

Supporting Information

Efficient Synthetic Method of Multisubstituted Allenes from the Reactions of Allylindium Reagents with 3°-Propargyl Alcohols

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Experimental Section

Typical experimental procedure : Reaction of 2-phenyl-3-butyn-2-ol with allylin-
dium reagents : Allyl bromide (97.4 μ L, 1.125 mmol) was added to suspension of
indium (86.1 mg, 0.75 mmol) in THF (1.0 mL). After being stirred for 30 min at room
temperature under nitrogen atmosphere, the solution of 2-phenyl-3-butyn-2-ol (73.1 mg,
0.5 mmol) in THF (1.0 mL) was added to reaction mixture and then, stirred at 35 °C for
4 h. The reaction mixture was quenched with aqueous 10 % HCl (5.0 mL). The aqueous
layer was extracted with ether (3 x 20 mL) and the combined organic phase was washed
with water and brine, dried with MgSO_4 , filtered and concentrated under reduced
pressure. The residue was purified by silica gel column chromatography using hexane
as an eluant to give 2-phenyl-hepta-2,3,6-triene (**2a**) (74.0 mg, 87%). ^1H NMR (400
MHz, CDCl_3) δ 7.41 (d, J = 7.79 Hz, 2H), δ 7.31 (t, J = 7.69 Hz, 2H), δ 7.19 (t, J = 7.28
Hz, 1H), δ 5.96-5.86 (m, 1H), δ 5.48-5.43 (m, 1H), δ 5.14 (d, J = 17.09 Hz, 1H), δ 5.04
(d, J = 10.09 Hz, 1H), δ 2.86 (t, J = 6.61 Hz, 2H), δ 2.09 (d, J = 2.86 Hz, 1H); ^{13}C NMR
(100 MHz, CDCl_3) δ 204.9, 137.8, 137.0, 128.6, 126.8, 126.0, 115.7, 101.2, 91.5, 33.8,
17.5; IR (film) 2977, 2867, 1382, 1350, 1125, 1076 cm^{-1} ; HRMS (EI) : m/z calcd. For
 $\text{C}_{13}\text{H}_{14}$: 170.1096; found: 170.1095.

6-Methyl-2-phenyl-hepta-2,3,6-triene (2b) ^1H NMR (400 MHz, CDCl_3) δ 7.41 (d, J =
7.42 Hz, 2H), δ 7.31 (t, J = 7.71 Hz, 2H), δ 7.19 (t, J = 7.29 Hz, 1H), δ 5.46-5.42 (m,
1H), δ 4.84 (s, 1H), δ 4.79 (s, 1H), δ 2.81 (d, J = 7.35 Hz, 2H), δ 2.10 (d, J = 2.82 Hz,
3H), δ 1.79 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.8, 144.4, 137.4, 128.2, 126.4,

125.8, 125.6, 110.9, 100.2, 90.9, 37.9, 22.3, 17.1; IR (film) 2970, 1649, 1493, 1443, 1370, 1026, 889 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 184.1252; found: 184.1248.

4-Methyl-2-phenyl-hepta-2,3,6-triene (2c) ^1H NMR (400 MHz, CDCl_3) δ 7.38 (d, J = 7.79 Hz, 2H), δ 7.30 (t, J = 7.73 Hz, 2H), δ 7.17 (t, J = 7.26 Hz, 1H), δ 5.91-5.81 (m, 1H), δ 5.11 (d, J = 17.02 Hz, 1H), δ 5.02 (d, J = 10.04 Hz, 1H), δ 2.82 (d, J = 6.83 Hz, 2H), δ 2.06 (s, 3H), δ 1.78 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 201.9, 138.4, 136.0, 128.1, 126.1, 125.6, 115.8, 99.8, 99.5, 39.0, 18.5, 17.3; IR (film) 2923, 1596, 1491, 1443, 1367, 1026, 912 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 184.1252; found: 184.1250.

4,6-Dimethyl-2-phenyl-hepta-2,3,6-triene (2d) ^1H NMR (400 MHz, CDCl_3) δ 7.39 (d, J = 7.99 Hz, 2H), δ 7.31 (t, J = 7.73 Hz, 2H), δ 7.17 (t, J = 7.28 Hz, 1H), δ 4.81 (s, 2H), δ 2.83-2.74 (m, 2H), δ 2.07 (s, 3H), δ 1.75 (s, 3H), δ 1.74 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 202.6, 143.1, 138.4, 128.1, 126.1, 125.7, 112.1, 98.8, 98.6, 43.8, 21.9, 18.0, 17.3; IR (film) 2978, 2868, 1444, 1382, 1350, 1128, 1076, 845 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 198.1409; found: 198.1407.

4-*n*-Butyl-2-phenyl-hepta-2,3,6-triene (2e) ^1H NMR (400 MHz, CDCl_3) δ 7.39 (d, J = 8.17 Hz, 2H), δ 7.30 (t, J = 7.72 Hz, 2H), δ 7.17 (t, J = 7.28 Hz, 1H), δ 5.90-5.80 (m, 1H), δ 5.09 (d, J = 17.04 Hz, 1H), δ 5.00 (d, J = 10.02 Hz, 1H), δ 2.82 (d, J = 6.85 Hz, 2H), δ 2.12-2.01 (m, 2H), δ 2.07 (s, 3H), δ 1.45-1.39 (m, 2H), δ 1.38-1.31 (m, 2H), δ 0.87 (t, J = 7.24 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 201.6, 138.4, 136.2, 128.2, 128.1, 126.0, 125.4, 115.6, 104.8, 100.9, 37.8, 32.1, 30.8, 29.7, 22.4, 17.3, 13.9; IR

(film) 2928, 1597, 1492, 1465, 1026, 912 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 226.1721; found: 226.1720.

4-*n*-Butyl-6-methyl-2-phenyl-hepta-2,3,6-triene (2f) ^1H NMR (400 MHz, CDCl_3) δ 7.40 (d, $J = 7.66$ Hz, 2H), δ 7.30 (t, $J = 7.73$ Hz, 2H), δ 7.17 (t, $J = 7.28$ Hz, 1H), δ 4.79 (s, 2H), δ 2.84-2.75 (m, 2H), δ 2.08 (s, 3H), δ 2.05-1.97 (m, 2H), δ 1.74 (s, 3H), δ 1.46-1.38 (m, 2H), δ 1.36-1.30 (m, 2H), δ 0.87 (t, $J = 7.22$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 202.2, 143.4, 138.4, 128.1, 126.0, 125.5, 112.0, 103.8, 100.1, 42.5, 31.5, 29.8, 22.5, 22.0, 17.3, 14.0; IR (film) 2928, 1597, 1492, 1444, 1371, 1065, 1026, 889 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 240.1878; found: 240.1879.

2,4-Diphenyl-hepta-2,3,6-triene (2g) ^1H NMR (400 MHz, CDCl_3) δ 7.46-7.41 (m, 4H), δ 7.34-7.29 (m, 4H), δ 7.24-7.18 (m, 2H), δ 6.03-5.93 (m, 1H), δ 5.19 (d, $J = 17.06$ Hz, 1H), δ 5.06 (d, $J = 10.09$ Hz, 1H), δ 3.33 (dd, $J = 5.00$ Hz, $J = 1.48$ Hz, 2H), δ 2.21 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 205.9, 136.9, 136.4, 135.7, 128.4, 128.4, 126.8, 126.0, 125.7, 116.2, 106.0, 103.9, 34.9, 16.8, 15.2; IR (film) 3082, 1596, 1491, 1445, 1026, 911 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 246.1409; found: 246.1408.

2,4-Diphenyl-6-methyl-hepta-2,3,6-triene (2h) ^1H NMR (400 MHz, CDCl_3) δ 7.46-7.42 (m, 4H), δ 7.34-7.27 (m, 4H), δ 7.23-7.17 (m, 2H), δ 4.90 (s, 1H), δ 4.85 (s, 1H), δ 3.28 (s, 2H), δ 2.21 (s, 3H), δ 1.80 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 206.6, 143.1, 136.9, 136.5, 128.3, 128.3, 126.7, 126.7, 126.2, 125.7, 112.4, 105.1, 103.0, 39.5, 22.5, 16.7; IR (film) 2915, 1596, 1492, 1445, 1371, 1065, 1026, 892 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 260.1565; found: 260.1564.

2-(*p*-Bromophenyl)-hepta-2,3,6-triene (2i) ^1H NMR (400 MHz, CDCl_3) δ 7.44-7.40 (m, 2H), δ 7.27-7.24 (m, 2H), δ 5.94-5.84 (m, 1H), δ 5.48-5.43 (m, 1H), δ 5.13 (d, J = 17.07 Hz, 1H), δ 5.04 (d, J = 10.08 Hz, 1H), δ 2.86 (t, J = 6.56 Hz, 2H), δ 2.06 (d, J = 2.93 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.5, 136.5, 136.3, 131.2, 127.2, 120.2, 115.5, 100.1, 91.5, 33.2, 17.0; IR (film) 2978, 2868, 1444, 1382, 1350, 1127, 845 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 248.0201; found: 248.0203.

2-(*p*-Bromophenyl)-6-methyl-hepta-2,3,6-triene (2j) ^1H NMR (400 MHz, CDCl_3) δ 7.44-7.40 (m, 2H), δ 7.28-7.24 (m, 2H), δ 5.46-5.42 (m, 1H), δ 4.83 (s, 1H), δ 4.79 (s, 1H), δ 2.80 (d, J = 7.36 Hz, 2H), δ 2.07 (d, J = 2.86 Hz, 3H), δ 1.78 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.7, 144.2, 136.5, 131.2, 127.2, 120.2, 111.0, 99.6, 91.3, 37.7, 22.3, 17.0; IR (film) 2977, 2866, 1382, 1350, 1125, 844 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 262.0357; found: 262.0359.

2-(*m*-Hydroxy-phenyl)-hepta-2,3,6-triene (2k) ^1H NMR (400 MHz, CDCl_3) δ 7.19 (t, J = 7.88 Hz, 1H), δ 6.99 (d, J = 7.87 Hz, 1H), δ 6.89 (t, J = 2.04 Hz, 1H), δ 6.68 (dd, J = 7.96 Hz, J = 2.43 Hz, 1H), δ 5.95-5.85 (m, 1H), 5.47-5.43 (m, 1H), δ 5.14 (d, J = 17.07 Hz, 1H), δ 5.04 (d, J = 10.11 Hz, 1H), δ 2.86 (t, J = 6.57 Hz, 2H), δ 2.06 (d, J = 2.87 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.6, 155.4, 139.4, 136.5, 129.4, 118.2, 115.4, 113.4, 112.5, 100.5, 91.2, 33.3, 17.1; IR (film) 3316, 2977, 2867, 1445, 1382, 1350, 1122, 1076 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 186.1045; found: 186.1045.

2-(*m*-Hydroxyphenyl)-6-methyl-hepta-2,3,6-triene (2l) ^1H NMR (400 MHz, CDCl_3) δ 7.19 (t, J = 7.91 Hz, 1H), δ 6.99 (d, J = 7.66 Hz, 1H), δ 6.89 (t, J = 1.81 Hz, 1H), δ

6.67 (dd, $J = 7.99$ Hz, $J = 2.42$ Hz, 1H), δ 5.46-5.41 (m, 1H), δ 4.84 (s, 1H), δ 4.79 (s, 1H), δ 4.75 (s, 1H), δ 2.80 (d, $J = 7.37$ Hz, 2H), δ 2.07 (d, $J = 2.84$ Hz, 3H), δ 1.79 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.8, 155.4, 144.3, 139.4, 129.4, 118.3, 113.4, 112.6, 110.9, 100.0, 91.0, 37.8, 22.3, 17.1; IR (film) 3365, 2968, 1648, 1584, 1486, 1444, 1283, 888 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 200.1201; found: 200.1205.

2-(*p*-Tolyl)-hepta-2,3,6-triene (2m) ^1H NMR (400 MHz, CDCl_3), δ 7.30 (d, $J = 8.2$ Hz, 2H), δ 7.12 (d, $J = 8.06$ Hz, 2H), δ 5.95-5.85 (m, 1H), δ 5.46-5.40 (m, 1H), δ 5.13 (d, $J = 17.07$ Hz, 1H), δ 5.03 (d, $J = 10.09$ Hz, 1H), δ 2.85 (t, $J = 6.56$ Hz, 2H), δ 2.33 (s, 3H), δ 2.07 (d, $J = 2.83$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.3, 136.6, 136.1, 134.5, 128.9, 125.5, 115.2, 100.6, 90.9, 33.4, 21.0, 17.1; IR (film) 2977, 2867, 1382, 1350, 1124, 845 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 184.1252; found: 184.1254.

6-Methyl-2-(*p*-tolyl)-hepta-2,3,6-triene (2n) ^1H NMR (400 MHz, CDCl_3), δ 7.30 (d, $J = 8.09$ Hz, 2H), δ 7.12 (d, $J = 8.00$ Hz, 2H), δ 5.43-5.39 (m, 1H), δ 4.83 (s, 1H), δ 4.78 (s, 1H), δ 2.80 (d, $J = 7.33$ Hz, 2H), δ 2.33 (s, 3H), δ 2.08 (d, $J = 2.78$ Hz, 3H), δ 1.79 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.5, 144.5, 136.1, 134.5, 128.9, 125.5, 110.8, 100.1, 90.7, 38.0, 22.3, 21.0, 17.2; IR (film) 2921, 1648, 1511, 1440, 1370, 1064, 1018, 889 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 198.1409; found: 198.1410.

1,1-Diphenyl-hexa-1,2,5-triene (2o) ^1H NMR (400 MHz, CDCl_3), δ 7.37-7.25 (m, 10H), δ 5.98-5.88 (m, 1H), δ 5.71 (t, $J = 6.77$ Hz, 1H), δ 5.16 (d, $J = 17.08$ Hz, 1H), δ 5.07 (d, $J = 10.07$ Hz, 1H), δ 2.95 (t, $J = 6.56$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 205.8, 137.0, 136.1, 128.4, 128.3, 127.0, 115.8, 110.2, 92.4, 33.3; IR (film) 3058, 1637,

1597, 1492, 1442, 1031, 992, 914 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 232.1252; found: 232.1252.

1,1-Diphenyl-5-methyl-hexa-1,2,5-triene (2p) ^1H NMR (400 MHz, CDCl_3), δ 7.39-7.24 (m, 10H), δ 5.69 (t, $J = 7.37$ Hz, 1H), δ 4.86 (s, 1H), δ 4.81 (s, 1H), δ 2.90 (d, $J = 7.36$ Hz, 2H), δ 1.76 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 206.5, 144.5, 137.4, 128.8, 128.7, 127.4, 111.7, 110.1, 92.6, 38.2, 22.8; IR (film) 2977, 2868, 1444, 1382, 1350, 1127, 1076, 845 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 246.1409; found: 246.1404.

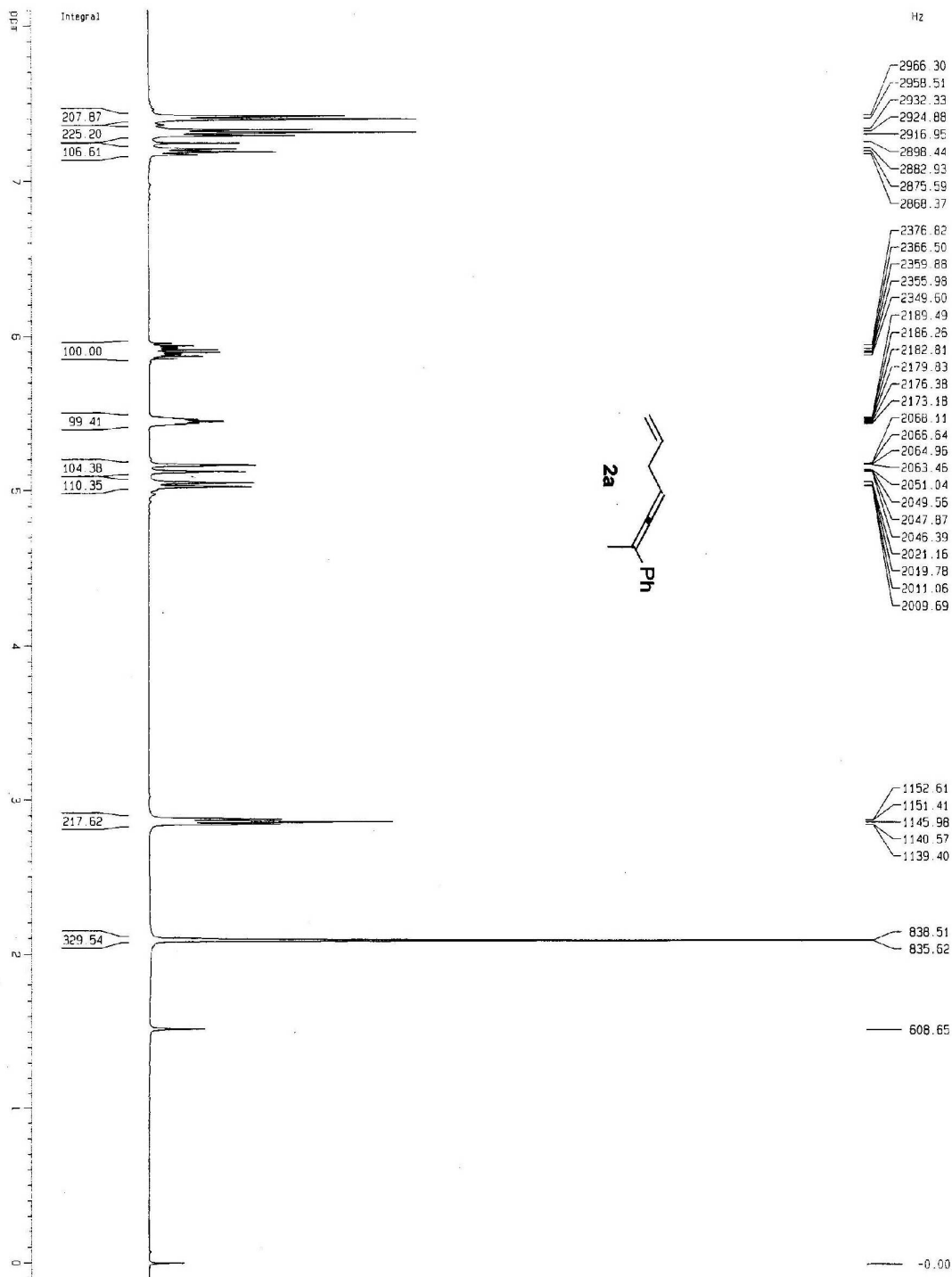
2-Methyl-4-(1-phenylpropyl)-hepta-2,3,6-triene (2q) ^1H NMR (400 MHz, CDCl_3) δ 7.29 (d, $J = 7.57$ Hz, 1H), δ 7.19-7.16 (m, 3H), δ 5.85-5.75 (m, 1H), δ 5.03 (d, $J = 17.06$ Hz, 1H), δ 4.98 (d, $J = 10.05$ Hz, 1H), δ 2.67 (d, $J = 6.82$ Hz, 2H), δ 2.62 (t, $J = 7.82$ Hz, 2H), δ 1.95 (t, $J = 7.23$ Hz, 2H), δ 1.74-1.67 (m, 2H), δ 1.68 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 199.0, 142.8, 136.8, 128.4, 128.2, 125.5, 115.0, 99.8, 95.9, 38.1, 35.5, 31.9, 29.5, 21.0; IR (film) 2980, 1742, 1446, 1374, 1240, 1119, 1047 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 226.1721; found: 226.1722.

2,6-Dimethyl-4-(1-phenylpropyl)-hepta-2,3,6-triene (2r) ^1H NMR (400 MHz, CDCl_3) δ 7.29 (d, $J = 7.59$ Hz, 2H), δ 7.19-7.17 (m, 3H), δ 4.75 (s, 1H), δ 4.72 (s, 1H), δ 2.64 (s, 2H), δ 2.61 (t, $J = 7.91$ Hz, 2H), δ 1.91 (t, $J = 7.21$ Hz, 2H), δ 1.73-1.66 (m, 2H), δ 1.71 (s, 3H), δ 1.69 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 199.7, 144.0, 142.9, 128.4, 128.2, 125.5, 111.4, 98.8, 94.9, 43.0, 35.5, 31.3, 29.5, 21.7, 20.8; IR (film) 2980, 1742, 1374, 1240, 1120, 1048, 846 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 240.1878; found: 240.1879.

1-Cyclohexyl-3-(1-phenylpropyl)-hexa-1,2,5-triene (2s) This compound was prepared in a fashion analogous to (**2a**) utilizing In (114.8 mg, 1.0 mmol) and allyl bromide (130 μl , 1.5 mmol) to give **2s** (106.4 mg, 80%). ^1H NMR (400 MHz, CDCl_3) δ 7.30-7.16 (m, 5H), δ 5.86-5.76 (m, 1H), δ 5.02 (d, $J = 17.18$ Hz, 1H), δ 4.98 (d, $J = 10.86$ Hz, 1H), δ 2.67 (d, $J = 6.76$ Hz, 2H), δ 2.63 (t, $J = 7.75$ Hz, 2H), δ 2.09 (t, $J = 5.86$ Hz, 4H), δ 1.95 (t, $J = 7.17$ Hz, 2H), δ 1.77-1.69 (m, 2H), δ 1.59-1.48 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 195.5, 142.8, 136.9, 128.4, 128.2, 125.5, 114.9, 103.7, 99.7, 38.2, 35.3, 32.1, 31.9, 29.3, 27.9, 26.3; IR (film) 2976, 2861, 1444, 1382, 1350, 1123 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 266.2034; found: 266.2034.

1-Cyclohexyl-5-methyl-4-(1-phenylpropyl)-hexa-1,2,5-triene (2t) This compound was prepared in a fashion analogous to (**2a**) utilizing In (114.8 mg, 1.0 mmol) and 3-bromide-2-methyl-propene (151 μl , 1.5 mmol) to give **2t** (116.2 mg, 83%). ^1H NMR (400 MHz, CDCl_3) δ 7.29-7.15 (m, 5H), δ 4.74 (s, 1H), δ 4.71 (s, 1H), δ 2.65 (s, 2H), δ 2.62 (t, $J = 7.92$ Hz, 2H), δ 2.10 (t, $J = 5.90$ Hz, 4H), δ 1.92 (t, $J = 7.16$ Hz, 2H), δ 1.76-1.68 (m, 2H), δ 1.70 (s, 3H), δ 1.60-1.49 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 196.5, 144.4, 143.3, 128.8, 128.6, 125.9, 111.8, 103.2, 99.1, 43.7, 35.8, 32.4, 31.8, 29.8, 28.2, 26.7, 22.2; IR (film) 2981, 1742, 1374, 1240, 1047 cm^{-1} ; HRMS (EI) : m/z calcd. For $\text{C}_{13}\text{H}_{14}$: 280.2191; found: 280.2194.

