Electronic Supplementary Material (ESI) for Chemical Communications

Supporting information

An Efficient Synthesis of Trisubstituted Oxazoles via Chemoselective *O*-acylations and Intramolecular Wittig Reactions

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I. Experimental procedures

General methods: *N*-acyl imines **2** were prepared according to the reported literature[1]. Other reagents were used directly from commercial suppliers without further purification. IR spectra were recorded on a Perkin Elmer 500 spectrometer. NMR spectra were recorded on a BrukerAvance 400/500 NMR spectrometer. Chemical shifts are reported in δ ppm referenced to an internal TMS standard for ^{1}H NMR and chloroform-d (δ 77.0 ppm) for ^{13}C NMR. HRMS spectra were recorded on JEOL SX-102A. The X-ray diffraction measurements were carried out at 298 K on a KAPPA APEX II CCD area detector system equipped with a graphite monochromator and a Mo-Kα fine-focus sealed tube (k = 0.71073 Å). Analytical thin layer chromatography (TLC) was performed using Merck 60 F254 precoated silica gel plate (0.2 mm thickness). Flash-chromatography was performed using Merck silica gel 60 (70–230 mesh).

Typical procedure :

TP1 Preparation of **1aa**: A flame dried and nitrogen-flushed 10-mL Schlenk tube, equipped with a magnetic stirring bar and a septum, was charged with a solution of **2a** (75.3 mg, 1.2 equiv) in anhydrous toluene (1.5 mL). To the stirred reaction mixture, **3a** (35 μL, 0.3 mmol), Bu_3P (103 μL, 1.1 equiv) and Et_3N (46 μL, 1.1 equiv) were added in sequence. The reaction mixture was further stirred for 2 hours at room temperature and was monitored by ^{1}H NMR data analysis. The solvent was removed by evaporation *in vacuo*. Purification by flash chromatography (ethyl acetate/hexanes = 1/50) furnished the desired adduct **1aa** as white solid (77.7 mg, 87% yield).

TP2 Preparation of **1ak**: A flame dried and nitrogen-flushed 10-mL Schlenk tube, equipped with a magnetic stirring bar and a septum, was charged with a solution of **2a** (62.8 mg, 0.3 mmol) and PPh_3 (87.1 mg, 1.1 equiv) in anhydrous toluene (1.5 mL). To the stirred reaction mixture, TFAA (46 μL, 1.1 equiv) and Et_3N (54 μL, 1.3 equiv) were added in sequence. The reaction mixture was further stirred for 10 min. at room temperature (monitored by ^{1}H NMR data analysis). The solvent was removed by evaporation *in vacuo*. Purification by flash chromatography (ethyl acetate/hexanes = 1/50) furnished the desired adduct **1ak** as white solid (75.4 mg, 87% yield).

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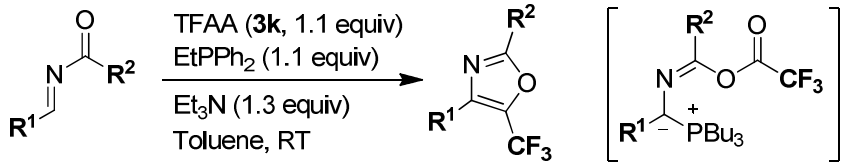
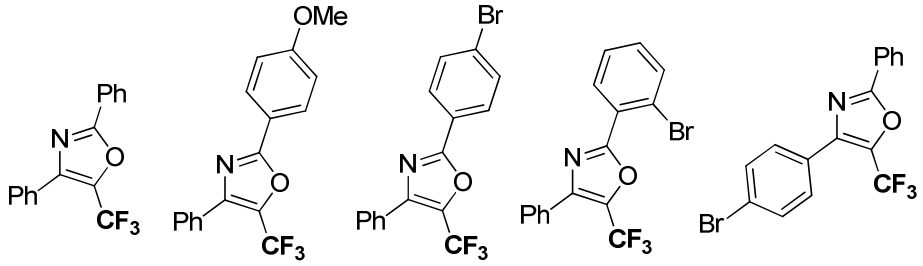
[1] B. J. Cowen, L. B. Saunders, S. J. Miller, *J. Am. Chem. Soc.* **2009,** *131***,** 6105.

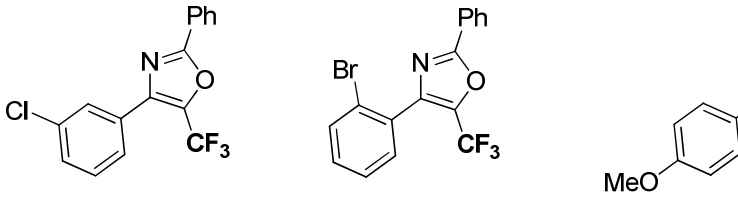
II. Preparation of trifluoromethyl-substituted oxazoles 1ak-1hk using $EtPPh_2$ (Scheme S1).



