

Supplementary Information

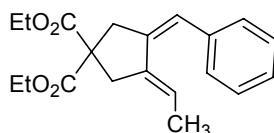
Rhodium Catalysed Chemo- and Stereoselective Arylative and Alkenylative Cyclisation Reactions of Unsymmetric Diynes Containing a Terminal Alkyne Moiety with Organoboronic Acids

Levent Artok,^{*a} Melih Kuş,^a Bağdagül N. Ürer,^a Gülşah Türkmen,^a Özge Aksın-Artok^b

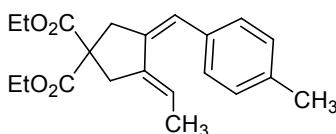
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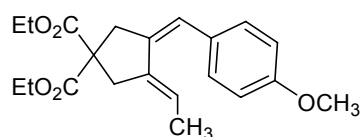
Data of Compounds



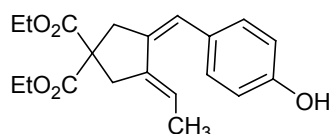
Compound 3aa: ¹H NMR (400 MHz, CDCl₃) δ: 1.26 (t, *J* = 7.0 Hz, 6H), 1.55 (d, *J* = 7.2 Hz, 3H), 3.01 (s, 2H), 3.08 (d, *J* = 2.0 Hz, 2H), 4.22 (q, *J* = 7.2 Hz, 4H), 5.73-5.78 (m, 1H), 6.33 (s, 1H), 7.14-7.34 (m, 5H); ¹³C NMR (100 MHz, CDCl₃) δ: 14.1, 15.1, 38.1, 43.4, 57.0, 61.6, 122.0, 122.2, 126.4, 128.2, 128.5, 135.2, 138.0, 138.2, 171.5; FTIR (ν_{max}/cm⁻¹): 2981, 1731, 1285, 1246, 1190, 1155, 1067, 861, 698; MS(EI, *m/z*): 328 (12 M⁺), 254 (92), 181 (100); HRMS (*m/z*, M⁺): 328.1669 (calculated), 328.1671 (found).



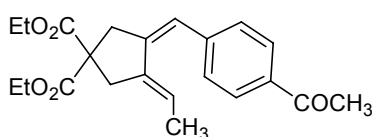
Compound 3ab: ^1H NMR (400 MHz, CDCl_3) δ : 1.26 (t, $J = 7.0$ Hz, 6H), 1.56 (d, $J = 7.2$ Hz, 3H), 2.32 (s, 3H), 3.00 (d, $J = 1.6$ Hz, 2H), 3.07 (d, $J = 1.6$ Hz, 2H), 4.22 (q, $J = 7.6$ Hz, 4H), 5.79-5.84 (m, 1H), 6.29 (s, 1H), 7.07 (d, $J = 8.0$ Hz, 2H), 7.22 (d, $J = 8.0$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.0, 15.1, 21.2, 38.1, 43.4, 57.0, 61.5, 121.9, 122.0, 128.4, 128.9, 134.9, 135.3, 136.0, 137.6, 171.5; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2980, 2923, 2856, 1732, 1286, 1246, 1191, 1156, 1068, 1054, 863, 804; MS(EI, m/z): 342 (15 M^+), 268 (100), 195 (99); HRMS (m/z , M^+): 342.1826 (calculated), 342.1818 (found).



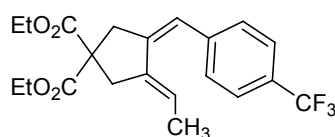
Compounds 3ac: ^1H NMR (400 MHz, CDCl_3) δ : 1.26 (t, $J = 7.2$ Hz, 6H), 1.57 (d, $J = 7.6$ Hz, 3H), 3.00 (s, 2H), 3.06 (d, $J = 2.0$ Hz, 2H), 3.80 (s, 3H), 4.21 (q, $J = 7.2$ Hz, 4H), 5.80-5.83 (m, 1H), 6.27 (s, 1H), 6.81 (d, $J = 8.8$ Hz, 2H), 7.26 (d, $J = 8.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.1, 15.1, 38.1, 43.4, 55.1, 55.2, 57.0, 61.5, 113.6, 121.6, 121.7, 129.7, 130.3, 135.4, 137.2, 158.1, 171.5; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2976, 2919, 2848, 1730, 1606, 1508, 1286, 1245, 1192, 1068, 910, 862, 731; MS(EI, m/z): 358 (53 M^+), 284 (38), 211 (72); HRMS (m/z , M^+): 358.1775 (calculated), 358.1776 (found).



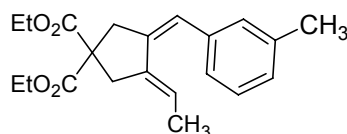
Compound 3ad: ^1H NMR (400 MHz, CDCl_3) δ : 1.22 (t, $J = 7.2$ Hz, 6H), 1.77 (d, $J = 6.8$ Hz, 3H), 3.00 (s, 2H), 3.29 (d, $J = 1.6$ Hz, 2H), 4.219 (q, $J = 7.2$ Hz, 2H), 4.221 (q, $J = 7.2$ Hz, 2H), 5.95-6.01 (m, 1H), 6.67 (s, 1H), 6.80 (d, $J = 8.4$ Hz, 2H), 7.19 (d, $J = 8.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.0, 15.0, 36.8, 39.5, 58.4, 61.7, 114.8, 115.3, 118.5, 130.1, 130.3, 136.2, 139.1, 154.6, 171.7; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2985, 2932, 2855, 1727, 1512, 1260, 1190, 1067, 910, 731; MS(EI, m/z): 344 (58 M^+), 270 (88), 197 (100); HRMS (m/z , M^+): 344.1618 (calculated), 344.1619 (found).



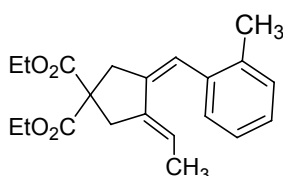
Compound 3ae: ^1H NMR (400 MHz, CDCl_3) δ : 1.27 (t, $J = 7.0$ Hz, 6H), 1.57 (d, $J = 7.2$ Hz, 3H), 2.58 (s, 3H), 3.02 (s, 2H), 3.09 (d, $J = 1.6$ Hz, 2H), 4.23 (q, $J = 7.2$ Hz, 4H), 5.76-5.81 (m, 1H), 6.32 (s, 1H), 7.44 (d, $J = 8.4$ Hz, 2H), 7.86 (d, $J = 8.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.0, 15.1, 26.5, 37.9, 43.3, 56.9, 61.6, 120.8, 123.3, 128.4, 128.7, 135.1, 135.2, 140.4, 143.3, 171.3, 197.7; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2981, 1730, 1681, 1600, 1250, 1191, 1068, 911, 863; MS(EI, m/z): 370 (33 M^+), 296 (93), 254 (100), 223 (54), 181 (49); HRMS (m/z , M^+): 370.1775 (calculated), 370.1771 (found).



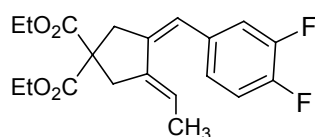
Compound 3af: ^1H NMR (400 MHz, CDCl_3) δ : 1.27 (t, $J = 7.2$ Hz, 6H), 1.57 (d, $J = 7.2$ Hz, 3H), 3.02 (s, 2H), 3.09 (d, $J = 1.6$ Hz, 2H), 4.23 (q, $J = 7.2$ Hz, 4H), 5.71-5.74 (m, 1H), 6.30 (s, 1H), 7.45 (d, $J = 8.4$ Hz, 2H), 7.51 (d, $J = 8.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.1, 15.1, 37.9, 43.3, 56.9, 61.6, 120.4, 123.2, 125.2 (q, $J=15.6$ Hz), 128.8, 135.1, 140.2, 141.8, 171.3; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2984, 1730, 1323, 1249, 1162, 1122, 1066, 909, 730, 832, 732; MS(EI, m/z): 396 (17 M^+), 322 (100), 249 (15); HRMS (m/z , M^+): 396.1543 (calculated), 396.1540 (found).



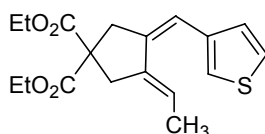
Compound 3ag: ^1H NMR (400 MHz, CDCl_3) δ : 1.26 (t, $J = 7.0$ Hz, 6H), 1.55 (d, $J = 7.2$ Hz, 3H), 2.30 (s, 3H), 3.00 (s, 2H), 3.08 (d, $J = 1.6$ Hz, 2H), 4.22 (q, $J = 7.2$ Hz, 4H), 5.75-5.80 (m, 1H), 6.31 (s, 1H), 6.99 (d, $J = 6.0$ Hz, 1H), 7.12-7.14 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.1, 15.1, 21.3, 38.1, 43.4, 57.0, 61.6, 122.1, 125.5, 127.2, 128.1, 129.1, 135.2, 137.8, 137.9, 171.5; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2983, 2930, 1729, 1254, 1187, 1070, 909, 725; MS(EI, m/z): 342 (21 M^+), 269 (100), 196 (79); HRMS (m/z , M^+): 342.1826 (calculated), 342.1825 (found).



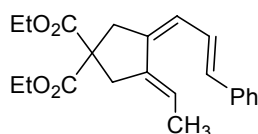
Compound 3ah: ^1H NMR (400 MHz, CDCl_3) δ : 1.27 (t, $J = 7.0$ Hz, 6H), 1.50 (d, $J = 6.8$ Hz, 3H), 2.20 (s, 3H), 3.0 (s, 2H), 3.12 (d, $J = 1.6$ Hz, 2H), 4.219 (q, $J = 7.2$ Hz, 2H), 4.22 (q, $J = 7.0$ Hz, 2H), 5.27-5.33 (m, 1H), 6.33 (s, 1H), 7.08-7.18 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ : 13.1, 14.2, 18.7, 37.3, 42.3, 56.3, 60.5, 120.2, 121.0, 124.6, 125.7, 127.7, 128.8, 134.7, 134.9, 136.5, 137.0, 170.5; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 3062, 2980, 2932, 1731, 1246, 1191, 1068, 861, 830, 758, 735; MS(EI, m/z): 342 (21 M^+), 269 (100), 196 (88); HRMS (m/z , M^+): 342.1826 (calculated), 342.1834 (found).



Compound 3ai: ^1H NMR (400 MHz, CDCl_3) δ : 1.26 (t, $J = 7.2$ Hz, 6H), 1.58 (d, $J = 6.8$ Hz, 3H), 3.00 (s, 2H), 3.06 (d, $J = 2.0$ Hz, 2H), 4.22 (q, $J = 7.2$ Hz, 4H), 5.70-5.73 (m, 1H), 6.21 (s, 1H), 6.99-7.17 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.1, 15.1, 37.9, 43.2, 56.9, 61.6, 116.9, 117.1, 117.2, 117.3, 119.7, 123.0, 124.67, 124.71, 124.73, 124.76, 135.9, 139.5, 147.6, 147.8, 148.8, 149.0, 150.2, 151.3, 150.1, 151.4, 171.3; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2983, 1731, 1513, 1285, 1245, 1192, 1191, 1068, 862, 768; MS(EI, m/z): 364 (25 M^+), 290 (100), 217 (27); HRMS (m/z , M^+): 364.1481 (calculated), 364.1488 (found).

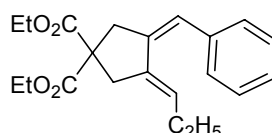


Compound 3aj: ^1H NMR (400 MHz, CDCl_3) δ : 1.25 (t, $J = 7$ Hz, 6H), 1.62 (d, $J = 6.8$ Hz, 3H), 3.02 (s, 2H), 3.06 (d, $J = 1.6$ Hz, 2H), 4.22 (q, $J = 7.2$ Hz, 4H), 5.89-5.95 (m, 1H), 6.23 (s, 1H), 7.10-7.22 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.1, 15.1, 38.0, 43.2, 57.0, 61.6, 116.1, 122.3, 122.5, 124.7, 128.0, 135.7, 138.4, 138.5, 171.5; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2980, 1729, 1366, 1250, 1185, 1067, 861, 774; MS(EI, m/z): 334 (7 M^+), 260 (24), 173 (100); HRMS (m/z , M^+): 334.1233 (calculated), 334.1227 (found).

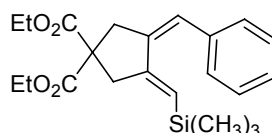


Compound 3ak: ^1H NMR (400 MHz, CDCl_3) δ : 1.25 (t, $J = 7.2$ Hz, 6H), 1.82 (d, $J = 8.8$ Hz, 3H), 3.04 (s, 2H), 3.07 (s, 2H), 4.20 (q, $J = 7.2$ Hz, 4H), 6.01-6.06 (m, 1H), 6.16 (d, $J =$

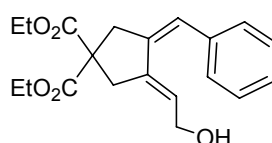
10.8 Hz, 1H), 6.53 (d, $J = 15.6$ Hz, 1H), 7.2 (q, $J = 8$ Hz, 1H), 7.25-7.45 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.0, 15.6, 38.2, 43.1, 57.2, 61.6, 123.3, 123.4, 125.7, 126.4, 127.3, 128.6, 132.6, 137.5, 137.7, 138.9, 171.4; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 3026, 2984, 2959, 2854, 1730, 1447, 1366, 1247, 1188, 1060, 964, 860, 749, 692; MS(EI, m/z): 354 (7 M^+), 279 (100), 206 (11); HRMS (m/z , M^+): 354.1826 (calculated), 354.1835 (found).



Compound 3ba: ^1H NMR (400 MHz, CDCl_3) δ : 0.83 (t, $J = 7.6$ Hz, 3H), 1.26 (t, $J = 7.2$ Hz, 6H), 1.95 (q, $J = 7.2$ Hz, 2H), 3.00 (s, 2H), 3.08 (d, $J = 2$ Hz, 2H), 4.22 (q, $J = 7.2$ Hz, 4H), 5.70 (tt, $J = 2.4, 7.6$ Hz, 1H), 6.33 (s, 1H), 7.10-7.40 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 13.2, 14.1, 23.0, 37.9, 43.2, 57.1, 61.5, 122.2, 126.4, 128.1, 128.5, 129.5, 133.6, 138.0, 138.3, 171.5; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2956, 2925, 2872, 1732, 1247, 1191, 1067, 863, 698; MS(EI, m/z): 342 (18 M^+), 268 (100), 239 (79), 195 (93), 165 (63); HRMS (m/z , M^+): 342.1826 (calculated), 342.1821 (found).

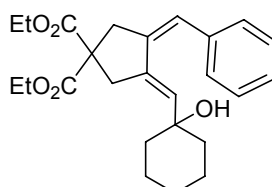


Compound 3ca: ^1H NMR (400 MHz, CDCl_3) δ : 0.2 (s, 9H), 1.45 (t, $J = 7.0$ Hz, 6H), 3.25 (d, $J = 2.0$ Hz, 2H), 3.28 ($J = 2.0$ Hz, 2H), 4.396 (q, $J = 7.2$ Hz, 2H), 4.402 (q, $J = 7.2$ Hz, 2H), 6.07 (t, $J = 2.0$ Hz, 1H), 6.62 (s, 1H), 7.35 (t, $J = 7.2$ Hz, 1H), 7.41-7.45 (m, 2H), 7.53 (d, $J = 7.2$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : -0.5, 14.2, 41.9, 42.4, 57.5, 61.7, 124.9, 126.5, 126.9, 128.2, 128.7, 137.5, 139.1, 149.8, 171.5; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2977, 2956, 2899, 1732, 1246, 1190, 1158, 1066, 861, 751, 696; MS(EI, m/z): 386 (7, M^+), 313 (89), 195 (100), 165 (27), 73 (30); HRMS (m/z , M^+): 386.1908 (calculated), 386.1911 (found).

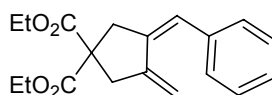


Compound 3da: ^1H NMR (400 MHz, CDCl_3) δ : 1.26 (t, $J = 7.2$ Hz, 6H), 1.68 (s, OH), 3.03 (s, 2H), 3.12 (d, $J = 1.6$ Hz, 2H), 4.07 (d, $J = 7.2$ Hz, 2H), 4.21 (q, $J = 7.2$ Hz, 4H), 5.80-

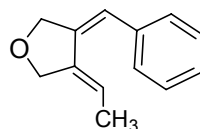
5.85 (m, 1H), 6.46 (s, 1H), 7.16-7.33 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.2, 38.2, 42.8, 57.2, 60.6, 61.9, 124.6, 125.3, 127.0, 128.53, 128.55, 137.3, 137.53, 137.58, 171.4; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2918, 2850, 1737, 1456, 908, 735, 699; MS(EI, m/z): 344 ($<1\text{ M}^+$), 326 (27), 253 (69), 207 (51), 179 (100), 165 (39); HRMS (m/z , M^+): 344.1618 (calculated), 344.1608 (found).



Compound 3ea: ^1H NMR (400 MHz, CDCl_3) δ : 1.10-1.60 (m, 10H), 1.26 (t, $J = 7.2\text{ Hz}$, 6H), 1.81(s, OH), 3.08 (d, $J = 2\text{ Hz}$, 2H), 3.29 (d, $J = 2\text{ Hz}$, 2H), 4.21 (q, $J = 7.2\text{ Hz}$, 4H), 5.79 (t, $J = 2\text{ Hz}$, 1H), 6.41 (s, 1H), 7.10-7.38 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.1, 22.3, 25.2, 38.6, 38.8, 57.6, 61.6, 72.1, 123.2, 126.6, 128.3, 128.6, 133.3, 135.3, 137.9, 139.4, 171.5, FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2930, 2853, 1732, 1448, 1553, 1184, 1068, 910, 733, 700; MS(EI, m/z): 394(39), 320 (62), 247 (62), 173 (100); HRMS (m/z , M^+): 412.2244 (calculated), 412.2251 (found).

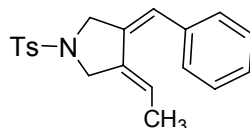


Compound 3fa: ^1H NMR (400 MHz, CDCl_3) δ : 1.26 (t, $J = 7.0\text{ Hz}$, 6H), 3.06 (t, $J = 2.0\text{ Hz}$, 2H), 3.15 (d, $J = 1.6\text{ Hz}$, 2H), 4.21 (q, $J = 7.0\text{ Hz}$, 4H), 4.91 (s, 1H), 5.12 (d, $J = 2.0\text{ Hz}$, 1H), 6.49 (s, 1H), 7.17-7.36 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.0, 42.8, 43.0, 57.1, 61.6, 111.0, 124.9, 126.8, 128.3, 128.4, 137.1, 137.6, 142.5, 171.3; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 3054, 2972, 1714, 1595, 1366, 1189, 910, 733, 698; MS(EI, m/z): 314 (16 M^+), 240 (94), 167 (100); HRMS (m/z , M^+): 314.1513 (calculated), 314.1517 (found).

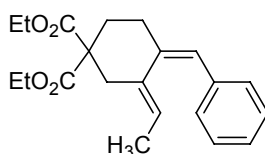


Compound 3ga: ^1H NMR (400 MHz, CDCl_3) δ : 0.87 (t, $J = 7.4\text{ Hz}$, 3H), 1.89 (q, $J = 8.4\text{ Hz}$, 2H), 4.52 (m, 4H), 5.8 (tt, $J = 2.4, 7.4\text{ Hz}$, 1H), 6.36 (s, 1H), 7.20-7.40 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 13.3, 23.3, 71.6, 74.7, 119.5, 126.8, 126.9, 128.3, 128.4, 133.8, 137.1;

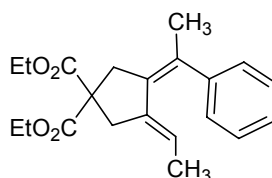
FTIR ($\nu_{\max}/\text{cm}^{-1}$): 3040, 1073, 739, 699; MS(EI, m/z): 200 (14 M^+), 185 (16), 170 (92), 155 (16), 141 (100), 128 (51), 115 (47), 105 (56), 91 (60), 77 (31); HRMS (m/z , M^+): 200.1187 (calculated), 200.1196 (found).



Compound 3ha: ^1H NMR (400 MHz, CDCl_3) δ : 1.49 (d, $J = 7.2$ Hz, 3H), 2.44 (s, 3H), 3.97 (s, 2H), 4.02 (d, $J = 2.0$ Hz, 2H), 5.67-5.76 (m, 1H), 6.31 (s, 1H), 7.19-7.30 (m, 5H), 7.34 (d, $J = 8.0$ Hz, 2H), 7.75 (d, $J = 8.0$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 15.3, 21.7, 51.8, 55.2, 122.3, 122.5, 127.2, 128.1, 128.3, 128.6, 129.9, 132.5, 132.8, 134.0, 136.9, 143.9; FTIR ($\nu_{\max}/\text{cm}^{-1}$): 3059, 3027, 2924, 2853, 1348, 1162, 1065, 815, 738, 699, 663; MS(EI, m/z): 339 (26 M^+), 281 (12), 207 (91), 183 (100), 168 (69), 155 (54), 141 (45), 129 (61), 115 (31), 91 (66); HRMS (m/z , $(M+H)^+$): 340.13658 (calculated), 340.13667 (found).

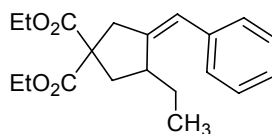


Compound 3ia: ^1H NMR (400 MHz, CDCl_3) δ : 1.26 (t, $J = 7.2$ Hz, 6H), 1.57 (d, $J = 7.0$ Hz, 3H), 2.26 (t, $J = 6.4$ Hz, 2H), 2.40 (t, $J = 6.4$ Hz, 2H), 2.94 (s, 2H), 4.20 (q, $J = 7.2$ Hz, 4H), 5.32 (t, $J = 3.2$ Hz, 1H), 6.14 (s, 1H), 7.05-7.32 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 13.2, 14.1, 32.8, 33.6, 34.7, 56.3, 61.4, 122.9, 124.5, 125.9, 127.8, 128.7, 132.2, 137.8, 142.6, 171.1; FTIR ($\nu_{\max}/\text{cm}^{-1}$): 2927, 1731, 1251, 1185, 1070, 861, 700; MS(EI, m/z): 342 (9, M^+), 268 (100), 196 (39); HRMS (m/z , M^+): 342.1826 (calculated), 342.1822 (found).

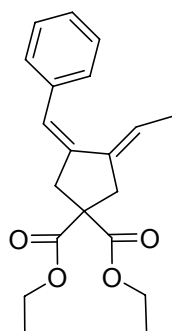


Compound 5a: ^1H NMR (400 MHz, CDCl_3) δ : 1.19 (t, $J=7.2$ Hz, 6H), 1.34, (d, $J=6.8$ Hz, 3H), 1.93 (s, 3H), 2.9 (s, 2H), 3.0 (s, 2H), 4.15 (q, $J=7.2$ Hz, 4H), 4.67-4.72 (m, 1H), 7.04-7.25 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.3, 15.4, 24.2, 38.2, 40.0, 57.3, 61.8, 121.3, 126.5, 128.2, 128.8, 130.3, 132.6, 136.5, 144.8, 172.0; FTIR ($\nu_{\max}/\text{cm}^{-1}$): 2982, 2816, 1730,

1248, 1192, 1054, 912, 861, 732, 701; MS(EI, m/z): 342 (19 M^+), 268 (100), 239 (69), 195 (96), 167 (44); HRMS (m/z , M^+): 342.1826 (calculated), 342.1822 (found).



Compound 7a: ^1H NMR (400 MHz, CDCl_3) δ : 1.26 (t, $J = 7.3$ Hz, 6H), 2.09 (dd, $J = 14.0, 6.2$ Hz, 1H), 2.17 (dd, $J = 15.6, 11.0$ Hz, 1H), 2.60 (dd, $J = 16.4, 3.4$ Hz, 1H), 2.80 (dd, $J = 13.6, 8.2$ Hz, 1H), 3.02 (d, $J = 16.4$ Hz, 1H), 3.23 (d, $J = 16.4$ Hz, 1H), 3.63 (s, 3H), 3.62-3.72 (m, 1H), 4.20 (q, $J = 7.2$ Hz, 2H), 4.21 (q, $J = 7.2$ Hz, 2H), 6.41 (s, 1H), 7.16-7.33 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 14.00, 14.04, 36.3, 37.4, 40.1, 43.1, 51.6, 58.3, 61.6, 61.7, 123.6, 126.6, 128.1, 128.4, 136.9, 143.7, 171.3, 171.7, 172.7; FTIR ($\nu_{\text{max}}/\text{cm}^{-1}$): 2982, 1728, 1245, 1176, 1068, 914, 731, 698; MS(EI, m/z): 374 (21 M^+), 300 (100), 254 (44), 240 (25), 227 (43), 194 (23), 167 (75), 153 (57), 91 (41); HRMS (m/z , M^+): 374.1724 (calculated), 374.1722 (found).