LJY-088



Current Data Parameters

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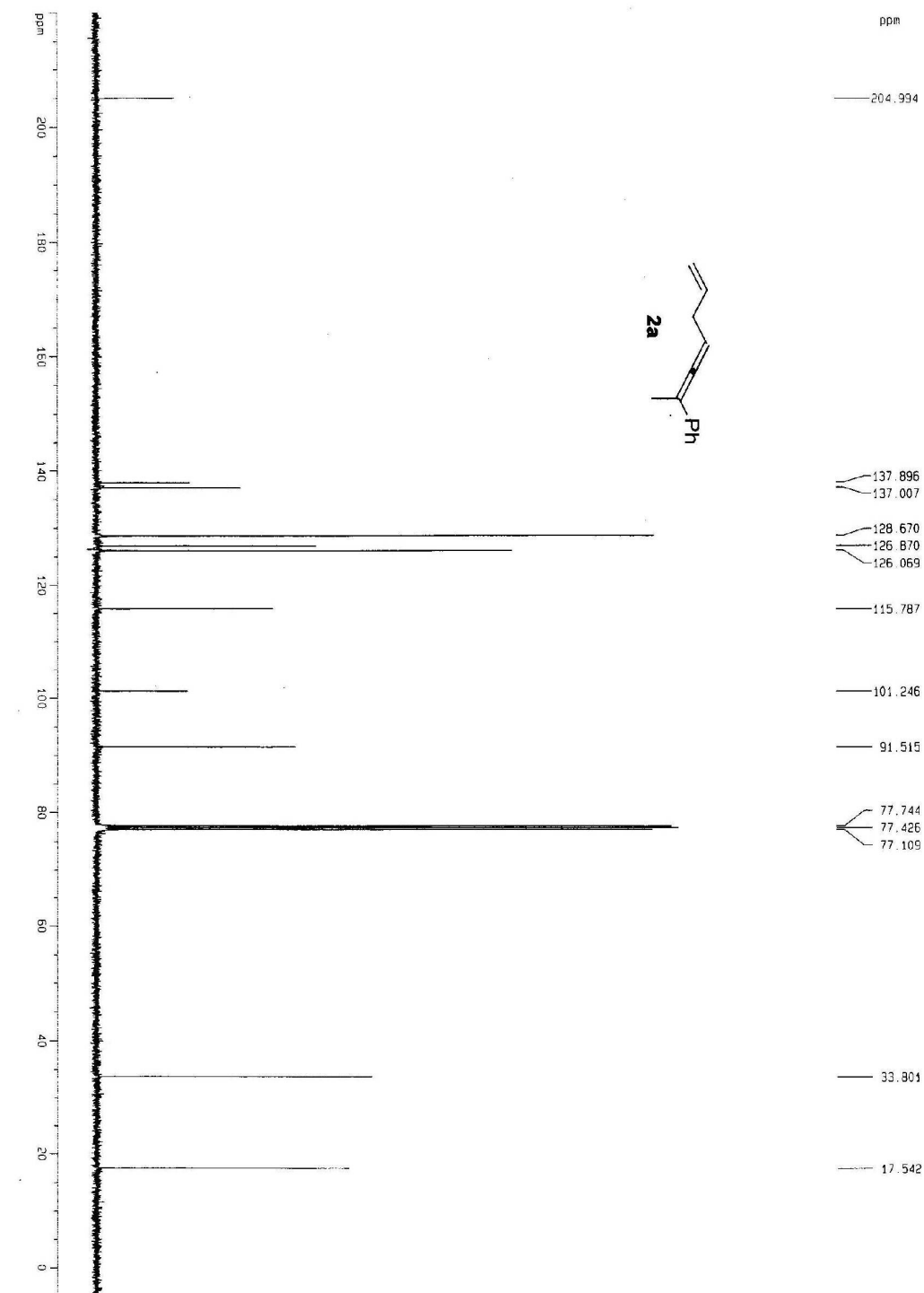
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LJY-088



Current Data Parameters
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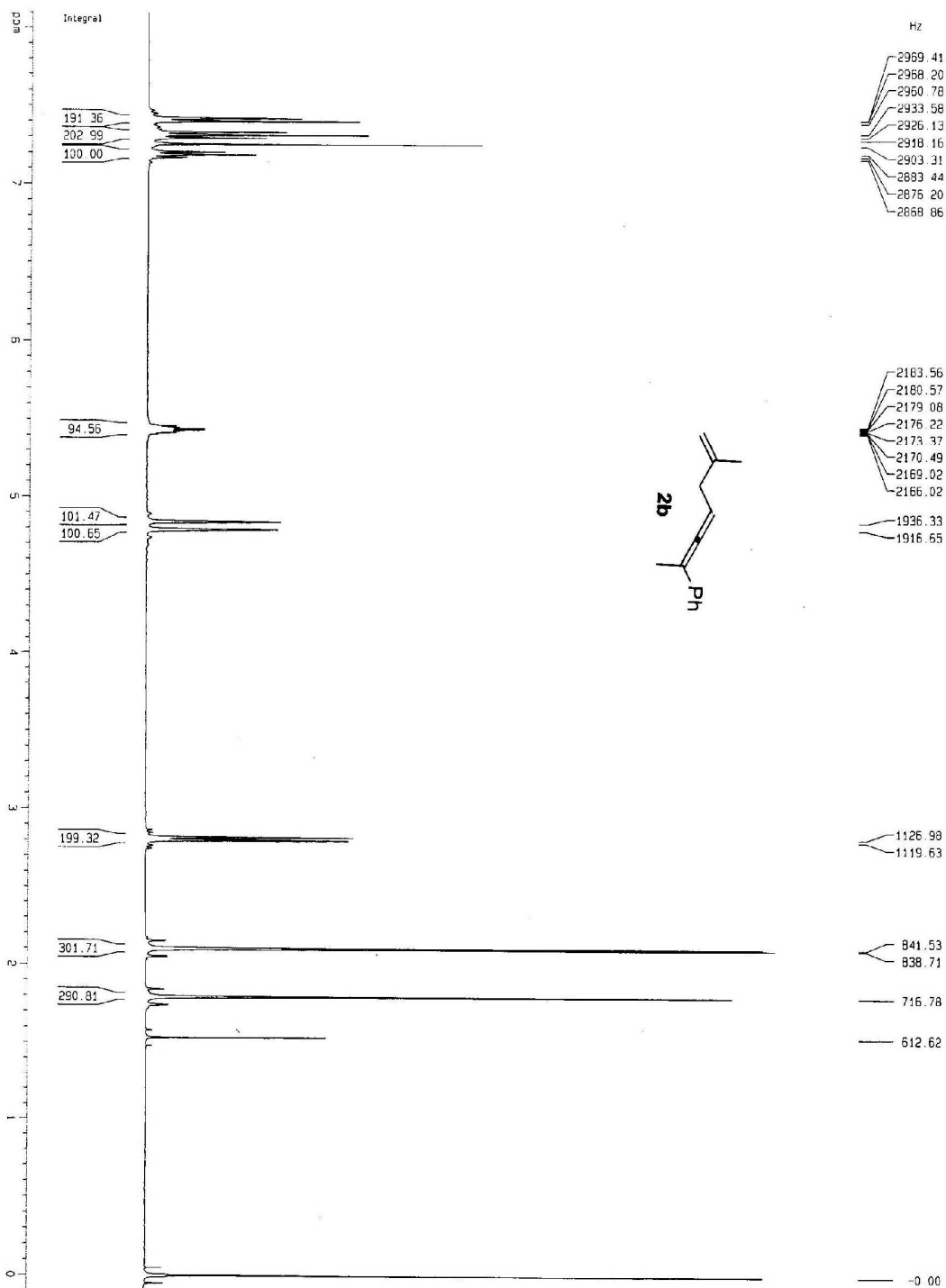
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PPHCK 734.59545 Hz/cm
HZCW

LJY-105



Current Data Parameters
 NAME LJY-105
 EXPNO 05
 PROCNO 1

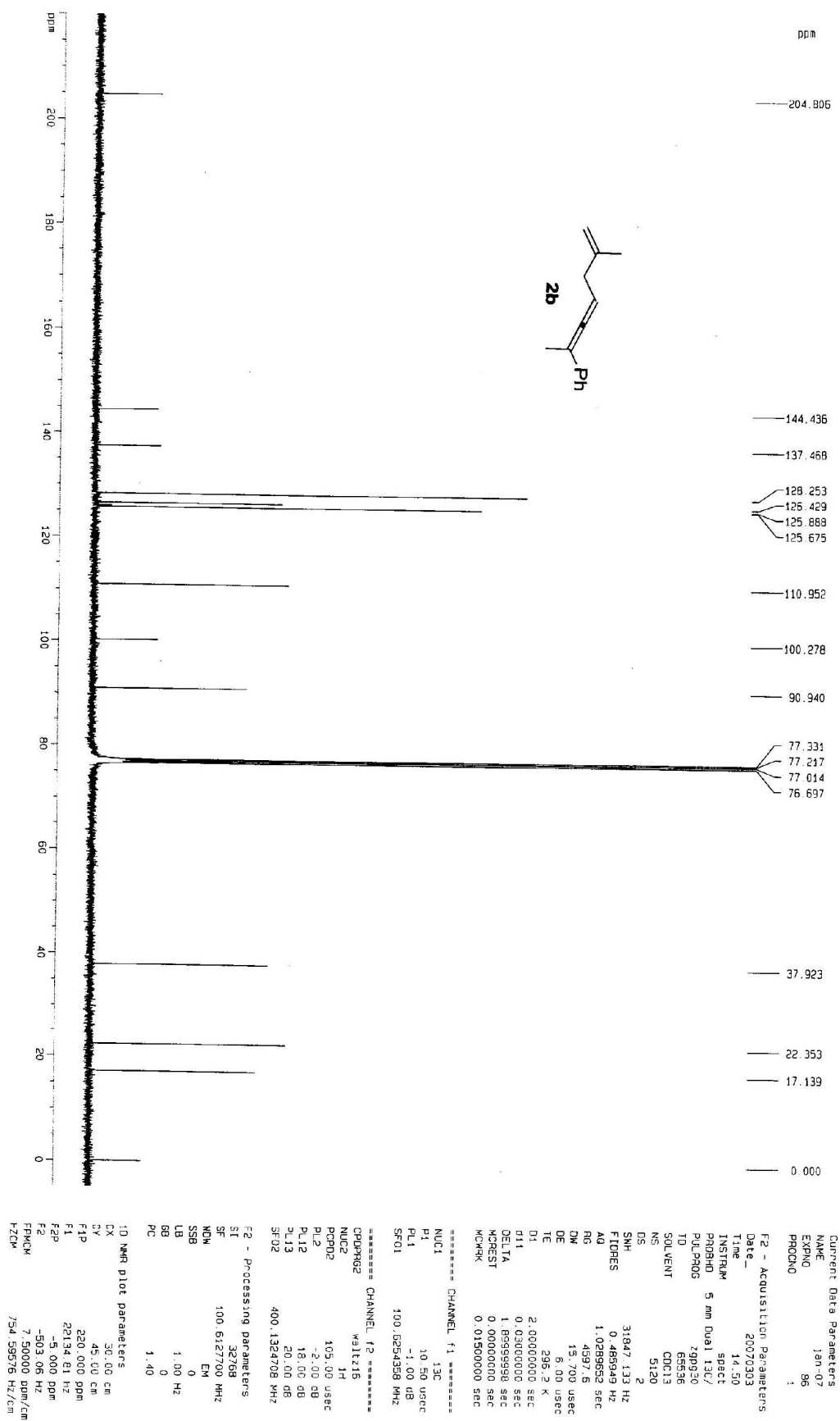
F2 - Acquisition Parameters
 Date_ 20070303
 Time 14.39
 INSTRUM spect
 PROBNM 5 mm QNP 13C/
 PULPROG zg30
 TO 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.250967 Hz
 AQ 1.5923444 sec
 RG 362
 JM 60.800 usec
 DE 6.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 ACQRES 0.00000000 sec
 MCNMR 0.01500000 sec

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

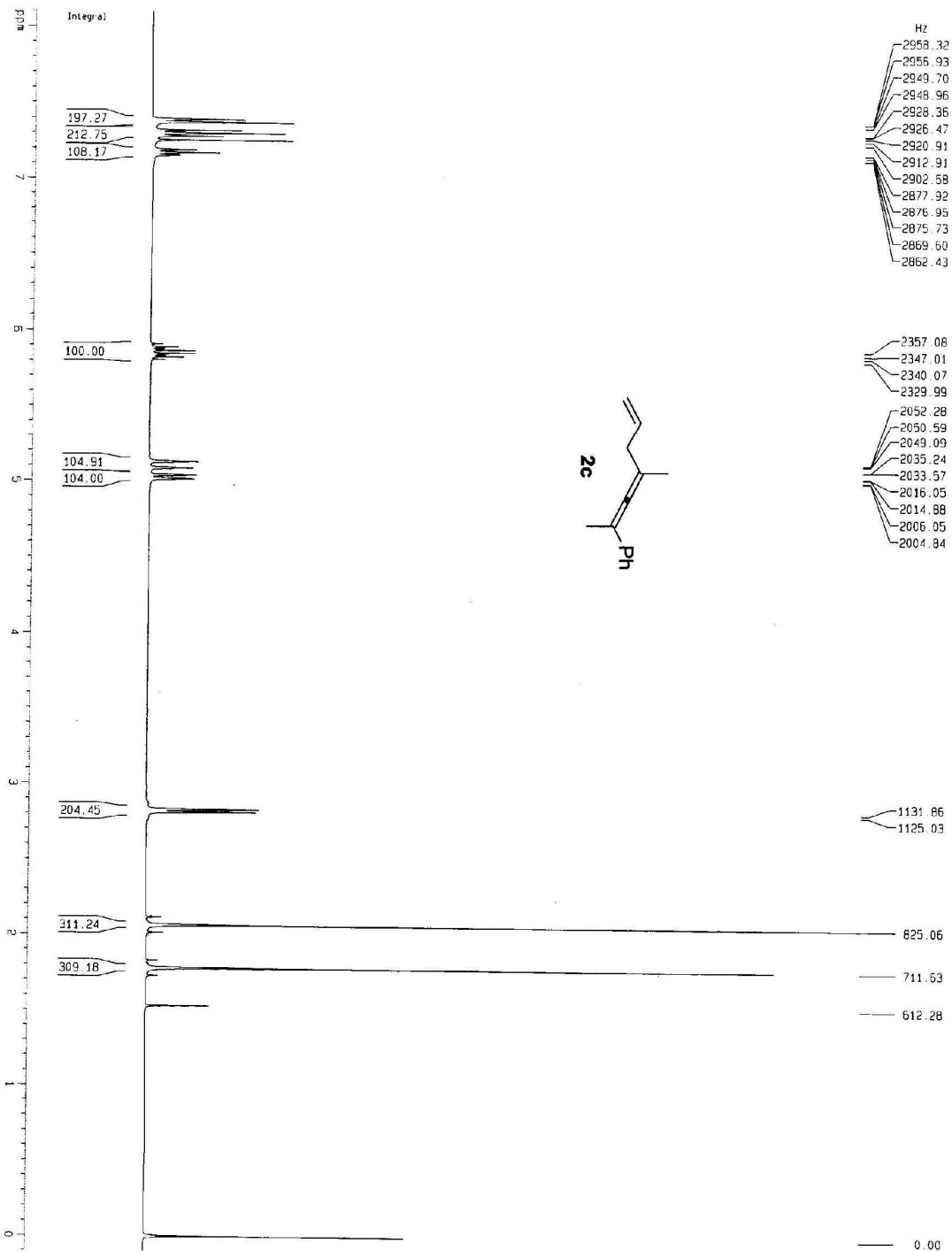
F2 - Processing parameters
 SI 16384
 SF 400.1300113 MHz
 KW EM
 SSR 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 CY 17.00 cm
 F1p 8.100 ppm
 F1 3241.05 Hz
 F2p -0.100 ppm
 F2 -40.01 Hz
 PPMCM 0.27333 ppm/cm
 HZCM 109.36897 Hz/cm

LJY-105



LJv-108



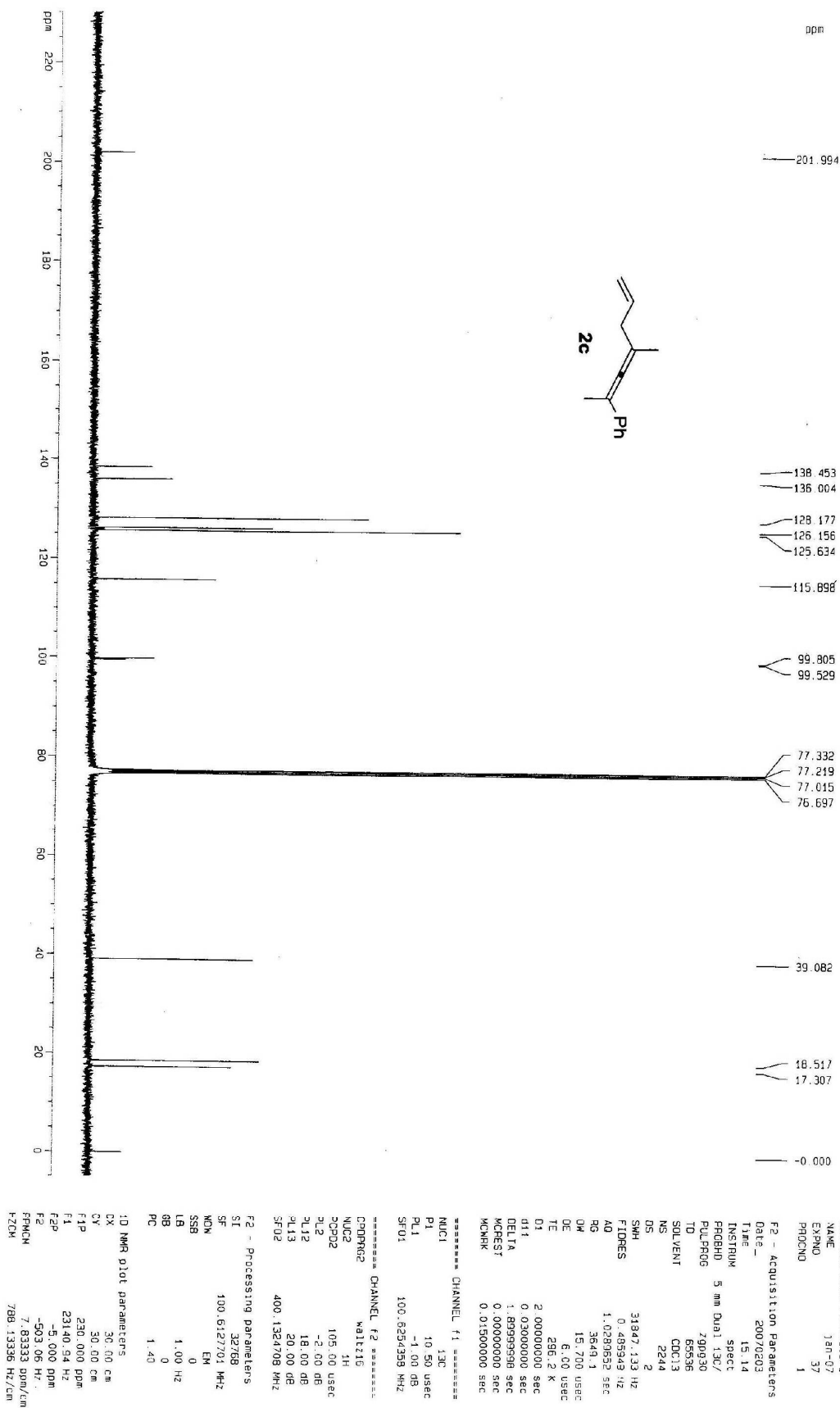
Current Data Parameters
 NAME: LJv-108
 EXPNO: 36
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 2007/02/03
 Time: 17:08
 INSTRUM: spect
 PROBRD: 5 mm Dual 13C/
 PULPROG: zgpg30
 TD: 32768
 SOLVENT: CDCl3
 NS: 32
 DS: 0
 SWH: 823.585 Hz
 FIDRES: 0.250957 Hz
 AQ: 1.5922444 sec
 RG: 322.5
 DM: 60.000 usec
 DE: 6.00 usec
 TE: 296.2 K
 D1: 1.00000000 sec
 MCREST: 0.00000000 sec
 MCPRK: 0.01500000 sec

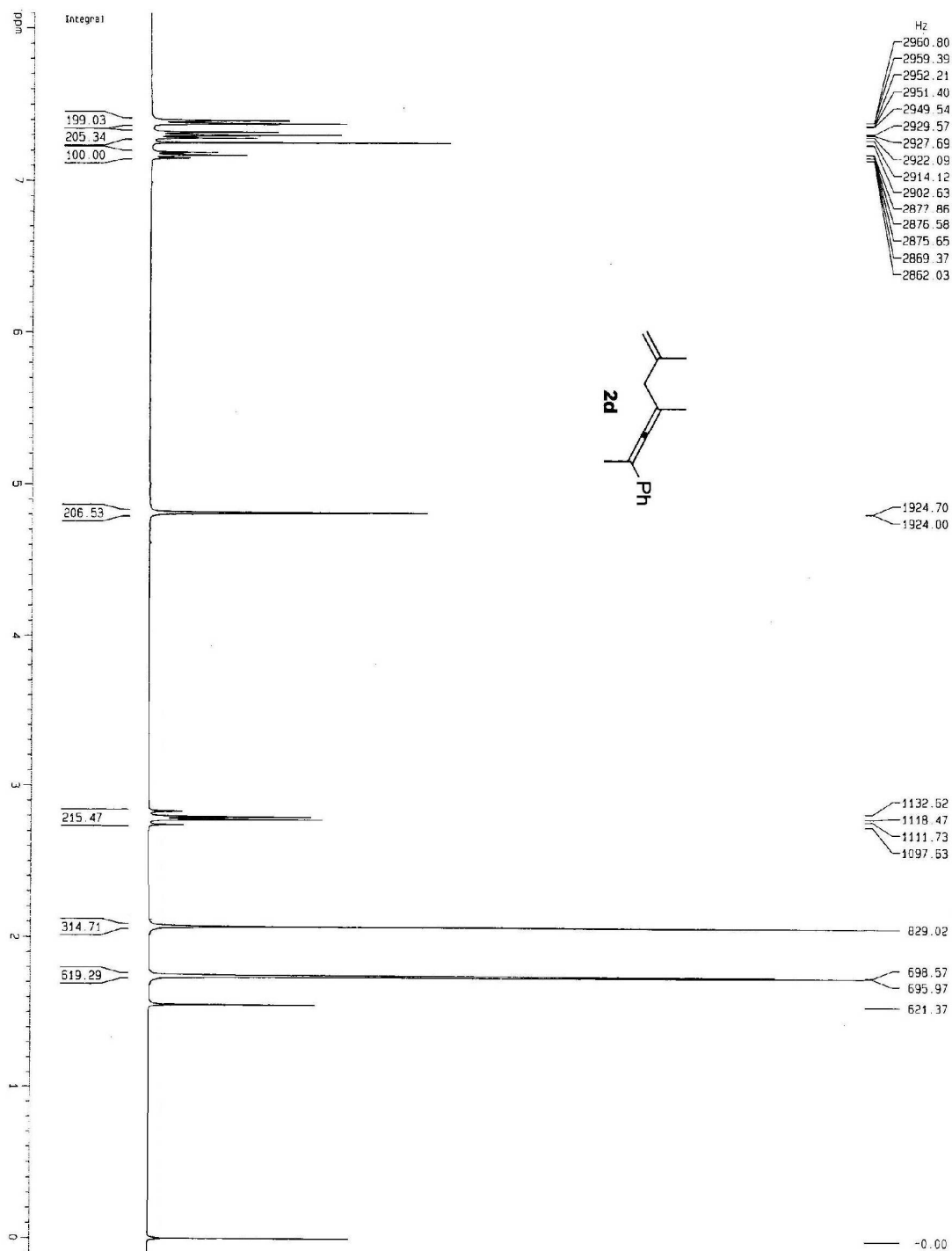
===== CHANNEL f1 =====
 NUC1: 13C
 P1: 11.00 usec
 PL1: -2.00 dB
 SFO1: 400.1324710 MHz

F2 - Processing parameters
 SI: 16384
 SF: 400.1300120 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
 FWHM: 0.27333 nm/cm
 HZCM: 109.35997 Hz/cm



