Supplementary Material (ESI) for Chemical Communications

Supporting Information

Palladium-catalyzed cross-couplings of 1,3-Butadien-2-yl Species with organoindiums generated from allenylmethyl bromide and indium

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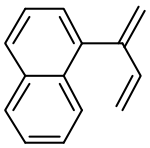
Contents

Experimental Section

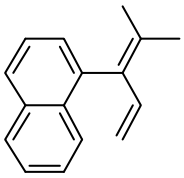
General: Reactions were carried out in oven-dried glassware under a nitrogen atmosphere. $Pd_2dba_3CHCl_3$ (dba = dibenzylideneacetone) were purchased from Strem Chemical Co. and were used as received. Indium, PPh_3, Xantphos, LiI were purchased from Aldrich Chemical Company. Commercial available reagents were used without purification. DMF and CH_2Cl_2 were dried with CaH_2 and Et_2O and THF were dried with Na-benzophenone. All reactions were monitored by TLC using Merck silica gel 60 F_{254} precoated glass plates and purifications were performed by column chromatography using Merck silica gel 60 (0.04-0.063 mm, 230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Brucker DPX FT (400 MHz) spectrometer using deuterated chloroform as solvent and chemical shift values (δ) are reported in part per million relative to TMS as an internal standard. Melting points were determined in open capillary tube using Electrothermal 9100 apparatus. High-resolution mass spectra were recorded on a Jeol JMS 700 high resolution mass spectrometer at the Korea Basic Science Institute (Daegu) and infrared spectra were recorded on a JASCO FT/IR-460 plus spectrometer.

General procedure of Pd-catalyzed 1,3-butadien-2-yl cross-coupling reactions using aryl halides and triflate

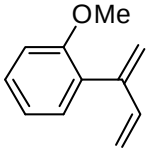
To a suspension of indium (114.8 mg, 2 mol %) and lithium iodide (66.9 mg, 0.5 mmol) in DMF (1 mL) was added allenyl bromide (199.5 mg, 1.5 mmol) at room temperature under a nitrogen atmosphere. After the solution was stirred at room temperature for 30 min, a suspension of $Pd_2dba_3CHCl_3$ (10.3 mg, 2 mol %) and phosphine lignads (PPh_3 or P(*p*-CF_3-C_6H_4)$_3$, 16 mol %) in DMF (1 mL) and aryl halides and triplates (0.5 mmol) was added and the mixture was stirred at 100 ^{o}C for 1 h. The reaction mixture was quenched with $NaHCO_3$ (sat. aq.). The aqueous layer was extracted with ether (3 × 20 mL), and the combined organics were washed with water and brine, dried with anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography to give cross-coupling products.



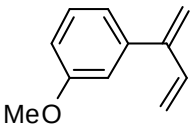
1-(Buta-1,3-dien-2-yl)naphthalene (3a)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78-7.88 (m, 3H), 7.38-7.46 (m, 3H), 7.29 (dd, *J* = 7.2, 1.6 Hz, 1H), 6.75 (dd, *J* = 17.2, 10.8 Hz, 1H), 5.58 (s, 1H), 5.24 (s, 1H), 5.11 (d, *J* = 9.6 Hz, 1H), 4.67 (d, *J* = 17.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 139.6, 138.2, 133.9, 132.3, 128.5, 128.1, 127.1, 126.8, 126.2, 126.1, 125.8, 120.1, 118.2; IR (neat) 3044, 2360, 1590, 1506, 1402, 1255, 987, 903, 801, 777 cm^{-1}; HRMS calcd. for $C_{14}H_{12}$: 180.0939. found: 180.0937.



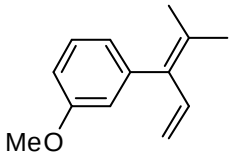
1-(2-Methyl-1-vinyl-propenyl)-naphthalene (3b)[2]: major isomer A; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* =7.5 Hz, 1H), 7.77 (d, *J* =8.3 Hz, 1H), 7.71 (d, *J* =8.1 Hz, 1H), 7.48-7.37 (m, 3H), 7.18 (d, *J* =6.9 Hz, 1H), 7.11 (dd, *J* =10.6, 17.1 Hz, 1H), 4.93 (d, *J* =10.6 Hz, 1H), 4.33 (d, *J* =17.1 Hz, 1H), 2.08 (s, 3H), 1.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 135.7, 135.0, 134.2, 134.0, 132.7, 128.6, 128.3, 127.9, 127.2, 126.4, 126.2, 126.0, 115.4, 23.5, 20.3; minor isomer B; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.80 (m, 3H), 7.48-7.37 (m, 3H), 7.22-7.20 (m, 1H), 7.04 (dd, *J* =10.7, 17.1 Hz, 1H), 5.02 (d, *J* =10.7 Hz, 1H), 4.53 (d, *J* =17.1 Hz, 1H), 2.00 (s, 3H), 1.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 136.1, 135.9, 134.2, 133.8, 132.7, 128.2, 128.1, 128.0, 126.3, 126.2, 126.1, 125.9, 115.5, 23.6, 20.3; IR (film) 3087, 3055, 3013, 2908, 2855, 1630, 1594, 1505, 1442, 902, 778 cm^{-1}; HRMS calcd. For $C_{16}H_{16}$: 208.1252. found: 208.1255.



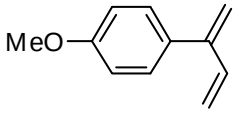
2-(*o*-Methoxyphenyl)-1,3-butadiene (3c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.28 (m, 1H), 7.12 (dd, *J* = 7.3, 1.7 Hz, 1H), 6.96 (dt, *J* = 7.5, 0.9 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 6.92 (dd, *J* = 17.3, 10.4 Hz, 1H), 5.42 (d, *J* = 1.64 Hz, 1H), 5.15 (d, *J* = 1.4 Hz, 1H), 5.11 (d, *J* = 10.5 Hz, 1H), 4.84 (d, *J* = 17.2 Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 146.3, 138.6, 131.3, 129.3, 129.2, 120.9, 118.9, 116.6, 111.3, 56.1; IR (neat) 3088, 3003, 1928, 1838, 1576, 1485, 1284, 1241, 1228, 1049, 1037, 783, 715 cm^{-1}; HRMS calcd. For $C_{11}H_{12}O$: 160.0888. found: 160.0889.



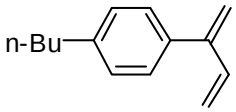
2-(*m*-Methoxyphenyl)-1,3-butadiene (3d)[3]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (t, *J* = 7.8 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 6.88-6.84 (m, 2H), 6.60 (dd, *J* = 17.3, 10.9 Hz, 1H), 5.28 (s, 1H), 5.22 (d, *J* = 17.6 Hz, 1H), 5.21 (d, *J* = 9.5 Hz, 1H), 5.21 (s, 1H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 148.5, 141.6, 138.4, 129.5, 121.2, 117.6, 117.3, 114.3, 113.4, 55.6; IR (neat) 3087, 3003, 2043, 1900, 1815, 1598, 1589, 1491, 1462, 1434, 1241, 1027, 902, 752 cm^{-1}; HRMS calcd. For $C_{11}H_{12}O$: 160.0888. found: 160.0890.



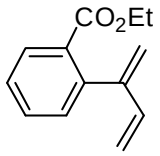
1-Methoxy-3-(2-methyl-1-vinyl-propenyl)benzene (e): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (dd, *J* =8.1, 7.5 Hz, 1H), 6.95 (dd, *J* =17.1, 10.6 Hz, 1H), 6.81 (d, *J* =8.1 Hz, 1H), 6.66 (d, *J* =7.5 Hz, 1H), 6.62 (s, 1H), 5.00 (d, *J* =10.6 Hz, 1H) 4.56 (d, *J* =17.1 Hz, 1H), 3.79 (s, 3H), 1.95 (s, 3H), 1.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 142.4, 135.9, 135.8, 133.2, 129.4, 122.9, 115.9, 115.3, 112.2, 55.5, 23.5, 20.2; IR (film) 3088, 2998, 2911, 2854, 2834, 1597, 1577, 1483, 1428, 1320, 1246, 1049, 706 cm^{-1}; HRMS calcd. For $C_{13}H_{16}O$: 188.1201. found: 188.1200.



2-(*p*-Methoxyphenyl)-1,3-butadiene (3f)[1a,1d,4]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.9 Hz, 2H), 6.89 (d, *J* = 8.6 Hz, 2H), 6.61 (dd, *J* = 16.9, 10.8 Hz, 1H), 5.24-5.16 (m, 4H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 148.0, 138.8, 132.5, 129.7, 117.4, 116.4, 113.9, 55.7; IR (neat) 3089, 3003, 1609, 1510, 1246, 1033, 835 cm^{-1}; HRMS calcd. For $C_{11}H_{12}O$: 160.0888. found: 160.0891.

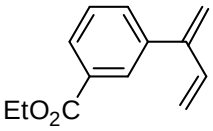


2-(*p*-*n*-Methylphenyl)-1,3-butadiene (3g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (d, *J* = 8.2 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 6.55 (dd, *J* = 17.4, 10.8 Hz, 1H), 5.21-5.13 (m, 4H), 2.56 (t, *J* = 7.7 Hz, 2H), 1.59-1.51 (m, 2H), 1.31 (sextet, *J* = 7.4 Hz, 2H), 0.87 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.5, 142.7, 138.7, 137.3, 128.6, 128.5, 117.4, 116.8, 35.8, 34.0, 22.8, 14.4; IR (neat) 3088, 3024, 3006, 2957, 2929, 2871, 2857, 1908, 1797, 1589, 1509, 990, 915, 893, 837, 745 cm^{-1}; HRMS calcd. For $C_{14}H_{18}$: 186.1409. found: 186.1409.

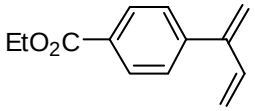


Ethyl 2-(buta-1,3-dien-2-yl)benzoate (3h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.49 (dt, *J* = 7.5, 1.4 Hz, 1H), 7.38 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.23 (dd, *J* = 7.6, 1.1 Hz, 1H), 6.65 (dd, *J* = 17.5, 10.7 Hz, 1H), 5.33 (d, *J* = 0.7 Hz, 1H), 5.10 (s, 1H), 5.10 (d, *J* = 9.9 Hz, 1H), 4.74 (d, *J* = 17.4 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 1.31 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz,

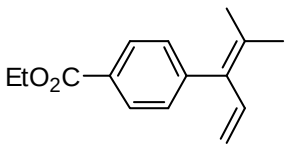
$CDCl_3$) δ 168.1, 149.0, 140.7, 139.5, 131.9, 131.5, 131.3, 130.0, 127.8, 117.6, 116.5, 61.4, 14.4; IR (neat) 3088, 2980, 2937, 1717, 1591, 1289, 1252, 1126, 1074, 903, 771, 717 cm^{-1}; HRMS calcd. For $C_{13}H_{14}O_2$: 202.0994. found: 202.0993.



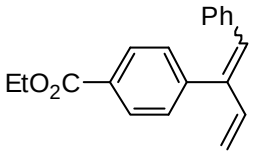
Ethyl 3-(buta-1,3-dien-2-yl)benzoate (3i): δ 8.01-7.98 (m, 2H), 7.50 (dt, *J* = 7.7, 1.5 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 6.63 (dd, *J* = 17.4, 10.8 Hz, 1H), 5.35 (s, 1H), 5.24 (s, 1H), 5.24 (d, *J* = 10.8 Hz, 1H), 5.14 (d, *J* = 17.8 Hz, 1H), 4.39 (q, *J* = 7.3 Hz, 2H), 1.40 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 147.4, 139.8, 137.8, 132.7, 130.5, 129.4, 128.6, 128.1, 117.7, 117.5, 61.0, 14.4; IR (neat) 3090, 2980, 2937, 1973, 1921, 1719, 1588, 1280, 1256 cm^{-1}; HRMS calcd. For $C_{13}H_{14}O_2$: 202.0994. found: 202.0991.



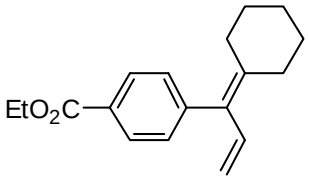
Ethyl 4-(buta-1,3-dien-2-yl)benzoate (3j): ^1H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 6.62 (dd, *J* = 10.9, 17.4 Hz, 1H), 5.36 (s, 1H), 5.25 (s, 1H), 5.24 (d, *J* = 10.9 Hz, 1H), 5.15 (d, *J* = 17.6 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 1.40 (t, *J* = 7.11 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 147.9, 144.8, 138.0, 129.9, 129.8, 128.7, 118.3, 117.9, 61.4, 14.8; IR (neat) 3090, 2980, 2943, 1718, 1608, 1273, 1103 cm^{-1}; HRMS calcd. For $C_{13}H_{14}NO_2$: 202.0994. found: 202.0992.



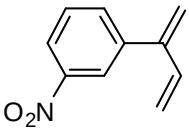
Ethyl 4-(2-methyl-1-vinyl-propenyl)benzoate (3k): ^1H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* =6.6 Hz, 2H), 7.15 (d, *J* =8.2 Hz, 2H), 6.96 (dd, *J* =10.8, 17.1 Hz, 1H), 5.01 (d, *J* =10.8 Hz, 1H), 4.46 (d, *J* =17.1 Hz, 1H), 4.39 (q, *J* =7.1 Hz, 2H), 1.97 (s, 3H), 1.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 145.7, 135.2, 134.9, 133.4, 130.1, 129.4, 128.6, 60.9, 23.0, 19.9, 14.4; IR (film) 3088, 2982, 2909, 2858, 1813, 1721, 1607, 1272, 1099, 777 cm^{-1}; HRMS calcd. For $C_{15}H_{18}O_2$: 230.1307. found: 230.1309.



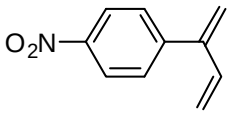
Ethyl 4-(1-benzylideneallyl)benzoate (3l): major isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.2 Hz, 2H), 7.48 (d, *J* = 8.3 Hz, 2H), 7.39-7.38 (m, 3H), 7.31-7.25 (m, 2H), 7.02 (dd, *J* = 17.3, 10.9 Hz, 1H), 6.63 (s, 1H), 5.39 (d, *J* = 10.9 Hz, 1H), 5.20 (d, *J* = 17.3 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 146.5, 140.5, 136.9, 134.3, 131.7, 129.6, 129.4, 129.2, 128.2, 127.4, 120.0, 60.9, 14.4; minor isomer B; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-8.04 (m, 2H), 7.31-7.25 (m, 2H), 7.10-7.08 (m, 3H), 6.90-6.87 (m, 2H), 6.73 (dd, *J* = 10.6, 17.2 Hz, 1H), 6.65 (s, 1H), 5.17 (d, *J* = 10.6 Hz, 1H), 4.78 (d, *J* = 17.2 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 143.0, 141.1, 140.7, 136.2, 132.0, 130.0, 129.8, 129.4, 128.1, 127.2, 61.0, 14.4; IR (film) 3087, 2980, 2904, 1717, 1606, 1274, 1176, 1101, 1021, 699 cm^{-1}; HRMS calcd. For $C_{19}H_{18}O_2$: 278.1307. found: 278.1308.



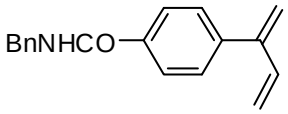
Ethyl 4-(1-cyclohexylideneallyl)benzoate (3m): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.2 Hz, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 7.01 (dd, *J* = 17.2, 10.8 Hz, 1H), 5.02 (dd, *J* = 10.8, 1.5 Hz, 1H), 4.46 (dd, *J* = 17.2, 1.6 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 2.47 (t, *J* = 5.7 Hz, 2H), 1.90 (t, *J* = 5.9 Hz, 2H), 1.69-1.64 (m, 2H), 1.61-1.56 (m, 2H), 1.48-1.43 (m, 2H), 1.40 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 145.6, 141.9, 137.7, 134.5, 130.2, 129.3, 128.5, 115.7, 60.8, 33.1, 30.1, 28.4, 28.3, 26.8, 14.4; IR (neat) 3089, 2982, 2903, 1710, 1607, 1265 1174, 1102, 1031, 701 cm^{-1}; HRMS calcd. For $C_{18}H_{22}O_2$: 270.1620. found: 270.1621.



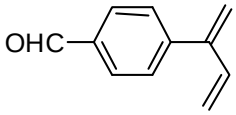
2-(*m*-Nitrophenyl)-1,3-butadiene (3n): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 8.18 (d, *J* = 7.4 Hz, 1H), 7.65 (d, *J* = 7.7 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 6.64 (dd, *J* = 17.4, 10.9 Hz, 1H), 5.43 (s, 1H), 5.29 (s, 1H), 5.29 (d, *J* = 10.3 Hz, 1H), 5.13 (d, *J* = 17.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 146.2, 141.4, 137.2, 134.4, 129.1, 123.25, 122.47, 118.7, 117.9; IR (neat) 3091, 1934, 1829, 1596, 1518, 1345, 992, 908, 861, 705 cm^{-1}; HRMS calcd. For $C_{10}H_9NO_2$: 175.0633. found: 175.0632.



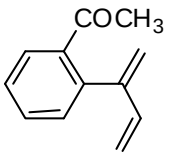
2-(*p*-Nitrophenyl)-1,3-butadiene (3o)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.8 Hz, 2H), 7.49 (d, *J* = 8.7 Hz, 2H), 6.62 (dd, *J* = 17.5, 10.9 Hz, 1H), 5.44 (s, 1H), 5.29 (s, 1H), 5.29 (d, *J* = 10.4 Hz, 1H), 5.13 (d, *J* = 17.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.5, 146.4, 137.1, 129.2, 123.5, 118.9, 118.0; IR (neat) 3090, 1967, 1832, 1738, 1589, 1530, 1350, 991, 903, 703 cm^{-1}; HRMS calcd. For $C_{10}H_9NO_2$: 175.0633. found: 175.0634.



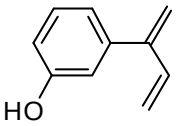
4-(Buta-1,3-dien-2-yl)phenyl *N*-benzylformimidate (3p): mp 114-115 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.3 Hz, 2H), 7.40-7.33 (m, 6H), 7.32-7.28 (m, 1H), 6.61 (dd, *J* = 17.4, 10.9 Hz, 1H), 6.40 (s, 1H), 5.35 (s, 1H), 5.23 (d, *J* = 10.5 Hz, 1H), 5.14 (d, *J* = 17.6 Hz, 1H), 4.67 (d, *J* = 5.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 147.4, 143.2, 138.2, 137.7, 133.4, 128.8, 128.5, 127.9, 127.7, 126.8, 117.8, 117.5, 44.17; IR (neat) 3351, 3063, 2926, 1644, 1537, 1321, 1017, 734, 699 cm^{-1}; HRMS calcd. For $C_{18}H_{17}NO$: 263.1310. found: 263.1313.



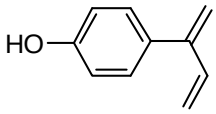
4-(Buta-1,3-dien-2-yl)benzaldehyde (3q): ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 7.88 (d, *J* = 8.3 Hz, 2H), 7.49 (d, *J* = 8.2 Hz, 2H), 6.63 (dd, *J* = 17.4, 10.8 Hz, 1H), 5.40 (s, 1H), 5.28 (s, 1H), 5.27 (d, *J* = 10.8 Hz, 1H), 5.16 (d, *J* = 17.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 147.7, 146.5, 137.8, 135.9, 130.1, 129.3, 118.7, 118.2; IR (neat) 3089, 2830, 2731, 1820, 1702, 1605, 1209, 837 cm^{-1}; HRMS calcd. For $C_{11}H_{10}O$: 158.0732. found: 158.0732.



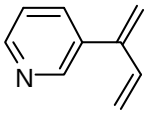
1-(2-(Buta-1,3-dien-2-yl)phenyl)ethanone (3r): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.46 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.38 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.24 (dd, , *J* = 7.5, 1.2 Hz, 1H), 6.67 (dd, *J* = 17.4, 10.6 Hz, 1H), 5.41 (s, 1H), 5.21 (d, *J* = 10.6 Hz, 1H), 5.14 (s, 1H), 4.89 (d, *J* = 17.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.6, 148.4, 140.8, 139.3, 138.5, 131.2, 131.0, 128.3, 128.1, 119.9, 118.2, 30.2; IR (neat) 3088, 1691, 1276, 1240, 909, 760 cm^{-1}; HRMS calcd. For $C_{12}H_{12}O$: 172.0888. found: 172.0887.



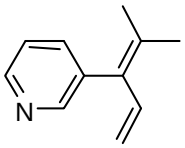
3-(Buta-1,3-dien-2-yl)phenol (3s): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (t, *J* = 8.1 Hz, 1H), 6.90 (d, *J* = 7.5 Hz, 1H), 6.80 (s, 1H), 6.81-6.77 (m, 1H), 6.58 (dd, *J* = 17.2, 10.5 Hz, 1H), 5.28-5.20 (m, 1H), 5.20 (s, 2H), 4.89 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 147.8, 141.4, 137.9, 129.4, 120.9, 117.2, 116.9, 115.2, 114.4; IR (neat) 3348, 3089, 1933, 1844, 1578, 1448, 1322, 1217, 901, 788 cm^{-1}; HRMS calcd. For $C_{10}H_{10}O$: 146.0732. found: 146.0730.



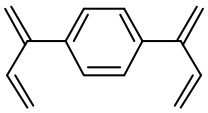
4-(Buta-1,3-dien-2-yl)phenol (3t): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.66 Hz, 2H), 6.82 (d, *J* = 8.68 Hz, 2H), 6.60 (dd, *J* = 17.2, 10.2Hz, 1H), 5.71 (s, 1H), 5.24-5.16 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.4, 147.9, 138.7, 129.9, 129.0, 117.4, 116.5, 115.4; IR (neat) 3365, 1611, 1510, 1231, 837 cm^{-1}; HRMS calcd. For $C_{10}H_{10}O$: 146.0732. found: 146.0730.



3-(Buta-1,3-dien-2-yl)pyridine (3u): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 1.1 Hz, 1H), 8.56 (d, *J* = 1.7 Hz, 1H), 7.63 (dt, *J* = 7.7, 1.9 Hz, 1H), 7.27-7.30 (m, 1H), 6.64 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.39 (s, 1H), 5.26 (d, *J* = 10.5 Hz, 1H), 5.25 (s, 1H), 5.13 (d, *J* = 17.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 148.8, 145.0, 137.6, 135.7, 135.3, 123.0, 118.6, 117.7; IR (neat) 3059, 1620, 1338, 1187, 1098 cm^{-1}; HRMS calcd. For C_9H_9N: 131.0735. found: 131.0734.



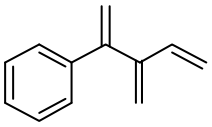
3-(2-Methyl-1-vinyl-propenyl)-pyridine (3v): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* =4.9 Hz, 1H), 8.33 (s, 1H), 7.41 (d, *J* =7.7 Hz, 1H), 7.29 (dd, *J* =4.9, 7.7 Hz, 1H), 6.98 (dd, *J* =10.7, 17.1 Hz, 1H), 5.03 (d, *J* =10.7 Hz, 1H), 4.46 (d, *J* =17.1 Hz, 1H), 1.99 (s, 3H), 1.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4, 148.1, 138.1, 136.4, 135.8, 135.3, 132.4, 123.5, 115.7, 23.4, 20.4; IR (film) 3088, 3024, 2988, 2913, 2857, 1630, 1473, 1408, 1027, 721 cm^{-1}; HRMS calcd. For $C_{11}H_{13}N$: 159.1048. found: 159.1048.



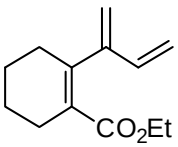
1,4-Bis(1-methylene-2-propenyl)benzene (3w)[5]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (s, 4 H), 6.63 (dd, *J* = 17.2, 11.0 Hz, 2H), 5.31-5.22 (m, 8 H); ^{13}C NMR ($CDCl_3$) δ 148.3, 139.3, 138.5, 128.4, 117.6, 117.2; IR (neat, cm^{-1}) 1578, 1510, 1313, 1107; HRMS calcd. For $C_{14}H_{14}$: 182.1096. found: 182.1095.

General experimental of Pd-catalyzed 1,3-butadien-2-yl cross-coupling reactions using vinyl bromides and triflates

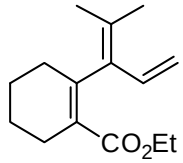
To a suspension of indium (114.8 mg, 2 mo l %) and lithium iodide (66.9 mg, 0.5 mmol) in DMF (1 mL) was added allenyl bromide (199.5 mg, 1.5 mmol) at room temperature under a nitrogen atmosphere. After the solution was stirred at room temperature for 30 min, a suspension of $Pd_2dba_3CHCl_3$ (10.3 mg, 2 mol %) and phosphine lignads (PPh_3 or P(*p*-CF_3-C_6H_4)$_3$, 16 mol %) in DMF (1 mL) and vinyl bromides and triflates (0.5 mmol) was added and the mixture was stirred at 100 ^{o}C for 1 h. The reaction mixture was quenched with $NaHCO_3$ (sat. aq.). The aqueous layer was extracted with ether (3 × 20 mL), and the combined organics were washed with water and brine, dried with anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography to give cross-coupling products.



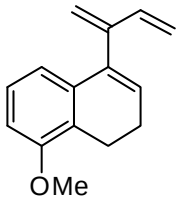
(3-Methylenepenta-1,4-dien-2-yl)benzene (4a)[6]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.39 (m, 2H), 7.32-7.23 (m, 3H), 6.45 (dd, *J* = 10.3, 15.7 Hz, 1H), 5.52 (d, *J* = 1.6 Hz 1H), 5.32 (d, *J* = 1.9 Hz, 1H), 5.18 (s, 1H), 5.05 (dd, *J* = 10.3, 15.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 148.5, 140.4, 137.7, 128.7, 128.0, 127.2, 118.8, 117.9, 115.3; IR (film) 3088, 3058, 3027, 2974, 1810, 1584, 1494, 902 cm^{-1}; HRMS calcd. For $C_{12}H_{12}$: 156.0939. found: 156.0938.



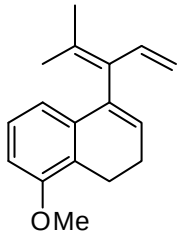
2-(1-Methylene-allyl)-cyclohex-1-enecarboxylic acid ethyl ester (4b): ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.35 (dd, *J* = 10.2, 17.6 Hz, 1H), 5.07 (dd, *J* = 11.1, 16.7 Hz, 2H), 5.04 (d, *J* =0.7 Hz, 1H), 4.88 (s, 1H), 4.07 (q, *J* =7.1 Hz, 2H), 2.39-2.35 (m, 2H), 2.23-2.19 (m, 2H), 1.71-1.63 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 150.7, 145.5, 137.5, 128.1, 115.4, 114.7, 60.4, 32.5, 26.3, 22.7, 22.5, 14.3; IR (film) 3087, 2979, 2936, 2860, 1709, 1368, 1279, 1255, 1230 cm^{-1}; HRMS calcd. For $C_{13}H_{18}O_2$: 206.1307. found: 206.1305.



2-(2-Methyl-1-vinyl-propenyl)-cyclohex-1-enecarboxylic acid ethyl ester (4c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.65 (dd, *J* = 10.7, 17.2 Hz, 1H), 4.93 (d, *J* = 10.7 Hz, 1H), 4.88 (d, *J* = 17.2 Hz, 1H), 4.04 (q, *J* = 7.1 Hz, 2H), 2.41-2.38 (m, 2H), 2.22-2.17 (m, 2H), 2.02-1.96 (m, 1H), 1.80 (s, 3H), 1.70-1.58 (m, 3H), 1.65 (s, 3H), 1.15 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 146.3, 136.5, 133.2, 129.6, 128.4, 112.8, 60.1, 31.4, 26.4, 22.8, 22.7, 22.5, 19.7, 14.5; IR (film) 3086, 2980, 2859, 1704, 1650, 1622, 1597, 1448, 1370, 1277, 1254, 1227, 824 cm^{-1}; HRMS calcd. For $C_{15}H_{22}O$: 234.1620. found: 234.1622.



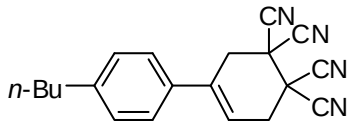
8-Methoxy-4-(1-methylene-allyl)-1,2-dihydro-naphthalene (4d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 (t, *J* = 7.95 Hz, 1H), 6.77 (d, *J* = 8.98 Hz, 1H), 6.75 (d, *J* = 8.57 Hz, 1H), 6.52 (dd, *J* = 10.58, 17.26 Hz, 1H), 5.99 (t, *J* = 4.57 Hz, 1H), 5.31 (s, 1H), 5.18 (s, 1H), 5.06 (d, *J* = 10.37 Hz, 1H), 5.04 (d, *J* = 17.28 Hz, 1H), 3.85 (s, 3H), 2.84 (t, *J* = 8.08 Hz, 2H), 2.33 (dt, *J* = 4.58, 8.43 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.3, 148.2, 138.4, 137.8, 135.9, 128.5, 126.6, 124.1, 118.6, 118.5, 117.3, 109.9, 56.0, 23.0, 20.3; IR (film) 3086, 3001, 2935, 2884, 2834, 1572, 1468, 1439, 1259 cm^{-1}; HRMS calcd. For $C_{15}H_{16}O$: 212.1201. found: 212.1203.



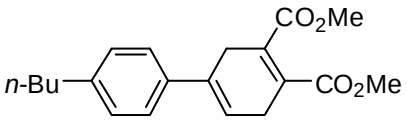
8-Methoxy-4-(2-methyl-1-vinyl-propenyl)-1,2-dihydro-naphthalene (4e): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (dd, *J* = 8.2, 6.6 Hz, 1H), 6.88 (dd, *J* = 10.6, 17.1 Hz, 1H), 6.75 (d, *J* = 8.2 Hz, 1H), 6.60 (d, *J* = 6.6 Hz, 1H), 5.75 (t, *J* = 4.5 Hz, 1H), 4.93 (dd, *J* = 10.6, 17.1 Hz, 2H), 3.82 (s, 3H), 2.96-2.88 (m, 1H), 2.81-2.73 (m, 1H), 2.37-2.32 (m, 2H), 1.94 (s, 3H), 1.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.4, 136.9, 136.3, 134.8, 134.1, 133.9, 128.7, 126.8, 124.2, 117.8, 114.3, 109.8, 55.9, 23.3, 23.1, 20.4, 20.0; IR (film) 3086, 2926, 2853, 2834, 1573, 1468, 1439, 1259, 1038 cm^{-1}; HRMS calcd. for $C_{17}H_{20}O$: 240.1514. found: 240.1510.

General experimental procedure of tandem cross-coupling/[4+2] cycloaddition

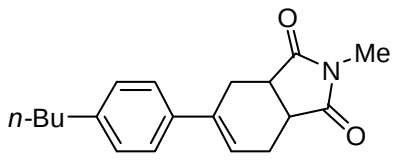
To a suspension of indium (114.8 mg, 1.0 mmol) and lithium iodide (66.9 mg, 0.5 mmol) in DMF (1 mL) was added allenyl bromide (199.5 mg, 1.5 mmol) at room temperature under a nitrogen atmosphere. After the solution was stirred at room temperature for 30 min, a suspension of $Pd_2dba_3CHCl_3$ (10.3 mg, 2 mol %) and triphenylphosphine (21.0 mg, 16 mol %) in DMF (1 mL) and *n*-butyl-4-iodobenzene (130.1 mg, 0.5 mmol) was added and the mixture was stirred at 100 ^oC for 1 h. The reaction mixture was cooled to room temperature and tetracyanoethylene (128.1 mg, 1.0 mmol) in DMF (0.5 mL) was added and stirred at room temperature for 30 min. The reaction mixture was quenched with $NaHCO_3$ (sat. aq.). The aqueous layer was extracted with ether (3 × 20 mL), and the combined organics were washed with water and brine, dried with anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (EtOAc:Hexane=1:5) to give desired product **5a** (130.5 mg, 83%).



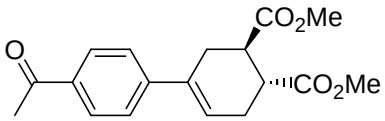
4-(4-Butylphenyl)cyclohex-4-ene-1,1,2,2-tetracarbonitrile (5a): ^1H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.5 Hz, 2H), 7.22 (d, *J* = 8.5 Hz, 2H), 6.10-6.08 (m, 1H), 3.48 (q, *J* = 1.9 Hz, 2H), 3.32 (quintet, *J* = 1.9 Hz, 2H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.60 (quintet, *J* = 7.3 Hz, 2H), 1.35 (sextet, *J* = 7.4 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$) δ 144.7, 137.1, 132.5, 129.1, 125.2, 115.5, 110.6, 110.6, 38.2, 37.3, 35.3, 34.5, 33.4, 32.9, 22.3, 13.9; IR (neat, cm^{-1}) 3028, 2931, 2249, 1910, 1794, 1618, 1515, 1436, 870, 839, 792; HRMS calcd. For $C_{20}H_{18}N_4$: 314.1531. found: 314.1534.



Dimethyl 4-(4-butylphenyl)cyclohexa-1,4-diene-1,2-dicarboxylate (5b): ^1H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.2 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 6.07 (quintet, *J* = 1.9 Hz, 1H), 3.82 (s, 3H), 3.81 (s, 3H), 3.39 (t, *J* = 8.2 Hz, 2H), 3.22 (dt, *J* = 7.9, 3.3 Hz, 2H), 2.60 (t, *J* = 7.6 Hz, 2H), 1.59 (quintet, *J* = 7.3 Hz, 2H), 1.36 (sextet, *J* = 7.4 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$) δ 168.4, 168.3, 142.4, 137.1, 132.8, 132.2, 132.1, 128.5, 124.8, 118.3, 52.3, 52.2, 35.3, 33.6, 29.7, 29.1, 22.4, 13.9; IR (neat, cm^{-1}) 3024, 2997, 2953, 2858, 2096, 1914, 1729, 1606, 1434, 1291, 1129, 1075, 773; HRMS calcd. For $C_{20}H_{24}O_4$: 328.1675. found: 328.1670.



5-(4-Butylphenyl)-2-methyl-3a,4,7,7a-tetrahydro-1H-isoindole-1,3(2H)-dione (5c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.2 Hz, 2H), 7.13 (d, *J* = 8.2 Hz, 2H), 6.09 (quintet, *J* = 3.3 Hz, 1H), 3.25 (ddd, *J* = 9.3, 7.0, 2.8 Hz, 1H), 3.14 (dd, *J* = 14.9, 2.7 Hz, 1H), 2.80 (ddd, *J* = 15.5, 7.0, 2.5 Hz, 1H), 2.58 (t, *J* = 7.6 Hz, 2H), 2.53 (ddt, *J* = 15.4, 6.9, 2.4 Hz, 1H), 2.40-2.32 (m, 1H), 1.58 (septet, *J* = 7.7 Hz, 2H), 1.35 (sextet, *J* = 7.5 Hz, 2H), 0.92 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$) δ 180.6, 180.3, 142.7, 139.9, 138.0, 128.9, 125.7, 122.6, 40.5, 39.8, 35.7, 34.0, 27.5, 25.4, 25.3, 22.8, 14.4; IR (neat, cm^{-1}) 3027, 2929, 1913, 1697, 1435, 1284, 1125; HRMS calcd. For $C_{19}H_{23}NO_2$: 297.1729. found: 297.1732.



Dimethyl 4-(4-acetylphenyl)cyclohex-4-ene-1,2-dicarboxylate (5d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.5 Hz, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 6.23-6.21 (m, 1H), 3.75 (s, 3H), 3.74 (s, 3H), 3.05 (dd, *J* = 10.6, 5.3 Hz, 1H), 2.96 (dd, *J* = 10.4, 5.6 Hz, 1H), 2.86-2.81 (m, 1H), 2.72-2.61 (m, 2H), 2.60 (s, 3H), 2.48-2.39 (m, 1H); ^{13}C NMR ($CDCl_3$) δ 197.6, 174.9, 174.8, 145.2, 135.8, 134.3, 128.6, 125.1, 124.4, 52.1, 52.1, 41.7, 40.8, 29.7, 28.6, 26.6; IR (neat, cm^{-1}) 2952, 1731, 1681, 1602, 1436, 1268, 1239, 1196, 1175, 1013, 801; HRMS calcd. For $C_{18}H_{20}O_5$: 316.1311. found: 316.1309.

References

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(2) T. Moriya, T. Furuuchi, N. Miyaura and A. Suzuki, *Tetrahedron,* **1994**, *50*, 7961.

(3) C. T. Lin and W. J. Hsu, *Can. J. Chem.,* **1989**, *67*, 2153.

