Efficent Synthesis of *N*-(buta-2,3-dienyl) Amides from Terminal *N*-Proparyl Amides and Their Synthetic Potential towards Oxazoline Derivatives

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Supporting Information

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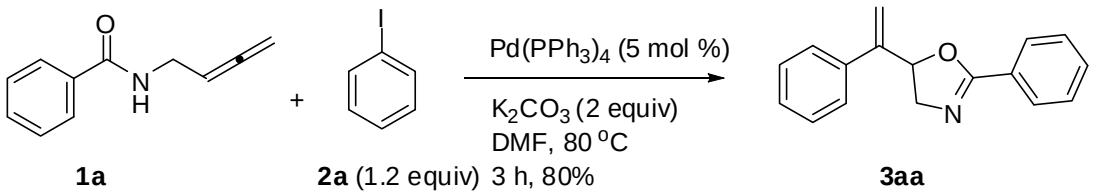
General Information: All reactions were carried out in oven-dried Schlenk tubes. DMSO, CH_3CN, DMA and DMF were dried over calcium hydride before distillation. 1,4-Dioxane and toluene were dried over Na wire before distillation. All the temperatures are referred to the bath temperature. All ^1H NMR experiments were measured relative to the signal of tetramethylsilane (0 ppm) in $CDCl_3$ and ^{13}C NMR experiments were measured in relative to the signal of residual chloroform (77.0 ppm) in $CDCl_3$. IR spectra were recorded on the infrared spectrometer. Melting points were measured without correction. Common reagents were purchased from commercial sources and were used without further purification. Column chromatography was performed using silica gel (300-400 mesh) eluting with ethyl acetate and petroleum ether. TLC was performed on glass-backed silica plates.

(1) Synthesis of 2-phenyl-5-(1-phenylvinyl)-4,5-dihydrooxazole (3aa).



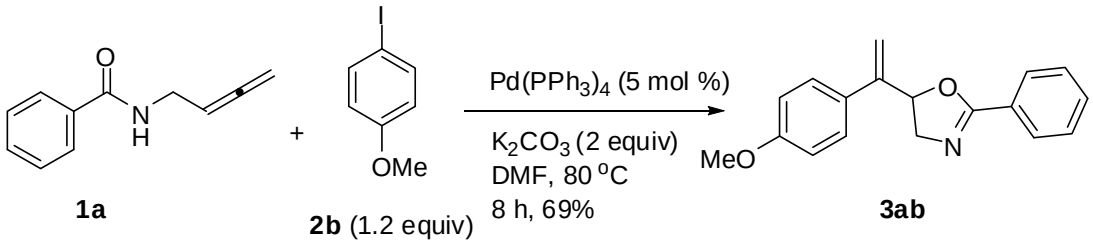
1a **2a** (1.2 equiv) 3 h, 80% **3aa**

Typical procedure: After the Schlenk tube containing K_2CO_3 (55.4 mg, 0.4 mmol) was flamed-dried and filled with nitrogen, $Pd(PPh_3)_4$ (11.7 mg, 0.01 mmol), **1a** (34.9 mg, 0.2 mmol), **2a** (49.7 mg, 0.24 mmol), and DMF (2 mL) were added sequentially. The resulting solution was stirred at 80 °C. When the reaction was completed as monitored by TLC, the mixture was diluted with diethyl ether (50 mL) and washed with water (5 mL×3). Then the combined organic layer was dried over anhydrous Na_2SO_4, filtrated and evaporated. The residue was purified by

chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 10:1) to afford **3aa** (40.3 mg, 80%): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06-7.97 (m, 2 H, ArH), 7.55-7.24 (m, 8 H, ArH), 5.61 (t, *J* = 9.0 Hz, 1 H, OCH), 5.46 (s, 1 H, one proton in C=CH_2), 5.42 (s, 1 H, one proton in C=CH_2), 4.29 (dd, *J* = 14.7, 10.2 Hz, 1 H, one proton in NCH_2), 3.80 (dd, *J* = 14.7, 7.8 Hz, 1 H, one proton in NCH_2) (for more detail about ^{1}HNMR, see Supporting Information); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.7, 146.8, 137.9, 131.3, 128.5, 128.3, 128.1, 128.0, 127.6, 126.5, 112.4, 80.0, 61.0; IR (neat) 3059, 2927, 2870, 1652, 1579, 1495, 1448, 1335, 1257, 1177, 1082, 1062, 1025 cm^{-1}; MS (EI) *m/z* (%) 249 (M^+, 21.13), 117 (100); HRMS calcd. for $C_{17}H_{15}NO$ [M^+]: 249.1154; Found: 249.1152.

The following compounds were prepared according to typical procedure.

(2) Synthesis of 5-(1-(4-methoxyphenyl)vinyl)-2-phenyl-4,5-dihydrooxazole (3ab) .

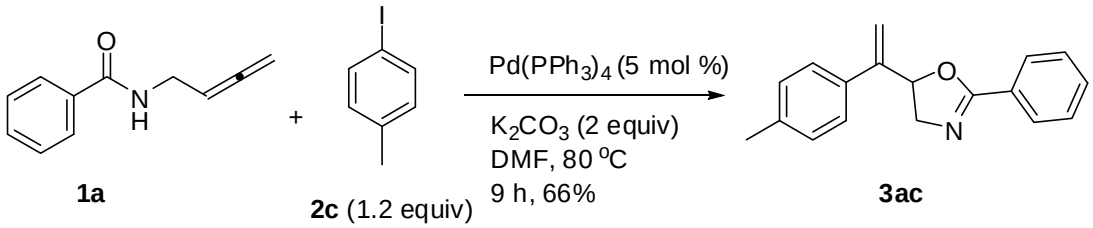


1a **2b** (1.2 equiv) **3ab**

The reaction of K_2CO_3 (55.3 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.7 mg, 0.01 mmol), **1a** (35.9 mg, 0.2 mmol), **2b** (57.3 mg, 0.24 mmol), and DMF (2 mL) afforded **3ab** (39.3 mg, 69%) (eluent: petroleum ether/ethyl acetate = 10:1): solid; mp 70-72 °C (*n*-hexane/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05-7.99 (m, 2 H, ArH), 7.54-7.40 (m, 3 H, ArH), 7.35-7.28 (m, 2 H, ArH), 6.91-6.85 (m, 2 H, ArH), 5.62-5.54 (m, 1 H, OCH), 5.38 (s, 1 H, one proton in C=CH_2), 5.34 (s, 1 H, one

proton in C=CH_2), 4.28 (dd, *J* = 14.4, 10.2 Hz, 1 H, one proton in NCH_2), 3.83-3.74 (m, 4 H, OCH_3 and one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 159.5, 146.1, 131.4, 130.2, 128.4, 128.1, 127.6, 114.0, 110.9, 80.2, 61.0, 55.2; IR (neat) 1651, 1604, 1512, 1450, 1369, 1331, 1311, 1293, 1247, 1185, 1084, 1063, 1026 cm^{-1}; MS (EI) *m/z* (%) 279 (M^+, 24.07), 117 (100); Anal. Calcd. for $C_{18}H_{17}NO_2$: C, 77.40; H, 6.13; N, 5.01; Found: C, 77.18, H, 6.18; N, 4.96.

(3) Synthesis of 2-phenyl-5-(1-*p*-tolylvinyl)-4,5-dihydrooxazole (3ac).

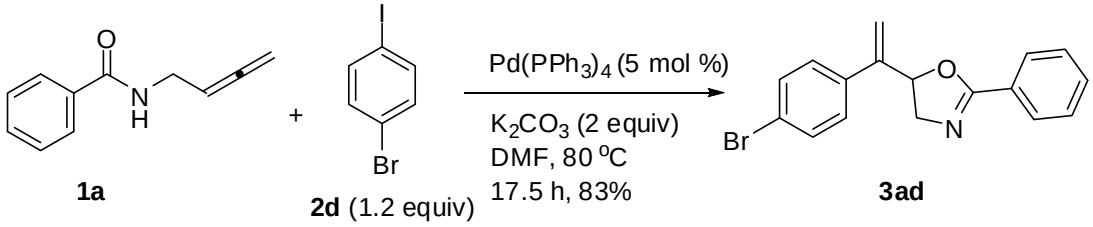


1a **2c** (1.2 equiv) **3ac**

The reaction of K_2CO_3 (55.5 mg, 0.4 mmol), $Pd(PPh_3)_4$ (12.1 mg, 0.01 mmol), **1a** (35.0 mg, 0.2 mmol), **2c** (52.2 mg, 0.24 mmol), and DMF (2 mL) afforded **3ac** (35.3 mg, 66%) (eluent: petroleum ether/ethyl acetate = 10:1): solid; mp 91.3-93 °C (*n*-hexane/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05-7.95 (m, 2 H, ArH), 7.55-7.36 (m, 3 H, ArH), 7.27 (d, *J* = 8.4 Hz, 2 H, ArH), 7.15 (d, *J* = 8.1 Hz, 2 H, ArH), 5.63-5.54 (m, 1 H, OCH), 5.42 (s, 1 H, one proton in C=CH_2), 5.37 (s, 1 H, one proton in C=CH_2), 4.28 (dd, *J* = 14.7, 10.5 Hz, 1 H, one proton in NCH_2), 3.78 (dd, *J* = 14.7, 7.8 Hz, 1 H, one proton in NCH_2), 2.34 (s, 3 H, $ArCH_3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 146.5, 137.9, 134.9, 131.3, 129.3, 128.3, 128.1, 127.6, 126.3, 111.5, 80.0, 61.0, 21.1; IR (neat) 2925, 2852, 1652, 1621, 1578, 1514, 1493, 1448, 1395, 1368, 1332, 1312, 1289, 1261, 1176, 1158, 1127, 1083, 1063, 1024, 1012 cm^{-1}; MS (EI) *m/z* (%) 263 (M^+, 24.85), 117 (100); Anal.

Calcd. for $C_{18}H_{17}NO$: C, 82.10; H, 6.51; N, 5.32; Found: C, 81.98, H, 6.41; N, 5.14.

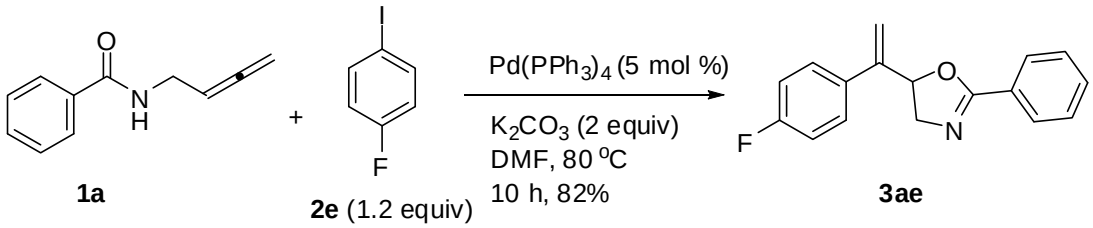
(4) Synthesis of 5-(1-(4-bromophenyl)vinyl)-2-phenyl-4,5-dihydrooxazole (3ad).



1a **2d** (1.2 equiv) **3ad**

The reaction of K_2CO_3 (55.9 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.8 mg, 0.01 mmol), **1a** (34.2 mg, 0.2 mmol), **2d** (68.5 mg, 0.24 mmol), and DMF (2 mL) afforded **3ad** (54.0 mg, 83%) (eluent: petroleum ether/ethyl acetate = 10:1): solid; mp 81-82 °C (*n*-hexane/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.5 Hz, 2 H, ArH), 7.60-7.30 (m, 5 H, ArH),7.25 (d, *J* = 8.1 Hz, 2 H, ArH), 5.54 (t, *J* = 7.4 Hz, 1 H, OCH), 5.44 (s, 2 H, C=CH_2), 4.27 (dd, *J* = 14.4, 10.5 Hz, 1 H, one proton in NCH_2), 3.81 (dd, *J* = 14.4, 7.8 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 145.8, 136.8, 131.7, 131.5, 128.4, 128.24, 128.15, 127.5, 122.2, 113.5, 79.9, 60.8; IR (neat) 2924, 2853, 1654, 1624, 1578, 1490, 1448, 1391, 1366, 1330, 1261, 1119, 1065, 1024, 1005 cm^{-1}; MS (EI) *m/z* (%) 329 ($M(^{81}Br)^+$, 12.43), 327 ($M(^{79}Br)^+$, 12.71), 117 (100); Anal. Calcd. for $C_{17}H_{14}BrNO$: C, 62.21; H, 4.30; N, 4.27; Found: C, 62.05, H, 4.54; N, 4.06.

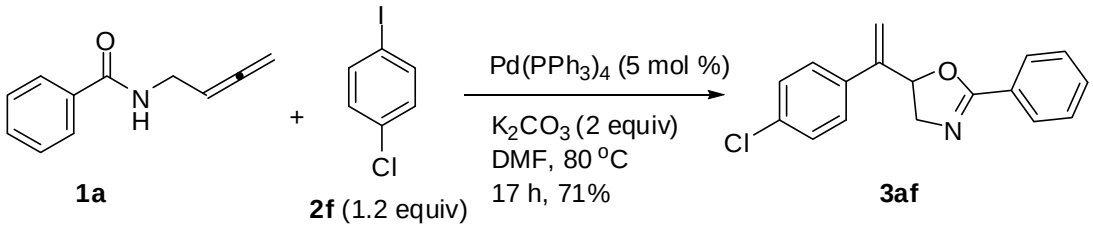
(5) Synthesis of 5-(1-(4-flurophenyl)vinyl)-2-phenyl-4,5-dihydrooxazole (3ae).



1a **2e** (1.2 equiv) **3ae**

The reaction of K_2CO_3 (55.7 mg, 0.4 mmol), $Pd(PPh_3)_4$ (12.1 mg, 0.01 mmol), **1a** (34.2 mg, 0.2 mmol), **2e** (56.2 mg, 0.24 mmol), and DMF (2 mL) afforded **3ae** (43.3 mg, 82%) (eluent: petroleum ether/ethyl acetate = 10:1): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05-7.97 (m, 2 H, ArH), 7.55-7.39 (m, 3 H, ArH), 7.37-7.30 (m, 2 H, ArH), 7.10-6.95 (m, 2 H, ArH), 5.61-5.50 (m, 1 H, OCH), 5.41 (s, 1 H, one proton in C=CH_2), 5.40 (s, 1 H, one proton in C=CH_2), 4.27 (dd, *J* = 14.7, 10.2 Hz, 1 H, one proton in NCH_2), 3.77 (dd, *J* = 14.7, 7.5 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 162.6 (d, *J* = 246.0 Hz), 145.8, 134.0 (d, *J* = 4.0 Hz), 131.5, 128.4, 128.283, 128.281 (d, *J* = 19.4 Hz), 127.5, 115.5 (d, *J* = 21.4 Hz), 113.0, 80.2, 60.8; ^{19}F NMR ($CDCl_3$, 282 MHz) -113.83; IR (neat) 1656, 1624, 1601, 1579, 1511, 1494, 1449, 1367, 1330, 1307, 1287, 1263, 1236, 1168, 1114, 1084, 1064, 1025, 1011 cm^{-1}; MS (EI) *m/z* (%) 267 (M^+, 28.51), 117 (100); HRMS calcd. for $C_{17}H_{14}NOF$ [M^+]: 267.1059; Found: 267.1058.

(6) Synthesis of 5-(1-(4-chlorophenyl)vinyl)-2-phenyl-4,5-dihydrooxazole (3af).

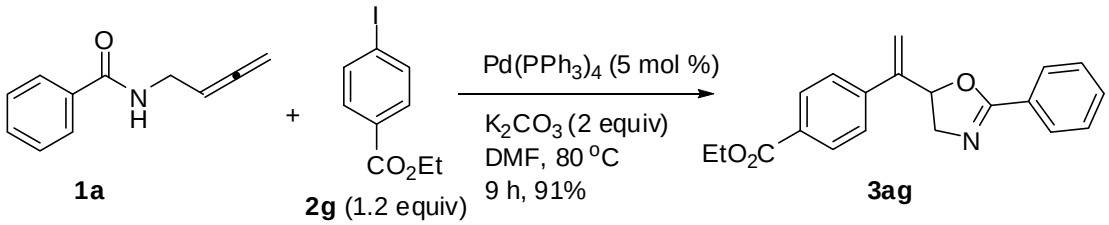


1a **2f** (1.2 equiv) **3af**

The reaction of K_2CO_3 (55.6 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.7 mg, 0.01 mmol), **1a** (36.1 mg, 0.2 mmol), **2f** (57.1 mg, 0.24 mmol), and DMF (2 mL) afforded **3af**

(42.0 mg, 71%) (eluent: petroleum ether/ethyl acetate = 10:1): solid; mp 84-85 °C (*n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0 Hz, 2 H, ArH), 7.58-7.40 (m, 3 H, ArH), 7.39-7.23 (m, 4 H, ArH), 5.54 (t, *J* = 9.0 Hz, 1 H, OCH), 5.43 (s, 2 H, C=CH_2), 4.27 (dd, *J* = 13.8, 11.0 Hz, 1 H, one proton in NCH_2), 3.78 (dd, *J* = 14.6, 7.8 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 145.8, 136.4, 134.0, 131.4, 128.8, 128.4, 128.1, 127.9, 127.5, 113.4, 80.0, 60.8; IR (neat) 1652, 1628, 1578, 1494, 1450, 1379, 1333, 1283, 1089, 1066, 1024, 1011 cm^{-1}; MS (EI) *m/z* (%) 285 (M(^{37}Cl)$^+$, 7.12), 283 (M(^{35}Cl)$^+$, 23.22), 117 (100); Anal. Calcd. for $C_{17}H_{14}ClNO$: C, 71.96; H, 4.97; N, 4.94; Found: C, 71.75, H, 5.04; N, 4.88.

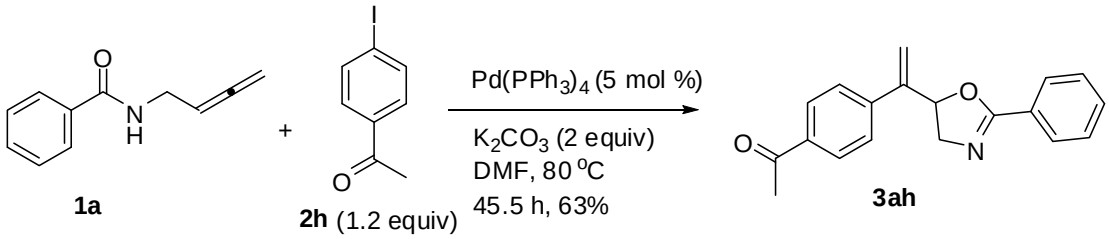
(7) Synthesis of ethyl 4-(1-(2-phenyl-4,5-dihydrooxazol-5-yl)vinyl)benzoate (3ag).



The reaction of K_2CO_3 (55.3 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.6 mg, 0.01 mmol), **1a** (35.1 mg, 0.2 mmol), **2g** (66.8 mg, 0.24 mmol), and DMF (2 mL) afforded **3ag** (59.0 mg, 91%) (eluent: petroleum ether/ethyl acetate = 15/1 to 5/1): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07-7.96 (m, 4 H, ArH), 7.55-7.36 (m, 5 H, ArH), 5.61 (t, *J* = 9.0 Hz, 1 H, OCH), 5.55 (s, 1 H, one proton in C=CH_2), 5.52 (s, 1 H, one proton in C=CH_2), 4.42-4.23 (m, 3 H, OCH_2 and one proton in NCH_2), 3.78 (dd, *J* = 15.0, 7.8 Hz, 1 H, one proton in NCH_2), 1.39 (t, *J* = 7.1 Hz, 3 H, CH_3 in CO_2Et); ^{13}C

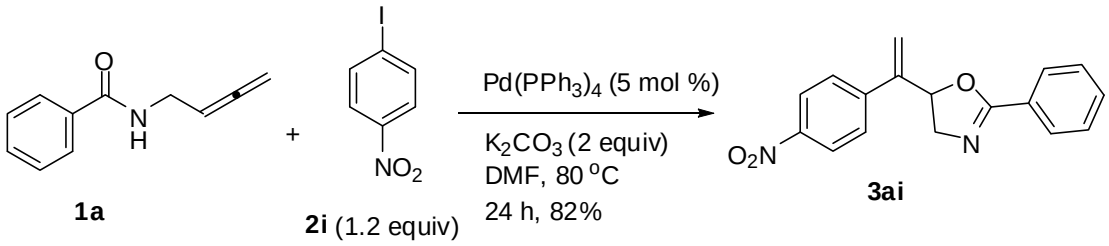
NMR (75 MHz, $CDCl_3$) δ 166.0, 163.7, 146.0, 142.2, 131.4, 129.9, 129.7, 128.3, 128.1, 127.3, 126.4, 114.3, 79.7, 60.9, 60.8, 14.2; IR (neat) 1708, 1650, 1607, 1579, 1493, 1446, 1406, 1365, 1334, 1275, 1192, 1124, 1109, 1095, 1081, 1065, 1021, 1009 cm^{-1}; MS (EI) *m/z* (%) 321 (M^+, 13.15), 117 (100); HRMS calcd. for $C_{20}H_{19}NO_3$ [M^+]: 321.1365; Found: 321.1364.

(8) Synthesis of 1-(4-(1-(2-phenyl-4,5-dihydrooxazol-5-yl)vinyl)phenyl)ethanone (3ah).



The reaction of K_2CO_3 (55.9 mg, 0.4 mmol), $Pd(PPh_3)_4$ (12.1 mg, 0.01 mmol), **1a** (35.5 mg, 0.2 mmol), **2h** (59.1 mg, 0.24 mmol), and DMF (2 mL) afforded **3ah** (37.7 mg, 63%) (eluent: petroleum ether/ethyl acetate = 5:1): solid; mp 149-150 °C (Et_2O/DCM); ^1H NMR (300 MHz, $CDCl_3$) δ 8.05-7.92 (m, 4 H, ArH), 7.56-7.40 (m, 5 H, ArH), 5.62 (t, *J* = 9.0 Hz, 1 H, OCH), 5.56 (s, 1 H, one proton in $C=CH_2$), 5.54 (s, 1 H, one proton in $C=CH_2$), 4.32 (dd, *J* = 14.6, 10.4 Hz, 1 H, one proton in NCH_2), 3.79 (dd, *J* = 14.7, 7.8 Hz, 1 H, one proton in NCH_2), 2.60 (s, 3 H, $ArCOCH_3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.5, 163.8, 146.0, 142.5, 136.5, 131.5, 128.6, 128.4, 128.2, 127.4, 126.8, 114.7, 79.8, 60.9, 26.6; IR (neat) 1671, 1649, 1603, 1578, 1560, 1493, 1446, 1406, 1359, 1334, 1268, 1198, 1131, 1081, 1060, 1025, 1008 cm^{-1}; MS (EI) *m/z* (%) 291 (M^+, 29.61), 117 (100); Anal. Calcd. for $C_{19}H_{17}NO_2$: C, 78.33; H, 5.88; N, 4.81; Found: C, 78.03, H, 5.87; N, 4.79.

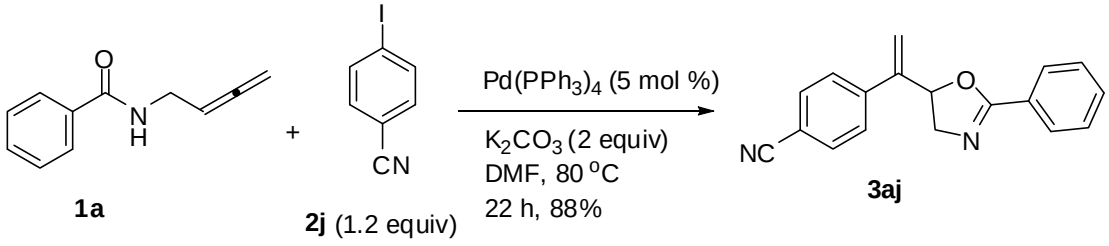
(9) Synthesis of 5-(1-(4-nitrophenyl)vinyl)-2-phenyl-4,5-dihydrooxazole (3ai).



1a **2i** (1.2 equiv) **3ai**

The reaction of K_2CO_3 (56.0 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.3 mg, 0.01 mmol), **1a** (34.1 mg, 0.2 mmol), **2i** (59.8 mg, 0.24 mmol), and DMF (2 mL) afforded **3ai** (47.4 mg, 82%) (eluent: petroleum ether/ethyl acetate = 10:1 to 8/1 to 5/1): solid; mp 136-137 °C (petroleum ether/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.25-8.15 (m, 2 H, ArH), 8.09-7.92 (m, 2 H, ArH), 7.58-7.39 (m, 5 H, ArH), 5.65-5.53 (m, 3 H, OCH and C=CH_2), 4.33 (dd, *J* = 14.9, 10.4 Hz, 1 H, one proton in NCH_2), 3.80 (dd, *J* = 14.9, 7.7 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.7, 147.4, 145.2, 144.4, 131.6, 128.5, 128.1, 127.5, 127.2, 123.8, 116.5, 79.7, 60.6; IR (neat) 2923, 2851, 1651, 1596, 1511, 1448, 1340, 1255, 1182, 1111, 1079, 1063, 1025, 1010 cm^{-1}; MS (EI) *m/z* (%) 294 (M, 20.09), 117 (100); Anal. Calcd. for $C_{17}H_{14}N_2O_3$: C 69.38; H, 4.79; N, 9.52; Found: C, 69.30, H, 4.91; N, 9.51.

(10) Synthesis of 4-(1-(2-phenyl-4,5-dihydrooxazol-5-yl)vinyl)benzonitrile (3aj).

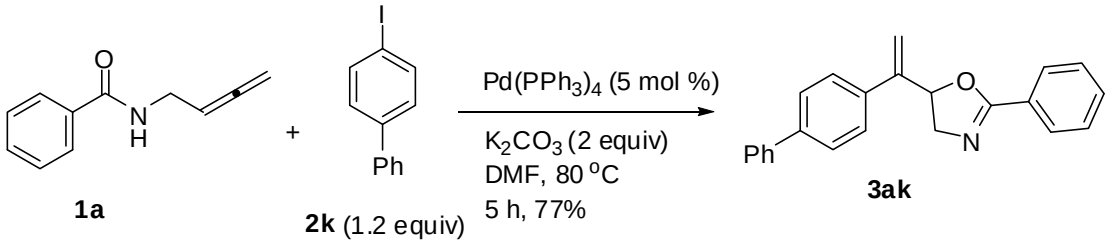


1a **2j** (1.2 equiv) **3aj**

The reaction of K_2CO_3 (54.9 mg, 0.4 mmol), $Pd(PPh_3)_4$ (12.1 mg, 0.01 mmol), **1a**

(34.6 mg, 0.2 mmol), **2j** (55.3 mg, 0.24 mmol), and DMF (2 mL) afforded **3aj** (48.4 mg, 88%) (eluent: petroleum ether/ethyl acetate = 5:1): solid; mp 125-127 °C (*n*-hexane/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02-7.96 (m, 2 H, ArH), 7.65 (d, *J* = 7.8 Hz, 2 H, ArH), 7.55-7.40 (m, 5 H, ArH), 5.62-5.53 (m, 3 H, OCH and C=CH_2), 4.31 (dd, *J* = 15.0, 10.5 Hz, 1 H, one proton in NCH_2), 3.79 (dd, *J* = 15.0, 8.1 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.6, 145.4, 142.4, 132.3, 131.5, 128.4, 128.0, 127.23, 127.18, 118.5, 115.8, 111.7, 79.5, 60.7; IR (neat) 2924, 2854, 2229, 1655, 1623, 1604, 1578, 1509, 1449, 1400, 1331, 1260, 1085, 1063, 1026, 1013 cm^{-1}; MS (EI) *m/z* (%) 274 (M^+, 22.20), 117 (100); Anal. Calcd. for $C_{18}H_{14}N_2O$: C, 78.81; H, 5.14; N, 10.21; Found: C, 78.48, H, 5.11; N, 10.10.

(11) Synthesis of 5-(1-(biphenyl-4-yl)vinyl)-2-phenyl-4,5-dihydrooxazole (3ak).



1a **2k** (1.2 equiv) **3ak**

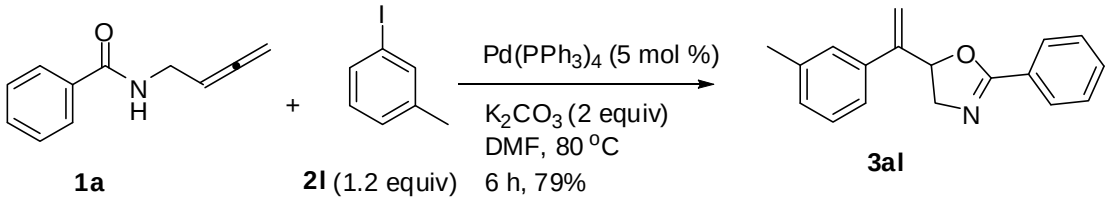
The reaction of K_2CO_3 (56.1 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.5 mg, 0.01 mmol), **1a** (34.2 mg, 0.2 mmol), **2k** (66.8 mg, 0.24 mmol), and DMF (2 mL) afforded **3ak** (49.3 mg, 77%) (eluent: petroleum ether/ethyl acetate = 10:1): solid; mp 128-129 °C (petroleum ether/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.2 Hz, 2 H, ArH), 7.59 (d, *J* = 7.5 Hz, 4 H, ArH), 7.53-7.30 (m, 8 H, ArH), 5.65 (t, *J* = 9.0 Hz, 1 H, OCH), 5.52 (s, 1 H, one proton in =CH_2), 5.46 (s, 1 H, one proton in =CH_2), 4.34 (dd, *J* = 14.6, 10.7 Hz, 1 H, one proton in NCH_2), 3.85 (dd, *J*

= 14.7, 7.8 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 146.3, 140.9, 140.4, 136.7, 131.4, 128.8, 128.4, 128.2, 127.6, 127.4, 127.3, 126.94, 126.87, 112.4, 80.0, 61.1; IR (neat) 3060, 2926, 2871, 1653, 1622, 1579, 1489, 1448, 1403, 1366, 1334, 1319, 1261, 1183, 1080, 1063, 1024, 1003 cm^{-1}; MS (EI) *m/z* (%) 325 (M^+,42.04), 117 (100); Anal. Calcd. for $C_{23}H_{19}NO$: C 84.89; H, 5.89; N, 4.30; Found: C, 84.79, H, 5.83; N, 4.23.

Gram scale synthesis of 3ak.

After the Schlenk tube containing K_2CO_3 (2.2062 g, 16 mmol) was flamed-dried and filled with nitrogen, $Pd(PPh_3)_4$ (9.3 mg, 0.008 mmol), **1a** (1.3836 g, 8 mmol), **2k** (2.6815 g, 9.6 mmol), and DMF (10 mL) were added sequentially. The resulting solution was heated to and stirred at 80 ^oC. When the reaction was completed after 69 hours as monitored by TLC, the solvent was diluted with diethyl ether (100 mL) and washed with water (15 mL×3). Then the organic layers were dried over anhydrous Na_2SO_4, filtrated and evaporated. Chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 5:1) afforded **3ak** (2.0021 g, 77%): solid; ^1H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.5 Hz, 2 H, ArH), 7.62-7.30 (m, 12 H, ArH), 5.65 (t, *J* = 9.0 Hz, 1 H, OCH), 5.52 (s, 1 H, one proton in $=CH_2$), 5.45 (s, 1 H, one proton in $=CH_2$), 4.34 (dd, *J* = 14.7, 10.2 Hz, 1 H, one proton in NCH_2), 3.85 (dd, *J* = 14.7, 7.8 Hz, 1 H, one proton in NCH_2).

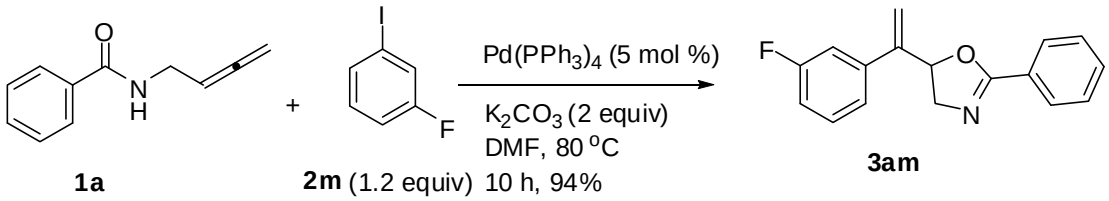
(12) Synthesis of 2-phenyl-5-(1-*m*-tolylvinyl)-4,5-dihydrooxazole (3al).



1a **2l** (1.2 equiv) **3al**

The reaction of K_2CO_3 (55.7 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.4 mg, 0.01 mmol), **1a** (35.8 mg, 0.2 mmol), **2l** (54.1 mg, 0.24 mmol), and DMF (2 mL) afforded **3al** (42.4 mg, 78%) (eluent: petroleum ether/ethyl acetate = 10:1): solid; mp 70-71 °C (*n*-hexane/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05-7.95 (m, 2 H, ArH), 7.55-7.37 (m, 3 H, ArH), 7.29-7.10 (m, 4 H, ArH), 5.64-5.53 (m, 1 H, OCH), 5.42 (s, 1 H, one proton in C=CH_2), 5.39 (s, 1 H, one proton in C=CH_2), 4.27 (dd, *J* = 14.7, 10.2 Hz, 1 H, one proton in NCH_2), 3.79 (dd, *J* = 14.7, 7.5 Hz, 1 H, one proton in NCH_2), 2.34 (s, 3 H, $ArCH_3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 146.9, 138.1, 137.8, 131.3, 128.8, 128.4, 128.3, 128.1, 127.6, 127.3, 123.5, 112.0, 80.0, 61.0, 21.4; IR (neat) 3097, 3057, 2928, 1653, 1602, 1579, 1493, 1446, 1373, 1333, 1277, 1262, 1175, 1086, 1066, 1023 cm^{-1}; MS (EI) *m/z* (%) 263 (M^+, 17.86), 117 (100); Anal. Calcd. for $C_{18}H_{17}NO$: C, 82.10; H, 6.51; N, 5.32; Found: C, 81.92, H, 6.47; N, 5.18.

(13) Synthesis of 5-(1-(3-flurophenyl)vinyl)-2-phenyl-4,5-dihydrooxazole (3am).

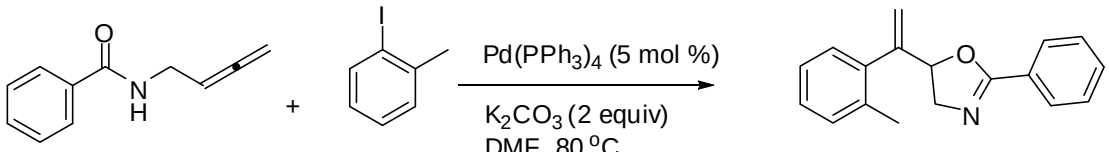


1a **2m** (1.2 equiv) **3am**

The reaction of K_2CO_3 (55.4 mg, 0.4 mmol), $Pd(PPh_3)_4$ (12.5 mg, 0.01 mmol), **1a** (34.9 mg, 0.2 mmol), **2m** (56.8 mg, 0.24 mmol), and DMF (2 mL) afforded **3am**

(50.8 mg, 94%) (eluent: petroleum ether/ethyl acetate = 10:1): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06-7.96 (m, 2 H, ArH), 7.59-7.38 (m, 3 H, ArH), 7.36-7.24 (m, 1 H, ArH), 7.17-6.95 (m, 3 H, ArH), 5.60-5.51 (m, 1 H, OCH), 5.48 (s, 1 H, one proton in C=CH_2), 5.46 (s, 1 H, one proton in C=CH_2), 4.30 (dd, *J* = 14.7, 10.2 Hz, 1 H, one proton in NCH_2), 3.79 (dd, *J* = 14.7, 7.8 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 162.8 (d, *J* = 245.1 Hz), 145.7 (d, *J* = 2.1 Hz), 140.1 (d, *J* = 8.0 Hz), 131.5, 130.1 (d, *J* = 8.6 Hz), 128.4, 128.1, 127.5, 122.2 (d, *J* = 3.3 Hz), 115.0 (d, *J* = 21.2 Hz), 113.65 (d, *J* = 21.1 Hz), 113.64, 79.8, 60.9; ^{19}F NMR ($CDCl_3$, 282 MHz) -112.58; IR (neat) 3062, 2935, 2873, 1653, 1613, 1579, 1488, 1448, 1371, 1332, 1263, 1199, 1172, 1084, 1062, 1026 cm^{-1}; MS (EI) *m/z* (%) 267 (M^+, 28.70), 117 (100); HRMS calcd. for $C_{17}H_{14}NOF$ [M^+]: 267.1059; Found: 267.1058.

(14) Synthesis of 2-phenyl-5-(1-(*o*-tolyl)vinyl)-4,5-dihydrooxazole (3an).

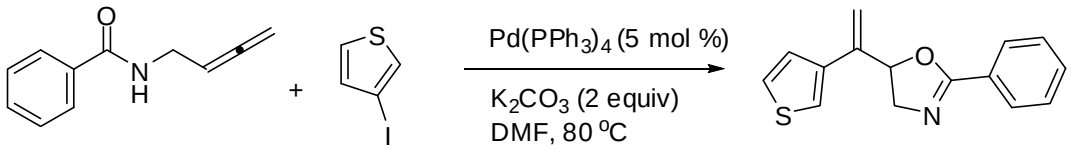


1a **2n** (1.2 equiv) **3an**

The reaction of K_2CO_3 (56.2 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.8 mg, 0.01 mmol), **1a** (34.6 mg, 0.2 mmol), **2n** (52.3 mg, 0.24 mmol), and DMF (2 mL) afforded **3an** (34.6 mg, 66%) (eluent: petroleum ether/ethyl acetate = 10:1): liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02-7.95 (m, 2 H, ArH), 7.53-7.39 (m, 3 H, ArH), 7.24-7.11 (m, 4 H, ArH), 5.56 (s, 1 H, one proton in C=CH_2), 5.43-5.35 (m, 1 H, OCH), 5.10 (s, 1 H, one proton in C=CH_2), 4.09 (dd, *J* = 14.7, 10.2 Hz, 1 H, one proton in NCH_2), 3.83 (dd, *J* = 15.0, 7.8 Hz, 1 H, one proton in NCH_2), 2.35 (s, 3 H, -CH_3);

^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 147.1, 138.2, 135.8, 131.3, 130.3, 129.1, 128.3, 128.1, 127.7, 127.6, 125.6, 114.9, 81.1, 59.7, 20.0; IR (neat) 3061, 2930, 2871, 1651, 1580, 1495, 1449, 1353, 1330, 1256, 1177, 1082, 1062, 1025 cm^{-1}; MS (EI) *m/z* (%) 263 (M^+, 5.94), 117 (100); HRMS calcd. for $C_{18}H_{17}NO$ [M^+]: 263.1310; Found: 263.1308.

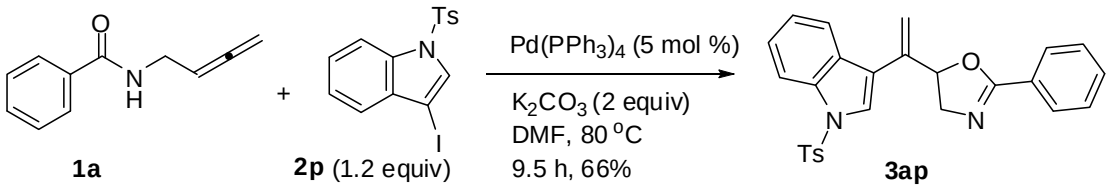
(15) Synthesis of 2-phenyl-5-(1-(thiophen-2-yl)vinyl)-4,5-dihydrooxazole (3ao).



1a **2o** (1.2 equiv) **3ao**

The reaction of K_2CO_3 (56.3 mg, 0.4 mmol), $Pd(PPh_3)_4$ (12.0 mg, 0.01 mmol), **1a** (35.2 mg, 0.2 mmol), **2o** (50.7 mg, 0.24 mmol), and DMF (2 mL) afforded **3ao** (41.1 mg, 79%) (eluent: petroleum ether/ethyl acetate = 10:1): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.5 Hz, 2 H, ArH), 7.55-7.36 (m, 3 H, ArH), 7.35-7.28 (m, 1 H, ArH), 7.26-7.16 (m, 1 H, ArH), 6.99 (s, 1 H, ArH), 5.54-5.45 (m, 2 H, OCH and one proton in $C=CH_2$), 5.31 (s, 1 H, one proton in $C=CH_2$), 4.36 (dd, *J* = 14.6, 10.7 Hz, 1 H, one proton in NCH_2), 3.90 (dd, *J* = 14.9, 8.0 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.7, 140.6, 140.3, 131.4, 128.3, 128.2, 127.4, 125.1, 124.0, 111.2, 79.9, 61.1; IR (neat) 3099, 2925, 2854, 1650, 1578, 1493, 1450, 1365, 1328, 1260, 1202, 1083, 1062, 1022 cm^{-1}; MS (EI) *m/z* (%) 255 (M^+, 34.17), 117 (100); HRMS calcd. for $C_{15}H_{13}NOS$ [M^+]: 255.0718; Found: 255.0719.

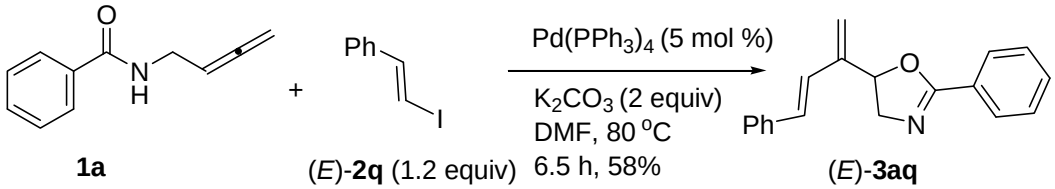
(16) Synthesis of 2-phenyl-5-(1-(1-tosyl-1*H*-indol-3-yl)vinyl)-4,5-dihydrooxazole (3ap).



1a **2p** (1.2 equiv) **3ap**

The reaction of K_2CO_3 (55.9 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.4 mg, 0.01 mmol), **1a** (35.3 mg, 0.2 mmol), **2p** (96.3 mg, 0.24 mmol), and DMF (2 mL) afforded **3ap** (60.0 mg, 66%) (eluent: petroleum ether/ethyl acetate = 5:1): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05-7.96 (m, 3 H, ArH), 7.69 (d, *J* = 7.8 Hz, 1 H, ArH), 7.62 (d, *J* = 8.1 Hz, 2 H, ArH), 7.58-7.42 (m, 4 H, ArH), 7.37-7.21 (m, 2 H, ArH), 7.13 (d, *J* = 7.8 Hz, 2 H, ArH), 5.61 (s, 1 H, one proton in C=CH_2), 5.58 (s, 1 H, one proton in C=CH_2), 5.51 (t, *J* = 9.2 Hz, 1 H, OCH), 4.28 (dd, *J* = 14.9, 10.4 Hz, 1 H, one proton in NCH_2), 3.73 (dd, *J* = 14.7, 7.8 Hz, 1 H, one proton in NCH_2), 2.30 (s, 3 H, $ArCH_3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.7, 145.0, 138.8, 135.0, 134.7, 131.5, 129.8, 129.5, 128.5, 128.2, 127.4, 126.7, 125.0, 123.6, 123.4, 120.5, 119.1, 114.9, 113.6, 80.9, 60.8, 21.5; IR (neat) 1650, 1447, 1371, 1306, 1255, 1172, 1136, 1115, 1090, 1062, 1024 cm^{-1}; MS (EI) *m/z* (%) 442 (M^+, 13.92), 91 (100); HRMS calcd. for $C_{26}H_{22}N_2O_3S$ [M^+]: 442.1351; Found: 442.1350.

(17) Synthesis of (*E*)-2-phenyl-5-(4-phenylbuta-1,3-dien-2-yl)-4,5-dihydrooxazole (3aq).

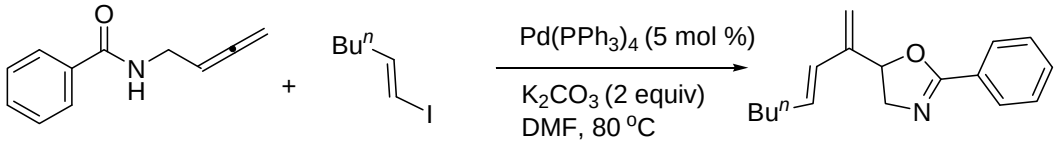


1a (*E*)-**2q** (1.2 equiv) (*E*)-**3aq**

The reaction of K_2CO_3 (55.5 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.6 mg, 0.01 mmol), **1a**

(35.2 mg, 0.2 mmol), (*E*)-**2q** (55.7 mg, 0.24 mmol), and DMF (2 mL) afforded (*E*)-**3aq** (32.3 mg, 58%) (eluent: petroleum ether/ethyl acetate = 10:1): solid; mp 100-101 °C (*n*-hexane/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, *J* = 6.9 Hz, 2 H, ArH), 7.53-7.21 (m, 8 H, ArH), 6.83 (d, *J* = 16.5 Hz, 1 H, one proton in CH=CHPh), 6.49 (d, *J* = 16.8 Hz, 1 H, one proton in CH=CHPh), 5.50 (t, *J* = 9.2 Hz, 1 H, OCH), 5.38 (s, 1 H, one proton in C=CH_2), 5.31 (s, 1 H, one proton in C=CH_2), 4.44 (dd, *J* = 14.6, 10.4 Hz, 1 H, one proton in NCH_2), 3.89 (dd, *J* = 14.7, 7.8 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 144.7, 136.6, 131.4, 129.2, 128.6, 128.4, 128.2, 127.9, 127.5, 127.2, 126.4, 114.5, 78.4, 61.4; IR (neat) 1650, 1603, 1578, 1495, 1449, 1339, 1262, 1179, 1080, 1065, 1024 cm^{-1}; MS (EI) *m/z* (%) 275 (M^+, 20.65), 117 (100); Anal. Calcd. for $C_{19}H_{17}NO$: C, 82.88; H, 6.22; N, 5.09; Found: C, 82.73, H, 6.25; N, 5.05.

(18) Synthesis of (*E*)-5-(octa-1,3-dien-2-yl)-2-phenyl-4,5-dihydrooxazole (3ar).