2 **1**[a,b] **5** (key intermediate)



1ak: 87%, 2 h **1ek**: 96%, 2 h **1fk**: 76%, 1 h **1hk**: 92%, 2 h **1ck**: 87%, 1 h

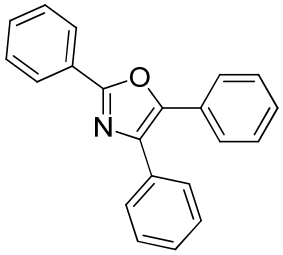


1gk: 89%, 2 h **1dk**: 28%, 2 h (38%)[c] **1bk**: 31%, 2 h (47%)[c, d]

[a] Reactions were performed with **2** (0.3 mmol), **3k** (1.1 equiv), $EtPPh_2$ (1.1 equiv), and Et3N (1.3 equiv) in dry toluene (1.5 mL) under nitrogen. [b] Isolated yield. [c] DMAP (10 mol%) was added after 2 h, and the resulting reaction mixture was stirred for 2 h. [d] **1'bk** was observed.

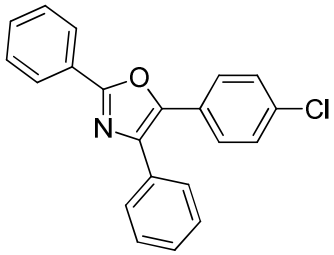
III. Spectra data of the substrates

2,4,5-triphenyloxazole (1aa):



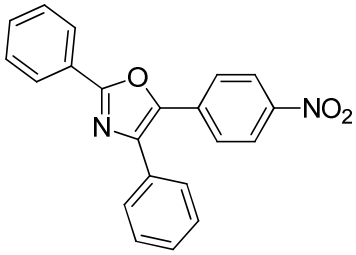
White solid;R_f 0.25 (ethyl acetate/hexanes: 1/20); mp.: 114.1-114.4 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.15 (dd, 2H, J = 8.0 Hz, 1.9 Hz), 7.73 (d, 2H, J =7.0 Hz), 7.66 (d, 2H, J =7.0 Hz), 7.48-7.42 (m, 3H), 7.41-7.29 (m, 6H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.1, 145.5, 136.7, 132.5, 130.3, 128.9, 128.7, 128.6, 128.5, 128.4, 128.2, 128.1, 127.3, 126.5, 126.4; **MS** (70 eV, EI) *m/z* (%): 297 $[M]^+$ (85), 269 (21), 165 (40), 105 (89), 77 (100); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (m), 1600 (w), 1501 (m), 1326 (m), 1067 (m); **HRMS** (MALDI) for **$C_{21}H_{16}NO$**, **$[M+H]^+$** (298.1232) found: 298.1238.

5-(4-chlorophenyl)-2,4-diphenyloxazole (1ab):



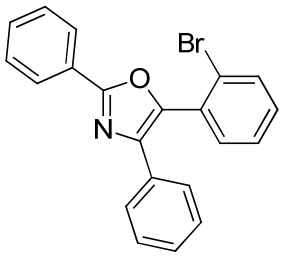
White solid; R_f 0.23 (ethyl acetate/hexanes: 1/20); mp.: 125.4-126.7 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.14 (dd, 2H, J = 7.5 Hz, 3.2 Hz), 7.69 (d, 2H, J = 7.0 Hz), 7.60 (d, 2H, J = 8.5 Hz), 7.50-7.46 (m, 3H), 7.42-7.36 (m, 3H), 7.34 (d, 2H, J = 8.5 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.3, 144.5, 137.2, 134.3, 132.3, 130.5, 129.0, 128.8, 128.7, 128.5, 128.1, 127.7, 127.4, 127.2, 126.5; **MS** (70 eV, EI) *m/z* (%): 333 $[M+2]^+$ (42), 331 $[M]^+$ (100), 305 (7), 303 (14), 244 (16), 190 (9), 165 (81), 139 (70), 105 (62), 89 (33), 77 (65); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 1637 (m), 1478 (m), 1094 (m), 684 (s); **HRMS** (MALDI) fo**r $C_{21}H_{15}ClNO$**, **$[M+H]^+$** (332.0842) found: 332.0852.

