dropwise *n*-BuLi (2.5 M in hexane, 1.9 mL, 4.8 mmol) at 0 °C in 10 minutes under N_2. After lithiation for 1 h at 0 °C, a solution of **13-^{18}O** (88% ^{18}O) (0.8652 g, 4.8 mmol) in THF (2 mL) was added dropwise at this temperature within 5 minutes. After being stirred at 0 °C for 1 h, the resulting mixture was warmed up to room temperature and stirred for 36 h as monitored by TLC (eluent: petroleum ether/ethyl acetate = 5/1) and quenched with a saturated aqueous solution of NH_4Cl (5 mL). The organic phase was separated and the acqueous phase was extracted with ether (20 mL × 3). The combined organic phase was washed with brine and dried over anhydrous Na_2SO_4. After filtration, evaporation of the solvent and chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10/1) afforded **2e-^{18}O** (0.7463 g, 71%, 86% ^{18}O) as an oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.17-7.09 (m, 2 H, Ar-H), 6.86-6.79 (m, 2 H, Ar-H), 3.78 (s, 3 H, OCH_3), 2.85-2.72 (m, 2 H, CH_2), 2.22 (t, J = 6.9 Hz, 2 H, CH_2), 2.09 (bs, 1 H, OH), 1.96-1.83 (m, 2 H, CH_2), 1.56-1.37 (m, 7 H, CH_3 + CH_2 × 2), 0.92 (t, J = 7.2 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.6, 134.1, 129.2, 113.7, 84.1, 83.7, 68.1, 55.2, 45.9,

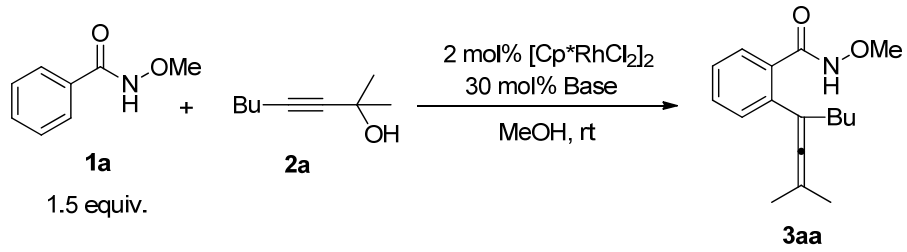
30.7, 30.33, 30.29, 21.9, 18.2, 13.5; IR (neat, cm^{-1}) 3431, 3028, 2955, 2929, 2873, 2858, 2835, 2236, 1612, 1584, 1513, 1465, 1455, 1442, 1368, 1327, 1300, 1246, 1177, 1109, 1083, 1037; MS (EI, 70 eV) *m*/*z* (%) 262 (M ($^{18}O)^+$, 6.50), 260 (M ($^{16}O)^+$, 1.03), 121 (100); HRMS Calcd for $C_{17}H_{24}{}^{16}O_2$ (M^+): 260.1776. Found: 260.1775. HRMS Calcd for $C_{17}H_{24}{}^{16}O^{18}O$ (M^+): 262.1819. Found: 262.1820.

The ^{18}O% incorporation of **2e-^{18}O** was determined via the analysis of MS spectrum. The natural abundances of the stable isotopes of C, H, and O are known. The naturally occurring isotopic ^{18}O will also produce $[M(^{18}O)]^+$ peak. According to the natural abundance of ^{18}O, the ratio $C_{17}H_{24}{}^{16}O_2$: $C_{17}H_{24}{}^{16}O^{18}O$ is 99.76:0.2. Thus, the intensity of $[M(^{18}O)^+]$ $(C_{17}H_{24}{}^{16}O^{18}O)^+$ peak will be 0.2% of the intensity of the molecular peak $[M(^{16}O)^+]$ ($C_{17}H_{24}{}^{16}O_2$). According to the MS spectrum of **2e-^{18}O**, the relative abundances of **2e-^{16}O** 260 $[M(^{16}O)^+]$ and **2e-^{18}O** 262 $[M(^{18}O)^+]$ are 1.03, 6.50, respectively. The ^{18}O% of **2e-^{18}O** can be calculated as follows: $([M(^{18}O)^+] - [M(^{16}O)^+] \times 0.2\%)/([M(^{18}O)^+] - [M(^{16}O)^+] \times 0.2\% + [M(^{16}O)^+]) = 6.50\text{-}6.50\times0.002/(6.50\text{-}6.50\times0.002+ 1.03) \approx 86.30\%$.

In addition, the contributions to the isotope peak intensities from background peaks or from impurities in the sample must be considered. According to the MS spectrum of **2e**, such contribution of **2e** to $[M(^{16}O)+2]^+$ is $(0.15\text{-}6.21\times0.002)\% (\approx 0.14\%)$.

So the ^{18}O% of **2e-^{18}O** is 86.30% - 0.14% ≈ 86%.

Table S1. The effect of base.[a]

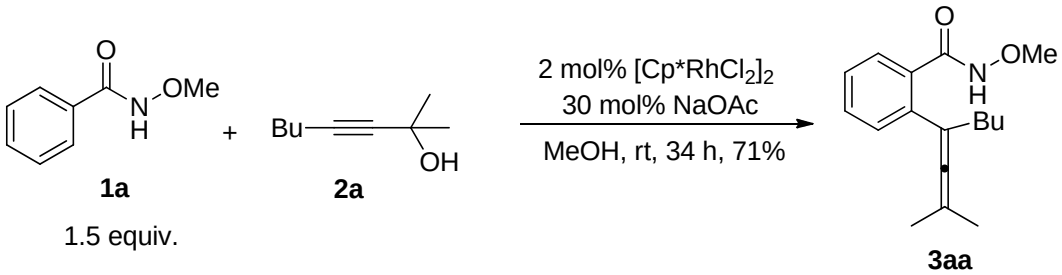


Entry	Base	Time/ h	NMR yield of **3aa**/ %
1[b]	Na_2CO_3	48	-
2[c]	K_2CO_3	48	10
3	NaOAc	24	65
4[d]	KOAc	24	22
5[e]	CsOAc	24	25
6[f]	K_3PO_4	48	18

[a] The reaction was conducted with **1a** (0.3 mmol), **2a** (0.2 mmol), $[Cp^*RhCl_2]_2$ (0.004 mmol), Base (0.06 mmol), MeOH (1.2 mL), and monitored by TLC. [b] The reaction only afforded a complicated mixture. [c] 21% of **2a** was recovered. [d] 20% of **2a** was recovered. [e] 10% of **2a** was recovered. [f] 27% of **2a** was recovered.

Rh(III)-Catalyzed Synthesis of of Tetra-substituted allenes 3

1. Preparation of *N*-methoxy-2-(7-methyl-5,6-octadien-5-yl)benzamide **3aa**. (Wsz-7-93)

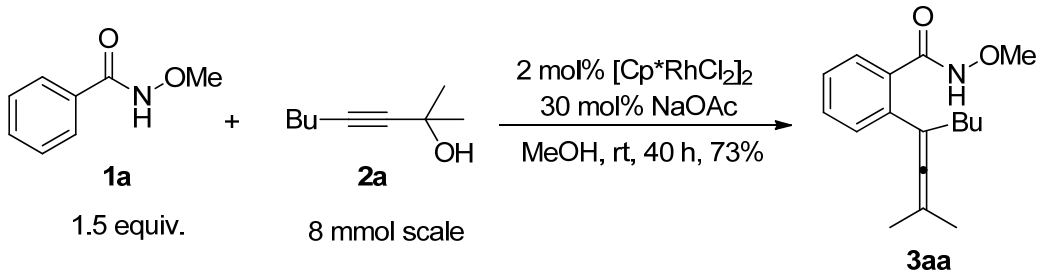


Typical Procedure I: To a dried Schlenk tube equipped with a Teflon-coated magnetic stirring bar were added *N*-methoxybenzamide **1a** (226.1 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (12.3

mg, 0.02 mmol), NaOAc (24.2 mg, 0.3 mmol), 2-methyloct-3-yn-2-ol **2a** (140.6 mg, 1 mmol), and MeOH (6 mL) sequentially at rt (29 ^{o}C). After being stirred for 34 h, the reaction was complete as monitored by TLC. Filtration through a short column of silica gel (eluent: ethyl acetate 20 mL × 3) and evaporation afforded the crude product, which was purified by flash column chromatography on silica gel (eluent: petroleum/ethyl acetate/dichloromethane = 8/1/0.1 (500 mL) to 5/1/0.1) to afford **3aa**[4] (195.6 mg, 71%): solid; m.p. 67.1-68.4 ^{o}C (hexane/ethyl acetate), reproted in the ref: 66.9-68.1 ^{o}C (hexane/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.86 (brs, 1 H, NH), 7.54 (d, J = 7.2 Hz, 1 H, Ar-H), 7.43-7.34 (m, 1 H, Ar-H), 7.32-7.19 (m, 2 H, Ar-H), 3.83 (s, 3 H, OCH_3), 2.29 (t, J = 7.1 Hz, 2 H, CH_2), 1.75 (s, 6 H, 2 × CH_3), 1.47-1.28 (m, 4 H, 2 × CH_2), 0.89 (t, J = 7.1 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.3, 167.9, 138.3, 131.5, 130.5, 129.0, 126.7, 102.8, 97.5, 64.3, 33.5, 30.0, 22.1, 20.3, 13.9; IR ν (neat, cm^{-1}) 3195, 3062, 2956, 2931, 2875, 2859, 2814, 1953, 1660, 1595, 1570, 1465, 1440, 1361, 1300, 1260, 1188, 1158, 1108, 1035; MS (EI, 70 eV) *m*/*z* (%) 273 (M^+, 1.13), 198 (100).

The following compounds were prepared according to the **Typical Procedure I**.

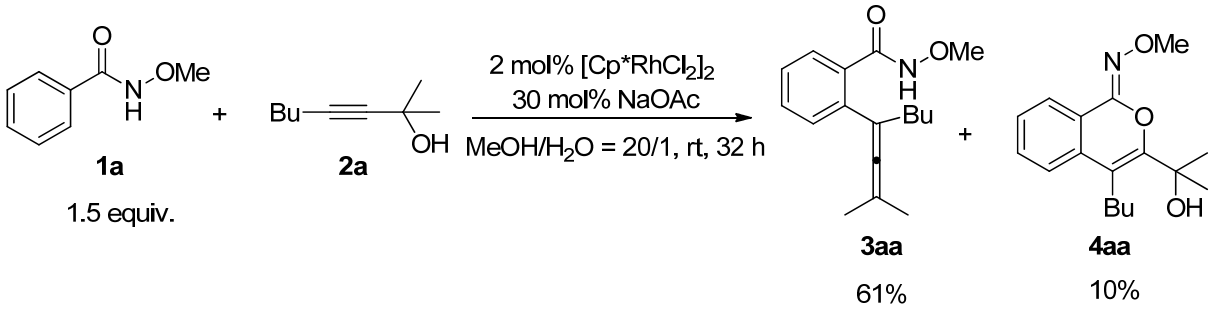
Preparation of **3aa** on 8 mmol scale. (Wsz-8-60)



The reaction of **1a** (1812.6 mg, 12 mmol), $[Cp^*RhCl_2]_2$ (98.3 mg, 0.16 mmol), NaOAc (196.7 mg, 2.4 mmol), **2a** (1122.1 mg, 8 mmol), and MeOH (50 mL) at rt (10 ^{o}C) afforded **3aa** (1590.4 mg, 73%) (eluent: petroleum/ethyl acetate/dichloromethane = 6/1/0.3): ^{1}H NMR

(300 MHz, $CDCl_3$) δ 8.82 (brs, 1 H, NH), 7.55 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.42-7.33 (m, 1 H, Ar-H), 7.32-7.18 (m, 2 H, Ar-H), 3.84 (s, 3 H, OCH_3), 2.29 (t, *J* = 7.2 Hz, 2 H, CH_2), 1.76 (s, 6 H, 2 × CH_3), 1.47-1.28 (m, 4 H, 2 × CH_2), 0.89 (t, *J* = 7.2 Hz, 3 H, CH_3).

2. Identification of the byproduct (Z)-4-butyl-3-(2-hydroxypropan-2-yl)-1H-isochromen-1-one O-methyl oxime **4aa** using mixed solvent ($MeOH/H_2O$, V/V = 20/1). (Wsz-6-197)

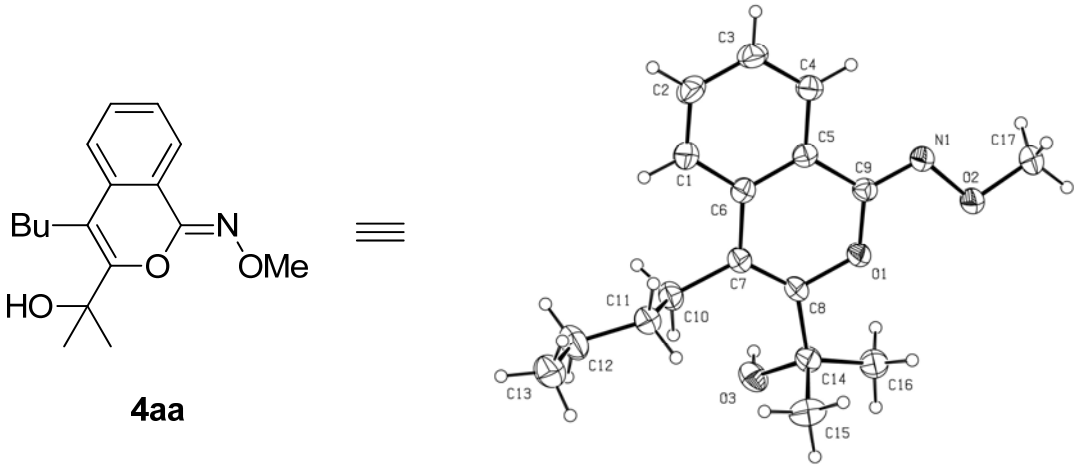


The reaction of **1a** (226.6 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (12.6 mg, 0.02 mmol), NaOAc (24.9 mg, 0.3 mmol), **2a** (140.8 mg, 1 mmol), MeOH (6 mL), and H_2O (0.3 mL) at rt (21 ^oC) afforded **4aa** (28.2 mg, 10%) and **3aa** (166.7 mg, 61%) (eluent: petroleum ether/ethyl acetate = 15/1 to petroleum ether/ethyl acetate/dichloromethane = 6/1/0.4).

3aa: solid, ^1H NMR (300 MHz, $CDCl_3$) δ 8.80 (brs, 1 H, NH), 7.56 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.42-7.33 (m, 1 H, Ar-H), 7.32-7.18 (m, 2 H, Ar-H), 3.85 (s, 3 H, OCH_3), 2.29 (t, *J* = 7.1 Hz, 2 H, CH_2), 1.76 (s, 6 H, 2 × CH_3), 1.47-1.28 (m, 4 H, 2 × CH_2), 0.89 (t, *J* = 7.1 Hz, 3 H, CH_3).

4aa: solid; m.p. 77.5-78.6 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.94 (dd, J_1 = 8.0 Hz, J_2 = 1.1 Hz, 1 H, Ar-H), 7.48-7.39 (m, 1 H, Ar-H), 7.39-7.33 (m, 1 H, Ar-H), 7.29-7.22 (m, 1 H, Ar-H), 3.92 (s, 3 H, OCH_3), 2.82 (t, *J* = 7.1 Hz, 2 H, CH_2), 2.28 (s, 1 H, OH), 1.63 (s, 6 H, 2 × CH_3), 1.58-1.40 (m, 4 H, 2 × CH_2), 0.97 (t, *J* = 7.1 Hz, 3 H, CH_3). ^{13}C

NMR (75 MHz, $CDCl_3$) δ 153.0, 148.6, 132.8, 130.8, 127.3, 123.8, 122.6, 121.3, 111.0, 74.1, 62.4, 32.4, 29.7, 25.0, 23.1, 13.9; IR ν (neat, cm^{-1}) 3463, 2958, 2933, 2872, 2816, 1638, 1616, 1593, 1486, 1457, 1345, 1191, 1140, 1056; MS (EI, 70 eV) *m*/*z* (%) 290 (M^++1, 15.46), 289 (M^+, 100); Anal. Calcd for $C_{17}H_{23}NO_3$: C 70.56, H 8.01, N 4.84. Found: C 70.35, H 8.19, N 4.50.



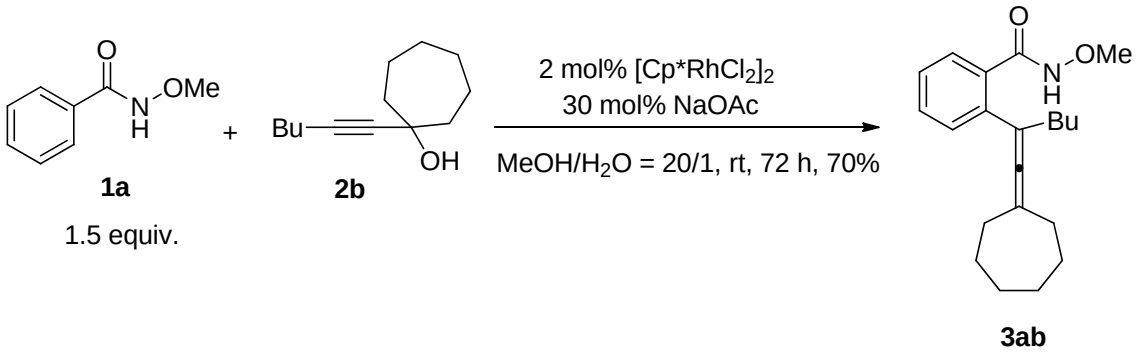
4aa

ORTEP representation of **4aa**

4aa: $C_{17}H_{23}NO_3$, MW = 289.36, monoclinic, space group P 1 21/c 1, final R indices [I > 2σ(I)], R1 = 0.0429, wR2 = 0.0980; Rindices (all data), R1 = 0.0708, wR2 = 0.1147; a = 16.5610(13) Å, b = 9.1887(6) Å, c = 10.5955(7) Å, α = 90.00°, β = 98.666(7)°, γ = 90.00°, V = 1593.94(19) $Å^3$, T = 293(2) K, Z = 4, reflections collected/unique 6042/2906 (R_{int} = 0.0321), number of observations [> 2σ(I)]: 1993, parameters: 195. Supplementary crystallographic data have been deposited at the Cambridge Crystallographic Data Centre, CCDC 1483457.

3. Preparation of *N*-methoxy-2-(1,1-hexamethylene-1,2-heptadien-3-yl)benzamide **3ab**.

(Wsz-7-200)



1a

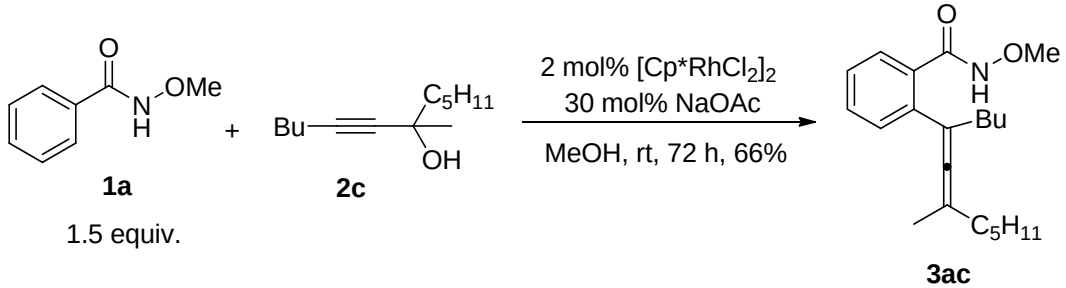
1.5 equiv.

2b

3ab

The reaction of **1a** (227.1 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (12.7 mg, 0.02 mmol), NaOAc (24.9 mg, 0.3 mmol), and **2b** (194.5 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (13 ^oC) afforded **3ab** (228.7 mg, 70%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 7/1/0.3): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.93 (s, 1 H, NH), 7.58 (d, J = 7.2 Hz, 1 H, Ar-H), 7.38 (td, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1 H, Ar-H), 7.32-7.17 (m, 2 H, Ar-H), 3.83 (s, 3 H, OCH_3), 2.43-2.18 (m, 6 H, $CH_2 \times 3$), 1.75-1.49 (m, 8 H, $CH_2 \times 4$), 1.48-1.28 (m, 4 H, $CH_2 \times 2$), 0.90 (t, J = 7.1 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.2, 167.7, 138.5, 131.2, 130.5, 129.3, 129.1, 126.7, 106.7, 102.8, 64.2, 33.7, 32.2, 30.1, 29.2, 28.3, 22.1, 13.9; IR ν (neat, cm^{-1}) 3187, 3063, 2953, 2926, 2852, 1947, 1658, 1594, 1569, 1499, 1462, 1440, 1376, 1349, 1302, 1156, 1035; MS (EI, 70 eV) m/z (%) 328 (M^++1, 11.16), 327 (M^+, 4.84), 296 (100); HRMS Calcd for $C_{21}H_{29}NO_2$ (M^+): 327.2198. Found: 327.2192.

4. Preparation of *N*-methoxy-2-(7-methyl-5,6-dodedien-5-yl)benzamide **3ac**. (Wsz-7-189)



1a

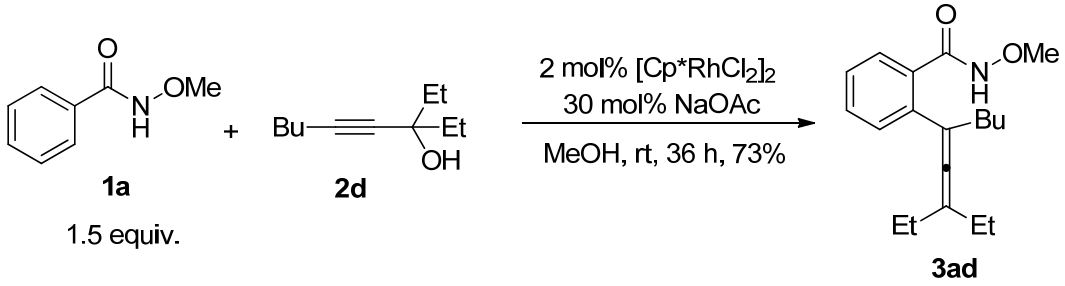
1.5 equiv.

2c

3ac

The reaction of **1a** (226.6 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (12.5 mg, 0.02 mmol), NaOAc (24.3 mg, 0.3 mmol), and **2c** (196.7 mg, 1 mmol) in MeOH (6 mL) at rt (17 ^oC) afforded **3ac** (218.3 mg, 66%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 7/1/0.3): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.96 (s, 1 H, NH), 7.61 (d, J = 7.5 Hz, 1 H, Ar-H), 7.39 (td, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1 H, Ar-H), 7.33-7.17 (m, 2 H, Ar-H), 3.85 (s, 3 H, OCH_3), 2.37-2.19 (m, 2 H, CH_2), 2.07-1.93 (m, 2 H, CH_2), 1.77 (s, 3 H, CH_3), 1.57-1.17 (m, 10 H, CH_2 × 5), 0.99-0.78 (m, 6 H, CH_3× 2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.8, 167.7, 138.4, 131.2, 130.6, 129.4, 129.2, 126.8, 104.6, 101.9, 64.3, 34.1, 33.9, 31.5, 30.2, 27.3, 22.4, 22.2, 18.8, 14.0, 13.9; IR ν (neat, cm^{-1}) 3189, 3063, 2956, 2929, 2869, 2857, 1950, 1659, 1590, 1566, 1499, 1465, 1439, 1373, 1299, 1159, 1035; MS (EI, 70 eV) *m*/*z* (%) 329 (M^+, 1.30), 130 (100); HRMS Calcd for $C_{21}H_{31}NO_2$ (M^+): 329.2355. Found: 329.2360.

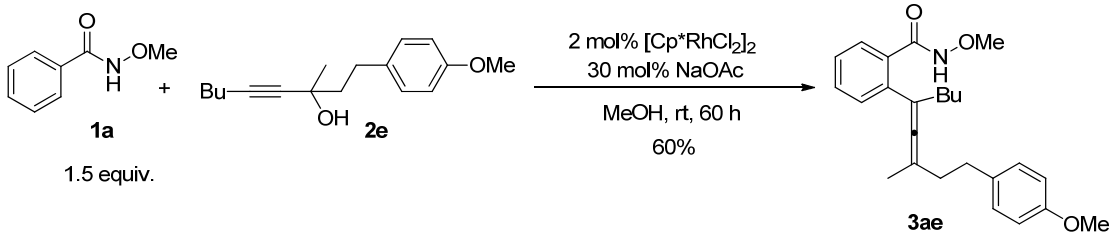
5. Preparation of *N*-methoxy-2-(3-ethyl-3,4-nonadien-5-yl)benzamide **3ad**. (Wsz-7-173)



The reaction of **1a** (226.8 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (12.5 mg, 0.02 mmol), NaOAc (24.3 mg, 0.3 mmol), and **2d** (167.9 mg, 1 mmol) in MeOH (6 mL) at rt (20 ^oC) afforded **3ad**[4] (220.5 mg, 73%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 7/1/0.2): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 9.08 (s, 1 H, NH), 7.67 (d, J = 7.5 Hz, 1 H, Ar-H), 7.39 (td, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1 H, Ar-H), 7.34-7.22 (m, 2 H, Ar-H), 3.85 (s, 3 H, OCH_3), 2.29 (t, J = 7.4 Hz, 2 H, CH_2), 2.08 (q, J = 7.4 Hz, 4 H, CH_2 × 2), 1.47-1.28 (m, 4 H, CH_2 × 2), 1.10 (t, J

= 7.4 Hz, 6 H, CH_3 × 2), 0.87 (t, *J* = 6.9 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.7, 167.5, 138.5, 130.8, 129.8, 129.3, 127.1, 110.4, 108.0, 64.3, 34.4, 30.4, 25.9, 22.3, 13.9, 12.6; IR ν (neat, cm^{-1}) 3193, 3061, 2962, 2932, 2873, 1953, 1659, 1594, 1572, 1498, 1459, 1439, 1376, 1305, 1153, 1035; MS (EI, 70 eV) *m*/*z* (%) 301 (M^+, 3.36), 270 (100).

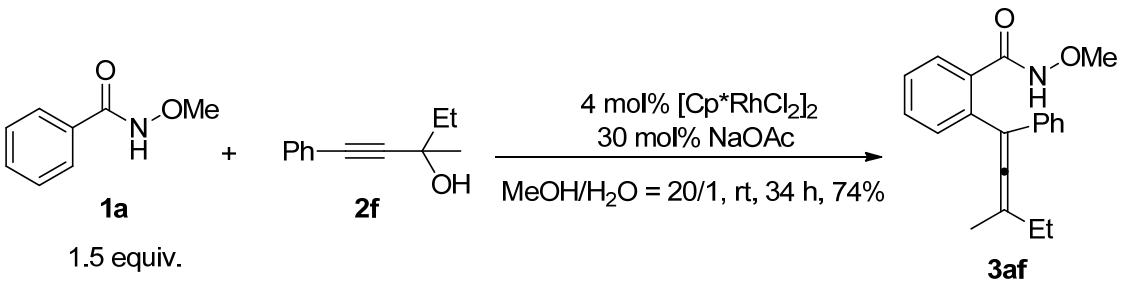
6. Preparation of *N*-methoxy-2-(3-methyl-9-(4-methoxylphenyl)-3,4-dodedien-5-yl) benzamide **3ae**. (Wsz-9-76)



The reaction of **1a** (226.7 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (12.6 mg, 0.02 mmol), NaOAc (24.3 mg, 0.3 mmol), and **2e** (260.1 mg, 1 mmol) in MeOH (6 mL) at rt (23 ^oC) afforded **3ae** (234.6 mg, 60%) (eluent: petroleum/ethyl acetate/dichloromethane = 8/1/0.3 to 5/1/0.3): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.32 (s, 1 H, NH), 7.47 (d, *J* = 7.5 Hz, 1 H, Ar-H), 7.37 (td, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1 H, Ar-H), 7.30-7.15 (m, 2 H, Ar-H), 7.01 (d, *J* = 8.7 Hz, 2 H, Ar-H), 6.65 (d, *J* = 8.7 Hz, 2 H, Ar-H), 3.78 (s, 3 H, OCH_3), 3.71 (s, 3 H, OCH_3), 2.69 (t, *J* = 7.2 Hz, 2 H, CH_2), 2.31 (t, *J* = 7.5 Hz, 2 H, CH_2), 2.28-2.16 (m, 2 H, CH_2), 1.80 (s, 3 H, CH_3), 1.38-1.25 (m, 4 H, CH_2 × 2), 0.87 (t, *J* = 7.1 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.2, 167.8, 157.5, 138.1, 133.6, 131.5, 130.4, 129.1, 129.0, 128.9, 126.6, 113.4, 104.5, 100.9, 64.2, 55.0, 36.0, 33.5, 32.5, 30.1, 22.2, 18.6, 13.9; IR ν (neat, cm^{-1}) 3207, 3061, 2955, 2932, 2870, 2857, 1953, 1661, 1611, 1512, 1465, 1440, 1368, 1300, 1246, 1178, 1158, 1106, 1036; MS (EI, 70 eV) *m*/*z* (%) 393 (M^+, 2.41), 121 (100); HRMS Calcd for $C_{25}H_{31}NO_3$ (M^+):

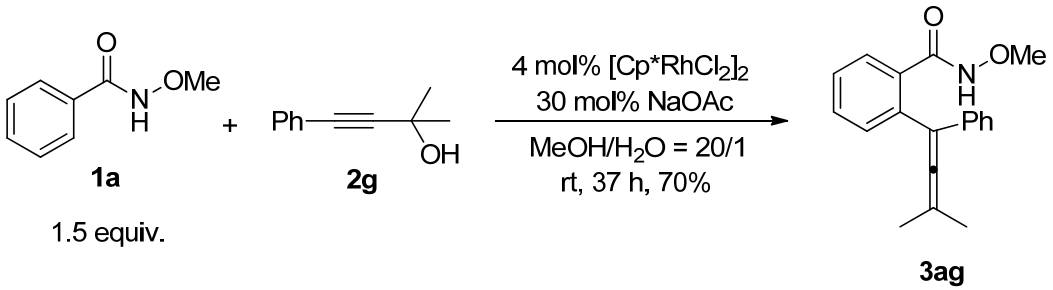
393.2304. Found: 393.2308.

7. Preparation of *N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadienyl)benzamide **3af**. (Wsz-7-6)



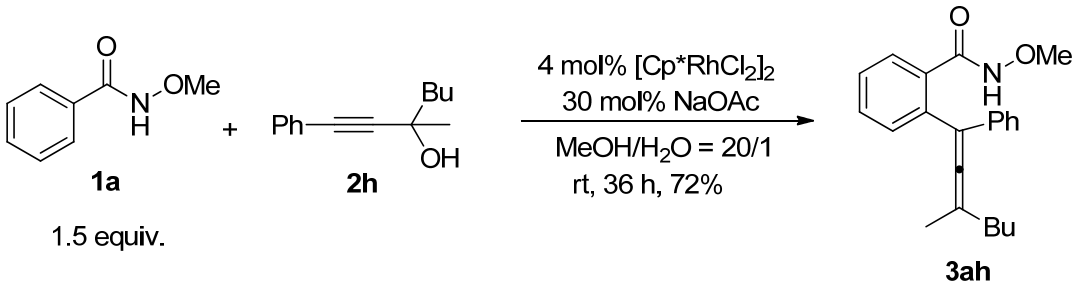
The reaction of **1a** (226.5 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.5 mg, 0.04 mmol), NaOAc (24.1 mg, 0.3 mmol), and **2f** (174.8 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (23 ^oC) afforded **3af**[4] (227.2 mg, 74%) (eluent: petroleum/ethyl acetate/dichloromethane = 6/1/0.3): solid; m.p. 104.9-106.2 ^oC (hexane/ethyl acetate), reproted in the ref: m.p. 105.9-107.5 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.69 (brs, 1 H, NH), 7.76 (d, *J* = 7.5 Hz, 1 H, Ar-H), 7.53-7.23 (m, 5 H, Ar-H), 7.22-7.16 (m, 3 H, Ar-H), 3.45 (s, 3 H, OCH_3), 2.25-2.08 (m, 2 H, CH_2), 1.89 (s, 3 H, CH_3), 1.13 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.0, 166.5, 137.3, 135.6, 132.5, 131.2, 131.1, 129.6, 128.6, 127.8, 127.0, 126.5, 107.5, 106.4, 63.8, 27.4, 18.7, 12.3; IR ν (neat, cm^{-1}) 3200, 3058, 3018, 2966, 2933, 1944, 1661, 1595, 1491, 1456, 1440, 1369, 1302, 1157, 1032; MS (EI, 70 eV) *m*/*z* (%) 308 (M^++1, 13.40), 307 (M^+, 10.81), 276 (100).

8. Preparation of *N*-methoxy-2-(1-phenyl-3-methyl-1,2-butadienyl)benzamide **3ag**. (Wsz-7-118)



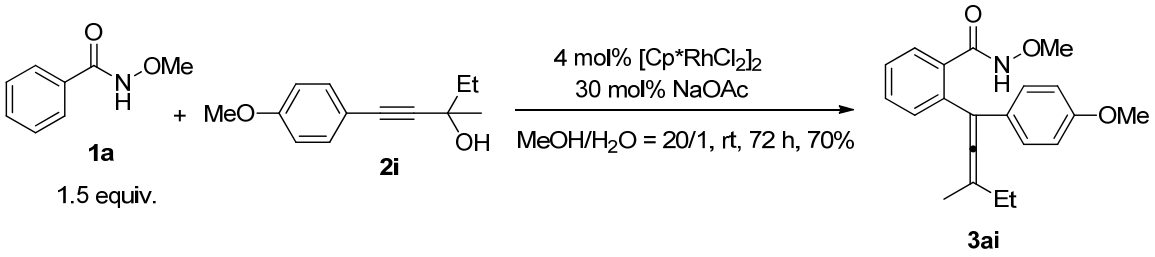
The reaction of **1a** (226.7 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.5 mg, 0.04 mmol), NaOAc (24.3 mg, 0.3 mmol), and **2g** (160.8 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (24 ^oC) afforded **3ag**[4] (205.6 mg, 70%) (eluent: petroleum/ethyl acetate/dichloromethane = 7/1/0.2): solid; m.p. 126.6-127.8 ^oC (hexane/ethyl acetate), reproted in the ref: 126.8-127.7 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.59 (brs, 1 H, NH), 7.73 (d, J = 7.2 Hz, 1 H, Ar-H), 7.53-7.37 (m, 2 H, Ar-H), 7.37-7.25 (m, 3 H, Ar-H), 7.24-7.15 (m, 3 H, Ar-H), 3.48 (s, 3 H, OCH_3), 1.88 (s, 6 H, 2 × CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.8, 166.8, 137.3, 135.6, 132.7, 131.1, 131.0, 129.5, 128.6, 127.8, 127.0, 126.8, 105.4, 99.9, 63.9, 20.1; IR ν (neat, cm^{-1}) 3199, 3057, 3022, 2977, 2934, 2911, 2856, 2814, 1950, 1659, 1595, 1491, 1440, 1376, 1361, 1301, 1182, 1158, 1101, 1033, 1017; MS (EI, 70 eV) m/z (%) 294 (M^++1, 6.50), 293 (M^+, 6.64), 262 (100).

9. Preparation of *N*-methoxy-2-(1-phenyl-3-methyl-1,2-heptadienyl)benzamide **3ah**. (Wsz-7-115)



The reaction of **1a** (226.6 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (25.1 mg, 0.04 mmol), NaOAc (25.2 mg, 0.3 mmol), and **2h** (201.9 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (24 ^oC) afforded **3ah** (241.7 mg, 72%) (eluent: petroleum/ethyl acetate/dichloromethane = 6/1/0.3 to 5/1/0.3): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.66 (brs, 1 H, NH), 7.78 (d, J = 7.2 Hz, 1 H, Ar-H), 7.53-7.47 (m, 2 H, Ar-H), 7.47-7.24 (m, 3 H, Ar-H), 7.24-7.14 (m, 3 H, Ar-H), 3.45 (s, 3 H, OCH_3), 2.15 (t, J = 7.5 Hz, 2 H, CH_2), 1.88 (s, 3 H, CH_3), 1.59-1.43 (m, 2 H, Ar-H), 1.42-1.26 (m, 2 H, Ar-H), 0.89 (t, J = 7.2 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.3, 166.5, 137.2, 135.5, 132.5, 131.2, 131.1, 129.6, 128.6, 127.9, 127.0, 126.5, 106.9, 104.7, 63.9, 34.0, 29.8, 22.4, 18.7, 13.9; IR ν (neat, cm^{-1}) 3197, 3058, 3024, 2956, 2930, 2871, 2861, 1950, 1659, 1599, 1492, 1465, 1439, 1376, 1301, 1153, 1032; MS (EI, 70 eV) m/z (%) 336 (M^++1, 3.25), 335 (M^+, 12.45), 304 (100); HRMS Calcd for $C_{22}H_{25}NO_2$ (M^+): 335.1885. Found: 335.1881.

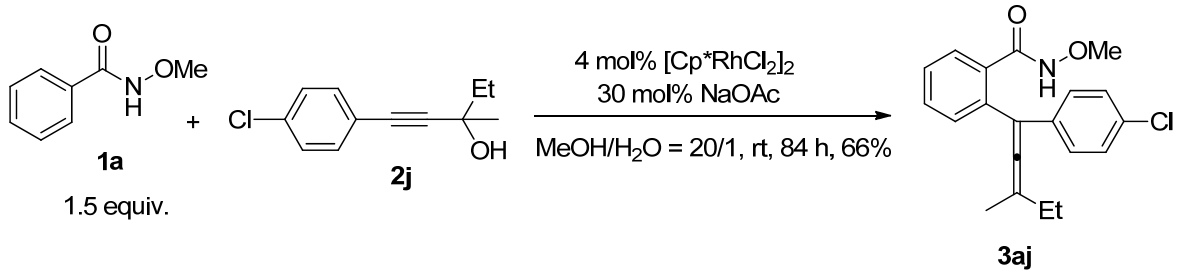
10. Preparation of *N*-methoxy-2-(1-(4-methoxylphenyl)-3-methyl-1,2-pentadienyl)-benzamide **3ai**. (Wsz-8-21)



The reaction of **1a** (226.1 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.5 mg, 0.04 mmol), NaOAc (24.9 mg, 0.3 mmol), and **2i** (204.6 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (10 ^oC) afforded **3ai** (236.1 mg, 70%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 4/1/0.3 to 2/1/0.3): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.74 (s, 1 H, NH), 7.79 (d, J = 7.2 Hz,

1 H, Ar-H), 7.54-7.37 (m, 2 H, Ar-H), 7.34 (d, J = 7.2 Hz, 1 H, Ar-H), 7.11 (d, J = 8.7 Hz, 2 H, Ar-H), 6.82 (d, J = 8.7 Hz, 2 H, Ar-H), 3.77 (s, 3 H, OCH_3), 3.50 (s, 3 H, OCH_3), 2.26-2.05 (m, 2 H, CH_2), 1.88 (s, 3 H, CH_3), 1.12 (t, J = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.2, 166.6, 158.8, 135.8, 132.4, 131.1, 129.7, 129.5, 127.8, 127.7, 114.1, 107.2, 106.3, 64.0, 55.2, 27.5, 18.8, 12.4; IR ν (neat, cm^{-1}) 3200, 3057, 2965, 2933, 2837, 1950, 1659, 1605, 1572, 1508, 1462, 1440, 1367, 1292, 1247, 1179, 1033; MS (EI, 70 eV) m/z (%) 337 (M^+, 1.98), 276 (100); HRMS calcd. for $C_{21}H_{23}NO_3$ (M^+): 337.1678; Found: 337.1671.

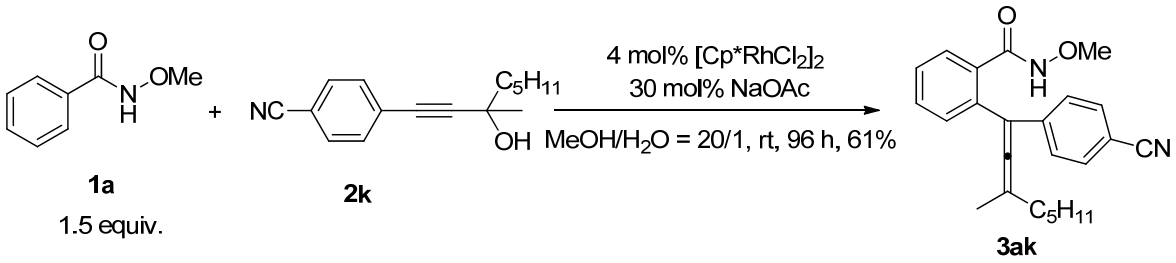
11. Preparation of *N*-methoxy-2-(1-(4-chlorophenyl)-3-methyl-1,2-pentadienyl)-benzamide **3aj**. (Wsz-7-184)



The reaction of **1a** (226.1 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.5 mg, 0.04 mmol), NaOAc (24.9 mg, 0.3 mmol), and **2j** (208.5 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (19 ^oC) afforded **3aj** (224.6 mg, 66%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 3.5/1/3.5): solid; m.p. 142.3-143.9 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.71 (s, 1 H, NH), 7.68 (d, J = 7.2 Hz, 1 H, Ar-H), 7.48 (td, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1 H, Ar-H), 7.44-7.37 (m, 1 H, Ar-H), 7.33 (dd, J_1 = 7.5 Hz, J_2 = 0.6 Hz, 1 H, Ar-H), 7.23 (d, J = 9.0 Hz, 2 H, Ar-H), 7.12 (d, J = 8.7 Hz, 2 H, Ar-H), 3.50 (s, 3 H, OCH_3), 2.24-2.06 (m, 2 H, CH_2), 1.88 (s, 3 H, CH_3), 1.11 (t, J = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.0,

166.6, 136.0, 135.4, 132.7, 132.6, 131.1, 129.4, 128.6, 127.9, 127.8, 106.75, 106.72, 64.0, 27.4, 18.6, 12.3; IR ν (KBr, cm^{-1}) 3436, 3268, 2973, 2931, 1953, 1659, 1492, 1465, 1439, 1385, 1364, 1275, 1086, 1031, 1010; MS (EI, 70 eV) *m*/*z* (%) 343 ($M(^{37}Cl)^+$, 0.06), 341 ($M(^{35}Cl)^+$, 0.21), 309 (100), 294 ($M(^{35}Cl)^+$-NH_2OMe, 67.23), 259 ($M(^{35}Cl)^+$-NH_2OMeCl, 85.07); Anal. Calcd for $C_{20}H_{20}ClNO_2$: C 70.27, H 5.90, N 4.10. Found: C 70.18, H 6.00, N 4.03.

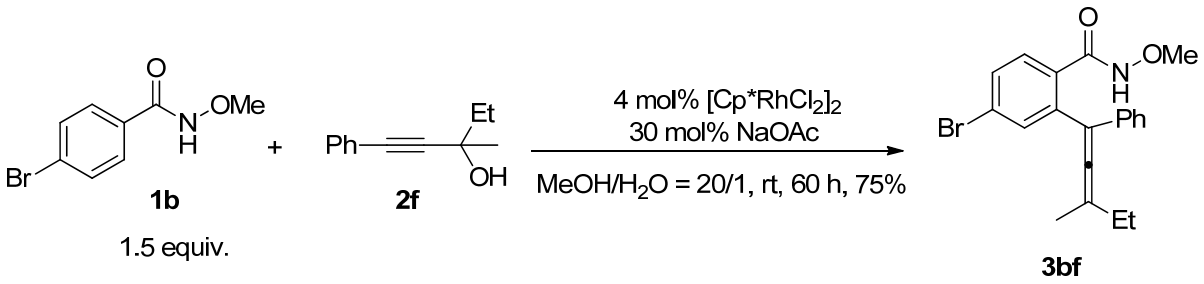
12. Preparation of N-methoxy-2-(1-(4-cyanophenyl)-3-methyl-1,2-octadienyl)benzamide **3ak**. (Wsz-8-158)



The reaction of **1a** (226.7 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.6 mg, 0.04 mmol), NaOAc (24.4 mg, 0.3 mmol), and **2k** (241.3 mg, 1 mmol) in MeOH (6 mL), and H_2O (0.3 mL) at rt (19 ^oC) afforded **3ak** (227.8 mg, 61%) (eluent: petroleum/ethyl acetate/dichloromethane = 4/1/0.3 to 3/1/0.3): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.56 (s, 1 H, NH), 7.64 (d, J = 7.5 Hz, 1 H, Ar-H), 7.56-7.46 (m, 3 H, Ar-H), 7.41 (td, J_1 = 7.4 Hz, J_2 = 1.2 Hz, 1 H, Ar-H), 7.36-7.20 (m, 3 H, Ar-H), 3.53 (s, 3 H, OCH_3), 2.16 (t, J = 7.7 Hz, 2 H, CH_2), 1.89 (s, 3 H, CH_3), 1.58-1.43 (m, 2 H, CH_2), 1.46-1.22 (m, 4 H, CH_2 × 2), 0.83 (t, J = 7.1 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.6, 166.6, 142.7, 134.9, 132.8, 132.2, 131.1, 129.0, 128.1, 127.1, 118.9, 109.9, 106.1, 105.5, 64.0, 34.0, 31.5, 27.2, 22.3, 18.3, 13.9; IR ν (neat, cm^{-1}) 3201, 2955, 2929, 2855, 2225, 1944, 1660, 1603, 1500, 1466, 1440, 1378, 1304, 1159, 1033;

MS (EI, 70 eV) *m*/*z* (%) 375 (M^++1, 3.31), 374 (M^+, 5.01), 57 (100); HRMS Calcd for $C_{24}H_{26}N_2O_2$ (M^+): 374.1994. Found: 374.1998.

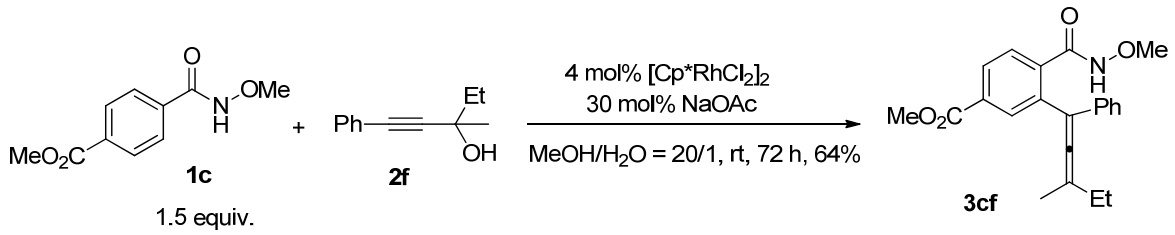
13. Preparation of *N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadienyl)-4-bromobenzamide **3bf**. (Wsz-7-8)



The reaction of **1b** (344.8 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.5 mg, 0.04 mmol), NaOAc (25.1 mg, 0.3 mmol), and **2f** (175.1 mg, 1 mmol) in MeOH (6 mL), and H_2O (0.3 mL) at rt (30 ^oC) afforded **3bf**[4] (290.2 mg, 75%) (eluent: petroleum/ethyl acetate/dichloromethane = 6/1/0.4): solid; m.p. 135.5-137.0 ^oC (hexane/ethyl acetate), reproted in the ref: 134.6-135.8 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.67 (s, 1 H, NH), 7.63 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.58-7.46 (m, 2 H, Ar-H), 7.36-7.13 (m, 5 H, Ar-H), 3.43 (s, 3 H, OCH_3), 2.28-2.08 (m, 2 H, CH_2), 1.90 (s, 3 H, CH_3), 1.13 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.1, 165.6, 137.6, 136.7, 133.9, 131.4, 131.2, 131.0, 128.7, 127.3, 126.4, 125.4, 107.2, 106.6, 63.9, 27.4, 18.6, 12.4; IR *ν* (neat, cm^{-1}) 3182, 2967, 2933, 1947, 1659, 1580, 1557, 1492, 1455, 1368, 1305, 1160, 1080, 1035; MS (EI, 70 eV) *m*/*z* (%) 388 ($M^+(Br^{81})$+1, 17.40), 387 ($M^+(Br^{81})$, 10.59), 386 ($M^+(Br^{79})$+1, 17.70), 385 ($M^+(Br^{79})$, 7.47), 356 (100).

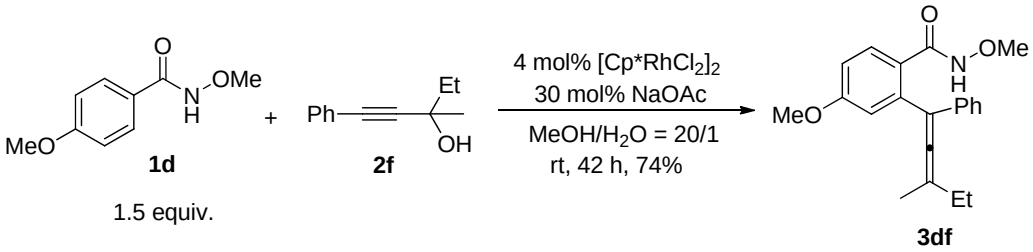
14. Preparation of *N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadienyl)-4-methoxycarbonyl-

benzamide **3cf**. (Wsz-8-47)



The reaction of **1c** (209.5 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.5 mg, 0.04 mmol), NaOAc (24.3 mg, 0.3 mmol), and **2f** (173.9 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (10 ^oC) afforded **3cf** (233.0 mg, 64%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 3/1/0.3): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.65 (s, 1 H, NH), 8.08-7.97 (m, 2 H, Ar-H), 7.81 (d, J = 7.8 Hz, 1 H, Ar-H), 7.33-7.24 (m, 2 H, Ar-H), 7.24-7.12 (m, 3 H, Ar-H), 3.93 (s, 3 H, OCH_3), 3.48 (s, 3 H, OCH_3), 2.27-2.08 (m, 2 H, CH_2), 1.90 (s, 3 H, CH_3), 1.13 (t, J = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.2, 166.1, 165.7, 136.9, 136.6, 136.2, 132.32, 132.26, 129.6, 128.7, 127.1, 126.5, 106.9, 106.7, 63.9, 52.3, 27.4, 18.5, 12.3; IR ν (neat, cm^{-1}) 3191, 2966, 2932, 1950, 1726, 1663, 1492, 1437, 1412, 1367, 1301, 1244, 1188, 1163, 1118, 1096, 1035; MS (EI, 70 eV) m/z (%) 365 (M^+, 4.40), 304 (100). HRMS calcd. for $C_{22}H_{23}NO_4$ (M^+): 365.1627; Found: 365.1622.

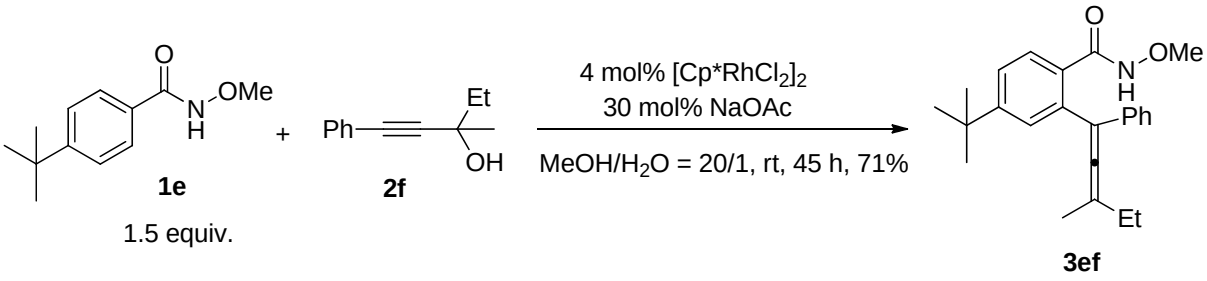
15. Preparation of *N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadienyl)-4-methoxy-benzamide **3df**. (Wsz-7-110)



The reaction of **1d** (271.2 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.5 mg, 0.04 mmol), NaOAc

(25.1 mg, 0.3 mmol), and **2f** (174.3 mg, 1 mmol) in MeOH (6 mL), and H_2O (0.3 mL) at rt (20 ^oC) afforded **3df**[4] (249.0 mg, 74%) (eluent: petroleum/ethyl acetate/dichloromethane = 3.5/1/1): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.76 (s, 1 H, NH), 7.81 (d, J = 8.7 Hz, 1 H, Ar-H), 7.33-7.24 (m, 2 H, Ar-H), 7.24-7.16 (m, 3 H, Ar-H), 6.94 (dd, J_1 = 8.9 Hz, J_2 = 2.6 Hz, 1 H, Ar-H), 6.85 (d, J = 2.4 Hz, 1 H, Ar-H), 3.83 (s, 3 H, OCH_3), 3.42 (s, 3 H, OCH_3), 2.28-2.07 (m, 2 H, CH_2), 1.90 (s, 3 H, CH_3), 1.14 (t, J = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.6, 166.2, 161.6, 137.3, 136.9, 131.7, 128.6, 127.1, 126.4, 124.7, 116.6, 113.0, 107.8, 106.6, 63.8, 55.3, 27.4, 18.7, 12.4; IR ν (neat, cm^{-1}) 3203, 2965, 2933, 1944, 1659, 1599, 1568, 1490, 1367, 1316, 1287, 1224, 1182, 1156, 1109, 1028; MS (EI, 70 eV) *m*/*z* (%) 337 (M^+, 5.76), 276 (100).

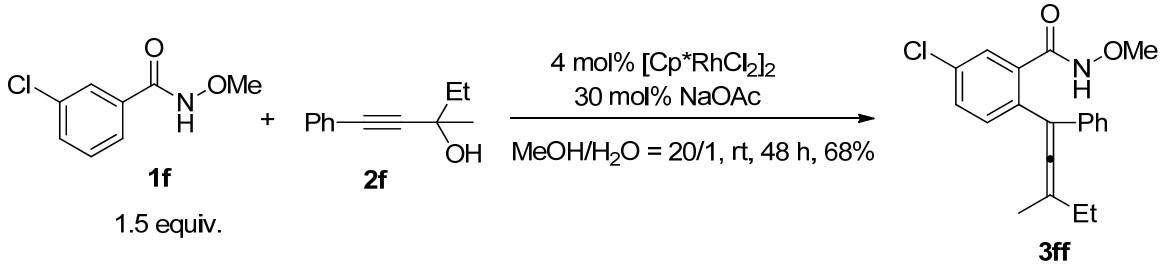
16. Preparation of *N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadienyl)-4-tert-butylbenzamide **3ef**. (Wsz-7-199)



The reaction of **1e** (311.2 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.6 mg, 0.04 mmol), NaOAc (24.1 mg, 0.3 mmol), and **2f** (174.5 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (13 ^oC) afforded **3ef**[4] (259.8 mg, 71%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 6/1/0.4): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.70 (s, 1 H, NH), 7.76 (d, J = 8.1 Hz, 1 H, Ar-H), 7.45 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1 H, Ar-H), 7.38-7.10 (m, 6 H, Ar-H), 3.43 (s, 3 H, OCH_3), 2.28-2.07 (m, 2 H, CH_2), 1.90 (s, 3 H, CH_3), 1.33 (s, 9 H, $CH_3\times$ 3), 1.15 (t, J = 7.4 Hz,

3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.9, 166.5, 154.7, 137.2, 135.0, 129.6, 129.5, 128.6, 128.2, 127.0, 126.4, 125.0, 108.2, 106.3, 63.8, 34.8, 31.1, 27.4, 18.7, 12.4; IR ν (neat, cm^{-1}) 3222, 2964, 2932, 2908, 2872, 1947, 1662, 1601, 1491, 1460, 1395, 1364, 1307, 1256, 1203, 1179, 1095, 1032; MS (EI, 70 eV) *m*/z (%) 364 (M^++1, 11.00), 363 (M^+, 7.19), 332 (100).

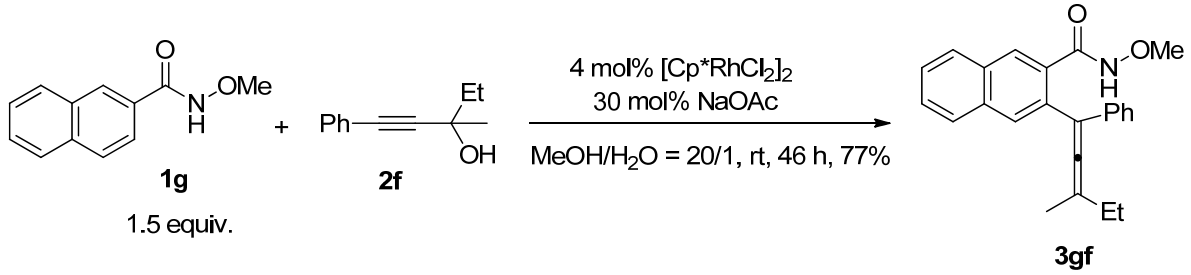
17. Preparation of *N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadienyl)-5-chlorobenzamide **3ff**. (Wsz-8-6)



The reaction of **1f** (278.3 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.8 mg, 0.04 mmol), NaOAc (24.1 mg, 0.3 mmol), and **2f** (174.5 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (27 ^oC) afforded **3ff** (233.7 mg, 68%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 7/1/0.3): solid; m.p. 106.2-107.5 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.70 (s, 1 H, NH), 7.74 (d, J = 1.5 Hz, 1 H, Ar-H), 7.44 (dd, J_1 = 8.1 Hz, J_2 = 2.4 Hz, 1 H, Ar-H), 7.35-7.29 (m, 3 H, Ar-H), 7.28-7.13 (m, 3 H, Ar-H), 3.45 (s, 3 H, OCH_3), 2.26-2.07 (m, 2 H, CH_2), 1.88 (s, 3 H, CH_3), 1.11 (t, J = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.1, 165.1, 136.9, 134.2, 134.0, 133.8, 132.6, 131.1, 129.5, 128.7, 127.2, 126.4, 106.8, 106.6, 63.9, 27.4, 18.6, 12.3; IR ν (neat, cm^{-1}) 3188, 3078, 3059, 3018, 2967, 2934, 2837, 2816, 1947, 1660, 1597, 1492, 1455, 1369, 1303, 1160, 1114, 1039; MS (EI, 70 eV) *m*/z (%) 343 ($M(^{37}Cl)^+$, 0.08), 341 ($M(^{35}Cl)^+$, 0.23), 311 ($M(^{35}Cl)^+$-OMe+H, 69.83), 280 (100); Anal.

Calcd for $C_{20}H_{20}ClNO_2$: C 70.27, H 5.90, N 4.10. Found: C 70.17, H 5.91, N 4.06.

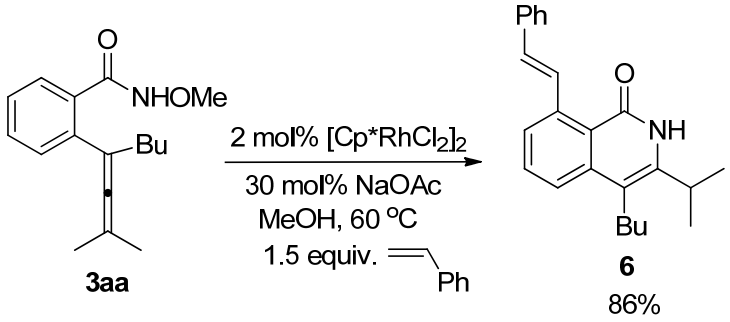
18. Preparation of *N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadienyl)-2-naphthamide **3gf**. (Wsz-8-40)



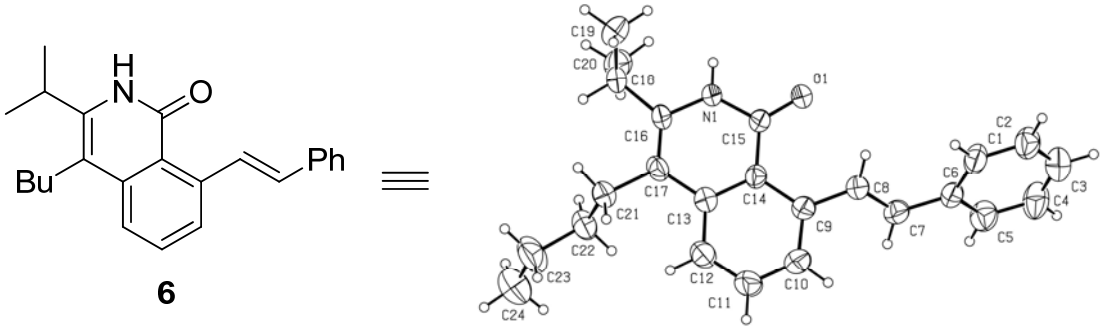
The reaction of **1g** (302.1 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (24.5 mg, 0.04 mmol), NaOAc (24.9 mg, 0.3 mmol), and **2f** (174.4 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt (10 ^oC) afforded **3gf** (275.1 mg, 77%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 5/1/0.5): solid; m.p. 146.4-147.9 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.80 (s, 1 H, NH), 8.31 (s, 1 H, Ar-H), 7.91 (d, J = 6.9 Hz, 1 H, Ar-H), 7.88-7.78 (m, 2 H, Ar-H), 7.62-7.48 (m, 2 H, Ar-H), 7.33-7.15 (m, 5 H, Ar-H), 3.46 (s, 3 H, OCH_3), 2.28-2.12 (m, 2 H, CH_2), 1.94 (s, 3 H, CH_3), 1.18 (t, J = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.4, 166.4, 137.6, 134.4, 132.4, 132.1, 130.5, 130.4, 128.6, 128.5, 127.9, 127.6, 127.0, 126.8, 126.7, 107.9, 106.2, 63.9, 27.5, 18.8, 12.5; IR ν (neat, cm^{-1}) 3189, 3055, 2966, 2932, 1947, 1658, 1596, 1491, 1456, 1438, 1373, 1300, 1260, 1194, 1147, 1095, 1025; MS (EI, 70 eV) *m*/*z* (%) 358 (M^++1, 7.11), 357 (M^+, 9.84), 326 (100); Anal. Calcd for $C_{24}H_{23}NO_2$: C 80.64, H 6.49, N 3.92. Found: C 80.39, H 6.47, N 3.81.

Synthetic applications

1. The synthesis of (*E*)-4-butyl-3-isopropyl-8-styrylisoquinolin-1(*2H*)-one **6**.[7] (Wsz-9-9)



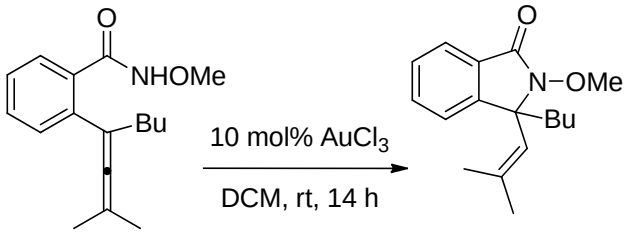
To a dried Schlenk tube equipped with a Teflon-coated magnetic stirring bar were added **3aa** (82.2 mg, 0.2 mmol), $[Cp^*RhCl_2]_2$ (3.8 mg, 0.006 mmol), NaOAc (7.1 mg, 0.09 mmol), styrene (46.9 mg, 0.45 mmol), and MeOH (1.5 mL) sequentially at rt. The Schlenk tube was then equipped with a condenser. After being stirred for 25 h at 60 °C, the reaction was complete as monitored by TLC (eluent: petroleum ether/ethyl acetate = 3/1). Filtration through a short column of silica gel (eluent: (dichloromethane/ethyl acetate = 1/1) (20 mL × 3)) and evaporation afforded the crude product, which was purified by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate/dichloromethane = 20/1/0.1) to afford **6** (89.1 mg, 86%): solid; m.p. 222.9-224.3 °C (dichloromethane/diethyl ether); ^{1}H NMR (300 MHz, $CDCl_3$) δ 11.00 (s, 1 H, NH), 8.74 (d, *J* = 16.2 Hz, 1 H, =CH), 7.70-7.49 (m, 5 H, Ar-H), 7.36 (t, *J* = 7.5 Hz, 2 H, Ar-H), 7.32-7.20 (m, 1 H, Ar-H), 6.85 (d, *J* = 16.2 Hz, 1 H, =CH), 3.17 (h, *J* = 6.7 Hz, 1 H, CH), 2.69 (t, *J* = 7.4 Hz, 2 H, CH_2), 1.58-1.37 (m, 4 H, CH_2 × 2), 1.20 (d, *J* = 6.9 Hz, 6 H, CH_3 × 2), 0.96 (t, *J* = 6.9 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.4, 143.1, 141.5, 140.0, 138.3, 132.0, 131.7, 129.8, 128.4, 127.2, 127.1, 125.1, 122.8, 122.2, 111.1, 32.6, 28.4, 26.5, 23.0, 20.6, 14.0; IR ν (neat, cm^{-1}) 3172, 3073, 3021, 2958, 2926, 1641, 1587, 1553, 1491, 1465, 1447, 1328, 1296; MS (EI, 70 eV) *m*/*z* (%) 346 (M^++1, 20.44), 345 (M^+, 77.71), 302 (100); Anal. Calcd for $C_{24}H_{27}NO$: C 83.44, H 7.88, N 4.05. Found: C 83.17, H 7.76, N 3.80.



ORTEP representation of **6**

6: $C_{24}H_{27}NO$, MW = 345.46, triclinic, space group P -1, final R indices I > 2\s(I), R1 = 0.0889, wR2 = 0.1758; Rindices (all data), R1 = 0.2693, wR2 = 0.2639; a = 8.316(2) Å, b = 10.229(2) Å, c = 13.179(3) Å, α = 69.905(18)°, β = 82.818(18)°, γ = 72.230(19)°, V = 1002.4(4) $Å^3$, T = 293(2) K, Z = 2, reflections collected/unique 6466/3643 (R_{int} = 0.0886), number of observations [> 2σ(I)]: 1151, parameters: 238. Supplementary crystallographic data have been deposited at the Cambridge Crystallographic Data Centre, CCDC 1526789.

2. The synthesis of 3-butyl-2-methoxy-3-(2-methylprop-1-en-1-yl)isoindolin-1-one **7**.[8] (Wsz-9-66)

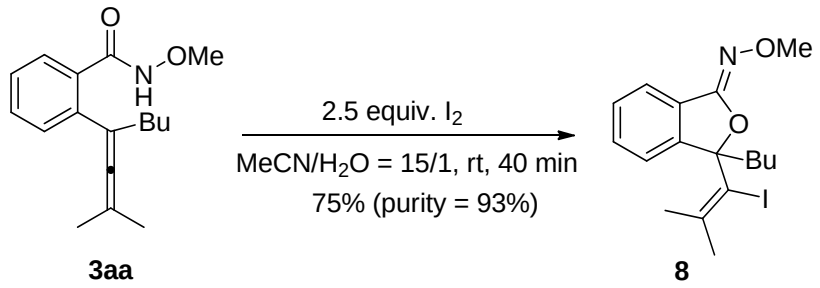


3aa **7** 83%

A dried Schlenk tube equipped with a Teflon-coated magnetic stirring bar was evacuated

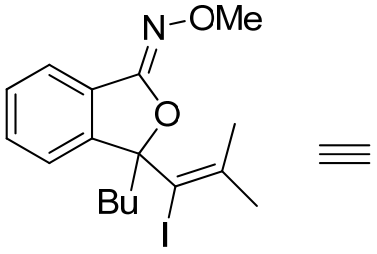
and backfilled with nitrogen for three times. Then $AuCl_3$ (9.4 mg, 0.03 mmol) was added to it in the glovebox. Then **3aa** (81.6 mg, 0.3 mmol) and DCM (2 mL) were added sequentially at rt. After being stirred for 14 h at rt, the reaction was complete as monitored by TLC. Filtration through a short column of silica gel (eluent: ethyl acetate 20 mL × 3) and evaporation afforded the crude product, which was purified by flash column chromatography on silica gel (eluent: petroleum/ethyl acetate = 15/1) to afford **7** (67.5 mg, 83%): solid; m.p. 47.3-48.8 ^{o}C (hexane/ethyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (d, J = 7.5 Hz, 1 H, Ar-H), 7.54 (td, J_1 = 7.6 Hz, J_2 = 1.1 Hz, 1 H, Ar-H), 7.42 (t, J = 7.4 Hz, 1 H, Ar-H), 7.22 (d, J = 7.5 Hz, 1 H, Ar-H), 5.45 (t, J = 1.4 Hz, 1 H, =CH), 3.97 (s, 3 H, OCH_3), 2.24-2.09 (m, 1 H, one proton of CH_2), 2.02-1.88 (m, 1 H, one proton of CH_2), 1.74 (d, J = 0.9 Hz, 3 H, CH_3), 1.31-1.05 (m, 5 H, $CH_2 + CH_3$), 1.03-0.87 (m, 1 H, one proton of CH_2), 0.75 (t, J = 7.4 Hz, 3 H, CH_3), 0.55-0.38 (m, 1 H, one proton of CH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.1, 147.1, 140.5, 132.3, 129.7, 127.7, 123.4, 123.3, 121.7, 67.6, 64.1, 39.5, 27.0, 24.4, 22.3, 18.2, 13.8; IR ν (neat, cm^{-1}) 2958, 2936, 2863, 1713, 1661, 1611, 1467, 1340, 1087, 1003; MS (EI, 70 eV) m/z (%) 273 (M^+, 3.75), 216 (100); Anal. Calcd for $C_{17}H_{23}NO_2$: C 74.69, H 8.48, N 5.12. Found: C 74.56, H 8.28, N 4.89.

3. The synthesis of (*Z*)-3-butyl-3-(1-iodo-2-methylprop-1-en-1-yl)isobenzofuran-1(3H)-one *O*-methyl oxime **8**.[9] (Wsz-9-97)

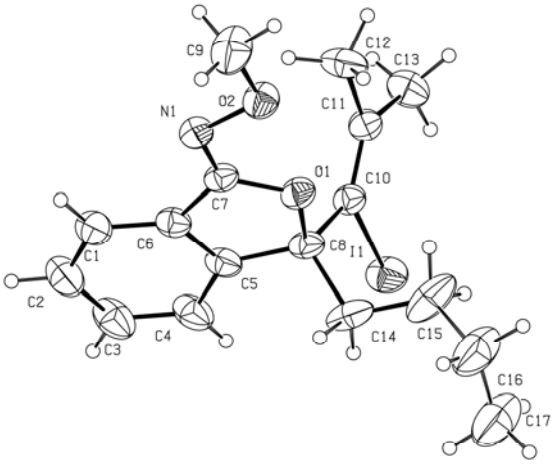


3aa **8**

To a dried Schlenk tube equipped with a Teflon-coated magnetic stirring bar were added **3aa** (164.2 mg, 0.6 mmol), MeCN (2 mL), H_2O (0.13 mL), and I_2 (380.5 mg, 1.5 mmol) sequentially at rt. After being stirred for 40 min at rt, the reaction was complete as monitored by TLC. H_2O (10 mL) was added to the resulting mixture with stirring. After another 10 min, a saturated aqueous solution of $Na_2S_2O_3$ (5 mL) was added to quench the reaction and the resulting mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. Filtration, evaporation, and purification by flash column chromatography on silica gel (eluent: petroleum/ethyl acetate = 100/1 to petrpleum/ethyl acetate/dichloromethane = 40/1/0.4) afforded **8** (193.7 mg, 75%, purity = 93%): soild; m.p. 85.2-86.7 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.65 (t, J = 8.4 Hz, 2 H, Ar-H), 7.50-7.34 (m, 2 H, Ar-H), 3.94 (s, 3 H, OCH_3), 2.61-2.46 (m, 1 H, one proton of CH_2), 2.28-2.12 (m, 1 H, one proton of CH_2), 2.08 (s, 3 H, CH_3), 1.92 (s, 3 H, CH_3), 1.43-1.19 (m, 3 H, CH_2 + one proton of CH_2), 1.04-0.89 (m, 1 H, one proton of CH_2), 0.83 (t, J = 7.1 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.9, 146.6, 142.9, 130.5, 128.7, 128.3, 123.4, 121.0, 100.3, 95.4, 62.6, 44.0, 37.0, 25.6, 22.4, 21.9, 13.9; IR ν (neat, cm^{-1}) 2956, 2932, 2871, 2814, 1773, 1659, 1609, 1468, 1347, 1306, 1272, 1189, 1158, 1130, 1092, 1052, 1019; MS (EI, 70 eV) m/z (%) 400 (M^++1, 2.25), 399 (M^+, 9.23), 184 (100); HRMS Calcd for $C_{17}H_{22}NO_2I$ (M^+): 399.0695. Found: 399.0694.



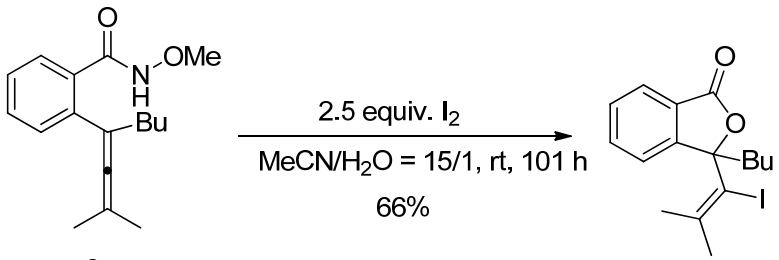
8



ORTEP representation of **8**

8: $C_{17}H_{22}INO_2$, MW = 399.26, monoclinic, space group P 1 21/n 1, final R indices [I > 2σ(I)], R1 = 0.0460, wR2 = 0.0999; Rindices (all data), R1 = 0.0708, wR2 = 0.1149; a = 11.7810(10) Å, b = 12.2621(7) Å, c = 12.7517(10) Å, α = 90.00°, β = 110.261(9)°, γ = 90.00°, V = 1728.1(2) $Å^3$, T = 293(2) K, Z = 4, reflections collected/unique 7006/3159 (R_{int} = 0.0326), number of observations [> 2σ(I)]: 2229, parameters: 214. Supplementary crystallographic data have been deposited at the Cambridge Crystallographic Data Centre, CCDC 1525866.

4. The synthesis of 3-butyl-3-(1-iodo-2-methylprop-1-en-1-yl)isobenzofuran-1(3H)-one **9**. (Wsz-9-109)

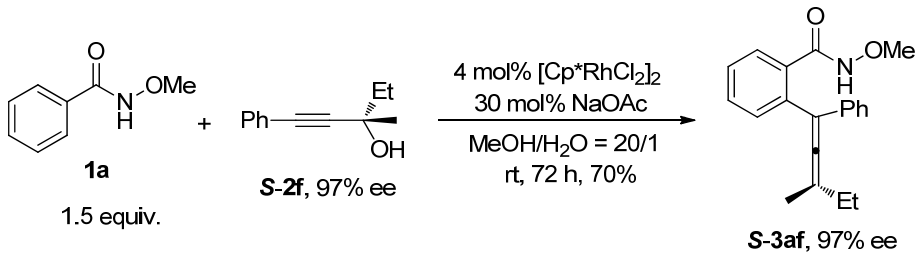


3aa **9**

To a dried Schlenk tube equipped with a Teflon-coated magnetic stirring bar were added **3aa** (164.3 mg, 0.6 mmol), MeCN (2 mL), H_2O (0.13 mL), and I_2 (380.5 mg, 1.5 mmol) sequentially at rt. After being stirred for 101 h at rt, the reaction was complete as monitored by TLC. H_2O (10 mL) was added to the resulting mixture with stirring for another 10 min. Then a saturated aqueous solution of $Na_2S_2O_3$ (5 mL) was added to quench the reaction and the resulting mixture was extracted with ethyl acetate (3 × 20 mL). The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. Filtration, evaporation, and purification by flash column chromatography on silica gel (eluent: petroleum/ethyl acetate = 50/1) afforded **9** (147.1 mg, 66%): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (d, J = 7.5 Hz, 1 H, Ar-H), 7.86 (d, J = 7.5 Hz, 1 H, Ar-H), 7.67 (td, J_1 = 7.5 Hz, J_2 = 1.1 Hz, 1 H, Ar-H), 7.53 (td, J_1 = 7.4 Hz, J_2 = 0.7 Hz, 1 H, Ar-H), 2.69-2.56 (m, 1 H, one proton of CH_2), 2.13-1.98 (m, 7 H, CH_3 × 2 + one proton of CH_2), 1.44-1.22 (m, 3 H, CH_2 + one proton of CH_2), 1.14-0.99 (m, 1 H, one proton of CH_2), 0.85 (t, J = 7.2 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.6, 152.5, 142.7, 133.5, 129.3, 125.7, 125.2, 124.5, 98.6, 91.5, 42.2, 37.0, 25.7, 22.8, 22.4, 13.8; IR ν (neat, cm^{-1}) 2956, 2929, 2870, 1770, 1610, 1592, 1465, 1379, 1364, 1336, 1286, 1266, 1243, 1216, 1159, 1128, 1079, 1017; MS (EI, 70 eV) *m*/*z* (%) 370 (M^+, 5.21), 186 (100); HRMS Calcd for $C_{16}H_{19}O_2I$ (M^+): 370.0430. Found: 370.0433.