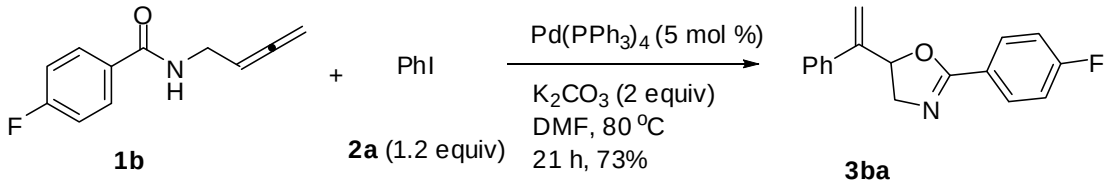


1a (*E*)-**2r** (1.2 equiv) (*E*)-**3ar**

The reaction of K_2CO_3 (55.3 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.9 mg, 0.01 mmol), **1a** (34.5 mg, 0.2 mmol), (*E*)-**2r** (50.5 mg, 0.24 mmol), and DMF (2 mL) afforded (*E*)-**3ar** (39.3 mg, 77%) (eluent: petroleum ether/ethyl acetate = 5:1): liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.2 Hz, 2 H, ArH), 7.52-7.31 (m, 3 H, ArH), 6.07 (d, *J* = 16.2 Hz, 1 H, CH=C), 5.68-5.55 (m, 1 H, C=CH), 5.31 (t, *J* = 9.0 Hz, 1 H, OCH), 5.16 (s, 1 H, one proton in C=CH_2), 5.03 (s, 1 H, one proton in C=CH_2), 4.30 (dd, *J* = 14.0, 11.0 Hz, 1 H, one proton in NCH_2), 3.79 (dd, *J* = 14.4, 8.1 Hz, 1

H, one proton in NCH_2), 2.18-2.01 (m, 2 H, -CH_2), 1.45-1.22 (m, 4 H, -CH_2CH_2), 0.89 (t, J = 6.6 Hz, 3 H, -CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.6, 144.6, 131.7, 131.1, 128.3, 128.2, 128.0, 127.6, 111.5, 78.6, 61.2, 32.6, 31.1, 22.0, 13.7; IR (neat) 2956, 2927, 2871, 1654, 1605, 1580, 1496, 1450, 1378, 1335, 1258, 1177, 1083, 1063, 1026 cm^{-1}; MS (EI) *m/z* (%) 255 (M^+, 14.83), 117 (100); HRMS calcd. for $C_{17}H_{21}NO$ [M^+]: 255.1623; Found: 255.1620.

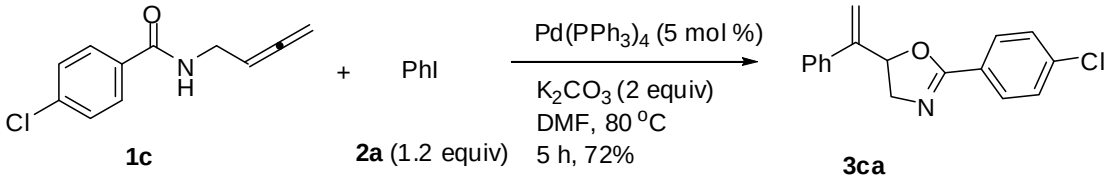
(19) Synthesis of 2-(4-flurophenyl)-5-(1-phenylvinyl)-4,5-dihydrooxazole (3ba).



The reaction of K_2CO_3 (56.0 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.5 mg, 0.01 mmol), **1b** (38.4 mg, 0.2 mmol), **2a** (50.0 mg, 0.24 mmol), and DMF (2 mL) afforded **3ba** (39.1 mg, 73%) (eluent: petroleum ether/ethyl acetate = 10:1): solid; mp 74-75 °C (petroleum ether/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (t, J = 6.5 Hz, 2 H, ArH), 7.42-7.28 (m, 5 H, ArH), 7.12 (t, J = 8.1 Hz, 2 H, ArH), 5.60 (t, J = 8.9 Hz, 1 H, OCH), 5.46 (s, 1 H, one proton in C=CH_2), 5.40 (s, 1 H, one proton in C=CH_2), 4.33-4.20 (m, 1 H, one proton in NCH_2), 3.79 (dd, J = 14.6, 7.7 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.7 (d, J = 250.7 Hz), 162.8, 146.7, 137.8, 130.4 (d, J = 8.6 Hz), 128.6, 128.1, 126.5, 123.8 (d, J = 2.9 Hz), 115.5 (d, J = 22.0 Hz), 112.4, 80.2, 61.0; ^{19}F NMR ($CDCl_3$, 282 MHz) -107.98; IR (neat) 1654, 1623, 1604, 1506, 1411, 1365, 1340, 1327, 1292, 1281, 1267, 1237, 1221, 1151, 1066, 1014 cm^{-1}; MS (EI) *m/z* (%) 267 (M^+, 27.08), 135 (100); Anal.

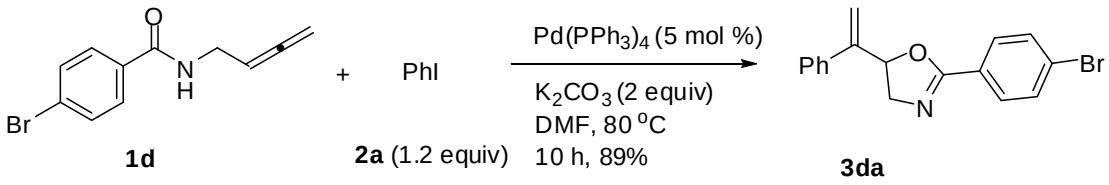
Calcd. for $C_{17}H_{14}FNO$: C, 76.39; H, 5.28; N, 5.24; Found: C, 76.45, H, 5.31; N, 5.28.

(20) Synthesis of 2-(4-chlorophenyl)-5-(1-phenylvinyl)-4,5-dihydrooxazole (3ca).



The reaction of K_2CO_3 (54.9 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.6 mg, 0.01 mmol), **1c** (42.0 mg, 0.2 mmol), **2a** (49.0 mg, 0.24 mmol), and DMF (2 mL) afforded **3ca** (41.2 mg, 72%) (eluent: petroleum ether/ethyl acetate = 5:1): solid; mp 61-62 °C (*n*-hexane/ethtyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.0 Hz, 2 H, ArH), 7.45-7.24 (m, 7 H, ArH), 5.60 (t, *J* = 8.8 Hz, 1 H, OCH), 5.45 (s, 1 H, one proton in C=CH_2), 5.39 (s, 1 H, one proton in C=CH_2), 4.33-4.22 (m, 1 H, one proton in NCH_2), 3.79 (dd, *J* = 14.6, 7.8 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 146.6, 137.8, 137.6, 129.5, 128.7, 128.6, 128.1, 126.5, 126.1, 112.6, 80.3, 61.0; IR (neat) 1654, 1596, 1489, 1403, 1375, 1341, 1262, 1108, 1090, 1073, 1010 cm^{-1}; MS (EI) *m/z* (%) 285 (M^+(^{37}Cl), 11.80), 283 (M^+(^{35}Cl), 34.92), 151 (100); Anal. Calcd. for $C_{17}H_{14}ClNO$: C, 71.96; H, 4.97; N, 4.94; Found: C, 71.81, H, 5.08; N, 4.90.

(21) Synthesis of 2-(4-bromophenyl)-5-(1-phenylvinyl)-4,5-dihydrooxazole (3da).

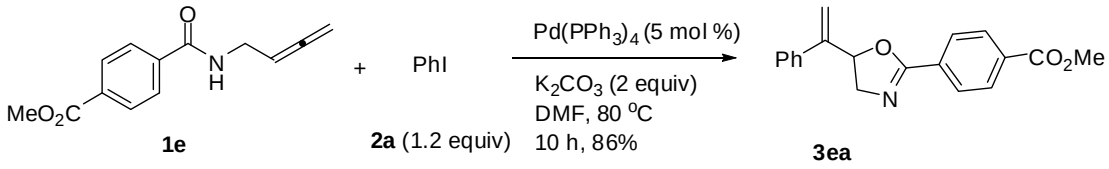


The reaction of K_2CO_3 (55.0 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.6 mg, 0.01 mmol), **1d** (50.2 mg, 0.2 mmol), **2a** (48.7 mg, 0.24 mmol), and DMF (2 mL) afforded **3da** (58.2 mg, 89%) (eluent: petroleum ether/ethyl acetate = 10:1): solid; mp 66-67 °C (*n*-hexane/ethtyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.0 Hz, 2 H, ArH), 7.56 (d, *J* = 8.0 Hz, 2 H, ArH), 7.41-7.32 (m, 5 H, ArH), 5.59 (t, *J* = 9.0 Hz, 1 H, OCH), 5.45 (s, 1 H, one proton in C=CH_2), 5.39 (s, 1 H, one proton in C=CH_2), 4.32-4.20 (m, 1 H, one proton in NCH_2), 3.78 (dd, *J* = 14.6, 7.8 Hz, 1 H, one proton in NCH_2).

The gram scale synthesis of 3da: After the Schlenk tube containing K_2CO_3 (1.1060 g, 8 mmol) was flamed-dried and filled with nitrogen, $Pd(PPh_3)_4$ (46.6 mg, 0.04 mmol), **1d** (1.0086 g, 4 mmol), **2a** (0.9797 g, 4.8 mmol), and DMF (10 mL) were added sequentially. The resulting solution was heated to and stirred at 80 °C. When the reaction was completed as monitored by TLC, the solvent was diluted with diethyl ether (50 mL) and washed with water (5 mL×3). Then the organic layers were dried over anhydrous Na_2SO_4 and evaporated. The residue was purified by chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 5:1) to afford **3da** (1.1476 g, 87%): solid; mp 66-67 °C (*n*-hexane/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93-7.83 (m, 2 H, ArH), 7.62-7.53 (m, 2 H, ArH), 7.41-7.30 (m, 5 H, ArH), 5.67-5.55 (m, 1 H, OCH), 5.45 (s, 1 H, one proton in C=CH_2), 5.39 (s, 1 H, one proton in C=CH_2), 4.27 (dd, *J* = 14.9, 10.1 Hz, 1 H, one

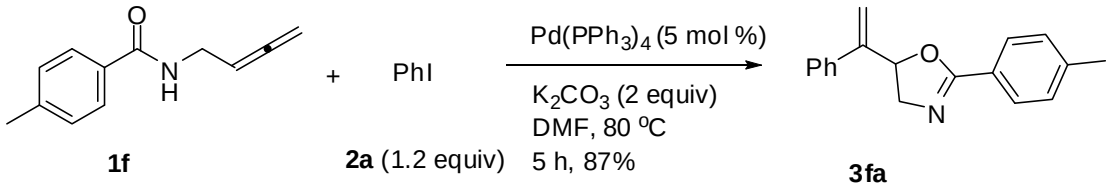
proton in NCH_2), 3.78 (dd, *J* = 14.9, 7.7 Hz, 1 H, one proton in NCH_2) ; ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.0, 146.6, 137.8, 131.7, 129.7, 128.6, 128.1, 126.6, 126.5, 126.1, 112.6, 80.3, 61.0; IR (neat) 1656, 1591, 1573, 1526, 1499, 1483, 1446, 1397, 1375, 1328, 1259, 1187, 1107, 1071 cm^{-1}; MS (EI) *m/z* (%) 329 (M^+(^{81}Br), 39.22), (M^+(^{79}Br), 38.39), 195 (100); Anal. Calcd. for $C_{17}H_{14}BrNO$: C, 62.21; H, 4.30; N, 4.27; Found: C, 62.27, H, 4.49; N, 4.29.

(22) Synthesis of methyl 4-(5-(1-phenylvinyl)-4,5-dihydrooxazol-2-yl)benzoate (3ea).



The reaction of K_2CO_3 (55.9 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.8 mg, 0.01 mmol), **1e** (47.0 mg, 0.2 mmol), **2a** (49.3 mg, 0.24 mmol), and DMF (2 mL) afforded **3ea** (53.5 mg, 86%) (eluent: petroleum ether/ethyl acetate = 5:1): solid; mp 97-98 °C (*n*-hexane/ethtyl acetate); ^1H NMR (300 MHz, $CDCl_3$) δ 8.15-8.03 (m, 4 H, ArH), 7.42-7.25 (m, 5 H, ArH), 5.63 (t, *J* = 9.0 Hz, 1 H, OCH), 5.46 (s, 1 H, one proton in $C=CH_2$), 5.41 (s, 1 H, one proton in $C=CH_2$), 4.31 (dd, *J* = 15.2, 10.4 Hz, 1 H, one proton in NCH_2), 3.93 (s, 3 H, OCH_3), 3.82 (dd, *J* = 15.2, 7.7 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.3, 163.0, 146.5, 137.7, 132.5, 131.6, 129.6, 128.6, 128.1, 126.5, 112.6, 80.3, 61.1, 52.2; IR (neat) 1714, 1652, 1609, 1571, 1497, 1440, 1410, 1277, 1264, 1192, 1112, 1075, 1020, 1010 cm^{-1}; MS (EI) *m/z* (%) 307 (M^+, 36.50), 175 (100); Anal. Calcd. for $C_{19}H_{17}NO_3$: C, 74.25; H, 5.58; N, 4.56; Found: C, 74.04, H, 5.68; N, 4.51.

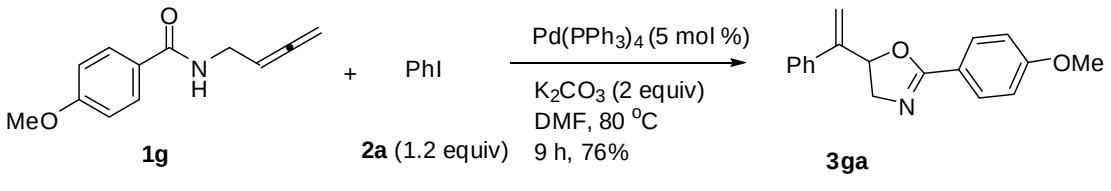
(23) Synthesis of 5-(1-phenylvinyl)-2-p-tolyl-4,5-dihydrooxazole (3fa).



1f **2a** (1.2 equiv) 5 h, 87% **3fa**

The reaction of K_2CO_3 (55.5 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.7 mg, 0.01 mmol), **1f** (37.0 mg, 0.2 mmol), **2a** (50.1 mg, 0.24 mmol), and DMF (2 mL) afforded **3fa** (45.2 mg, 87%) (eluent: petroleum ether/ethyl acetate = 10:1): oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.1 Hz, 2 H, ArH), 7.42-7.26 (m, 5 H, ArH), 7.23 (d, *J* = 7.8 Hz, 2 H, ArH), 5.63-5.51 (m, 1 H, OCH), 5.44 (s, 1 H, one proton in $C=CH_2$), 5.41 (s, 1 H, one proton in $C=CH_2$), 4.26 (dd, *J* = 14.7, 10.2 Hz, 1 H, one proton in NCH_2), 3.78 (dd, *J* = 14.7, 7.8 Hz, 1 H, one proton in NCH_2), 2.39 (s, 3 H, $ArCH_3$); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 146.8, 141.7, 137.9, 129.1, 128.5, 128.1, 128.0, 126.5, 124.8, 112.3, 79.9, 60.9, 21.5; IR (neat) 2922, 2851, 1651, 1622, 1573, 1511, 1498, 1460, 1404, 1364, 1339, 1326, 1282, 1266, 1175, 1110, 1068, 1018 cm^{-1}; MS (EI) *m/z* (%) 263 (M^+, 30.74), 131(100); HRMS calcd. for $C_{18}H_{17}NO$ [M^+]: 263.1310; Found: 263.1311.

(24) Synthesis of 2-(4-methoxyphenyl)-5-(1-phenylvinyl)-4,5-dihydrooxazole (3ga).

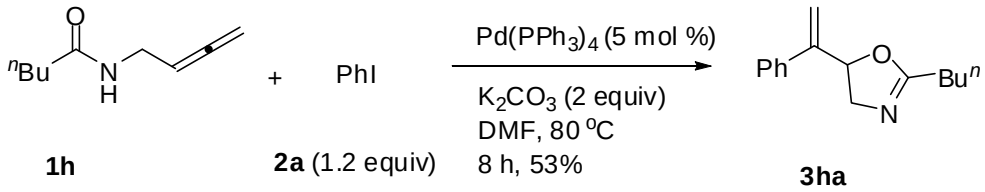


1g **2a** (1.2 equiv) 9 h, 76% **3ga**

The reaction of K_2CO_3 (55.8 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.6 mg, 0.01 mmol), **1g** (38.0 mg, 0.2 mmol), **2a** (49.0 mg, 0.24 mmol), and DMF (2 mL) afforded **3ga**

(39.7 mg, 76%) (eluent: petroleum ether/ethyl acetate = 5:1): solid; mp 104-106 °C (hexane/ethtyl acetate); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.4 Hz, 2 H, ArH), 7.40-7.28 (m, 5 H, ArH), 6.94 (d, *J* = 8.7 Hz, 2 H, ArH), 5.58 (t, *J* = 8.9 Hz, 1 H, OCH), 5.45 (s, 1 H, one proton in C=CH_2), 5.41 (s, 1 H, one proton in C=CH_2), 4.26 (dd, *J* = 14.4, 10.2 Hz, 1 H, one proton in NCH_2), 3.86 (s, 3 H, OMe), 3.77 (dd, *J* = 14.6, 7.7 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.5, 162.0, 146.8, 137.9, 129.8, 128.5, 128.0, 126.5, 120.1, 113.7, 112.3, 79.9, 60.9, 55.3; IR (neat) 2926, 2852, 1650, 1634, 1606, 1510, 1455, 1371, 1338, 1328, 1309, 1254, 1169, 1072, 1024 cm^{-1}; MS (EI) *m/z* (%) 279 (M^+, 33.63), 147 (100); Anal. Calcd. for $C_{18}H_{17}NO_2$: C, 77.40; H, 6.13; N, 5.01; Found: C, 77.06, H, 6.07; N, 4.98.

(25) Synthesis of 5-(hex-1-en-2-yl)-2-phenyl-4,5-dihydrooxazole (3ha).

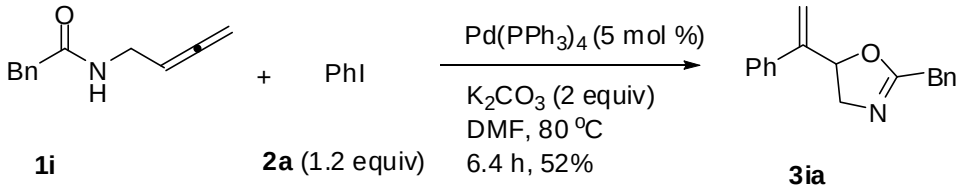


1h **2a** (1.2 equiv) **3ha**

The reaction of K_2CO_3 (55.5 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.5 mg, 0.01 mmol), **1h** (30.3 mg, 0.2 mmol), **2a** (49.5 mg, 0.24 mmol), and DMF (2 mL) afforded **3ha** (24.2 mg, 53%) (eluent: petroleum ether/ethyl acetate/Et_3N = 10:1:0.1): liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38-7.25 (m, 5 H, ArH), 5.43-5.31 (m, 3 H, OCH and C=CH_2), 4.05 (dd, *J* = 14.0, 10.4 Hz, 1 H, one proton in NCH_2), 3.56 (dd, *J* = 14.1, 8.1 Hz, 1 H, one proton in NCH_2), 2.35 (t, *J* = 7.7 Hz, 2 H, CH_2), 1.74-1.60 (m, 2 H, CH_2), 1.50-1.32 (m, 2 H, CH_2), 0.94 (t, *J* = 7.4 Hz, 3 H, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.9, 147.1, 138.0, 128.5, 128.0, 126.5, 112.1, 79.7, 60.5, 28.0,

27.9, 22.3, 13.7; IR (neat) 2958, 2931, 2873, 1673, 1633, 1497, 1466, 1380, 1290, 1234, 1172, 1107 cm^{-1}; MS (EI) *m/z* (%) 229 (M^+, 3.60), 187 (100); HRMS calcd. for $C_{15}H_{19}NO$ [M^+]: 229.1467; Found: 229.1468.

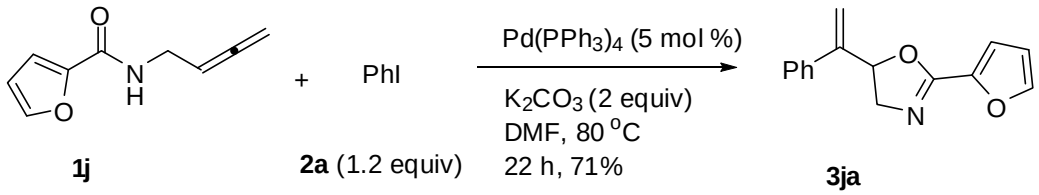
(26) Synthesis of 2-benzyl-5-(1-phenylvinyl)-4,5-dihydrooxazole (3ia).



1i **2a** (1.2 equiv) **3ia**

The reaction of K_2CO_3 (55.9 mg, 0.4 mmol), $Pd(PPh_3)_4$ (11.5 mg, 0.01 mmol), **1i** (36.9 mg, 0.2 mmol), **2a** (48.5 mg, 0.24 mmol), and DMF (2 mL) afforded **3ia** (27.1 mg, 52%) (eluent: *n*-pentane/ethyl acetate/Et_3N = 5:1:0.1): liquid; ^1H NMR (300 MHz, $CDCl_3$) δ 7.37-7.22 (m, 10 H, ArH), 5.44-5.34 (m, 1 H, OCH), 5.31 (s, 1 H, one proton in $C=CH_2$), 5.14 (s, 1 H, one proton in $C=CH_2$), 4.06 (dd, *J* = 14.1, 10.5 Hz, 1 H, one proton in NCH_2), 3.71 (d, *J* = 15.0 Hz, 1 H, one proton in CH_2Ph), 3.65 (d, *J* = 15.0 Hz, 1 H, one proton in CH_2Ph), 3.56 (dd, *J* = 14.1, 7.8 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.2, 146.7, 137.8, 134.9, 129.1, 128.6, 128.5, 128.0, 127.0, 126.5, 112.4, 80.2, 60.5, 35.0; IR (neat) 3030, 2930, 1671, 1496, 1455, 1238, 1161, 1075 cm^{-1}; MS (EI) *m/z* (%) 263 (M^+, 18.81), 91 (100); HRMS calcd. for $C_{18}H_{17}NO$ [M^+]: 263.1310; Found: 263.1313.

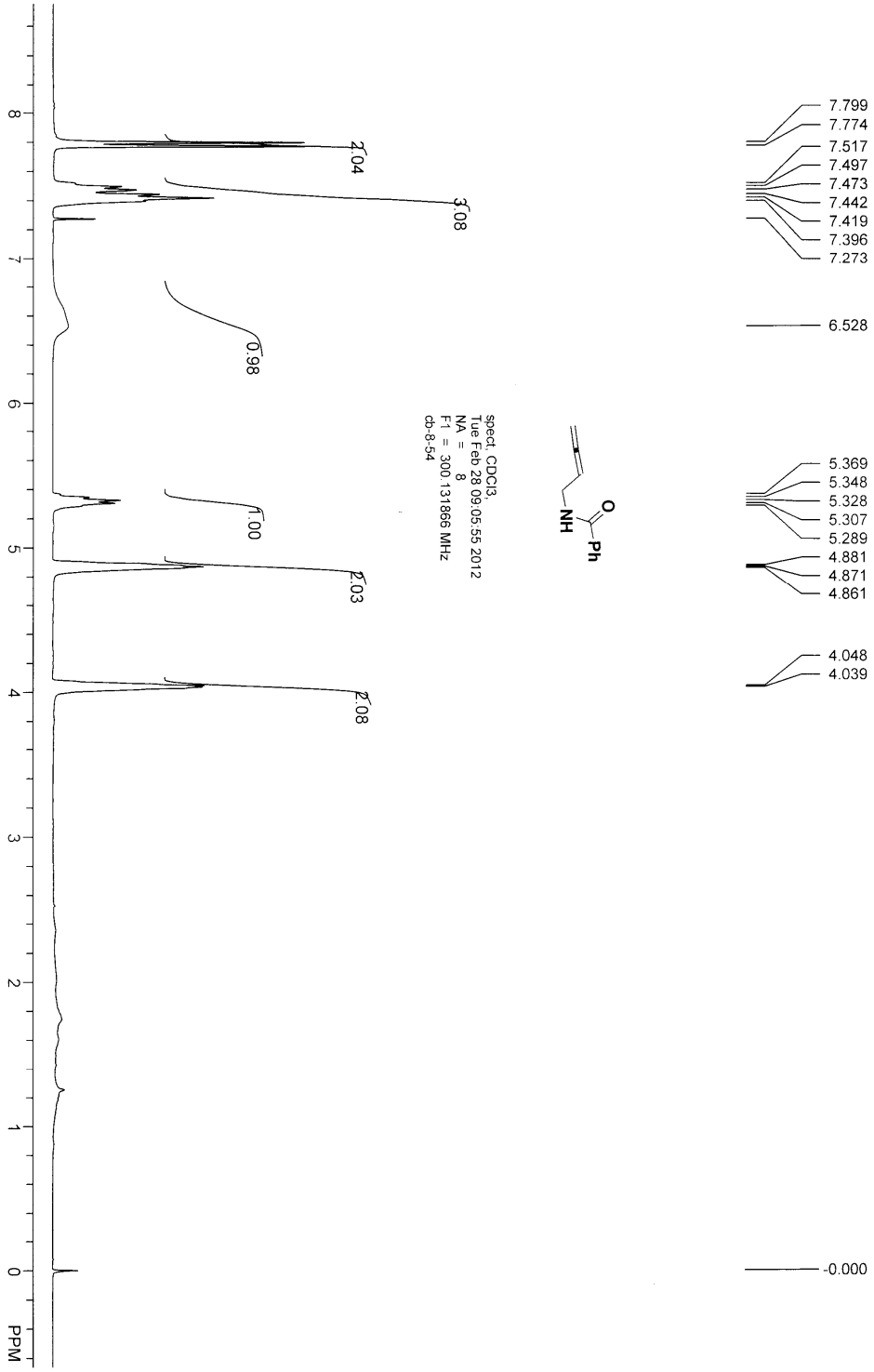
(27) Synthesis of 5-(1-(furan-2-yl)vinyl)-2-phenyl-4,5-dihydrooxazole (3ja).

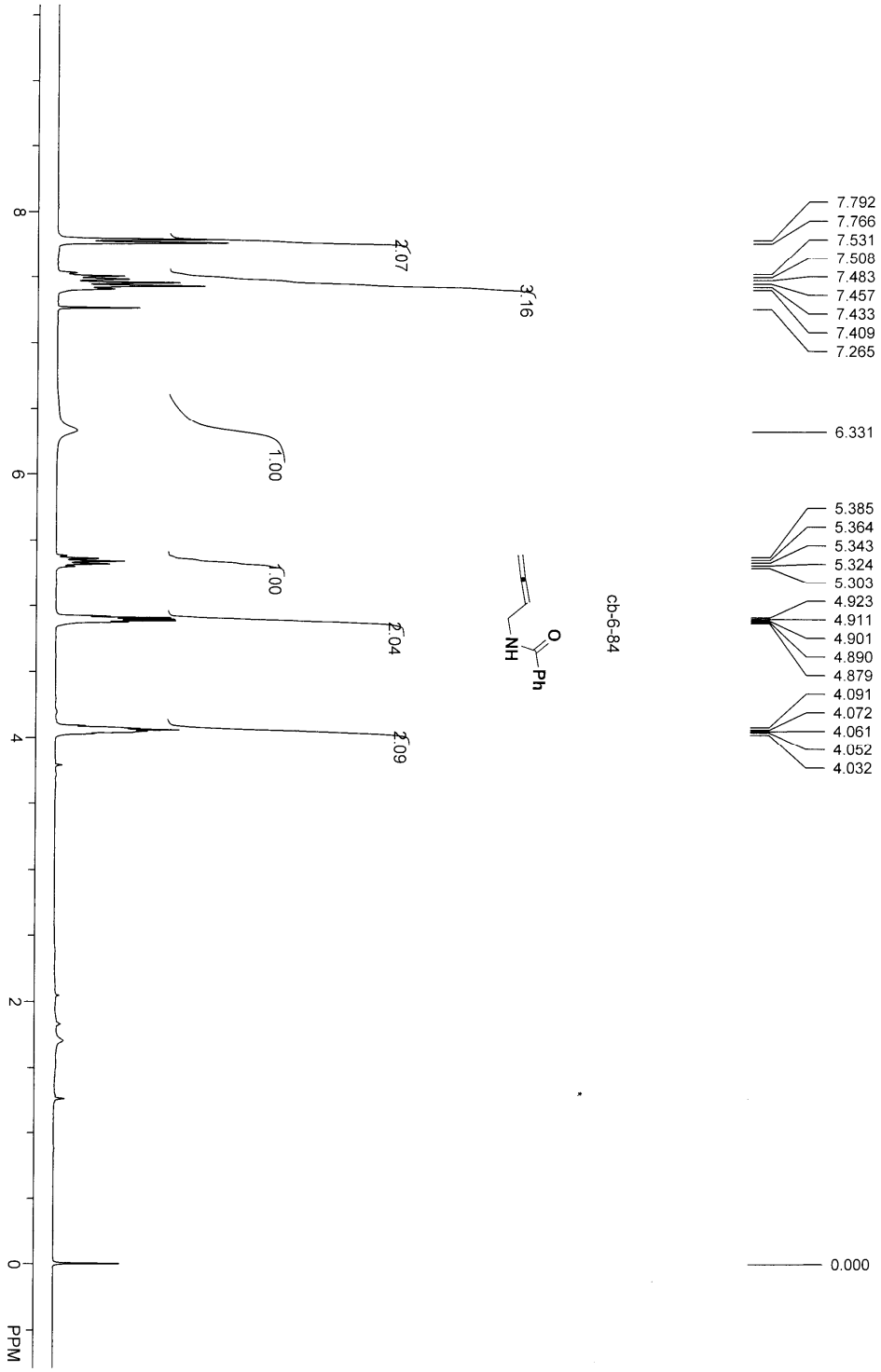


1j **2a** (1.2 equiv) **3ja**

The reaction of K_2CO_3 (56.2 mg, 0.4 mmol), $Pd(PPh_3)_4$ (12.2 mg, 0.01 mmol),

1j (32.2 mg, 0.2 mmol), **2a** (50.1 mg, 0.24 mmol), and DMF (2 mL) afforded **3ja** (33.8 mg, 71%) (eluent: petroleum ether/ethyl acetate = 5:1): liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57 (d, *J* = 0.9 Hz, 1 H, ArH), 7.38-7.28 (m, 5 H, ArH), 7.03 (d, *J* = 3.6 Hz, 1 H, ArH), 6.51 (dd, *J* = 3.5, 2.0 Hz, 1 H, ArH), 5.58 (t, *J* = 8.9 Hz, 1 H, OCH), 5.46 (s, 1 H, one proton in $C=CH_2$), 5.41 (s, 1 H, one proton in $C=CH_2$), 4.28 (dd, *J* = 14.9, 10.2 Hz, 1 H, one proton in NCH_2), 3.79 (dd, *J* = 14.7, 7.8 Hz, 1 H, one proton in NCH_2); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.2, 146.3, 145.3, 142.8, 137.7, 128.6, 128.1, 126.5, 114.3, 112.8, 111.5, 80.3, 60.8; IR (neat) 2932, 2872, 1673, 1582, 1562, 1482, 1404, 1327, 1264, 1228, 1169, 1089, 1010 cm^{-1}; MS (EI) *m/z* (%) 239 (M^+, 39.83), 107 (100); HRMS calcd. for $C_{15}H_{13}NO_2$ [M^+]: 239.0946; Found: 239.0947.

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4.890
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4.061
4.052
4.032
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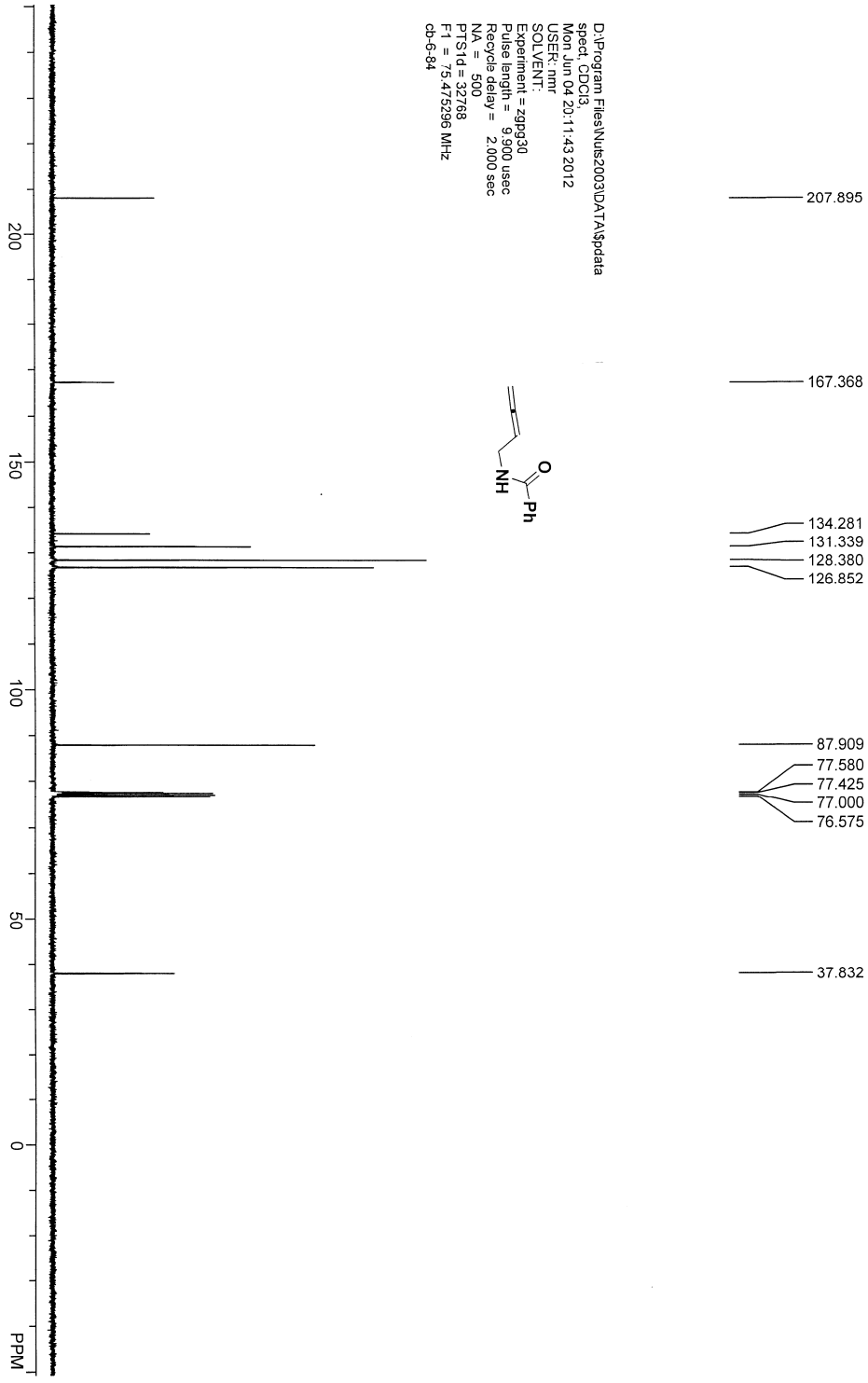
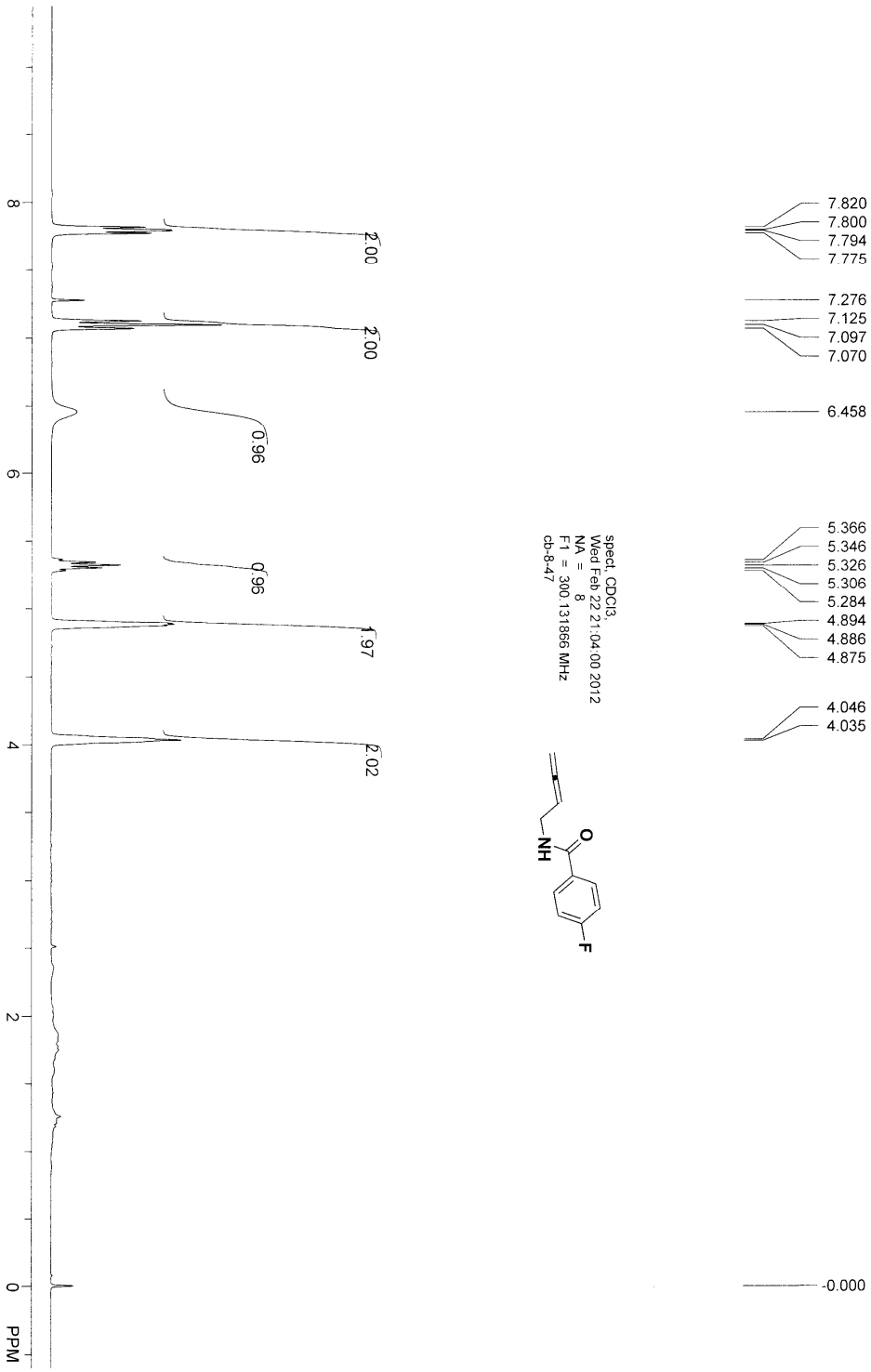
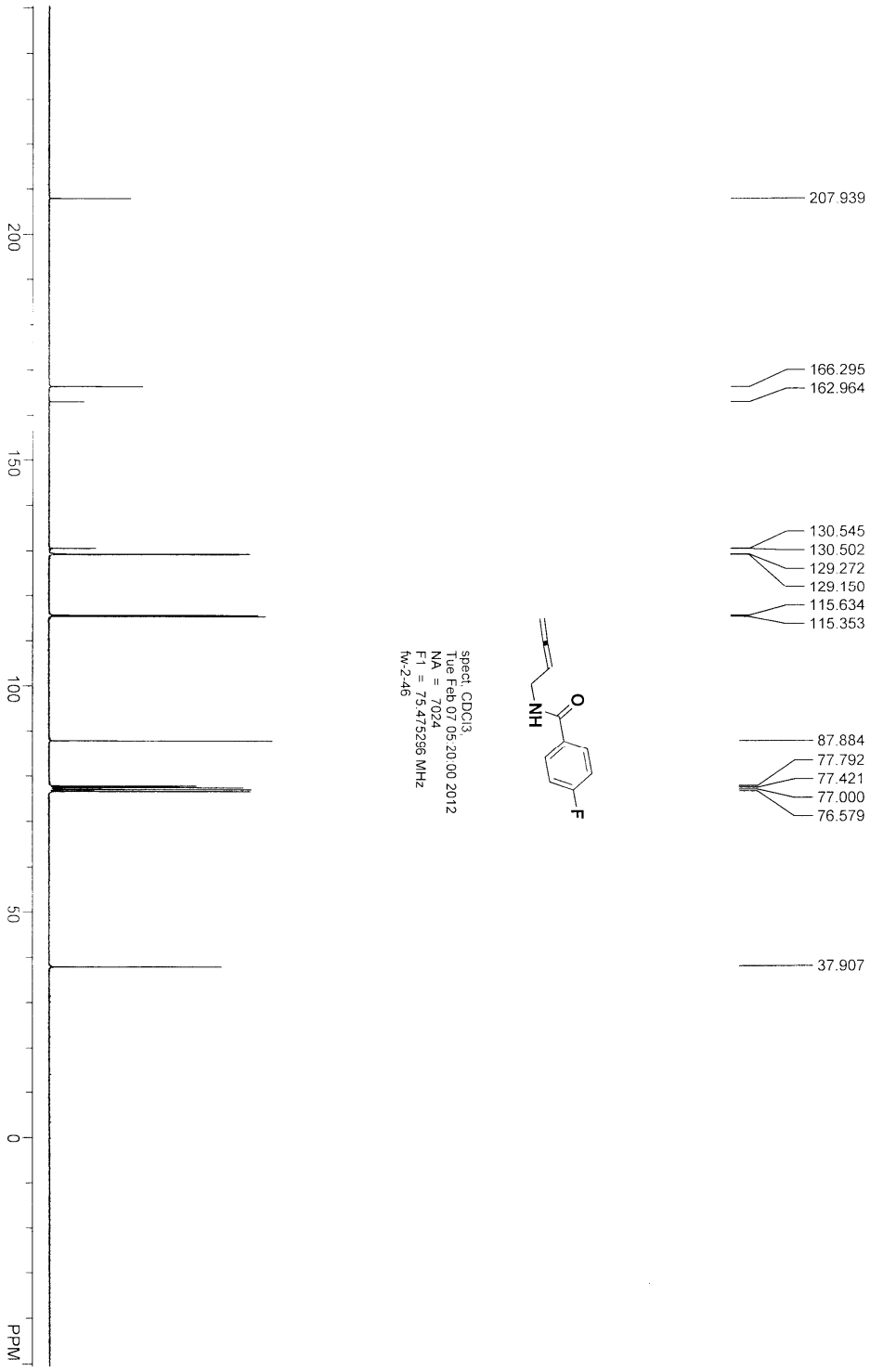
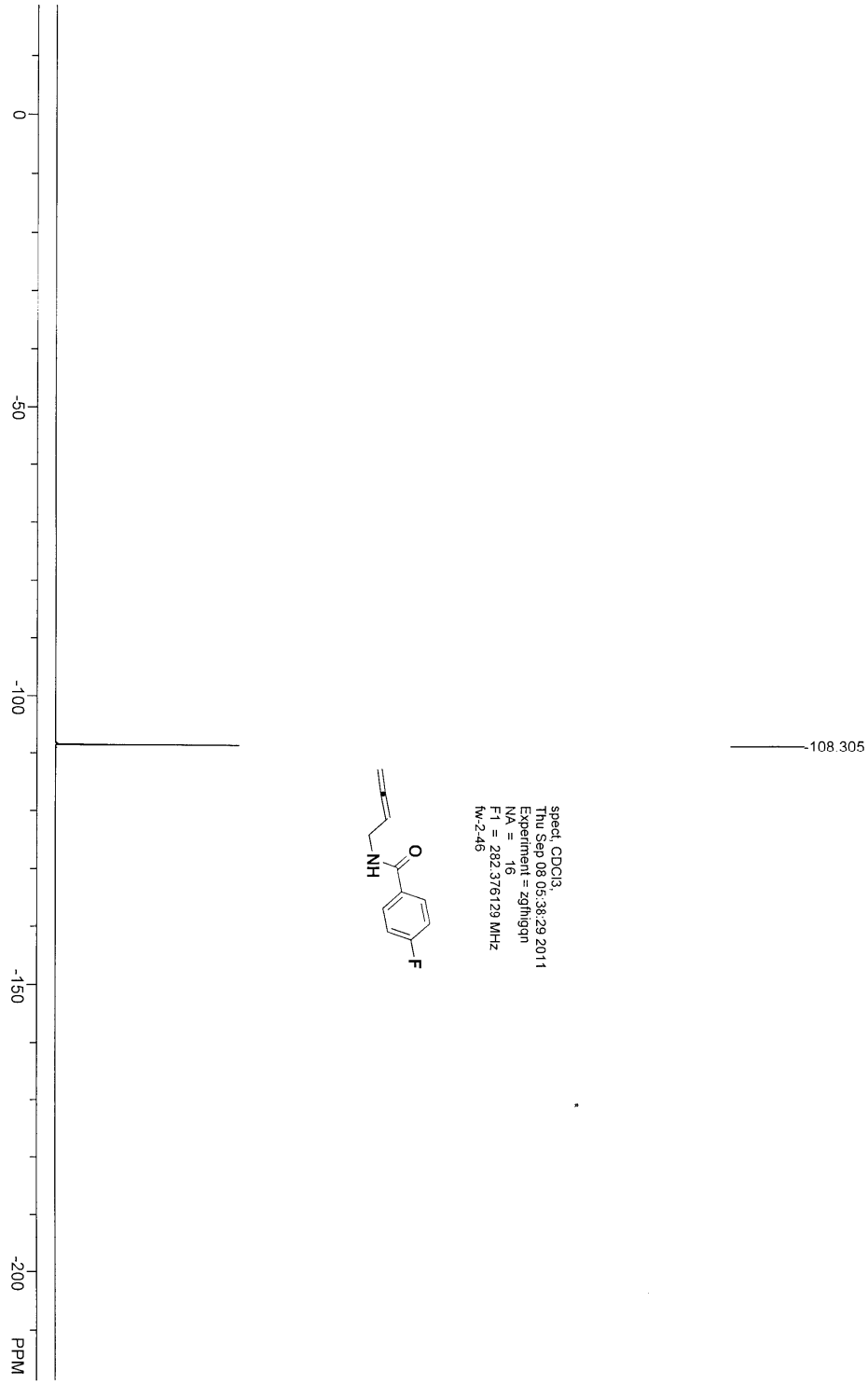
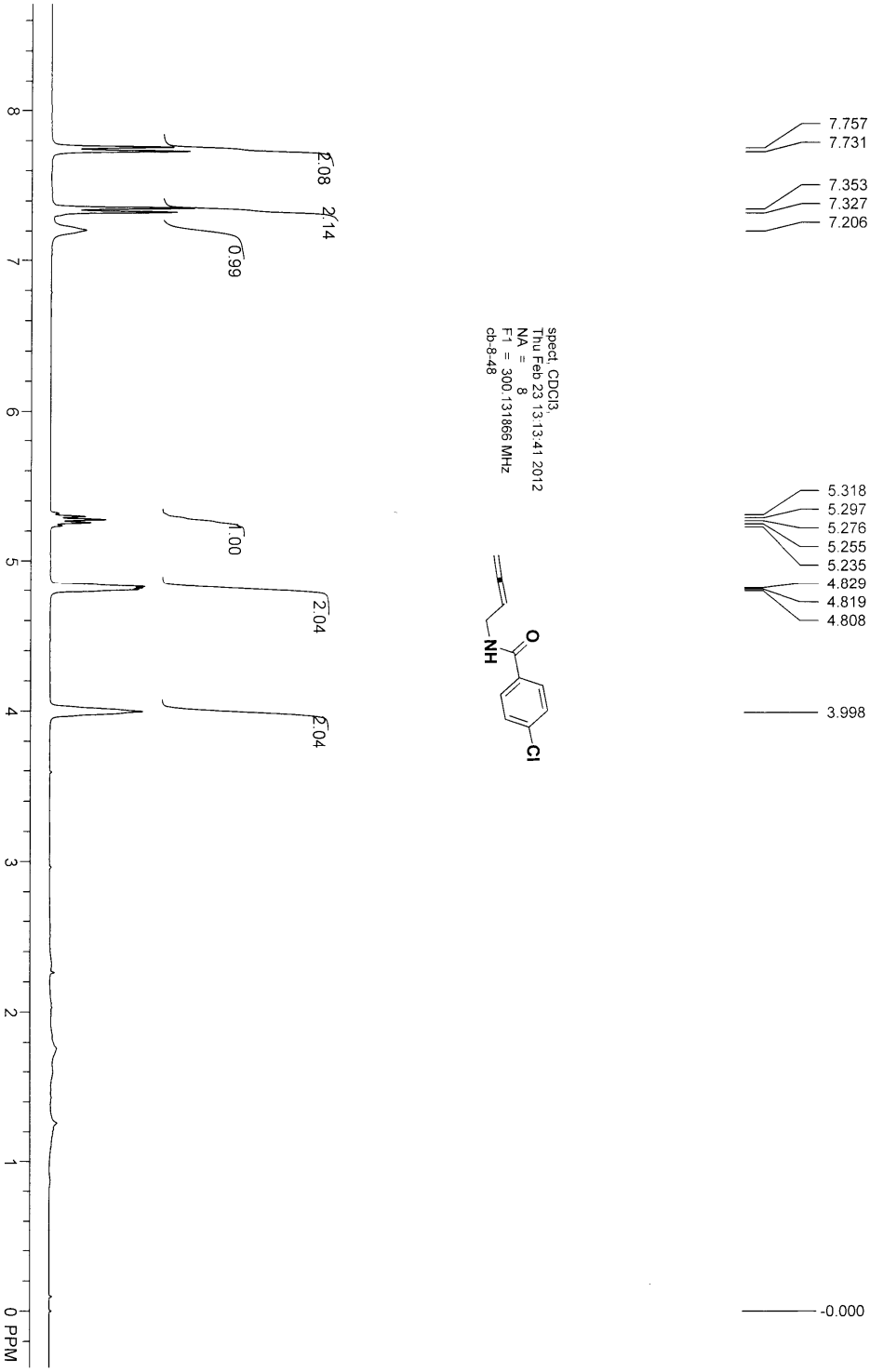
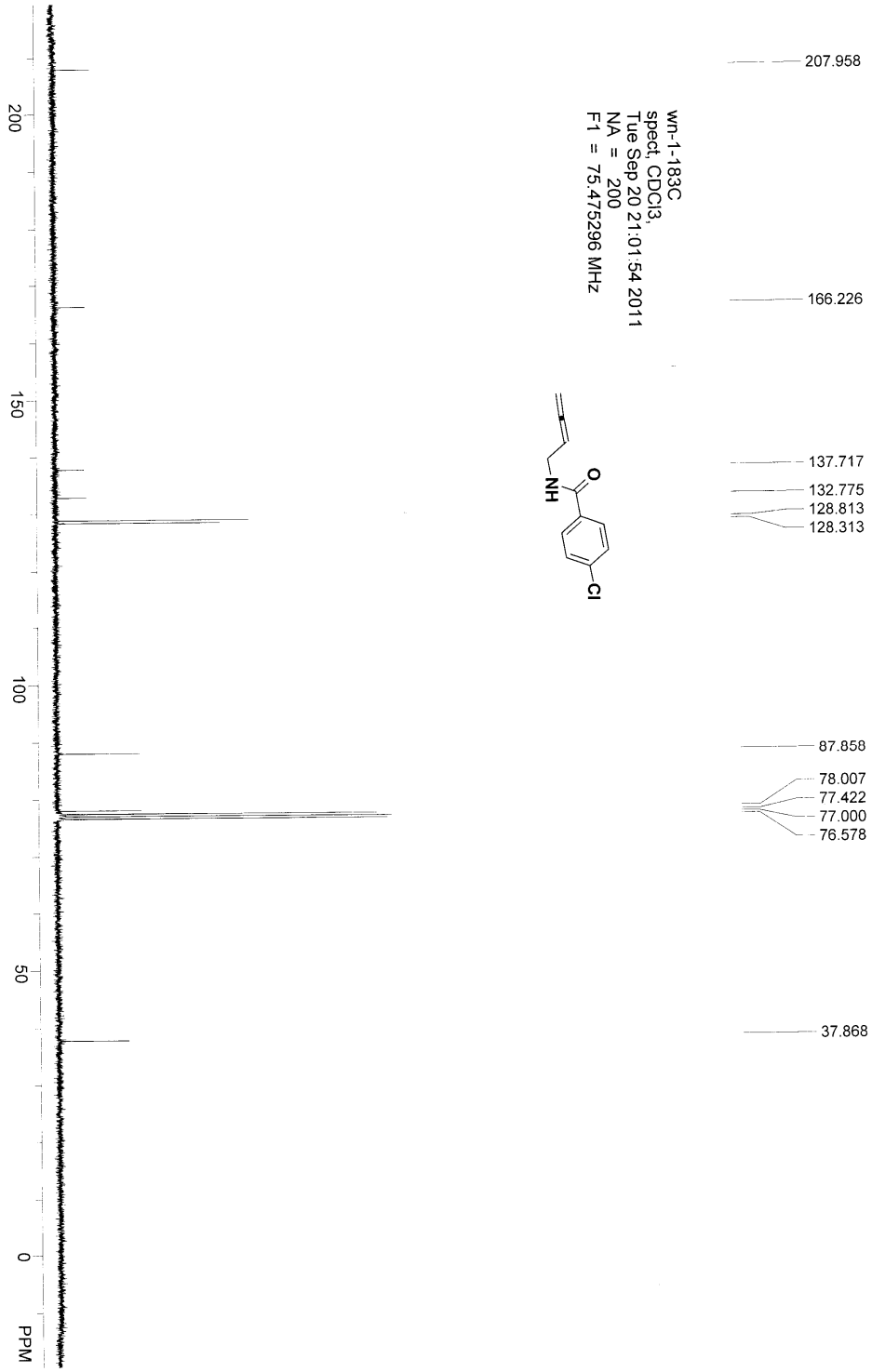