LJY-206

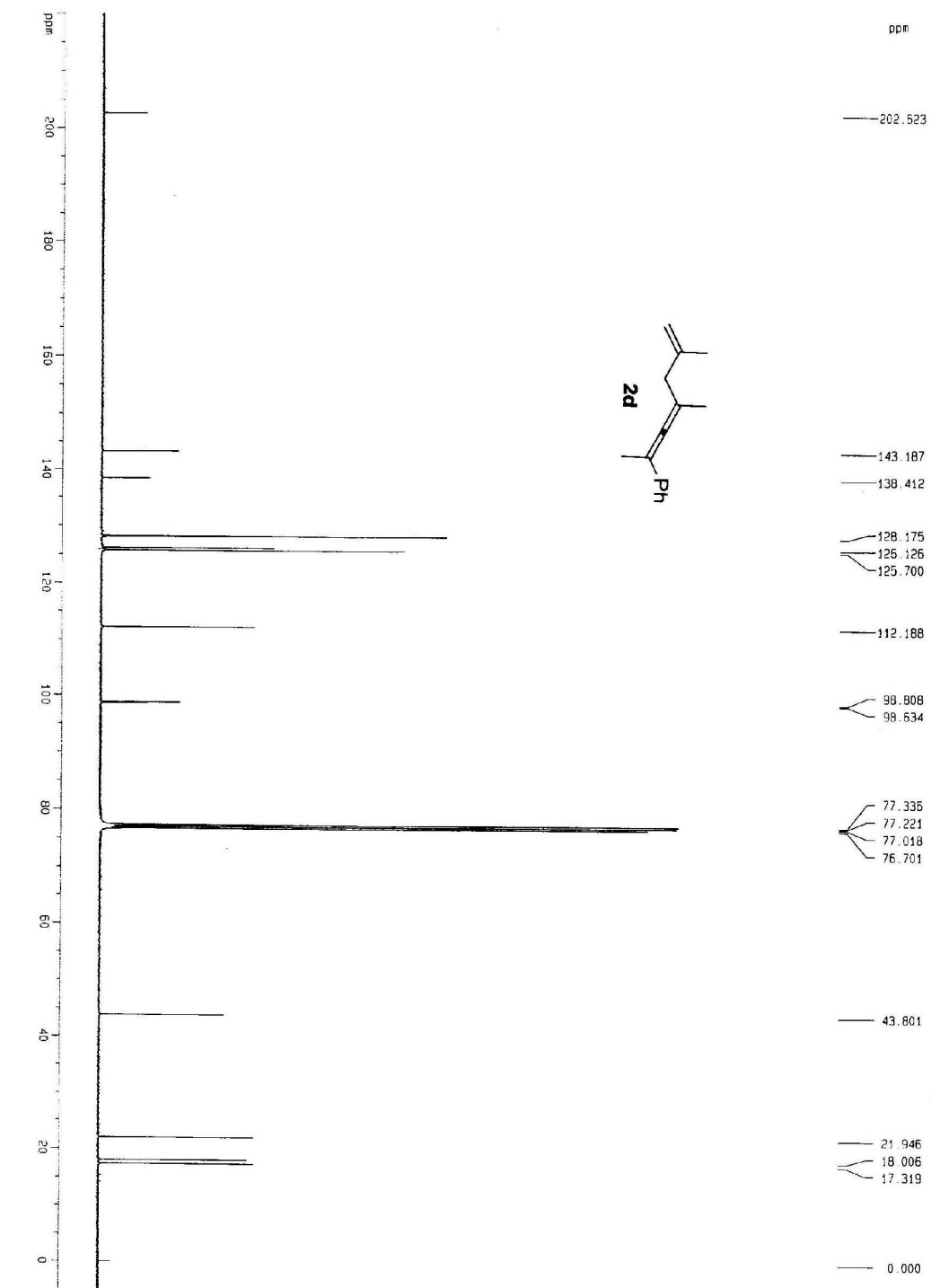


Current Data Parameters
NAME LJY-206
EXPNO 132
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070815
Time 22.37
INSTRUM spect
PROBHD 5 mm QNP1 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.5923444 sec
RG 326
FM 60.800 usec
DE 6.00 usec
TE 295.2 K
NUC1 13C
NUC2 1H
PC 1.00
F2 - Processing parameters
SI 16384
SF 400.130120 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
F1 8.100 ppm
F2 3241.05 Hz
F3 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM 109.36837 Hz/cm

LJY-206



Current Data Parameters
NAME LJY-206
EXPNO 133
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070815
Time 22:41
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 12532
DS 2
SWH 31847.133 Hz
FIDRES 0.485943 Hz
AQ 1.028952 sec
RG 256
DW 15.700 usec
DE 5.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.88999998 sec
ACQRES 0.00000000 sec
NCMRK 0.01500000 sec

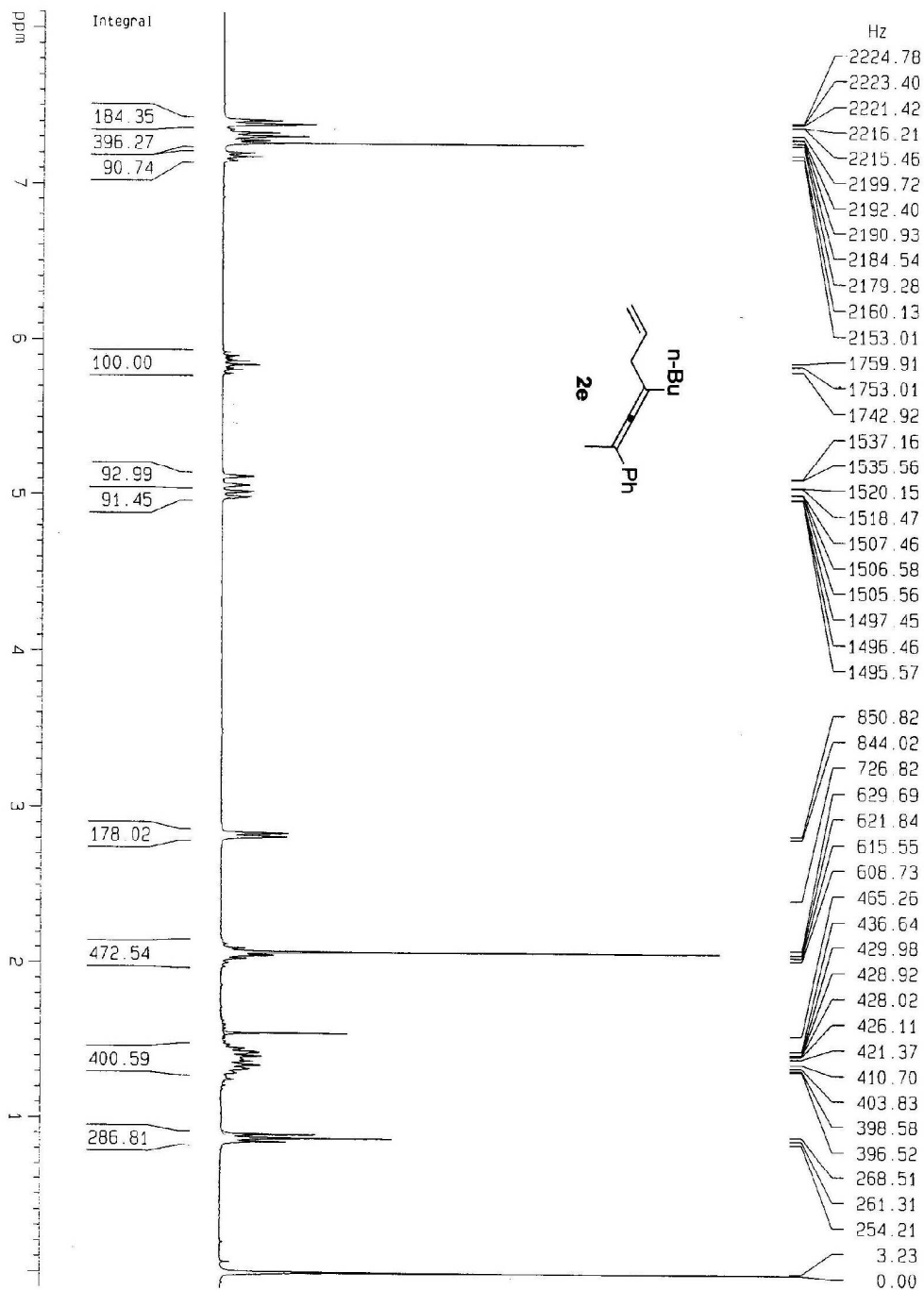
===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.625456 MHz

===== 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 100.6127701 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13 NMR pilot parameters
CX 30.00 cm
CY 15.00 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPKCM 7.50000 ppm/cm
H2CM 754.59576 Hz/cm

LJY-129



Current Data Parameters

NAME: Jm-07
EXPNO: 247
PROCNO: 1

F2 - Acquisition Parameters

Date_: 20070226
Time: 9.34
INSTRUM: spect
PROBHD: 5 mm GNP 1H/1
PULPROG: zg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 0
SWH: 6172.839 Hz
FIDRES: 0.18880 Hz
AQ: 2.6542580 sec
RG: 1024
DM: 81.000 uSec
DE: 6.00 uSec
TE: 0.0 K
D1: 1.00000000 sec

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

NUC1: 1H
P1: 10.20 uSec
PL1: 0.00 dB
SFO1: 300.1318534 MHz

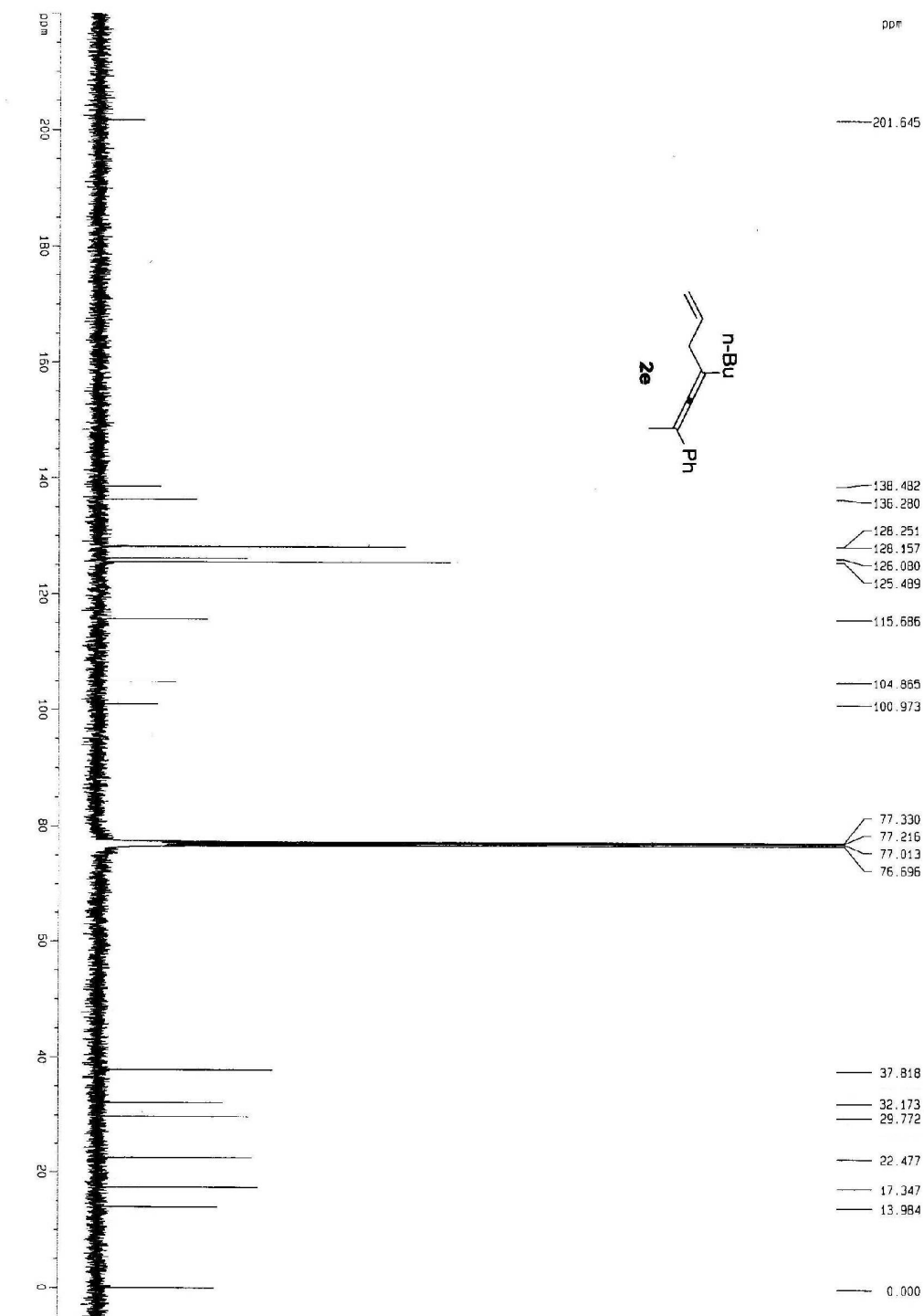
F2 - Processing parameters

SF: 300.1300062 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

ID NMR plot parameters

CX: 20.00 cm
CY: 13.00 cm
FJP: 8.100 ppm
F1: 2431.05 Hz
F2P: -0.100 ppm
F2: -30.01 Hz
PPMCM: 0.41000 ppm/cm
HZCM: 123.05531 Hz/cm

LJY-129



Current Data Parameters

NAME	EXPNO	PROCNO
NAME	Jan-07	80
EXPNO	1	1
PROCNO	1	1

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DM	DE	TE	D1	d11	DELTA	NCREST	NAME
20070226	16:50	spect	5 mm DuJ 13C/	zgpg30	65536	CDCl3	4695	2	31847.133 Hz	0.485949 Hz	1.028962 sec	3549.1	15.700 usec	5.000 usec	296.2 K	2.00000000 sec	0.03000000 sec	1.89999998 sec	0.00000000 sec	0.01500000 sec

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

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

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

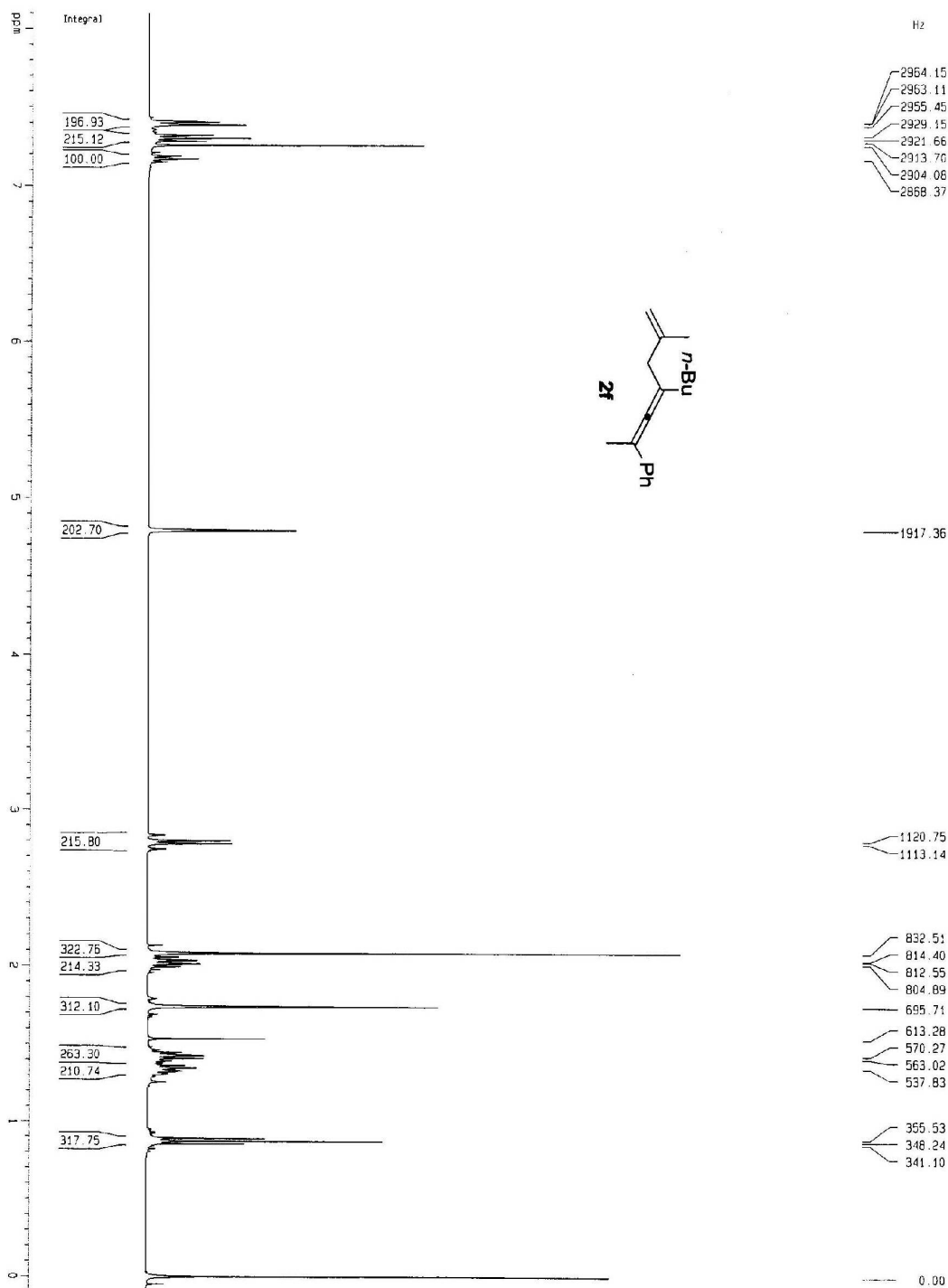
CPDPRG2	WALTZ16	NUC2	PCPD2	PL2	PL12	PL13	SFO2
WALTZ16	1H	105.00 usec	-2.00 dB	18.00 dB	20.00 dB	400.1324708 MHz	

F2 - Processing parameters

SI	SF	WDW	SSB	LB	GB	PC
32768	100.6127701 MHz	EM	0	1.00 Hz	0	1.40

1D NMR plot parameters

CX	F1P	F2	PPMCH	HZCM
30.00 cm	220.000 ppm	22134.81 Hz	-5.000 ppm	7.50000 ppm/cm
				754.59576 Hz/cm



Current Data Parameters
NAME Jan-07
EXPNO 83
PROCNO 1

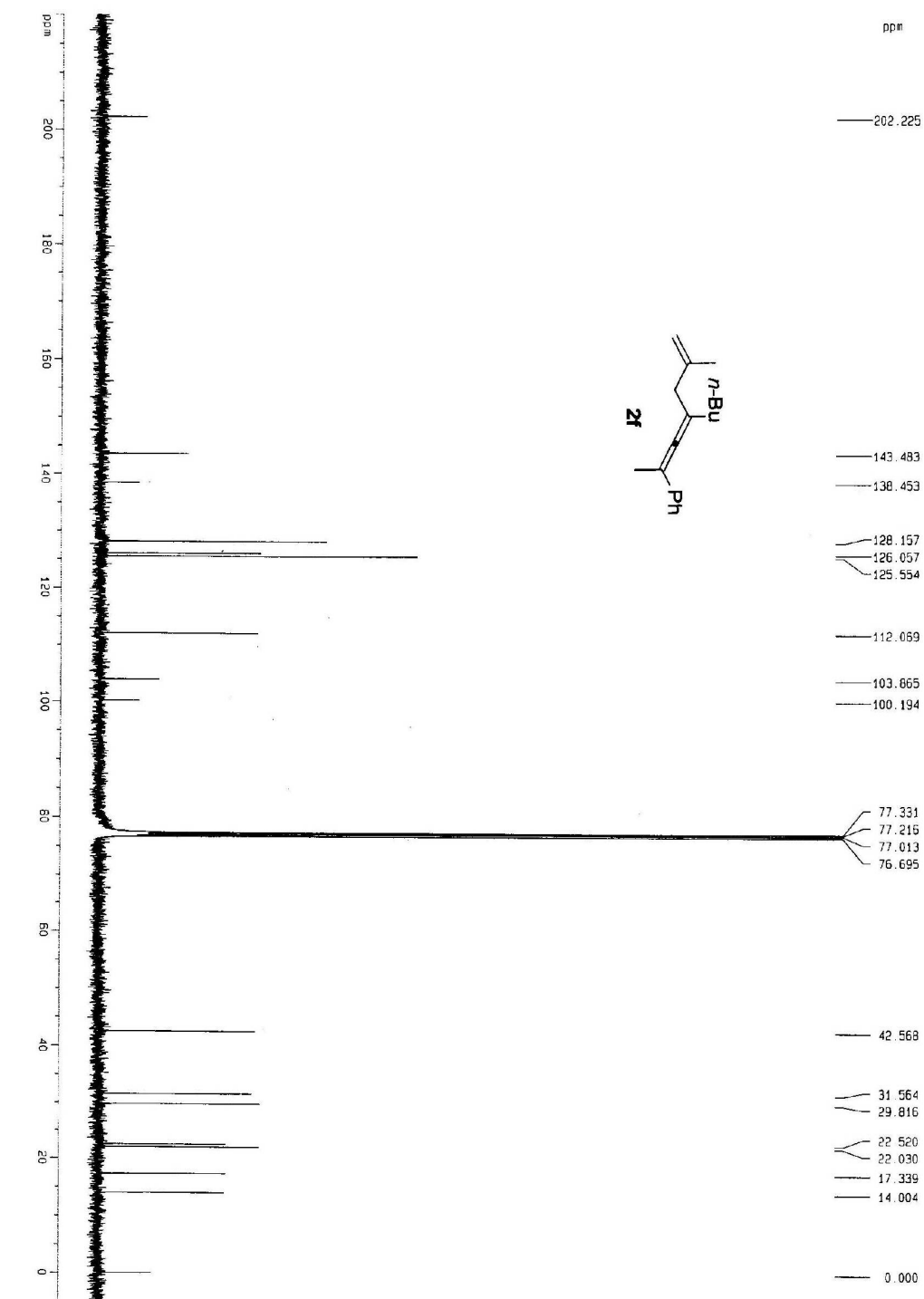
F2 - Acquisition Parameters
Date_ 20070303
Time 10:37
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 362
DM 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1362710 MHz

F2 - Processing parameters
SI 16384
SF 400.1360106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 30.00 cm
CY 14.00 cm
F1P 8.100 ppm
F2P 3241.05 Hz
F2 -40.100 dB
PHICH 0.27333 DDV/cm
H2OH 109.36687 Hz/cm

LJY-130



Current Data Parameters
 NAME LJY-130
 EXPNO 1
 PROCNO 1

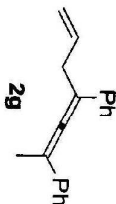
F2 - Acquisition Parameters
 Date_ 20070303
 Time 14.31
 INSTRUM spect
 PROBO 5 mm DuJ 13C/
 PULPROG zgpg30
 TD 65536
 ID C0C13
 SOLVENT CDCl3
 NS 4469
 DS 2
 SWH 31847.133 Hz
 FIDRES 0.465649 Hz
 AQ 1.028952 sec
 RG 114
 DM 15.700 usec
 DE 6.00 usec
 TE 296.2 K
 D3 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MEMRK 0.01500000 sec

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

===== CHANNEL f2 =====
 CPOPRG2 waltz16
 NUC2 1H
 P2 105.00 usec
 PL2 -2.00 dB
 PL12 18.00 dB
 PL13 20.00 dB
 SFO2 400.1324708 MHz