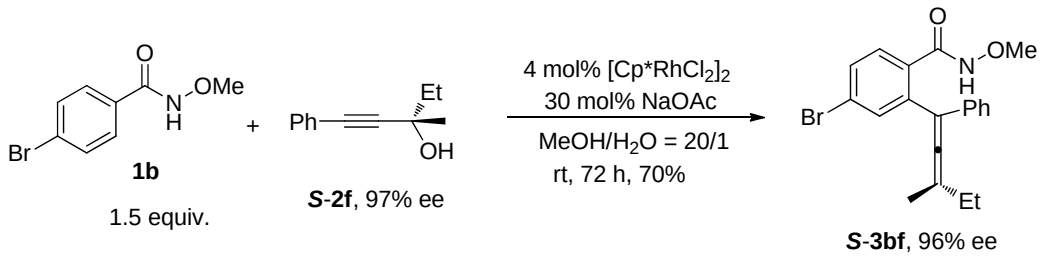
Asymmetric synthesis of tetral-substituted allenes by chirality transfer

1. Preparation of *S*-*N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadien-1-yl)benzamide ***S*-3af**. (Wsz-8-17)



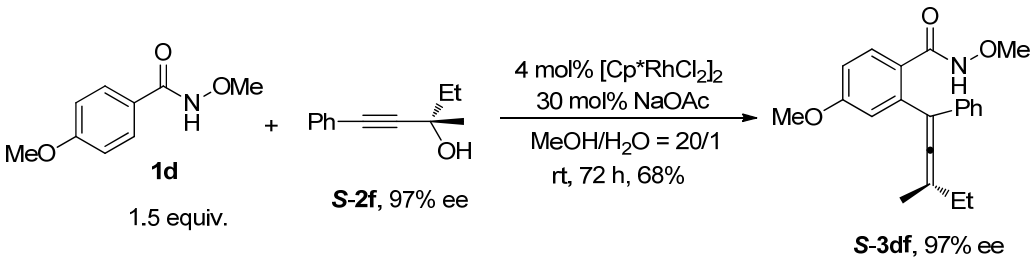
The reaction of **1a** (68.2 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.3 mg, 0.012 mmol), NaOAc (7.7 mg, 0.09 mmol), and ***S*-2f** (97% ee, 52.5 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 mL) at rt (8 ^oC) afforded ***S*-3af**[4] (64.5 mg, 70%) (eluent: petroleum/ethyl acetate/dichloromethane = 5/1/0.3): 97% ee (HPLC conditions: Chiralcel AD-H column, hexane/*i*-PrOH = 10/1, 1.0 mL/min, λ = 207 nm, t_R(minor) = 19.892 min, t_R(major) = 21.832 min); $[\alpha]_D^{20}$ = +12.3 (*c* = 0.75, $CHCl_3$); solid; m.p. 100.2-101.2 ^oC (hexane/ethyl acetate), reproted in the ref: 99.9-101.1 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.64 (s, 1 H, NH), 7.78 (dd, J_1 = 7.4 Hz, J_2 = 1.1 Hz, 1 H, Ar-H), 7.52-7.39 (m, 2 H, Ar-H), 7.38-7.24 (m, 3 H, Ar-H), 7.23-7.16 (m, 3 H, Ar-H), 3.46 (s, 3 H, OCH_3), 2.27-2.08 (m, 2 H, CH_2), 1.89 (s, 3 H, CH_3), 1.13 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.0, 166.6, 137.3, 135.6, 132.5, 131.2, 131.1, 129.6, 128.7, 127.9, 127.1, 126.5, 107.6, 106.4, 63.9, 27.4, 18.7, 12.4; IR ν(neat, cm^{-1}) 3200, 3058, 3024, 2966, 2932, 1944, 1659, 1596, 1492, 1439, 1370, 1301, 1153, 1099, 1032; MS (EI, 70 eV) *m*/*z* (%) 308 (M^++1, 4.12), 307 (M^+, 4.29), 276 (100).

2. Preparation of *S*-*N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadien-1-yl)-4-bromo-benzamide ***S*-3bf**. (Wsz-8-20)



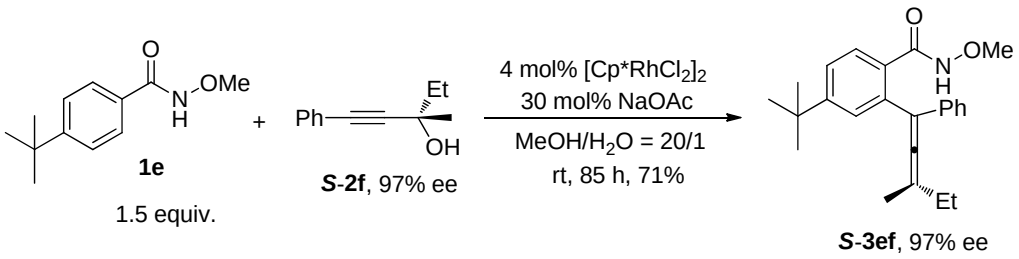
The reaction of **1b** (103.7 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.3 mg, 0.012 mmol), NaOAc (7.7 mg, 0.09 mmol), and ***S*-2f** (97% ee, 52.8 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 mL) at rt (12 ^oC)afforded ***S*-3bf**[4] (81.6 mg, 70%) (eluent: petroleum/ethyl acetate/dichloromethane = 5/1/0.3): 96% ee (HPLC conditions: Chiralcel AD-H column, hexane/*i*-PrOH = 10/1, 0.7 mL/min, λ = 207 nm, t_R(minor) = 26.202 min, t_R(major) = 28.337 min); $[\alpha]_D^{20}$ = +0.1 (*c* = 0.77, $CHCl_3$); solid; m.p. 134.4-135.7 ^oC (hexane/ethyl acetate), reproted in the ref: 121.7-123.1 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.73 (s, 1 H, NH), 7.61 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.56-7.46 (m, 2 H, Ar-H), 7.34-7.04 (m, 5 H, Ar-H), 3.42 (s, 3 H, OCH_3), 2.25-2.09 (m, 2 H, CH_2), 1.90 (s, 3 H, CH_3), 1.13 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.1, 165.5, 137.7, 136.7, 133.8, 131.4, 131.1, 130.9, 128.7, 127.2, 126.4, 125.3, 107.1, 106.6, 63.8, 27.4, 18.6, 12.3; IR ν (neat, cm^{-1}) 3181, 2966, 2933, 1944, 1659, 1580, 1557, 1492, 1455, 1367, 1305, 1160, 1080, 1035; MS (EI, 70 eV) *m*/*z* (%) 387 ($M^+(Br^{81})$, 3.42), 385 ($M^+(Br^{79})$, 3.74), 245 (100).

3. Preparation of *S*-*N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadien-1-yl)-4-methoxy-benzamide ***S*-3df**. (Wsz-8-22)



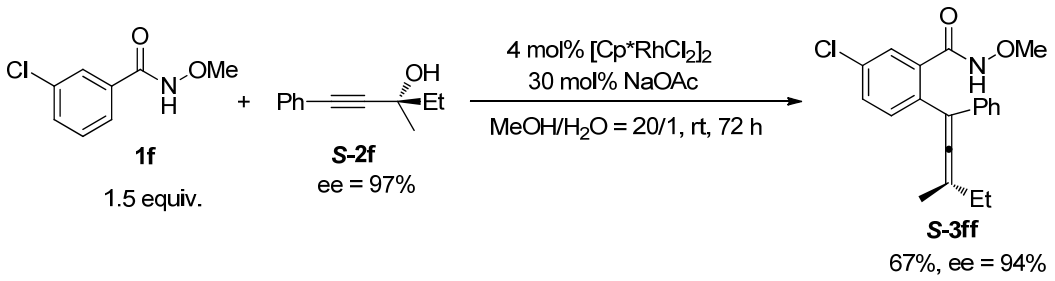
The reaction of **1d** (81.7 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.2 mg, 0.012 mmol), NaOAc (7.5 mg, 0.09 mmol), and ***S*-2f** (97% ee, 52.6 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 mL) at rt (10 ^oC) afforded ***S*-3df**[4] (69.1 mg, 68%) (eluent: petroleum/ethyl acetate/dichloromethane = 3.5/1/1): 97% ee (HPLC conditions: Chiralcel AD-H column, hexane/*i*-PrOH = 10/1, 1.0 mL/min, λ = 207 nm, t_R(minor) = 28.880 min, t_R(major) = 32.365 min); $[\alpha]_D^{20}$ = +1.4 (*c* = 1.05, $CHCl_3$); oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.74 (s, 1 H, NH), 7.83 (d, *J* = 8.7 Hz, 1 H, Ar-H), 7.33-7.24 (m, 2 H, Ar-H), 7.24-7.16 (m, 3 H, Ar-H), 6.95 (dd, J_1 = 8.6 Hz, J_2 = 2.6 Hz, 1 H, Ar-H), 6.85 (d, *J* = 2.4 Hz, 1 H, Ar-H), 3.85 (s, 3 H, OCH_3), 3.43 (s, 3 H, OCH_3), 2.28-2.08 (m, 2 H, CH_2), 1.90 (s, 3 H, CH_3), 1.14 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.7, 166.2, 161.6, 137.3, 136.9, 131.8, 128.7, 127.1, 126.4, 124.7, 116.6, 113.1, 107.9, 106.7, 63.8, 55.4, 27.5, 18.7, 12.4; IR ν (neat, cm^{-1}) 3204, 2965, 2934, 1949, 1658, 1599, 1569, 1491, 1460, 1368, 1288, 1225, 1110, 1029; MS (EI, 70 eV) *m*/*z* (%) 338 (M^++1, 8.11), 337 (M^+, 5.09), 306 (100).

4. Preparation of *S*-*N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadien-1-yl)-4-*tert*-butyl-benzamide ***S*-3ef**. (Wsz-8-27)



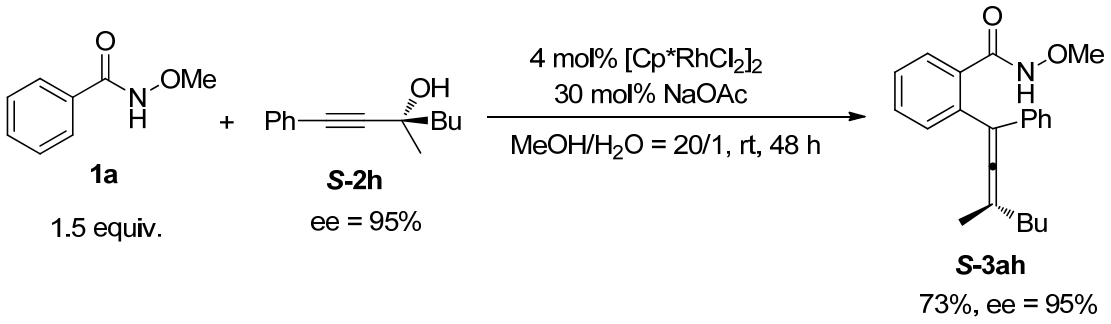
The reaction of **1e** (92.5 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.4 mg, 0.012 mmol), NaOAc (7.3 mg, 0.09 mmol), and ***S*-2f** (52.8 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 ml) at rt (14 ^oC) afforded ***S*-3ef**[4] (78.1 mg, 71%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 6/1/0.4): 97% ee (HPLC conditions: Chiralcel AD-H column, hexane/*i*-PrOH = 10/1, 0.8 mL/min, λ = 207 nm, t_R(minor) = 19.643 min, t_R(major) = 21.573 min); $[\alpha]_D^{20}$ = +1.4 (*c* = 2.0, $CHCl_3$); oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.86 (s, 1 H, NH), 7.72 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.43 (dd, J_1 = 8.3 Hz, J_2 = 2.0 Hz, 1 H, Ar-H), 7.36 (d, *J* = 1.5 Hz, 1 H, Ar-H), 7.32-7.13 (m, 5 H, Ar-H), 3.41 (s, 3 H, OCH_3), 2.26-2.08 (m, 2 H, CH_2), 1.90 (s, 3 H, CH_3), 1.32 (s, 9 H, CH_3× 3), 1.15 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.8, 166.3, 154.4, 137.2, 135.1, 129.5, 129.3, 128.4, 128.1, 126.8, 126.3, 124.8, 108.1, 106.0, 63.6, 34.6, 30.9, 27.3, 18.6, 12.3; IR ν (neat, cm^{-1}) 3216, 3060, 3030, 2964, 2935, 2905, 2866, 1944, 1661, 1601, 1491, 1460, 1394, 1364, 1302, 1257, 1095, 1033; MS (EI, 70 eV) *m*/*z* (%) 364 (M^++1, 6.99), 363 (M^+, 5.12), 332 (100).

5. Preparation of *S*-*N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadien-1-yl)-5-chloro-benzamide ***S*-3ff**. (Wsz-8-96)



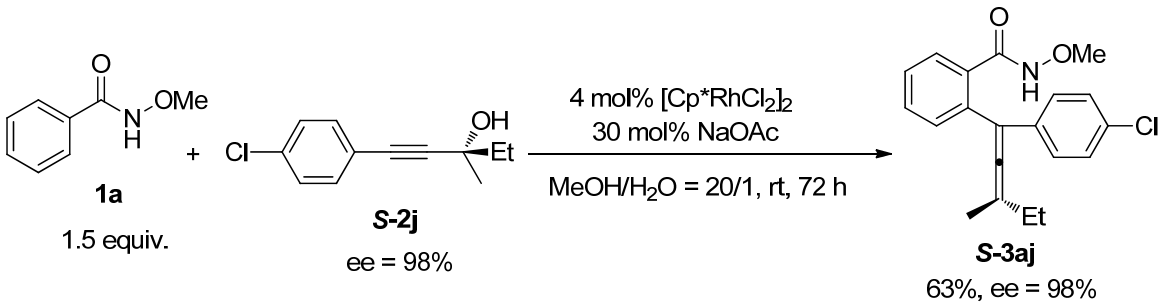
The reaction of **1f** (83.8 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.1 mg, 0.012 mmol), NaOAc (7.5 mg, 0.09 mmol), and ***S*-2f** (97% ee, 52.6 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 mL) at rt (17 ^oC) afforded ***S*-3ff** (68.9 mg, 67%) (eluent: petroleum/ethyl acetate/dichloromethane = 7/1/0.3): 94% ee (HPLC conditions: Chiralcel AD-H column, hexane/*i*-PrOH = 10/1, 1.0 mL/min, λ = 207 nm, t_R(minor) = 13.458 min, t_R(major) = 19.063 min); $[\alpha]_D^{20}$ = +11.00 (*c* = 1.92, $CHCl_3$); solid; m.p. 106.4-107.7 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.76 (s, 1 H, NH), 7.72 (s, 1 H, Ar-H), 7.44 (dd, J_1 = 8.1 Hz, J_2 = 2.4 Hz, 1 H, Ar-H), 7.33-7.23 (m, 3 H, Ar-H), 7.23-7.15 (m, 3 H, Ar-H), 3.44 (s, 3 H, OCH_3), 2.26-2.07 (m, 2 H, CH_2), 1.88 (s, 3 H, CH_3), 1.11 (t, J = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.1, 165.1, 136.9, 134.2, 134.0, 133.7, 132.5, 131.1, 129.5, 128.7, 127.2, 126.4, 106.8, 106.6, 63.9, 27.4, 18.5, 12.3; IR ν (neat, cm^{-1}) 3192, 2966, 2933, 1947, 1662, 1596, 1492, 1456, 1370, 1301, 1160, 1113, 1040; MS (EI, 70 eV) *m*/*z* (%) 343 ($M(^{37}Cl)^+$, 0.85), 341 ($M(^{35}Cl)^+$, 1.37), 310 (100); Anal. Calcd for $C_{20}H_{20}ClNO_2$: C 70.27, H 5.90, N 4.10. Found: C 70.00, H 6.01, N 3.91.

6. Preparation of *S*-*N*-methoxy-2-(1-phenyl-3-methyl-1,2-heptadien-1-yl)benzamide ***S*-3ah**. (Wsz-8-35)



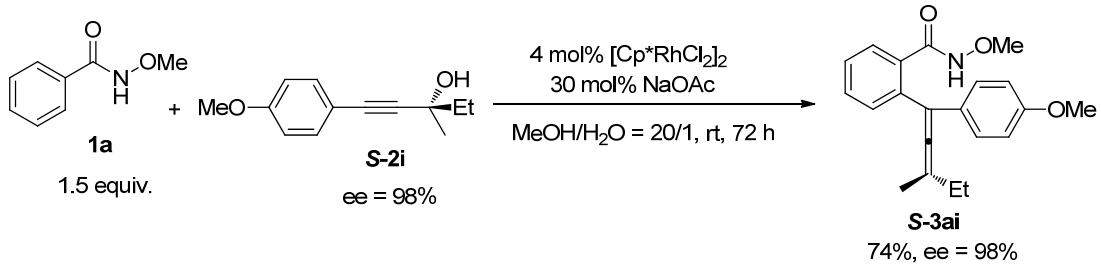
The reaction of **1a** (60.8 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.4 mg, 0.012 mmol), NaOAc (7.1 mg, 0.09 mmol), and ***S*-2h** (95% ee, 58.6 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 mL) at rt (8 ^oC) afforded ***S*-3ah** (73.3 mg, 73%) (eluent: petroleum/ethyl acetate/dichloromethane = 5/1/0.3): 95% ee (HPLC conditions: Chiralcel AS-H column, hexane/*i*-PrOH = 10/1, 1.0 mL/min, λ = 207 nm, t_R(minor) = 43.928 min, t_R(major) = 51.062 min); $[\alpha]_D^{20}$ = +14.00 (*c* = 2.90, $CHCl_3$); oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.64 (s, 1 H, NH), 7.79 (d, *J* = 6.6 Hz, 1 H, Ar-H), 7.53-7.37 (m, 2 H, Ar-H), 7.36-7.24 (m, 3 H, Ar-H), 7.24-7.13 (m, 3 H, Ar-H), 3.46 (s, 3 H, OCH_3), 2.22-2.07 (m, 2 H, CH_2), 1.88 (s, 3 H, CH_3), 1.59-1.43 (m, 2 H, Ar-H), 1.42-1.26 (m, 2 H, Ar-H), 0.89 (t, *J* = 7.2 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.3, 166.6, 137.2, 135.6, 132.5, 131.2, 131.1, 129.7, 128.6, 127.9, 127.0, 126.5, 106.9, 104.7, 63.9, 34.0, 29.8, 22.4, 18.7, 13.9; IR ν (neat, cm^{-1}) 3201, 2956, 2928, 2875, 2855, 1949, 1659, 1599, 1492, 1463, 1437, 1376, 1307, 1154, 1032; MS (EI, 70 eV) *m*/*z* (%) 336 (M^++1, 12.46), 335 (M^+, 49.33), 246 (100); HRMS Calcd for $C_{22}H_{25}NO_2$ (M^+): 335.1885. Found: 335.1882.

7. Preparation of *S*-*N*-methoxy-2-(1-(4-chloro-phenyl)-3-methyl-1,2-pentadien-1-yl) benzamide ***S*-3aj**. (Wsz-8-59)



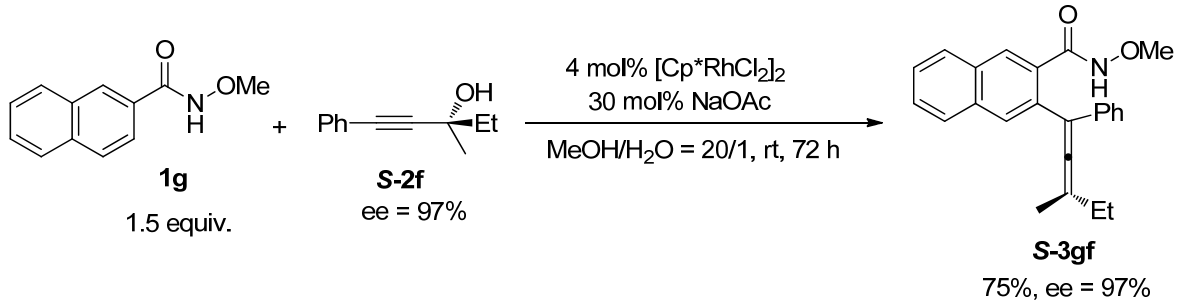
The reaction of **1a** (68.3 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.3 mg, 0.012 mmol), NaOAc (7.7 mg, 0.09 mmol), and ***S*-2j** (98% ee, 62.9 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 mL) at rt (10 ^oC) afforded ***S*-3aj** (64.7 mg, 63%) (eluent: petroleum/ethyl acetate/dichloromethane = 3.5/1/3.5): 98% ee (HPLC conditions: Chiralcel AD-H column, hexane/*i*-PrOH = 10/1, 1.0 mL/min, λ = 207 nm, t_R(minor) = 20.938 min, t_R(major) = 26.005 min); $[\alpha]_D^{20}$ = +5.00 (*c* = 1.06, $CHCl_3$); solid; m.p. 141.9-143.2 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.56 (s, 1 H, NH), 7.73 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.53-7.37 (m, 2 H, Ar-H), 7.33 (dd, J_1 = 7.4 Hz, J_2 = 1.4 Hz, 1 H, Ar-H), 7.28-7.20 (m, 2 H, Ar-H), 7.16-7.07 (m, 2 H, Ar-H), 3.53 (s, 3 H, OCH_3), 2.25-2.07 (m, 2 H, CH_2), 1.89 (s, 3 H, CH_3), 1.12 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.0, 166.6, 136.0, 135.4, 132.8, 132.6, 131.2, 131.1, 129.5, 128.7, 128.0, 127.8, 106.8, 64.1, 27.4, 18.6, 12.4; IR *ν* (neat, cm^{-1}) 3203, 2965, 2931, 1944, 1659, 1488, 1453, 1439, 1368, 1299, 1272, 1088, 1032, 1012; MS (EI, 70 eV) *m*/*z* (%) 343 ($M(^{37}Cl)^+$, 20.57), 341 ($M(^{35}Cl)^+$, 57.90), 312 (100); Anal. Calcd for $C_{20}H_{20}ClNO_2$: C 70.27, H 5.90, N 4.10. Found: C 69.92, H 5.90, N 3.94.

8. Preparation of *S*-*N*-methoxy-2-(1-(4-methoxyl-phenyl)-3-methyl-1,2-pentadien-1-yl) benzamide ***S*-3ai**. (Wsz-8-69)



The reaction of **1c** (68.3 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.4 mg, 0.012 mmol), NaOAc (7.7 mg, 0.09 mmol), and ***S*-2i** (98% ee, 61.1 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 mL) at rt (8 ^oC) afforded ***S*-3ci** (74.3 mg, 74%) (eluent: petroleum/ethyl acetate/dichloromethane = 4/1/0.3 (600 mL) to 2/1/0.3): 98% ee (HPLC conditions: Chiralcel AD-H column, hexane/*i*-PrOH = 10/1, 1.0 mL/min, λ = 207 nm, t_R(minor) = 14.268 min, t_R(major) = 16.853 min); $[\alpha]_D^{20}$ = +6.30 (*c* = 1.10, $CHCl_3$); oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.84 (s, 1 H, NH), 7.75 (d, *J* = 7.5 Hz, 1 H, Ar-H), 7.52-7.30 (m, 3 H, Ar-H), 7.16-7.07 (m, 2 H, Ar-H), 6.86-6.73 (m, 2 H, Ar-H), 3.75 (s, 3 H, OCH_3), 3.49 (s, 3 H, OCH_3), 2.23-2.09 (m, 2 H, CH_2), 1.88 (s, 3 H, CH_3), 1.12 (t, *J* = 7.5 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.1, 166.5, 158.6, 135.8, 132.4, 130.94, 130.88, 129.5, 129.4, 127.6, 107.0, 113.9, 107.0, 106.0, 63.7, 55.1, 27.4, 18.6, 12.2; IR ν (neat, cm^{-1}) 3199, 2965, 2933, 2837, 1950, 1660, 1605, 1578, 1508, 1462, 1440, 1364, 1292, 1247, 1179, 1033; MS (EI, 70 eV) *m*/*z* (%) 338 (M^++1, 12.39), 337 (M^+, 55.43), 308 (100). HRMS calcd. for $C_{21}H_{23}NO_3$ (M^+): 337.1678; Found: 337.1678.

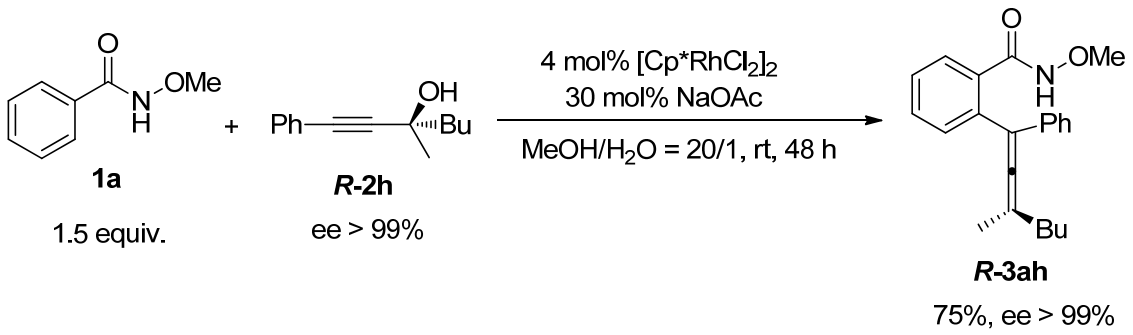
9. Preparation of *S*-*N*-methoxy-2-(1-phenyl-3-methyl-1,2-pentadien-1-yl)-2-naphthamide ***S*-3gf**. (Wsz-8-104)



The reaction of **1g** (90.8 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.3 mg, 0.012 mmol), NaOAc (7.6 mg, 0.09 mmol), and ***S*-2f** (97% ee, 52.5 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 mL) at rt (10 ^oC) afforded ***S*-3gf** (80.7 mg, 75%) (eluent: petroleum/ethyl acetate/dichloromethane = 5/1/0.5): 97% ee (HPLC conditions: Chiralcel AD-H column, hexane/*i*-PrOH = 10/1, 1.0 mL/min, λ = 207 nm, t_R(minor) = 39.578 min, t_R(major) = 53.270 min); $[\alpha]_D^{20}$ = +10.10 (*c* = 2.80, $CHCl_3$); solid; m.p. 146.2-147.8 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.86 (s, 1 H, NH), 8.29 (s, 1 H, Ar-H), 7.89 (d, *J* = 7.5 Hz, 1 H, Ar-H), 7.86-7.76 (m, 2 H, Ar-H), 7.61-7.46 (m, 2 H, Ar-H), 7.33-7.13 (m, 5 H, Ar-H), 3.44 (s, 3 H, OCH_3), 2.28-2.09 (m, 2 H, CH_2), 1.93 (s, 3 H, CH_3), 1.17 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.3, 166.3, 137.6, 134.3, 132.4, 132.0, 130.5, 130.3, 130.2, 128.5, 128.4, 127.8, 127.5, 127.0, 126.7, 126.6, 107.8, 106.1, 63.8, 27.5, 18.7, 12.4; IR ν (neat, cm^{-1}) 3191, 3055, 2966, 2932, 1947, 1659, 1596, 1491, 1456, 1438, 1368, 1300, 1263, 1197, 1146, 1095, 1025; MS (EI, 70 eV) *m*/*z* (%) 358 (M^++1, 3.43), 357 (M^+, 2.64), 326 (100); Anal. Calcd for $C_{24}H_{23}NO_2$: C 80.64, H 6.49, N 3.92. Found: C 80.27, H 6.59, N 3.72.

10. Preparation of *R*-*N*-methoxy-2-(1-phenyl-3-methyl-1,2-heptadien-1-yl)benzamide ***R*-3ah**.

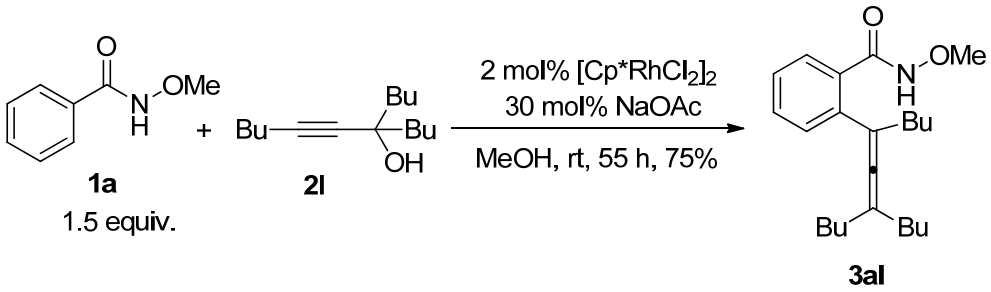
(Wsz-8-30)



The reaction of **1a** (60.6 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (7.3 mg, 0.012 mmol), NaOAc (7.8 mg, 0.09 mmol), and ***R*-2h** (>99% ee, 59.1 mg, 0.3 mmol) in MeOH (2 mL) and H_2O (0.1 mL) at rt (12 ^oC) afforded ***R*-3ah** (75.6 mg, 75%) (eluent: petroleum/ethyl acetate/dichloromethane = 5/1/0.3): >99% ee (HPLC conditions: Chiralcel AS-H column, hexane/*i*-PrOH = 10/1, 1.0 mL/min, λ = 207 nm, t_R(major) = 47.442 min); $[\alpha]_D^{20}$ = -14.00 (*c* = 1.81, $CHCl_3$); oil; ^1H NMR (300 MHz, $CDCl_3$) δ 8.64 (s, 1 H, NH), 7.79 (d, *J* = 7.5 Hz, 1 H, Ar-H), 7.52-7.47 (m, 2 H, Ar-H), 7.46-7.24 (m, 3 H, Ar-H), 7.24-7.13 (m, 3 H, Ar-H), 3.46 (s, 3 H, OCH_3), 2.15 (t, *J* = 7.5 Hz, 2 H, CH_2), 1.88 (s, 3 H, CH_3), 1.59-1.43 (m, 2 H, Ar-H), 1.42-1.25 (m, 2 H, Ar-H), 0.89 (t, *J* = 7.2 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 202.3, 166.6, 137.2, 135.6, 132.5, 131.2, 131.1, 129.7, 128.6, 127.9, 127.0, 126.5, 106.9, 104.7, 63.9, 34.0, 29.8, 22.4, 18.7, 13.9; IR ν (neat, cm^{-1}) 3200, 3058, 3021, 2954, 2929, 2872, 2858, 1944, 1660, 1596, 1492, 1459, 1439, 1379, 1301, 1158, 1032; MS (EI, 70 eV) *m*/*z* (%) 336 (M^++1, 11.96), 335 (M^+, 49.94), 246 (100); HRMS Calcd for $C_{22}H_{25}NO_2$ (M^+): 335.1885. Found: 335.1880.

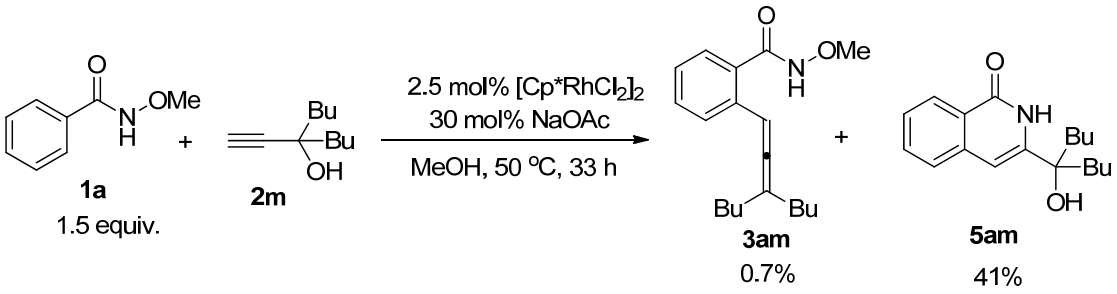
Control experiments with non-terminal propargylic alcohol

1. The reaction of **1a** with **2l**: formation of 2-(7-butylundeca-5,6-dien-5-yl)-*N*-methoxy benzamide **3al** (Wsz-10-13).



Following **Typical Procedure I**, the reaction of **1a** (226.8 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (12.6 mg, 0.02 mmol), NaOAc (24.3 mg, 0.3 mmol), and **2l** (224.3 mg, 1 mmol) in MeOH (6 mL) at rt (27 ^oC) afforded **3al** (267.2 mg, 75%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 10/1/0.3): oil; ^1H NMR (300 MHz, $CDCl_3$) δ 9.11 (s, 1 H, NH), 7.66 (d, J = 7.5 Hz, 1 H, Ar-H), 7.39 (td, J_1 = 7.5 Hz, J_2 = 1.4 Hz, 1 H, Ar-H), 7.33-7.19 (m, 2 H, Ar-H), 3.86 (s, 3 H, OCH_3), 2.28 (t, J = 7.4 Hz, 2 H, CH_2), 2.13-1.96 (m, 4 H, $CH_2 \times 2$), 1.55-1.25 (m, 12 H, $CH_2 \times 6$), 0.99-0.82 (m, 9 H, $CH_3 \times 3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.3, 167.4, 138.3, 130.8, 130.6, 129.7, 129.1, 126.8, 106.6, 64.0, 34.2, 32.5, 30.3, 30.0, 22.4, 22.2, 13.8, 13.7; IR ν (neat, cm^{-1}) 3193, 3061, 2956, 2930, 2869, 2855, 1952, 1659, 1595, 1570, 1498, 1465, 1439, 1377, 1300, 1258, 1193, 1158, 1105, 1035; MS (EI, 70 eV) *m*/*z* (%) 357 (M^+, 20.35), 188 (100); HRMS Calcd for $C_{23}H_{35}NO_2$ (M^+): 357.2668. Found: 357.2669.

2. The reaction of **1a** with **2m**: formation of 2-(3-butylhepta-1,2-dien-1-yl)-*N*-methoxy benzamide **3am** and 3-(5-hydroxynonan-5-yl)isoquinolin-1(*2H*)-one **5am** (Wsz-10-10).



Following **Typical Procedure I**, the reaction of **1a** (679.3 mg, 4.5 mmol), $[Cp^*RhCl_2]_2$ (46.2 mg, 0.075 mmol), NaOAc (73.4 mg, 0.9 mmol), and **2m** (504.6 mg, 3 mmol) in MeOH (18 mL) at 50 °C afforded **3am** (6.2 mg, 0.7%) and **5am** (356.3 mg, 41%) (eluent: petroleum ether/ethyl acetate/dichloromethane = 6/1/0.2 to 4/1/0.3):

3am: oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.43 (s, 1 H, NH), 7.54-7.46 (m, 1 H, Ar-H), 7.42-7.33 (m, 2 H, Ar-H), 7.18 (t, *J* = 7.5 Hz, 1 H, Ar-H), 6.52-6.45 (m, 1 H, =CH), 3.91 (s, 3 H, OCH_3), 2.17-2.02 (m, 4 H, $CH_2 \times 2$), 1.53-1.24 (m, 8 H, $CH_2 \times 4$), 0.89 (t, *J* = 7.1 Hz, 6 H, $CH_3 \times 2$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.6, 167.5, 134.9, 130.6, 130.5, 127.7, 127.4, 126.1, 109.0, 91.7, 64.7, 32.3, 29.8, 22.5, 13.9; IR ν (neat, cm^{-1}) 3192, 2957, 2930, 2873, 2856, 1947, 1654, 1597, 1500, 1466, 1445, 1378, 1302, 1156, 1035; MS (EI, 70 eV) *m*/*z* (%) 301 (M^+, 10.76), 143 (100); HRMS Calcd for $C_{19}H_{27}NO_2$ (M^+): 301.2042. Found: 301.2039.

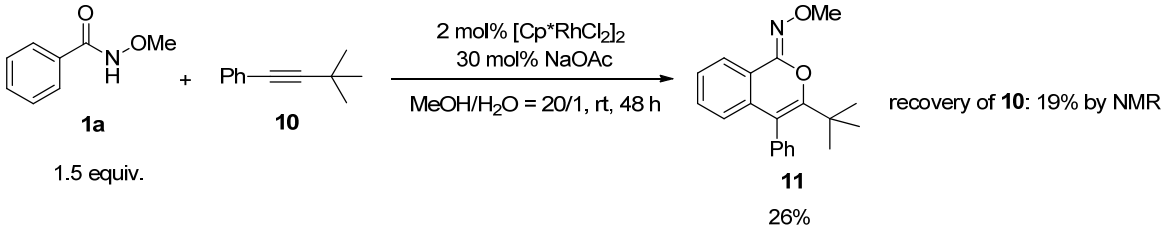
5am: oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.59 (s, 1 H, NH), 8.39 (d, *J* = 8.1 Hz, 1 H, Ar-H), 7.67-7.60 (m, 1 H, Ar-H), 7.54 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.47-7.40 (m, 1 H, Ar-H), 6.39 (s, 1 H, =CH), 4.76 (s, 1 H, OH), 1.97-1.83 (m, 4 H, $CH_2 \times 2$), 1.51-1.10 (m, 8 H, $CH_2 \times 4$), 0.80 (t, *J* = 7.2 Hz, 6 H, $CH_3 \times 2$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.5, 145.0, 138.4, 132.5, 127.1, 126.2, 126.0, 124.1, 101.6, 75.3, 41.8, 25.5, 22.8, 13.9; IR ν (neat, cm^{-1}) 3325, 3184, 3057, 2956, 2934, 2870, 2860, 1633, 1605, 1556, 1467, 1379, 1346, 1307, 1253, 1229, 1170, 1108, 1029, 1006; MS (EI, 70 eV) *m*/*z* (%) 287 (M^+, 38.15), 230 (100); HRMS Calcd

for $C_{18}H_{25}NO_2$ (M^+): 287.1885. Found: 287.1889.

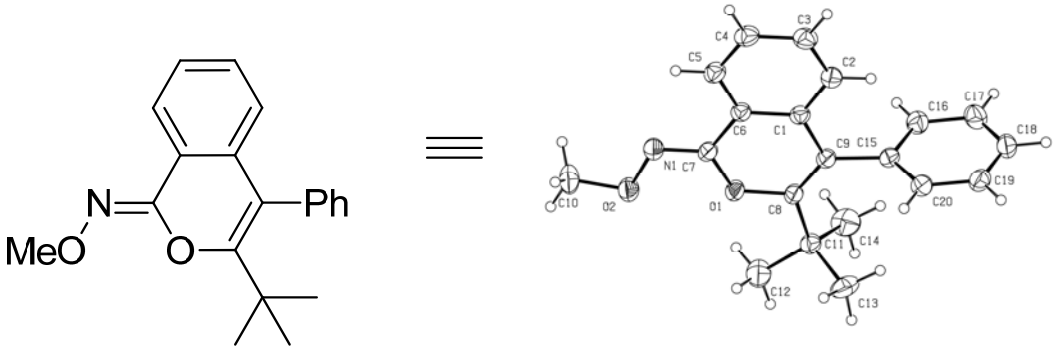
Mechanistic studies

1. Steric effect

(1) The reaction of **1a** with **10**: formation of (Z)-3-(*tert*-butyl)-4-phenyl-1*H*-isochromen-1-one *O*-methyl oxime **11**. (Wsz-8-51)



The reaction of **1a** (226.7 mg, 1.5 mmol), $[Cp^*RhCl_2]_2$ (12.5 mg, 0.02 mmol), NaOAc (24.7 mg, 0.3 mmol), and **10** (158.3 mg, 1 mmol) in MeOH (6 mL) and H_2O (0.3 mL) at rt afforded **11** (80.9 mg, 26%) (eluent: petroleum/ethyl acetate = 30/1): solid; m.p. 150.0-151.2 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 7.99-7.90 (m, 1 H, Ar-H), 7.46-7.35 (m, 3 H, Ar-H), 7.24-7.16 (m, 4 H, Ar-H), 6.50-6.42 (m, 1 H, Ar-H), 3.97 (s, 3 H, OCH_3); 1.10 (s, 9 H, $CH_3 \times 3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.7, 148.8, 135.9, 134.7, 131.6, 130.5, 128.2, 127.6, 127.1, 124.7, 123.2, 120.3, 113.0, 62.6, 38.4, 30.0; IR ν (neat, cm^{-1}) 3078, 3024, 2991, 2965, 2934, 2816, 1632, 1615, 1591, 1482, 1457, 1344, 1299, 1251, 1197, 1141, 1107, 1055; MS (EI, 70 eV) *m*/*z* (%) 308 (M^++1, 64.60), 307 (M^+, 100); Anal. Calcd for $C_{20}H_{21}NO_2$: C 78.15, H 6.89, N 4.56. Found: C 78.13, H 6.81, N 4.36.

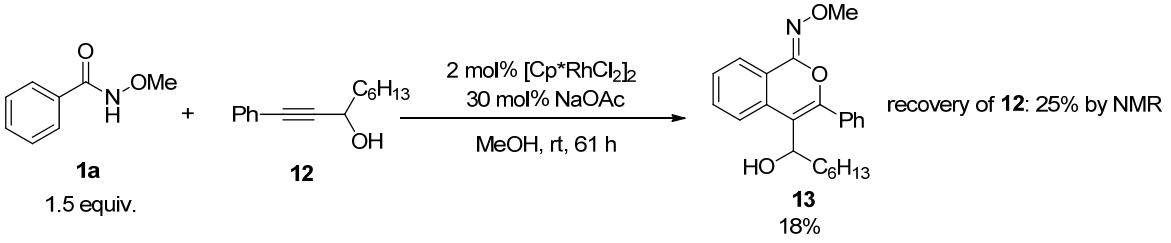


11

ORTEP representation of **11**

11: $C_{20}H_{21}NO_2$, MW = 307.38, monoclinic, space group P 1 21/n 1, final R indices [I > 2σ(I)], R1 = 0.0489, wR2 = 0.1144; Rindices (all data), R1 = 0.0821, wR2 = 0.1394; a = 11.8310(8) Å, b = 8.4718(5) Å, c = 16.4581(10) Å, α = 90.00°, β = 90.759(6)°, γ = 90.00°, V = 1649.45(17) $Å^3$, T = 293(2) K, Z = 4, reflections collected/unique 6441/3018 (R_{int} = 0.0375), number of observations [> 2σ(I)]: 2013, parameters: 212. Supplementary crystallographic data have been deposited at the Cambridge Crystallographic Data Centre, CCDC 1483579.

(2) The reaction of **1a** with **12**: the formation of (*Z*)-4-(1-hydroxyheptyl)-3-phenyl-1*H*-isochromen-1-one *O*-methyl oxime **13**. (Wsz-8-198)



1a
1.5 equiv.

12

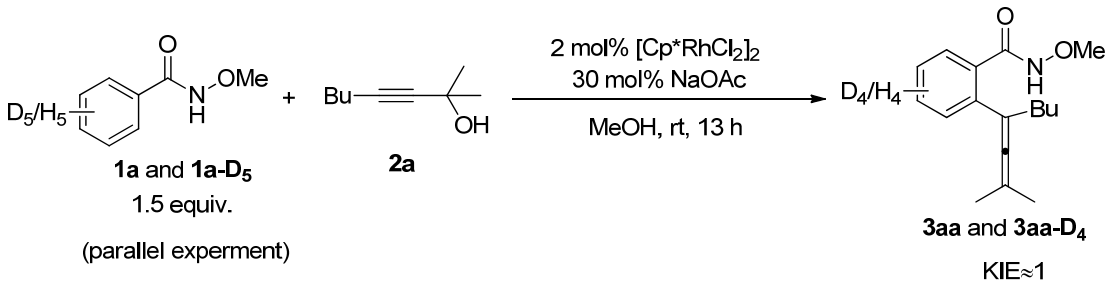
13
18%

The reaction of **1a** (453.3 mg, 3 mmol), $[Cp^*RhCl_2]_2$ (24.6 mg, 0.04 mmol), NaOAc (49.5 mg, 0.6 mmol), and **12** (432.2 mg, 2 mmol) in MeOH (12 mL) at rt afforded **13** (131.3 mg,

18%) (eluent: petroleum/ethyl acetate = 20/1 to 10/1): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.09 (d, J = 7.8 Hz, 1 H, Ar-H), 7.98 (dd, J_1 = 8.0 Hz, J_2 = 1.1 Hz, 1 H, Ar-H), 7.55-7.46 (m, 2 H, Ar-H), 7.46-7.34 (m, 4 H, Ar-H), 7.31-7.20 (m, 1 H, Ar-H), 4.74 (dd, J_1 = 7.8 Hz, J_2 = 6.6 Hz, 1 H, OCH), 3.91 (s, 3 H, OCH_3), 2.41 (bs, 1 H, OH), 2.06-1.77 (m, 2 H, CH_2), 1.33-1.02 (m, 8 H, $CH_2 \times 4$), 0.81 (d, J = 6.9 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.4, 148.5, 133.1, 130.4, 129.9, 129.5, 129.2, 128.4, 127.7, 125.7, 124.2, 122.0, 113.7, 71.3, 62.6, 35.9, 31.6, 28.8, 26.2, 22.5, 14.0; IR ν (neat, cm^{-1}) 3428, 3061, 3027, 2953, 2930, 2856, 2816, 1639, 1616, 1601, 1592, 1482, 1456, 1446, 1378, 1341, 1324, 1299, 1237, 1190, 1145, 1129, 1112, 1054; MS (EI, 70 eV) m/z (%) 365 (M^+, 22.83), 105 (100); HRMS Calcd for $C_{23}H_{27}NO_3$ (M^+): 365.1991. Found: 365.1994.

2. Kinetic isotope effect by parallel experiments

(1) The measurement of the KIE of **1a** and **1a-d$_4$**.[4,10] (Wsz-9-1, Wsz-9-2)

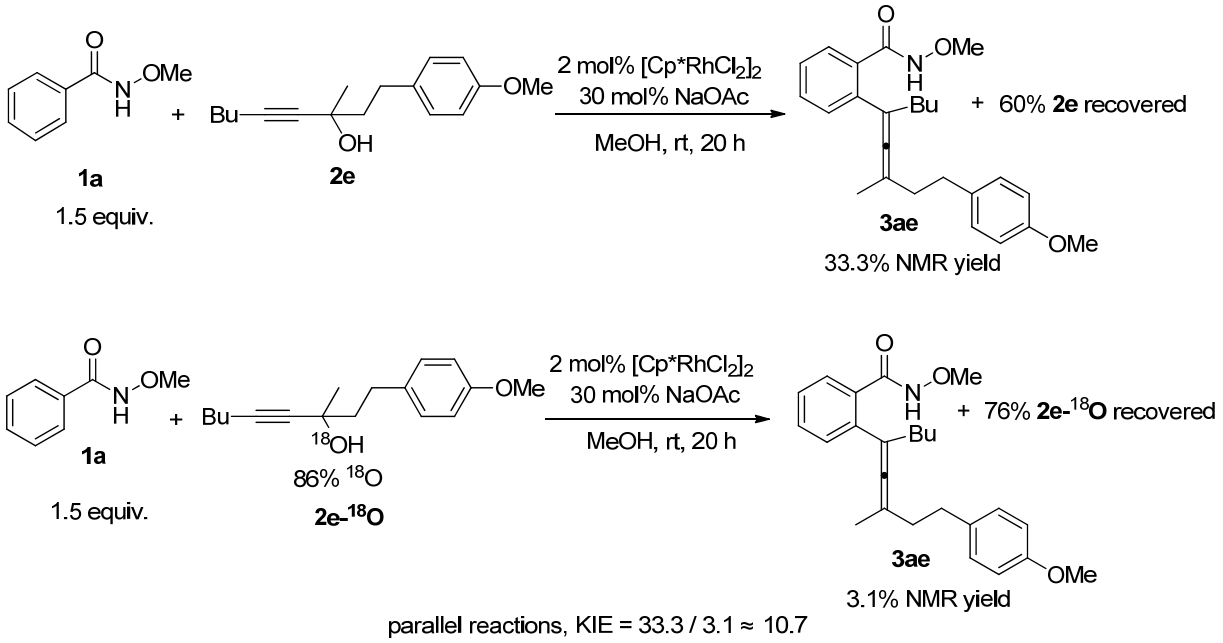


To a dried Schlenk tube equipped with a Teflon-coated magnetic stirring bar were added **1a** (68.2 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (3.7 mg, 0.006 mmol), NaOAc (7.6 mg, 0.09 mmol), **2a** (42.1 mg, 0.3 mmol), and MeOH (2 mL) sequentially at rt (Wsz-9-1). After being stirred for 13 h at rt, the resulting mixture was mixed with the resulting mixture of the subsequent reaction (Wsz-9-2).

In another dried Schlenk tube, the reaction of **1a-D_5** (70.3 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (3.7 mg, 0.006 mmol), NaOAc (7.5 mg, 0.09 mmol), **2a** (41.8 mg, 0.3 mmol), and MeOH (2 mL) at rt was stirred for 13 h at rt, and then the resulting mixture was mixed with the resulting mixture of the above reaction (Wsz-9-1).

The mixed resulting mixture was evaporated to afford the crude product, which was purified by flash column chromatography on silica gel (eluent: petroleum/ethyl acetate/dichloromethane = 7/1/0.3) to afford **3aa** and **3aa-D_4** (61.8 mg, 38%): solid; m.p. 68.7-69.9 ^oC (hexane/ethyl acetate), reproted in the ref: 68.1-68.9 ^oC (hexane/ethyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.82 (s, 1 H, NH), 3.85 (s, 3 H, OCH_3), 2.29 (t, *J* = 7.1 Hz, 2 H, CH_2), 1.76 (s, 6 H, 2 × CH_3), 1.53-1.28 (m, 4 H, 2 × CH_2), 0.89 (t, *J* = 7.1 Hz, 3 H, CH_3), the following signal is discernible for **3aa**: δ 7.56 (d, *J* = 7.2 Hz, 0.50 H, Ar-H), 7.39 (t, *J* = 7.4 Hz, 0.53 H, Ar-H), 7.32-7.20 (m, 1.12 H, Ar-H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.3, 167.9, 138.2, 131.4, 130.0, 129.7, 128.6, 128.4, 126.3, 125.9, 102.9, 97.6, 64.3, 33.6, 30.1, 22.2, 20.4, 13.9; the following signal is discernible for **3aa**: 138.3, 131.5, 130.5, 129.1, 128.6, 128.4, 126.8; IR ν (neat, cm^{-1}) 3193, 3061, 2956, 2931, 2869, 2859, 2816, 1956, 1659, 1594, 1570, 1495, 1465, 1440, 1376, 1361, 1300, 1259, 1188, 1158, 1108, 1035; MS (EI, 70 eV) *m*/*z* (%) 277 ($M^+(D_4)$, 28.01), 273 (M^+, 40.35), 198 (100).

2. The measurement of the KIE of **2e** and **2e-^{18}O**. (Wsz-9-153, Wsz-9-154)



To a dried Schlenk tube equipped with a Teflon-coated magnetic stirring bar were added **1a** (68.1 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (3.7 mg, 0.006 mmol), NaOAc (7.1 mg, 0.09 mmol), **2e** (78.2 mg, 0.3 mmol), and MeOH (2 mL) sequentially at rt (Wsz-9-153). After being stirred for 20 h, the reaction was stopped. Filtration through a short column of silica gel (eluent: ethyl acetate 20 mL × 3) and evaporation afforded the crude product. **3ae (**33.3%) was formed as determined by NMR analysis of the crude product.

In another dried Schlenk tube, the reaction of **1a** (68.3 mg, 0.45 mmol), $[Cp^*RhCl_2]_2$ (3.7 mg, 0.006 mmol), NaOAc (7.5 mg, 0.09 mmol), **2e-^{18}O** (78.7 mg, 0.3 mmol), and MeOH (2 mL) reacted at rt (Wsz-9-154). After being stirred for 20 h, the reaction was stopped. Filtration through a short column of silica gel (eluent: ethyl acetate 20 mL × 3) and evaporation afforded the crude product. **3ae (**3.1%) was formed as determined by NMR analysis of the crude product.

The KIE value was determined by the ratio of the NMR yield of **3ae** in these two reactions

using CH_2Br_2 as the internal standard: KIE = 33.3 / 3.1 ≈ 10.7.

The crude product of Wsz-9-154 was was purified by flash column chromatography on silica gel (eluent: petroleum/ethyl acetate = 10/1 to petroleum/ethyl acetate/dichloromethane = 5/1/0.3) to afford recovered **2e-^{18}O** (57.6 mg, 73%, 87% ^{18}O) and product **3ae** (3.8 mg, 3%).

2e-^{18}O: oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.17-7.09 (m, 2 H, Ar-H), 6.86-6.79 (m, 2 H, Ar-H), 3.78 (s, 3 H, OCH_3), 2.84-2.73 (m, 2 H, CH_2), 2.25-2.17 (m, 3 H, CH_2 + OH), 1.97-1.84 (m, 2 H, CH_2), 1.56-1.36 (m, 7 H, CH_3 + CH_2 × 2), 0.92 (t, *J* = 7.1 Hz, 3 H, CH_3); MS (EI, 70 eV) *m*/*z* (%) 262 (M (^{18}O)$^+$, 16.37), 260 (M (^{16}O)$^+$, 2.45), 121 (100).

The ^{18}O% incorporation of **2e-^{18}O** was determined via the analysis of MS spectrum. The natural abundances of the stable isotopes of C, H, and O are known. The naturally occurring isotopic ^{18}O will also produce [M(^{18}O)]$^+$ peak. According to the natural abundance of ^{18}O, the ratio $C_{17}H_{24}{}^{16}O_2$: $C_{17}H_{24}{}^{16}O^{18}O$ is 99.76:0.2. Thus, the intensity of [M(^{18}O)$^+$] ($C_{17}H_{24}{}^{16}O^{18}O)^+$ peak will be 0.2% of the intensity of the molecular peak [M(^{16}O)$^+$] ($C_{17}H_{24}{}^{16}O_2$). According to the MS spectrum of **2e-^{18}O**, the relative abundances of **2e-^{16}O** 260 [M(^{16}O)$^+$] and **2e-^{18}O** 262 [M(^{18}O)$^+$] are 2.45, 16.37, respectively. The ^{18}O% of **2e-^{18}O** can be calculated as follows: ([M(^{18}O)$^+$] - [M(^{16}O)$^+$] × 0.2%)/([M(^{18}O)$^+$] - [M(^{16}O)$^+$] × 0.2% + [M(^{16}O)$^+$]) = 16.37-16.37×0.002/(16.37-16.37×0.002+ 2.45) ≈ 86.96%.

In addition, the contributions to the isotope peak intensities from background peaks or from impurities in the sample must be considered. According to the MS spectrum of **2e**, such contribution of **2e** to [M(^{16}O)+2]$^+$ is (0.15-6.21×0.002)% (≈ 0.14%).

So the ^{18}O% of **2e-^{18}O** is 86. 96% - 0.14% ≈ 87%.

3ae: oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17 (s, 1 H, NH), 7.52 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.39 (td, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1 H, Ar-H), 7.33-7.22 (m, 1 H, Ar-H), 7.19 (d, *J* = 7.5 Hz, 1 H, Ar-H), 7.02 (d, *J* = 8.7 Hz, 1 H, Ar-H), 6.66 (d, *J* = 8.4 Hz, 2 H, Ar-H), 3.80 (s, 3 H, OCH_3), 3.74 (s, 3 H, OCH_3), 2.70 (t, *J* = 7.1 Hz, 2 H, CH_2), 2.32 (t, *J* = 7.4 Hz, 2 H, CH_2), 2.28-2.16 (m, 2 H, CH_2), 1.81 (s, 3 H, CH_3), 1.39-1.25 (m, 4 H, CH_2 × 2), 0.87 (t, *J* = 6.8 Hz, 3 H, CH_3).

References:

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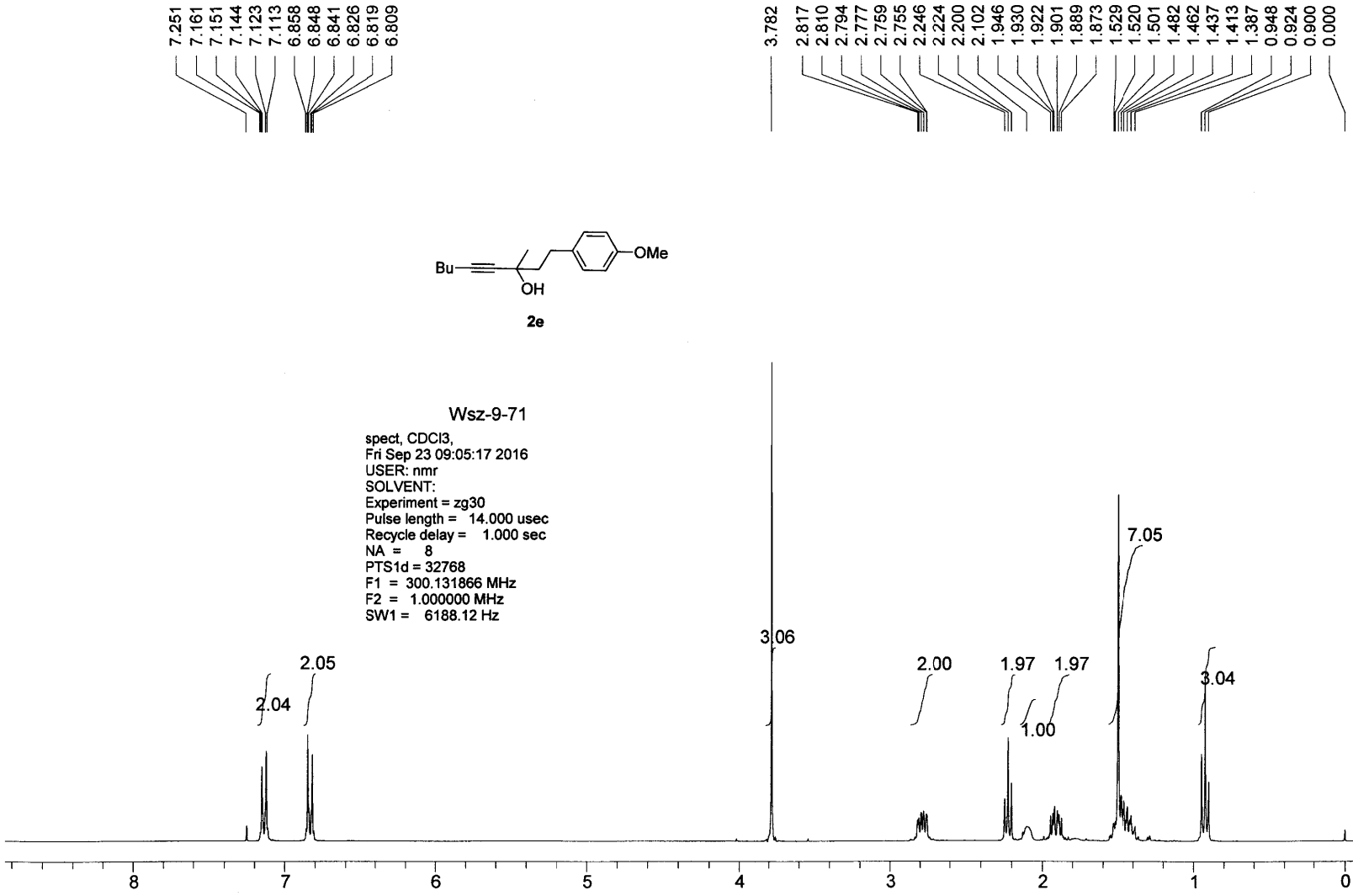
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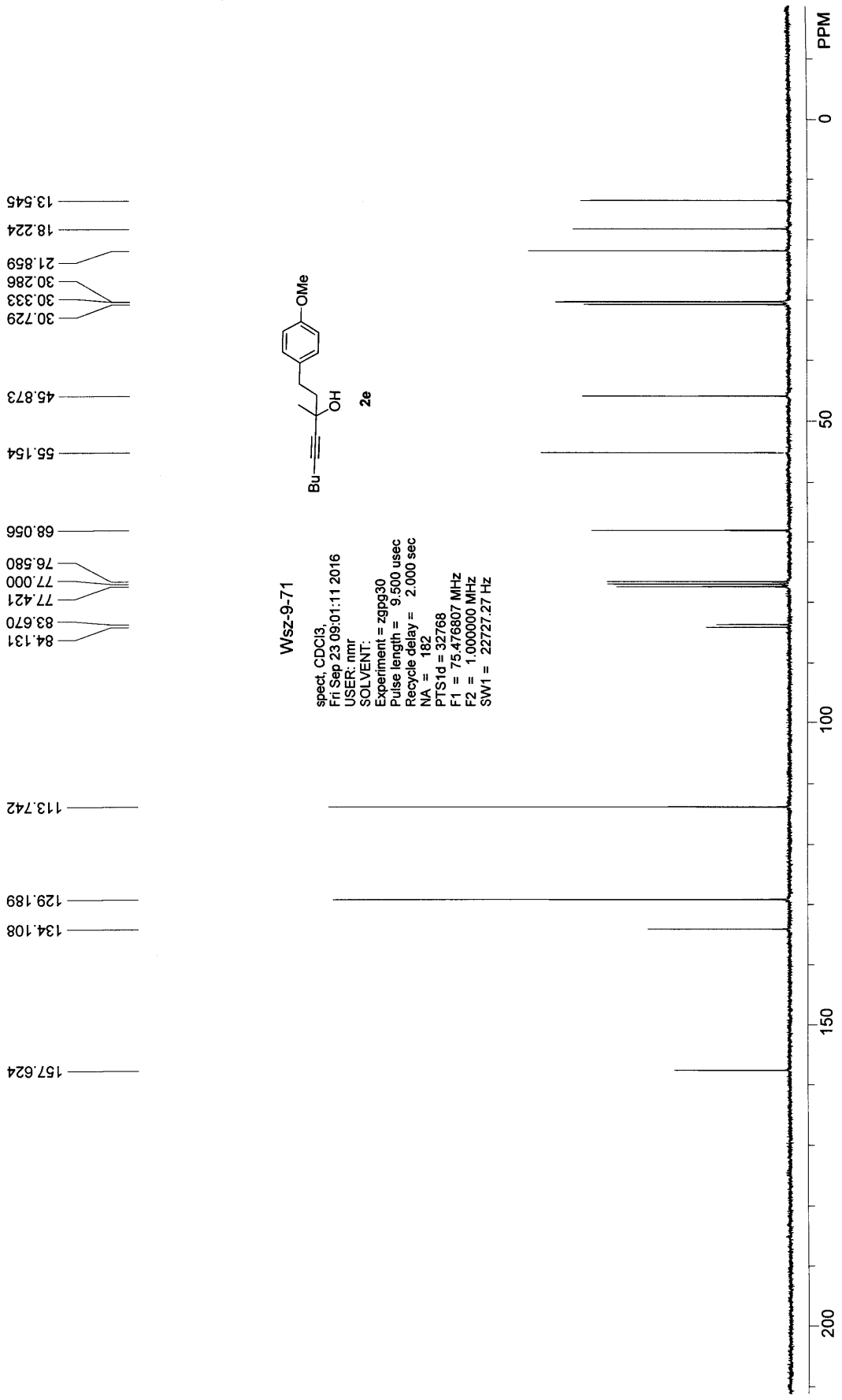
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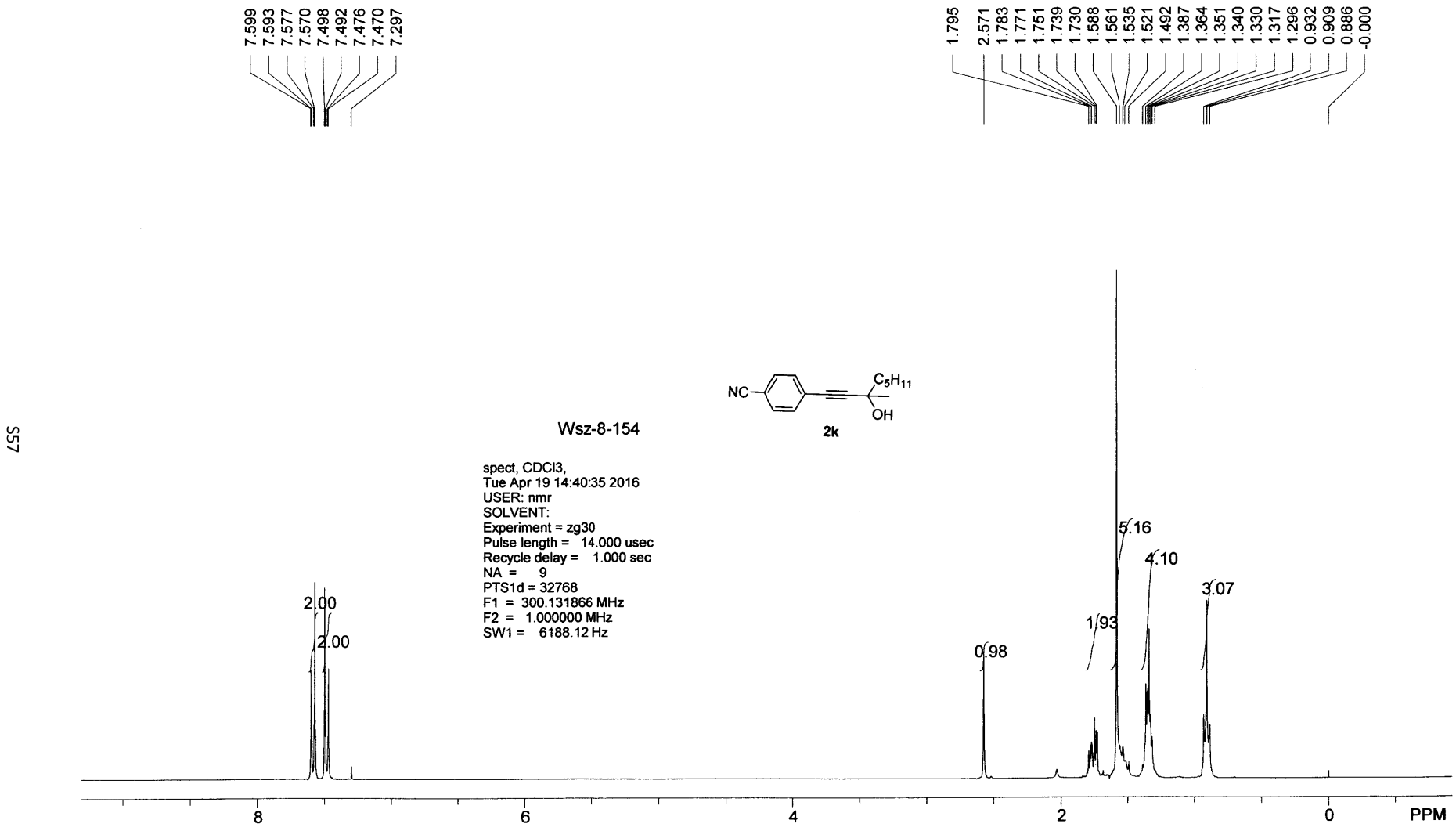
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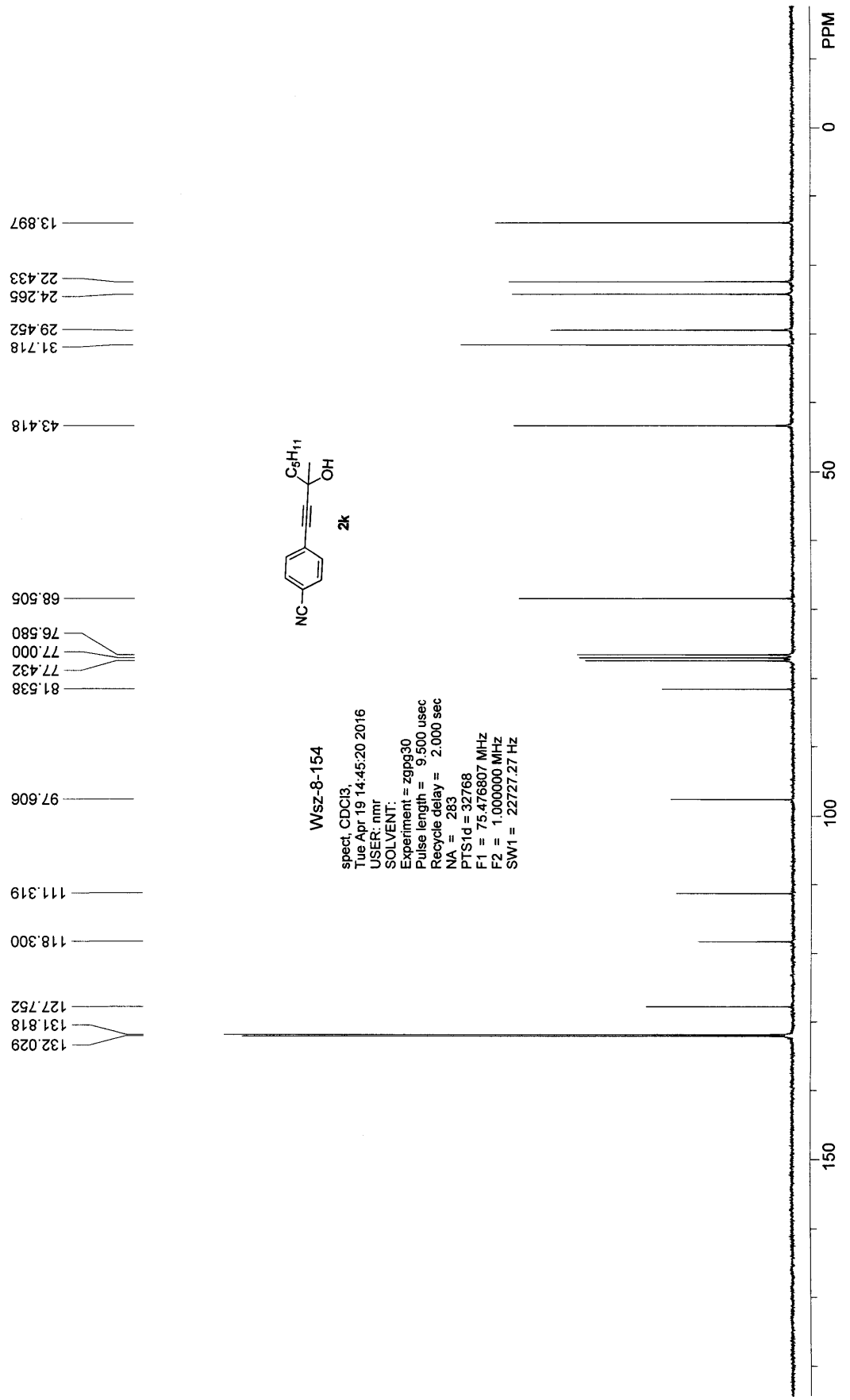
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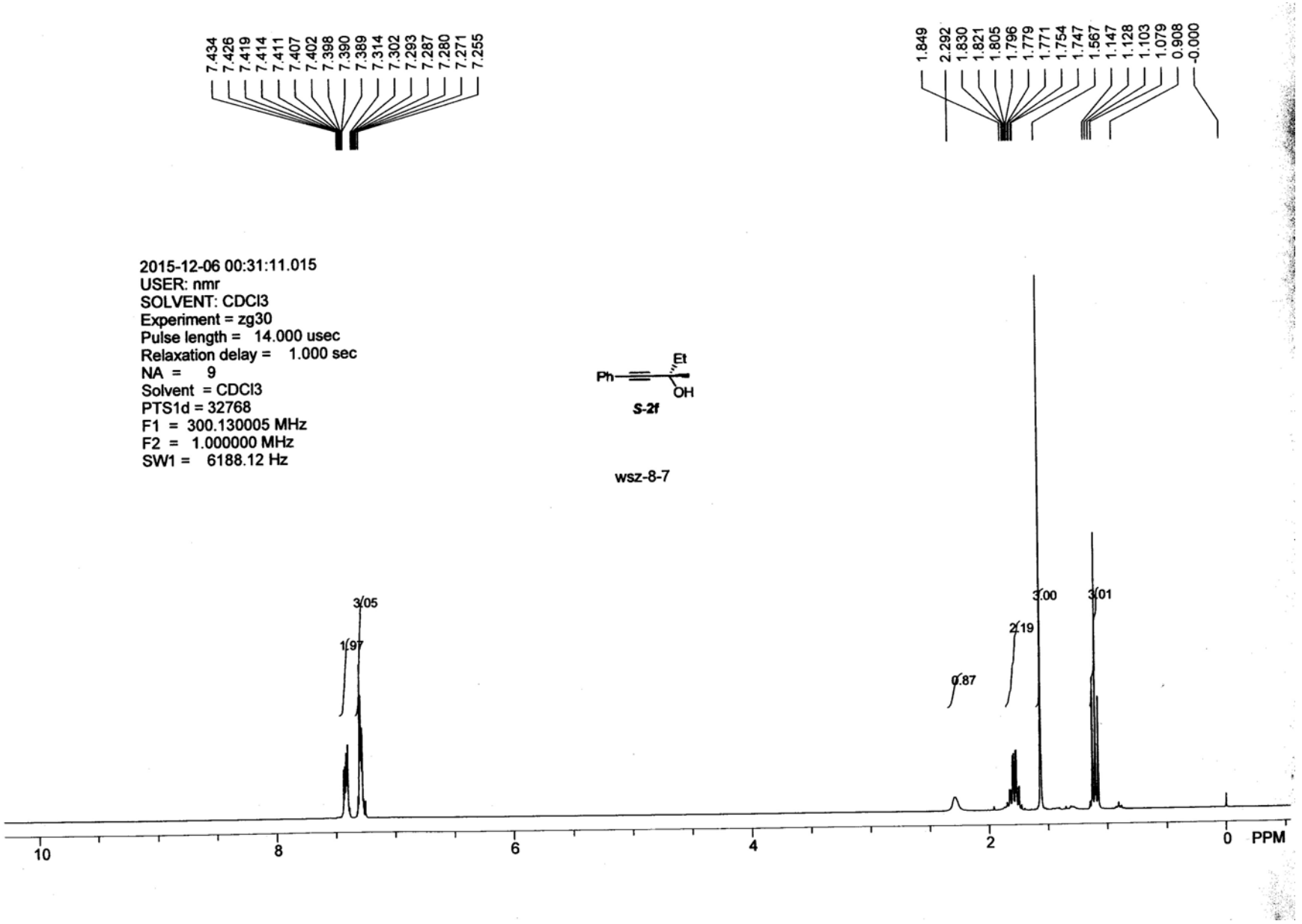
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Wsz-8-7