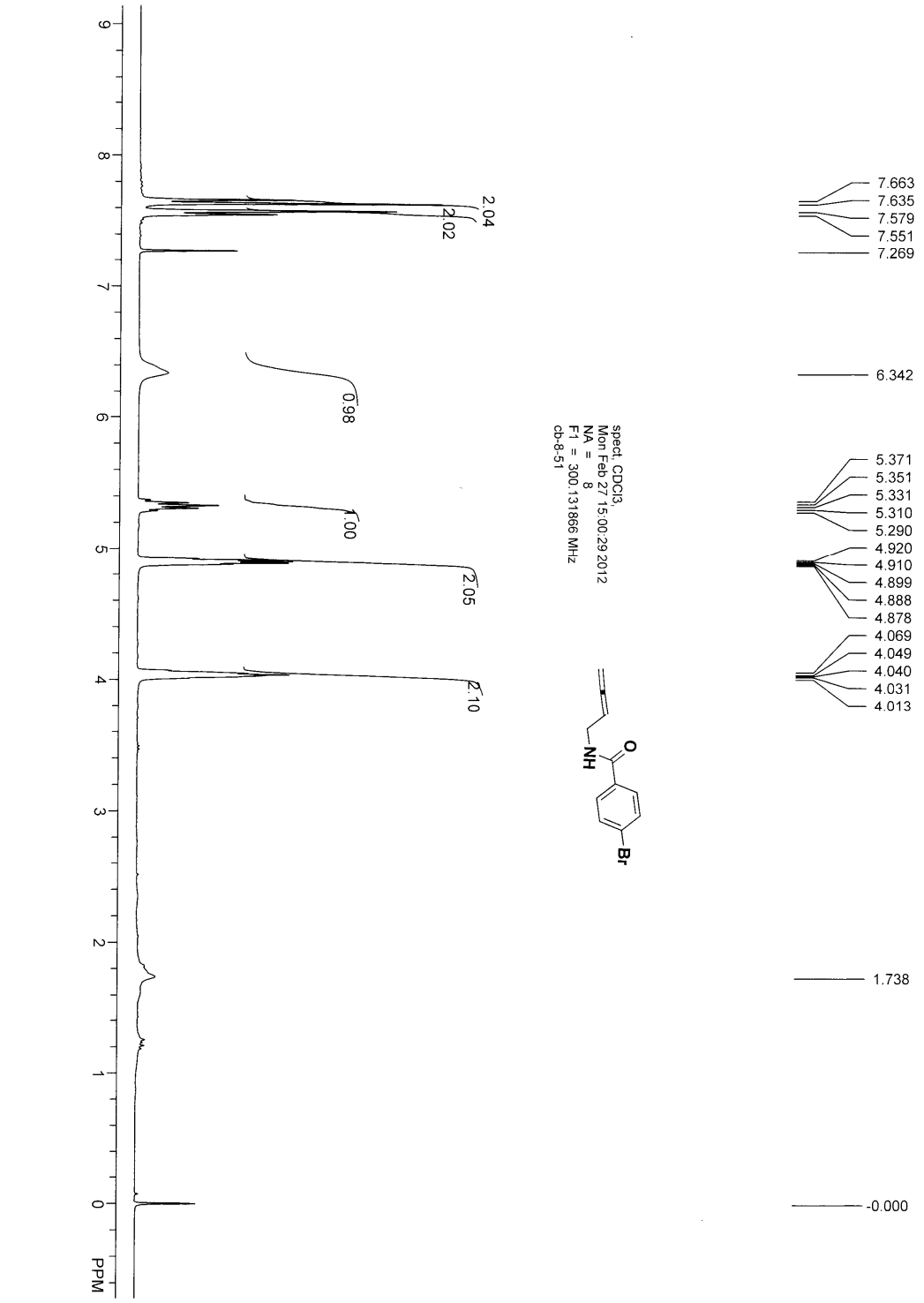


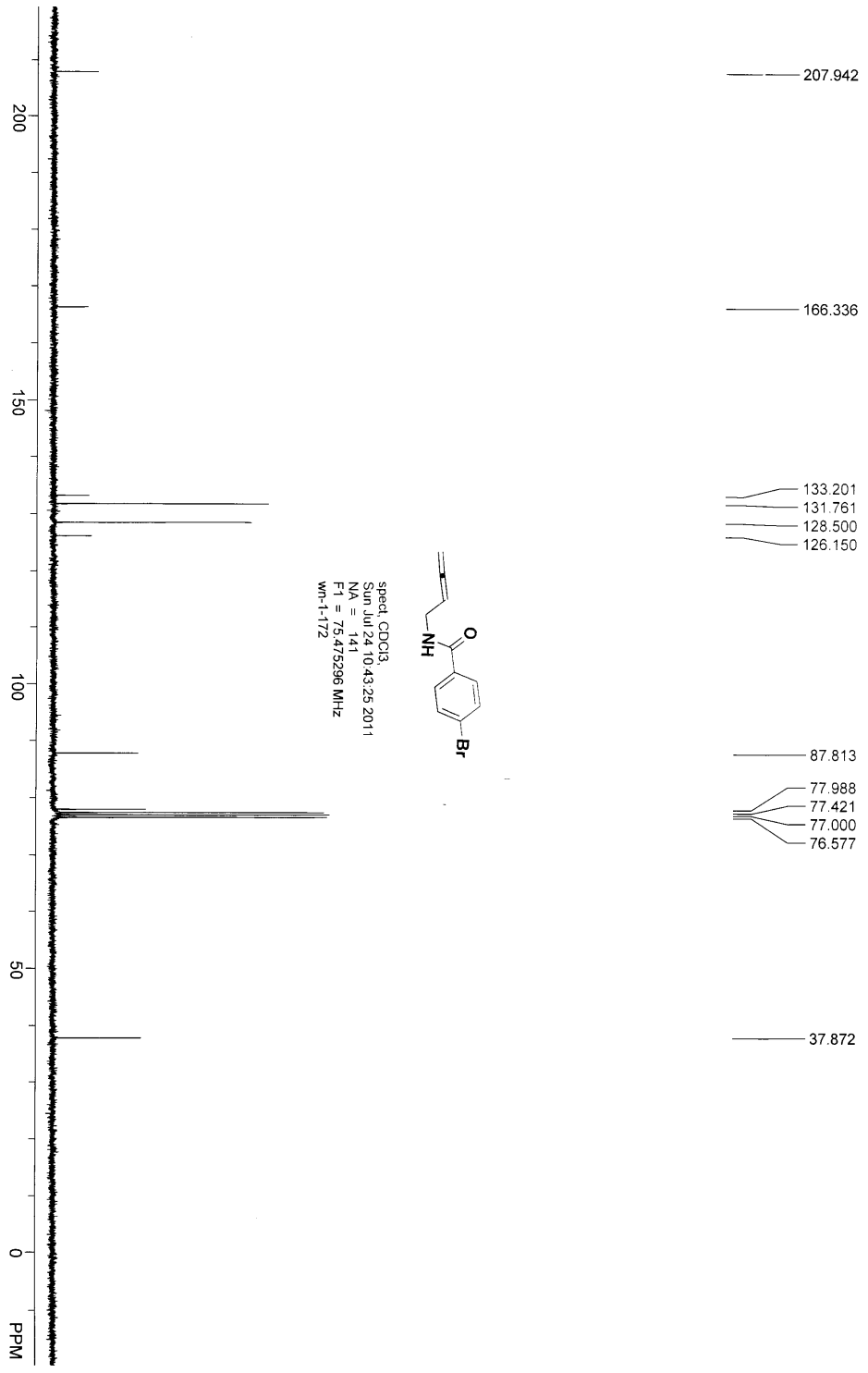


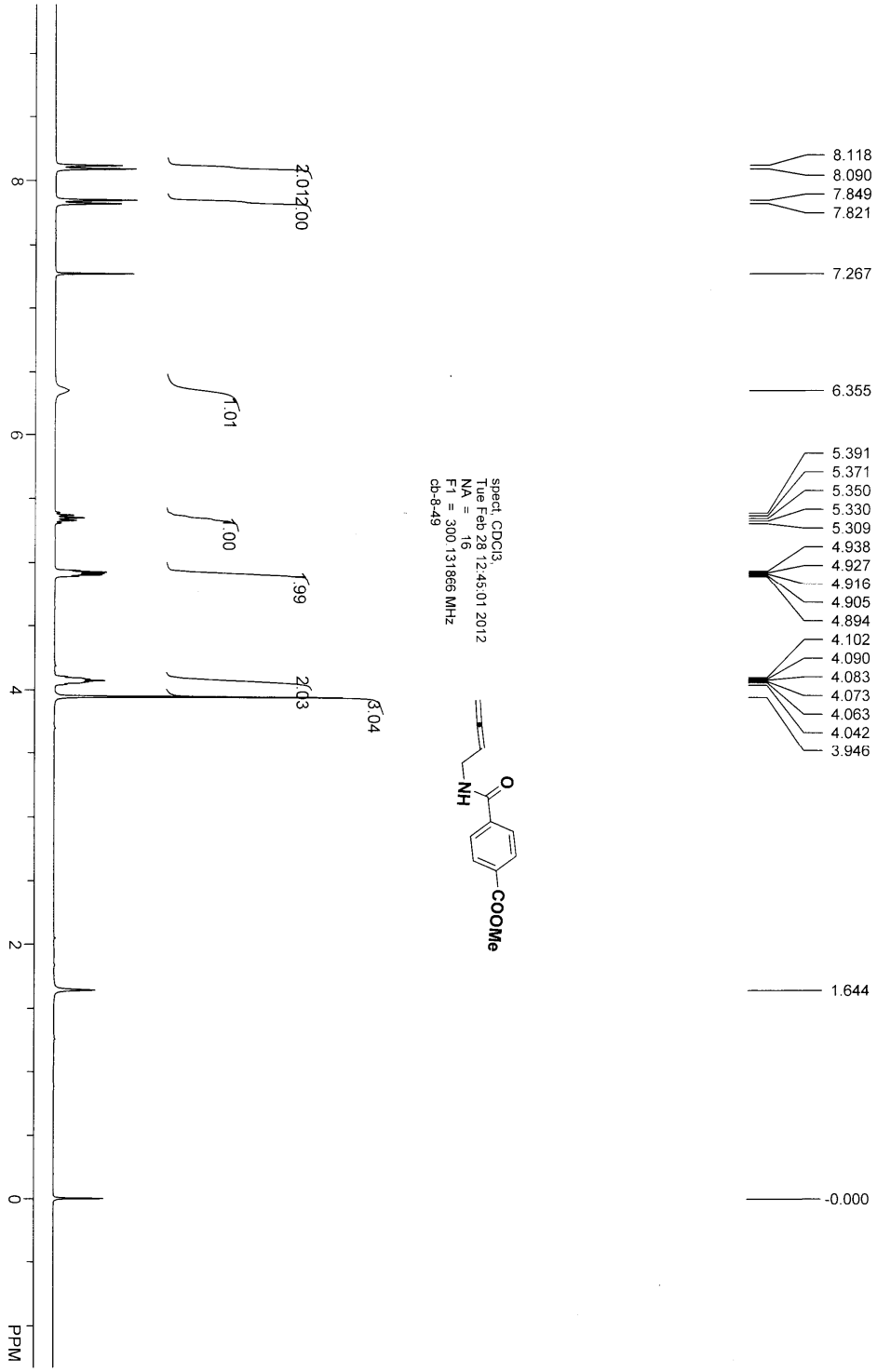


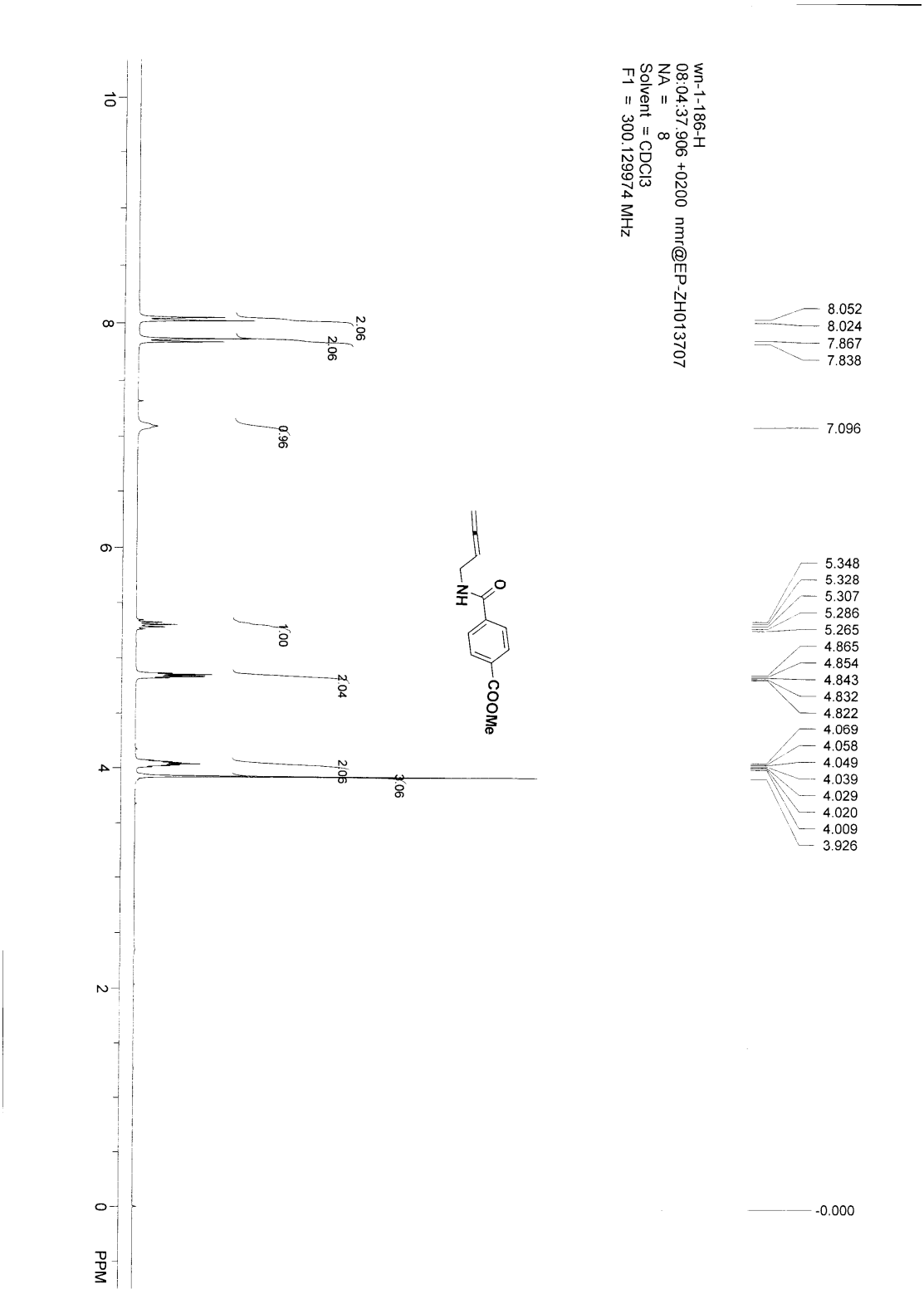


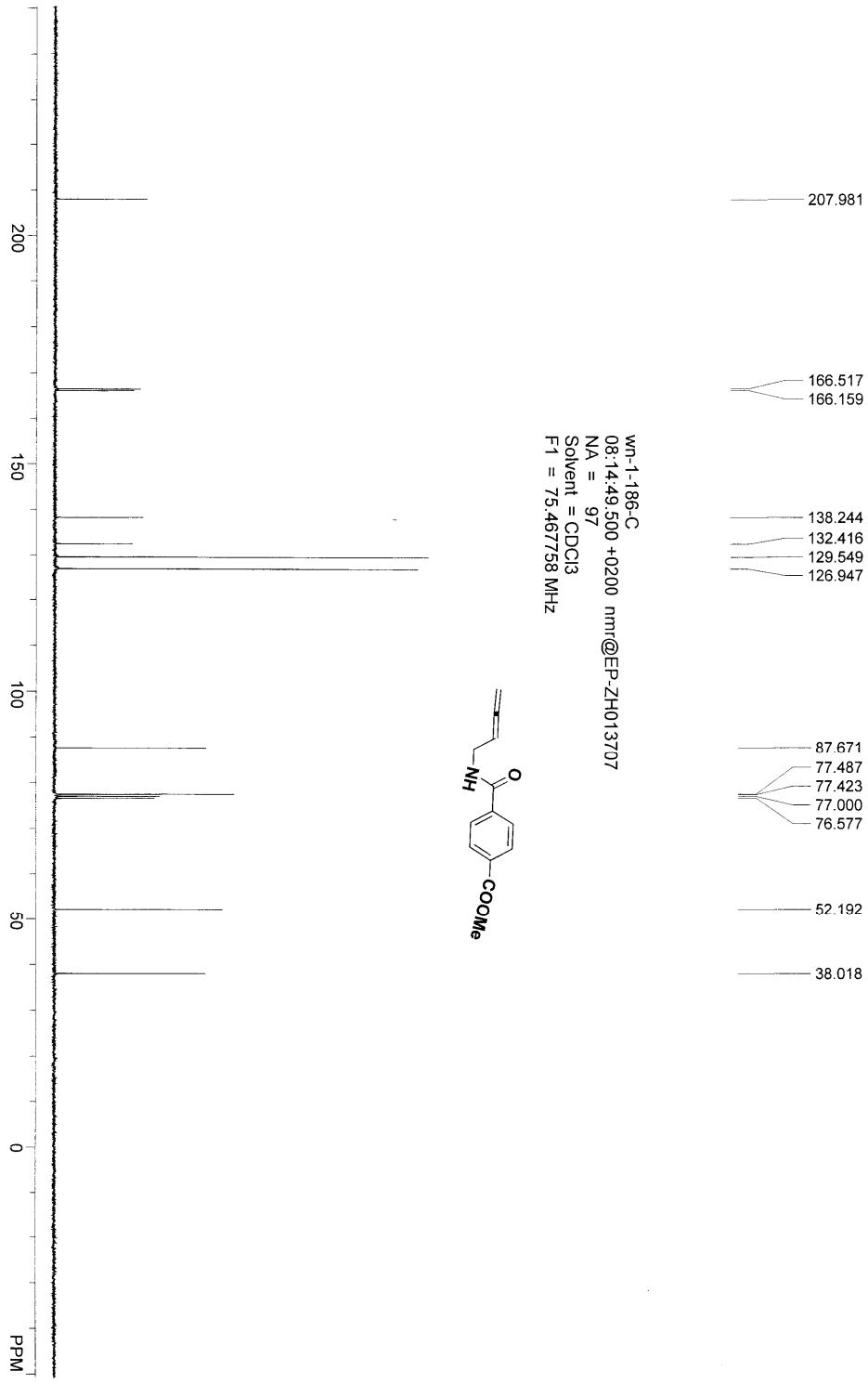


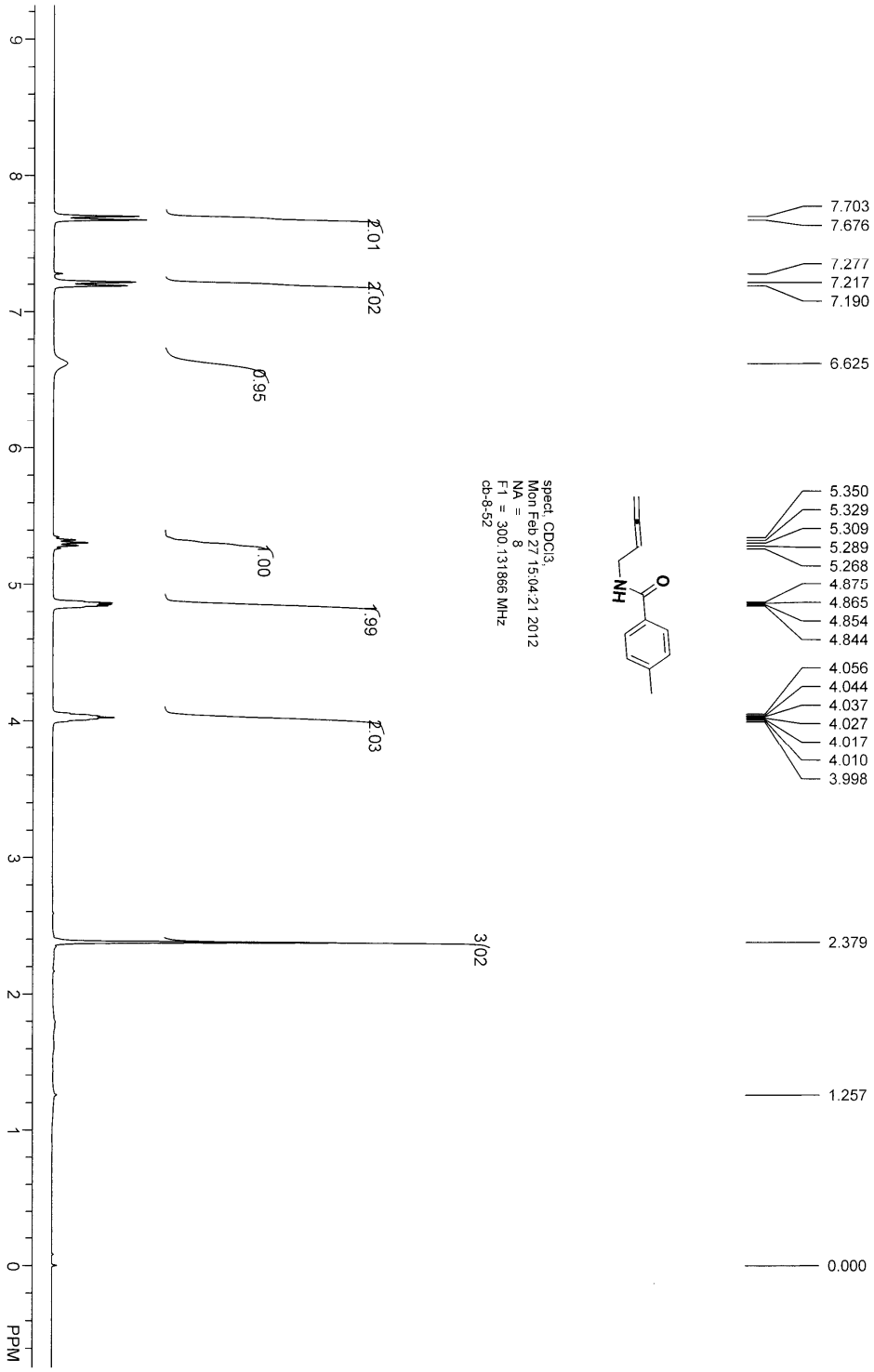


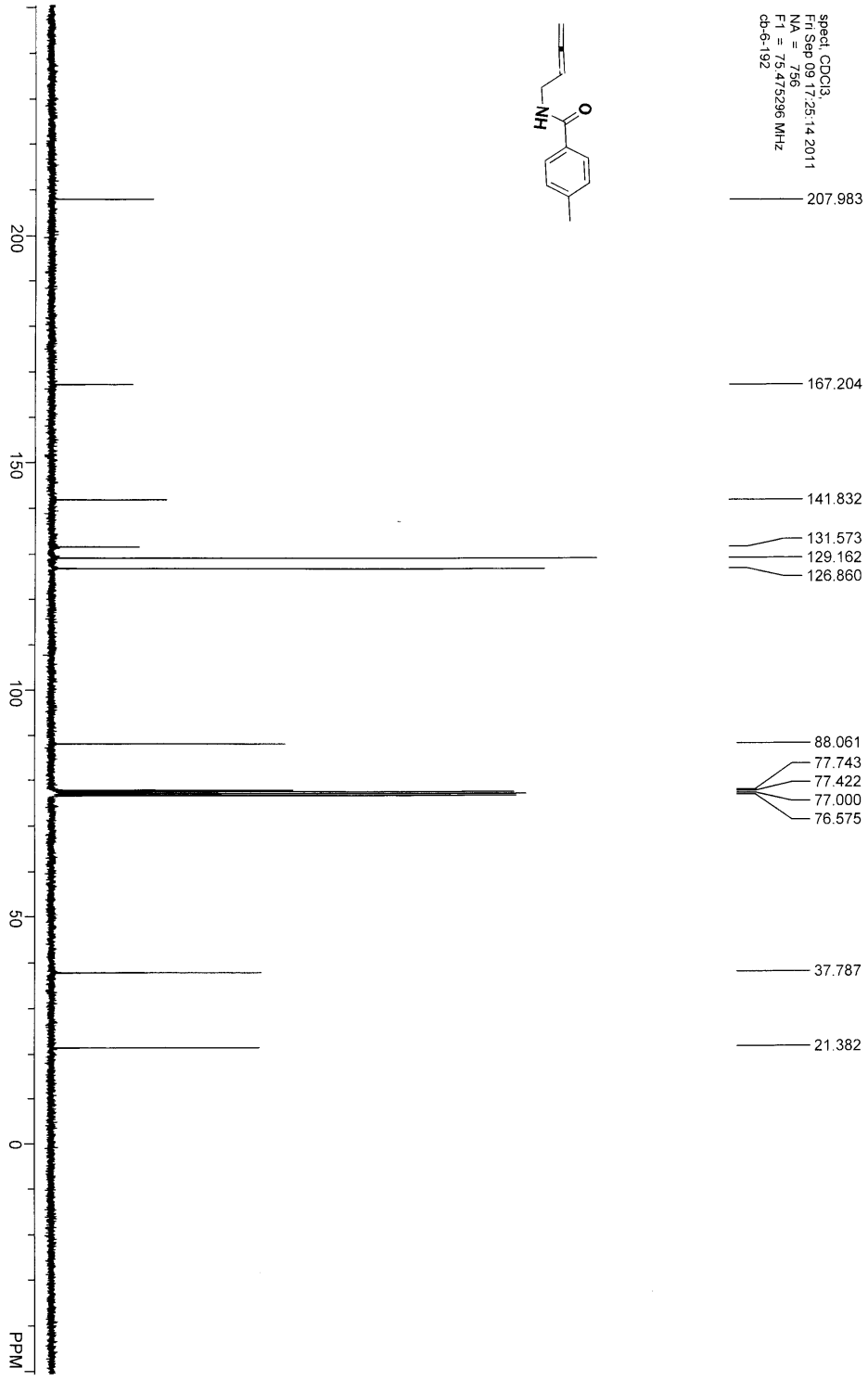


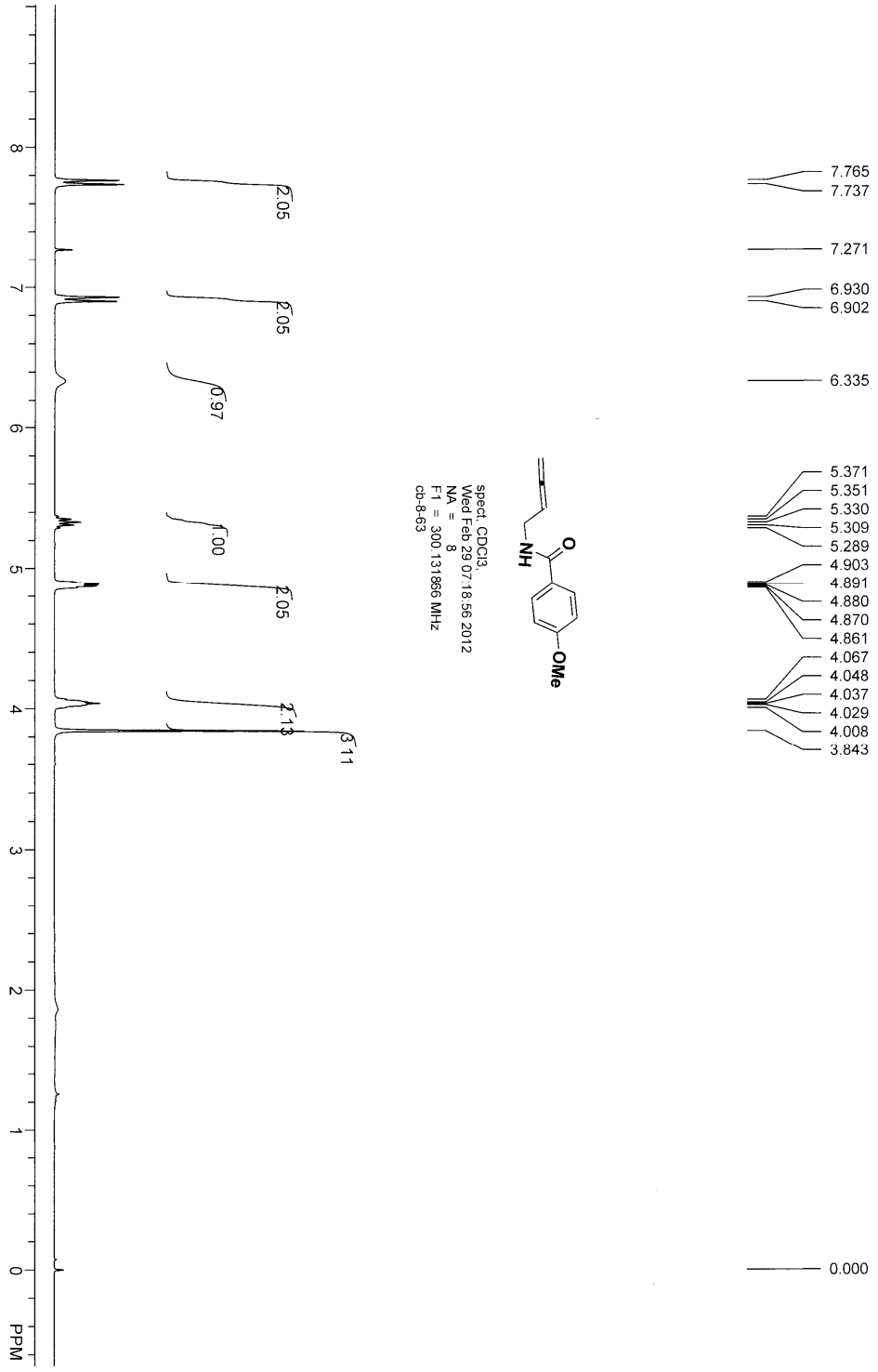


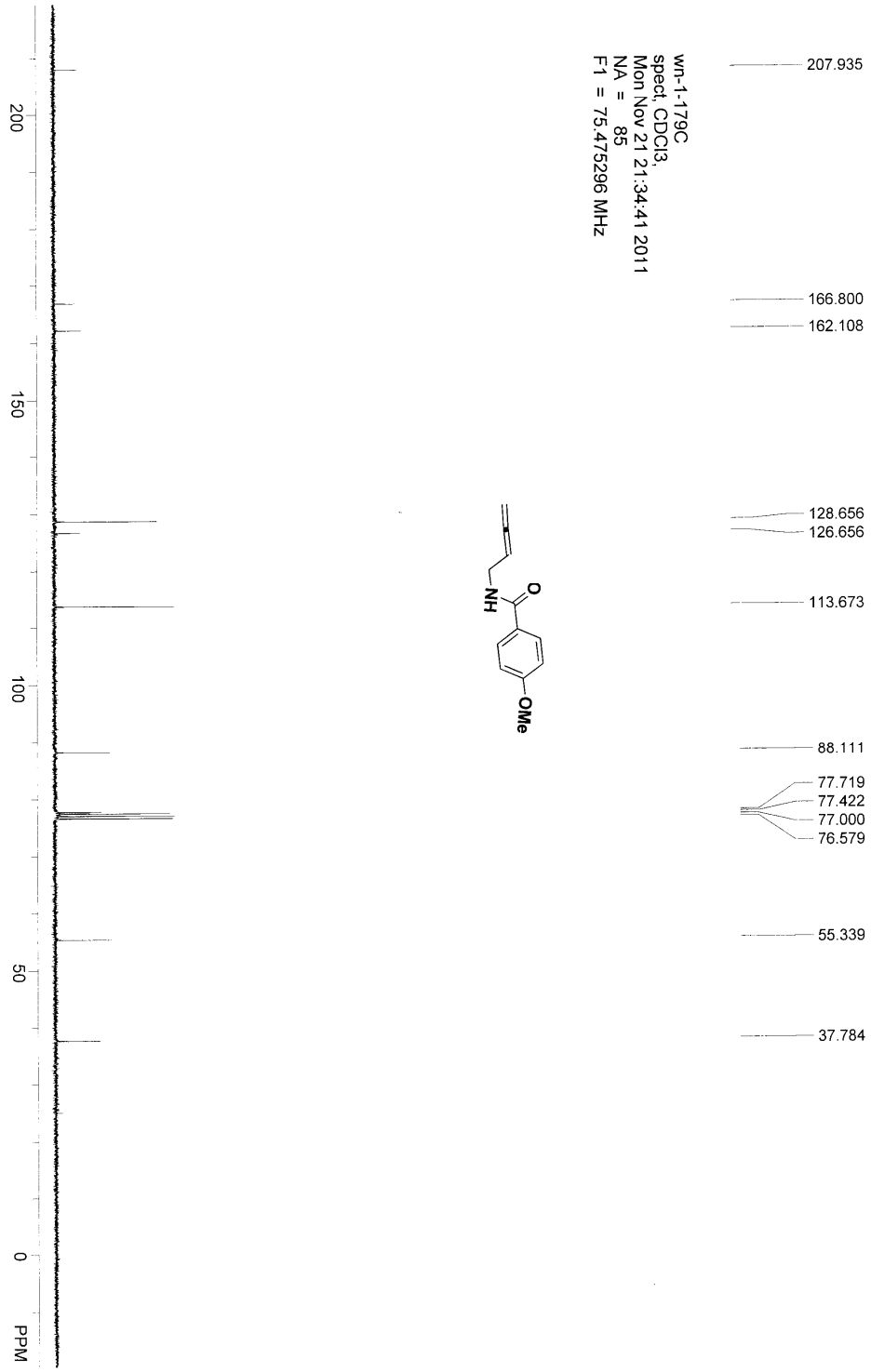


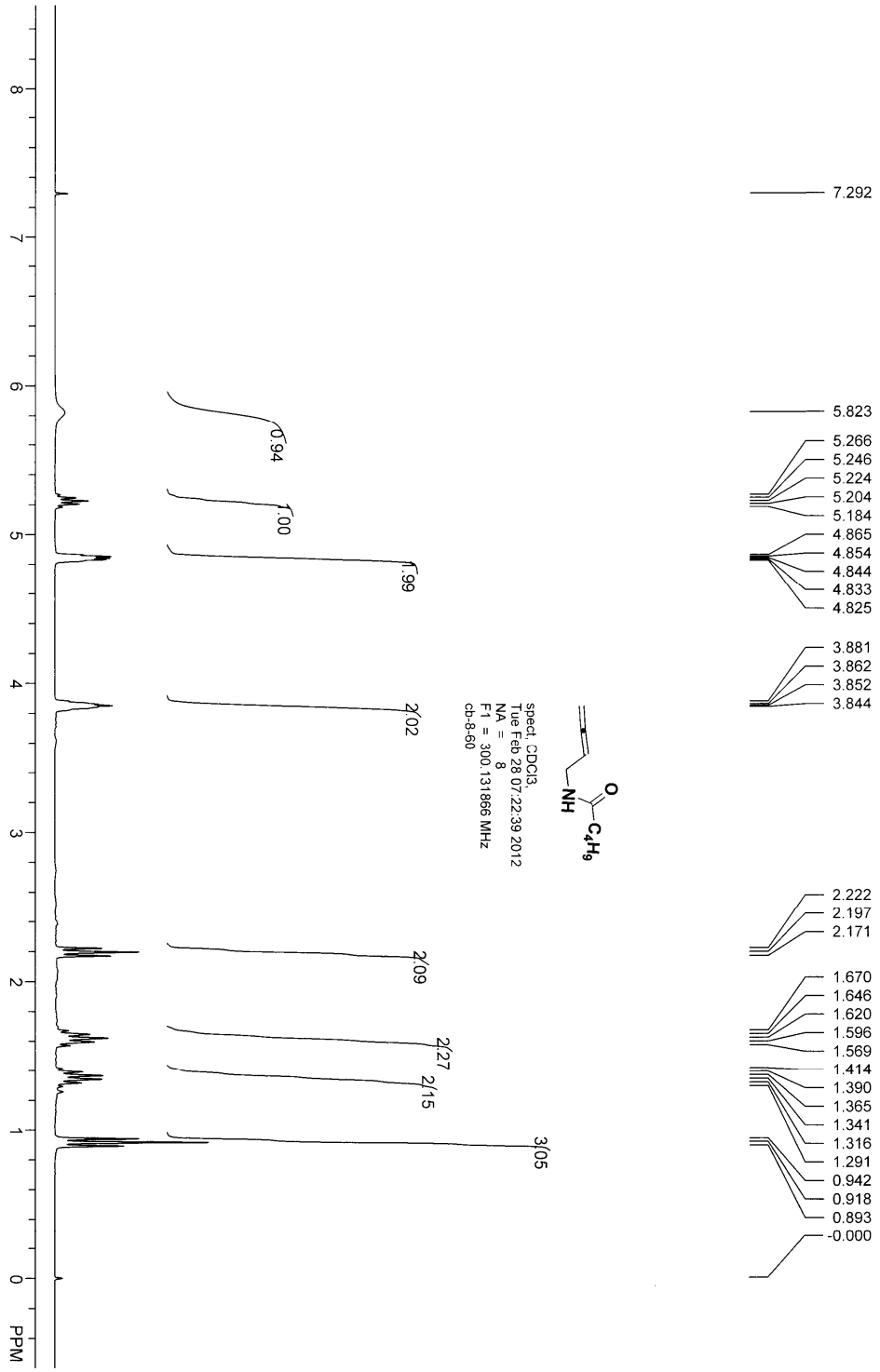


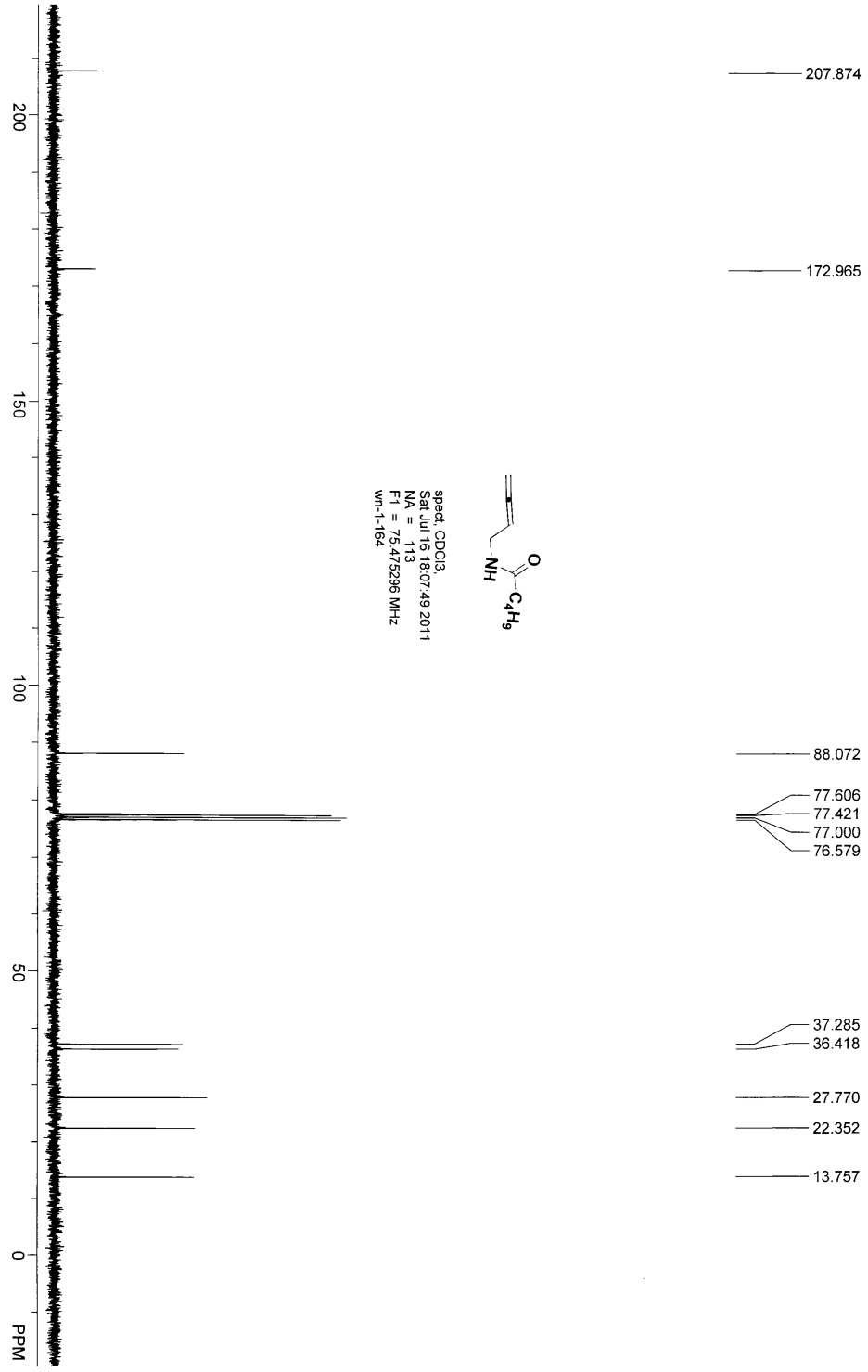


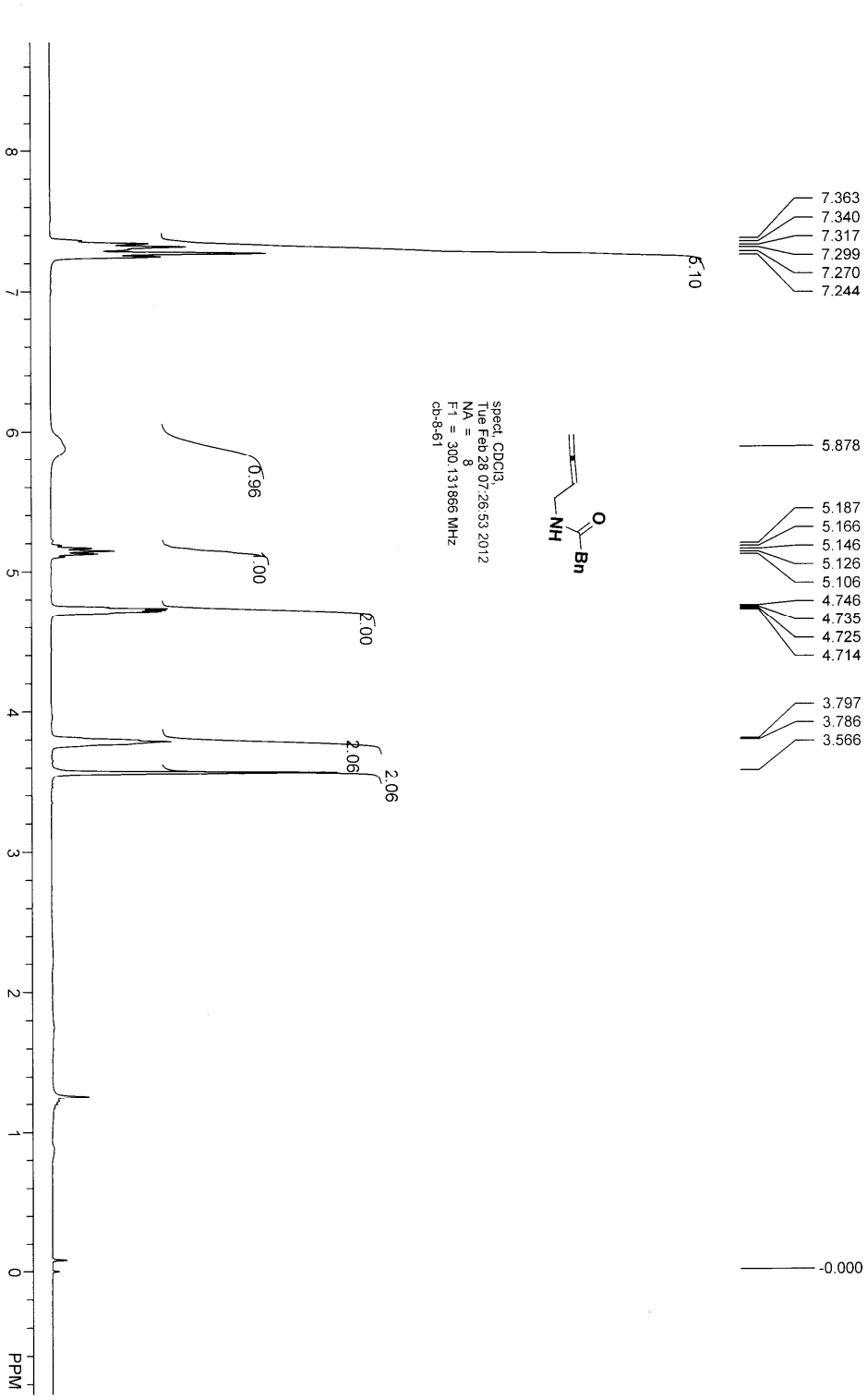


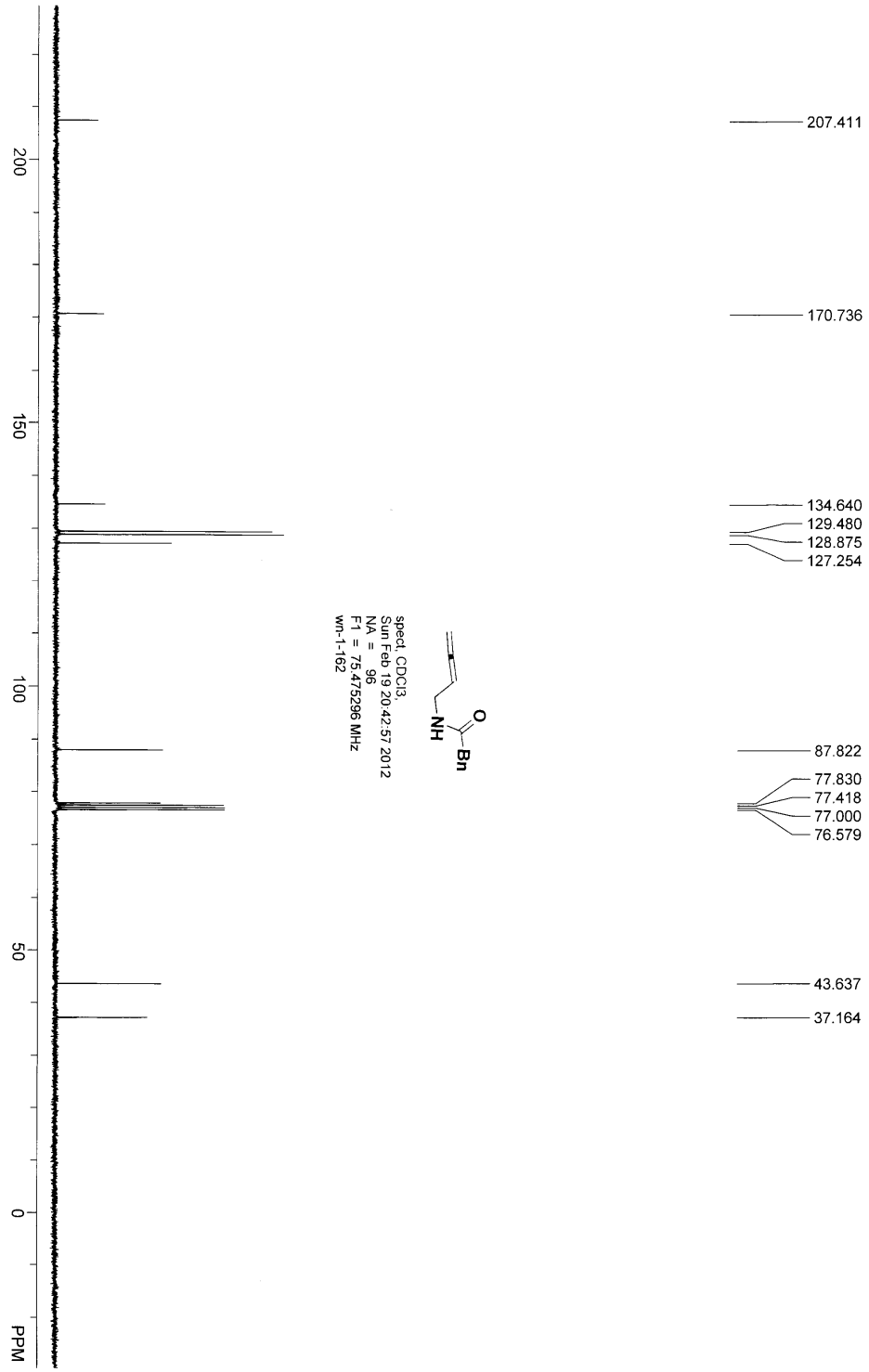


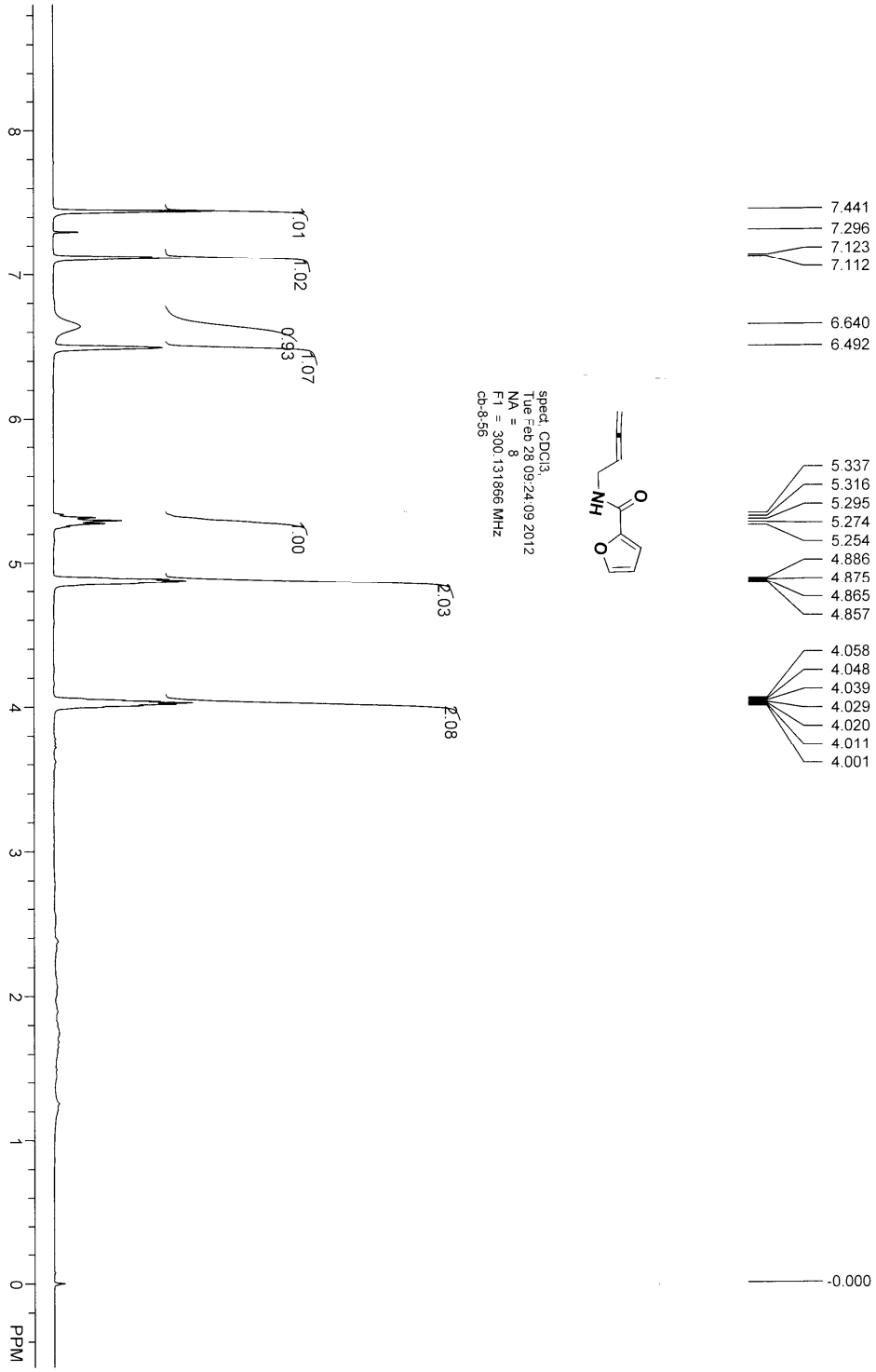


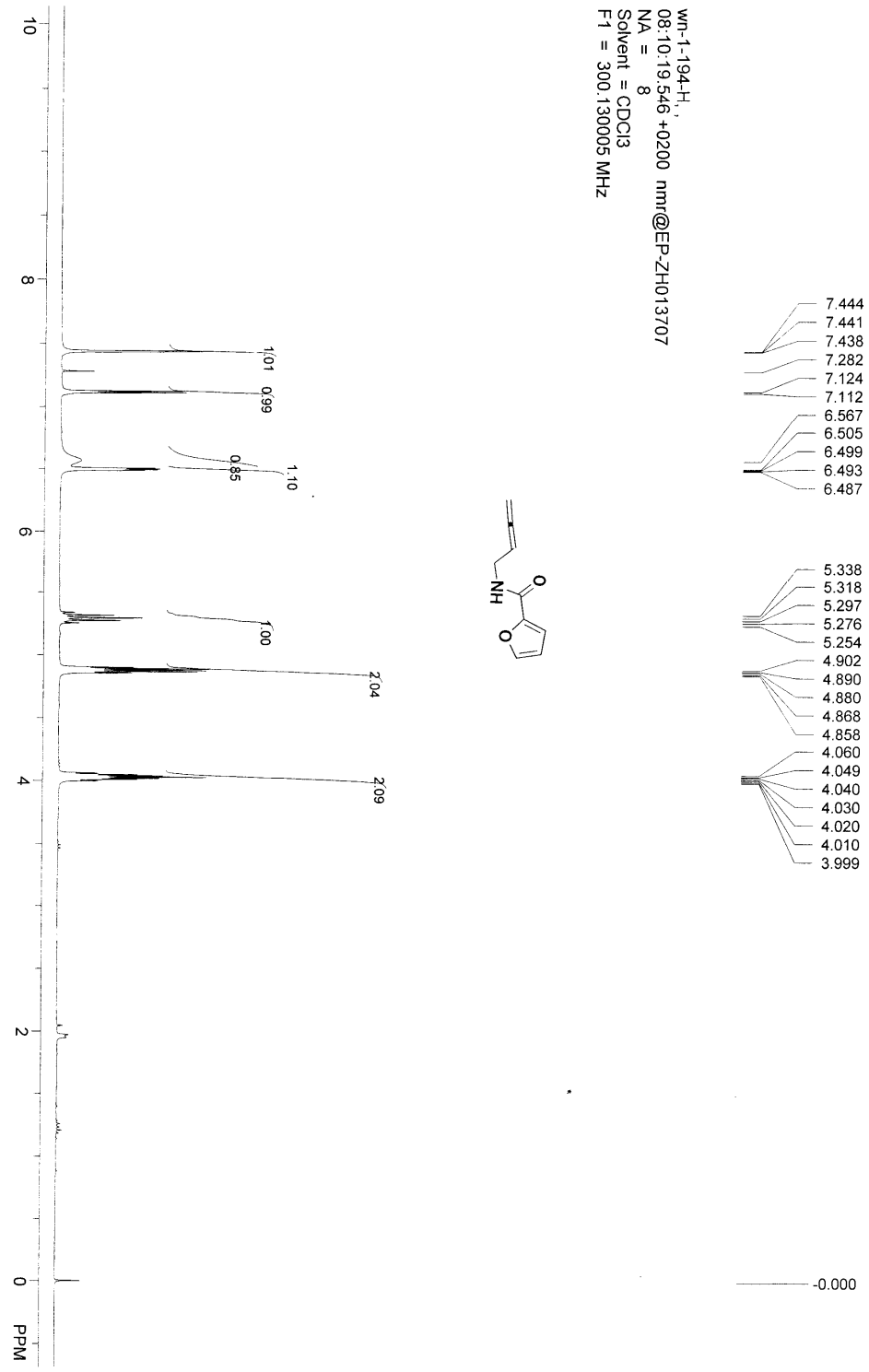


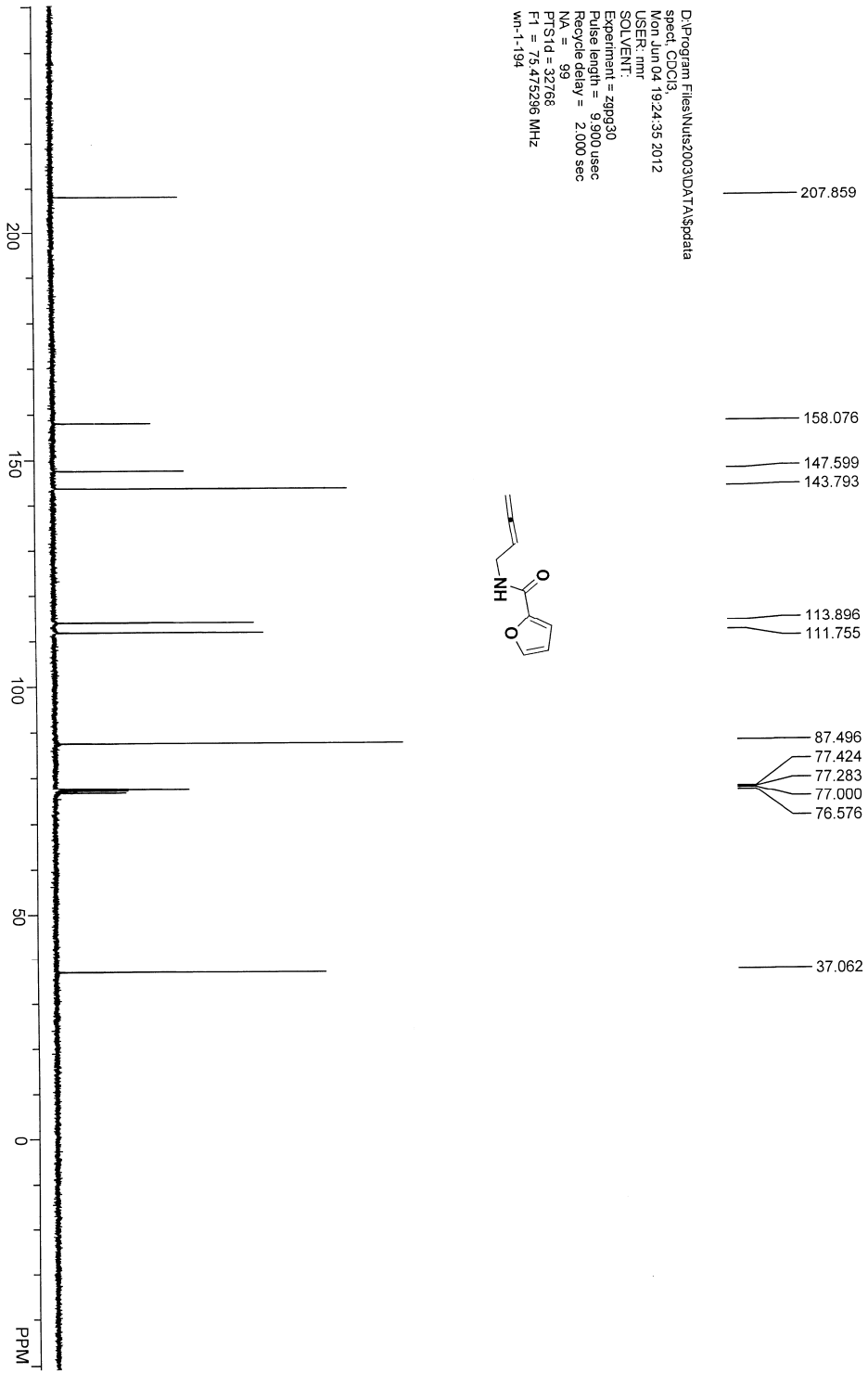


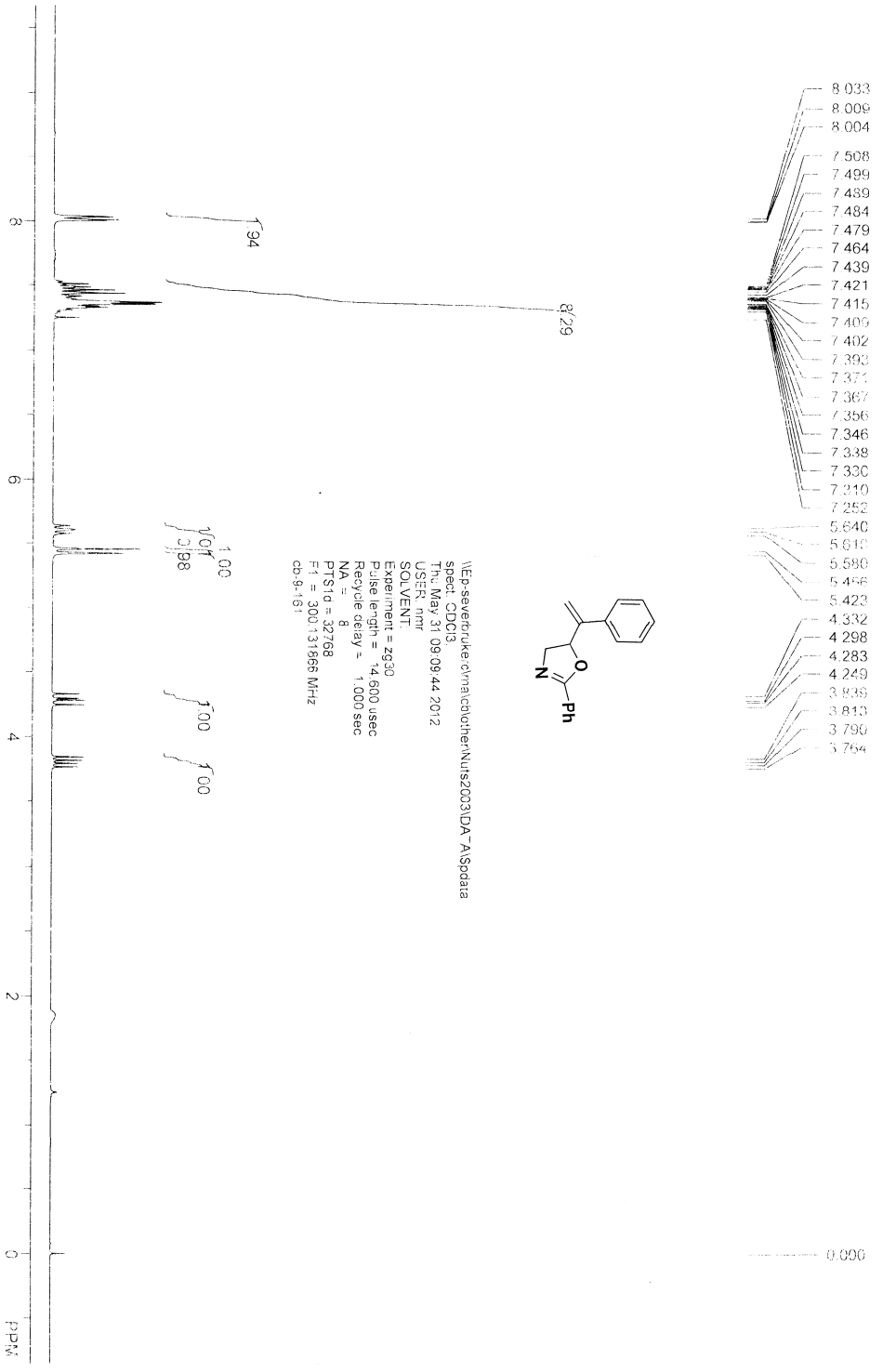