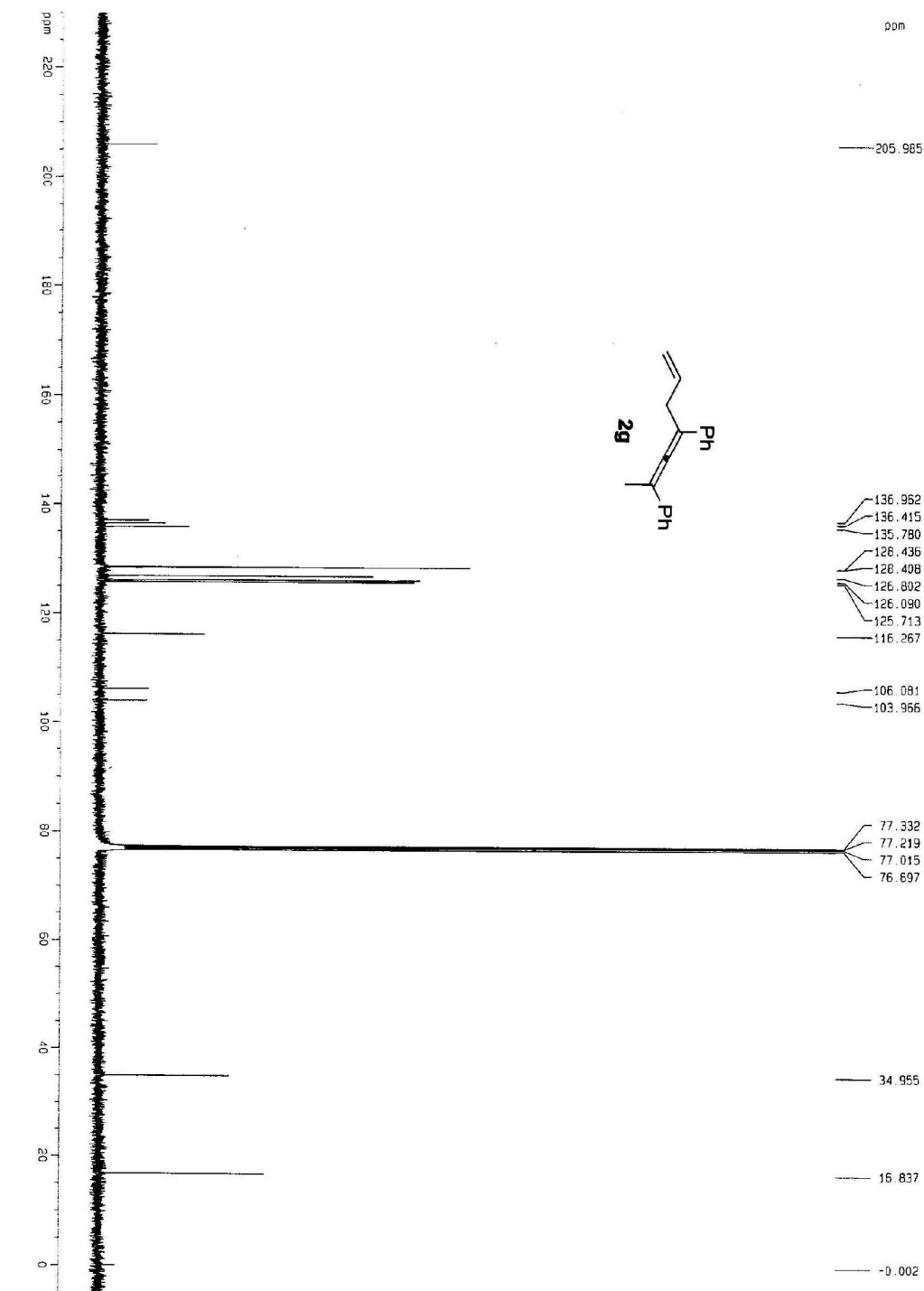
F2 - Processing Parameters
 SI 32768
 SF 100.6127694 MHz
 KCM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 MHz plot parameters
 CX 50.00 cm
 CY 56.00 cm
 FIP 220.000 ppm
 F1 22134.81 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 FPCN 754.59576 Hz/cm
 HZCN



Current Data Parameters	
NAME	Value
EXPNO	13
PROCNO	1
F2 - Acquisition Parameters	
Date_	20070327
Time	15.28
INSTRUM	spec
PROBHD	5 mm QNP1 1H/
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	362
CM	60.800 usec
CE	6.00 usec
TE	295.2 K
CL	1.00000000 sec
MOREST	0.00000000 sec
MONRR	0.01500006 sec
===== CHANNEL f1 =====	
NUC1	1H
PL1	11.00 usec
PI1	-2.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	16384
MD	400.1300121 MHz
SSB	EM
3	0
53	0.30 Hz
63	0
P2	1.00
10 NMR plot parameters	
CX	30.00 cm
CP	30.00 cm
F1P	8.100 cpm
F2P	3241.05 Hz
F2	-40.01 Hz
PRMCM	0.27132 PRM/cm
HZCM	109.36687 Hz/cm

LY-140



Current Data Parameters

NAME	EXPNO	PROCNO	DATE_	TIME	INSTRUM	SPECT	PROBHD	PULPROG	TO	SOLVENT	NS	DS	SNH	FIDRES	AC	RG	DM	DE	TE	D1	d11	DELTA	MICEST	MCMRK
LY-140	14	1	20070327	13.57	5 mm QNP 13C/	zgpg30	zpgp30	65536	2048	2	31847.133 Hz	0.485049 Hz	1.0289552 sec	3849.1	13.700 usec	296.2 K	2.00000000 sec	0.03000000 sec	1.89599988 sec	0.00000000 sec	0.01500000 sec			

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

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

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

NUC2	P2	PL2	SFO2
1H	105.00 usec	-2.00 dB	400.1324708 MHz

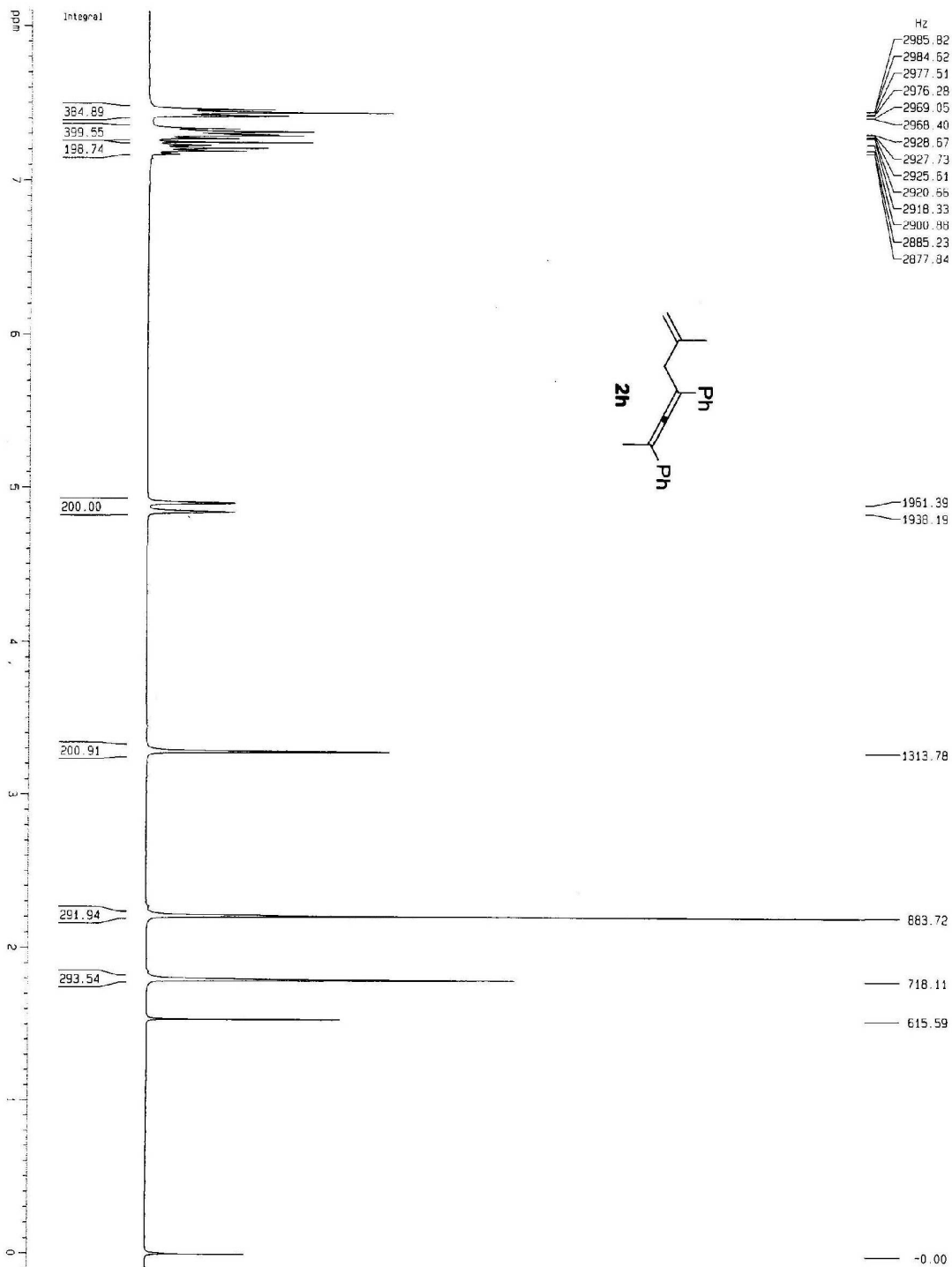
F2 - Processing parameters

SI	SF	WDW	SSB	LB	GB	PC
32768	100.6127710 MHz	CM	0	1.00 Hz	0	1.40

1D NMR plot parameters

CX	CY	F1P	F2P	PRNCH
30.00 cm	34.00 cm	230.000 ppm	-5.000 ppm	788.13356 Hz/cm

LJY-141



Current Data Parameters
 NAME mar-07
 EXPNO 15
 PROCNO 1

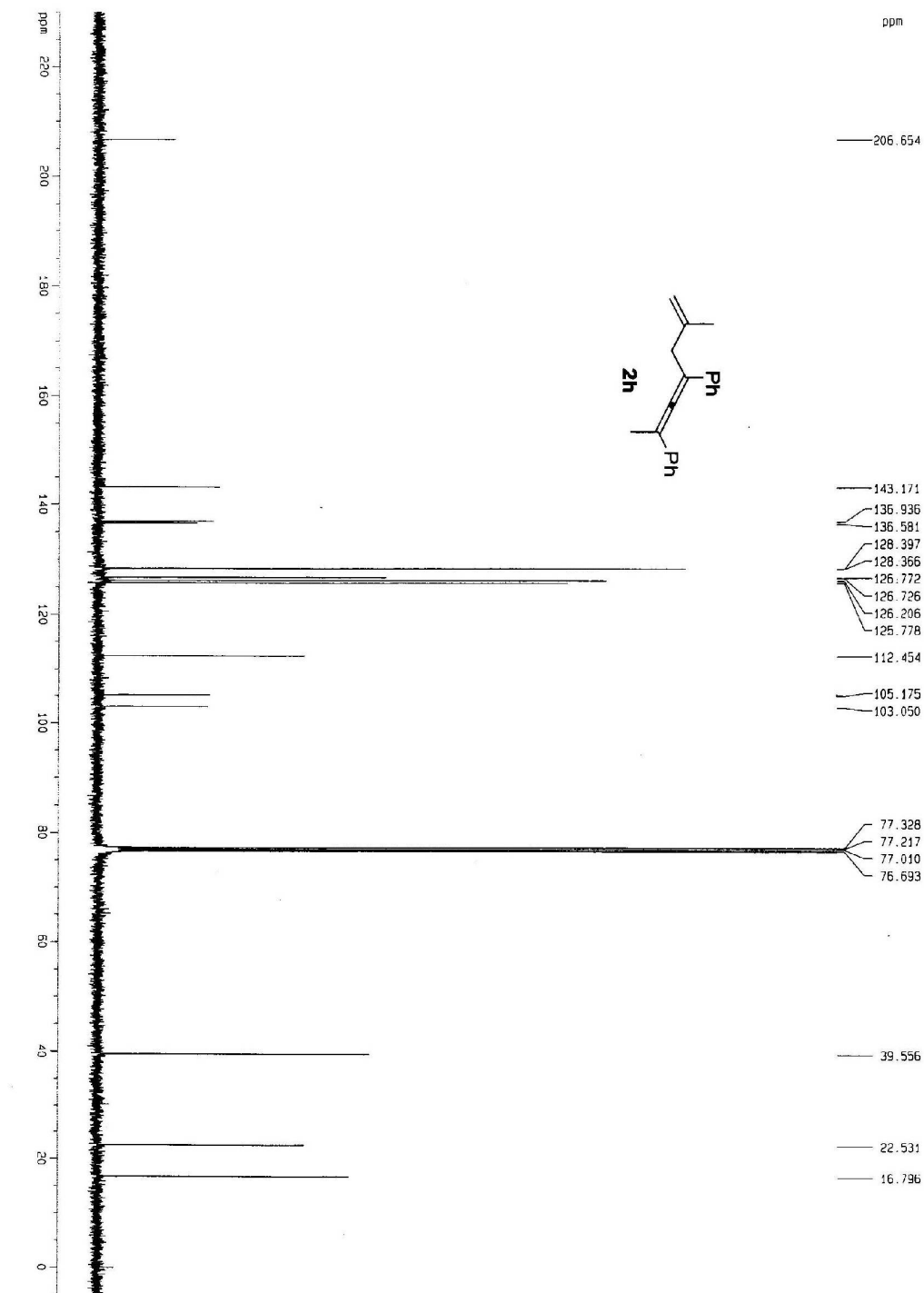
F2 - Acquisition Parameters
 Date_ 20070327
 Time 17.36
 INSTRUM spect
 PROBHD 5 mm Duet 13C/
 PULPROG zg30
 TO 32768
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 8023.685 Hz
 FIDRES 0.250957 Hz
 AQ 1.9923444 sec
 F3 228.1
 D4 50.800 usec
 DE 6.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 MCEST 0.00000000 sec
 MCMRK 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 400.1300138 MHz
 NDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 30.00 cm
 CY 20.00 cm
 F1P 8.100 DDM
 F1 3241.05 Hz
 F2P -40.01 Hz
 F2 0.27333 GHz/cm
 PPMCM 109.36887 Hz/cm

LJY-141



Current Data Parameters

NAME	EXPNO	PROCNO	DATE_	TIME	INSTRUM	PROBHD	PULPROG	TD	TE	DE	DM	DC	SC	SMH	FTRES	AC	RG	DE	TE	DELTA	MOESET	WCHRG
NAME	EXPNO	PROCNO	DATE_	TIME	INSTRUM	PROBHD	PULPROG	TD	TE	DE	DM	DC	SC	SMH	FTRES	AC	RG	DE	TE	DELTA	MOESET	WCHRG
			20070327	15:57	spec	5 mm Dual 13C/	zgpg30	299430	299.2 K	13.700 us	13.700 us	574.7	2	316.7, 133 Hz	0.489949 Hz	1.0289652 sec	574.7	13.700 us	299.2 K	0.03000000 sec	1.89999998 sec	0.01500000 sec

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

NUC1	PC1	PL1	SFO1
13C	10.50 us	-1.00 dB	100.626455 MHz

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

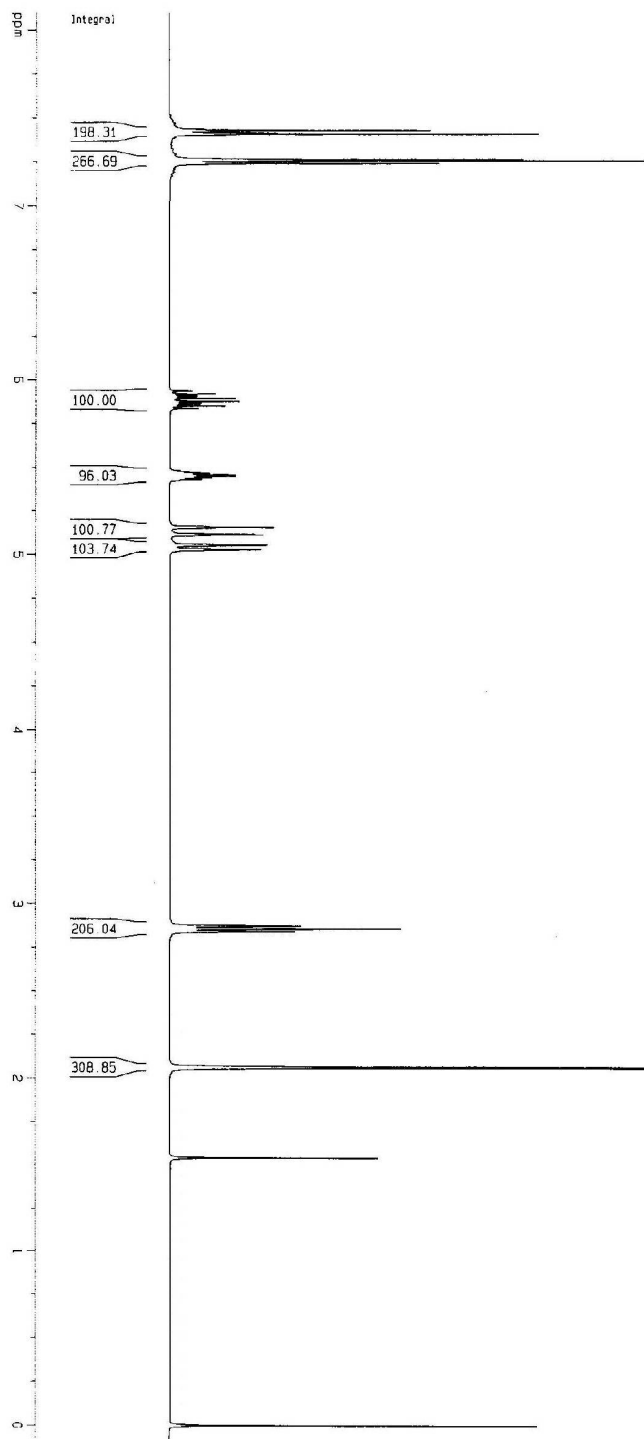
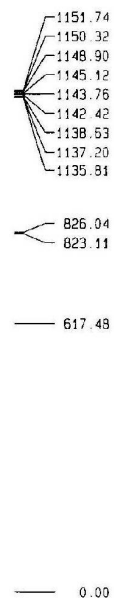
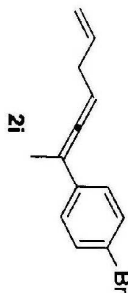
NUC2	PC2	PL2	SFO2
1H	105.00 us	-2.00 dB	400.1324706 MHz

===== Processing Parameters =====

SI	SF	WDW	SSB	LB	GB	PC
32768	100.612719 MHz	EM	0	1.00 Hz	0	1.40

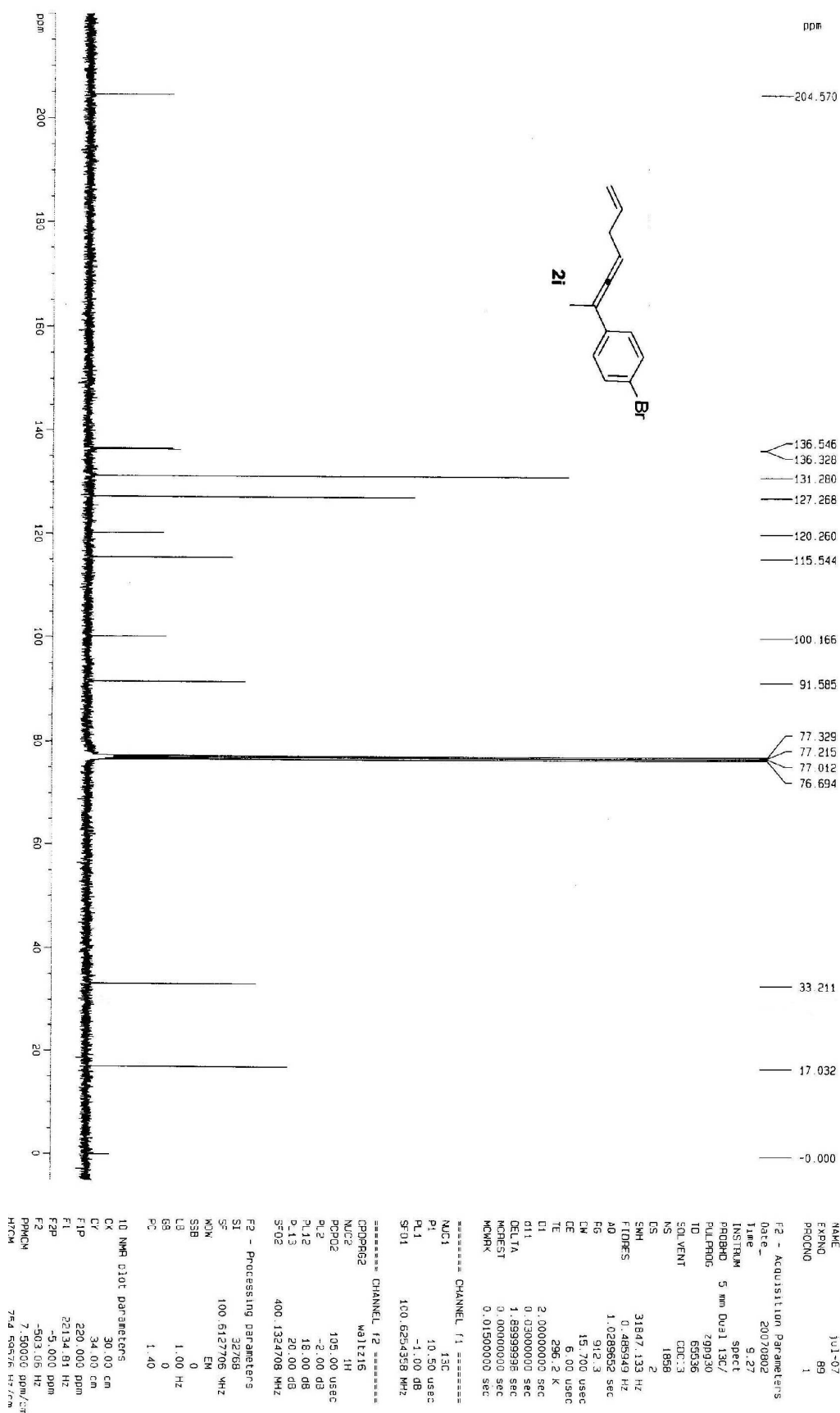
1D NMR plot parameters

CV	F1	F2	PPMCM	HZCM
30.00 cm	230.000 ppm	23140.94 Hz	-5.000 ppm	-503.06 Hz
			7.8333 ppm/cm	789.13336 Hz/cm