3aa

BC-DB3-KISIM1

Sample Name:

BC-DB3-KISIM1

Data Collected on:

nmr400-vnmr400

Archive directory:

/home/walkup1/vnmr400/data

Sample directory:

BC-DB3-KISIM1.18aug2008

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 18 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.356 sec

Width 6410.3 Hz

32 repetitions

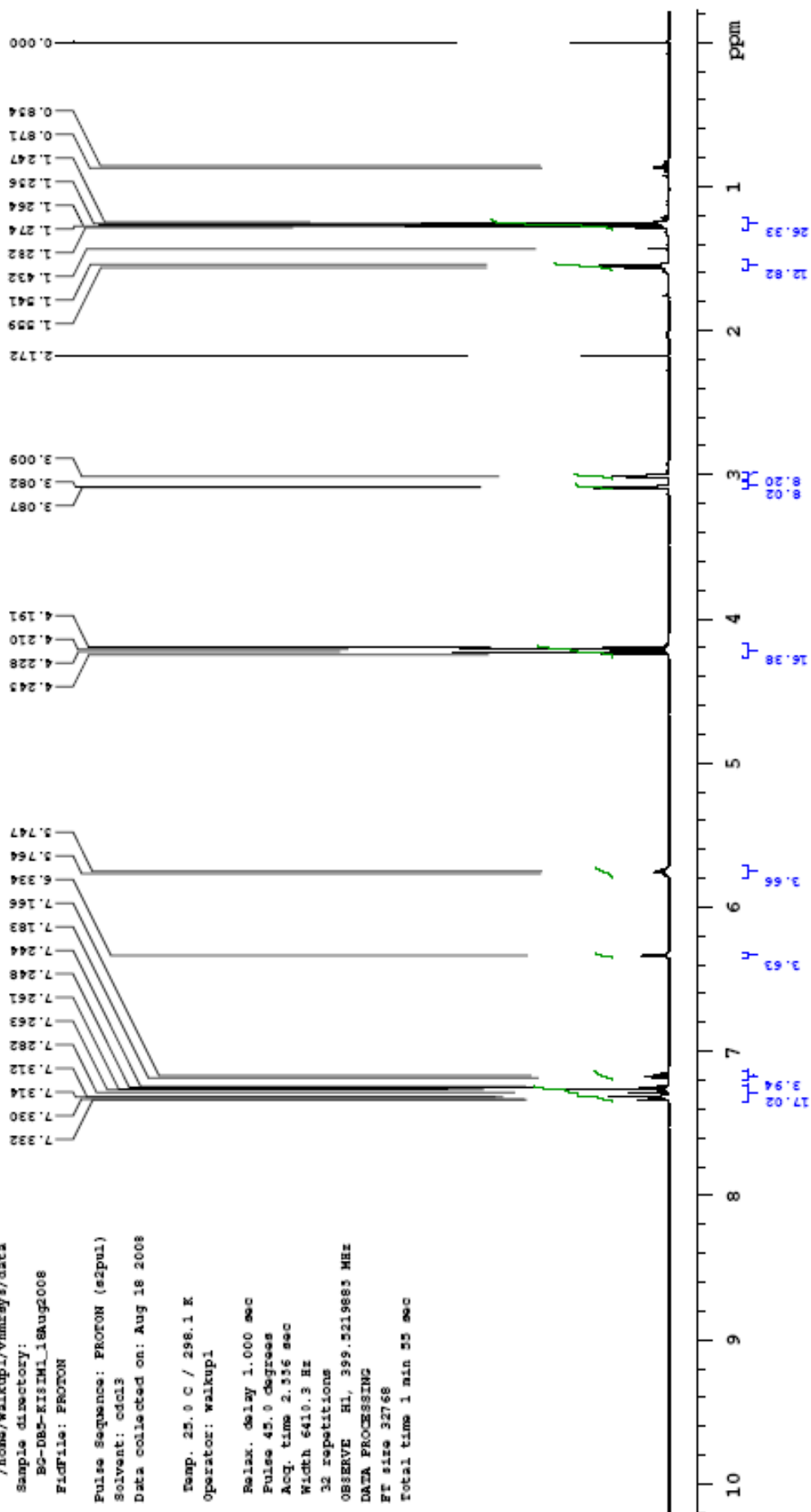
OBSERVE H1, 399.5219683 MHz

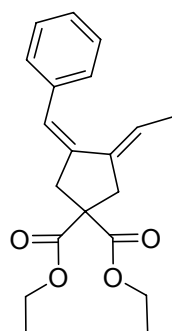
DATA PROCESSING

FT size 32768

Total time 1 min 55 sec

VARIAN





3aa

BO-DB3-KISIM1

Sample Name:

BO-DB3-KISIM1

Data Collected on:

nmr400-vnmr400

Archive directory:

/home/walkup/vnmr400/data

Sample directory:

BO-DB3-KISIM1_18Aug2008

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 18 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25310.2 Hz

256 repetitions

OBSERVE C13, 100.459839 MHz

DECOUPLE H1, 399.523962 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

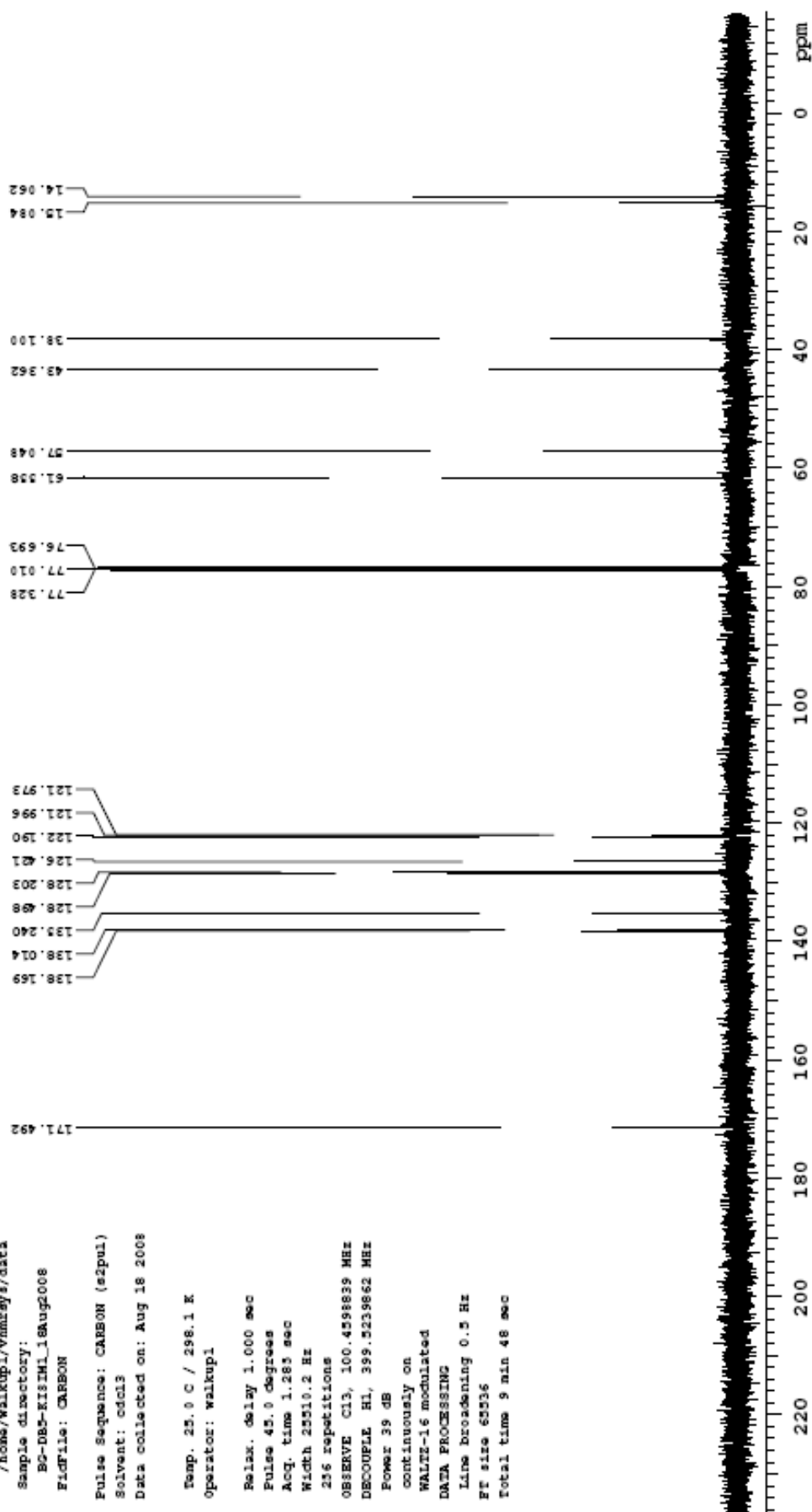
DATA PROCESSING

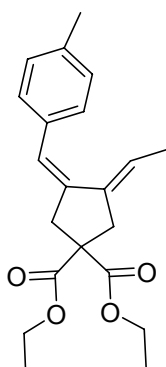
Line broadening 0.5 Hz

FT size 65536

Total time 9 min 48 sec

VARIAN





3ab

BC-DB9T-14-17KISIM

Sample Name:

BC-DB9T-14-17KISIM

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkup/vnmrsws/data

Sample directory:

BC-DB9T-14-17KISIM_26Aug2008

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 26 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

64 repetitions

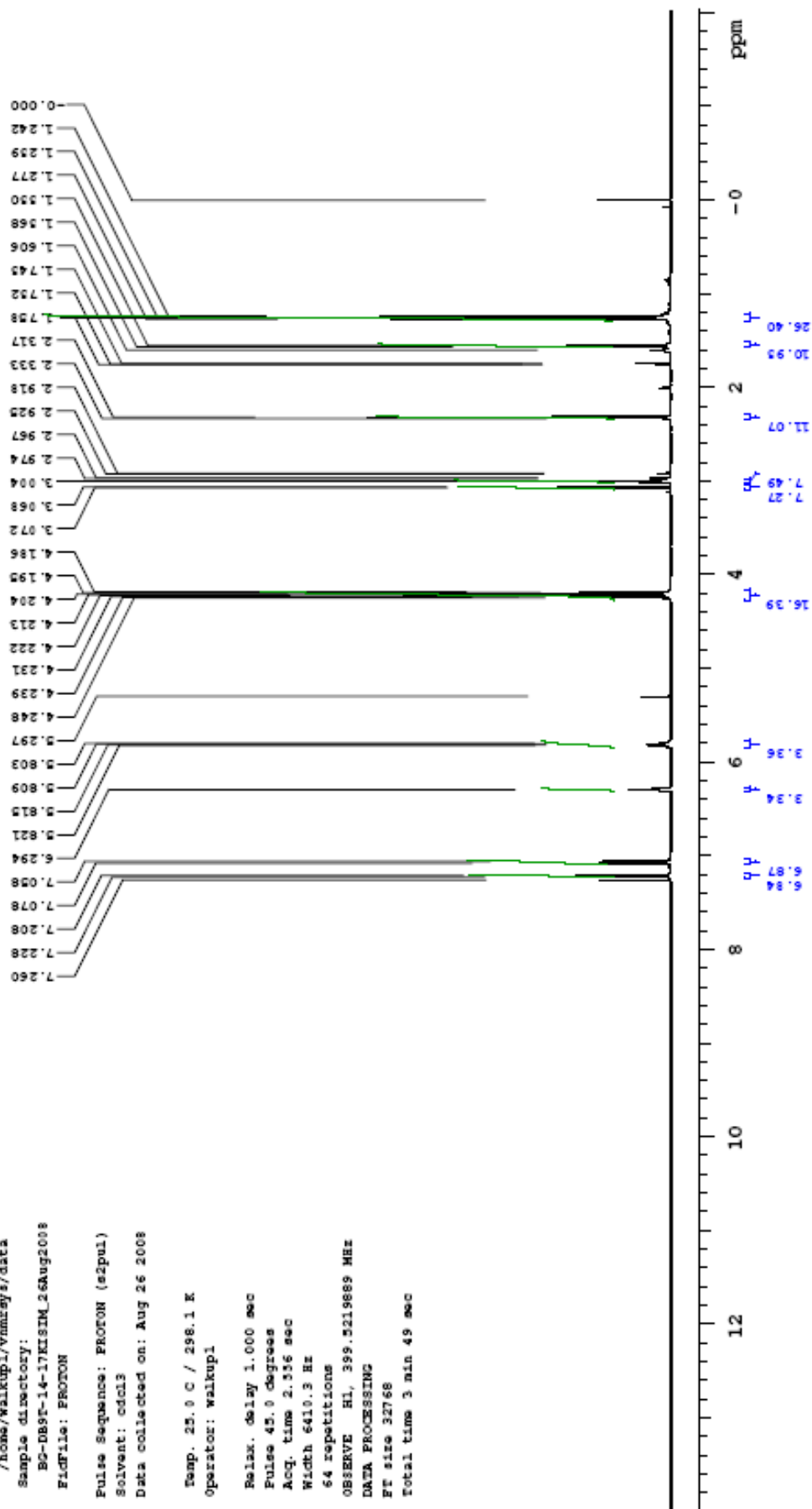
OBSERVE H1, 399.3219889 MHz

DATA PROCESSING

FF size 32768

Total time 3 min 49 sec

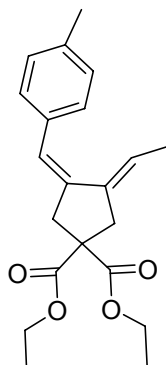
VARIAN



BG-DB9T-14-17KISIM

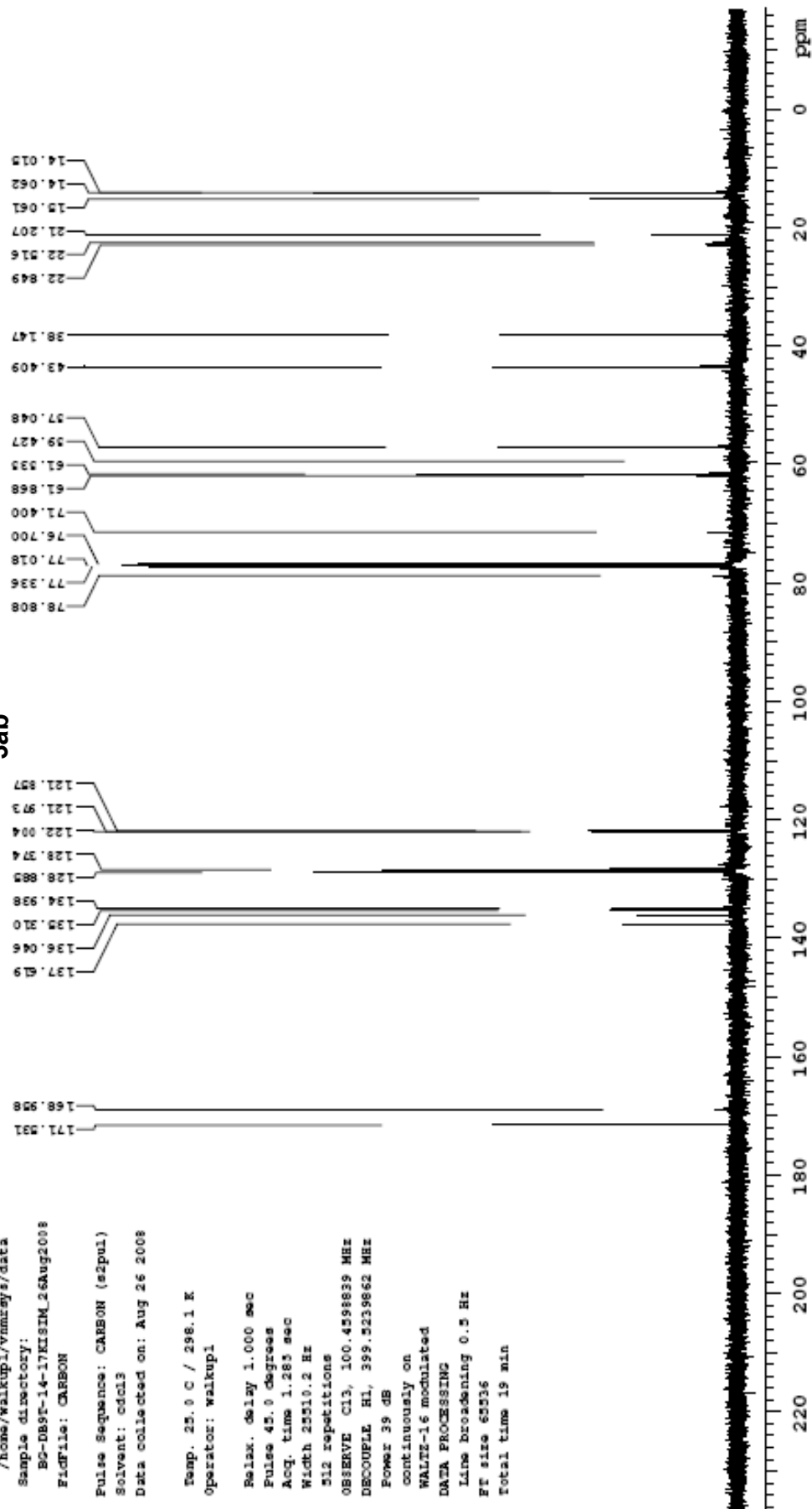
Sample Name:
BG-DB9T-14-17KISIM
Data Collected on:
nmr400-vnmr400
Archive directory:
/home/walkup/vnmr400/data
Sample directory:
BG-DB9T-14-17KISIM_26Aug2008
FidFile: CARBON
Pulse Sequence: CARBON (zgpg3)
Solvent: cdcl3
Data collected on: Aug 26 2008

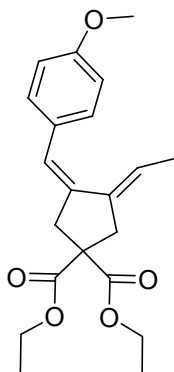
Temp. 25.0 C / 298.1 K
Operator: walkup
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.283 sec
Width 25510.2 Hz
312 repetitions
OBSERVE C13, 100.4598839 MHz
DECOUPLE H1, 399.5239862 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
Ft size 65536
Total time 19 min



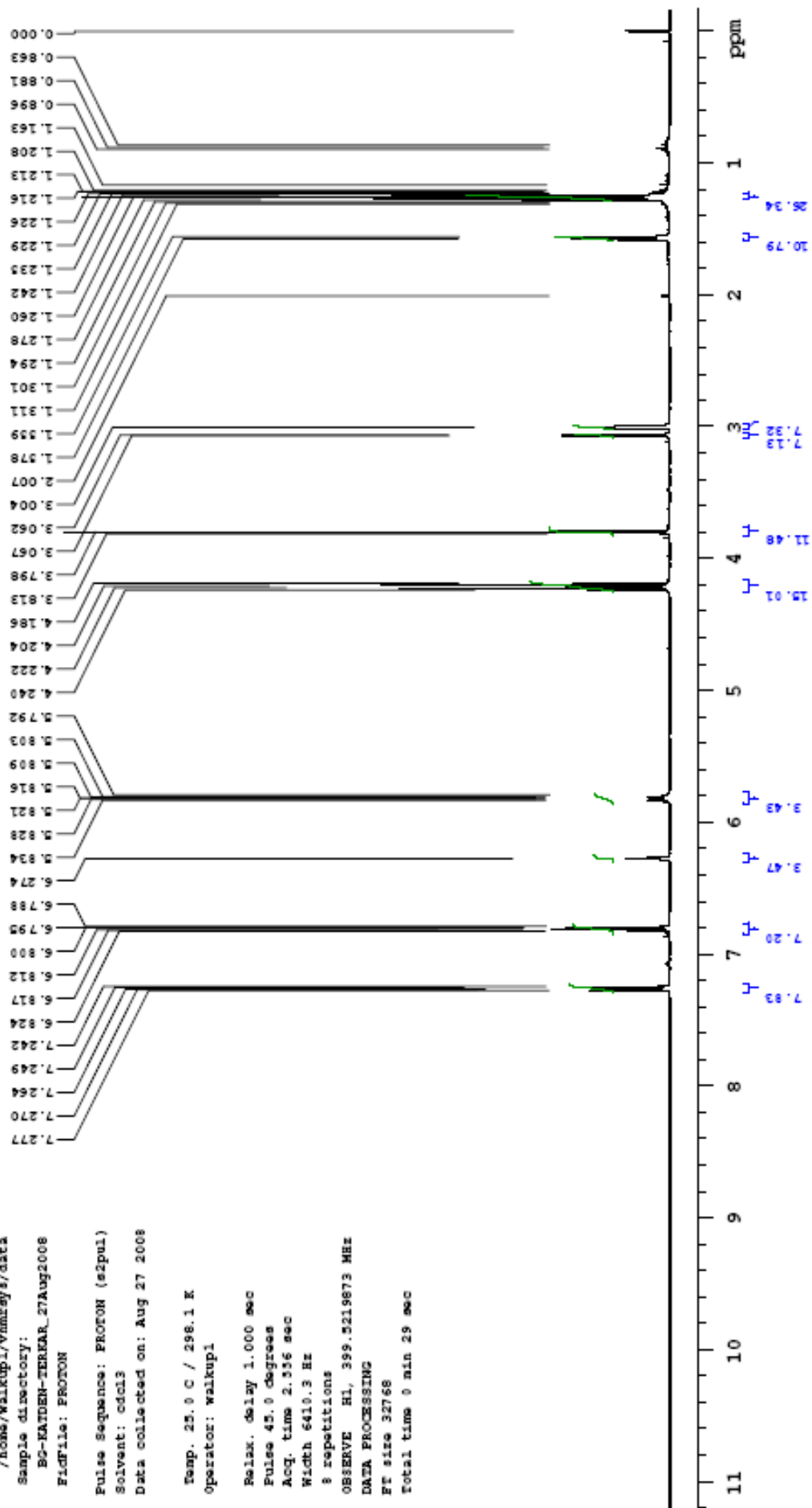
3ab

VARIAN





3ac



BO-KATDEN-TERKAR.

Sample Name:

BC-KATDEN-TERKAR.