5-(4-nitrophenyl)-2,4-diphenyloxazole (1ac):



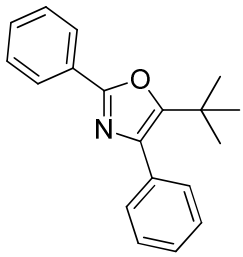
Yellow solid; R_f 0.24 (dichloromethane/hexanes: 1/1); mp.: 192.1-192.6 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.22 (d, 2H, J = 9.1 Hz), 8.18 (dd, 2H, J = 6.1 Hz, 2.5 Hz), 7.83 (d, 2H, J = 8.8 Hz), 7.70 (dd, 2H, J = 7.5 Hz, 2.2 Hz), 7.52-7.50 (m, 3H), 7.49-7.43 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 161.4, 147.0, 143.3, 140.3, 134.9, 131.8, 131.1, 129.2, 129.0, 128.9, 128.4, 126.7, 126.3, 124.1; **MS** (70 eV, EI) *m/z* (%): 342 $[M]^+$ (100), 165 (58), 150 (16), 139 (8), 104 (87), 91 (76), 76 (69); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 1596 (s), 1543 (m), 1509 (s), 1333 (s), 1105 (m); **HRMS** (FAB) for **$C_{21}H_{15}N_2O_3$**, **$[M+H]^+$** (343.1083) found: 343.1085.

5-(2-bromophenyl)-2,4-diphenyloxazole (1ad):



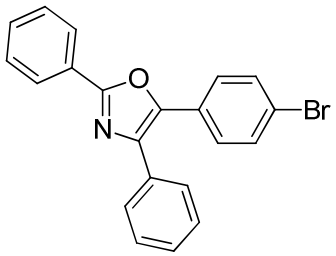
White solid; R_f 0.27 (ethyl acetate/hexanes: 1/20); mp.: 88.4-89.1 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.17 (dd, 2H, J = 7.8 Hz, 2.5 Hz), 7.73 (d, 1H, J =8.0 Hz), 7.62 (d, 2H, J =7.1 Hz), 7.49-7.44 (m, 4H), 7.38 (t, 1H, J = 7.5 Hz), 7.33-7.24 (m, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.6, 144.0, 137.9, 133.5, 132.4, 131.6, 131.0, 130.7, 130.4, 128.7, 128.4, 127.8, 127.5, 127.3, 126.7, 126.5, 124.4; **MS** (70 eV, EI) *m/z* (%): 377 $[M+2]^+$ (52), 375 $[M]^+$ (70), 190 (19), 185 (28), 165 (100), 157 (34), 155 (24), 103 (39), 89 (38), 77 (25); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3061 (w), 1637 (m), 1501 (w), 1440 (w), 1022 (m), 689 (m); **HRMS** (MALDI) for **$C_{21}H_{15}BrNO$**, **$[M+H]^+$** (376.0337) found: 376.0348.

5-(*tert*-butyl)-2,4-diphenyloxazole (1ae):



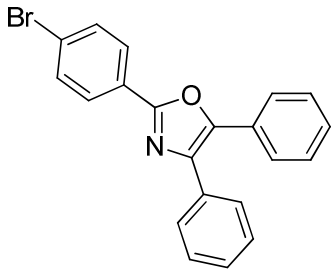
White solid; R_f 0.32 (ethyl acetate/hexanes: 1/20); mp.: 63.1-63.6 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.06 (dd, 2H, J = 7.5 Hz, 1.2 Hz), 7.48-7.33 (m, 8H), 1.32 (s, 9H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 158.1, 154.5, 135.2, 134.2, 130.1, 129.8, 128.6, 127.9, 127.7, 126.1, 32.7, 29.8; **MS** (70 eV, EI) *m/z* (%): 277 $[M]^+$ (36), 262 (100), 234 (1), 192 (3), 129 (6), 115 (15), 105 (41), 77 (40), 69 (45), 57 (74); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (m), 2962 (s), 2924 (s), 1623 (w), 1493 (m), 1459 (w), 1345 (m), 1109 (s); **HRMS** (MALDI) for **$C_{19}H_{20}NO$**, **$[M+H]^+$** (278.1545) found: 278.1551.

5-(4-bromophenyl)-2,4-diphenyloxazole (1af, 1'fa):



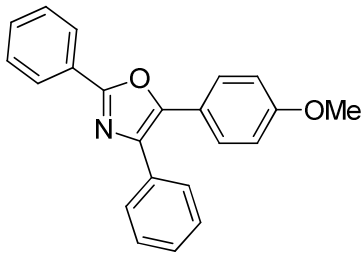
White solid; R_f 0.25 (dichloromethane/hexanes: 1/1); mp.: 123.1-123.4 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.14 (dd, 2H, J = 7.7 Hz, 3.8 Hz), 7.69 (d, 2H, J = 7.0 Hz), 7.53-7.46 (m, 7H), 7.42-7.34 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm:160.3, 144.4, 137.3, 132.2, 131.9, 130.5, 128.8, 128.7, 128.5, 128.1, 127.8, 127.1, 126.6, 126.5, 122.5; **MS** (70 eV, EI) *m/z* (%): 377 $[M+2]^+$ (90), 375 (100), 183 (36), 165 (74), 157 (42), 155 (38), 103 (37), 89 (72), 76 (50); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3061 (m), 1596 (w), 1486 (s), 1444 (s), 1067 (s), 686 (s); **HRMS**(ESI) for **$C_{21}H_{15}BrNO$**, **$[M+H]^+$** (376.0337) found: 376.0338.