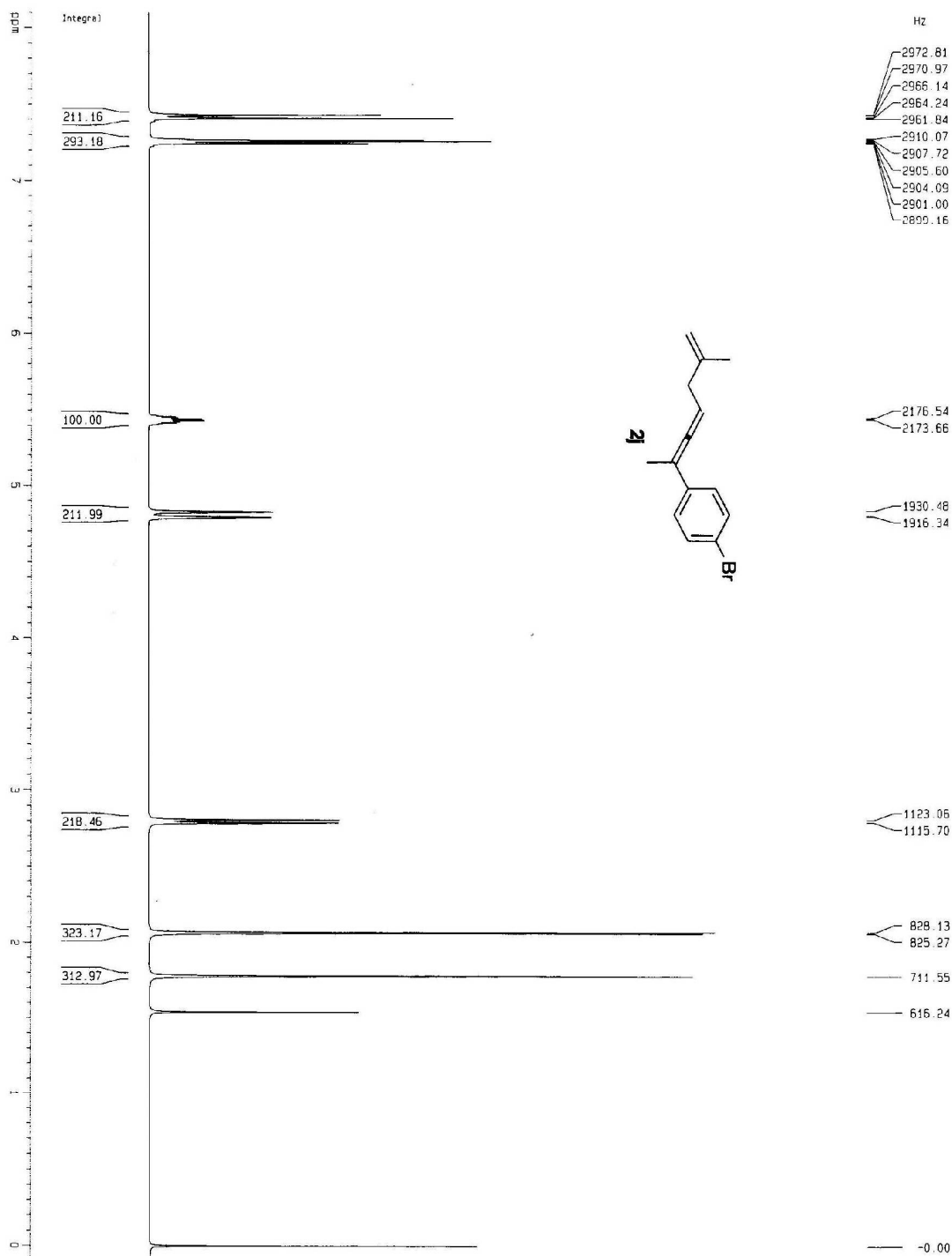


- S25 -

LJY-201



LJY-202



Current Data Parameters

NAME	LJY-202
EXPNO	90
PROCNO	1

F2 - Acquisition Parameters

Date_	20070802
Time	12.28
INSTRUM	INVTM
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	322.5
DN	60.800 usec
DE	6.00 usec
TE	297.2 K
DI	1.0000000 sec
MCREST	0.0000000 sec
MCPRK	0.01500000 sec

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

NUC1	13C
P1	11.00 usec
PL1	-2.00 dB
SFO1	400.1324710 MHz

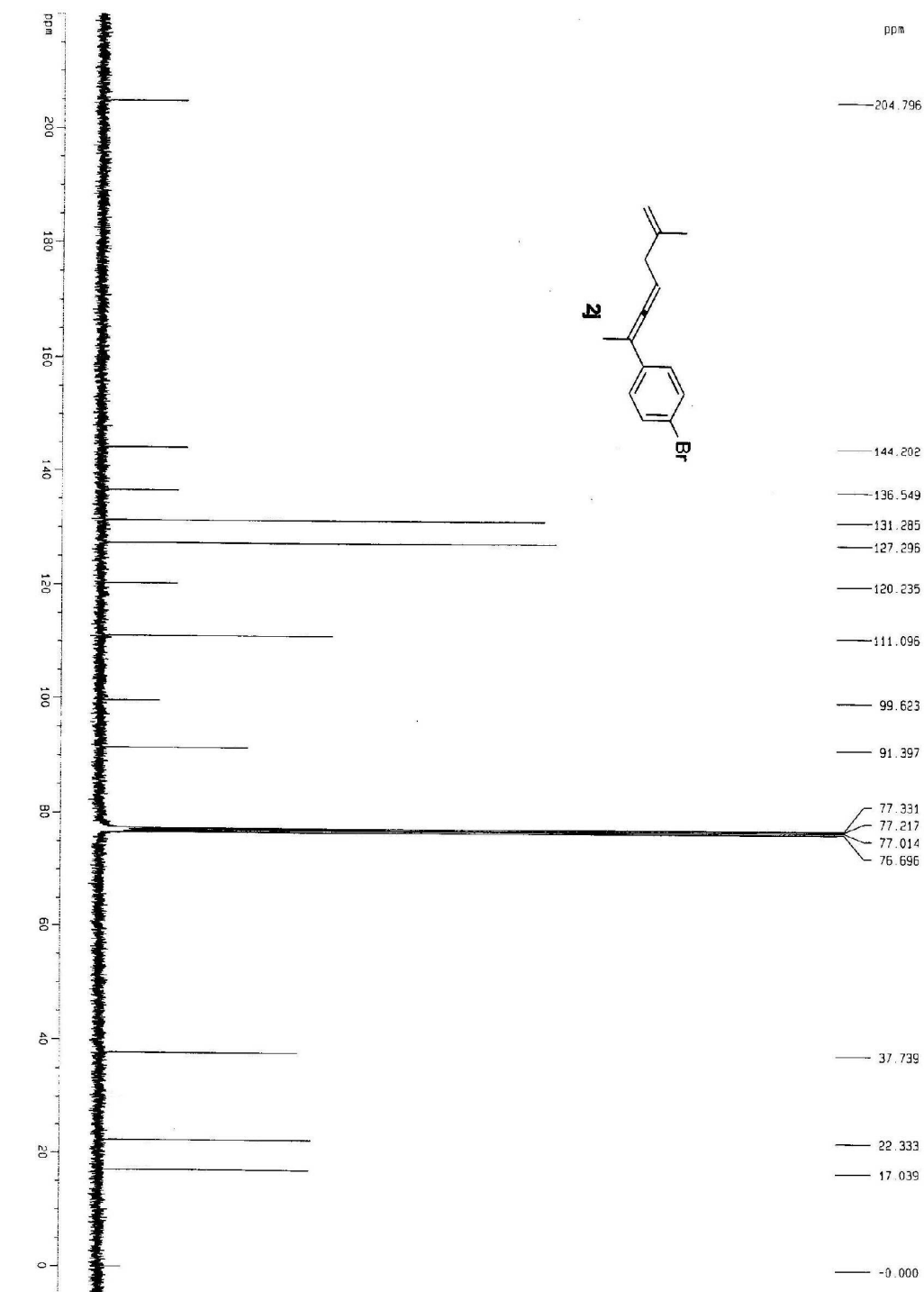
F2 - Processing parameters

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
CV	15.00 cm
F1P	8.100 ppm
F1	3241.05 Hz
F2P	-40.100 ppm
F2	-40.01 Hz
PPMCM	0.27333 ppm/cm
HZCM	109.36687 Hz/cm

LJY-202



Current Data Parameters

NAME	Jui-07
EXPNO	91
PROCNO	1

F2 - Acquisition Parameters

Date_	20070802
Time	11.19
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1643
DS	2
SWH	31847.133 Hz
FIDRES	0.480949 Hz
AQ	1.0289652 sec
RG	2580.3
UN	15.700 usec
DE	6.00 usec
TE	297.2 K
CI	2.00000000 sec
CH	0.03000000 sec
DELTA	1.89999998 sec
RGREST	0.00000000 sec
RGMRK	0.01500000 sec

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

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

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

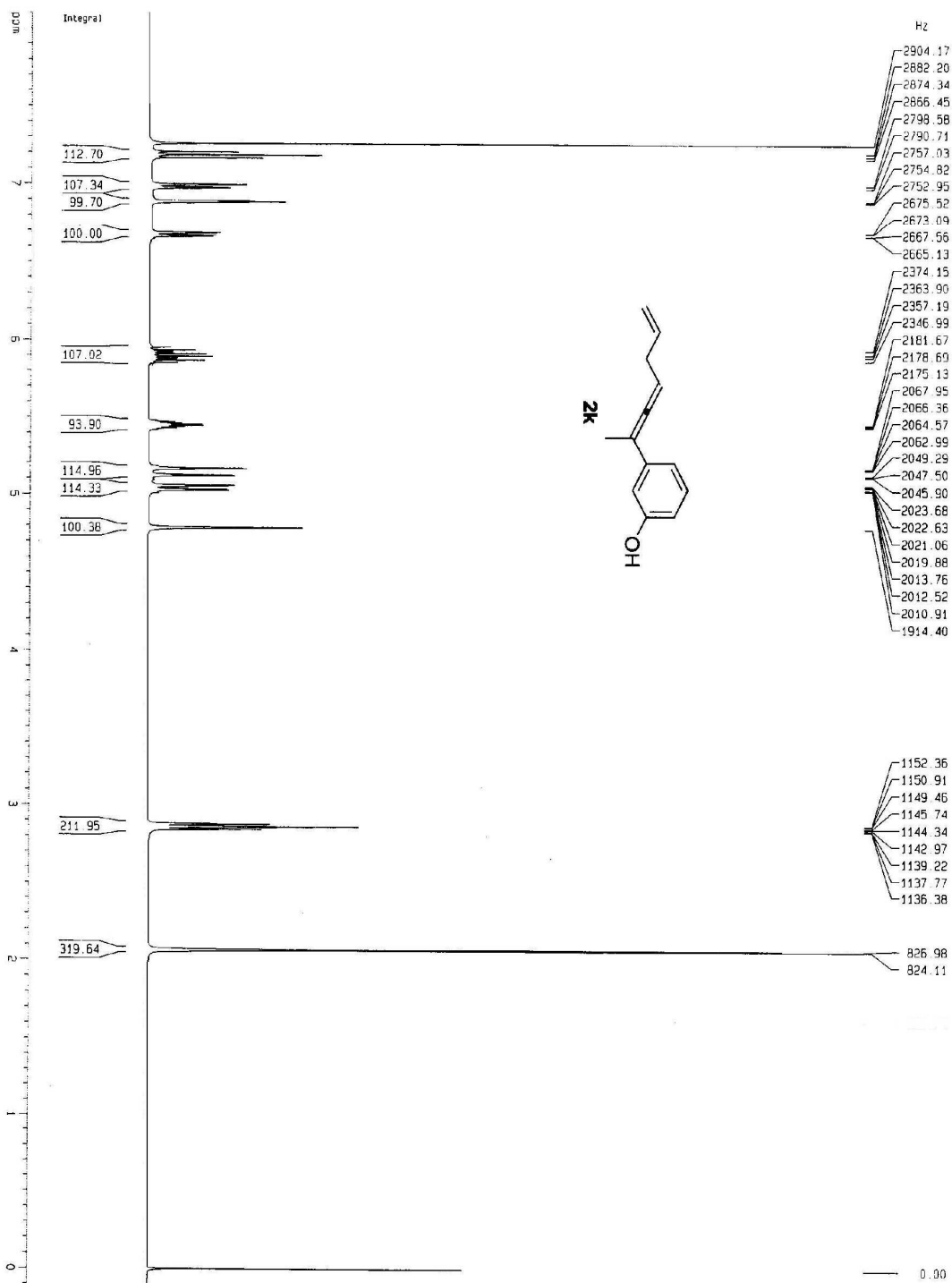
CPDPRG2	waltz16
NUC2	1H
PCPD2	105.00 usec
PL2	-2.00 dB
PL12	18.00 dB
PL13	20.00 dB
SFO2	400.1324708 MHz

F2 - Processing parameters

SI	32768
ST	100.6127701 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

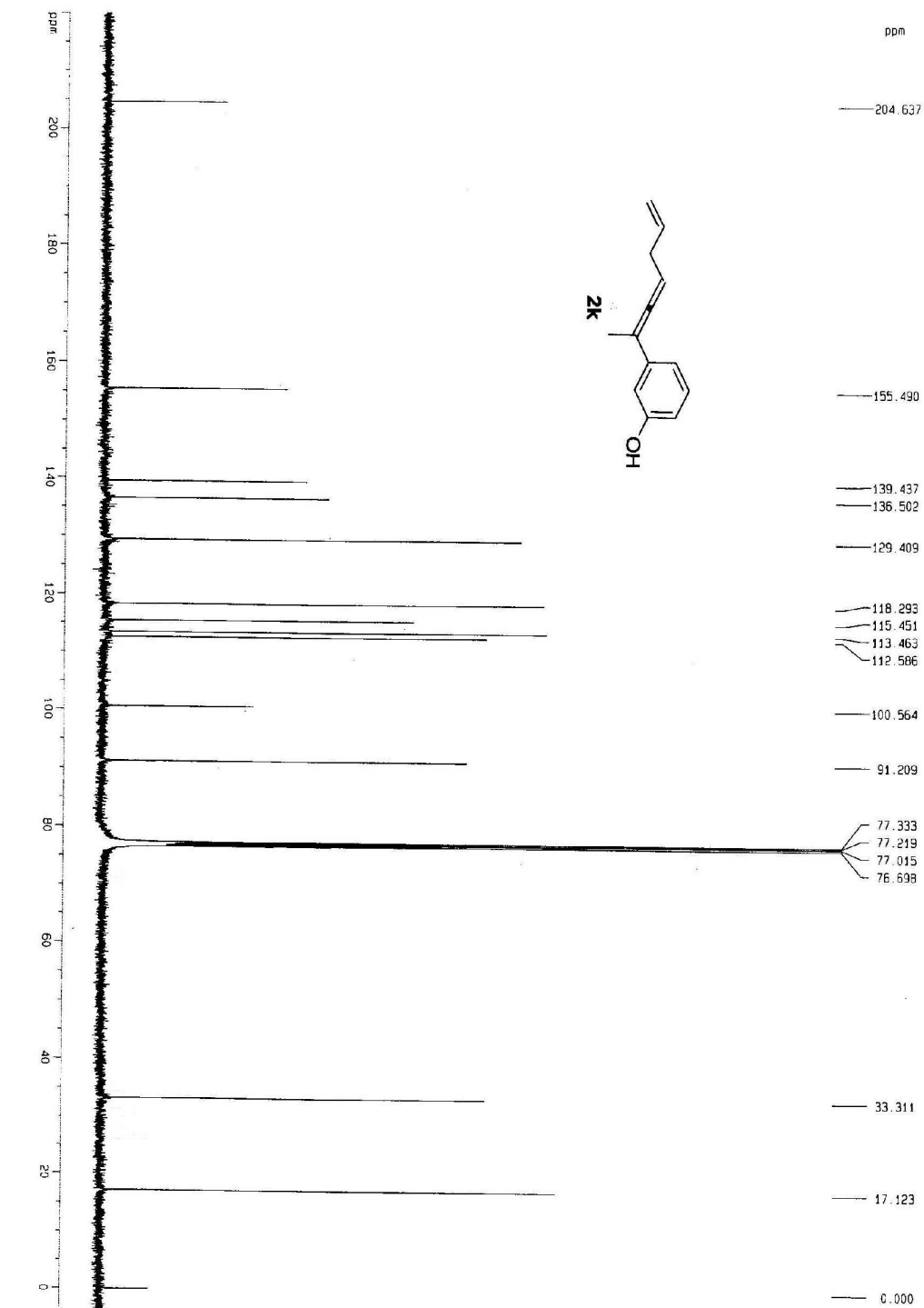
CX	30.00 cm
CV	34.00 cm
FLP	220.000 ppm
F1	221.24 Hz
F2P	-5.000 ppm
F2	-503.06 Hz
PPMCM	7.50000 ppm/cm
HZCM	754.59576 Hz/cm



LJY-200

Current Data Parameters
 NAME: sep-07
 EXPNO: 25
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20070909
 Time: 11.01
 INSTRUM: spect
 PROBHD: 5 mm Dui-13C/
 PULPROG: zgpg30
 TO: 32768
 SOLVENT: CDCl3
 NS: 16
 DS: 0
 SWH: 8223.685 Hz
 FIDRES: 0.25067 Hz
 AQ: 1.9922444 sec
 RG: 362
 DM: 60.800 usec
 DE: 6.00 usec
 TE: 296.2 K
 D1: 1.0000000 sec
 ACQRES: 0.0000000 sec
 MCWAK: 0.0150000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 11.00 usec
 PL1: -2.00 dB
 SFO1: 400.1327710 MHz
 F2 - Processing parameters
 SI: 16384
 SF: 400.1300105 MHz
 MDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00
 ID 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: 109.36687 Hz/cm

LJY-200



Current Data Parameters
 NAME sep-07
 EXPNO 26
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070907
 Time 18.26
 INSTRUM spect
 PROBRD 5 mm DAI 13C/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 20480
 DS 2
 SWH 31847.133 Hz
 FIDRES 0.465949 Hz
 AQ 1.0289552 sec
 RG 101.6
 SF 15.700 usrc
 DE 5.00 usrc
 TE 296.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 DELTA 1.89595958 sec
 ACQEST 0.00000000 sec
 ICNMRK 0.01500000 sec

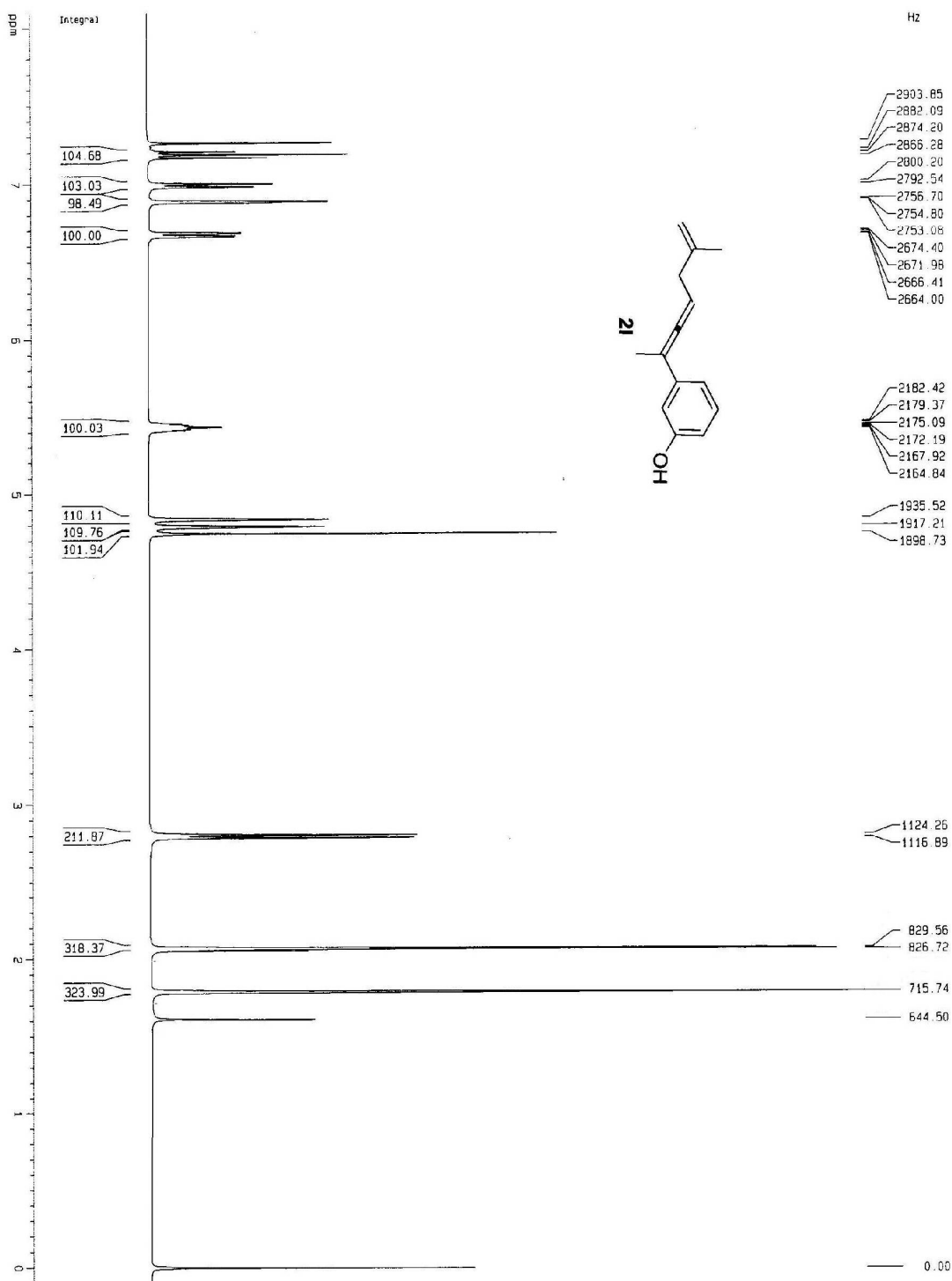
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usrc
 PL1 -1.00 dB
 SFO1 100.6261258 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 105.00 usrc
 PL2 -2.00 dB
 PL12 18.00 dB
 PL13 20.00 dB
 SFO2 400.1324708 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127702 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

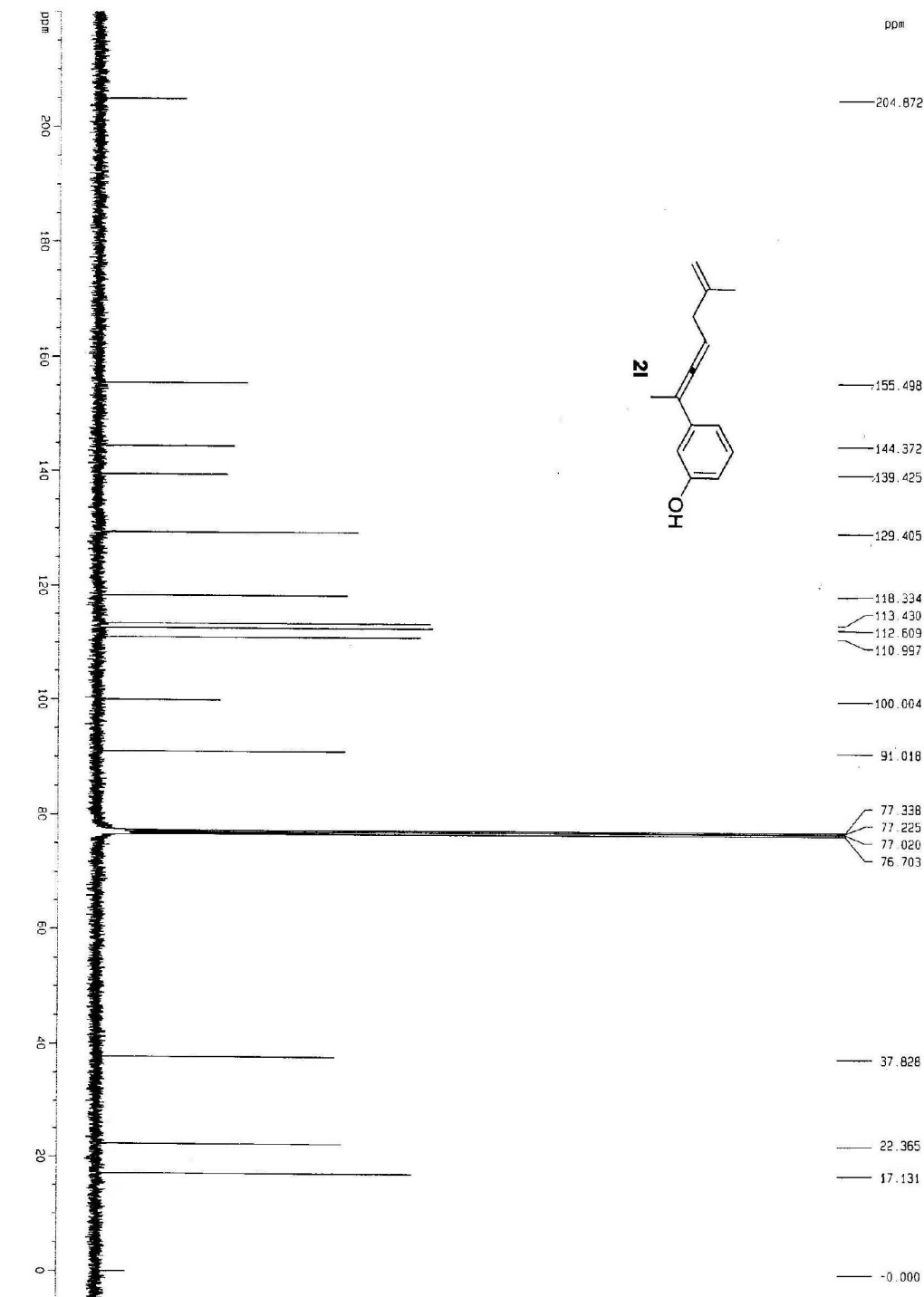
1D NMR plot parameters
 CX 30.00 cm
 CY 89.00 cm
 F1P 220.000 ppm
 F1 22134.81 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCH 754.55676 Hz/cm
 HZCM