Data Collected on:

nnr400-vnars400

Archive directory:

```
/home/walkup1/vnmrsws/data
```

sample director:

BC-KATDEN-TERKAR 27AUG2008

NOTED: PROTON
B2-BALANCE-28

Pulse sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 27 2008

Temp. 25.0 C / 298.1 K

operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

8 repetitions

OBSERVE H1, 399.5219873 MHz

DATA PROCESSING

FT 5120 32768

Total time 0 min 29 sec



BC-KATDEN-TERKEAR

Sample Name:

BC-KATDEN-TERKEAR

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkup1/vnmrsws/data

Sample directory:

BC-KATDEN-TERKEAR_27Aug2008

File: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 27 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.283 sec

Width 25510.2 Hz

256 repetitions

OBSERVE C13, 100.4598839 MHz

DECOUPLE H1, 399.5239862 MHz

Power 39 dB

continuously on

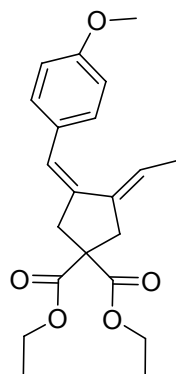
WALTZ-16 modulated

DATA PROCESSING

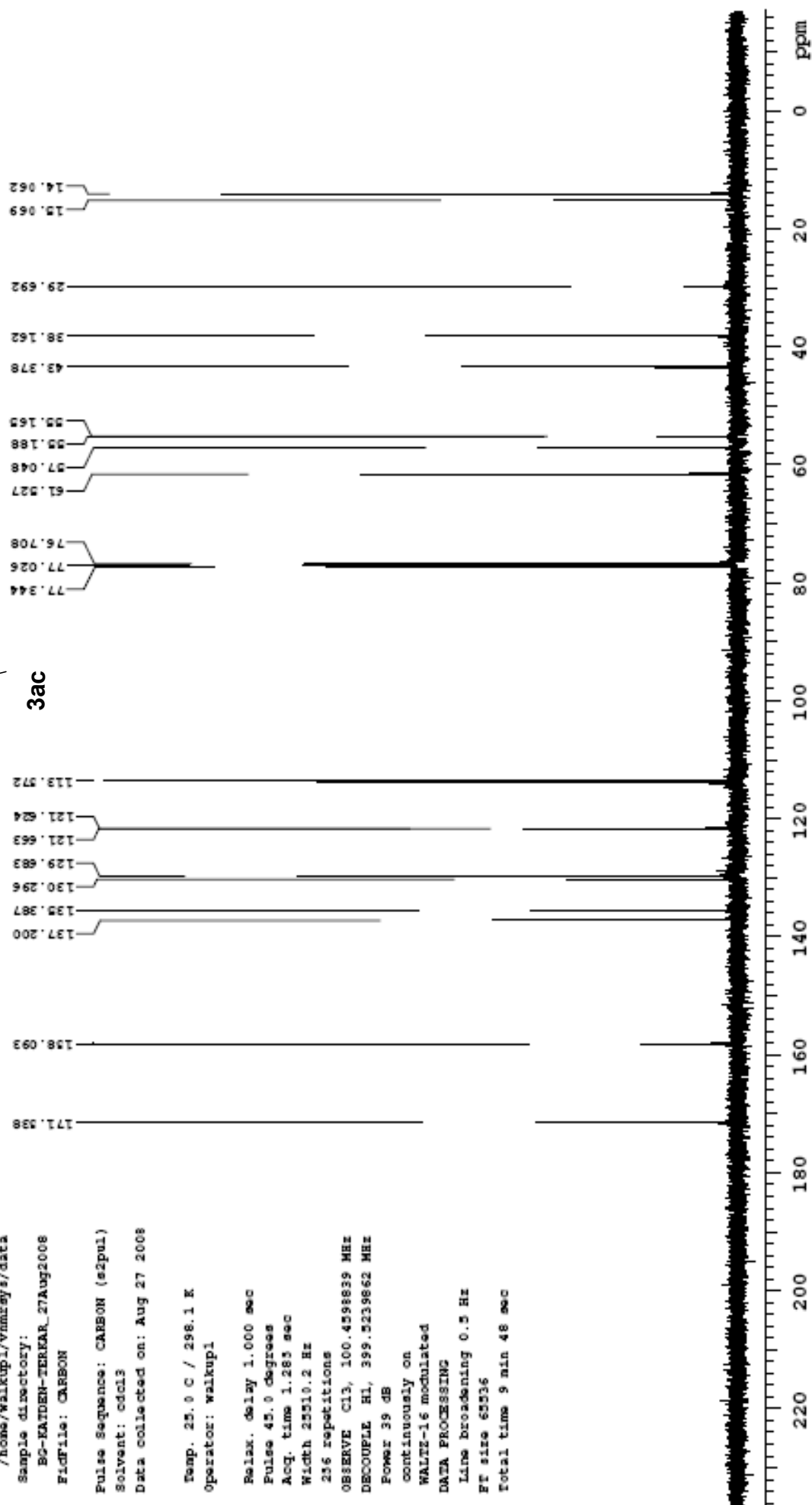
Line broadening 0.5 Hz

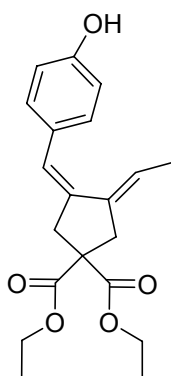
FT size 65536

Total time 9 min 48 sec



3ac

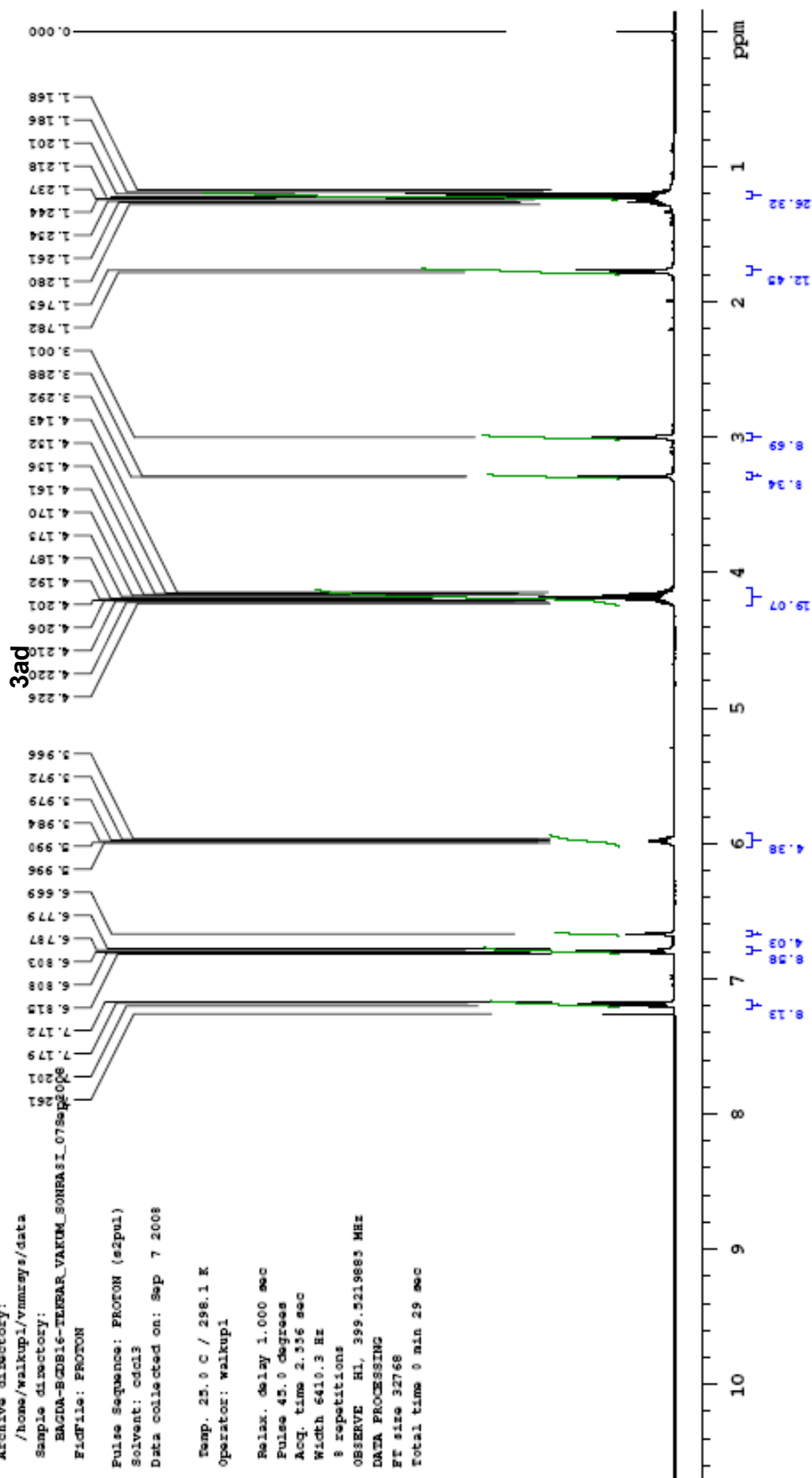


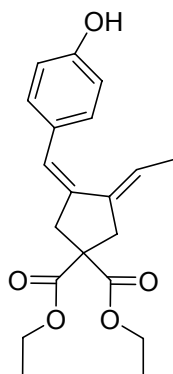


```

8 repetitions
OBSERVE HI, 399.5219885 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 29 sec

```





3ad

BAGDA-B2B16-TEKAR VAKUM SONHESI

Sample Name:

BAGDA-B2B16-TEKAR VAKUM SONHESI

Data Collected on:

nmr400-vnmr400

Archive directory:

/home/walkup1/vnmr400/data

Sample directory:

BAGDA-B2B16-TEKAR VAKUM SONHESI_079822008

FidFile: CARBON

Pulse Sequence: CARBON (zgpg3)

Solvent: cdcl3

Data collected on: Sep 7 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.283 sec

Width 25510.2 Hz

512 repetitions

OBSERVE CH3, 100.4598839 MHz

DECOUPLE H1, 399.5239862 MHz

Power 39 dB

continuously on

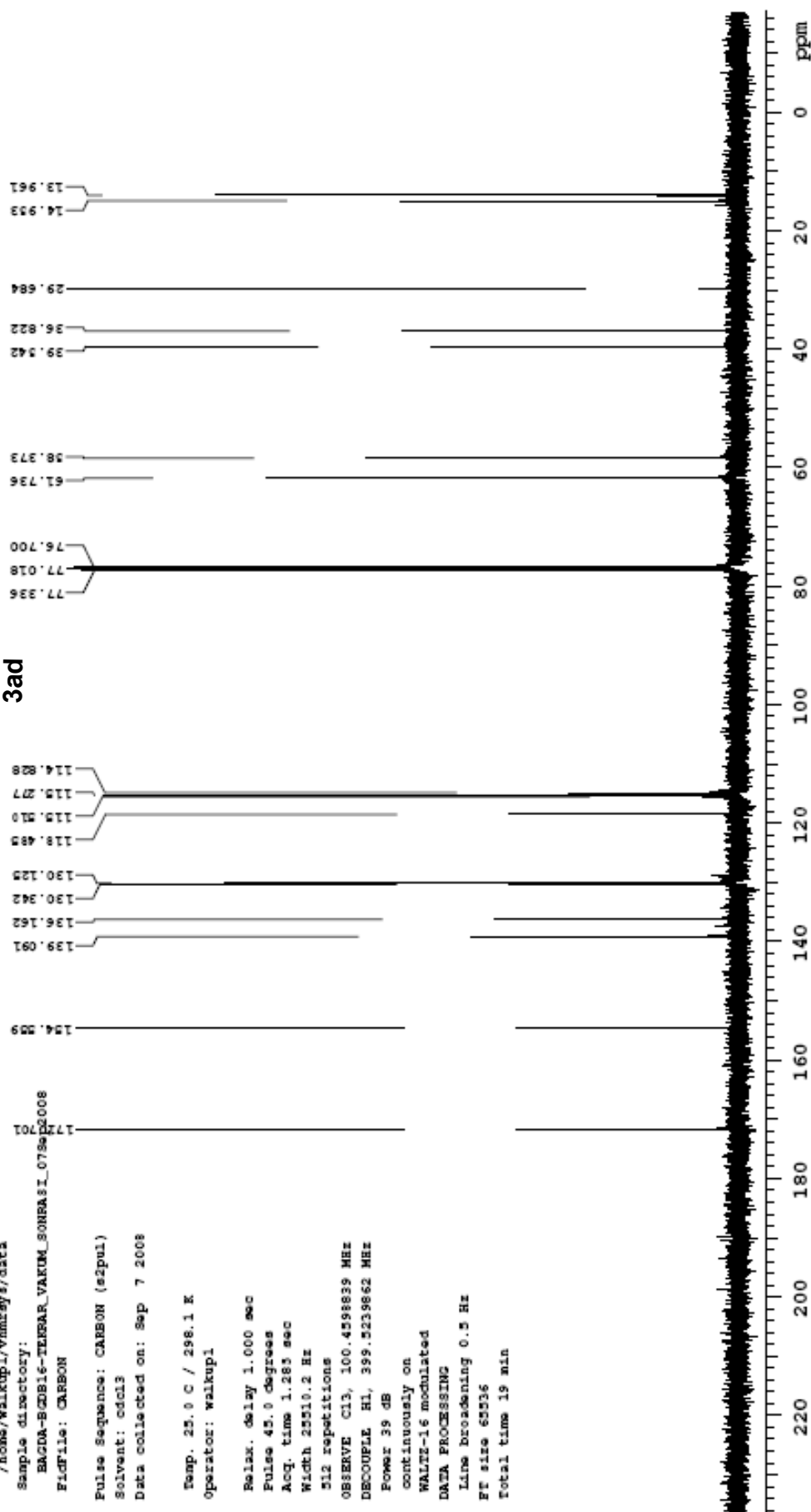
WALTZ-16 modulated

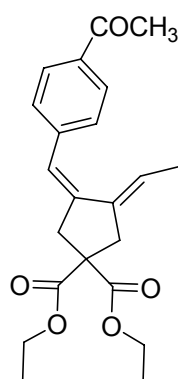
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 19 min





3ae

KUSHER

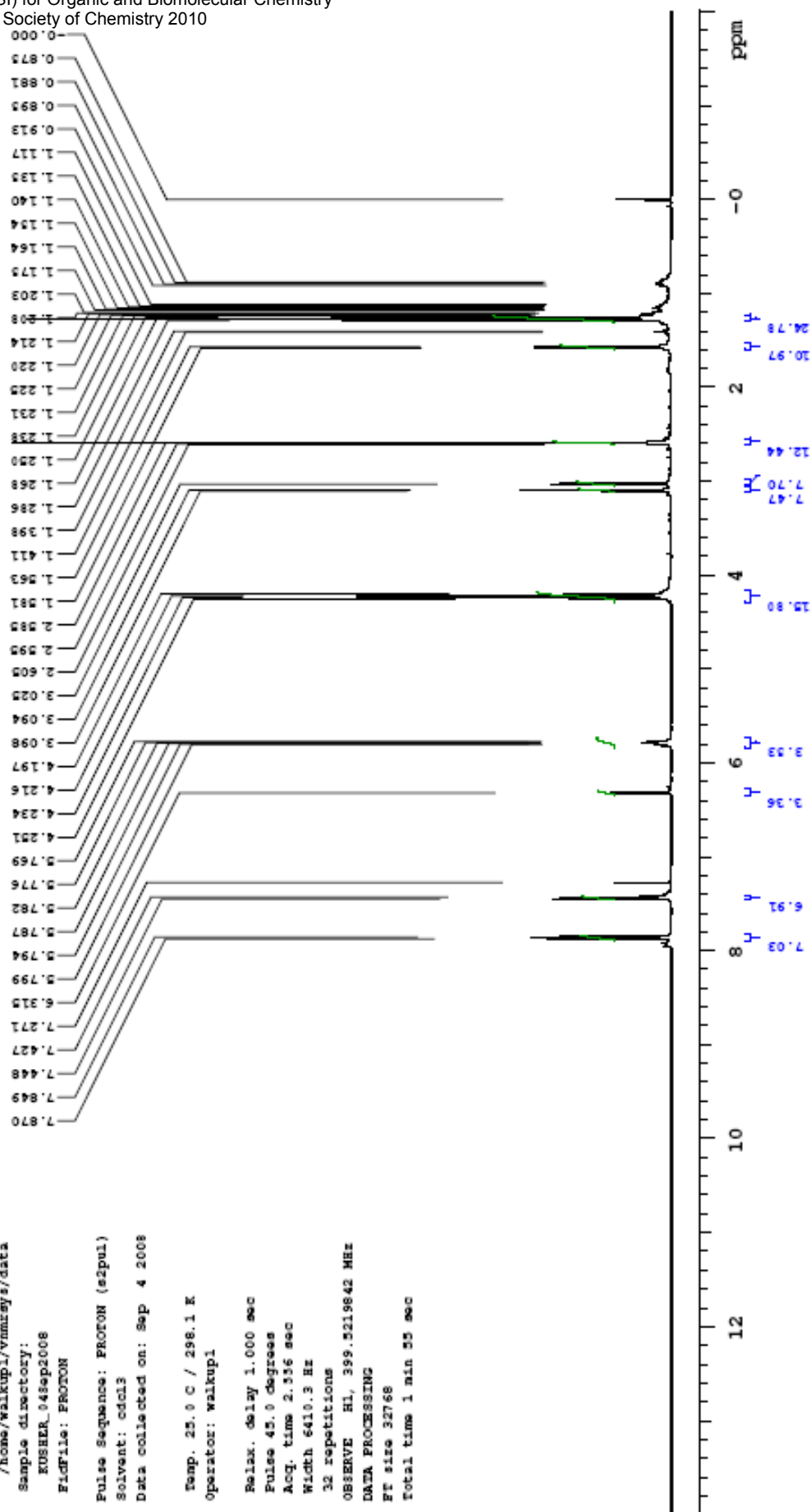
Sample Name:
KUSHER
Data Collected on:
nmr400-vnmr400
Archive directory:
/home/walkup1/vnmr400/data
Sample directory:
KUSHER_04sep2008
FidFile: PROTON

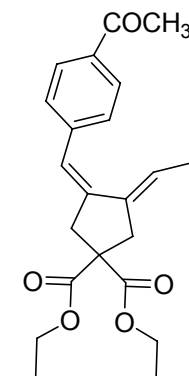
Pulse Sequence: PROTON (e2pul)
Solvent: cdcl3
Data collected on: Sep 4 2008

Temp. 25.0 C / 298.1 K
Operator: walkup1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
32 repetitions

OBSERVE H1, 399.5219642 MHz
DATA PROCESSING
Ft size 32768
Total time 1 min 55 sec





3ae

KUSHER

Sample Name:
KUSHER

Data Collected on:
mar400-vnmr400

Archive directory:
/home/walkup1/vnmrsw/data

Sample directory:
KUSHER_04sep2008

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 4 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.283 sec

Width 25510.2 Hz

512 repetitions

OBSERVE C13, 100.459833 MHz

DECOUPLE H1, 399.523962 MHz

Power 39 dB

continuously on

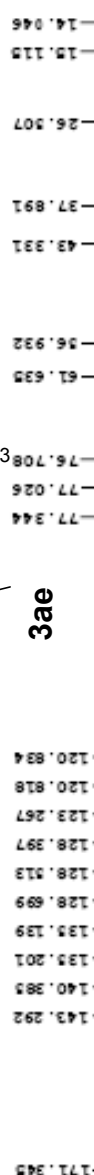
WALTZ-16 modulated

DATA PROCESSING

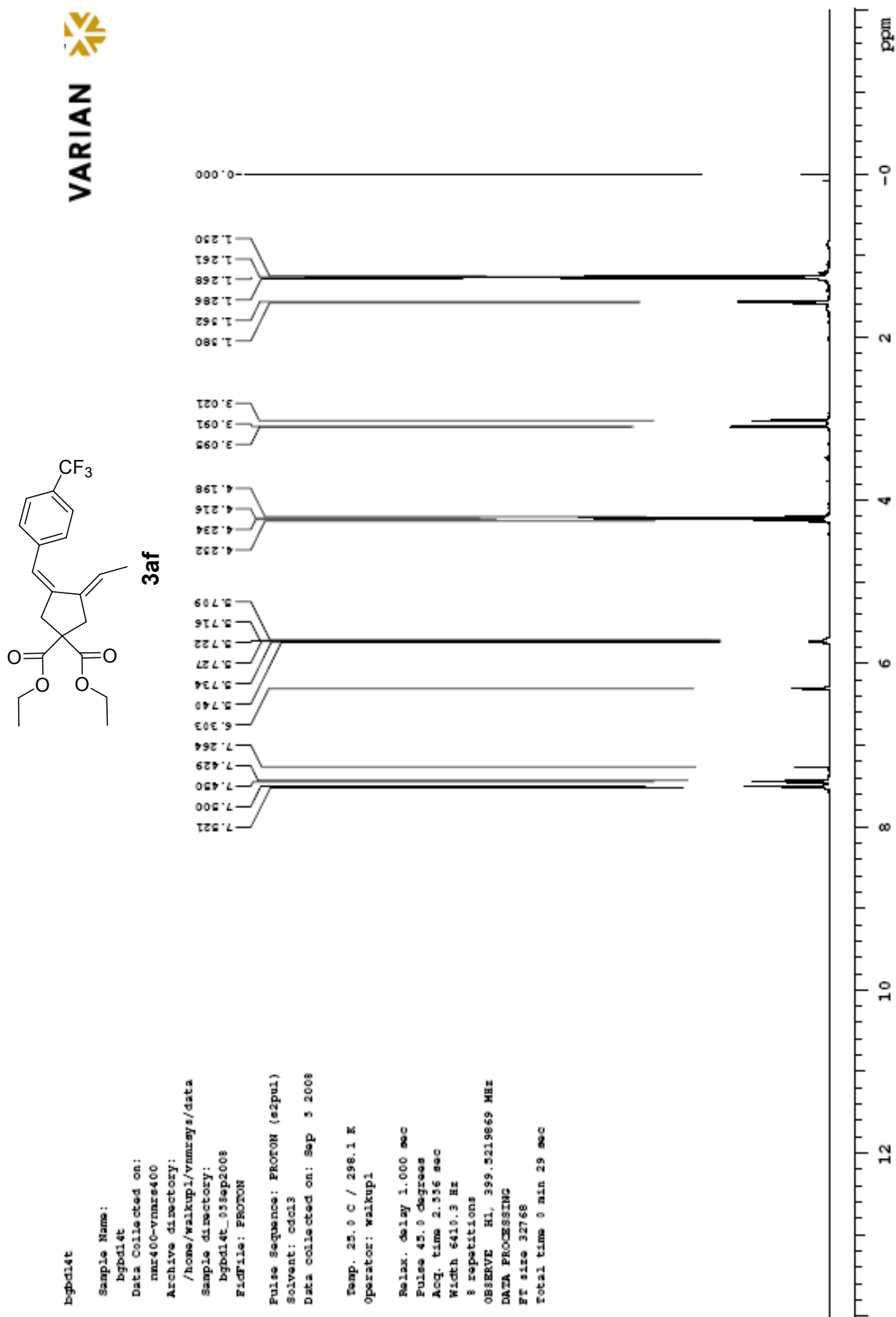
Line broadening 0.5 Hz

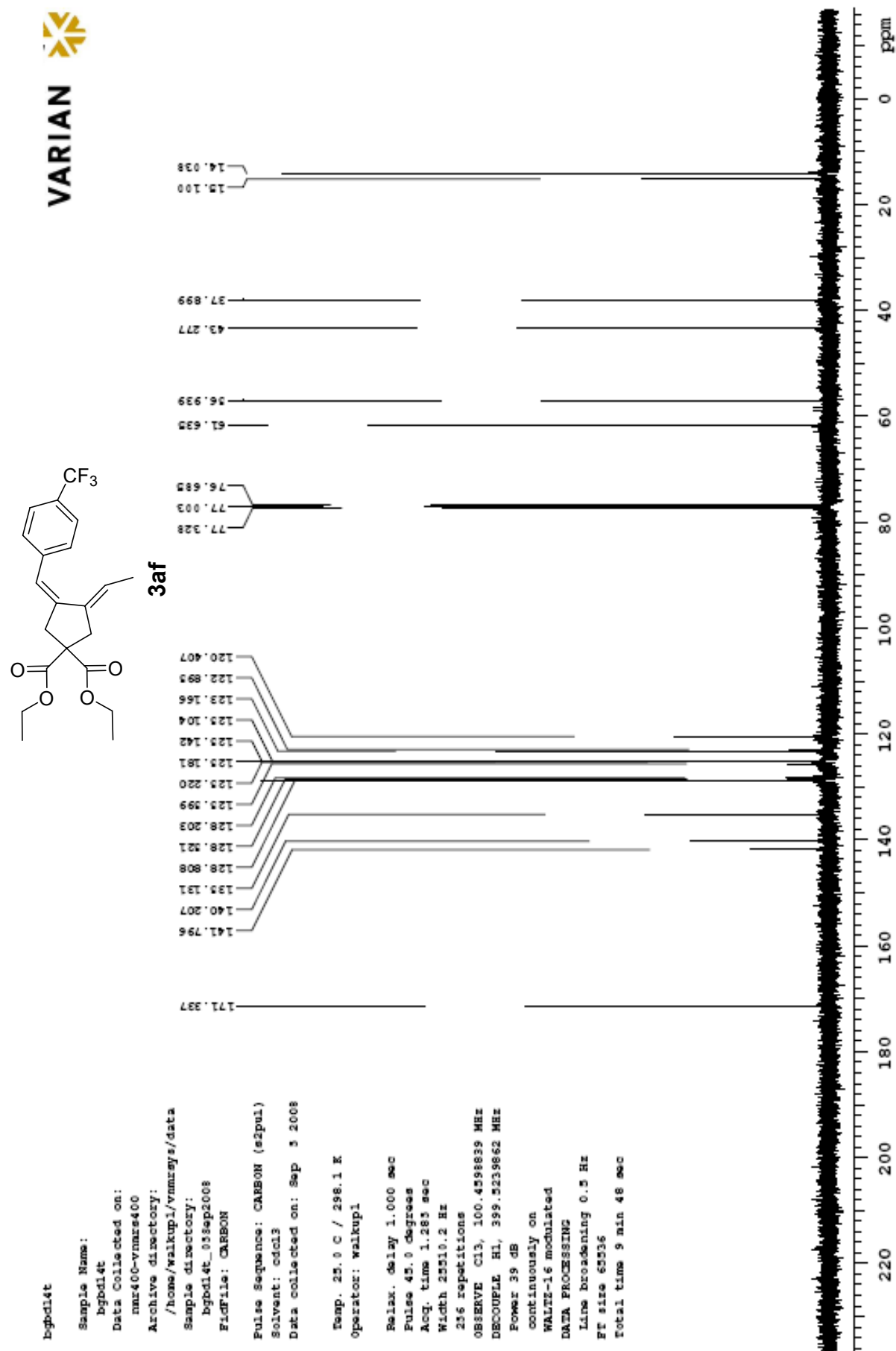
FT size 65536

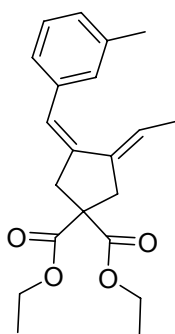
Total time 19 min



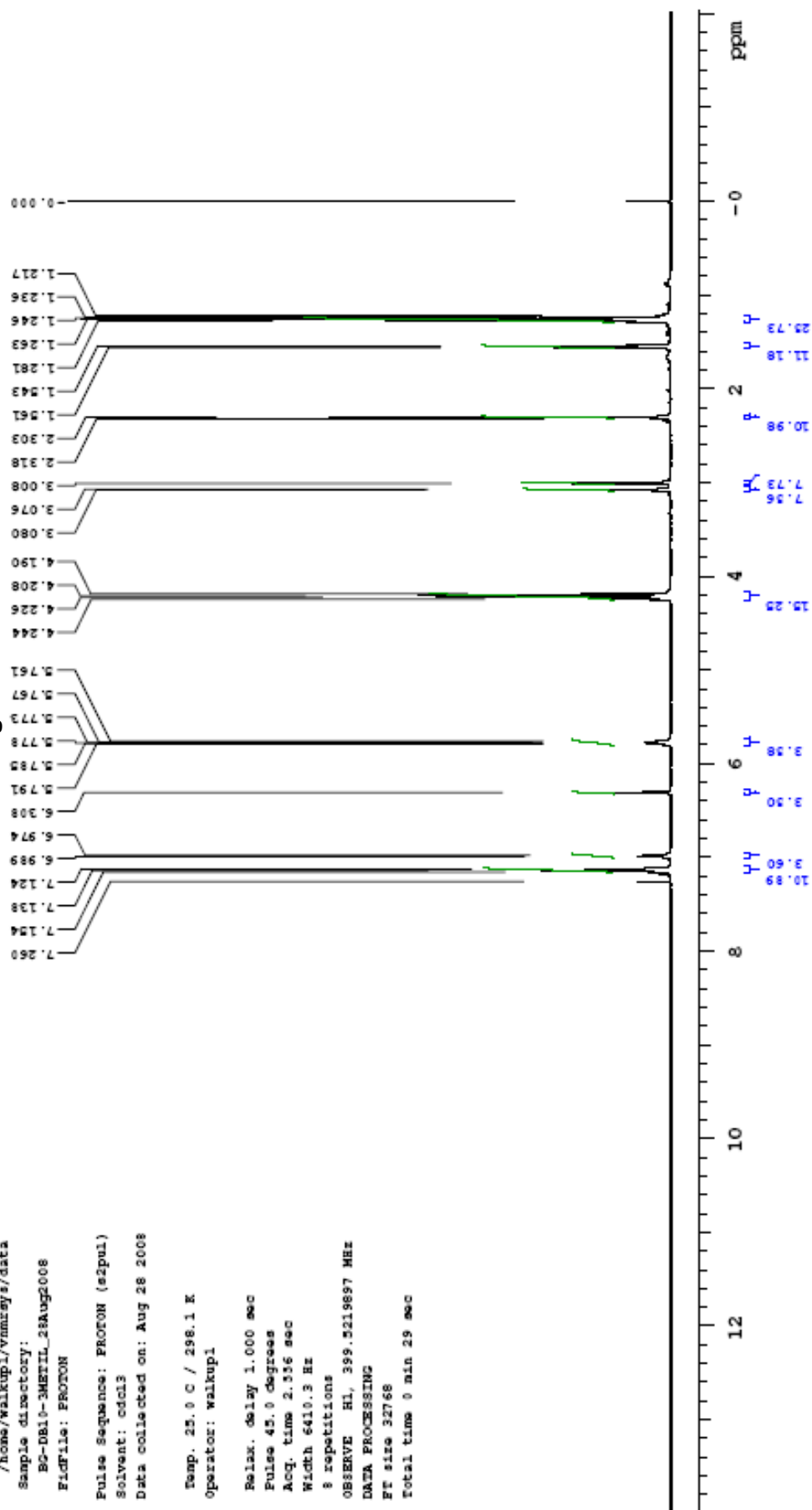
ppm







3ag



8G-DB10-3MERIL

Sample Name:

8G-DB10-3MERIL

Data Collected on:

nmr400-vnmr400

Archive directory:

/home/walkup/vnmr400/data

Sample directory:

8G-DB10-3MERIL_28Aug2008

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 28 2008

Temp. 25.0 C / 298.1 K

Operator: walkup

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

8 repetitions

OBSERVE H1, 399.5219697 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 29 sec



BO-DB10-3METIL

Sample Name:

BO-DB10-3METIL

Data Collected on:

mar400-vnmr400

Archive directory:

/home/walkup1/vnmrsws/data

Sample directory:

BO-DB10-3METIL_28Aug2008

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 28 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.283 sec

Width 25510.2 Hz

256 repetitions

OBSERVE C13, 100.459839 MHz

DECOUPLE H1, 399.521962 MHz

Power 39 dB

continuously on

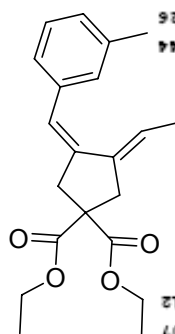
WALTZ-16 modulated

DATA PROCESSING

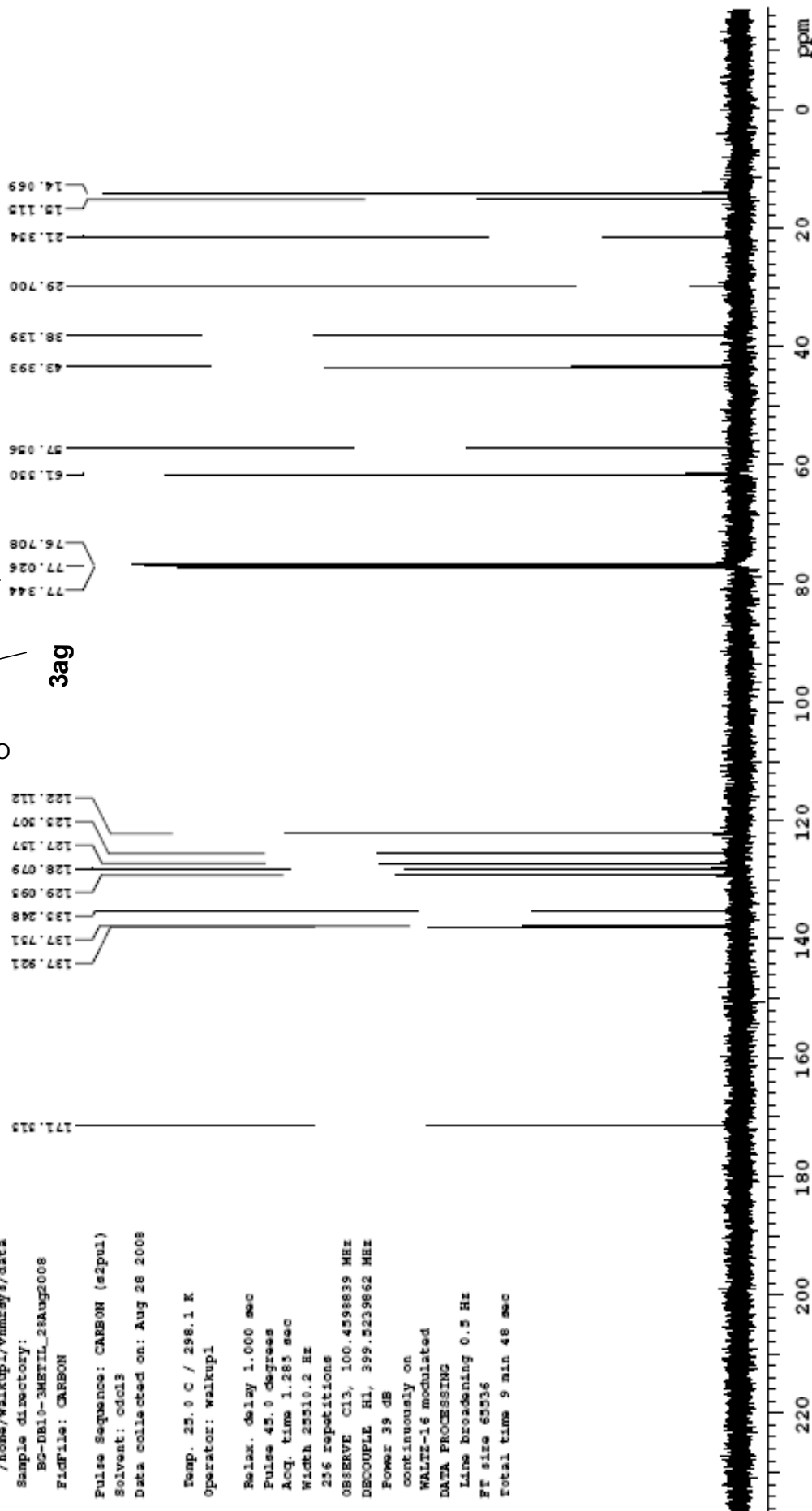
Line broadening 0.5 Hz

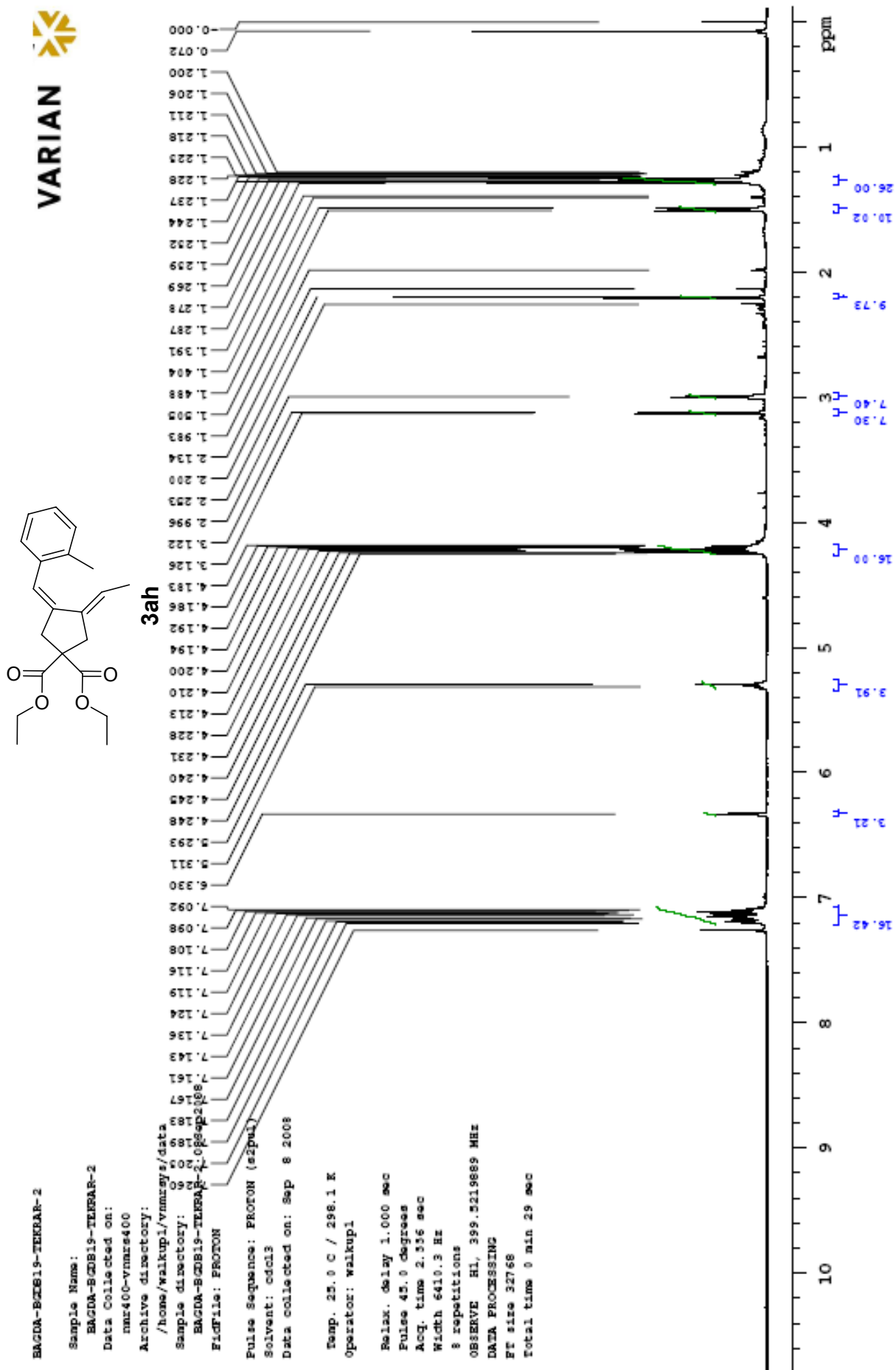
FT size 65536

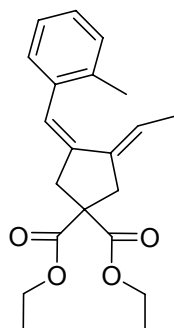
Total time 9 min 48 sec



3ag







3ah

BACDA-BGDB19-TEKAR-2

Sample Name:
BACDA-BGDB19-TEKAR-2
Data Collected on:
nmr400-vnmr400
Archive directory:
/home/walkup1/vnmr400/data
Sample directory:
BACDA-BGDB19-TEKAR-2_08sep2008
Fidfile: CARBON

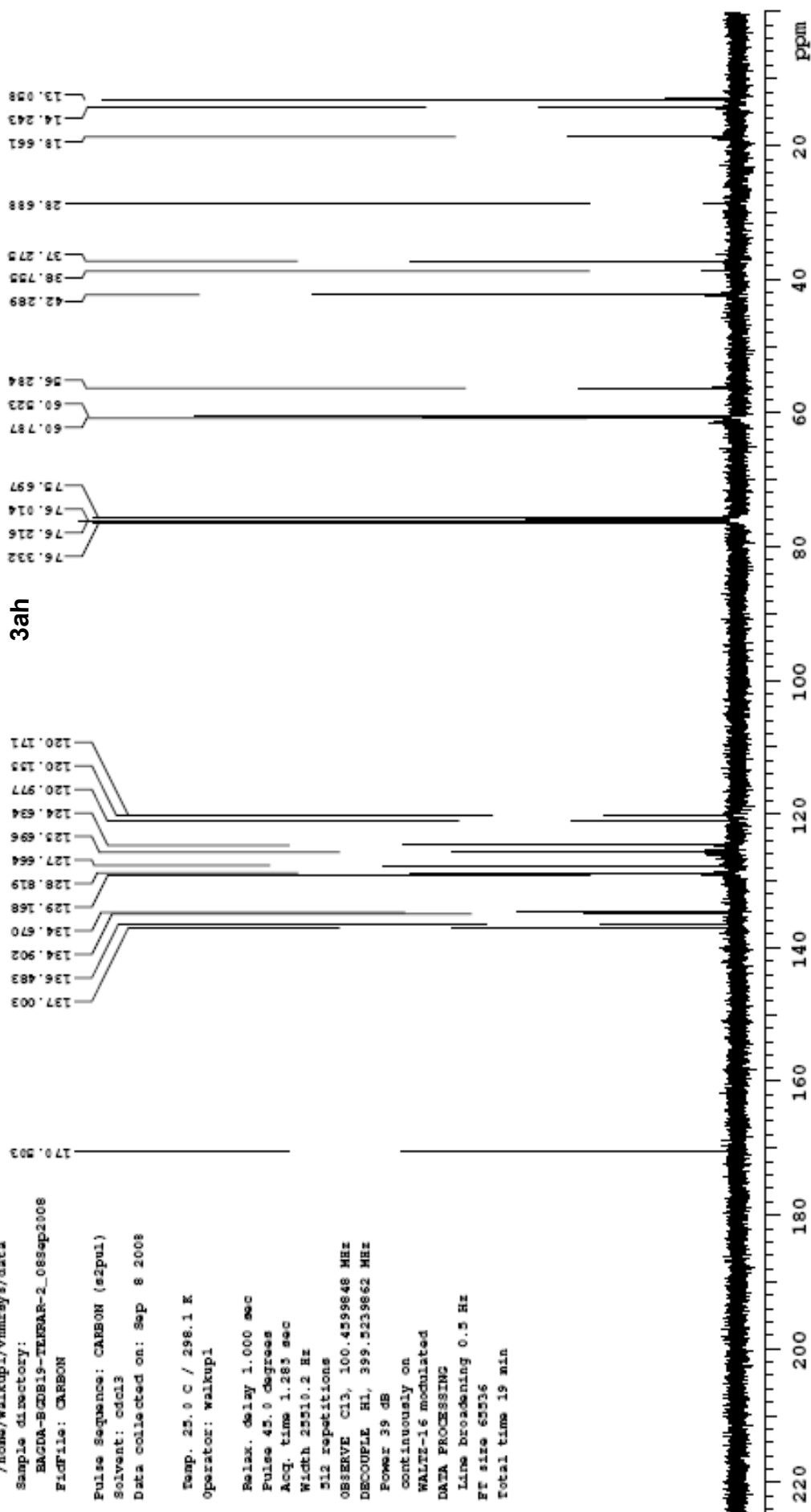
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 8 2008

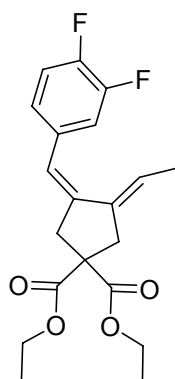
Temp. 25.0 C / 298.1 K
Operator: walkup1

Relax. delay 1.000 sec
Pulse 42.0 degrees
Acq. time 1.283 sec
Width 25510.2 Hz
312 repetitions

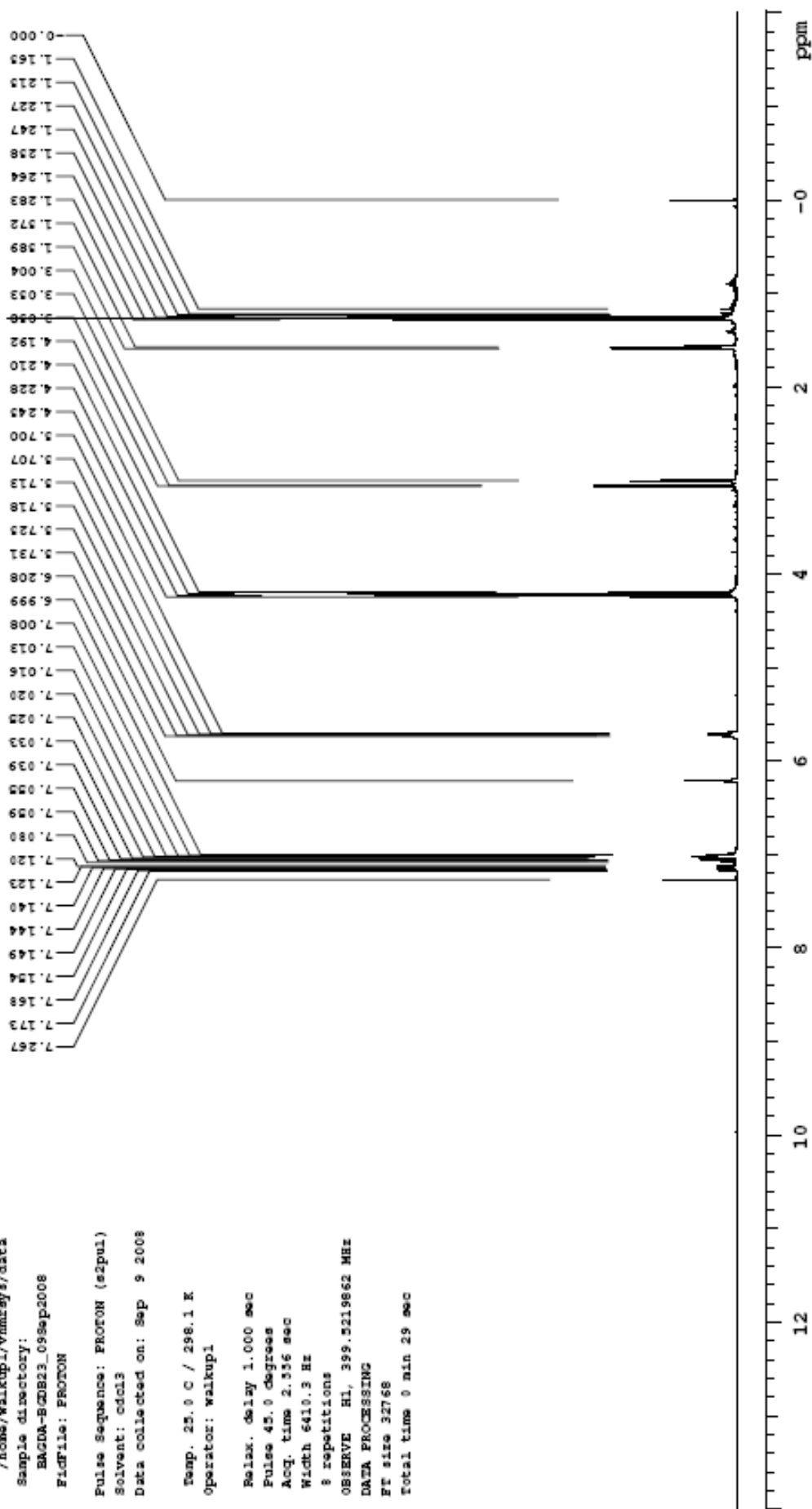
OBSERVE C13, 100.459848 MHz
DECOUPLE H1, 399.523862 MHz
Power 39 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 19 min





Ai



BAGDA-BCTB 23

Sample Memo:

BA/DA-B/DB23

Data Collected on:

nmr400-vnars400

Archive directory:

```
/home/walkup1/vnmrsys/data
```

Sample directory:

BACDA-BGDB23_09Sep2008

NOTES: 617JPTB
F1dF119: PROTON
0_2700000-012000

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Sep 9 2008

Temp. 25.0 C / 298.1 K

operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degre

Acq. time 2.556 sec

Width 6410.3 Hz

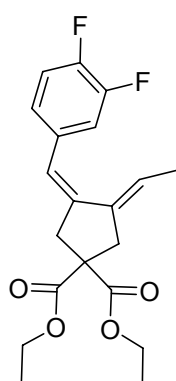
3 repetitions

OBSERVE H1, 399.5219862 MHz

DATA PROCESSING

FT 0120 32768

Total time 0 min 29 sec



3ai

BAGDA-BJIS23

Sample Name:

BAGDA-BJIS23

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkup1/vnmrs400/data

Sample directory:

BAGDA-BJIS23_09sep2008

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 9 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

256 repetitions

OBSERVE C13, 100.4598839 MHz

DECOUPLE H1, 399.5239662 MHz

Power 39 dB

continuously on

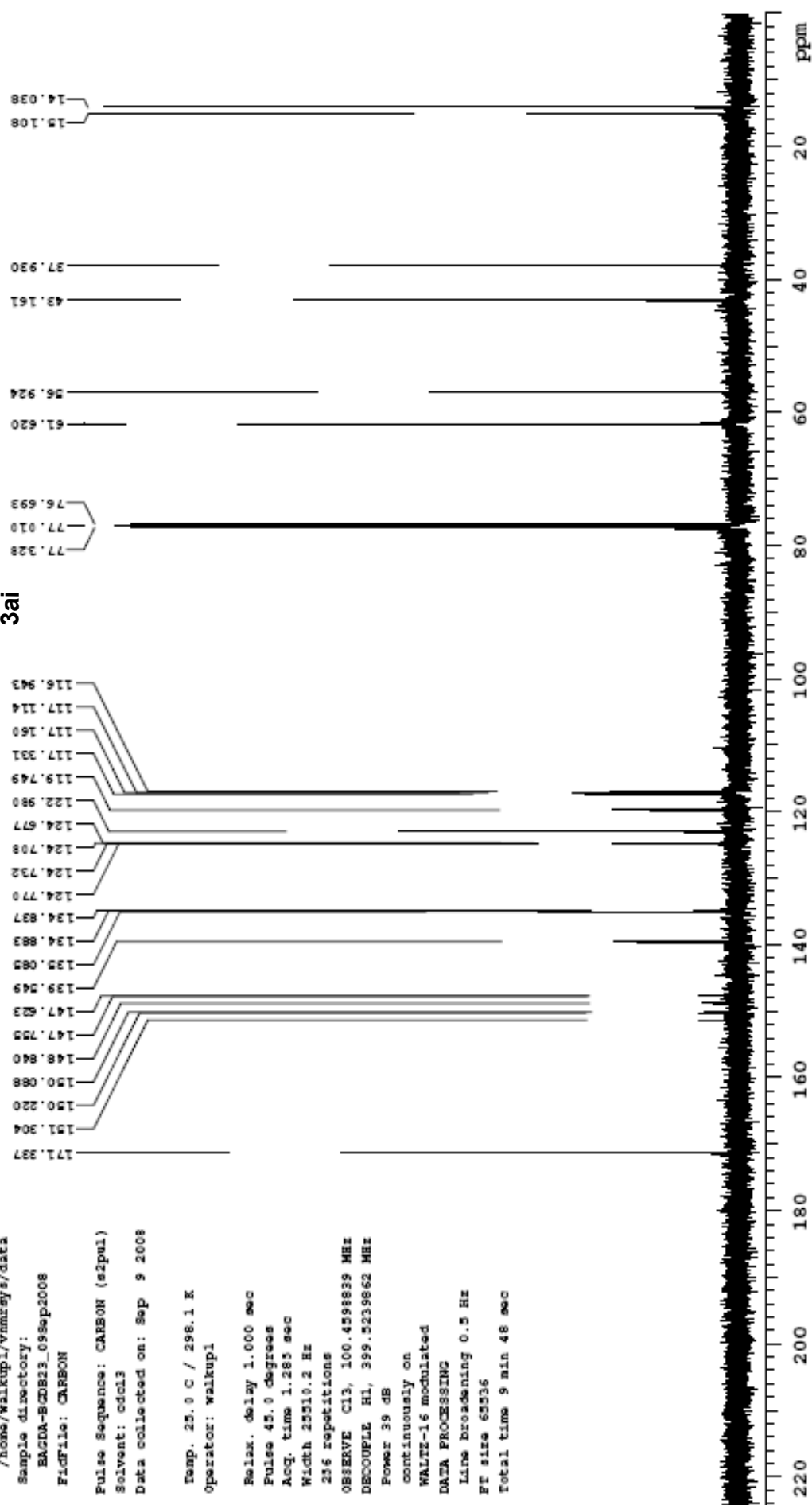
WALTZ-16 modulated

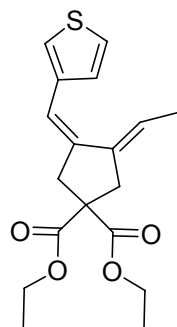
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min 48 sec