2-(4-bromophenyl)-4,5-diphenyloxazole (1'af, 1fa):



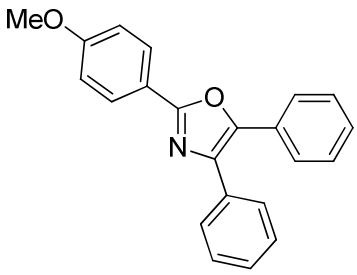
White solid; R_f 0.33 (ethyl acetate/hexanes: 1/20); mp.: 145.6-146.1 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.02 (d, 2H, J = 8.4 Hz), 7.71 (d, 2H, J = 7.9 Hz), 7.67 (d, 2H, J = 8.1 Hz), 7.62 (d, 2H, J = 8.4 Hz), 7.43-7.35 (m, 6H); **^{13}C-NMR** (125 MHz, $CDCl_3$, 25 °C) δ/ppm:159.3, 145.8, 136.9, 132.3, 132.0, 128.8, 128.7, 128.6, 128.3, 128.1, 127.9, 126.6, 126.3, 124.8; **MS** (70 eV, EI) *m/z* (%): 377 $[M+2]^+$ (18), 375 $[M]^+$ (24), 296 (2), 165 (56), 105 (58), 77 (100); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3031 (m), 2924 (s), 1600 (m), 1501 (s), 1474 (s), 1090 (m), 686 (s); **HRMS** (MALDI) for **$C_{21}H_{15}BrNO$**, **$[M+H]^+$** (376.0337) found: 376.0350.

5-(4-methoxyphenyl)-2,4-diphenyloxazole (1ag, 1'ea):



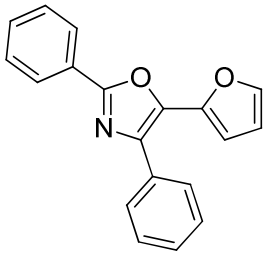
White solid; R_f 0.12 (ethyl acetate/hexanes: 1/60); mp.: 101.2-101.9 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.14 (dd, 2H, J = 8.0 Hz, 1.4 Hz), 7.72 (d, 2H, J =7.7 Hz), 7.59 (d, 2H, J =8.5 Hz), 7.48-7.42 (m, 3H), 7.38 (t, 2H, J = 7.6 Hz), 7.31-7.31 (m, 1H), 6.90 (d, 2H, J = 8.7Hz), 3.81 (s, 3H); **^{13}C-NMR** (125 MHz, $CDCl_3$, 25 °C) δ/ppm: 159.8, 159.6, 145.6, 135.5, 132.7, 130.1, 128.7, 128.5, 128.2, 127.9, 127.5, 126.3, 121.5, 114.1, 55.2; **MS** (70 eV, EI) *m/z* (%): 327 $[M]^+$ (100), 299 (10), 196 (17), 181 (16), 152 (20), 135 (57), 105 (11), 89 (13), 77 (16); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 2962 (w), 1615 (m), 1512 (s), 1444 (m), 1253 (s); **HRMS** (MALDI) for **$C_{22}H_{17}NO_2$**, **$[M]^+$** (327.1259) found: 327.1271.

2-(4-methoxyphenyl)-4,5-diphenyloxazole (1'ag, 1ea):



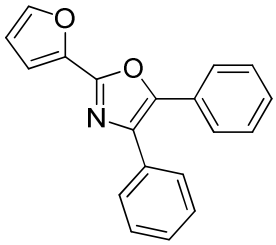
White solid; R_f 0.17 (ethyl acetate/hexanes: 1/20); mp.: 118.2-118.7 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.08 (d, 2H, J = 8.9 Hz), 7.72 (dd, 2H, J = 6.8 Hz, 1.4 Hz), 7.65 (dd, 2H, J = 7.0 Hz, 1.4 Hz), 7.41-7.28 (m, 6H), 6.97 (d, 2H, J = 8.9 Hz), 3.83 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 161.3, 160.2, 144.9, 136.5, 132.7, 129.1, 128.6, 128.5, 128.3, 128.1, 126.4, 120.1, 114.1, 55.3; **MS** (70 eV, EI) *m/z* (%): 327 $[M]^+$ (74), 181 (19), 165 (65), 133 (18), 105 (77), 77 (100); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (m), 2939 (m), 1611 (s), 1493 (s), 1250 (s), 1170 (s);**HRMS** (MALDI) for **$C_{22}H_{17}NO_2$**, **$[M]^+$** (327.1259) found: 327.1270.