LJY-154



Current Data Parameters
 NAME mar-07
 EXPNO 53
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20070423
 Time 13:57
 INSTRUM spect
 PROBN 5 mm Dual 13C/
 PULPROG zgpg30
 TD 65536
 FIDRES 0.250967 Hz
 AQ 1.9923444 sec
 RG 256
 DK 60.800 usec
 DE 6.00 usec
 TE 297.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCMRK 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 400.1300107 MHz
 MDW 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 6.100 ppm
 F1 3241.05 Hz
 F2P -40.01 Hz
 F2 0.27333 ppm/cm
 PPMCM 109.36587 Hz/cm

LY-154



Current Data Parameters

NAME	EXPNO	PROCNO	PROBHD	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FTRES	RG	RG	DM	DE	TE	D1	DELTA	MCREST	MCMRK
20070423	1	1	5 mm QNP 13C/	13C/	zgpg30	65536	65536	CDCl3	2048	2	31947.133 Hz	0.485949 Hz	1.0299652 sec	362	15.700 usec	5.00 usec	295.2 K	2.00000000 sec	0.03000000 sec	1.87999998 sec	0.00000000 sec

F2 - Acquisition Parameters

Date_ 20070423

Time 12.05

INSTRUM 13C/

PROBHD 5 mm QNP 13C/

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 2048

DS 2

SWH 31947.133 Hz

FTRES 0.485949 Hz

RG 1.0299652 sec

RG 362

DM 15.700 usec

DE 5.00 usec

TE 295.2 K

D1 2.00000000 sec

DELTA 0.03000000 sec

MCREST 1.87999998 sec

MCMRK 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 100.6127705 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

ID NMR plot parameters

CX 30.00 cm

CY 45.00 cm

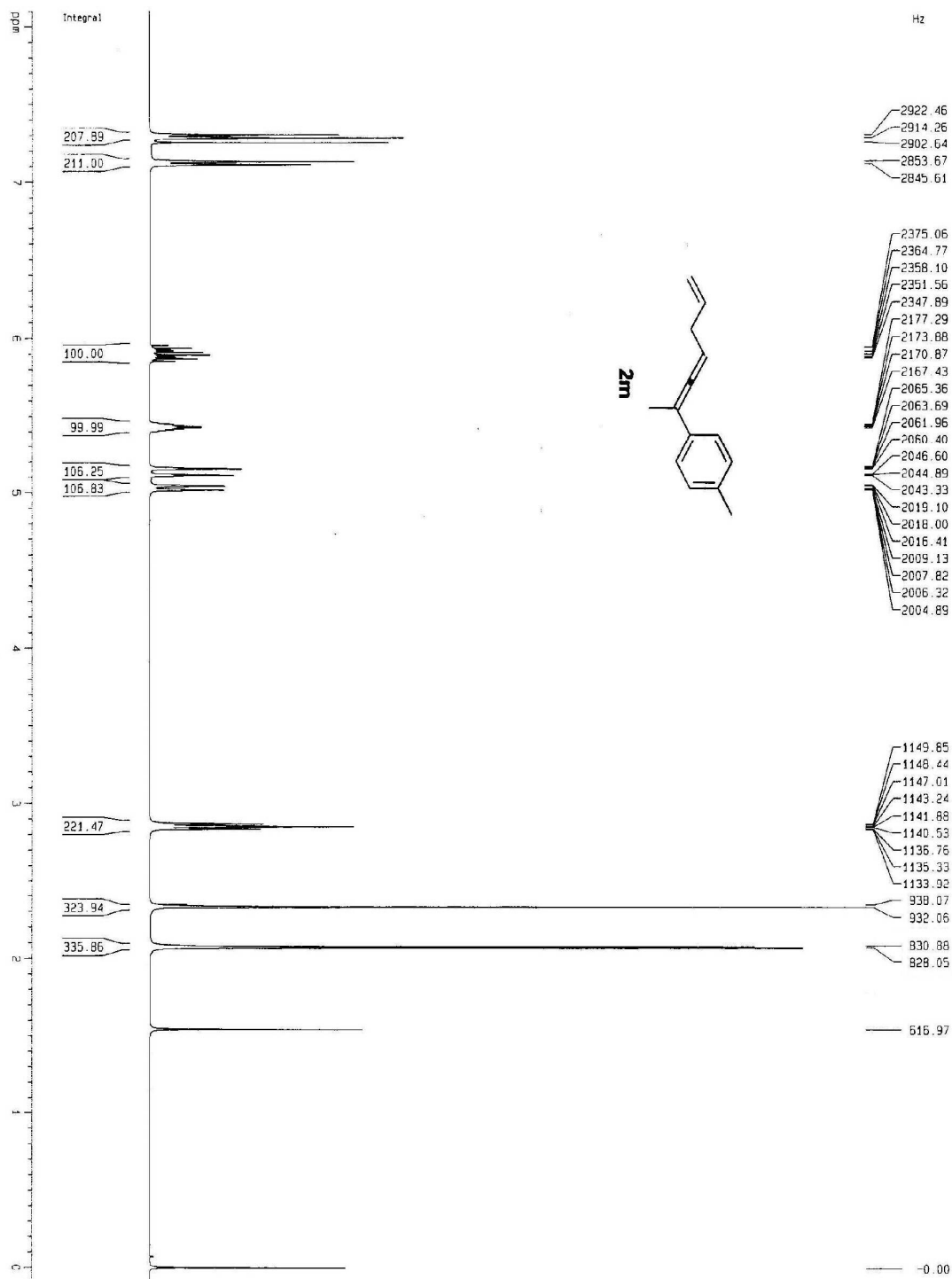
FLP 220.000 ppm

F1 22134.81 Hz

F2P -503.06 Hz

PRNCK 7.50000 ppm/cm

NCKM 754.55976 Hz/cm



LJY-144

Current Data Parameters
NAME: map-07
EXPNO: 20
PROCNO: 1

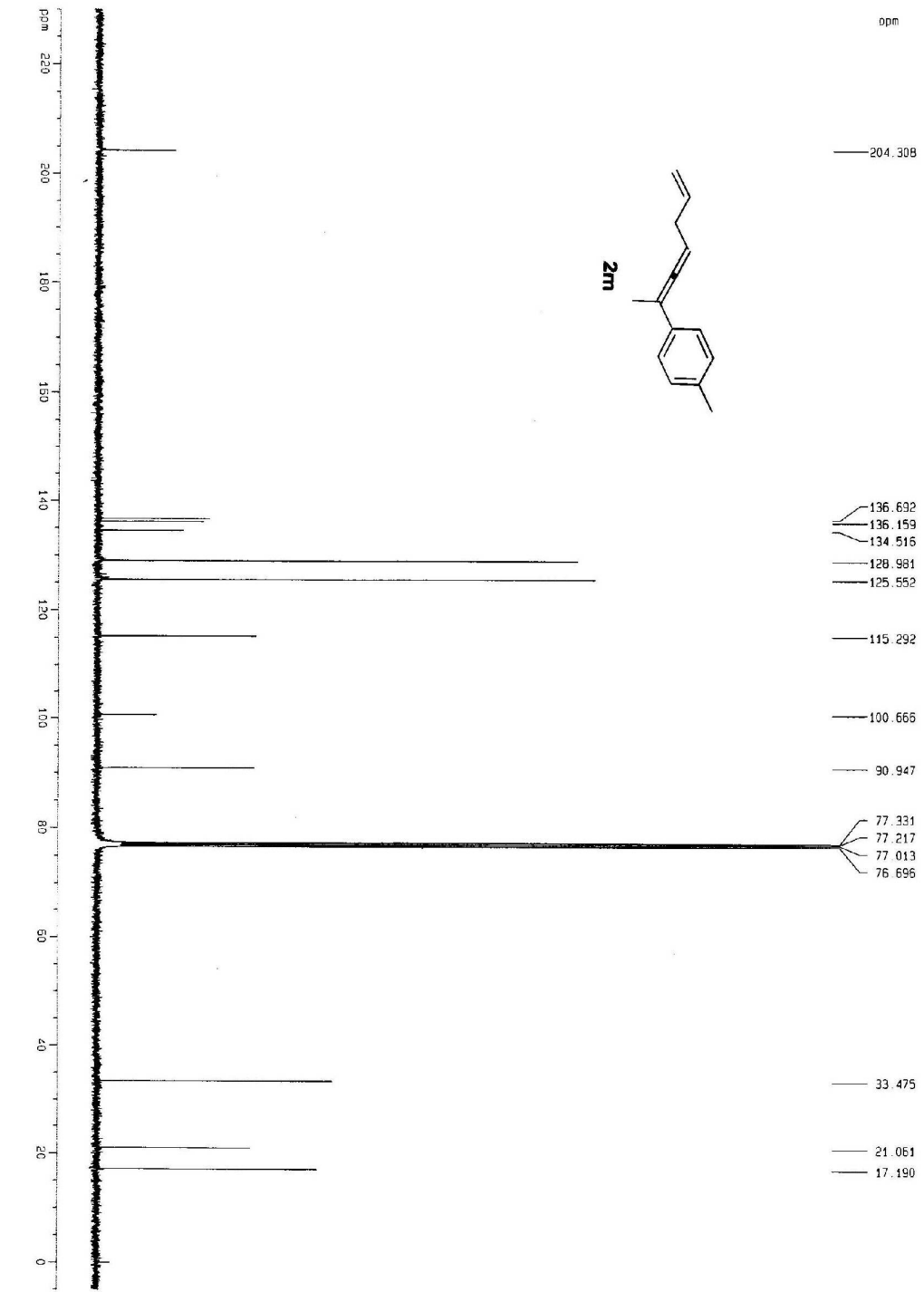
F2 - Acquisition Parameters
Date_: 20070330
Time: 17.06
INSTRUM: spect
PROBHD: 5 mm Dual 13C/
PULPROG: zg30
TO: 32768
SOLVENT: CDCl3
NS: 32
DS: 0
SWH: 8223.685 Hz
FIDRES: 0.250957 Hz
AQ: 1.5923444 sec
RG: 256
DM: 60.8104 usec
DE: 6.00 usec
TE: 296.2 K
J1: 1.00000000 sec
JCREST: 0.00000000 sec
JCMRK: 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: 400.1300120 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
PPMCK: 0.27333 ppm/cm
HZCN: 109.36687 Hz/cm

LJY-144



Current Data Parameters
NAME: mar-07
EXPNO: 21
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20070330
Time: 12.02
INSTRUM: spect
PROBHD: 5 mm Dual 13C/
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 3181
DS: 2
SWH: 31647.133 Hz
FIDRES: 0.485949 Hz
AQ: 1.028952 sec
RG: 1
DM: 228.1
DE: 15.700 usec
TE: 296.2 K
D1: 2.00000000 sec
d11: 0.03000000 sec
DELTA: 1.89999999 sec
MCREST: 0.00000000 sec
MCWK: 0.01500000 sec

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

===== CHANNEL f2 =====
CDEPRG2: waltz16
NUC2: 1H
PCPD2: 105.00 usec
PL2: -2.00 dB
PL12: 19.00 dB
PL13: 20.00 dB
SFO2: 400.1364708 MHz

F2 - Processing parameters
SI: 32768
SF: 100.612706 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: 230.000 ppm
F1: 23140.94 Hz
F2p: -5.000 ppm
F2: -503.06 Hz
PPMCH: 7.83333 ppm/cm
HZCM: 788.13336 Hz/cm

Hz

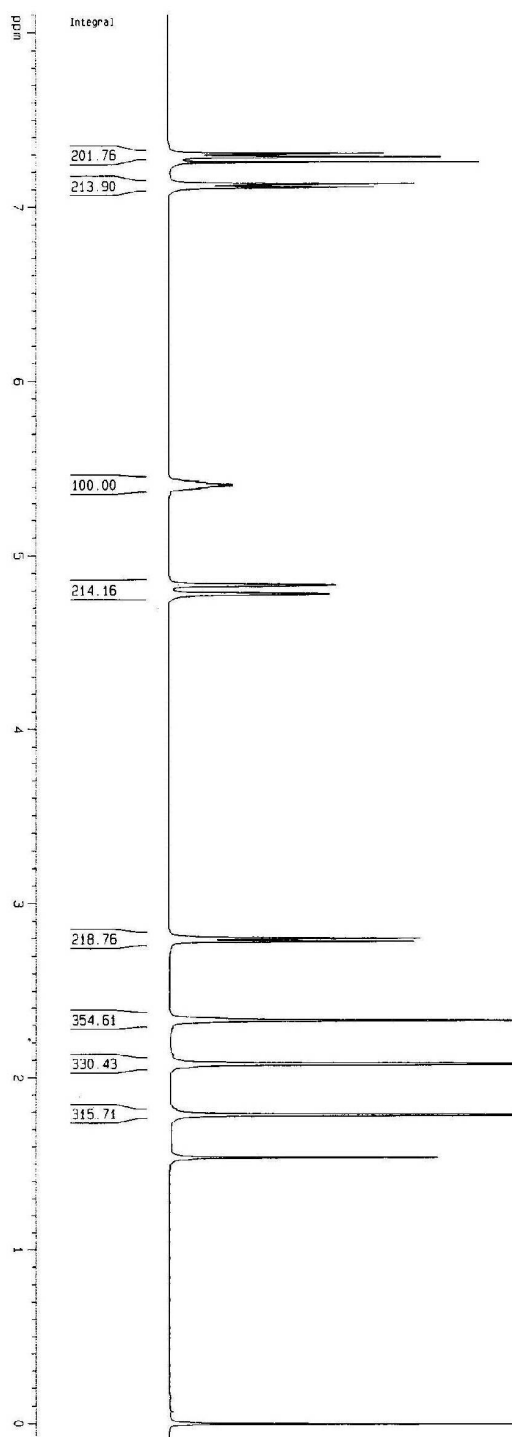
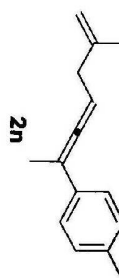
2173.09
2169.44
2165.91
2163.05
2159.05
2155.86

1933.08
1912.93

$\begin{array}{l} \diagup \\ \diagdown \end{array} \begin{array}{l} 1121.83 \\ 1114.50 \end{array}$

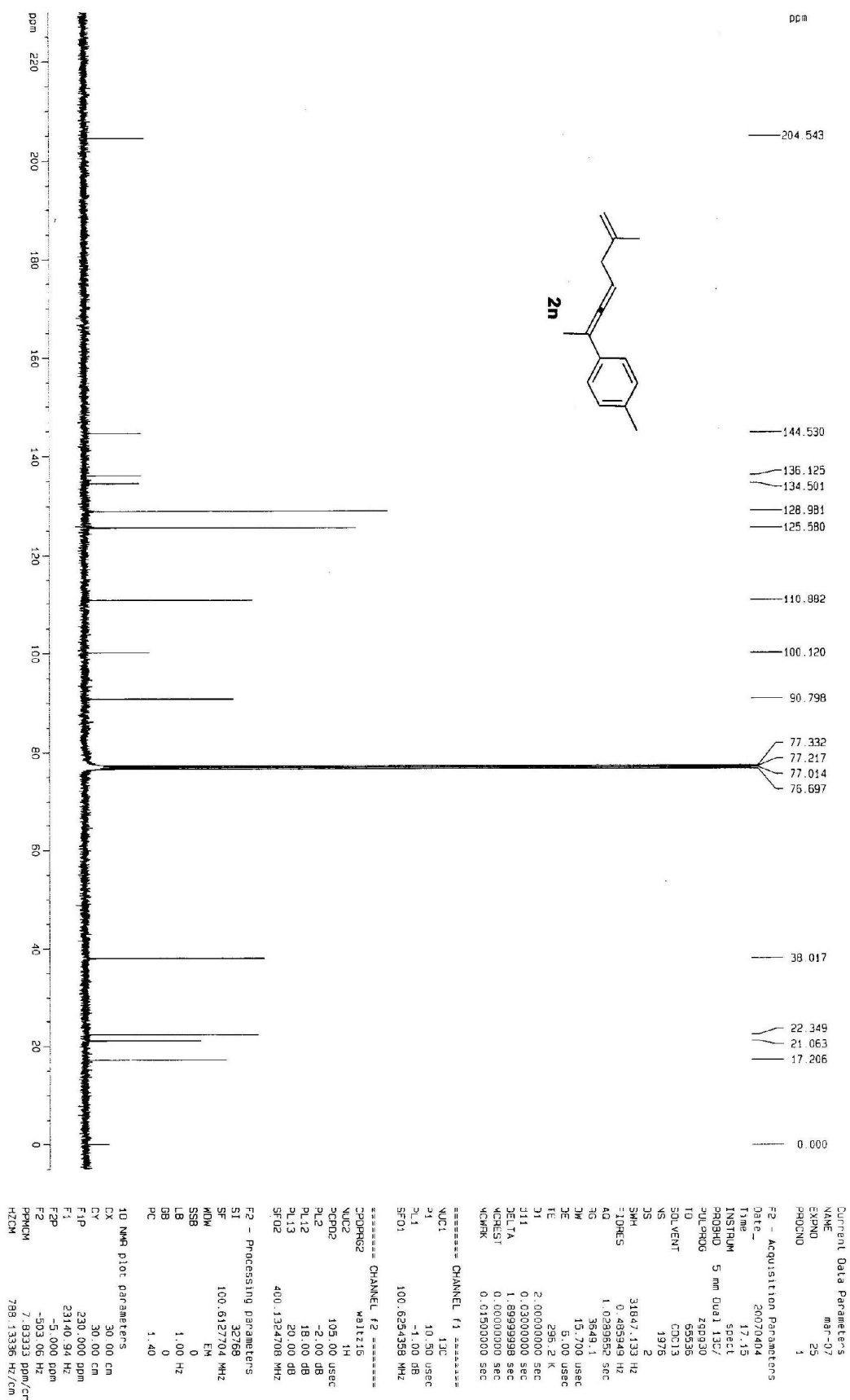
931.86
833.19
830.41
714.30
615.88

0.00

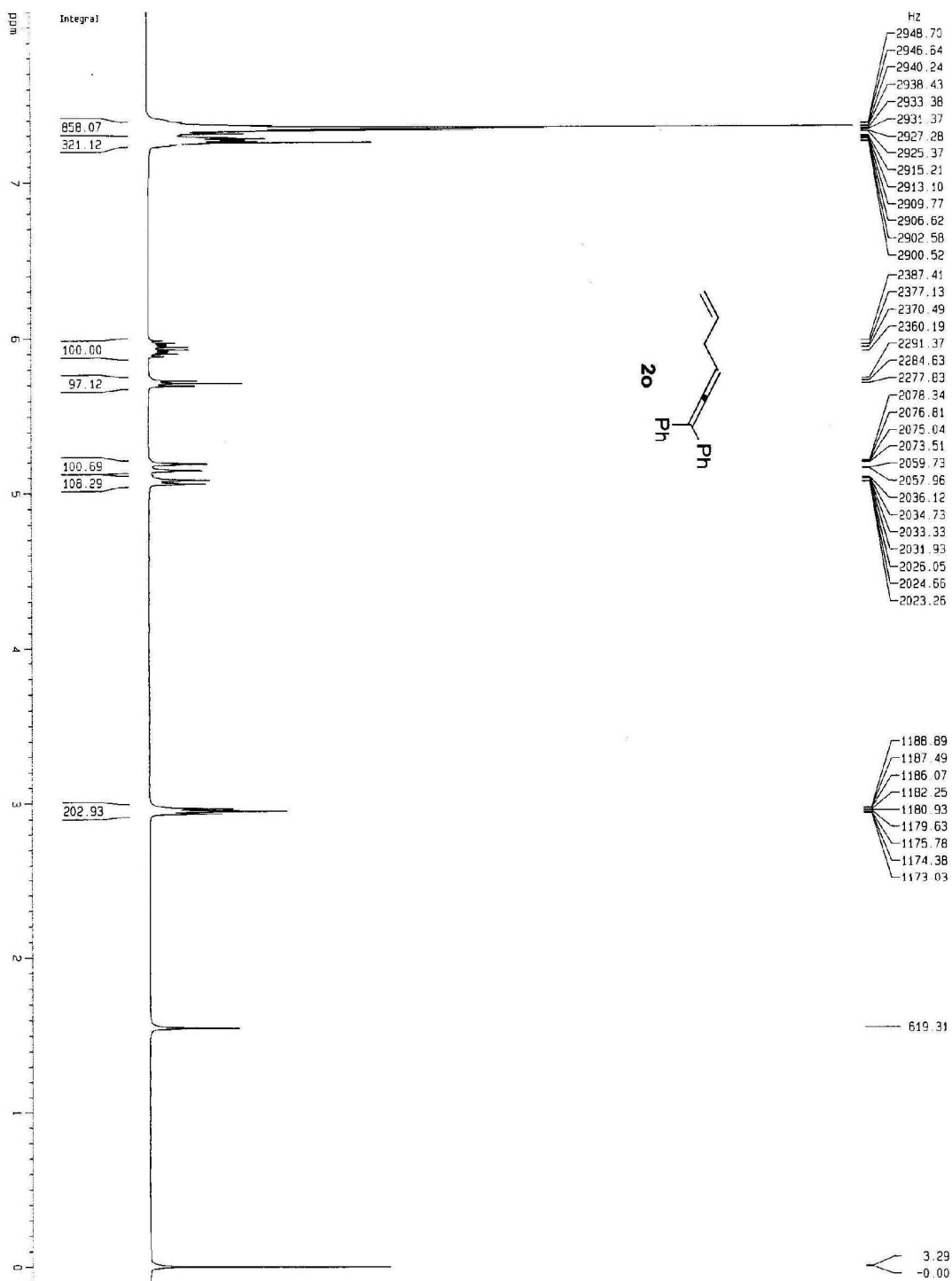


F2 - Acquisition Parameters		
Date_	Time	2007/04/05 9:54
INSTRUM	Spect	
PROBHD	5 mm DUB13C/	
PULPROG	zg30	
TD	32768	
NAME	COC13	
NS	32	
DS	0	
SMF	8223.665 Hz	
FIDRES	0.250567 Hz	
AQ	1.9923444 sec	
RG	362	
DM	60.000 usec	
DE	5.00 usec	
TE	296.2 K	
Q1	1.00000000 sec	
MCREST	0.00000000 sec	
MCNMR	0.01500000 sec	
----- CHANNEL f1 -----		
NUCL1	1H	
P1	11.00 usec	
PL1	-2.00 dB	
PR01	400.1324710 MHz	
F2 - Processing Parameters		
SI	16384	
SF	400.1300111 MHz	
MIM	FM	
SSB	0	
LB	0.30 Hz	
GB	0	
PC	1.00	
10 NMR plot parameters		
CX	30.00 cm	
CV	20.00 cm	
F1P	8.100 ppm	
F1	3241.05 Hz	
FPP	-0.100 ppm	
F2	-40.01 Hz	
P0MCM	0.27333 ppm/cm	
PCZCM	109.36887 Hz/cm	