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实验者：wsz
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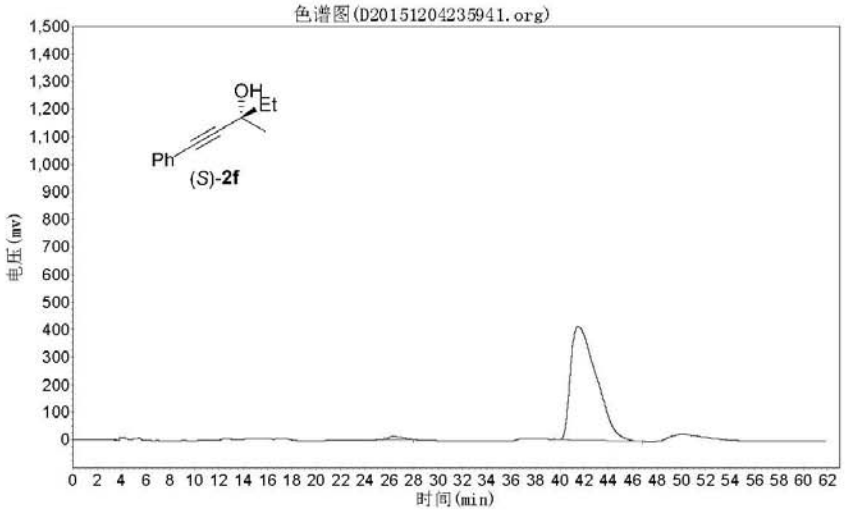

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Wsz-5-189 for 8-7

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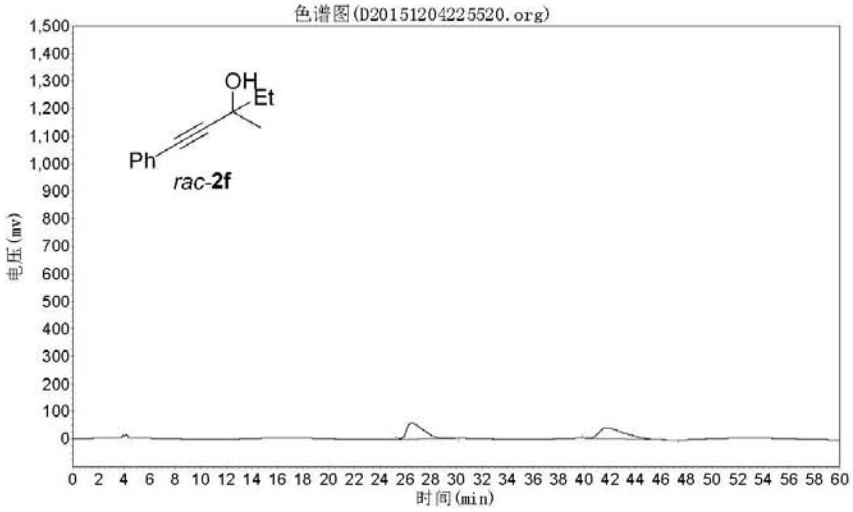

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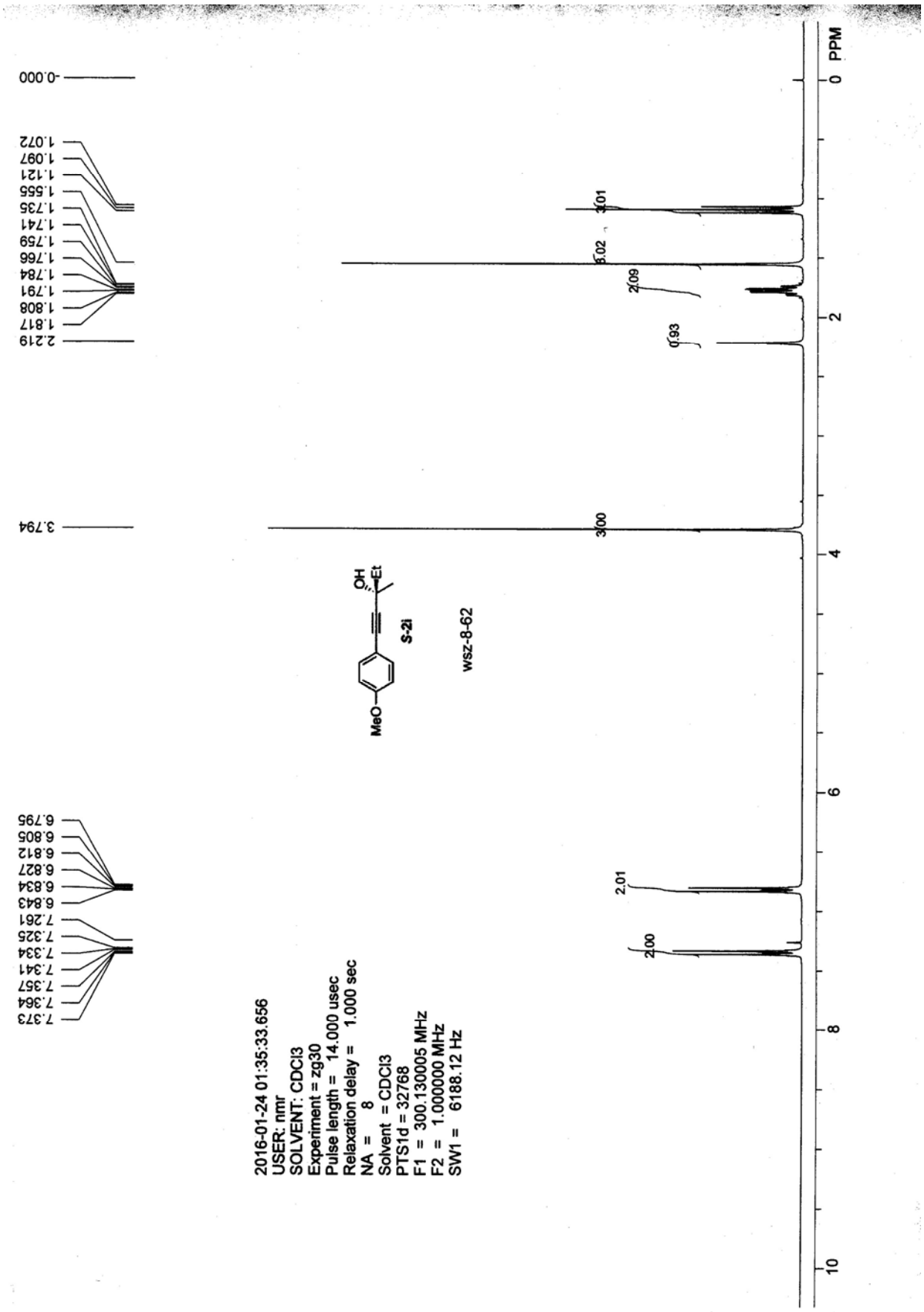
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wsz-8-62

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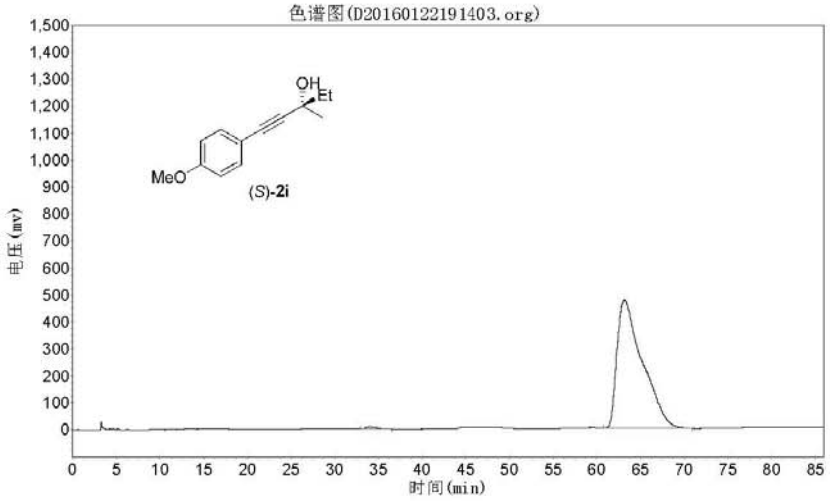

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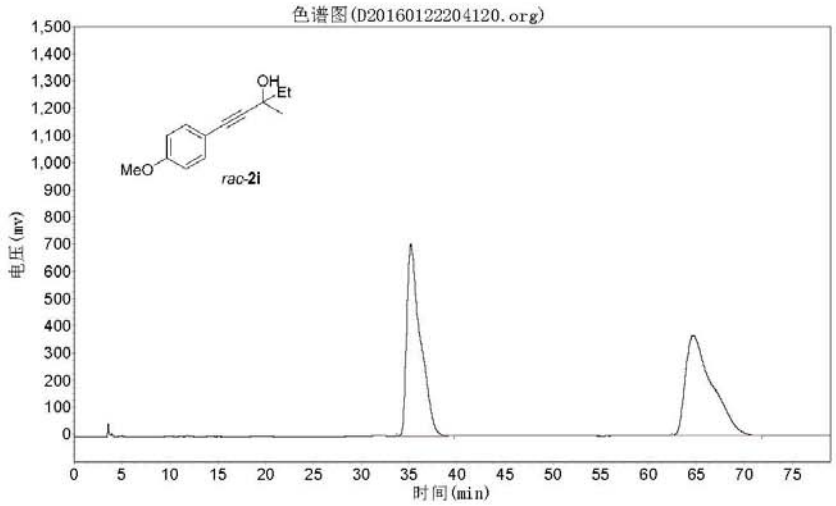

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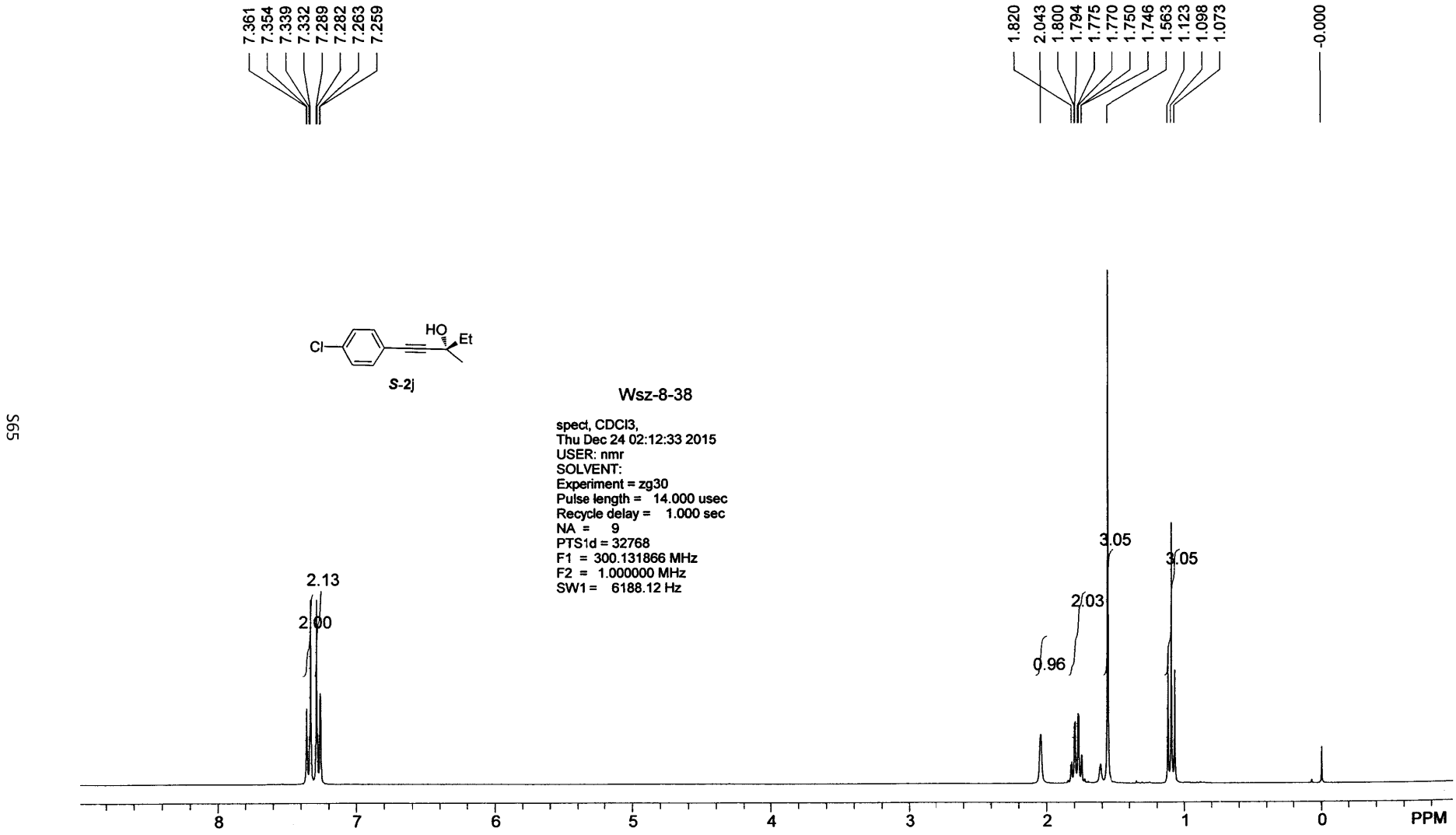
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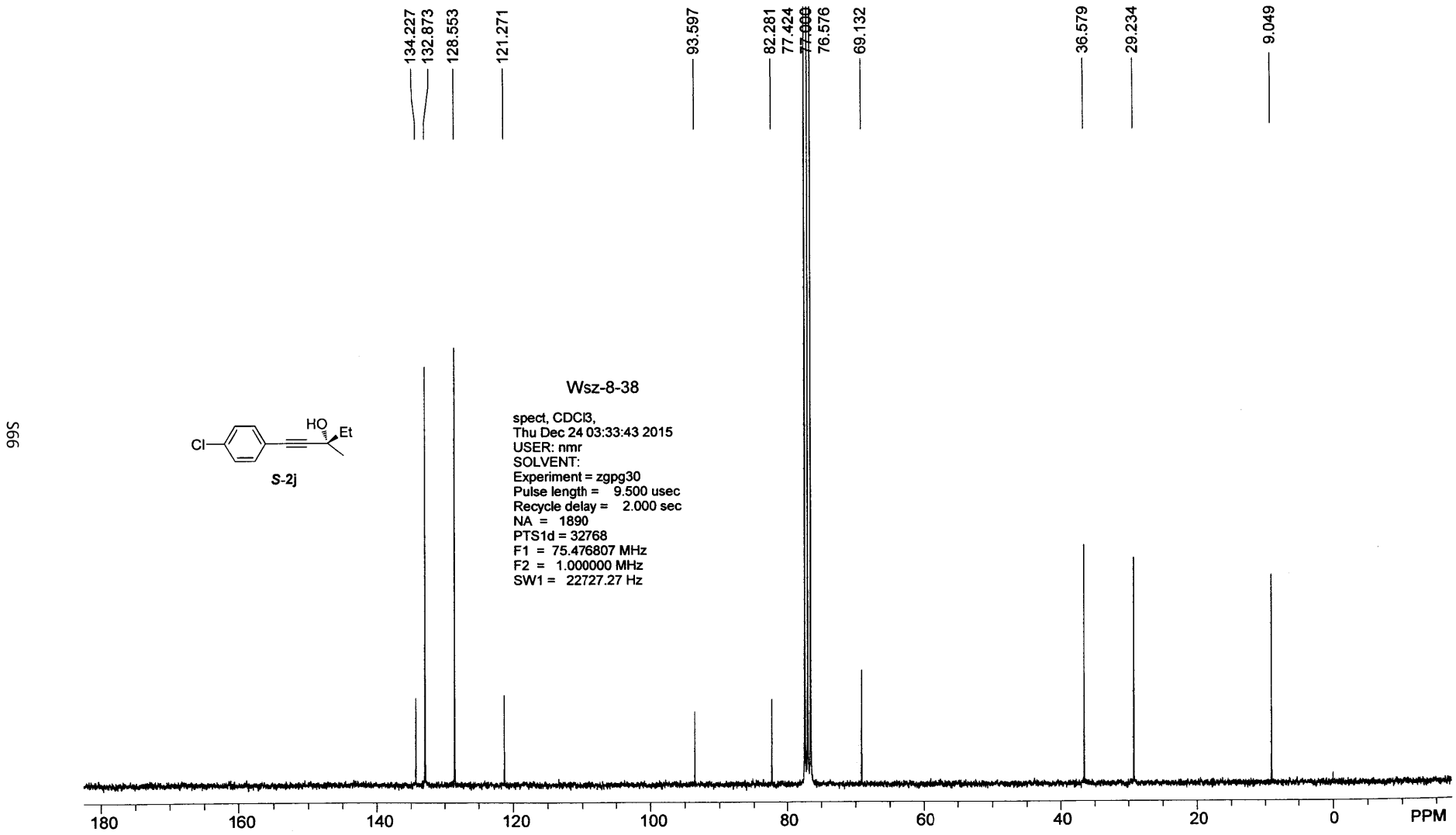
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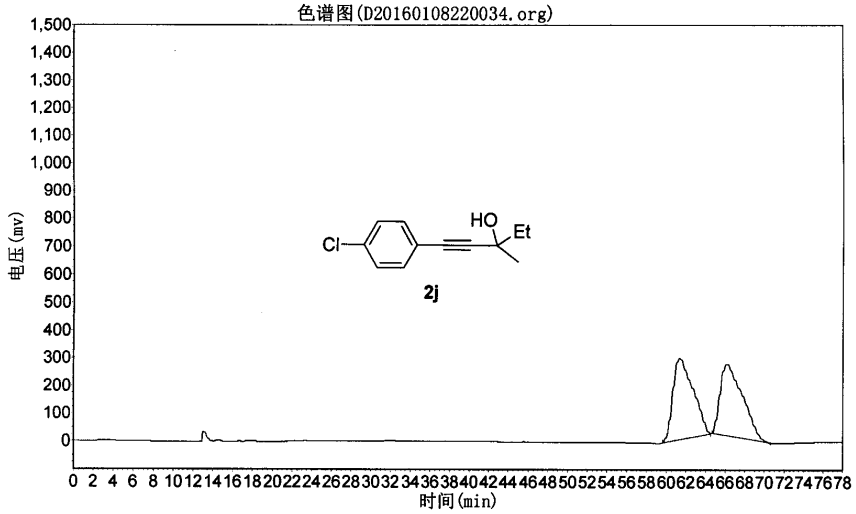
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
Cl
HO
Et
S-2j
180
160
140
120
100
80
60
40
20
0
PPM

wsz-7-128

实验单位：zju
实验时间：2016-01-08,22:00:34
谱图文件:D:\浙大智达\N2000\样品\D20160108220034.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2016-01-08,23:21:32
积分方法:面积归一法

实验内容简介：
OD-H, n-hexane/i-PrOH =100/1, 207 nm,0.5 ml/min



分析结果表

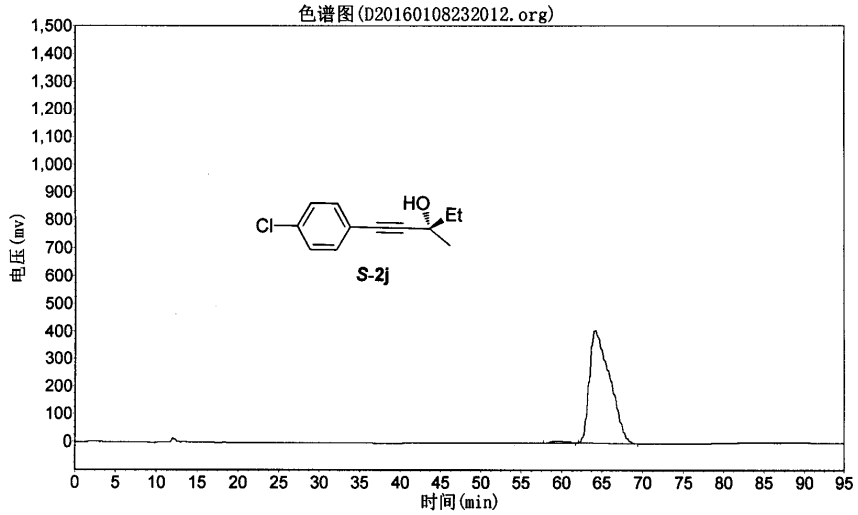
峰号	峰名	保留时间	峰高	峰面积	含量
1		61.388	291966.844	41325260.000	50.4636
2		66.135	256253.766	40566032.000	49.5364
总计			548220.609	81891292.000	100.0000

WSZ-8-38

实验单位：zju
实验时间：2016-01-08,23:20:11
谱图文件:D:\浙大智达\N2000\样品\D20160108232012.org
方法文件:D:\浙大智达\N2000\djx.mtd

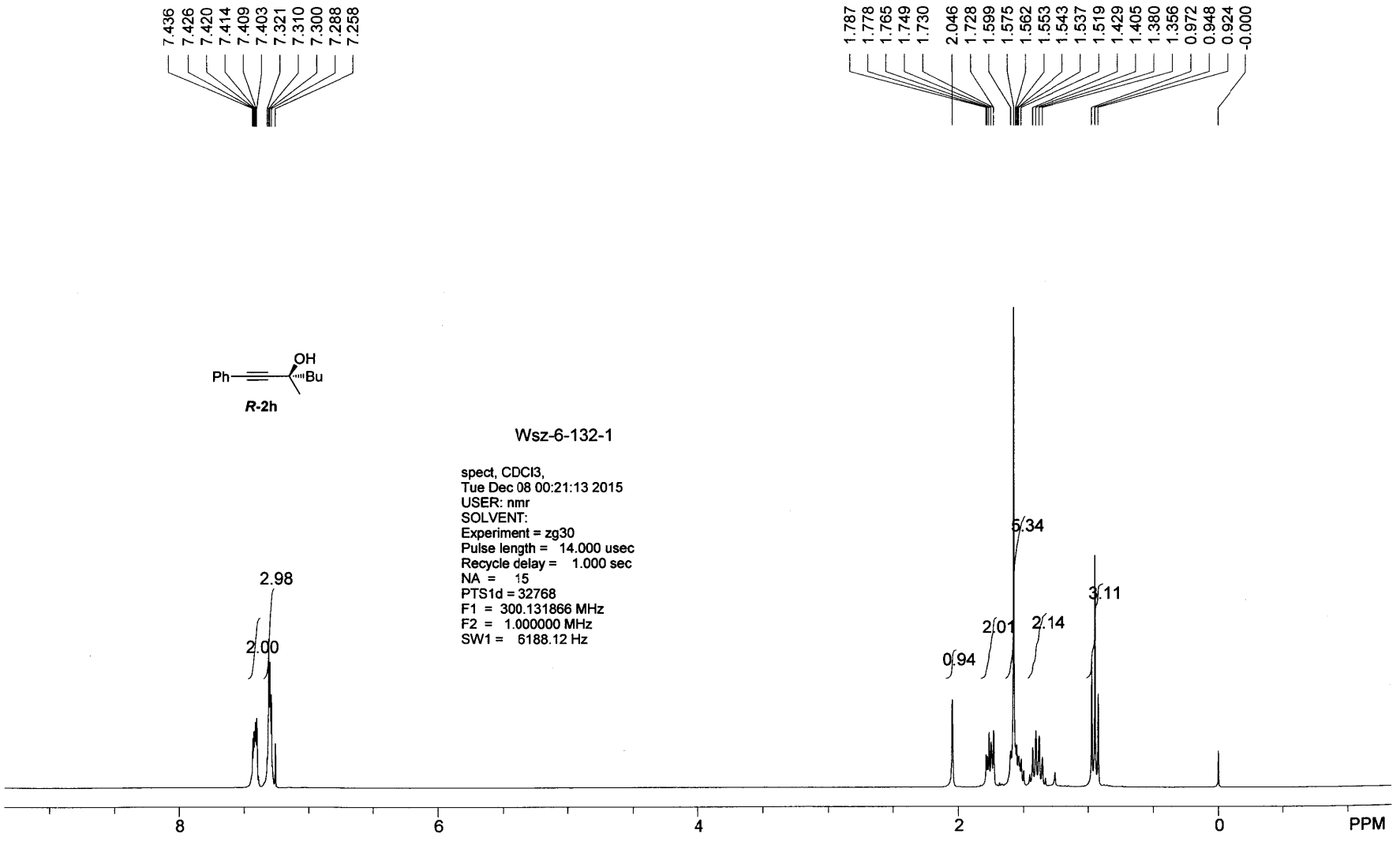
实验者：wsz
报告时间：2016-01-09,13:16:44
积分方法:面积归一法

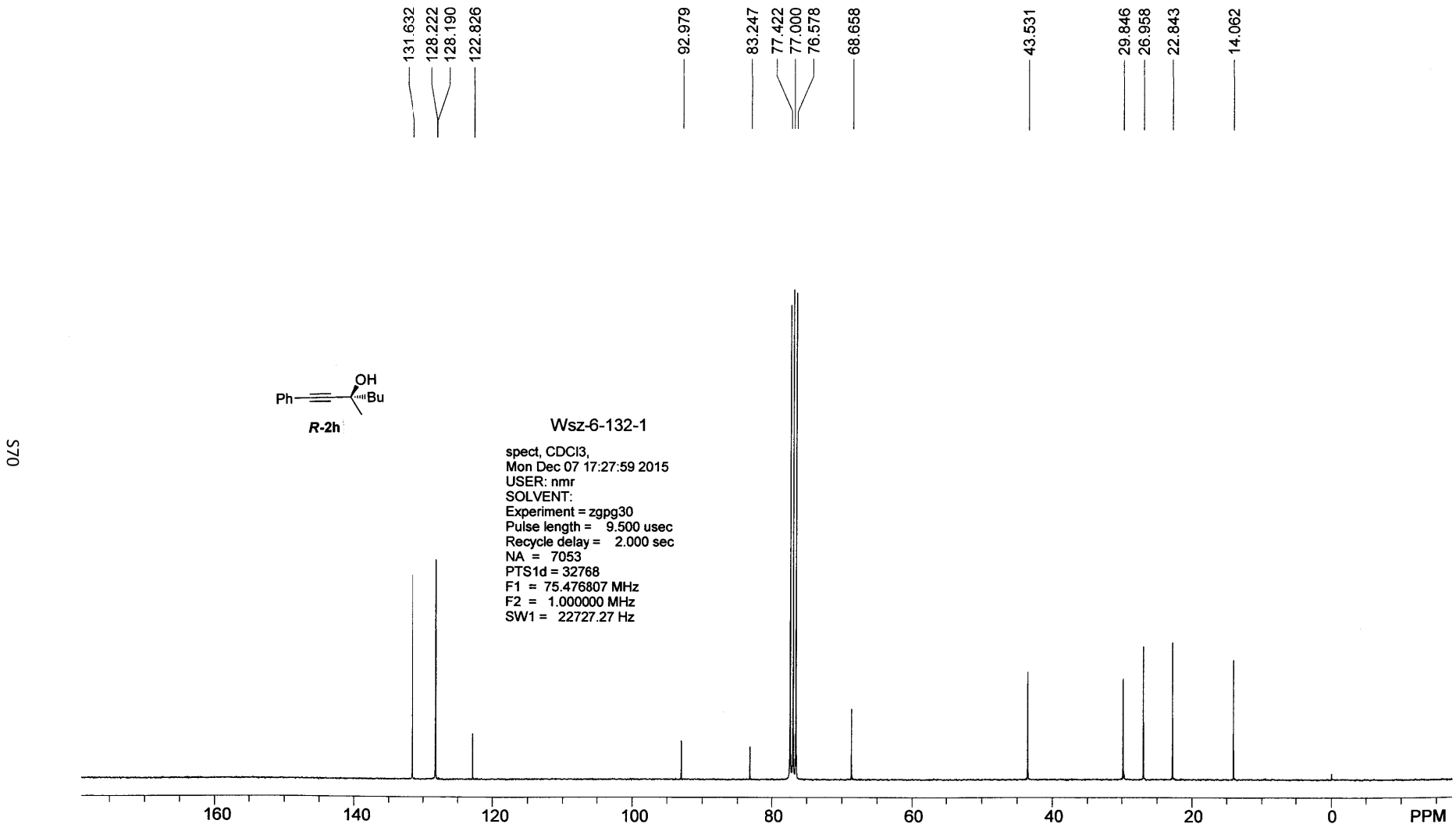
实验内容简介：
OD-H, n-hexane/i-PrOH =100/1, 207 nm,0.5 ml/min

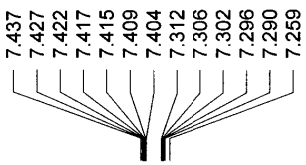


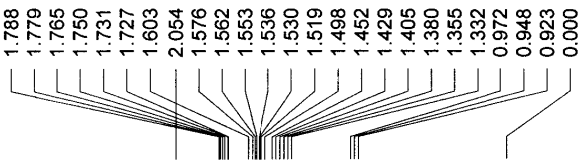
分析结果表

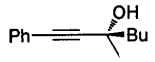
峰号	峰名	保留时间	峰高	峰面积	含量
1		59.320	5725.615	707455.313	0.9900
2		64.290	407751.250	70752168.000	99.0100
总计			413476.865	71459623.313	100.0000


7.436
7.426
7.420
7.414
7.409
7.403
7.321
7.310
7.300
7.288
7.258
1.787
1.778
1.765
1.749
1.730
2.046
1.728
1.599
1.575
1.562
1.553
1.543
1.537
1.519
1.429
1.405
1.380
1.356
0.972
0.948
0.924
-0.000
OH
Ph
Bu
R-2h
Wsz-6-132-1
spect, CDCl3,
Tue Dec 08 00:21:13 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 15
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
2.98
2.00
5.34
3.11
2.01
2.14
0.94
8
6
4
2
0
PPM


131.632
128.222
128.190
122.826
92.979
83.247
77.422
77.000
76.578
68.658
43.531
29.846
26.958
22.843
14.062
OH
Ph
Bu
R-2h
Wsz-6-132-1
spect, CDCl3,
Mon Dec 07 17:27:59 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 7053
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
160
140
120
100
80
60
40
20
0
PPM

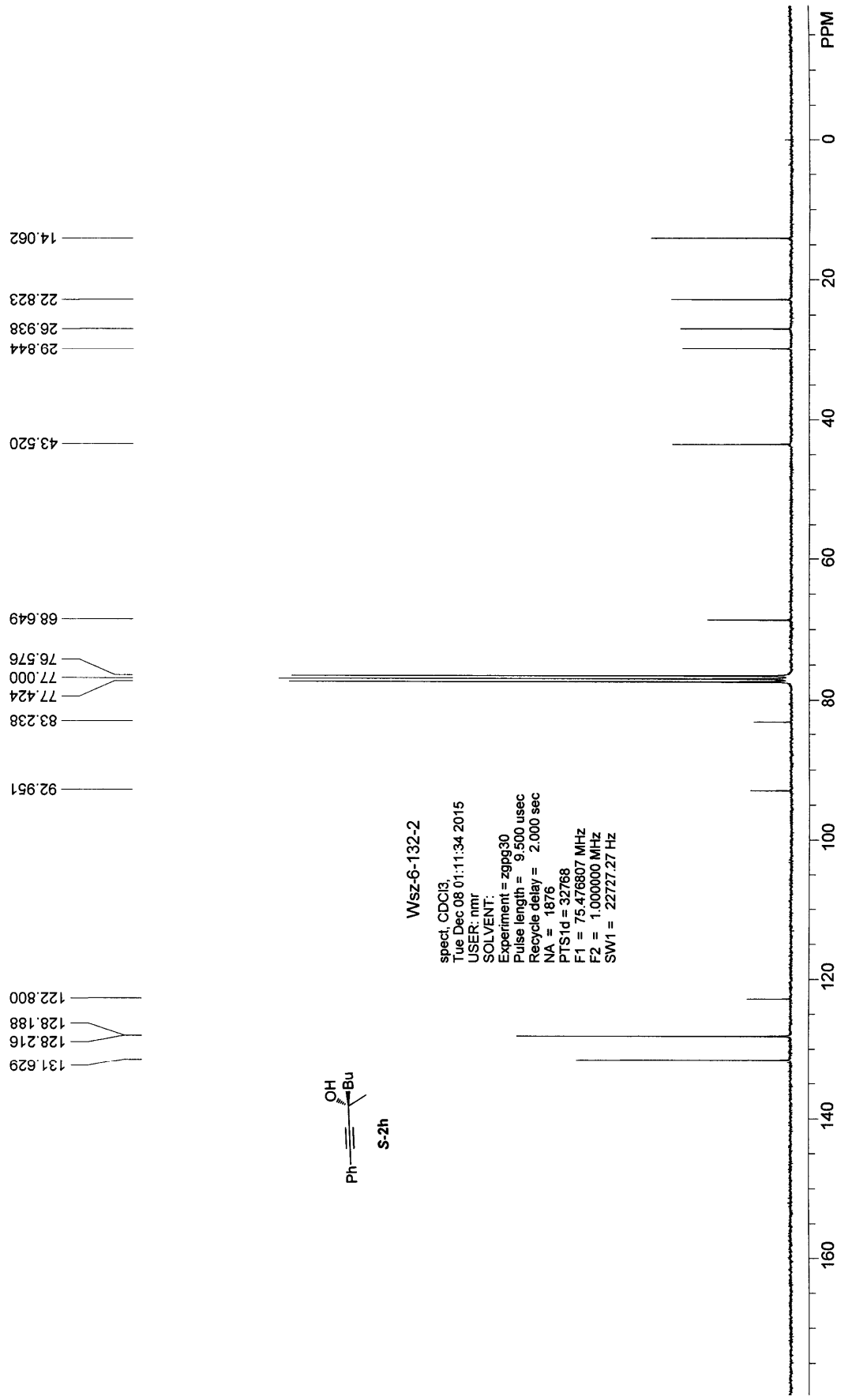

7.437
7.427
7.422
7.417
7.415
7.409
7.404
7.312
7.306
7.302
7.296
7.290
7.259


1.788
1.779
1.765
1.750
1.731
1.727
1.603
2.054
1.576
1.562
1.553
1.536
1.530
1.519
1.498
1.452
1.429
1.405
1.380
1.355
1.332
0.972
0.948
0.923
0.000


OH
Ph
Bu

***S*-2h**

Wsz-6-132-2
spect, CDCl3,
Tue Dec 08 00:27:16 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
3.01
2.00
0.93
2.00
5.36
2.15
3.11
8
6
4
2
0
PPM

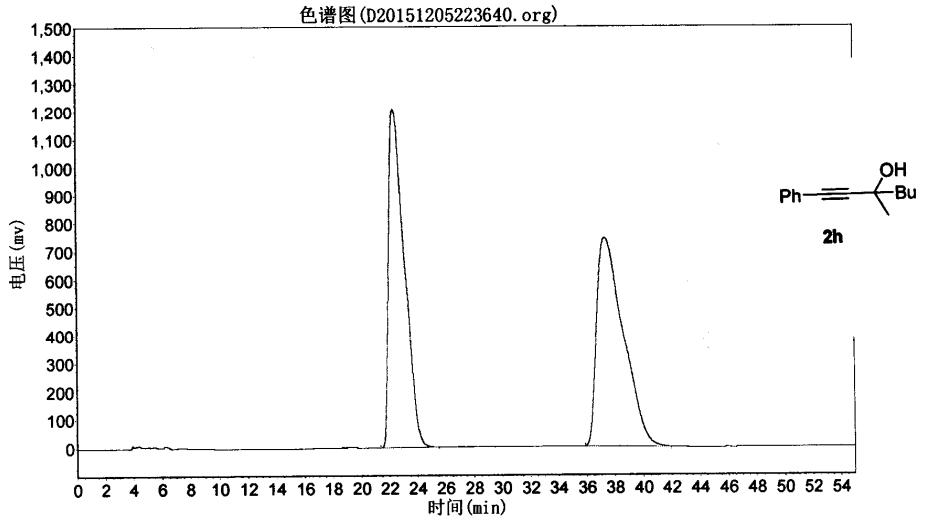

14.062
22.823
26.938
29.844
43.520
68.649
76.576
77.000
77.424
83.238
92.951
122.800
128.188
128.216
131.629
OH
Bu
Ph
S-2h
Wsz-6-132-2
spect, CDCl3,
Tue Dec 08 01:11:34 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1876
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
PPM
0
20
40
60
80
100
120
140
160

Wsz-6-132

实验单位：zju
实验时间：2015-12-05,22:36:40
谱图文件:D:\浙大智达\N2000\样品\D20151205223640.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2015-12-05,23:37:48
积分方法:面积归一法

实验内容简介：
OD-H, n-hexane/i-PrOH = 100/1, 207 nm,1.5 ml/min



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		22.332	1209642.750	93413992.000	49.1741
2		37.298	742860.688	96551848.000	50.8259
总计			1952503.438	189965840.000	100.0000

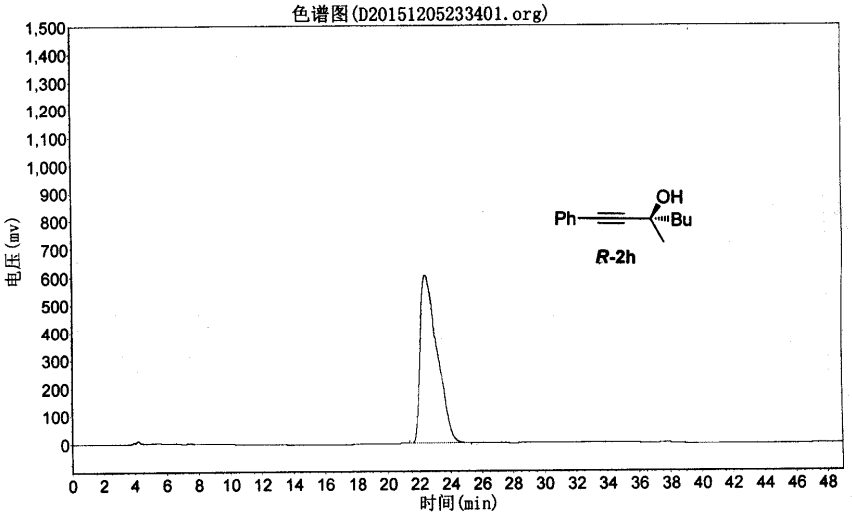
Wsz-6-132-1

实验单位：zju
实验时间：2015/12/5,23:34:01
谱图文件:D:\浙大智达\N2000\样品\D20151205233401.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2015/12/6,0:32:35
积分方法:面积归一法

实验内容简介：
OD-H, n-hexane/i-PrOH = 100/1, 207 nm,1.5 ml/min

色谱图(D20151205233401.org)



分析结果表

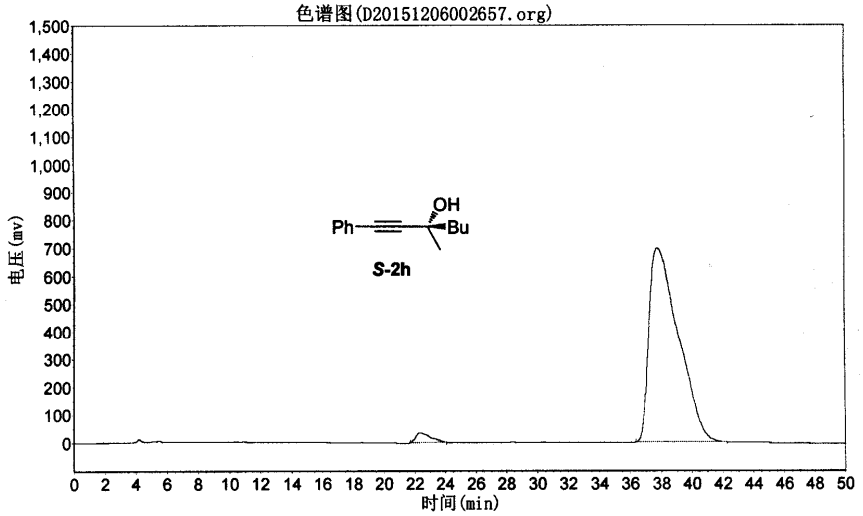
峰号	峰名	保留时间	峰高	峰面积	含量
1		22.408	603372.938	45338112.000	100.0000
总计			603372.938	45338112.000	100.0000

Wsz-6-132-2

实验单位：zju
实验时间：2015/12/6,0:26:57
谱图文件:D:\浙大智达\N2000\样品\D20151206002657.org
方法文件:D:\浙大智达\N2000\djx.mtd

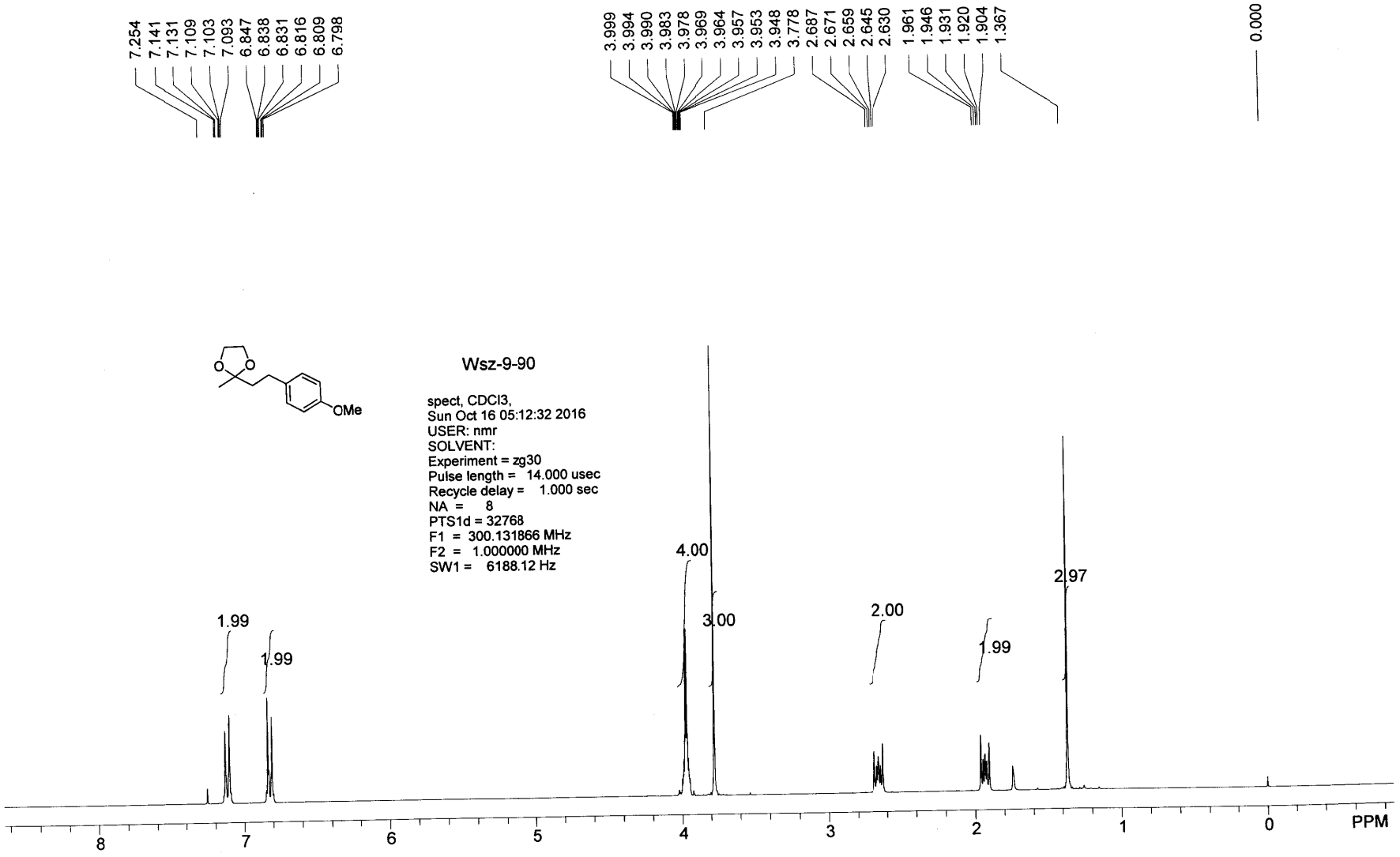
实验者：wsz
报告时间：2015/12/6,1:21:55
积分方法:面积归一法

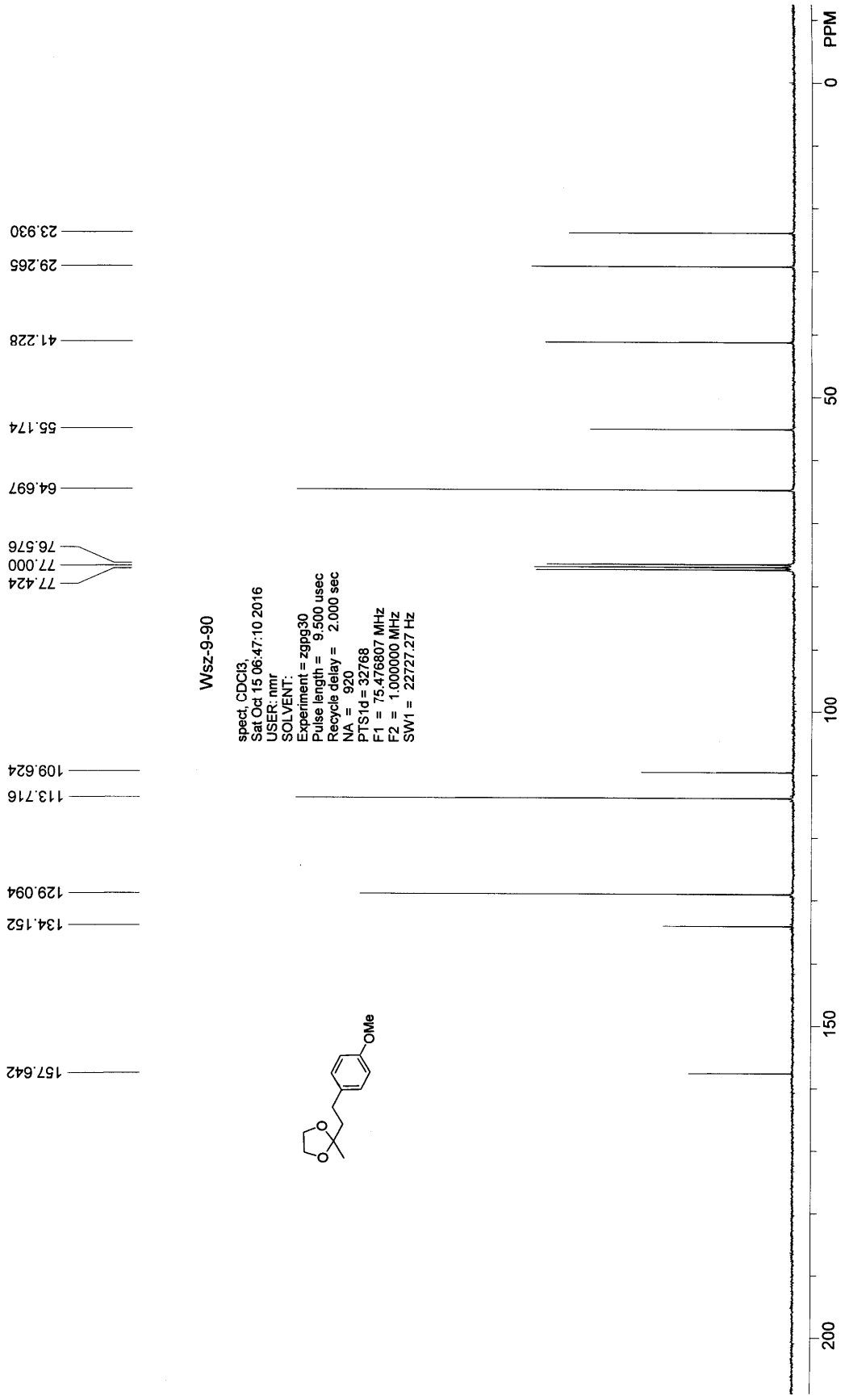
实验内容简介：
OD-H, n-hexane/i-PrOH = 100/1, 207 nm,1.5 ml/min

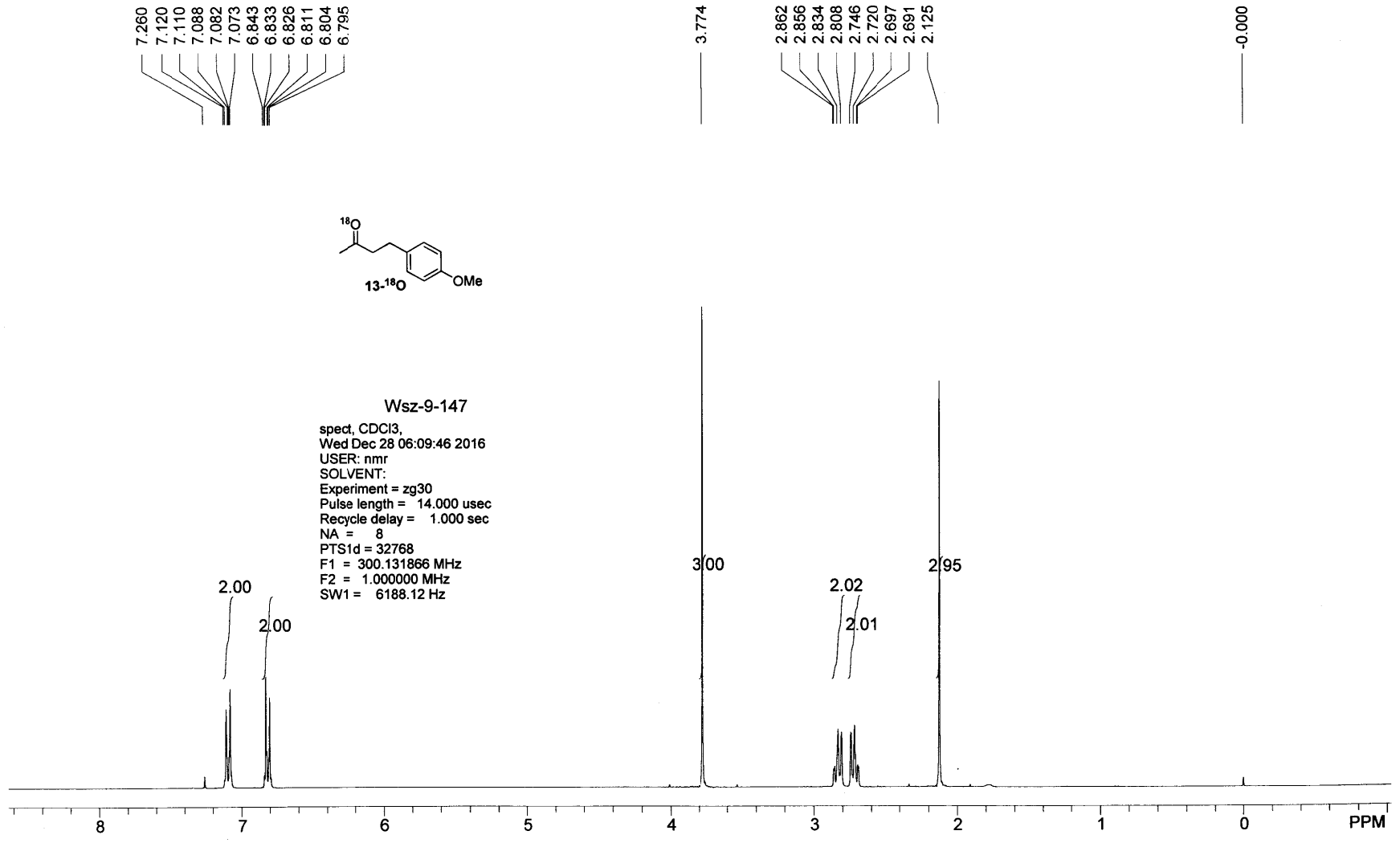


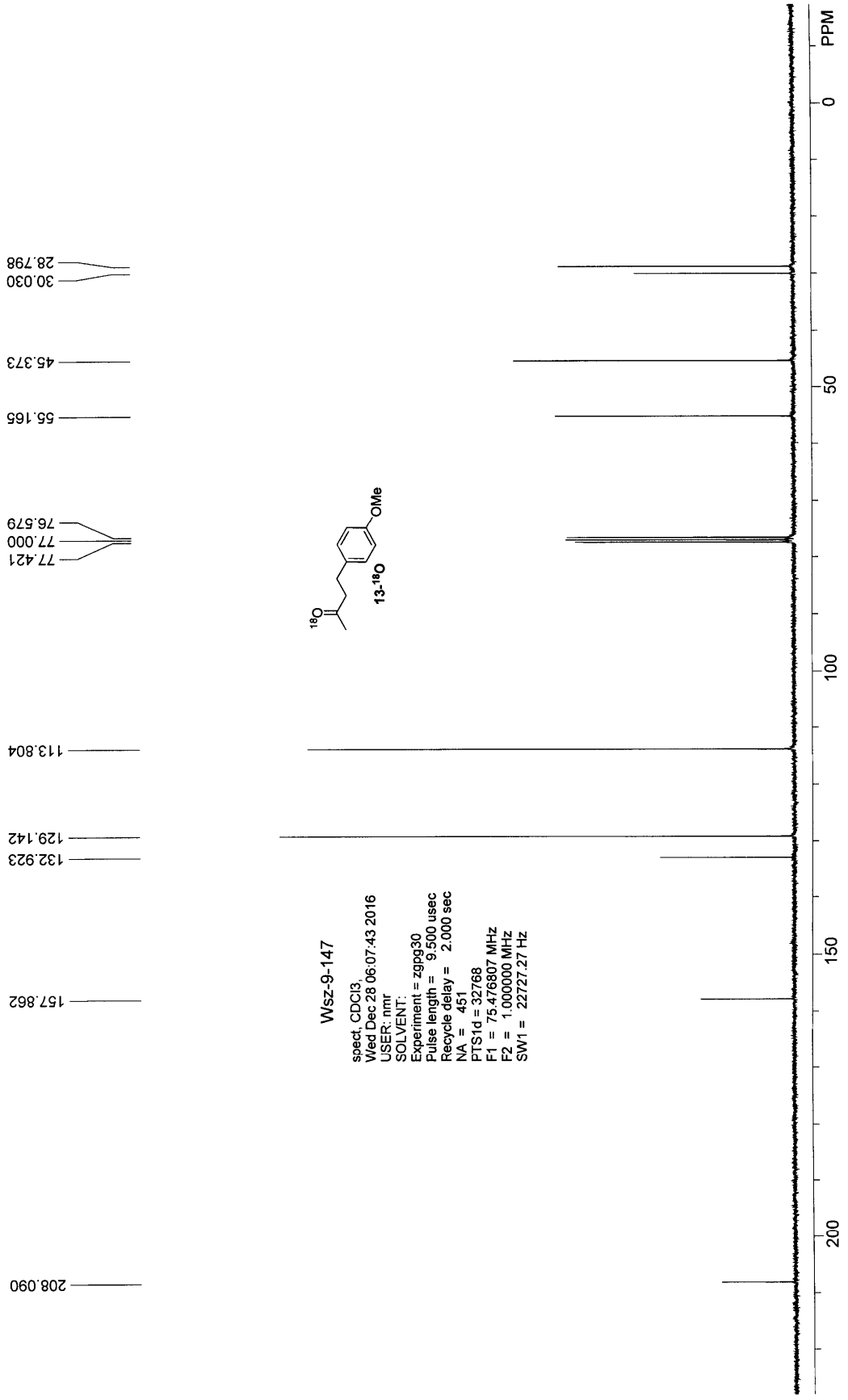
分析结果表

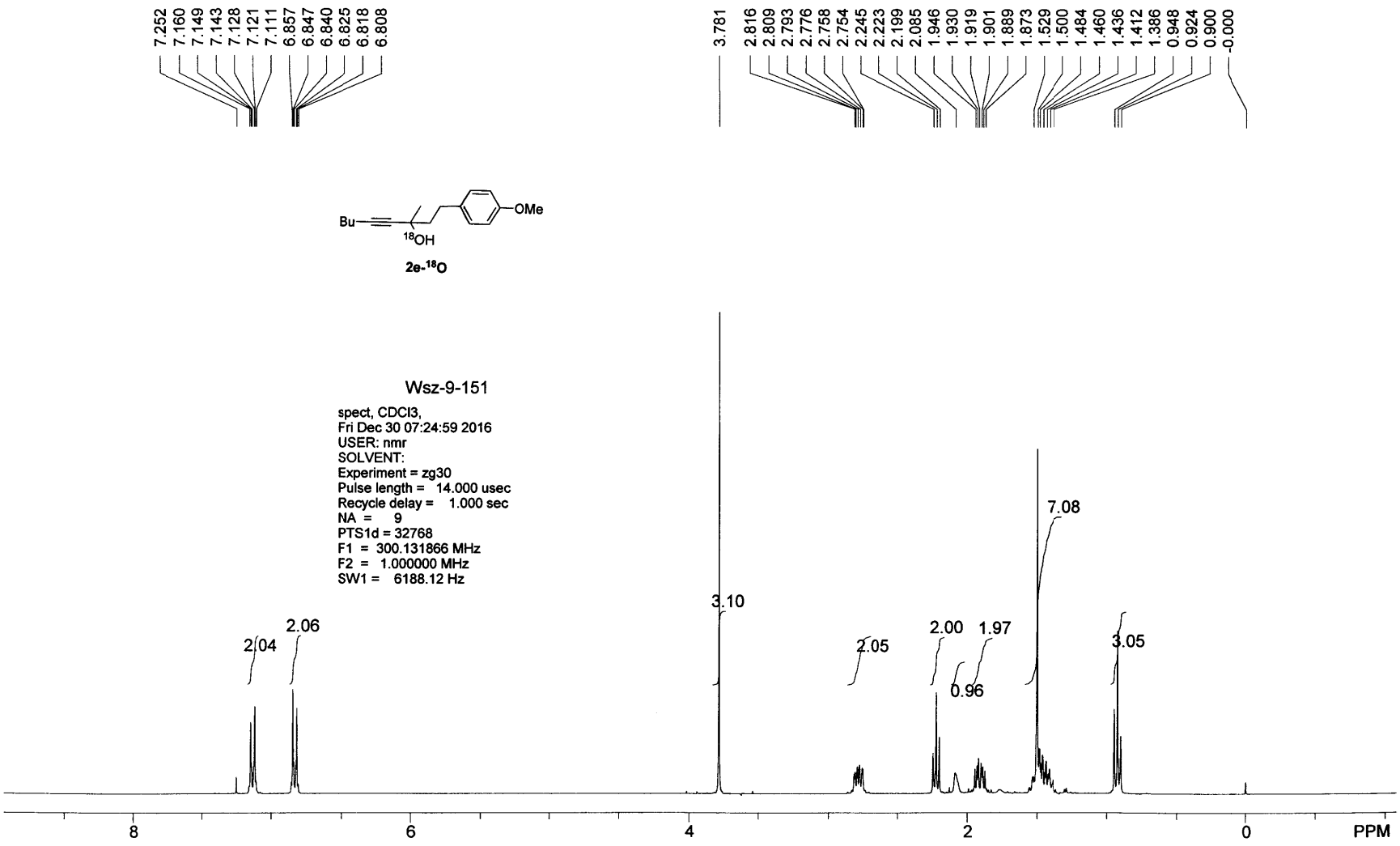
峰号	峰名	保留时间	峰高	峰面积	含量
1		22.343	33615.535	2317805.750	2.4709
2		37.828	695521.188	91486824.000	97.5291
总计			729136.723	93804629.750	100.0000

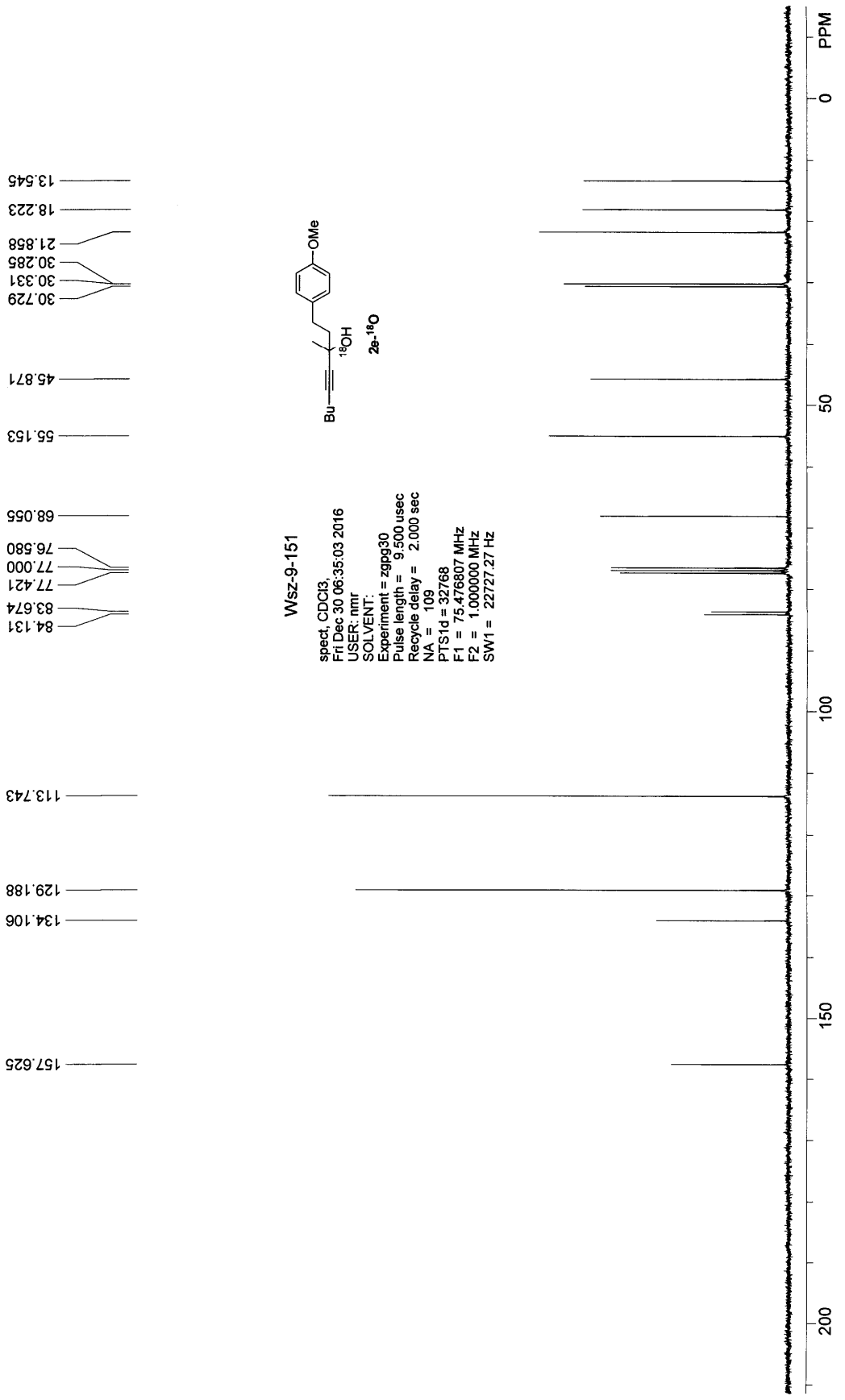

7.254
7.141
7.131
7.109
7.103
7.093
6.847
6.838
6.831
6.816
6.809
6.798
3.999
3.994
3.990
3.983
3.978
3.969
3.964
3.957
3.953
3.948
3.778
2.687
2.671
2.659
2.645
2.630
1.961
1.946
1.931
1.920
1.904
1.367
0.000
OMe
Wsz-9-90
spect, CDCl3,
Sun Oct 16 05:12:32 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
1.99
1.99
4.00
3.00
2.00
1.99
2.97
8
7
6
5
4
3
2
1
0
PPM

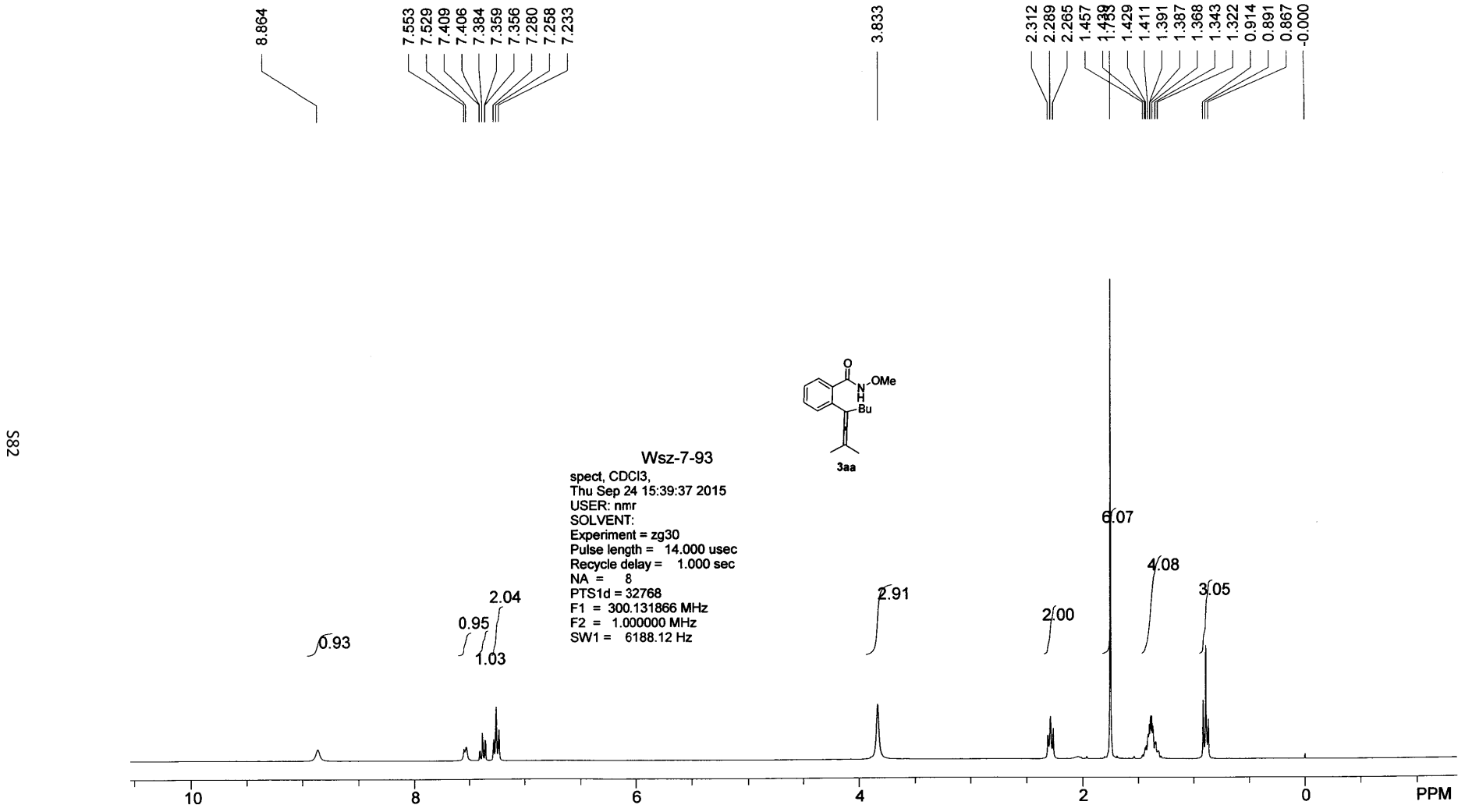

Wsz-9-90
spect, CDCl3,
Sat Oct 15 06:47:10 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 920
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
157.642
134.152
129.094
113.716
109.624
77.424
77.000
76.576
64.697
55.174
41.228
29.265
23.930
PPM
0
50
100
150
200

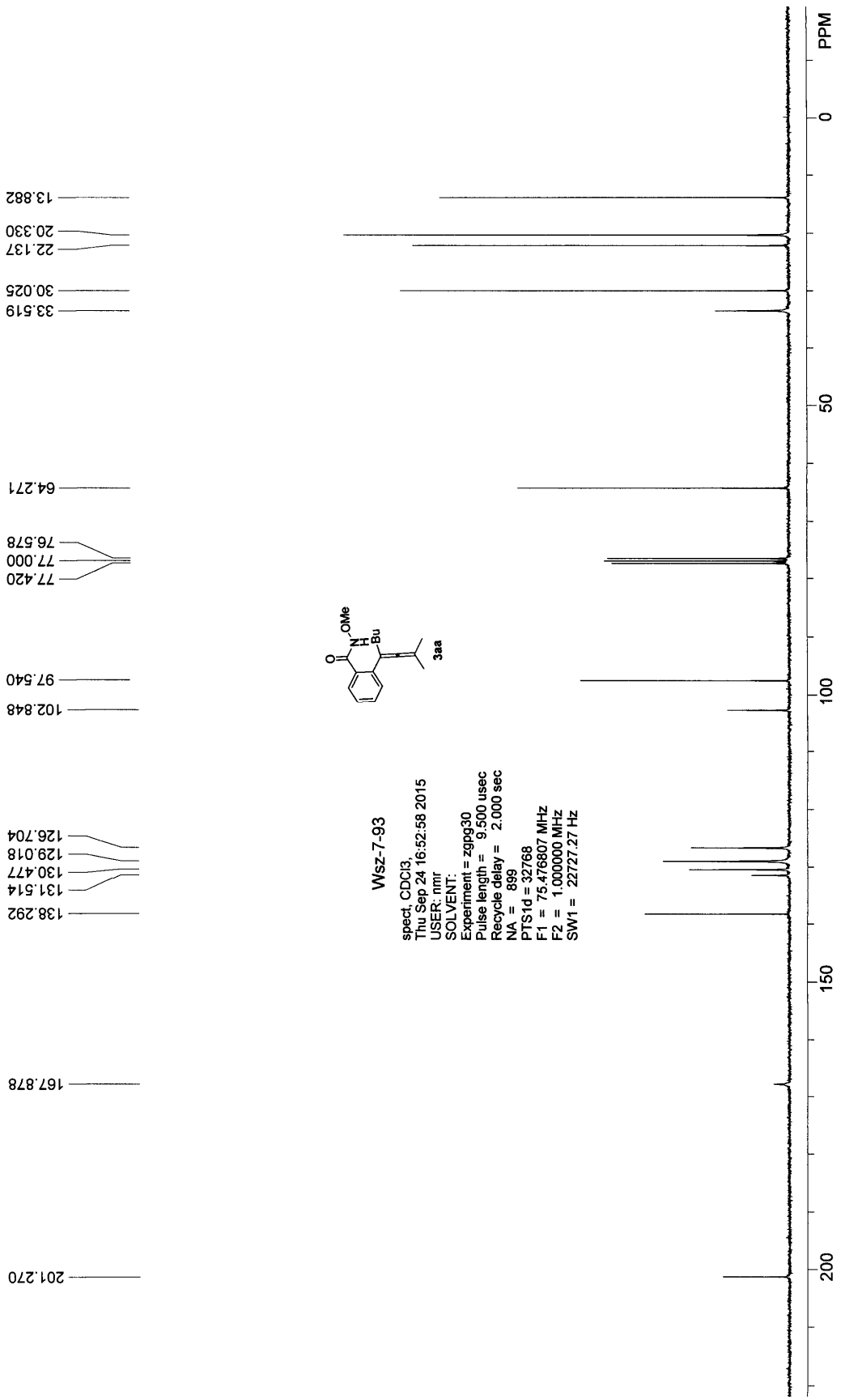

7.260
7.120
7.110
7.088
7.082
7.073
6.843
6.833
6.826
6.811
6.804
6.795
3.774
2.862
2.856
2.834
2.808
2.746
2.720
2.697
2.691
2.125
-0.000
18O
13-18O
OMe
Wsz-9-147
spect, CDCl3,
Wed Dec 28 06:09:46 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
2.00
2.00
3.00
2.02
2.01
2.95
8
7
6
5
4
3
2
1
0
PPM

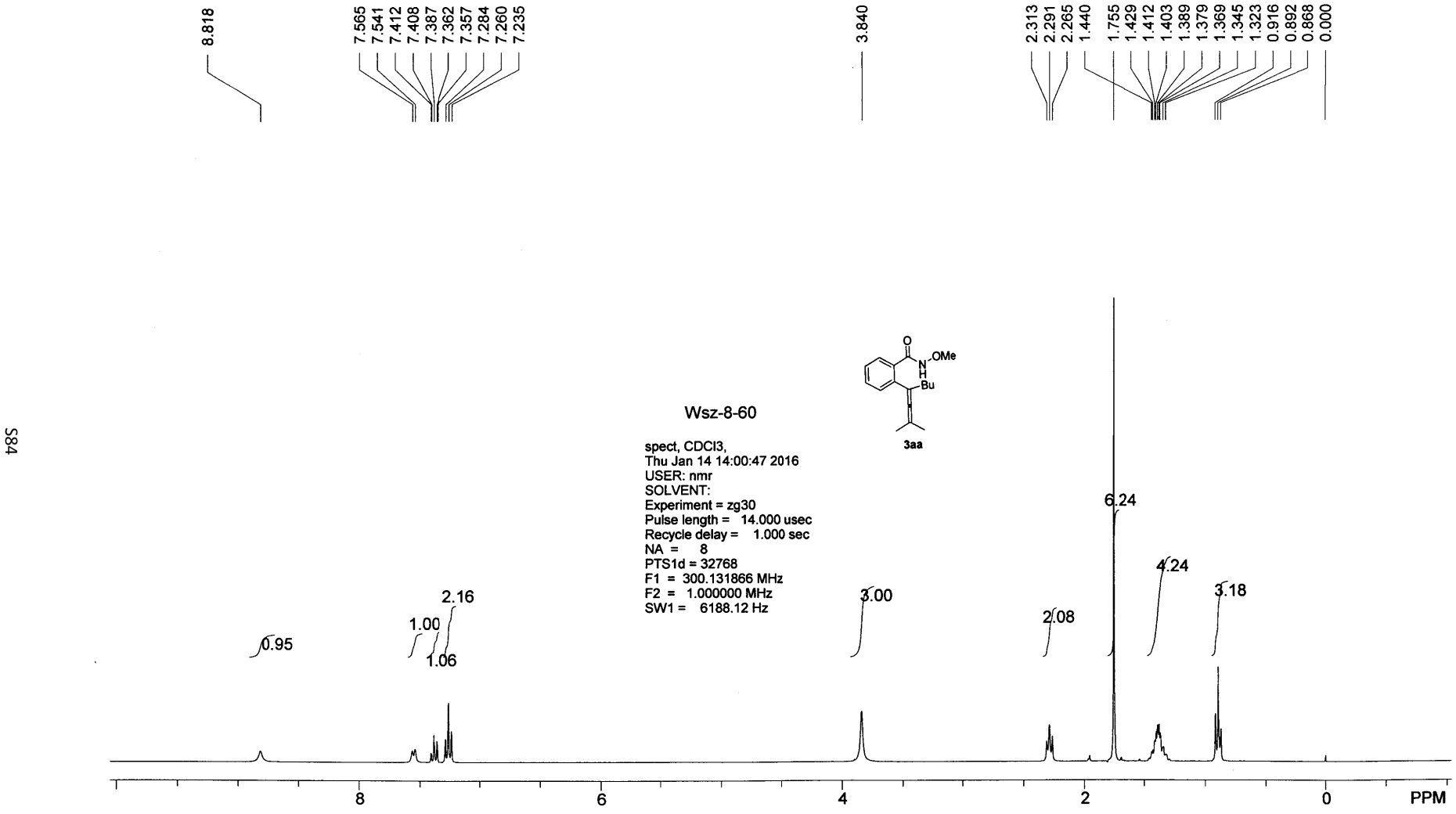

Wsz-9-147
spect, CDCl3,
Wed Dec 28 06:07:43 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 451
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
13-18O
OMe
208.090
157.862
132.923
129.142
113.804
77.421
77.000
76.579
55.165
45.373
30.030
28.798
PPM
0
50
100
150
200