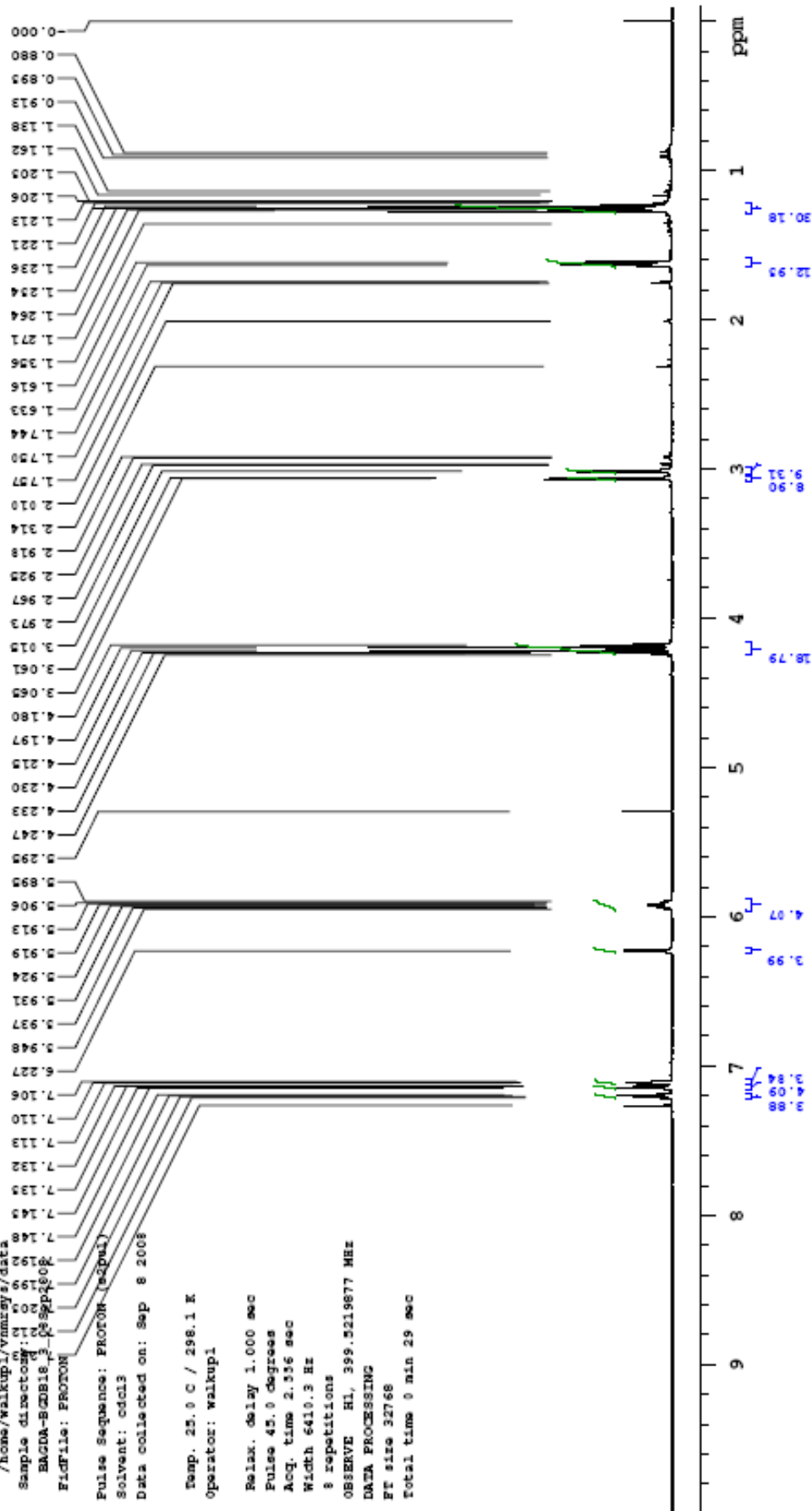


3aj

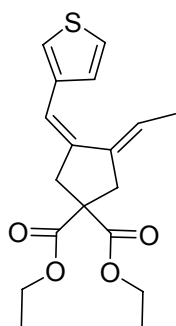


BACDA-BGDB18_3

Sample Name:
BACDA-BGDB18_3
Data Collected on:
nmr400-vnmr400
Archive directory:
/home/walkup/vnmr400/data
Sample directory: 110618
BACDA-BGDB18_3-080108
Fidfile: PROTON
Pulse Sequence: PROTON (zgpg3)
Solvent: cdcl3
Data collected on: Sep 8 2008
Temp. 25.0 C / 298.1 K
Operator: walkup1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.336 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.5219877 MHz
DATA PROCESSING
Ft size 32768
Total time 0 min 29 sec



VARIAN



3aj

BACDA-B0018_3

Sample Name:

BACDA-B0018_3

Data Collected on:

mar400-vnmr400

Archive directory:

/home/walkup/vnmr400/data

Sample directory:

BACDA-B0018_3_08Sep2008

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 8 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25310.2 Hz

512 repetitions

OBSERVE C13, 100.459839 MHz

DECOUPLE H1, 399.223862 MHz

Power 39 dB

continuously on

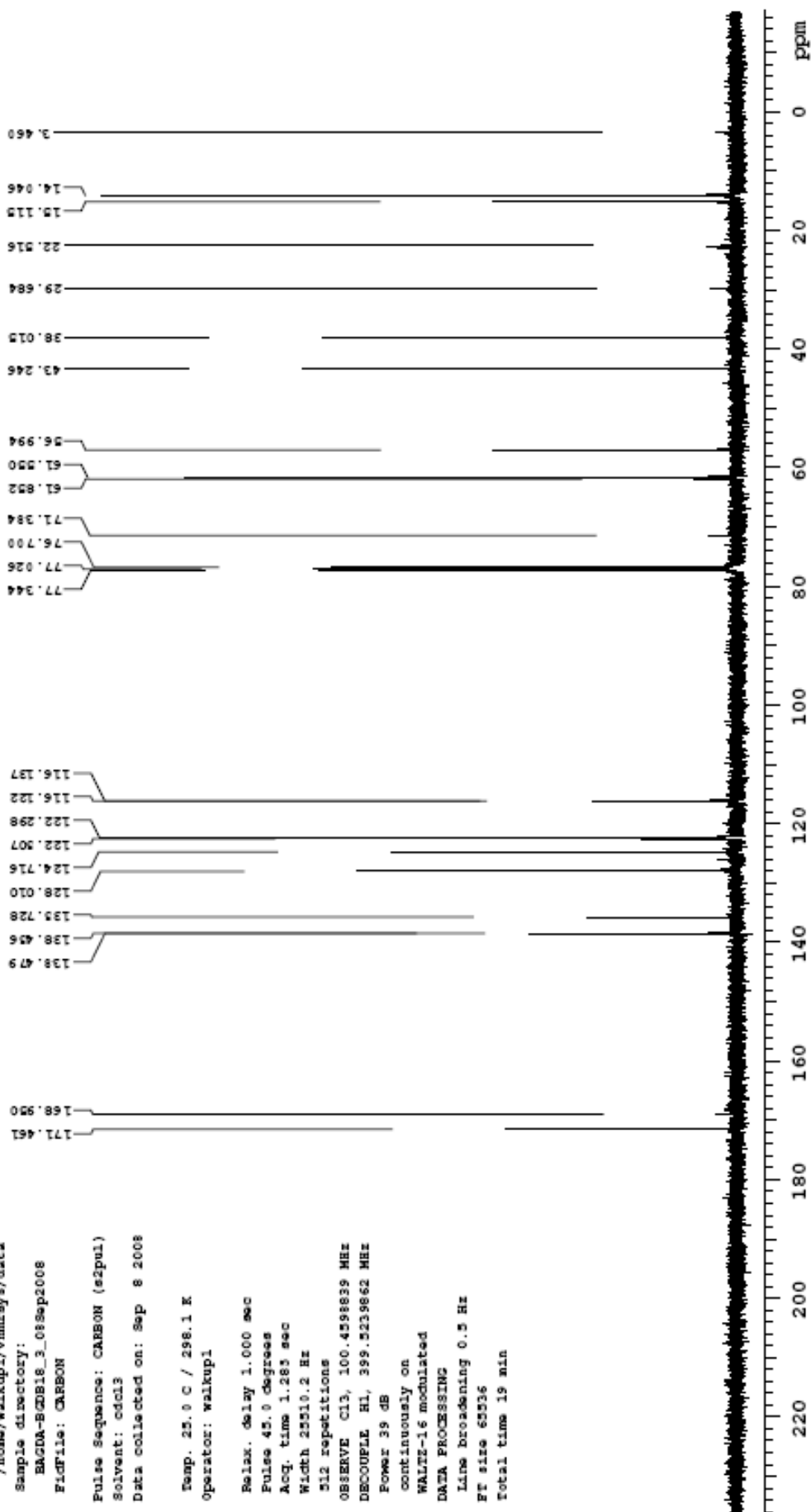
WALTZ-16 modulated

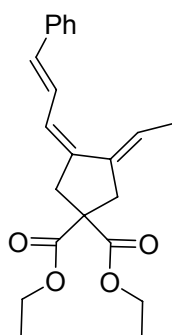
DATA PROCESSING

Line broadening 0.5 Hz

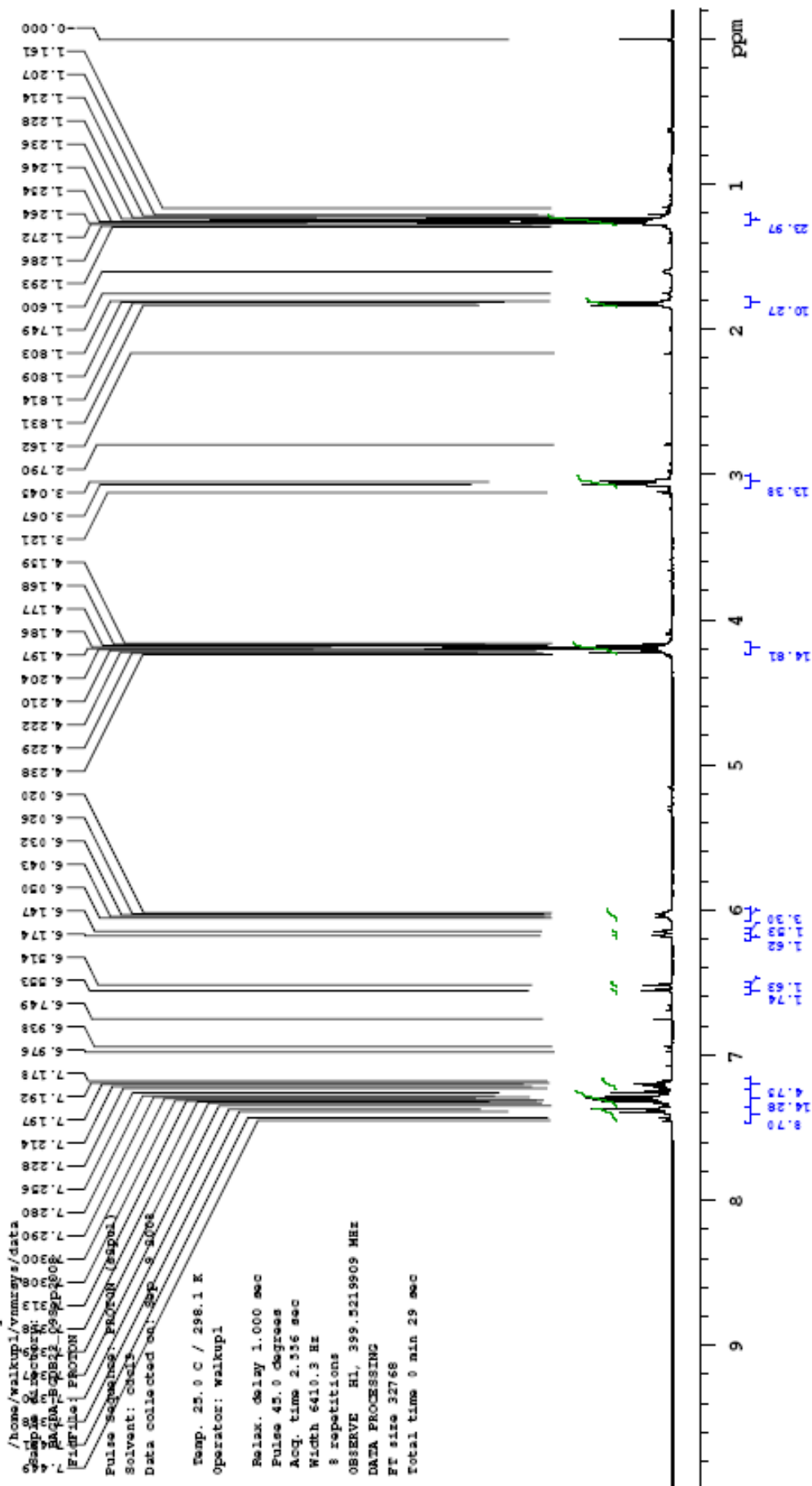
FT size 62536

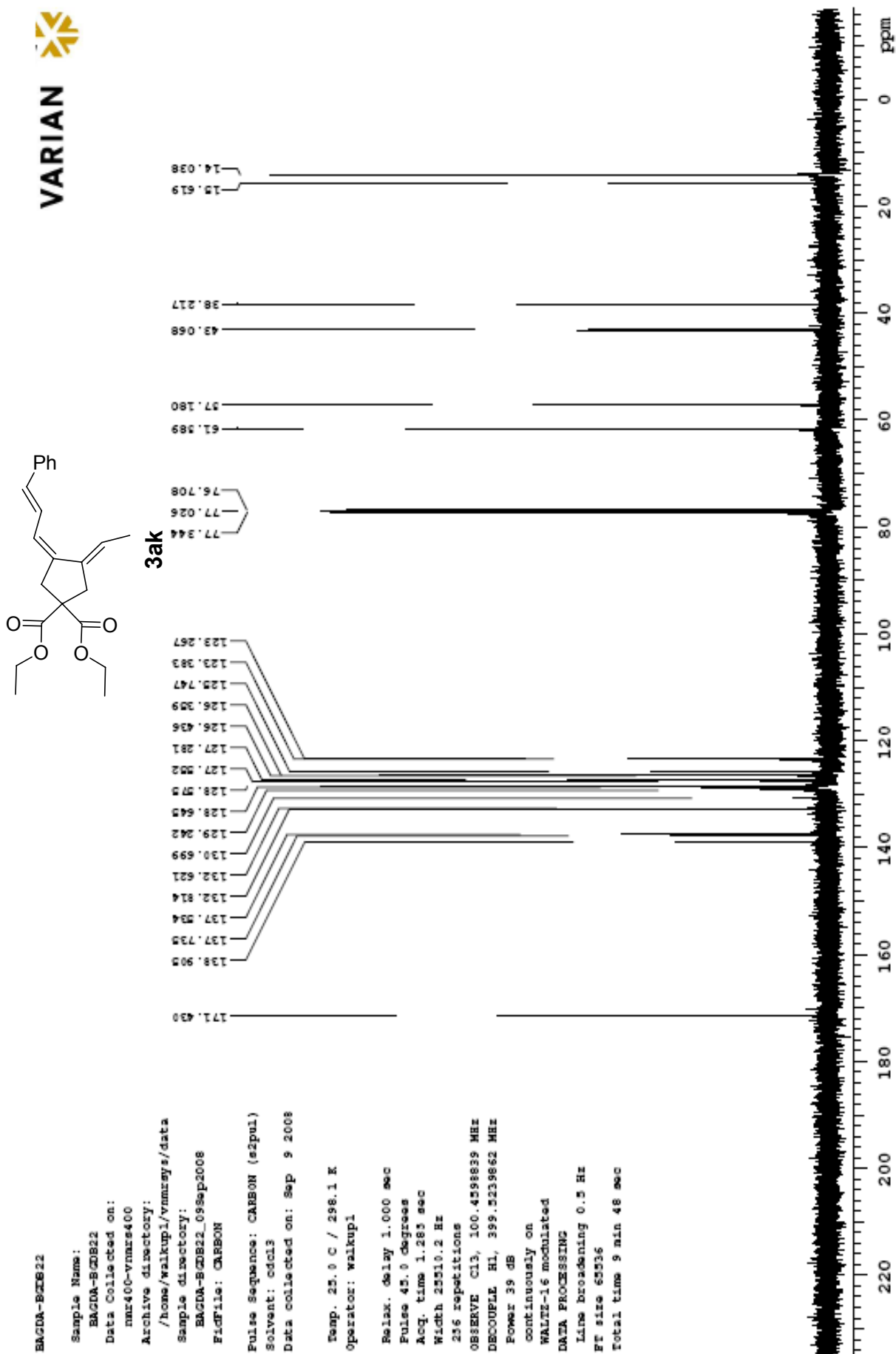
Total time 19 min

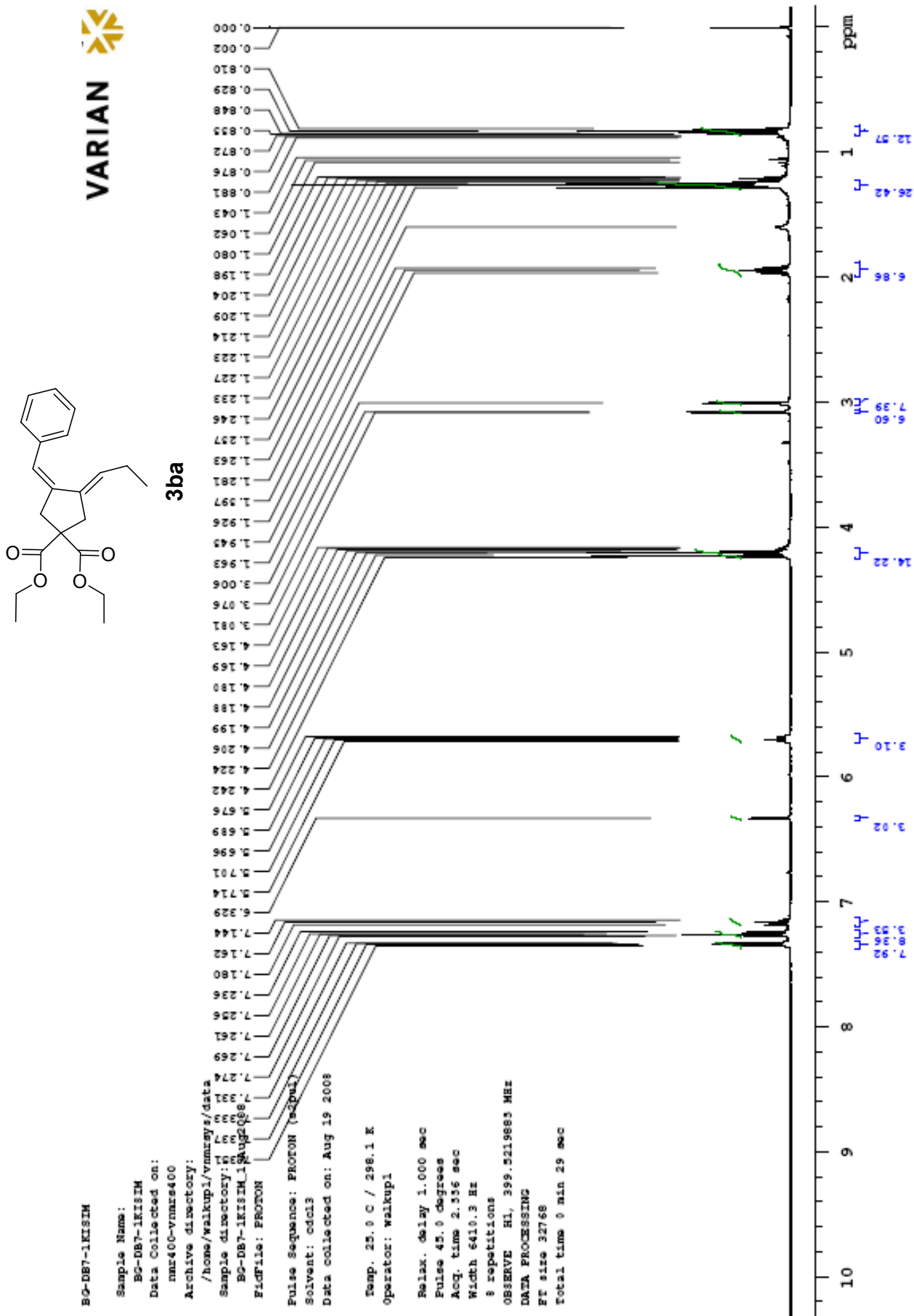


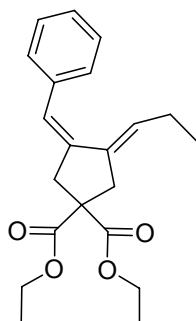


3ak









3ba

BO-DB7-1KISIM

Sample Name:

BO-DB7-1KISIM

Data Collected on:

mar400-vnmr400

Archive directory:

/home/walkup/vnmr400/data

Sample directory:

BO-DB7-1KISIM_18Aug2008

FIDFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 19 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.283 sec