LJY-146



LJY-152



Current Data Parameters

NAME	EXPNO	PROCNO	PROCNO
NAME	EXPNO	PROCNO	PROCNO
NAME	EXPNO	PROCNO	PROCNO

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TO	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DM	DE	TE	U1	MCREST	MCNMR
Date_	Time	INSTRUM	PROBHD	PULPROG	TO	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DM	DE	TE	U1	MCREST	MCNMR
2007/04/21	15.15	Spect	5 mm DUA1 15C/	ZQ30	32768	CDCl3	32	0	8223.666 Hz	0.250937 Hz	1.9923444 sec	207.4	60.800 usec	6.00 usec	297.2 K	1.00000000 sec	0.00000000 sec	0.01500000 sec

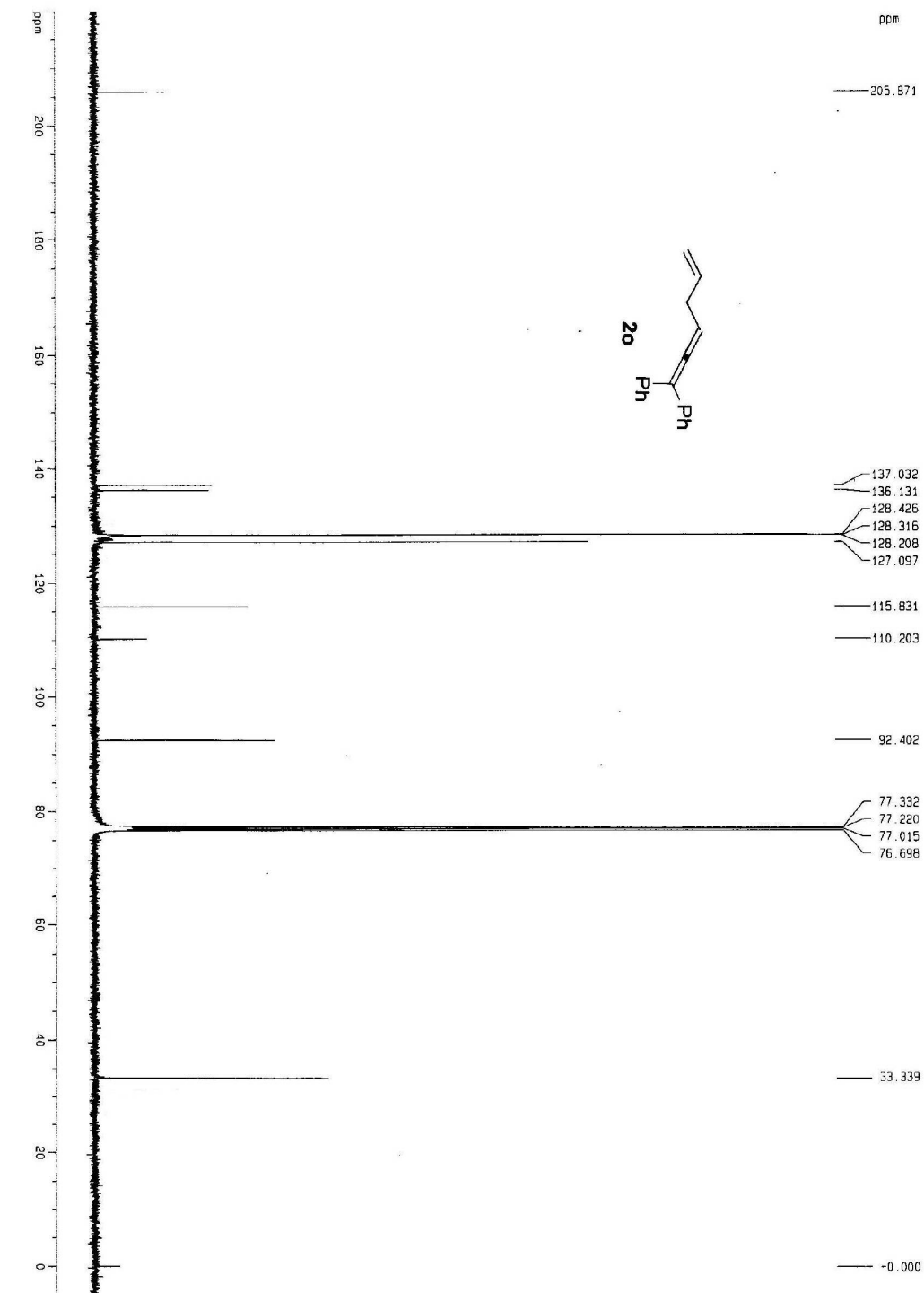
F2 - Processing parameters

SI	SF	WDW	SSB	LB	GB	PC
SI	SF	WDW	SSB	LB	GB	PC
36384	400.1300121 MHz	EM	0	0.30 Hz	0	1.00

1D NMR plot parameters

CX	CY	F1P	F2P	PPMCM	HZCM
CX	CY	F1P	F2P	PPMCM	HZCM
30.00 cm	20.00 cm	8.100 ppm	32.41, 05 Hz	-40.01 Hz	0.27333 ppm/cm
					109.36887 Hz/cm

LY-152



Current Data Parameters
NAME mar-07
EXPNO 52
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070421
Time 15:23
INSTRUM spect
PROBHD 5 mm Dui1 13C/
PULPROG zgpg30
TD 65536
FIDRES 0.485948 Hz
AQ 1.0288652 sec
RG 161.3
DM 15.700 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999995 sec
MCREST 0.00000000 sec
MCNRC 0.01500000 sec

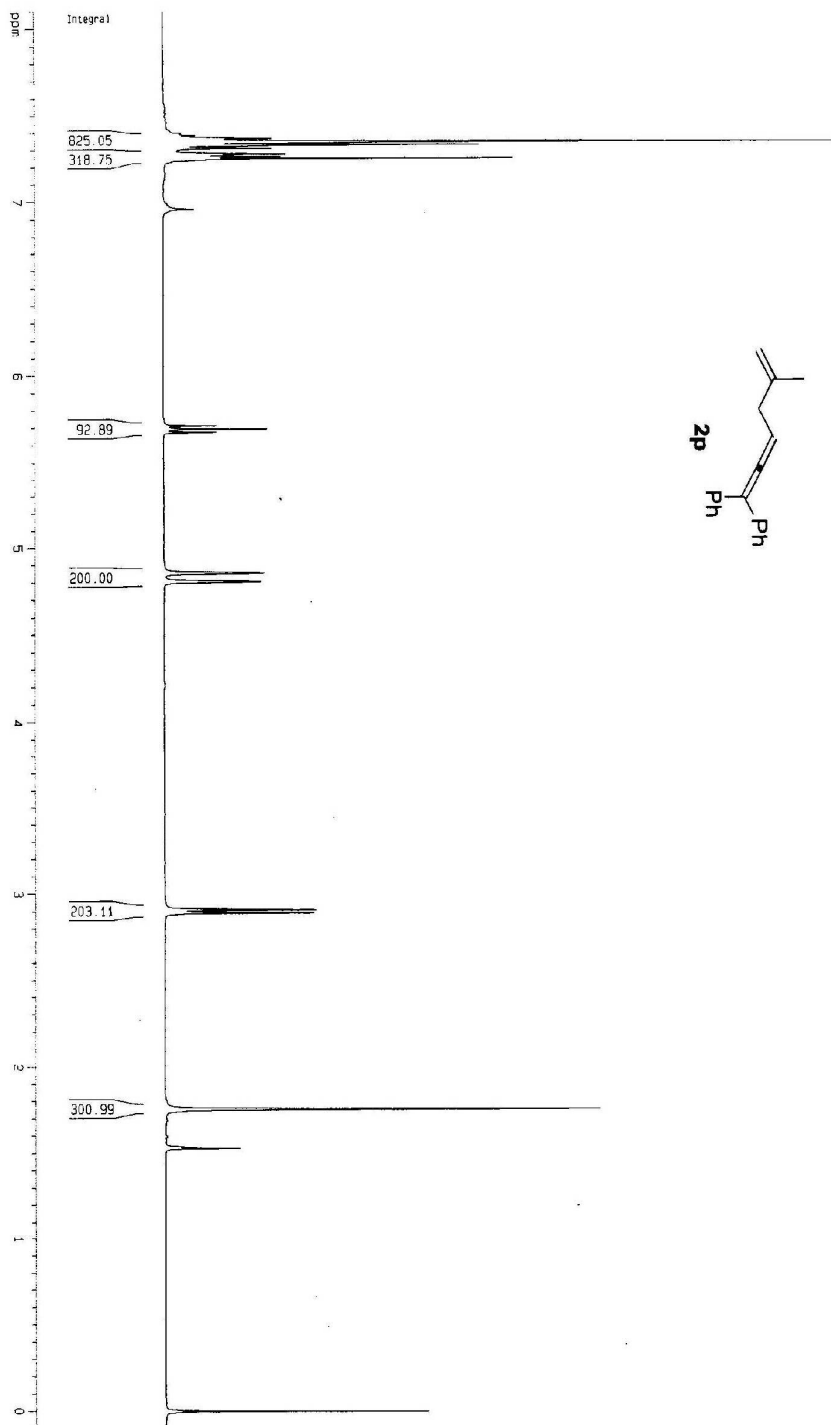
===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6264358 MHz

===== 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 40.00 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

LJY-203



Current Data Parameters
NAME LJY-203
EXPNO 102
PROCNO 1

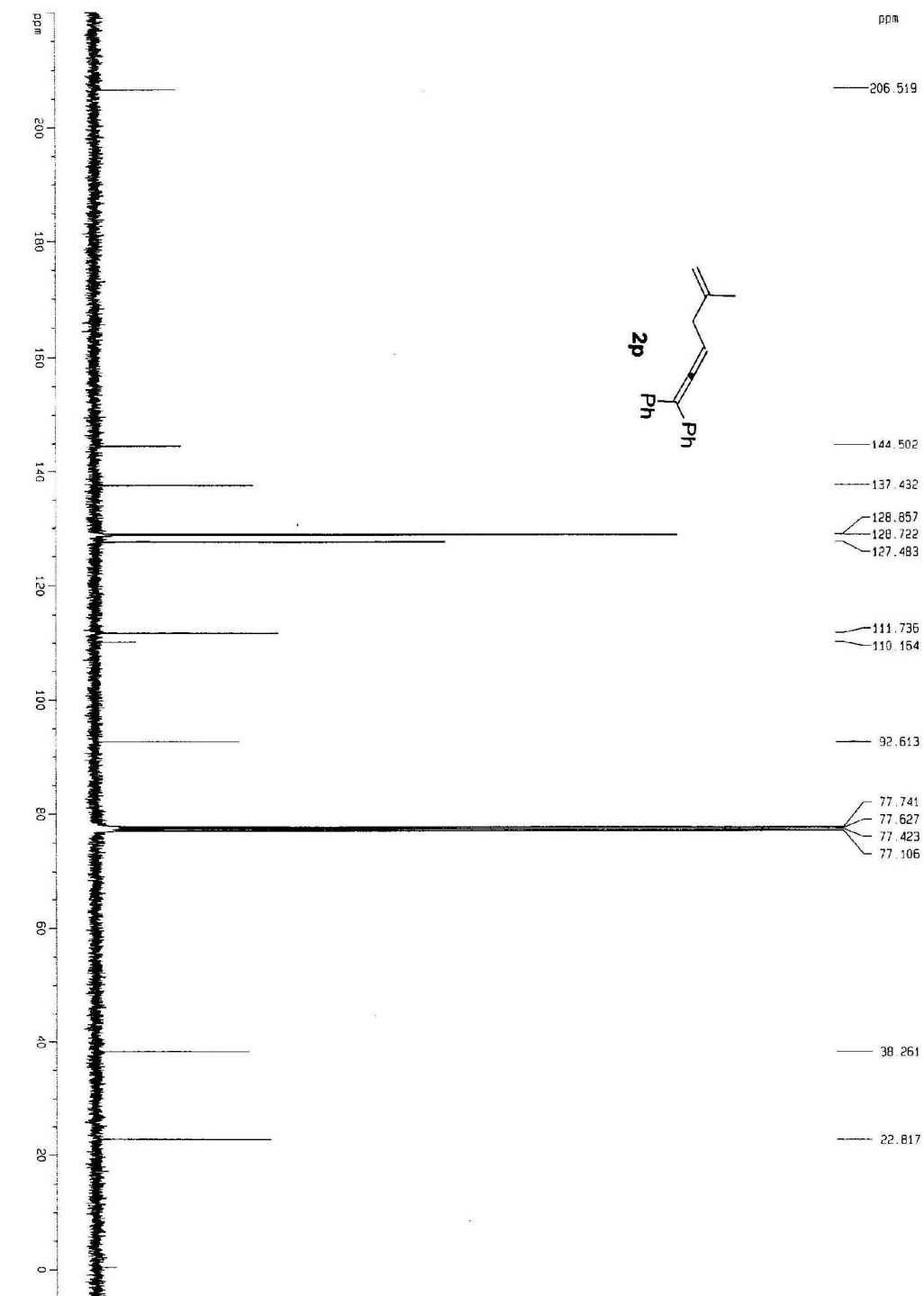
F2 - Acquisition Parameters
Date_ 20070610
Time 18.07
INSTRUM spect
PROBHD 5 mm Dvnl 13C/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.695 Hz
FIDRES 0.250667 Hz
AQ 1.9823444 sec
RG 322.5
BW 60.800 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWPR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13H
P1 11.00 usec
PL1 -2.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 16394
SF 400.130126 MHz
KW 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 8.100 ppm
F1 3241.05 Hz
F2P -40.01 Hz
F2 -40.01 Hz
PRNCH 0.27333 ppm/cm
HZCM 109.36887 Hz/cm

LJY-203



Current Data Parameters

NAME	VALUE
EXPNO	103
PROCNO	1

F2 - Acquisition Parameters

NAME	VALUE
Date_	20070813
Time	18:15
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1203
DS	2
SWH	31847.133 Hz
FIDRES	0.485943 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	1.89999999 sec
MCPRST	0.00000000 sec
MCNRC	0.01500000 sec

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

NAME	VALUE
NUC1	13C
Q1	10.50 usec
PL1	-1.00 dB
SFO1	100.6254359 MHz

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

NAME	VALUE
PROBHD	nm12115
NUC2	1H
PCPD2	105.00 usec
PL2	-2.00 dB
PL12	18.00 dB
PL13	20.00 dB
SFO2	400.1324709 MHz

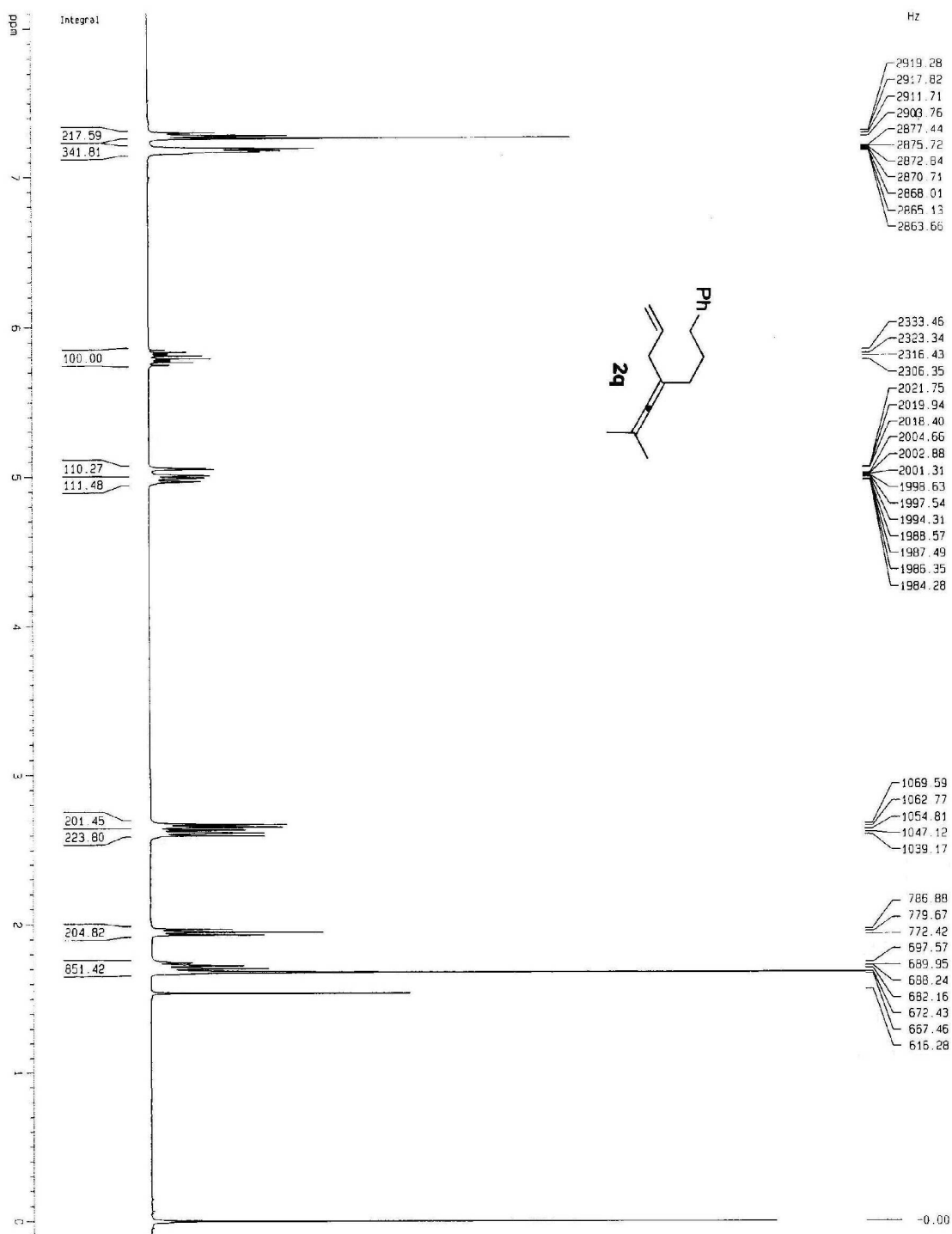
F2 - Processing Parameters

NAME	VALUE
SI	32768
SF	100.6127250 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

NAME	VALUE
CX	30.00 cm
CV	30.00 cm
FLP	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

LJY-165



Current Data Parameters

NAME	EXPNO	PROCNO
NAME	61	1

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS	DS	SWH	FIDRES	AQ	RG	DM	DE	TE	D1	MCHEST	MCWIK
20070607	11.46	spec	5 mm QNP 13C/	zg30	32768	CDCl3	32	0	8223.685 Hz	0.250957 Hz	1.9923444 sec	322.5	60.800 usec	6.00 usec	296.2 K	1.00000000 sec	0.00000000 sec	0.01500000 sec

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

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

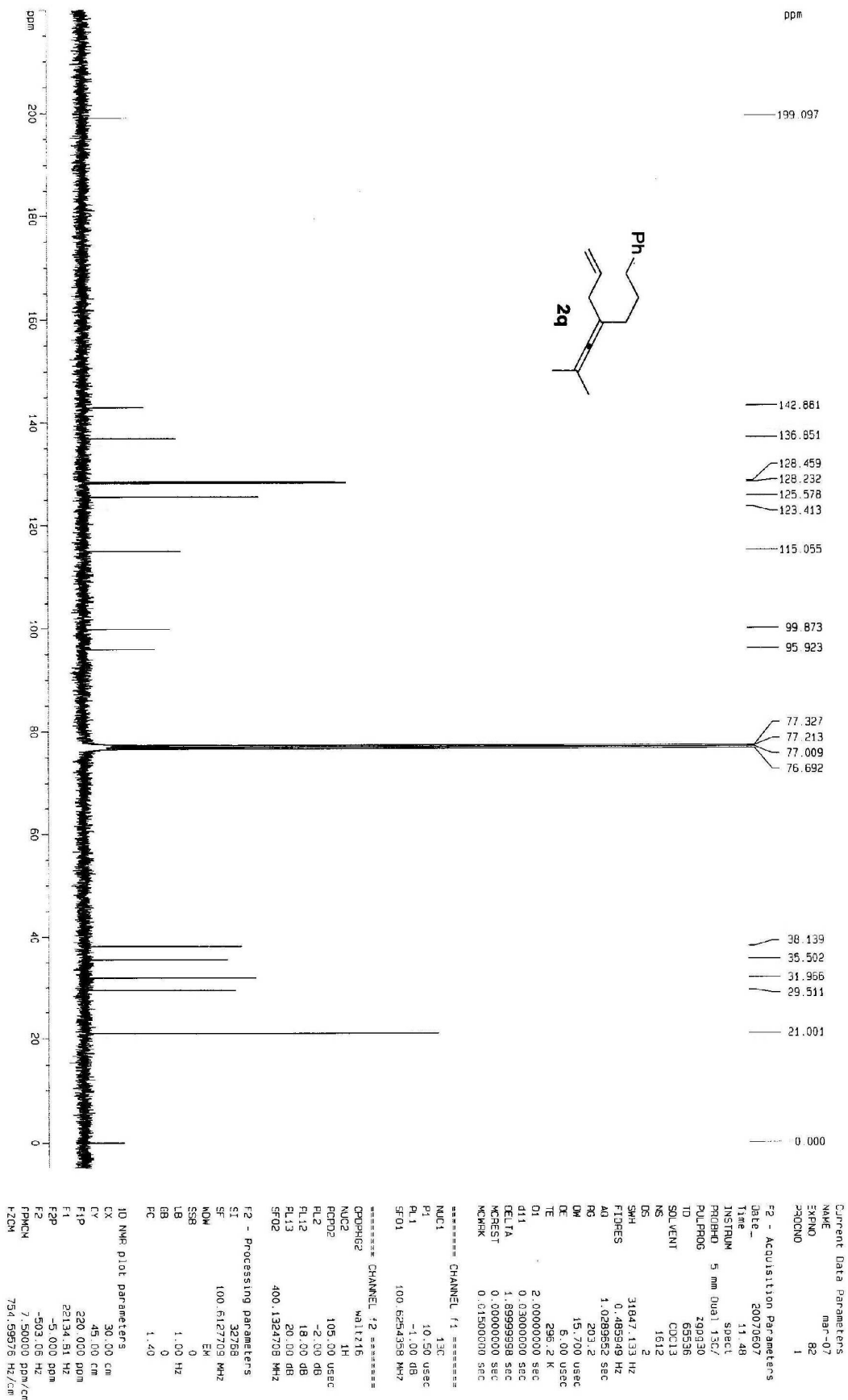
F2 - Processing parameters

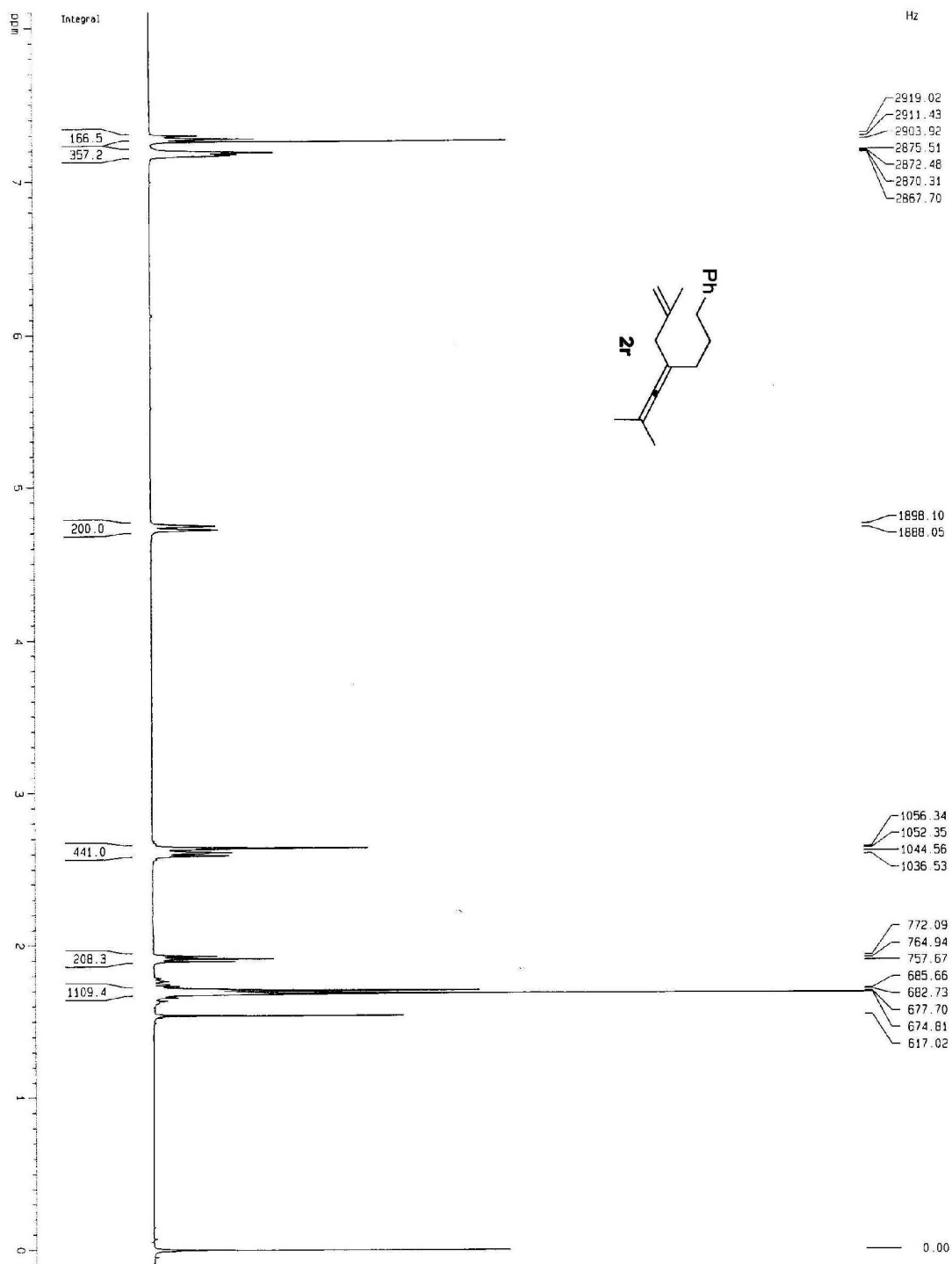
SF	SI	SF	WDW	SSB	LB	GB	PC
400.130110 MHz	16384	400.130110 MHz	EM	0	0.30 Hz	0	1.00