5-(furan-2-yl)-2,4-diphenyloxazole (1ah):



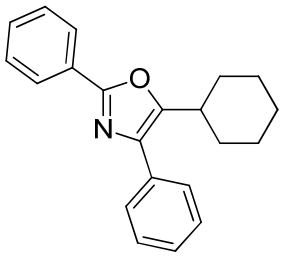
Brown oil; R_f 0.15 (ethyl acetate/hexanes: 1/60); **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.15 (dd, 2H, J = 7.8 Hz, 2.8 Hz), 7.91 (d, 2H, J = 7.4 Hz), 7.51-7.50 (m, 1H), 7.48-7.42 (m, 5H), 7.36 (t, 1H, J = 7.3 Hz), 6.76 (d, 1H, J = 3.4 Hz), 6.52 (dd, 1H, J = 3.1 Hz, 1.8 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.0, 143.9, 142.9, 137.8, 137.0, 131.6, 130.5, 128.7, 128.3, 128.2, 127.9, 127.1, 126.6, 111.5, 109.3; **MS** (20 eV, EI) *m/z* (%): 287 $[M]^+$ (95), 156 (42), 128 (100), 95 (58), 89 (49), 77 (43); **IR** (CH_2Cl_2) $\tilde{\nu}$ (cm^{-1}): 3054 (m), 1606 (m), 1493 (s), 1449 (s), 1071 (m); **HRMS** (MALDI) fo**r $C_{19}H_{14}NO_2$**, **$[M+H]^+$** (288.1024) found: 288.1036.

2-cyclohexyl-4,5-diphenyloxazole (1'ah):



Brown solid; R_f 0.1 (ethyl acetate/hexanes: 1/20); mp.: 61.7 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.72 (dd, 2H, J = 8.2 Hz, 1.3 Hz), 7.66 (dd, 2H, J = 8.2 Hz, 1.3 Hz), 7.60 (dd, 1H, J = 1.6 Hz, 0.8 Hz), 7.42-7.31 (m, 6H), 7.13 (d, 1H, J = 3.5 Hz), 6.58 (dd, 1H, J = 3.4 Hz, 1.8 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 153.0, 145.1, 144.5, 142.8, 136.4, 132.0, 128.73, 128.70, 128.6, 128.4, 128.2, 126.7, 111.9, 111.8, 111.7; **MS** (70 eV, EI) *m/z* (%): 287 $[M]^+$ (100), 259 (23), 230 (19), 185 (4), 182 (5), 165 (66), 156 (49), 128 (78), 105 (59), 77 (45); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3107 (s), 1600 (m), 1501 (m), 1303 (m), 1013 (m); **HRMS** (FAB) for **$C_{19}H_{14}NO_2$**, **$[M+H]^+$** (288.1025) found: 288.1024.

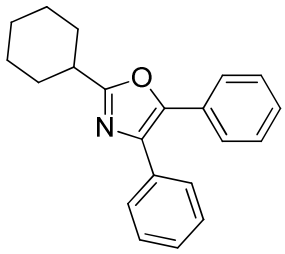
5-cyclohexyl-2,4-diphenyloxazole (1ai):



White solid; R_f 0.13 (ethyl acetate/hexanes: 1/60); mp.: 63.3-64.1 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.08 (dd, 2H, J = 7.5 Hz, 0.9 Hz), 7.68 (d, 2H, J = 7.5 Hz), 7.46-7.39 (m, 5H), 7.34 (t, 1H, J = 7.5 Hz), 3.03 (tt, 1H, J = 11.8 Hz, 6.8 Hz), 1.95 (d, 2H, J = 13.2 Hz), 1.88 (d, 2H, J = 11.5 Hz), 1.77-1.70 (m, 3H), 1.45-1.32 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 159.2, 152.1, 134.6, 132.7, 129.8, 128.6, 128.5, 127.8, 127.3, 127.2, 126.1, 35.7, 31.6, 26.2, 25.8; **MS** (70 eV, EI) *m/z* (%): 303 $[M]^+$ (100), 260 (23), 234 (17), 221 (5), 199 (5), 157 (14), 129 (11), 105 (39), 89 (27), 55 (13); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3076 (w), 2919 (s), 2915 (s), 1630 (m), 1448

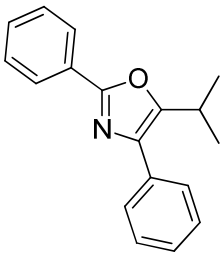
(m), 1069 (w); **HRMS** (MALDI) for **$C_{21}H_{22}NO$**, **$[M+H]^+$** (304.1701) found: 304.1705.