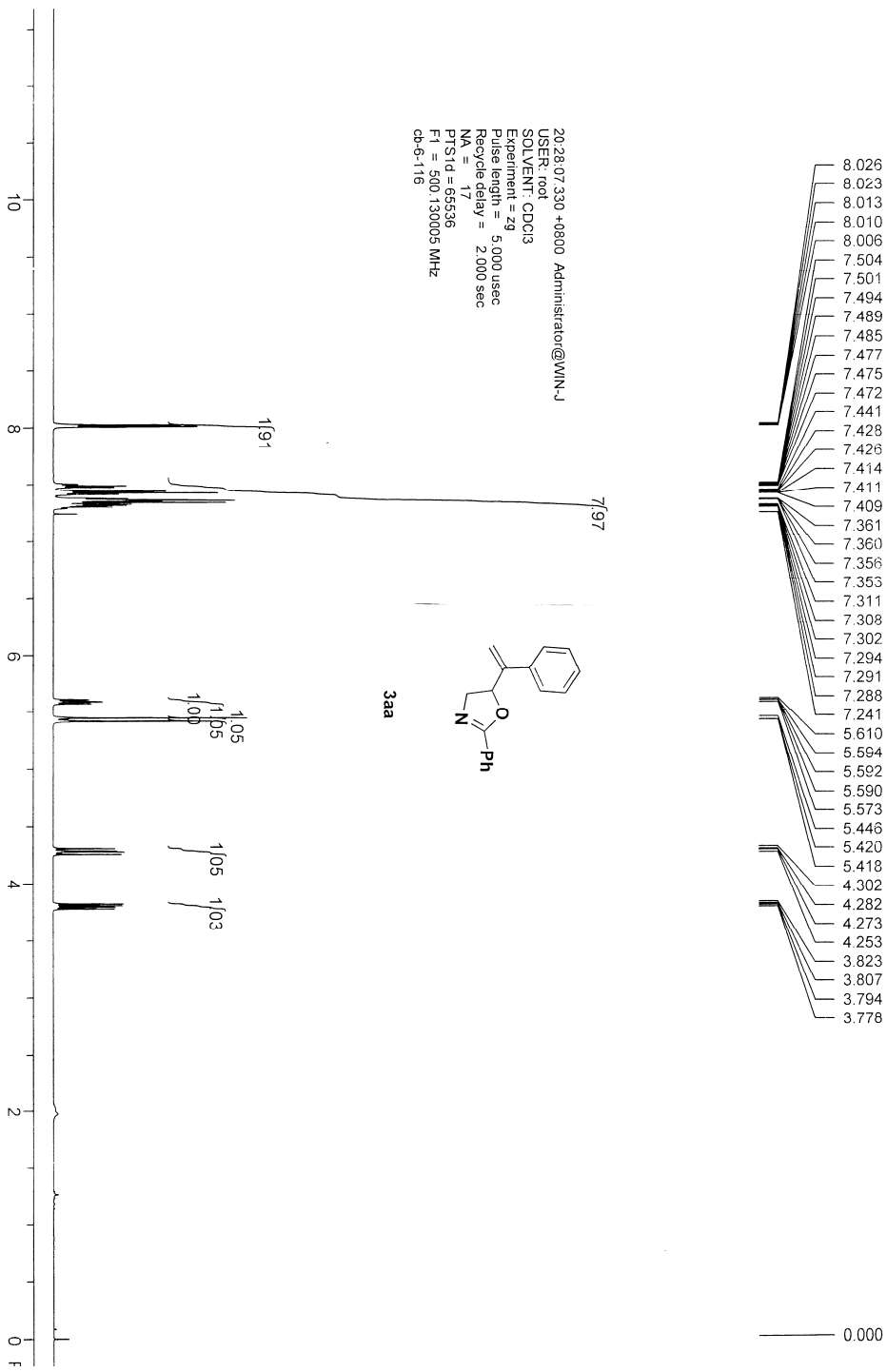


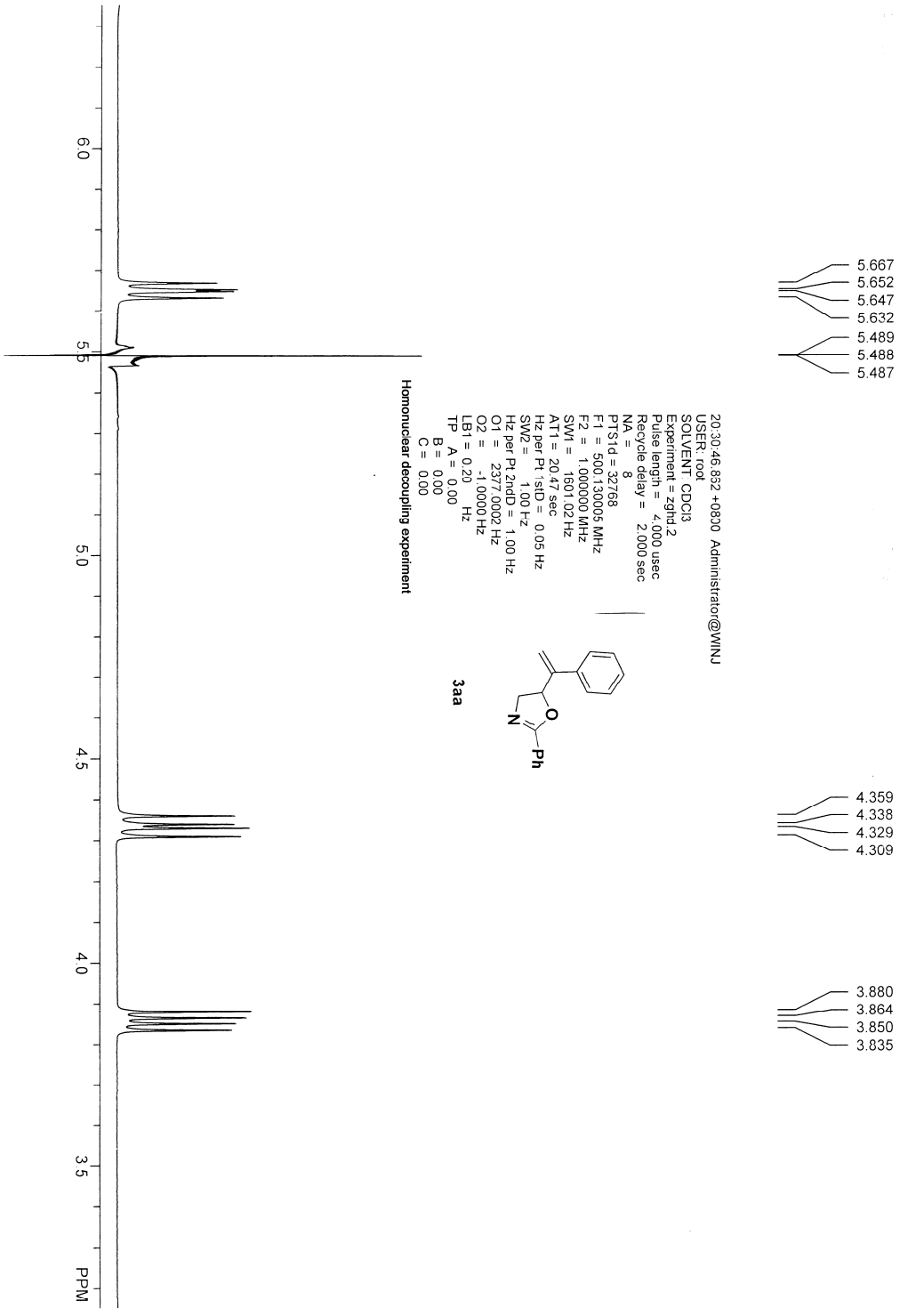


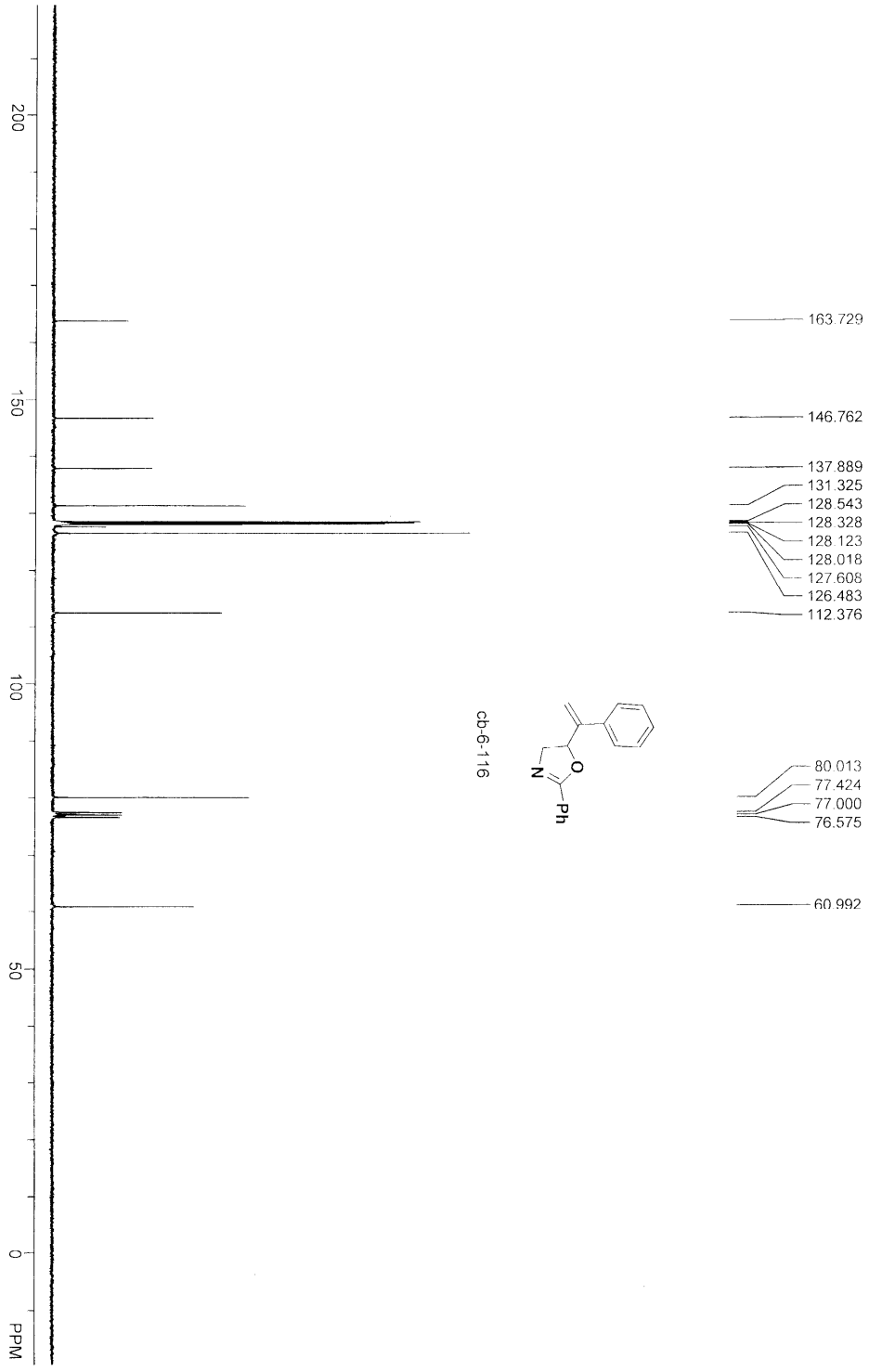


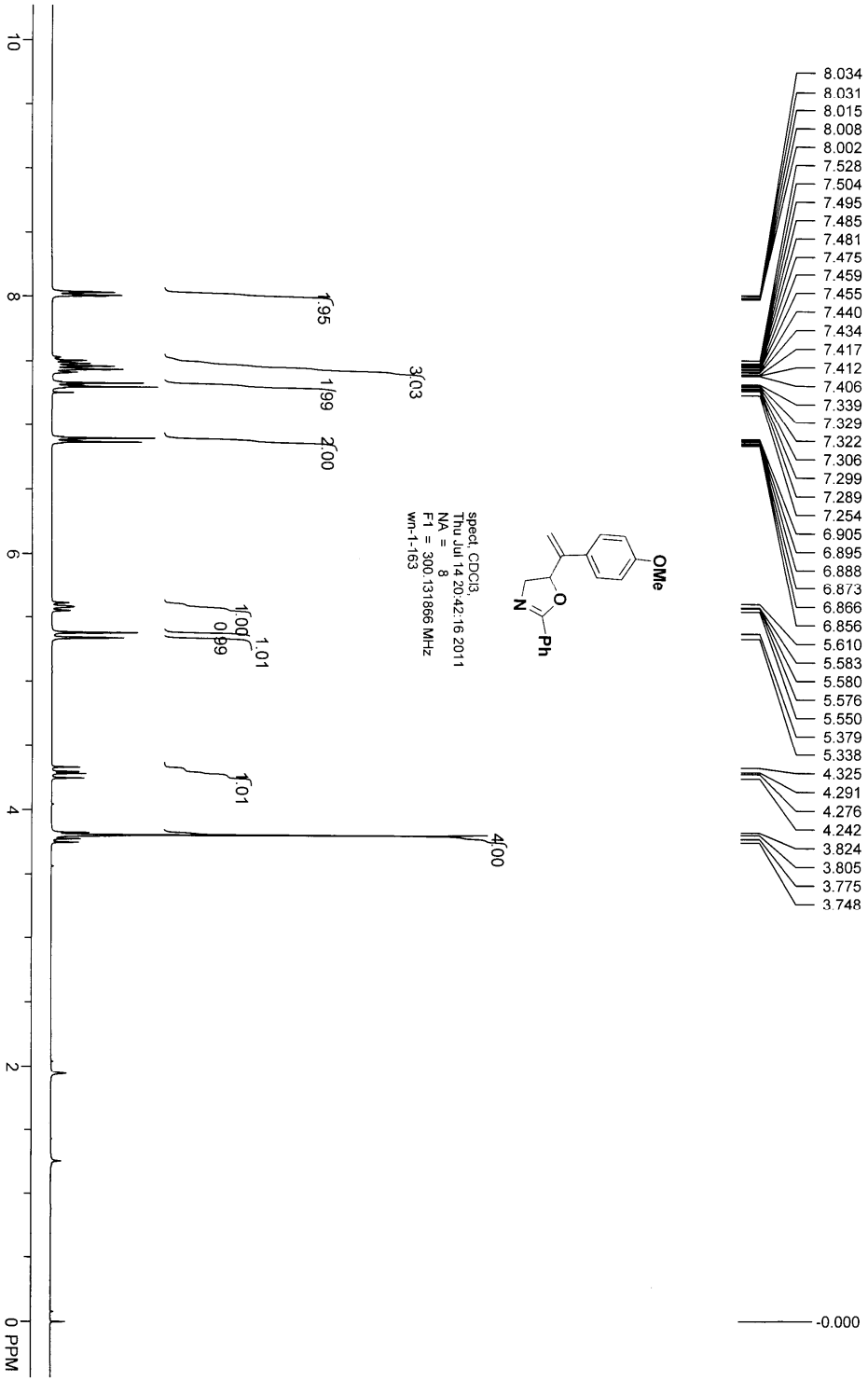


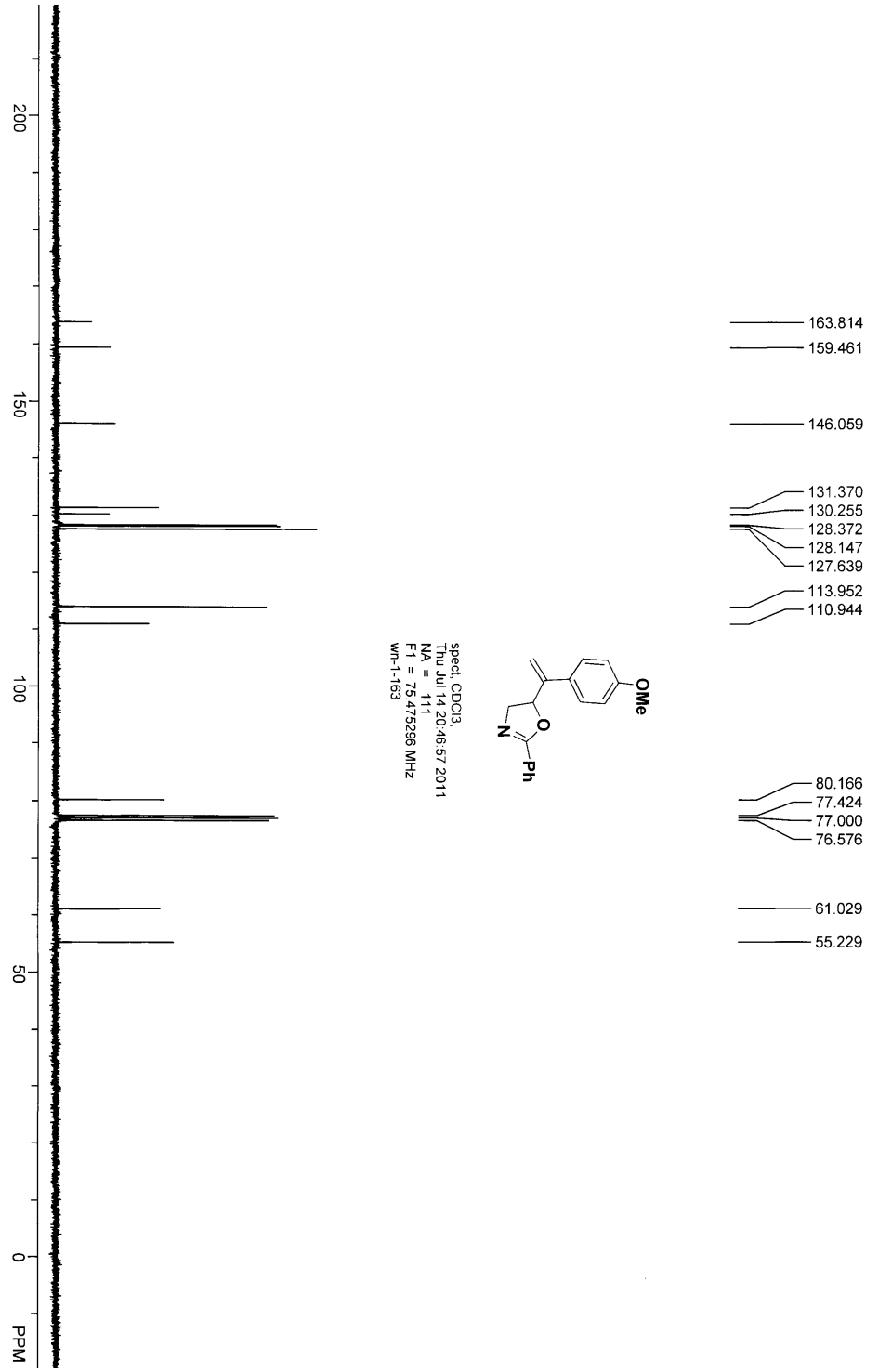

8.033
8.009
8.004
7.508
7.499
7.489
7.484
7.479
7.464
7.439
7.421
7.415
7.409
7.402
7.393
7.371
7.367
7.356
7.346
7.338
7.330
7.210
7.252
5.640
5.610
5.580
5.456
5.423
4.332
4.298
4.283
4.249
3.836
3.810
3.790
3.764
0.000
1.94
8.29
1.00
1.01
0.98
1.00
1.00
\\Ep-severbruker\chmlab\bother\Nuts2003\DATA\Spdata
spect CDCl3
Thu May 31 09:09:44 2012
USER nmr
SOLVENT
Experiment = zg30
Pulse length = 14.600 usec
Recycle delay = 1.000 sec
NA = 8
PTS1d = 32768
F1 = 300.131866 MHz
cb-9-161
O
N
Ph
8
6
4
2
0
PPM