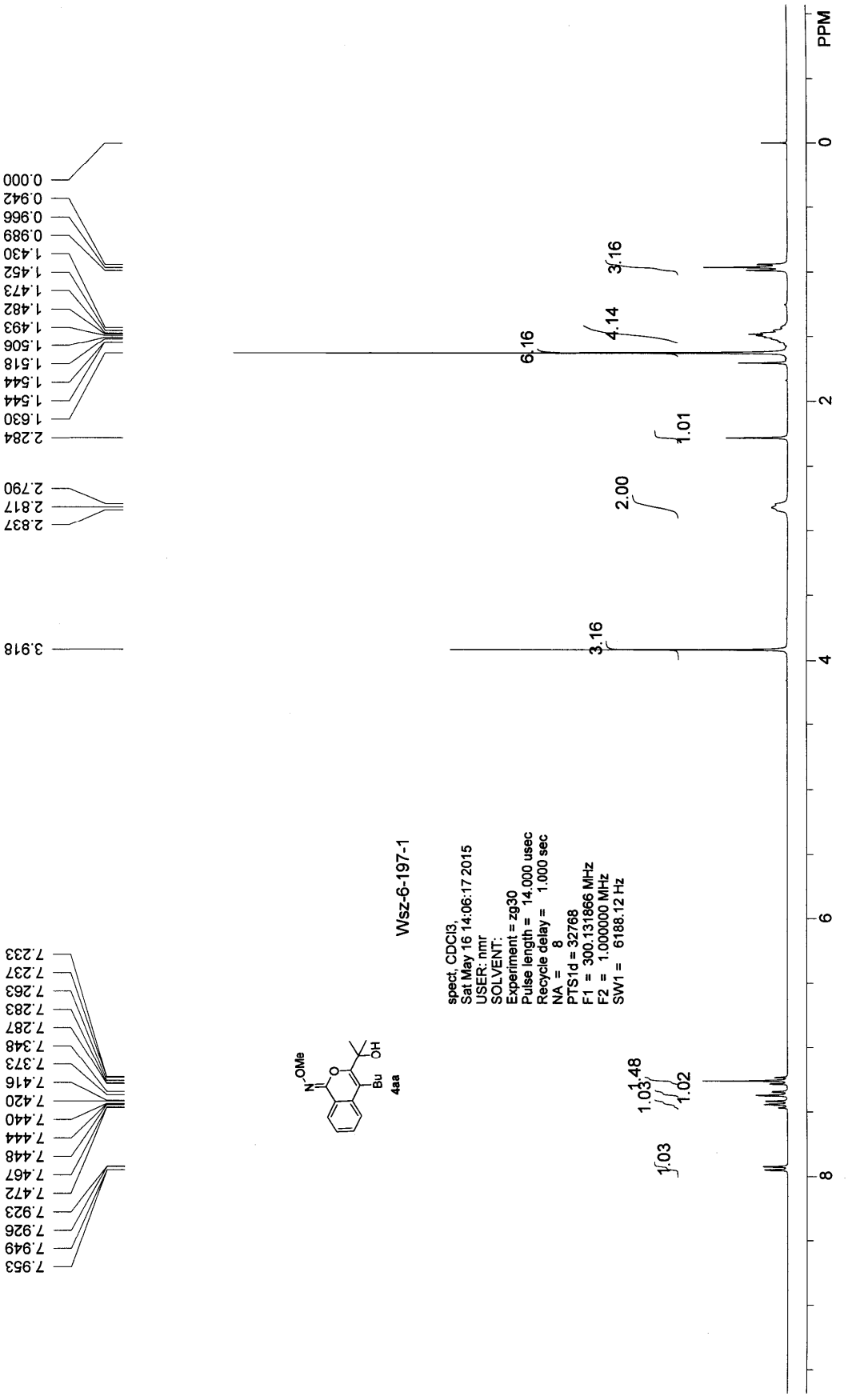

7.252
7.160
7.149
7.143
7.128
7.121
7.111
6.857
6.847
6.840
6.825
6.818
6.808
3.781
2.816
2.809
2.793
2.776
2.758
2.754
2.245
2.223
2.199
2.085
1.946
1.930
1.919
1.901
1.889
1.873
1.529
1.500
1.484
1.460
1.436
1.412
1.386
0.948
0.924
0.900
-0.000
Bu
OMe
18OH
2e-18O
Wsz-9-151
spect, CDCl3,
Fri Dec 30 07:24:59 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
2.04
2.06
3.10
2.05
2.00
1.97
0.96
7.08
3.05
8
6
4
2
0
PPM

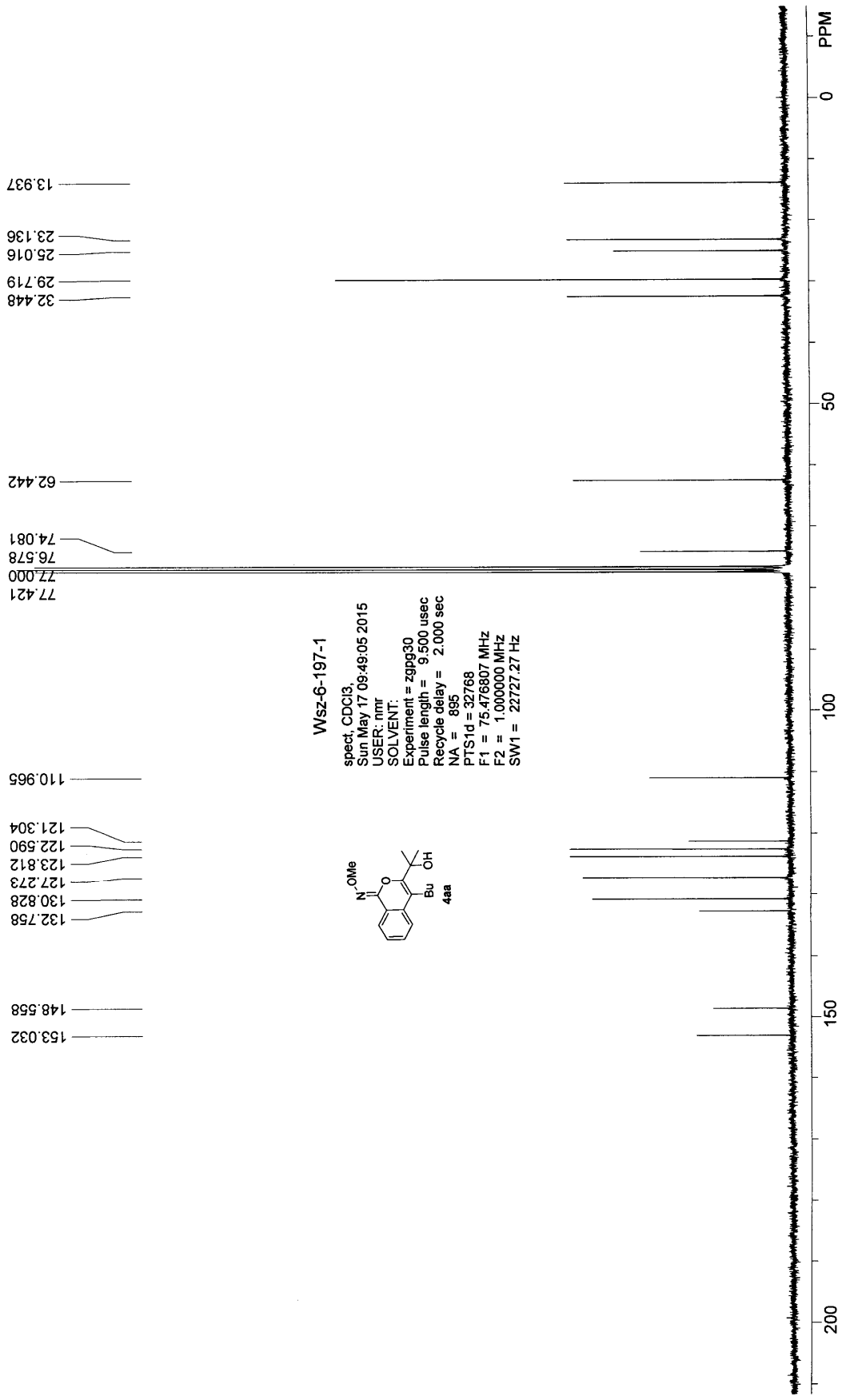

Wsz-9-151
spect, CDCl3,
Fri Dec 30 06:35:03 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 109
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
Bu
^{18}OH
2e-^{18}O
13.545
18.223
21.858
30.285
30.331
30.729
45.871
55.153
68.055
76.580
77.000
77.421
83.674
84.131
113.743
129.188
134.106
157.625
PPM
0
50
100
150
200

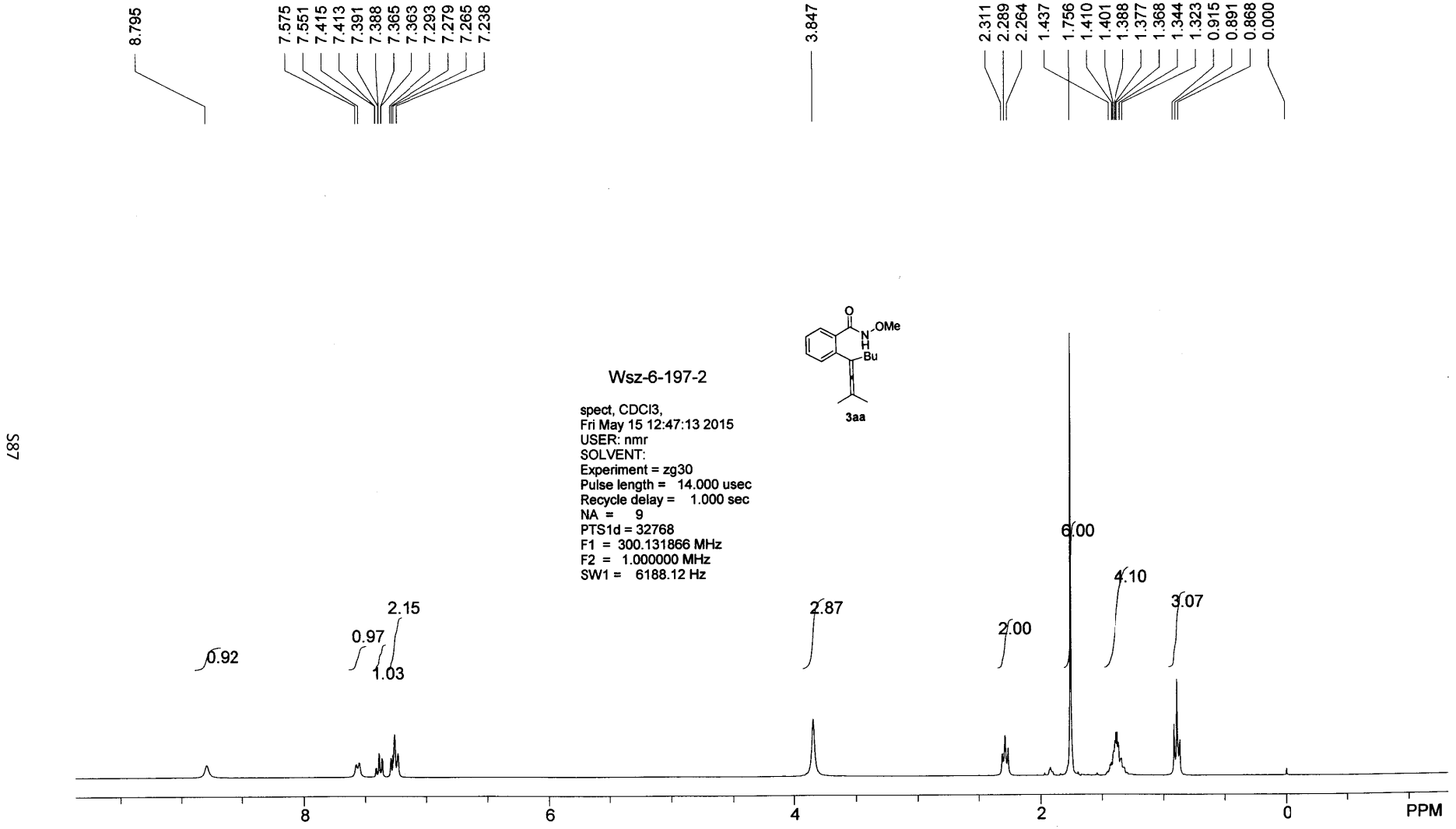

8.864
7.553
7.529
7.409
7.406
7.384
7.359
7.356
7.280
7.258
7.233
3.833
2.312
2.289
2.265
1.457
1.429
1.411
1.391
1.387
1.368
1.343
1.322
0.914
0.891
0.867
-0.000
Wsz-7-93
spect, CDCl3,
Thu Sep 24 15:39:37 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
OMe
N
H
Bu
3aa
0.93
0.95
2.04
1.03
2.91
2.00
6.07
4.08
3.05
10
8
6
4
2
0
PPM

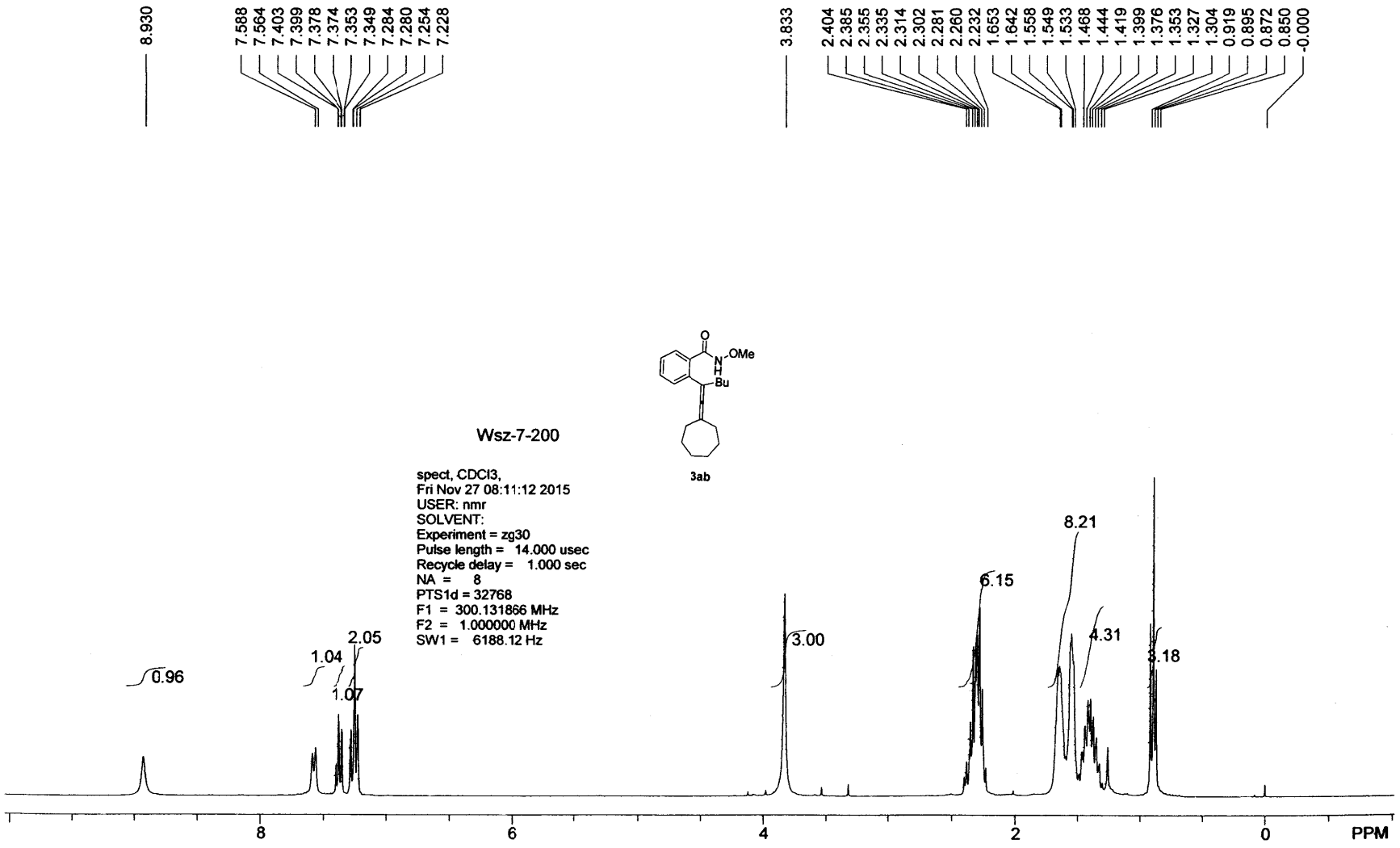

13.882
20.330
22.137
30.025
33.519
64.271
76.578
77.000
77.420
97.540
102.848
126.704
129.018
130.477
131.514
138.292
167.878
201.270
Wsz-7-93
spect, CDCl3,
Thu Sep 24 16:52:58 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 899
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
N
H
Bu
O
3aa
PPM
0
50
100
150
200

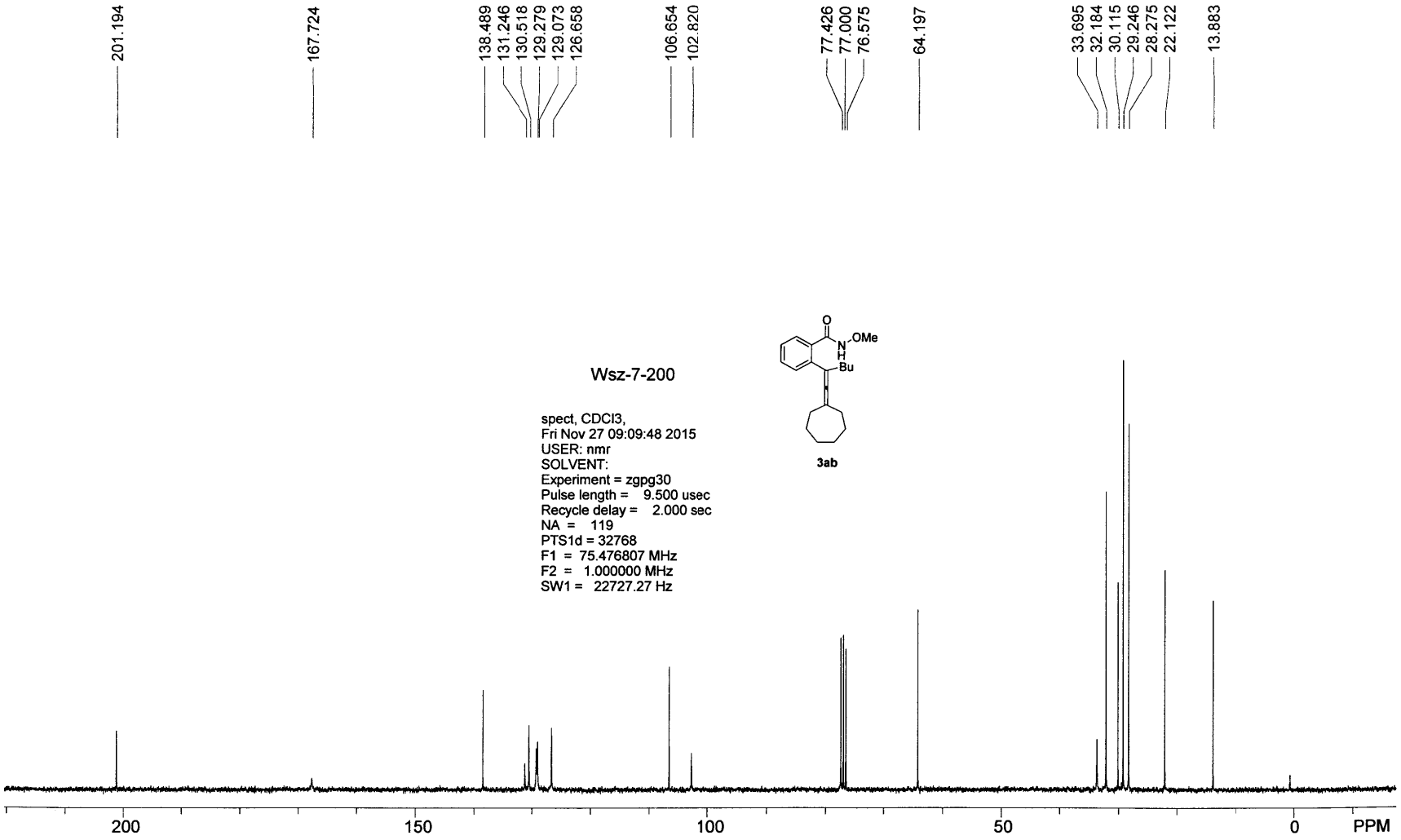

8.818
7.565
7.541
7.412
7.408
7.387
7.362
7.357
7.284
7.260
7.235
3.840
2.313
2.291
2.265
1.440
1.755
1.429
1.412
1.403
1.389
1.379
1.369
1.345
1.323
0.916
0.892
0.868
0.000
Wsz-8-60
spect, CDCl3,
Thu Jan 14 14:00:47 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
OMe
Bu
3aa
0.95
1.00
2.16
1.06
3.00
2.08
6.24
4.24
3.18
8
6
4
2
0
PPM


Wsz-6-197-1
spect, CDCl3,
Sat May 16 14:06:17 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
4aa
PPM
0
2
4
6
8
3.16
6.16
4.14
3.16
1.01
2.00
3.16
1.03
1.48
1.02
1.03
7.953
7.949
7.926
7.923
7.472
7.467
7.448
7.444
7.440
7.420
7.416
7.373
7.348
7.287
7.283
7.263
7.237
7.233
3.918
2.837
2.817
2.790
2.284
1.630
1.544
1.544
1.518
1.506
1.493
1.482
1.473
1.452
1.430
0.989
0.966
0.942
0.000

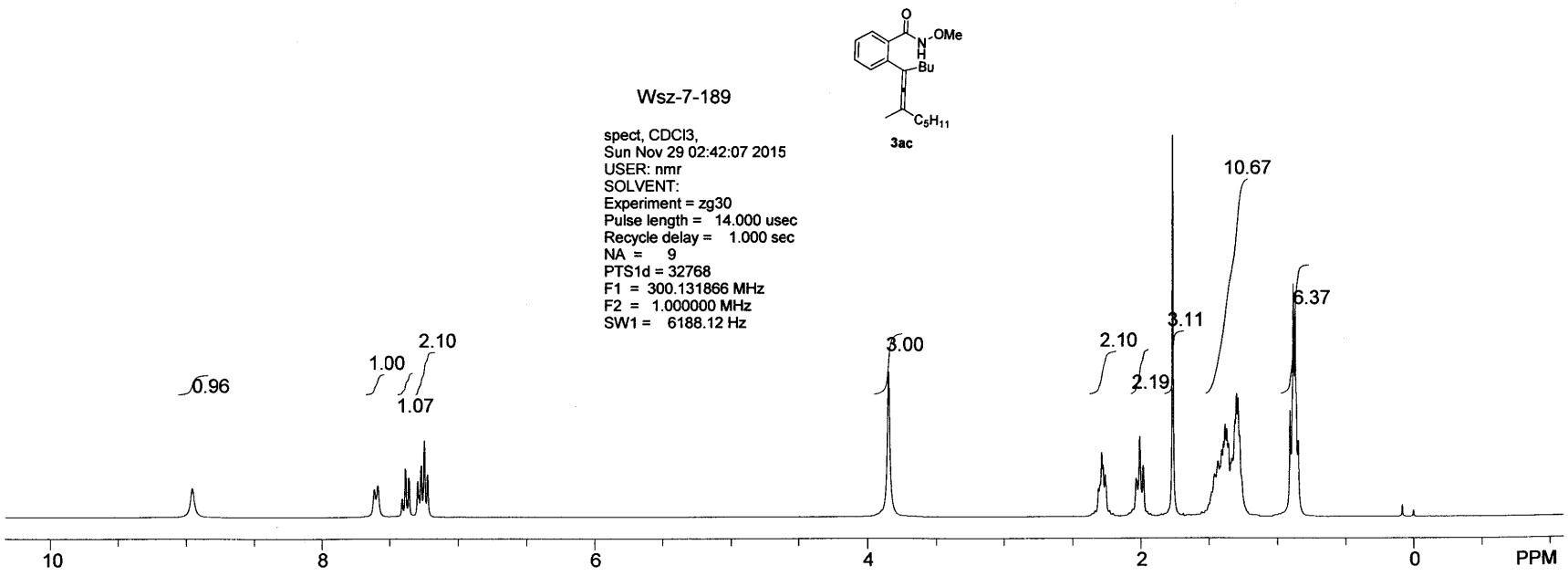

Wsz-6-197-1
spect, CDCl3,
Sun May 17 09:49:05 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 895
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
OH
Bu
4aa
13.937
23.136
25.016
29.719
32.448
62.442
74.081
76.578
77.000
77.421
110.965
121.304
122.590
123.812
127.273
130.828
132.758
148.558
153.032
PPM
0
50
100
150
200

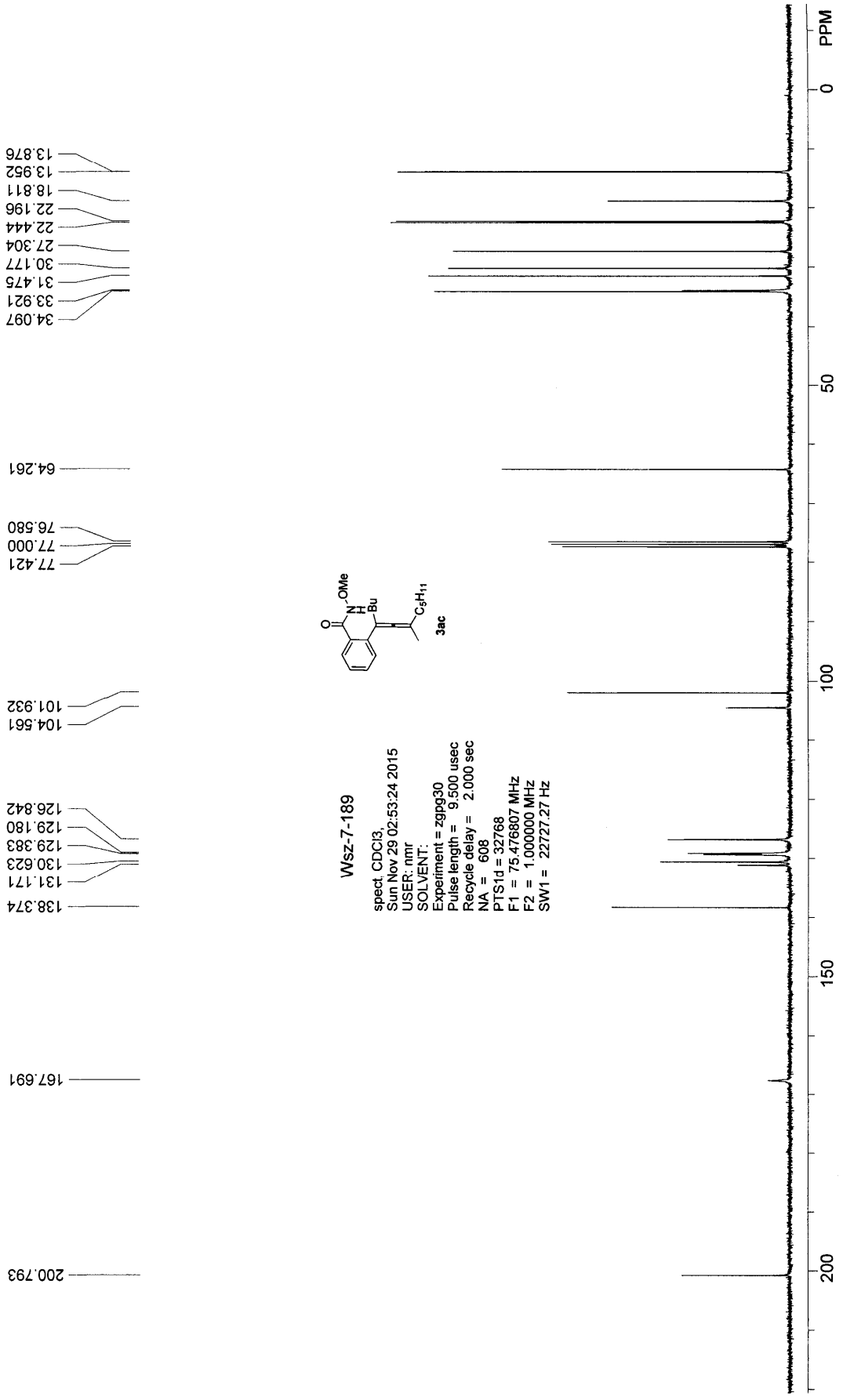

8.795
7.575
7.551
7.415
7.413
7.391
7.388
7.365
7.363
7.293
7.279
7.265
7.238
3.847
2.311
2.289
2.264
1.437
1.756
1.410
1.401
1.388
1.377
1.368
1.344
1.323
0.915
0.891
0.868
0.000
Wsz-6-197-2
spect, CDCl3,
Fri May 15 12:47:13 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
OMe
N
H
Bu
3aa
0.92
2.15
0.97
1.03
2.87
2.00
6.00
4.10
3.07
8
6
4
2
0
PPM

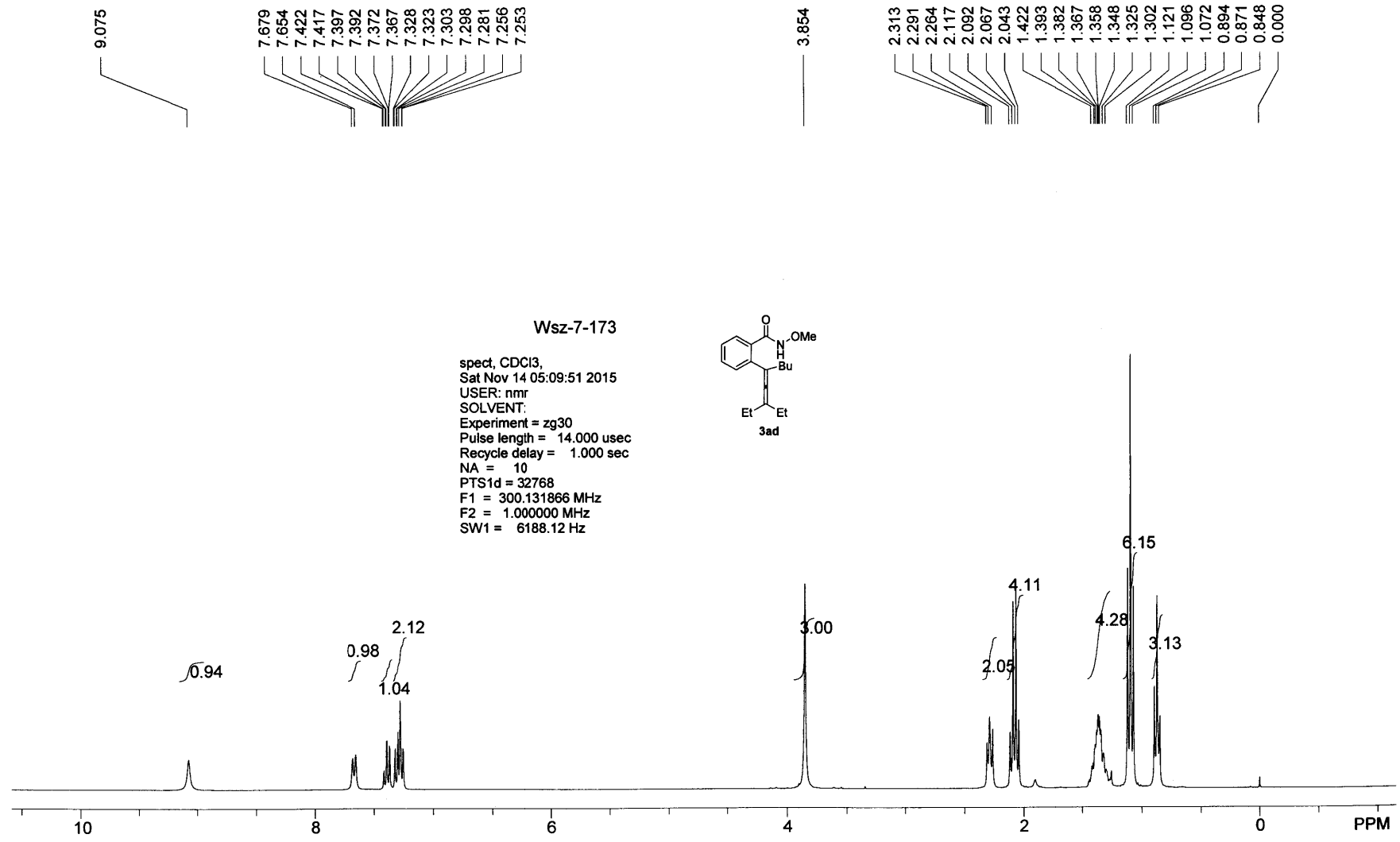

8.930
7.588
7.564
7.403
7.399
7.378
7.374
7.353
7.349
7.284
7.280
7.254
7.228
3.833
2.404
2.385
2.355
2.335
2.314
2.302
2.281
2.260
2.232
1.653
1.642
1.558
1.549
1.533
1.468
1.444
1.419
1.399
1.376
1.353
1.327
1.304
0.919
0.895
0.872
0.850
-0.000
O
N
H
OMe
Bu
3ab
Wsz-7-200
spect, CDCl3,
Fri Nov 27 08:11:12 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.96
1.04
1.07
2.05
3.00
6.15
8.21
4.31
3.18
8
6
4
2
0
PPM

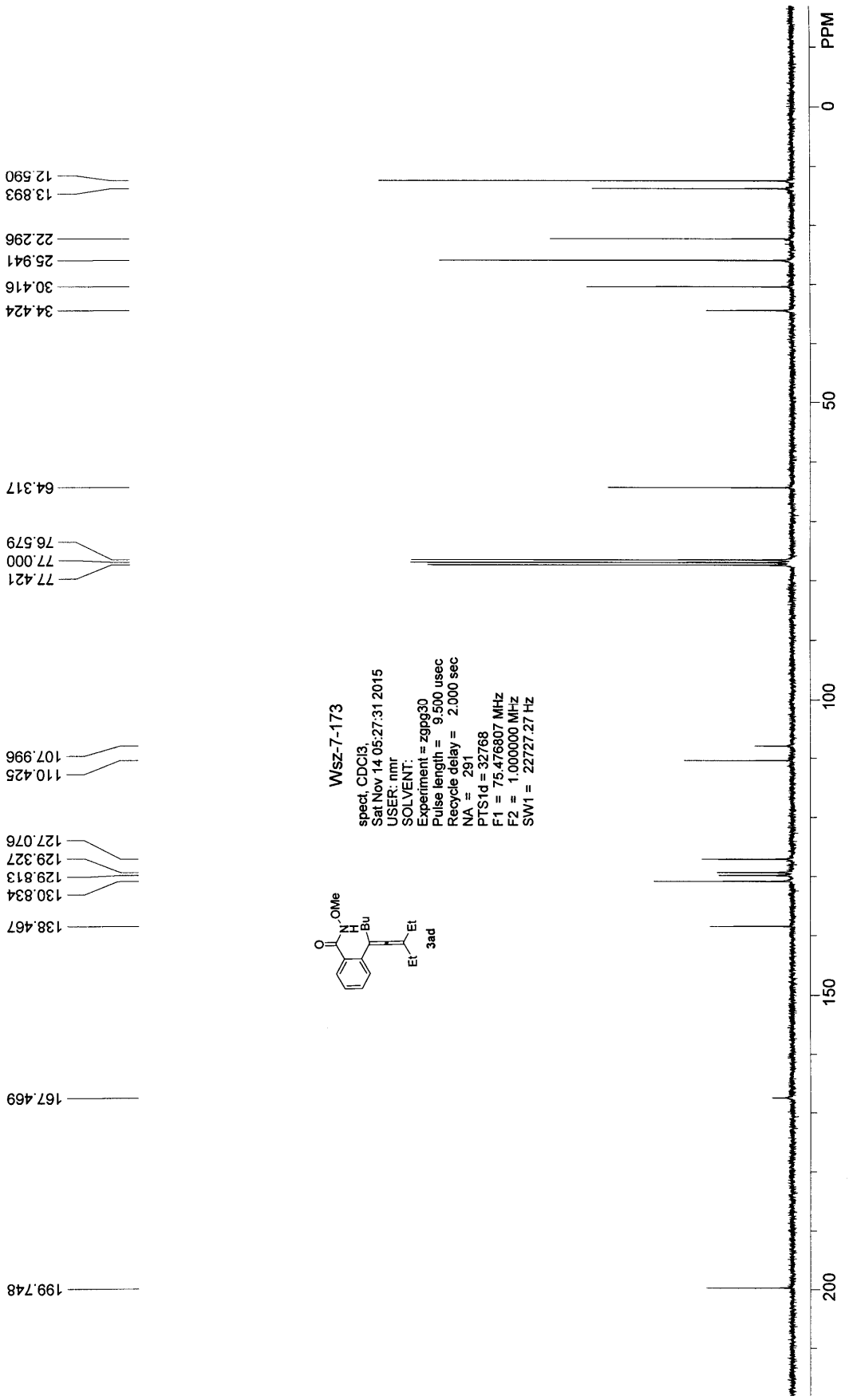

201.194
167.724
138.489
131.246
130.518
129.279
129.073
126.658
106.654
102.820
77.426
77.000
76.575
64.197
33.695
32.184
30.115
29.246
28.275
22.122
13.883
Wsz-7-200
spect, CDCl3,
Fri Nov 27 09:09:48 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 119
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
O
N
H
OMe
Bu
3ab
200
150
100
50
0
PPM

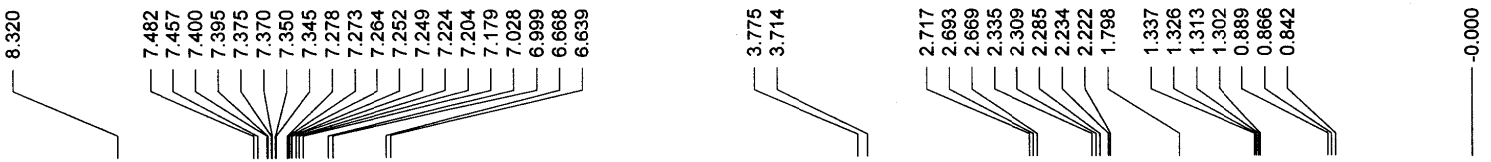

8.957
7.618
7.593
7.412
7.408
7.387
7.383
7.362
7.358
7.296
7.272
7.250
7.225
3.847
2.338
2.311
2.301
2.288
2.278
2.263
2.227
2.036
2.009
1.984
1.768
1.479
1.459
1.432
1.407
1.393
1.381
1.370
1.358
1.312
1.301
1.289
1.278
0.906
0.882
0.867
0.845
0.000

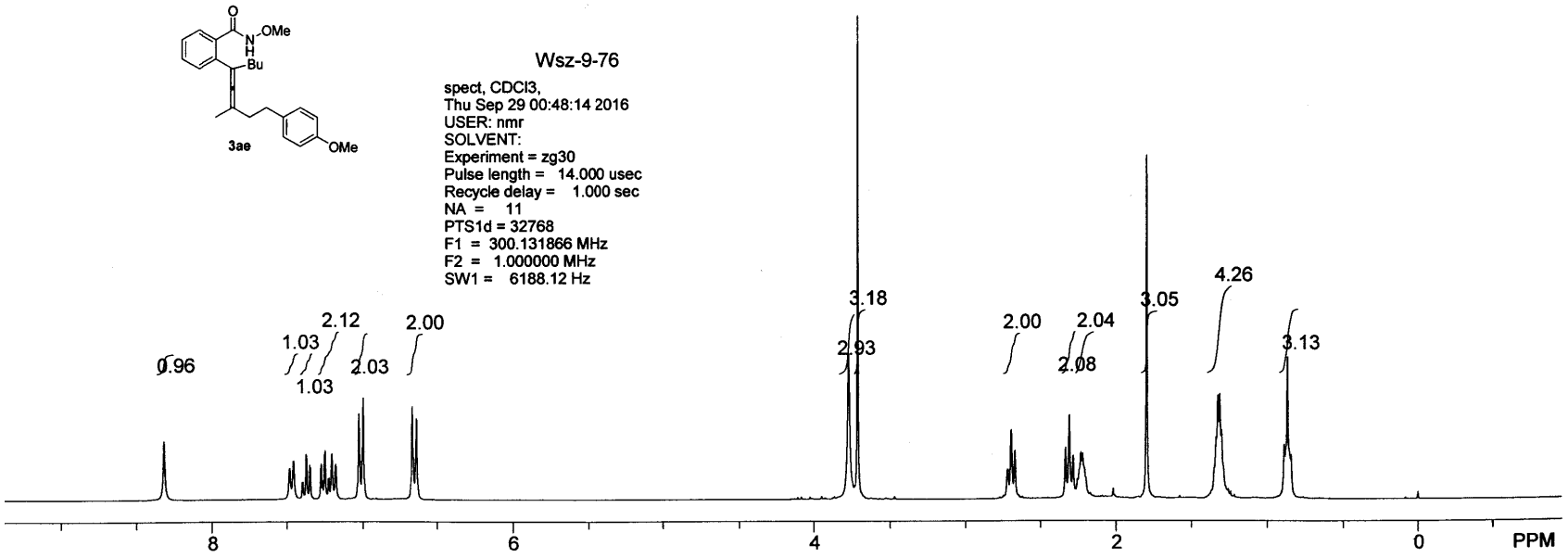

Wsz-7-189
spect, CDCl3,
Sun Nov 29 02:42:07 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
O
OMe
N
H
Bu
C5H11
3ac
0.96
1.00
2.10
1.07
3.00
2.10
2.19
3.11
10.67
6.37
10
8
6
4
2
0
PPM

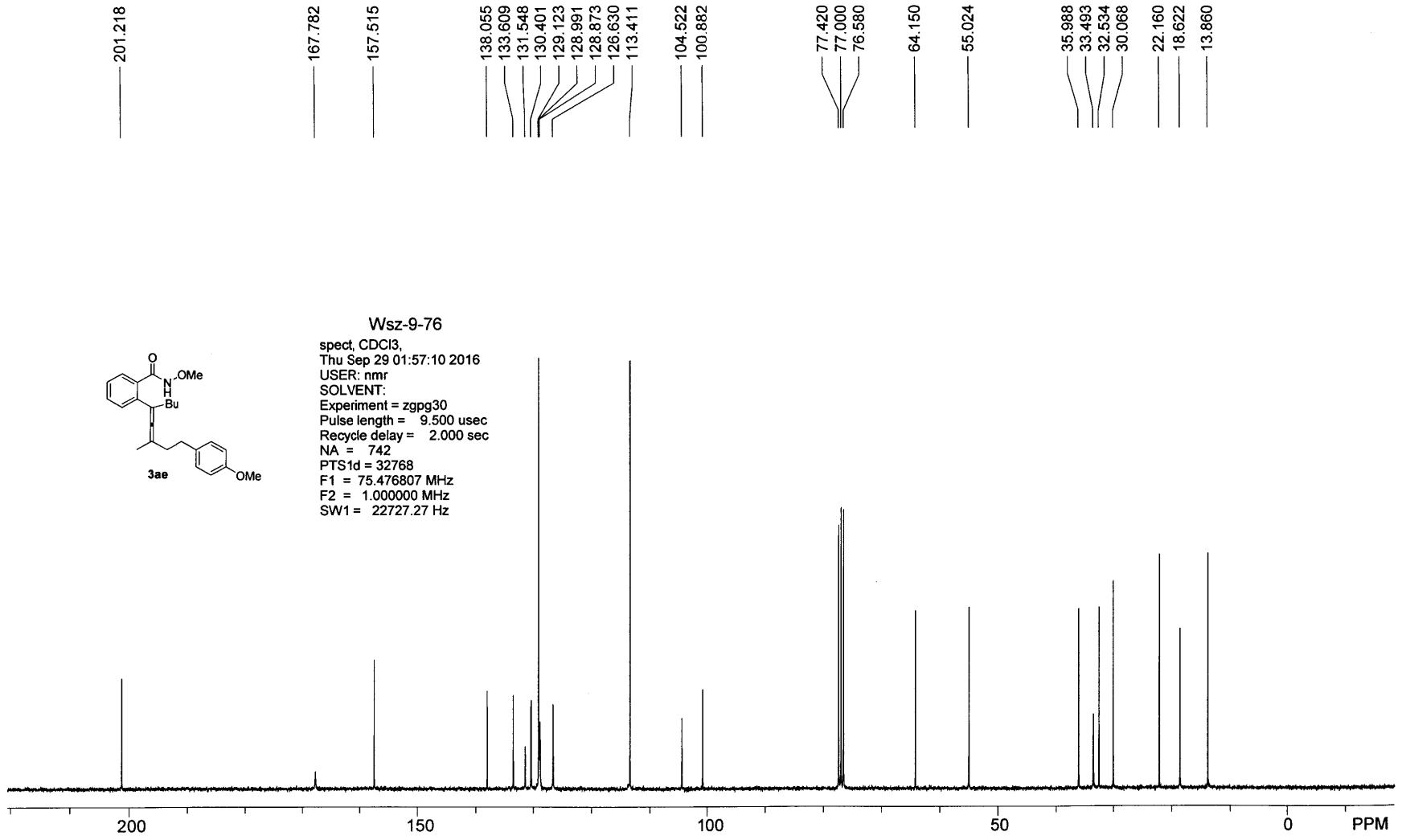

13.876
13.952
18.811
22.196
22.444
27.304
30.177
31.475
33.921
34.097
64.261
76.580
77.000
77.421
101.932
104.561
126.842
129.180
129.383
130.623
131.171
138.374
167.691
200.793
Wsz-7-189
spect CDCl3,
Sun Nov 29 02:53:24 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 608
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
3ac
PPM
0
50
100
150
200

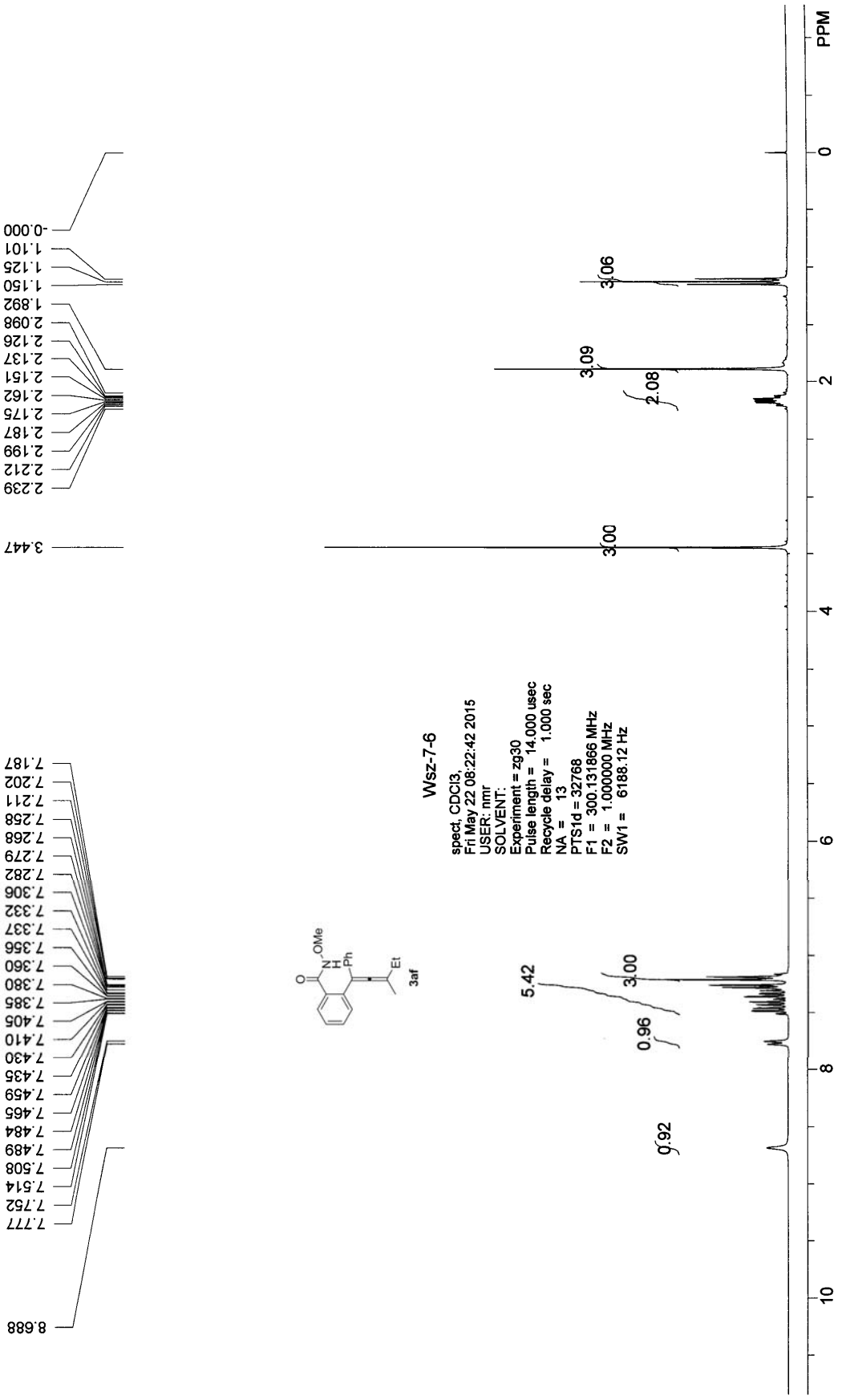

9.075
7.679
7.654
7.422
7.417
7.397
7.392
7.372
7.367
7.328
7.323
7.303
7.298
7.281
7.256
7.253
3.854
2.313
2.291
2.264
2.117
2.092
2.067
2.043
1.422
1.393
1.382
1.367
1.358
1.348
1.325
1.302
1.121
1.096
1.072
0.894
0.871
0.848
0.000
Wsz-7-173
spect, CDCl3,
Sat Nov 14 05:09:51 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 10
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
O
N
OMe
H
Bu
Et
Et
3ad
0.94
0.98
2.12
1.04
3.00
2.05
4.11
4.28
6.15
3.13
10
8
6
4
2
0
PPM

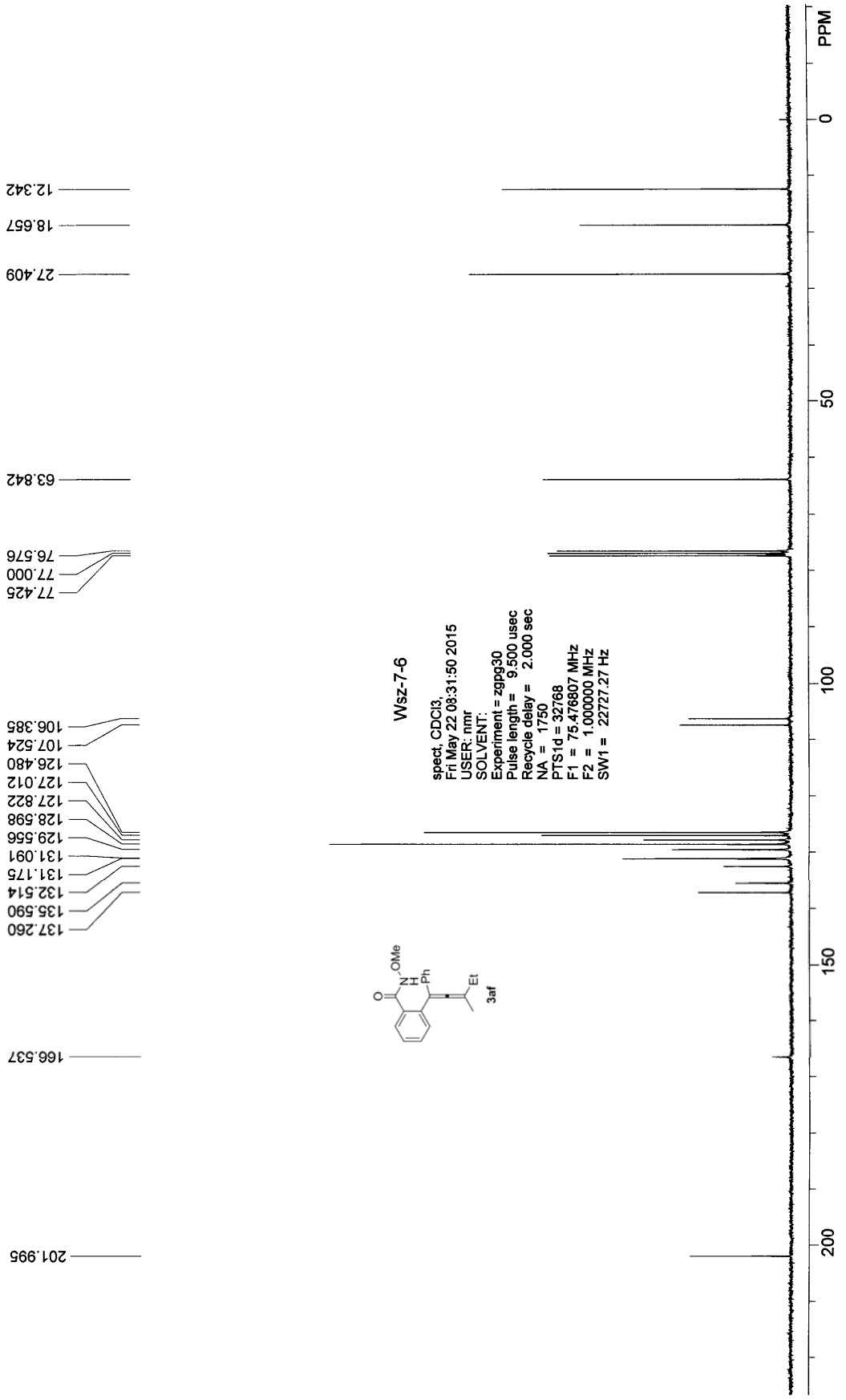

Wsz-7-173
spect, CDCl3,
Sat Nov 14 05:27:31 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 291
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
N
H
Bu
Et
Et
3ad
199.748
167.469
138.467
130.834
129.813
129.327
127.076
110.425
107.996
77.421
77.000
76.579
64.317
34.424
30.416
25.941
22.296
13.893
12.590
PPM
0
50
100
150
200

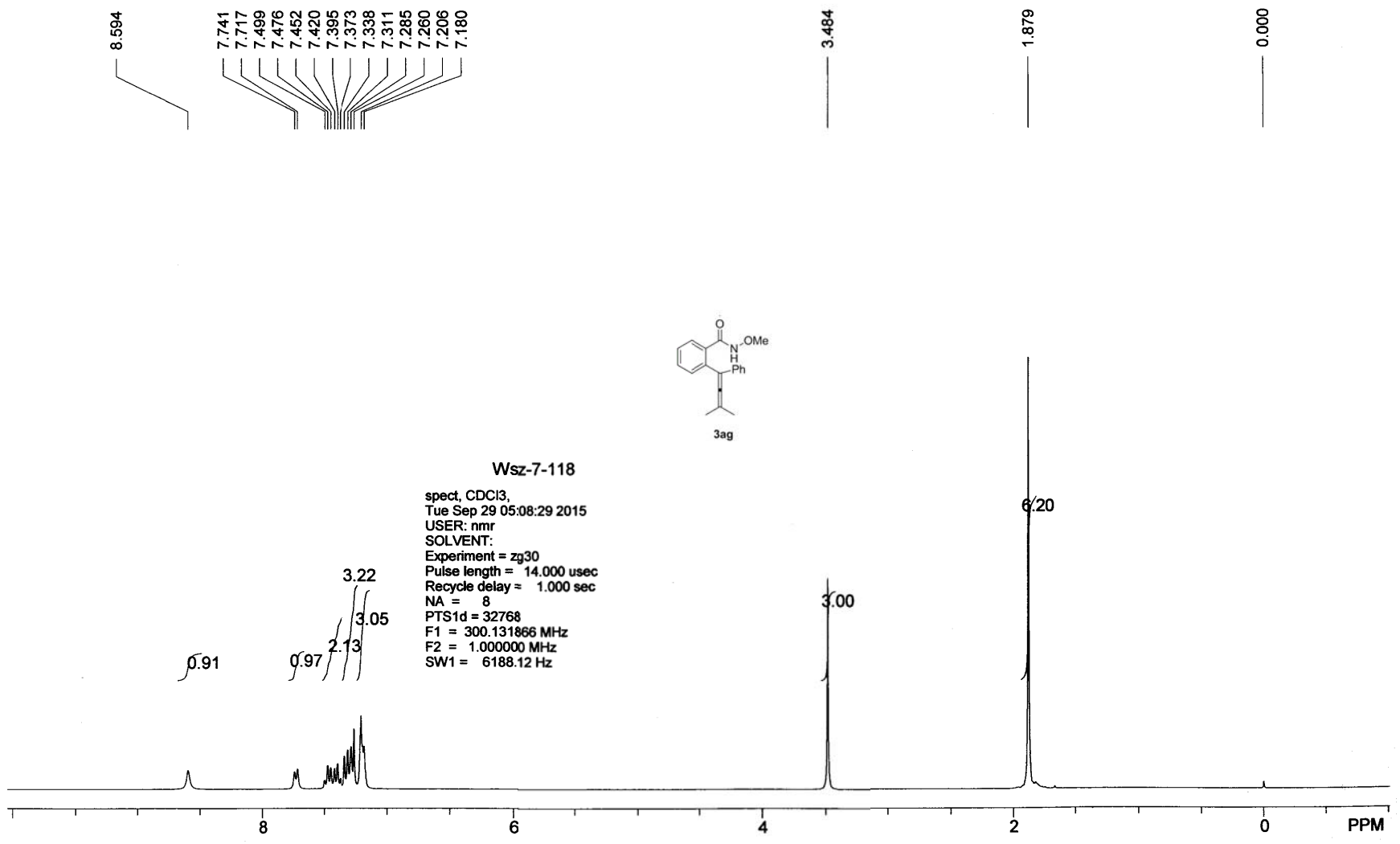

8.320
7.482
7.457
7.400
7.395
7.375
7.370
7.350
7.345
7.278
7.273
7.264
7.252
7.249
7.224
7.204
7.179
7.028
6.999
6.668
6.639
3.775
3.714
2.717
2.693
2.669
2.335
2.309
2.285
2.234
2.222
1.798
1.337
1.326
1.313
1.302
0.889
0.866
0.842
-0.000

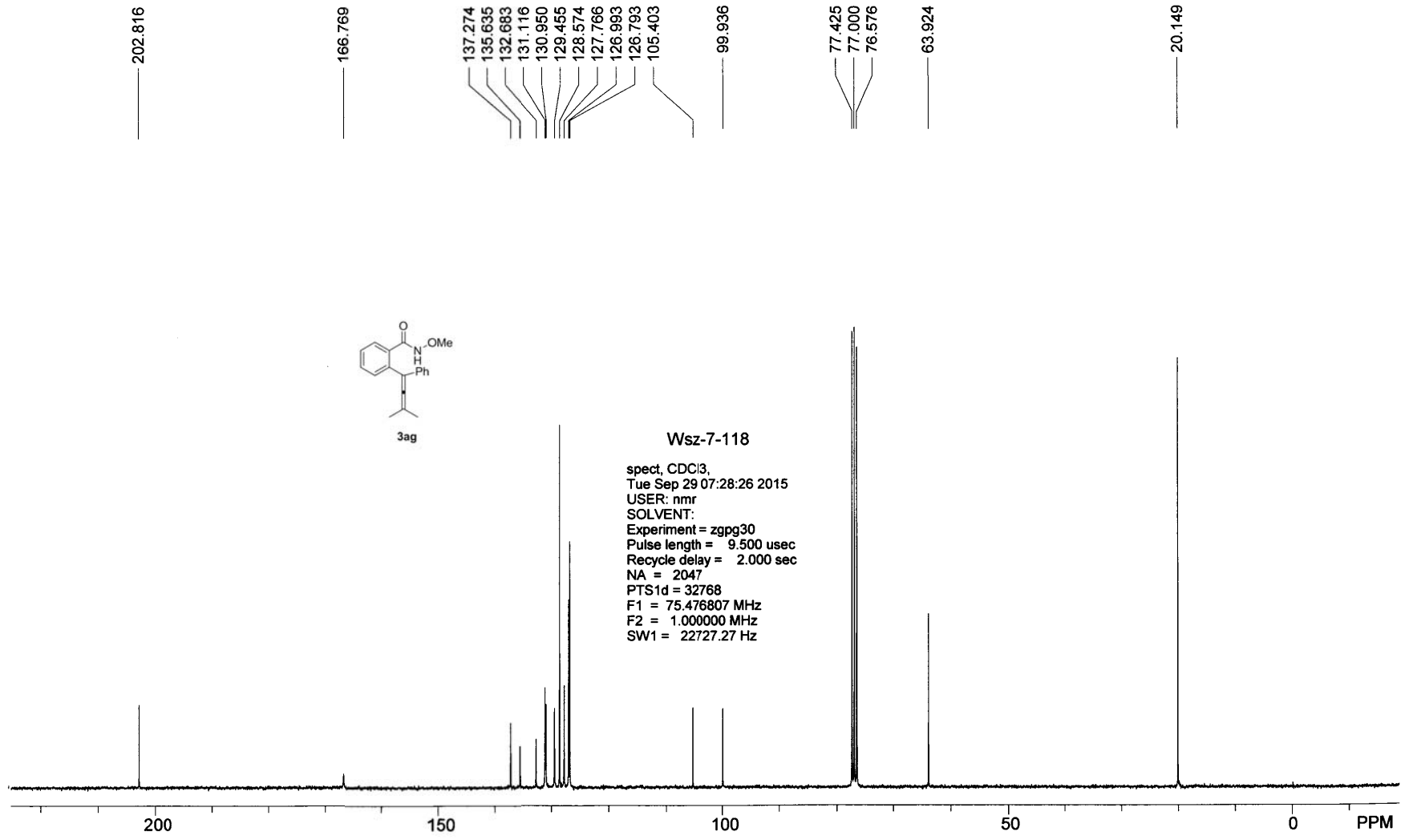

O
N
H
OMe
Bu
3ae
OMe
Wsz-9-76
spect, CDCl3,
Thu Sep 29 00:48:14 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 11
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.96
1.03
2.12
1.03
2.03
2.00
3.18
2.93
2.00
2.04
2.08
3.05
4.26
3.13
8
6
4
2
0
PPM

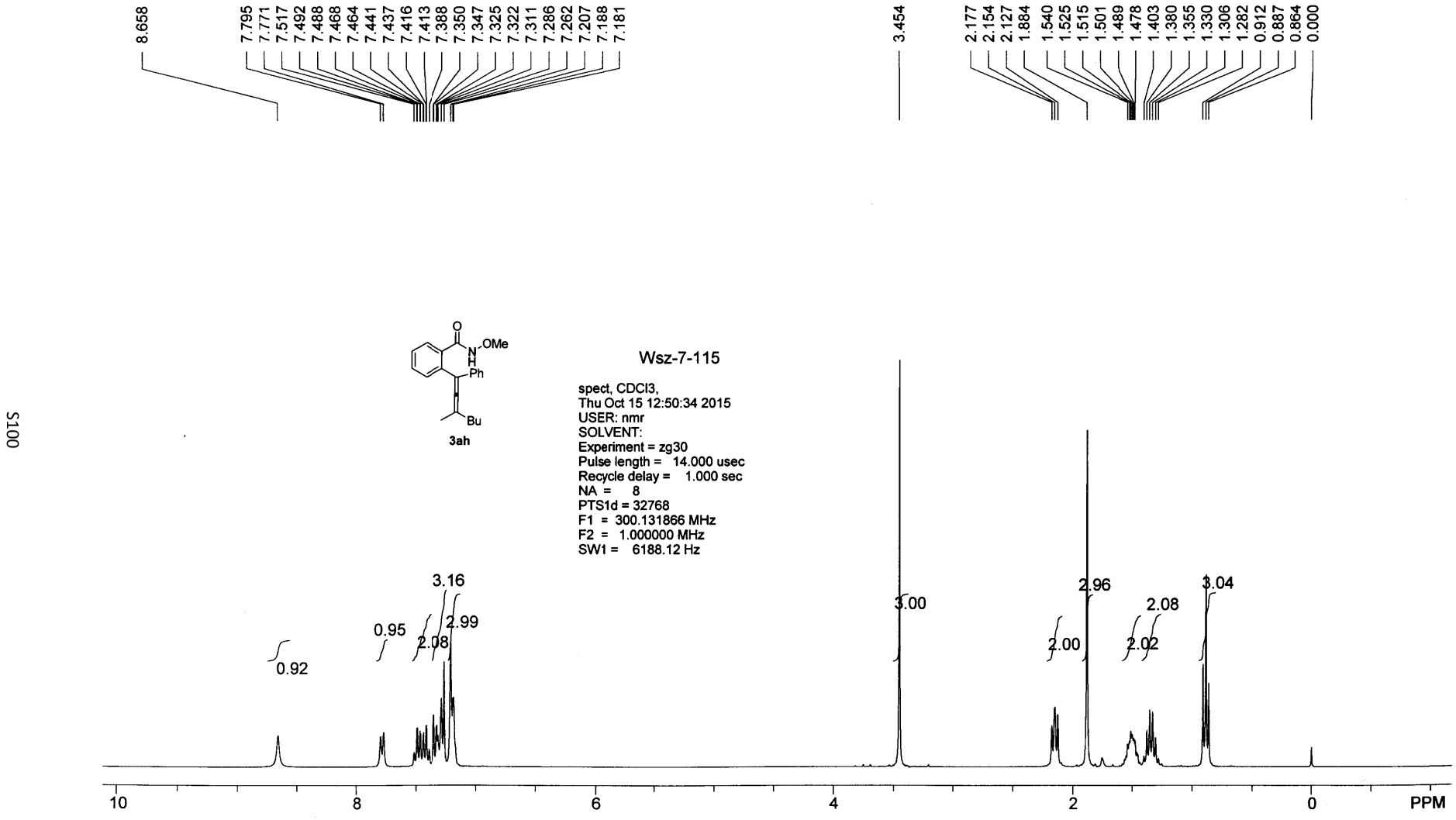

201.218
167.782
157.515
138.055
133.609
131.548
130.401
129.123
128.991
128.873
126.630
113.411
104.522
100.882
77.420
77.000
76.580
64.150
55.024
35.988
33.493
32.534
30.068
22.160
18.622
13.860
Wsz-9-76
spect, CDCl3,
Thu Sep 29 01:57:10 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 742
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
O
N
OMe
H
Bu
OMe
3ae
200
150
100
50
0
PPM

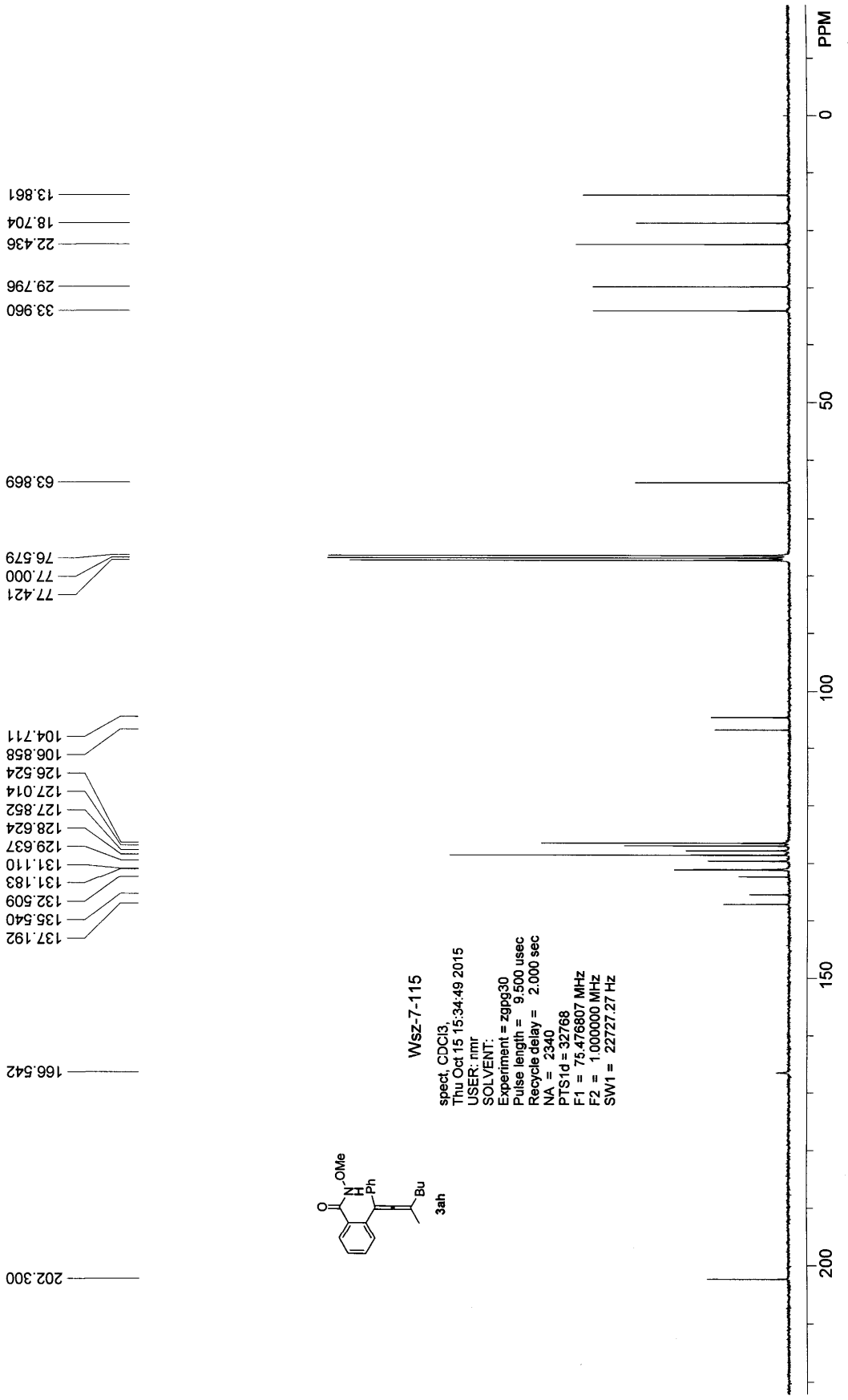

Wsz-7-6
spect, CDCl3,
Fri May 22 08:22:42 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 13
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
OMe
N
H
Ph
Et
3af
PPM
0
2
4
6
8
10
5.42
3.00
0.96
0.92
3.09
2.08
3.06
3.00
-0.000
1.101
1.125
1.150
1.892
2.098
2.126
2.137
2.151
2.162
2.175
2.187
2.199
2.212
2.239
3.447
7.187
7.202
7.211
7.258
7.268
7.279
7.282
7.306
7.332
7.337
7.356
7.360
7.380
7.385
7.405
7.410
7.430
7.435
7.459
7.465
7.484
7.489
7.508
7.514
7.752
7.777
8.688

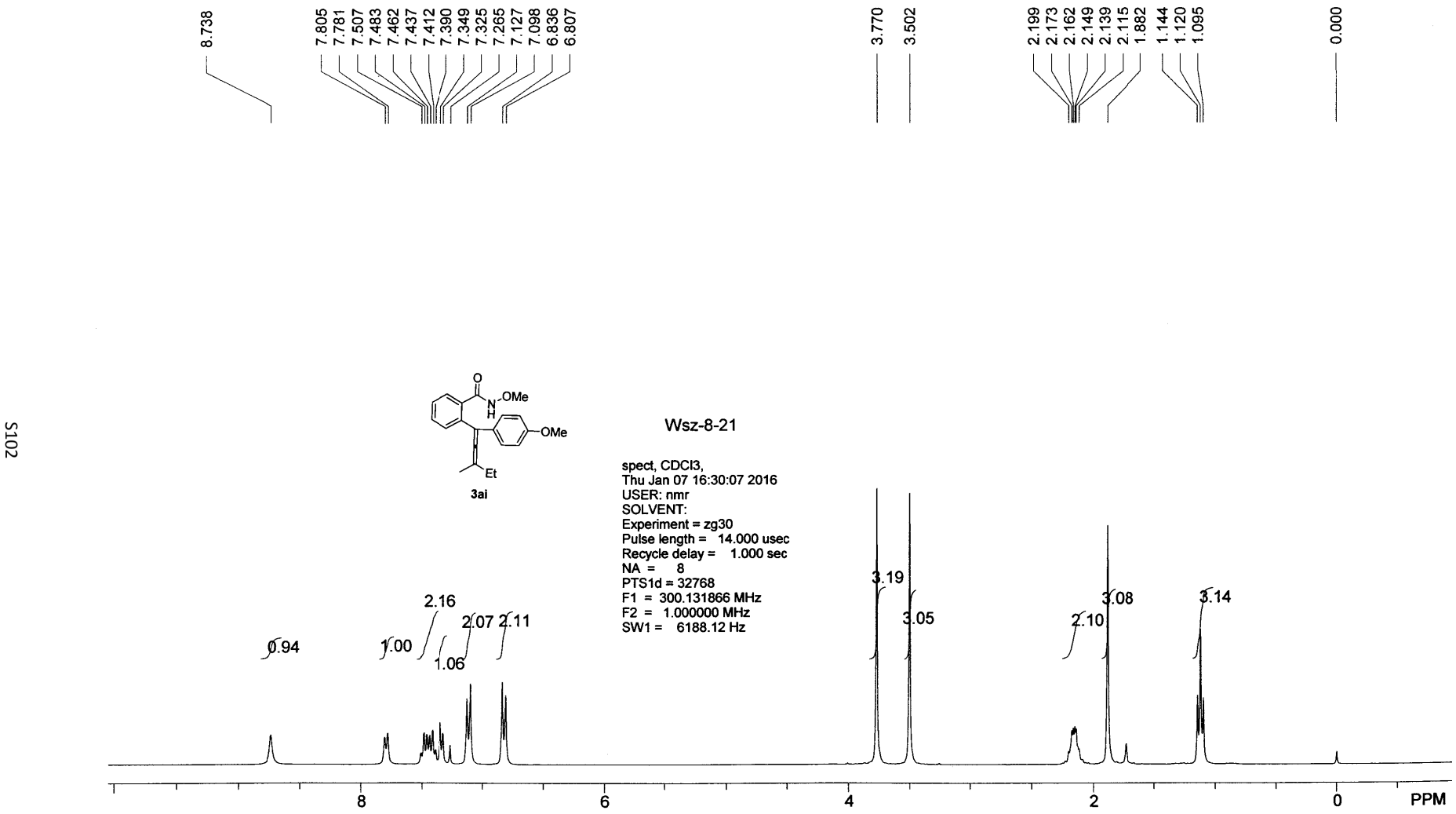

Wsz-7-6
spect, CDCl3,
Fri May 22 08:31:50 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1750
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
N
Ph
Et
O
3af
PPM
0
50
100
150
200
12.342
18.657
27.409
63.842
76.576
77.000
77.425
106.385
107.524
126.480
127.012
127.822
128.598
129.556
131.091
131.175
132.514
135.590
137.260
166.537
201.995