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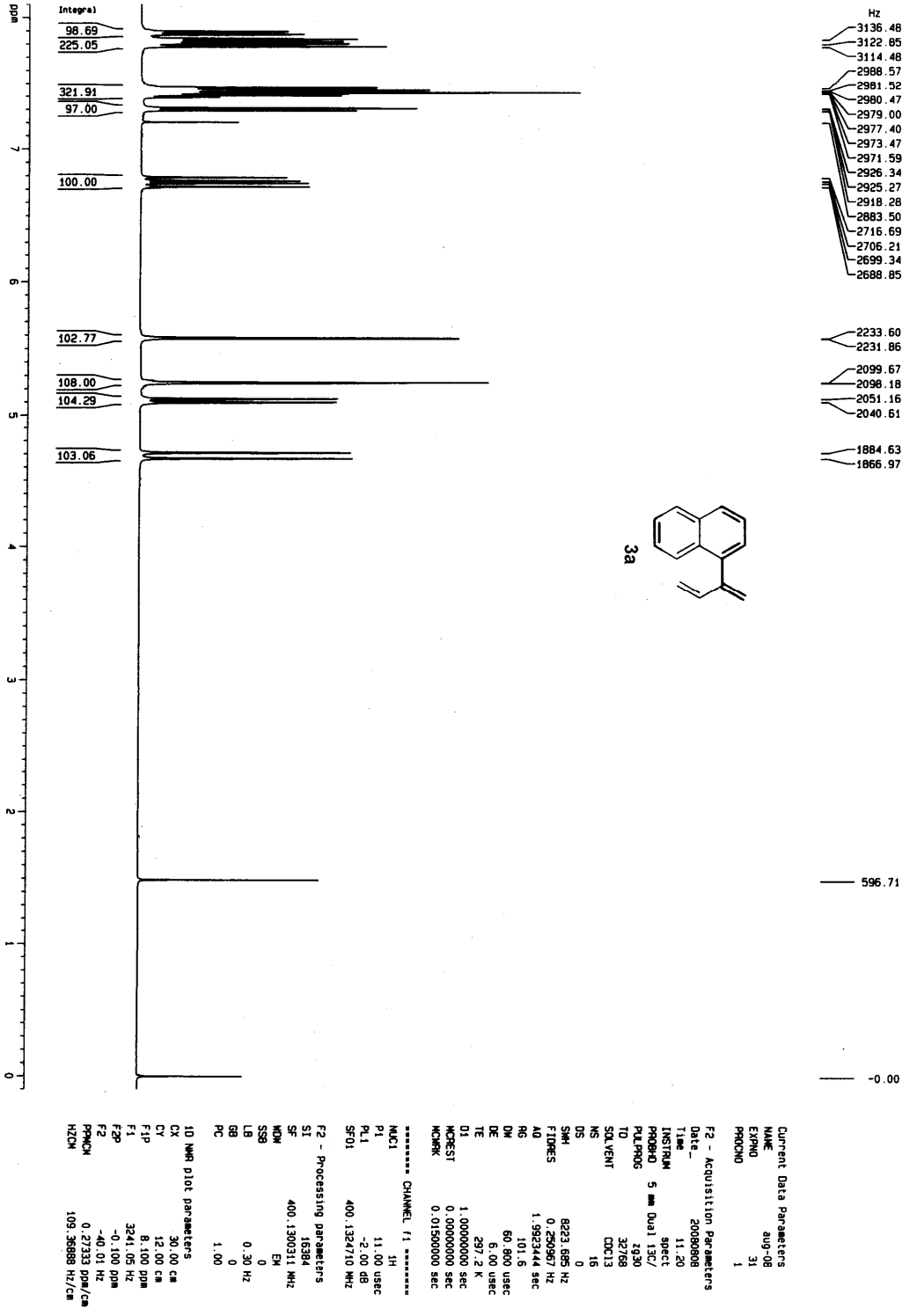
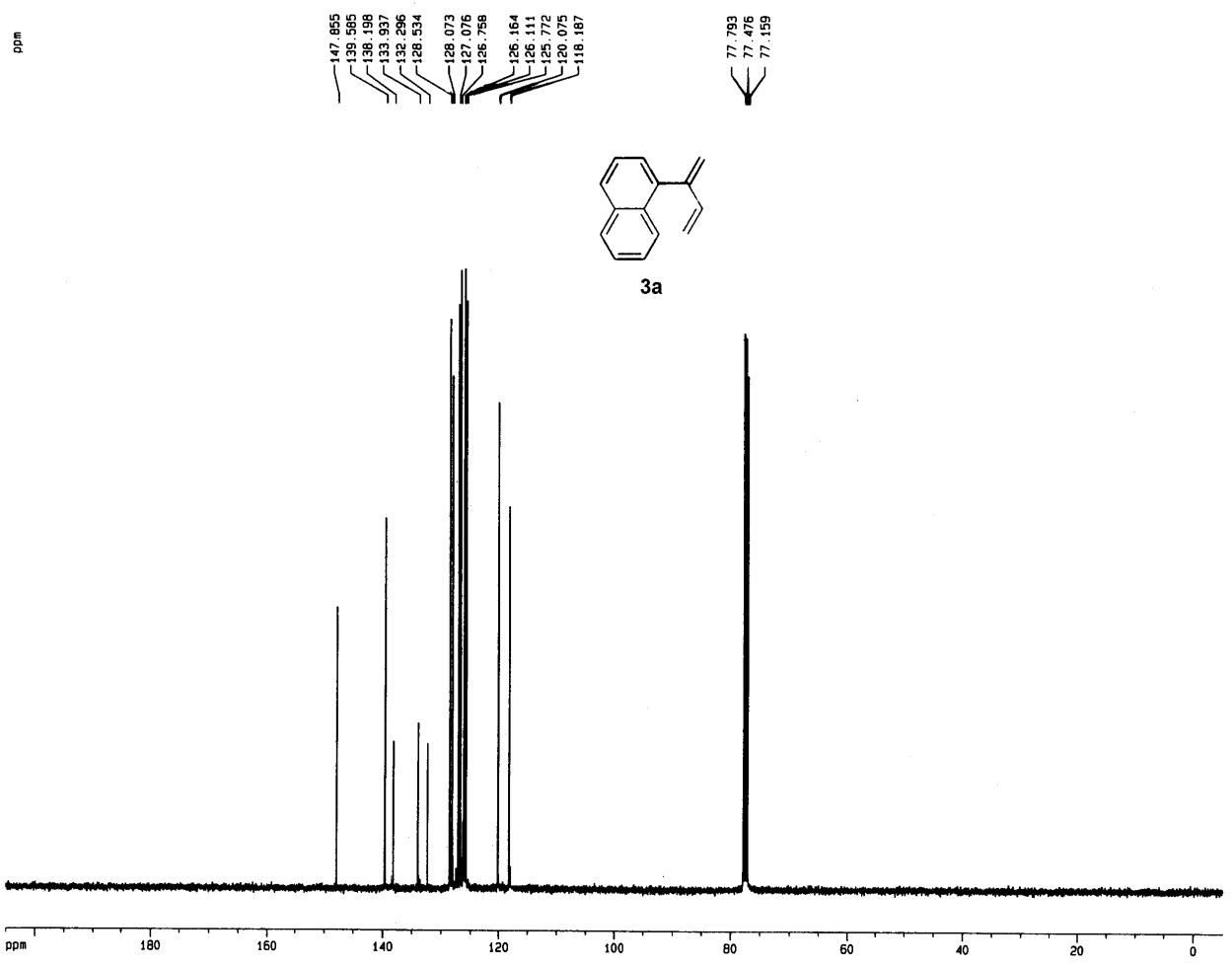
(6) T. A. Bradford, A. D. Payne, A. C. Willis, M. N. Paddon-Row and M. S. Sherburn, *Org. Lett.,* **2007**, *9*, 4861.

^{1}H and ^{13}C NMR Spectra of Products



YHS-388

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PROCNO                     1

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PULPROG                zgpg30
TD                      65536
SOLVENT                CDCl3
NS                       1035
DS                          2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                    3649.1
DW                   15.700 usec
DE                    6.00 usec
TE                    297.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2              400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF                100.6127290 MHz
WDW                         EM
SSB                          0
LB                     1.00 Hz
GB                           0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    15.00 cm
F1P                  205.000 ppm
F1                 20625.61 Hz
F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.00000 ppm/cm
HZCM               704.28906 Hz/cm
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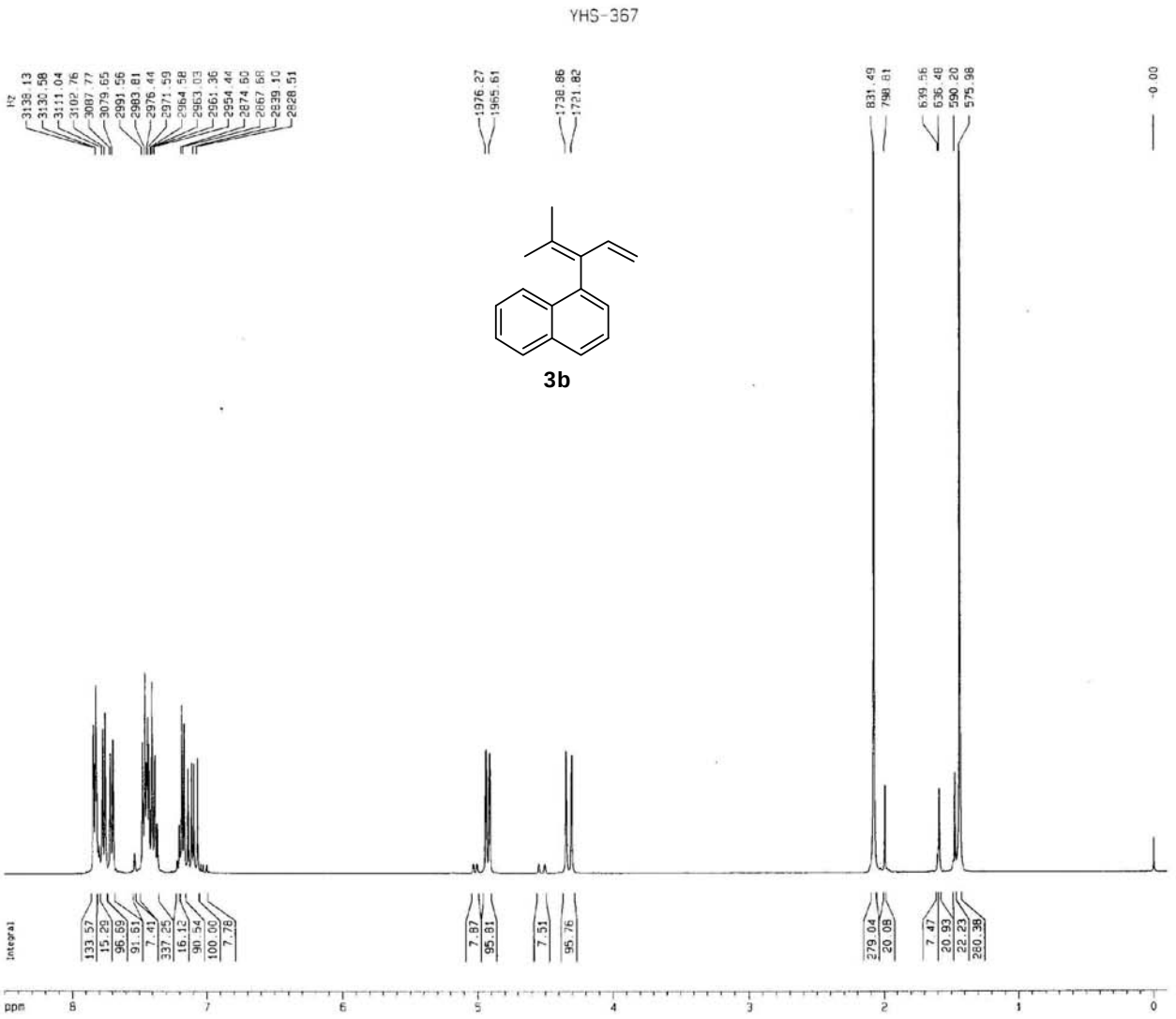

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NAME jul-08
EXPNO 93
PROCNO 1

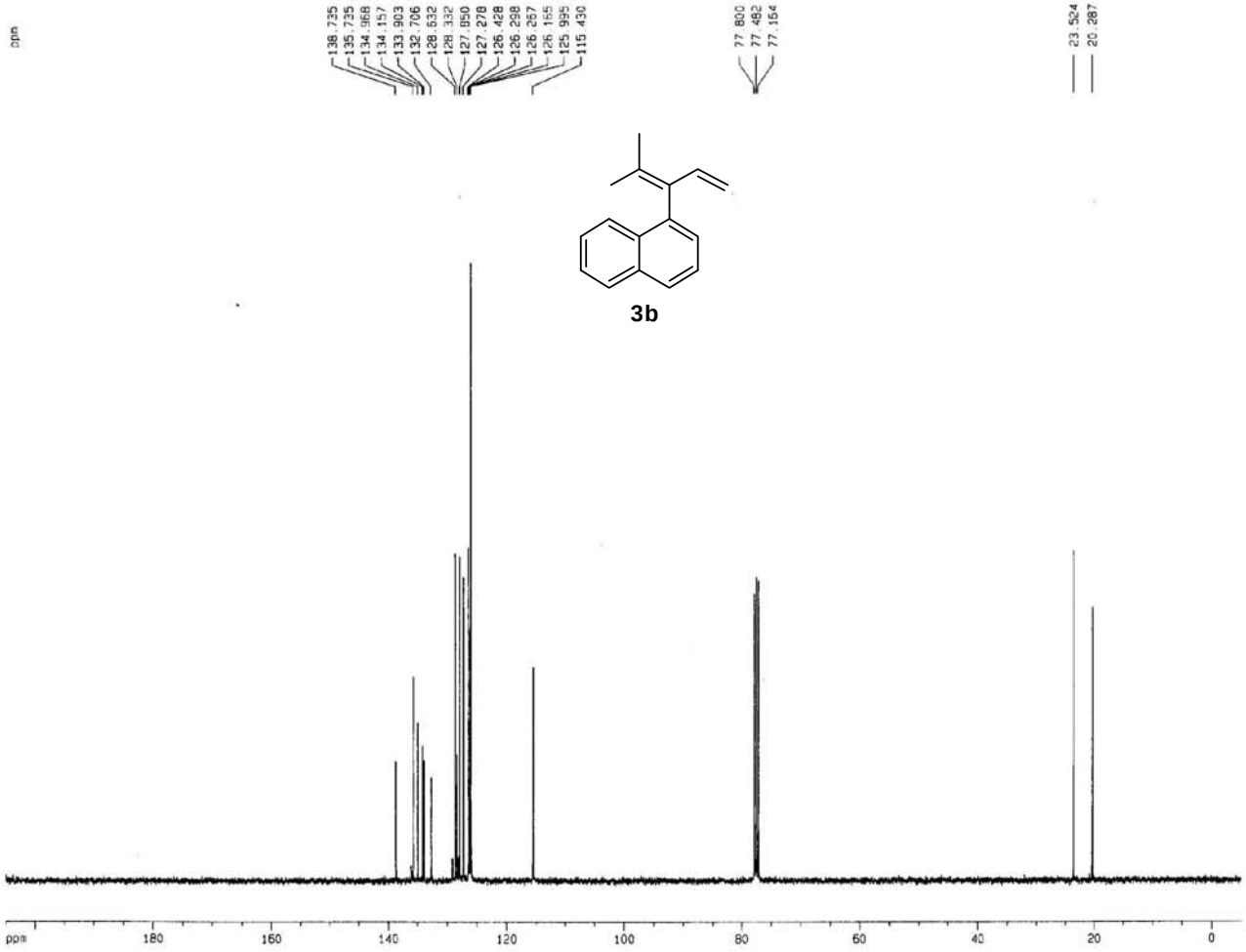
F2 - Acquisition Parameters
Date_ 20080718
Time 17.06
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 71.8
DW 60.800 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
WCREST 0.00000000 sec
WCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300326 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 30.00 cm
F1P 8.500 ppm
F1 3401.11 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.28667 ppm/cm
HZCM 114.70394 Hz/cm

YHS-367



3b

Current Data Parameters
NAME jul-08
EXPNO 94
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080718
Time 17.14
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 379
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 9195.2
DW 15.700 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

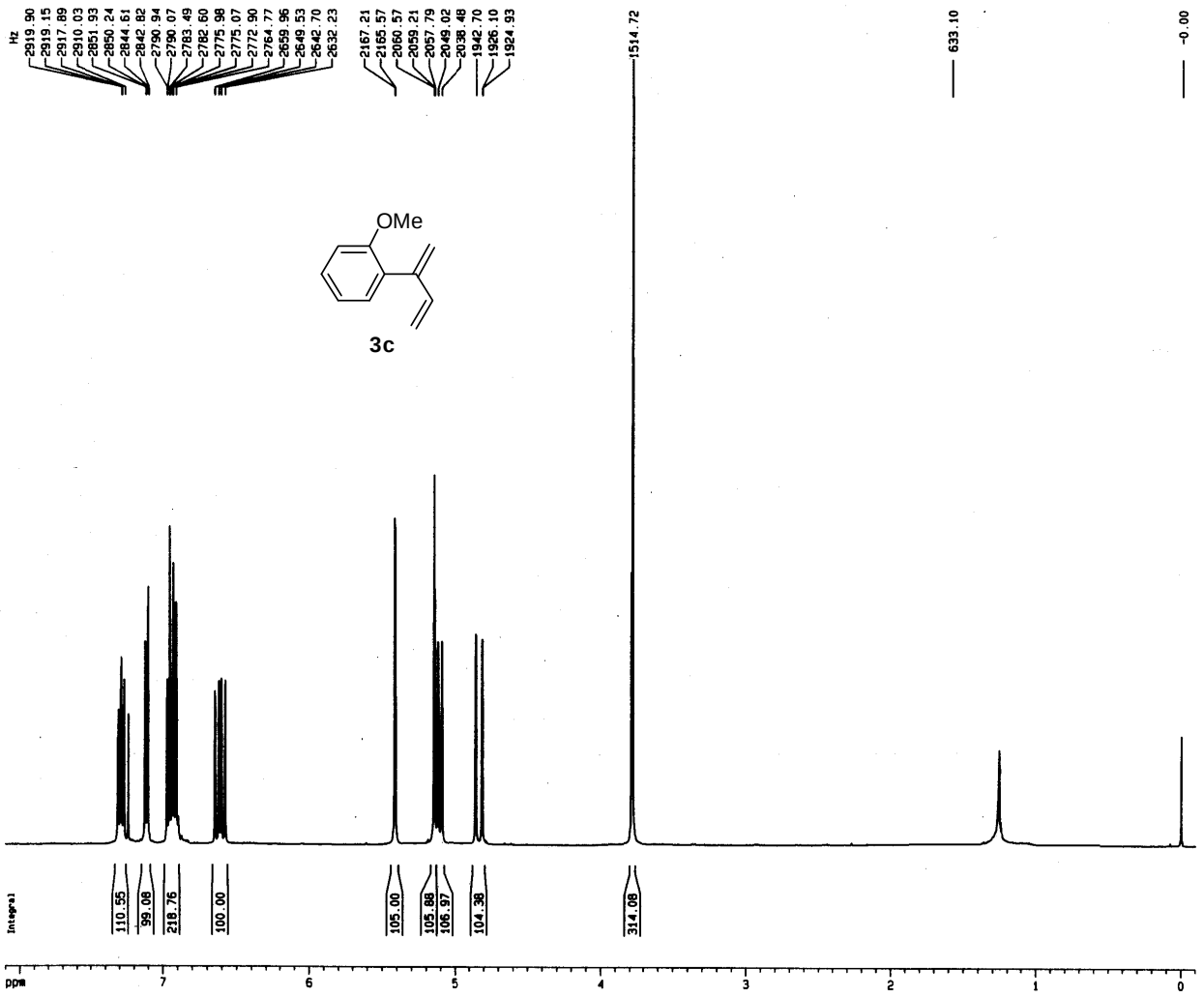
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SF01 100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SF02 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 30.00 cm
CY 15.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28906 Hz/cm

YHS-377

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Current Data Parameters
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EXPNO                     17
PROCNO                     1

F2 - Acquisition Parameters
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Time                   11.12
INSTRUM                spect
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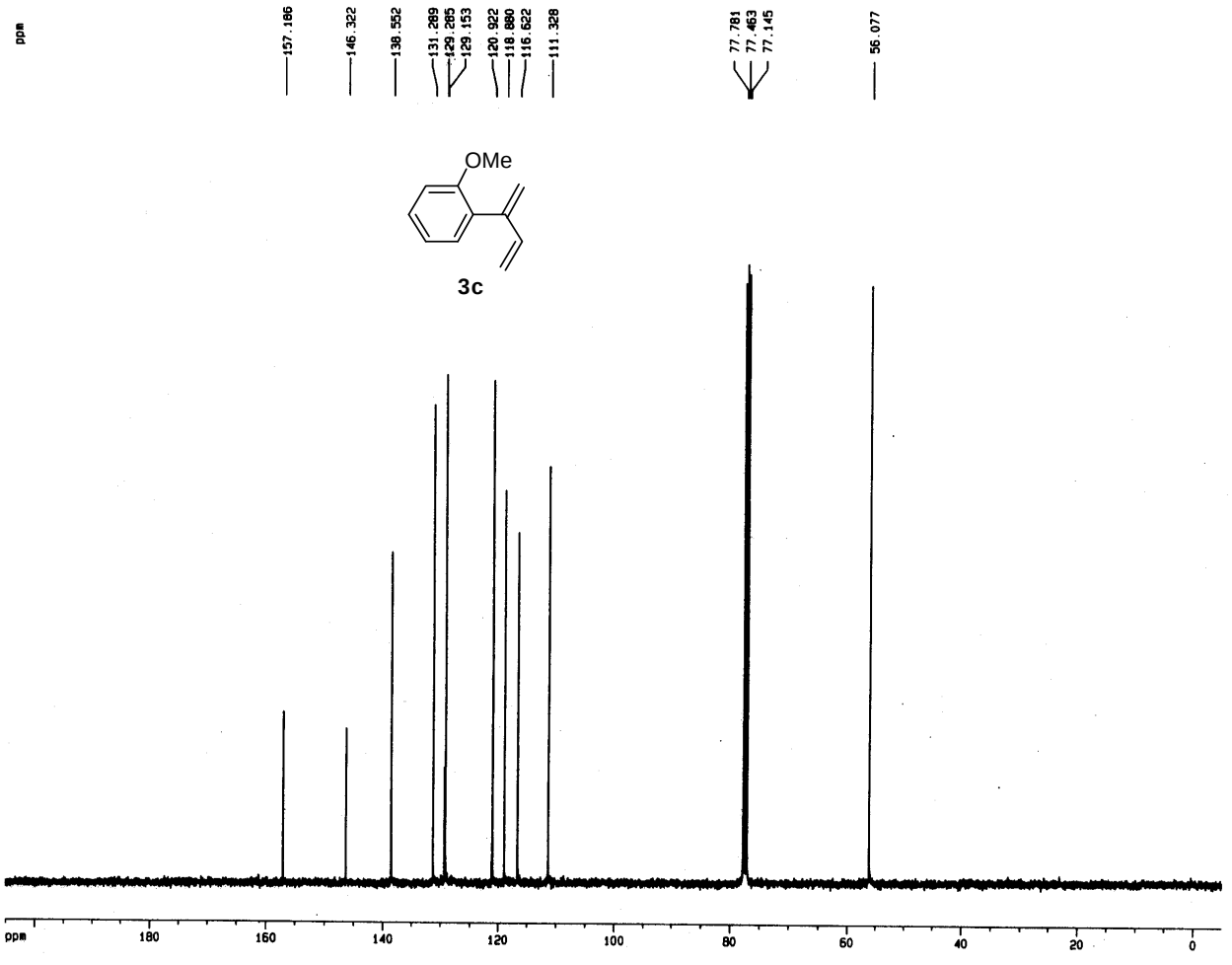
PULPROG                zg30
TD                    32768
SOLVENT                CDCl3
NS                        32
DS                         0
SWH                 8223.685 Hz
FIDRES              0.250967 Hz
AQ                  1.9923444 sec
RG                      101.6
DW                     60.800 usec
DE                      6.00 usec
TE                     296.2 K
D1                  1.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.00 usec
PL1                    -2.00 dB
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF                 400.1300166 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     30.00 cm
CY                     78.00 cm
F1P                     8.100 ppm
F1                   3241.05 Hz
F2P                    -0.100 ppm
F2                     -40.01 Hz
PPMCM                0.27333 ppm/cm
HZCM                 109.36887 Hz/cm
```

YHS-377

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Current Data Parameters
NAME                  aug-08
EXPNO                     18
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080807
Time                  11.59
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG               zgpg30
TD                     65536
SOLVENT               CDCl3
NS                       874
DS                         2
SWH               31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                    1625.5
DW                   15.700 usec
DE                    6.00 usec
TE                    297.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                 105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2              400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127290 MHz
WDW                          EM
SSB                           0
LB                       1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                       30.00 cm
CY                       15.00 cm
F1P                     205.000 ppm
F1                    20625.61 Hz
F2P                      -5.000 ppm
F2                     -503.06 Hz
PPMCM                 7.00000 ppm/cm
HZCM                704.28906 Hz/cm
```
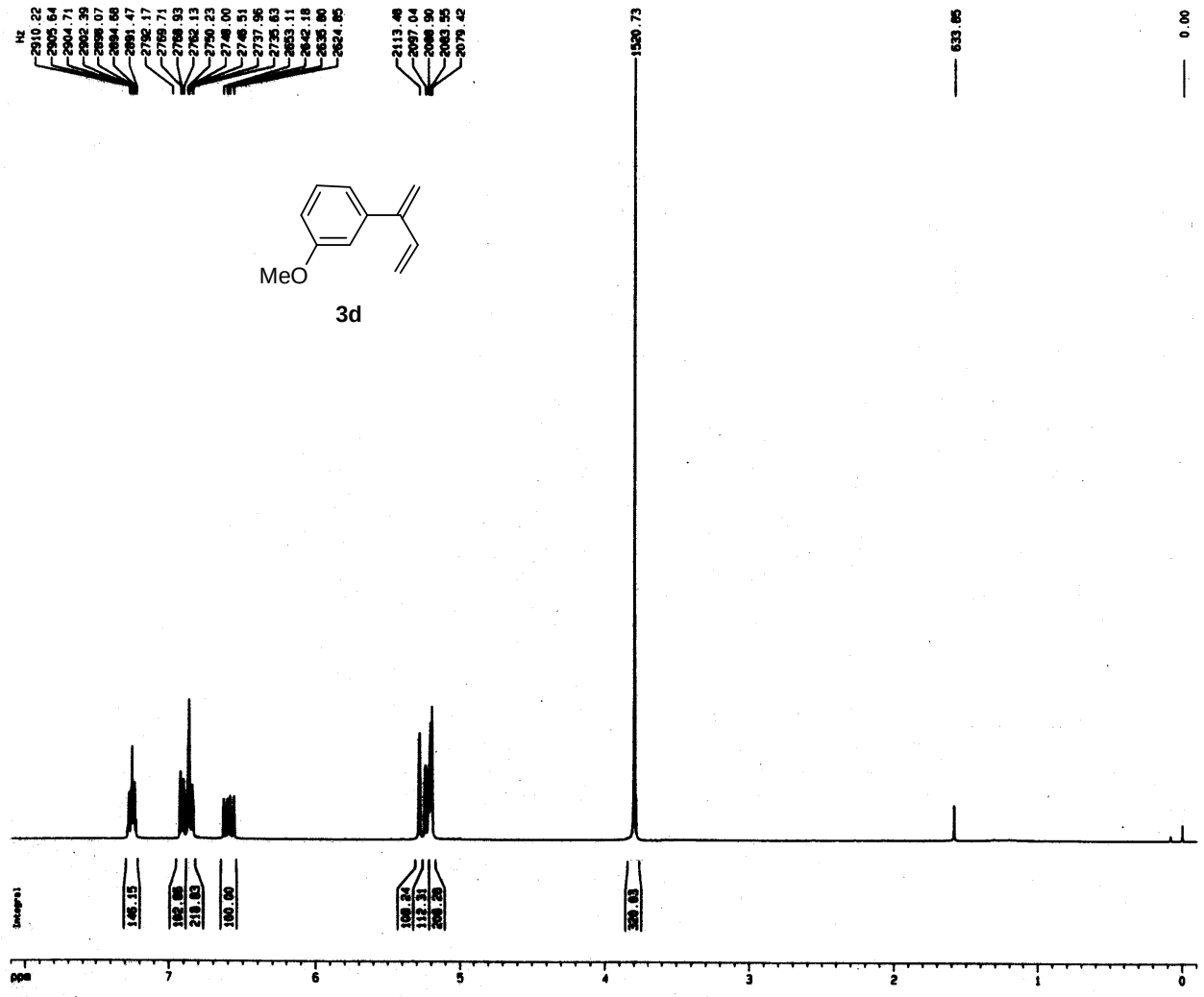

YHS-378




```
Current Data Parameters
NAME                  aug-08
EXPNO                     19
PROCNO                     1

F2 - Acquisition Parameters
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Time                   12.07
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zg30
TD                    32768
SOLVENT                CDCl3
NS                        32
DS                         0
SWH               8223.685 Hz
FIDRES            0.250967 Hz
AQ                1.9923444 sec
RG                        64
DW                  60.800 usec
DE                   6.00 usec
TE                  297.2 K
D1                1.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                   11.00 usec
PL1                  -2.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF                400.1300230 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                    1.00

1D NMR plot parameters
CX                   30.00 cm
CY                   20.00 cm
F1P                   8.100 ppm
F1                 3241.05 Hz
F2P                  -0.100 ppm
F2                  -40.01 Hz
PPMCM                0.27333 ppm/cm
HZCM               109.38088 Hz/cm
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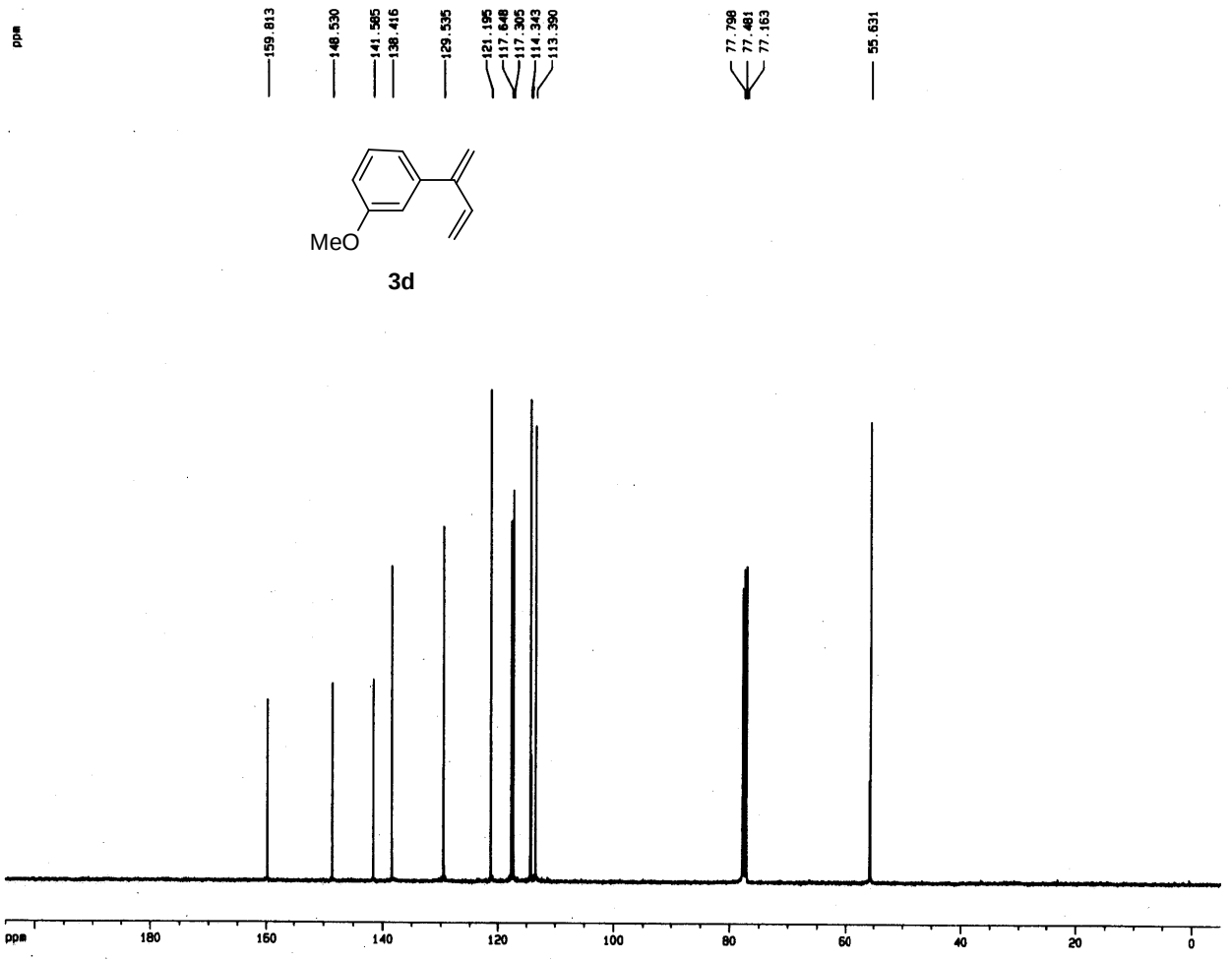
YHS-378



3d

```
Current Data Parameters
NAME                  aug-08
EXPNO                     20
PROCNO                     1

F2 - Acquisition Parameters
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Time                  13.58
INSTRUM               spect
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PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      2048
DS                         2
SWH               31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                       181
DW                    15.700 usec
DE                     6.00 usec
TE                    297.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2             400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127290 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                        30.00 cm
CY                        12.00 cm
F1P                      205.000 ppm
F1                     20625.61 Hz
F2P                       -5.000 ppm
F2                      -503.06 Hz
PPMCM                  7.00000 ppm/cm
HZCM                 704.28906 Hz/cm
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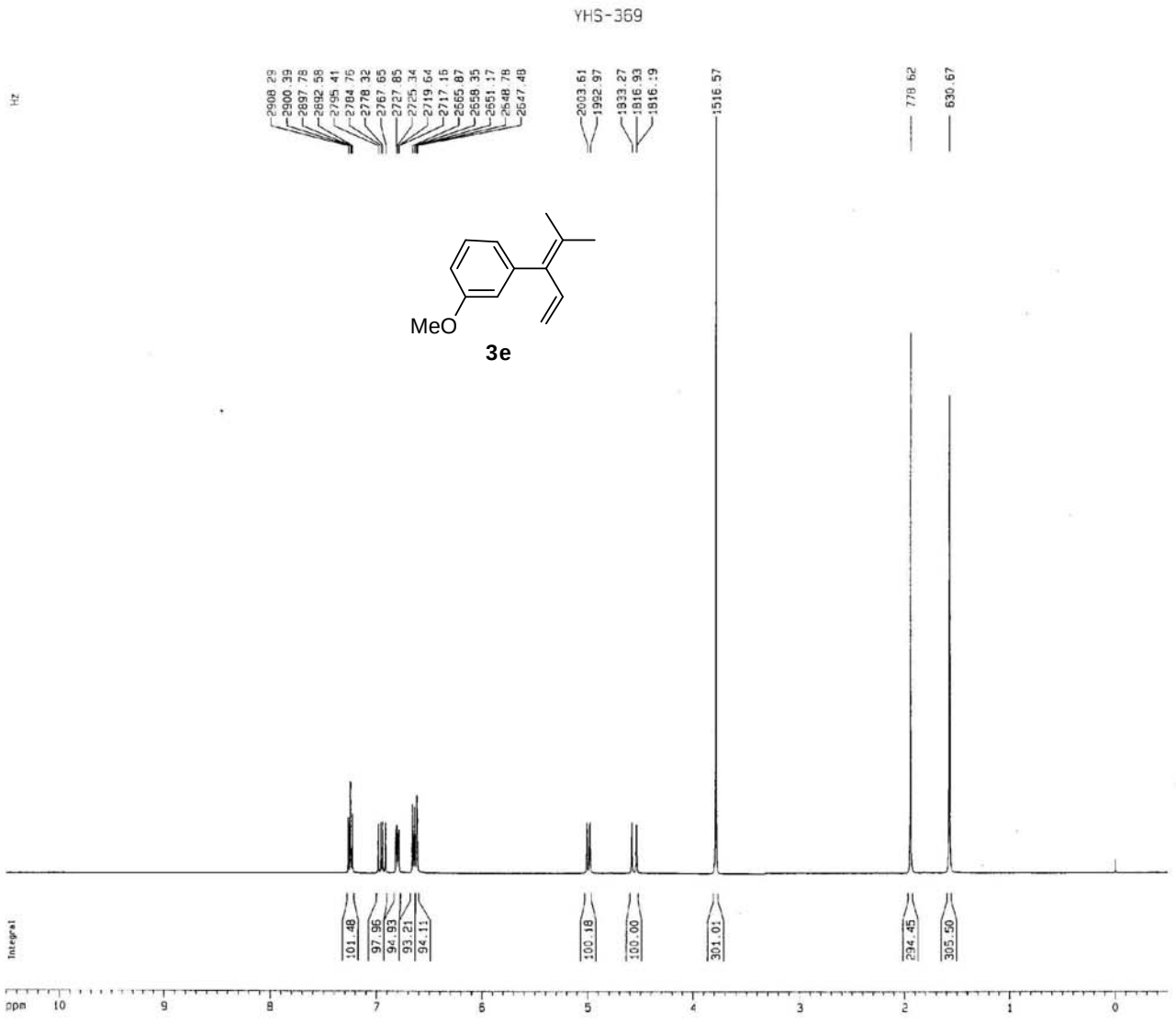


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Current Data Parameters
NAME                  jul-08
EXPNO                    107
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080722
Time                   15.30
INSTRUN                spect
PROBHD   5 mm Dual 13C/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        32
DS                         0
SWH                8223.685 Hz
FIDRES             0.250967 Hz
AQ                 1.9923444 sec
RG                        64
DW                   60.800 usec
DE                    6.00 usec
TE                   297.2 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    11.00 usec
PL1                   -2.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF               400.1300168 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                    30.00 cm
CY                    20.00 cm
F1P                  10.500 ppm
F1                  4201.37 Hz
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F2                  -200.06 Hz
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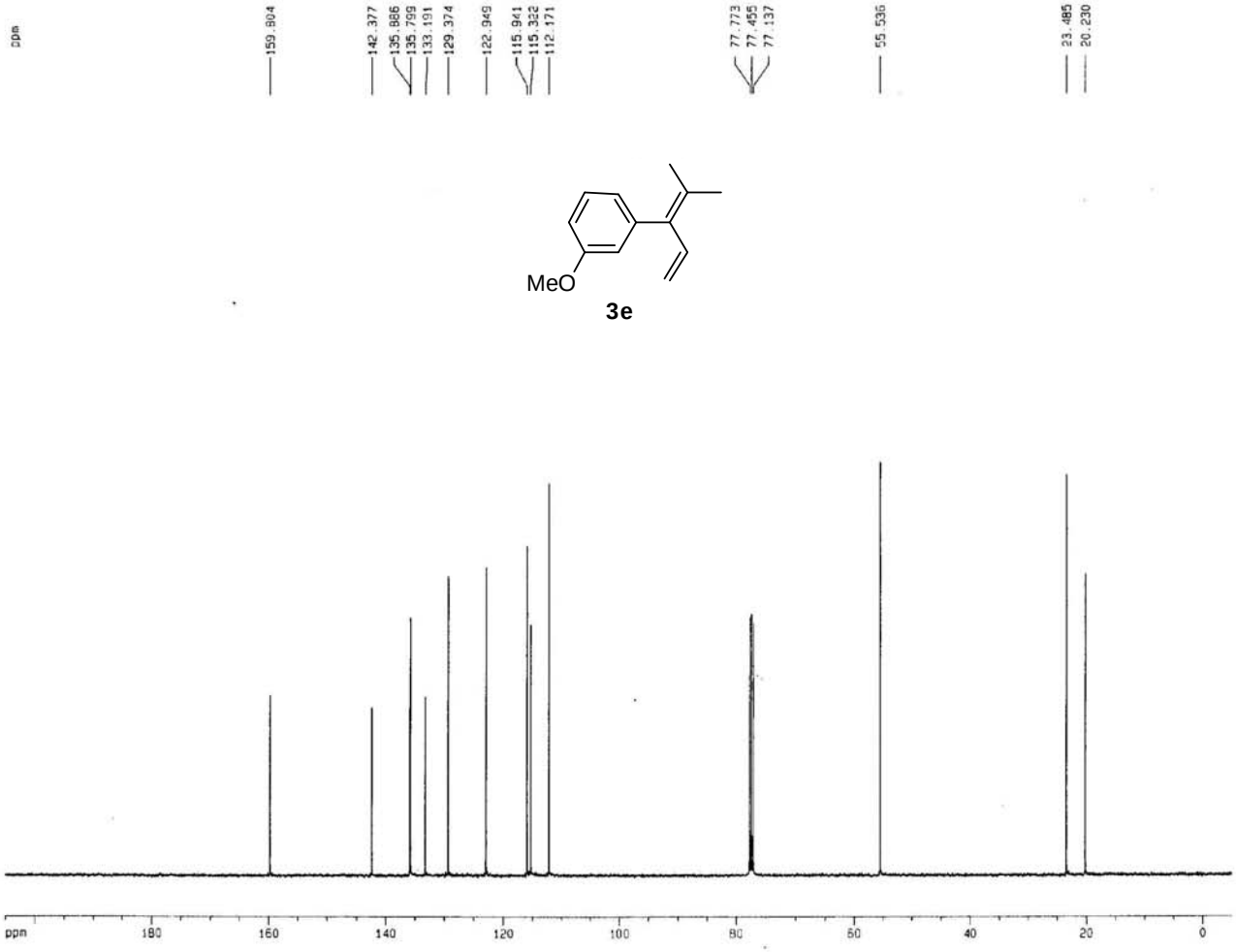
```

YHS-369