2-cyclohexyl-4,5-diphenyloxazole (1'ai):



White solid; R_f 0.1 (ethyl acetate/hexanes: 1/20); mp.: 111.1-111.8 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.64 (d, 2H, J = 7.1 Hz), 7.58 (d, 2H, J = 6.9 Hz), 7.38-7.28 (m, 6H), 2.89 (tt, 1H, J = 11.5 Hz, 7.2 Hz), 2.14 (dd, 2H, J = 13.2 Hz, 2.7 Hz), 1.86 (dt, 2H, J = 13.0 Hz, 3.5 Hz), 1.77-1.62 (m, 2H), 1.46-1.24 (m, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 166.9, 144.6, 134.8, 132.7, 129.3, 128.6, 128.5, 128.2, 128.0, 127.9, 126.4, 37.6, 30.7, 25.8, 25.7; **MS** (70 eV, EI) *m/z* (%): 303 $[M]^+$ (62), 262 (12), 248 (62), 235 (100), 234 (20), 198 (14), 165 (60), 115 (5), 105 (52), 68 (20), 55 (39); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 2924 (s), 2847 (s), 1600 (w), 1444 (m), 1055 (m); **HRMS** (MALDI) for **$C_{21}H_{22}NO$**, **$[M+H]^+$** (304.1701) found: 304.1706.

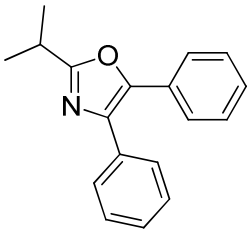
5-isopropyl-2,4-diphenyloxazole (1aj):



Colorless oil; R_f 0.18 (ethyl acetate/hexanes: 1/60); **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.09 (dd, 2H, J = 8.0 Hz, 1.6 Hz), 7.70 (d, 2H, J = 8.1 Hz), 7.47-7.39 (m, 5H), 7.33 (t, 1H, J = 7.5 Hz), 3.45 (sep, 1H, J = 7.0 Hz), 1.41 (s, 3H), 1.39 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 159.2, 152.4, 134.4, 132.6, 129.9, 128.6, 128.5, 127.8, 127.4, 127.3, 126.1, 26.0, 21.4; **MS** (70 eV, EI) *m/z* (%): 263 $[M]^+$ (39), 248 (35), 220 (2), 105 (21), 89 (100), 77 (22); **IR** (CH_2Cl_2) $\tilde{\nu}$ (cm^{-1}): 3039 (m), 2968

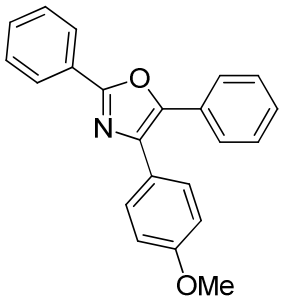
(s), 1597 (m), 1494 (s), 1445 (s), 1068 (s); **HRMS** (MALDI) for **$C_{18}H_{18}NO$**, **$[M+H]^+$** (264.1388) found: 264.1395.

2-isopropyl-4,5-diphenyloxazole (1'aj):



Colorless oil; R_f 0.13 (ethyl acetate/hexanes: 1/20); **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.64 (d, 2H, J = 7.2 Hz), 7.58 (d, 2H, J = 7.2 Hz), 7.38-7.27 (m, 6H), 3.18 (sep, 1H, J = 6.9 Hz), 1.45 (s, 3H),1.43 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 167.6, 144.8,134.9, 132.8, 129.3, 128.6, 128.5, 128.2, 128.0, 127.9, 126.4, 28.5, 20.5; **MS** (70 eV, EI) *m/z* (%): 263 $[M]^+$ (59), 248 (23), 193 (12), 165 (64), 158 (14), 117 (80), 105 (55),77 (100); **IR** (CH_2Cl_2) $\tilde{\nu}$ (cm^{-1}): 3045 (m), 2923 (s), 1603 (m), 1500 (m), 1442 (m), 1061 (m); **HRMS** (FAB) for **$C_{18}H_{18}NO$**, **$[M+H]^+$** (264.1388) found: 264.1382.