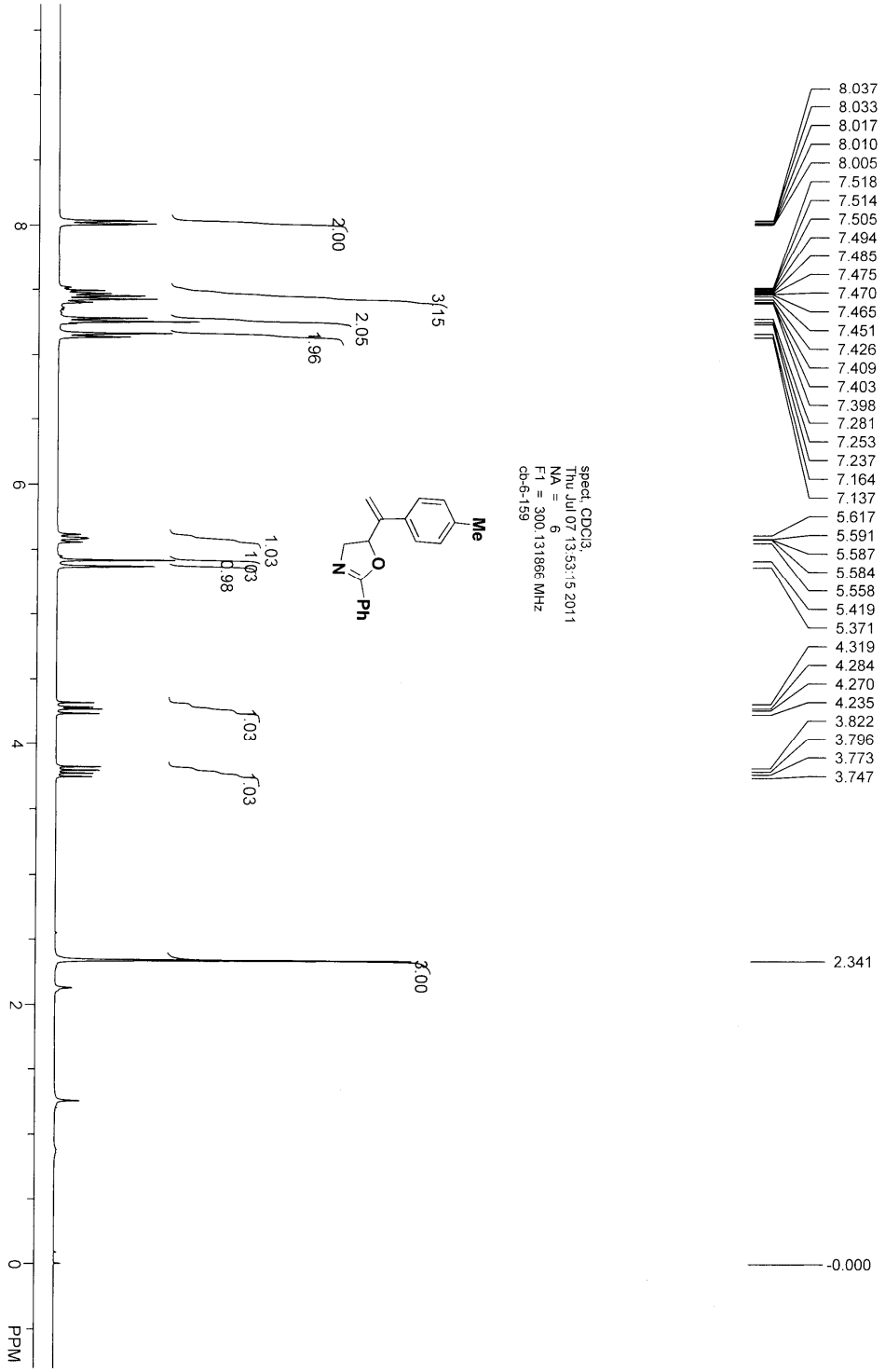


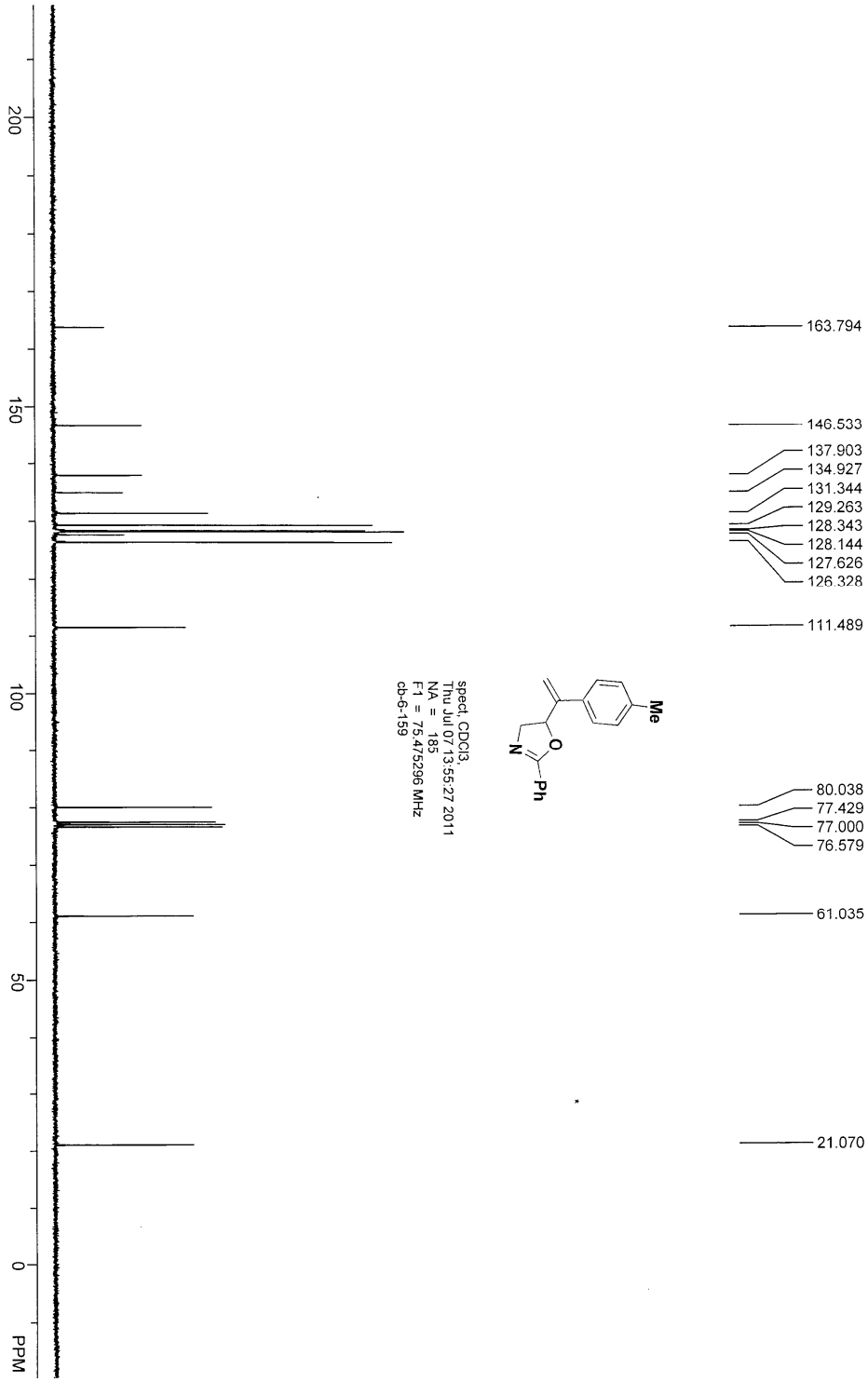


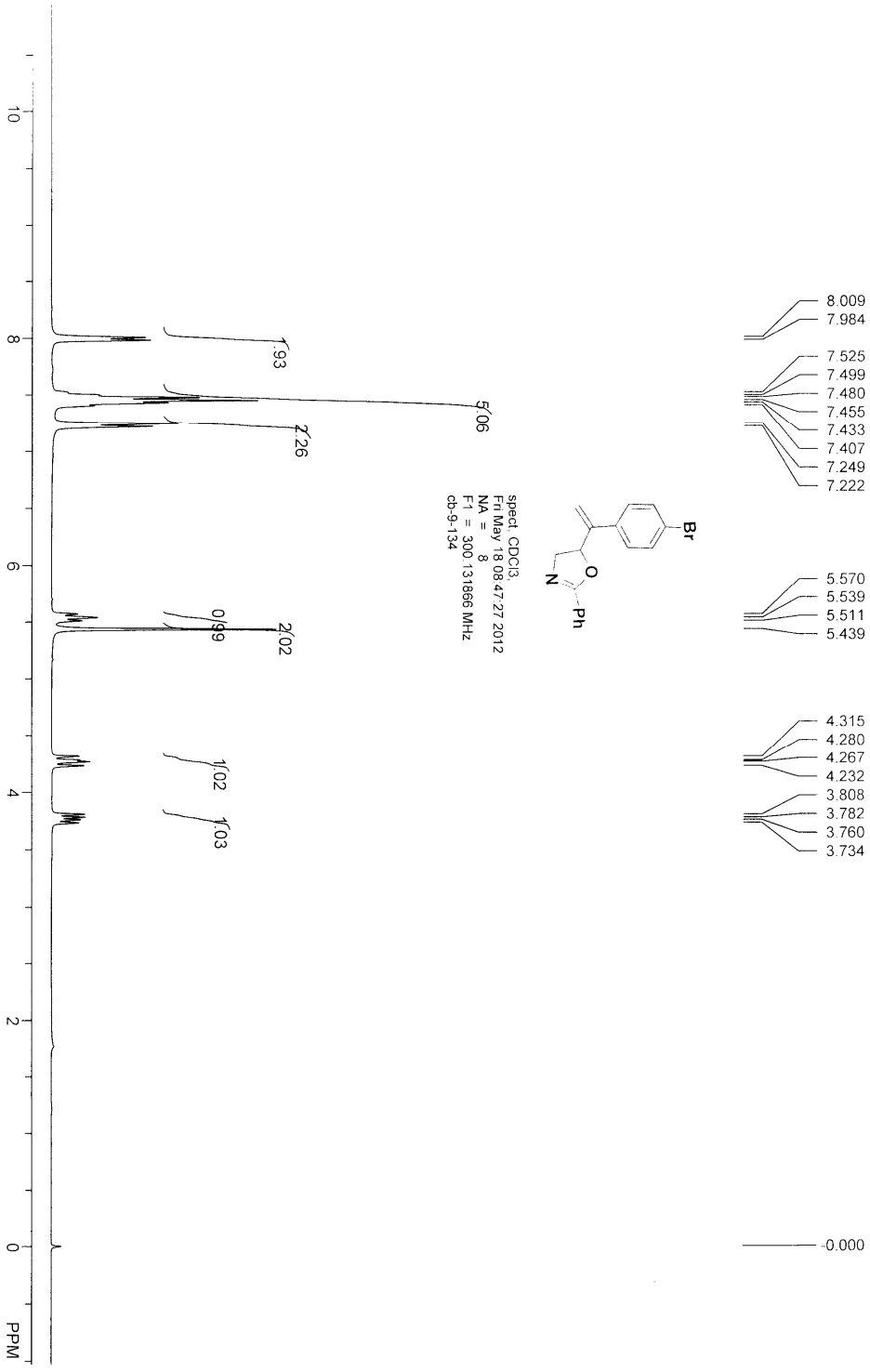


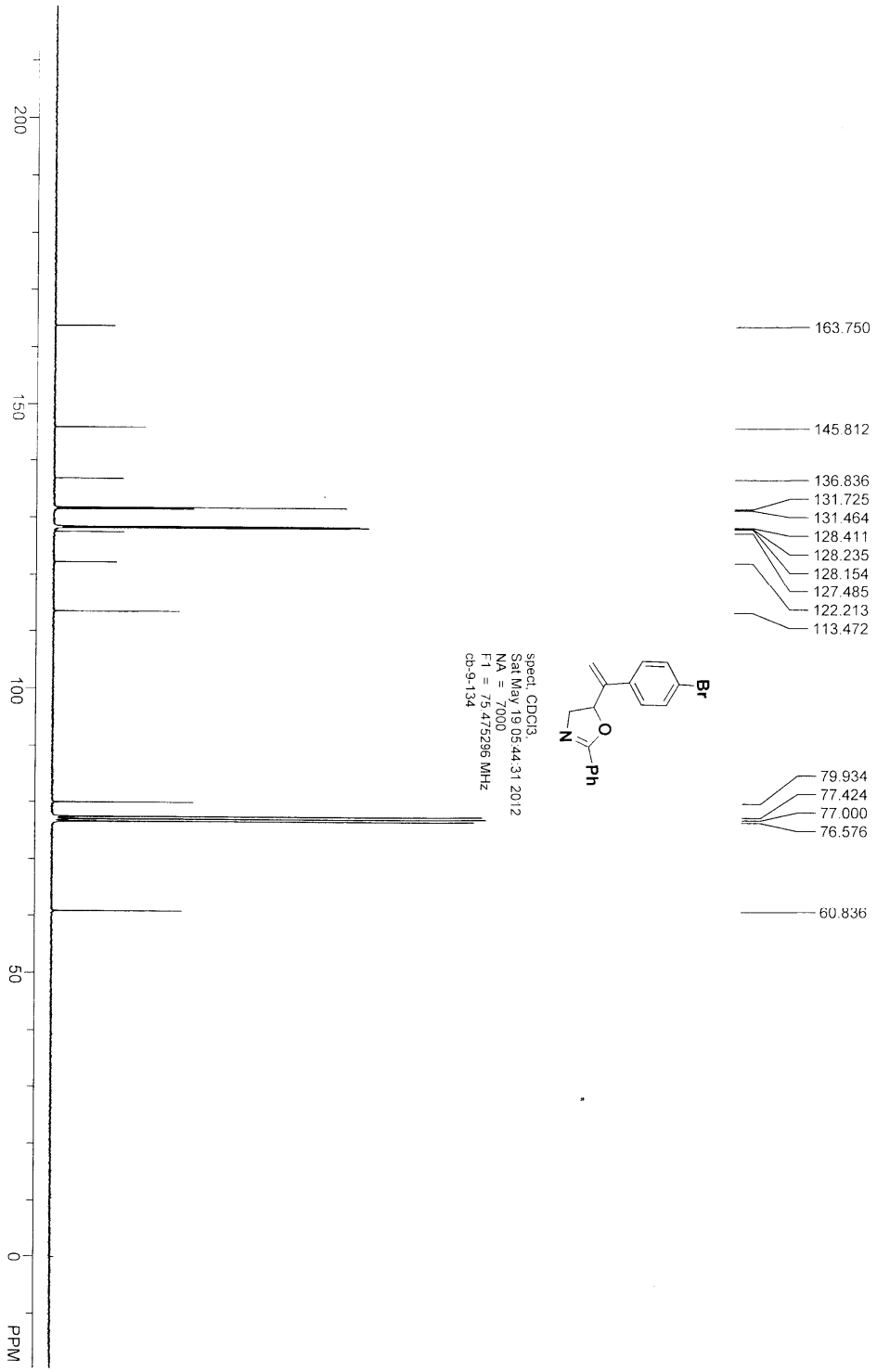


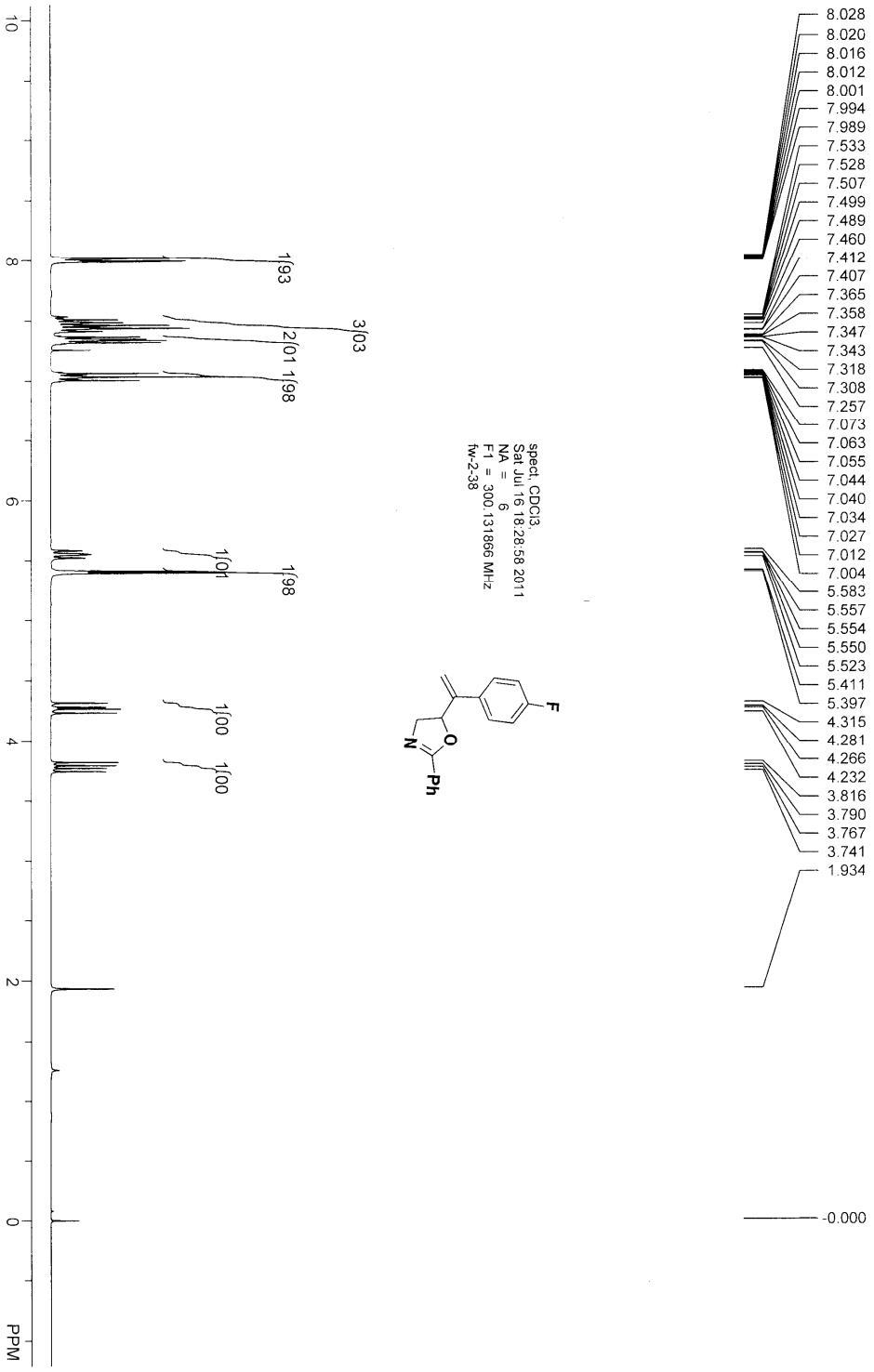


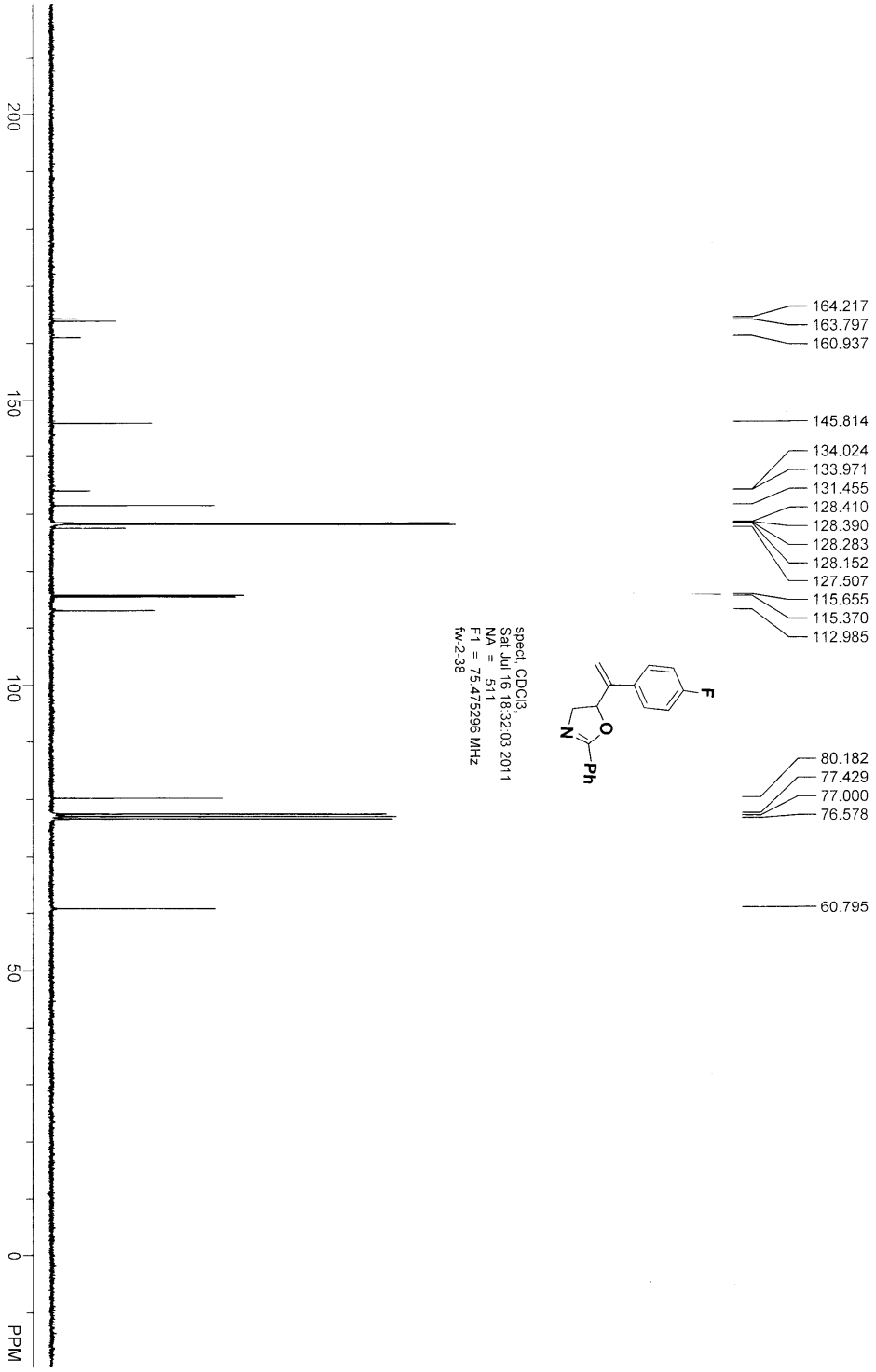

8.037
8.033
8.017
8.010
8.005
7.518
7.514
7.505
7.494
7.485
7.475
7.470
7.465
7.451
7.426
7.409
7.403
7.398
7.281
7.253
7.237
7.164
7.137
5.617
5.591
5.587
5.584
5.558
5.419
5.371
4.319
4.284
4.270
4.235
3.822
3.796
3.773
3.747
2.341
-0.000
spect_CDCl3_
Thu Jul 07 13:53:15 2011
NA = 6
F1 = 300.13186 MHz
cb-6-159
Me
O
N
Ph
2.00
3.15
2.05
1.96
1.03
1.03
0.98
1.03
1.03
3.00
8
6
4
2
0
PPM

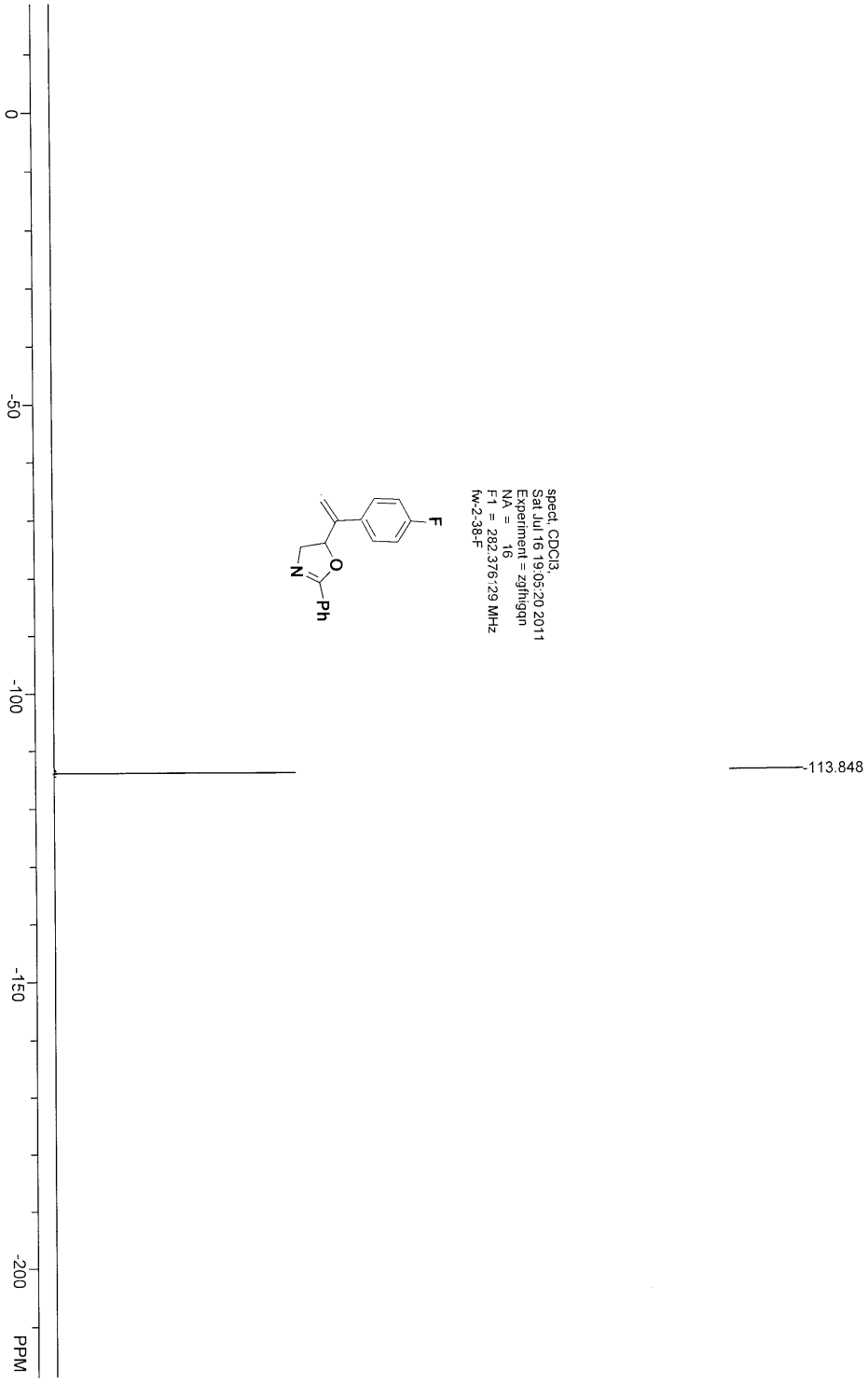

200
150
100
50
0
PPM
163.794
146.533
137.903
134.927
131.344
129.263
128.343
128.144
127.626
126.328
111.489
80.038
77.429
77.000
76.579
61.035
21.070
spect, CDCl3,
Thu Jul 07 13:55:27 2011
NA = 185
F1 = 75.475296 MHz
cb-6-159
Me
O
N
Ph

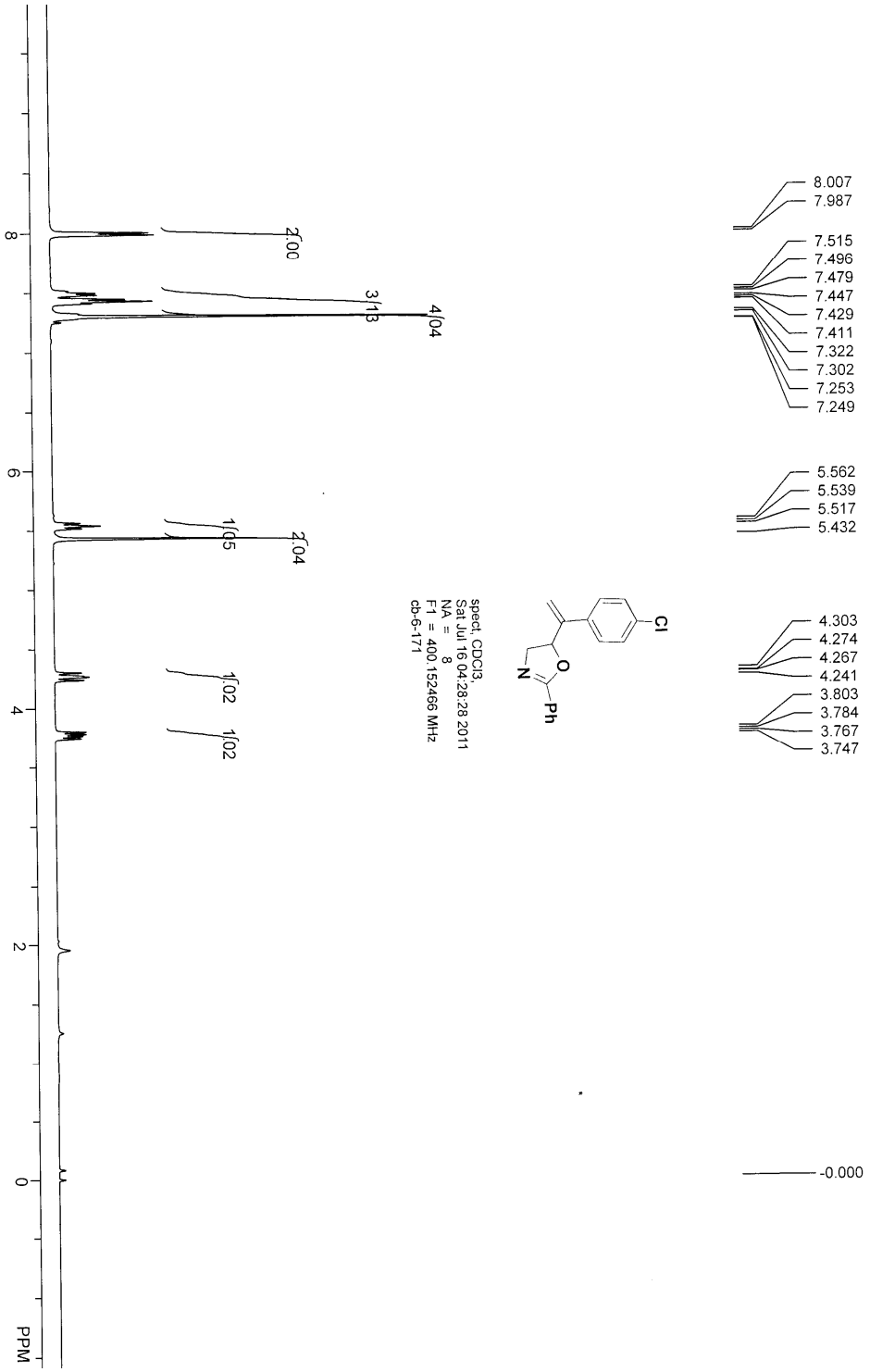


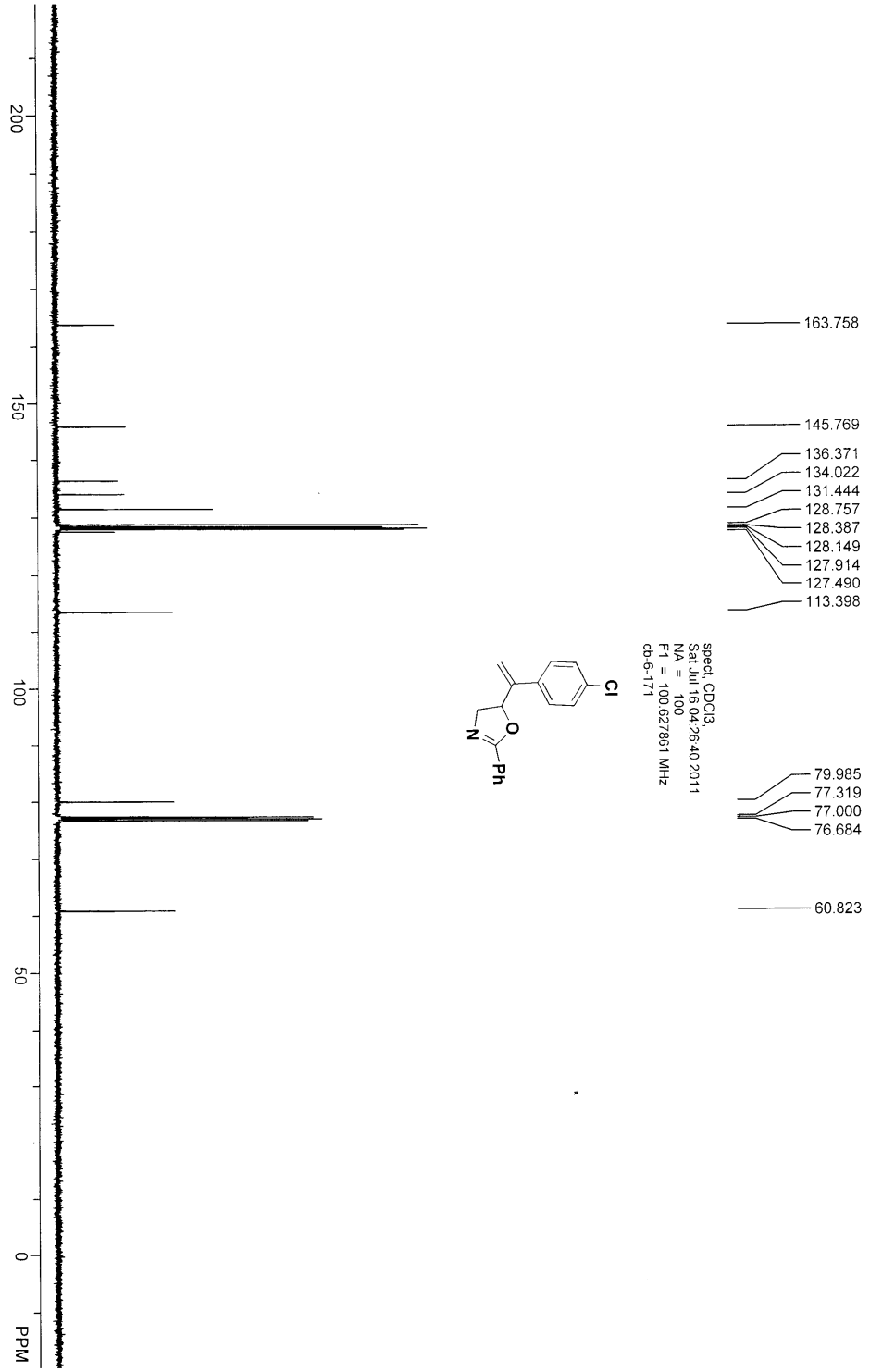


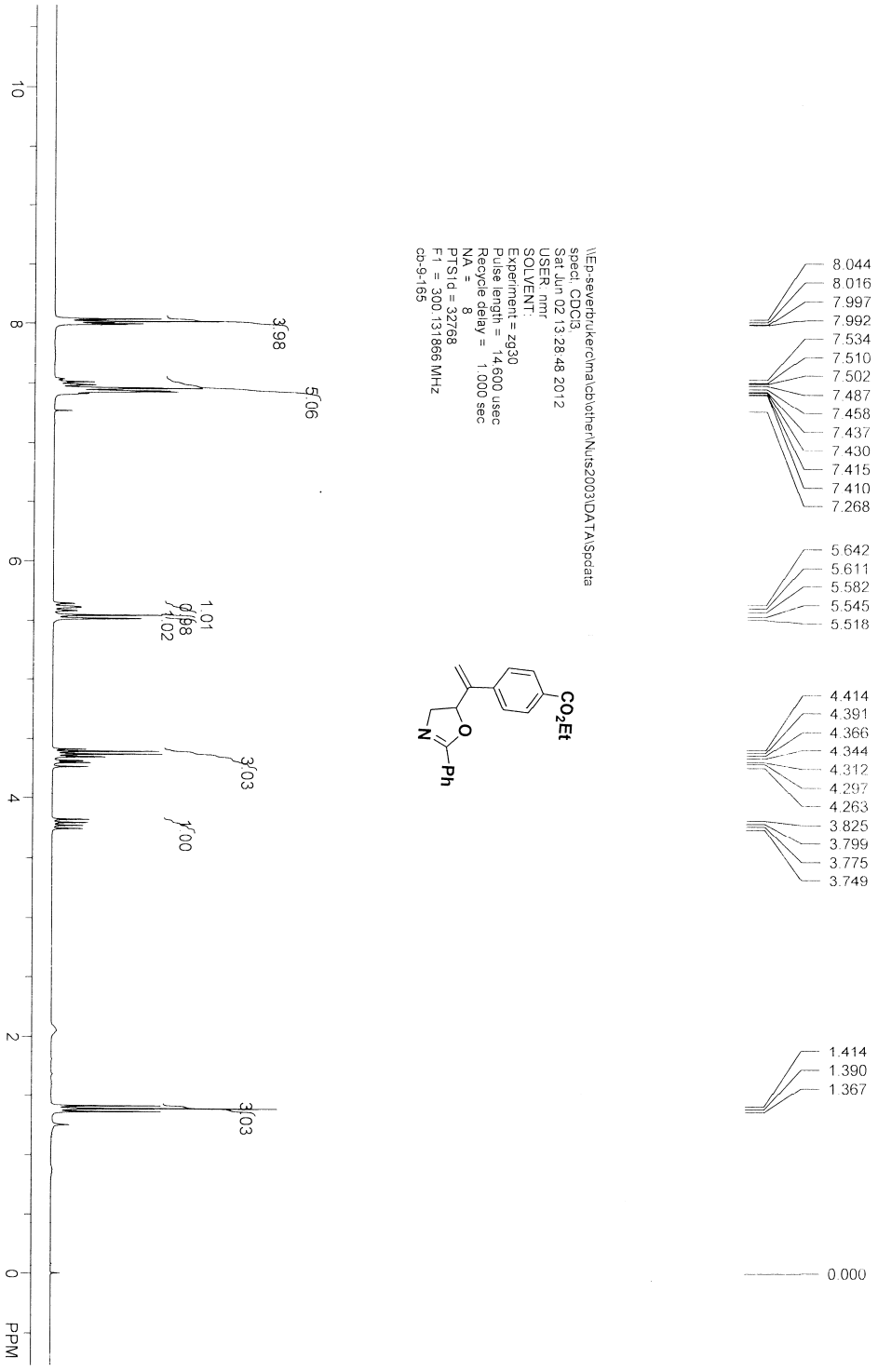

8.028
8.020
8.016
8.012
8.001
7.994
7.989
7.533
7.528
7.507
7.499
7.489
7.460
7.412
7.407
7.365
7.358
7.347
7.343
7.318
7.308
7.257
7.073
7.063
7.055
7.044
7.040
7.034
7.027
7.012
7.004
5.583
5.557
5.554
5.550
5.523
5.411
5.397
4.315
4.281
4.266
4.232
3.816
3.790
3.767
3.741
1.934
-0.000
spect, CDCl3
Sat Jul 16 18:28:58 2011
NA = 6
F1 = 300.131866 MHz
fw-2-38
F
O
N
Ph
1.93
3.03
2.01
1.98
1.01
1.98
1.00
1.00
10
8
6
4
2
0
PPM

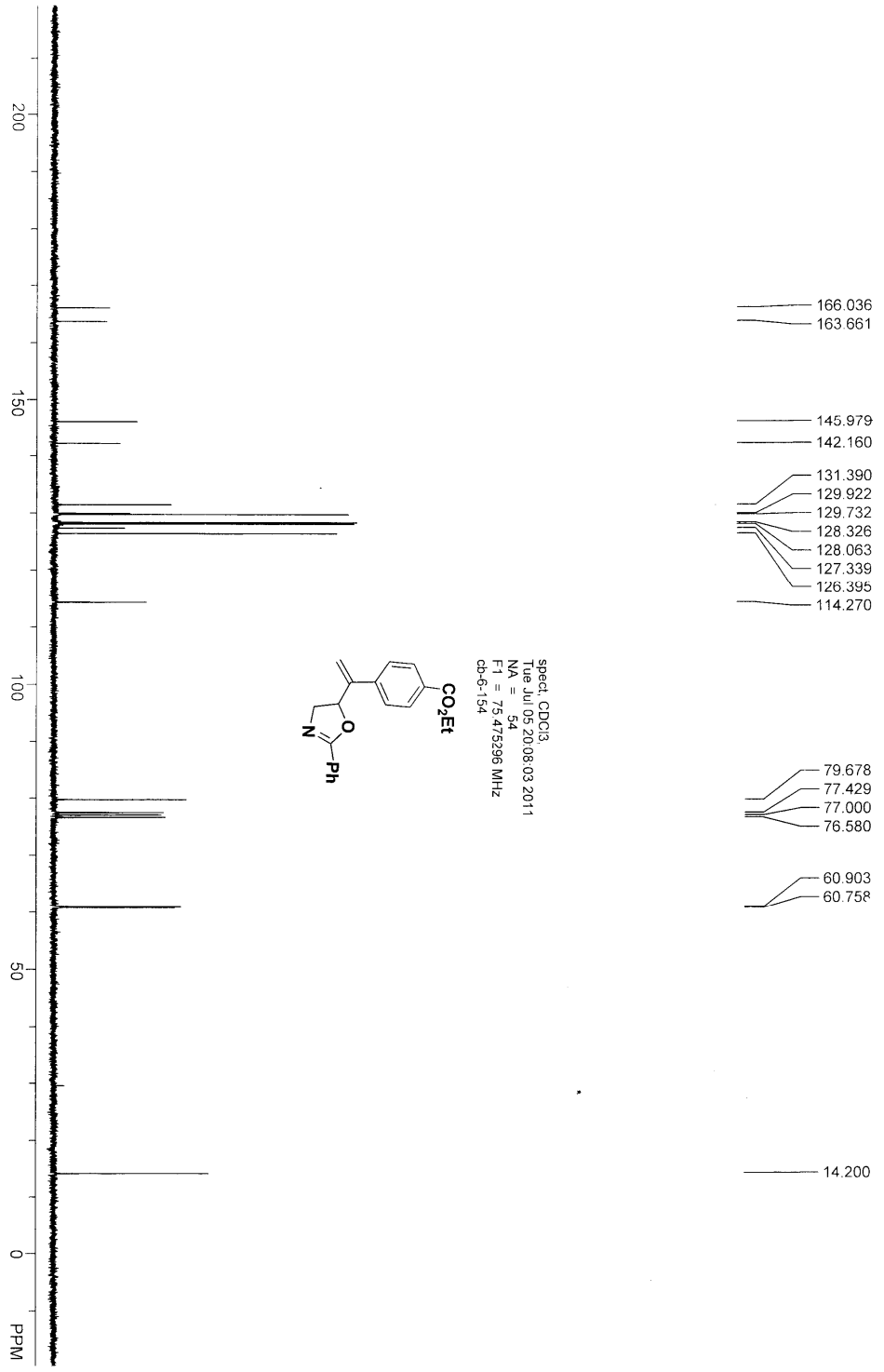


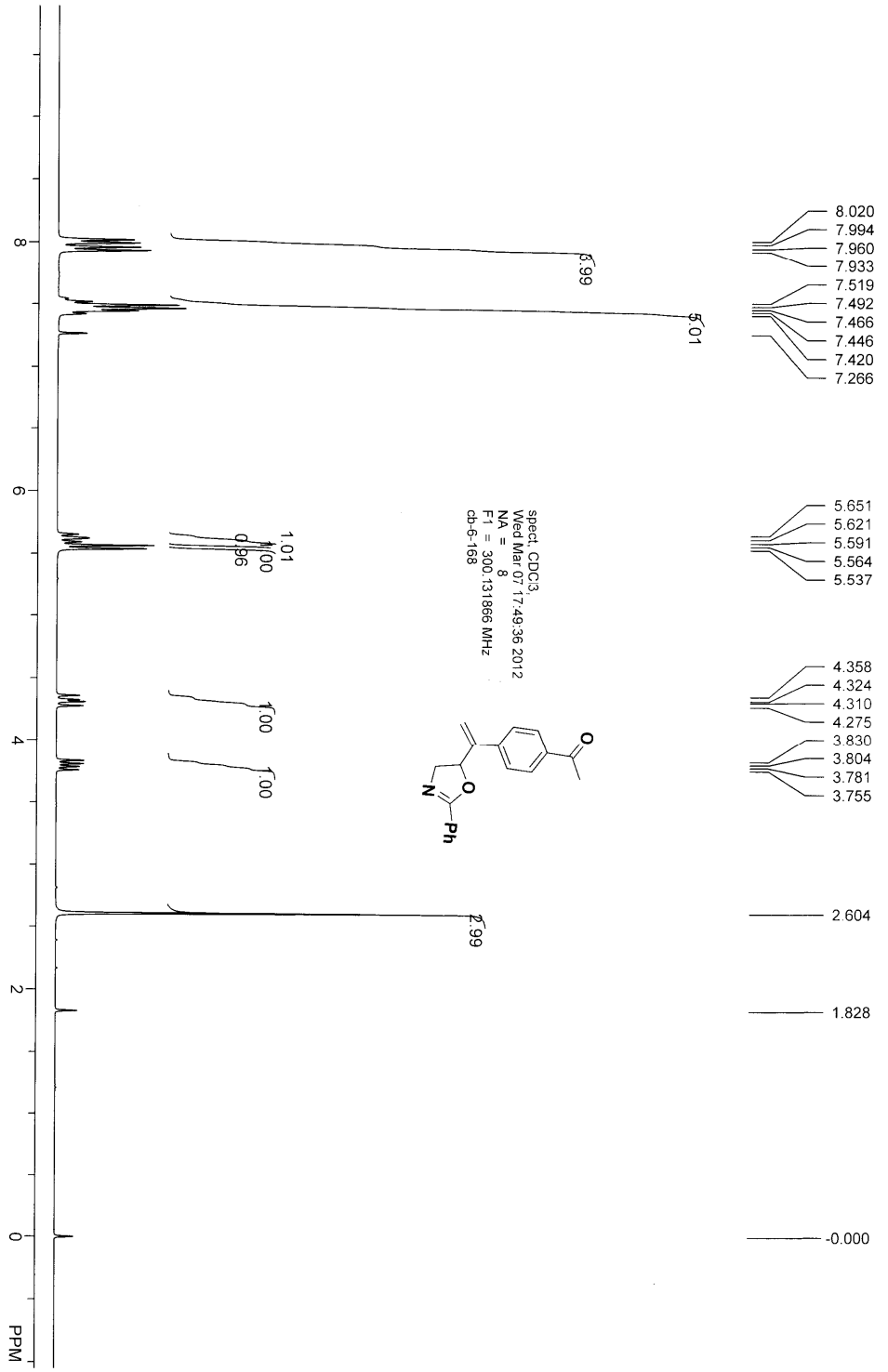

spect, CDCl3,
Sat Jul 16 19:05:20 2011
Experiment = zgfhigqn
NA = 16
F1 = 282.376129 MHz
fw-2-38-F
F
O
N
Ph
-113.848
0
-50
-100
-150
-200
PPM