```
Current Data Parameters
NAME                  jul-08
EXPNO                    108
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080722
Time                   16.31
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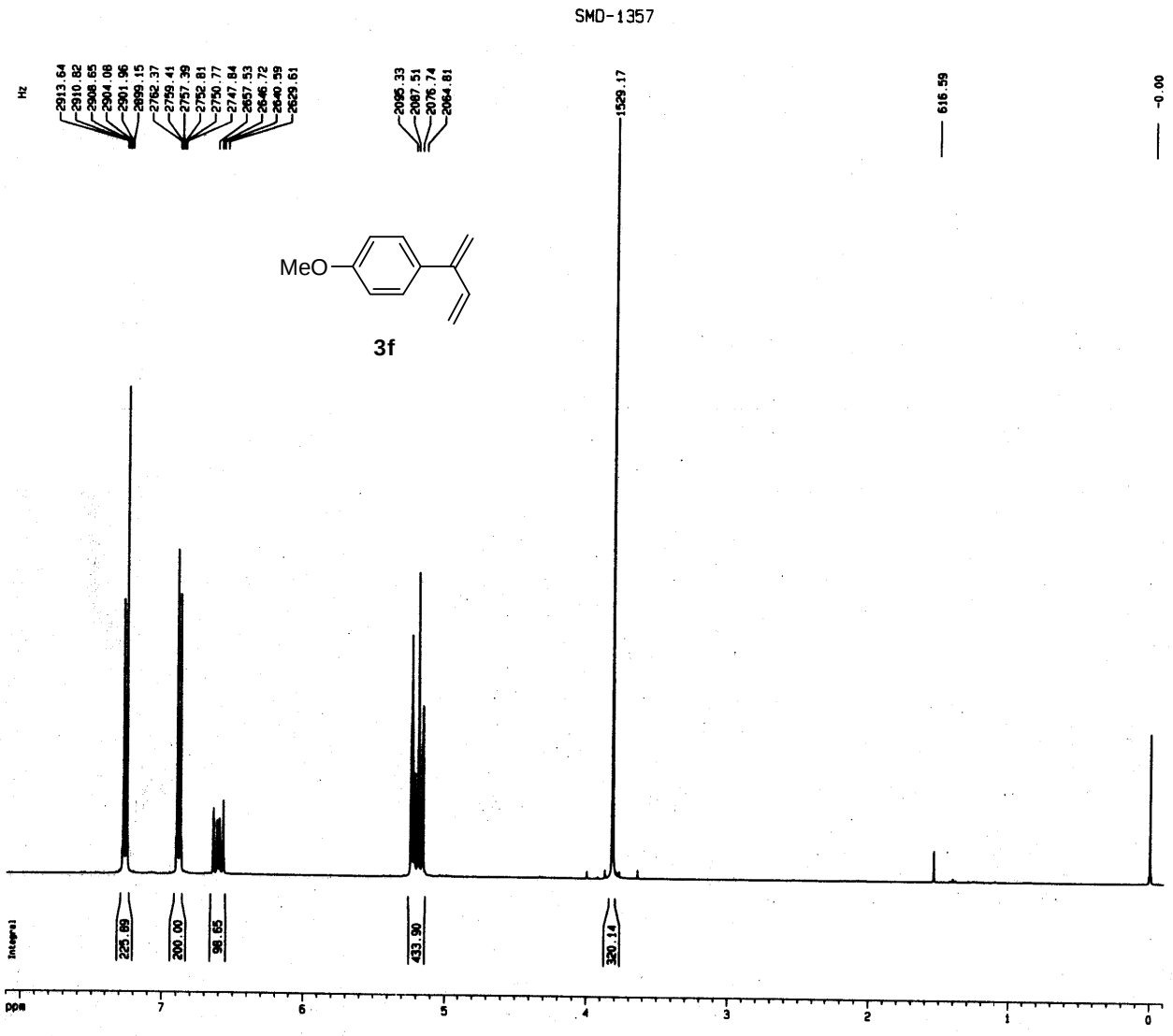
PULPROG                zgpg30
TD                      65536
SOLVENT                CDCl3
NS                      1167
DS                         2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                     228.1
DW                    15.700 usec
DE                     6.00 usec
TE                     297.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2              400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF                100.6127290 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                      30.00 cm
CY                      10.00 cm
F1P                   205.000 ppm
F1                  20625.61 Hz
F2P                    -5.000 ppm
F2                   -503.06 Hz
PPMCM                7.00000 ppm/cm
HZCM               704.28906 Hz/cm
```



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EXPNO 84
PROCNO 1

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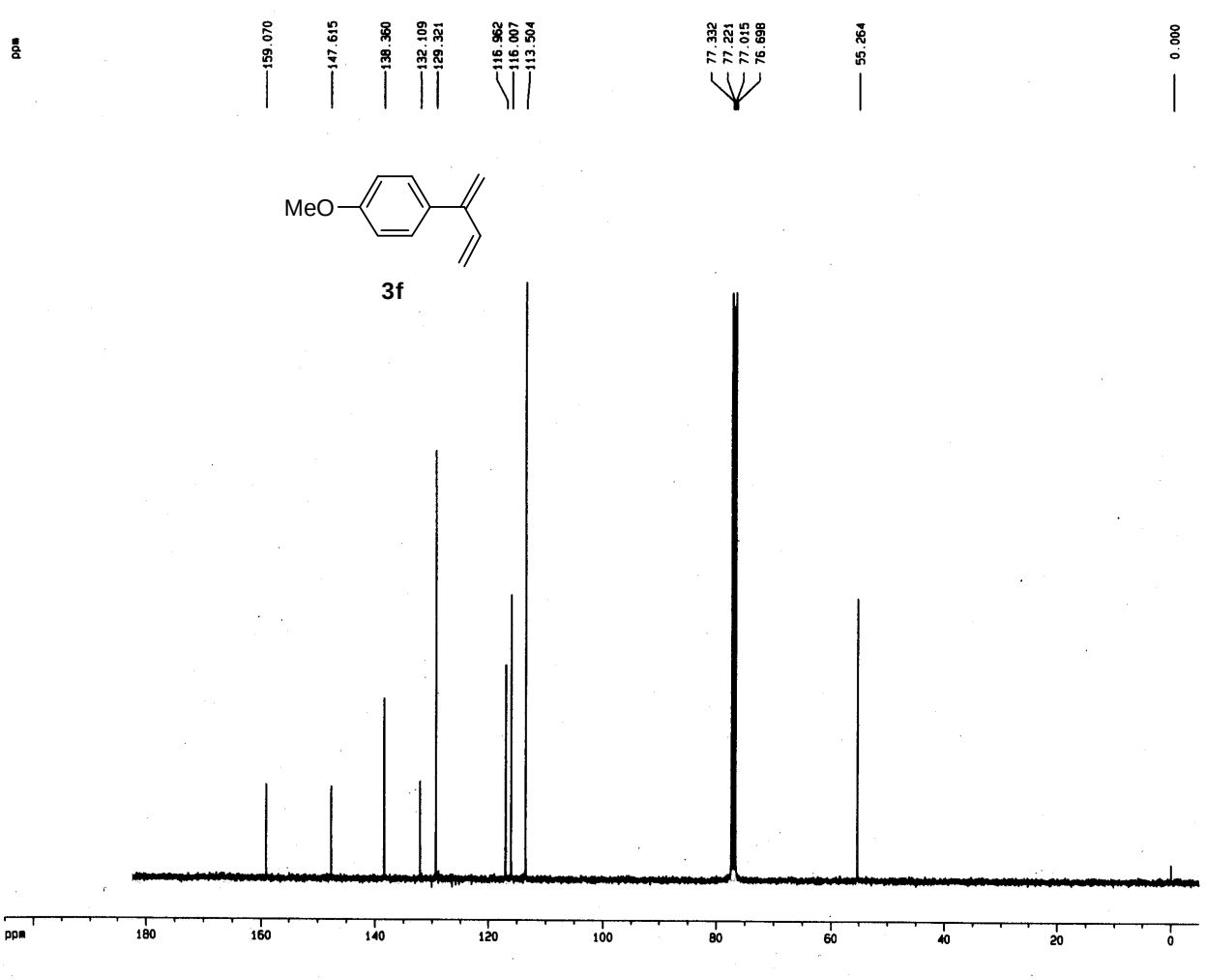
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 203.2
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 40.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36887 Hz/cm

SMD-1357



Current Data Parameters
NAME oct-07
EXPNO 85
PROCNO 1

F2 - Acquisition Parameters
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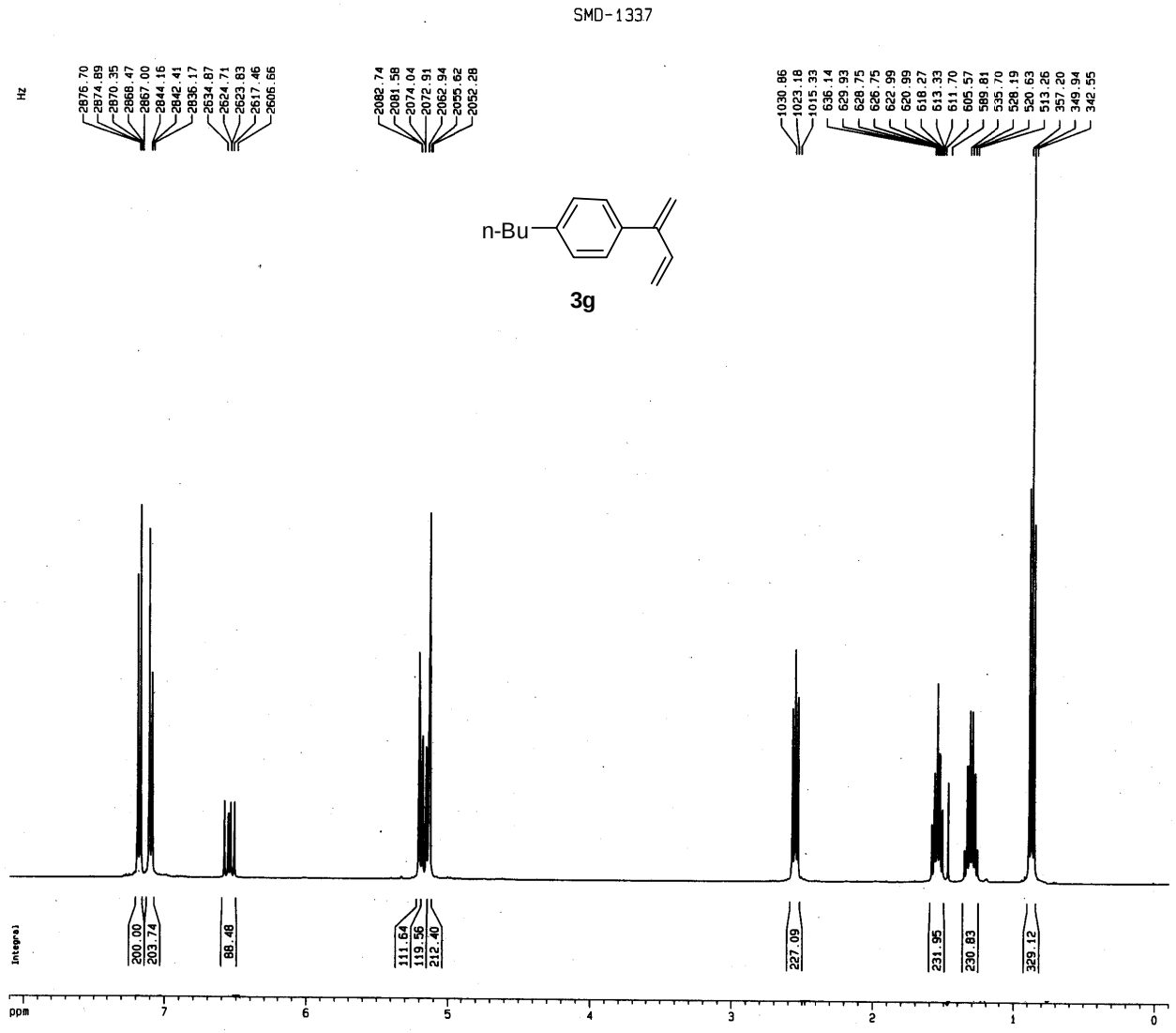
Time 16.22
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 80.6
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127707 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 30.00 cm
CY 15.00 cm
F1P 205.000 ppm
F1 20625.62 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28937 Hz/cm

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Current Data Parameters
NAME                  oct-07
EXPNO                     50
PROCNO                     1

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PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        0
SWH                8223.685 Hz
FIDRES             0.250967 Hz
AQ                 1.9923444 sec
RG                     161.3
DW                    60.800 usec
DE                     6.00 usec
TE                    296.2 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.00 usec
PL1                    -2.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF                400.1300379 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00

1D NMR plot parameters
CX                    30.00 cm
CY                    20.00 cm
F1P                    8.100 ppm
F1                  3241.05 Hz
F2P                   -0.100 ppm
F2                    -40.01 Hz
PPMCM              0.27333 ppm/cm
HZCM             109.36888 Hz/cm
```
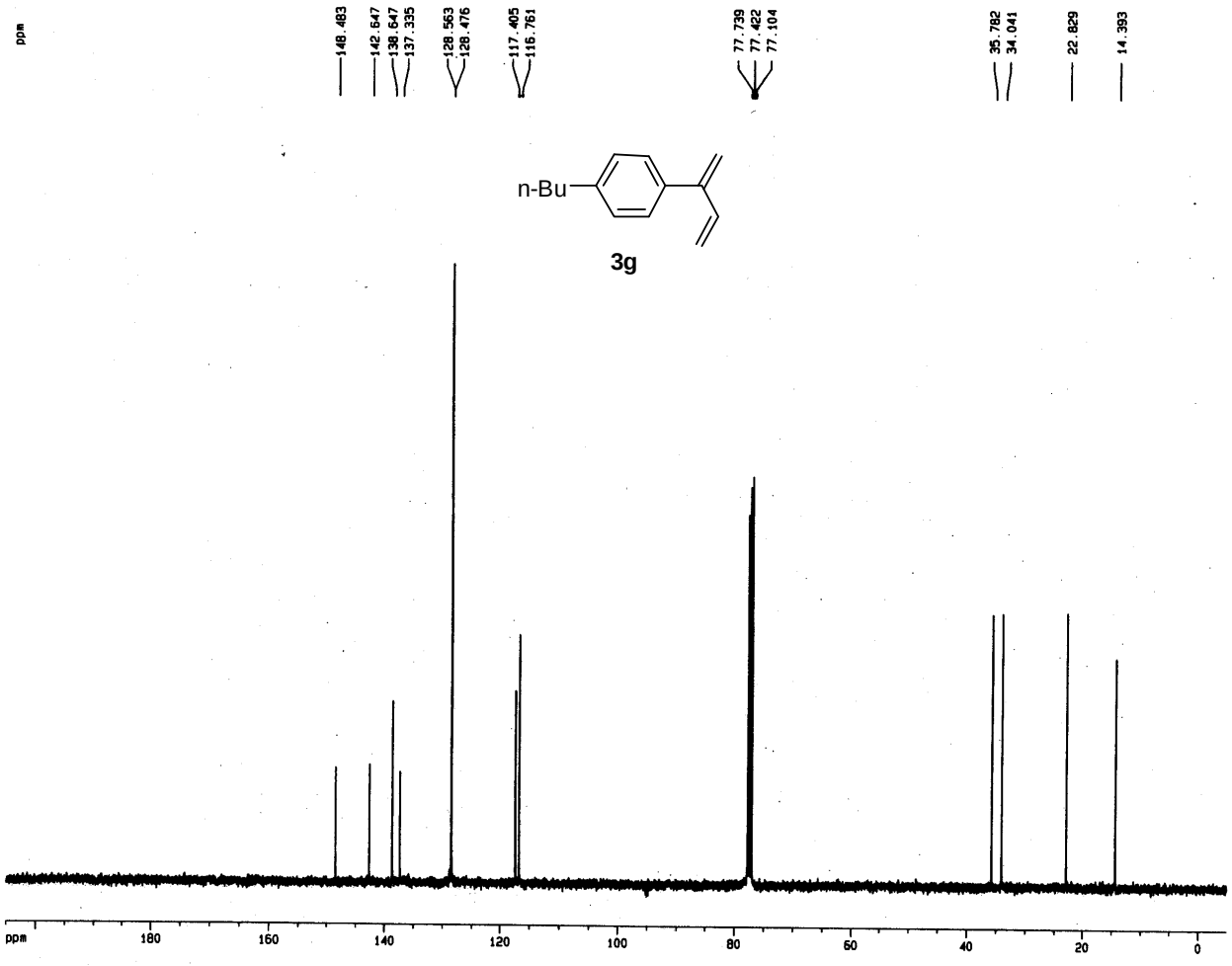
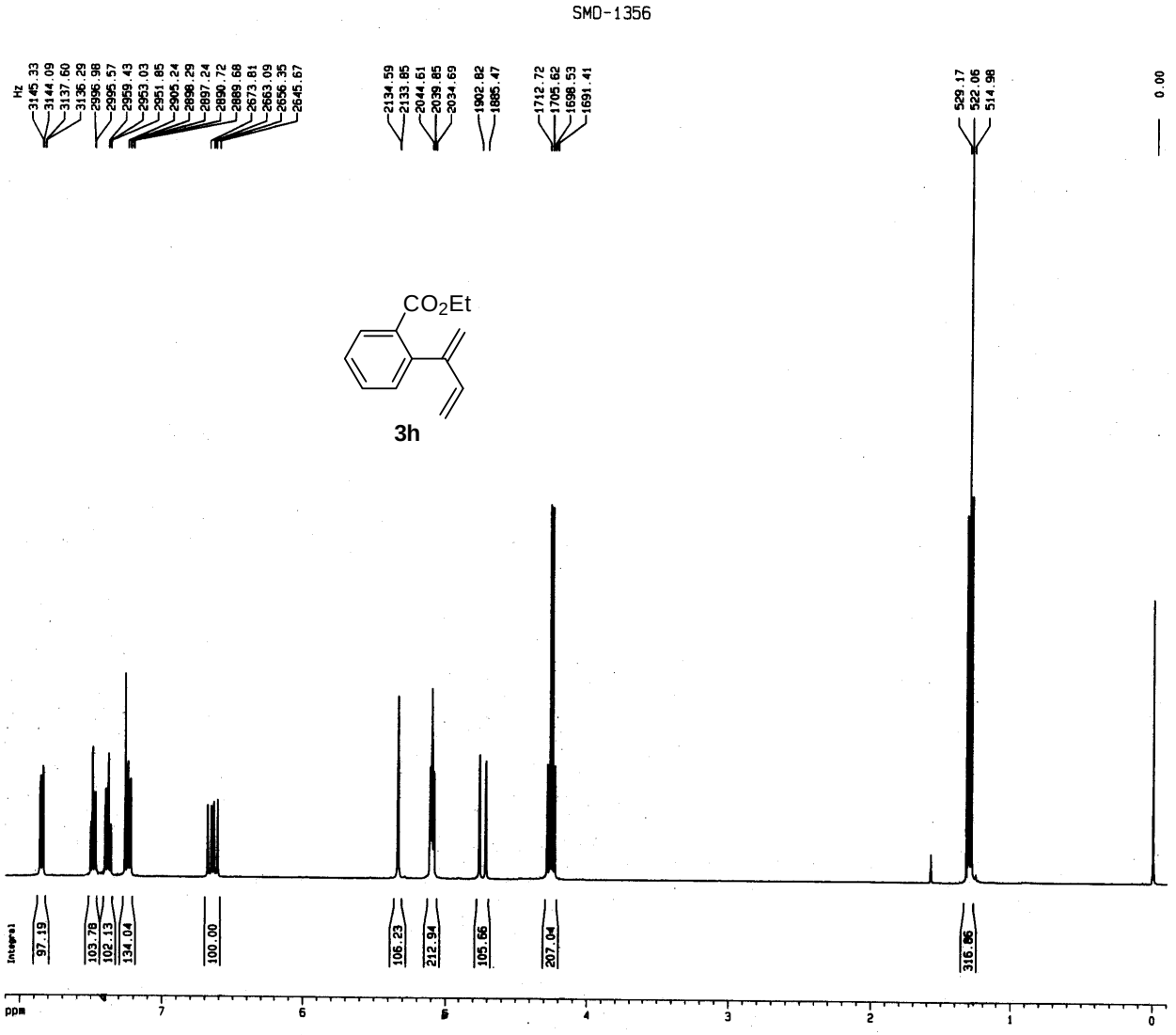

SMD-1337




```
Current Data Parameters
NAME                  oct-07
EXPNO                     51
PROCNO                     1

F2 - Acquisition Parameters
Date_              20071029
Time                  15.20
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       824
DS                         2
SWH               31847.133 Hz
FIDRES                0.485949 Hz
AQ                1.0289652 sec
RG                    3649.1
DW                   15.700 usec
DE                    6.00 usec
TE                    296.2 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                   10.50 usec
PL1                  -1.00 dB
SFO1            100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                105.00 usec
PL2                  -2.00 dB
PL12                 18.00 dB
PL13                 20.00 dB
SFO2            400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF              100.6127290 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                   30.00 cm
CY                   15.00 cm
F1P                 205.000 ppm
F1                20625.61 Hz
F2P                  -5.000 ppm
F2                 -503.06 Hz
PPMCM                7.00000 ppm/cm
HZCM               704.28906 Hz/cm
```



Current Data Parameters
NAME oct-07
EXPNO 59
PROCNO 1

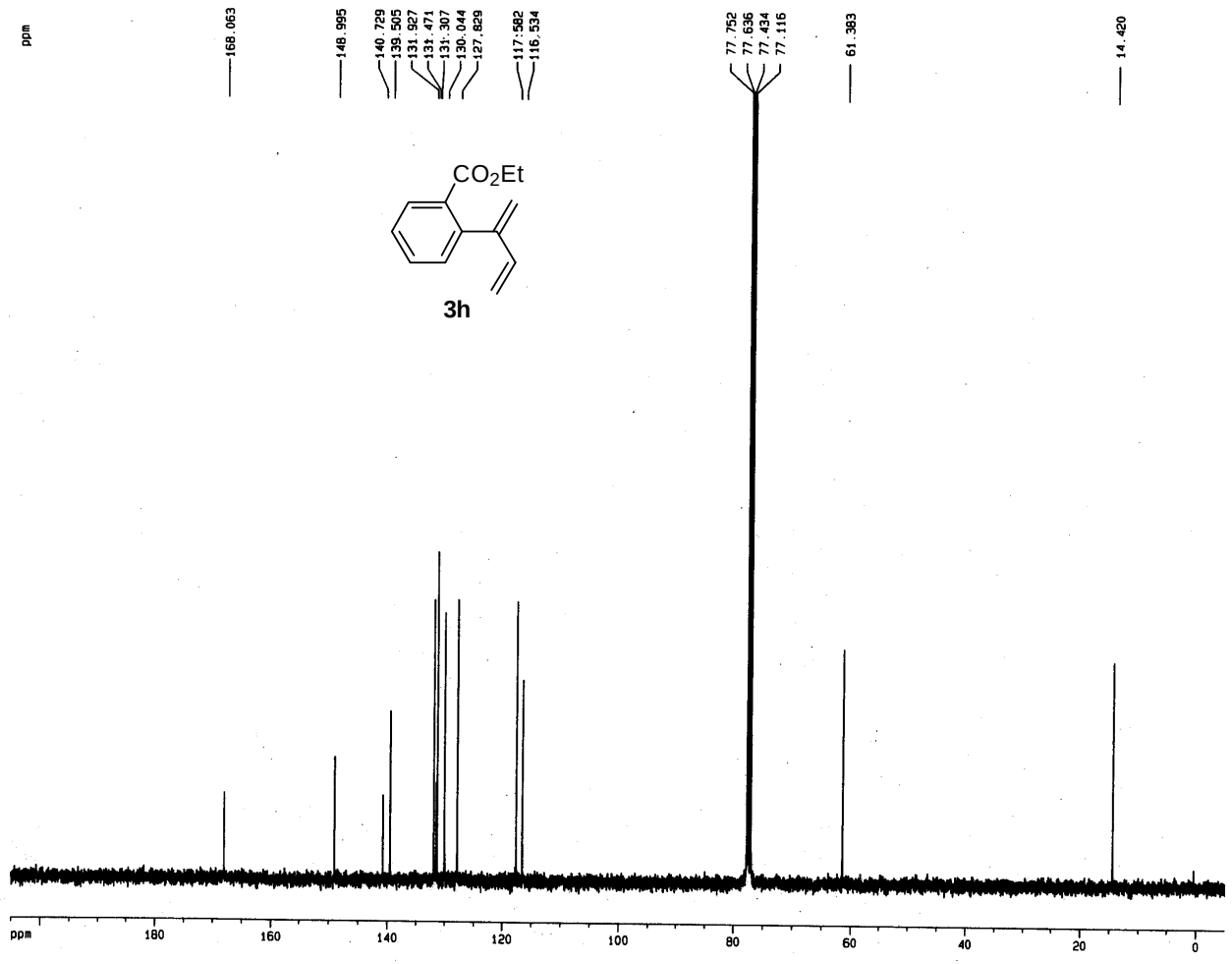
F2 - Acquisition Parameters
Date_ 20071031
Time 13.27
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 228.1
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

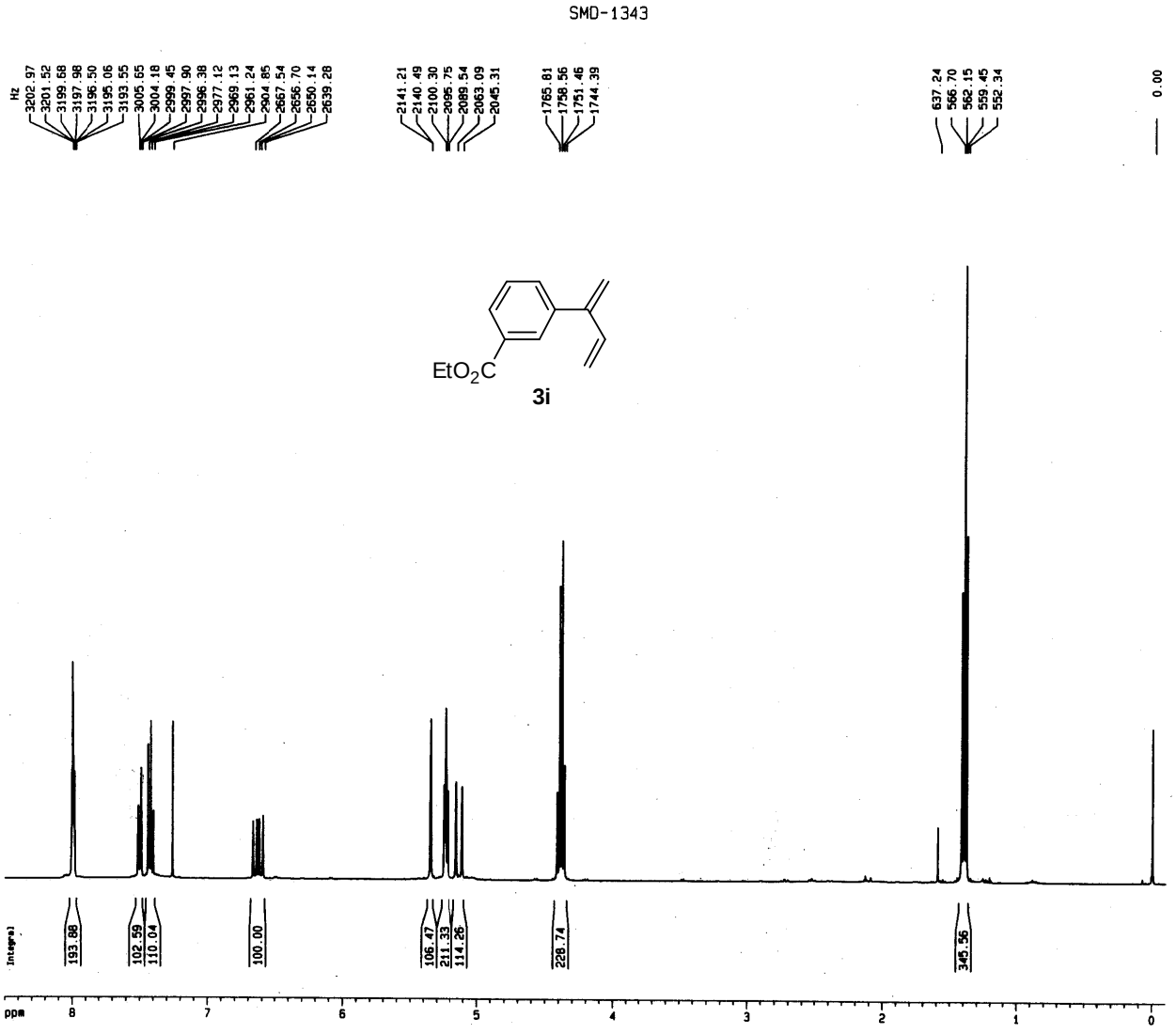
F2 - Processing parameters
SI 16384
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36887 Hz/cm

SMD-1356

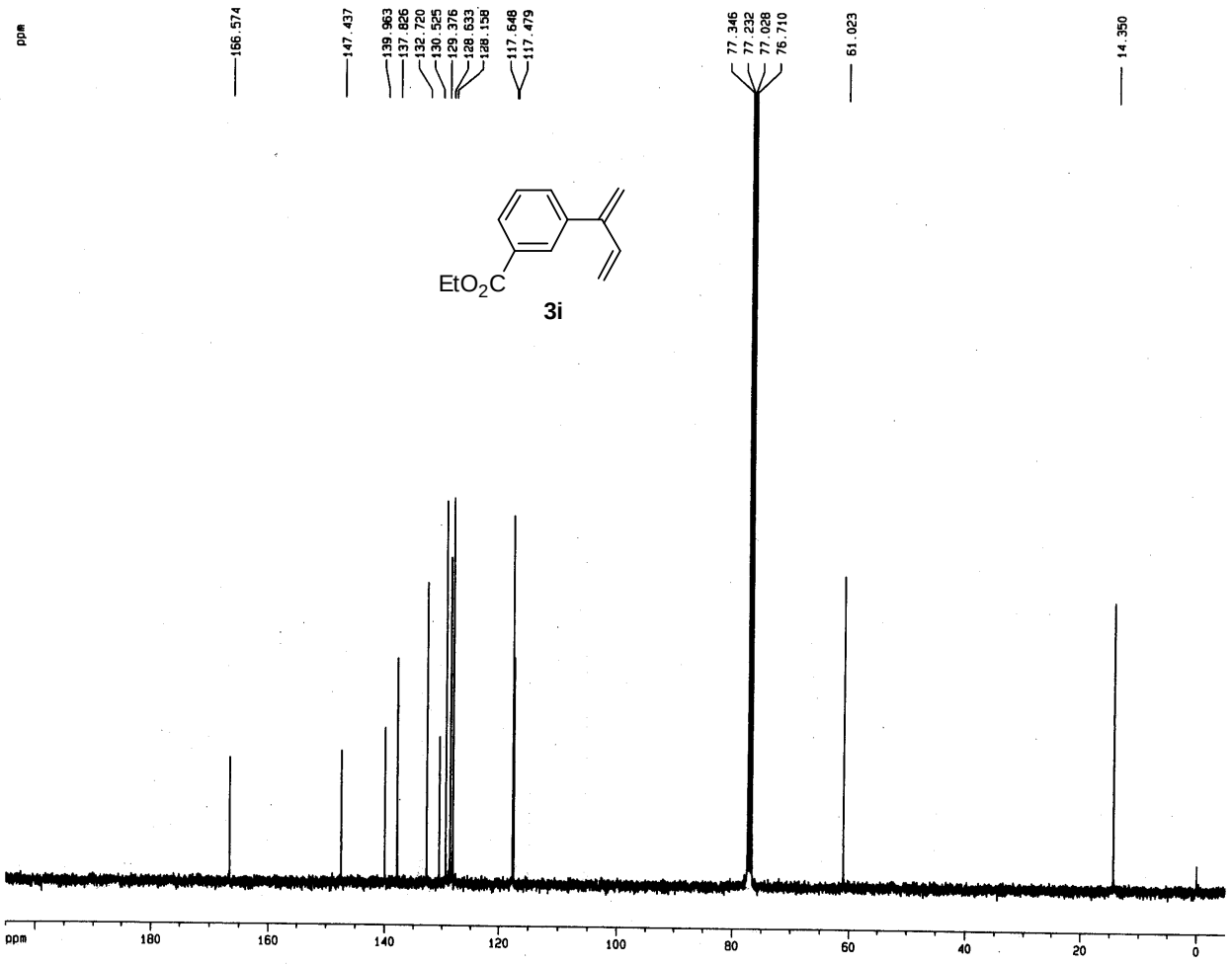



```
Current Data Parameters
NAME                  oct-07
EXPNO                     60
PROCNO                     1

F2 - Acquisition Parameters
Date_               20071031
Time                   13.50
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zgpg30
TD                      65536
SOLVENT                CDCl3
NS                        584
DS                          2
SWH                31847.133 Hz
FIDRES                0.485949 Hz
AQ                 1.0289652 sec
RG                        406.4
DW                    15.700 usec
DE                     6.00 usec
TE                     296.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                    10.50 usec
PL1                    -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2              400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127290 MHz
WDW                        EM
SSB                         0
LB                     1.00 Hz
GB                          0
PC                      1.40

1D NMR plot parameters
CX                     30.00 cm
CY                     23.00 cm
F1P                  205.000 ppm
F1                 20625.61 Hz
F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.00000 ppm/cm
HZCM               704.28906 Hz/cm
```




```
Current Data Parameters
NAME                  oct-07
EXPNO                     97
PROCNO                     1

F2 - Acquisition Parameters
Date_               20071112
Time                   10.46
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zg30
TD                     32768
SOLVENT                CDCl3
NS                        32
DS                         0
SWH                 8223.685 Hz
FIDRES              0.250967 Hz
AQ                  1.9923444 sec
RG                       181
DW                    60.800 usec
DE                     6.00 usec
TE                    296.2 K
D1                  1.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                    11.00 usec
PL1                   -2.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                       16384
SF                400.1300098 MHz
WDW                        EM
SSB                         0
LB                     0.30 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                    30.00 cm
CY                    16.00 cm
F1P                    8.500 ppm
F1                  3401.10 Hz
F2P                   -0.100 ppm
F2                    -40.01 Hz
PPMCM                 0.28667 ppm/cm
HZCM                114.70393 Hz/cm
```

SMD-1343



Current Data Parameters

NAME	oct-07
EXPNO	98
PROCNO	1

F2 - Acquisition Parameters

Date_	20071112
Time	11.40
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1018
DS	2
SWH	31847.133 Hz
FIDRES	0.485949 Hz
AQ	1.0289652 sec
RG	203.2
DW	15.700 usec
DE	6.00 usec
TE	296.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	10.50 usec
PL1	-1.00 dB
SFO1	100.6254358 MHz

======== CHANNEL f2 ========

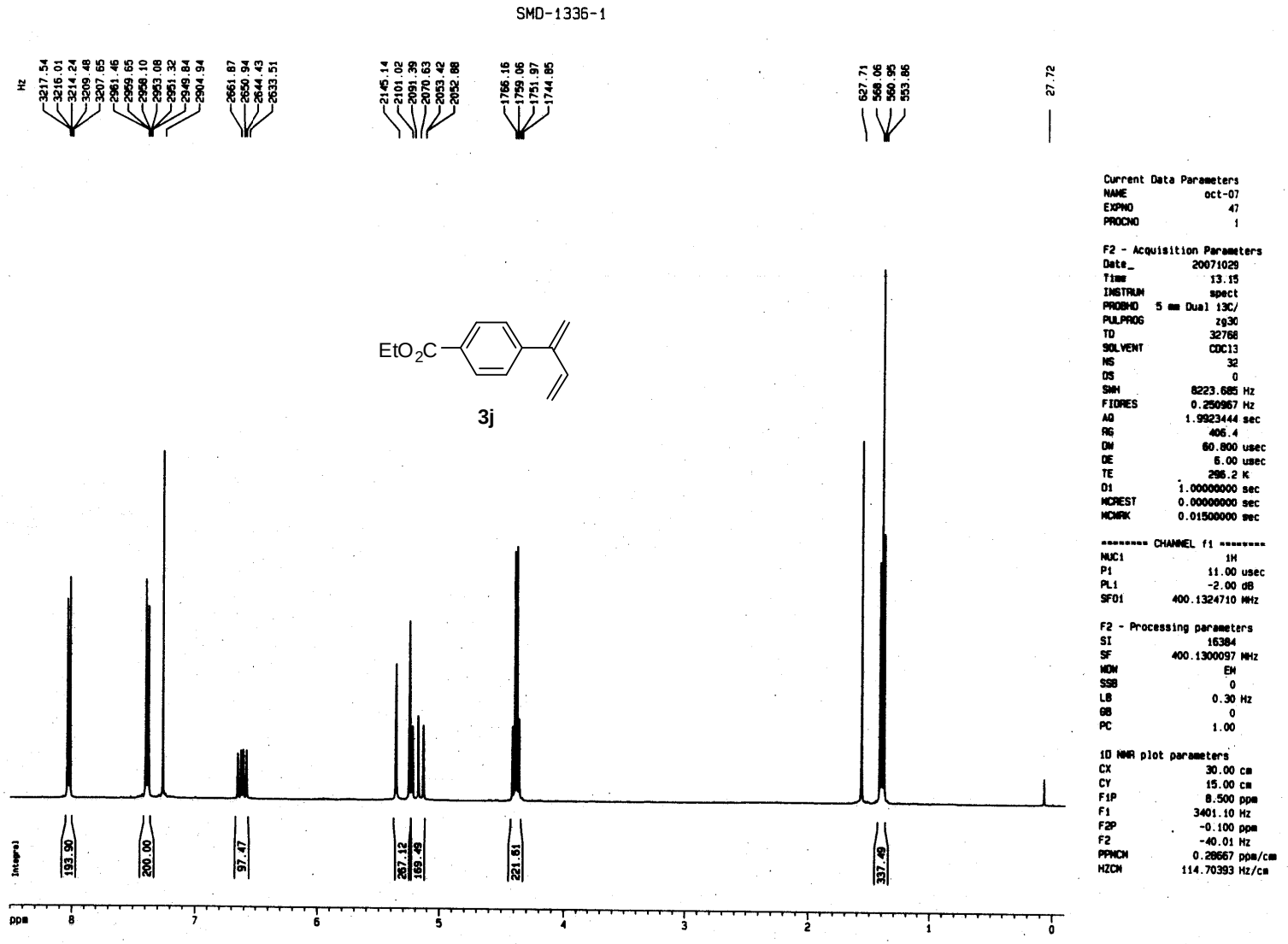
CPDPRG2	waltz16
NUC2	1H
PCPD2	105.00 usec
PL2	-2.00 dB
PL12	18.00 dB
PL13	20.00 dB
SFO2	400.1324708 MHz