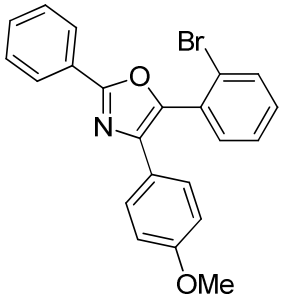
4-(4-methoxyphenyl)-2,5-diphenyloxazole (1ba):



White solid; R_f 0.18 (ethyl acetate/hexanes: 1/50); mp.: 127.7-128.5 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.15 (dd, 2H, J = 7.9 Hz, 1.9 Hz), 7.67-7.63 (m, 4H), 7.48-7.40 (m, 3H), 7.36 (t, 2H, J = 7.4 Hz), 7.31-7.28 (m, 1H), 6.94 (d, 2H, J= 8.7 Hz), 3.82 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 159.9, 159.6, 144.8, 136.6, 130.2, 129.4, 129.1, 128.7, 128.6, 128.3, 127.4, 126.4, 126.3, 124.9, 114.0, 55.2; **MS** (70 eV, EI) *m/z* (%): 327 $[M]^+$ (80), 196 (15), 181 (52), 165 (61), 152 (100), 119 (23), 105 (56), 77(23); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (m), 2962 (m), 1615 (m),

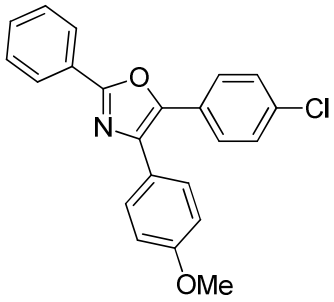
1509 (s), 1246 (s), 1177 (m); **HRMS** (ESI) for **$C_{22}H_{18}NO_2$**, **$[M+H]^+$** (328.1338) found: 328.1334.

5-(2-bromophenyl)-4-(4-methoxyphenyl)-2-phenyloxazole (1bd):



White solid; R_f 0.43 (ethyl acetate/hexanes: 1/20); mp.: 90.7-91.8 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.16-8.14 (m, 2H), 7.74 (dd, 1H, J = 7.9 Hz, 1.2 Hz), 7.56 (d, 2H, J = 8.9 Hz), 7.51-7.46 (m, 4H), 7.39 (td, 1H, J = 7.5 Hz, 1.2 Hz), 7.34 (td, 1H, J = 7.8 Hz, 1.9 Hz), 6.85 (d, 2H, J = 8.9 Hz), 3.79 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.6, 159.4, 143.1, 137.8, 133.6, 132.5, 131.0, 130.9, 130.3, 128.7, 128.1, 127.5, 127.4, 126.5, 124.5, 124.3, 113.9, 55.2; **MS** (70 eV, EI) *m/z* (%): 407 $[M+2]^+$ (83), 405 $[M]^+$ (100), 377 (15), 222 (9), 195 (30), 185 (77), 183 (93), 155 (79), 133 (24), 103(49), 77 (55); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 2923 (m), 1624 (m), 1515 (m), 1247 (s), 1027 (m), 689 (m); **HRMS** (MALDI) for **$C_{22}H_{17}BrNO_2$**, **$[M+H]^+$** (406.0443) found: 406.0456.

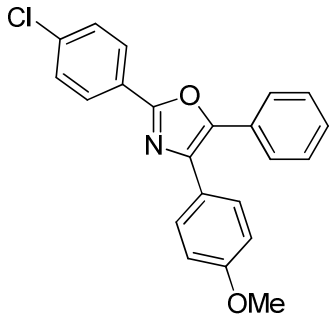
5-(4-chlorophenyl)-4-(4-methoxyphenyl)-2-phenyloxazole (1bb):



White solid; R_f 0.32 (ethyl acetate/hexanes: 1/20); mp.: 138.1-138.9 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.13-8.10 (m, 2H), 7.60 (dt, 2H, J = 8.8 Hz, 2.5 Hz), 7.58 (dt, 2H, J = 8.7 Hz, J = 8.7 Hz, 2.1 Hz), 7.48-7.42 (m, 3H), 7.32 (dt, 2H, J = 8.6 Hz, 2.1 Hz), 6.93 (dt, 2H, J= 8.8 Hz, 2.5 Hz), 3.82 (s, 3H); **^{13}C-NMR** (125 MHz,

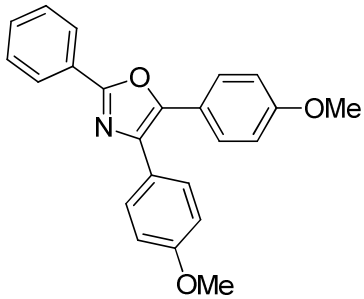
$CDCl_3$, 25 °C) δ/ppm: 160.1, 159.8, 143.8, 136.9, 134.1, 130.5, 129.5, 128.9, 128.7, 127.5, 127.4, 127.1, 126.5, 124.5, 114.1, 55.3; **MS** (70 eV, EI) *m/z* (%): 363 $[M+2]^+$ (35), 361 $[M]^+$ (99), 298 (4), 230 (5), 195 (20), 152 (65), 139 (88), 111 (100); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 2931 (w), 1618 (m), 1509 (s), 1488 (s), 1249 (s), 693 (s); **HRMS** (MALDI) for **$C_{22}H_{16}ClNO_2$**, **$[M]^+$** (361.0869) found: 361.0883.