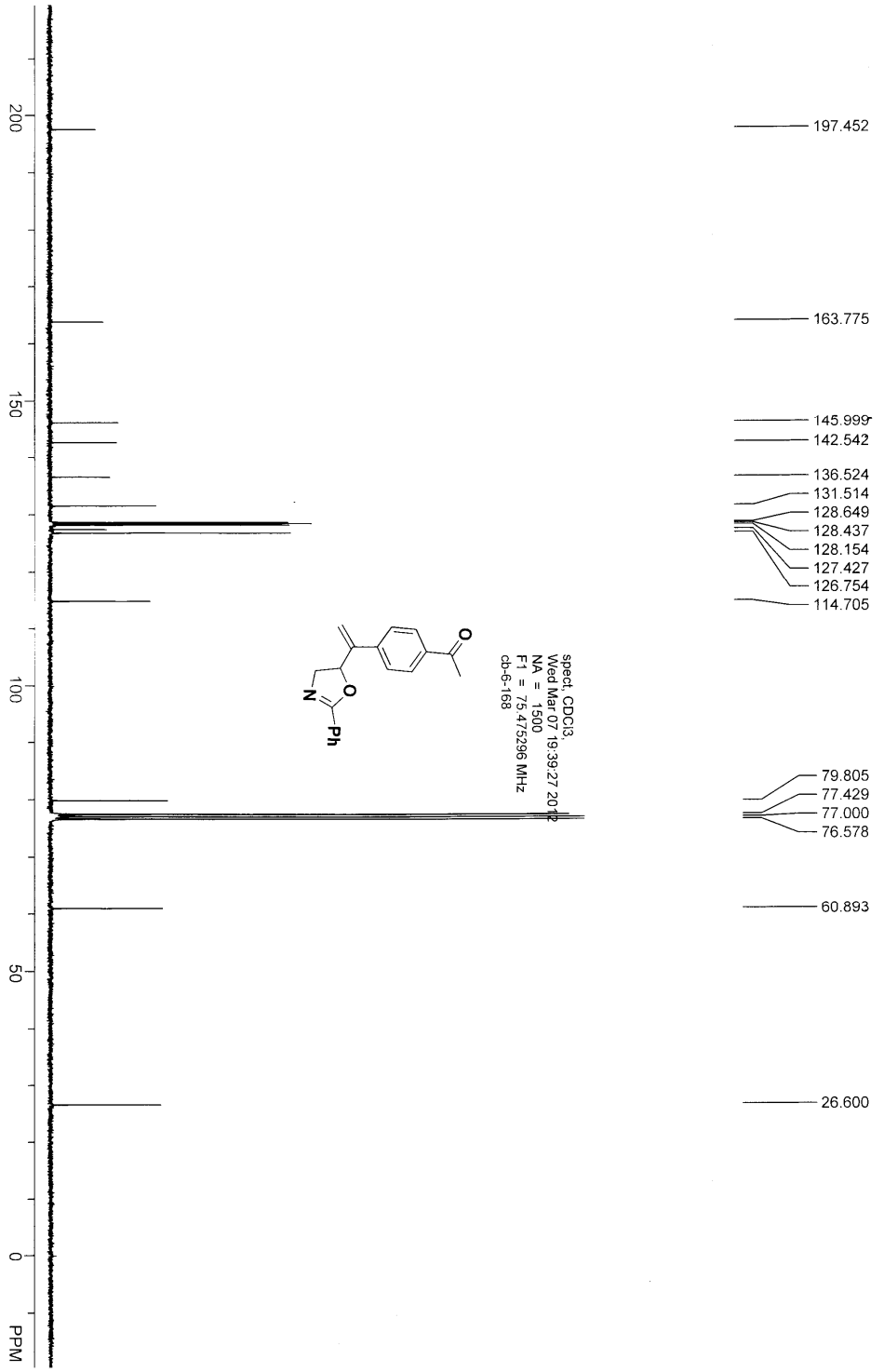

8.007
7.987
7.515
7.496
7.479
7.447
7.429
7.411
7.322
7.302
7.253
7.249
5.562
5.539
5.517
5.432
4.303
4.274
4.267
4.241
3.803
3.784
3.767
3.747
-0.000
2.00
3.13
4.04
1.05
2.04
1.02
1.02
8
6
4
2
0
PPM
spect, CDCl3,
Sat Jul 16 04:28:28 2011
NA = 8
F1 = 400.152466 MHz
cb-6-171
Cl
O
N
Ph

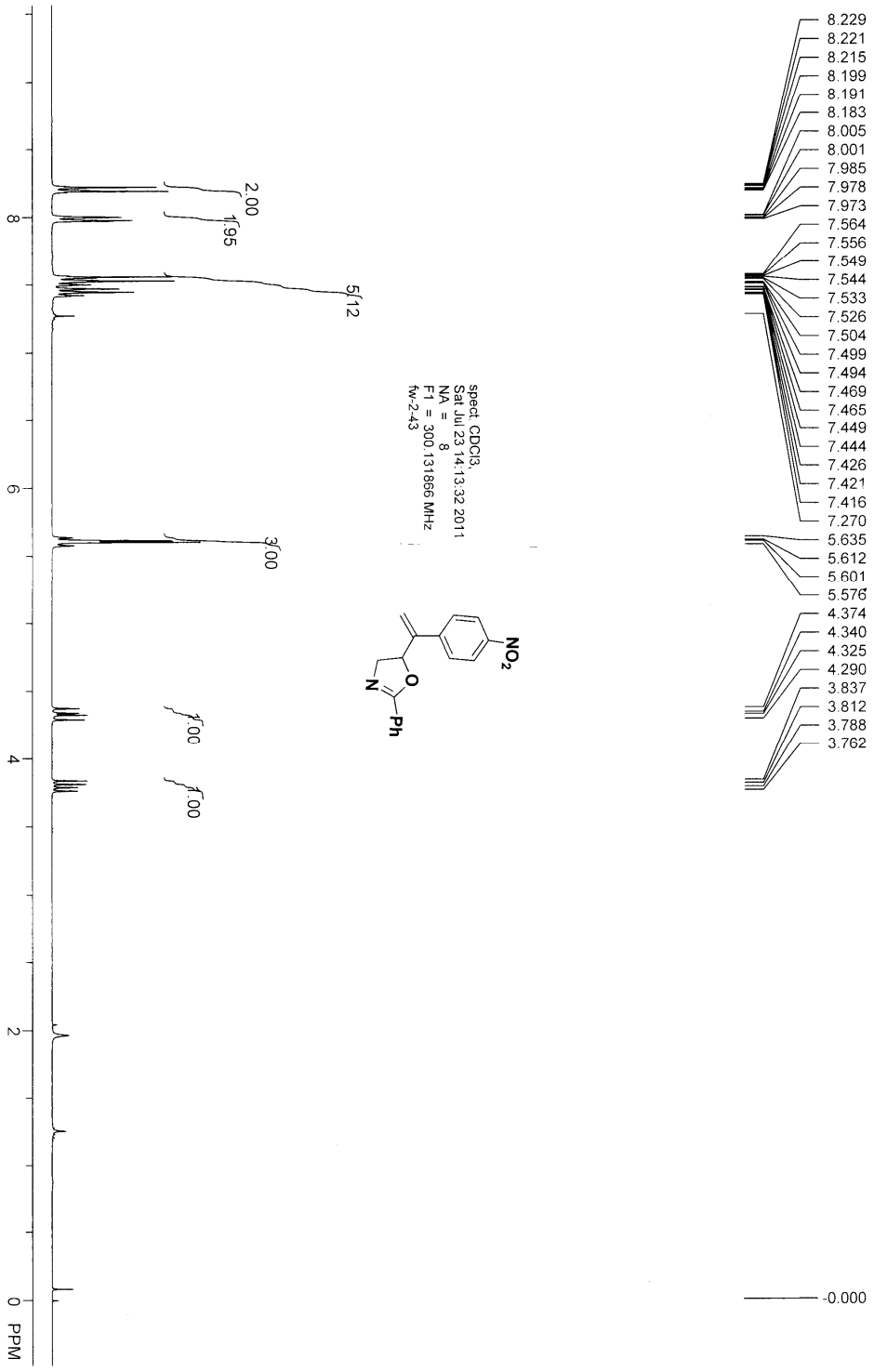


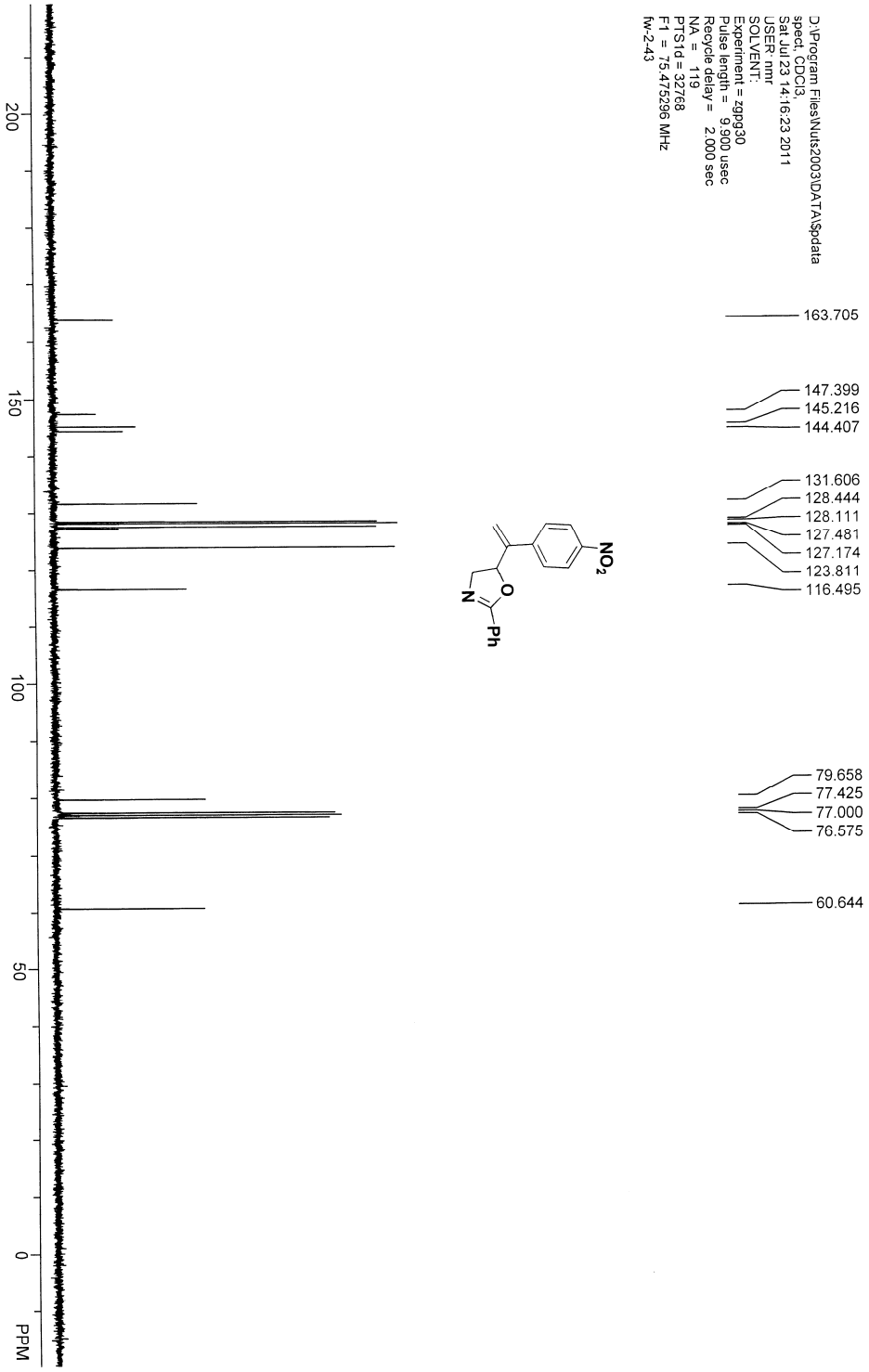


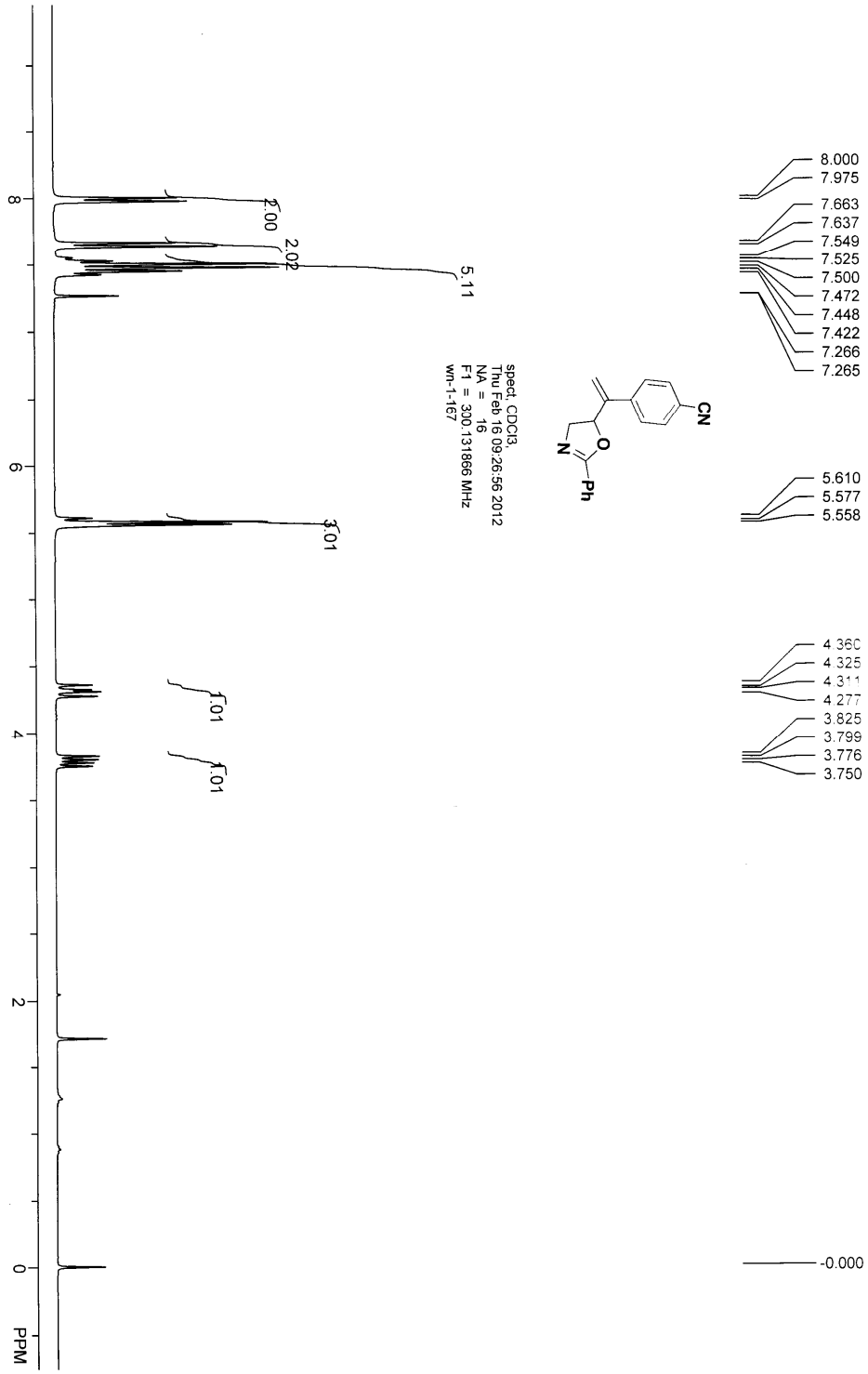


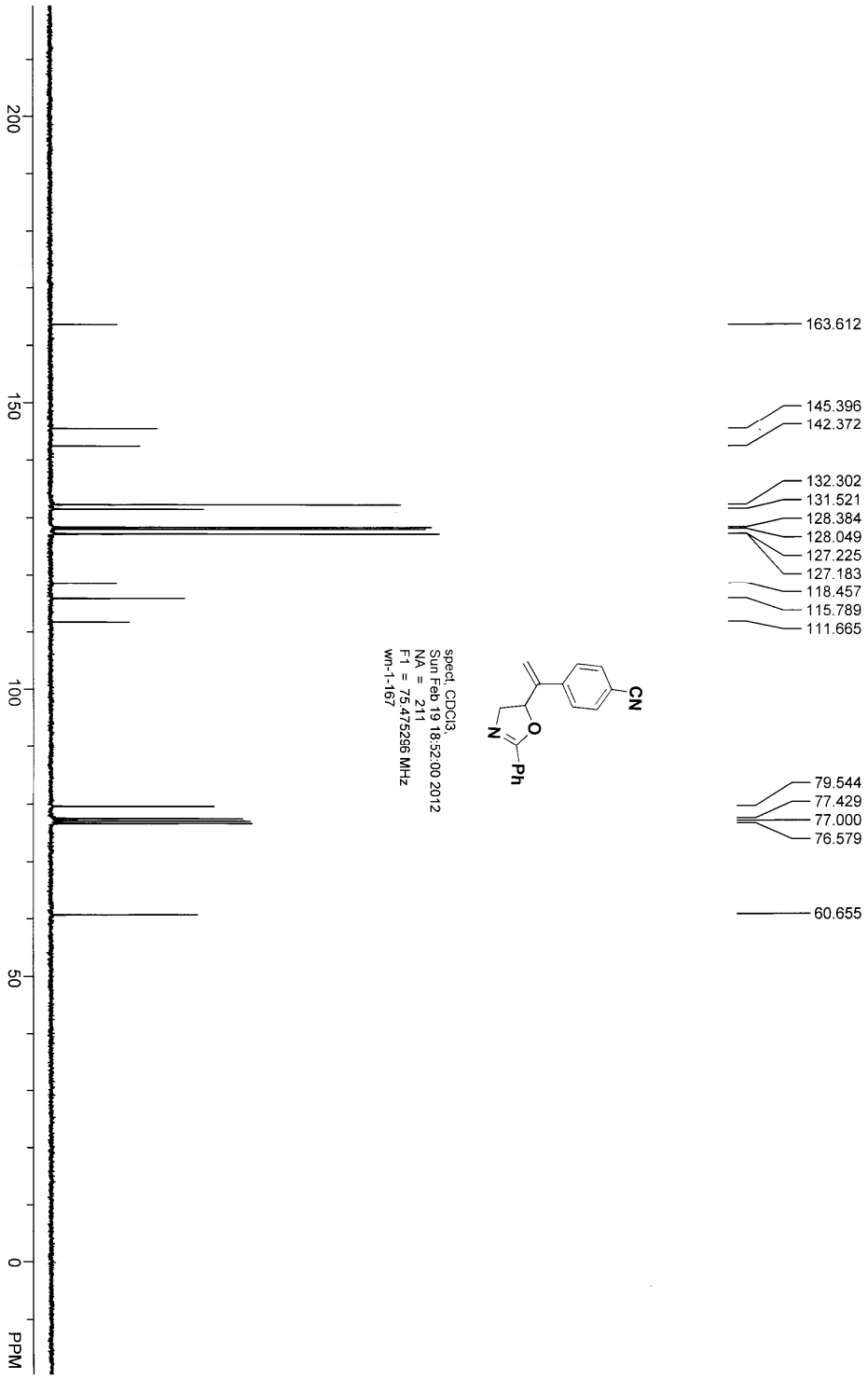

8.020
7.994
7.960
7.933
7.519
7.492
7.466
7.446
7.420
7.266
5.651
5.621
5.591
5.564
5.537
4.358
4.324
4.310
4.275
3.830
3.804
3.781
3.755
2.604
1.828
-0.000
3.99
5.01
1.01
1.00
0.96
1.00
1.00
2.99
spect, CDCl3,
Wed Mar 07 17:49:36 2012
NA = 8
F1 = 300.131866 MHz
cb-6-168
O
N
O
Ph
8
6
4
2
0
PPM

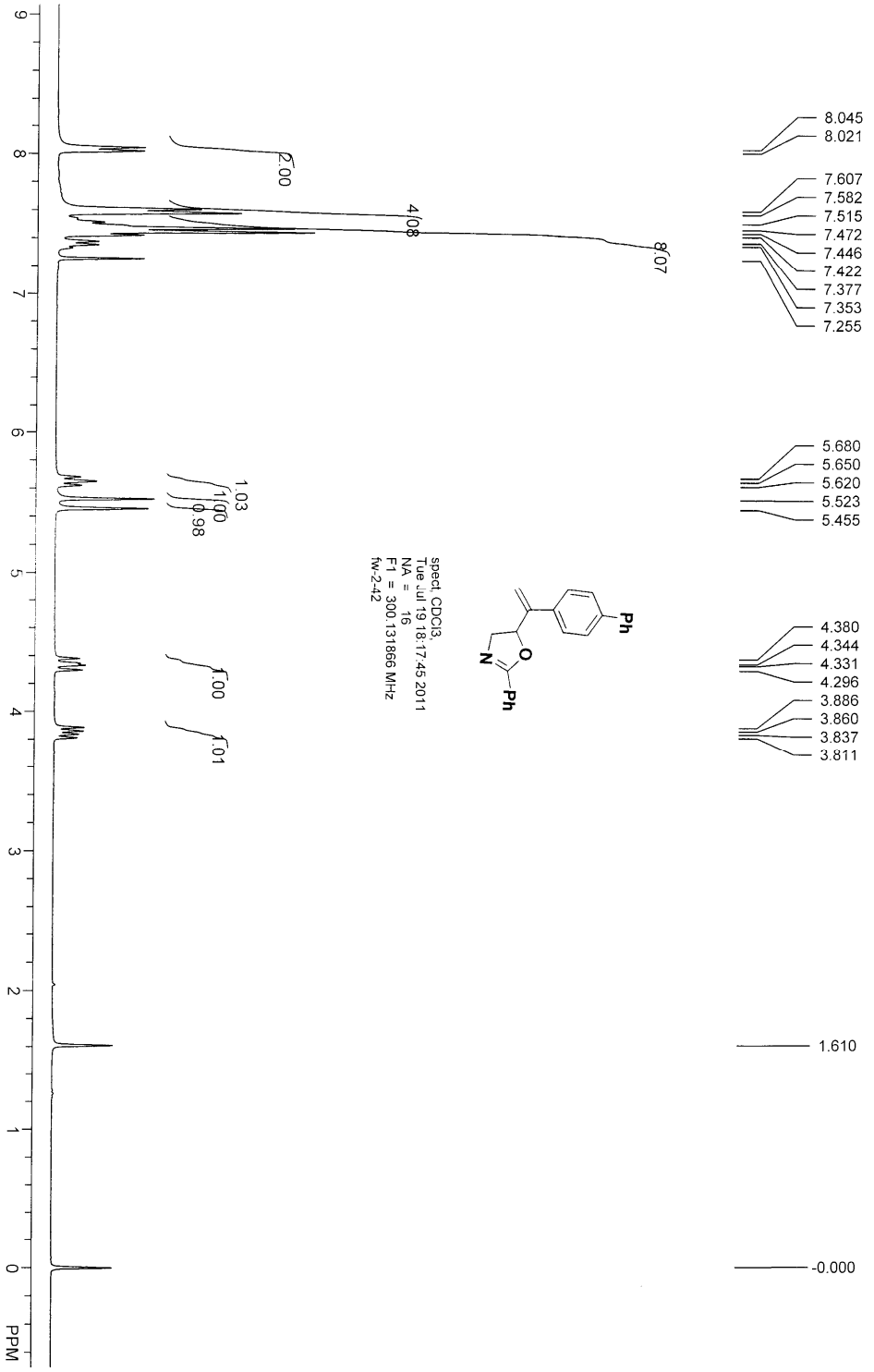


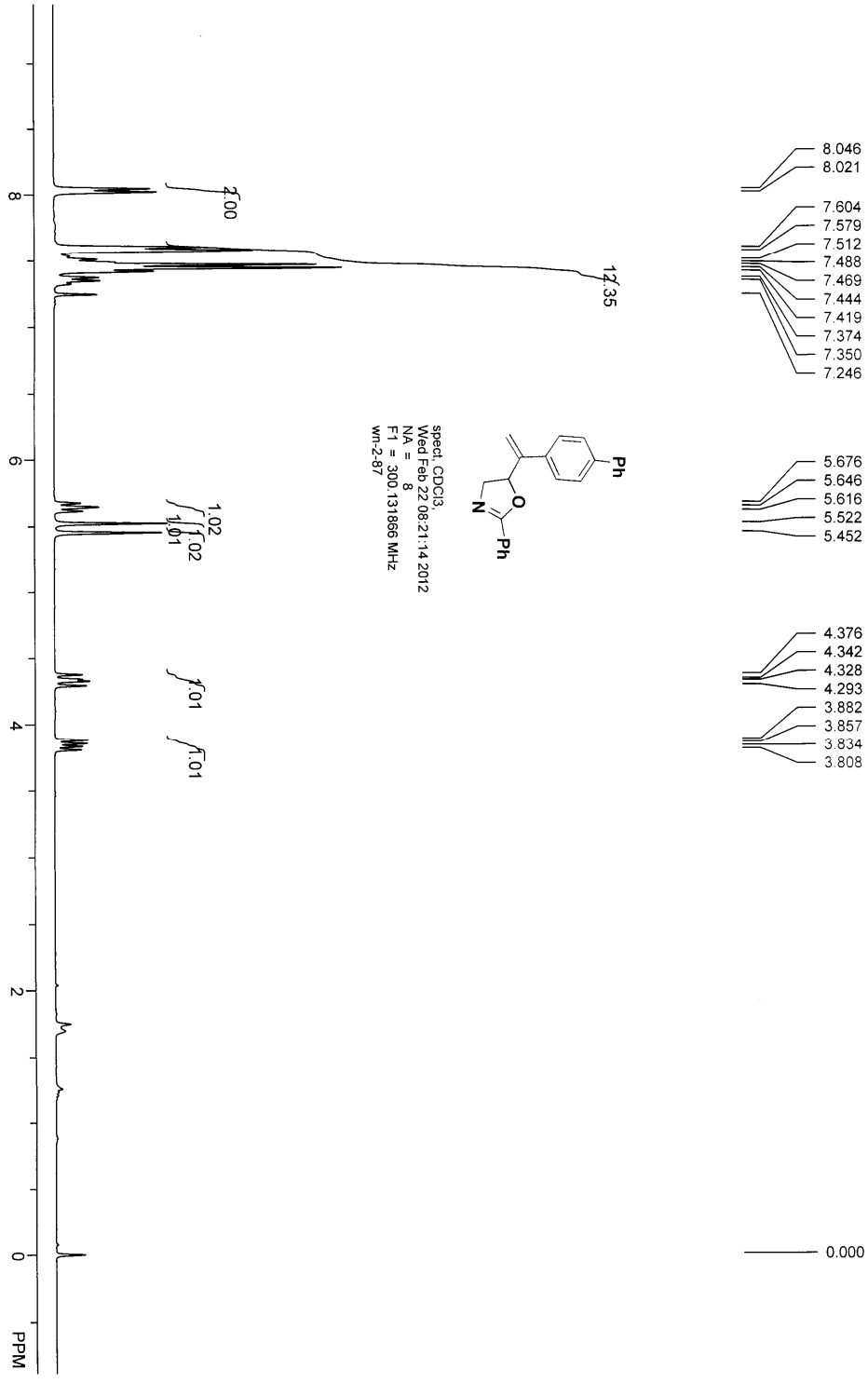


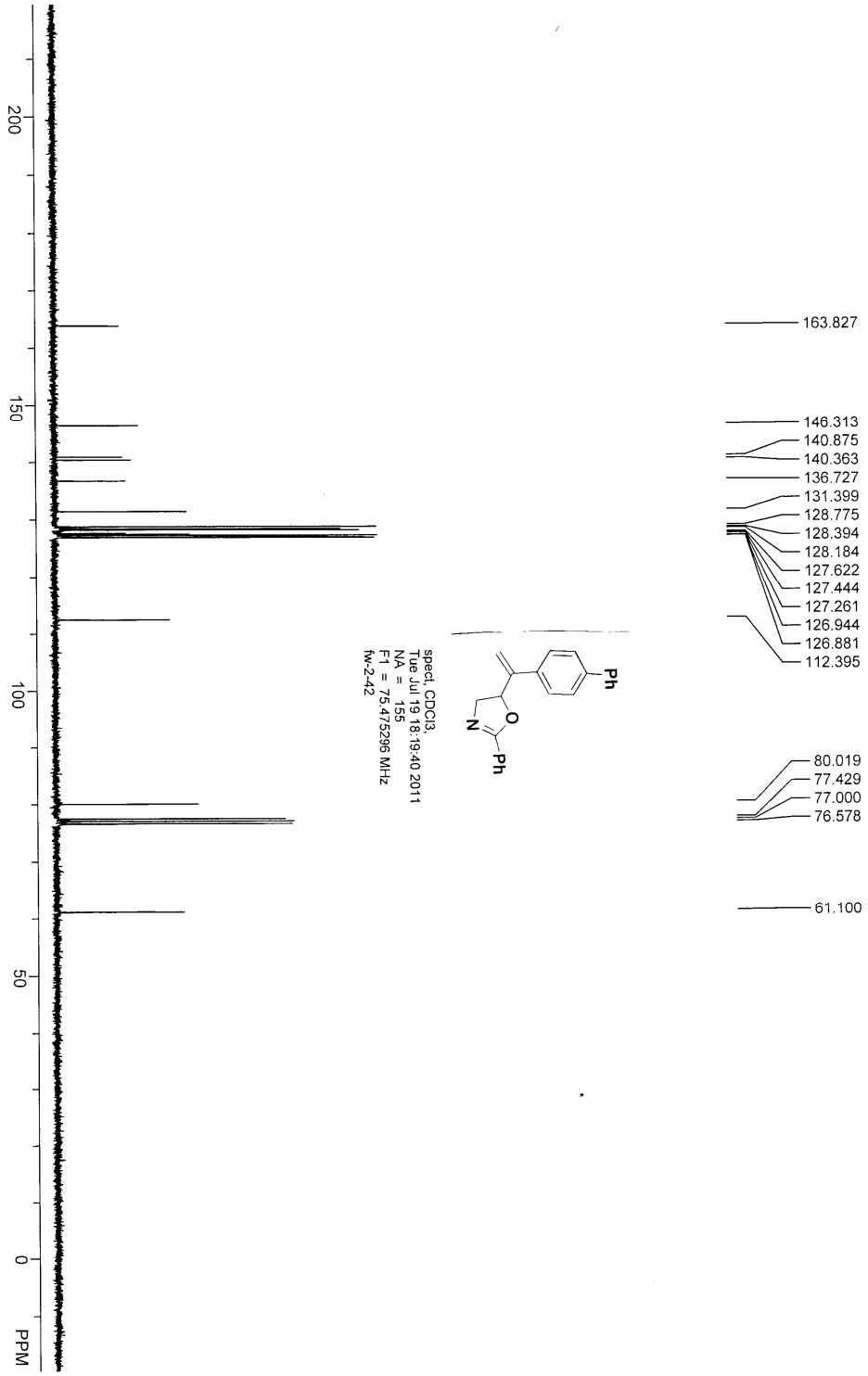


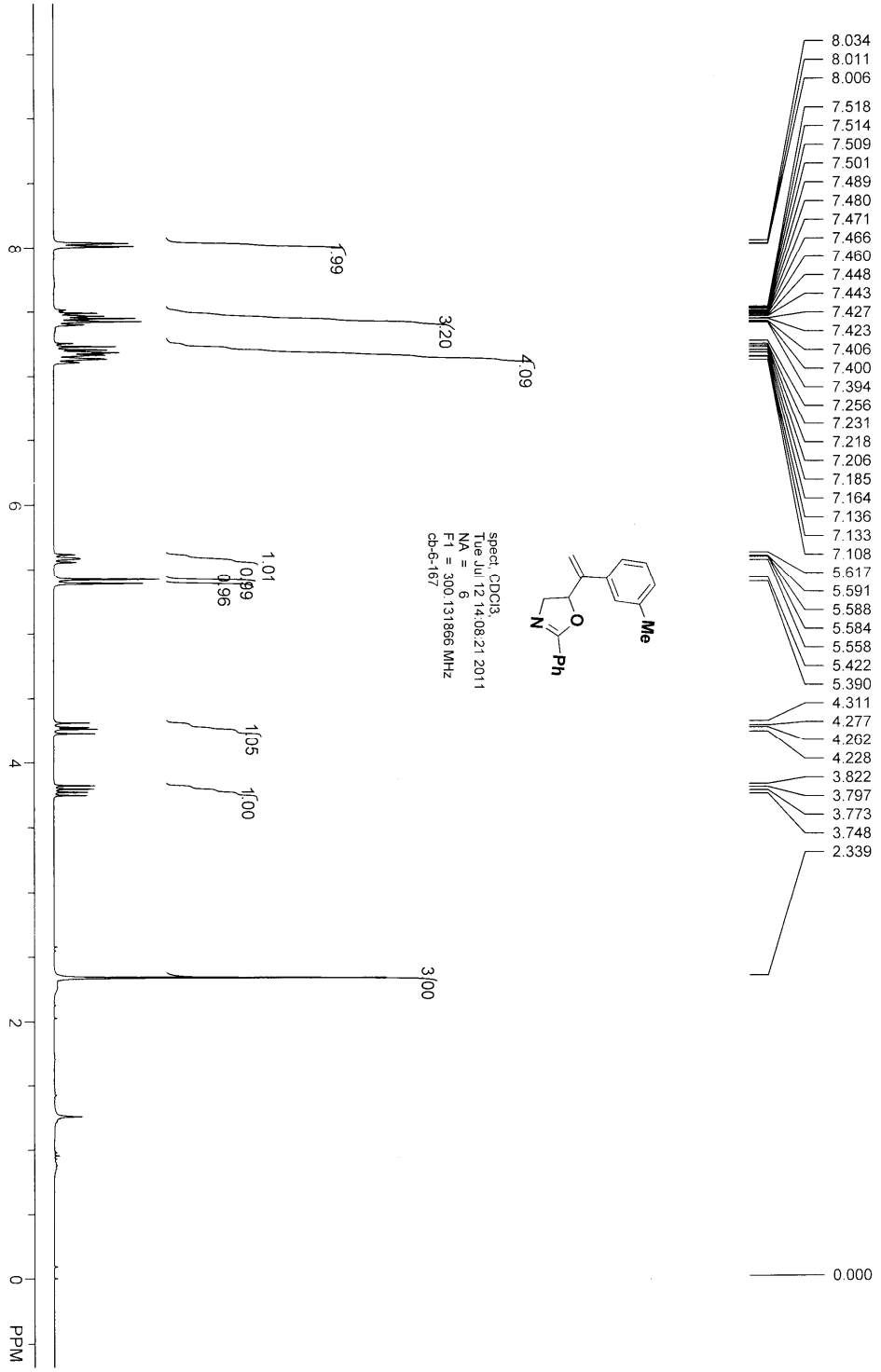


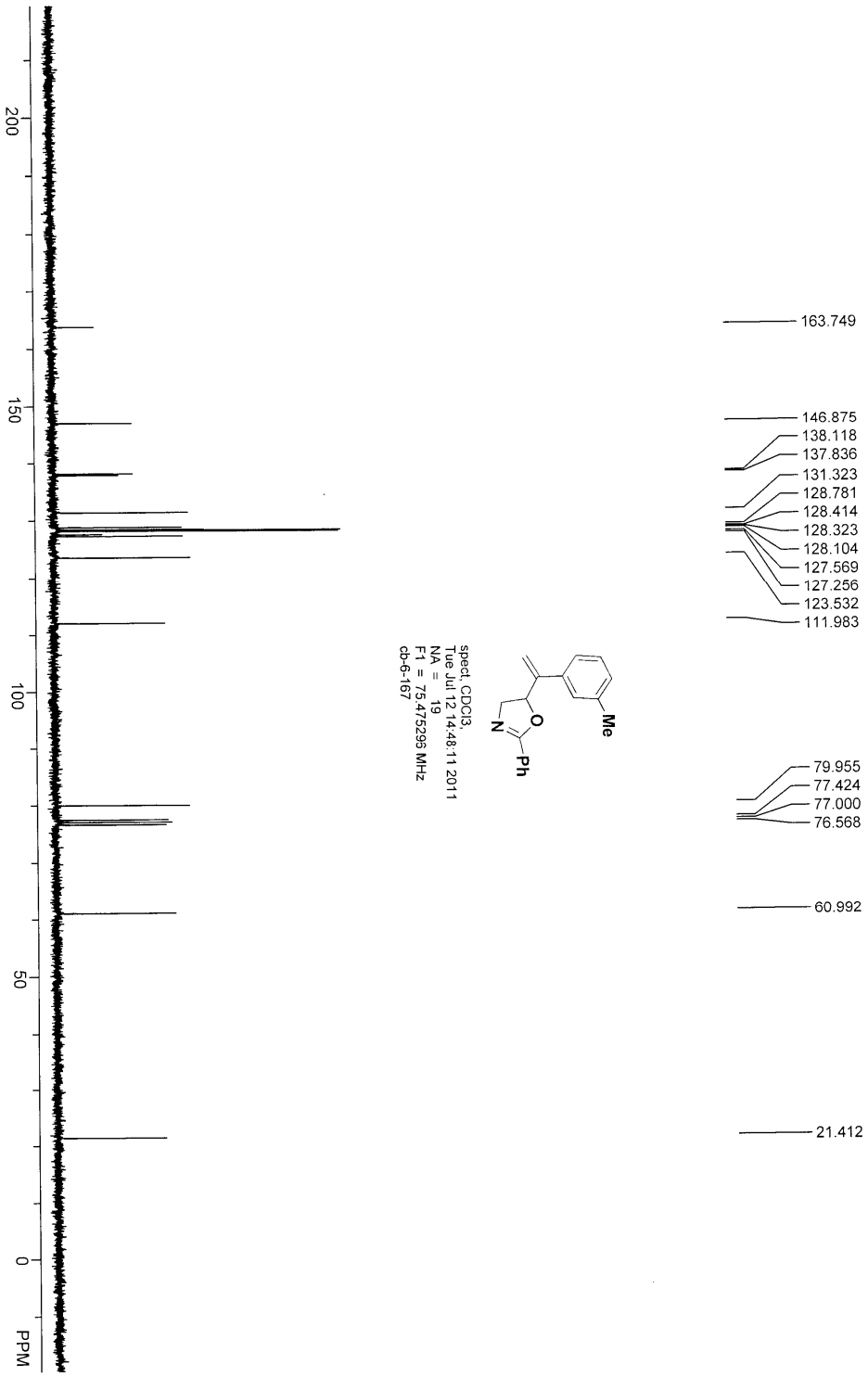


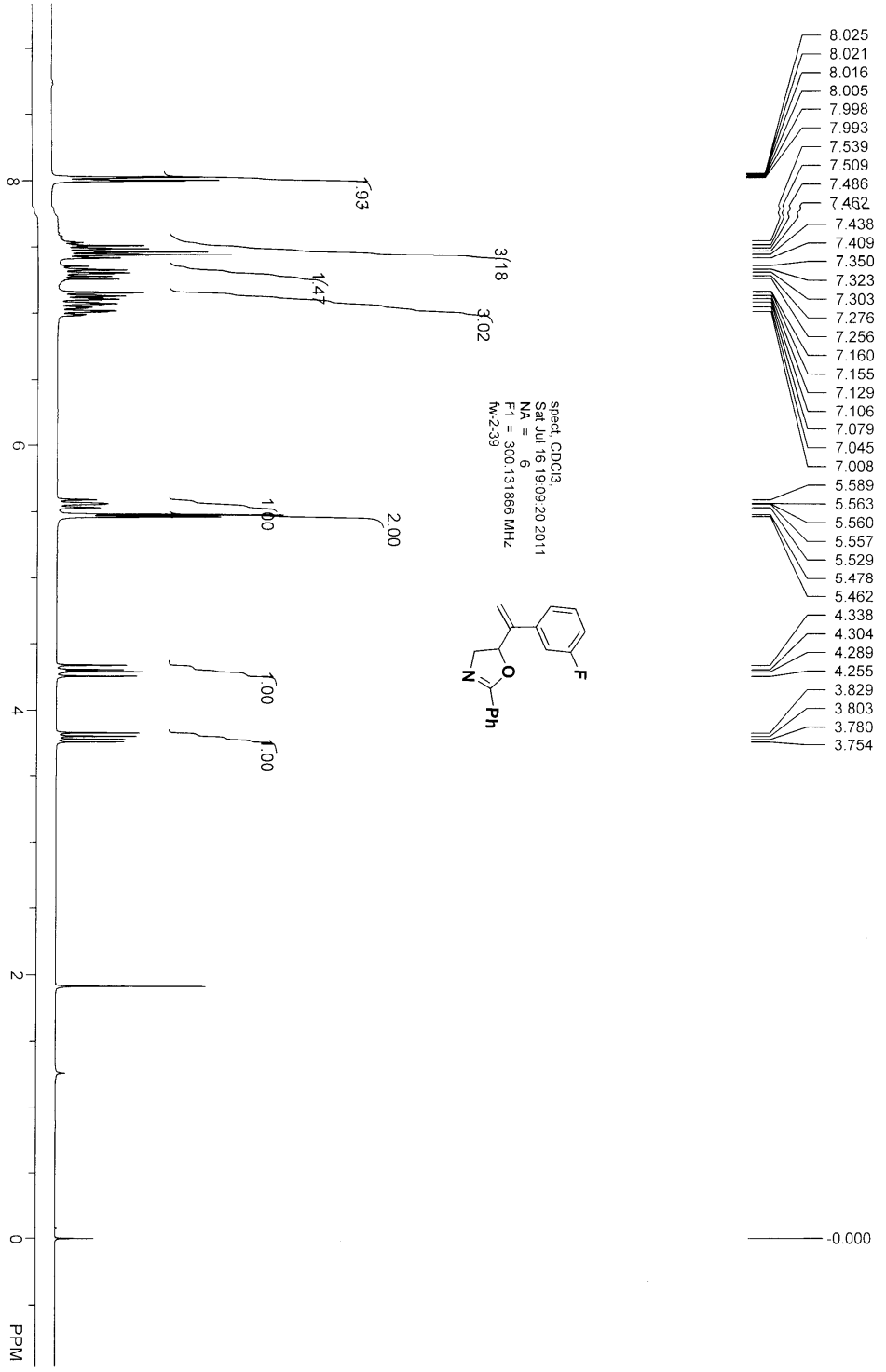


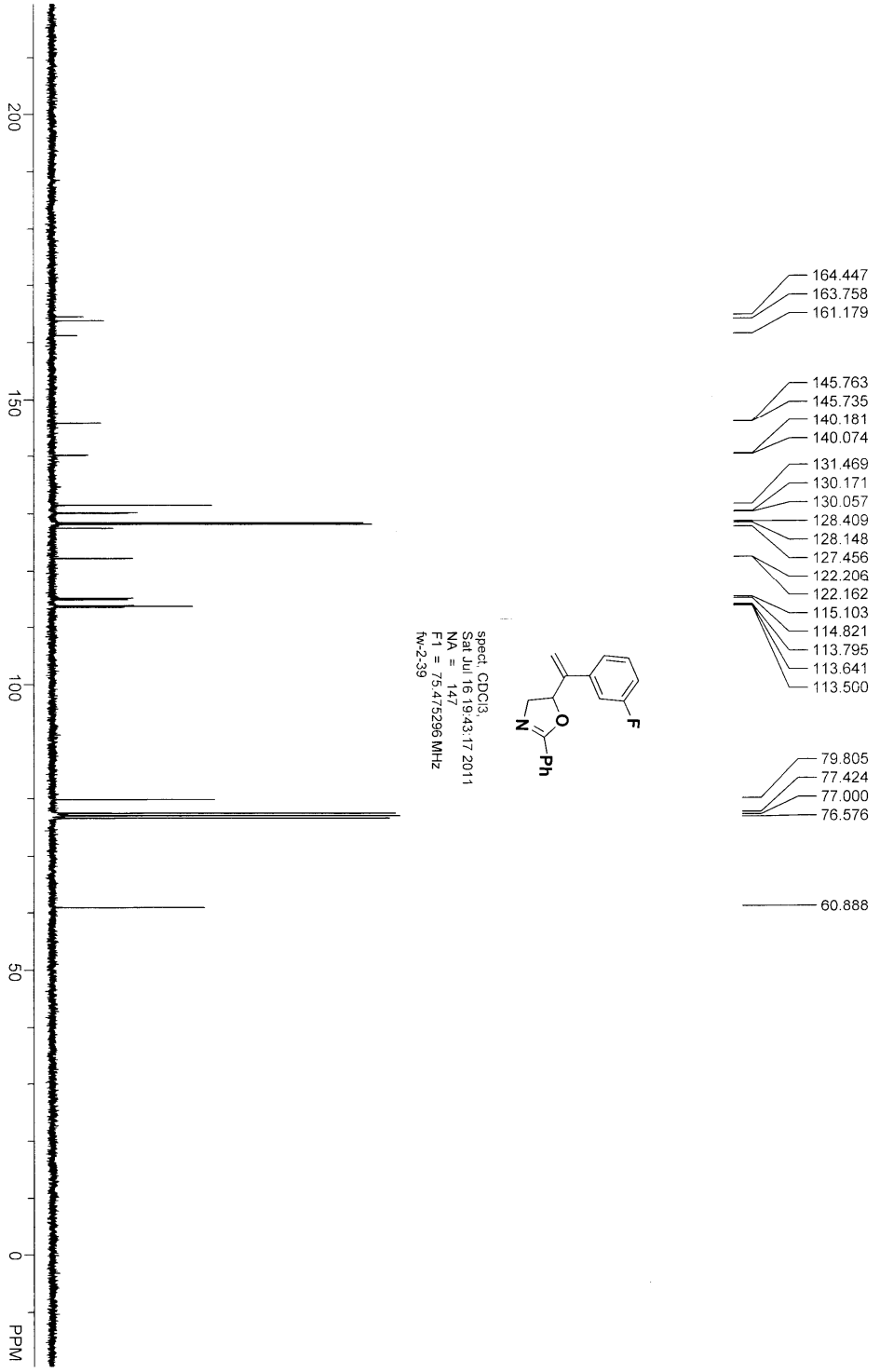

8.046
8.021
7.604
7.579
7.512
7.488
7.469
7.444
7.419
7.374
7.350
7.246
5.676
5.646
5.616
5.522
5.452
4.376
4.342
4.328
4.293
3.882
3.857
3.834
3.808
0.000
2.00
12.35
1.02
1.01
1.02
1.01
1.01
spect, CDCl3,
Wed Feb 22 08:21:14 2012
NA = 8
F1 = 300.131866 MHz
wn-2-87
Ph
O
N
Ph
8
6
4
2
0
PPM