F2 - Processing parameters

SI	32768
SF	100.6127699 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	30.00 cm
CY	23.00 cm
F1P	205.000 ppm
F1	20625.62 Hz
F2P	-5.000 ppm
F2	-503.06 Hz
PPMCM	7.00000 ppm/cm
HZCM	704.28937 Hz/cm



Current Data Parameters
NAME oct-07
EXPNO 47
PROCNO 1

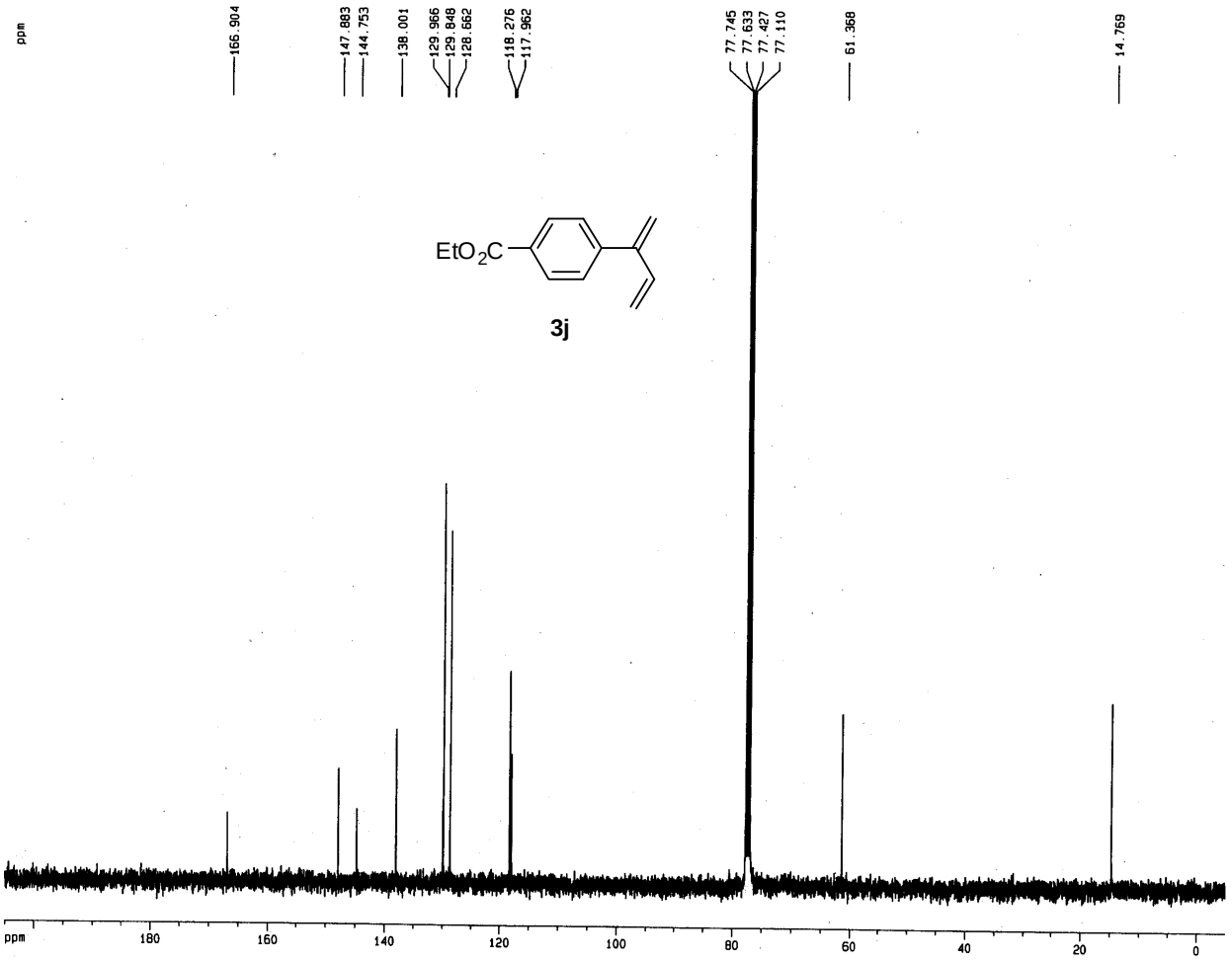
F2 - Acquisition Parameters
Date_ 20071029
Time 13.15
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 406.4
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

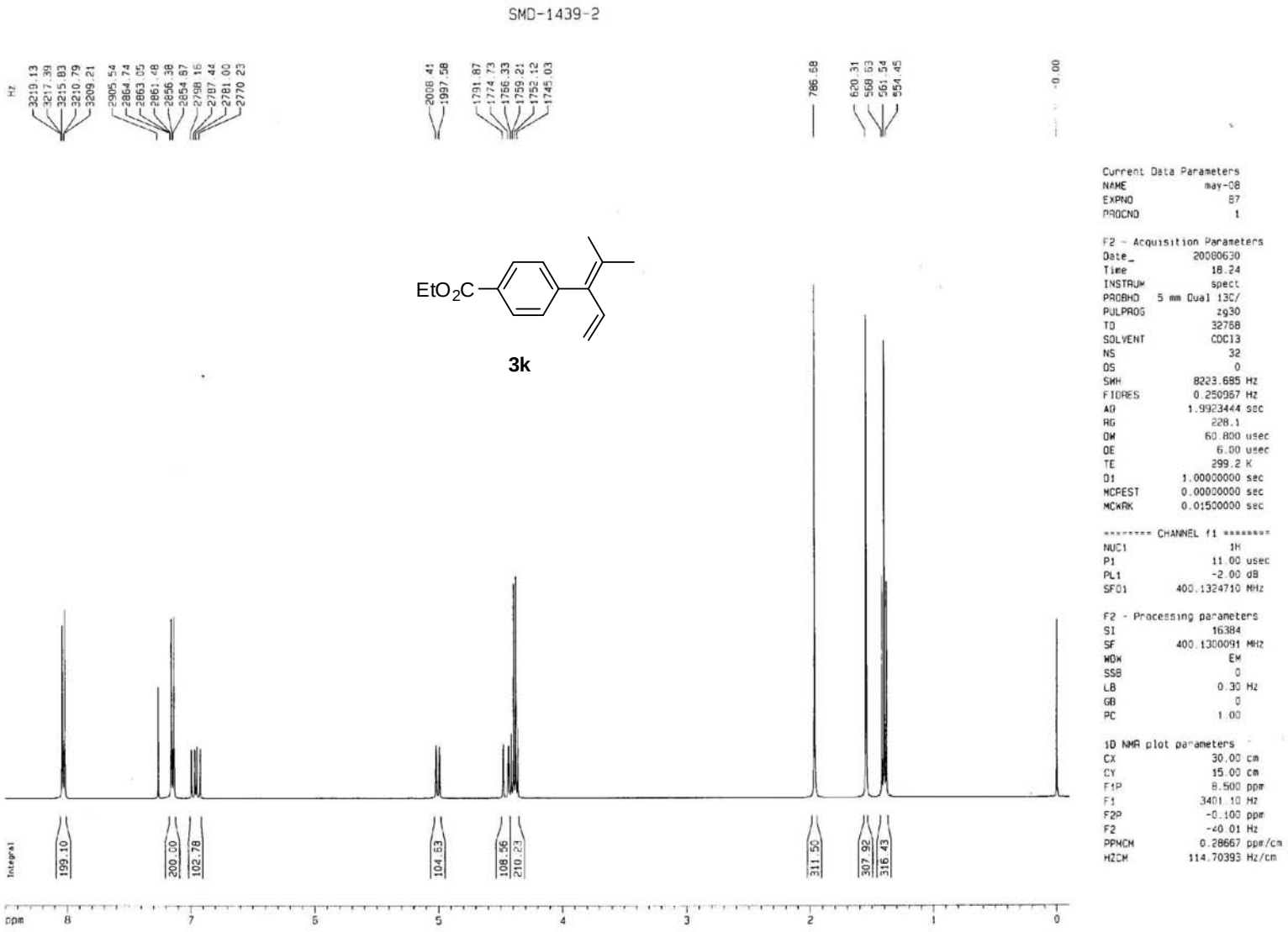
F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 15.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.28667 ppm/cm
HZCM 114.70393 Hz/cm

SMD-1336-1




```
Current Data Parameters
NAME                  oct-07
EXPNO                     48
PROCNO                     1

F2 - Acquisition Parameters
Date_               20071029
Time                   13.24
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zgpg30
TD                      65536
SOLVENT                CDCl3
NS                       1176
DS                          2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                    3649.1
DW                   15.700 usec
DE                    6.00 usec
TE                   296.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                 105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2              400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127290 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    45.00 cm
F1P                  205.000 ppm
F1                 20625.61 Hz
F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                 7.00000 ppm/cm
HZCM               704.28906 Hz/cm
```



Current Data Parameters
NAME may-08
EXPNO 87
PROCNO 1

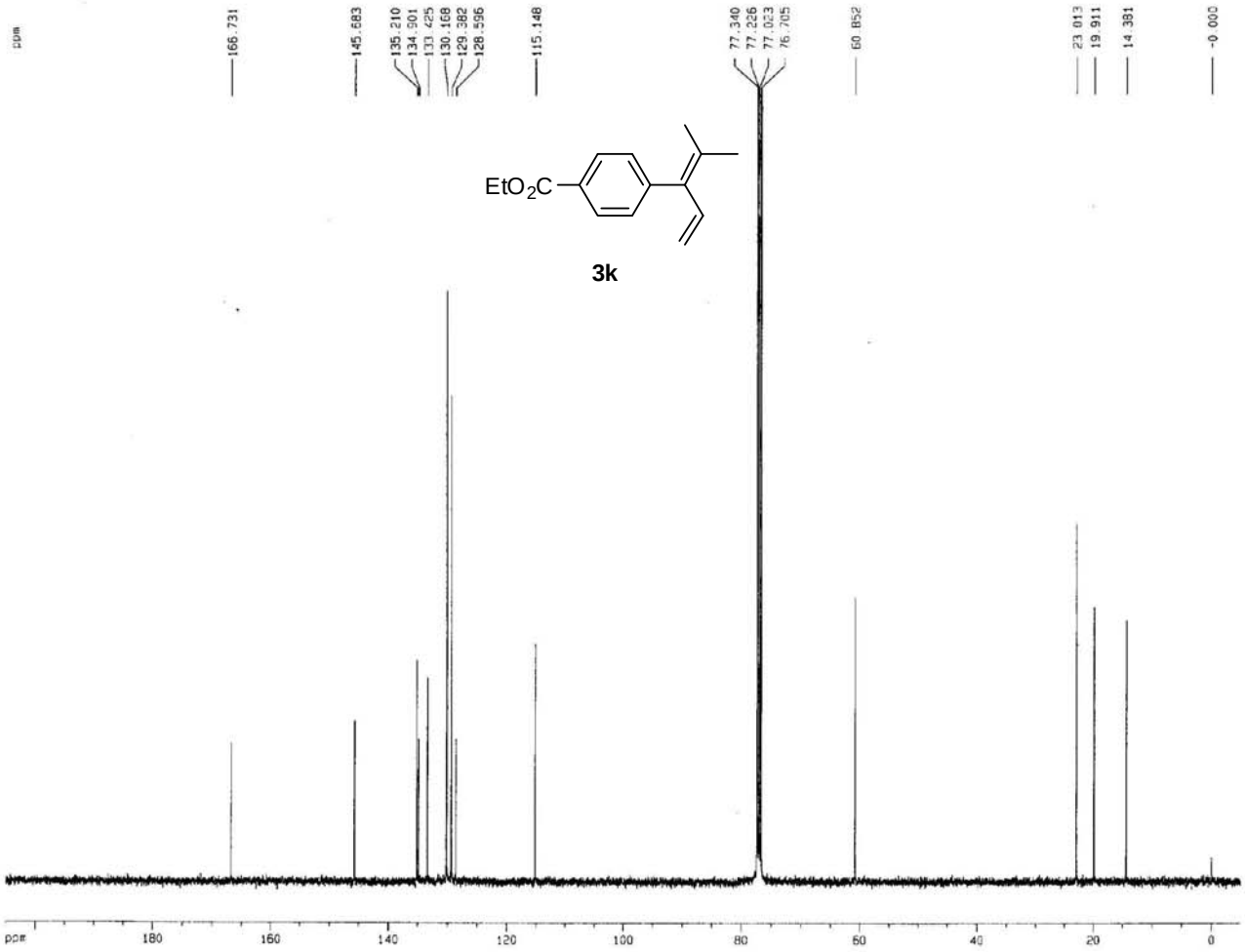
F2 - Acquisition Parameters
Date_ 20080630
Time 18.24
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250957 Hz
AQ 1.9923444 sec
RG 228.1
DW 60.800 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 15.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.28667 ppm/cm
HZCM 114.70393 Hz/cm

SMD-1439-2



Current Data Parameters
NAME may-08
EXPNO 86
PROCNO 1

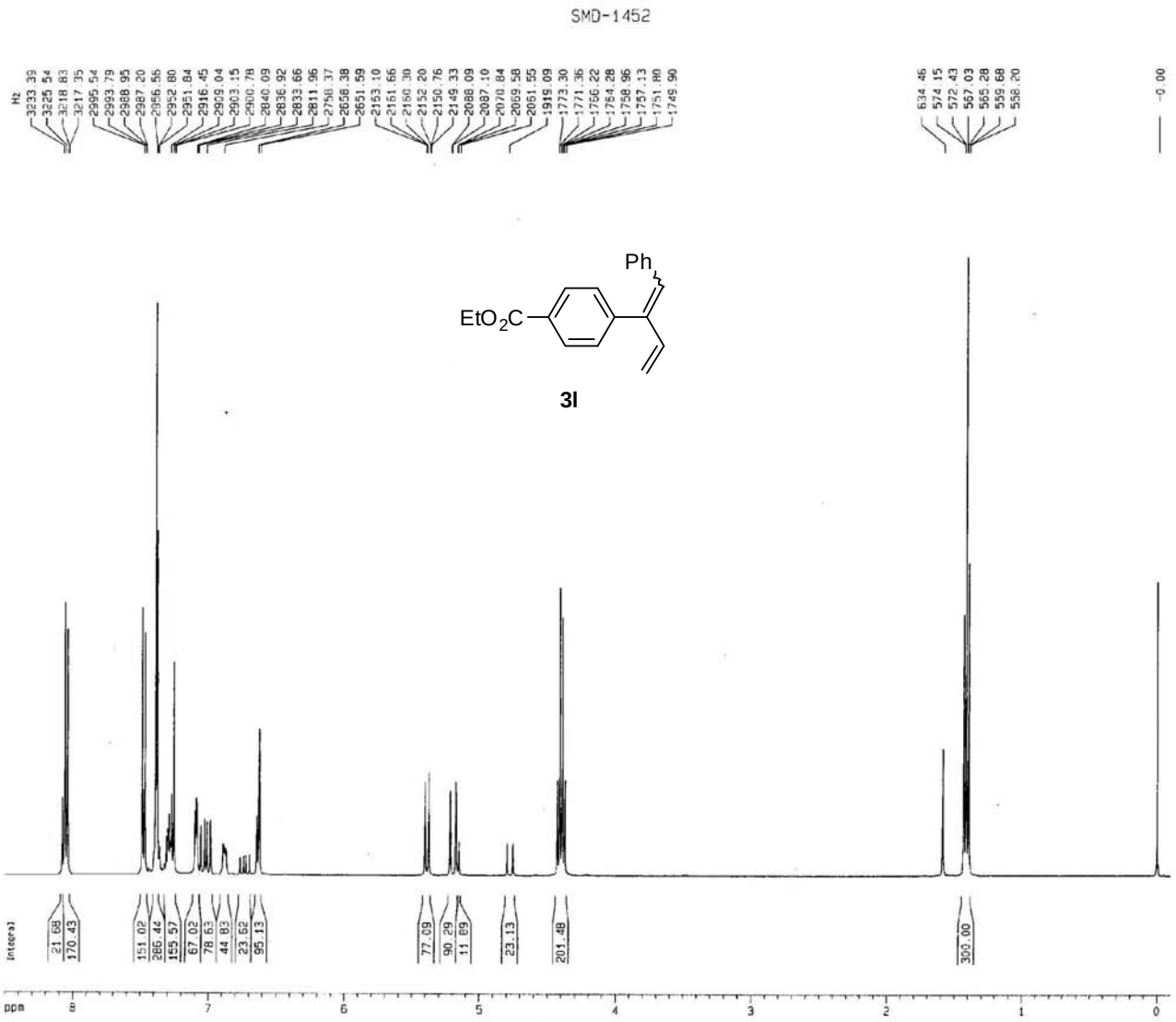
F2 - Acquisition Parameters
Date_ 20080630
Time 21.06
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 456.1
DW 15.700 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127687 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 30.00 cm
CY 30.00 cm
F1P 205.000 ppm
F1 20625.62 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28937 Hz/cm



Current Data Parameters

NAME	aug-08
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20080801
Time	8.59
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	8223.685 Hz
FIDRES	0.250957 Hz
AQ	1.9923444 sec
RG	203.2
DW	60.800 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	11.00 usec
PL1	-2.00 dB
SFO1	400.1324710 MHz

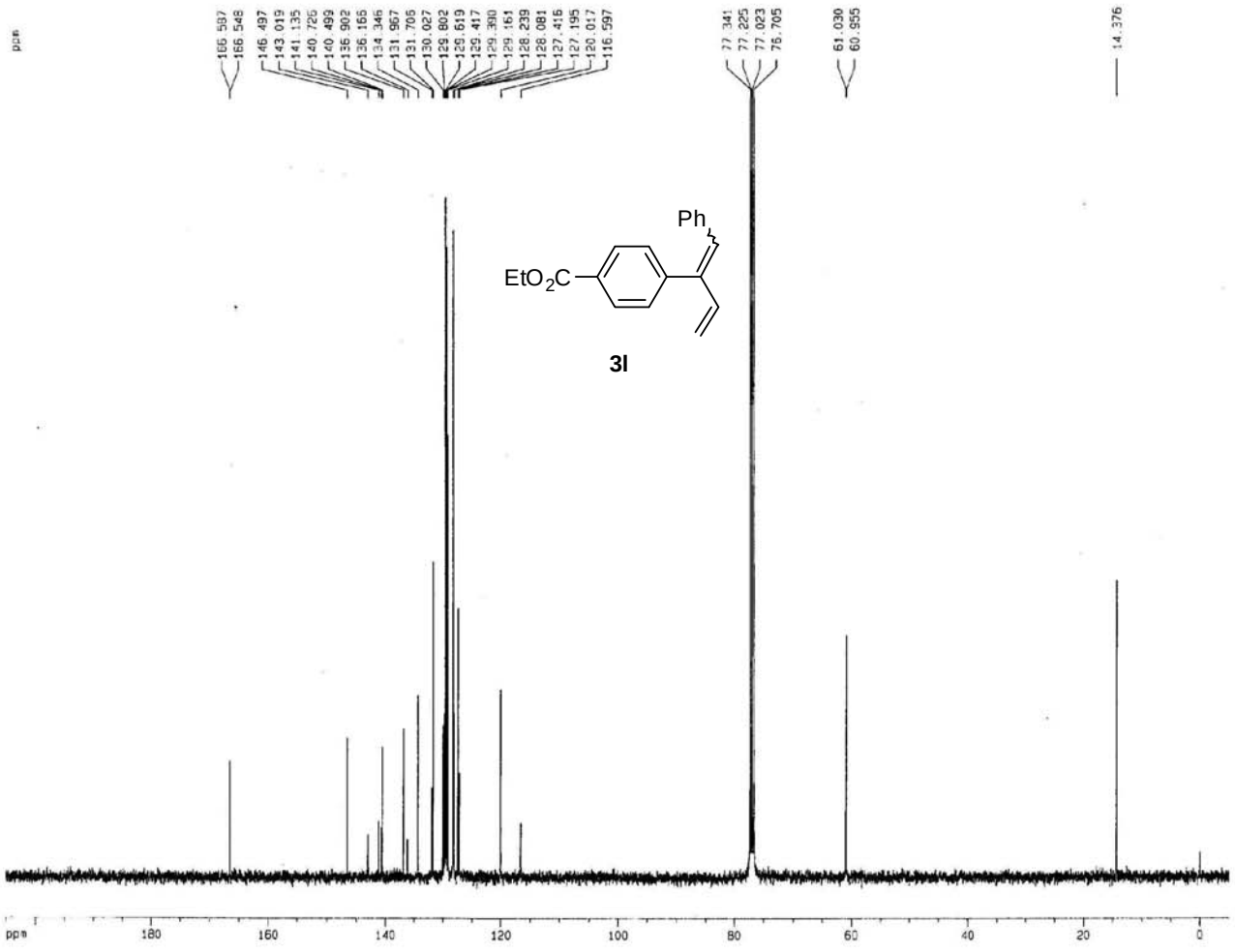
F2 - Processing parameters

SI	16384
SF	400.1300115 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

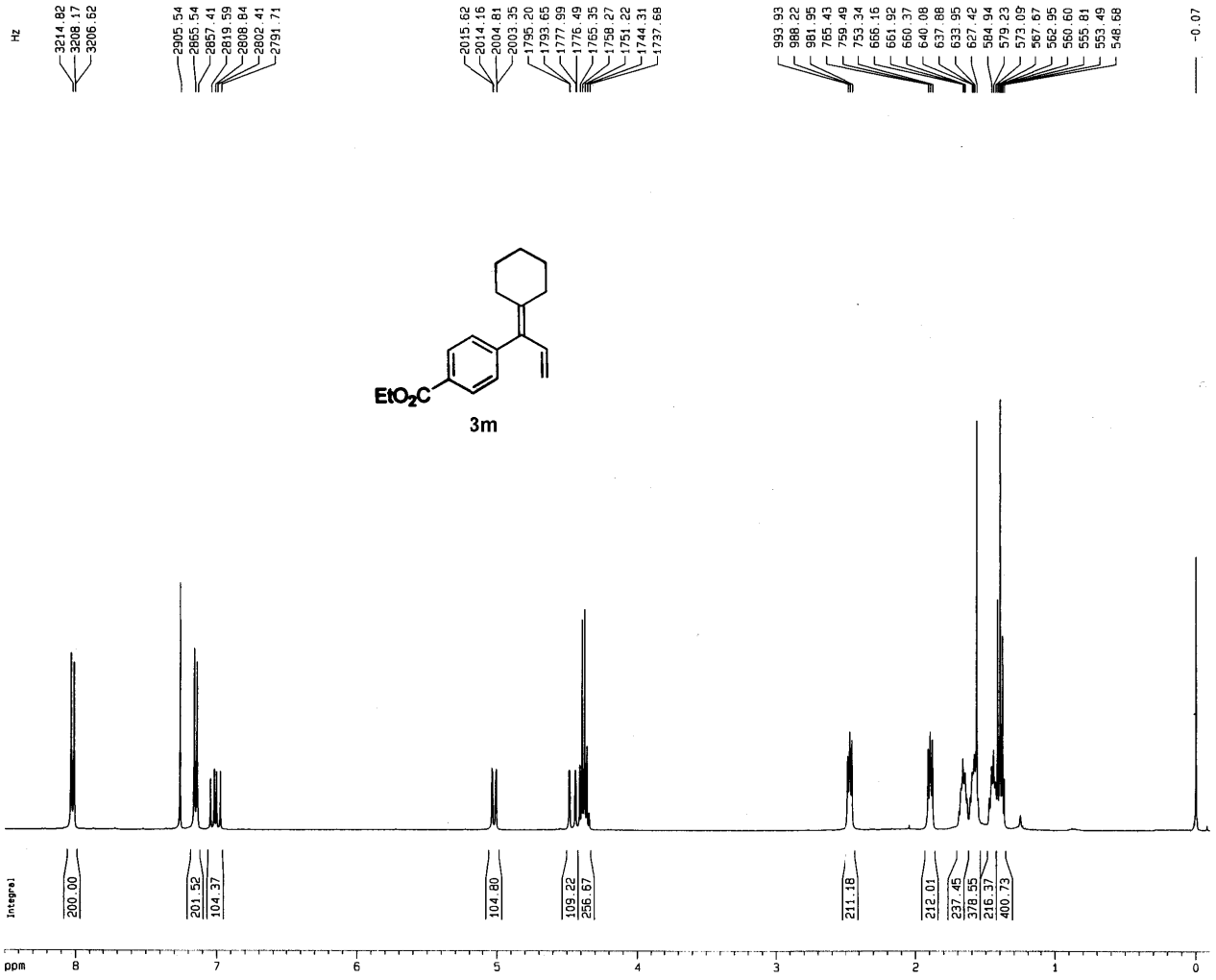
CX	30.00 cm
CY	16.00 cm
F1P	8.500 ppm
F1	3401.10 Hz
F2P	-0.100 ppm
F2	-40.01 Hz
PPMCM	0.28667 ppm/cm
HZCM	114.70393 Hz/cm

SMD-1452




```
Current Data Parameters
NAME                  aug-08
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080801
Time                   9.55
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        2
SWH               31847.133 Hz
FIDRES            0.485949 Hz
AQ                1.0289652 sec
RG                    101.6
DW                   15.700 usec
DE                    6.00 usec
TE                   297.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1           100.6254356 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2           400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF             100.6127705 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    34.00 cm
F1P                  205.000 ppm
F1                 20625.62 Hz
F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                 7.00000 ppm/cm
HZCM               704.28937 Hz/cm
```

SMD-1488-2



Current Data Parameters
NAME sep-08
EXPNO 95
PROCNO 1

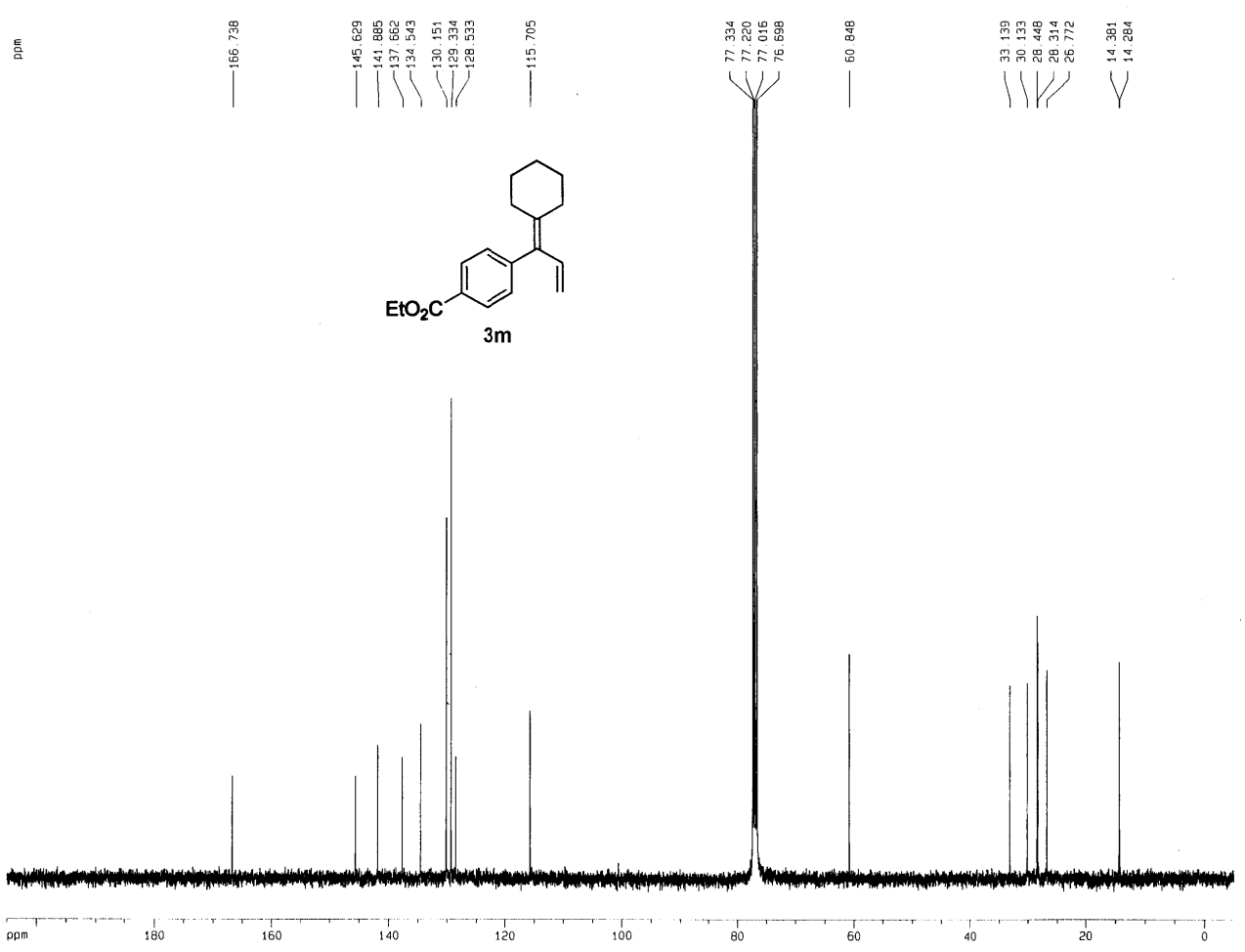
F2 - Acquisition Parameters
Date_ 20081022
Time 9.53
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 287.4
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

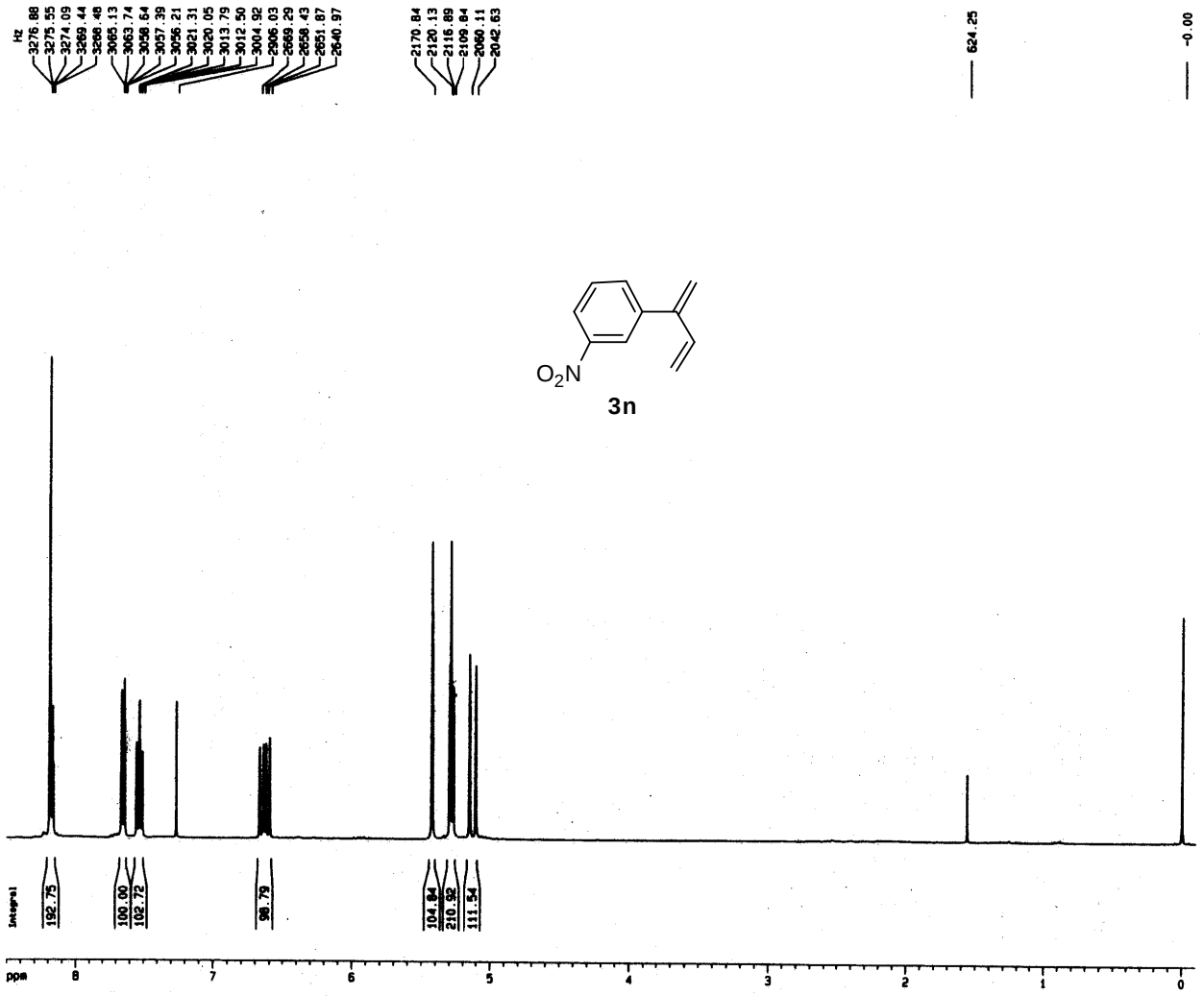
1D NMR plot parameters
CX 30.00 cm
CY 30.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.28667 ppm/cm
HZCM 114.70393 Hz/cm

SMD-1488-2




```
Current Data Parameters
NAME                  sep-08
EXPNO                     96
PROCNO                     1

F2 - Acquisition Parameters
Date_               20081022
Time                   10.11
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       4542
DS                          2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                        256
DW                   15.700 usec
DE                    6.00 usec
TE                    296.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                    10.50 usec
PL1                   -1.00 dB
SF01              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                105.00 usec
PL2                   -2.00 dB
PL12                  18.00 dB
PL13                  20.00 dB
SF02              400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127700 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    67.00 cm
F1P                  205.000 ppm
F1                 20625.62 Hz
F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.00000 ppm/cm
HZCM               704.28937 Hz/cm
```

SMD-1373



Current Data Parameters
NAME dec-07
EXPNO 1
PROCNO 1

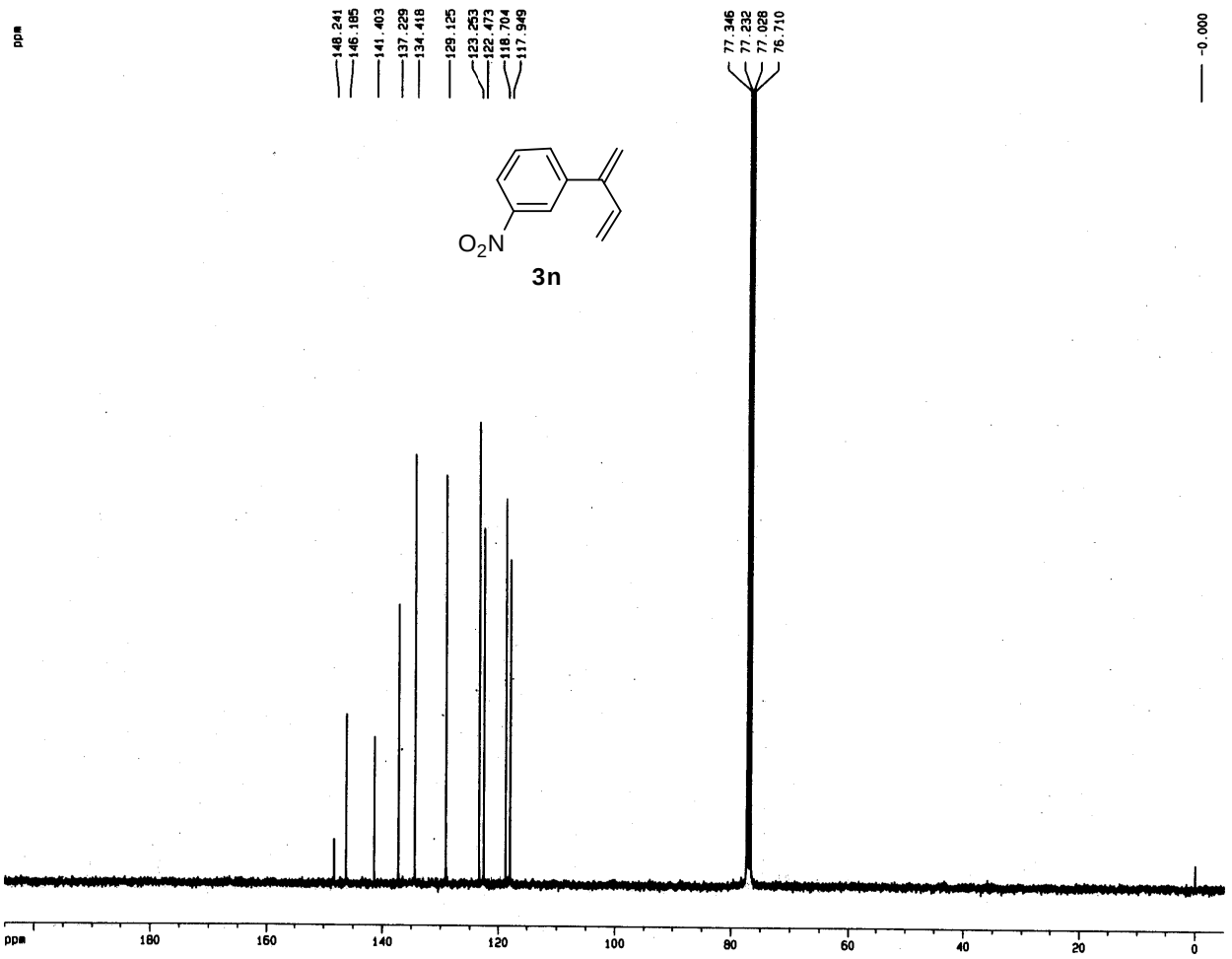
F2 - Acquisition Parameters
Date_ 20071203
Time 11.13
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250867 Hz
AQ 1.9923444 sec
RG 203.2
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