Width 25510.2 Hz

256 repetitions

OBSERVE C13, 100.459839 MHz

DECOUPLE H1, 399.523862 MHz

Power 39 dB

continuously on

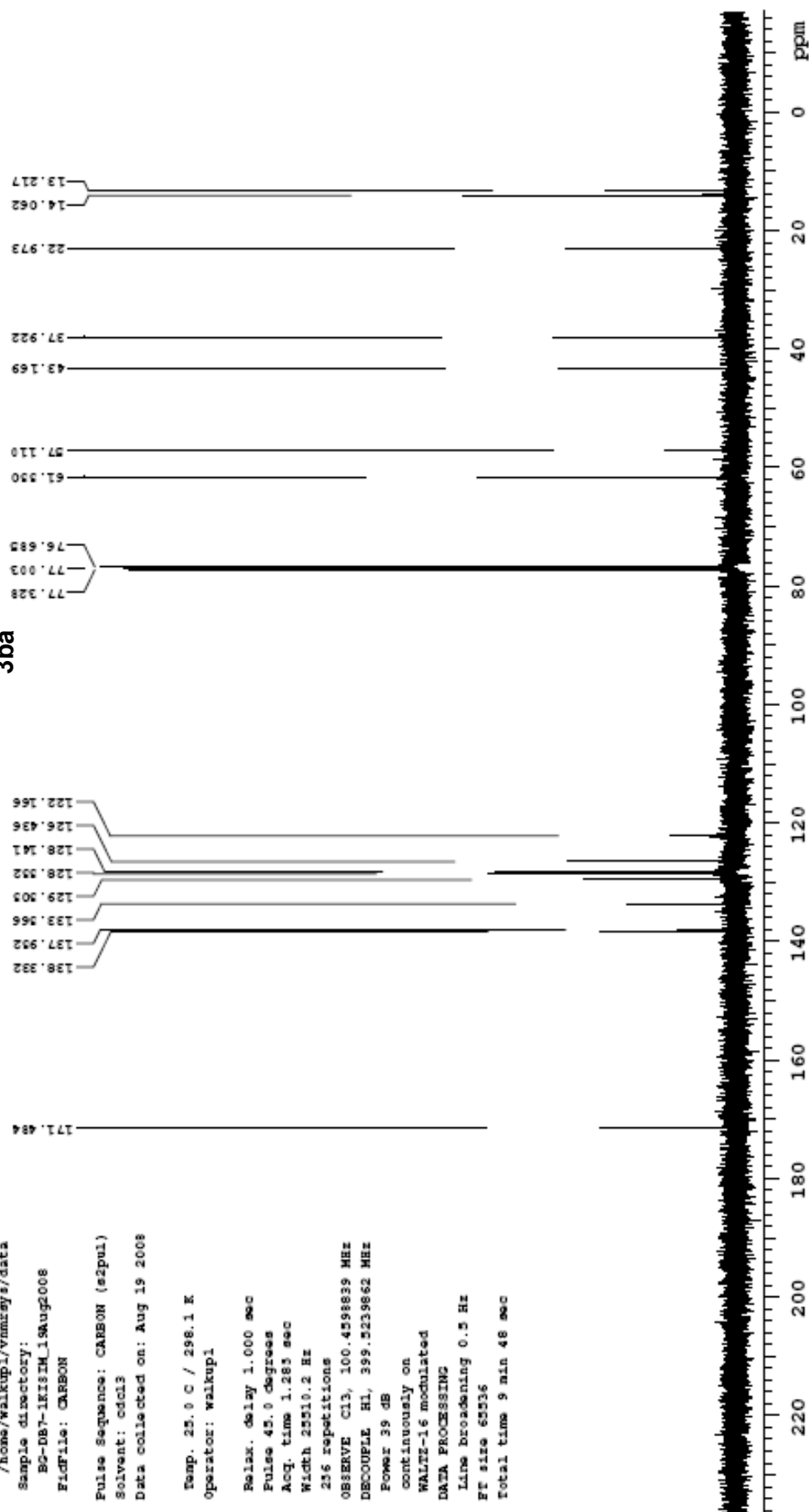
WALTZ-16 modulated

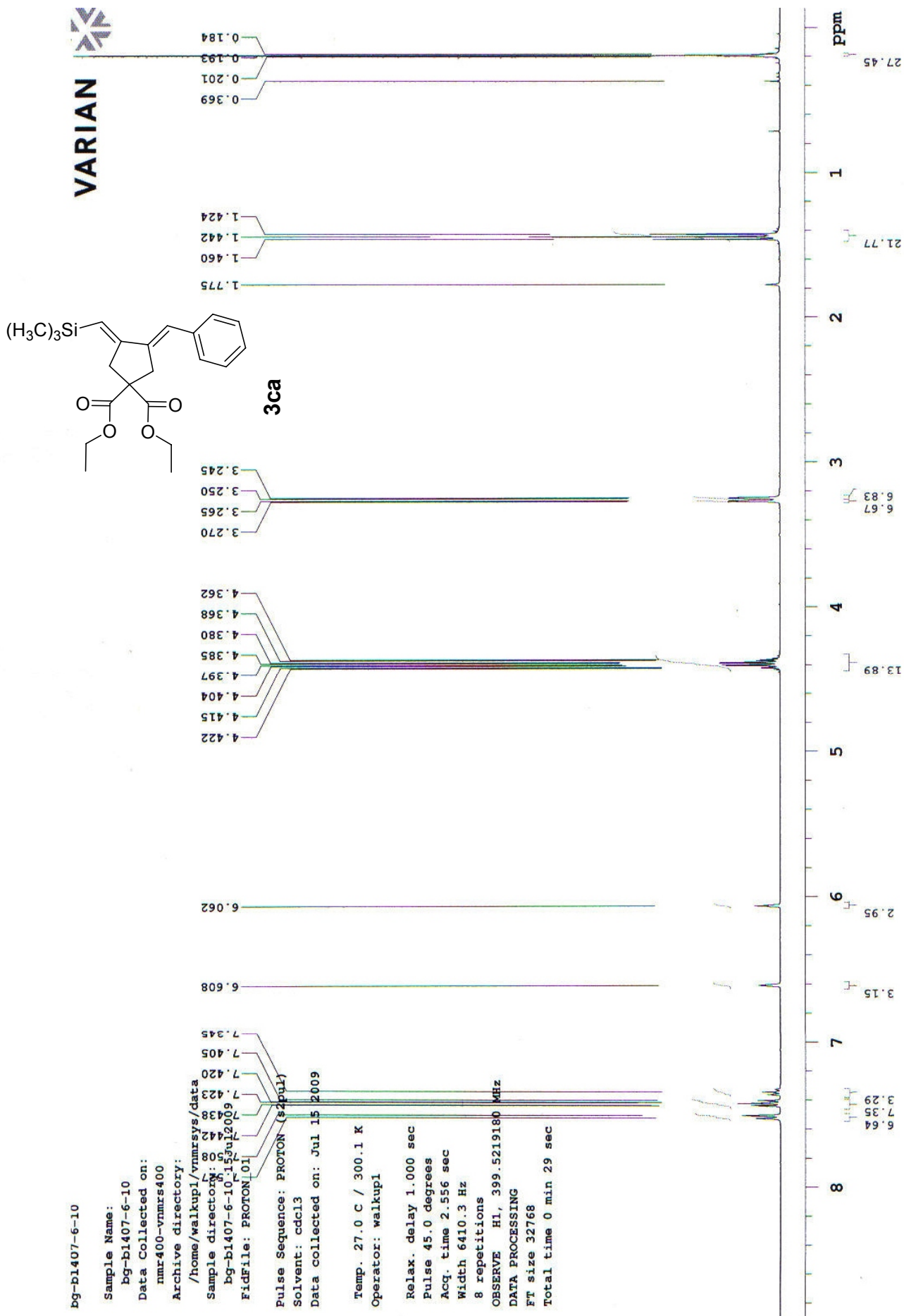
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min 48 sec





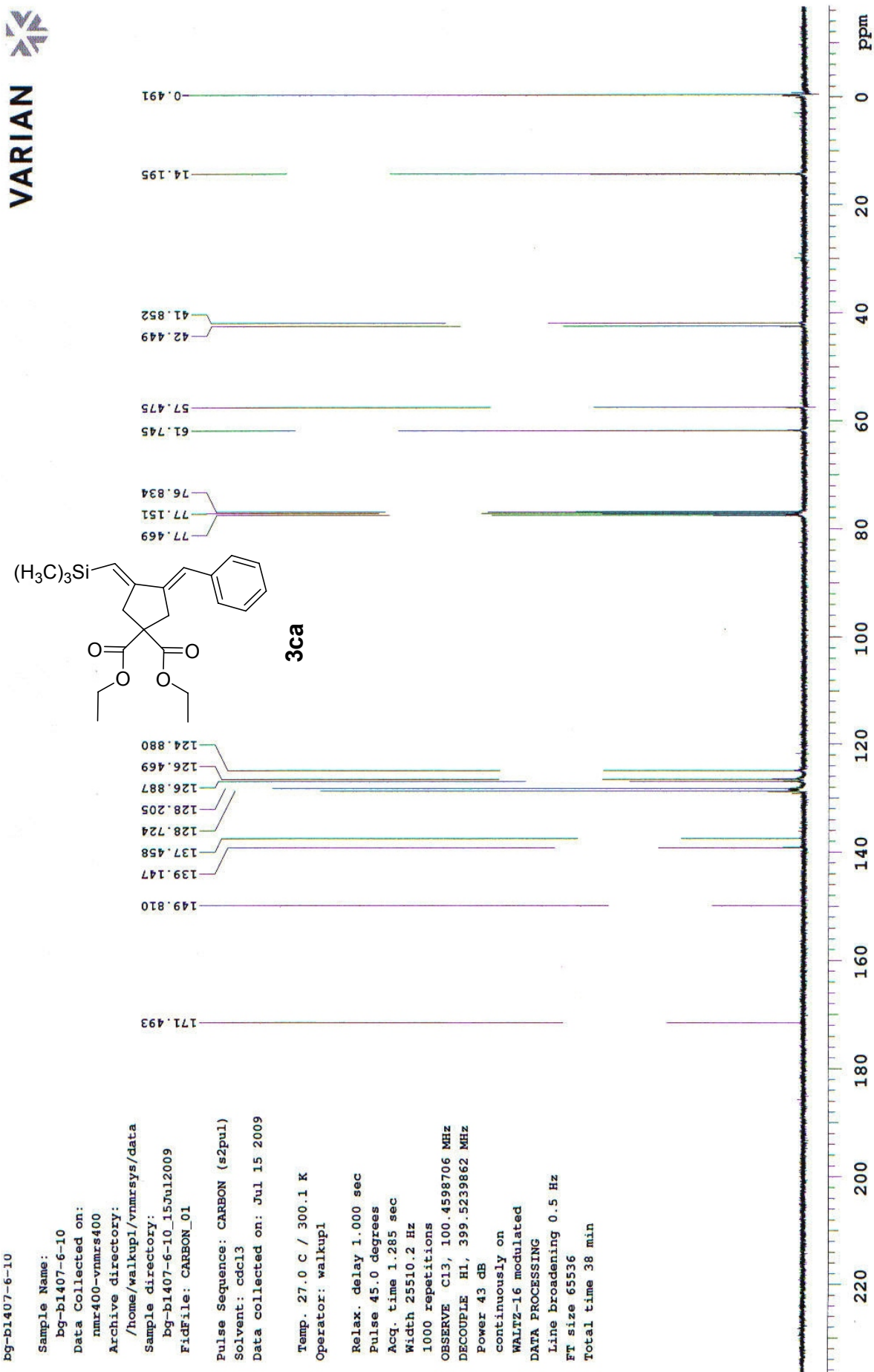
Plotname: --Not assigned--

bg-b1407-6-10

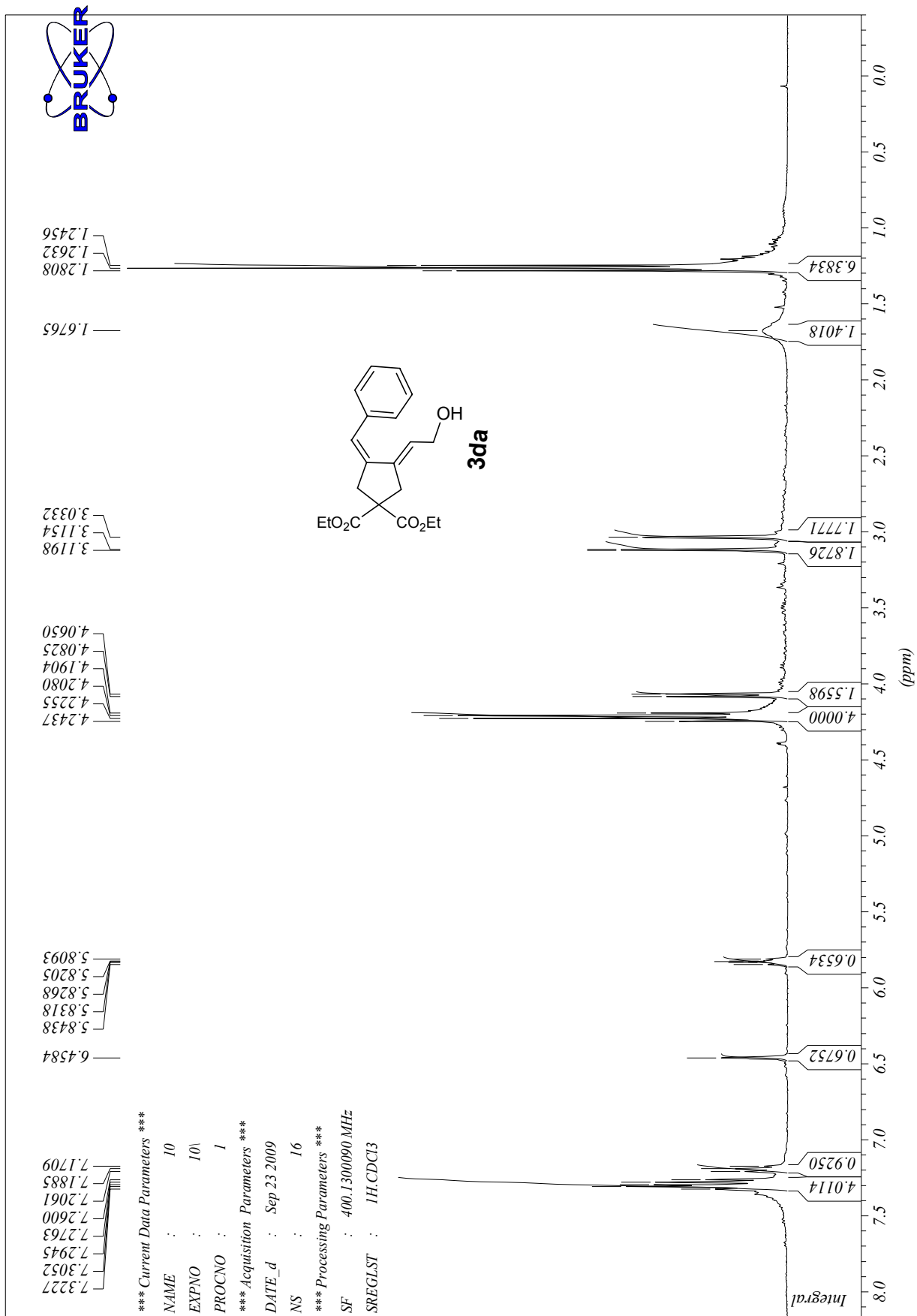
Sample Name:
bg-b1407-6-10
Data Collected on:
nmr400-vnmrs400
Archive directory:
/home/walkup/vnmrsys/data
Sample directory:
bg-b1407-6-10_15Jul2009
FidFile: CARBON_01
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 15 2009

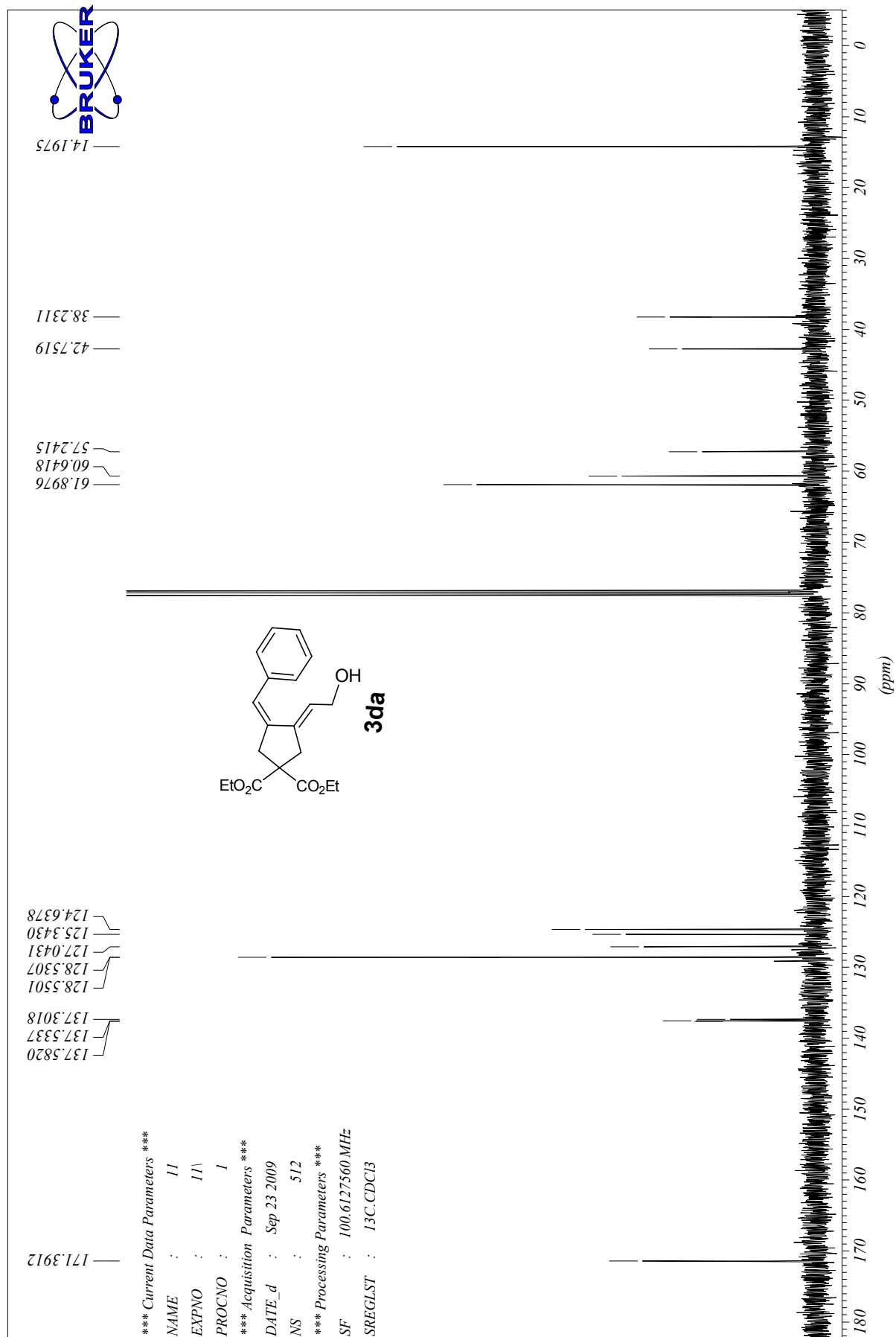
Temp. 27.0 C / 300.1 K
Operator: walkup

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
1000 repetitions
OBSERVE C13, 100.4598706 MHz
DECOUPLE H1, 399.5239862 MHz
Power 43 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 38 min



Plotname: --Not assigned--





VARIAN

BG-B31607

Sample Name:

BG-B31607

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkup/vnmrsys/data

USample directory:

USample directory:

USample directory:

USample directory:

USample directory:

USample directory:

USample directory:

USample directory:

USample directory:

USample directory:

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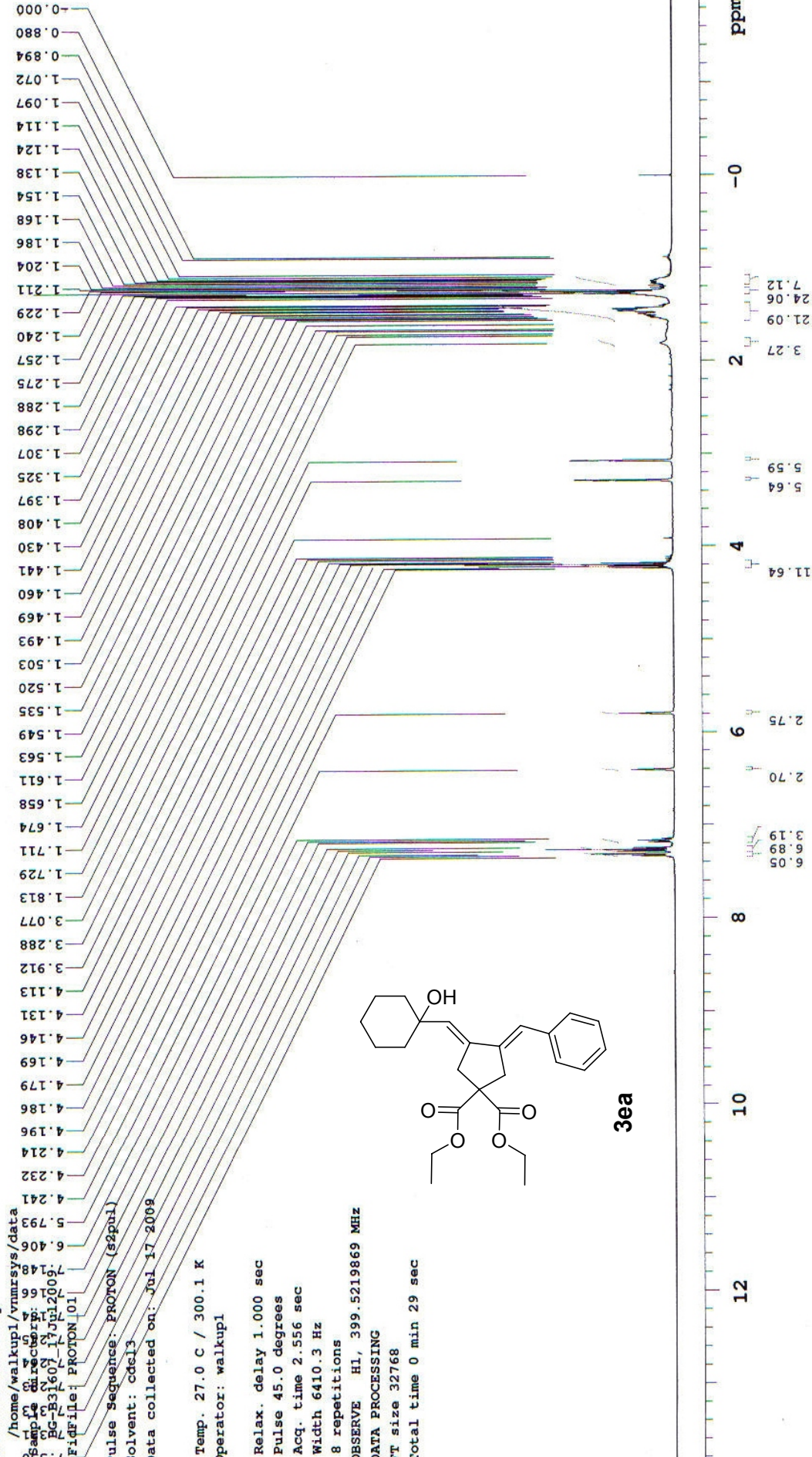
USample directory:

USample directory:

USample directory:

USample directory:

USample directory:



Plotname: ---Not assigned---

VARIAN

BG-B31607

Sample Name:

BG-B31607

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkup/vnmrsys/data

Sample directory:

BG-B31607_17Jul2009

FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 17 2009

Temp. 27.0 C / 300.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

512 repetitions

OBSERVE C13, 100.4598839 MHz

DECOUPLE H1, 399.5239862 MHz

Power 43 dB

continuously on

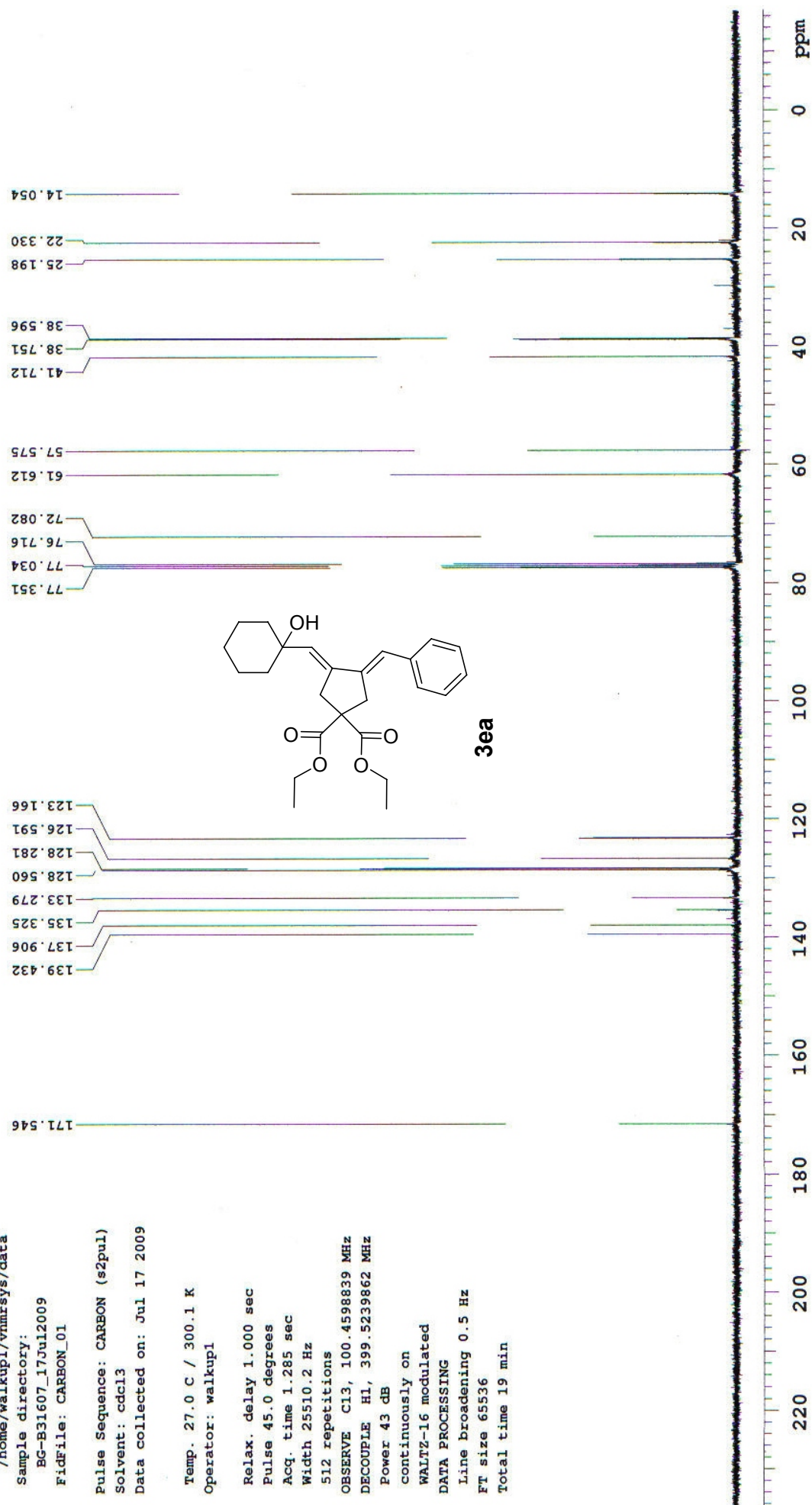
WALTZ-16 modulated

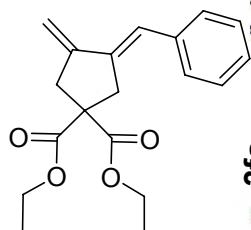
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 19 min