1D NMR Plot Parameters

EX	CV	FLP	F1	F2P	FMCH	FZCM
30.00 cm	50.00 cm	8.100 ppm	3241.05 Hz	-40.01 Hz	0.27353 ppm/cm	109.36887 Hz/cm

LJY-165





Current Data Parameters

NAME	nan-07
EXPNO	63
PROCNO	1

F2 - Acquisition Parameters

Date_	20070607
Time	13.20
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	8223.695 Hz
FIDRES	0.250957 Hz
AQ	1.9923444 sec
RG	287.4
W	60.800 usec
TE	296.2 K
DE	1.00000000 sec
MCREST	0.00000000 sec
MCNMR	0.01500000 sec

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

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

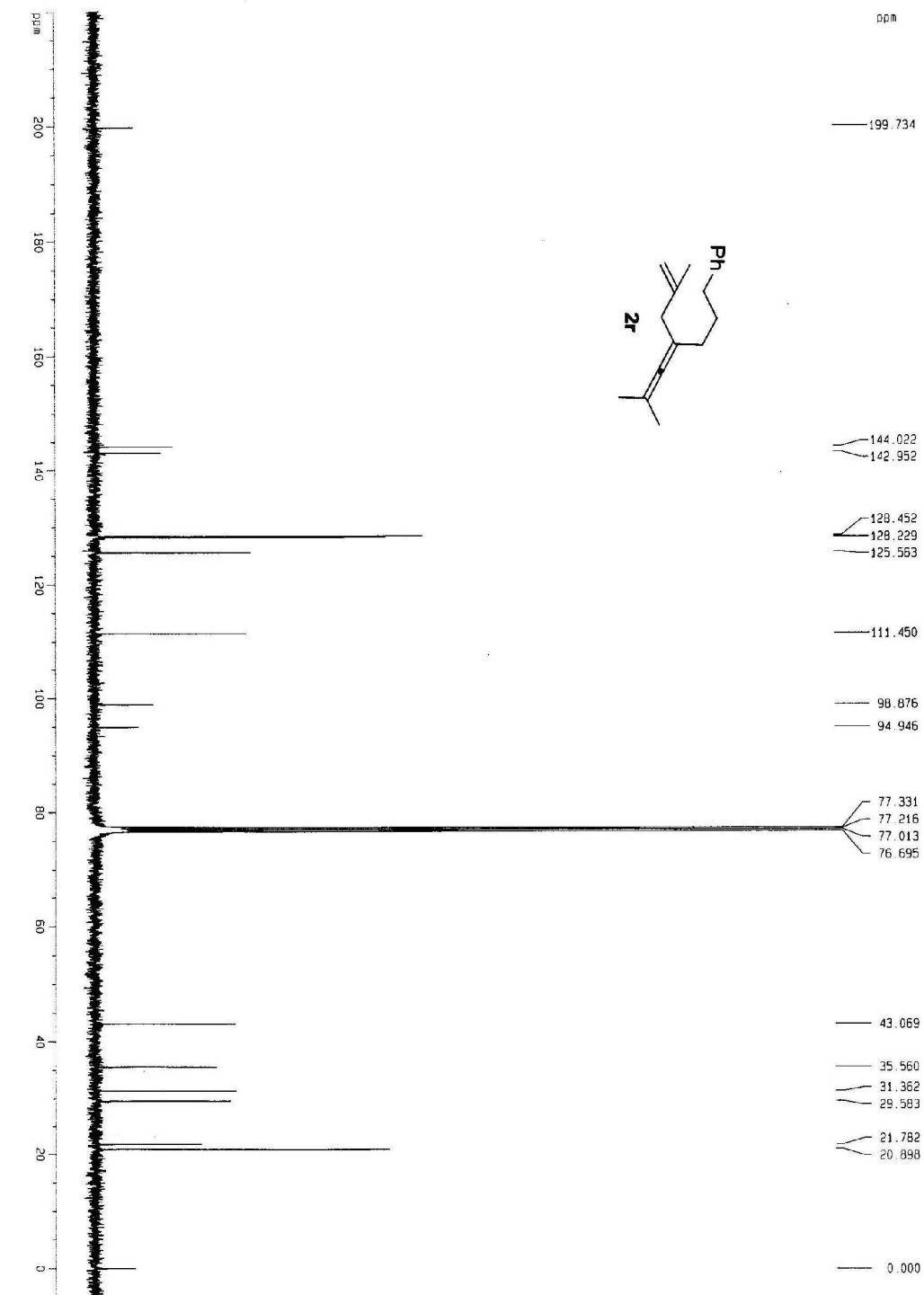
F2 - Processing parameters

SI	16384
SF	400.1300108 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
PPMCK	0.27333 ppm/cm
HZCM	109.36887 Hz/cm

LJY-166



Current Data Parameters
 NAME mar-07
 EXPNO 84
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070607
 Time 13.28
 INSTRUM spect
 PULPROG 5 mm Dual 13C/
 PULPROG zgpg30
 TD 65536
 ID C013
 SOLVENT CDCl3
 NS 2441
 DS 2
 SMH 31847.133 Hz
 FIDRES 0.465949 Hz
 AQ 1.0289652 sec
 RG 3649.1
 DK 15.700 usec
 DE 5.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCMRK 0.01500000 sec

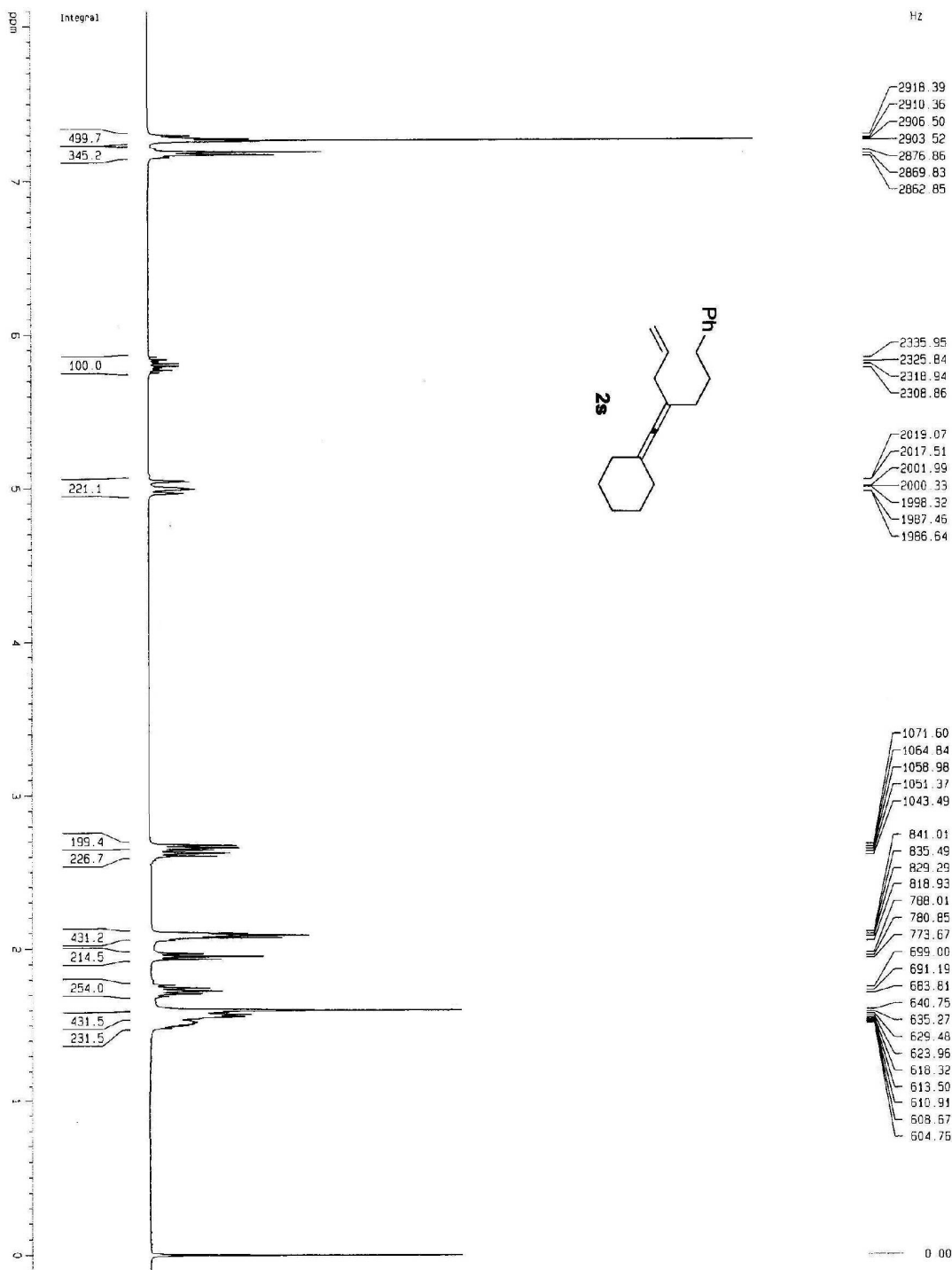
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 -1.00 dB
 SFO1 100.6264359 MHz

===== 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 100.6127704 MHz
 AOK EN
 SSB 0
 LB 1.00 Hz
 SB 0
 GC 1.40

1D NMR plot parameters
 CX 30.00 cm
 CY 45.00 cm
 F1P 220.000 ppm
 F1 223.481 Hz
 F2P -5.000 ppm
 F2 -503.66 Hz
 PHEN 7.5000000000000000
 HZCM 754.59376 Hz/cm

LJY-205



Current Data Parameters
NAME LJY-07
EXPNO 130
PROCNO 1

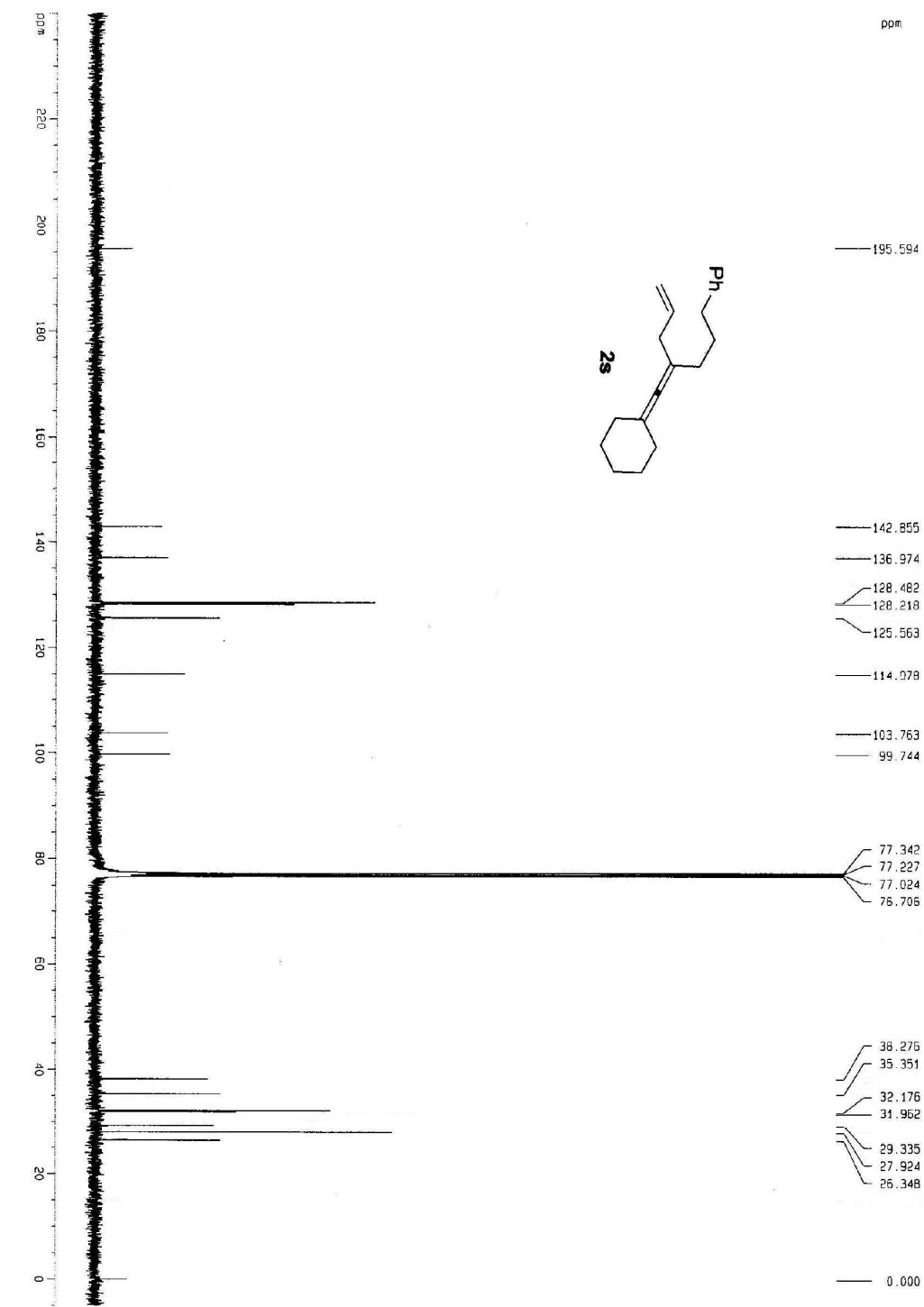
F2 - Acquisition Parameters
Date_ 20070815
Time 12.04
INSTRUM spect
PROBHD 5 mm Drel 13C/
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250667 Hz
AQ 1.9923444 sec
RG 382
JM 60.800 usec
JE 6.00 usec
TE 296.2 K
J1 1.00000000 sec
NOREST 0.00000000 sec
MCNMR 0.01500000 sec

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

F2 - Processing parameters
SI 16384
SF 400.130062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

===== NMR Plot Parameters =====
CX 30.00 cm
CY 100.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -40.100 ppm
F2 -40.01 Hz
PPMCM 0.27333 ppm/cm
HZCM :09.36887 Hz/cm

LJY-205



Current Data Parameters

NAME	VALUE
EXPNO	131
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20070815	12:57

INSTRUM spect

PROBHD 5 mm Dual 13C/

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 5118

DS 2

SWH 31847.133 Hz

FIDRES 0.465949 Hz

AQ 1.0286652 sec

RG 114

DW 15.700 usec

DE 6.00 usec

TE 256.2 K

31 2.00000000 sec

311 0.03000000 sec

DELTA 1.86599998 sec

ACQRES 0.00000000 sec

NCNRC 0.01500000 sec

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

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

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

OPPRG2	waltz16
NUC2 <td>1H</td>	1H
PCPD2	105.00 usec
PL2	-2.00 dB
PL12	18.00 dB
PL13	20.00 dB
SFO2	400.1324708 MHz

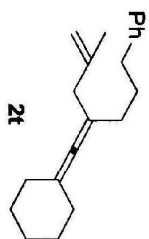
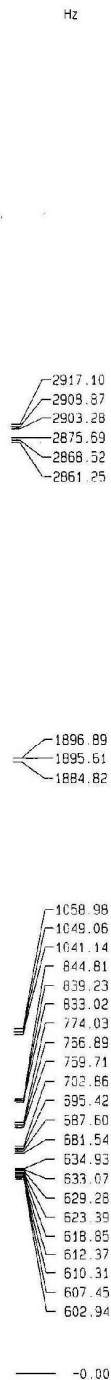
F2 - Processing parameters

SI	32768
SF	100.6127693 MHz
KON	EM
SSB	0
LB	1.00 Hz
GB	0
FC	1.40

1D NMR plot parameters

CX	30.00 cm
CV <td>56.00 cm</td>	56.00 cm
FLP <td>240.000 ppm</td>	240.000 ppm
F1 <td>24147.05 Hz</td>	24147.05 Hz
F2p <td>-5.000 ppm</td>	-5.000 ppm
F2 <td>-503.07 Hz</td>	-503.07 Hz
PPMCM <td>8.16657 ppm/cm</td>	8.16657 ppm/cm
HZTM <td>821.67062 Hz/cm</td>	821.67062 Hz/cm

LJY-1/1



Current Data Parameters
NAME mar-07
EXPNO 95
PROCNO 1

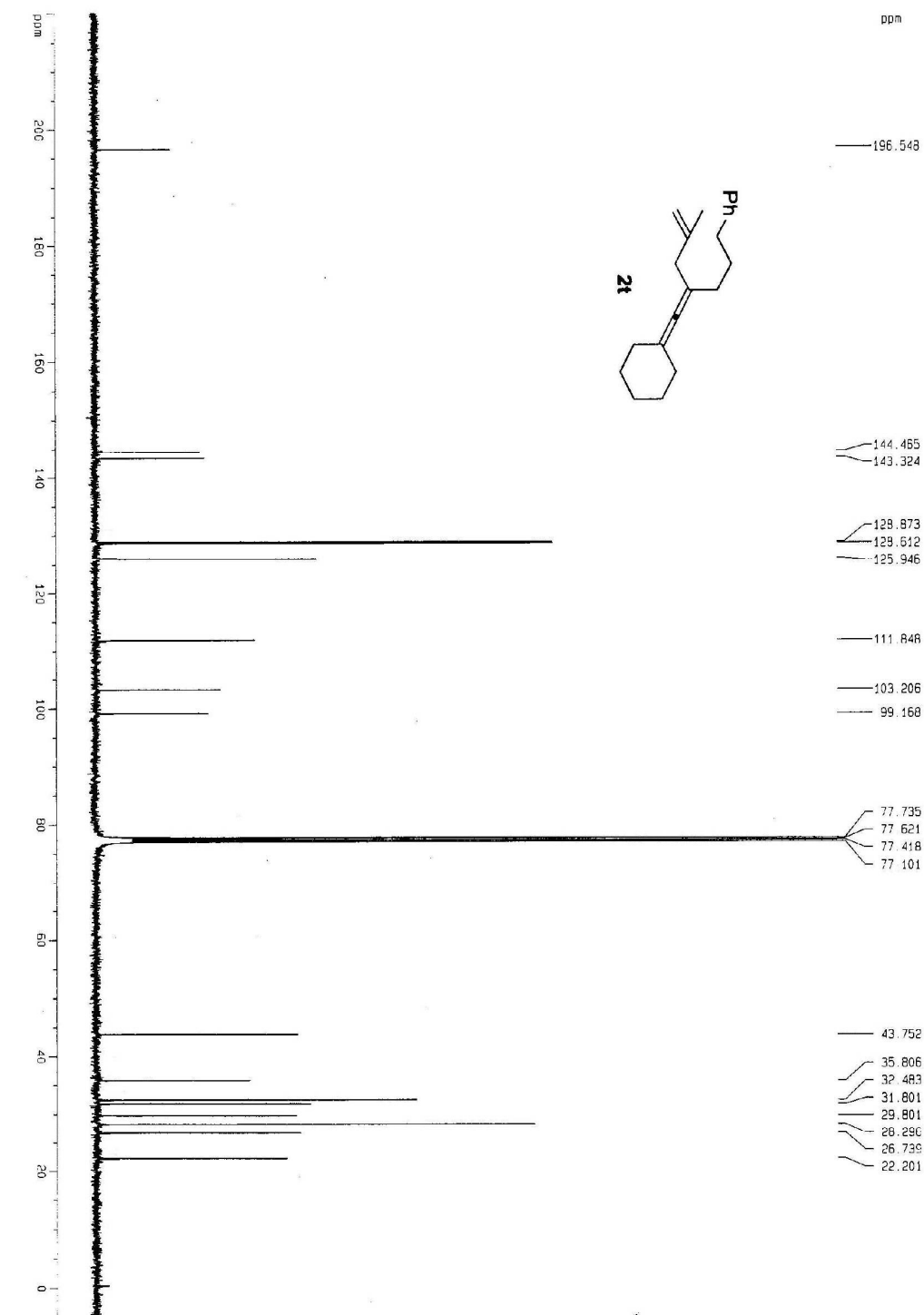
F2 - Acquisition Parameters
Date_ 20070612
Time 15.18
INSTRUM spect
PROBHD 5 mm QNP 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 228.1
RG 60.800 usec
DE 6.000 usec
TE 299.2 K
D1 1.00000000 sec
MORFEST 0.00000000 sec
MORF 0.01500000 sec

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

F2 - Processing parameters
SI 16384
SF 400.1300114 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 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

LJY-172



Current Data Parameters

NAME	Mar-07
EXPNO	96
PROCNO	1

F2 - Acquisition Parameters

Date_	20070612
Time	16.23
INSTRUM	spect
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	7577
DS	2
SWH	31647.133 Hz
FIDRES	0.485949 Hz
AQ	1.0289562 sec
RG	3649.1
OW	15.700 usec
DE	6.00 usec
TE	299.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.8898988 sec
MCOREST	0.00000000 sec
MCNPRK	0.01500000 sec

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

NUC1	13C
P1	10.80 usec
PL1	-1.00 dB
SFO1	100.6254358 MHz

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

OPDPFG2	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
SR	100.6127290 MHz
MW	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	220.000 ppm
F1	22134.80 Hz
F2P	-5.000 ppm
F2	-503.06 Hz
PPMCK	7.50000 ppm/cm
HZCK	754.59546 Hz/cm