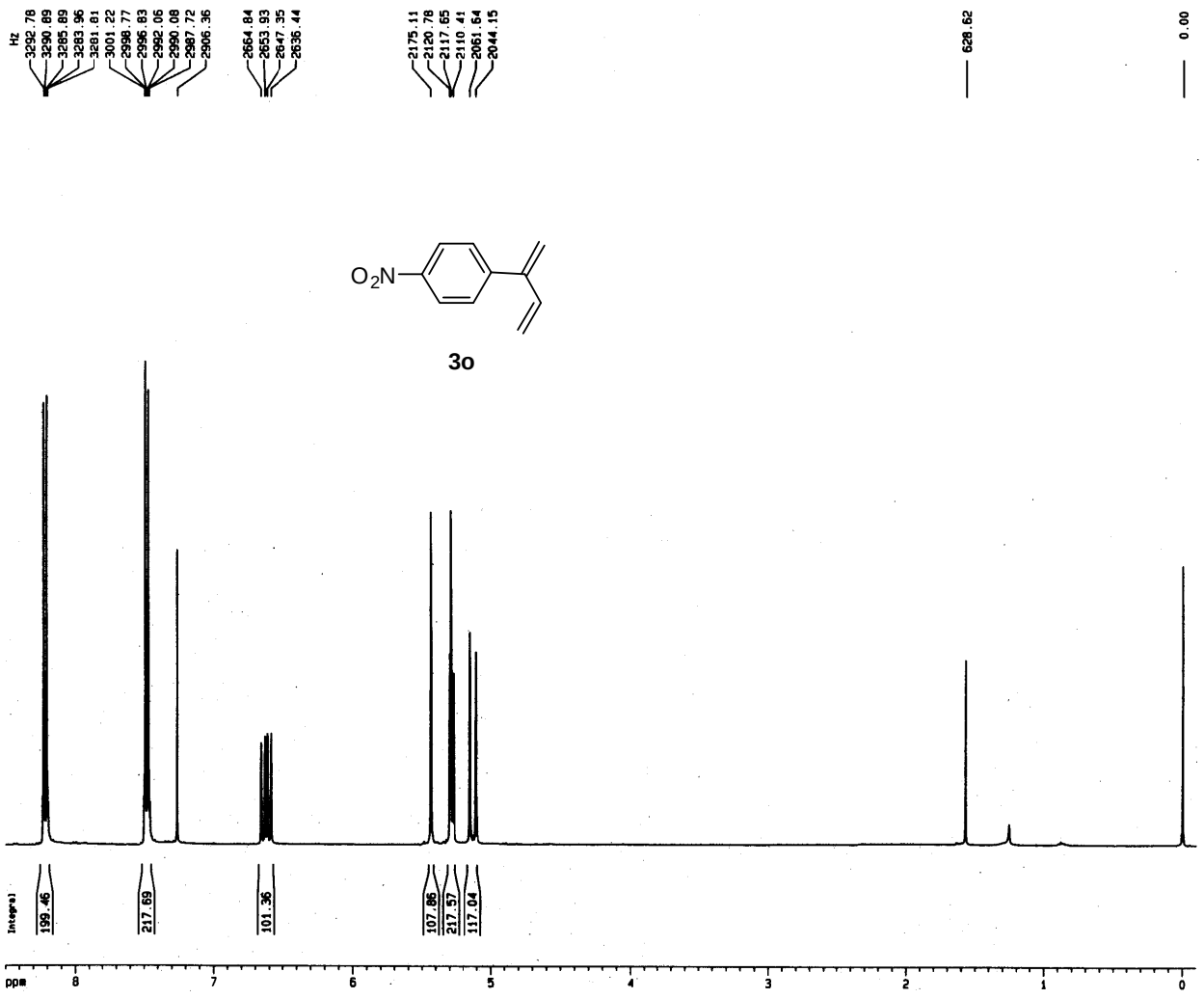
1D NMR plot parameters
CX 30.00 cm
CY 12.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.28667 ppm/cm
HZCM 114.70393 Hz/cm

SMD-1373



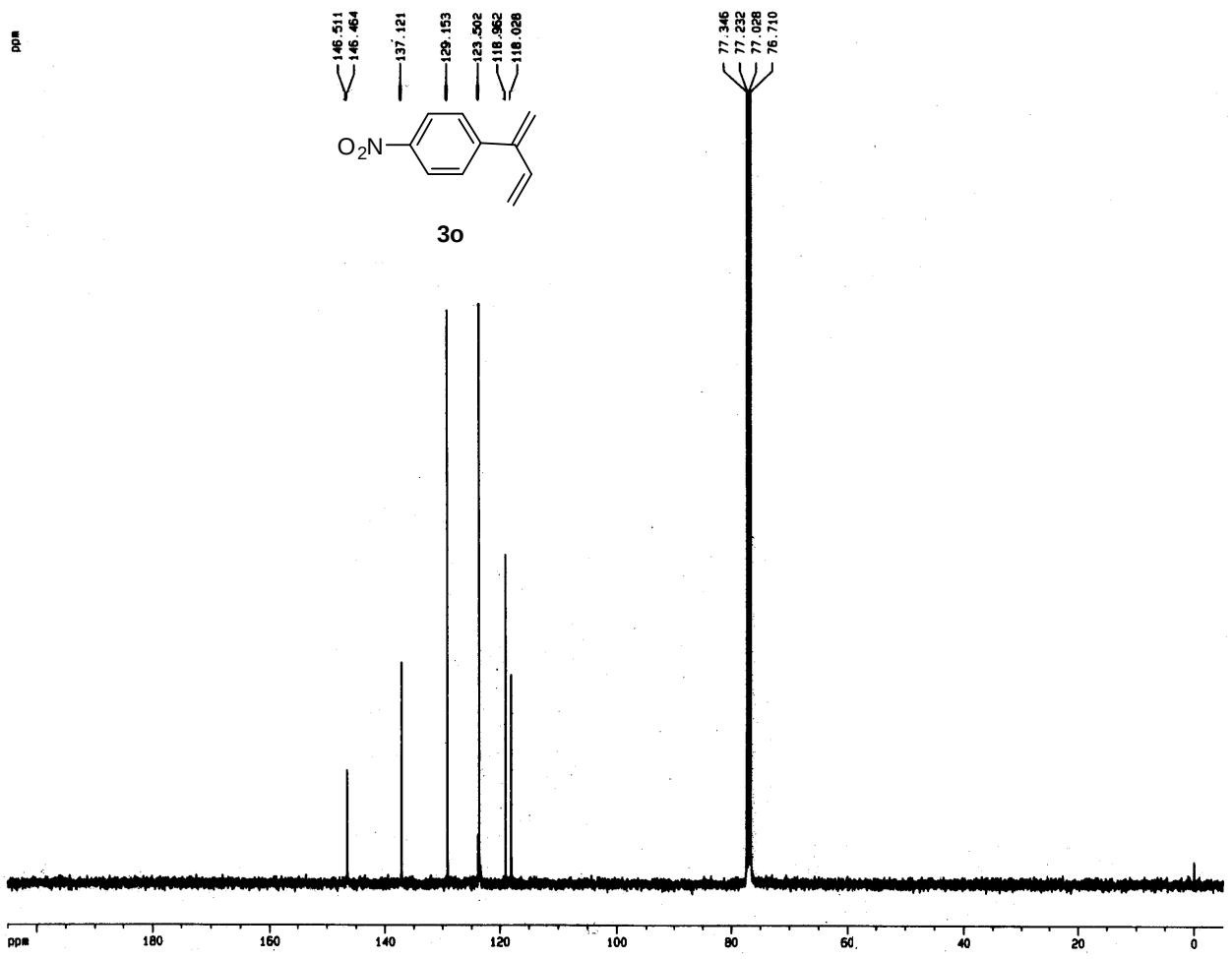

```
Current Data Parameters
NAME                  dec-07
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20071203
Time                  12.10
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      2048
DS                         2
SWH               31847.133 Hz
FIDRES            0.485949 Hz
AQ                1.0289652 sec
RG                       512
DW                  15.700 usec
DE                   6.00 usec
TE                   296.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                   10.50 usec
PL1                   -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                105.00 usec
PL2                   -2.00 dB
PL12                  18.00 dB
PL13                  20.00 dB
SFO2             400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127697 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    24.00 cm
F1P                  205.000 ppm
F1                  20625.62 Hz
F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.00000 ppm/cm
HZCM                704.28937 Hz/cm
```

SMD-1340



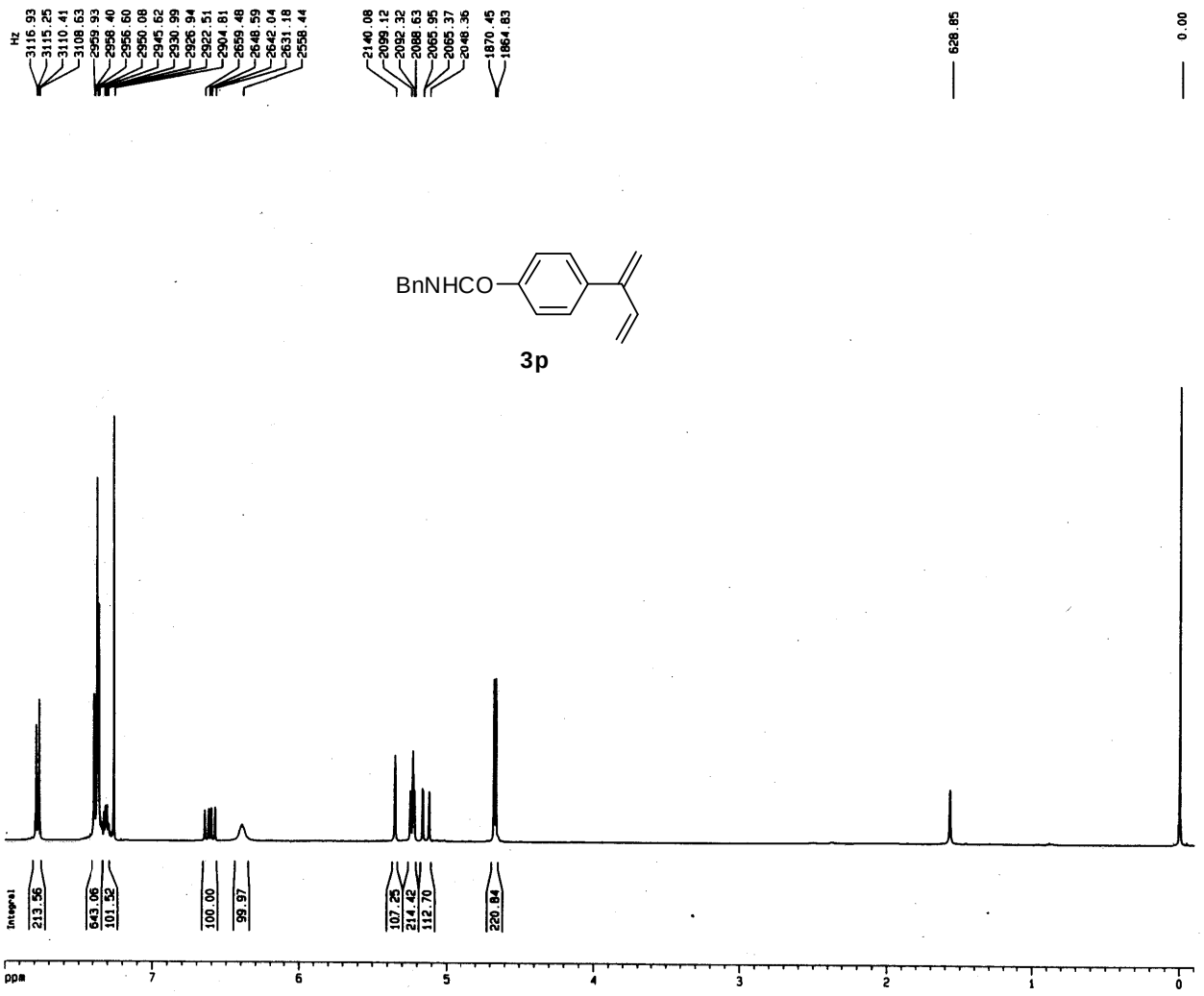

```
Current Data Parameters
NAME                  oct-07
EXPNO                     57
PROCNO                     1

F2 - Acquisition Parameters
Date_               20071031
Time                   12.06
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        0
SWH                8223.685 Hz
FIDRES             0.250967 Hz
AQ                 1.9923444 sec
RG                      256
DW                   60.800 usec
DE                    6.00 usec
TE                   296.2 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.00 usec
PL1                    -2.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF                400.1300083 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     30.00 cm
CY                     12.00 cm
F1P                     8.500 ppm
F1                   3401.10 Hz
F2P                    -0.100 ppm
F2                     -40.01 Hz
PPMCM                0.28667 ppm/cm
HZCM               114.70393 Hz/cm
```

SMD-1340



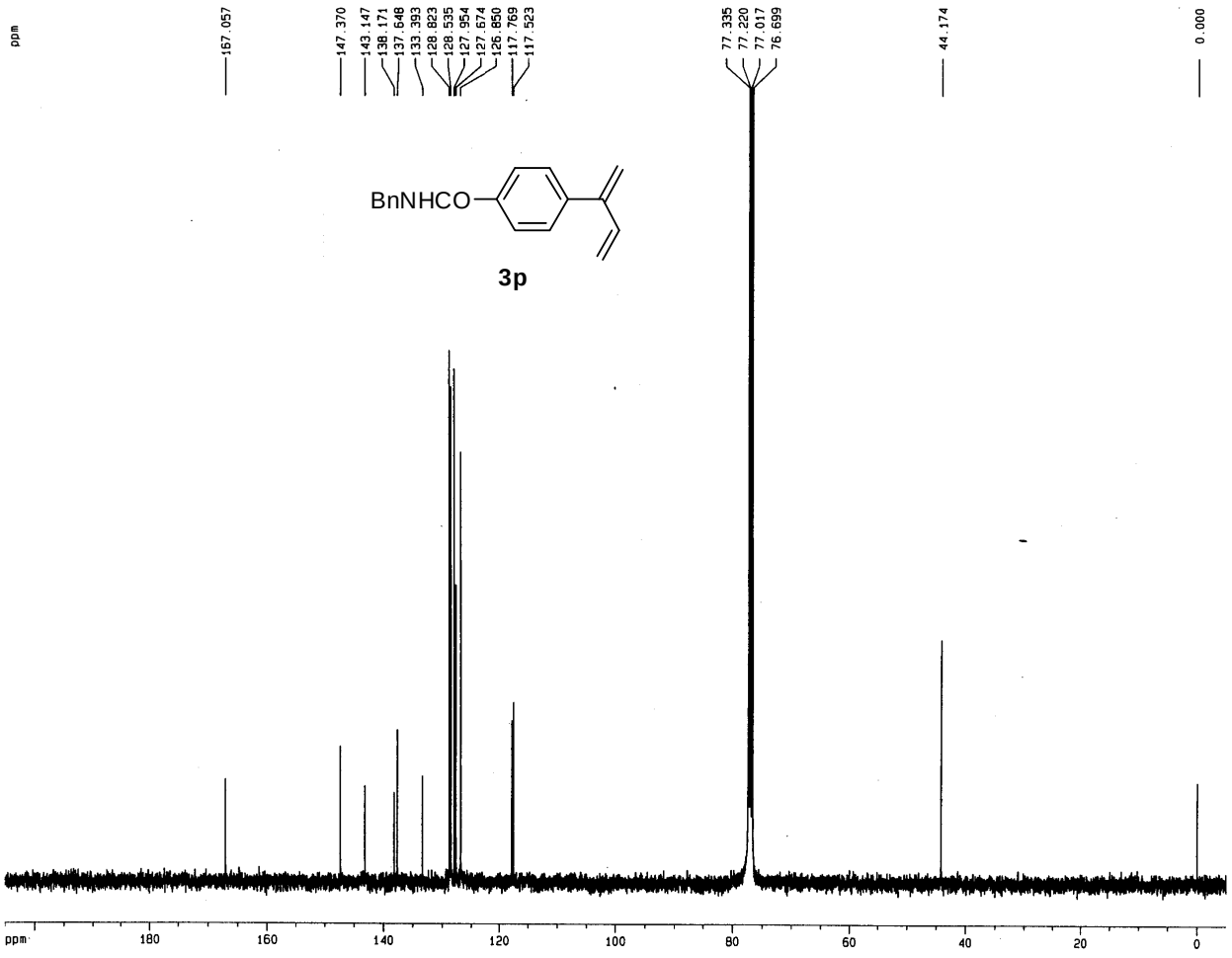

```
Current Data Parameters
NAME                  oct-07
EXPNO                     58
PROCNO                     1

F2 - Acquisition Parameters
Date_              20071031
Time                  13.21
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG               zgpg30
TD                     65536
SOLVENT               CDCl3
NS                      1427
DS                         2
SWH               31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                     228.1
DW                  15.700 usec
DE                   6.00 usec
TE                   296.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                   10.50 usec
PL1                  -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2               105.00 usec
PL2                  -2.00 dB
PL12                 18.00 dB
PL13                 20.00 dB
SFO2             400.1324708 MHz

F2 - Processing parameters
SI                      32768
SF               100.6127699 MHz
WDW                        EM
SSB                         0
LB                   1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                   30.00 cm
CY                   26.00 cm
F1P                 205.000 ppm
F1                20625.62 Hz
F2P                  -5.000 ppm
F2                 -503.06 Hz
PPMCM                7.00000 ppm/cm
HZCM               704.28937 Hz/cm
```

SMD-1388




```
Current Data Parameters
NAME                  dec-07
EXPNO                    127
PROCNO                     1

F2 - Acquisition Parameters
Date_              20071229
Time                  15.14
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        0
SWH                8223.685 Hz
FIDRES             0.250967 Hz
AQ                 1.9923444 sec
RG                      362
DW                   60.800 usec
DE                    6.00 usec
TE                   296.2 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.00 usec
PL1                    -2.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF                400.1300098 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00

1D NMR plot parameters
CX                    30.00 cm
CY                    12.00 cm
F1P                    8.000 ppm
F1                  3201.04 Hz
F2P                   -0.100 ppm
F2                   -40.01 Hz
PPMCM                 0.27000 ppm/cm
HZCM                108.03510 Hz/cm
```

SMD-1388



Current Data Parameters
NAME dec-07
EXPNO 128
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071229
Time 21.25
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7168
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 322.5
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

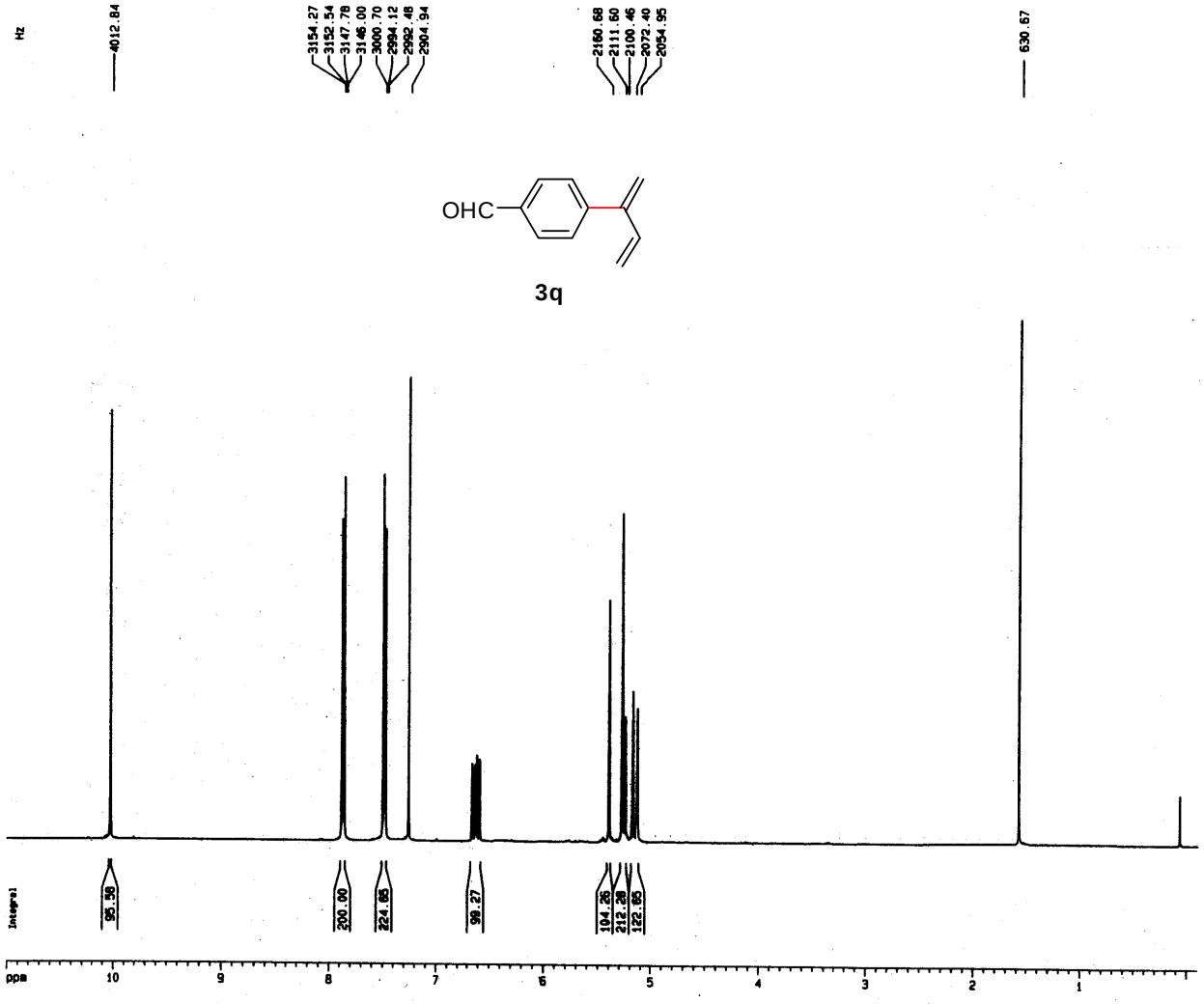
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127699 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 30.00 cm
CY 89.00 cm
F1P 205.000 ppm
F1 20625.62 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28937 Hz/cm

SMD-1341-1



Current Data Parameters
NAME oct-07
EXPNO 41
PROCNO 1

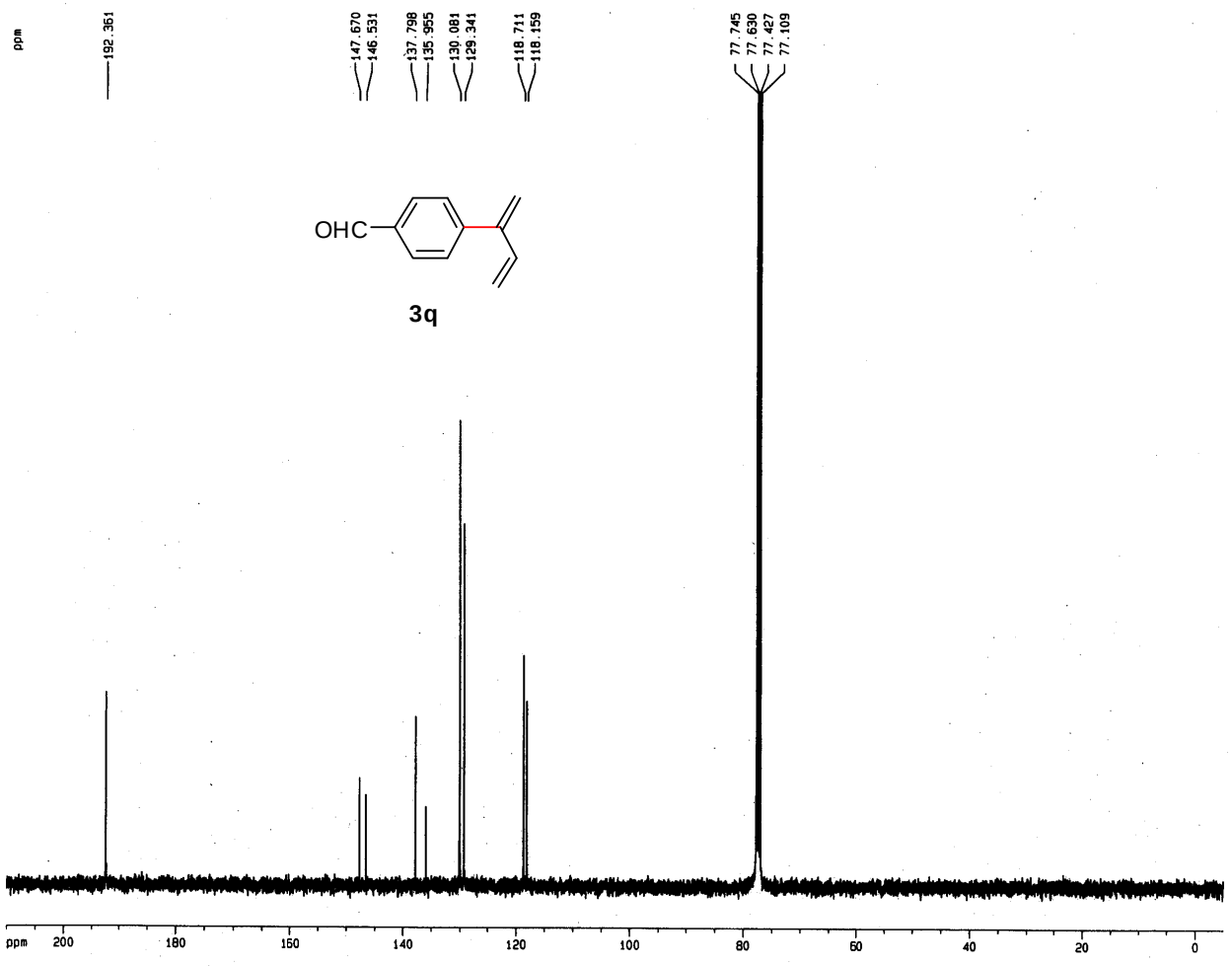
F2 - Acquisition Parameters
Date_ 20071026
TIME 13.28
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 322.5
DW 60.800 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

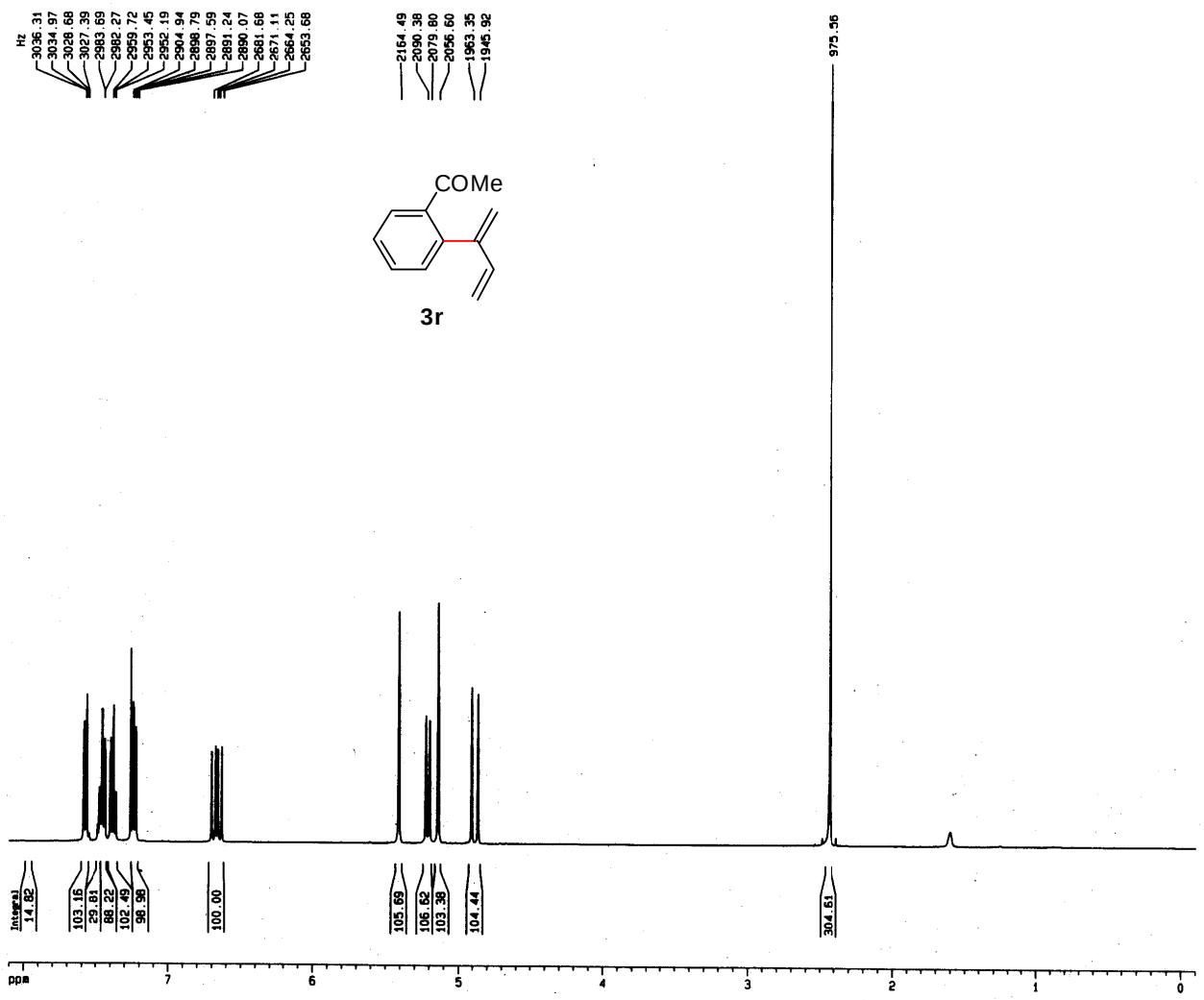
1D NMR plot parameters
CX 30.00 cm
CY 13.00 cm
F1P 11.000 ppm
F1 4401.43 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.37000 ppm/cm
HZCM 148.04810 Hz/cm

SMD-1341-1




```
Current Data Parameters
NAME                  oct-07
EXPNO                     42
PROCNO                     1

F2 - Acquisition Parameters
Date_              20071026
Time                  13.36
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2048
DS                        2
SWH              31847.133 Hz
FIDRES            0.485949 Hz
AQ                1.0289652 sec
RG                   3649.1
DW                  15.700 usec
DE                   6.00 usec
TE                  297.2 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                   10.50 usec
PL1                  -1.00 dB
SFO1            100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               105.00 usec
PL2                  -2.00 dB
PL12                 18.00 dB
PL13                 20.00 dB
SFO2            400.1324708 MHz

F2 - Processing parameters
SI                      32768
SF              100.6127290 MHz
WDW                        EM
SSB                         0
LB                   1.00 Hz
GB                          0
PC                   1.40

1D NMR plot parameters
CX                   30.00 cm
CY                   45.00 cm
F1P                 210.000 ppm
F1                21128.67 Hz
F2P                 -5.000 ppm
F2                -503.06 Hz
PPMCM              7.16667 ppm/cm
HZCM             721.05786 Hz/cm
```

SMD-1338



Current Data Parameters
NAME oct-07
EXPNO 39
PROCNO 1

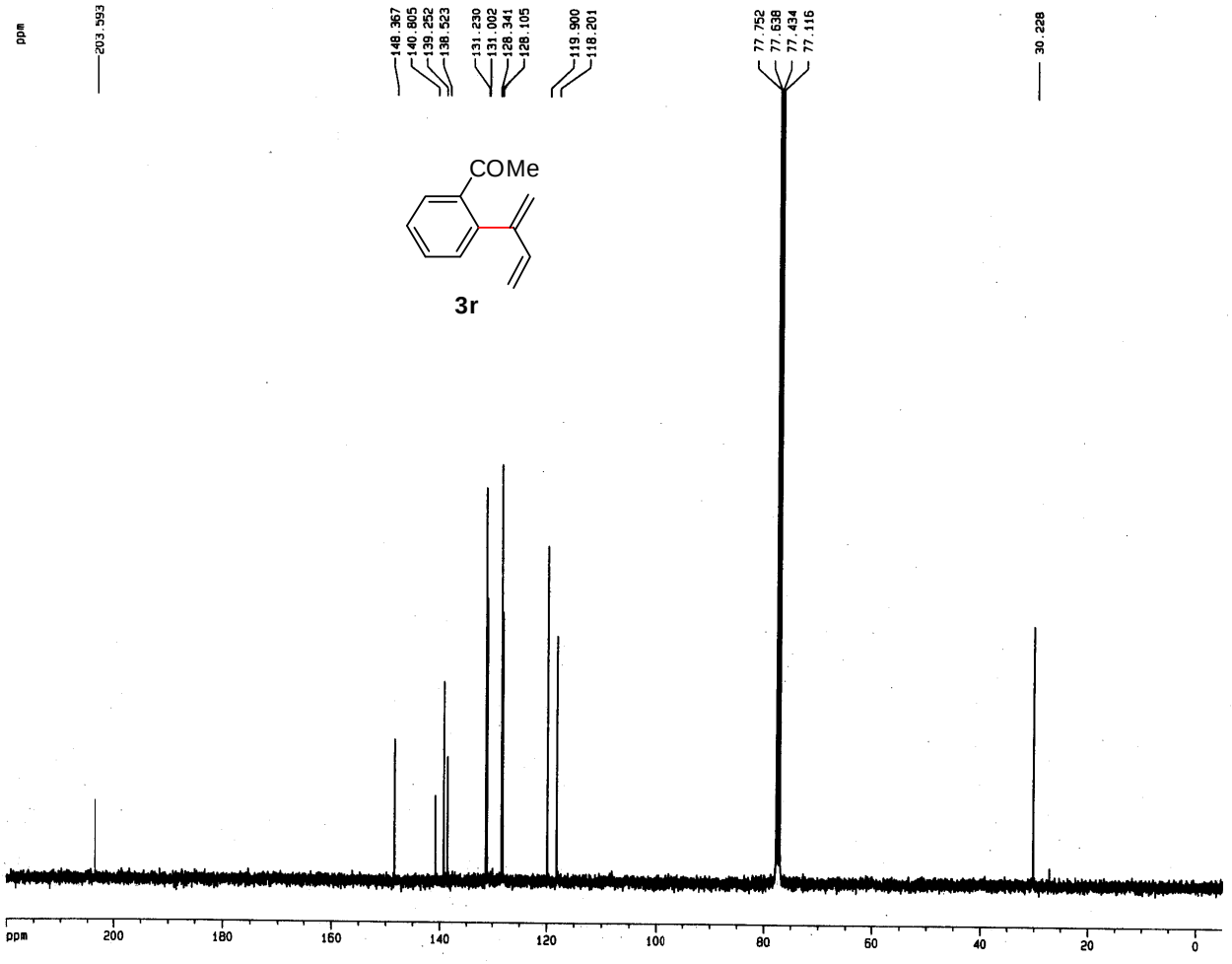
F2 - Acquisition Parameters
Date_ 20071026
Time 12.23
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 256
DW 60.800 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

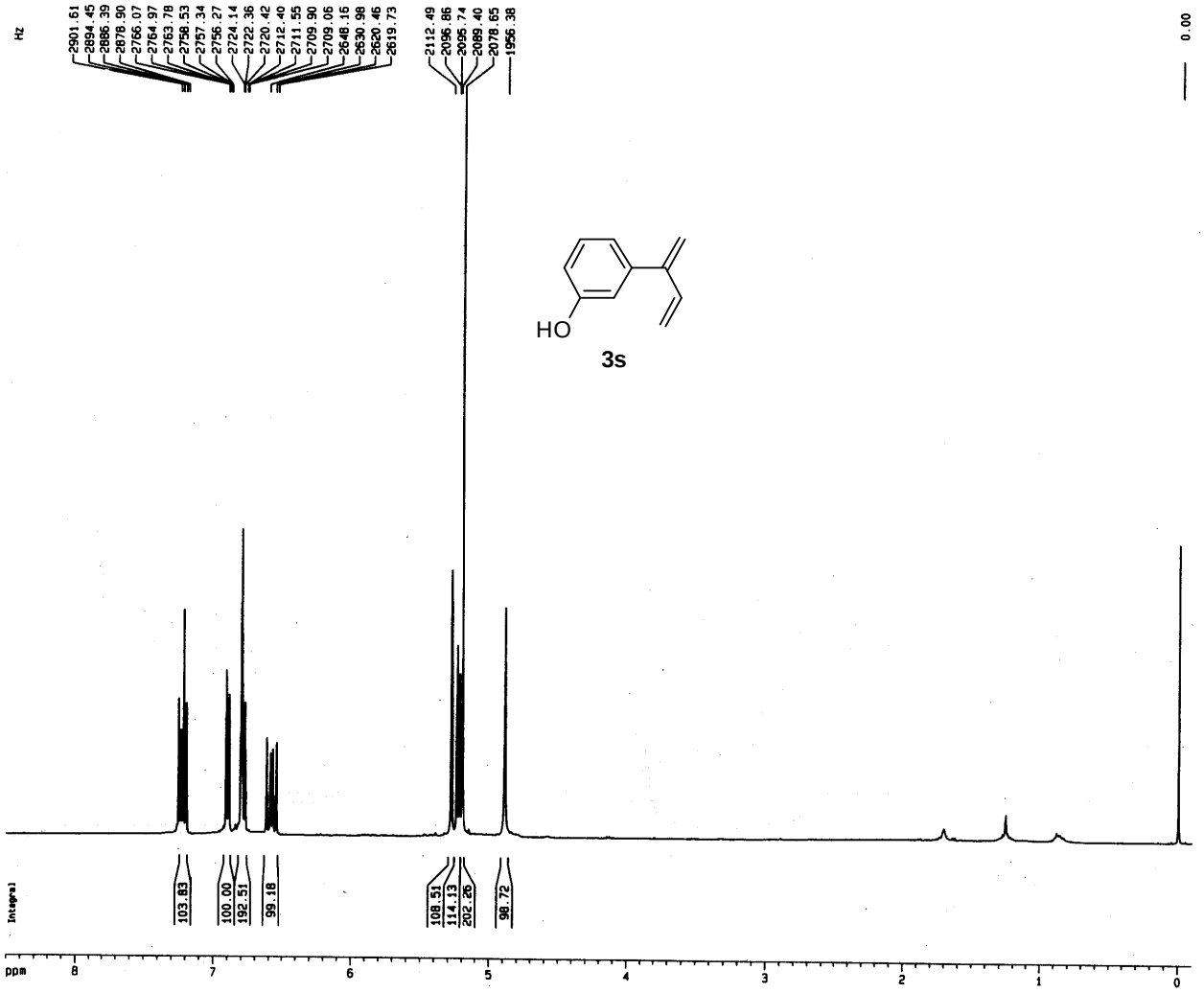
1D NMR plot parameters
CX 30.00 cm
CY 45.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36887 Hz/cm