3fa

BG-B1307-VAKUMSONRASI

Sample Name:

BG-B1307-VAKUMSONRASI

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkup1/vnmrsys/data

Sample directory:

BG-B1307-VAKUMSONRASI_13Jul2009

FidFile: PROTON_01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 13 2009

Temp. 27.0 C / 300.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

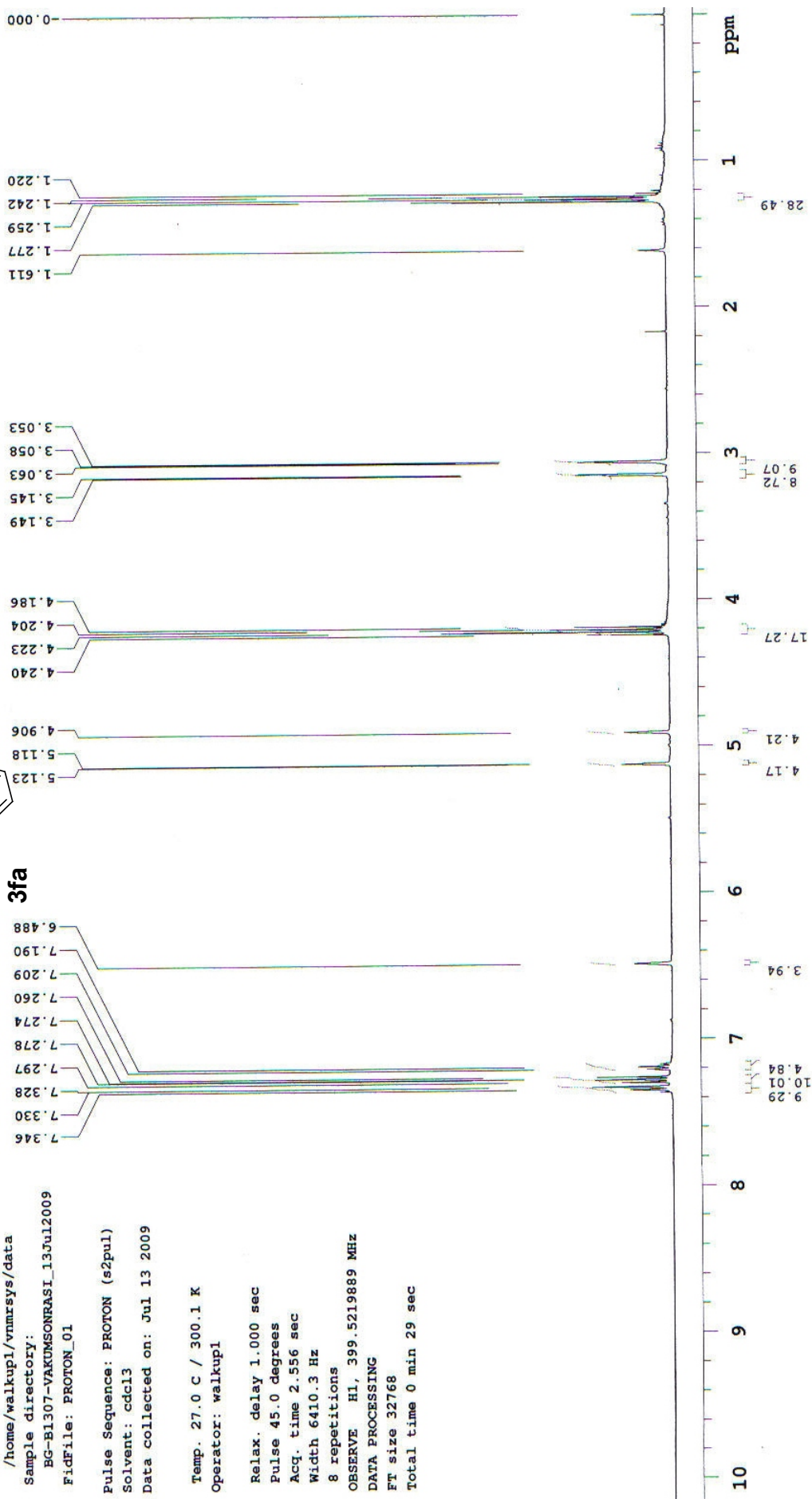
8 repetitions

OBSERVE H1, 399.5219889 MHz

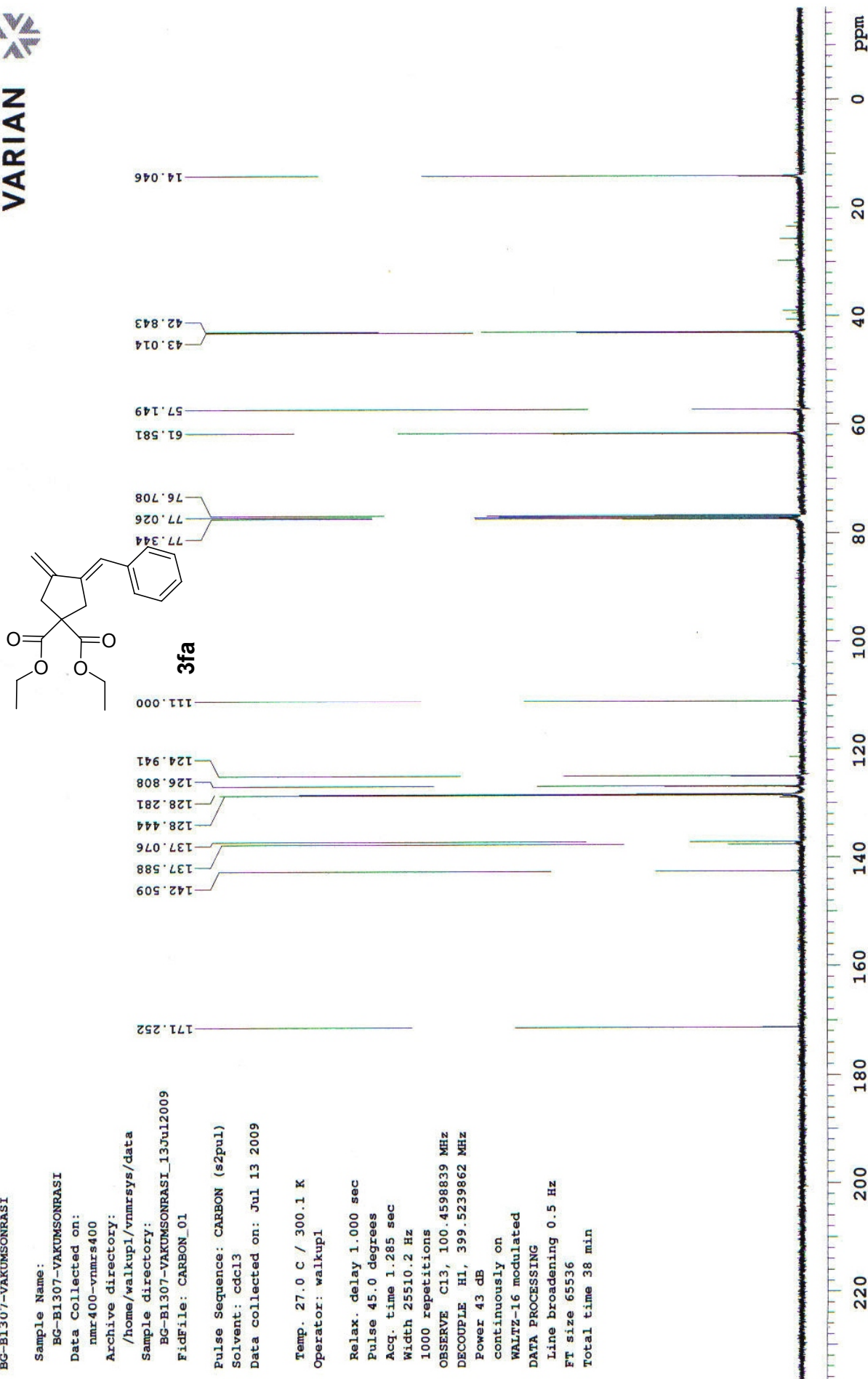
DATA PROCESSING

FT size 32768

Total time 0 min 29 sec



Plotname: --Not assigned--



BG-B1307-VAKUMSONRASI

Sample Name:

BG-B1307-VAKUMSONRASI

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkupl/vnmrsys/data

Sample directory:

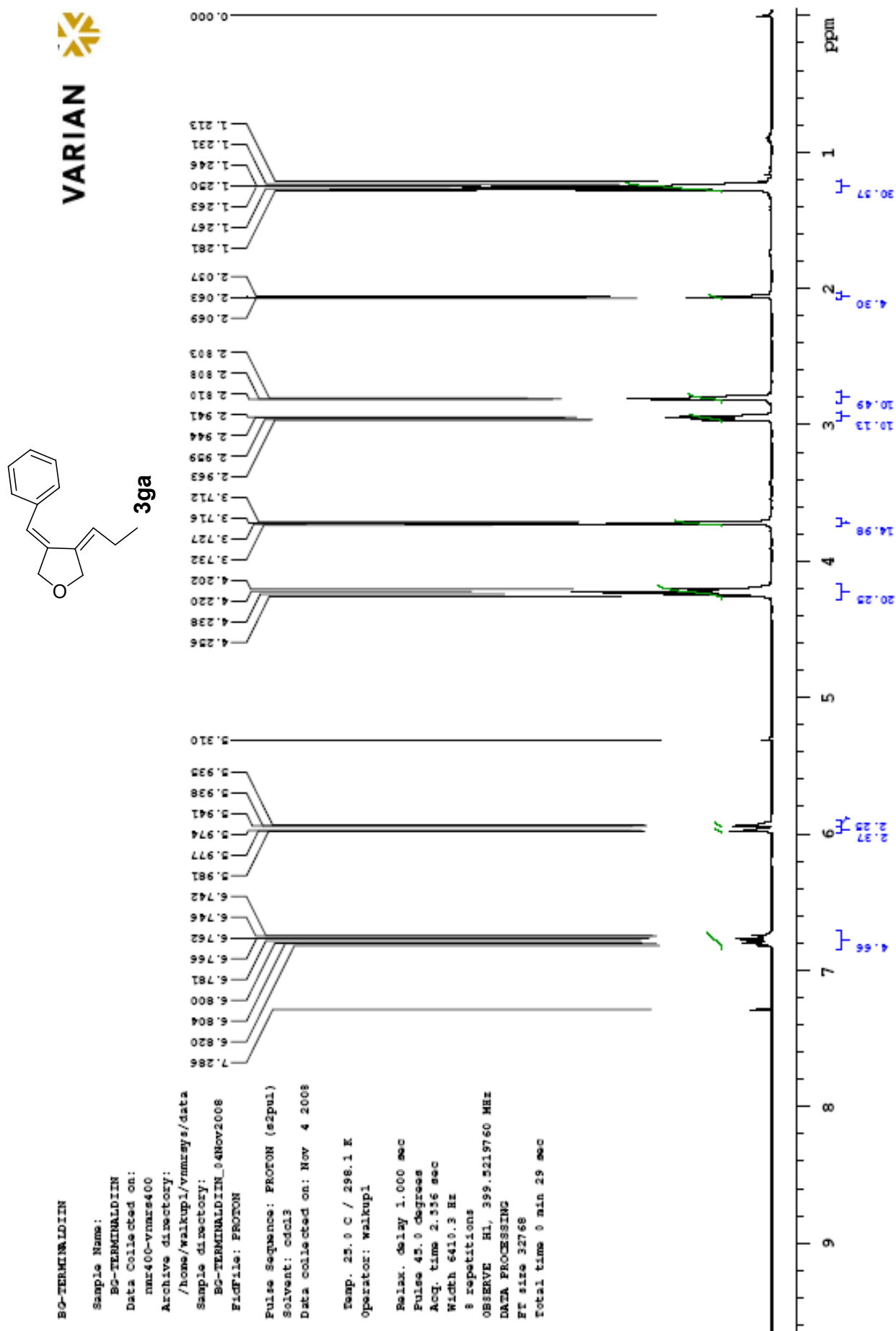
BG-B1307-VAKUMSONRASI_13Jul2009

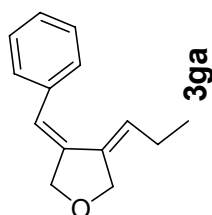
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

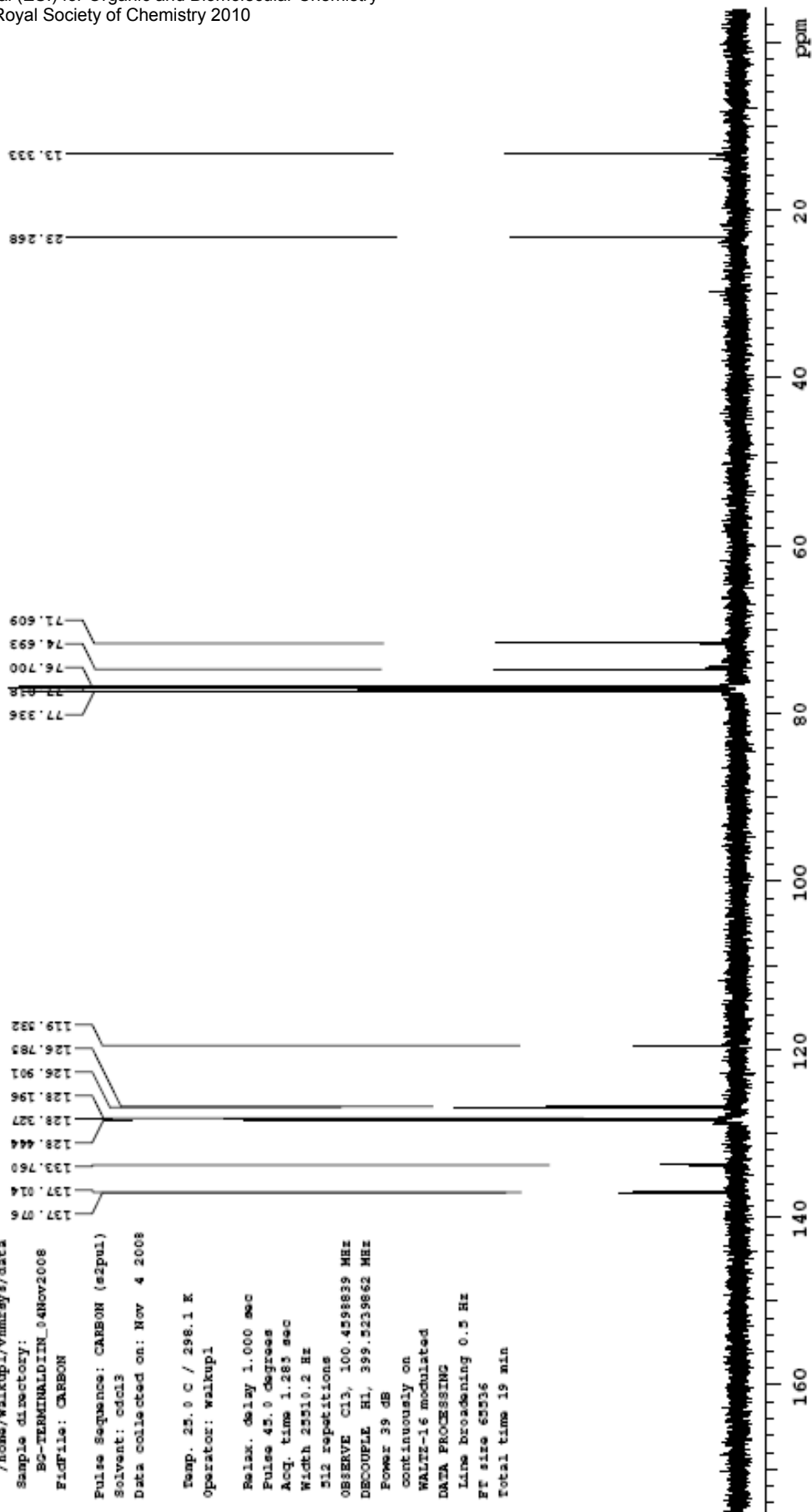
Data collected on: Jul 13 2009

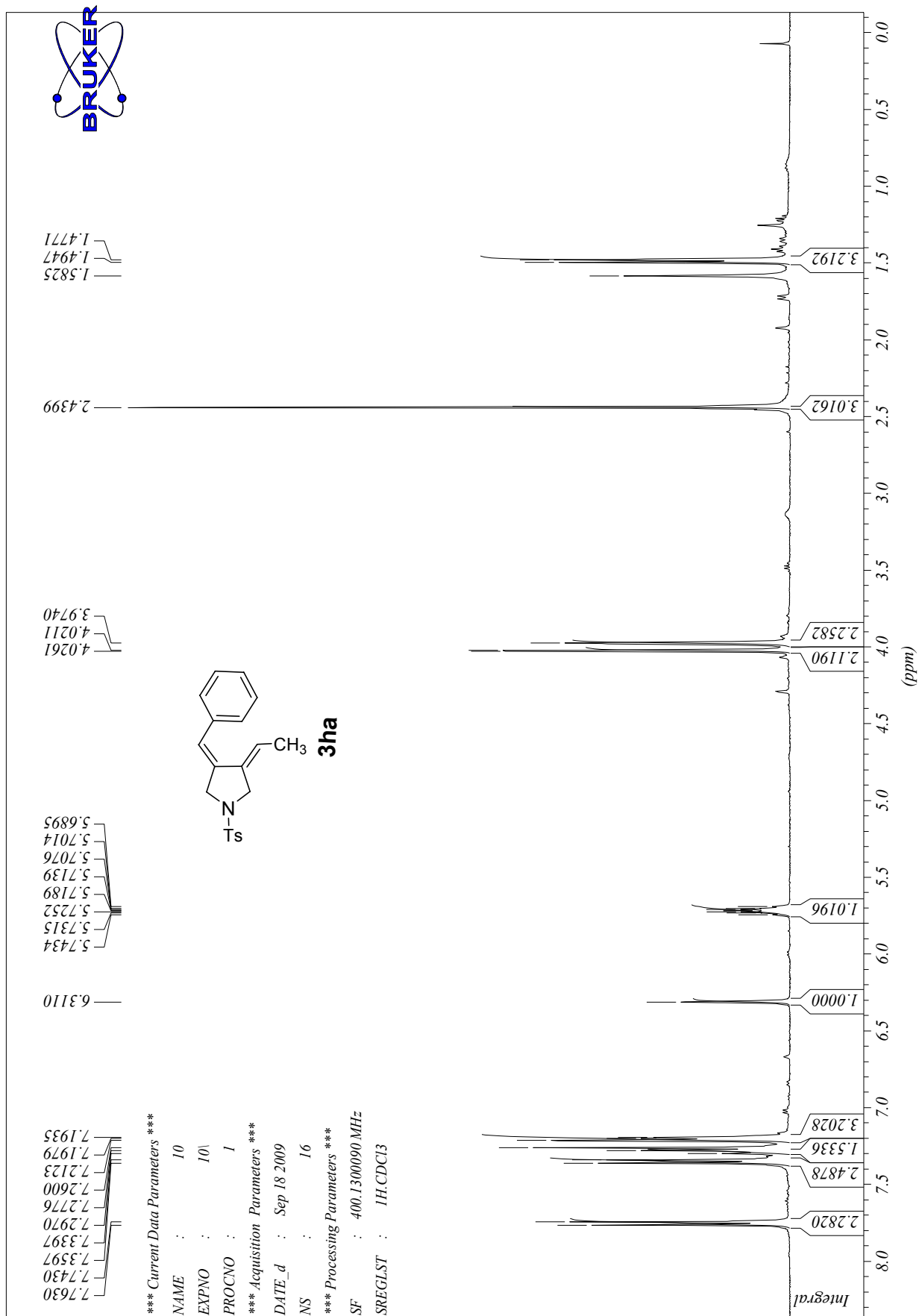


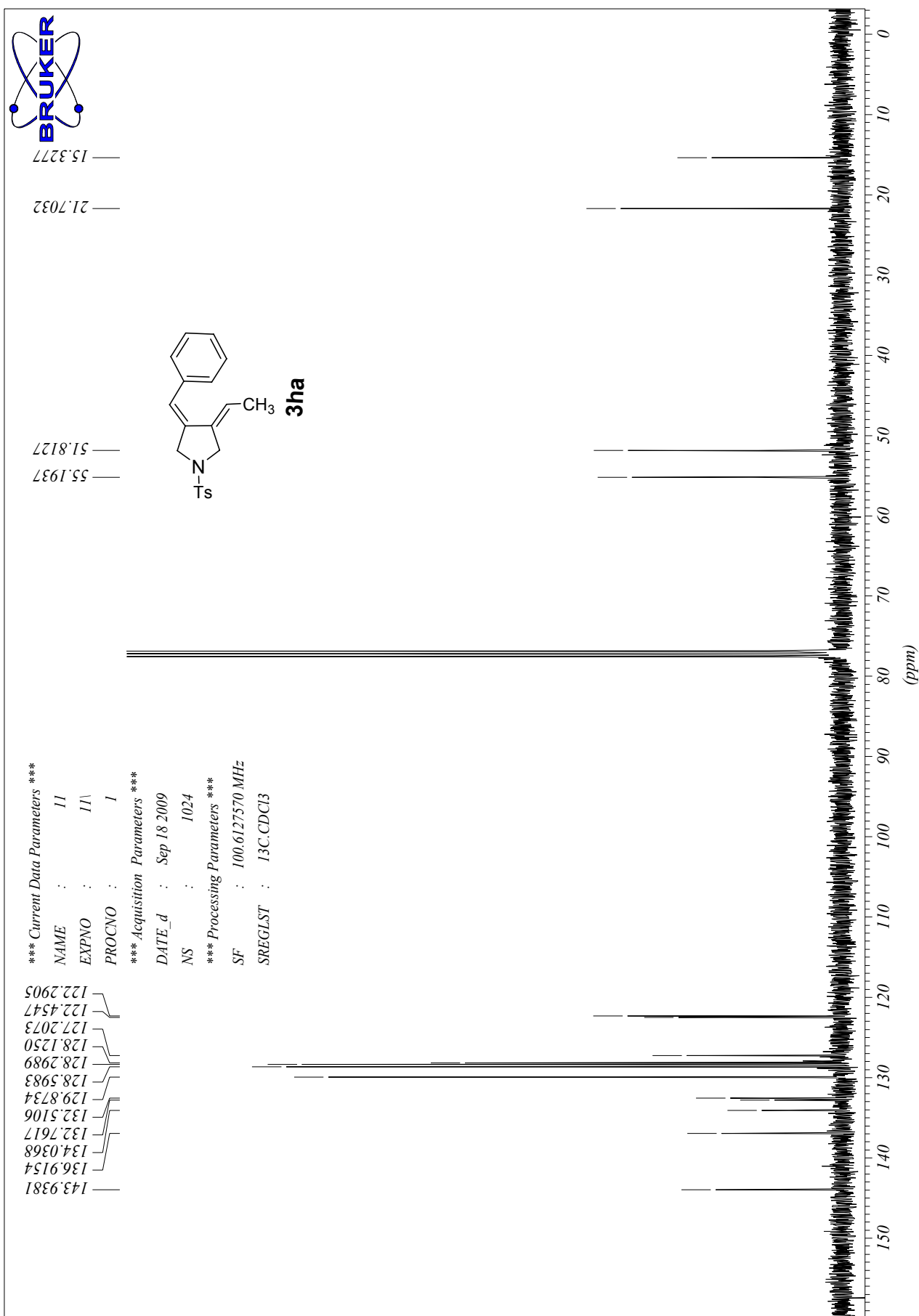


8G-TERMINALDIIN

Sample Name:
8G-TERMINALDIIN
Data Collected on:
nmr400-vnmr400
Archive directory:
/home/walkup/vnmr400/data
Sample directory:
8G-TERMINALDIIN_04Nov2008
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 4 2008
Temp. 25.0 C / 298.1 K
Operator: walkup
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.283 sec
Width 23510.2 Hz
312 repetitions
OBSERVE C13, 100.4598839 MHz
DECOUPLE H1, 399.5239862 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 19 min







BG-B21607

Sample Name:

BG-B21607

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkup1/vnmrsys/data

Sample directory:

BG-B21607_17Jul2009

FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 17 2009

Temp. 27.0 C / 300.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

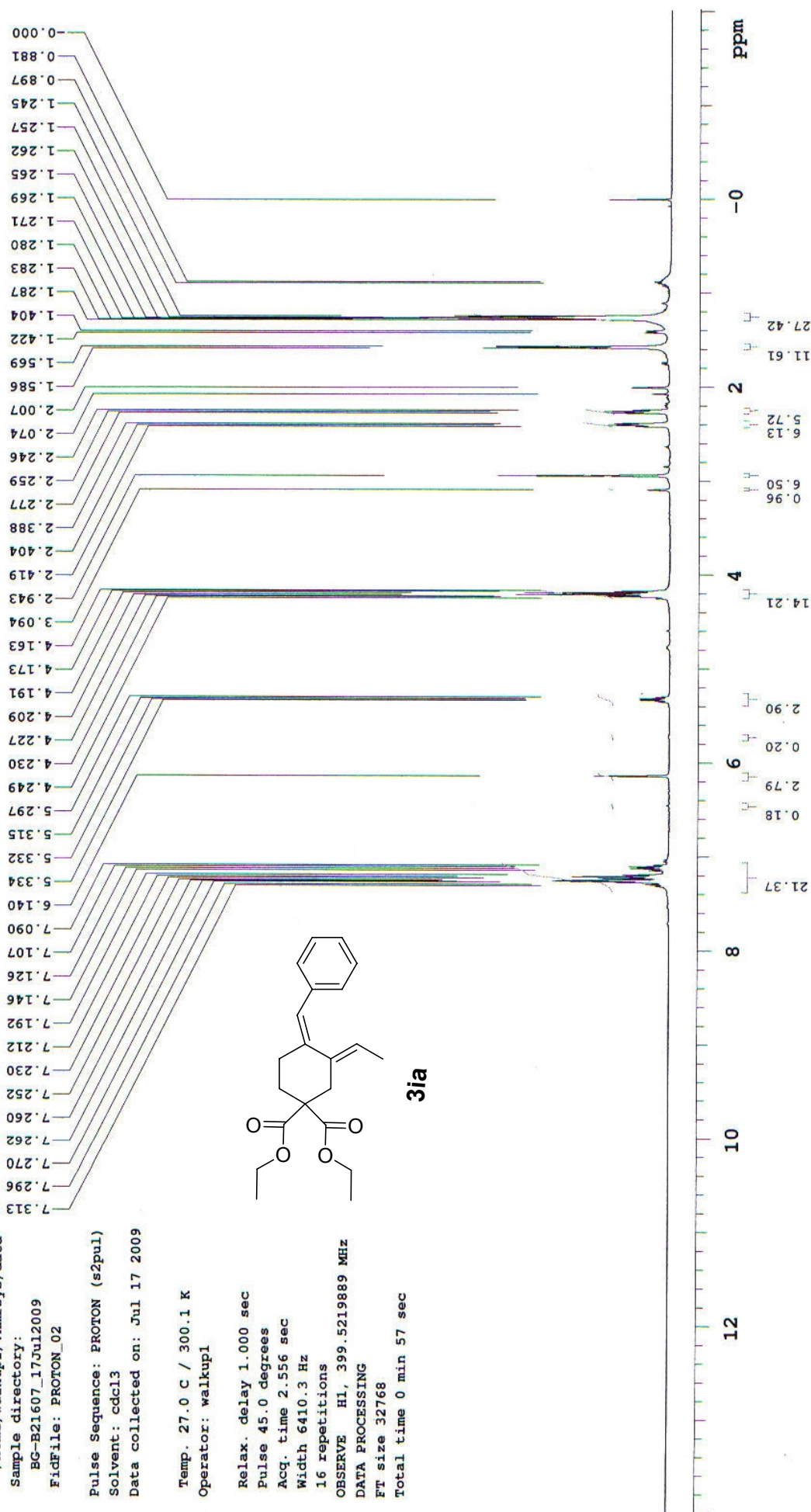
16 repetitions

OBSERVE H1, 399.5219889 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 57 sec



Plotname: --Not assigned--



VARIAN

BG-B21607

Sample Name:

BG-B21607

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkup/vnmrsys/data

Sample directory:

BG-B21607_17Jul2009

FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 17 2009

Temp. 27.0 C / 300.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

3000 repetitions

OBSERVE C13, 100.4598839 MHz

DECOUPLE H1, 399.5239862 MHz

Power 43 dB

continuously on

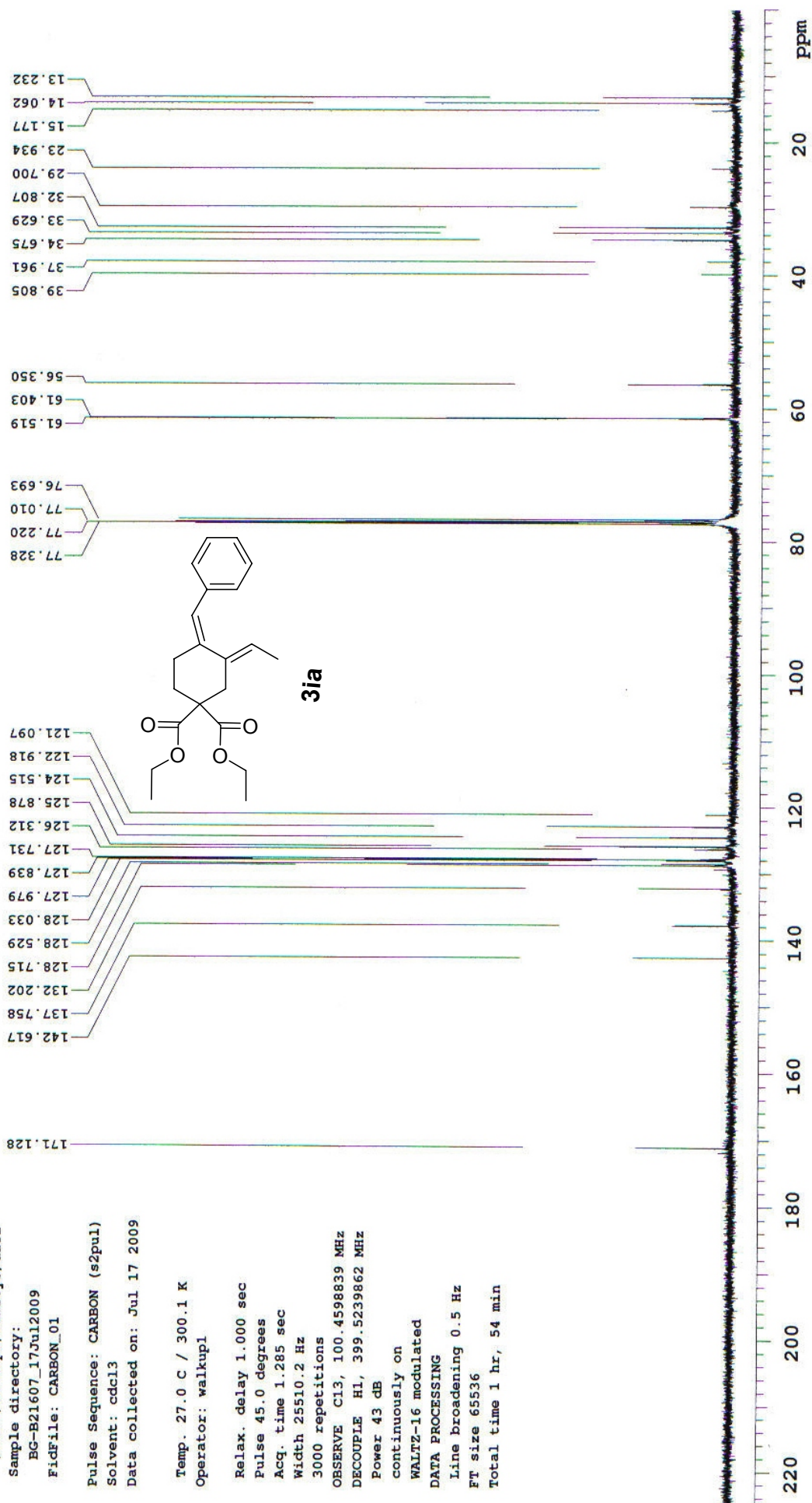
WALTZ-16 modulated

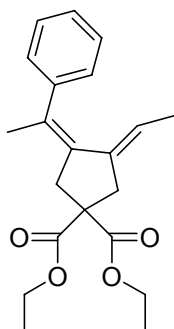
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

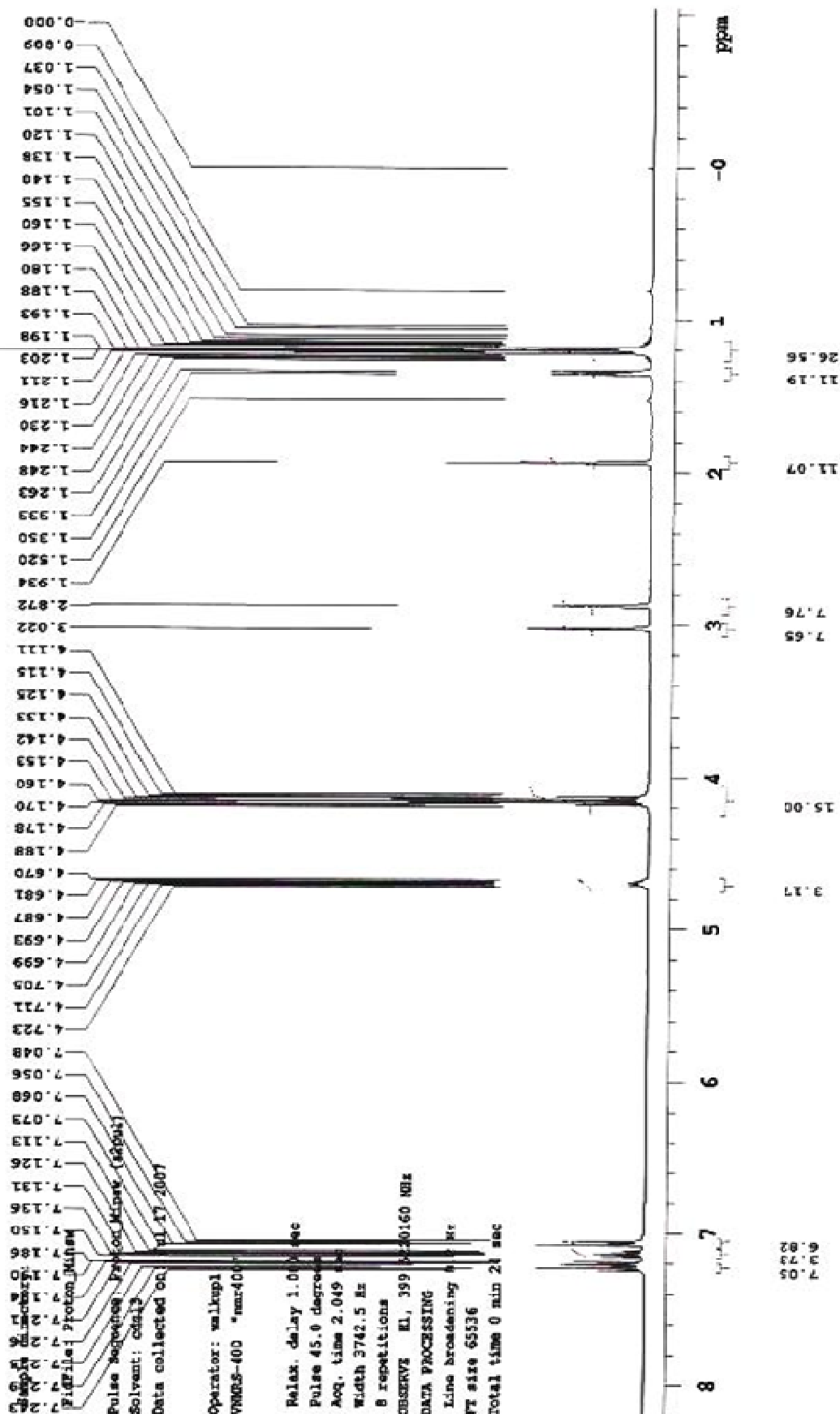
Total time 1 hr, 54 min

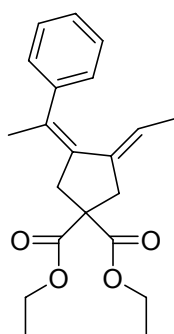




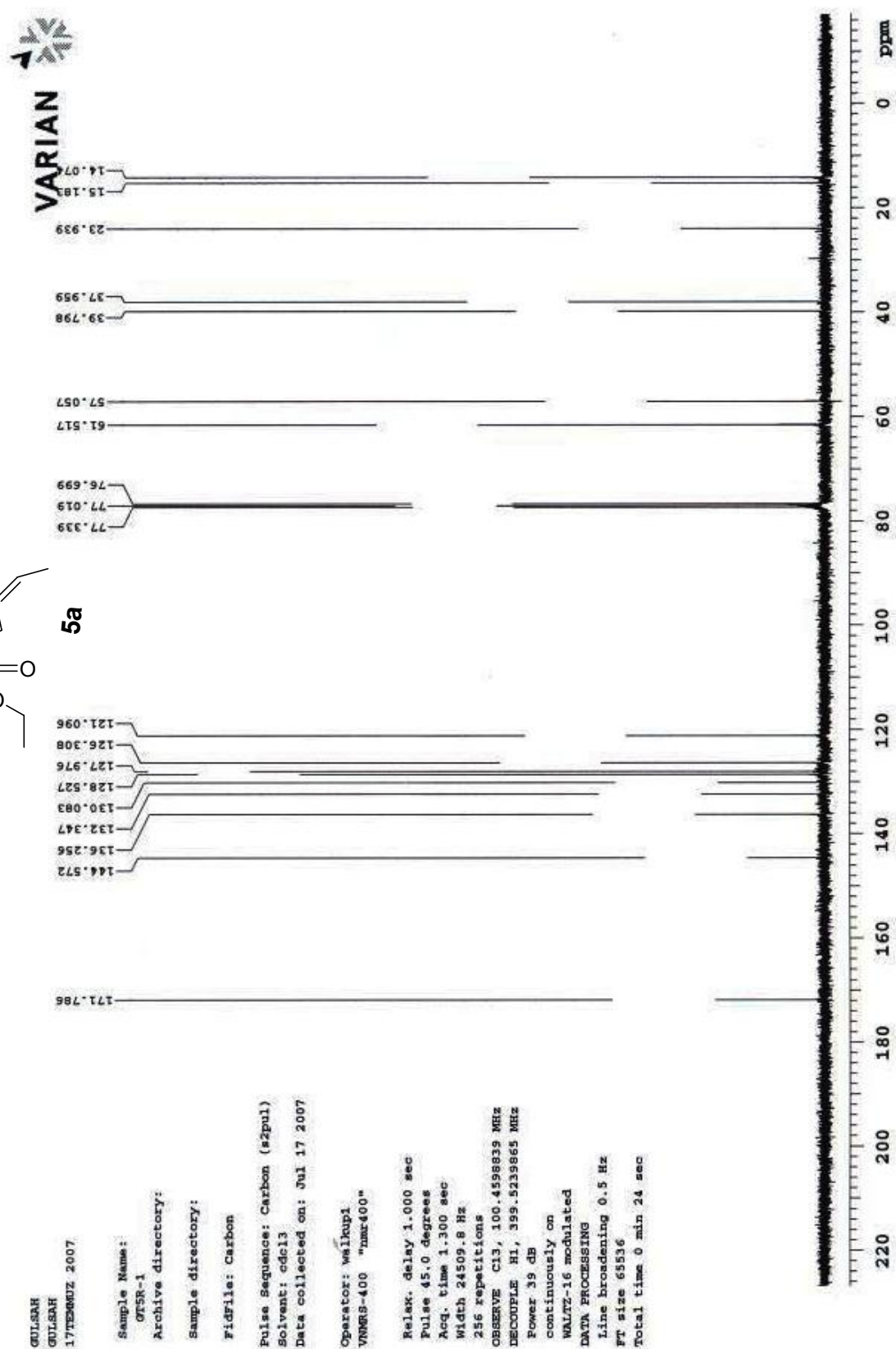
5a

Total time 0 min 24 sec





5a





BG-DB73--TEKRR

Sample Name:

BG-DB73--TEKRR

Data Collected on:

nmr400--vnmrs400

Archive directory:

/home/walkup1/vnmrsys/data

Sample Name: BG-DB73--TEKRR

Data Collected on: Nov 26 2008

File Name: PR0TON

Pulse Sequence: PR0TON (s2pul)

Solvent: cdcl3

Data collected on: Nov 26 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

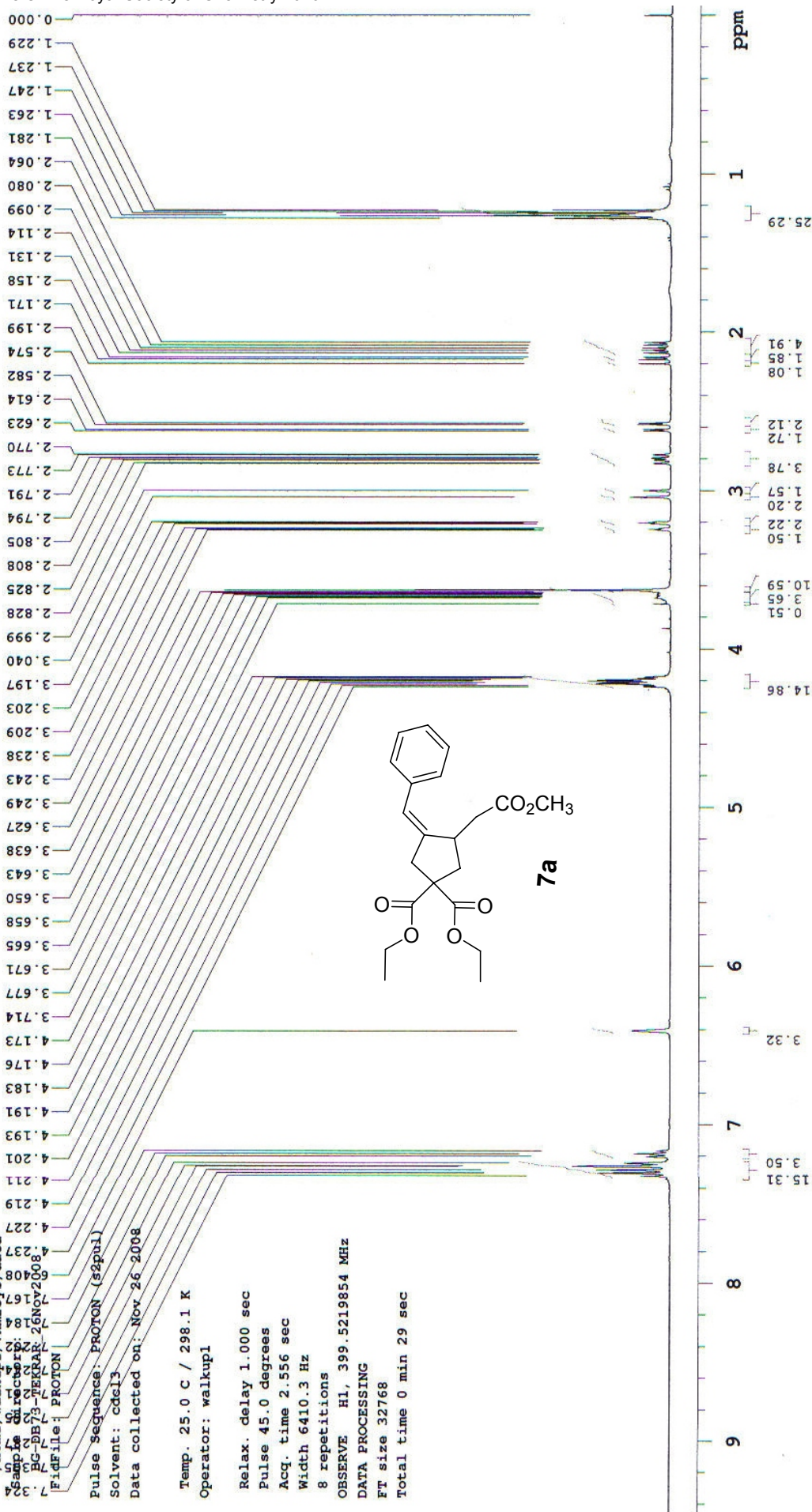
8 repetitions

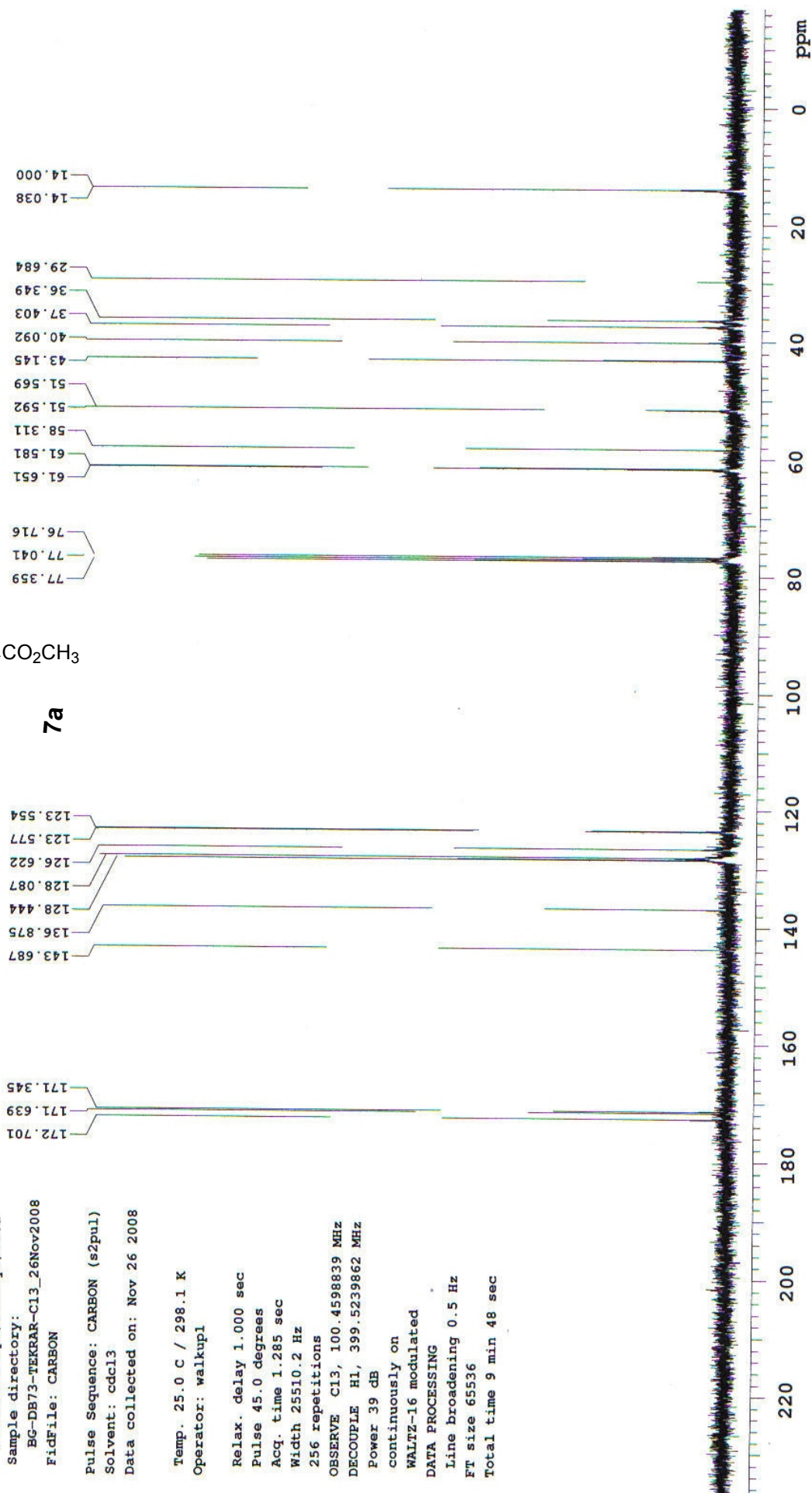
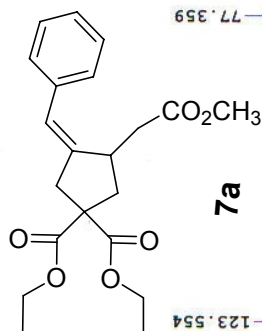
OBSERVE H1, 399.5219854 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 29 sec





BG-DB73-TEKRAR-C13

Sample Name:

BG-DB73-TEKRAR-C13

Data Collected on:

nmr400-vnmrs400

Archive directory:

/home/walkup1/vnmrsys/data

Sample directory:

BG-DB73-TEKRAR-C13_26Nov2008

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Nov 26 2008

Temp. 25.0 C / 298.1 K

Operator: walkup1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

256 repetitions

OBSERVE C13, 100.4598839 MHz

DECOUPLE H1, 399.5239862 MHz

Power 39 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min 48 sec