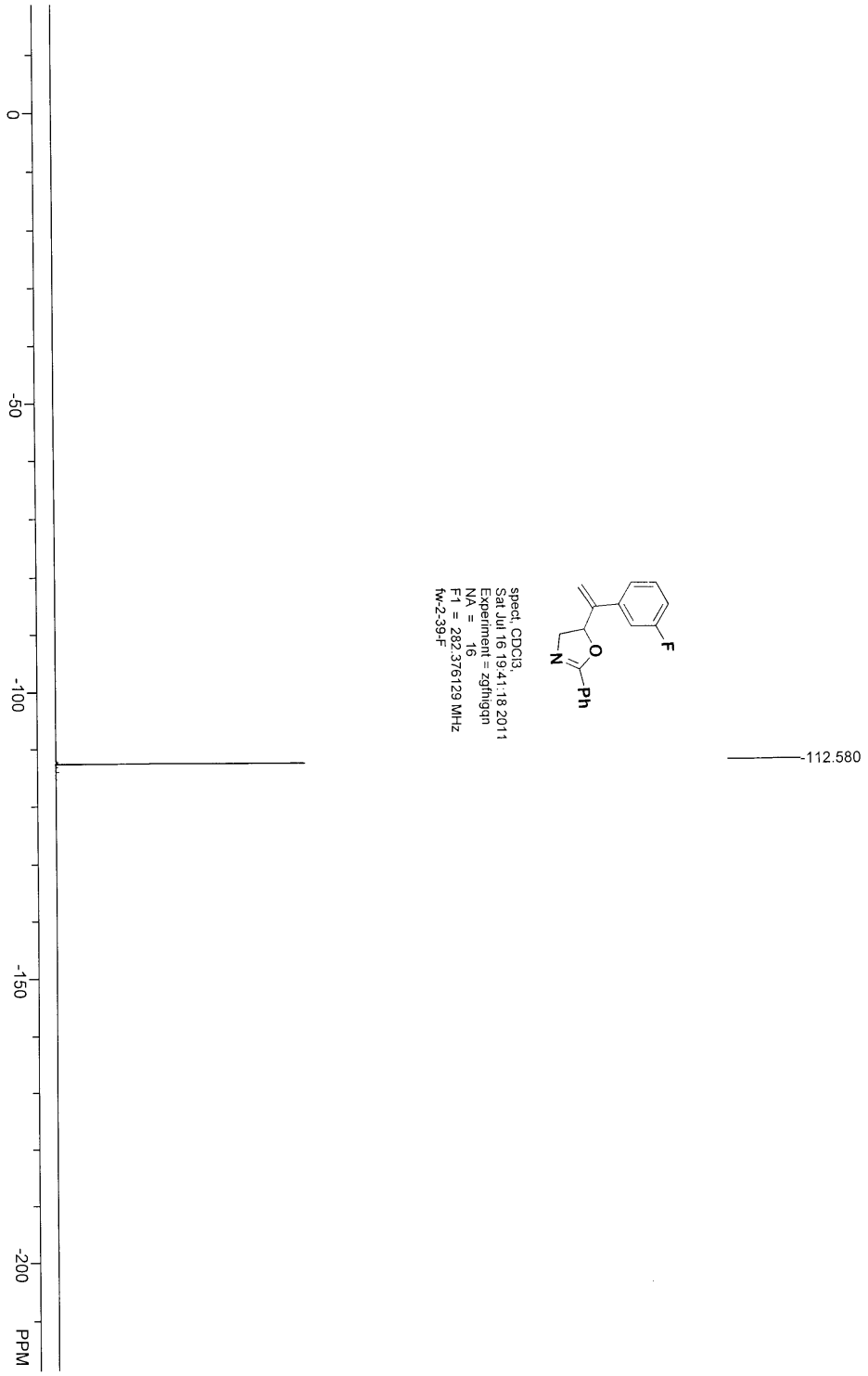


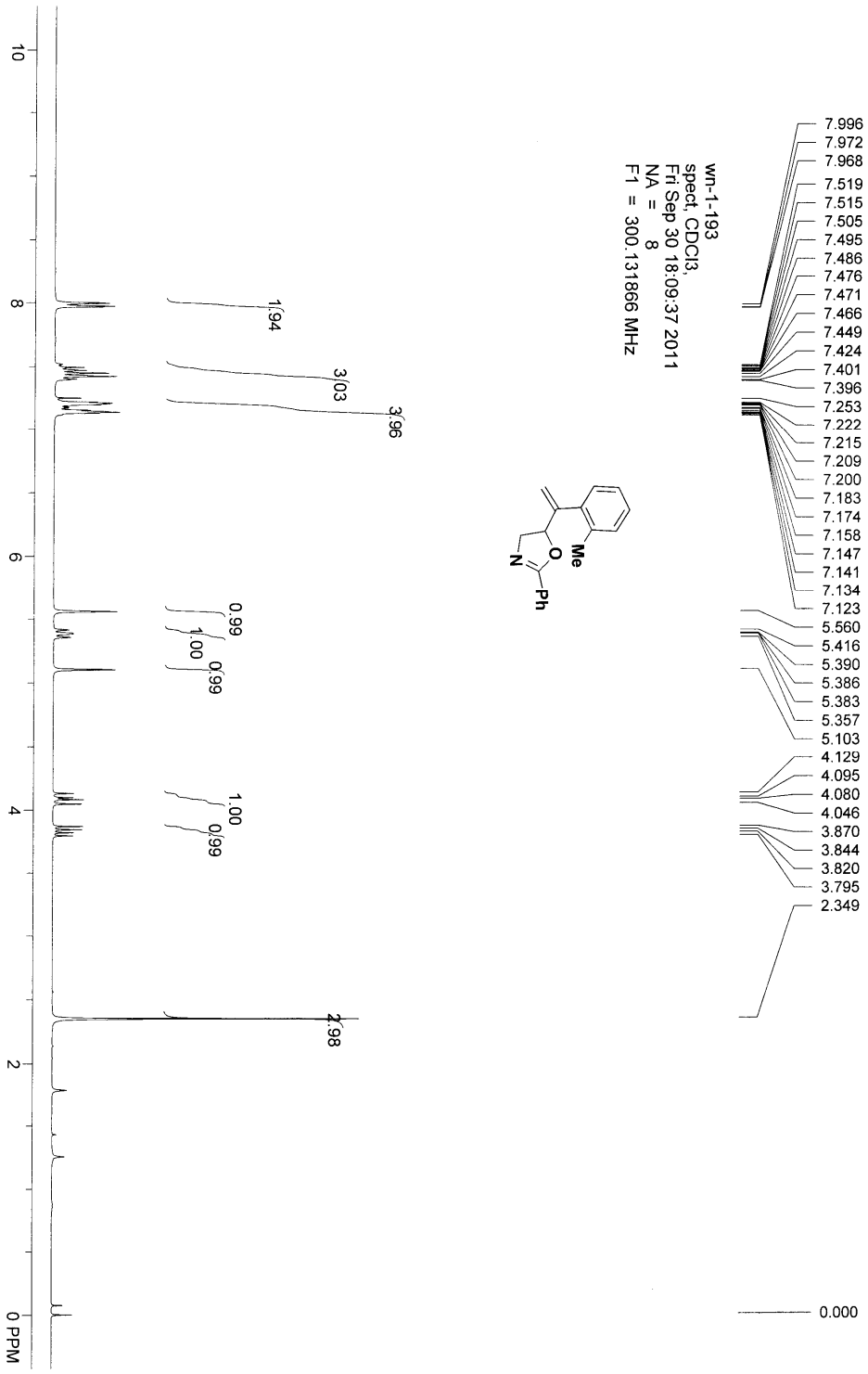


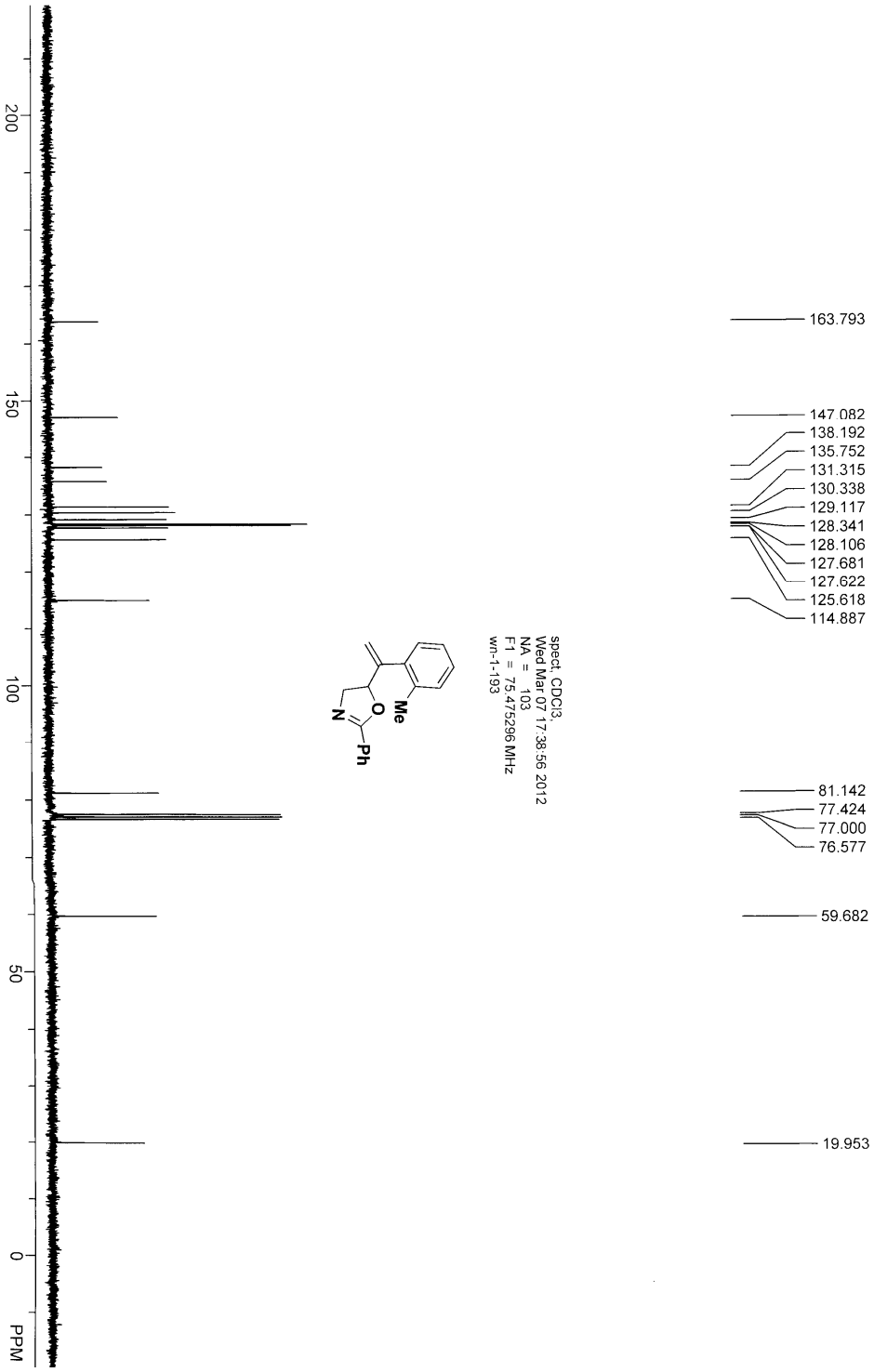


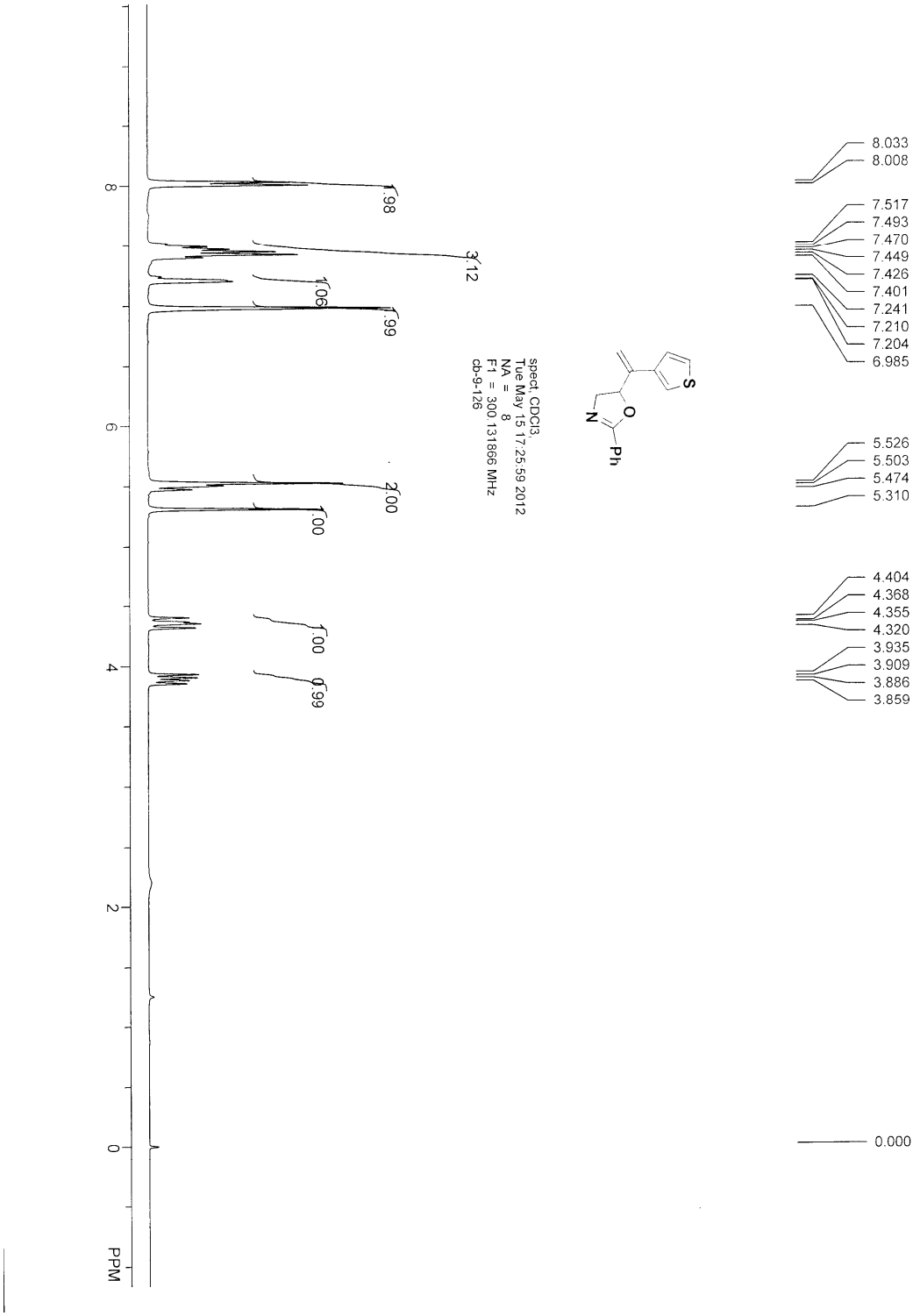

8.025
8.021
8.016
8.005
7.998
7.993
7.539
7.509
7.486
7.462
7.438
7.409
7.350
7.323
7.303
7.276
7.256
7.160
7.155
7.129
7.106
7.079
7.045
7.008
5.589
5.563
5.560
5.557
5.529
5.478
5.462
4.338
4.304
4.289
4.255
3.829
3.803
3.780
3.754
-0.000
1.93
3.18
1.47
3.02
1.00
2.00
1.00
1.00
spect, CDCl3,
Sat Jul 16 19:09:20 2011
NA = 6
F1 = 300.131866 MHz
fw-2-39
N
O
Ph
F
8
6
4
2
0
PPM

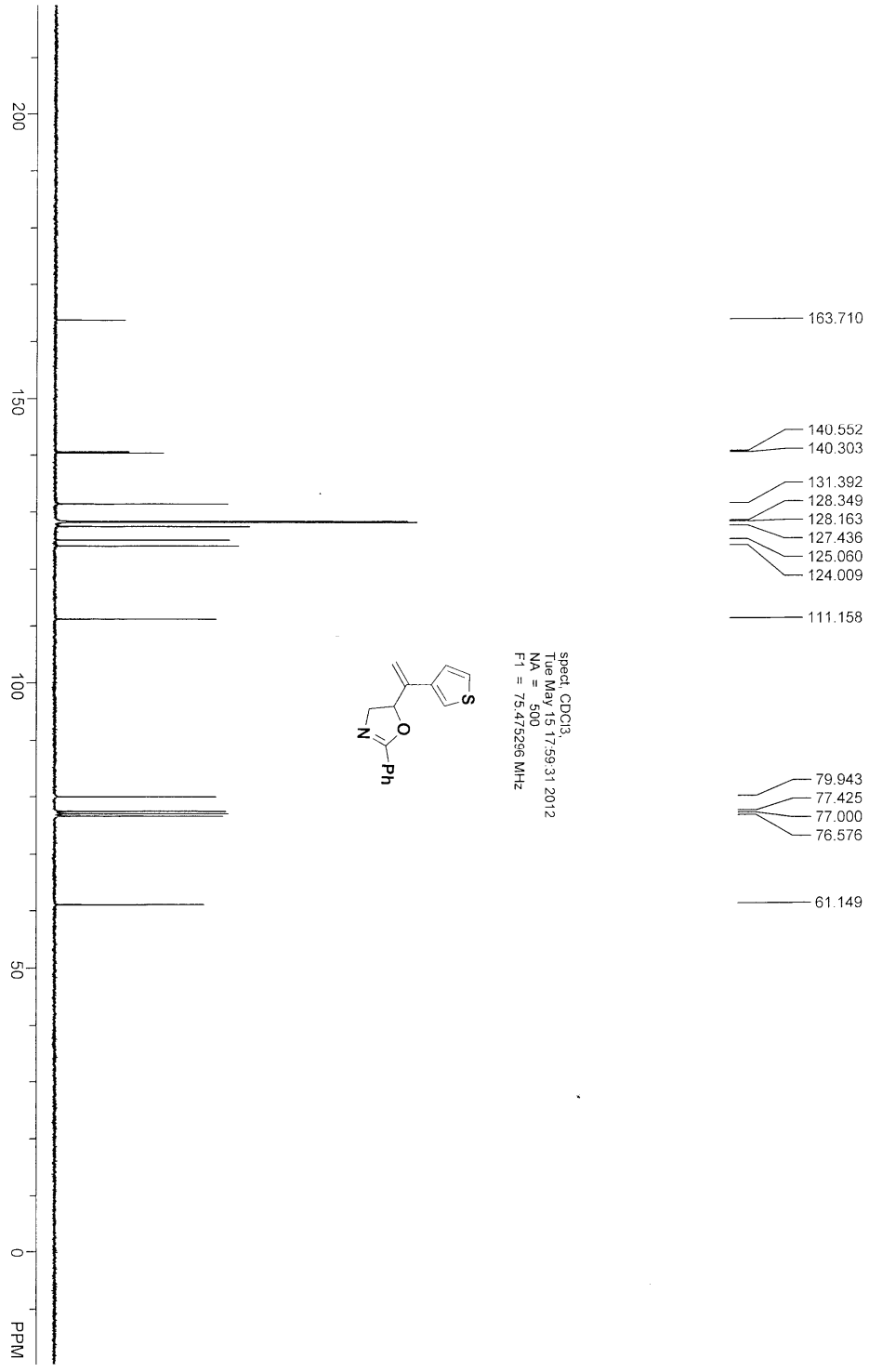


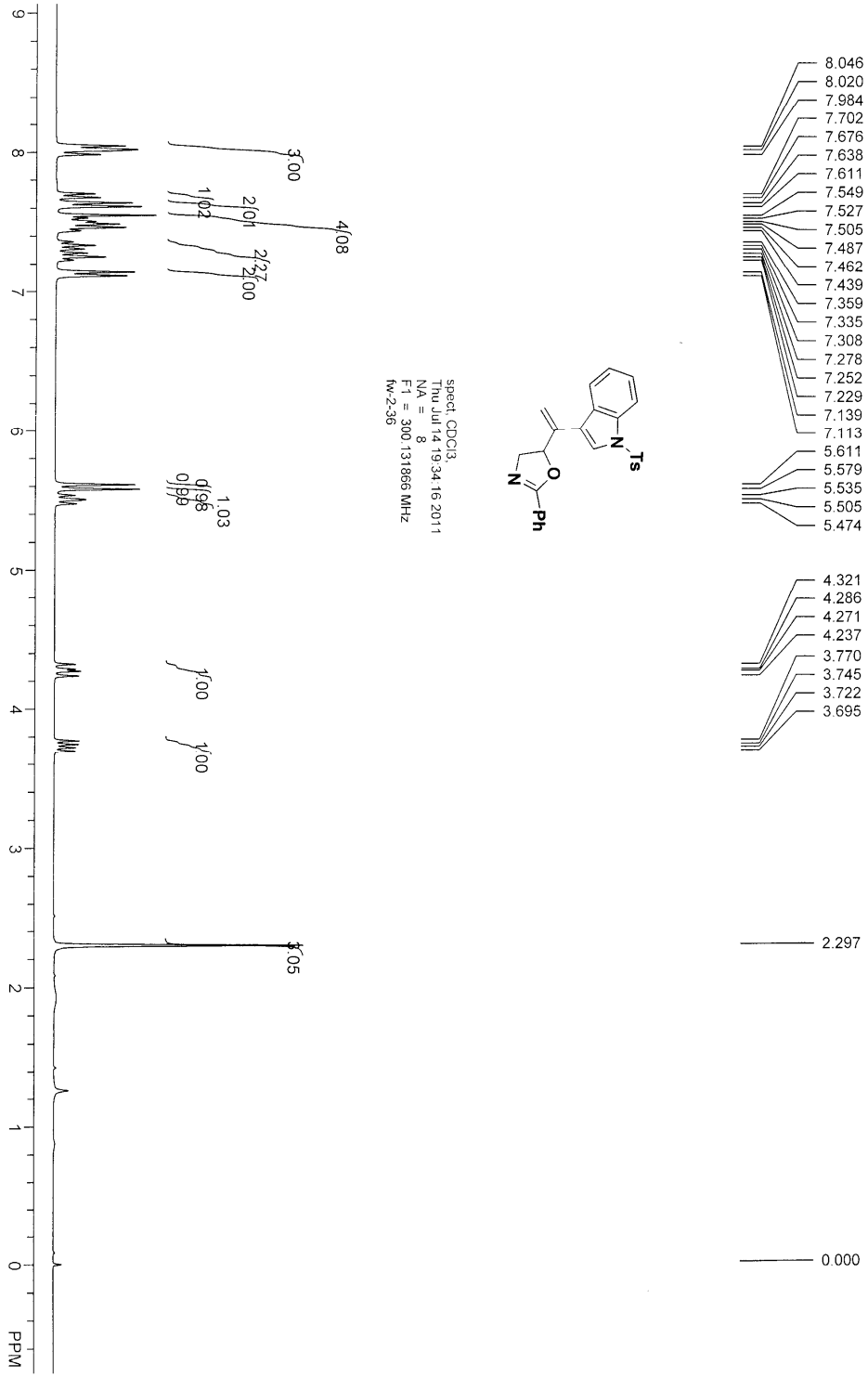

spect_CDCl3
Sat Jul 16 19:41:18 2011
Experiment = zgfhigqn
NA = 16
F1 = 282.376129 MHz
fw-2-39-F
F
O
N
Ph
-112.580
0
-50
-100
-150
-200
PPM

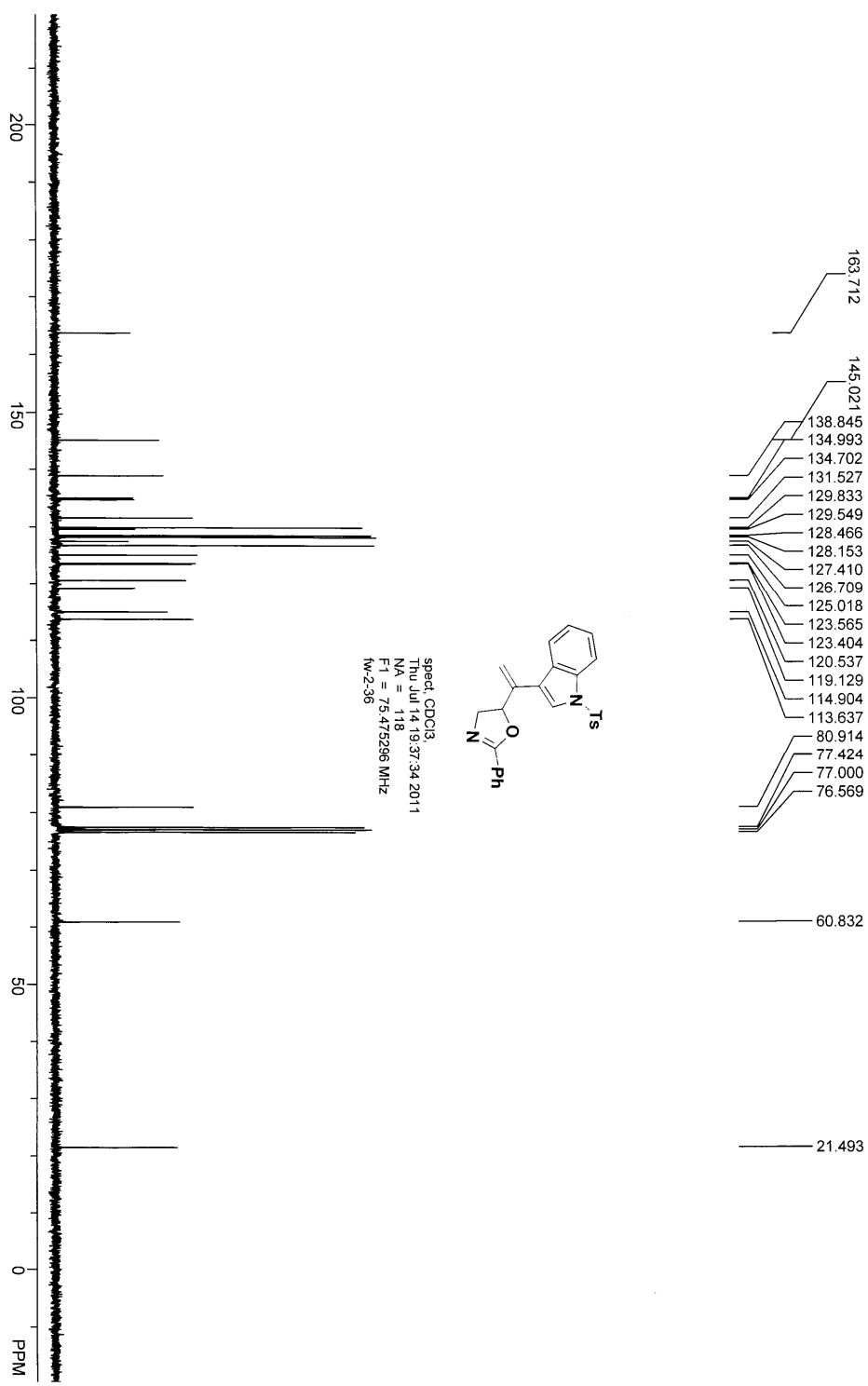


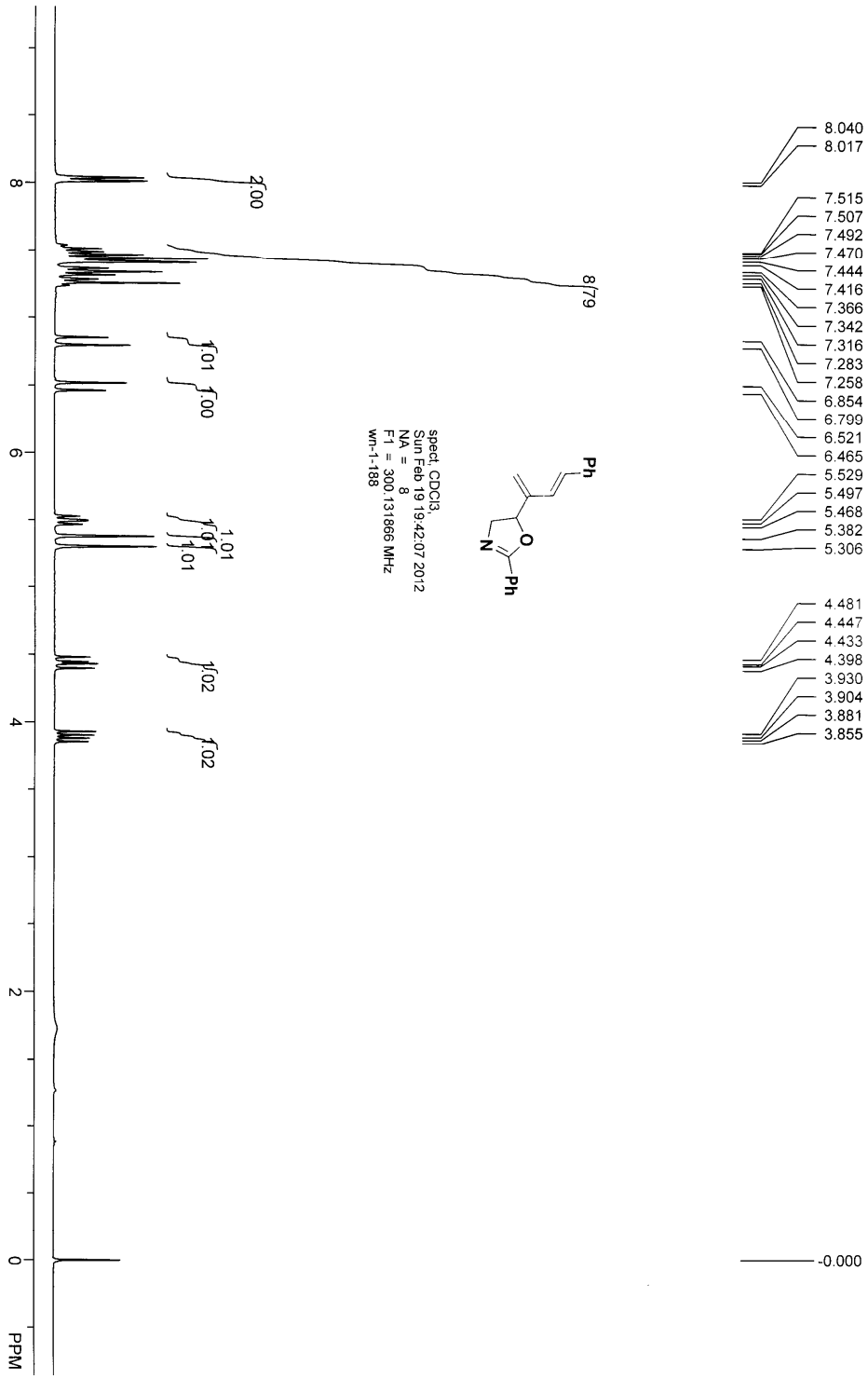


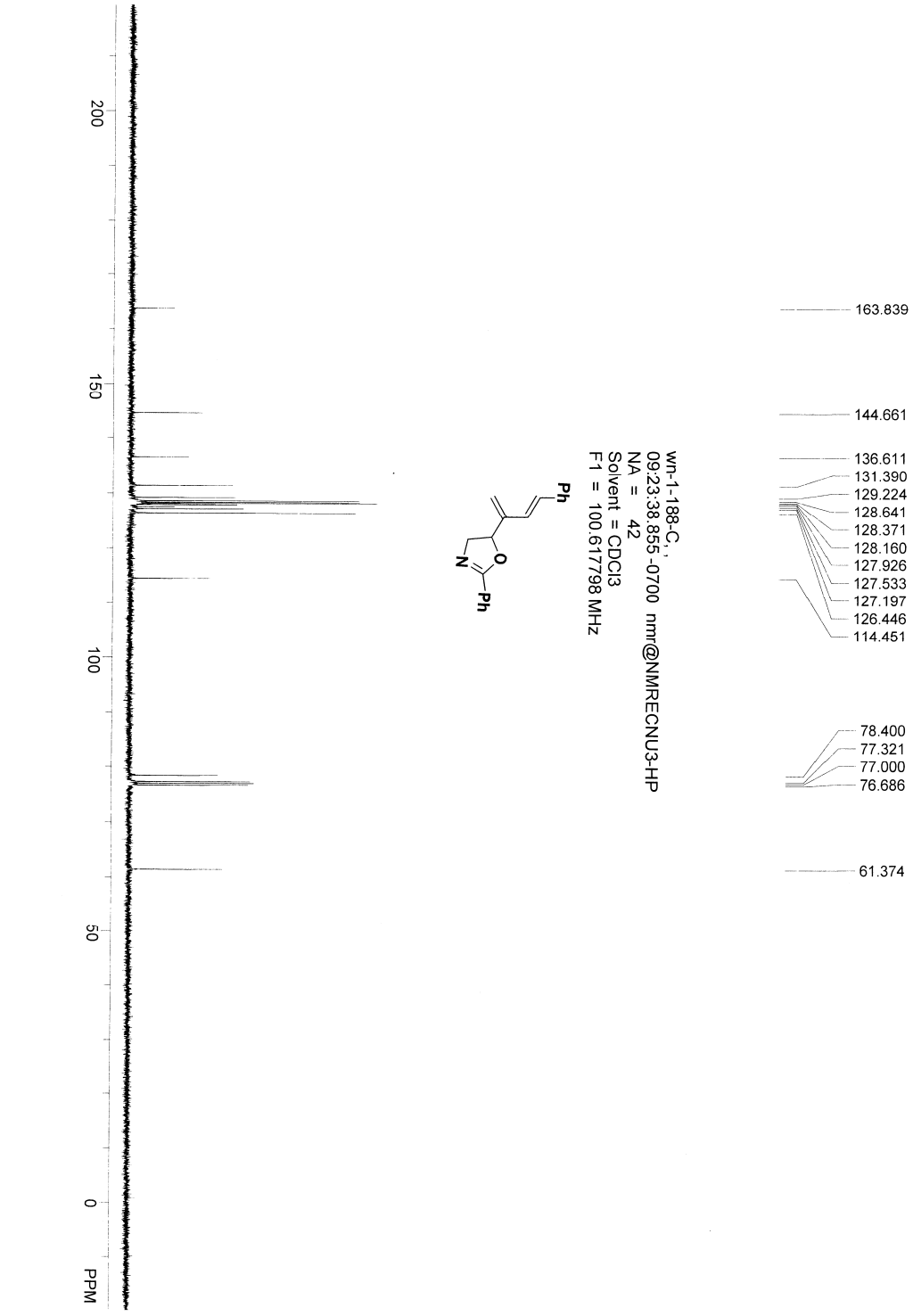


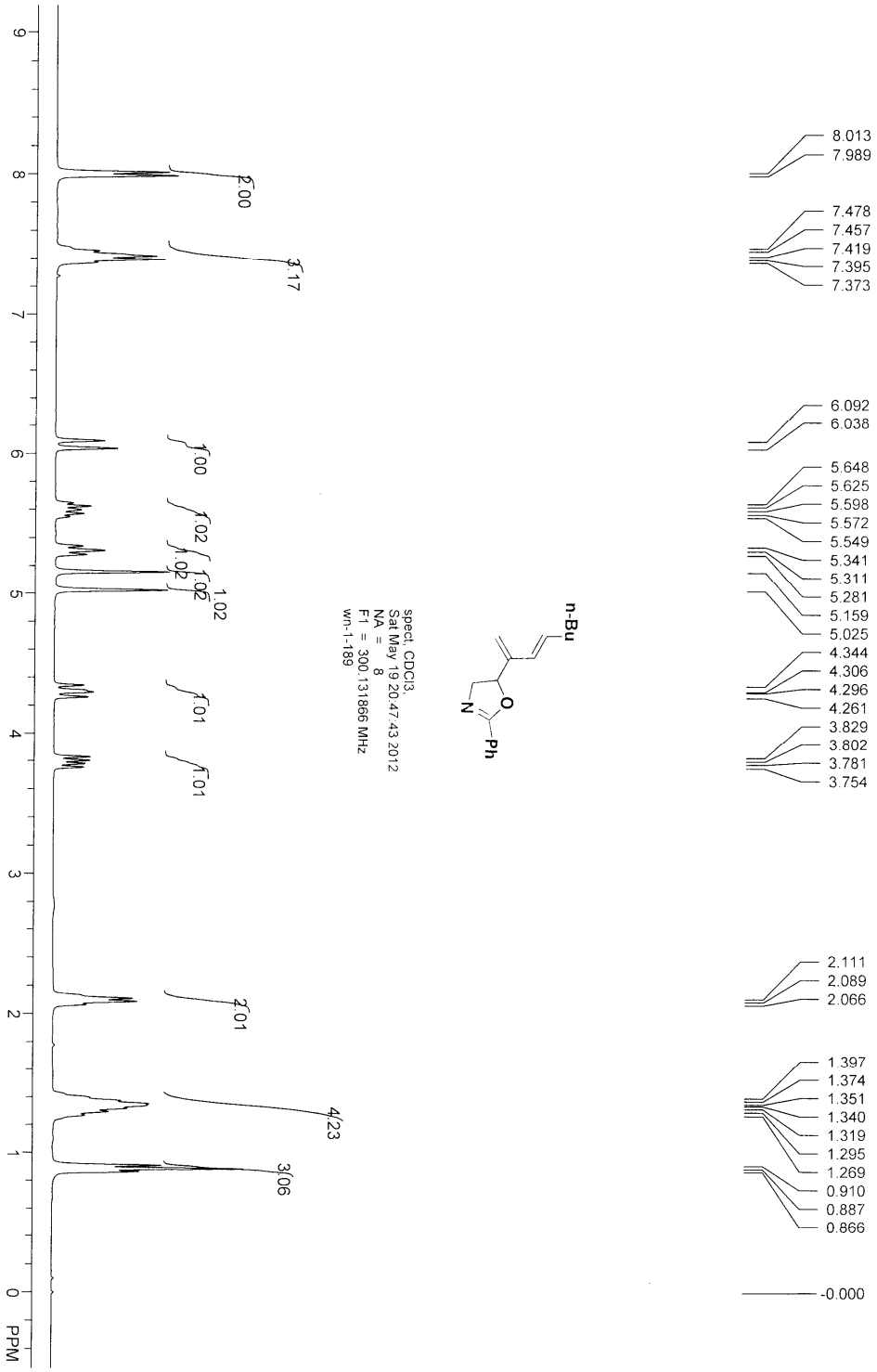


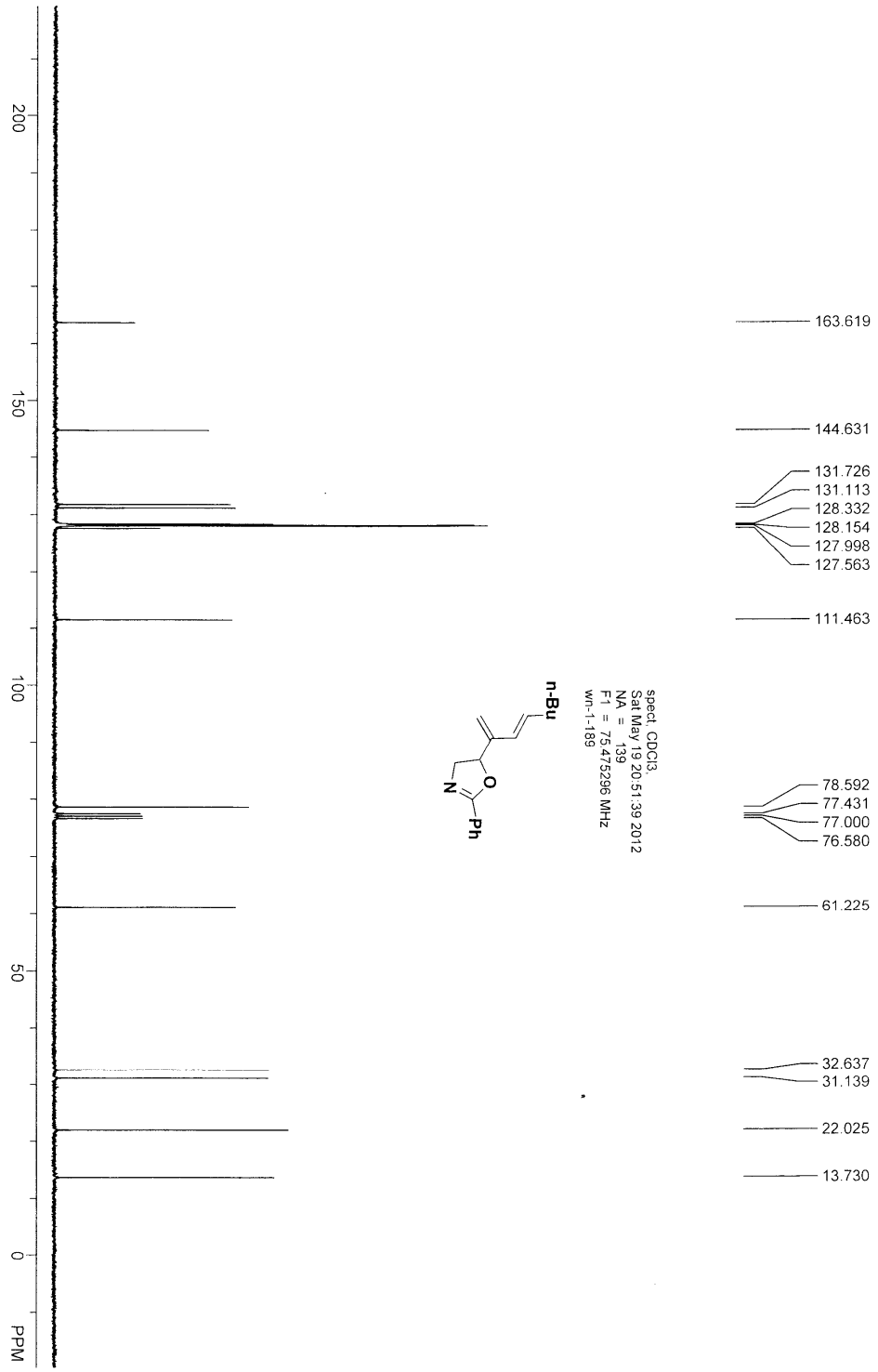


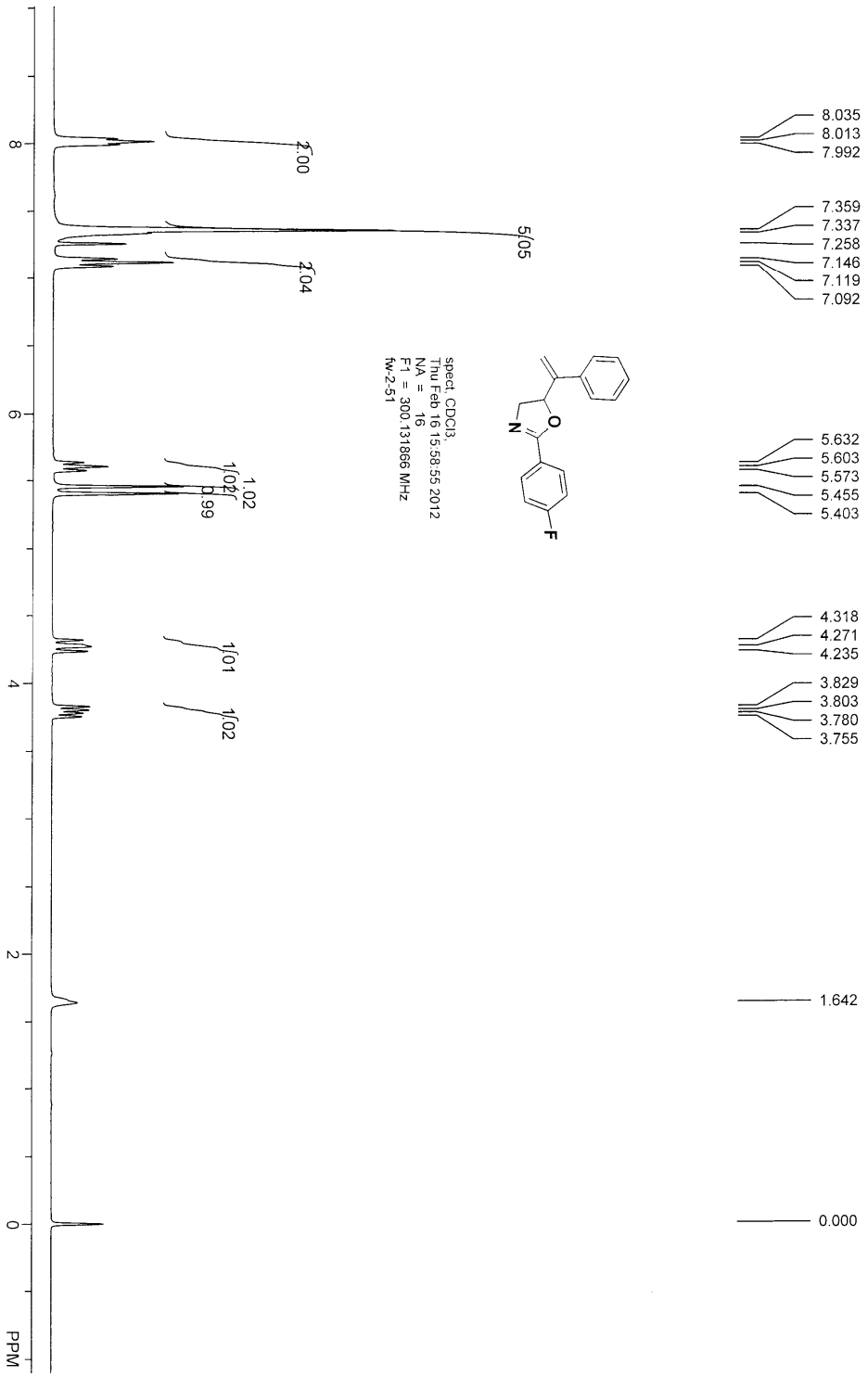


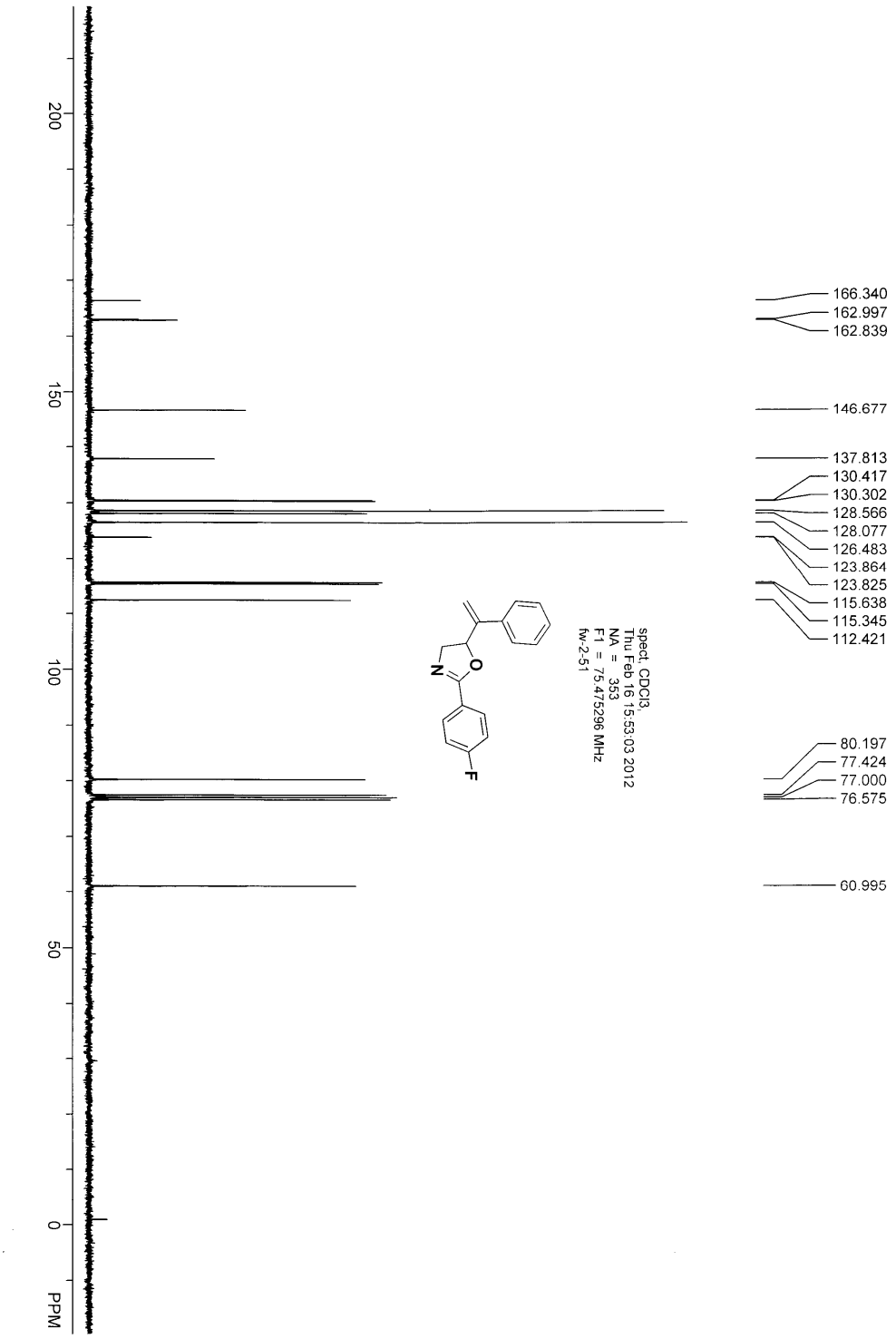

8.040
8.017
7.515
7.507
7.492
7.470
7.444
7.416
7.366
7.342
7.316
7.283
7.258
6.854
6.799
6.521
6.465
5.529
5.497
5.468
5.382
5.306
4.481
4.447
4.433
4.398
3.930
3.904
3.881
3.855
-0.000
2.00
8.79
1.01
1.00
1.01
1.01
1.01
1.02
1.02
spect_CDCl3_
Sun Feb 19 19:42:07 2012
NA = 8
F1 = 300.131866 MHz
wn-1-188
Ph
O
N
Ph
8
6
4
2
0
PPM