SMD-1338



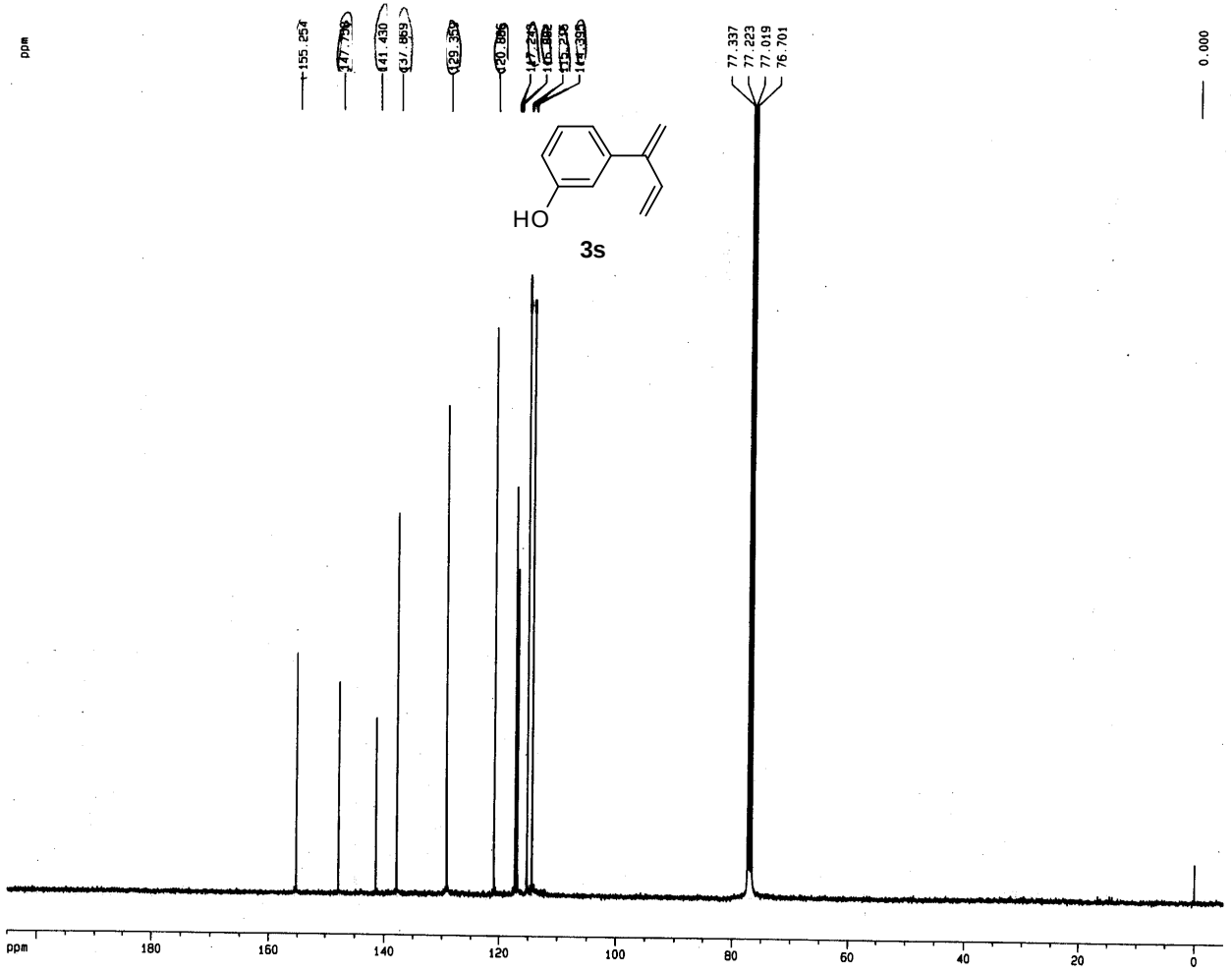

```
Current Data Parameters
NAME                  oct-07
EXPNO                     40
PROCNO                     1

F2 - Acquisition Parameters
Date_               20071026
Time                   13.13
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zgpg30
TD                      65536
SOLVENT                CDCl3
NS                        953
DS                          2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                    3649.1
DW                   15.700 usec
DE                    6.00 usec
TE                    297.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                 105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2              400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127290 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    25.00 cm
F1P                 220.000 ppm
F1                  22134.80 Hz
F2P                  -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.50000 ppm/cm
HZCM               754.59546 Hz/cm
```

SMD-1374



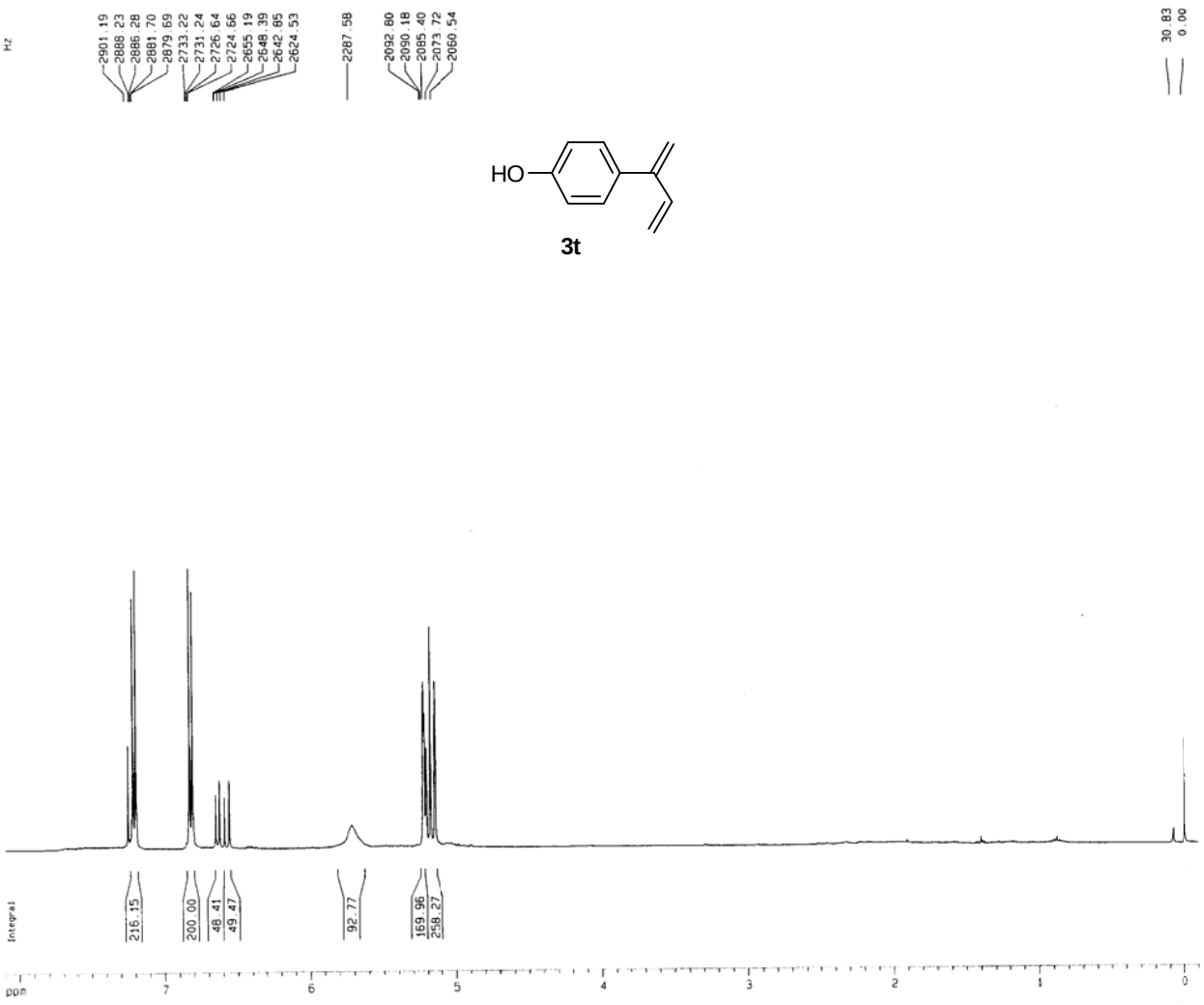

```
Current Data Parameters
NAME                  dec-07
EXPNO                      9
PROCNO                     1

F2 - Acquisition Parameters
Date_                20071204
Time                     9.44
INSTRUM                 spect
PROBHD   5 mm Dual 13C/
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        32
DS                         0
SWH                8223.685 Hz
FIDRES             0.250967 Hz
AQ                 1.9923444 sec
RG                       181
DW                    60.800 usec
DE                     6.00 usec
TE                    296.2 K
D1                 1.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    11.00 usec
PL1                   -2.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF               400.1300130 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                    30.00 cm
CY                    20.00 cm
F1P                    8.500 ppm
F1                  3401.10 Hz
F2P                   -0.100 ppm
F2                    -40.01 Hz
PPMCM                0.28667 ppm/cm
HZCM               114.70393 Hz/cm
```

SMD-1374




```
Current Data Parameters
NAME                  dec-07
EXPNO                     10
PROCNO                     1

F2 - Acquisition Parameters
Date_              20071204
Time                   9.13
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                     17639
DS                         2
SWH              31847.133 Hz
FIORES            0.485949 Hz
AQ                1.0289652 sec
RG                     406.4
DW                  15.700 usec
DE                   6.00 usec
TE                   296.2 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                   10.50 usec
PL1                  -1.00 dB
SFO1           100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2               105.00 usec
PL2                  -2.00 dB
PL12                 18.00 dB
PL13                 20.00 dB
SFO2           400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF             100.6127708 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                   30.00 cm
CY                   34.00 cm
F1P                205.000 ppm
F1                20625.62 Hz
F2P                 -5.000 ppm
F2                 -503.06 Hz
PPMCM              7.00000 ppm/cm
HZCM             704.28937 Hz/cm
```

YHS-410



Current Data Parameters
NAME sep-08
EXPNO 23
PROCNO 1

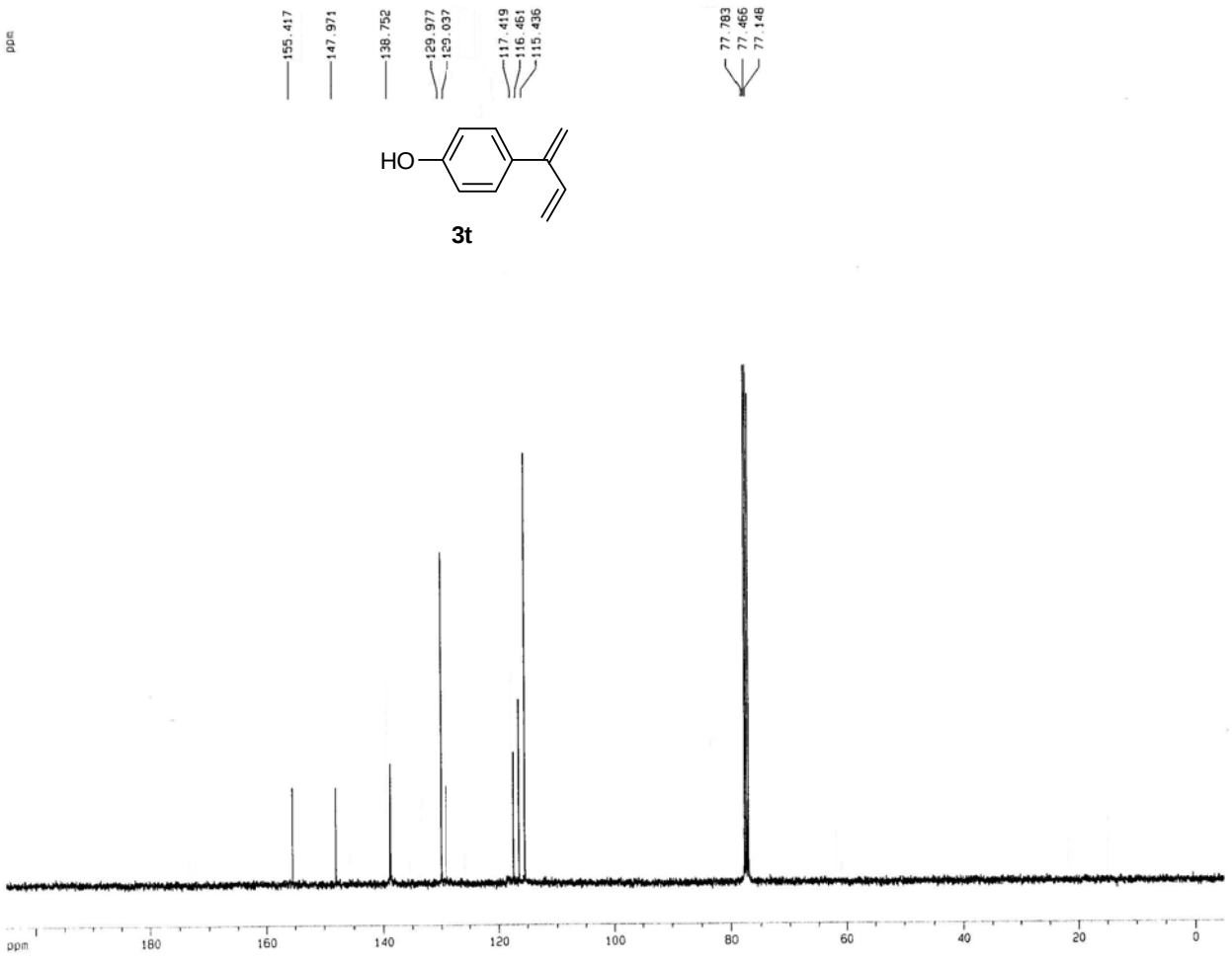
F2 - Acquisition Parameters
Date_ 20080910
Time 10.40
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 128
DW 60.800 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

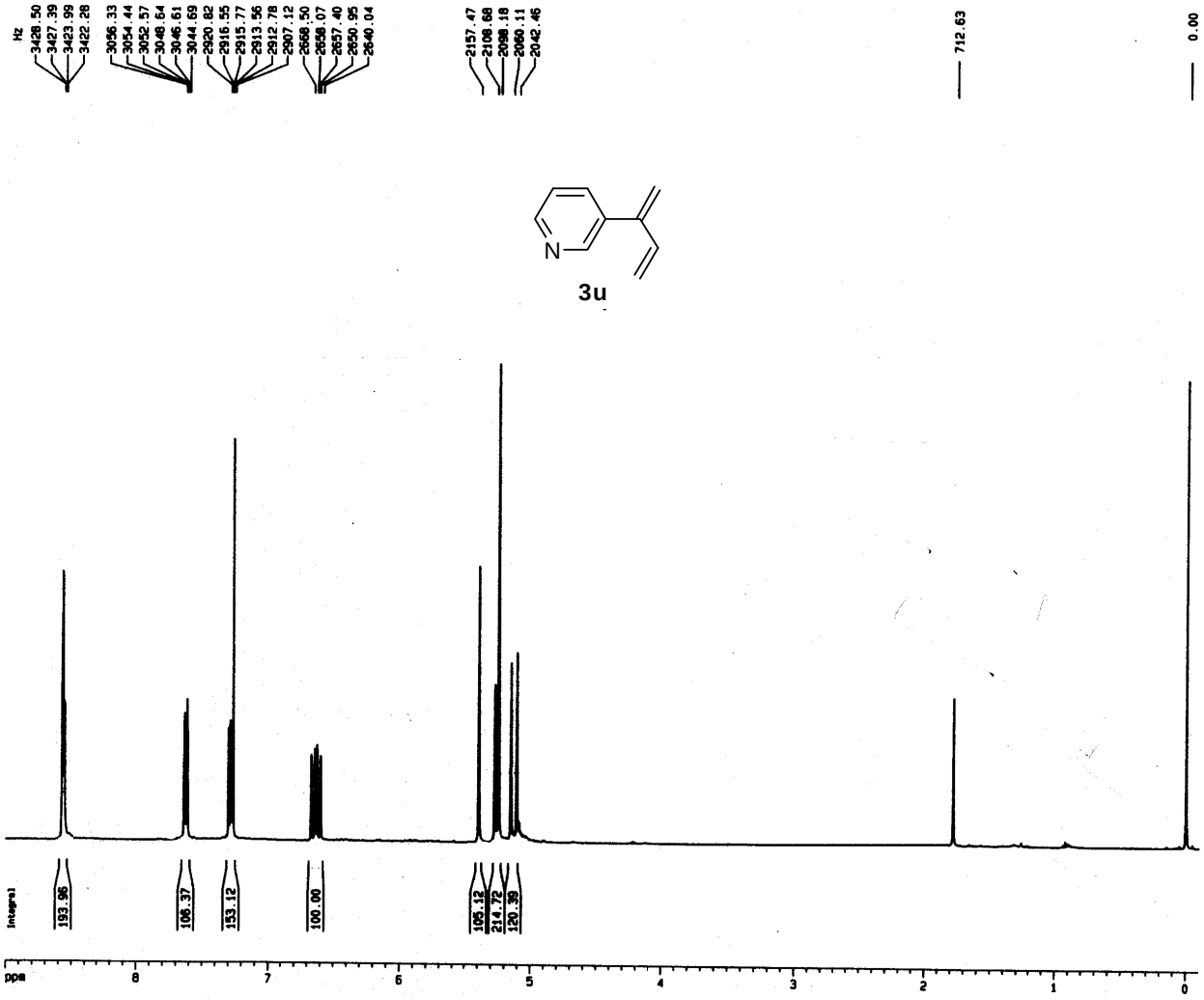
1D NMR plot parameters
CX 30.00 cm
CY 12.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36887 Hz/cm

YHS-410




```
Current Data Parameters
NAME                  sep-08
EXPNO                     24
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080910
Time                   11.00
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zgpg30
TD                      65536
SOLVENT                CDCl3
NS                        817
DS                          2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                    3649.1
DW                   15.700 usec
DE                    6.00 usec
TE                   298.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1               100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2               400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127290 MHz
WDW                          EM
SSB                           0
LB                       1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                       30.00 cm
CY                       15.00 cm
F1P                     205.000 ppm
F1                    20625.61 Hz
F2P                      -5.000 ppm
F2                     -503.06 Hz
PPMCM                  7.00000 ppm/cm
HZCM                 704.26906 Hz/cm
```

SMD-1387



Current Data Parameters
NAME dec-07
EXPNO 125
PROCNO 1

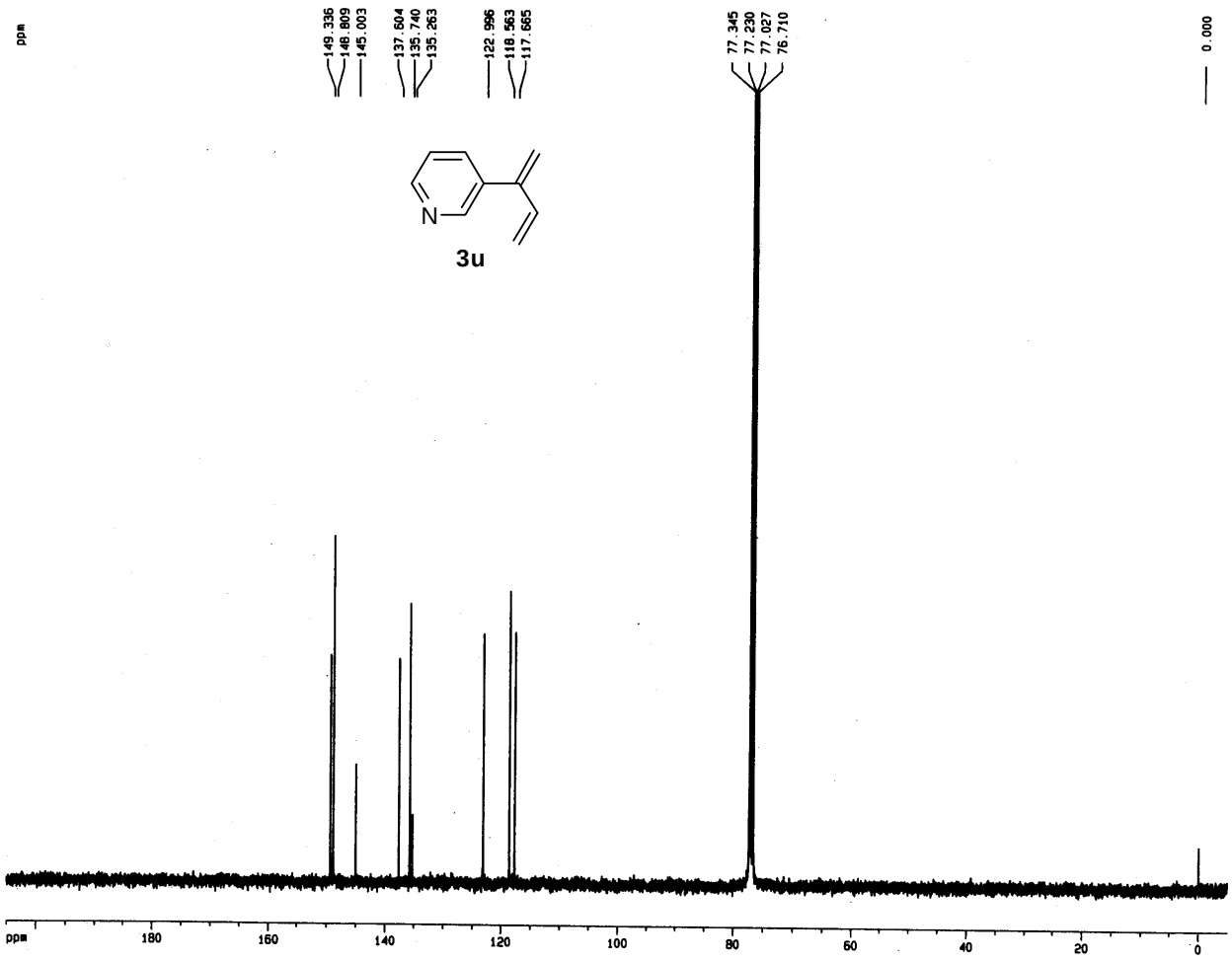
F2 - Acquisition Parameters
Date_ 20071229
Time 13.13
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 287.4
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

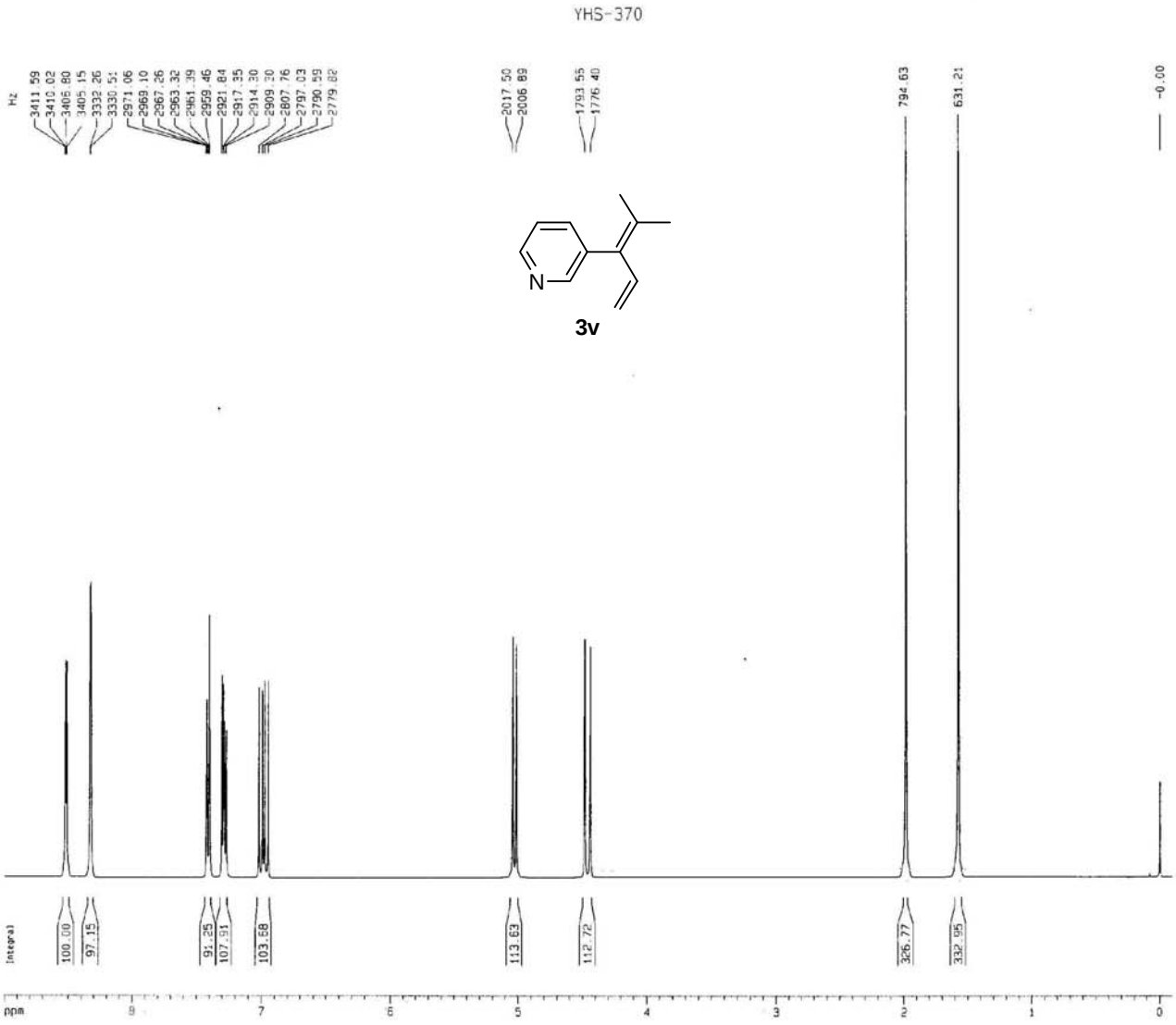
F2 - Processing parameters
SI 16384
SF 400.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 12.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.30333 ppm/cm
HZCM 121.37276 Hz/cm

SMD-1387




```
Current Data Parameters
NAME                  dec-07
EXPNO                    126
PROCNO                     1

F2 - Acquisition Parameters
Date_                20071229
Time                    14.17
INSTRUM                 spect
PROBHD   5 mm Dual 13C/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       2048
DS                          2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                      574.7
DW                     15.700 usec
DE                      6.00 usec
TE                      296.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SF01               100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SF02               400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127691 MHz
WDW                          EM
SSB                           0
LB                       1.00 Hz
GB                            0
PC                         1.40

1D NMR plot parameters
CX                       30.00 cm
CY                       35.00 cm
F1P                     205.000 ppm
F1                     20625.62 Hz
F2P                      -5.000 ppm
F2                     -503.06 Hz
PPMCM                  7.00000 ppm/cm
HZCM                 704.28937 Hz/cm
```



Current Data Parameters
NAME jul-08
EXPNO 117
PROCNO 1

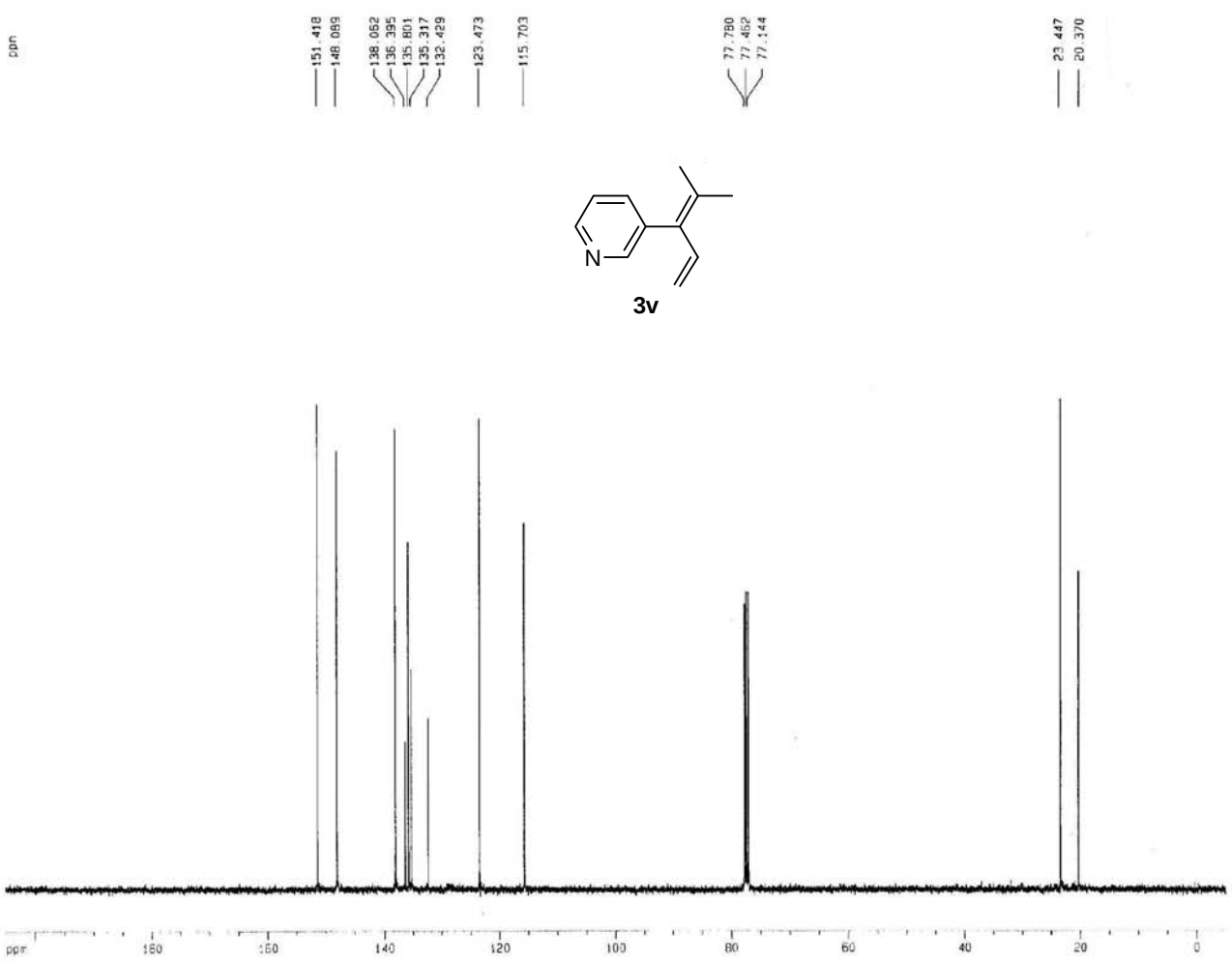
F2 - Acquisition Parameters
Date_ 20080725
Time 10.49
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250987 Hz
AQ 1.9923444 sec
RG 80.6
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

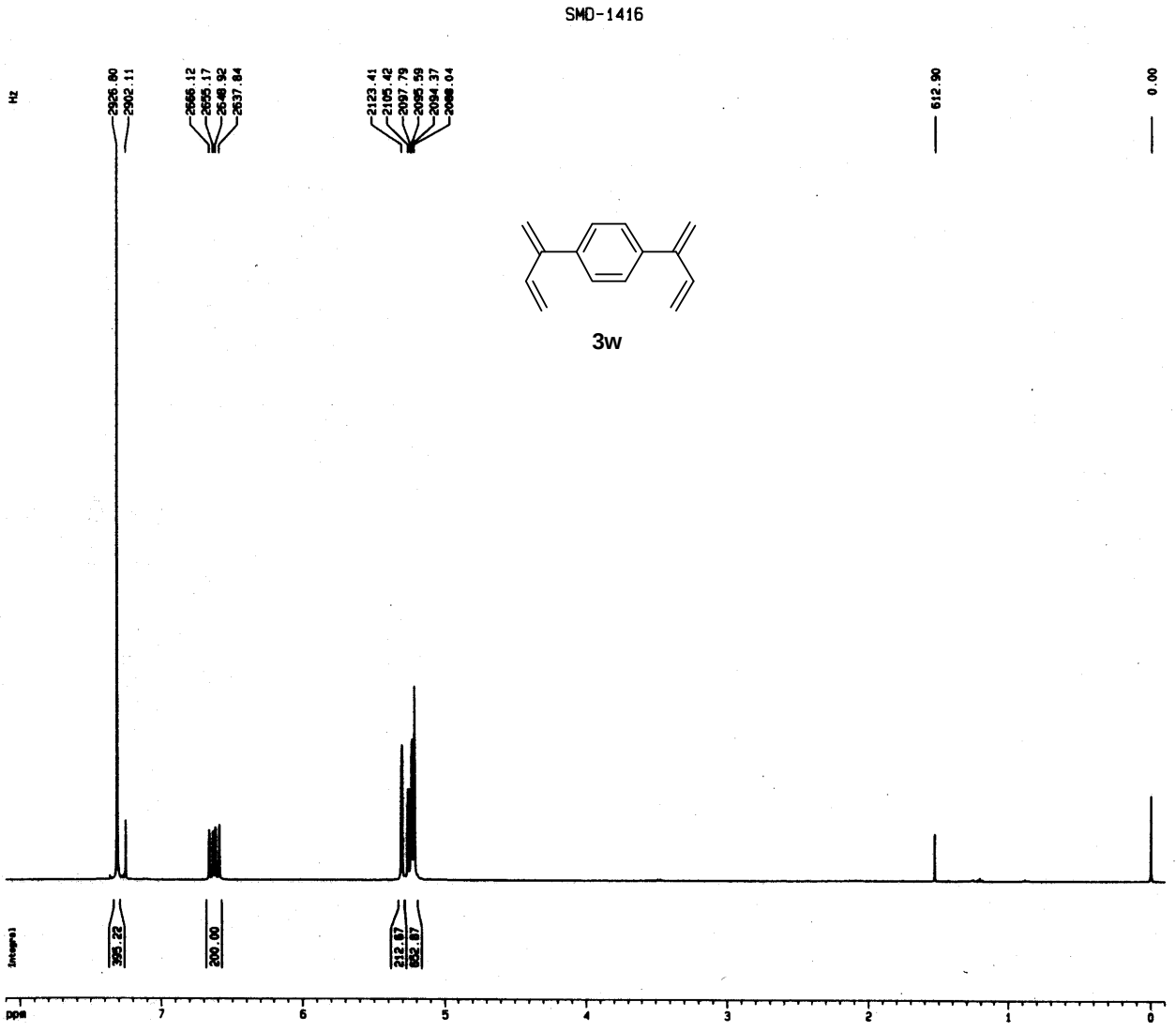
F2 - Processing parameters
SI 16384
SF 400.1299965 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 56.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.30333 ppm/cm
HZCM 121.37276 Hz/cm

YHS-370

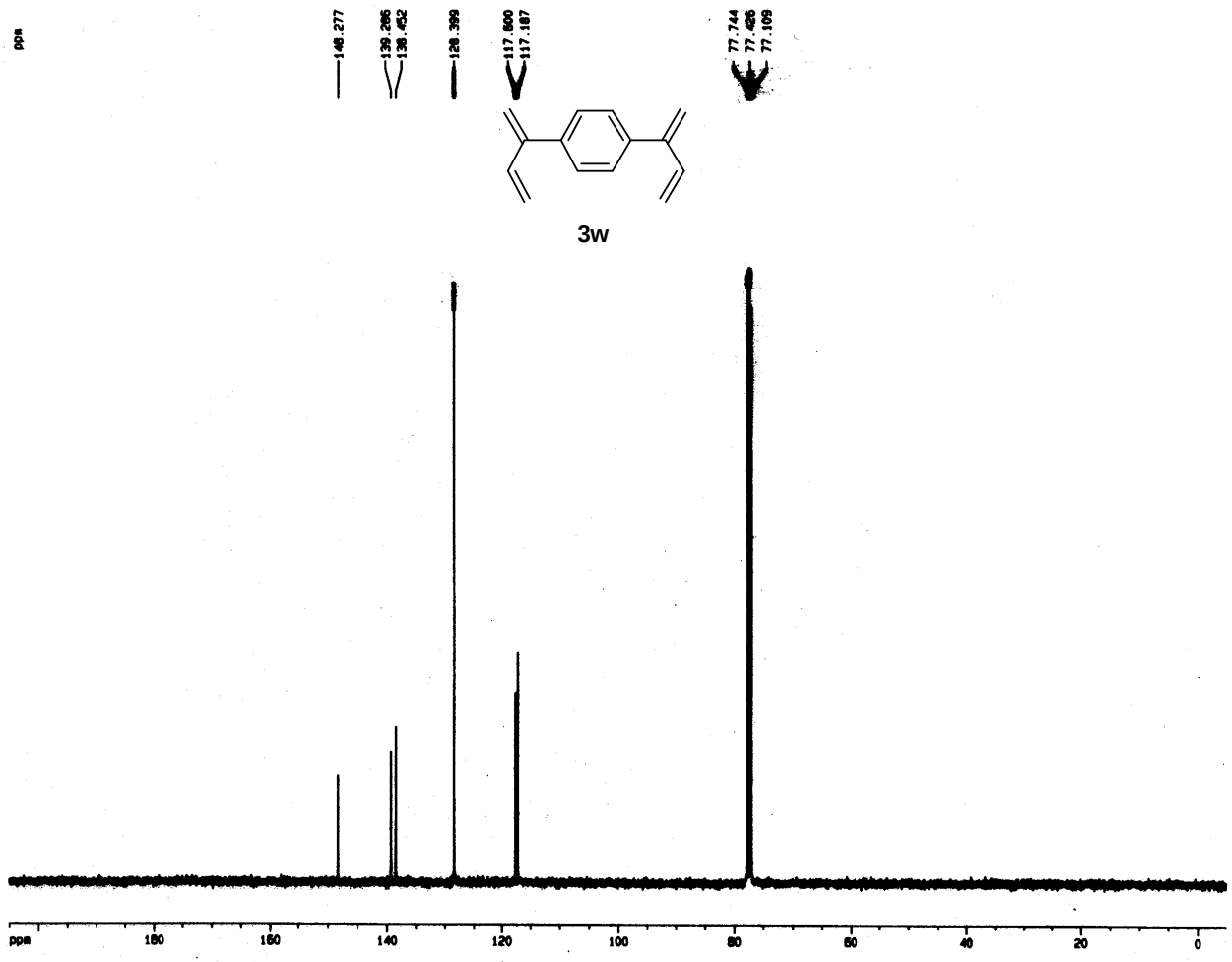



```
Current Data Parameters
NAME                  jul-08
EXPNO                    118
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080725
Time                  11.09
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG               zgpg30
TD                     65536
SOLVENT               CDCl3
NS                       695
DS                         2
SWH               31847.133 Hz
FIDRES            0.485949 Hz
AQ                1.0289652 sec
RG                     143.7
DW                  15.700 usec
DE                   6.00 usec
TE                   296.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                   10.50 usec
PL1                  -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2               105.00 usec
PL2                  -2.00 dB
PL12                 18.00 dB
PL13                 20.00 dB
SFO2             400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF               100.6127290 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                   30.00 cm
CY                   12.00 cm
F1P                205.000 ppm
F1                 20625.61 Hz
F2P                 -5.000 ppm
F2                   503.06 Hz
PPMCM              7.00000 ppm/cm
HZCM             704.28906 Hz/cm
```



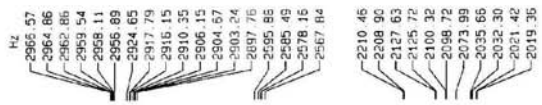

```
Current Data Parameters
NAME                  mar-08
EXPNO                     45
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080403
Time                   17.32
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       32
DS                        0
SWH               8223.685 Hz
FIDRES            0.250987 Hz
AQ                1.9923444 sec
RG                      362
DW                 60.800 usec
DE                  6.00 usec
TE                   296.2 K
D1                1.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.00 usec
PL1                    -2.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF               400.1300124 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     30.00 cm
CY                     20.00 cm
F1P                     8.100 ppm
F1                   3241.05 Hz
F2P                    -0.100 ppm
F2                     -40.01 Hz
PPMCM                0.27333 ppm/cm
HZCM               109.36887 Hz/cm
```