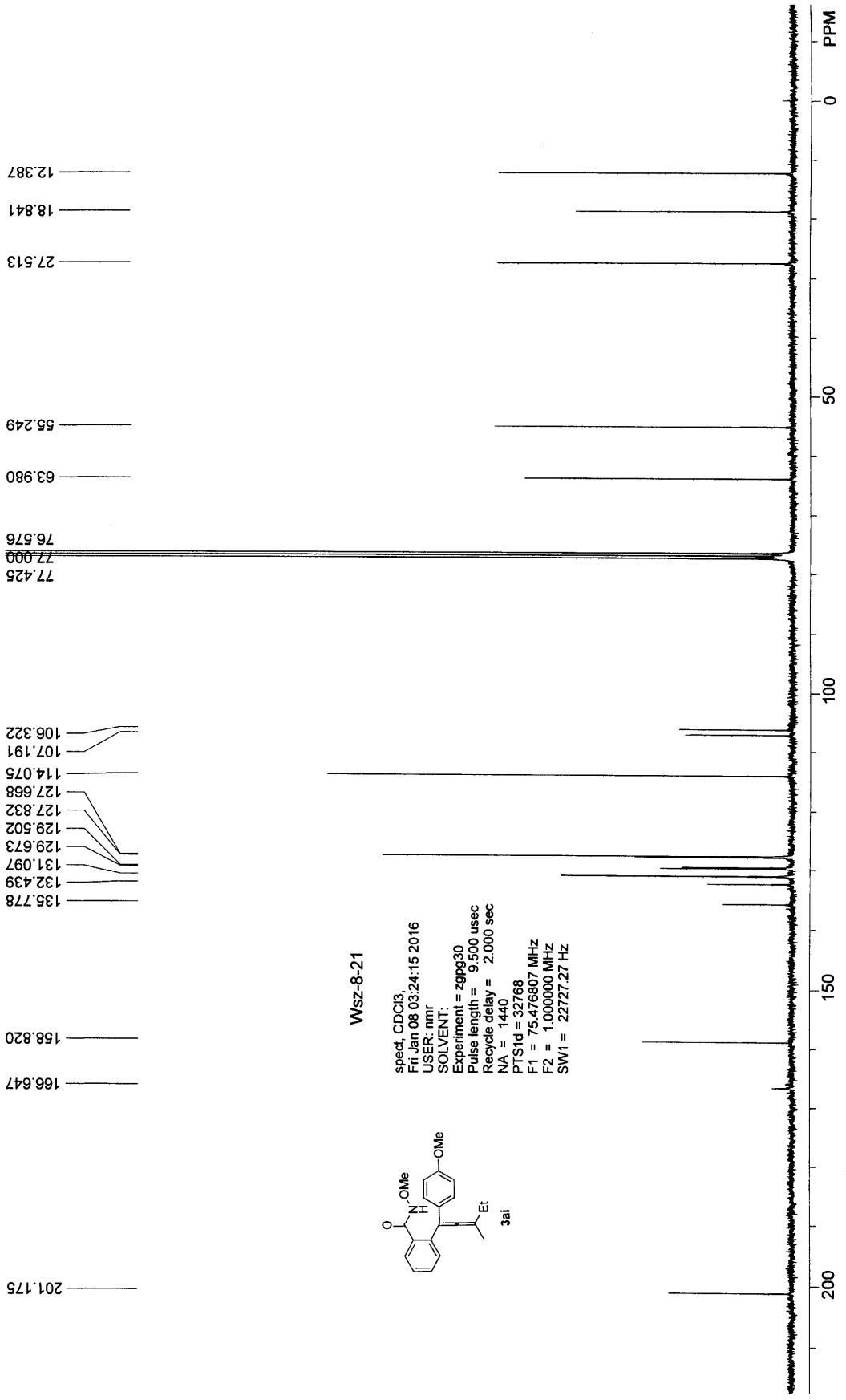

8.594
7.741
7.717
7.499
7.476
7.452
7.420
7.395
7.373
7.338
7.311
7.285
7.260
7.206
7.180
3.484
1.879
0.000
O
N
H
OMe
Ph
3ag
Wsz-7-118
spect, CDCl3,
Tue Sep 29 05:08:29 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.91
0.97
2.13
3.05
3.22
3.00
6.20
8
6
4
2
0
PPM

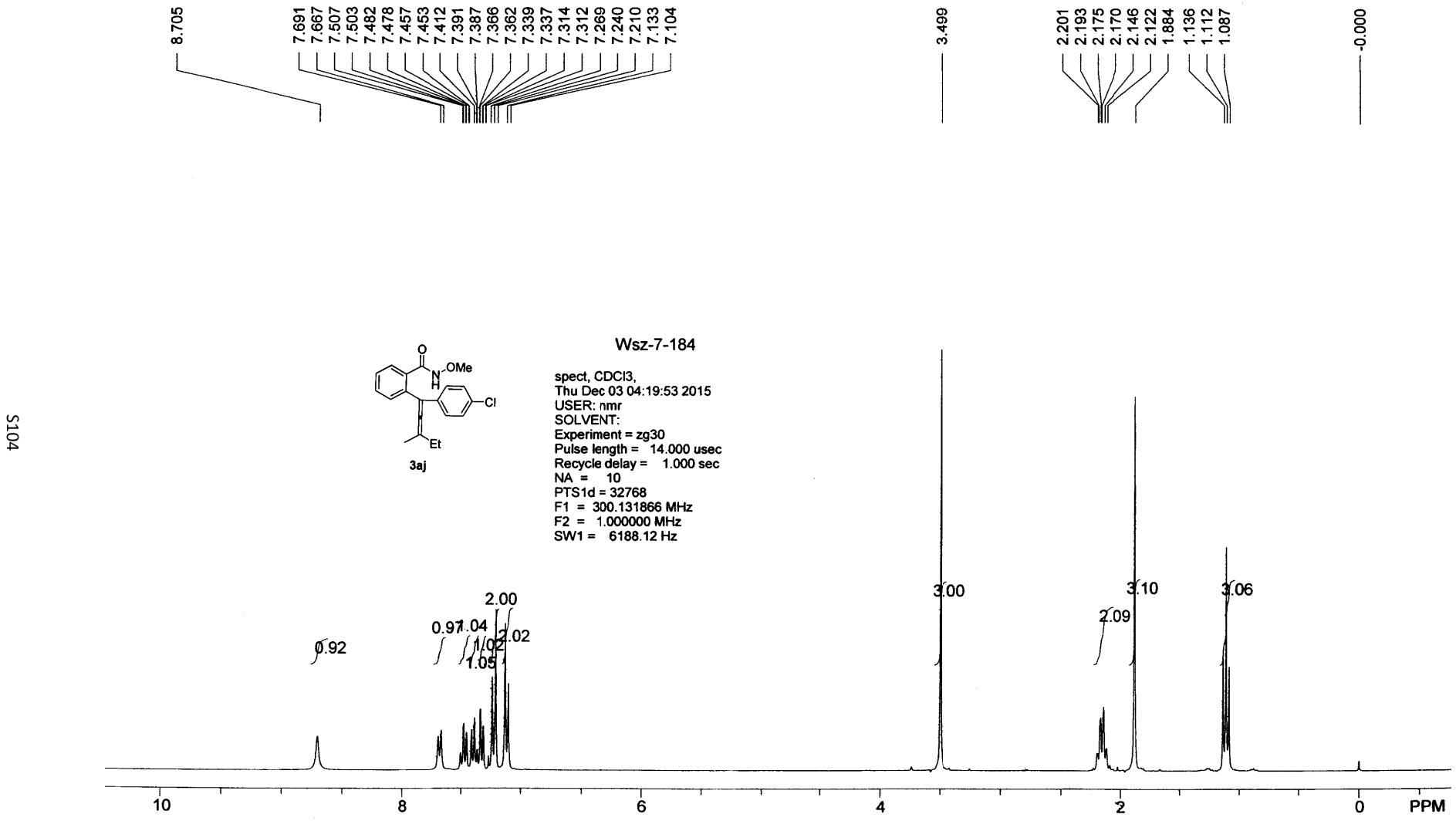

202.816
166.769
137.274
135.635
132.683
131.116
130.950
129.455
128.574
127.766
126.993
126.793
105.403
99.936
77.425
77.000
76.576
63.924
20.149
O
N
H
OMe
Ph
3ag
Wsz-7-118
spect, CDCl3,
Tue Sep 29 07:28:26 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 2047
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
200
150
100
50
0
PPM

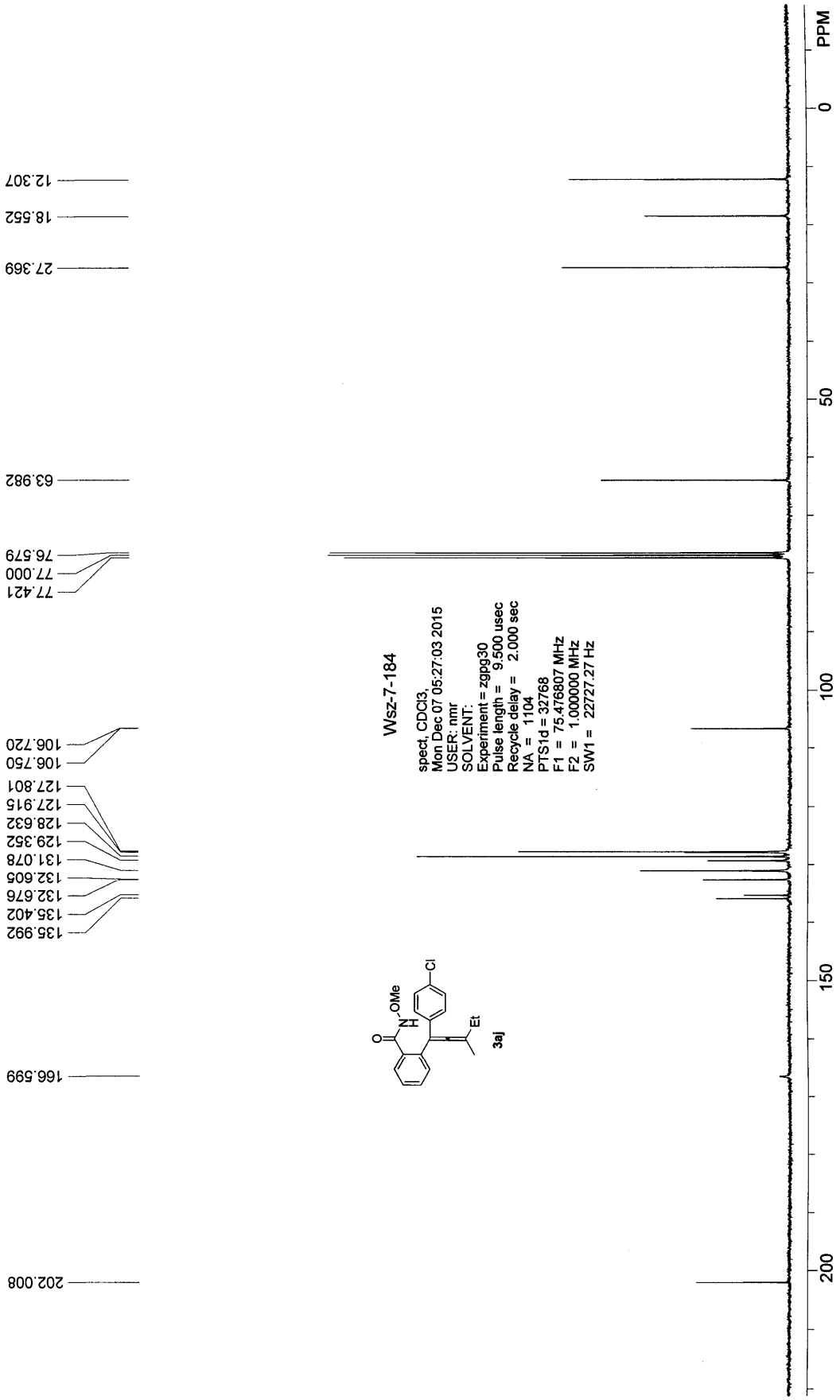

8.658
7.795
7.771
7.517
7.492
7.488
7.468
7.464
7.441
7.437
7.416
7.413
7.388
7.350
7.347
7.325
7.322
7.311
7.286
7.262
7.207
7.188
7.181
3.454
2.177
2.154
2.127
1.884
1.540
1.525
1.515
1.501
1.489
1.478
1.403
1.380
1.355
1.330
1.306
1.282
0.912
0.887
0.864
0.000
O
N
OMe
H
Ph
Bu
3ah
Wsz-7-115
spect, CDCl3,
Thu Oct 15 12:50:34 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.92
0.95
2.08
3.16
2.99
3.00
2.00
2.96
2.02
2.08
3.04
10
8
6
4
2
0
PPM

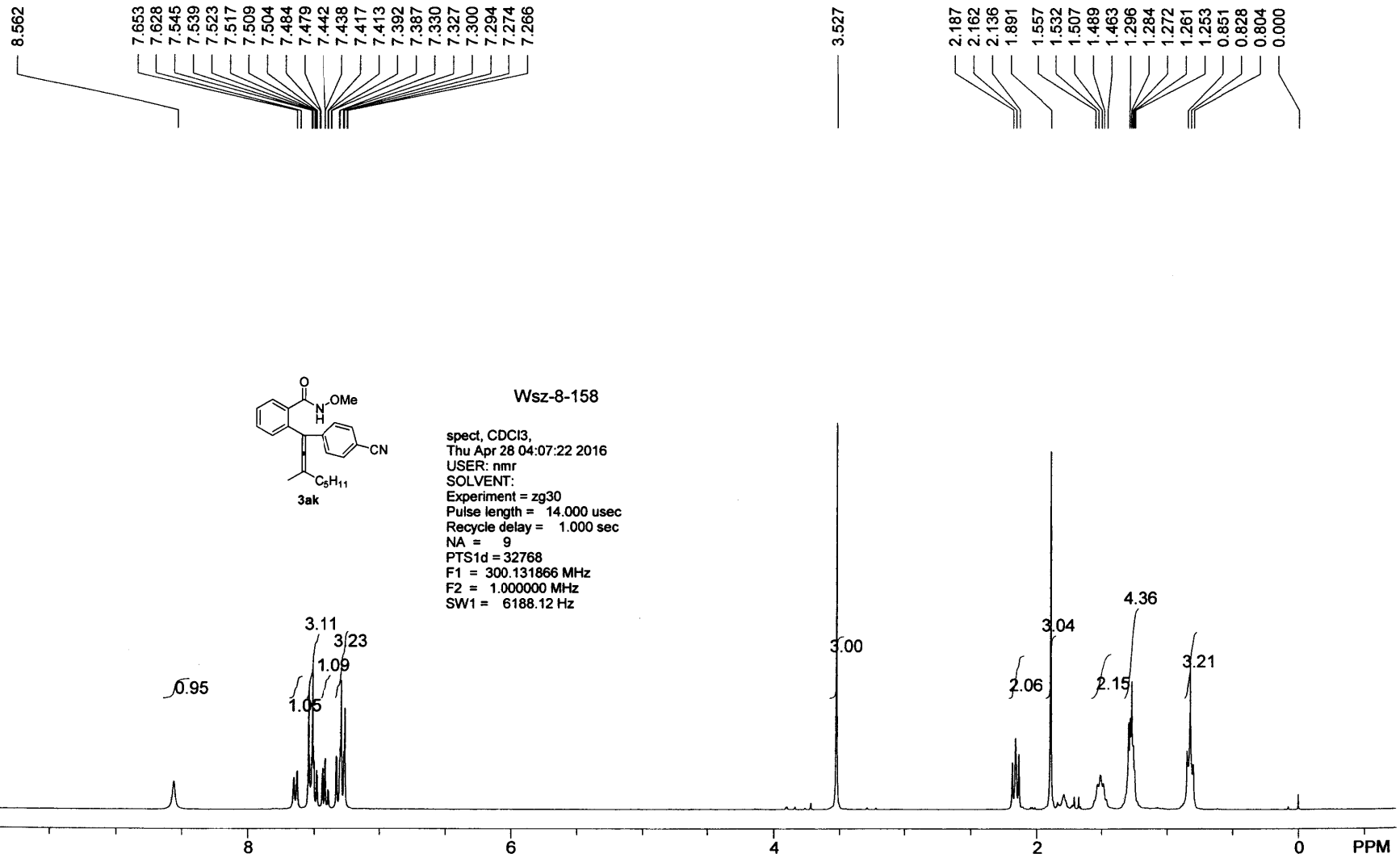

13.861
18.704
22.436
29.796
33.960
63.869
76.579
77.000
77.421
104.711
106.858
126.524
127.014
127.852
128.624
129.637
131.110
131.183
132.509
135.540
137.192
166.542
202.300
Wsz-7-115
spect, CDCl3,
Thu Oct 15 15:34:49 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 2340
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
N
H
Ph
O
Bu
3ah
PPM
0
50
100
150
200

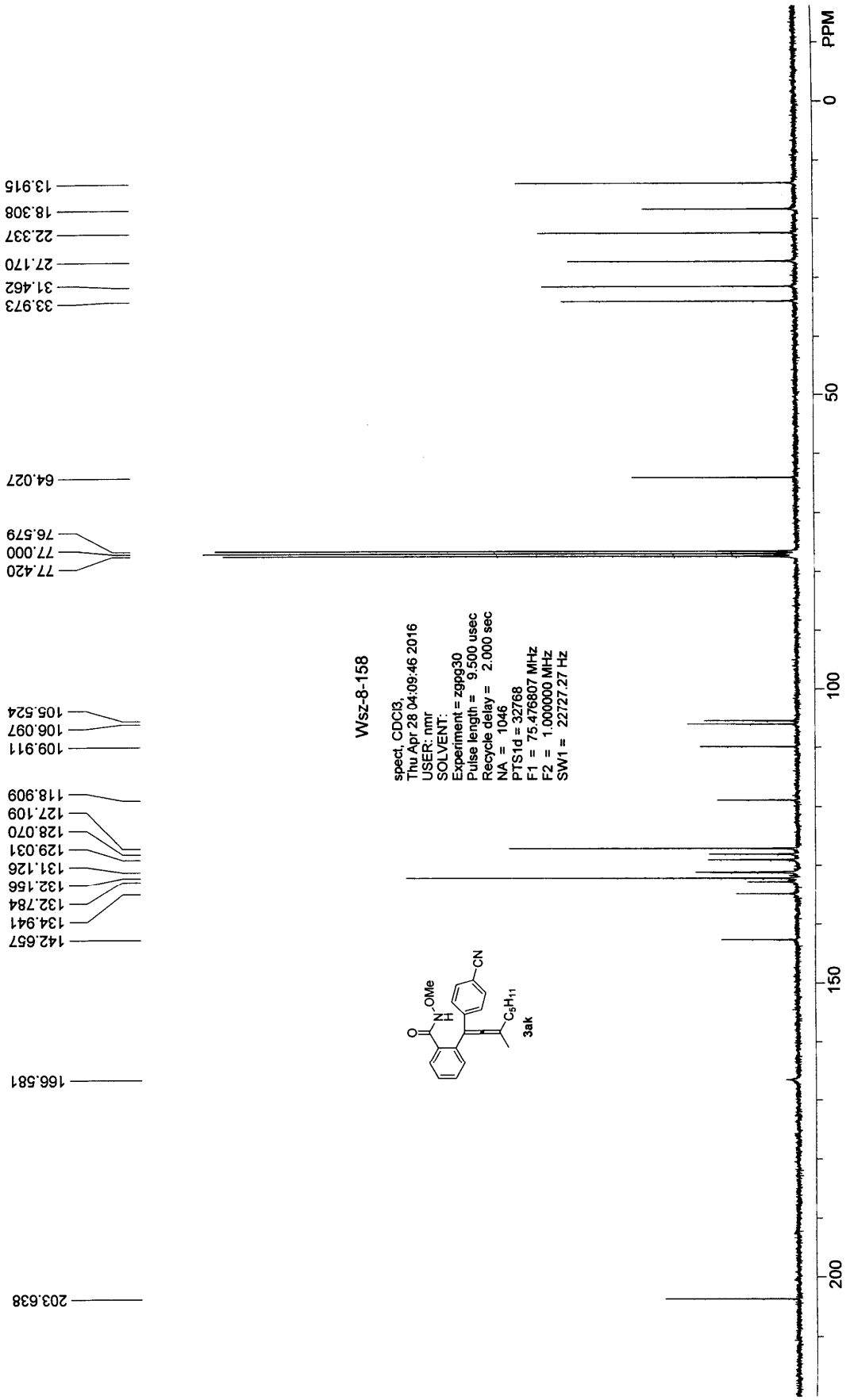

8.738
7.805
7.781
7.507
7.483
7.462
7.437
7.412
7.390
7.349
7.325
7.265
7.127
7.098
6.836
6.807
3.770
3.502
2.199
2.173
2.162
2.149
2.139
2.115
1.882
1.144
1.120
1.095
0.000
O
N
H
OMe
OMe
Et
3ai
Wsz-8-21
spect, CDCl3,
Thu Jan 07 16:30:07 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.94
1.00
2.16
1.06
2.07
2.11
3.19
3.05
2.10
3.08
3.14
8
6
4
2
0
PPM

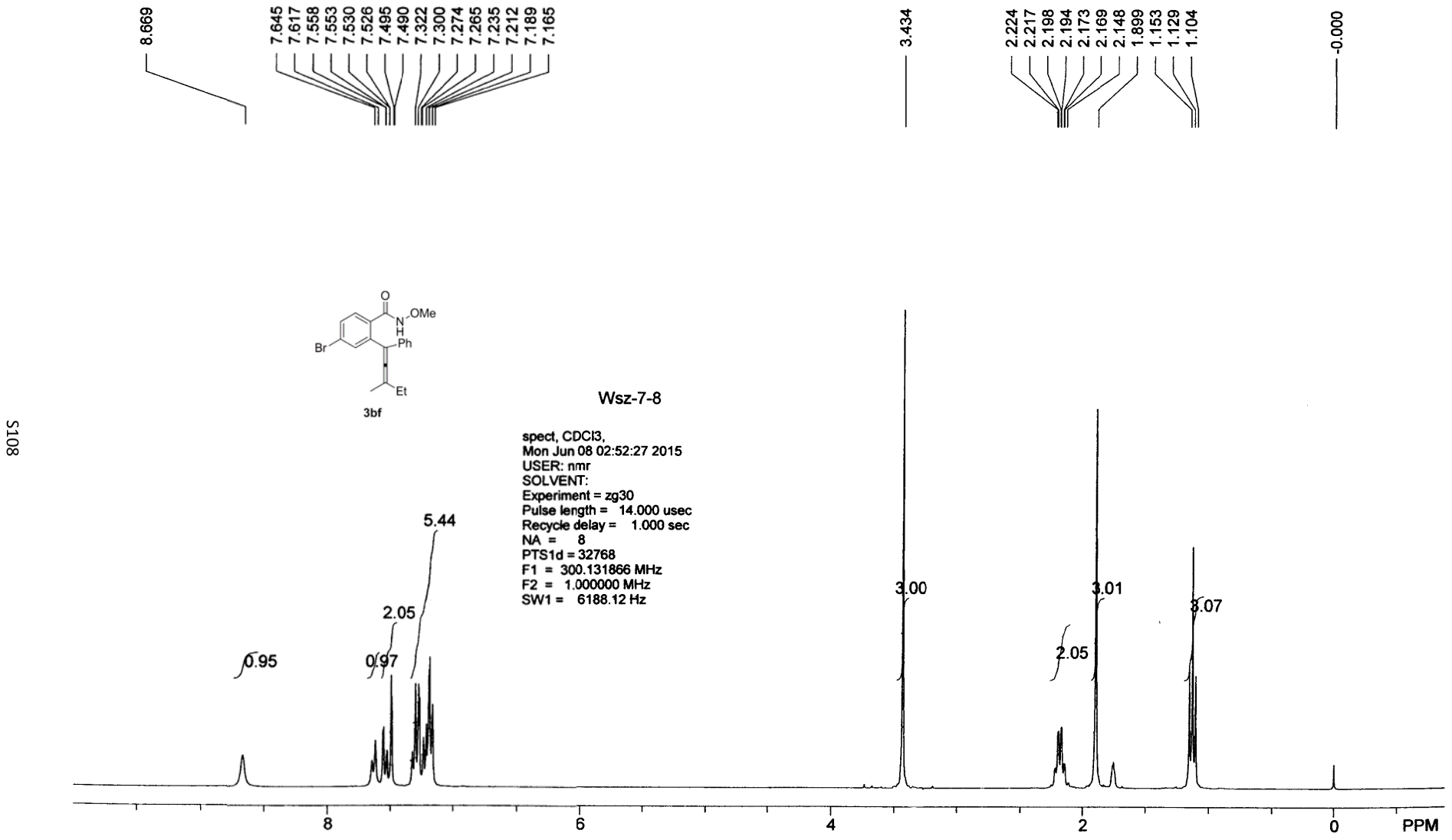

Wsz-8-21
spect, CDCl3,
Fri Jan 08 03:24:15 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1440
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
3ai
PPM
0
50
100
150
200
12.387
18.841
27.513
55.249
63.980
76.576
77.000
77.425
106.322
107.191
114.075
127.668
127.832
129.502
129.673
131.097
132.439
135.778
158.820
166.647
201.175

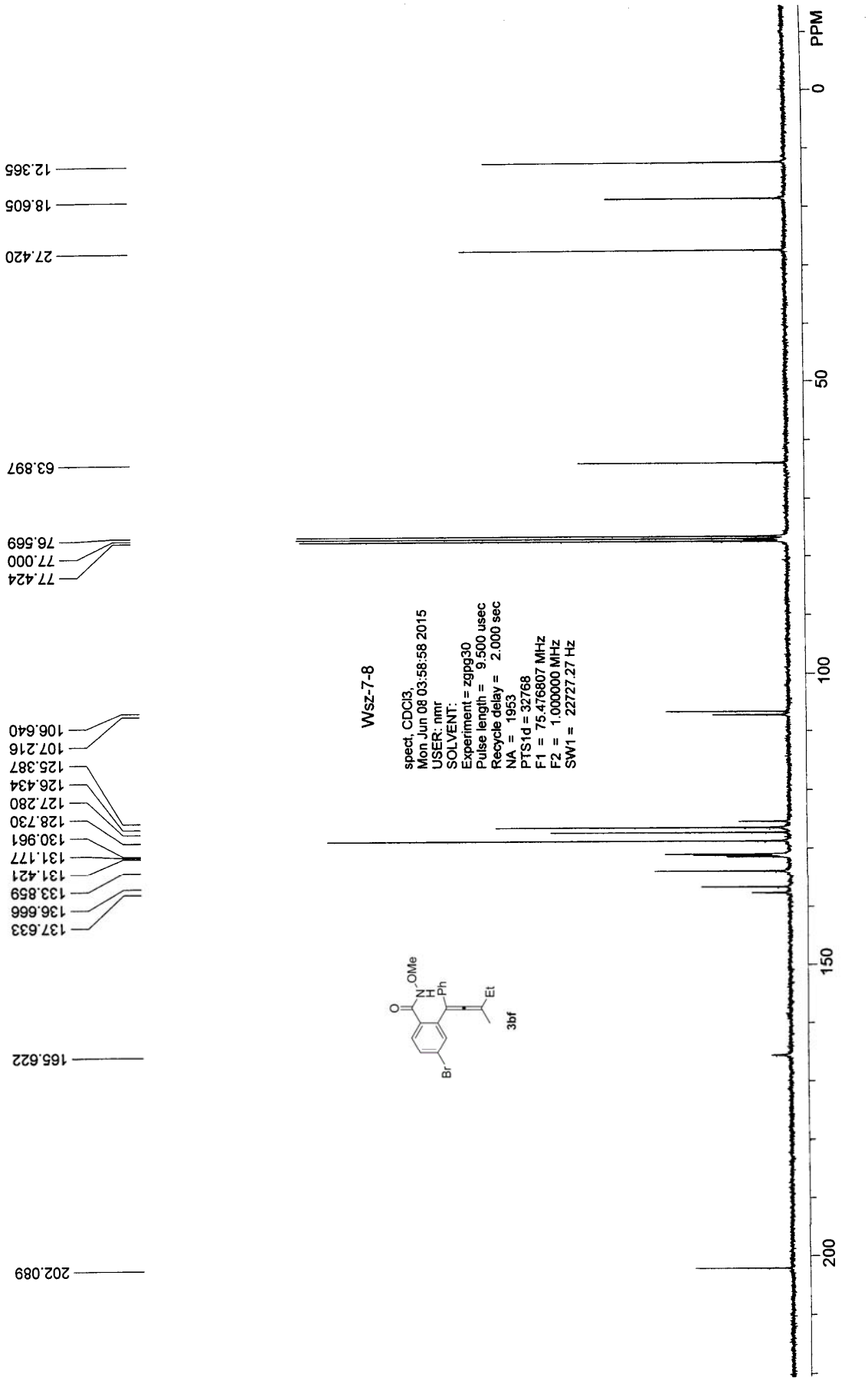

8.705
7.691
7.667
7.507
7.503
7.482
7.478
7.457
7.453
7.412
7.391
7.387
7.366
7.362
7.339
7.337
7.314
7.312
7.269
7.240
7.210
7.133
7.104
3.499
2.201
2.193
2.175
2.170
2.146
2.122
1.884
1.136
1.112
1.087
-0.000
Wsz-7-184
spect, CDCl3,
Thu Dec 03 04:19:53 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 10
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
3aj
0.92
0.97
1.04
2.00
1.02
1.05
2.02
3.00
2.09
3.10
3.06
10
8
6
4
2
0
PPM

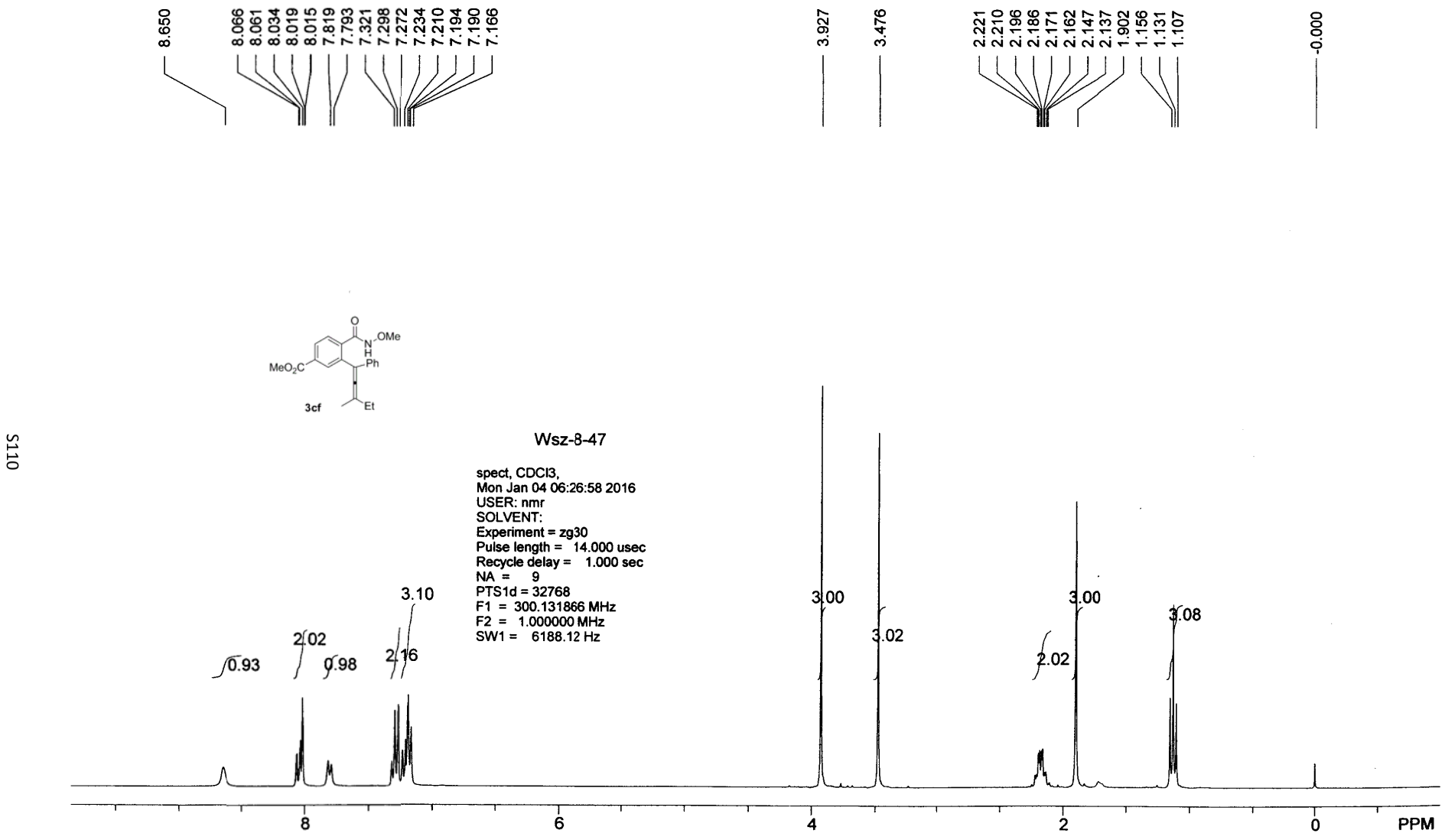

12.307
18.552
27.369
63.982
76.579
77.000
77.421
106.720
106.750
127.801
127.915
128.632
129.352
131.078
132.605
132.676
135.402
135.992
166.599
202.008
Wsz-7-184
spect, CDCl3,
Mon Dec 07 05:27:03 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1104
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
N
H
O
Cl
Et
3aj
PPM
0
50
100
150
200

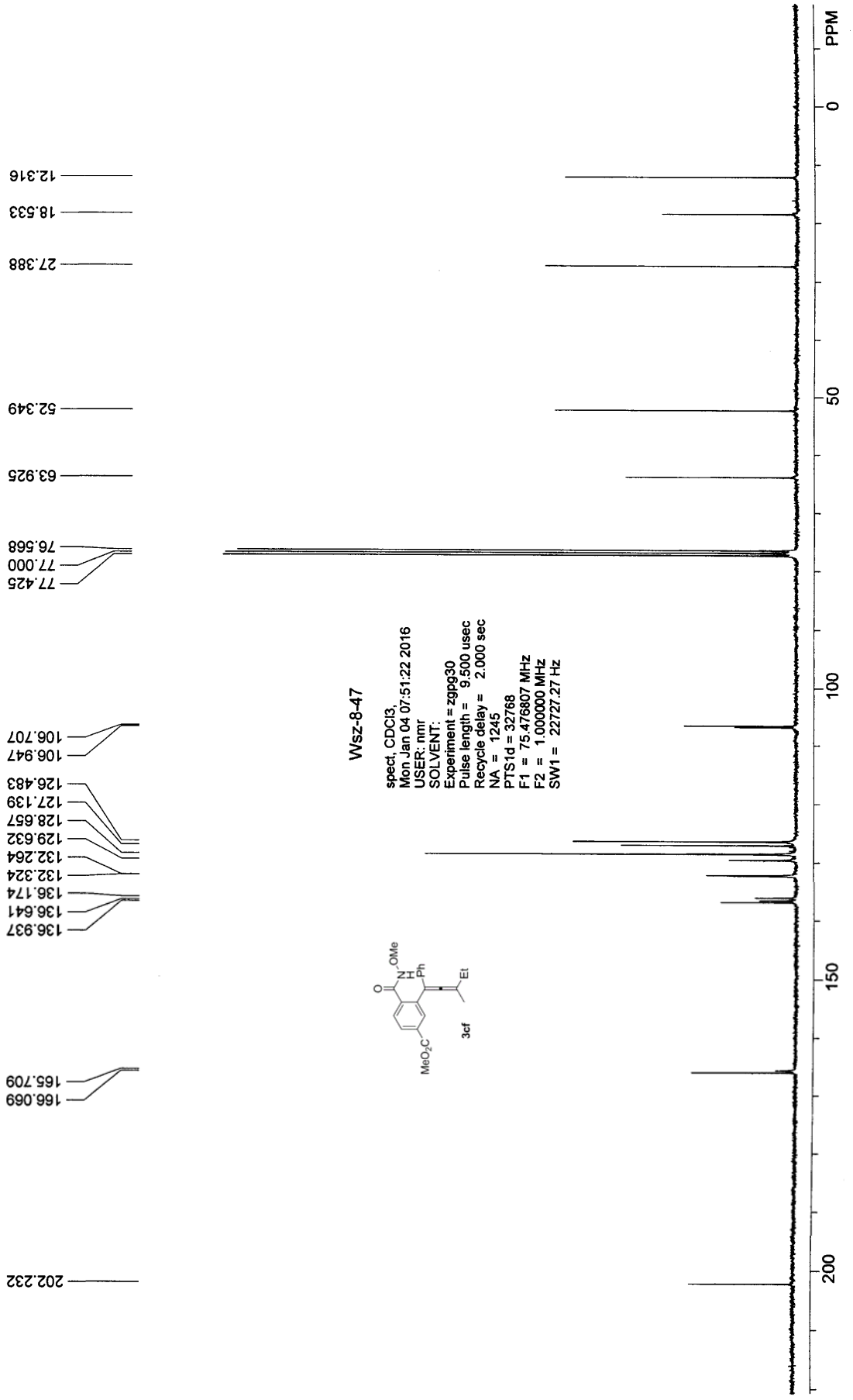

8.562
7.653
7.628
7.545
7.539
7.523
7.517
7.509
7.504
7.484
7.479
7.442
7.438
7.417
7.413
7.392
7.387
7.330
7.327
7.300
7.294
7.274
7.266
3.527
2.187
2.162
2.136
1.891
1.557
1.532
1.507
1.489
1.463
1.296
1.284
1.272
1.261
1.253
0.851
0.828
0.804
0.000
Wsz-8-158
spect, CDCl3,
Thu Apr 28 04:07:22 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
3ak
0.95
3.11
3.23
1.09
1.05
3.00
3.04
2.06
2.15
4.36
3.21
8
6
4
2
0
PPM

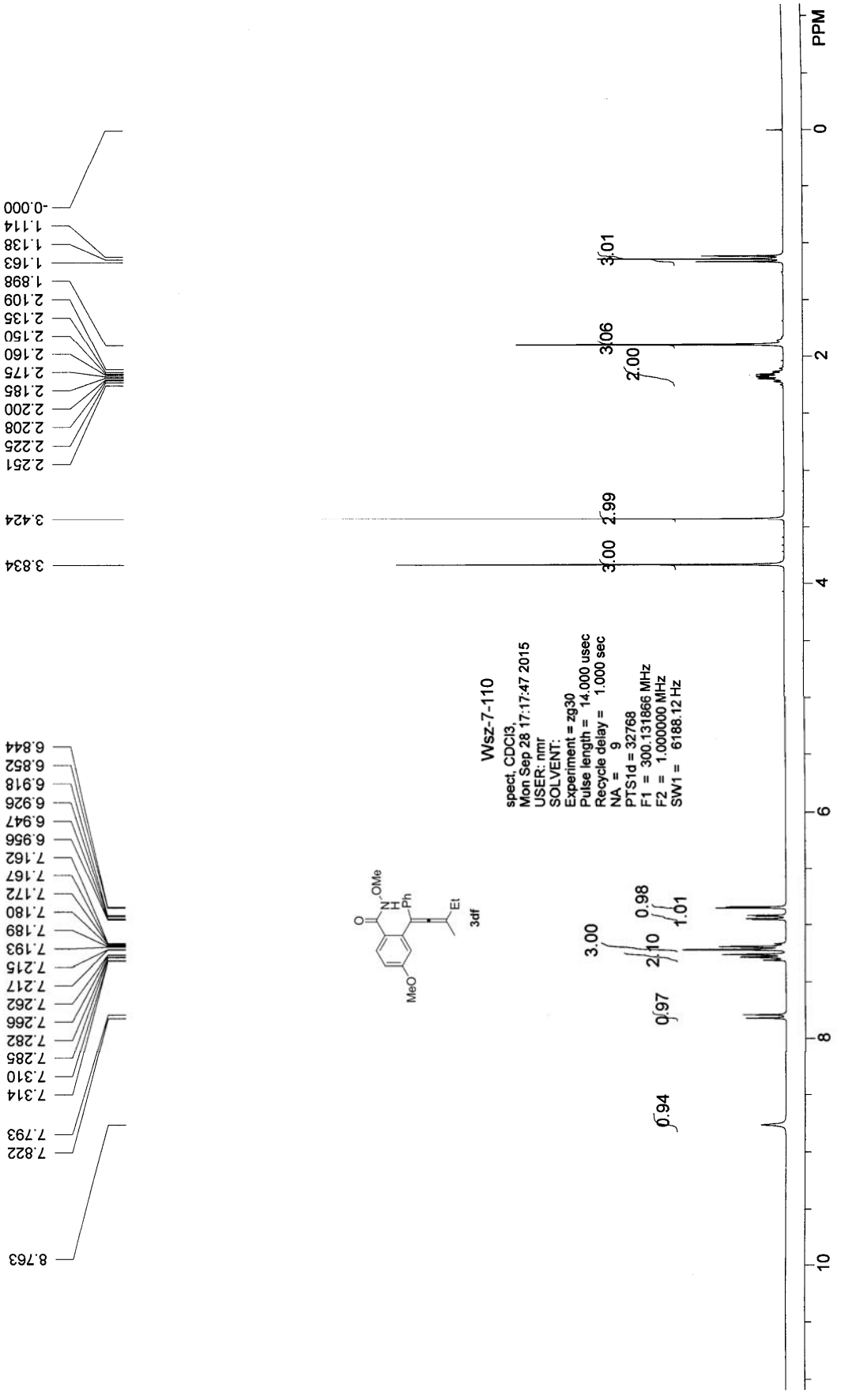

Wsz-8-158
spect, CDCl3,
Thu Apr 28 04:09:46 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1046
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
N
H
O
CN
C_5H_{11}
3ak
203.638
166.581
142.657
134.941
132.784
132.166
131.126
129.031
128.070
127.109
118.909
109.911
106.097
105.524
77.420
77.000
76.579
64.027
33.973
31.462
27.170
22.337
18.308
13.915
PPM
0
50
100
150
200

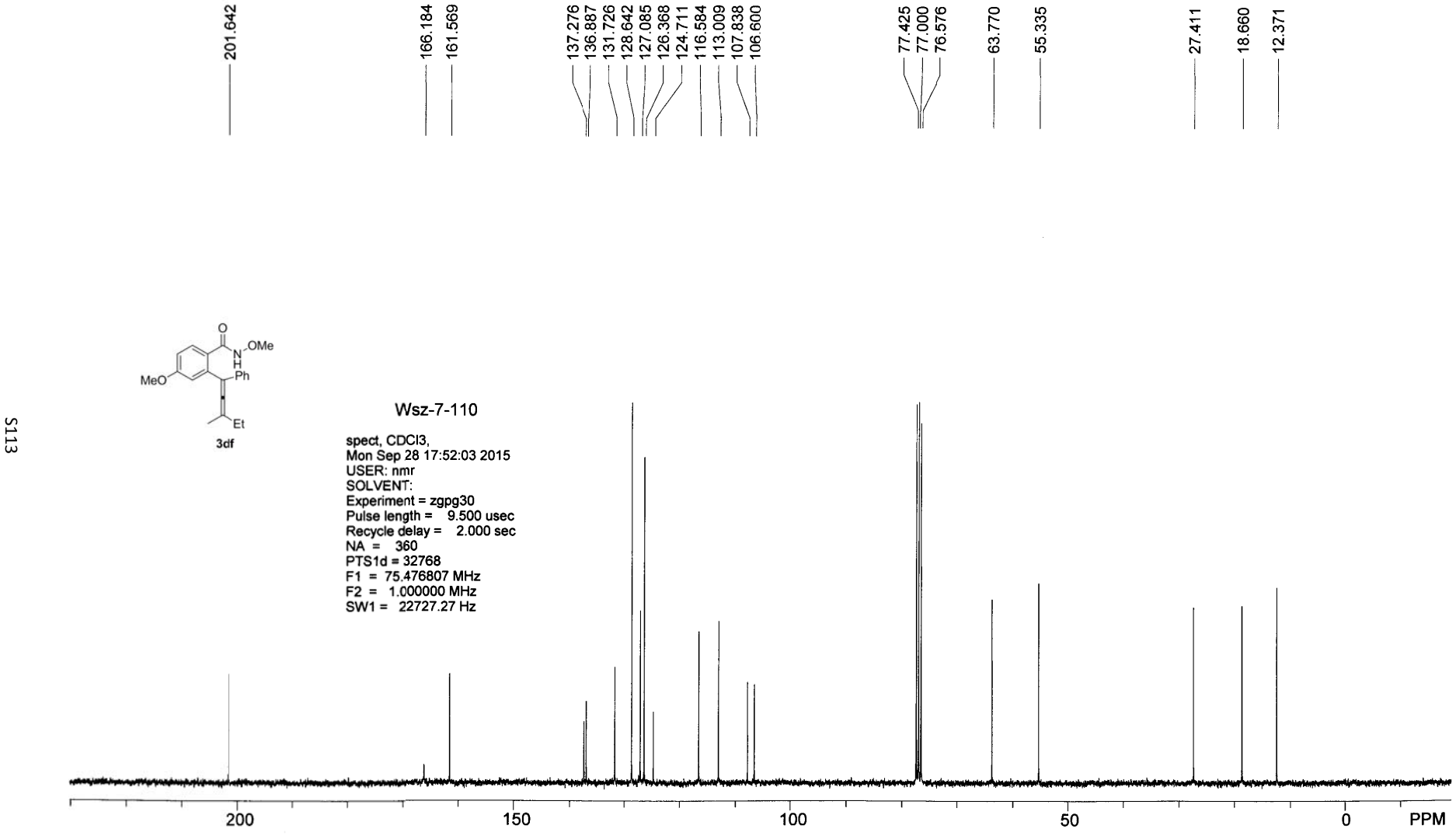

8.669
7.645
7.617
7.558
7.553
7.530
7.526
7.495
7.490
7.322
7.300
7.274
7.265
7.235
7.212
7.189
7.165
3.434
2.224
2.217
2.198
2.194
2.173
2.169
2.148
1.899
1.153
1.129
1.104
-0.000
O
N
OMe
H
Br
Ph
Et
3bf
Wsz-7-8
spect, CDCl3,
Mon Jun 08 02:52:27 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
5.44
2.05
0.95
0.97
3.00
3.01
3.07
2.05
8
6
4
2
0
PPM

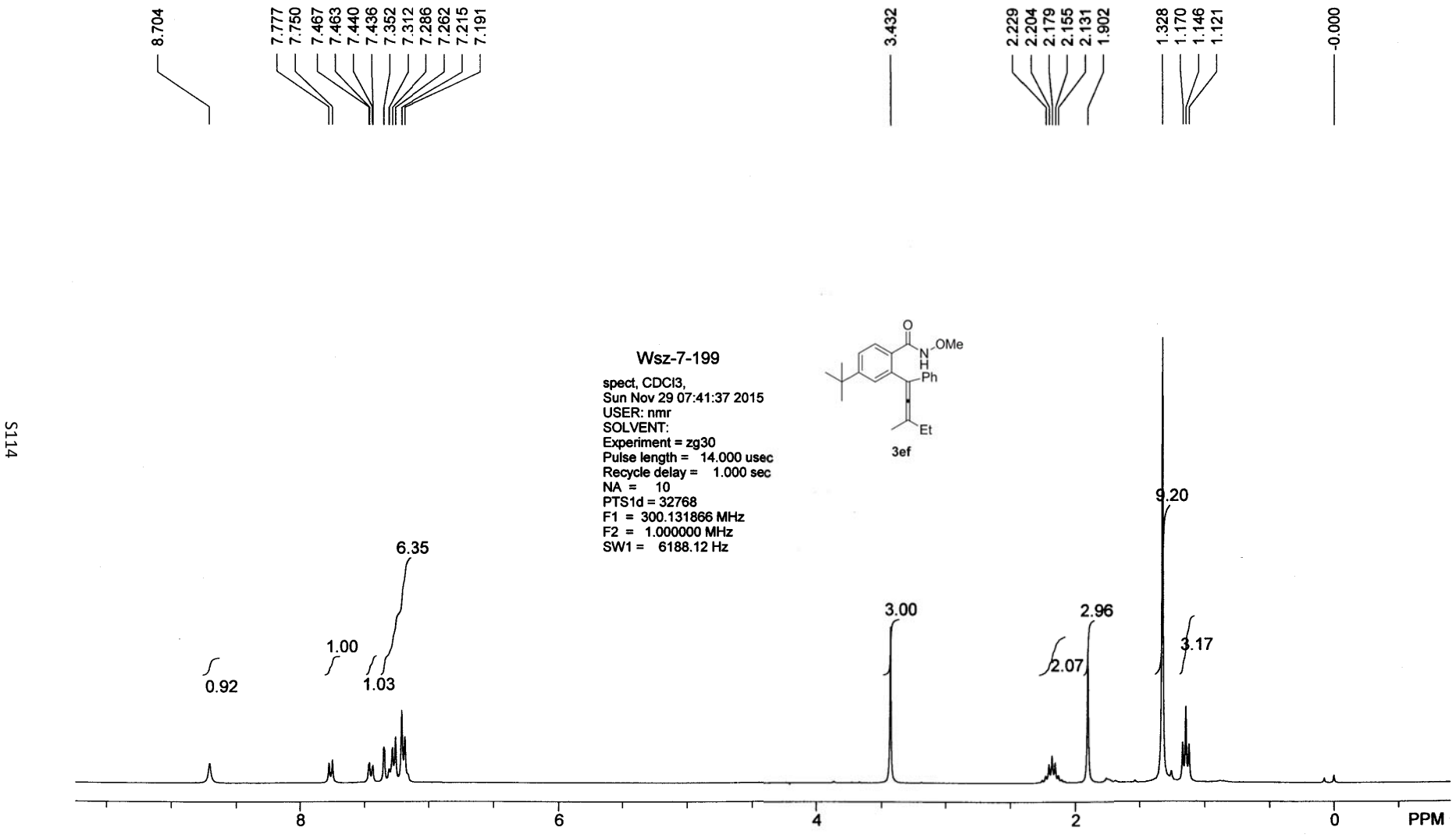

Wsz-7-8
spect. CDCl3.
Mon Jun 08 03:58:58 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1953
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
3bf
PPM
0
50
100
150
200
12.365
18.605
27.420
63.897
76.569
77.000
77.424
106.640
107.216
125.387
126.434
127.280
128.730
130.961
131.177
131.421
133.859
136.666
137.633
165.622
202.089

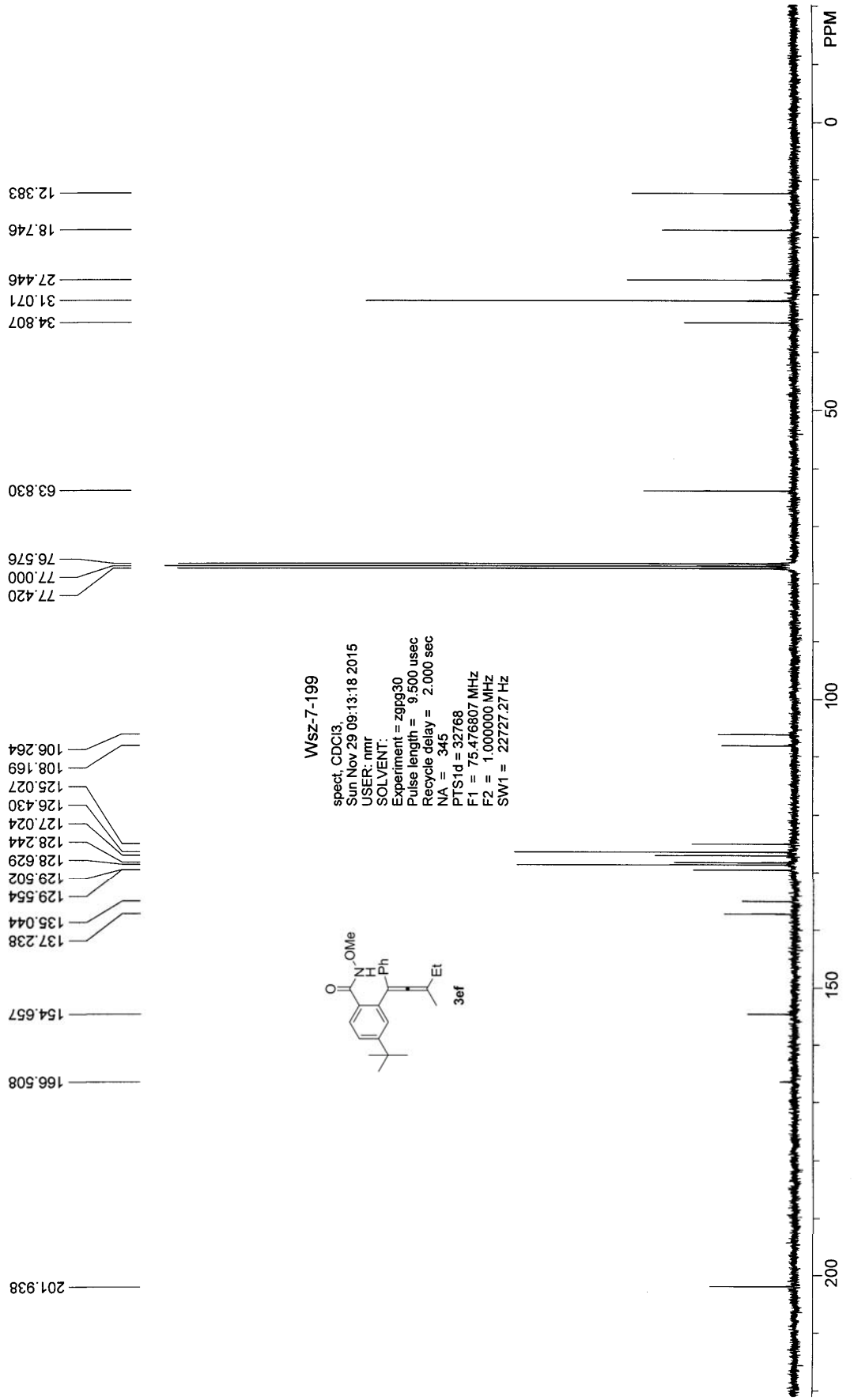

8.650
8.066
8.061
8.034
8.019
8.015
7.819
7.793
7.321
7.298
7.272
7.234
7.210
7.194
7.190
7.166
3.927
3.476
2.221
2.210
2.196
2.186
2.171
2.162
2.147
2.137
1.902
1.156
1.131
1.107
-0.000
MeO2C
N
H
OMe
Ph
Et
3cf
Wsz-8-47
spect, CDCl3,
Mon Jan 04 06:26:58 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.93
2.02
0.98
2.16
3.10
3.00
3.02
2.02
3.00
3.08
8
6
4
2
0
PPM

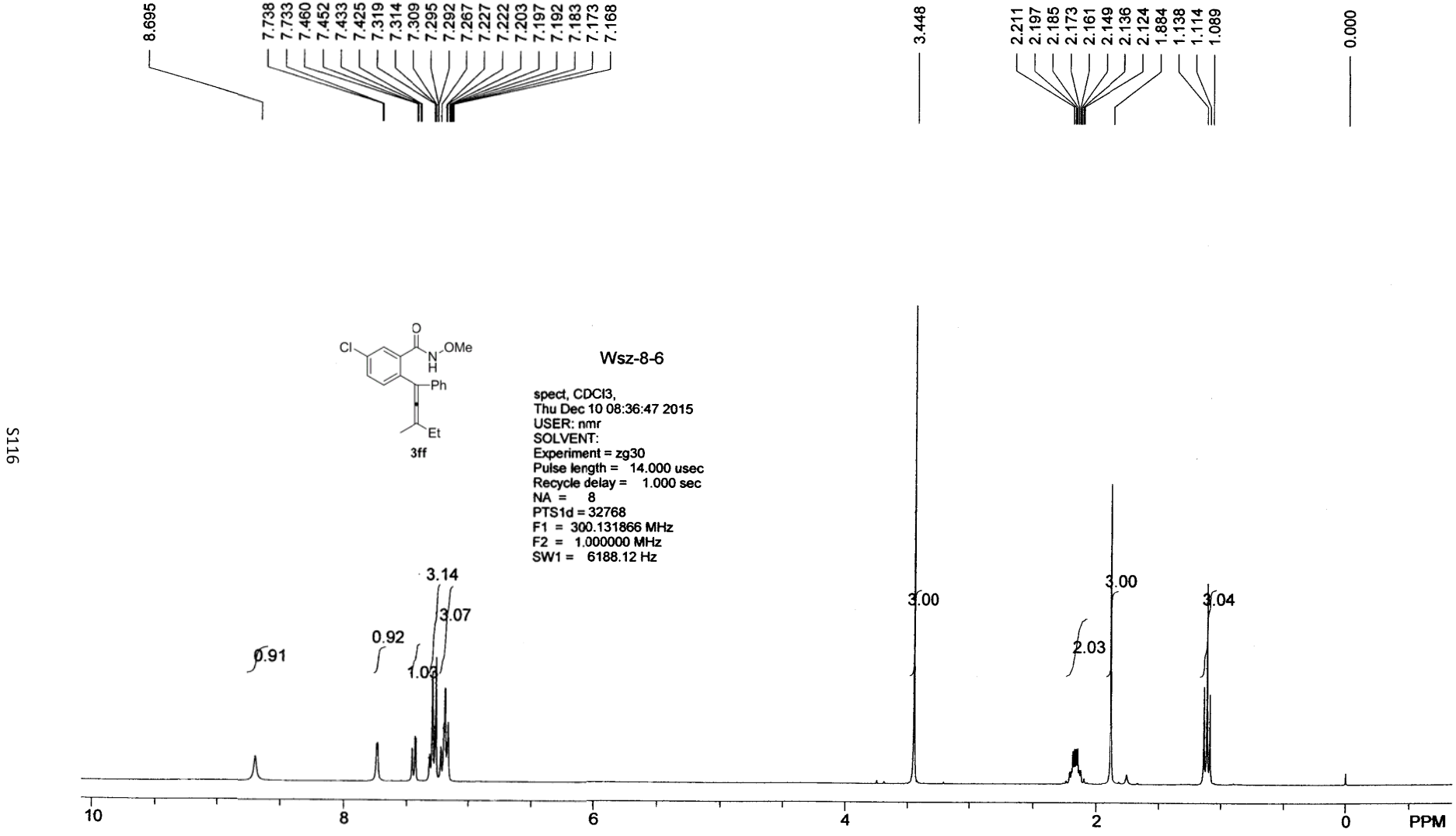

12.316
18.533
27.388
52.349
63.925
76.568
77.000
77.425
106.707
106.947
126.483
127.139
128.657
129.632
132.264
132.324
136.174
136.641
136.937
165.709
166.069
202.232
Wsz-8-47
spect, CDCl3,
Mon Jan 04 07:51:22 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1245
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
Ph
Et
MeO2C
3cf
PPM
0
50
100
150
200

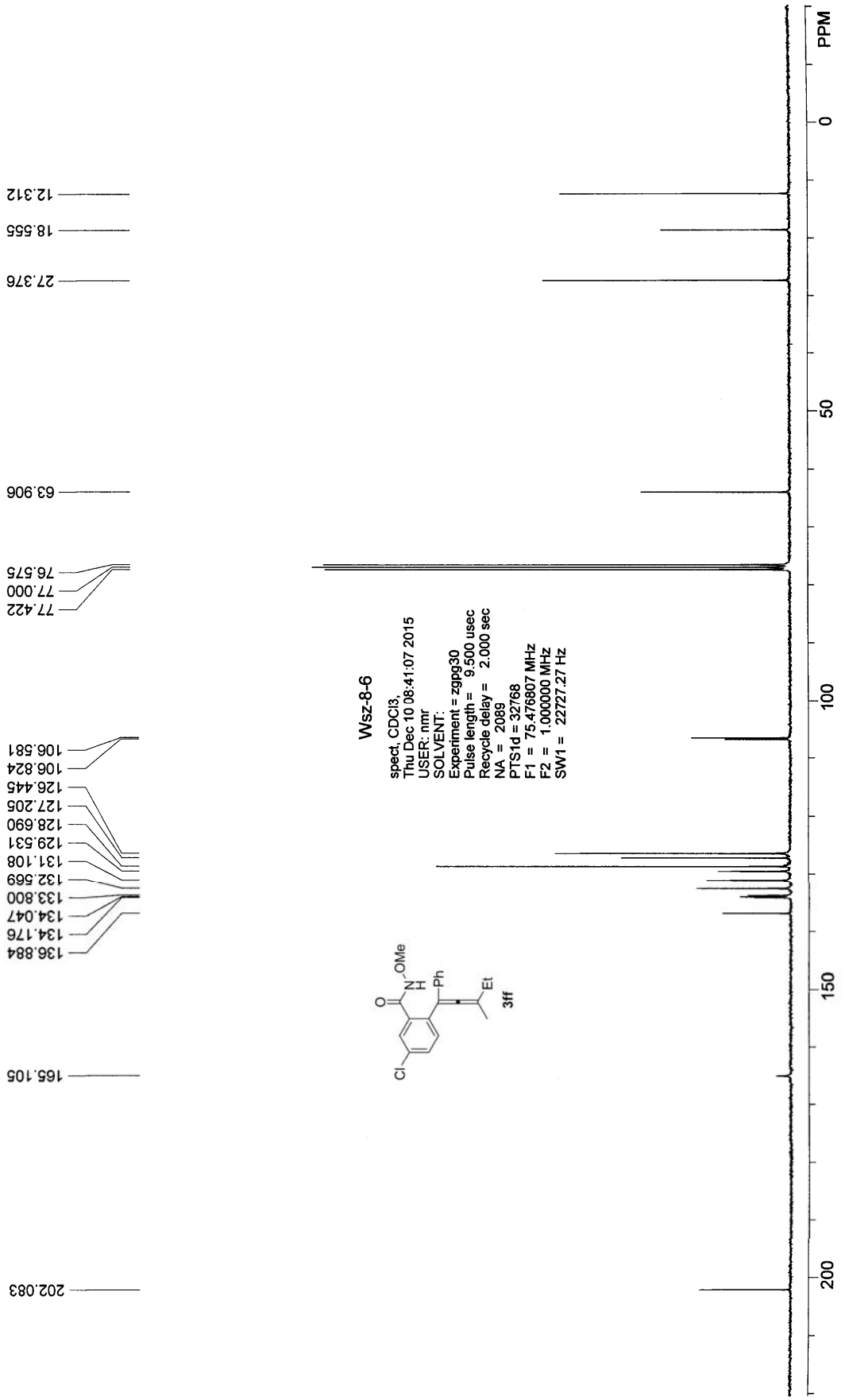

Wsz-7-110
spect, CDCl3,
Mon Sep 28 17:17:47 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
3df
OMe
Ph
Et
MeO
PPM
0
2
4
6
8
10
3.00
0.98
1.01
2.10
0.97
0.94
3.01
3.06
2.00
2.99
3.00
3.834
3.424
2.251
2.225
2.208
2.200
2.185
2.175
2.160
2.150
2.135
2.109
1.898
1.163
1.138
1.114
-0.000
8.763
7.822
7.793
7.314
7.310
7.285
7.282
7.266
7.262
7.217
7.215
7.193
7.189
7.180
7.172
7.167
7.162
6.956
6.947
6.926
6.918
6.852
6.844

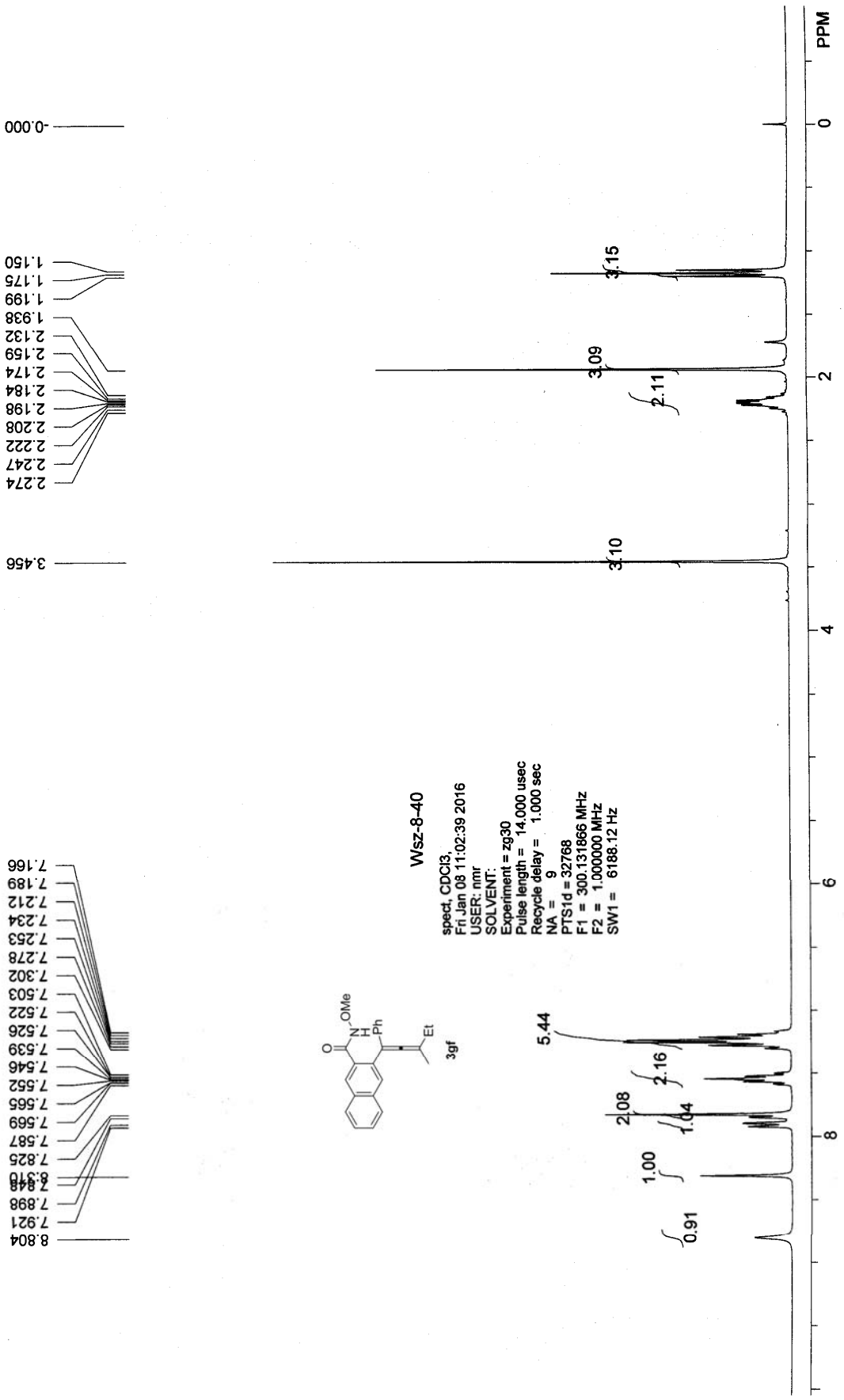

201.642
166.184
161.569
137.276
136.887
131.726
128.642
127.085
126.368
124.711
116.584
113.009
107.838
106.600
77.425
77.000
76.576
63.770
55.335
27.411
18.660
12.371
MeO
OMe
N
H
Ph
Et
3df
Wsz-7-110
spect, CDCl3,
Mon Sep 28 17:52:03 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 360
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
200
150
100
50
0
PPM

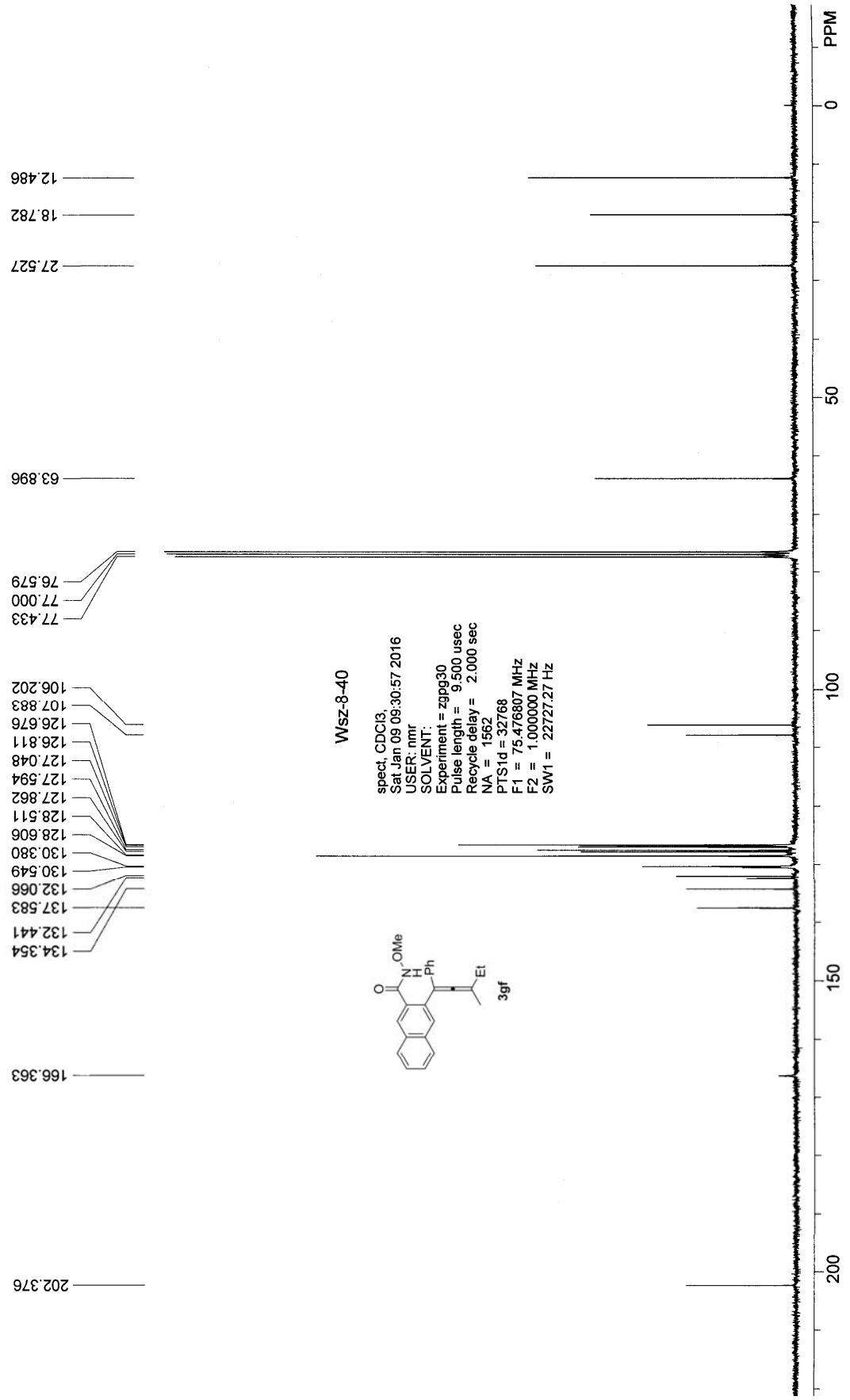

8.704
7.777
7.750
7.467
7.463
7.440
7.436
7.352
7.312
7.286
7.262
7.215
7.191
3.432
2.229
2.204
2.179
2.155
2.131
1.902
1.328
1.170
1.146
1.121
-0.000
Wsz-7-199
spect, CDCl3,
Sun Nov 29 07:41:37 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 10
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
O
N
OMe
H
Ph
Et
3ef
6.35
1.00
1.03
0.92
3.00
2.07
2.96
9.20
3.17
8
6
4
2
0
PPM

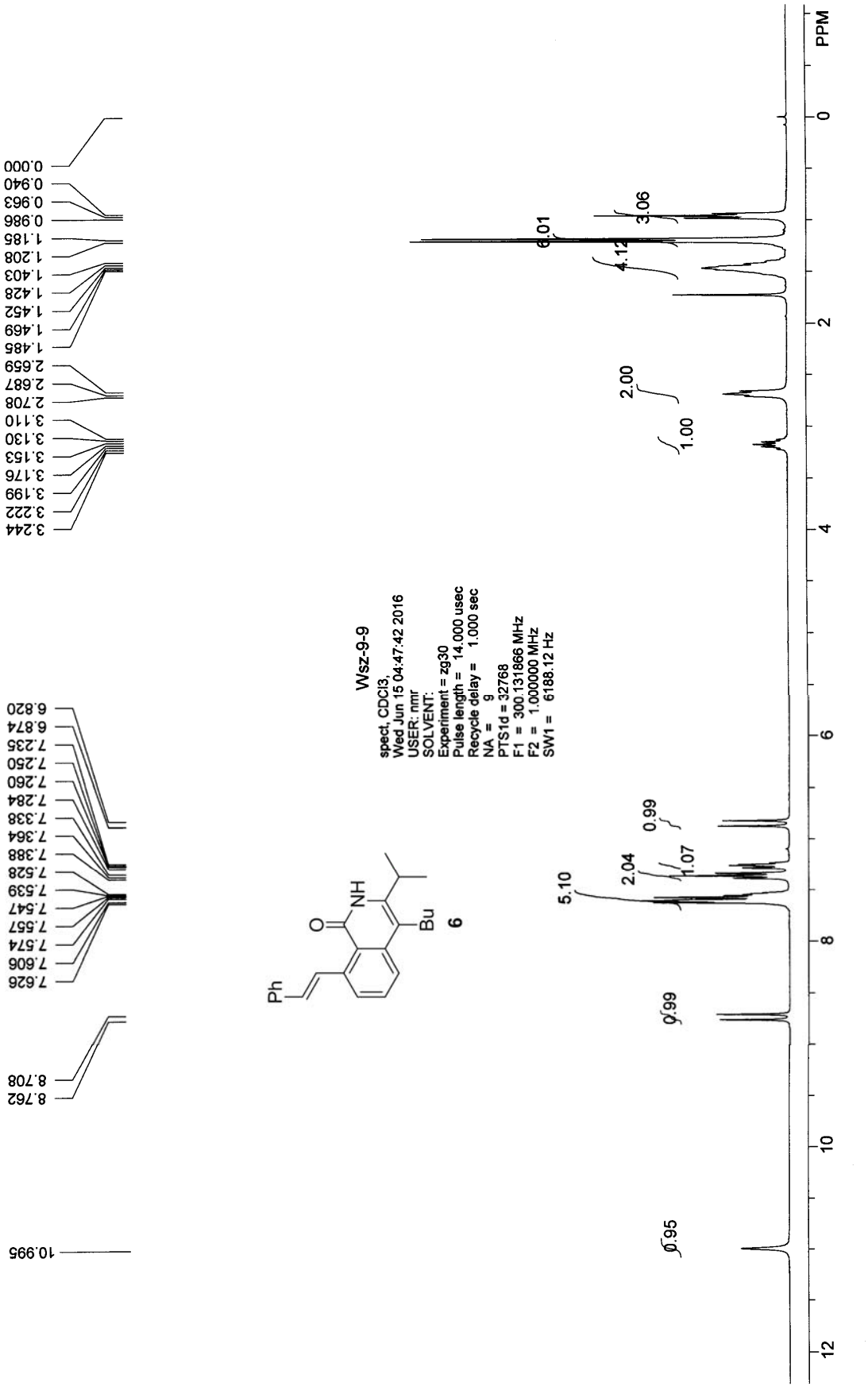

12.383
18.746
27.446
31.071
34.807
63.830
76.576
77.000
77.420
106.264
108.169
125.027
126.430
127.024
128.244
128.629
129.502
129.554
135.044
137.238
154.657
166.508
201.938
Wsz-7-199
spect, CDCl3,
Sun Nov 29 09:13:18 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 345
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
NH
Ph
Et
3ef
PPM
0
50
100
150
200