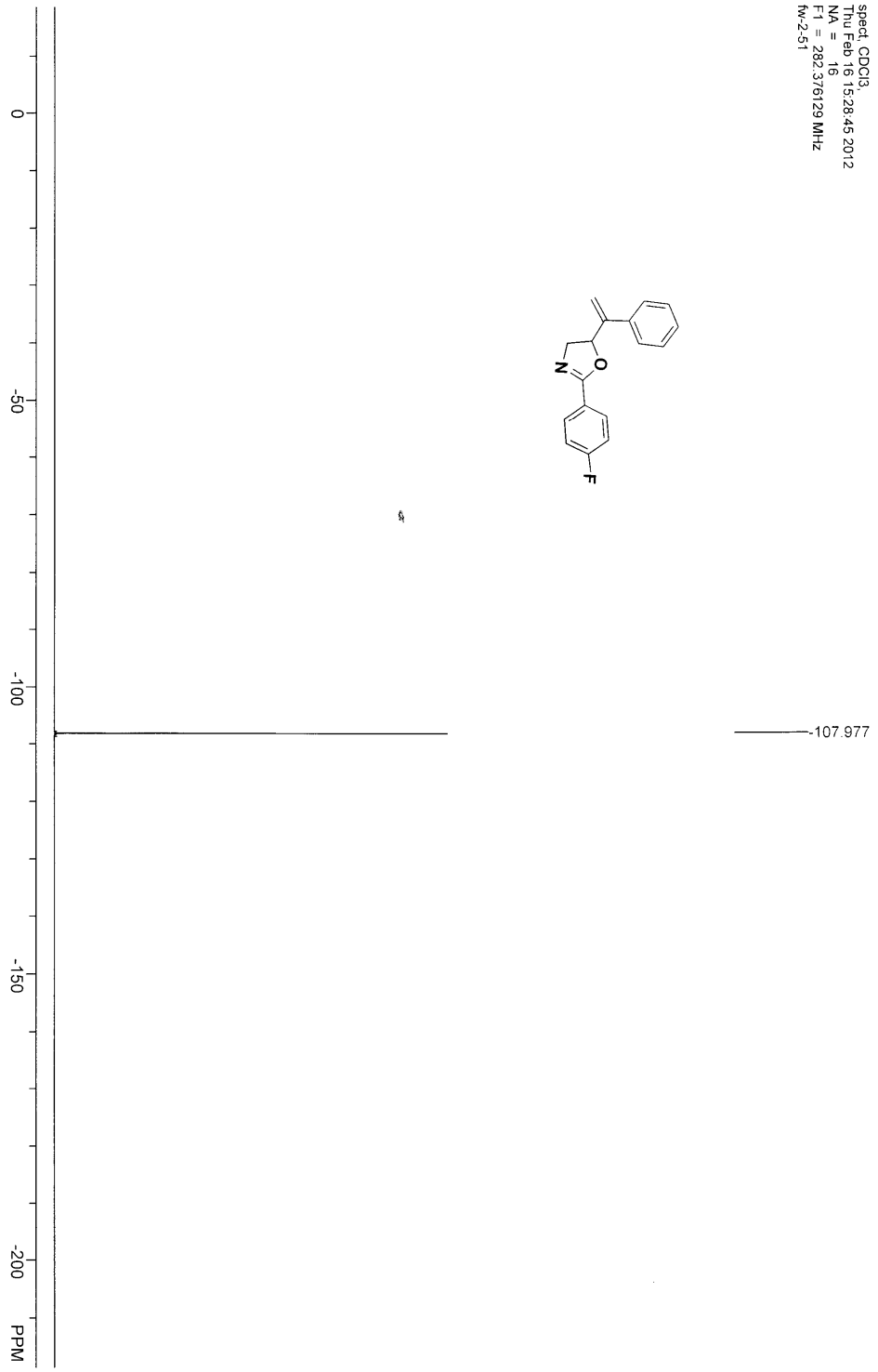


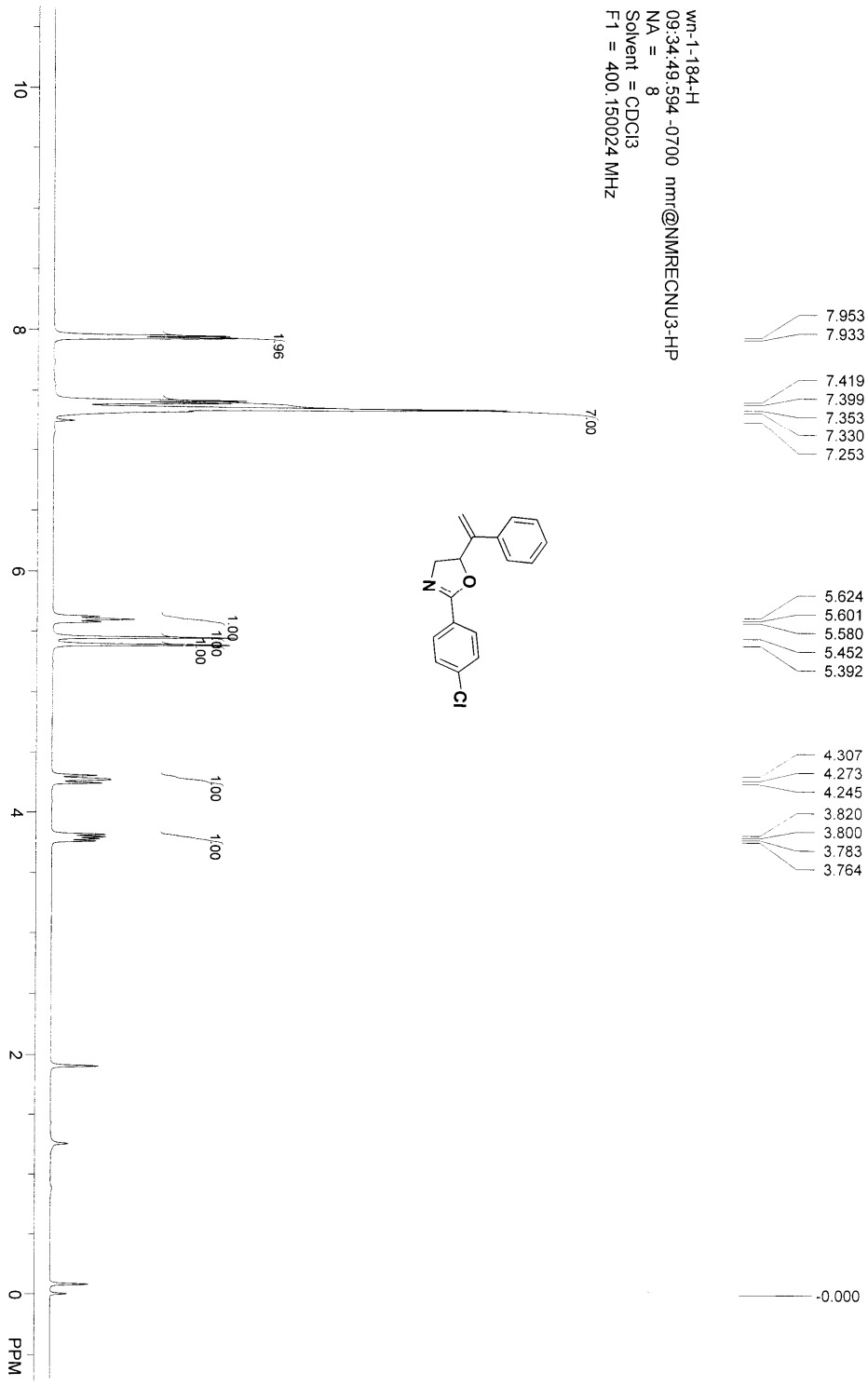








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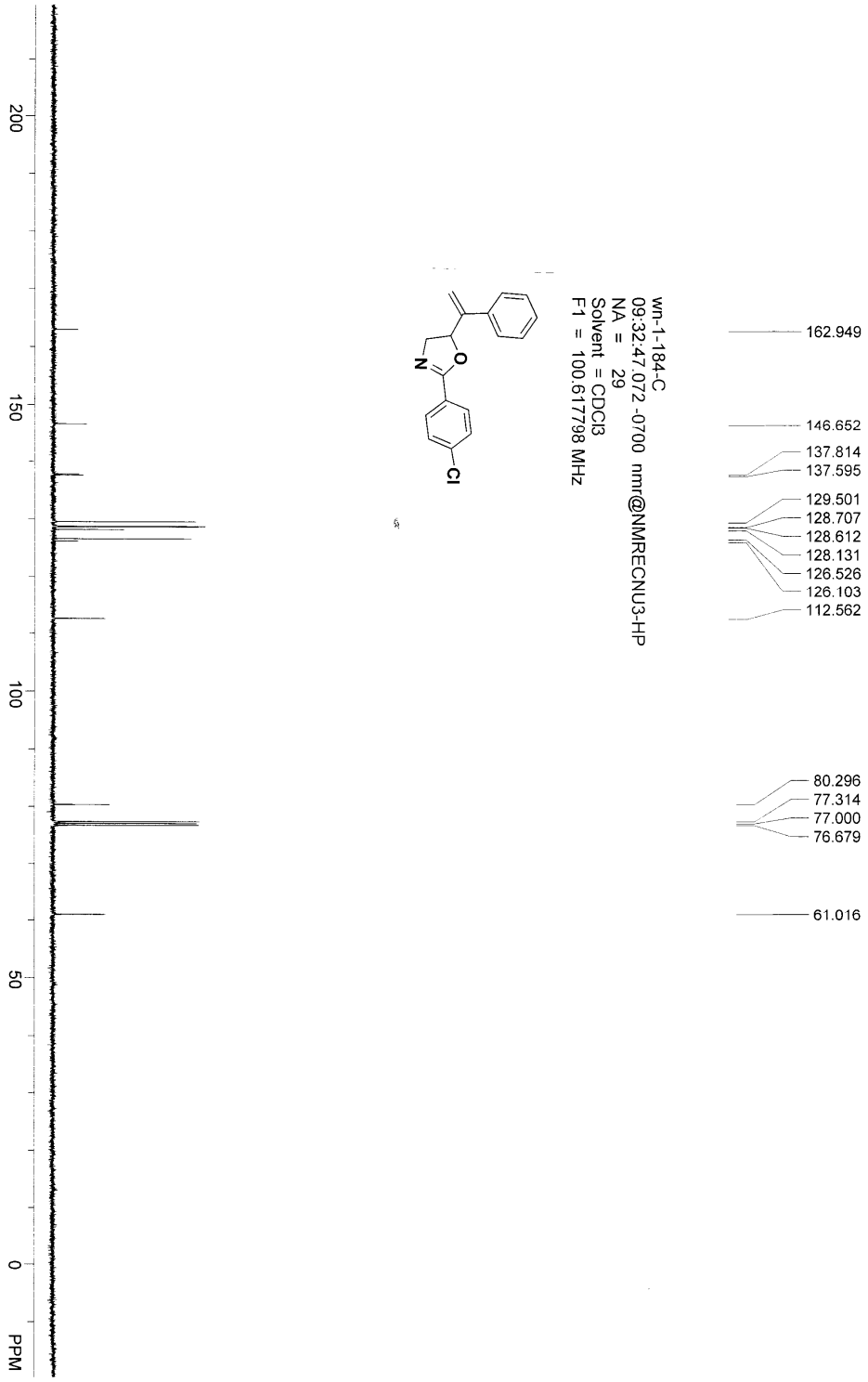

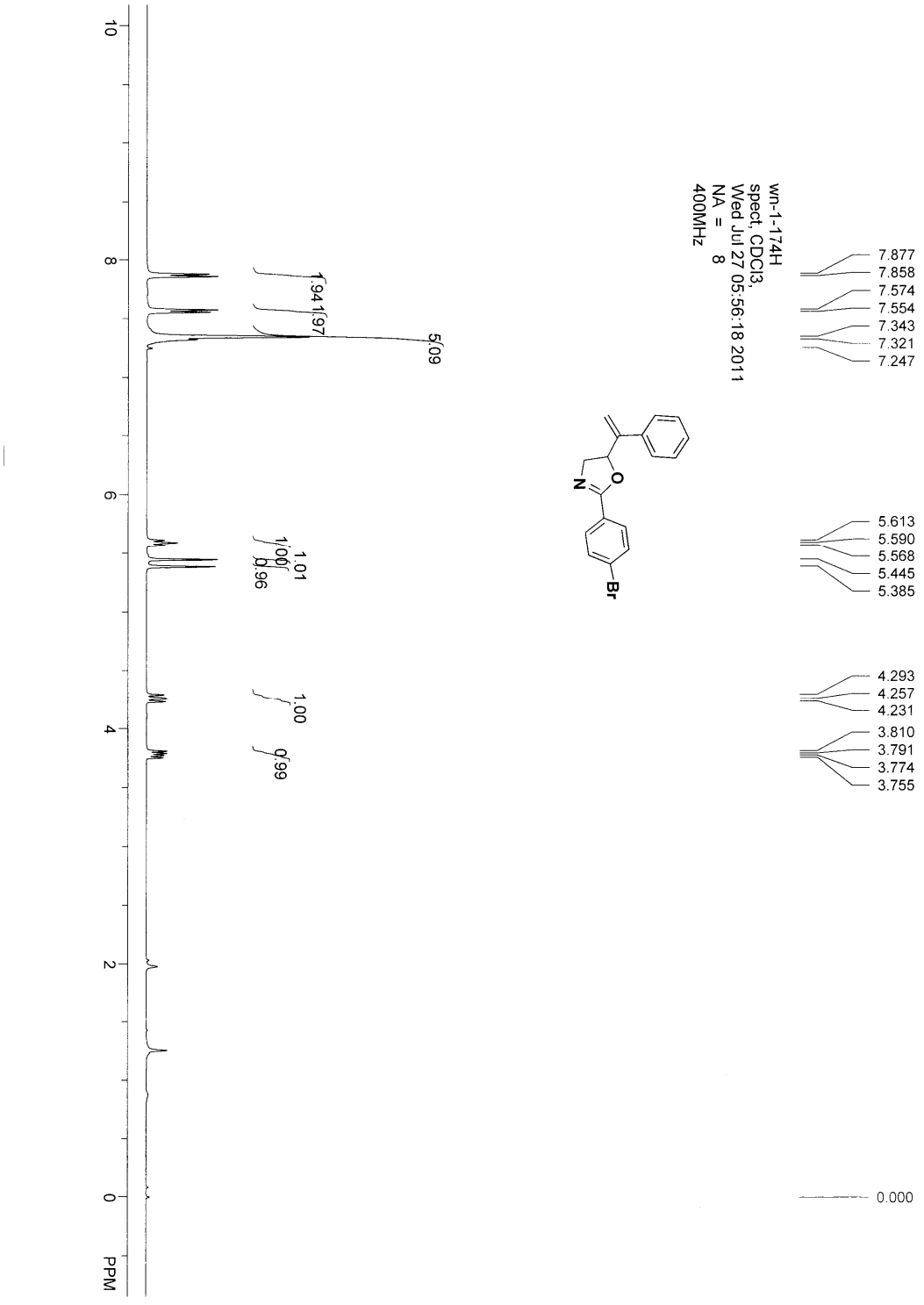

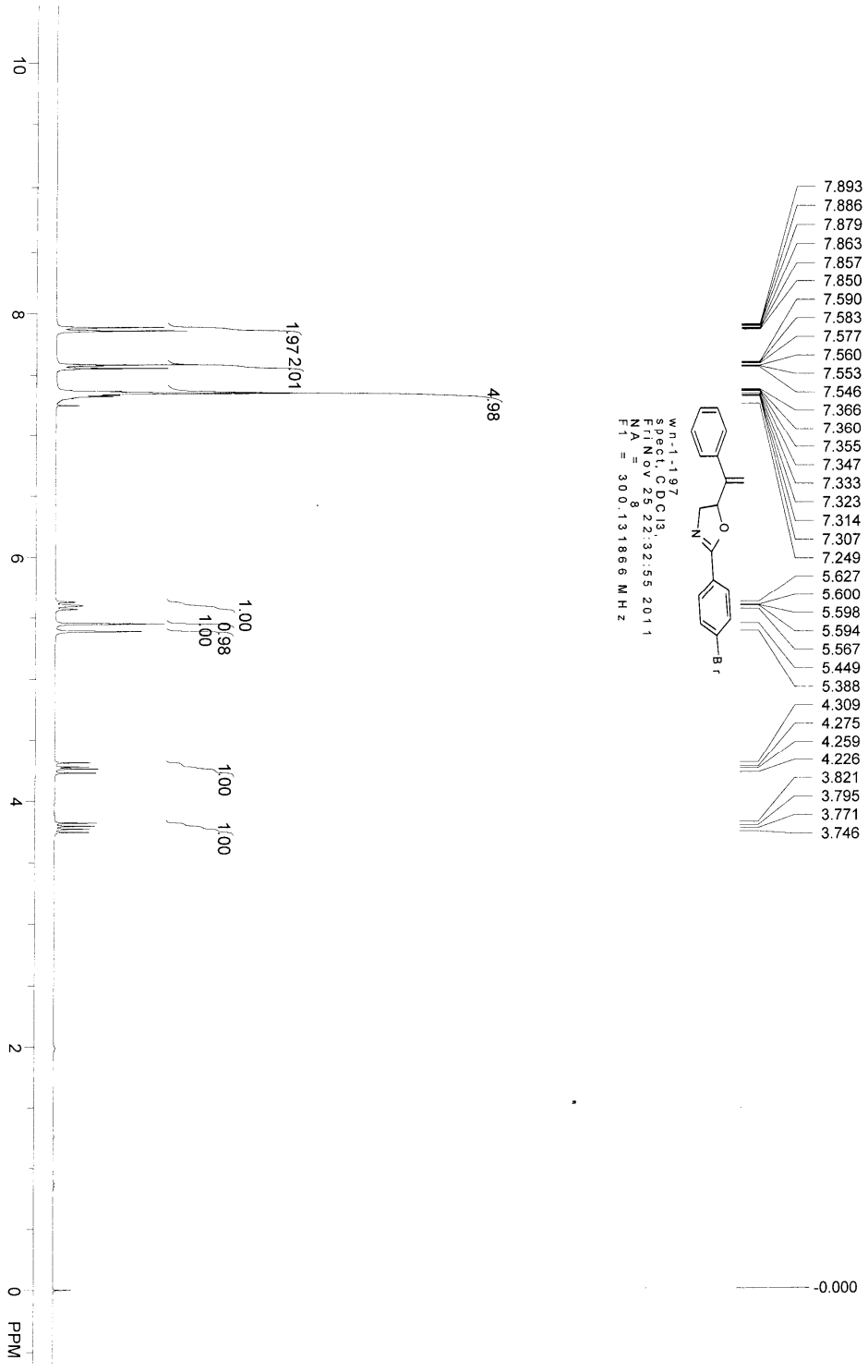

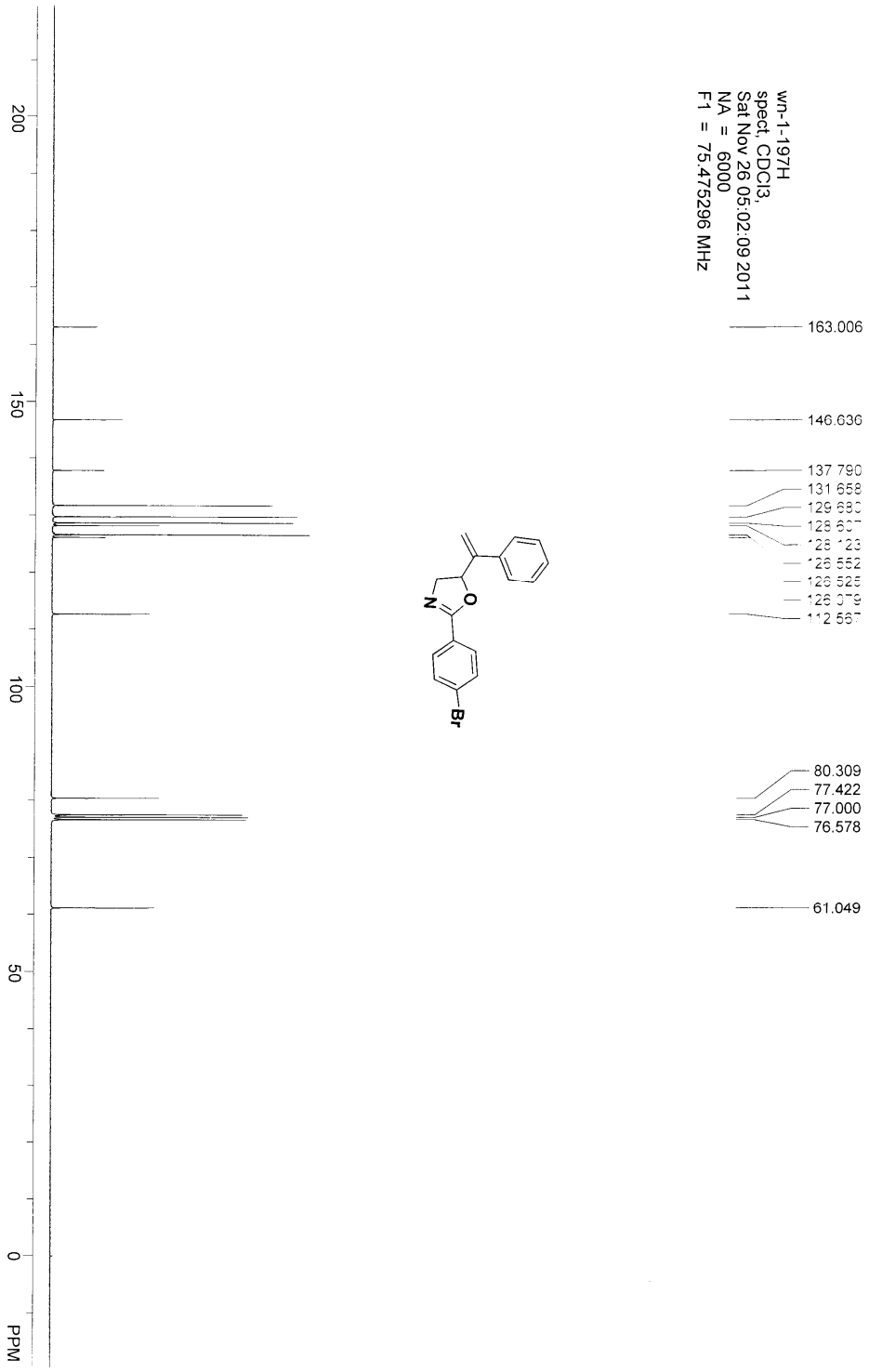

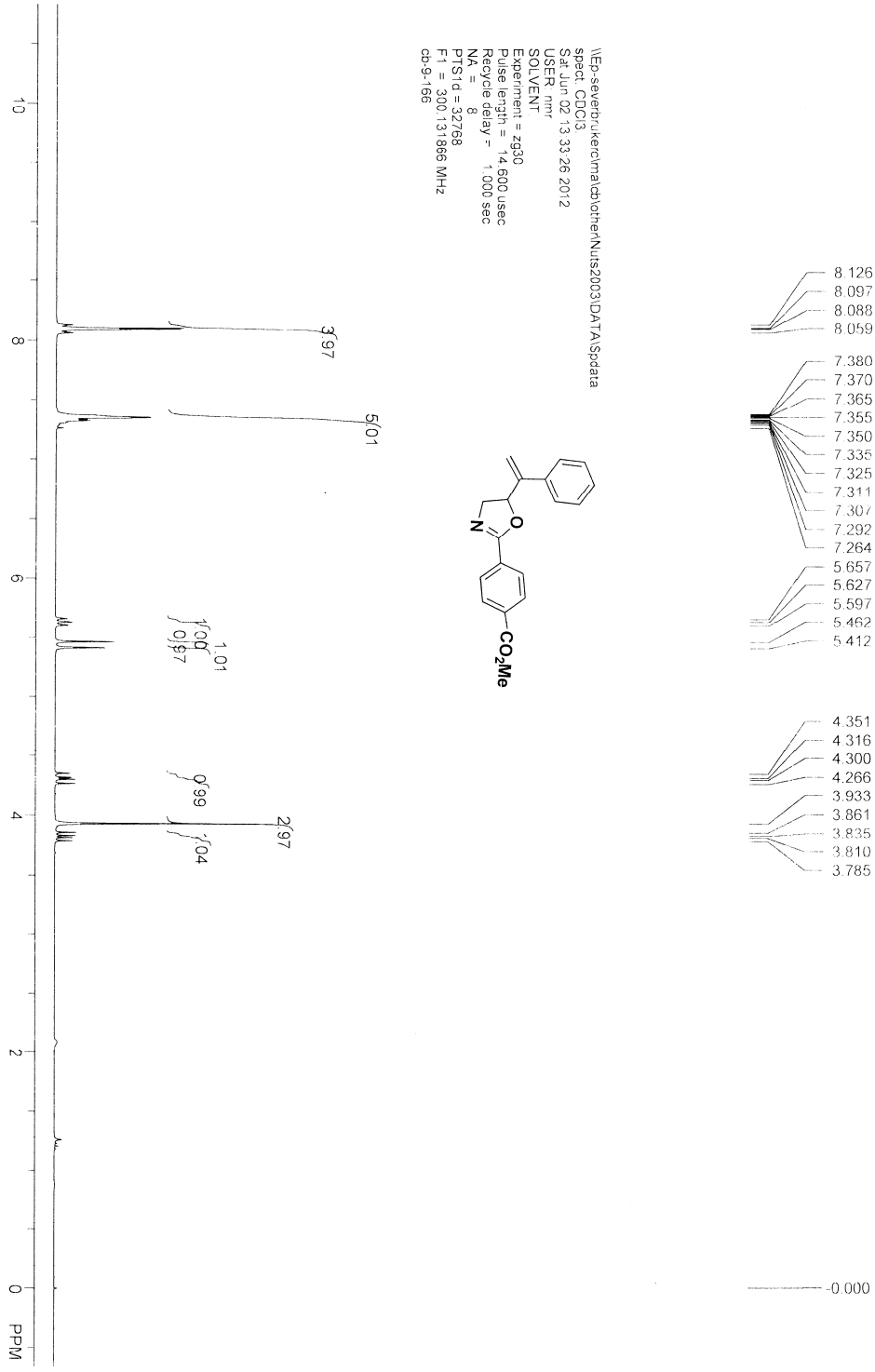

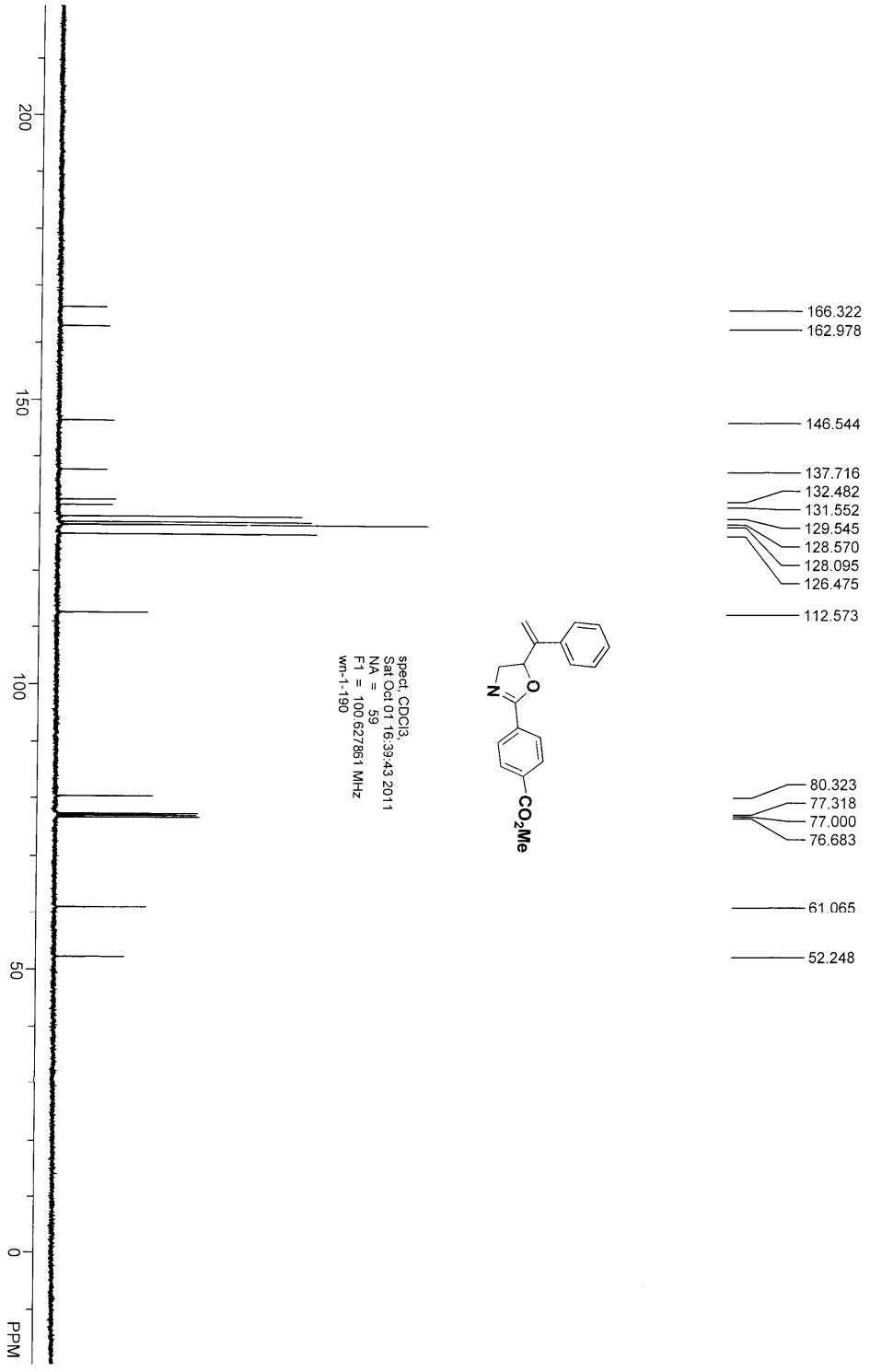

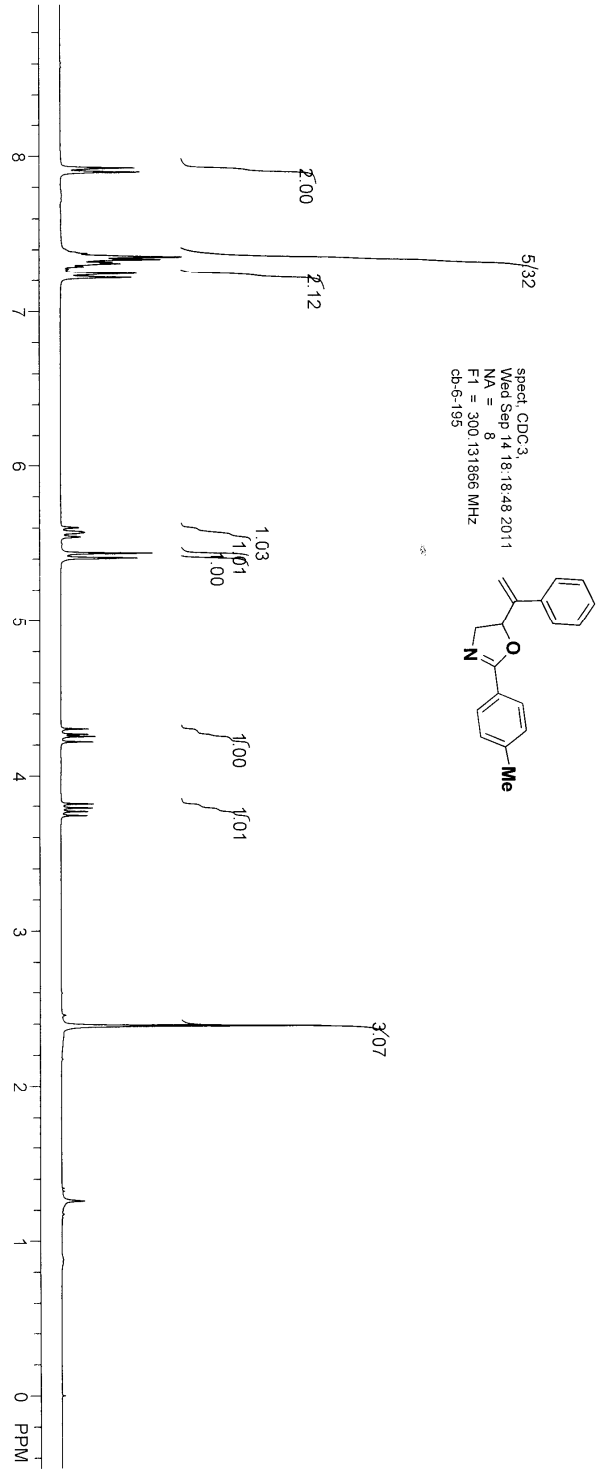

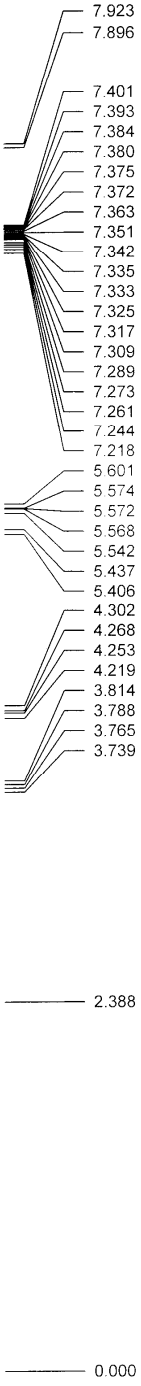

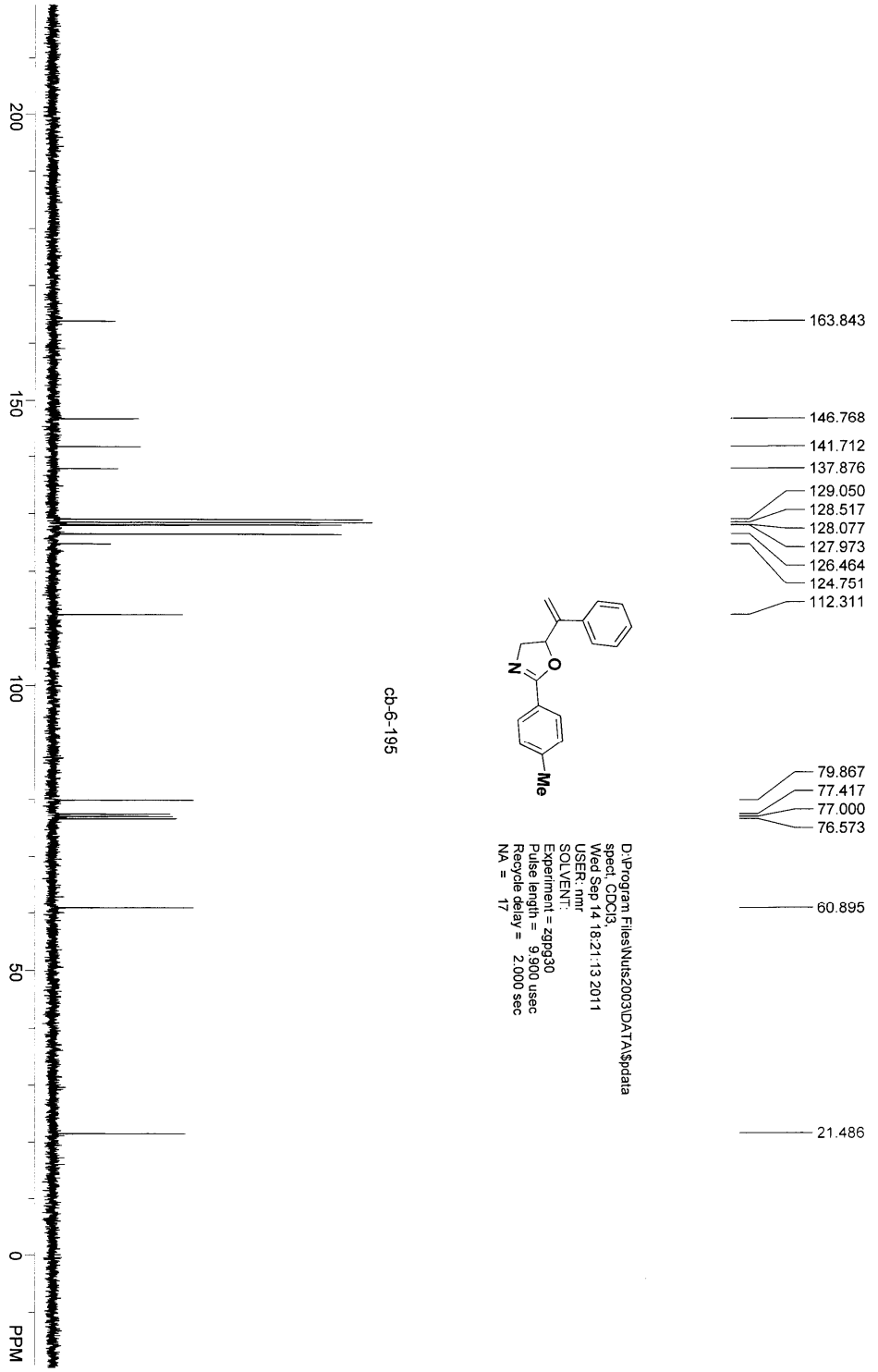

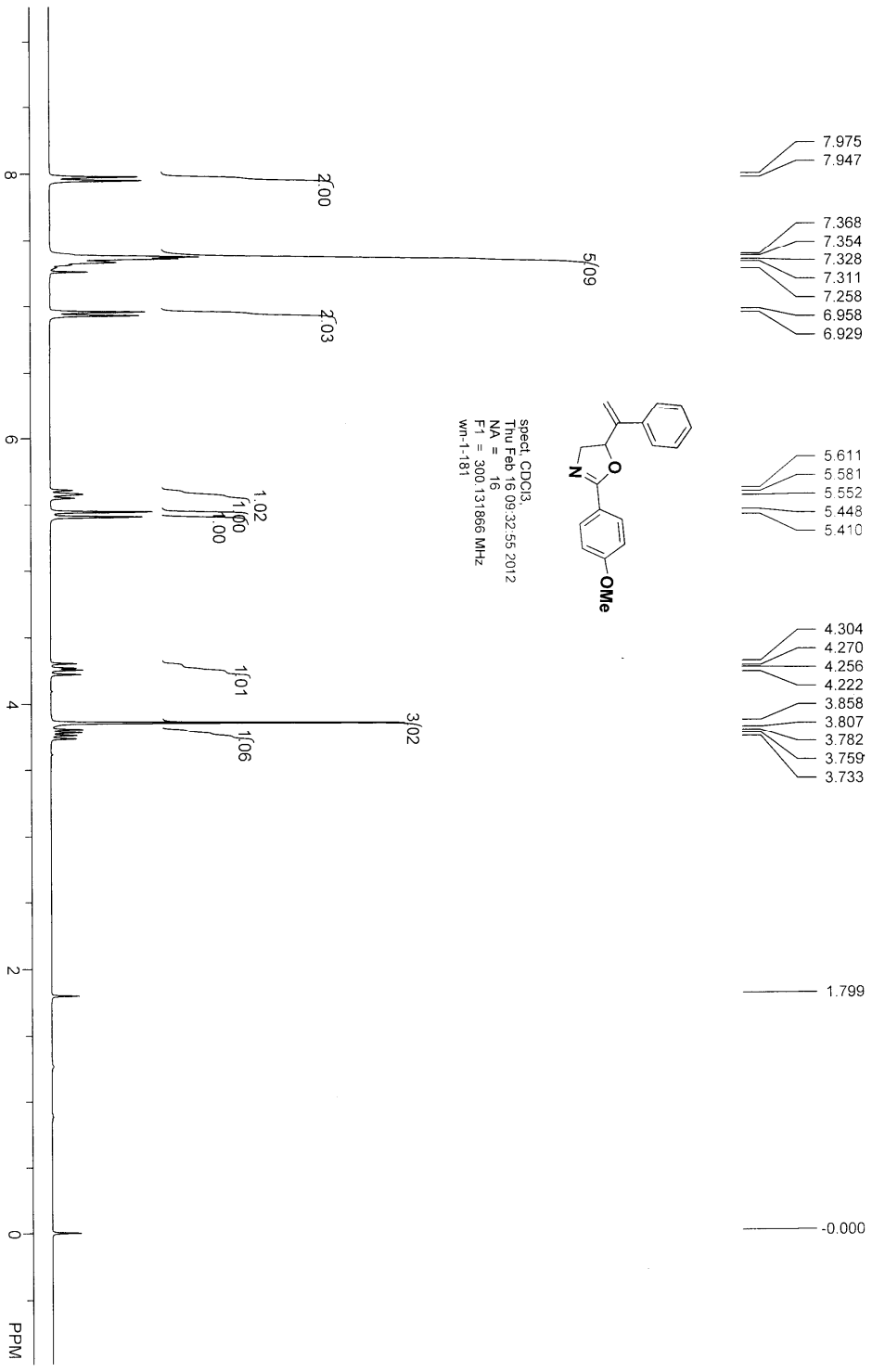
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