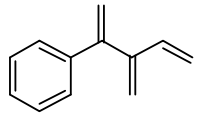
SMD-1416



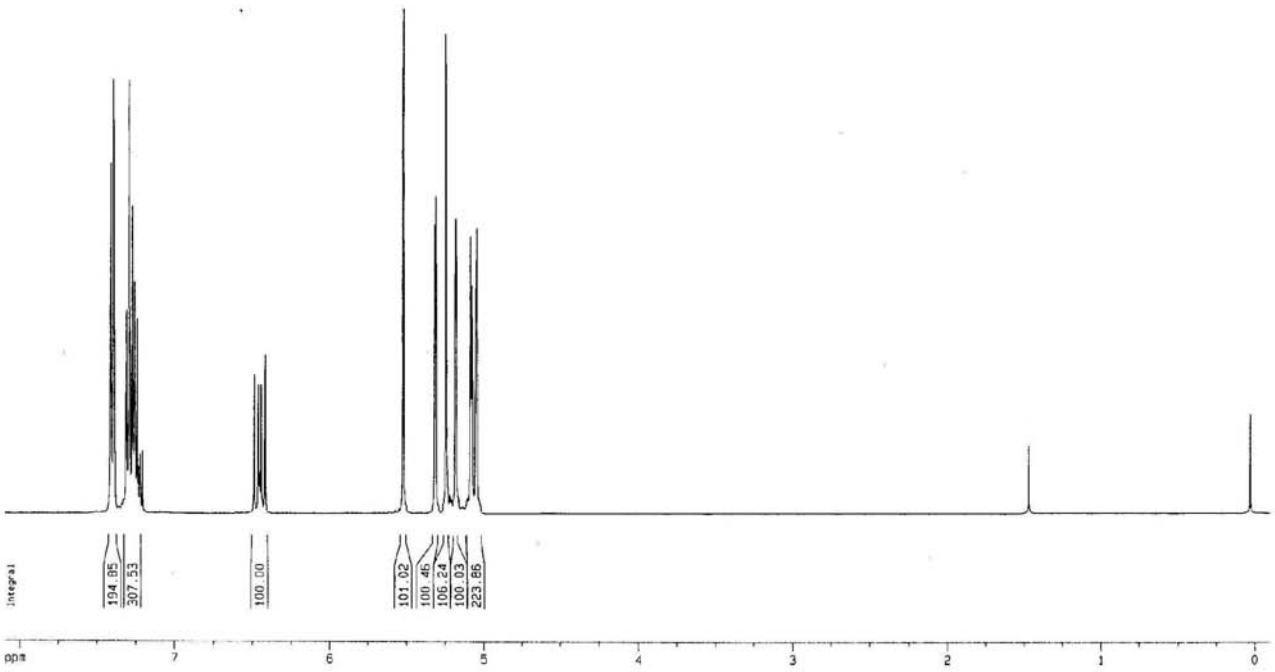

```
Current Data Parameters
NAME                  mar-08
EXPNO                     46
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080403
Time                   17.43
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      698
DS                        2
SWH               31847.133 Hz
FIDRES             0.485848 Hz
AQ                 1.0288852 sec
RG                     287.4
DW                  15.700 usec
DE                   6.00 usec
TE                   298.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.88888888 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.50 usec
PL1                    -1.00 dB
SF01              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SF02              400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127290 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    15.00 cm
F1P                  205.000 ppm
F1                 20625.61 Hz
F2P                   -5.000 ppm
F2                  -503.06 Hz
PPMCM                 7.00000 ppm/cm
HZCM                704.28906 Hz/cm
```

YHS-349



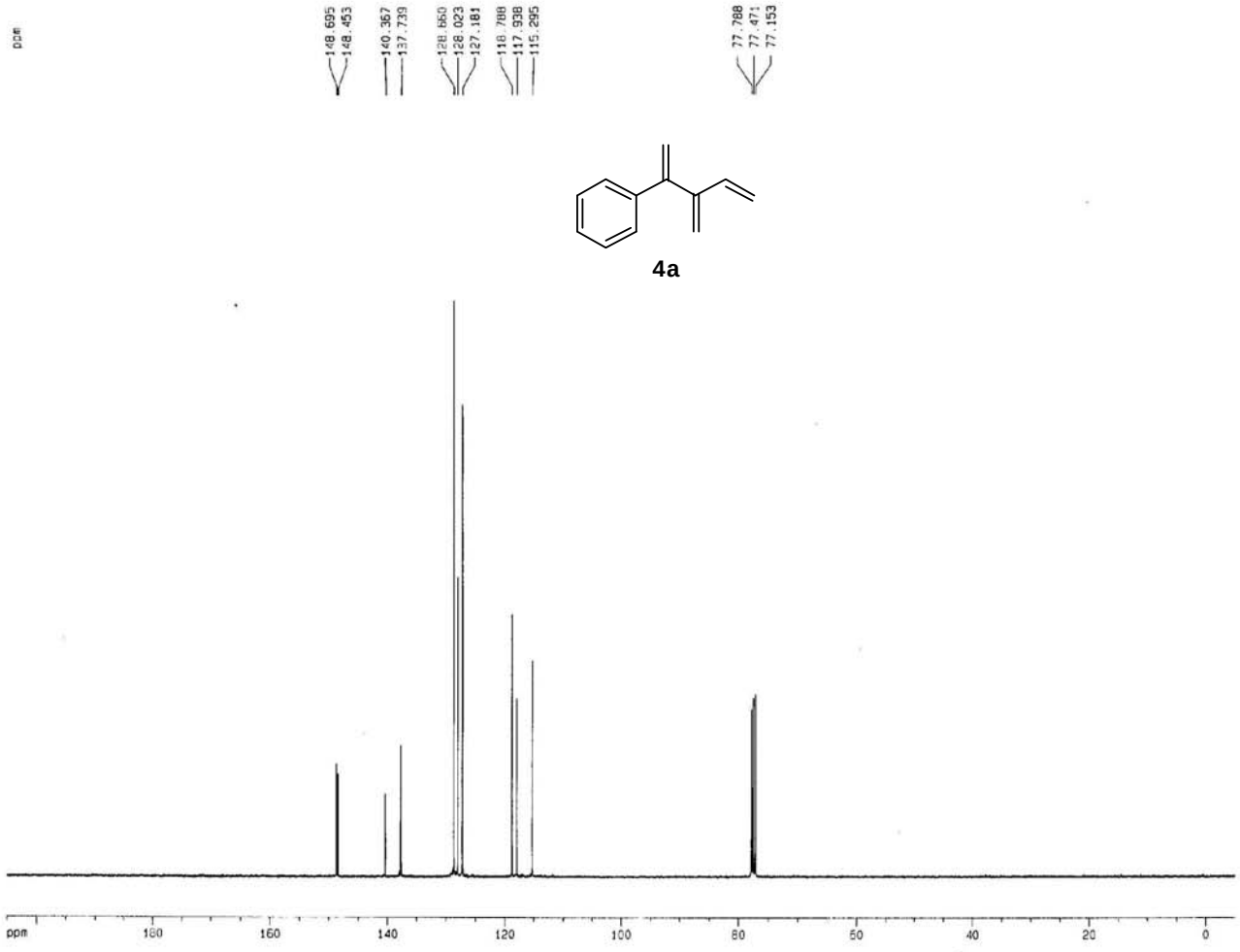


4a



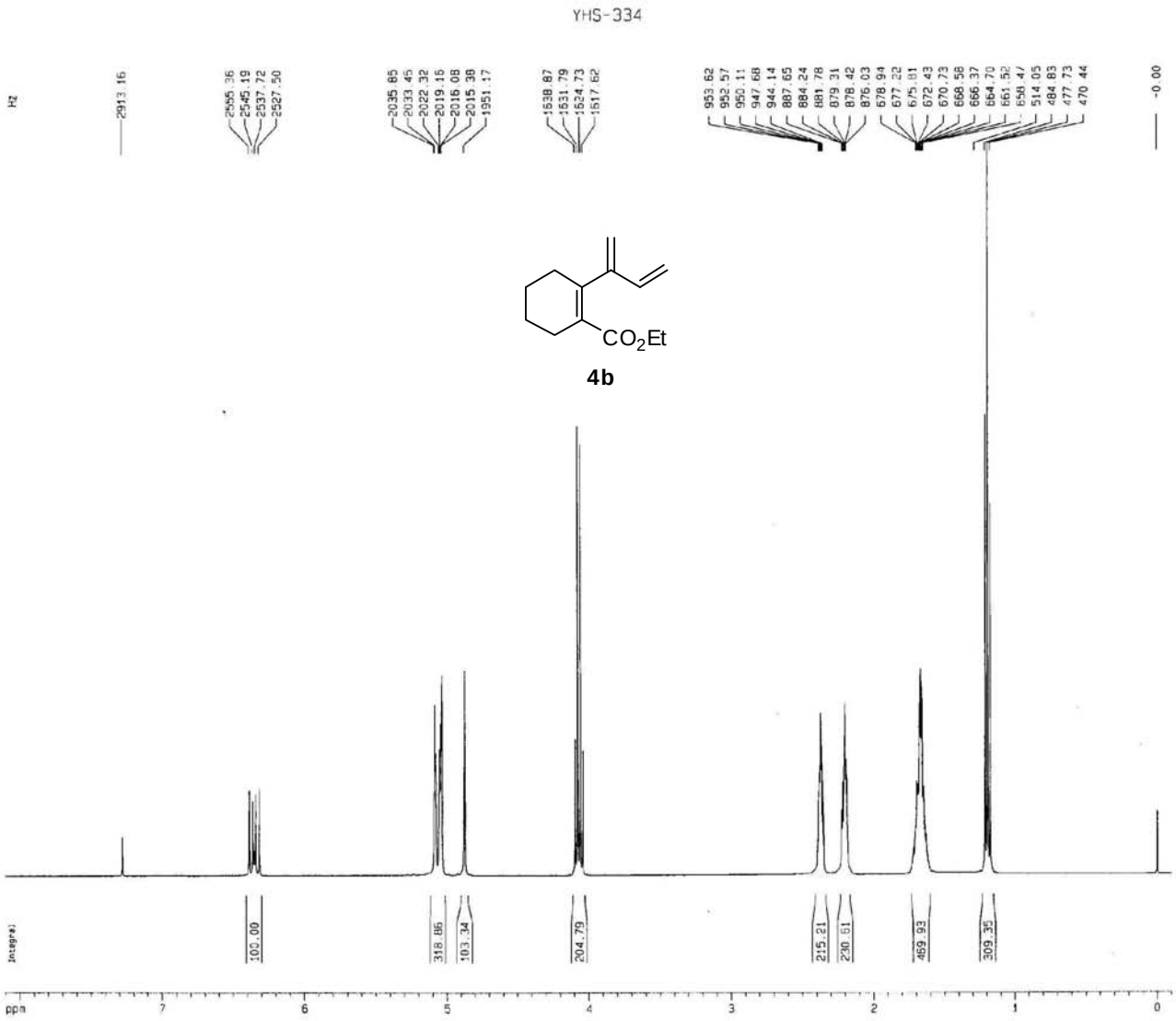

```
Current Data Parameters
NAME                  may-08
EXPNO                     89
PROCNO                     1

F2 - Acquisition Parameters
Date_               20080701
Time                   12.31
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zg30
TD                    32768
SOLVENT                CDCl3
NS                        22
DS                         0
SWH                 8223.685 Hz
FIDRES              0.250967 Hz
AQ                  1.9923444 sec
RG                       71.8
DW                     60.800 usec
DE                      6.00 usec
TE                     299.2 K
D1                  1.00000000 sec
NCREST              0.00000000 sec
NCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.00 usec
PL1                    -2.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF                400.1300307 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
.X                     30.00 cm
.Y                     12.00 cm
F1P                     8.100 ppm
F1                   3241.05 Hz
F2P                    -0.100 ppm
F2                     -40.01 Hz
PPMCM                0.27333 ppm/cm
HZCM               109.35888 Hz/cm
```

YHS-349



4a

```
Current Data Parameters
NAME                  may-08
EXPNO                     90
PROCNO                     1

F2 - Acquisition Parameters
Date_               20080701
Time                   13.08
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                      256
DW                  15.700 usec
DE                   6.00 usec
TE                  299.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                    10.50 usec
PL1                   -1.00 dB
SF01            100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                105.00 usec
PL2                   -2.00 dB
PL12                  18.00 dB
PL13                  20.00 dB
SF02            400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF              100.6127290 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    14.00 cm
F1P                 205.000 ppm
F1                  20625.61 Hz
F2P                  -5.000 ppm
F2                  -503.06 Hz
PPMCM                7.00000 ppm/cm
HZCM               704.28906 Hz/cm
```



Current Data Parameters
NAME may-08
EXPNO 37
PROCNO 1

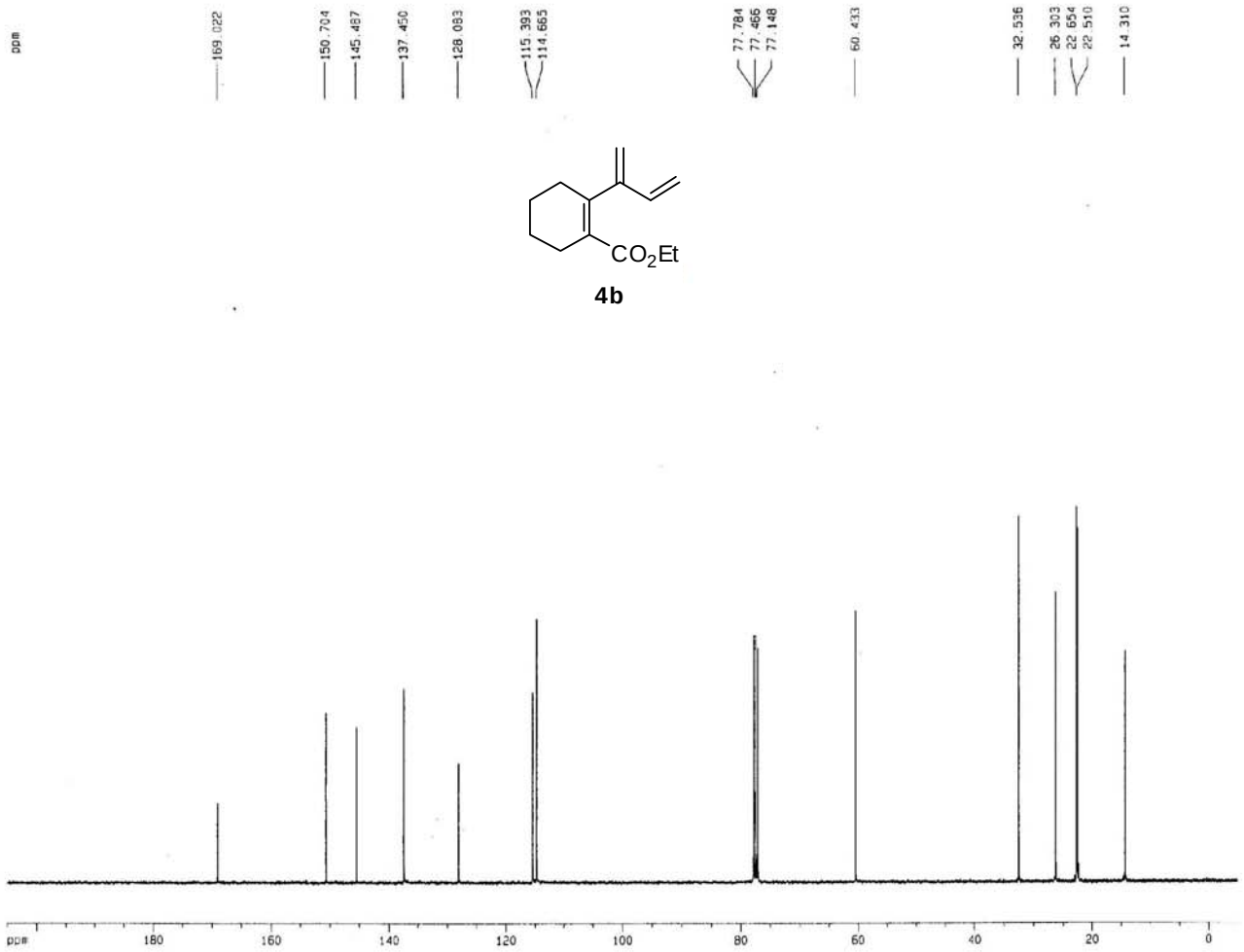
F2 - Acquisition Parameters
Date_ 20080610
Time 11.18
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 57
DW 60.800 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300015 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

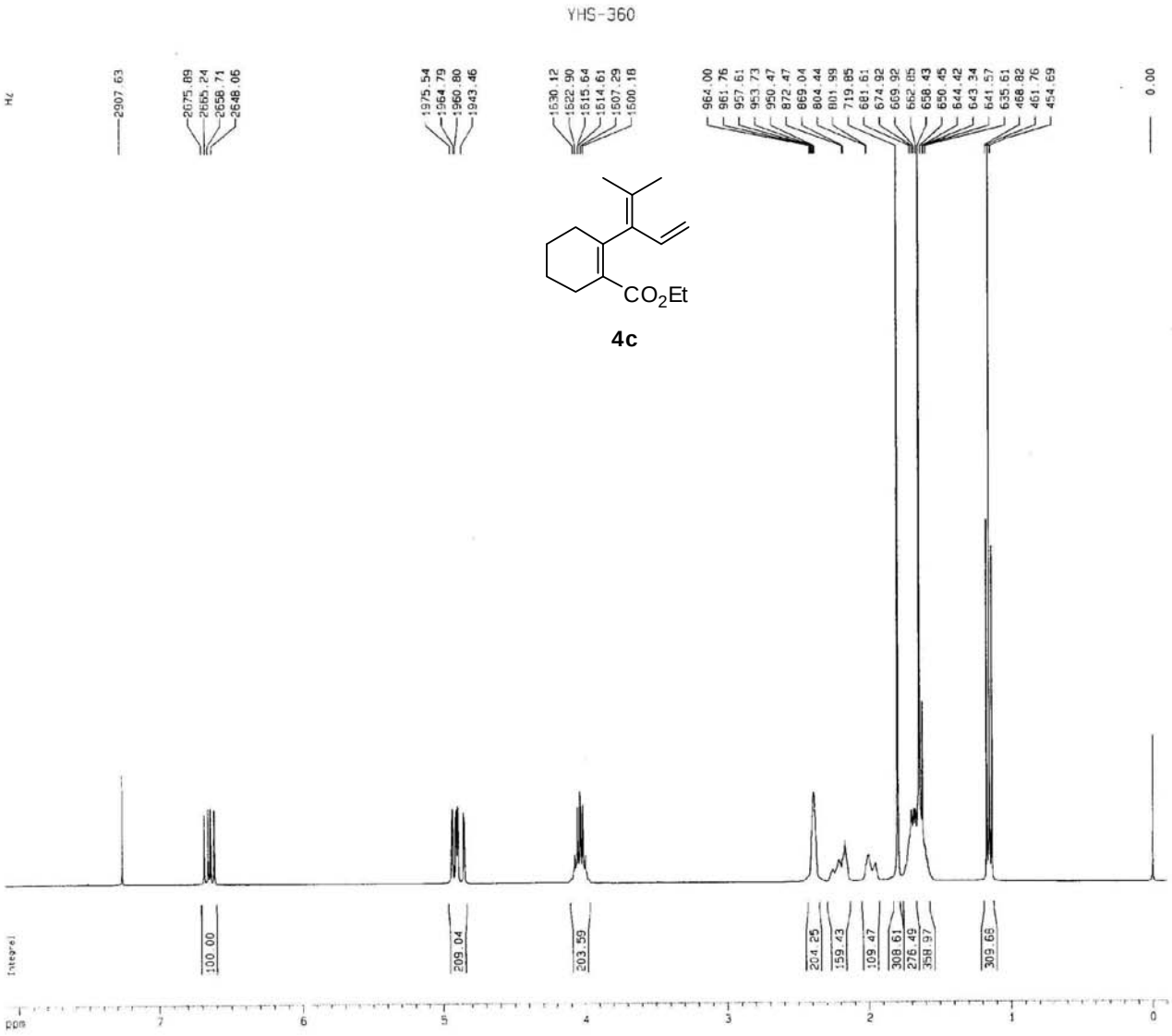
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36887 Hz/cm

YHS-334



4b

```
Current Data Parameters
NAME                  may-08
EXPNO                     38
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080610
Time                  11.50
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG             zgpg30
TD                   65536
SOLVENT               CDCl3
NS                      871
DS                        2
SWH               31847.133 Hz
FIDRES            0.485949 Hz
AQ                1.0289652 sec
RG                      114
DW                 15.700 usec
DE                  6.00 usec
TE                  298.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                  10.50 usec
PL1                 -1.00 dB
SFO1           100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz15
NUC2                      1H
PCPD2              105.00 usec
PL2                 -2.00 dB
PL12                18.00 dB
PL13                20.00 dB
SFO2           400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF            100.6127290 MHz
WDW                      EM
SSB                       0
LB                  1.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                   30.00 cm
CY                    9.00 cm
F1P                205.000 ppm
F1                20625.61 Hz
F2P                 -5.000 ppm
F2                -503.06 Hz
PPMCM               7.00000 ppm/cm
HZCM              704.28906 Hz/cm
```



Current Data Parameters
NAME sep-08
EXPNO 25
PROCNO 1

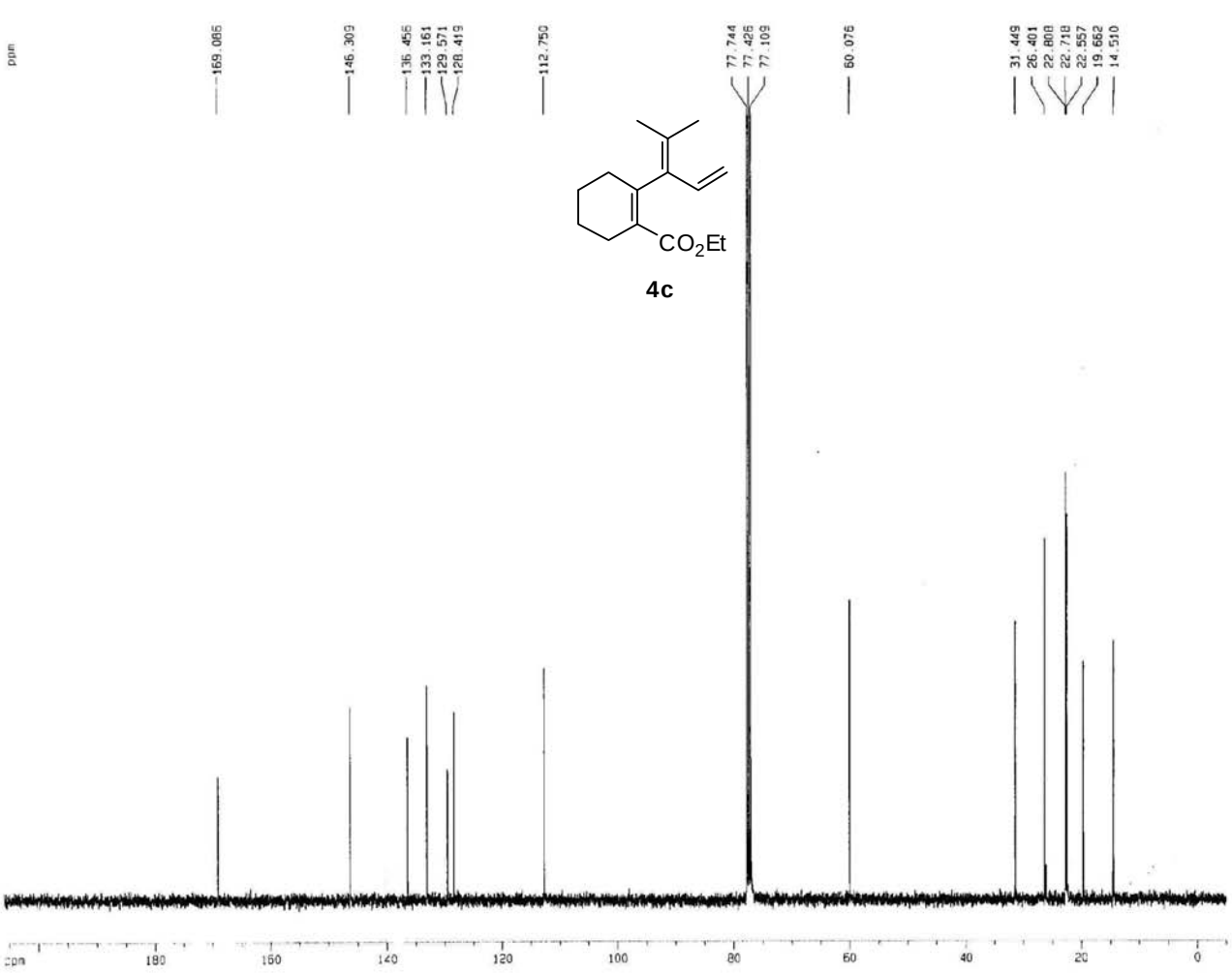
F2 - Acquisition Parameters
Date_ 20080910
Time 12.13
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 143.7
DW 60.800 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

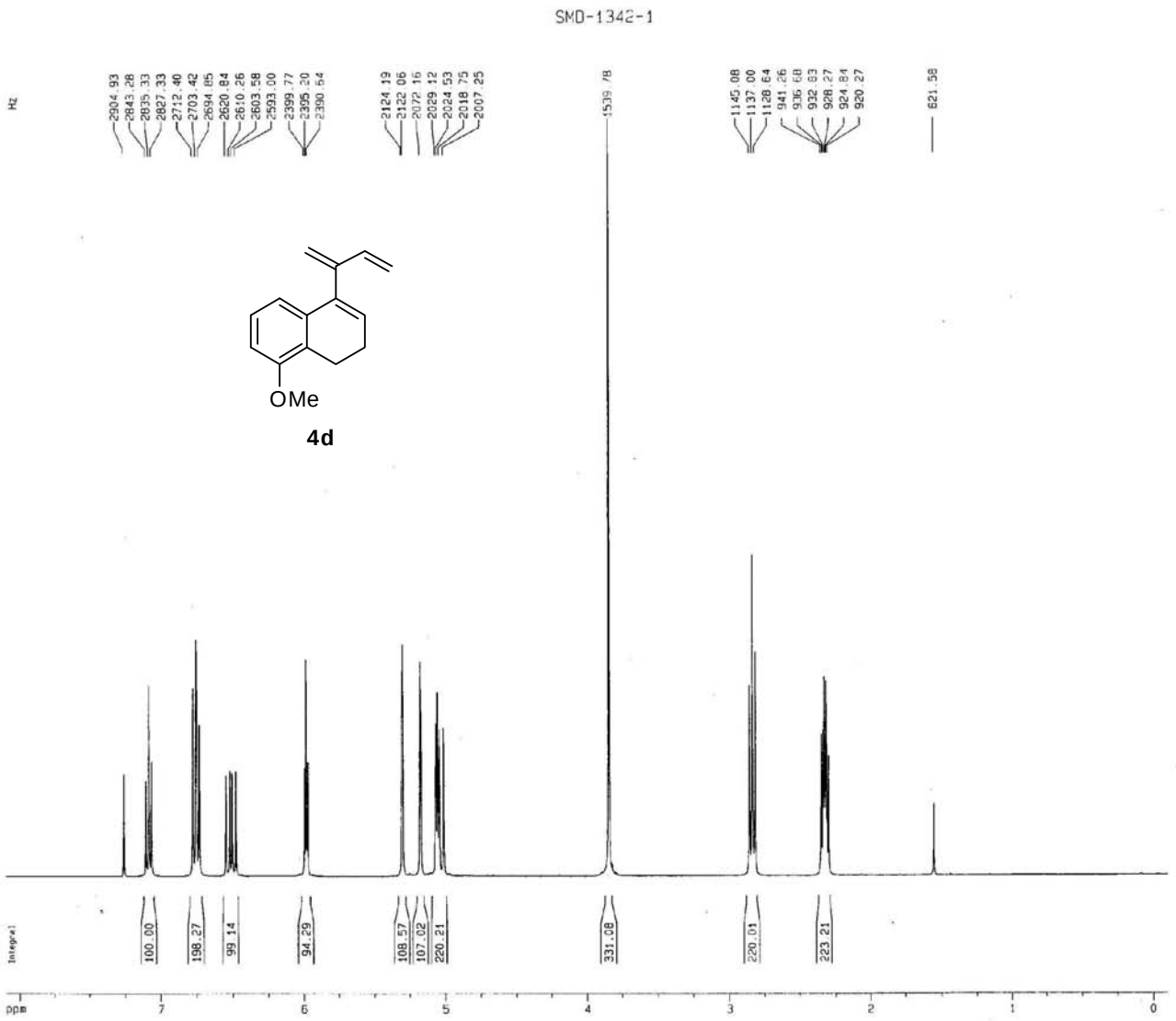
F2 - Processing parameters
SI 16384
SF 400.1300070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36887 Hz/cm

YHS-360




```
Current Data Parameters
NAME                  sep-08
EXPNO                     26
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080910
Time                  12.32
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG               zgpg30
TD                     65536
SOLVENT               CDCl3
NS                       748
DS                         2
SWH               31847.133 Hz
FIDRES            0.485949 Hz
AQ                1.0289652 sec
RG                   3649.1
DW                  15.700 usec
DE                   6.00 usec
TE                   299.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1             100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2             400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF               100.6127290 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                       30.00 cm
CY                       23.00 cm
F1P                     206.000 ppm
F1                    20726.22 Hz
F2P                      -5.000 ppm
F2                     -503.06 Hz
PPMCM                 7.03333 ppm/cm
HZCM                707.64288 Hz/cm
```



Current Data Parameters
NAME oct-07
EXPNO 44
PROCNO 1

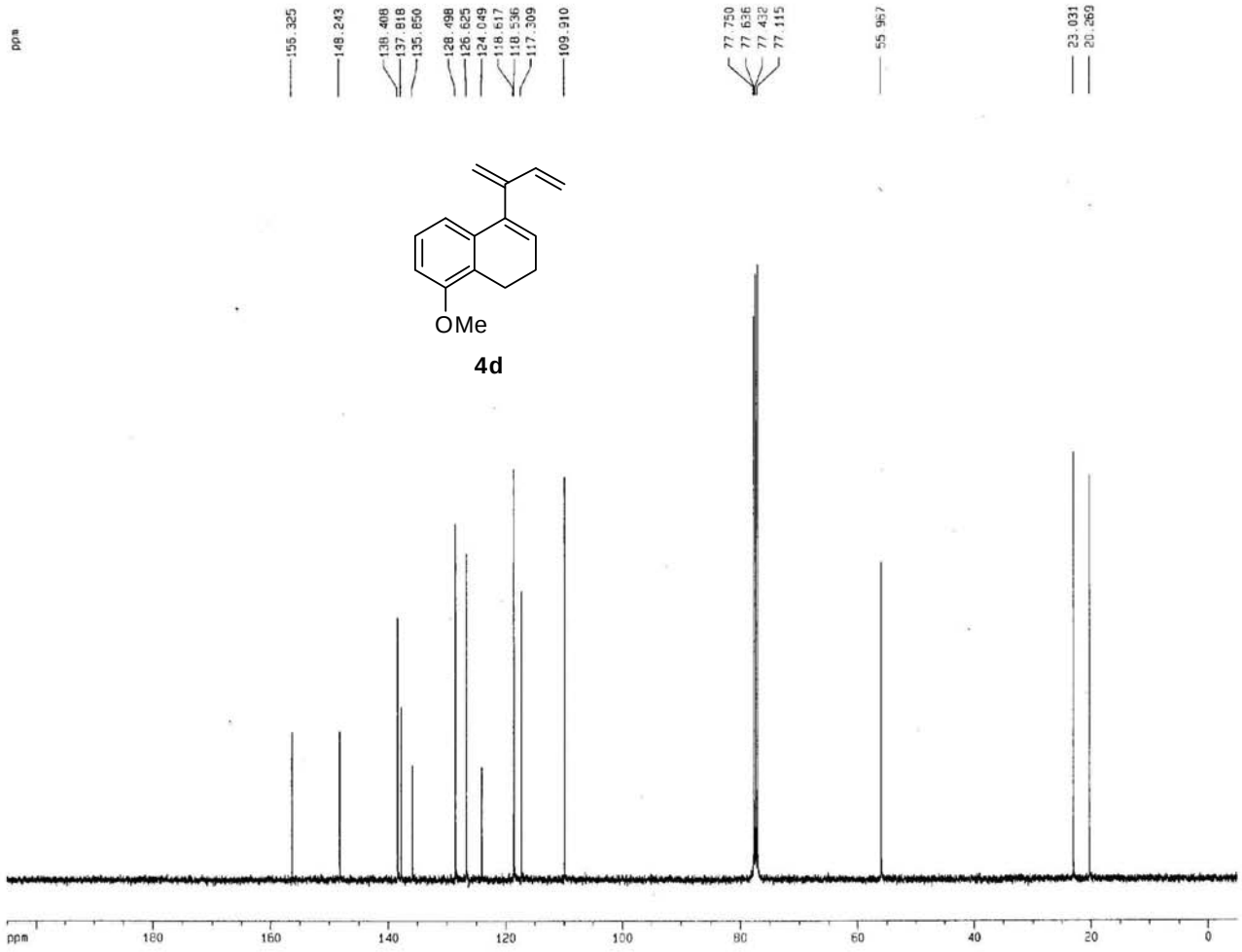
F2 - Acquisition Parameters
Date_ 20071026
Time 16.50
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 161.3
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

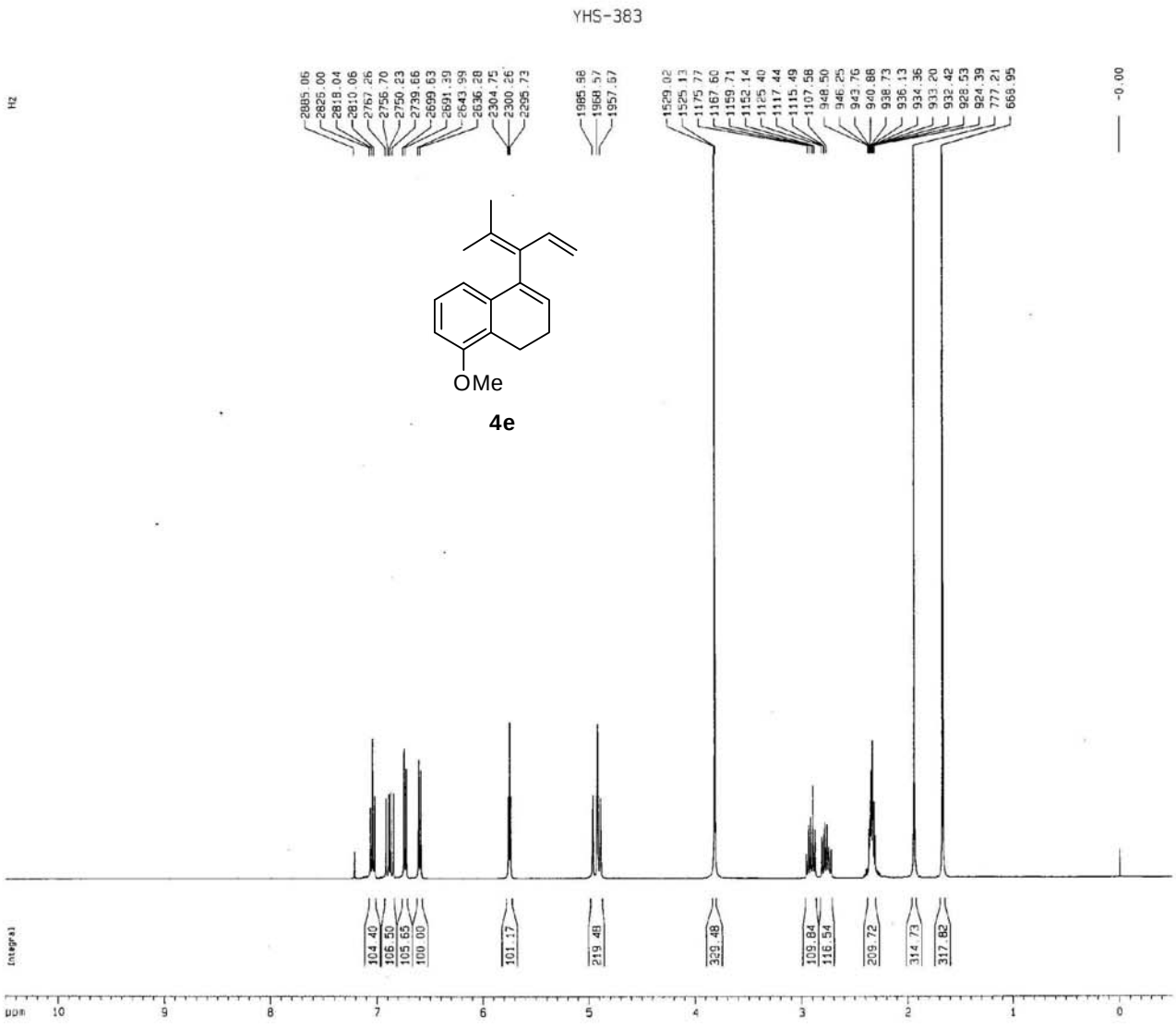
1D NMR plot parameters
CX 30.00 cm
CY 45.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36887 Hz/cm