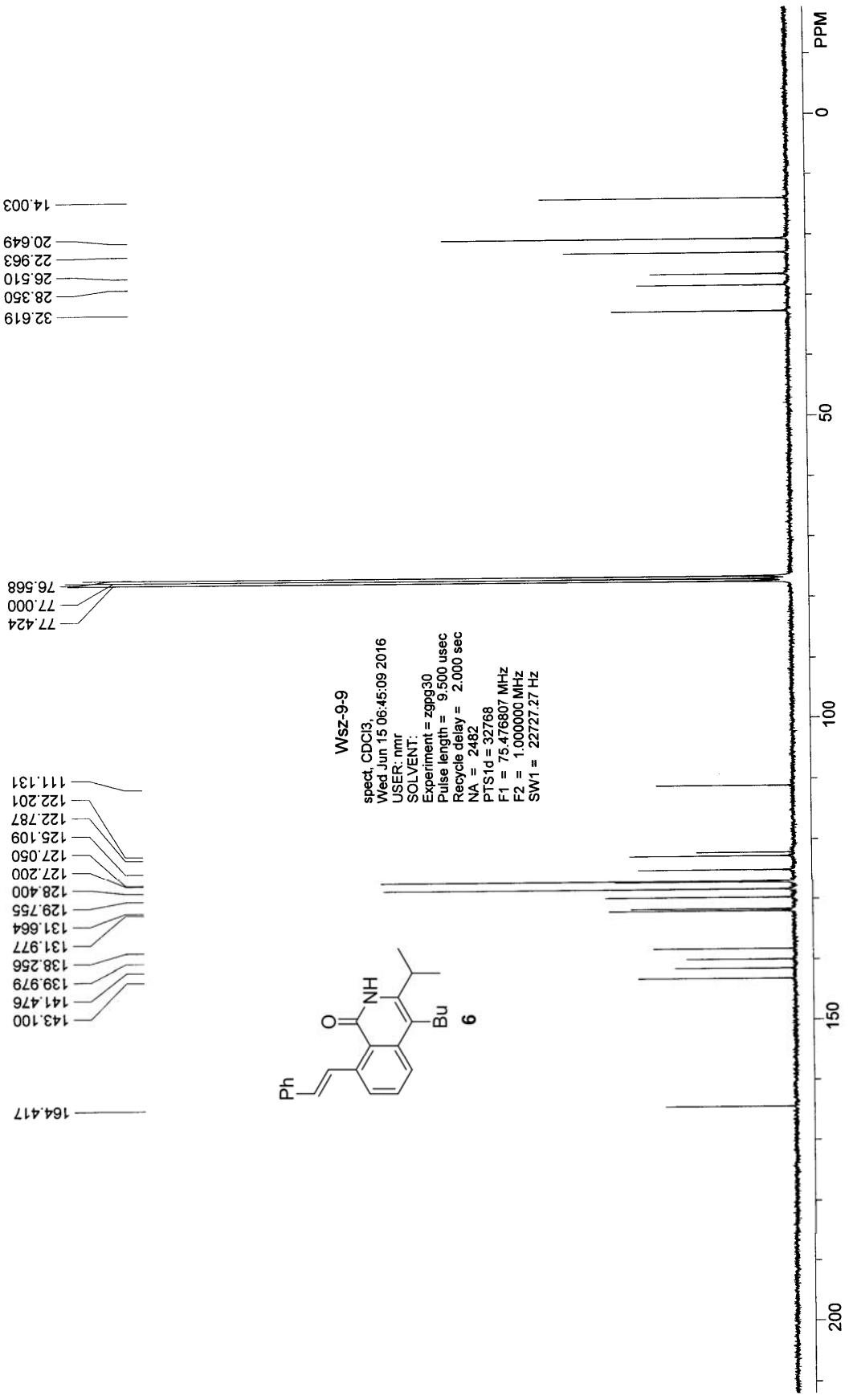

8.695
7.738
7.733
7.460
7.452
7.433
7.425
7.319
7.314
7.309
7.295
7.292
7.267
7.227
7.222
7.203
7.197
7.192
7.183
7.173
7.168
3.448
2.211
2.197
2.185
2.173
2.161
2.149
2.136
2.124
1.884
1.138
1.114
1.089
0.000
Cl
O
N
H
OMe
Ph
Et
3ff
Wsz-8-6
spect, CDCl3,
Thu Dec 10 08:36:47 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.91
0.92
1.03
3.14
3.07
3.00
2.03
3.00
3.04
10
8
6
4
2
0
PPM

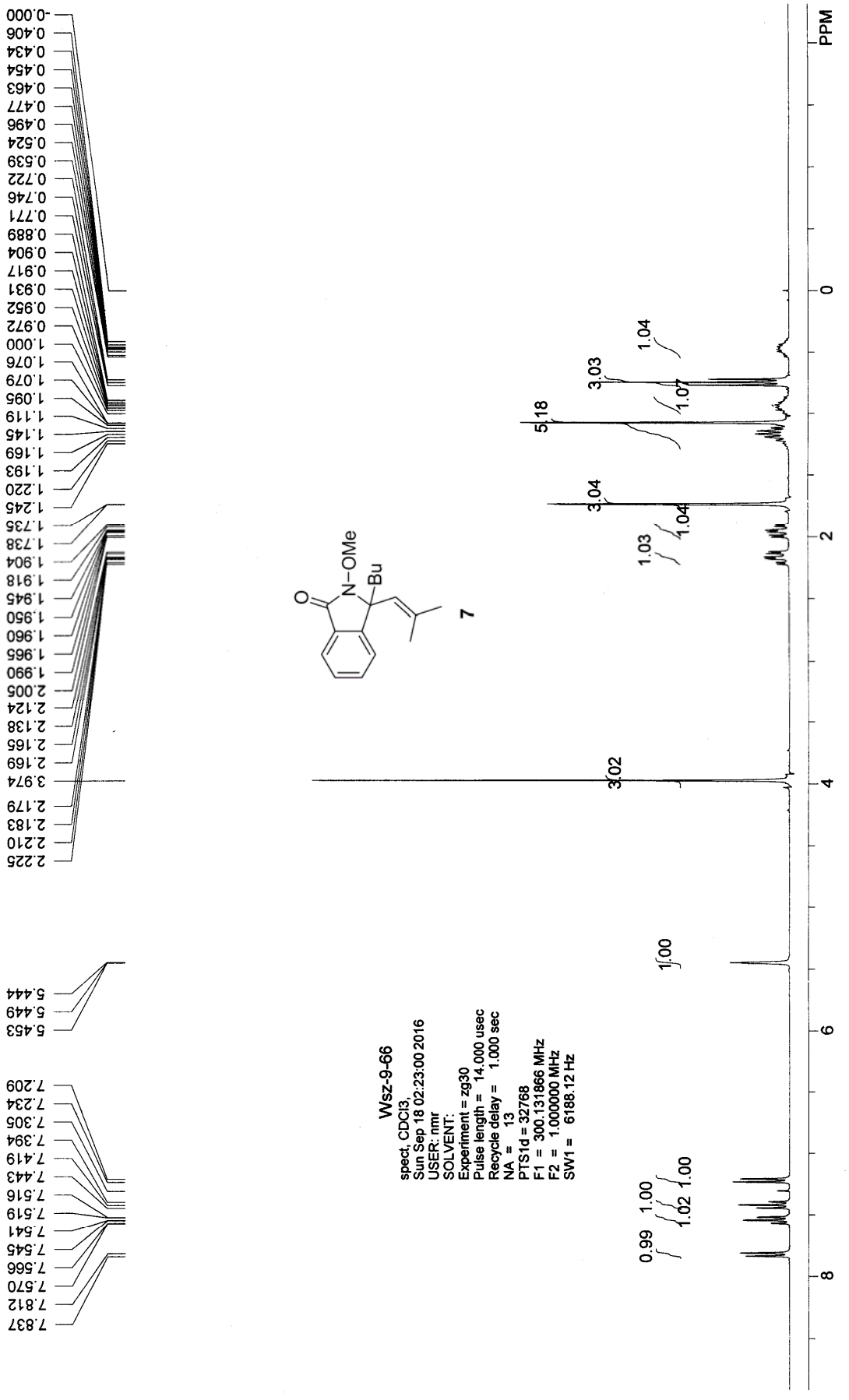

Wsz-8-6
spect, CDCl3,
Thu Dec 10 08:41:07 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 2089
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
3ff
PPM
0
50
100
150
200
12.312
18.555
27.376
63.906
76.575
77.000
77.422
106.581
106.824
126.445
127.205
128.690
129.531
131.108
132.569
133.800
134.047
134.176
136.884
165.105
202.083

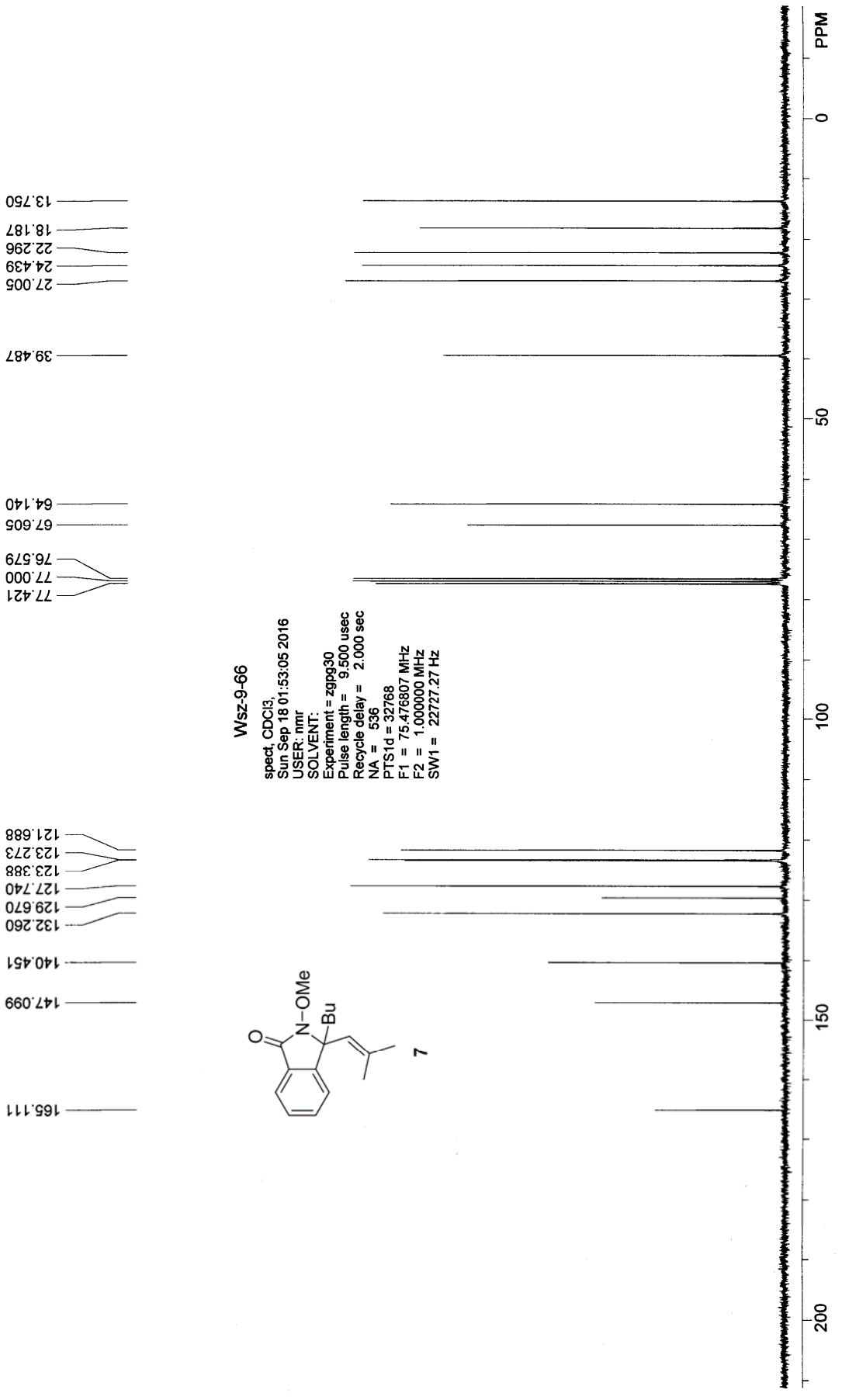

Wsz-8-40
spect, CDCl3,
Fri Jan 08 11:02:39 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
3gf
PPM
0
2
4
6
8
0.91
1.00
2.08
1.04
2.16
5.44
2.11
3.09
3.10
3.15
-0.000
1.150
1.175
1.199
1.938
2.132
2.159
2.174
2.184
2.198
2.208
2.222
2.247
2.274
3.456
7.166
7.189
7.212
7.234
7.253
7.278
7.302
7.503
7.522
7.526
7.539
7.546
7.552
7.565
7.569
7.587
7.825
8.310
7.848
7.898
7.921
8.804

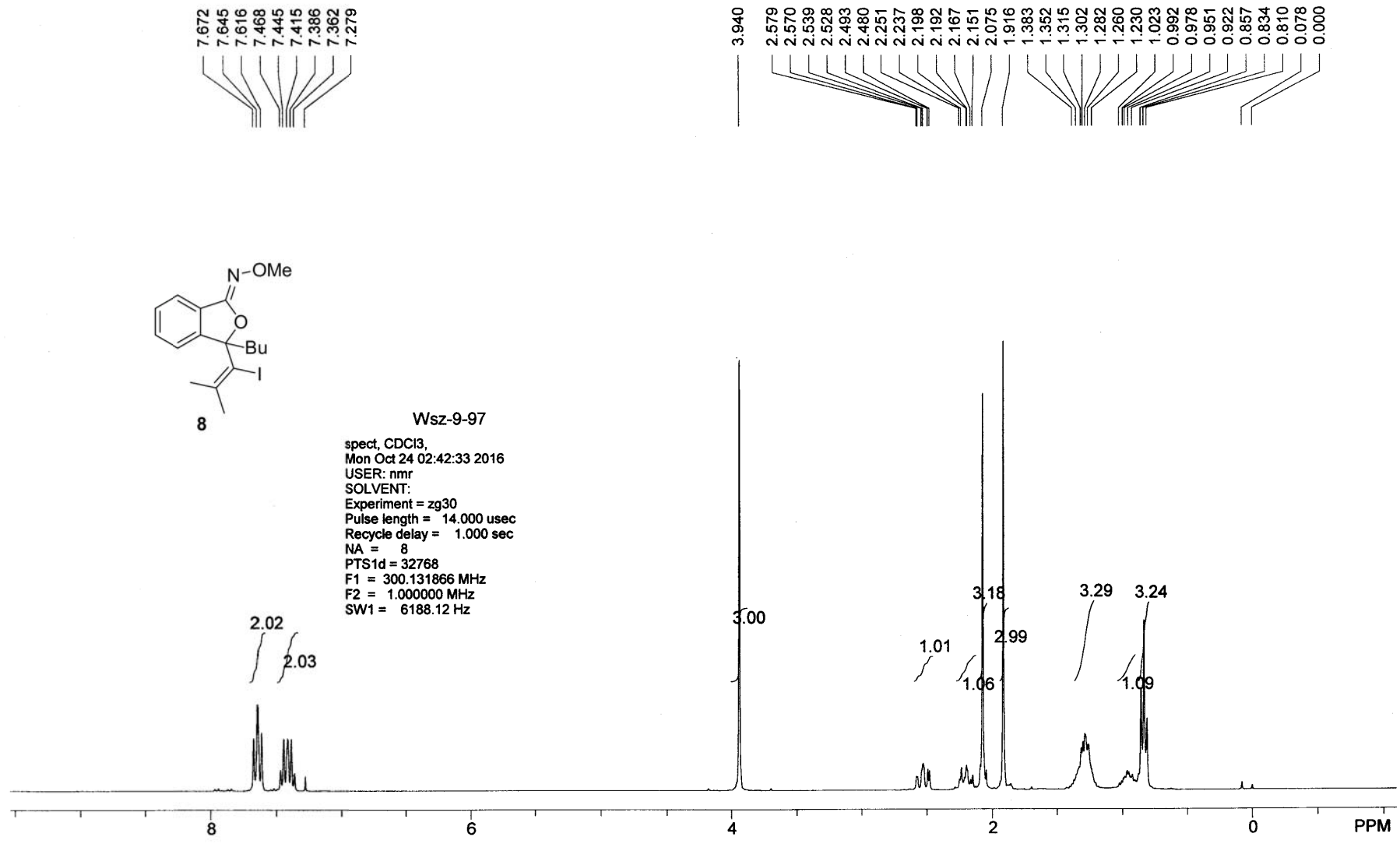

Wsz-8-40
spect, CDCl3,
Sat Jan 09 09:30:57 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1562
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
3gf
PPM
0
50
100
150
200
12.486
18.782
27.527
63.896
76.579
77.000
77.433
106.202
107.883
126.676
126.811
127.048
127.594
127.862
128.511
128.606
130.380
130.549
132.066
132.441
137.583
134.354
166.363
202.376

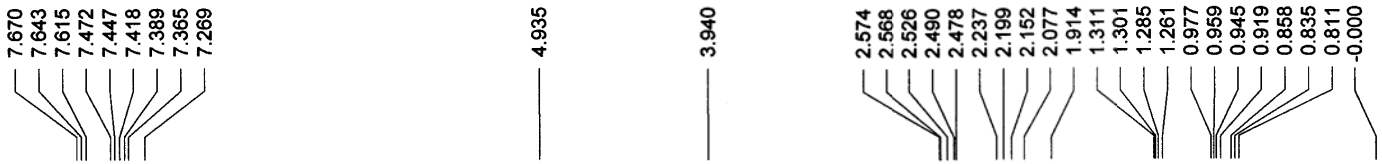

Wsz-9-9
spect, CDCl3,
Wed Jun 15 04:47:42 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
Ph
NH
O
Bu
6
PPM
0
2
4
6
8
10
12
0.95
0.99
5.10
2.04
0.99
1.07
2.00
1.00
4.12
6.01
3.06
10.995
8.762
8.708
7.626
7.606
7.574
7.557
7.547
7.539
7.528
7.388
7.364
7.338
7.284
7.260
7.250
7.235
6.874
6.820
3.244
3.222
3.199
3.176
3.153
3.130
3.110
2.708
2.687
2.659
1.485
1.469
1.452
1.428
1.403
1.208
1.185
0.986
0.963
0.940
0.000

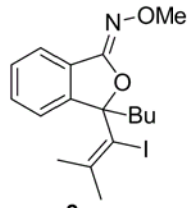

Wsz-9-9
spect, CDCl3,
Wed Jun 15 06:45:09 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 2482
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
PPM
0
50
100
150
200
14.003
20.649
22.963
26.510
28.350
32.619
76.568
77.000
77.424
111.131
122.201
122.787
125.109
127.050
127.200
128.400
129.755
131.664
131.977
138.256
139.979
141.476
143.100
164.417
NH
O
Bu
Ph
6


Wsz-9-66
spect, CDCl3,
Sun Sep 18 02:23:00 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 13
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
N–OMe
Bu
O
7
PPM


Wsz-9-66
spect, CDCl3,
Sun Sep 18 01:53:05 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 536
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
N-OMe
Bu
O
7
13.750
18.187
22.296
24.439
27.005
39.487
64.140
67.605
76.579
77.000
77.421
121.688
123.273
123.388
127.740
129.670
132.260
140.451
147.099
165.111
PPM
0
50
100
150
200

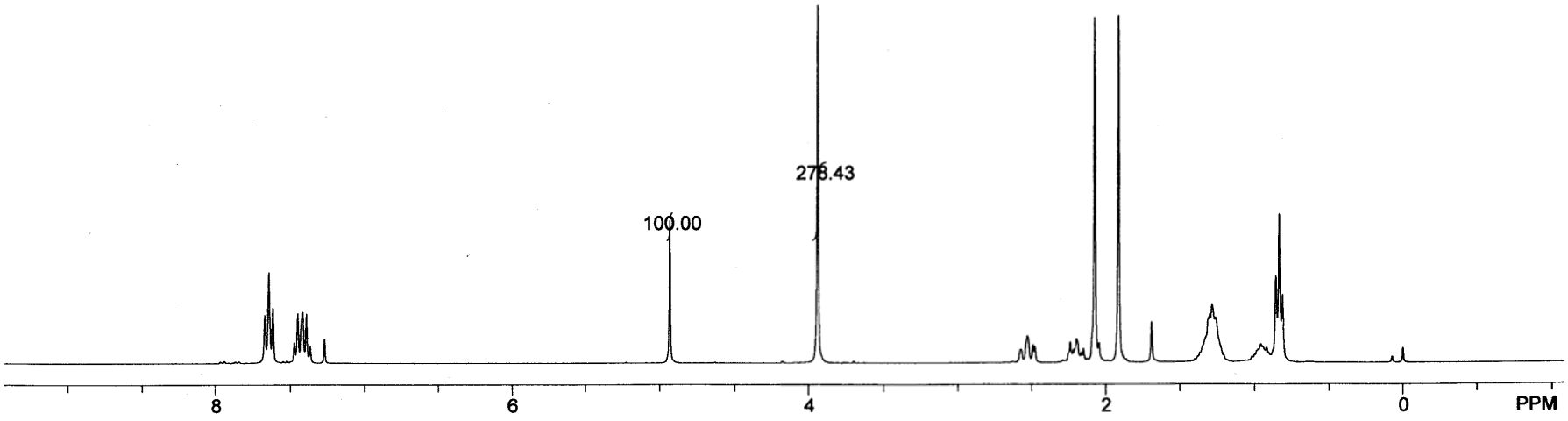

7.672
7.645
7.616
7.468
7.445
7.415
7.386
7.362
7.279
3.940
2.579
2.570
2.539
2.528
2.493
2.480
2.251
2.237
2.198
2.192
2.167
2.151
2.075
1.916
1.383
1.352
1.315
1.302
1.282
1.260
1.230
1.023
0.992
0.978
0.951
0.922
0.857
0.834
0.810
0.078
0.000
N–OMe
O
Bu
I
8
Wsz-9-97
spect, CDCl3,
Mon Oct 24 02:42:33 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
2.02
2.03
3.00
1.01
1.06
3.18
2.99
3.29
3.24
1.09
8
6
4
2
0
PPM

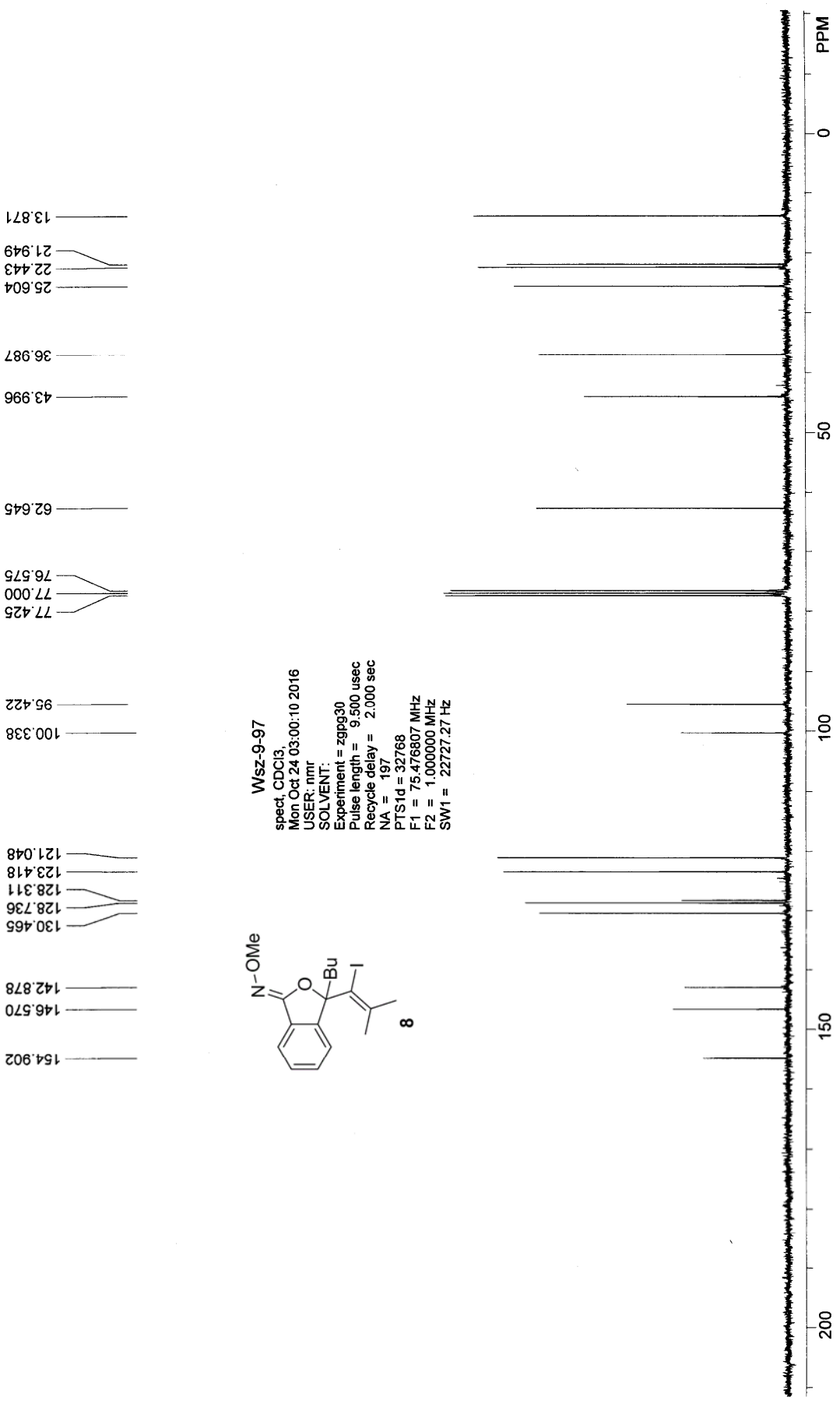


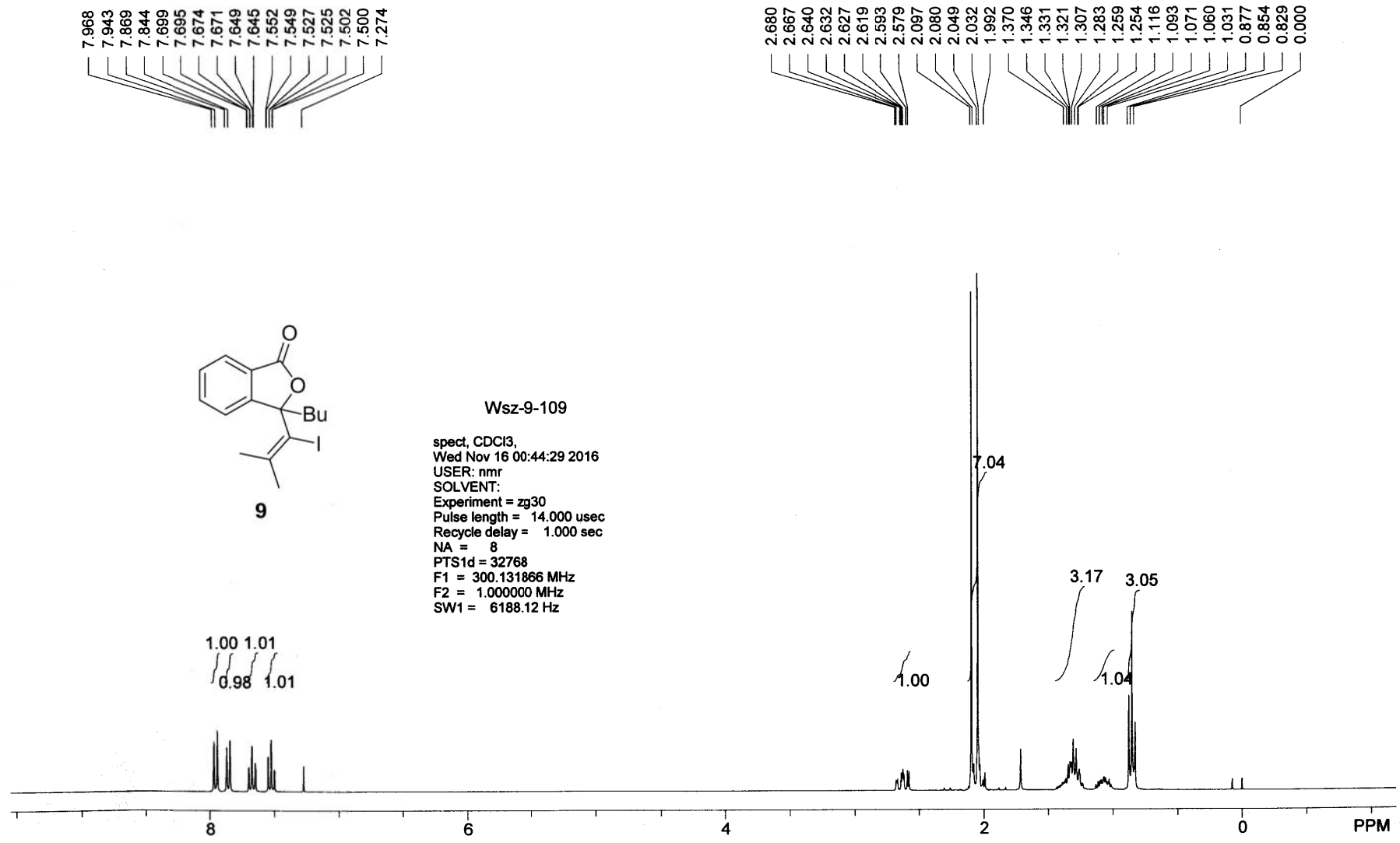


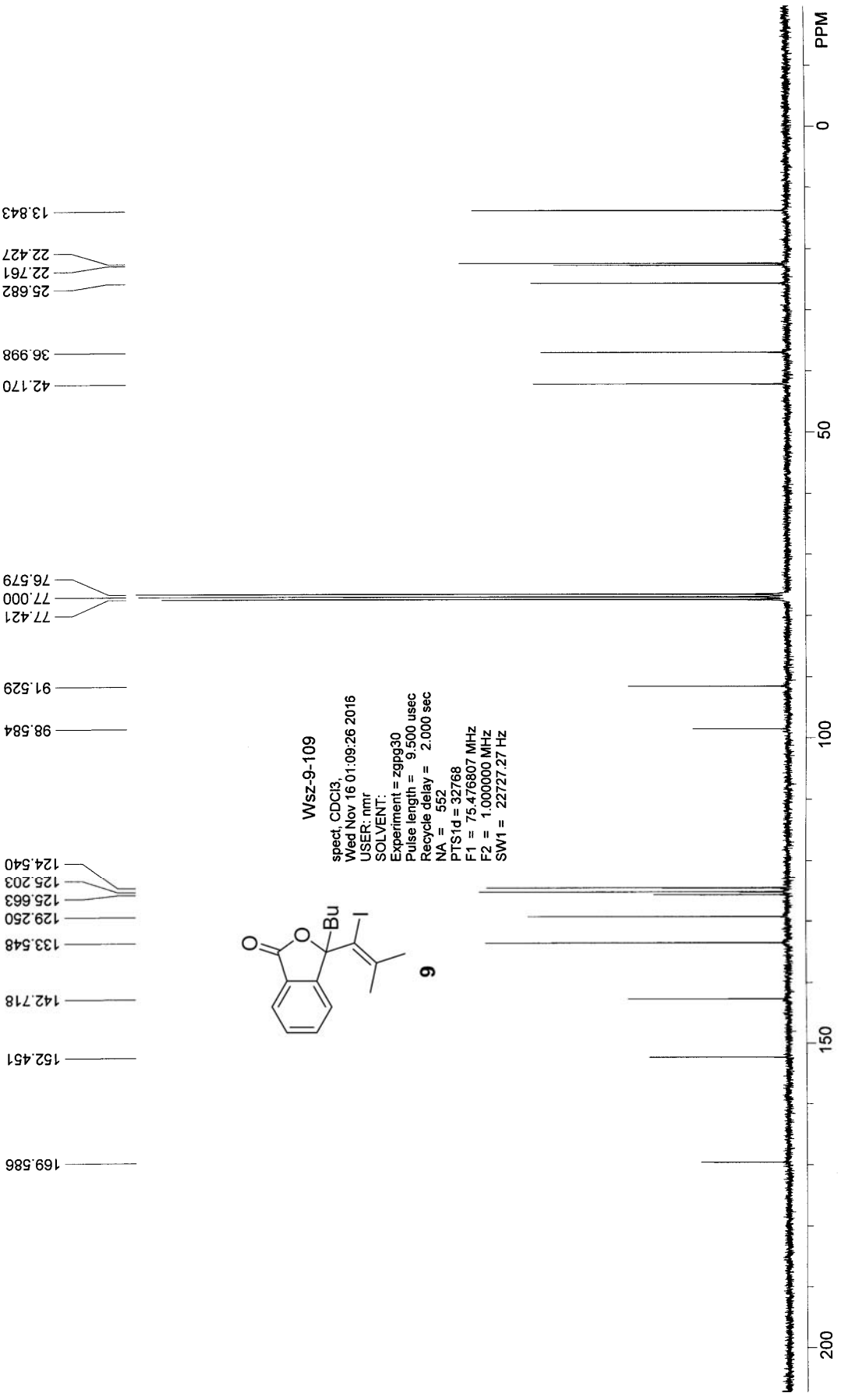
8

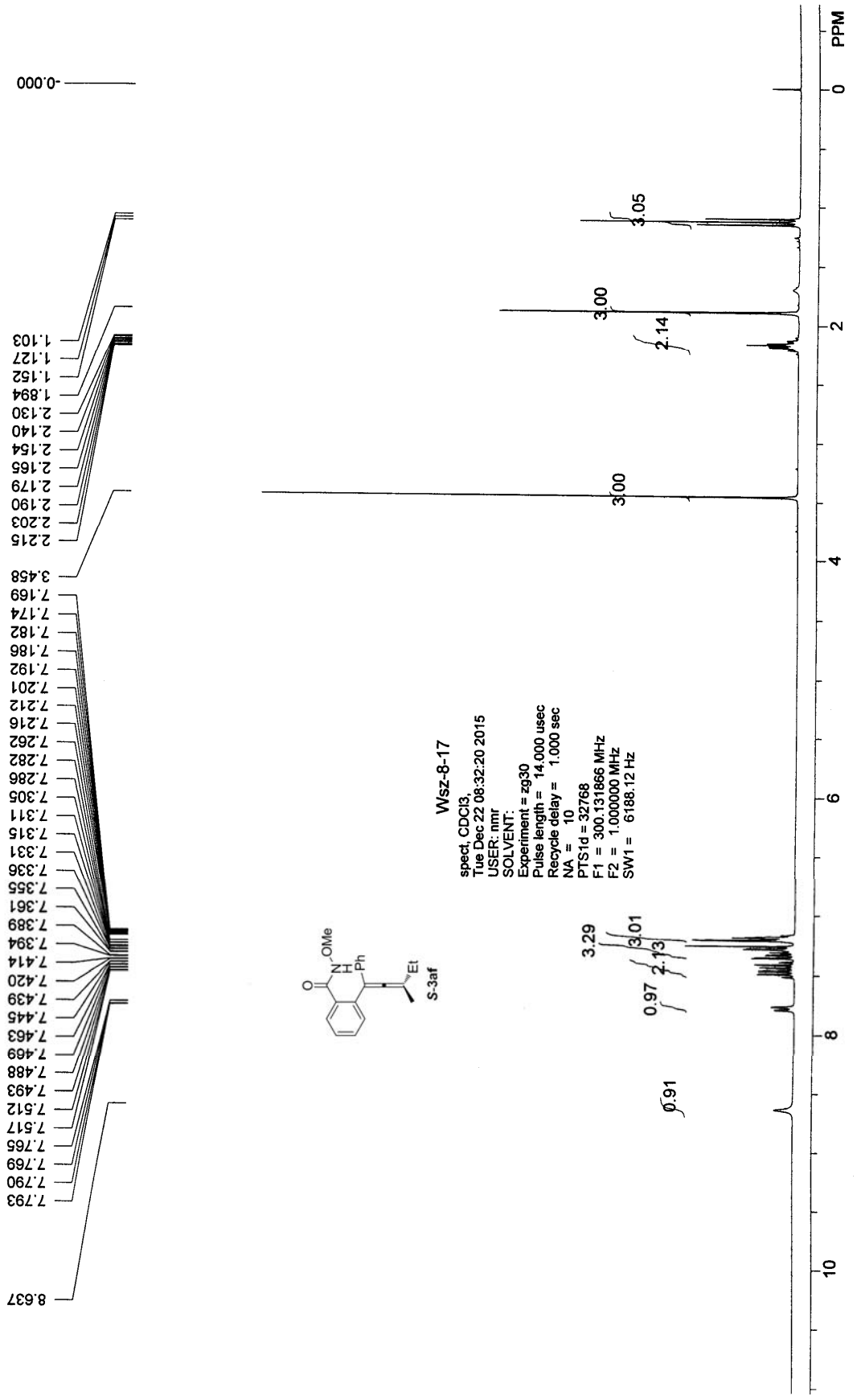
Wsz-9-97-purity
adding 7 uL CH2Br2 (0.1 mmol) to 79.9 mg sample

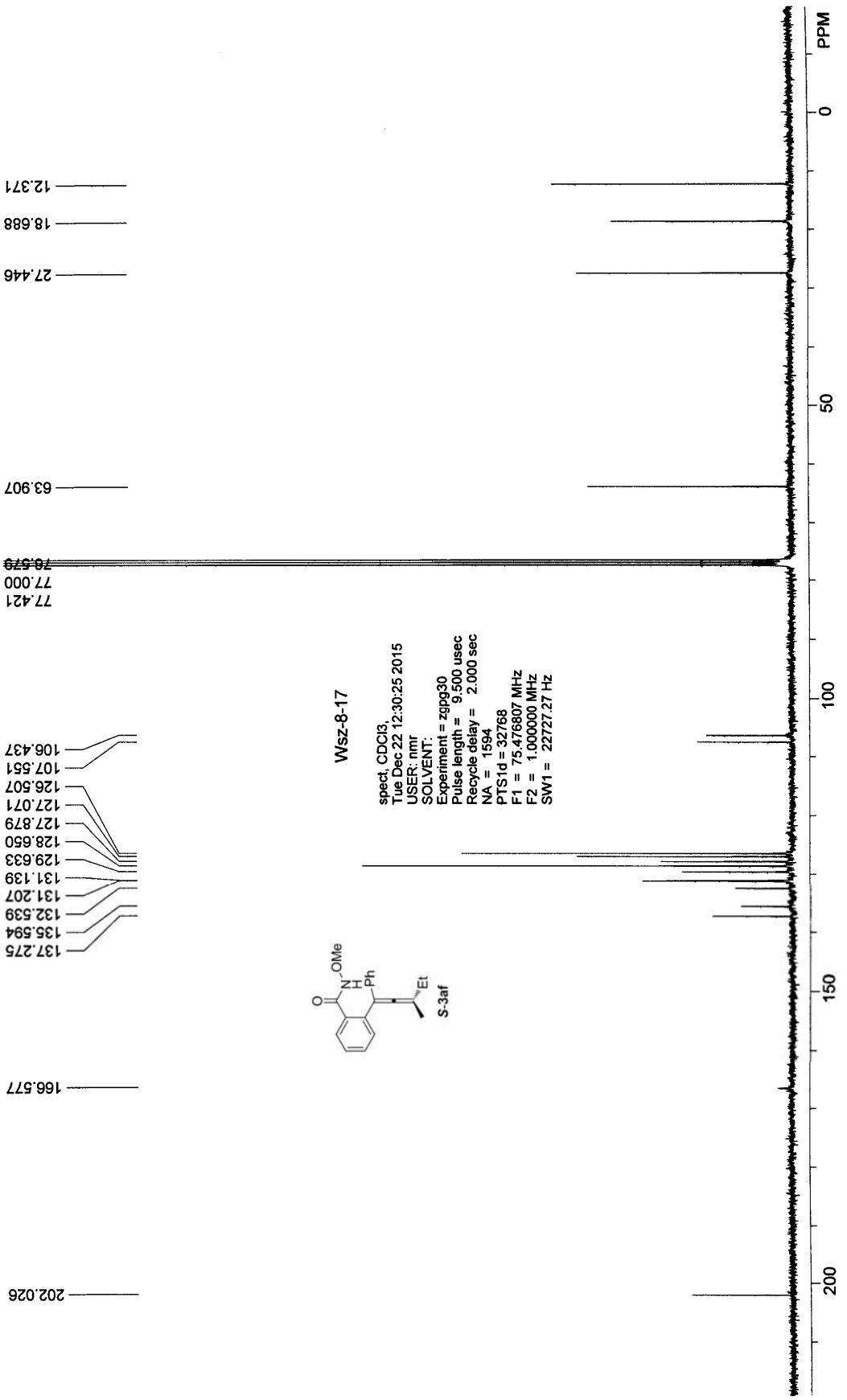



13.871
21.949
22.443
25.604
36.987
43.996
62.645
76.575
77.000
77.425
95.422
100.338
121.048
123.418
128.311
128.736
130.465
142.878
146.570
154.902
Wsz-9-97
spect, CDCl3,
Mon Oct 24 03:00:10 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 197
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
N–OMe
O
Bu
I
8
PPM
0
50
100
150
200


7.968
7.943
7.869
7.844
7.699
7.695
7.674
7.671
7.649
7.645
7.552
7.549
7.527
7.525
7.502
7.500
7.274
2.680
2.667
2.640
2.632
2.627
2.619
2.593
2.579
2.097
2.080
2.049
2.032
1.992
1.370
1.346
1.331
1.321
1.307
1.283
1.259
1.254
1.116
1.093
1.071
1.060
1.031
0.877
0.854
0.829
0.000
O
O
Bu
I
9
Wsz-9-109
spect, CDCl3,
Wed Nov 16 00:44:29 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
1.00 1.01
0.98 1.01
1.00
7.04
3.17
3.05
1.04
8
6
4
2
0
PPM


Wsz-9-109
spect, CDCl3,
Wed Nov 16 01:09:26 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 552
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
Bu
I
O
O
9
13.843
22.427
22.761
25.682
36.998
42.170
76.579
77.000
77.421
91.529
98.584
124.540
125.203
125.663
129.250
133.548
142.718
152.451
169.586
PPM
0
50
100
150
200


Wsz-8-17
spect, CDCl3,
Tue Dec 22 08:32:20 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 10
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
S-3af
PPM
0
2
4
6
8
10
3.29
3.01
2.13
0.97
0.91
3.00
3.00
2.14
3.05
-0.000
1.103
1.127
1.152
1.894
2.130
2.140
2.154
2.165
2.179
2.190
2.203
2.215
3.458
7.169
7.174
7.182
7.186
7.192
7.201
7.212
7.216
7.262
7.282
7.286
7.305
7.311
7.315
7.331
7.336
7.355
7.361
7.389
7.394
7.414
7.420
7.439
7.445
7.463
7.469
7.488
7.493
7.512
7.517
7.765
7.769
7.790
7.793
8.637


Wsz-8-17
spect, CDCl3,
Tue Dec 22 12:30:25 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1594
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
N
H
Ph
Et
O
S-3af
PPM
0
50
100
150
200
12.371
18.688
27.446
63.907
76.579
77.000
77.421
106.437
107.551
126.507
127.071
127.879
128.650
129.633
131.139
131.207
132.539
135.594
137.275
166.577
202.026

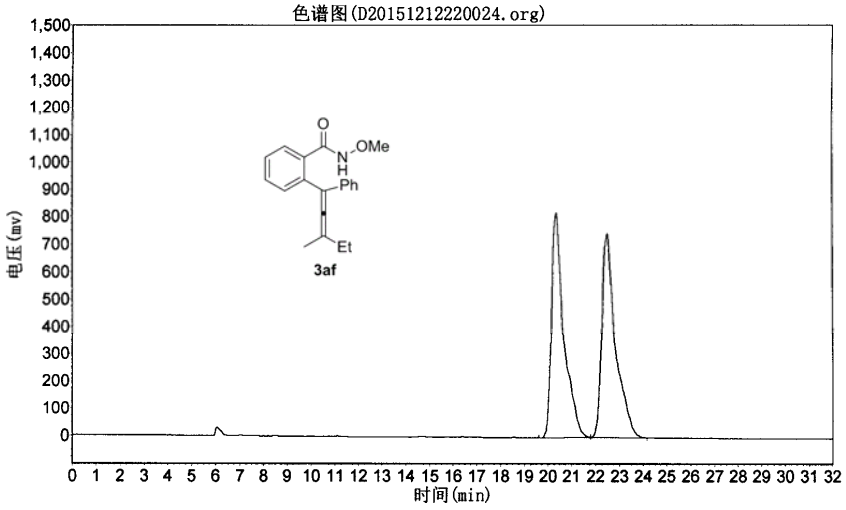
Wsz-7-6

实验单位：zju
实验时间：2015-12-12,22:00:24
谱图文件:D:\浙大智达\N2000\样品\D20151212220024.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2015-12-12,22:34:00
积分方法:面积归一法

实验内容简介：
AD-H, n-hexane/i-PrOH = 10/1, 207 nm,1.0 ml/min

色谱图(D20151212220024.org)



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		20.343	819713.188	29445186.000	49.9340
2		22.487	741909.313	29522970.000	50.0660
总计			1561622.500	58968156.000	100.0000

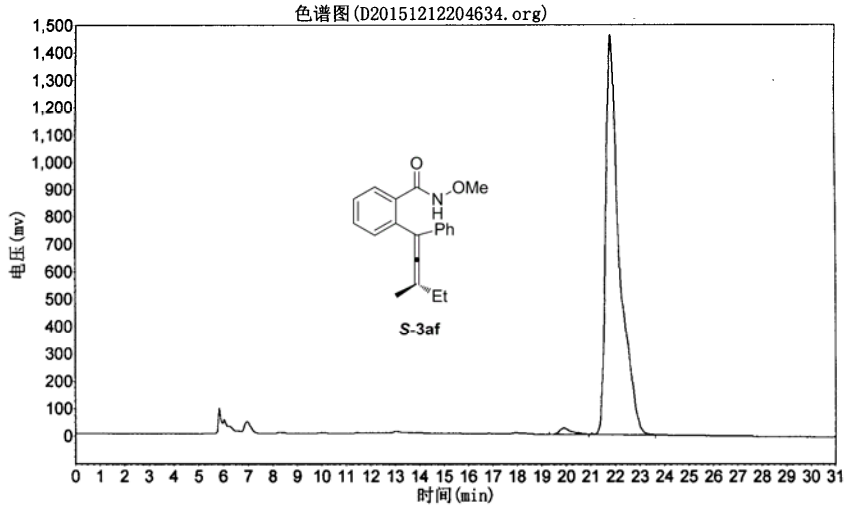
Wsz-8-17

实验单位：zju
实验时间：2015-12-12,20:46:34
谱图文件:D:\浙大智达\N2000\样品\D20151212204634.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2015-12-12,21:23:12
积分方法:面积归一法

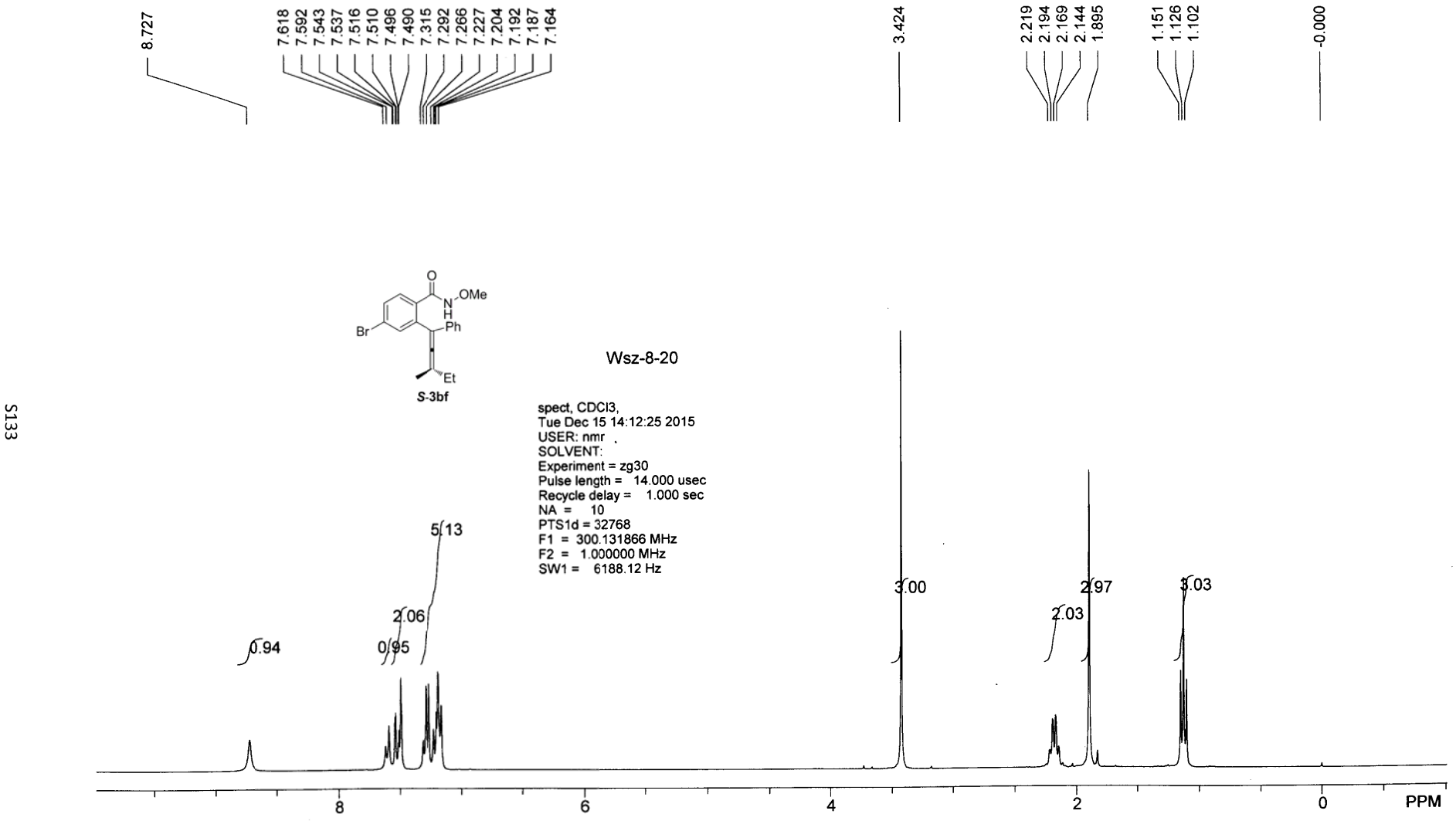
实验内容简介：
AD-H, n-hexane/i-PrOH = 10/1, 207 nm,1.0 ml/min

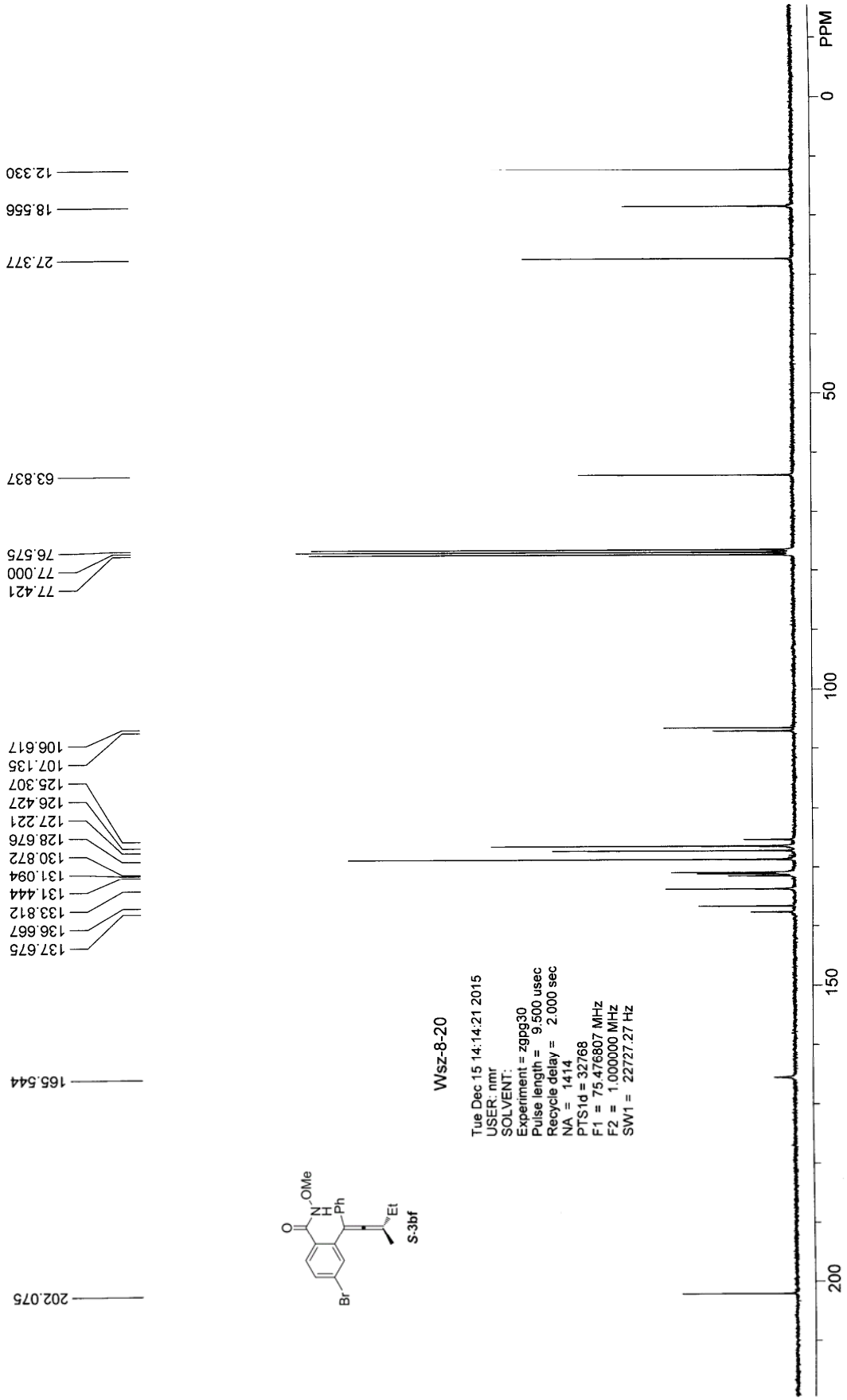
色谱图(D20151212204634.org)



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		19.892	22877.059	798620.813	1.4026
2		21.832	1459998.250	56140976.000	98.5974
总计			1482875.309	56939596.813	100.0000


8.727
7.618
7.592
7.543
7.537
7.516
7.510
7.496
7.490
7.315
7.292
7.266
7.227
7.204
7.192
7.187
7.164
3.424
2.219
2.194
2.169
2.144
1.895
1.151
1.126
1.102
-0.000
O
N
OMe
H
Br
Ph
Et
S-3bf
Wsz-8-20
spect, CDCl3,
Tue Dec 15 14:12:25 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 10
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
5.13
2.06
0.94
0.95
3.00
2.97
2.03
3.03
8
6
4
2
0
PPM


12.330
18.556
27.377
63.837
76.575
77.000
77.421
106.617
107.135
125.307
126.427
127.221
128.676
130.872
131.094
131.444
133.812
136.667
137.675
165.544
202.075
Wsz-8-20
Tue Dec 15 14:14:21 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1414
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
N
H
Ph
Et
O
Br
S-3bf
PPM
0
50
100
150
200

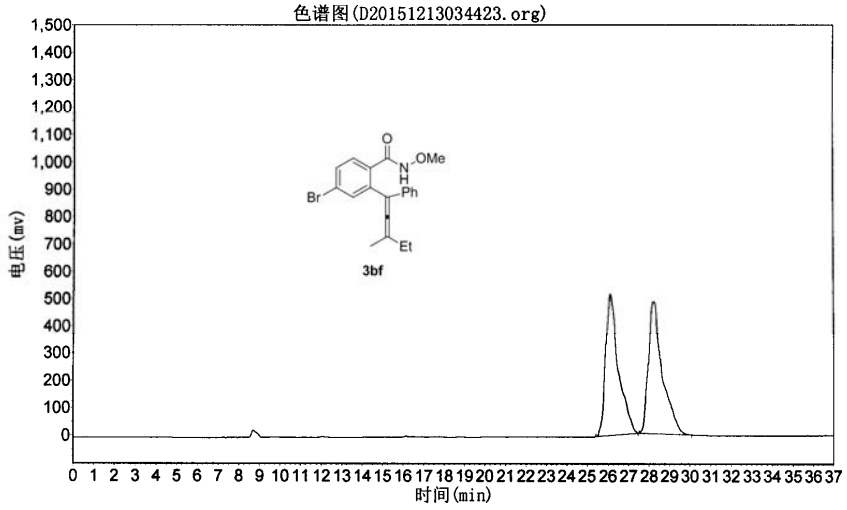
Wsz-7-8

实验单位：zju
实验时间：2015-12-13,3:44:23
谱图文件:D:\浙大智达\N2000\样品\D20151213034423.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2015-12-13,4:23:41
积分方法:面积归一法

实验内容简介：
AD-H, n-hexane/i-PrOH = 10/1, 207 nm,0.7 ml/min

色谱图(D20151213034423.org)



分析结果表

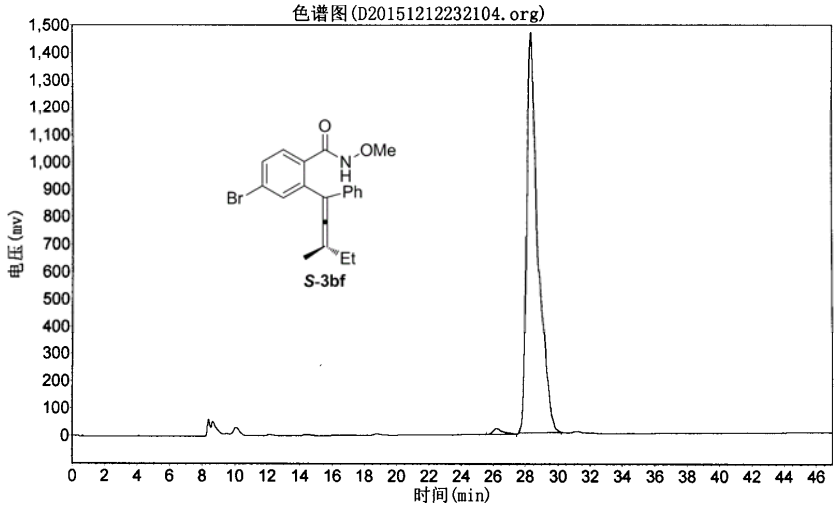
峰号	峰名	保留时间	峰高	峰面积	含量
1		26.107	517944.375	22303628.000	49.4844
2		28.210	484011.156	22768448.000	50.5156
总计			1001955.531	45072076.000	100.0000

Wsz-8-20

实验单位：zju
实验时间：2015-12-12,23:21:04
谱图文件:D:\浙大智达\N2000\样品\D20151212232104.org
方法文件:D:\浙大智达\N2000\djx.mtd

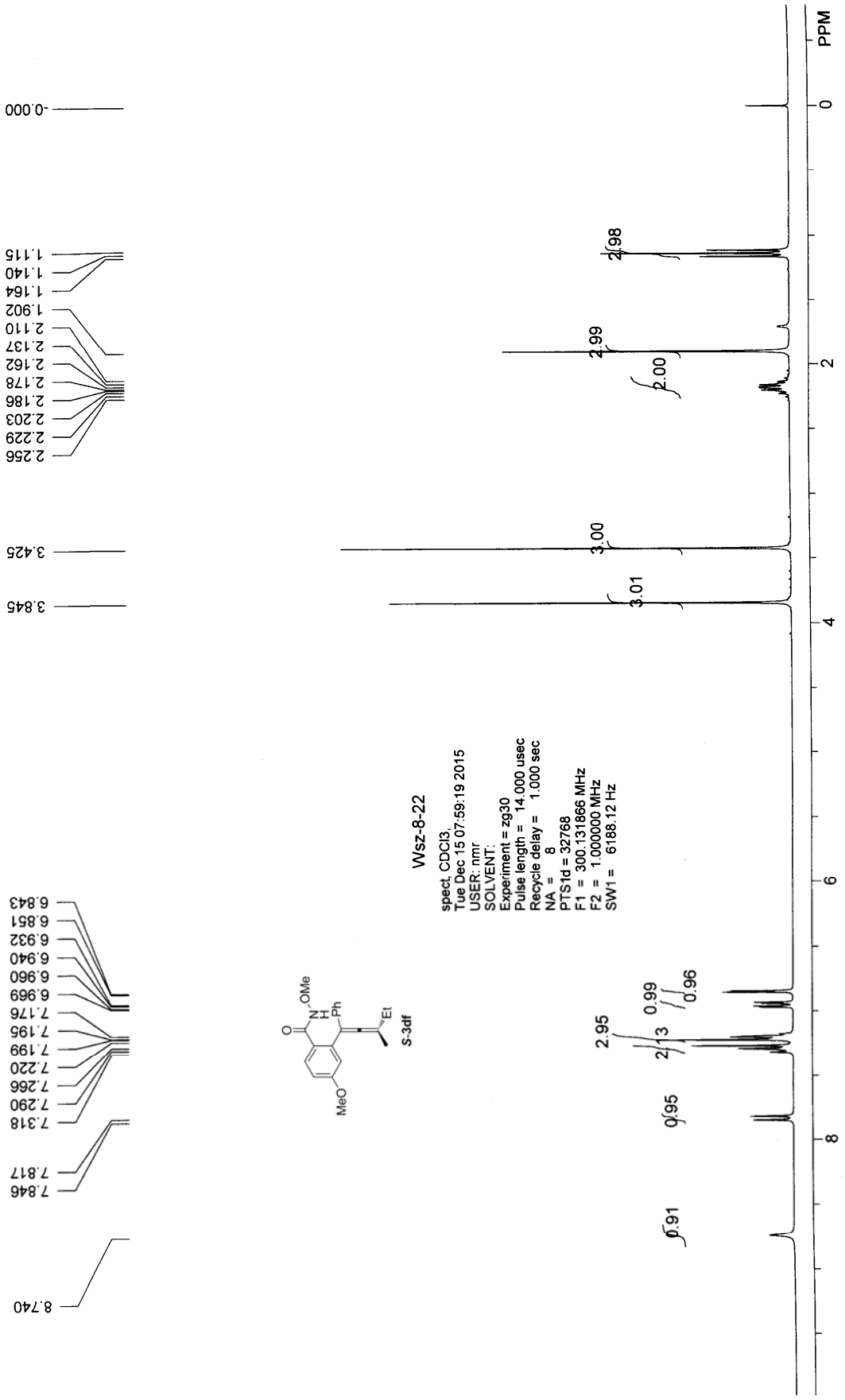
实验者：wsz
报告时间：2015-12-13,0:20:22
积分方法:面积归一法

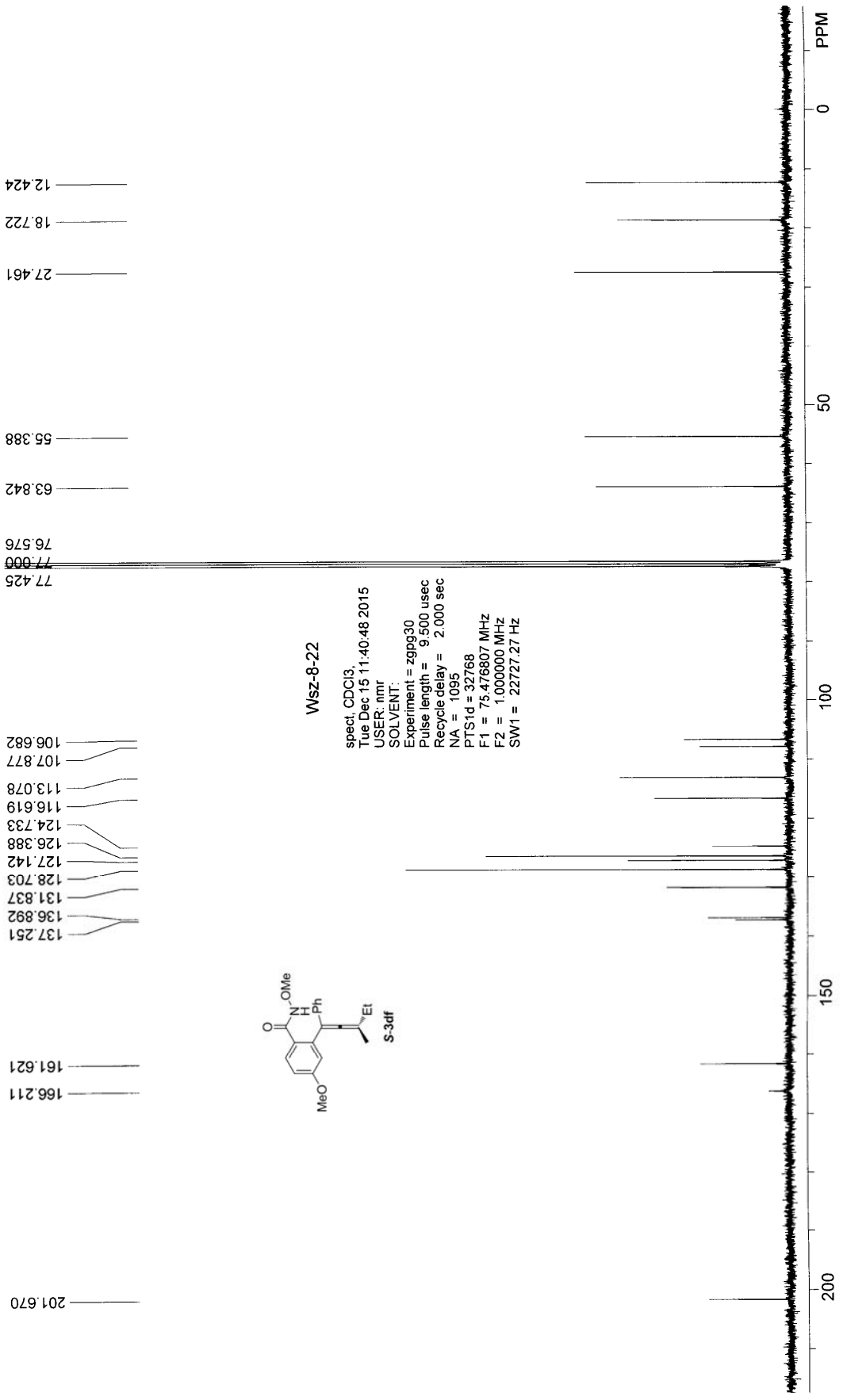
实验内容简介：
AD-H, n-hexane/i-PrOH = 10/1, 207 nm,0.7 ml/min



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		26.202	20459.438	895618.063	1.2513
2		28.337	1462053.000	70682032.000	98.7487
总计			1482512.438	71577650.063	100.0000


Wsz-8-22
spect, CDCl3,
Tue Dec 15 07:59:19 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
S-3df
PPM
0
2
4
6
8
-0.000
1.115
1.140
1.164
1.902
2.110
2.137
2.162
2.178
2.186
2.203
2.229
2.256
3.425
3.845
6.843
6.851
6.932
6.940
6.960
6.969
7.176
7.195
7.199
7.220
7.266
7.290
7.318
7.817
7.846
8.740
2.98
2.99
2.00
3.00
3.01
2.95
0.99
2.13
0.96
0.95
0.91


Wsz-8-22
spect, CDCl3,
Tue Dec 15 11:40:48 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1095
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
S-3df
OMe
N
H
Ph
Et
O
MeO
PPM
0
50
100
150
200
12.424
18.722
27.461
55.388
63.842
76.576
77.000
77.425
106.682
107.877
113.078
116.619
124.733
126.388
127.142
128.703
131.837
136.892
137.251
161.621
166.211
201.670

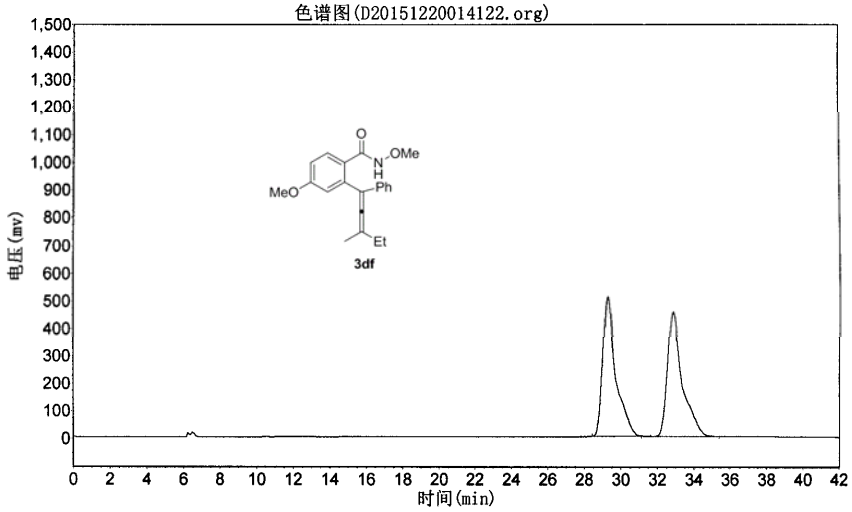
wsz-7-110

实验单位：zju
实验时间：2015-12-20,1:41:22
谱图文件:D:\浙大智达\N2000\样品\D20151220014122.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2015-12-20,2:25:21
积分方法:面积归一法

实验内容简介：
AD-H, n-hexane/i-PrOH = 10/1, 207 nm,1.0 ml/min

色谱图(D20151220014122.org)



分析结果表

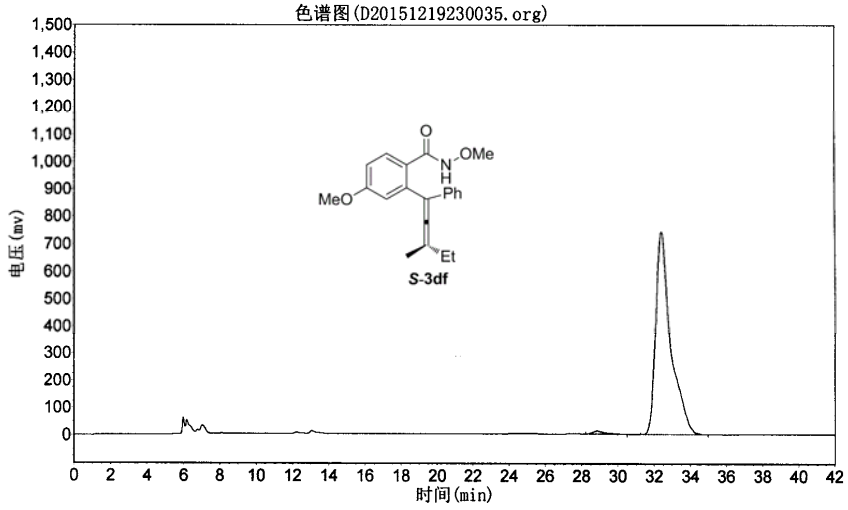
峰号	峰名	保留时间	峰高	峰面积	含量
1		29.260	508773.938	25207528.000	49.8214
2		32.830	452127.625	25388224.000	50.1786
总计			960901.563	50595752.000	100.0000

wsz-8-22

实验单位：zju
实验时间：2015-12-19,23:00:35
谱图文件:D:\浙大智达\N2000\样品\D20151219230035.org
方法文件:D:\浙大智达\N2000\djx.mtd

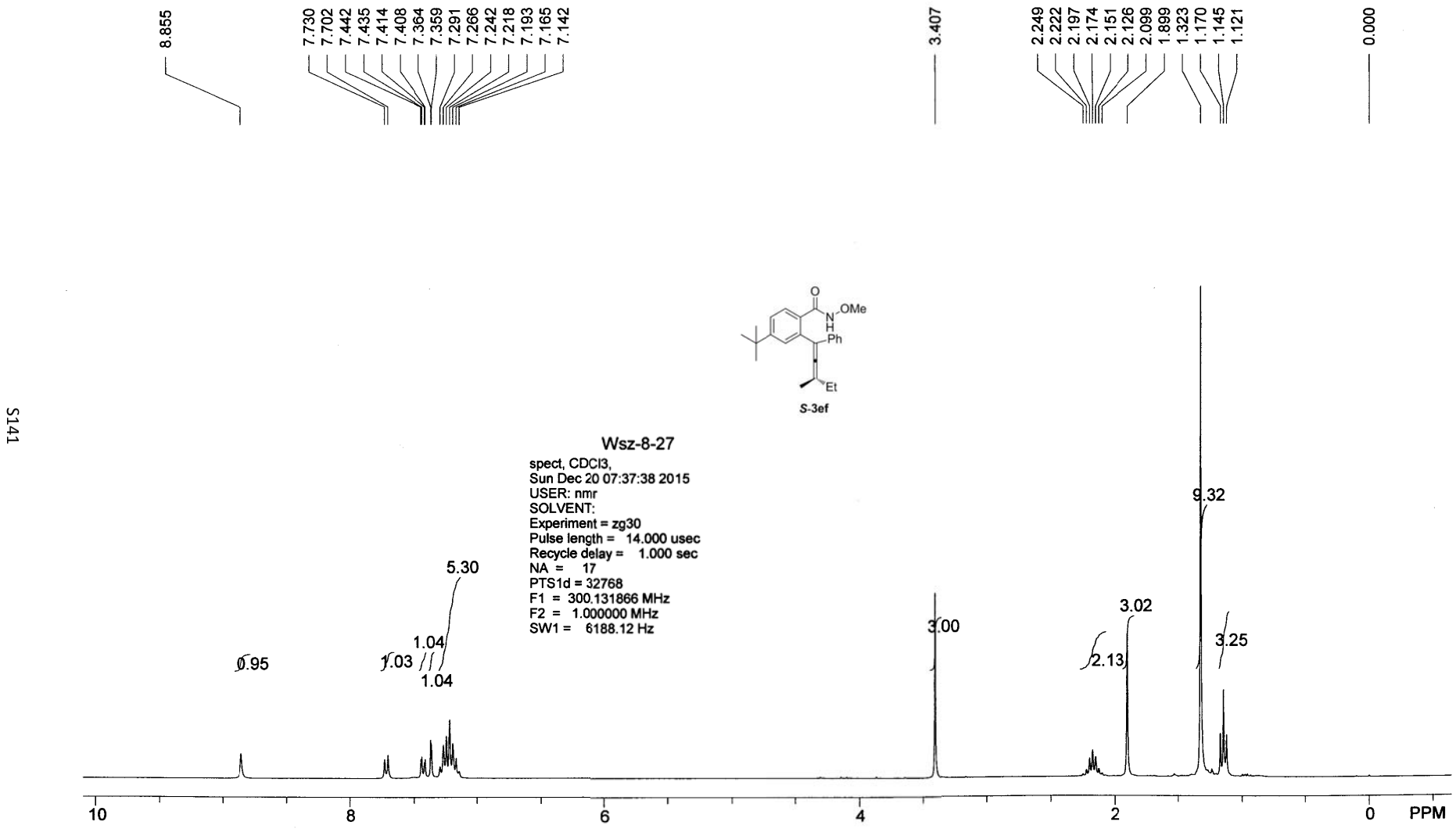
实验者：wsz
报告时间：2015-12-19,23:46:26
积分方法:面积归一法

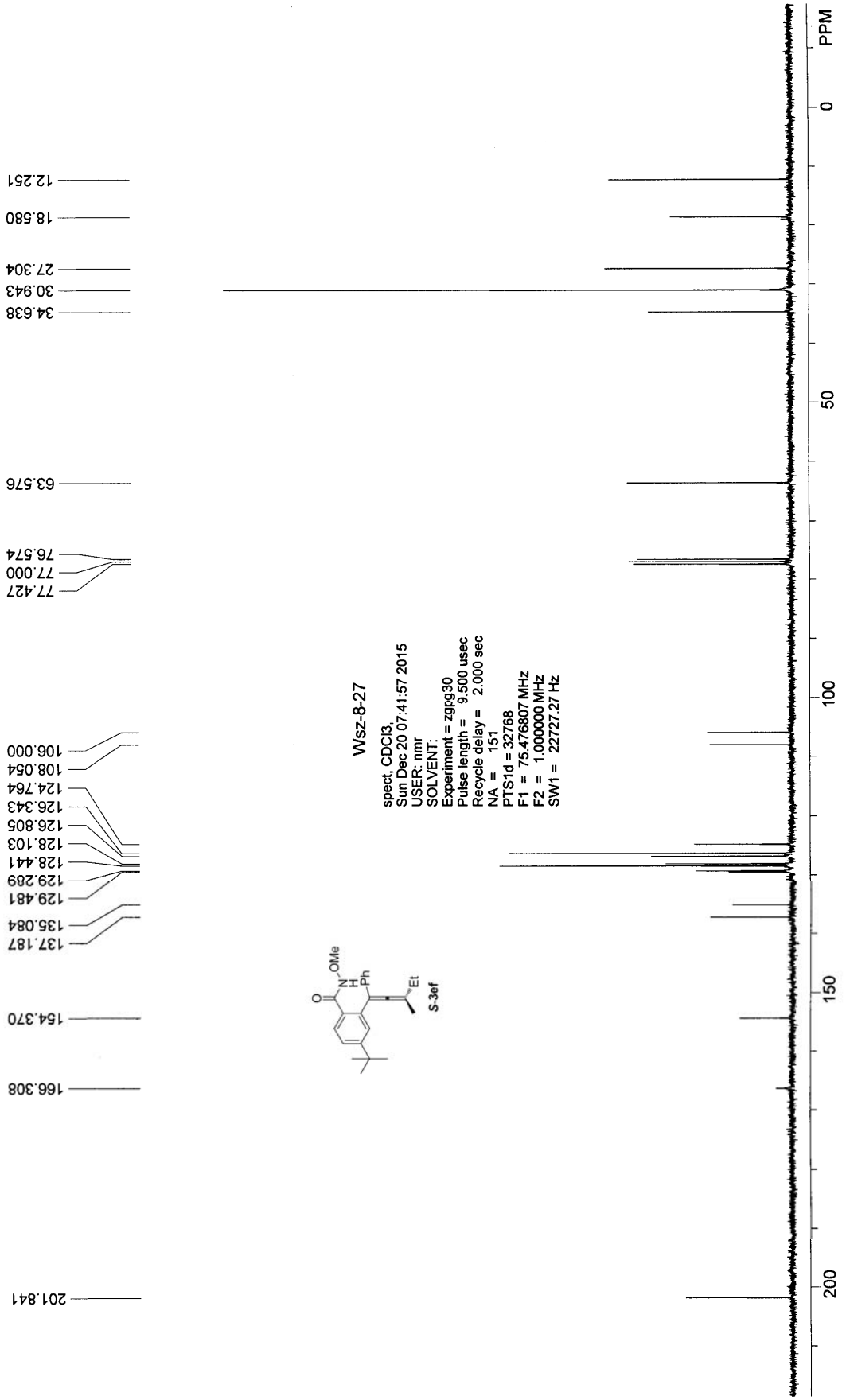
实验内容简介：
AD-H, n-hexane/i-PrOH = 10/1, 207 nm,1.0 ml/min



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		28.880	11733.245	569516.063	1.3265
2		32.365	740021.813	42365788.000	98.6735
总计			751755.058	42935304.063	100.0000


8.855
7.730
7.702
7.442
7.435
7.414
7.408
7.364
7.359
7.291
7.266
7.242
7.218
7.193
7.165
7.142
3.407
2.249
2.222
2.197
2.174
2.151
2.126
2.099
1.899
1.323
1.170
1.145
1.121
0.000
O
N
H
OMe
Ph
Et
S-3ef
Wsz-8-27
spect, CDCl3,
Sun Dec 20 07:37:38 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 17
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.95
1.03
1.04
1.04
5.30
3.00
2.13
3.02
9.32
3.25
10
8
6
4
2
0
PPM

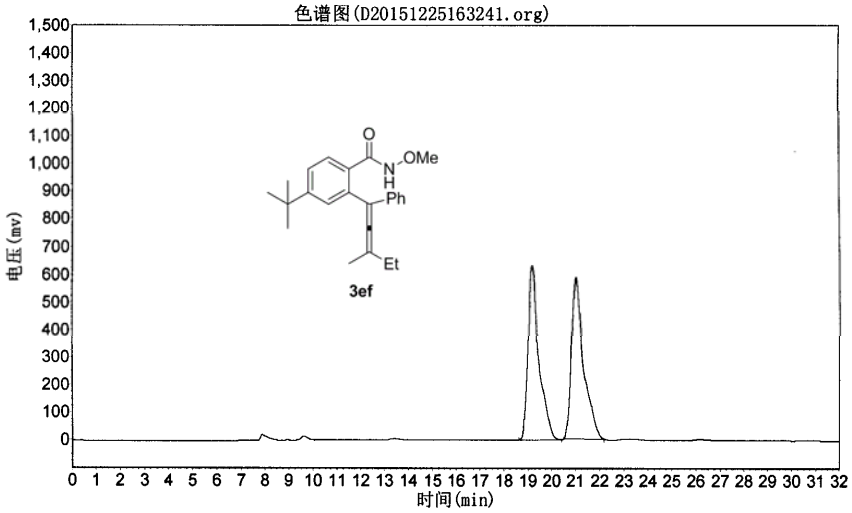

Wsz-8-27
spect, CDCl3,
Sun Dec 20 07:41:57 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 151
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
S-3ef
PPM
0
50
100
150
200
12.251
18.580
27.304
30.943
34.638
63.576
76.574
77.000
77.427
106.000
108.054
124.764
126.343
126.805
128.103
128.441
129.289
129.481
135.084
137.187
154.370
166.308
201.841

wsz-7-199

实验单位：zju
实验时间：2015-12-25,16:32:41
谱图文件:D:\浙大智达\N2000\样品\D20151225163241.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2015-12-25,20:18:51
积分方法:面积归一法

实验内容简介：
AD-H, n-hexane/i-PrOH = 10/1, 207 nm,0.8 ml/min



分析结果表

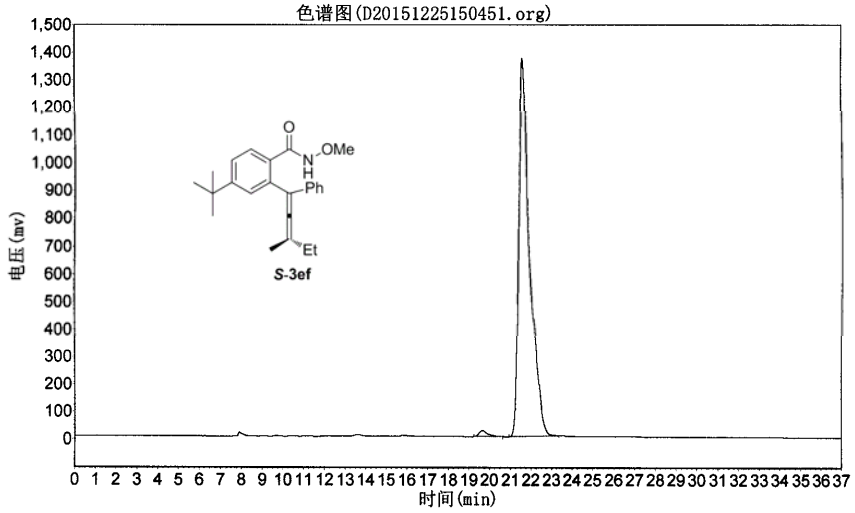
峰号	峰名	保留时间	峰高	峰面积	含量
1		19.152	633647.688	20044502.000	49.4640
2		20.985	588146.000	20478898.000	50.5360
总计			1221793.688	40523400.000	100.0000

wsz-8-27

实验单位：zju
实验时间：2015-12-25,15:04:51
谱图文件:D:\浙大智达\N2000\样品\D20151225150451.org
方法文件:D:\浙大智达\N2000\djx.mtd

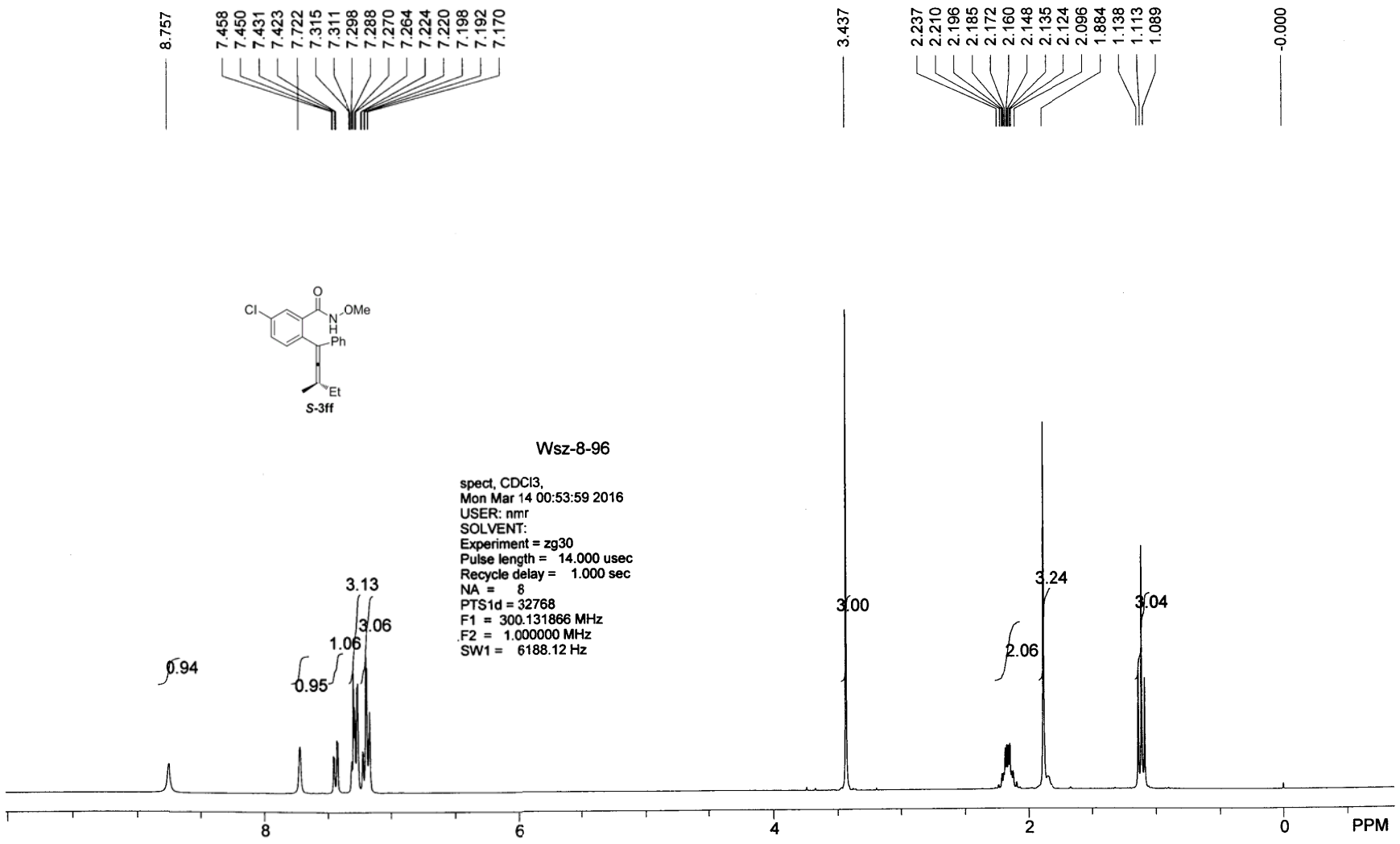
实验者：wsz
报告时间：2015-12-25,15:44:52
积分方法:面积归一法

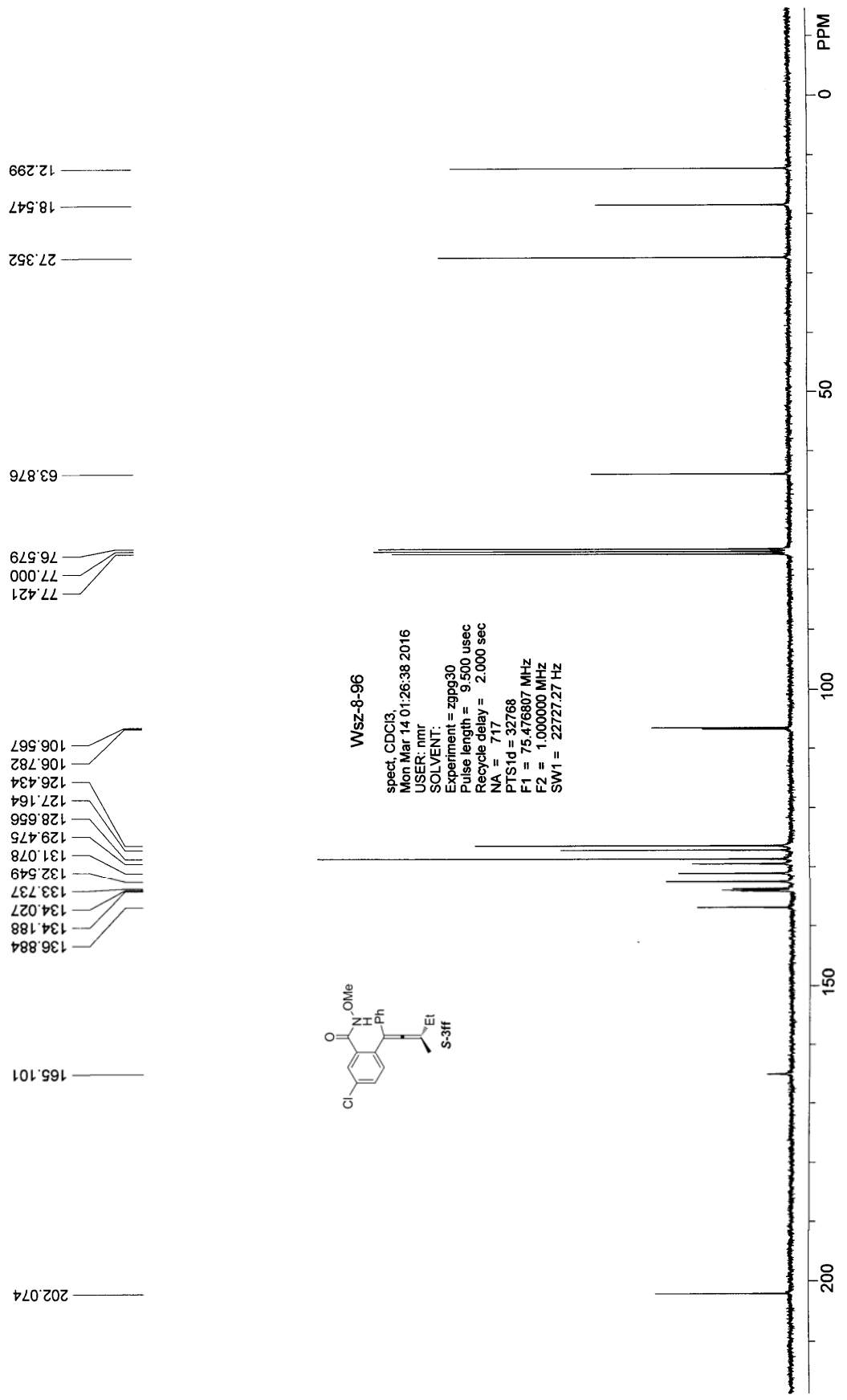
实验内容简介：
AD-H, n-hexane/i-PrOH = 10/1, 207 nm,0.8 ml/min



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		19.643	21648.209	672907.063	1.3296
2		21.573	1366786.000	49936248.000	98.6704
总计			1388434.209	50609155.063	100.0000


8.757
7.458
7.450
7.431
7.423
7.722
7.315
7.311
7.298
7.288
7.270
7.264
7.224
7.220
7.198
7.192
7.170
3.437
2.237
2.210
2.196
2.185
2.172
2.160
2.148
2.135
2.124
2.096
1.884
1.138
1.113
1.089
-0.000
Cl
O
N
H
OMe
Ph
Et
S-3ff
Wsz-8-96
spect, CDCl3,
Mon Mar 14 00:53:59 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.94
0.95
1.06
3.13
3.06
3.00
2.06
3.24
3.04
8
6
4
2
0
PPM

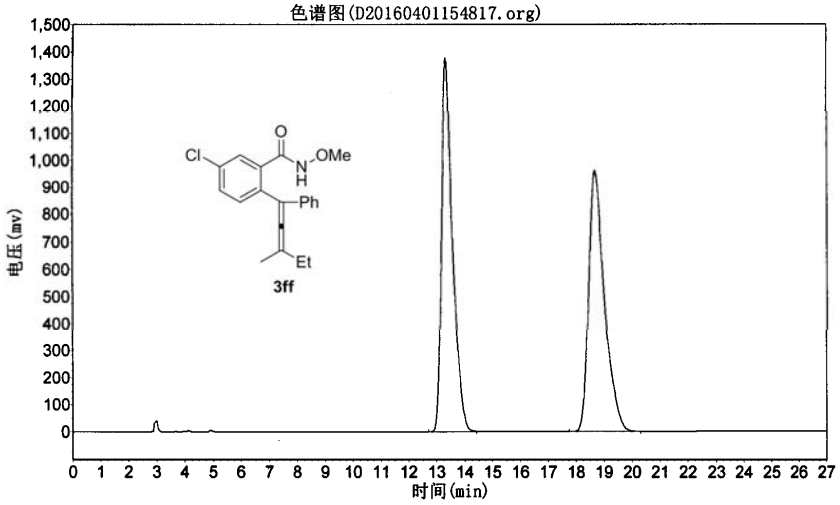

Wsz-8-96
spect, CDCl3,
Mon Mar 14 01:26:38 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 717
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
S-3ff
OMe
N
H
Ph
Et
O
Cl
PPM
0
50
100
150
200
12.299
18.547
27.352
63.876
76.579
77.000
77.421
106.567
106.782
126.434
127.164
128.656
129.475
131.078
132.549
133.737
134.027
134.188
136.884
165.101
202.074

wsz-8-6

实验单位：zju
实验时间：2016-04-01,15:48:17
谱图文件:D:\浙大智达\N2000\样品\D20160401154817.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2016-04-01,16:20:53
积分方法:面积归一法

实验内容简介：
AD-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

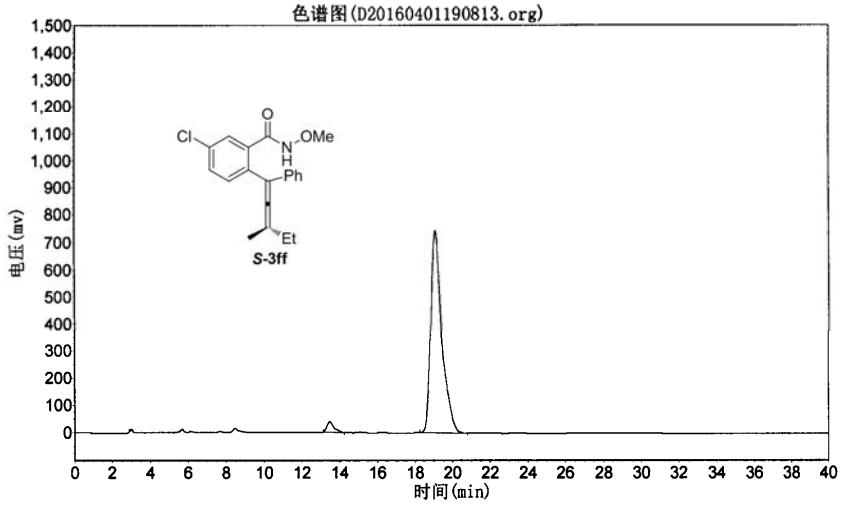
峰号	峰名	保留时间	峰高	峰面积	含量
1		13.323	1376926.625	37447000.000	49.9036
2		18.655	960959.063	37591636.000	50.0964
总计			2337885.688	75038636.000	100.0000

wsz-8-96

实验单位：zju
实验时间：2016-04-01,19:08:13
谱图文件:D:\浙大智达\N2000\样品\D20160401190813.org
方法文件:D:\浙大智达\N2000\djx.mtd

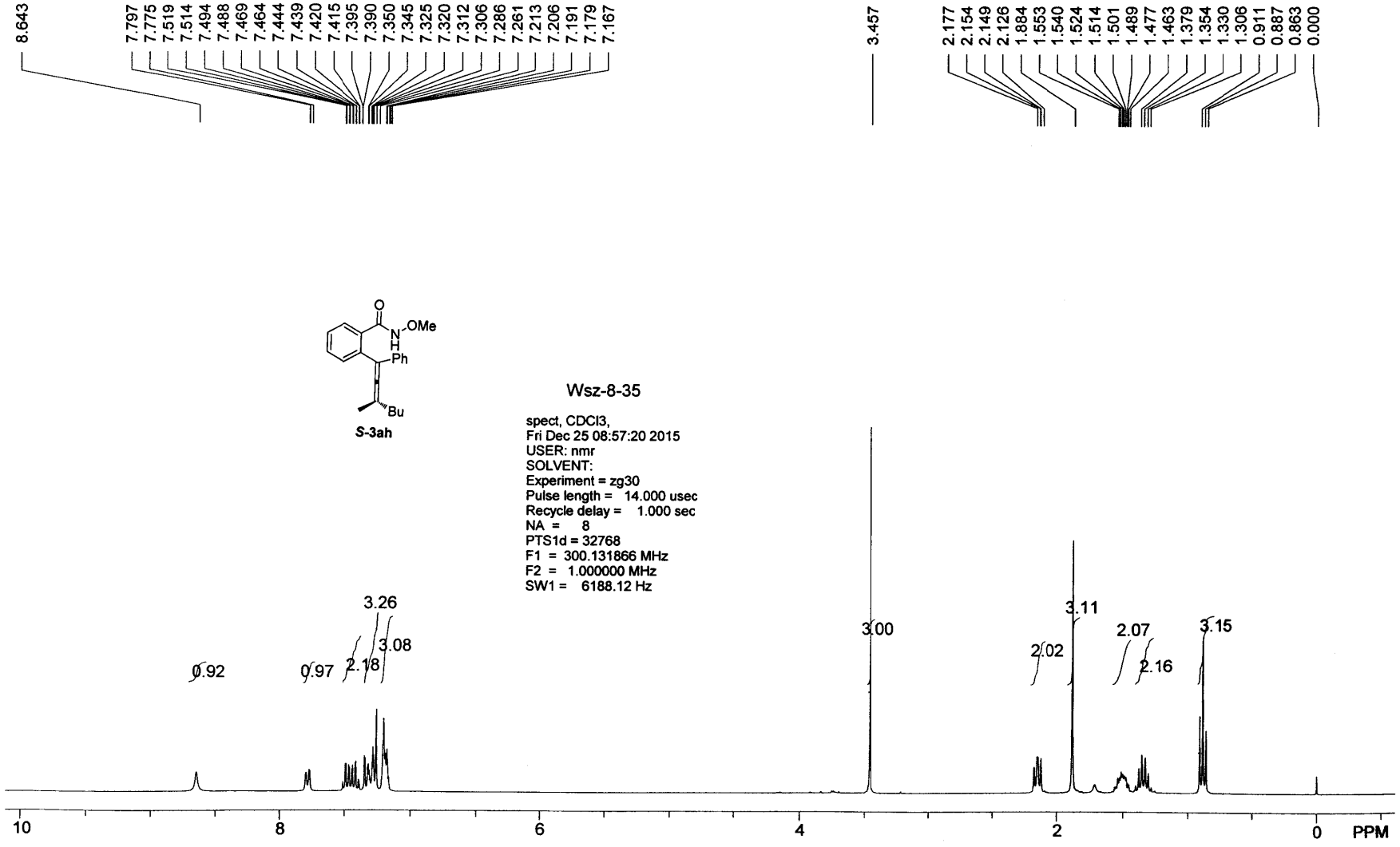
实验者：wsz
报告时间：2016-04-01,19:52:02
积分方法:面积归一法

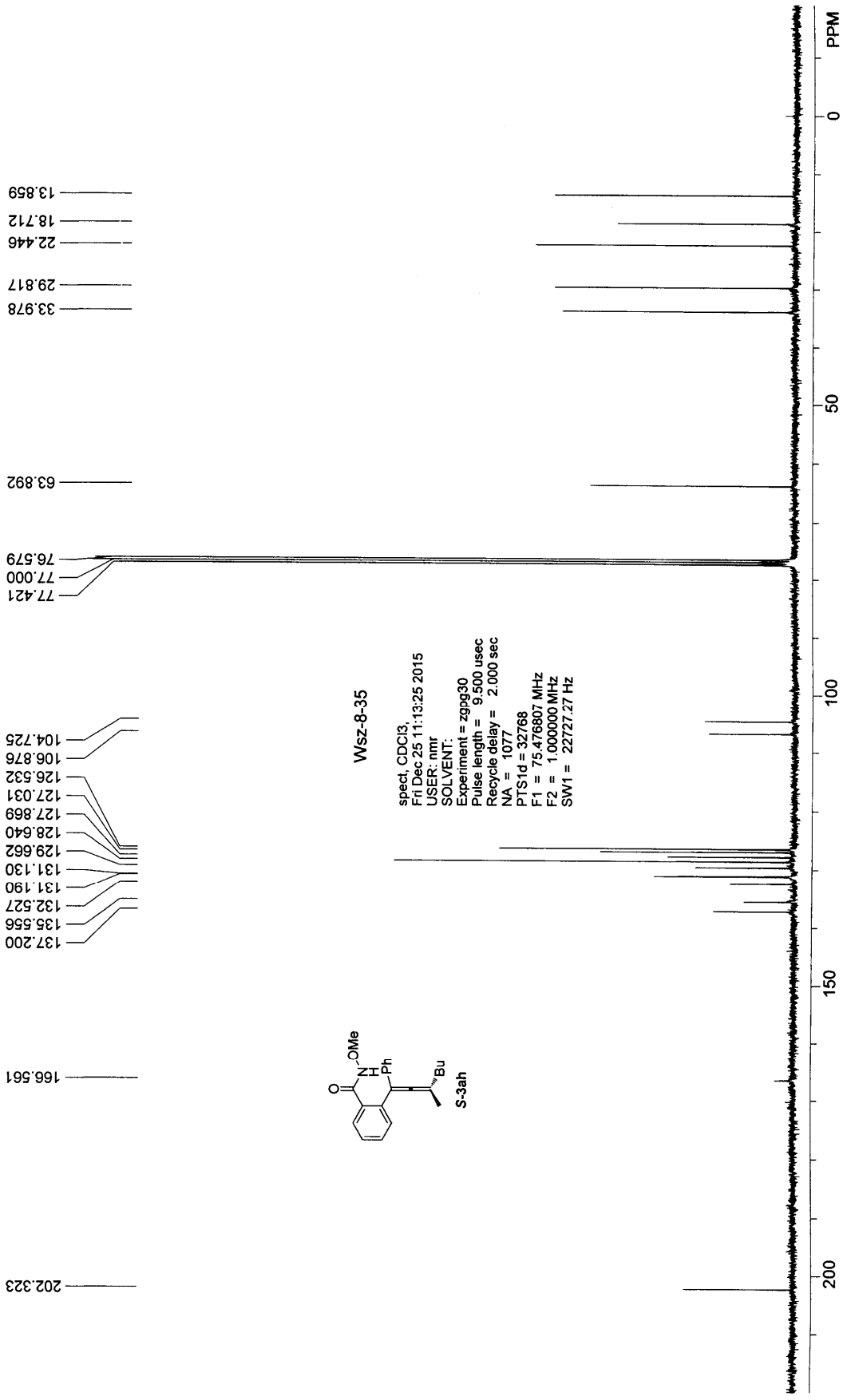
实验内容简介：
AD-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		13.458	37738.883	972598.188	3.1147
2		19.063	744657.375	30253720.000	96.8853
总计			782396.258	31226318.188	100.0000


8.643
7.797
7.775
7.519
7.514
7.494
7.488
7.469
7.464
7.444
7.439
7.420
7.415
7.395
7.390
7.350
7.345
7.325
7.320
7.312
7.306
7.286
7.261
7.213
7.206
7.191
7.179
7.167
3.457
2.177
2.154
2.149
2.126
1.884
1.553
1.540
1.524
1.514
1.501
1.489
1.477
1.463
1.379
1.354
1.330
1.306
0.911
0.887
0.863
0.000
O
N
OMe
H
Ph
Bu
S-3ah
Wsz-8-35
spect, CDCl3,
Fri Dec 25 08:57:20 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.92
0.97
2.18
3.26
3.08
3.00
2.02
3.11
2.07
2.16
3.15
10
8
6
4
2
0
PPM

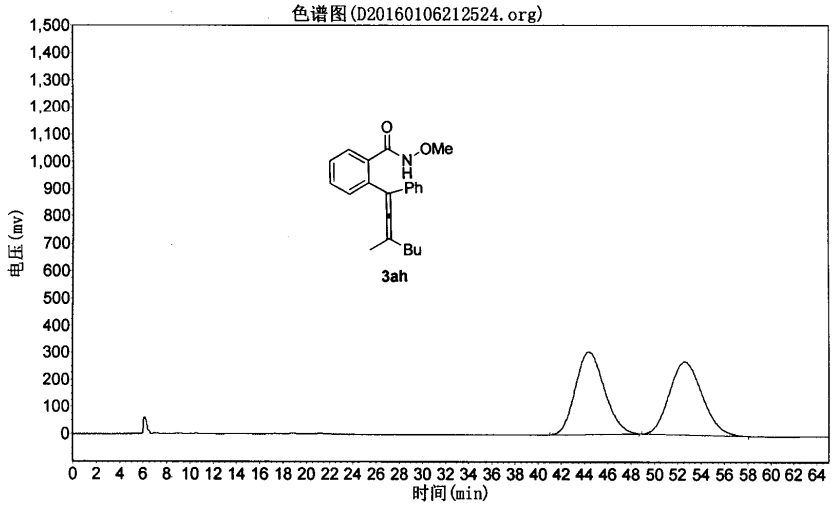

Wsz-8-35
spect, CDCl3,
Fri Dec 25 11:13:25 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1077
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
13.859
18.712
22.446
29.817
33.978
63.892
76.579
77.000
77.421
104.725
106.876
126.532
127.031
127.869
128.640
129.662
131.130
131.190
132.527
135.556
137.200
166.561
202.323
OMe
N
H
Ph
Bu
O
S-3ah
PPM
0
50
100
150
200

wsz-7-115

实验单位：zju
实验时间：2016-01-06,21:25:24
谱图文件:D:\浙大智达\N2000\样品\D20160106212524.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2016-01-06,22:33:16
积分方法:面积归一法

实验内容简介：
AS-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

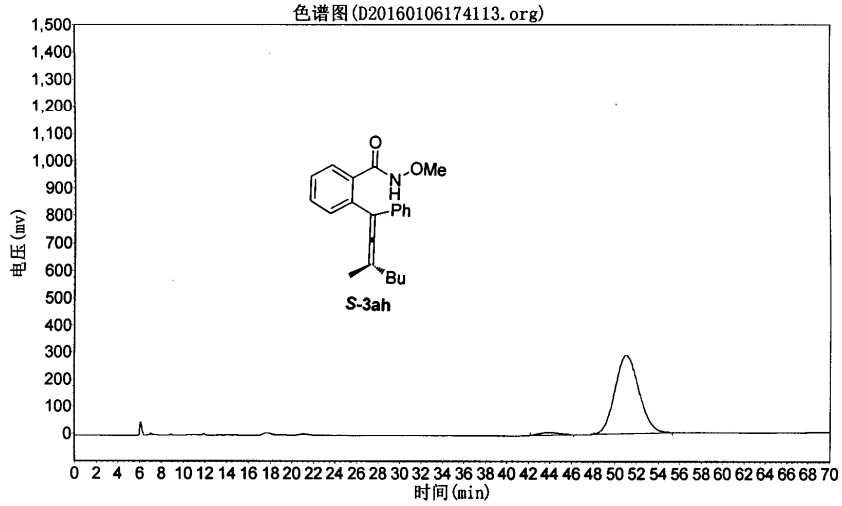
峰号	峰名	保留时间	峰高	峰面积	含量
1		44.358	302893.813	52123456.000	49.9982
2		52.585	267209.656	52127296.000	50.0018
总计			570103.469	104250752.000	100.0000

wsz-8-35

实验单位：zju
实验时间：2016-01-06,17:41:13
谱图文件:D:\浙大智达\N2000\样品\D20160106174113.org
方法文件:D:\浙大智达\N2000\djx.mtd

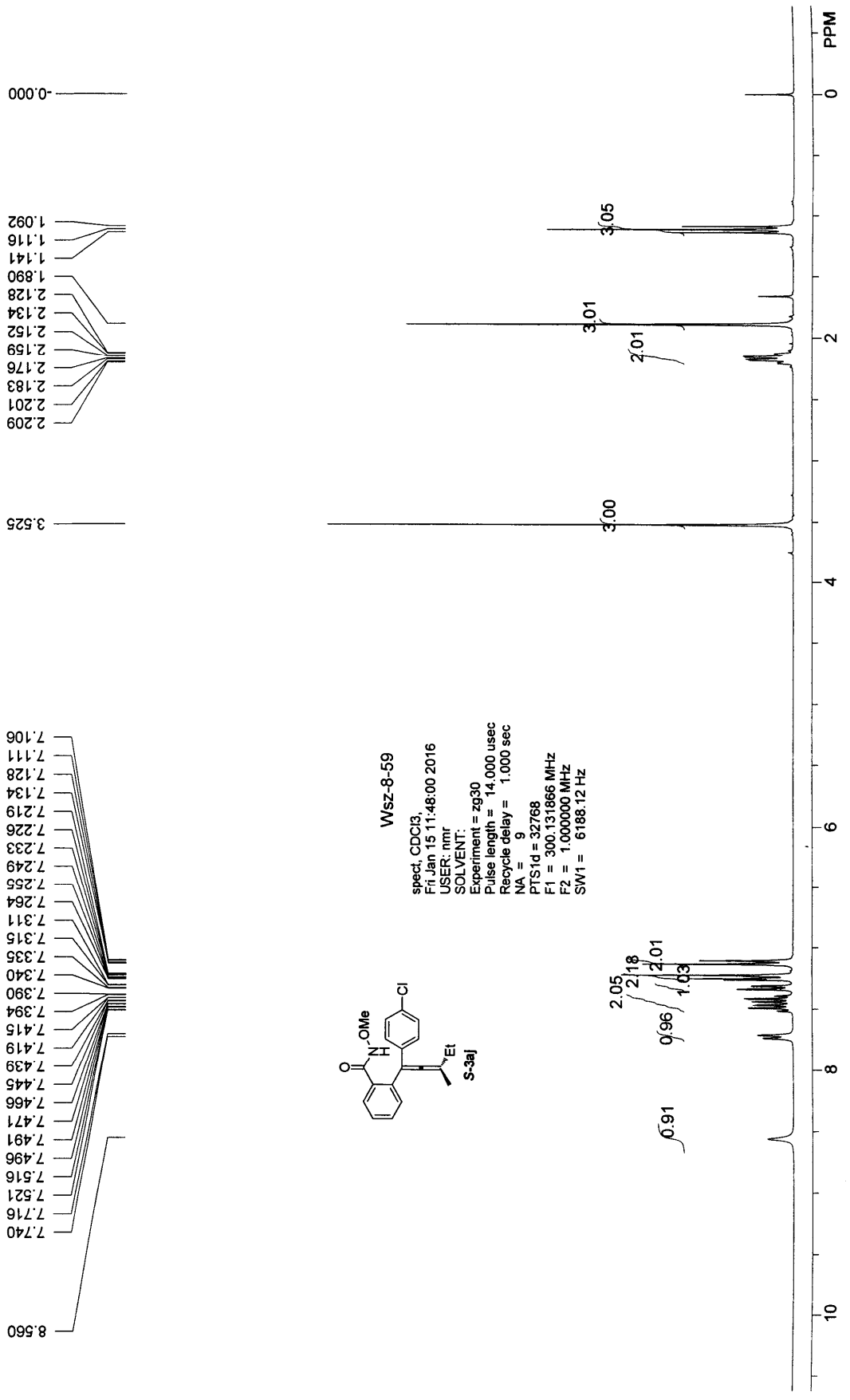
实验者：wsz
报告时间：2016-01-06,18:58:15
积分方法:面积归一法

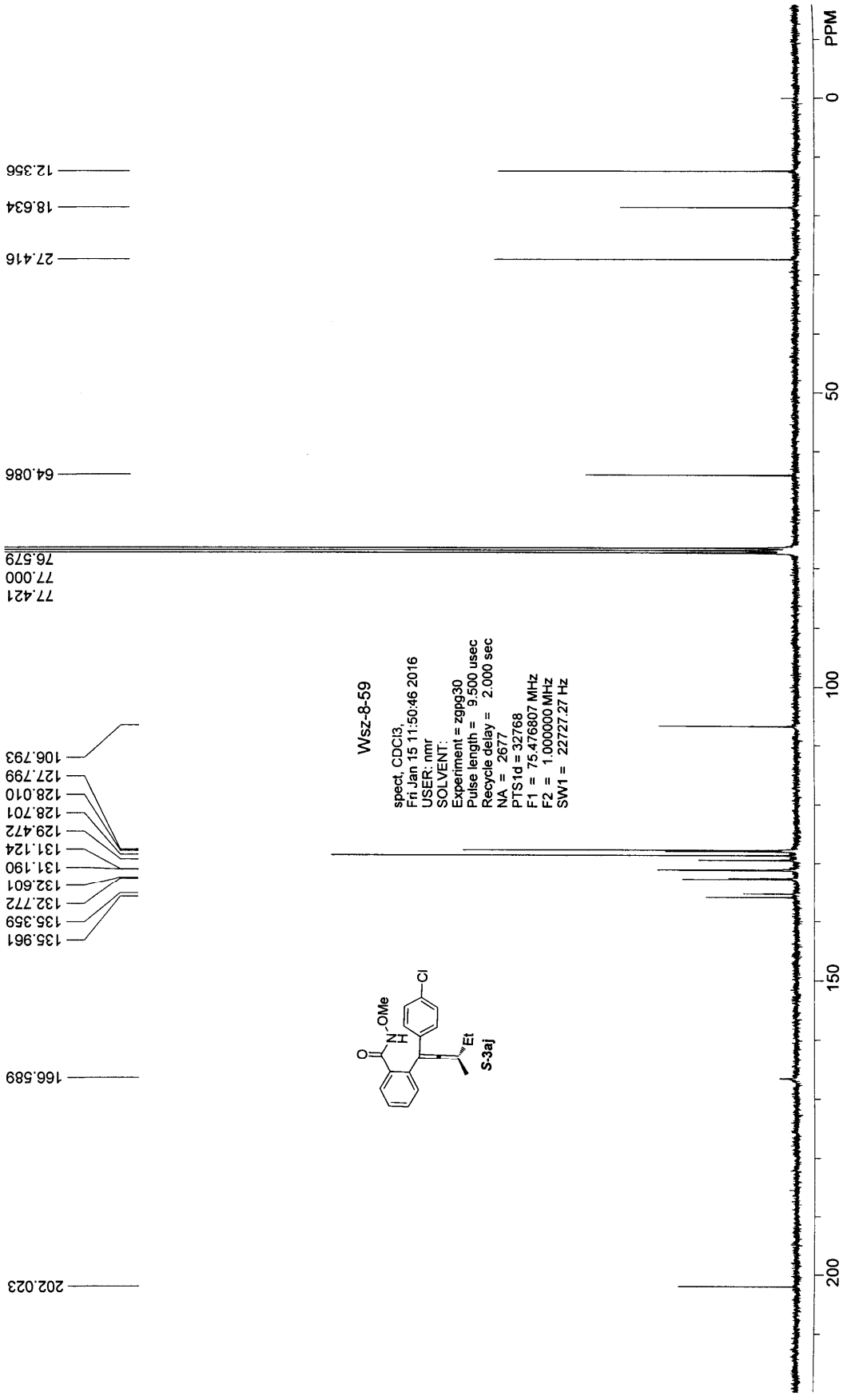
实验内容简介：
AS-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		43.928	8926.055	1119581.250	2.4769
2		51.062	285535.375	44081196.000	97.5231
总计			294461.430	45200777.250	100.0000


Wsz-8-59
spect, CDCl3,
Fri Jan 15 11:48:00 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
OMe
N
H
O
Cl
Et
S-3aj
PPM
0
2
4
6
8
10
3.00
3.01
2.01
3.05
2.05
2.18
2.01
1.03
0.96
0.91
-0.000
1.092
1.116
1.141
1.890
2.128
2.134
2.152
2.159
2.176
2.183
2.201
2.209
3.525
7.106
7.111
7.128
7.134
7.219
7.226
7.233
7.249
7.255
7.264
7.311
7.315
7.335
7.340
7.390
7.394
7.415
7.419
7.439
7.445
7.466
7.471
7.491
7.496
7.516
7.521
7.716
7.740
8.560

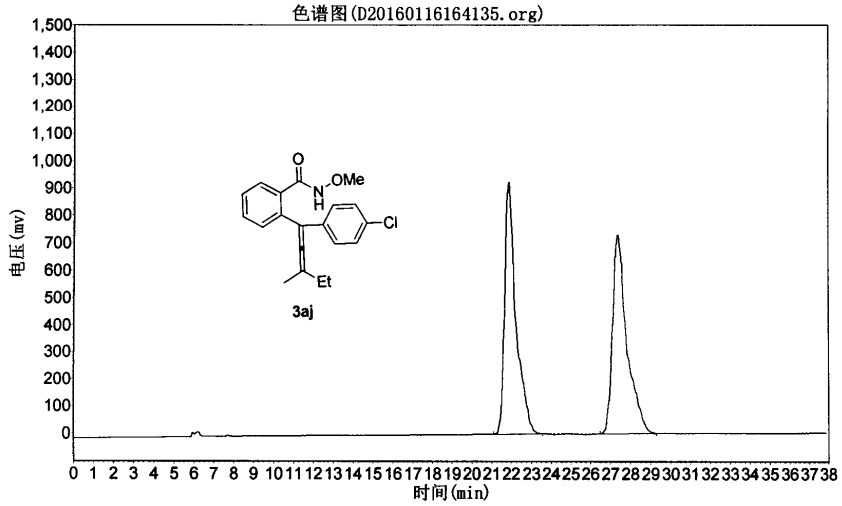

Wsz-8-59
spect, CDCl3,
Fri Jan 15 11:50:46 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 2677
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
S-3aj
PPM
0
50
100
150
200
12.356
18.634
27.416
64.086
76.579
77.000
77.421
106.793
127.799
128.010
128.701
129.472
131.124
131.190
132.601
132.772
135.359
135.961
166.589
202.023

wsz-7-184

实验单位：zju
实验时间：2016-01-16,16:41:35
谱图文件:D:\浙大智达\N2000\样品\D20160116164135.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2016-01-16,17:22:00
积分方法:面积归一法

实验内容简介：
AD-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

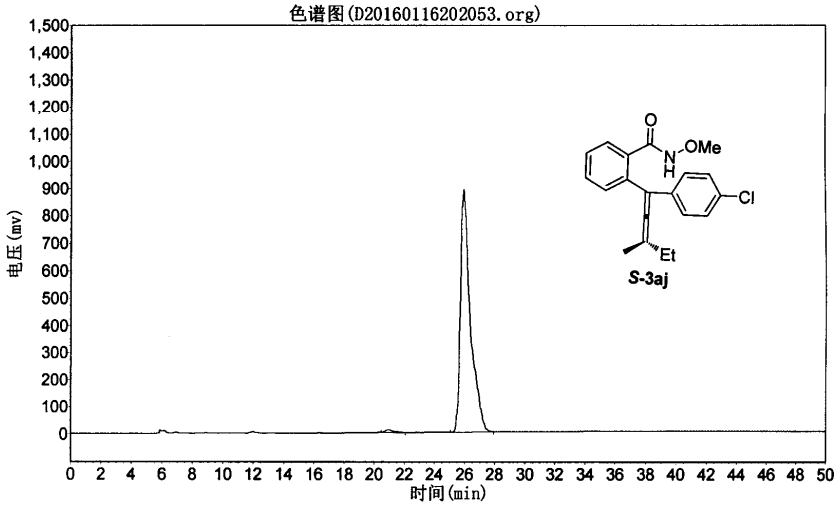
峰号	峰名	保留时间	峰高	峰面积	含量
1		21.870	921752.438	36254628.000	49.9583
2		27.345	727245.750	36315220.000	50.0417
总计			1648998.188	72569848.000	100.0000

wsz-8-59

实验单位：zju
实验时间：2016-01-16,20:20:53
谱图文件:D:\浙大智达\N2000\样品\D20160116202053.org
方法文件:D:\浙大智达\N2000\djx.mtd

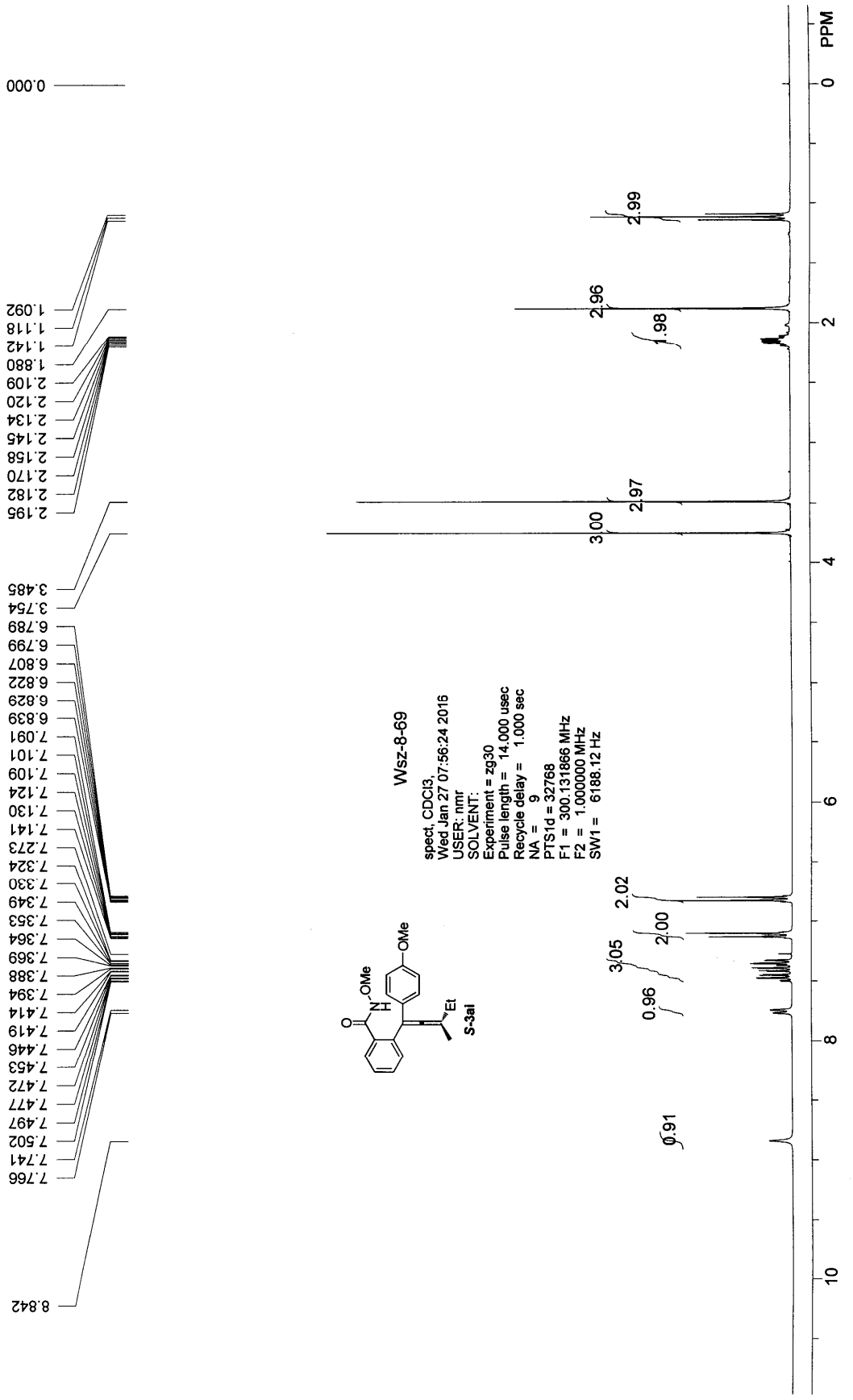
实验者：wsz
报告时间：2016-01-16,21:14:57
积分方法:面积归一法

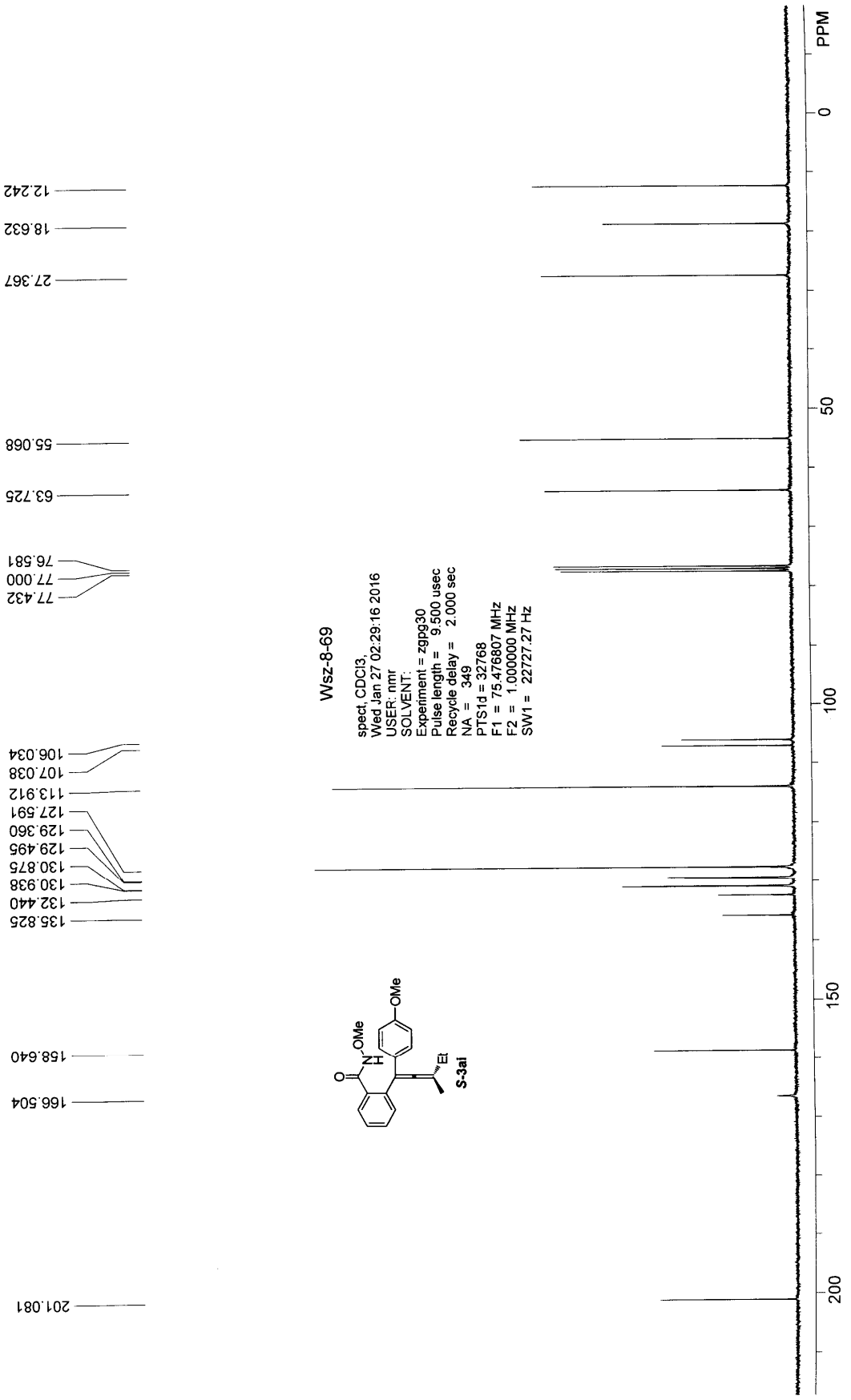
实验内容简介：
AD-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		20.938	10720.200	374647.719	0.9097
2		26.005	889514.625	40811192.000	99.0903
总计			900234.825	41185839.719	100.0000


Wsz-8-69
spect, CDCl3,
Wed Jan 27 07:56:24 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
OMe
OMe
Et
S-3al
PPM
0
2
4
6
8
10
2.99
2.96
1.98
2.97
3.00
2.02
2.00
3.05
0.96
0.91
0.000
1.092
1.118
1.142
1.880
2.109
2.120
2.134
2.145
2.158
2.170
2.182
2.195
3.485
3.754
6.789
6.799
6.807
6.822
6.829
6.839
7.091
7.101
7.109
7.124
7.130
7.141
7.273
7.324
7.330
7.349
7.353
7.364
7.369
7.388
7.394
7.414
7.419
7.446
7.453
7.472
7.477
7.497
7.502
7.741
7.766
8.842

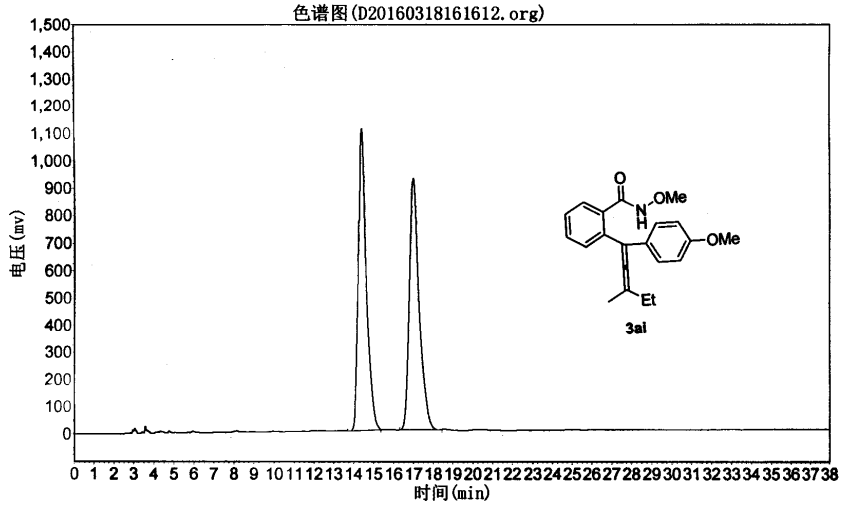

Wsz-8-69
spect.CDCl3.
Wed Jan 27 02:29:16 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 349
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
N
H
OMe
Et
S-3ai
PPM
0
50
100
150
200
12.242
18.632
27.367
55.068
63.725
76.581
77.000
77.432
106.034
107.038
113.912
127.591
129.360
129.495
130.875
130.938
132.440
135.825
158.640
166.504
201.081

Wsz-8-21

实验单位：zju
实验时间：2016-03-18,16:16:12
谱图文件:D:\浙大智达\N2000\样品\D20160318161612.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2016-03-18,16:58:07
积分方法:面积归一法

实验内容简介：
AD-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

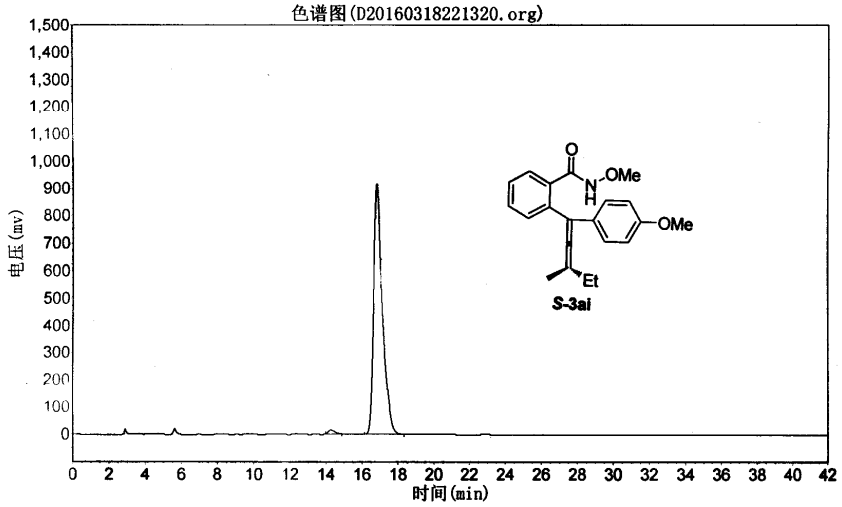
峰号	峰名	保留时间	峰高	峰面积	含量
1		14.390	1103135.750	31112882.000	49.8855
2		16.998	920120.750	31255670.000	50.1145
总计			2023256.500	62368552.000	100.0000

Wsz-8-69

实验单位：zju
实验时间：2016-03-18,22:13:20
谱图文件:D:\浙大智达\N2000\样品\D20160318221320.org
方法文件:D:\浙大智达\N2000\djx.mtd

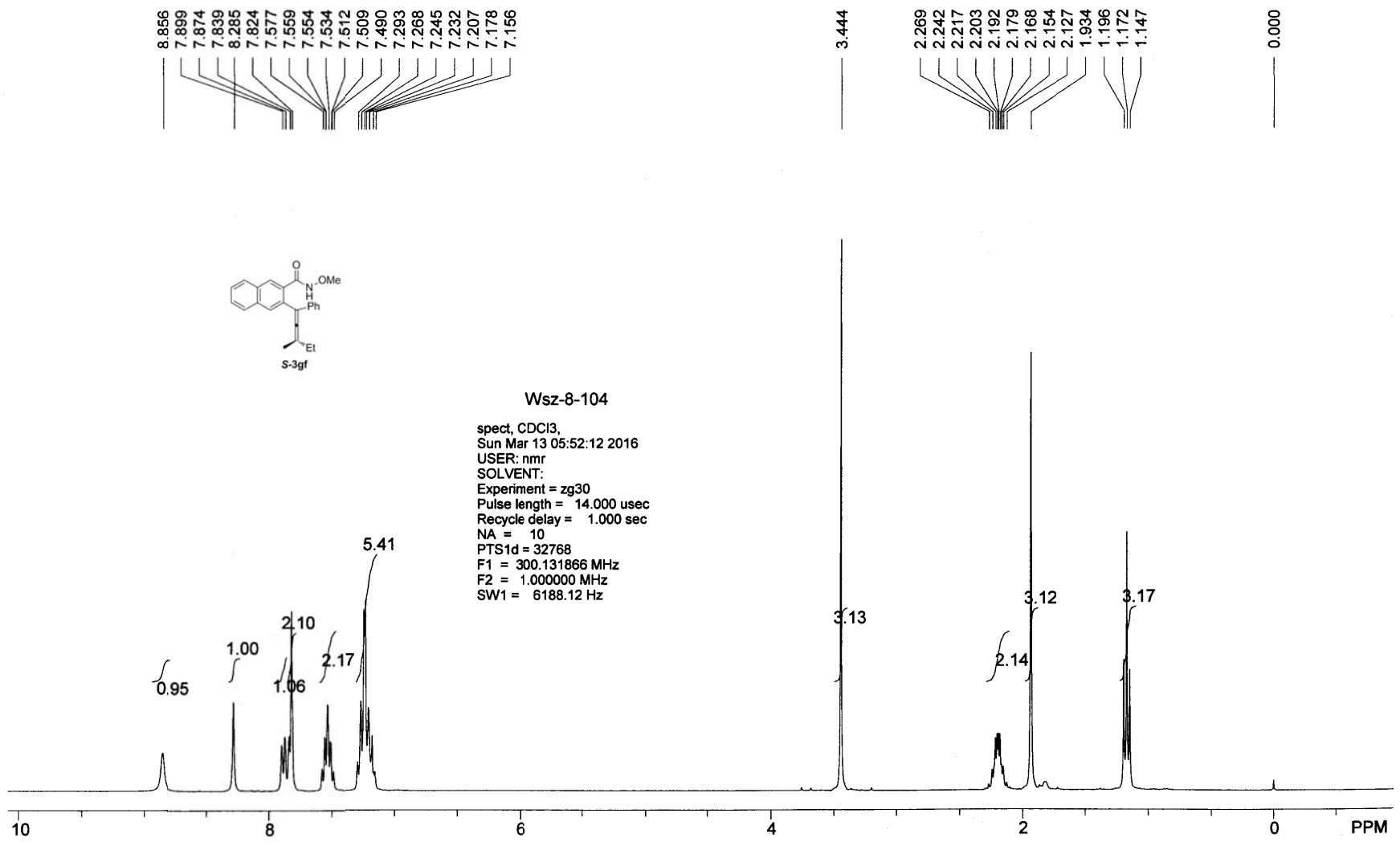
实验者：wsz
报告时间：2016-03-18,23:04:17
积分方法:面积归一法

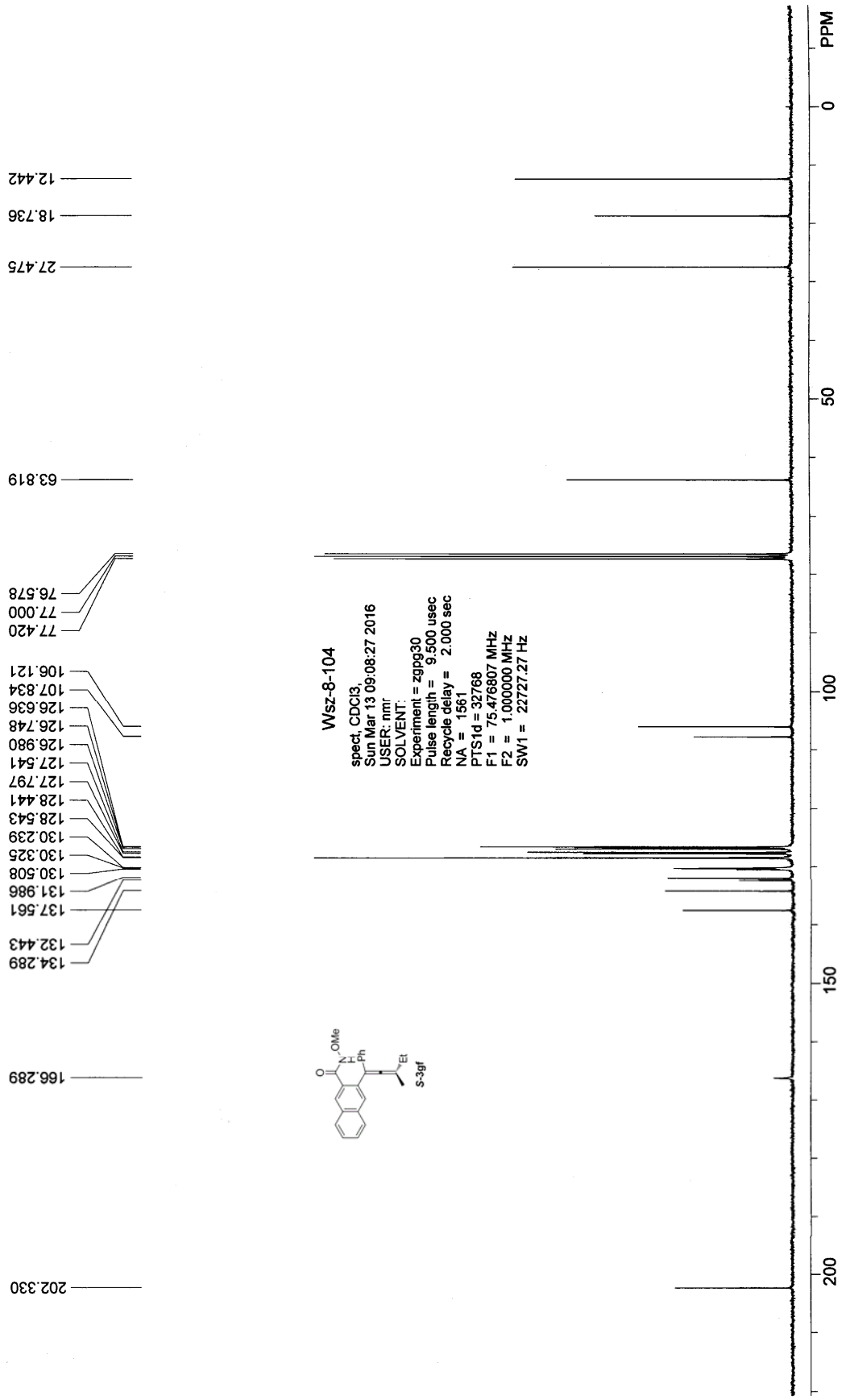
实验内容简介：
AD-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		14.268	15592.575	379630.094	1.2064
2		16.853	916951.625	31088348.000	98.7936
总计			932544.200	31467978.094	100.0000


8.856
7.899
7.874
7.839
8.285
7.824
7.577
7.559
7.554
7.534
7.512
7.509
7.490
7.293
7.268
7.245
7.232
7.207
7.178
7.156
3.444
2.269
2.242
2.217
2.203
2.192
2.179
2.168
2.154
2.127
1.934
1.196
1.172
1.147
0.000
OMe
N
H
Ph
Et
S-3gf
Wsz-8-104
spect, CDCl3,
Sun Mar 13 05:52:12 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 10
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.95
1.00
1.06
2.10
2.17
5.41
3.13
2.14
3.12
3.17
10
8
6
4
2
0
PPM

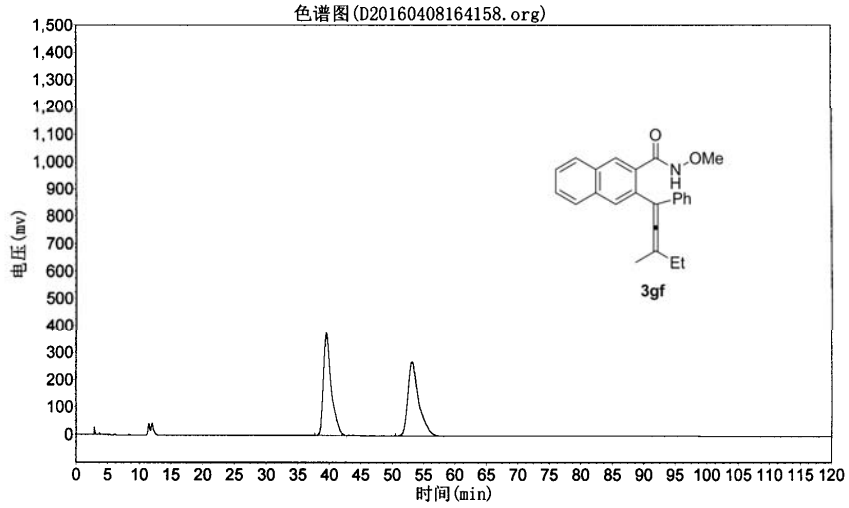

Wsz-8-104
spect, CDCl3,
Sun Mar 13 09:08:27 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1561
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
PPM
0
50
100
150
200
12.442
18.736
27.475
63.819
76.578
77.000
77.420
106.121
107.834
126.636
126.748
126.980
127.541
127.797
128.441
128.543
130.239
130.325
130.508
131.986
137.561
132.443
134.289
166.289
202.330
OMe
Ph
Et
S-3gf

wsz-8-40

实验单位：zju
实验时间：2016-04-08,16:41:58
谱图文件:D:\浙大智达\N2000\样品\D20160408164158.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2016-04-08,19:02:43
积分方法:面积归一法

实验内容简介：
AD-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		39.557	373760.094	31951060.000	49.9936
2		53.198	268537.656	31959218.000	50.0064
总计			642297.750	63910278.000	100.0000

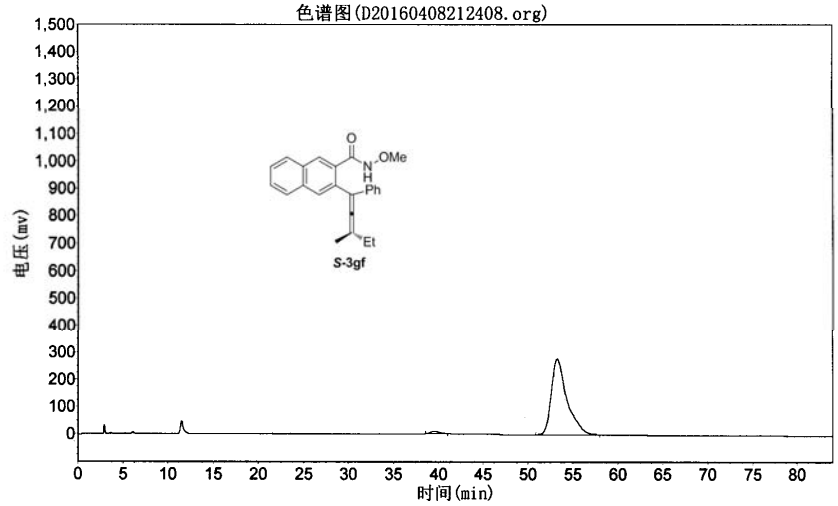
wsz-8-104

实验单位：zju
实验时间：2016-04-08,21:24:08
谱图文件:D:\浙大智达\N2000\样品\D20160408212408.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2016-04-08,22:54:24
积分方法:面积归一法

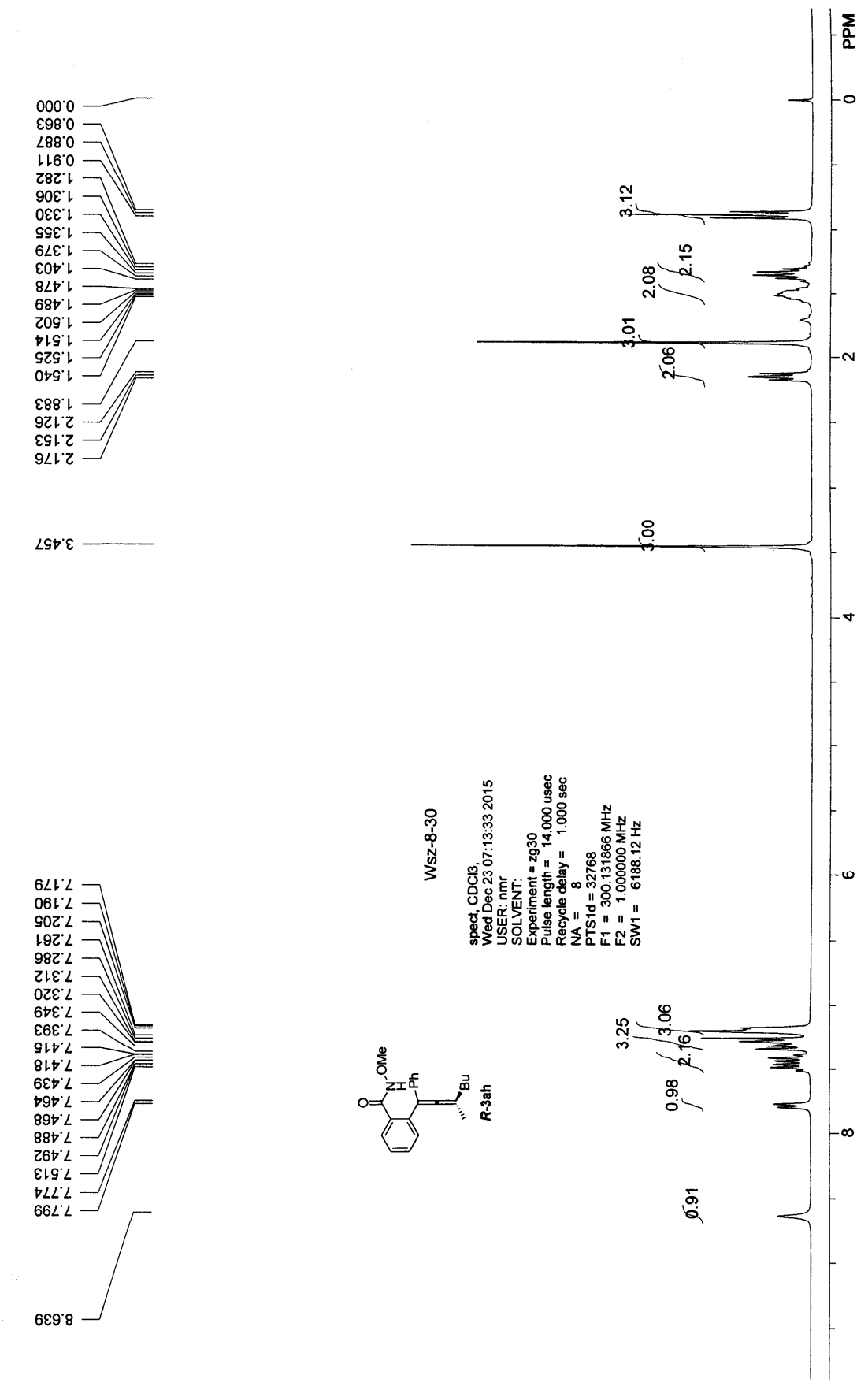
实验内容简介：
AD-H, n-hexane/i-PrOH = 10/1, 207 nm,1.0 ml/min

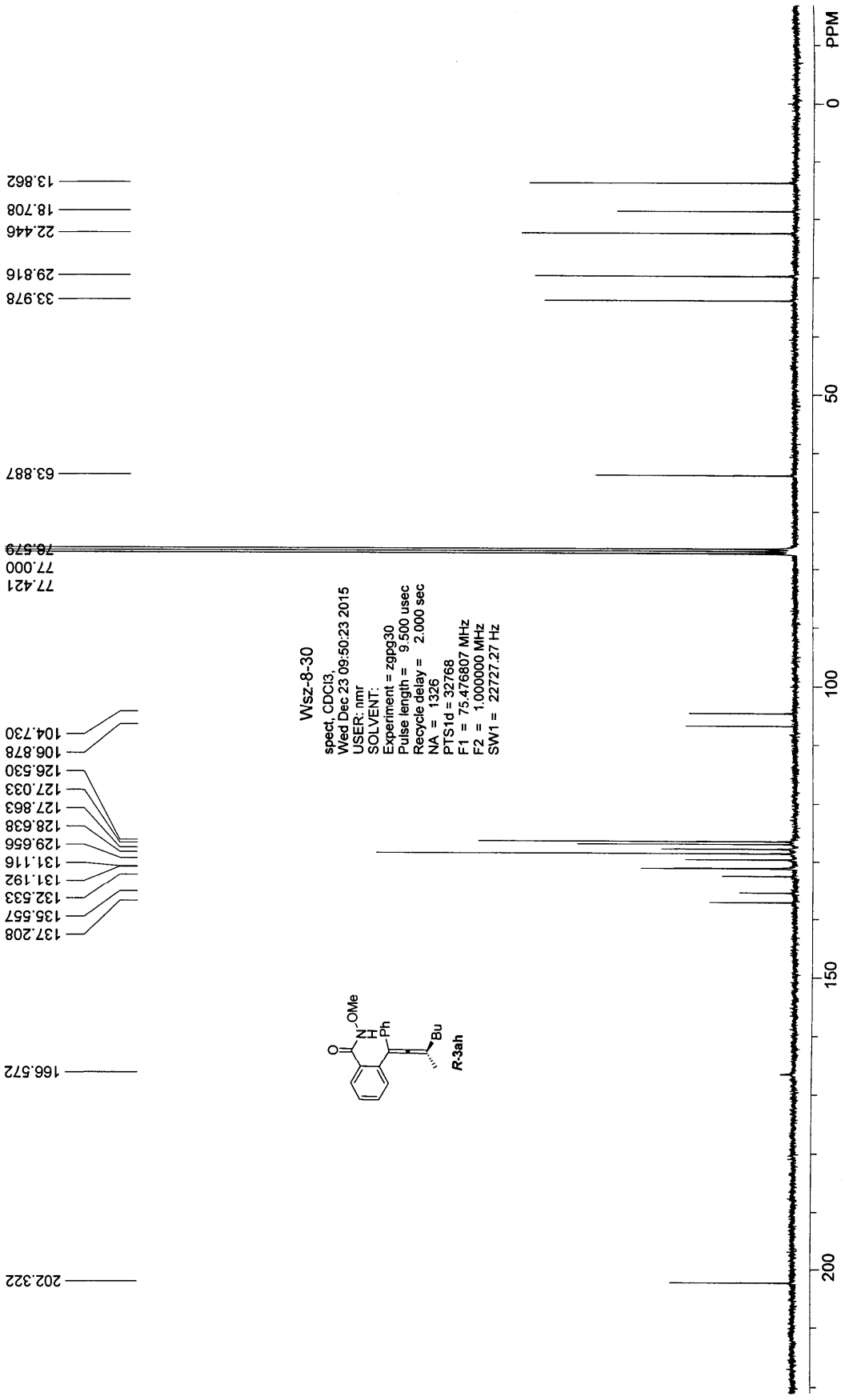
色谱图(D20160408212408.org)