SMD-1342-1



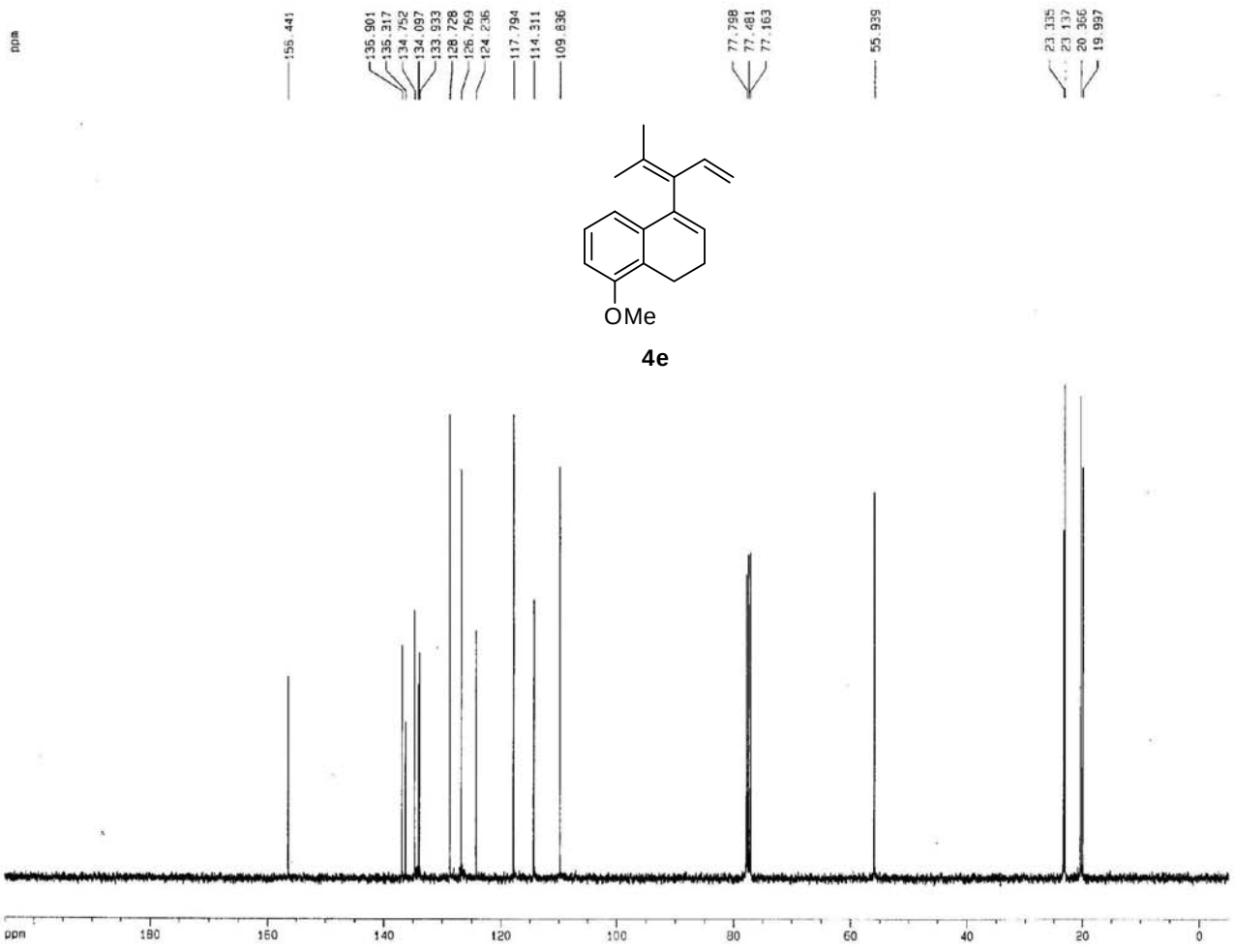
4d

```
Current Data Parameters
NAME                 oct-07
EXPNO                    45
PROCNO                    1

F2 - Acquisition Parameters
Date_              20071026
Time                  17.05
INSTRUM               spect
PROBHD   5 mm Dual 13C/
PULPROG              zgpg30
TD                    65536
SOLVENT                CDCl3
NS                      2048
DS                         2
SWH               31847.133 Hz
FIDRES            0.485949 Hz
AQ                1.0289652 sec
RG                     228.1
DW                15.700 usec
DE                 6.00 usec
TE                 296.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                  10.50 usec
PL1                 -1.00 dB
SFO1           100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2               105.00 usec
PL2                 -2.00 dB
PL12                18.00 dB
PL13                20.00 dB
SFO2           400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF             100.6127290 MHz
WDW                       EM
SSB                        0
LB                  1.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                  30.00 cm
CY                  15.00 cm
F1P               205.000 ppm
F1              20625.61 Hz
F2P                -5.000 ppm
F2               -503.06 Hz
PPMCM              7.00000 ppm/cm
HZCM             704.28906 Hz/cm
```




```
Current Data Parameters
NAME                  aug-08
EXPNO                     43
PROCNO                     1

F2 - Acquisition Parameters
Date_               20080811
Time                   16.37
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zg30
TD                    32768
SOLVENT                CDCl3
NS                        32
DS                         0
SWH                 8223.685 Hz
FIDRES              0.250967 Hz
AQ                  1.9923444 sec
RG                        57
DW                    60.800 usec
DE                     6.00 usec
TE                    299.2 K
D1                  1.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.00 usec
PL1                    -2.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                        16384
SF                400.1300294 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00

1D NMR plot parameters
CX                    30.00 cm
CY                    34.00 cm
F1P                   10.500 ppm
F1                  4201.37 Hz
F2P                   -0.500 ppm
F2                  -200.06 Hz
PPMCM                 0.36667 ppm/cm
HZCM                146.71434 Hz/cm
```

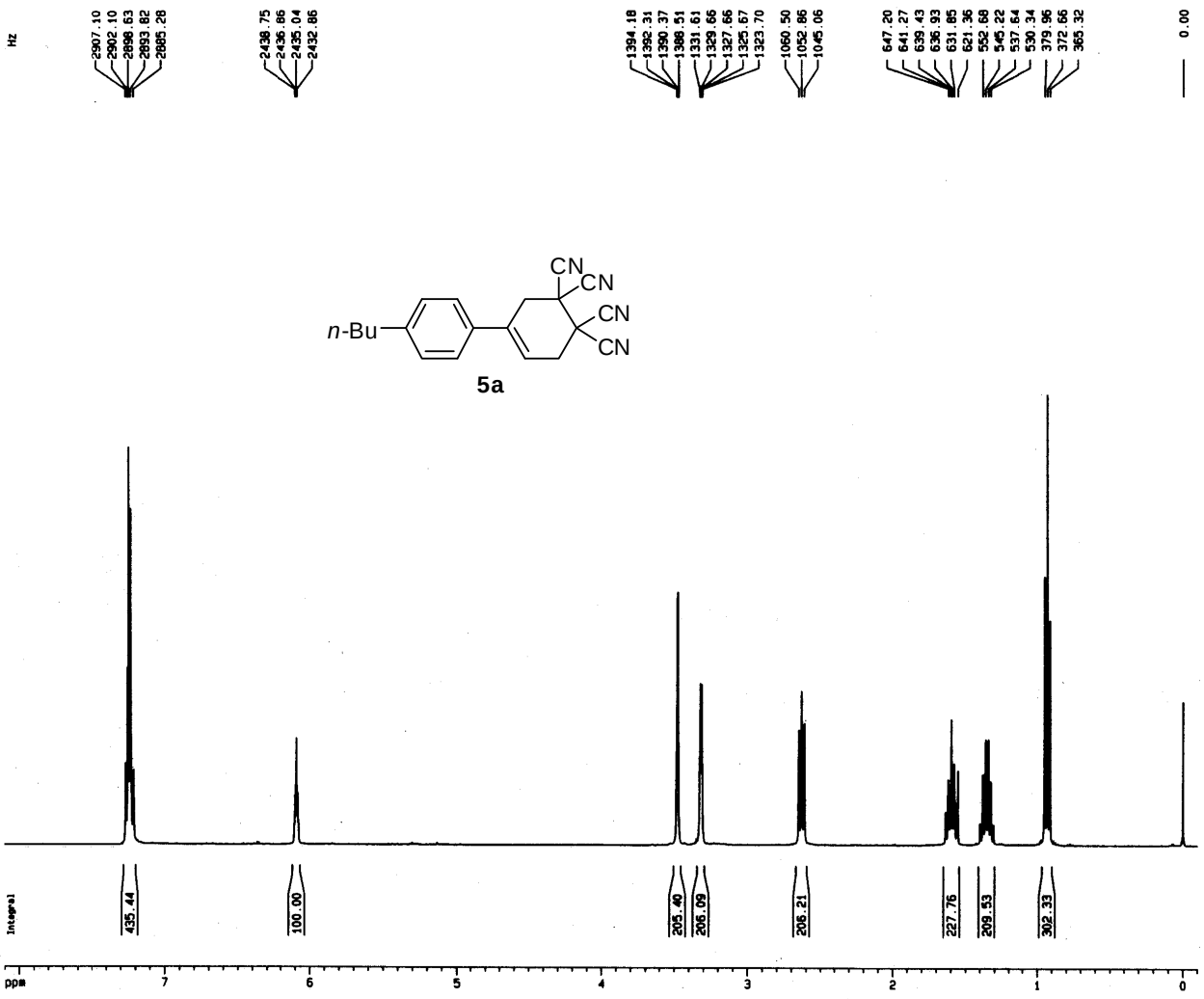
YHS-383



4e

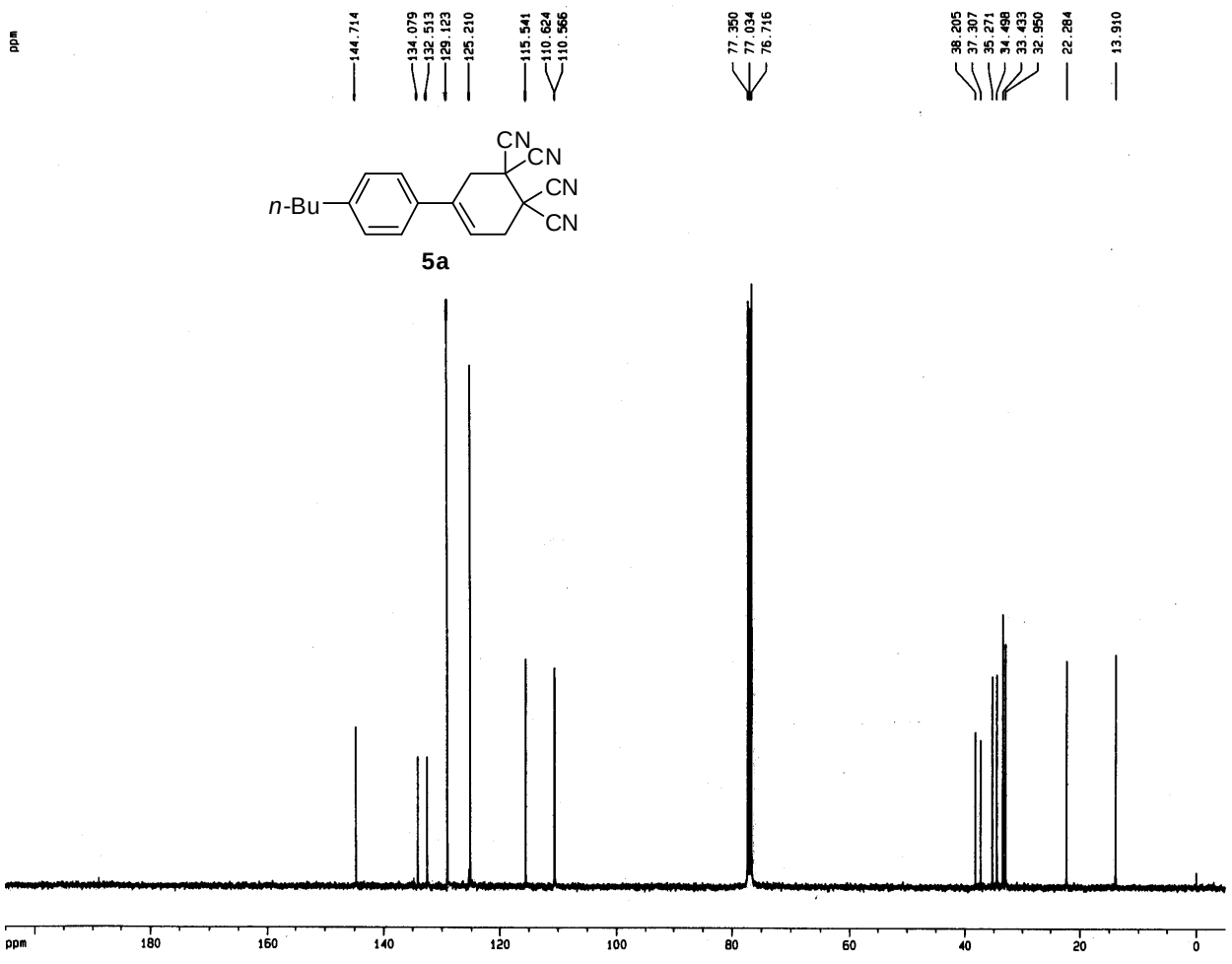
```
Current Data Parameters
NAME                  aug-08
EXPNO                     44
PROCNO                     1

F2 - Acquisition Parameters
Date_              20080811
Time                  16.47
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       288
DS                         2
SWH               31847.133 Hz
FIDRES            0.485949 Hz
AQ                1.0289652 sec
RG                    3649.1
DW                  15.700 usec
DE                   6.00 usec
TE                   299.2 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                     1H
PCPD2                 105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2              400.1324708 MHz

F2 - Processing parameters
SI                       32768
SF                100.6127290 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                        1.40

1D NMR plot parameters
CX                      30.00 cm
CY                      12.00 cm
F1P                   205.000 ppm
F1                  20625.61 Hz
F2P                    -5.000 ppm
F2                   -503.06 Hz
PPMCM                 7.00000 ppm/cm
HZCM                704.28906 Hz/cm
```

SMD-1380-2




```
Current Data Parameters
NAME                dec-07
EXPNO                   53
PROCNO                   1

F2 - Acquisition Parameters
Date_             20071217
Time                 11.03
INSTRUM              spect
PROBHD   5 mm Dual 13C/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH              8223.685 Hz
FIDRES           0.250967 Hz
AQ               1.9923444 sec
RG                   143.7
DW                  60.800 usec
DE                   6.00 usec
TE                  296.2 K
D1               1.00000000 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   11.00 usec
PL1                  -2.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                      16384
SF             400.1300125 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00

1D NMR plot parameters
CX                   30.00 cm
CY                   12.00 cm
F1P                   8.100 ppm
F1                 3241.05 Hz
F2P                  -0.100 ppm
F2                   -40.01 Hz
PPMCM             0.27333 ppm/cm
HZCM             109.36887 Hz/cm
```

SMD-1380-2



Current Data Parameters
NAME dec-07
EXPNO 54
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071217
Time 11.47
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1774
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 101.6
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

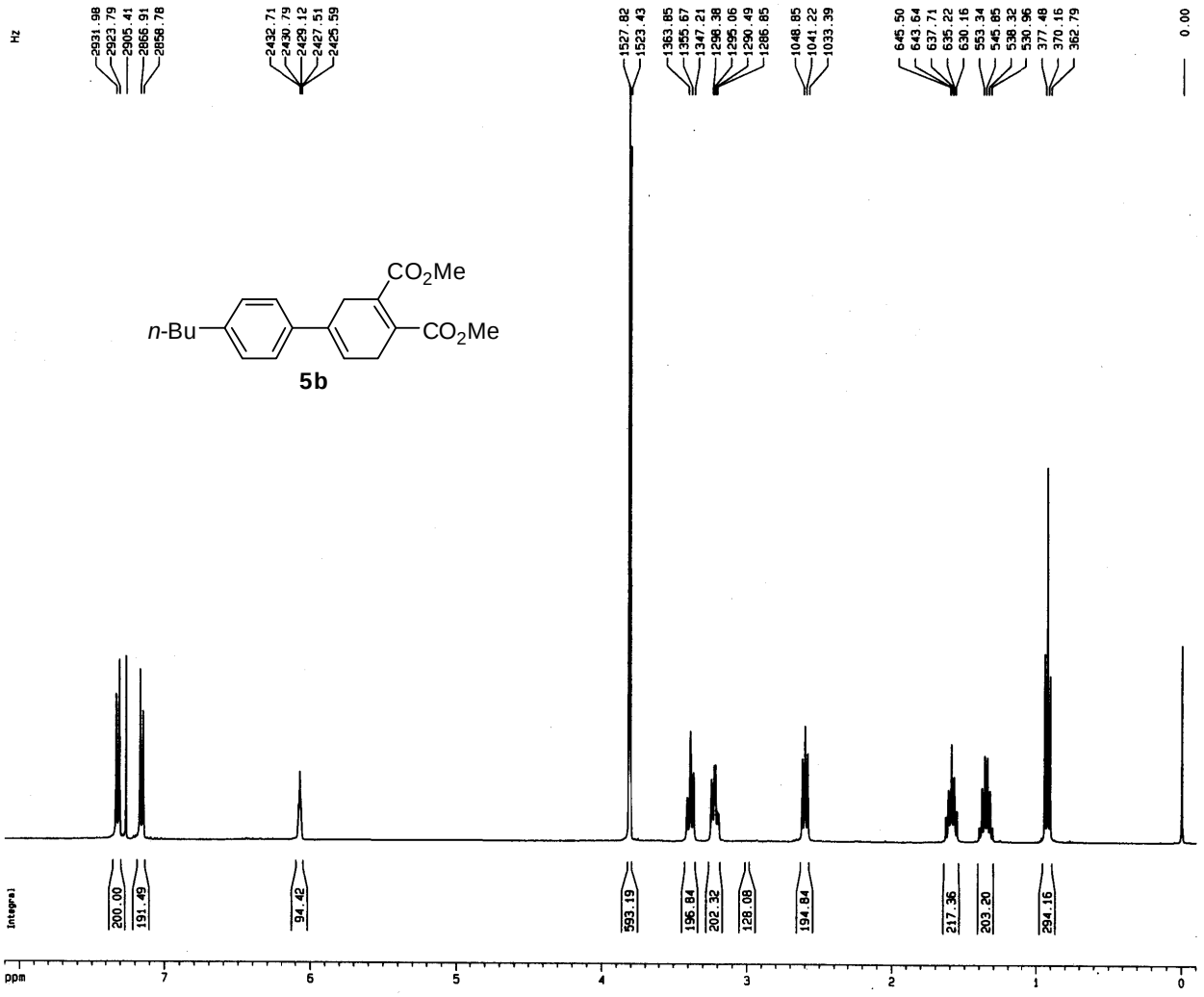
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SF01 100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SF02 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127709 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 30.00 cm
CY 15.00 cm
F1P 205.000 ppm
F1 20625.62 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28937 Hz/cm

SMD-1392



Current Data Parameters
NAME jan-08
EXPNO 37
PROCNO 1

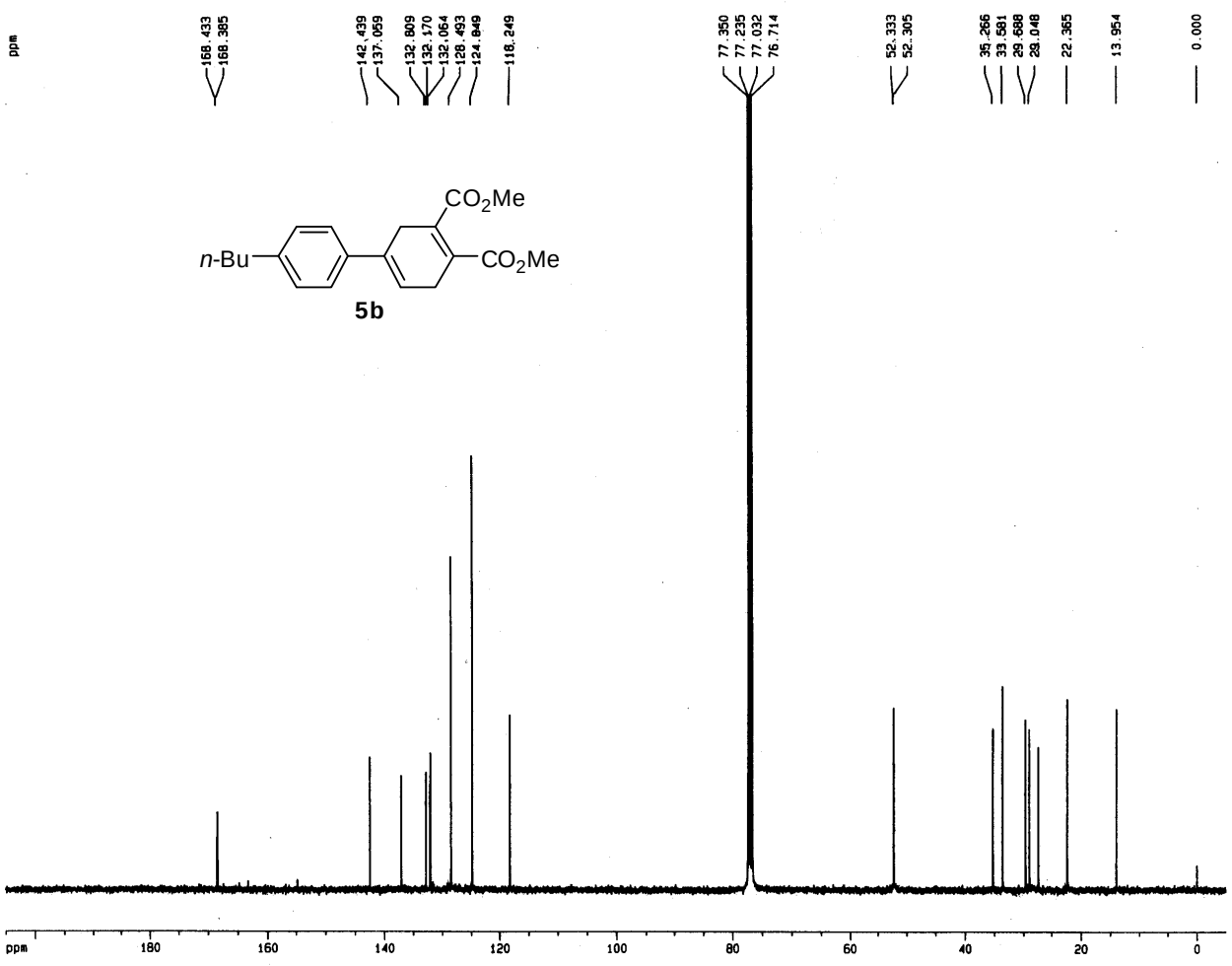
F2 - Acquisition Parameters
Date_ 20080115
Time 17.30
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

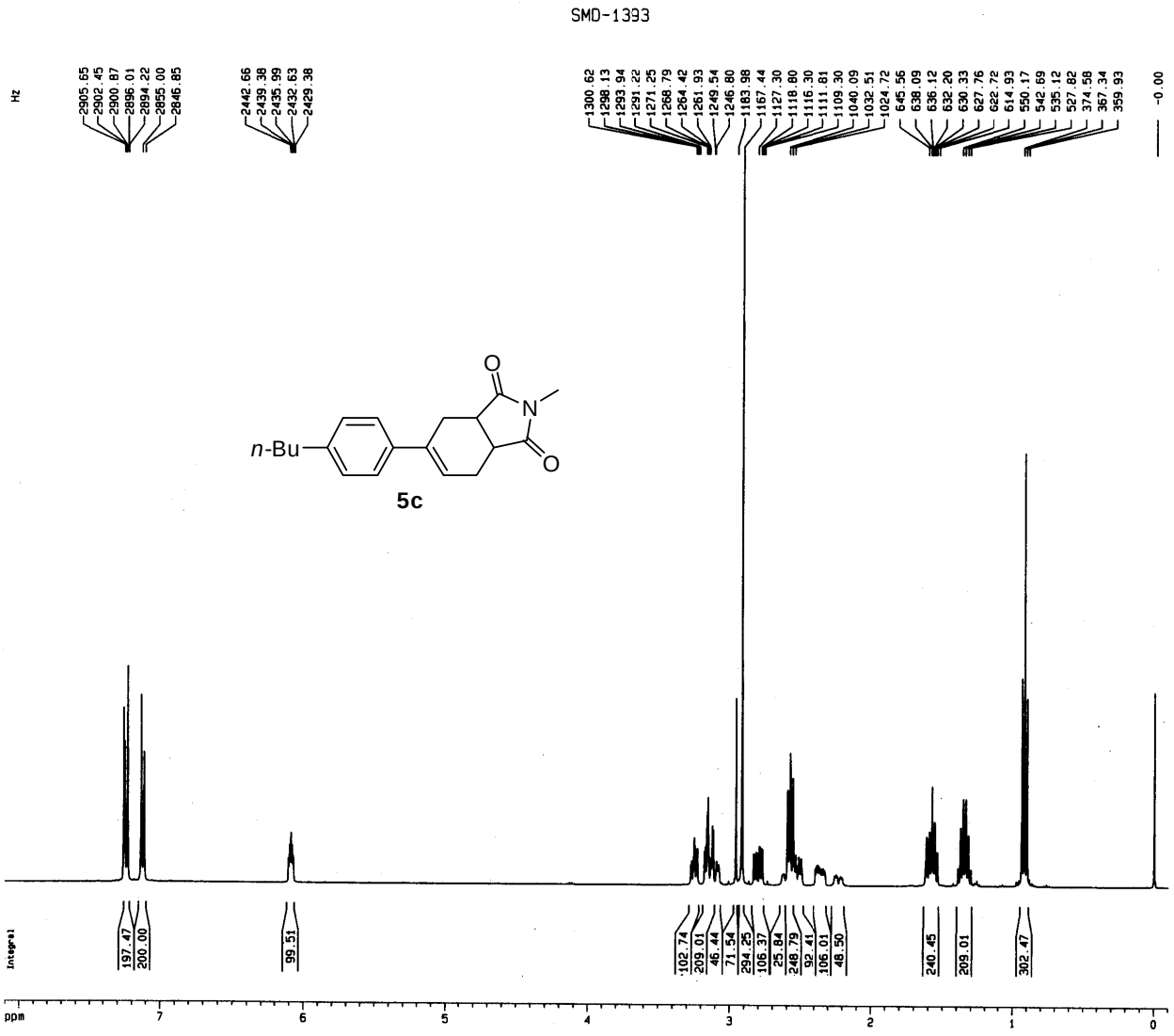
F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36887 Hz/cm

SMD-1392

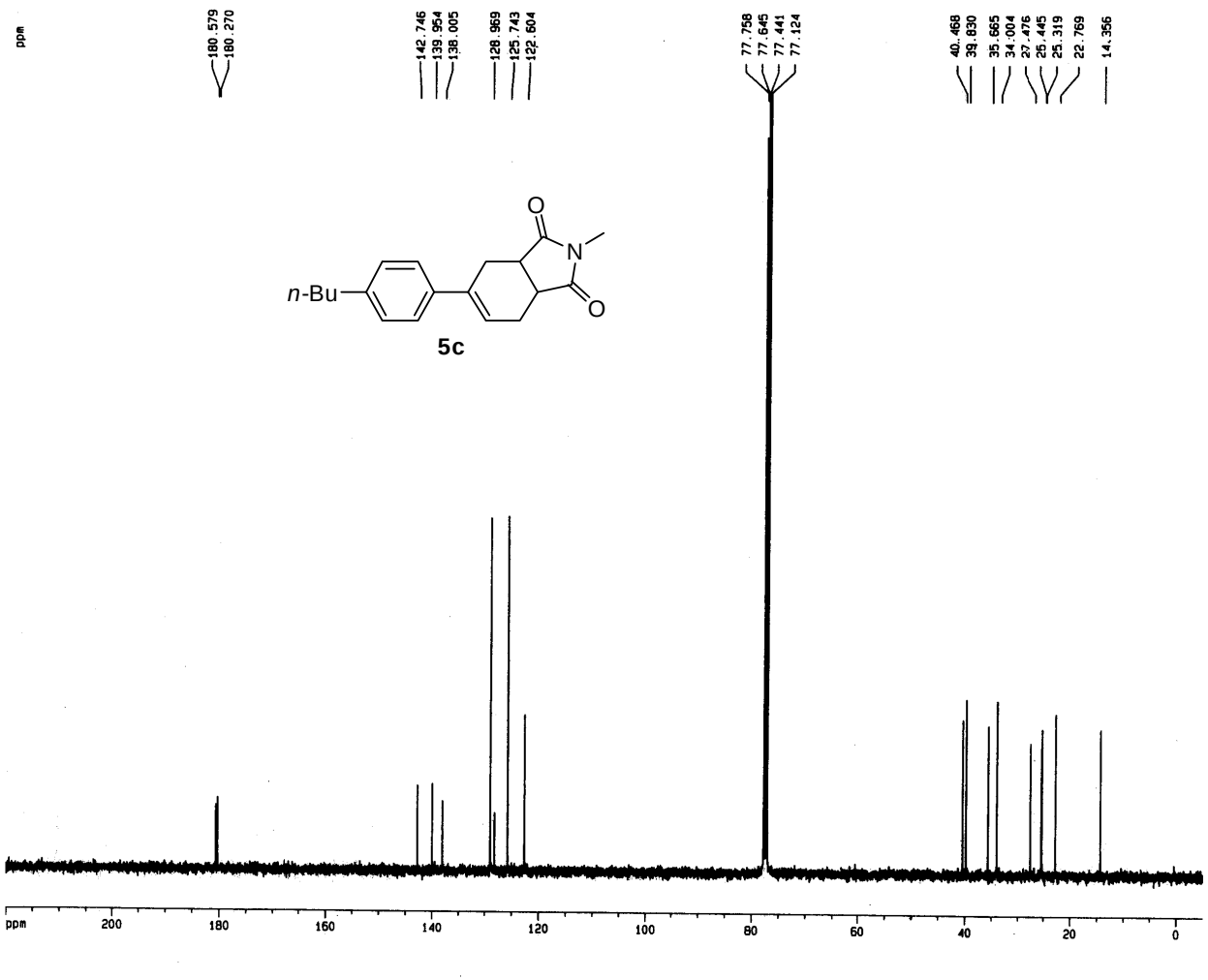



```
Current Data Parameters
NAME                  jan-08
EXPNO                     38
PROCNO                     1

F2 - Acquisition Parameters
Date_               20080115
Time                   18.12
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       7231
DS                          2
SWH                31847.133 Hz
FIDRES             0.485949 Hz
AQ                 1.0289652 sec
RG                      3649.1
DW                     15.700 usec
DE                      6.00 usec
TE                     296.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                     10.50 usec
PL1                    -1.00 dB
SFO1              100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                 105.00 usec
PL2                    -2.00 dB
PL12                   18.00 dB
PL13                   20.00 dB
SFO2              400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127695 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                     1.40

1D NMR plot parameters
CX                    30.00 cm
CY                    34.00 cm
F1P                  205.000 ppm
F1                 20625.62 Hz
F2P                   -5.000 ppm
F2                  -503.05 Hz
PPMCM                 7.00000 ppm/cm
HZCM               704.28937 Hz/cm
```




```
Current Data Parameters
NAME                  jan-08
EXPNO                     73
PROCNO                     1

F2 - Acquisition Parameters
Date_               20080123
Time                   13.45
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8223.685 Hz
FIDRES              0.250967 Hz
AQ                  1.9923444 sec
RG                       181
DW                    60.800 usec
DE                     6.00 usec
TE                     296.2 K
D1                  1.00000000 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.00 usec
PL1                    -2.00 dB
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                       16384
SF                400.1300090 MHz
WDW                        EM
SSB                         0
LB                     0.30 Hz
GB                          0
PC                      1.00

1D NMR plot parameters
CX                     30.00 cm
CY                     20.00 cm
F1P                    8.100 ppm
F1                   3241.05 Hz
F2P                   -0.100 ppm
F2                    -40.01 Hz
PPMCM                0.27333 ppm/cm
HZCM               109.36887 Hz/cm
```

SMD-1393



Current Data Parameters

NAME	jan-08
EXPNO	74
PROCNO	1

F2 - Acquisition Parameters

Date_	20080123
Time	14.04
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	840
DS	2
SWH	31847.133 Hz
FIDRES	0.485949 Hz
AQ	1.0289652 sec
RG	3649.1
DW	15.700 usec
DE	6.00 usec
TE	296.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	10.50 usec
PL1	-1.00 dB
SFO1	100.6254358 MHz

======== CHANNEL f2 ========

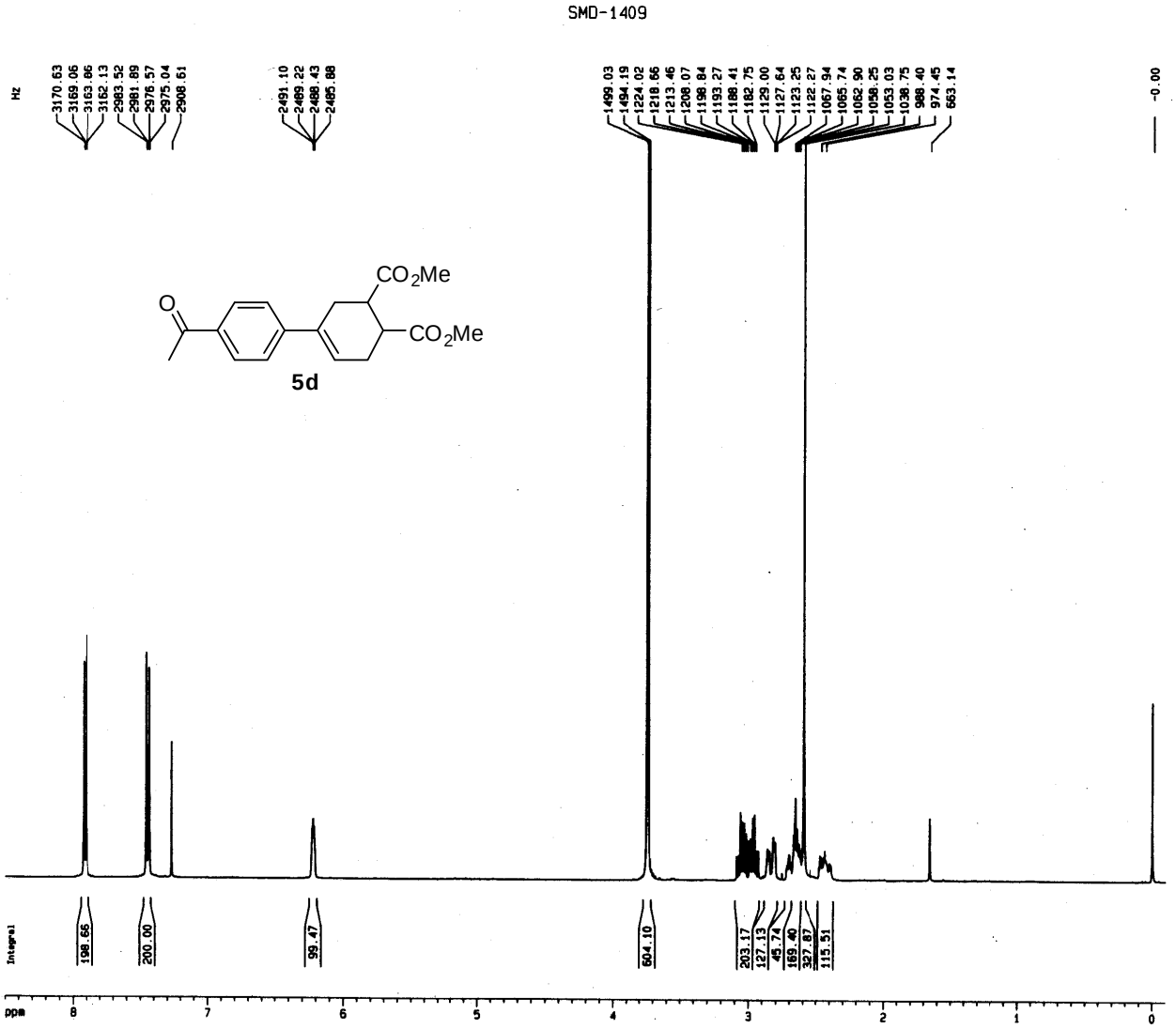
CPDPRG2	waltz16
NUC2	1H
PCPD2	105.00 usec
PL2	-2.00 dB
PL12	18.00 dB
PL13	20.00 dB
SFO2	400.1324708 MHz

F2 - Processing parameters

SI	32768
SF	100.6127290 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	30.00 cm
CY	20.00 cm
F1P	220.000 ppm
F1	22134.80 Hz
F2P	-5.000 ppm
F2	-503.06 Hz
PPMCM	7.50000 ppm/cm
HZCM	754.59546 Hz/cm



Current Data Parameters
NAME mar-08
EXPNO 31
PROCNO 1

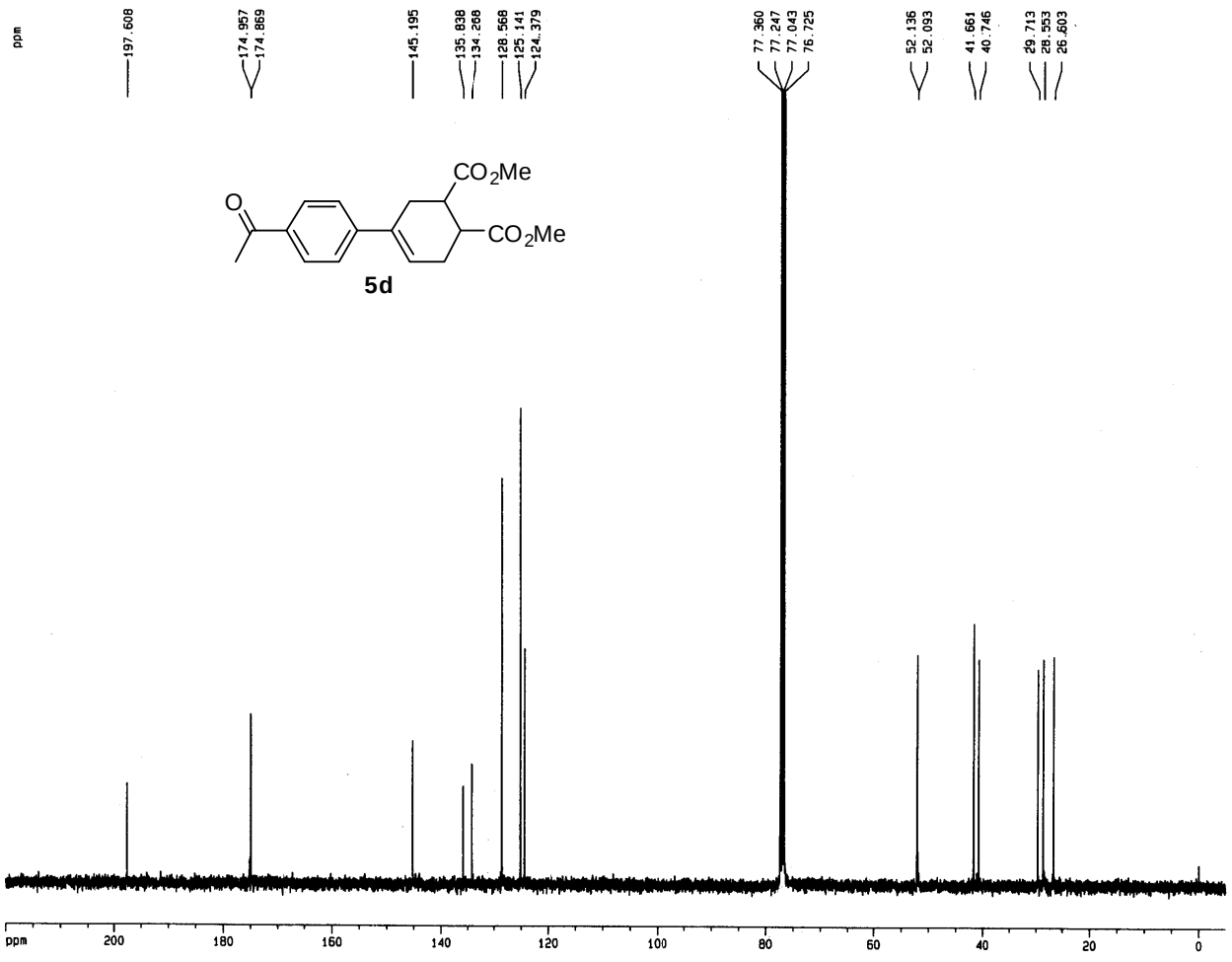
F2 - Acquisition Parameters
Date_ 20080401
Time 10.53
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300057 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
CY 34.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.28667 ppm/cm
HZCM 114.70393 Hz/cm

SMD-1409




```
Current Data Parameters
NAME                  mar-08
EXPNO                     32
PROCNO                     1

F2 - Acquisition Parameters
Date_               20080401
Time                   11.10
INSTRUM                spect
PROBHD   5 mm Dual 13C/
PULPROG                zgpg30
TD                      65536
SOLVENT                CDCl3
NS                      1124
DS                         2
SWH                31847.133 Hz
FIDRES                 0.485949 Hz
AQ                     1.0289652 sec
RG                      3649.1
DW                     15.700 usec
DE                      6.00 usec
TE                      296.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.50 usec
PL1                     -1.00 dB
SFO1               100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  105.00 usec
PL2                     -2.00 dB
PL12                    18.00 dB
PL13                    20.00 dB
SFO2               400.1324708 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6127691 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40

1D NMR plot parameters
CX                      30.00 cm
CY                      30.00 cm
F1P                    220.000 ppm
F1                   22134.81 Hz
F2P                     -5.000 ppm
F2                    -503.06 Hz
PPMCM                  7.50000 ppm/cm
HZCM                 754.59576 Hz/cm
```