分析结果表

峰号	峰名	保留时间	峰高	峰面积	含量
1		39.578	8782.203	584341.000	1.7299
2		53.270	276050.250	33194750.000	98.2701
总计			284832.453	33779091.000	100.0000


Wsz-8-30
spect, CDCl3,
Wed Dec 23 07:13:33 2015
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
R-3ah
PPM
0
2
4
6
8
3.12
2.15
2.08
3.01
2.06
3.00
3.25
3.06
2.16
0.98
0.91
8.639
7.799
7.774
7.513
7.492
7.488
7.468
7.464
7.439
7.418
7.415
7.393
7.349
7.320
7.312
7.286
7.261
7.205
7.190
7.179
3.457
2.176
2.153
2.126
1.883
1.540
1.525
1.514
1.502
1.489
1.478
1.403
1.379
1.355
1.330
1.306
1.282
0.911
0.887
0.863
0.000

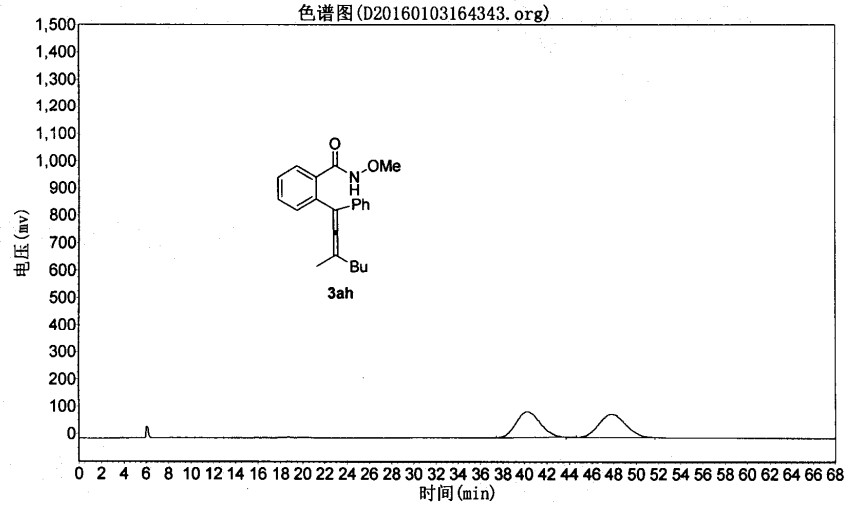

Wsz-8-30
spect, CDCl3,
Wed Dec 23 09:50:23 2015
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 1326
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
R-3ah
PPM
0
50
100
150
200
13.862
18.708
22.446
29.816
33.978
63.887
77.421
77.000
76.579
104.730
106.878
126.530
127.033
127.863
128.638
129.656
131.116
131.192
132.533
135.557
137.208
166.572
202.322

wsz-7-115

实验单位：zju
实验时间：2016-01-03,16:43:43
谱图文件:D:\浙大智达\N2000\样品\D20160103164343.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2016-01-03,17:57:55
积分方法:面积归一法

实验内容简介：
AS-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

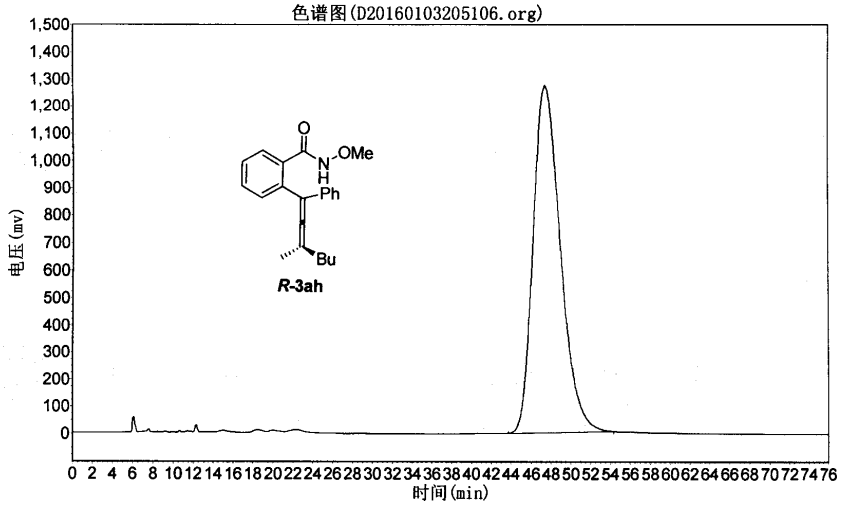
峰号	峰名	保留时间	峰高	峰面积	含量
1		40.257	94416.000	14155514.000	49.7555
2		47.875	84207.688	14294630.000	50.2445
总计			178623.688	28450144.000	100.0000

wsz-8-30

实验单位：zju
实验时间：2016-01-03,20:51:06
谱图文件:D:\浙大智达\N2000\样品\D20160103205106.org
方法文件:D:\浙大智达\N2000\djx.mtd

实验者：wsz
报告时间：2016-01-03,22:10:49
积分方法:面积归一法

实验内容简介：
AS-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min



分析结果表

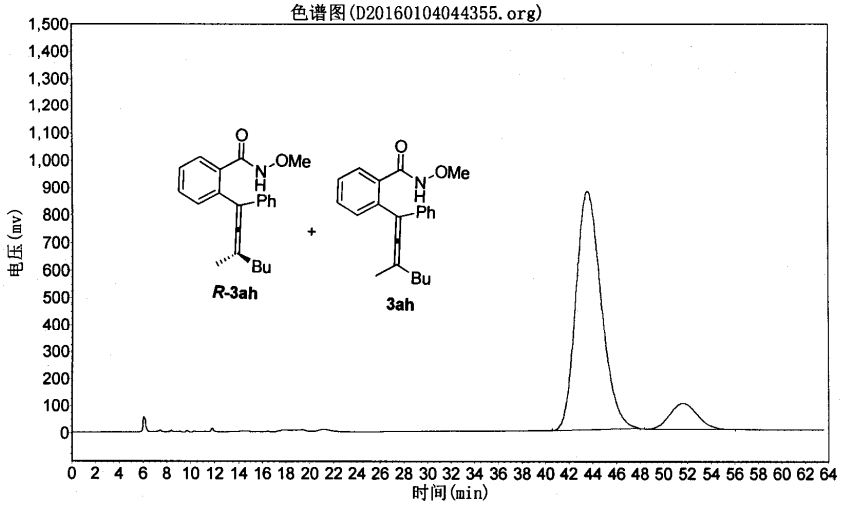
峰号	峰名	保留时间	峰高	峰面积	含量
1		47.442	1271058.250	242387136.000	100.0000
总计			1271058.250	242387136.000	100.0000

wsz-8-30 + wsz-7-115

实验单位：zju
实验时间：2016-01-04,4:43:55
谱图文件:D:\浙大智达\N2000\样品\D20160104044355.org
方法文件:D:\浙大智达\N2000\djx.mtd

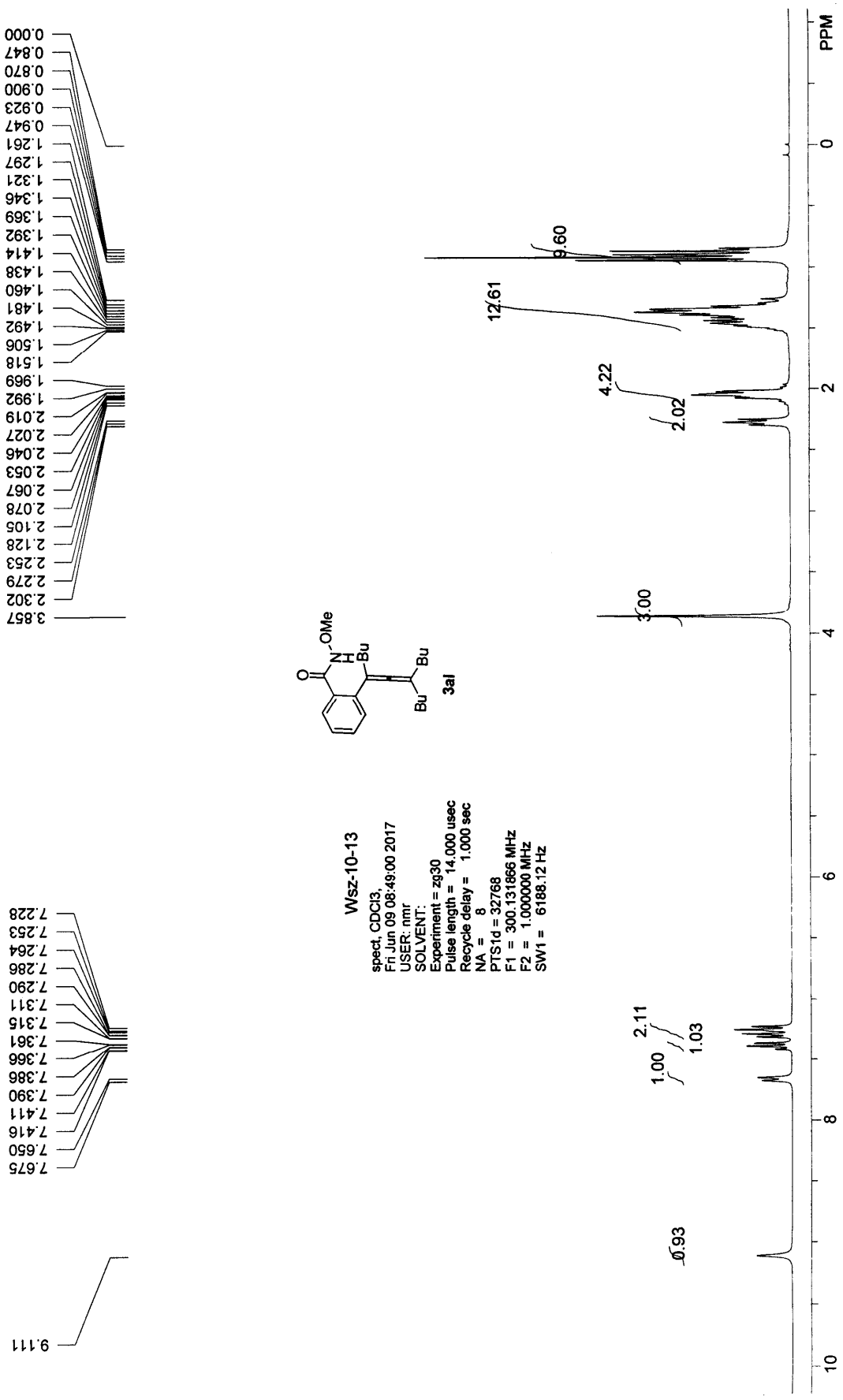
实验者：wsz
报告时间：2016-01-04,5:50:19
积分方法:面积归一法

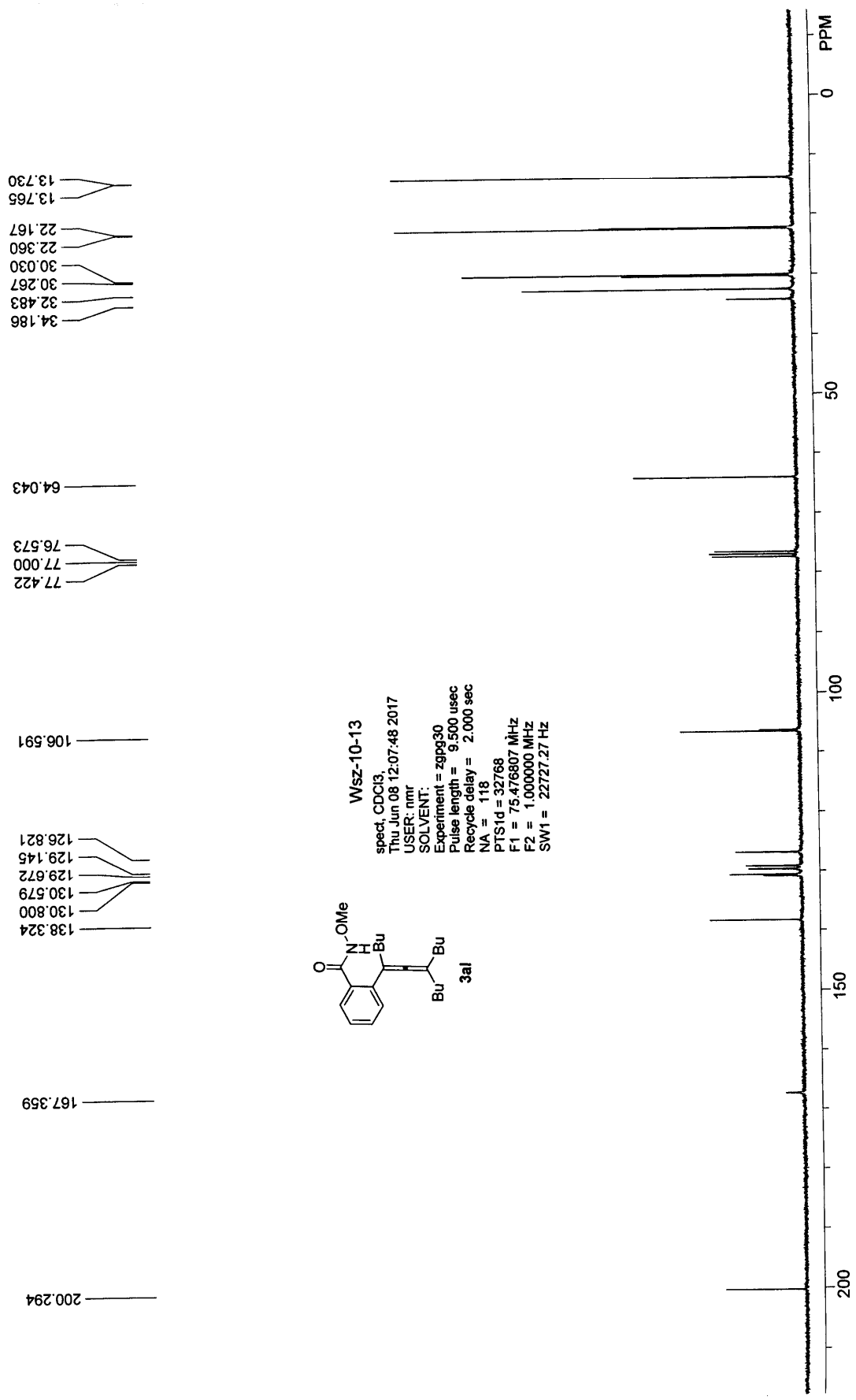
实验内容简介：
AS-H, n-hexane/i-PrOH =10/1, 207 nm,1.0 ml/min

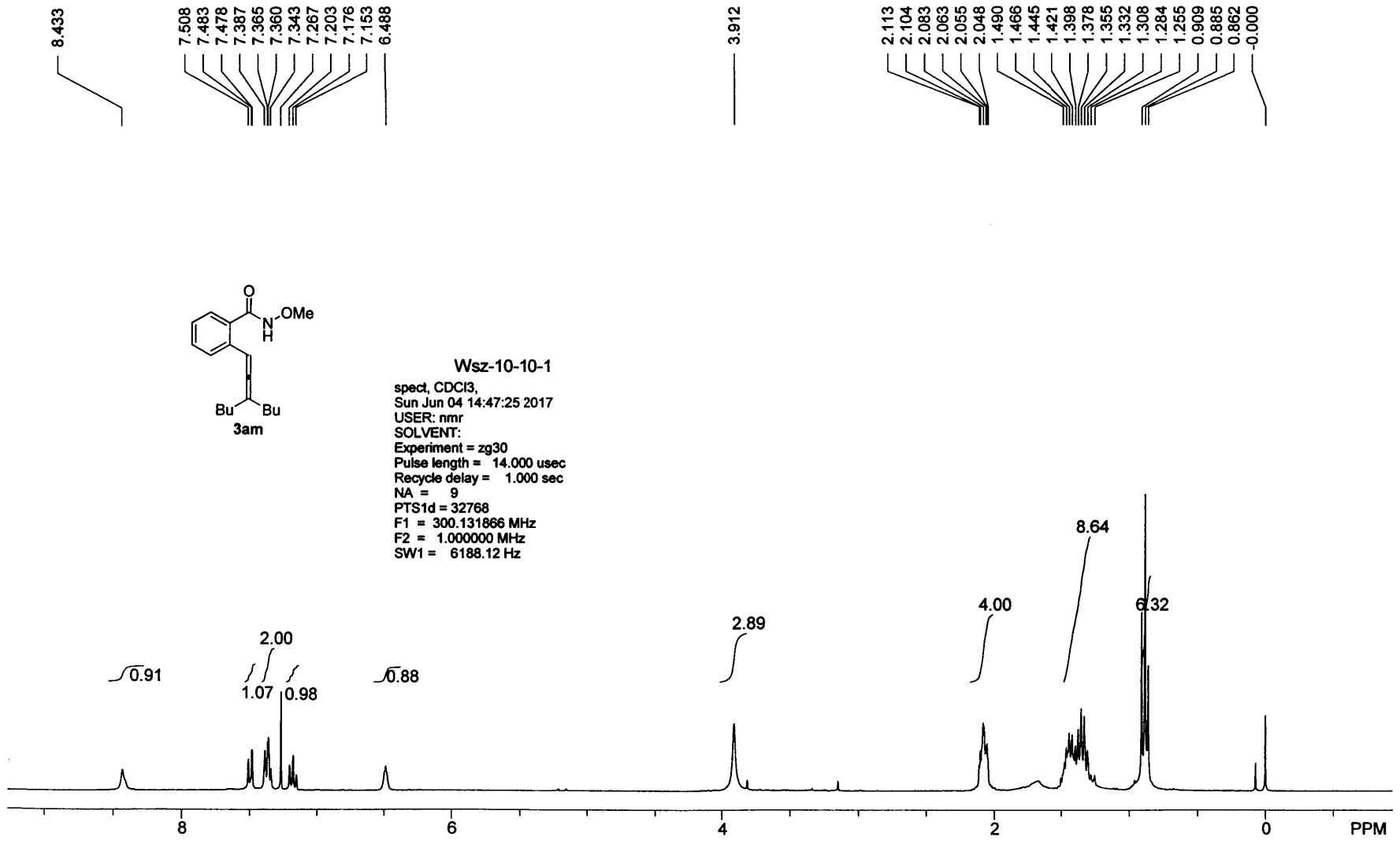


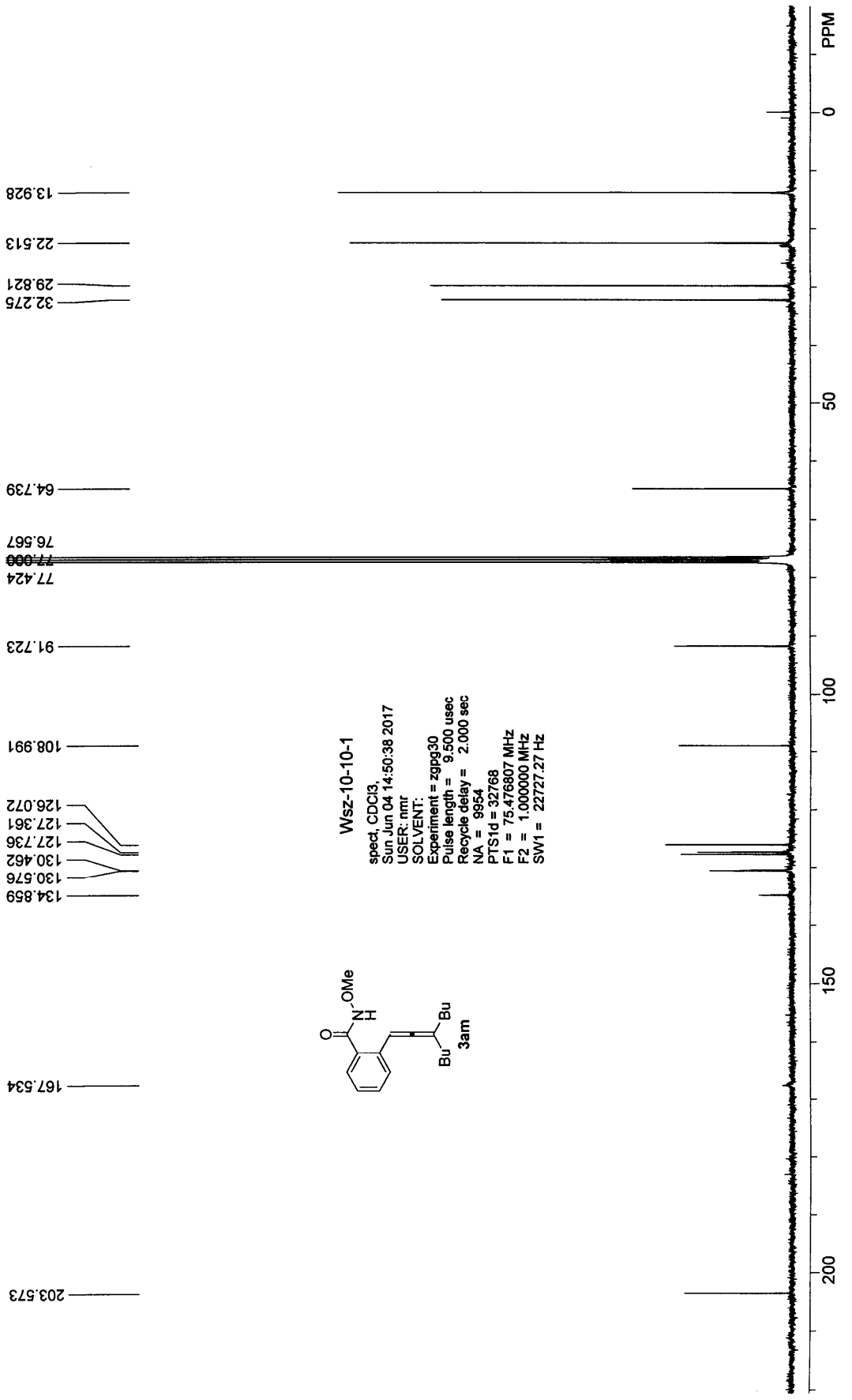
分析结果表

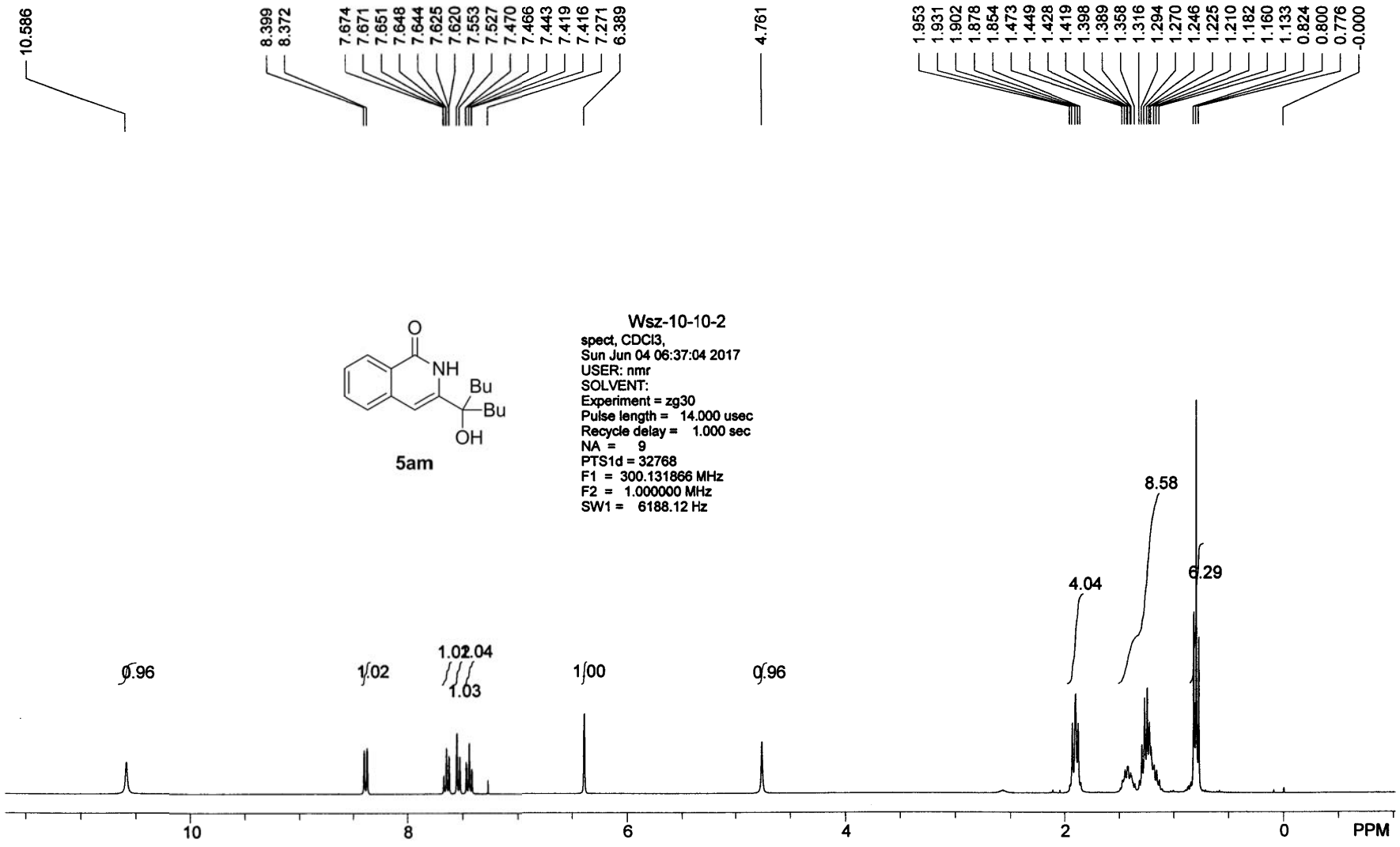
峰号	峰名	保留时间	峰高	峰面积	含量
1		43.545	872166.000	130359624.000	89.6488
2		51.647	94059.906	15051890.000	10.3512
总计			966225.906	145411514.000	100.0000

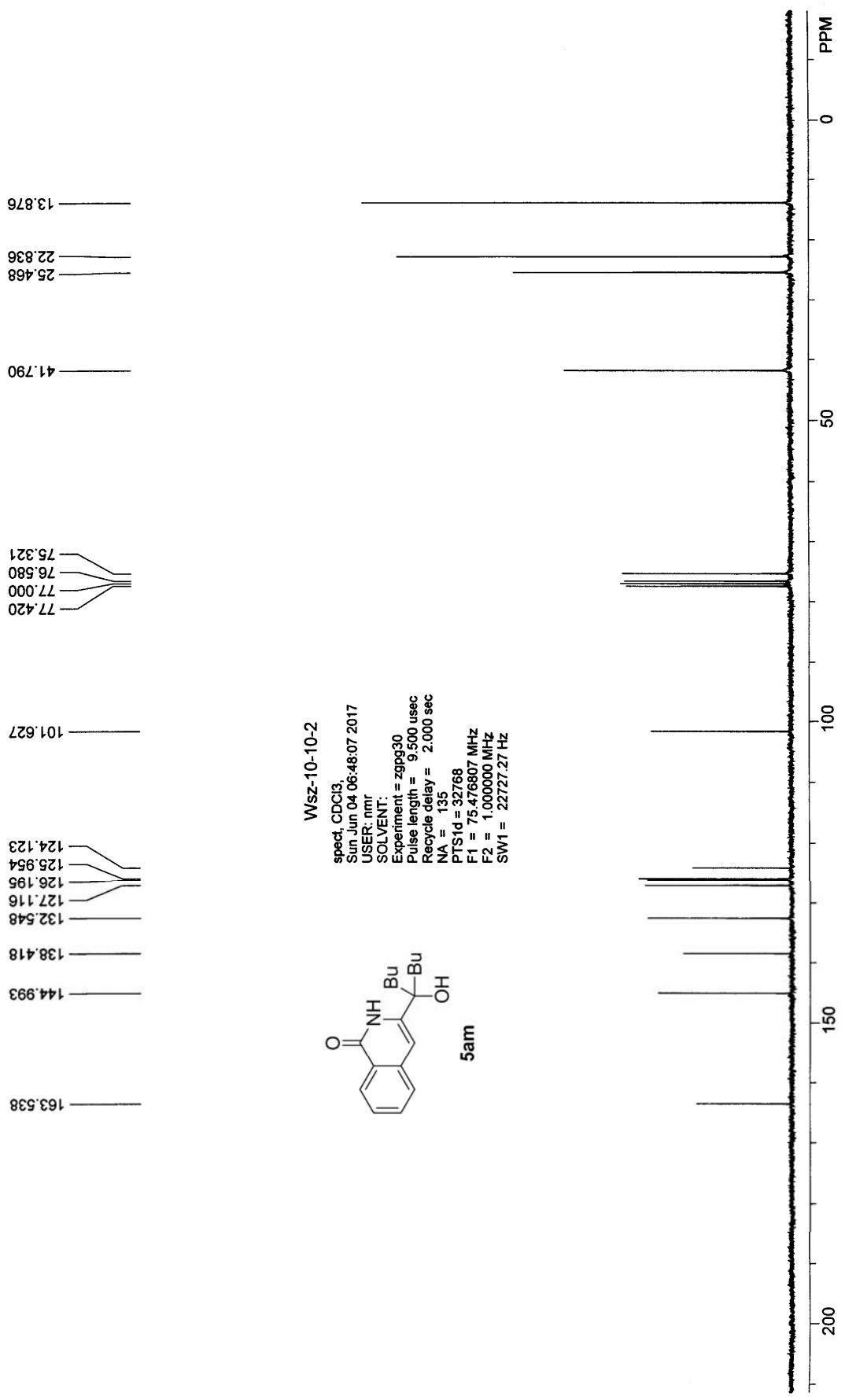

Wsz-10-13
spect, CDCl3,
Fri Jun 09 08:49:00 2017
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
3al
PPM

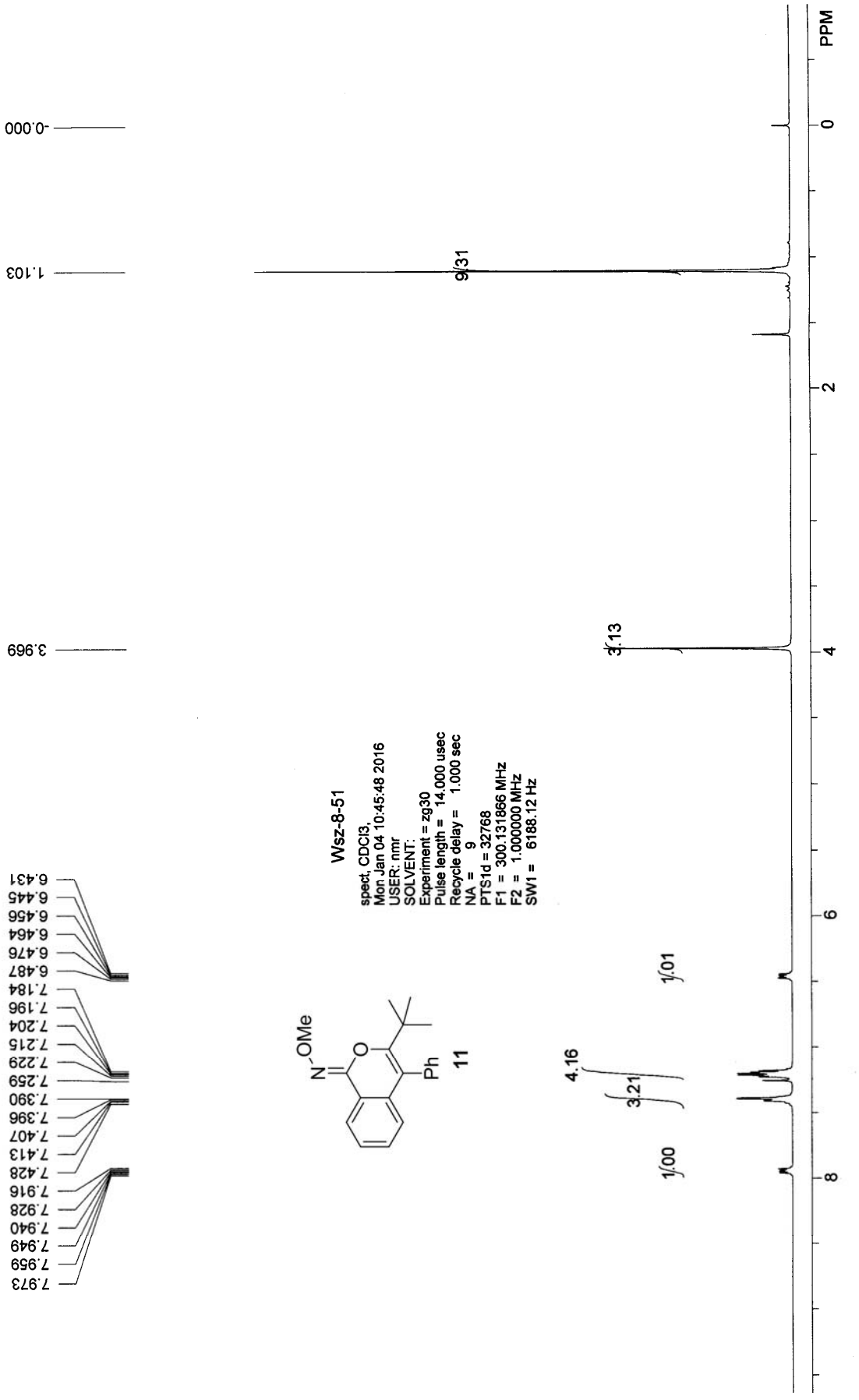

Wsz-10-13
spect, CDCl3,
Thu Jun 08 12:07:48 2017
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 118
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
3al
PPM
0
50
100
150
200
13.730
13.765
22.167
22.360
30.030
30.267
32.483
34.186
64.043
76.573
77.000
77.422
106.591
126.821
129.145
129.672
130.579
130.800
138.324
167.359
200.294

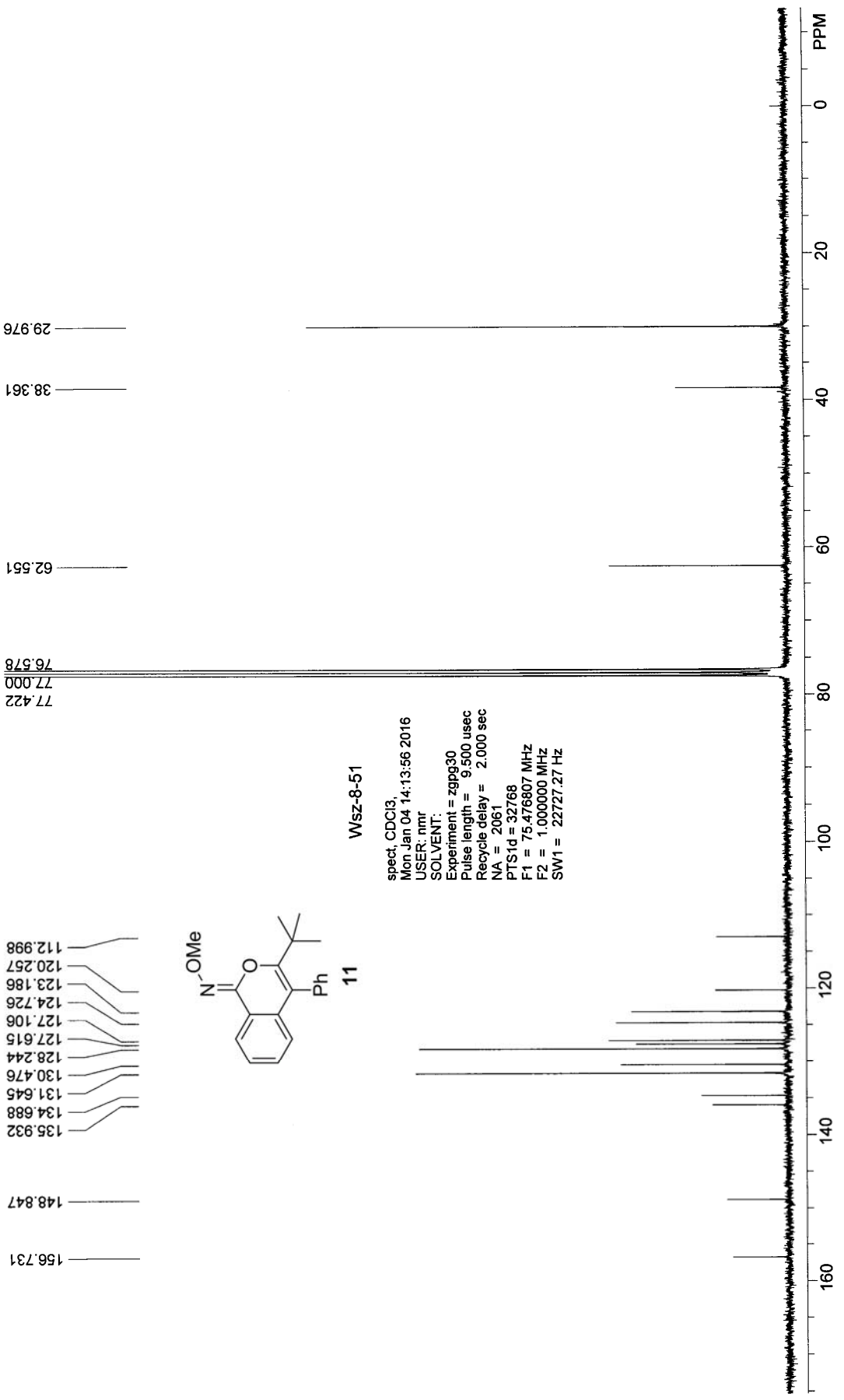

8.433
7.508
7.483
7.478
7.387
7.365
7.360
7.343
7.267
7.203
7.176
7.153
6.488
3.912
2.113
2.104
2.083
2.063
2.055
2.048
1.490
1.466
1.445
1.421
1.398
1.378
1.355
1.332
1.308
1.284
1.255
0.909
0.885
0.862
-0.000
O
N
H
OMe
Bu
Bu
3am
Wsz-10-10-1
spect, CDCl3,
Sun Jun 04 14:47:25 2017
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.91
2.00
1.07
0.98
0.88
2.89
4.00
8.64
6.32
8
6
4
2
0
PPM

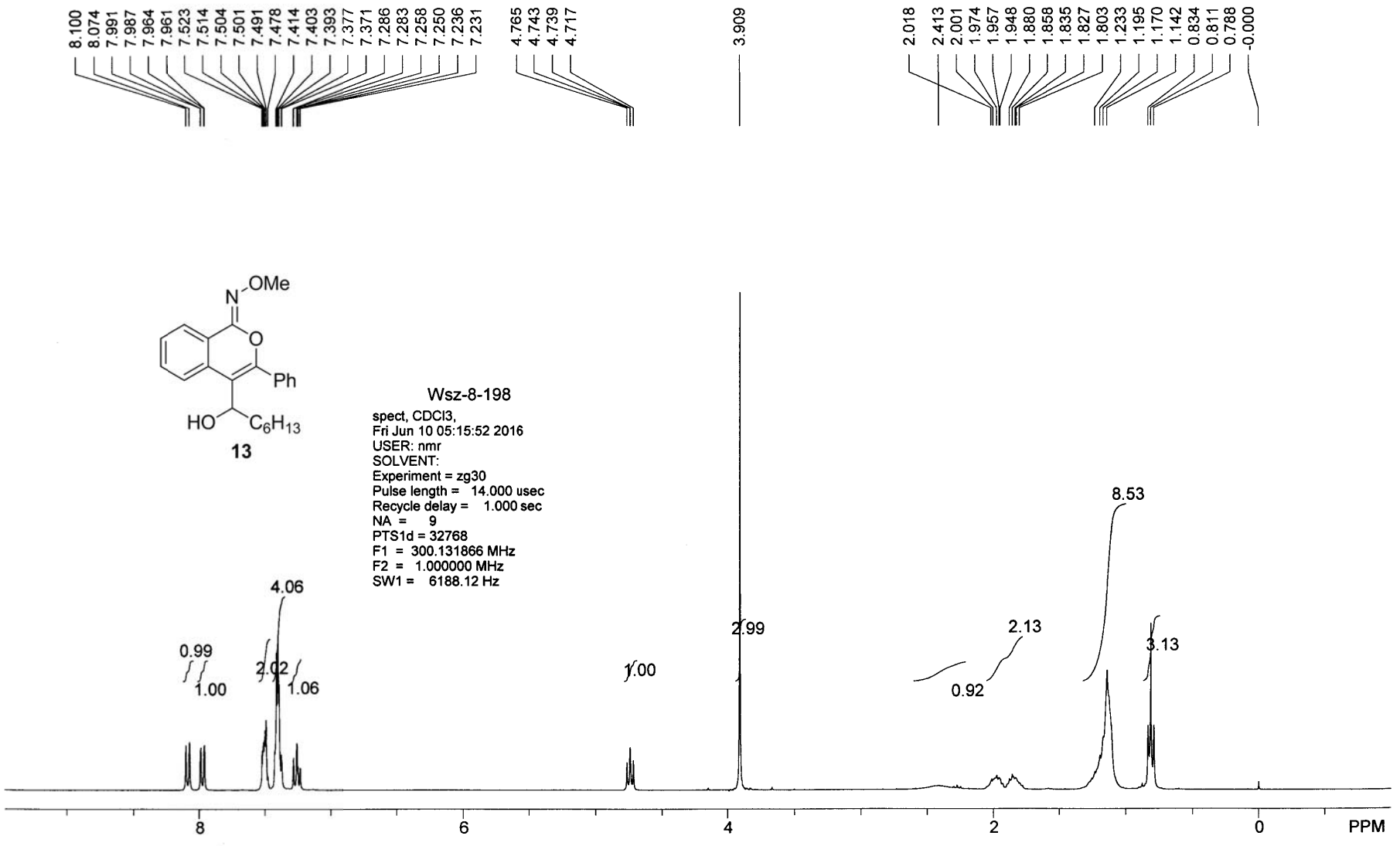

PPM
0
50
100
150
200
13.928
22.513
29.821
32.275
64.739
76.567
77.000
77.424
91.723
108.991
126.072
127.361
127.736
130.462
130.576
134.859
167.534
203.573
Wsz-10-1-1
spect, CDCl3,
Sun Jun 04 14:50:38 2017
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 9954
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
OMe
NH
O
Bu
Bu
3am

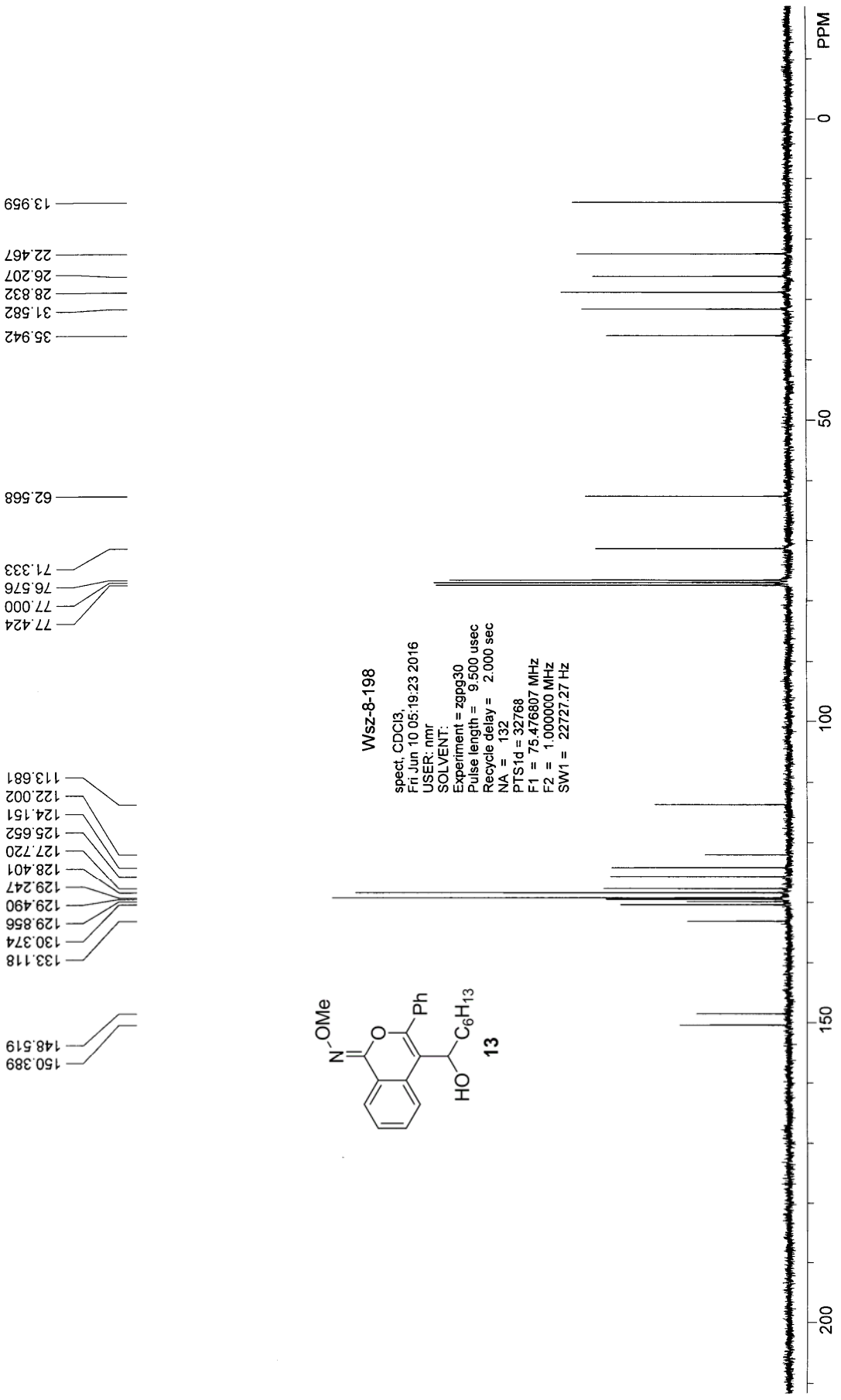

10.586
8.399
8.372
7.674
7.671
7.651
7.648
7.644
7.625
7.620
7.553
7.527
7.470
7.466
7.443
7.419
7.416
7.271
6.389
4.761
1.953
1.931
1.902
1.878
1.854
1.473
1.449
1.428
1.419
1.398
1.389
1.358
1.316
1.294
1.270
1.246
1.225
1.210
1.182
1.160
1.133
0.824
0.800
0.776
-0.000
O
NH
Bu
Bu
OH
5am
Wsz-10-10-2
spect, CDCl3,
Sun Jun 04 06:37:04 2017
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
0.96
1.02
1.02
2.04
1.03
1.00
0.96
4.04
8.58
6.29
10
8
6
4
2
0
PPM

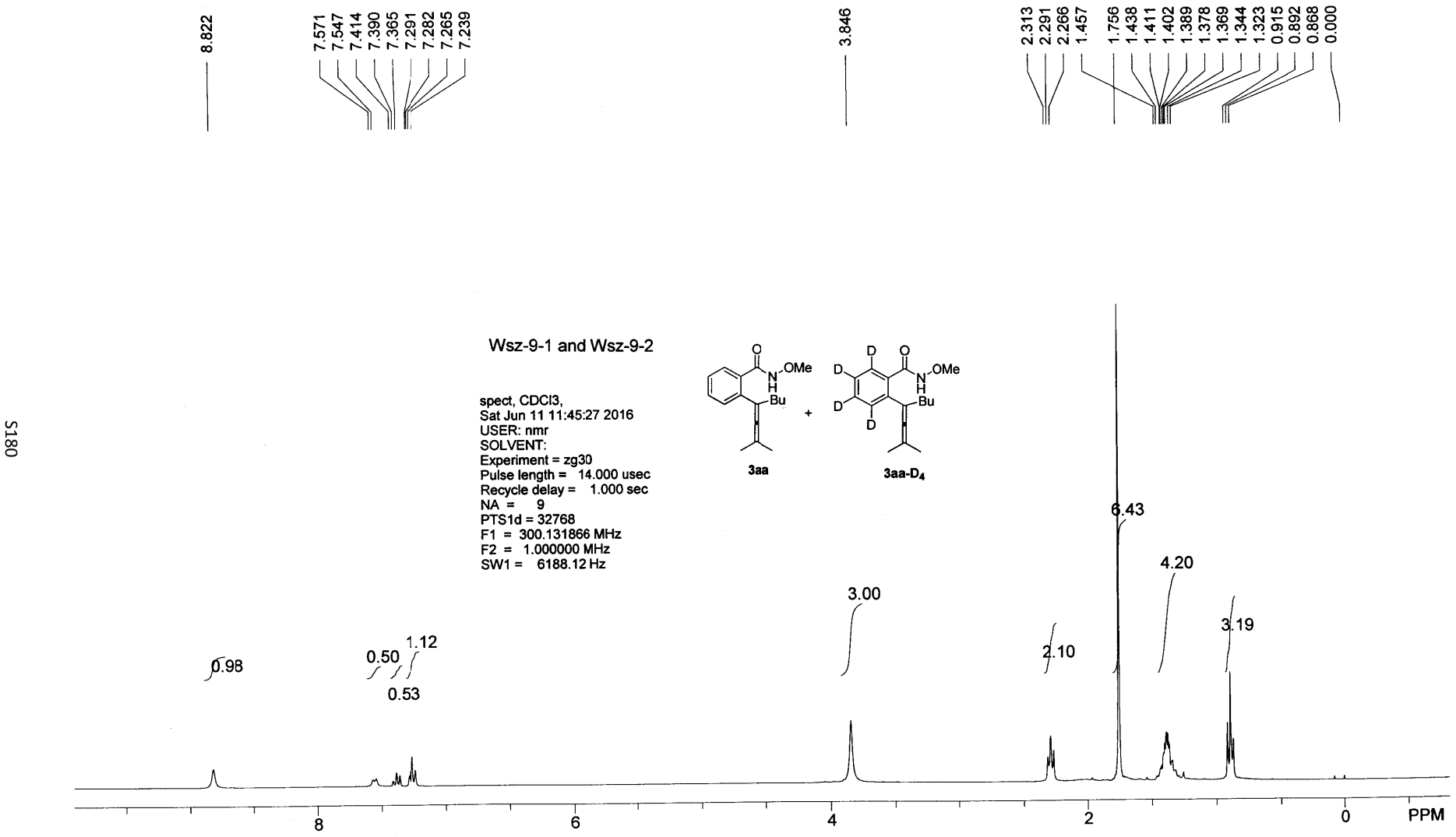

13.876
22.836
25.468
41.790
75.321
76.580
77.000
77.420
101.627
124.123
125.954
126.195
127.116
132.548
138.418
144.993
163.538
Wsz-10-10-2
spect, CDCl3,
Sun Jun 04 06:48:07 2017
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 135
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
Bu
Bu
OH
NH
O
5am
PPM
0
50
100
150
200

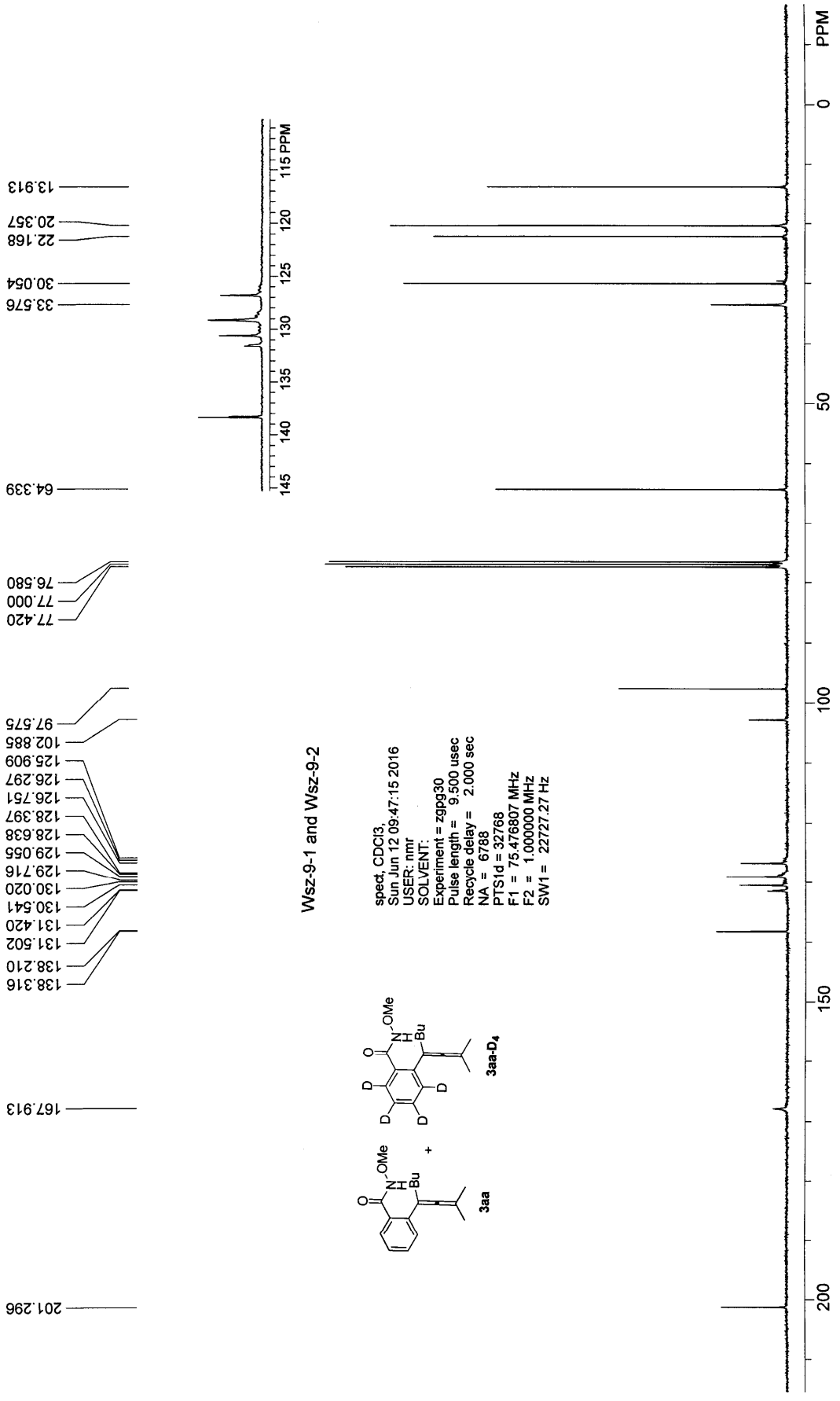

Wsz-8-51
spect, CDCl3,
Mon Jan 04 10:45:48 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
11
OMe
N
O
Ph
9.31
3.13
1.01
4.16
3.21
1.00
PPM
0
2
4
6
8
-0.000
1.103
3.969
6.431
6.445
6.456
6.464
6.476
6.487
7.184
7.196
7.204
7.215
7.229
7.259
7.390
7.396
7.407
7.413
7.428
7.916
7.928
7.940
7.949
7.959
7.973

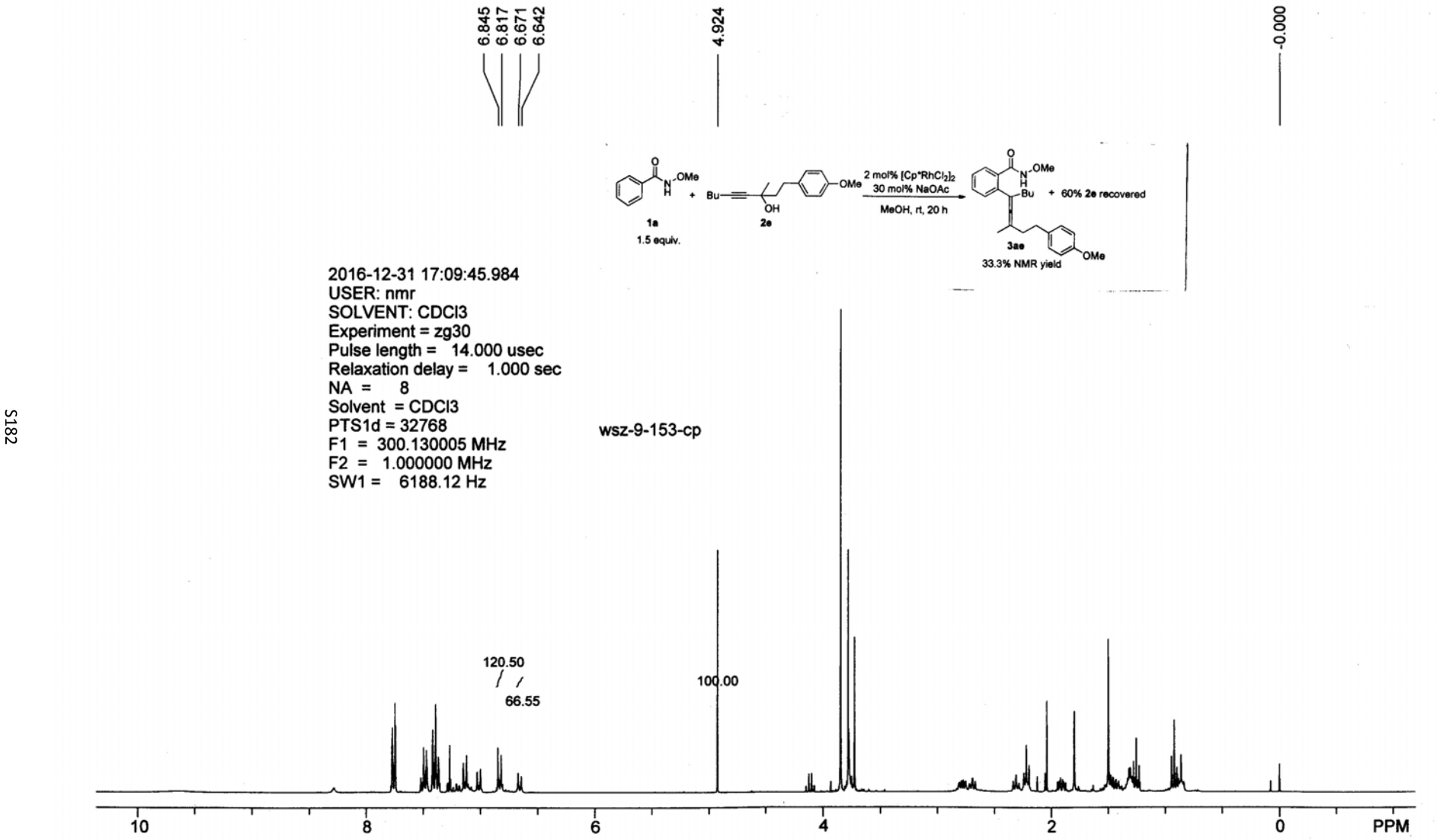

PPM
0
20
40
60
80
100
120
140
160
29.976
38.361
62.551
76.578
77.000
77.422
112.998
120.257
123.186
124.726
127.106
127.615
128.244
130.476
131.645
134.688
135.932
148.847
156.731
N
OMe
O
Ph
11
Wsz-8-51
spect, CDCl3,
Mon Jan 04 14:13:56 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 2061
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz

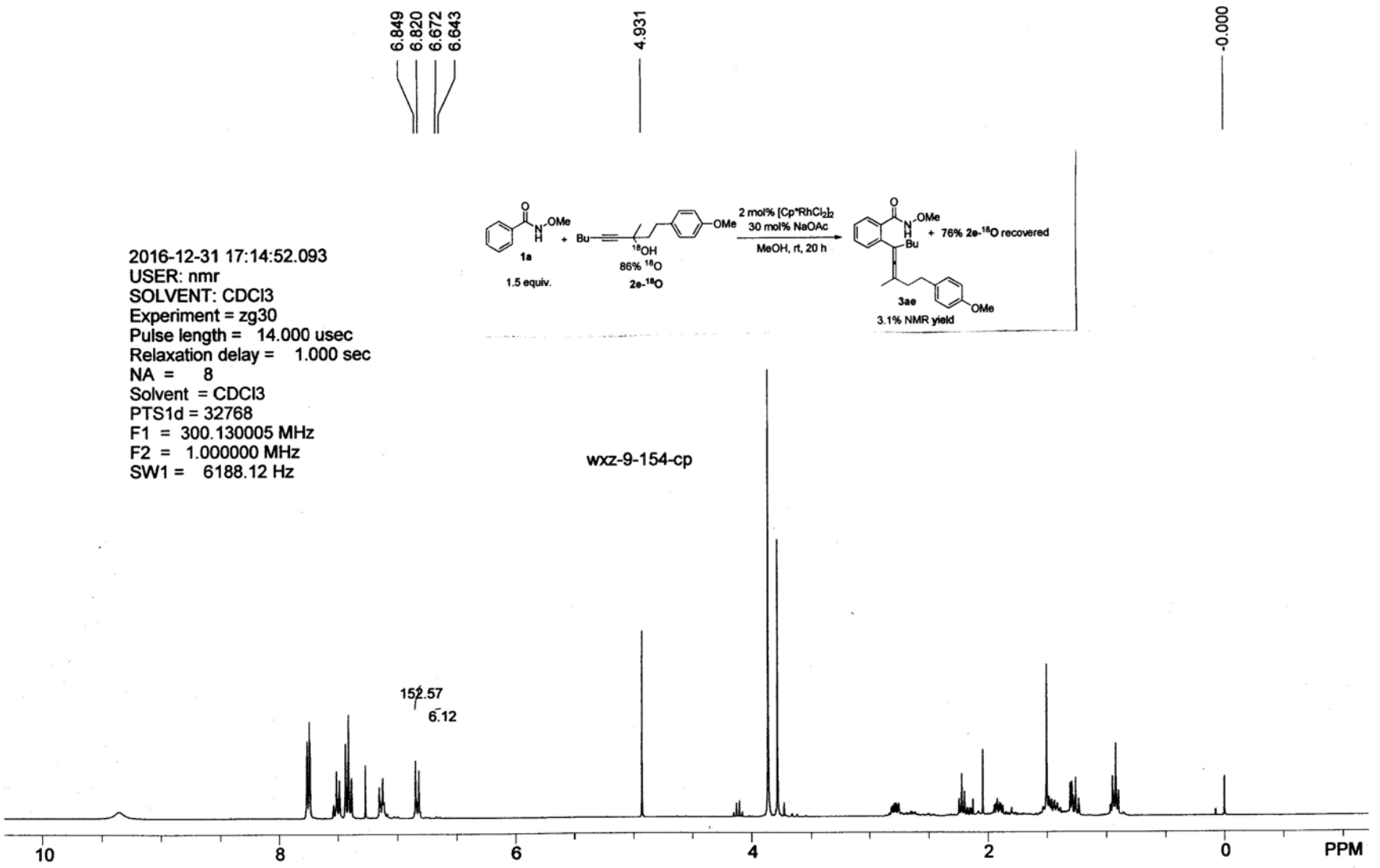

8.100
8.074
7.991
7.987
7.964
7.961
7.523
7.514
7.504
7.501
7.491
7.478
7.414
7.403
7.393
7.377
7.371
7.286
7.283
7.258
7.250
7.236
7.231
4.765
4.743
4.739
4.717
3.909
2.018
2.413
2.001
1.974
1.957
1.948
1.880
1.858
1.835
1.827
1.803
1.233
1.195
1.170
1.142
0.834
0.811
0.788
-0.000
N
OMe
O
Ph
HO
C6H13
13
Wsz-8-198
spect, CDCl3,
Fri Jun 10 05:15:52 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
4.06
0.99
1.00
2.02
1.06
1.00
2.99
0.92
2.13
8.53
3.13
8
6
4
2
0
PPM

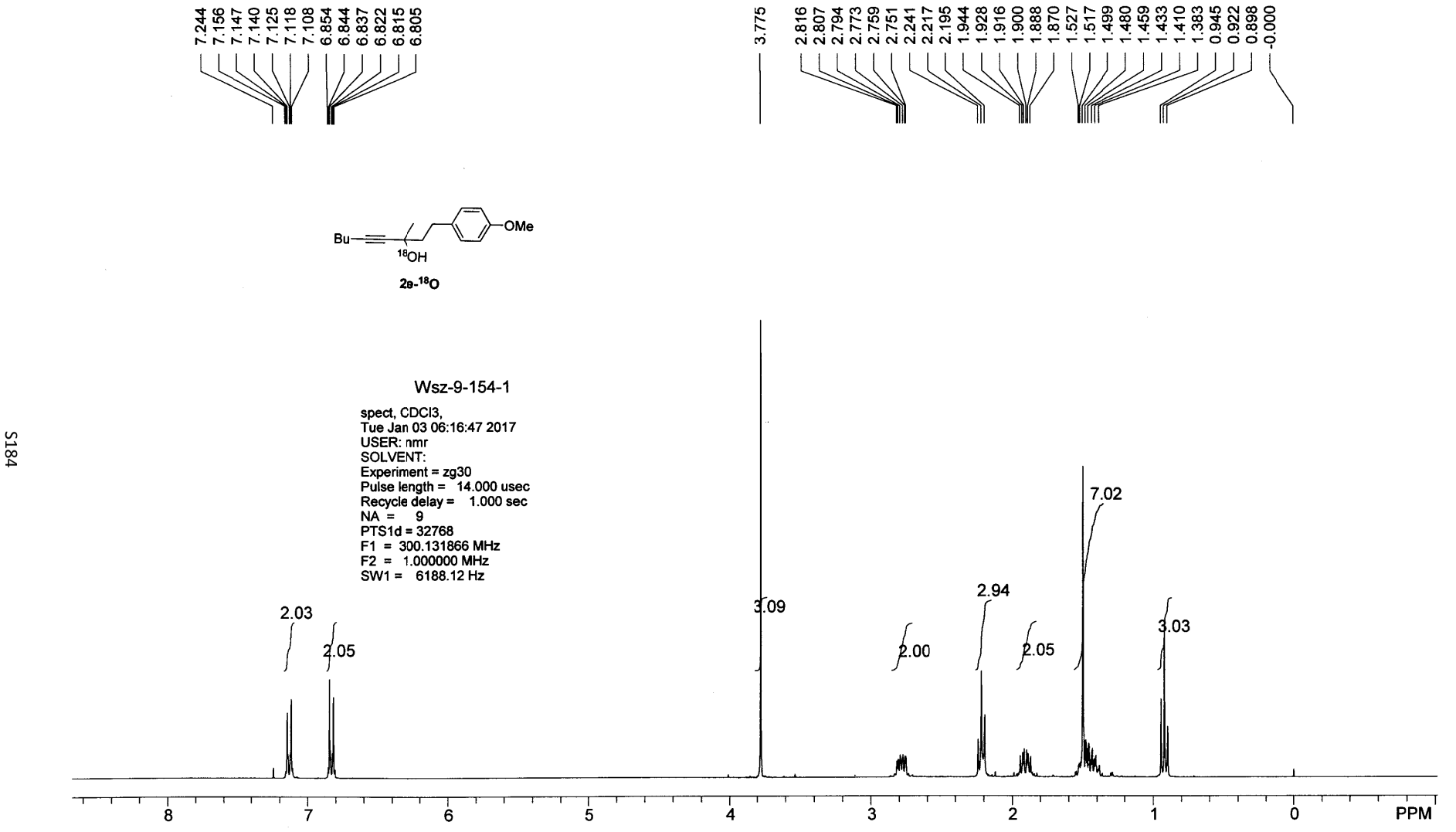

Wsz-8-198
spect, CDCl3,
Fri Jun 10 05:19:23 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 132
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
PPM
0
50
100
150
200
13.959
22.467
26.207
28.832
31.582
35.942
62.568
71.333
76.576
77.000
77.424
113.681
122.002
124.151
125.652
127.720
128.401
129.247
129.490
129.856
130.374
133.118
148.519
150.389
OMe
N
O
Ph
HO
C6H13
13

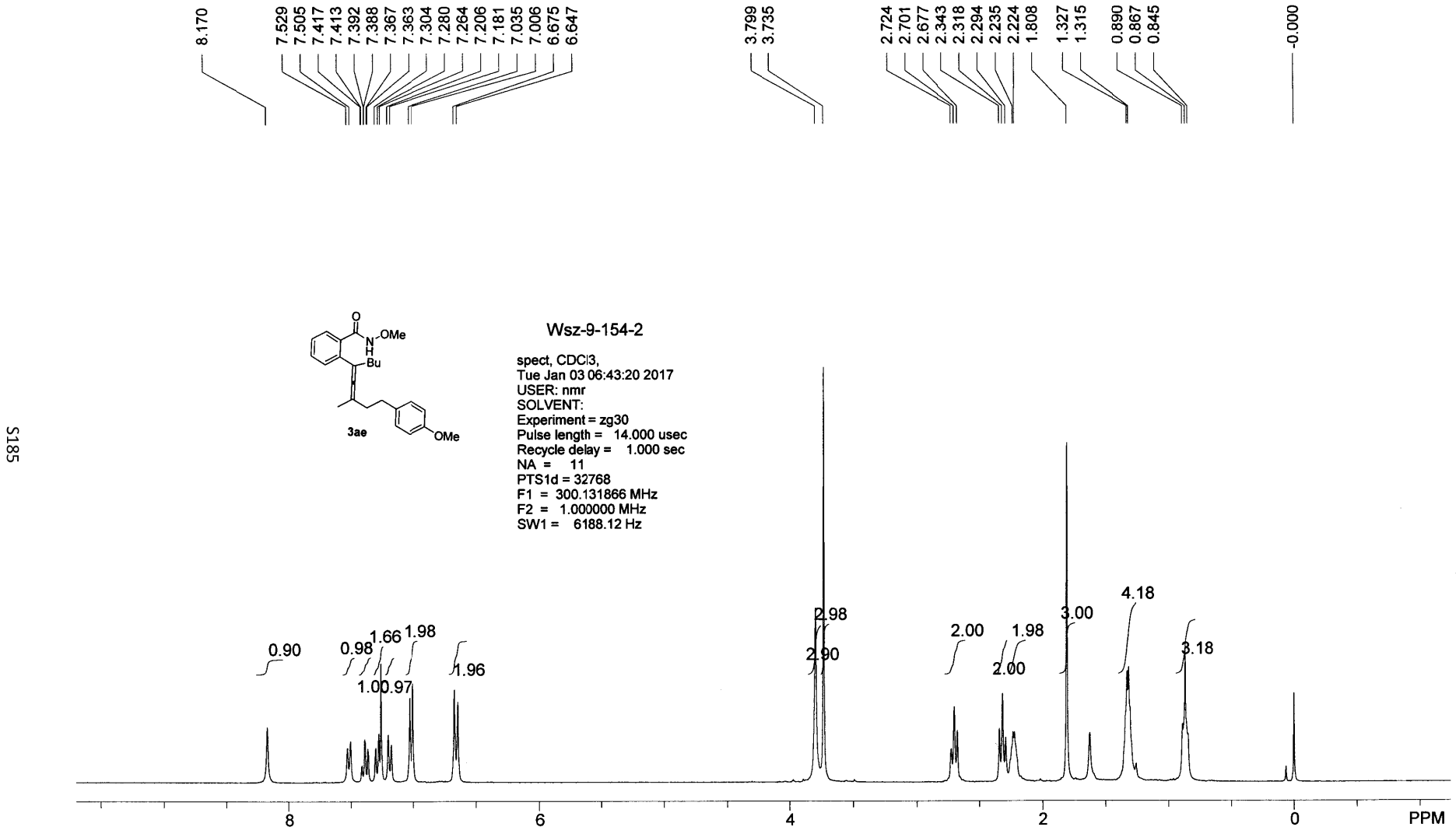

8.822
7.571
7.547
7.414
7.390
7.365
7.291
7.282
7.265
7.239
3.846
2.313
2.291
2.266
1.457
1.756
1.438
1.411
1.402
1.389
1.378
1.369
1.344
1.323
0.915
0.892
0.868
0.000
Wsz-9-1 and Wsz-9-2
spect, CDCl3,
Sat Jun 11 11:45:27 2016
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
OMe
Bu
3aa
3aa-D4
0.98
0.50
1.12
0.53
3.00
2.10
6.43
4.20
3.19
8
6
4
2
0
PPM


Wsz-9-1 and Wsz-9-2
spect, CDCl3,
Sun Jun 12 09:47:15 2016
USER: nmr
SOLVENT:
Experiment = zgpg30
Pulse length = 9.500 usec
Recycle delay = 2.000 sec
NA = 6788
PTS1d = 32768
F1 = 75.476807 MHz
F2 = 1.000000 MHz
SW1 = 22727.27 Hz
3aa
3aa-D4
PPM
115 PPM
13.913
20.357
22.168
30.054
33.576
64.339
76.580
77.000
77.420
97.575
102.885
125.909
126.297
126.751
128.397
128.638
129.055
129.716
130.020
130.541
131.420
131.502
138.210
138.316
167.913
201.296


6.845
6.817
6.671
6.642
4.924
-0.000
1a
1.5 equiv.
2e
2 mol% [Cp*RhCl2]2
30 mol% NaOAc
MeOH, rt, 20 h
60% 2e recovered
3ae
33.3% NMR yield
2016-12-31 17:09:45.984
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.000 usec
Relaxation delay = 1.000 sec
NA = 8
Solvent = CDCl3
PTS1d = 32768
F1 = 300.130005 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
wsz-9-153-cp
120.50
66.55
100.00
10
8
6
4
2
0
PPM


6.849
6.820
6.672
6.643
4.931
-0.000
2016-12-31 17:14:52.093
USER: nmr
SOLVENT: CDCl3
Experiment = zg30
Pulse length = 14.000 usec
Relaxation delay = 1.000 sec
NA = 8
Solvent = CDCl3
PTS1d = 32768
F1 = 300.130005 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
1a
1.5 equiv.
2e-18O
86% 18O
2 mol% [Cp*RhCl2]2
30 mol% NaOAc
MeOH, rt, 20 h
3ae
3.1% NMR yield
+ 76% 2e-18O recovered
wxz-9-154-cp
152.57
6.12
10
8
6
4
2
0
PPM


7.244
7.156
7.147
7.140
7.125
7.118
7.108
6.854
6.844
6.837
6.822
6.815
6.805
3.775
2.816
2.807
2.794
2.773
2.759
2.751
2.241
2.217
2.195
1.944
1.928
1.916
1.900
1.888
1.870
1.527
1.517
1.499
1.480
1.459
1.433
1.410
1.383
0.945
0.922
0.898
-0.000
Bu
OMe
18OH
2e-18O
Wsz-9-154-1
spect, CDCl3,
Tue Jan 03 06:16:47 2017
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 9
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
2.03
2.05
3.09
2.00
2.94
2.05
7.02
3.03
8
7
6
5
4
3
2
1
0
PPM


8.170
7.529
7.505
7.417
7.413
7.392
7.388
7.367
7.363
7.304
7.280
7.264
7.206
7.181
7.035
7.006
6.675
6.647
3.799
3.735
2.724
2.701
2.677
2.343
2.318
2.294
2.235
2.224
1.808
1.327
1.315
0.890
0.867
0.845
-0.000
Wsz-9-154-2
spect, CDCl3,
Tue Jan 03 06:43:20 2017
USER: nmr
SOLVENT:
Experiment = zg30
Pulse length = 14.000 usec
Recycle delay = 1.000 sec
NA = 11
PTS1d = 32768
F1 = 300.131866 MHz
F2 = 1.000000 MHz
SW1 = 6188.12 Hz
3ae
0.90
0.98
1.66
1.98
1.96
1.00
0.97
2.98
2.90
2.00
1.98
2.00
3.00
4.18
3.18
8
6
4
2
0
PPM