2-(4-chlorophenyl)-4-(4-methoxyphenyl)-5-phenyloxazole (1'bb):



White solid; R_f 0.36 (ethyl acetate/hexanes: 1/20); mp.: 122.2-122.5 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.11 (d, 2H, *J* = 8.5 Hz), 7.63-7.69 (m, 4H), 7.47 (d, 2H, *J* = 8.5 Hz), 7.43-7.31 (m, 3H), 6.95 (d, 2H, *J* = 8.7 Hz), 3.86 (s, 3H); **^{13}C-NMR** (125 MHz, $CDCl_3$, 25 °C) δ/ppm: 159.7, 159.1, 145.1, 136.8, 136.4, 129.4, 129.1, 129.0, 128.7, 128.5, 127.7, 126.4, 126.0, 124.8, 114.1, 55.3; **MS** (70 eV, EI) *m/z* (%): 363 $[M+2]^+$ (36), 362 $[M]^+$ (100), 280 (18), 196 (5), 182 (9), 167 (22), 149 (38), 97 (12); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 2924 (m), 1600 (m), 1509 (m), 1242 (s), 1173 (m), 686 (m); **HRMS** (FAB) for **$C_{22}H_{17}ClNO_2$**, **$[M+H]^+$** (362.0948) found: 362.0945.

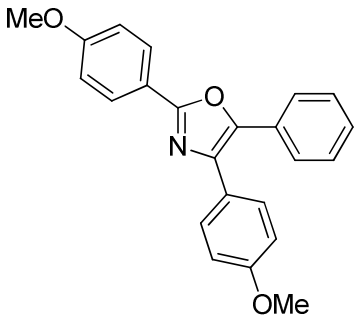
4,5-bis(4-methoxyphenyl)-2-phenyloxazole (1bg):



White solid; R_f 0.36 (ethyl acetate/hexanes: 1/20); mp.: 124.5-125.1 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.13 (dd, 2H, *J* = 8.0 Hz, 1.7 Hz), 7.64 (d, 2H, *J* = 8.8 Hz), 7.59 (d, 2H, *J* = 8.8 Hz), 7.48-7.40 (m, 3H), 6.93 (d, 2H, *J* = 8.6 Hz), 6.90 (d,

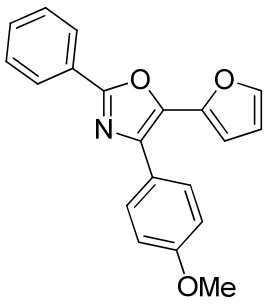
2H, *J* = 8.6 Hz), 3.83 (s, 3H), 3.82 (s, 3H); **^{13}C-NMR** (125 MHz, $CDCl_3$, 25 °C) *δ*/ppm: 159.6, 159.5, 159.4, 144.9, 135.3, 130.0, 129.2, 128.6, 128.0, 127.5, 126.2, 125.1, 121.7, 114.1, 114.0, 55.3, 55.2; **MS** (70 eV, EI) *m/z* (%): 357 $[M]^+$ (100), 225 (2), 211 (17), 196 (41), 181 (28), 135 (67), 133 (27), 92 (31), 77 (67); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3046 (w), 2954 (m), 1611 (m), 1497 (s), 1246 (s), 1177 (s); **HRMS** (ESI) for **$C_{23}H_{20}NO_3$**, **$[M+H]^+$** (358.1443) found: 358.1440.

2,4-bis(4-methoxyphenyl)-5-phenyloxazole (1'bg):



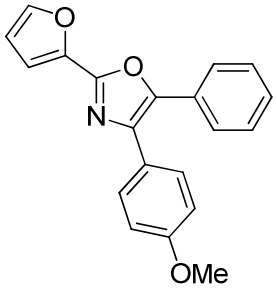
White solid; R_f 0.3 (ethyl acetate/hexanes: 1/20); mp.: 122.8-123.4 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) *δ*/ppm: 8.09 (d, 2H, *J* = 8.4Hz), 7.65 (td, 4H, *J* = 7.0 Hz, 2.0 Hz), 7.37 (t, 2H, *J* = 7.7 Hz), 7.33-7.29 (m, 1H), 6.99 (d, 2H, *J* = 8.4 Hz), 6.94 (d, 2H, *J* = 8.4 Hz), 3.87 (s, 3H), 3.85 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) *δ*/ppm: 161.4, 160.1, 159.6, 144.3, 136.3, 129.5, 129.3, 128.6, 128.2, 126.3, 125.0, 120.2, 114.2, 114.1, 55.4, 55.3; **MS** (70 eV, EI) *m/z* (%): 357 $[M]^+$ (100), 314 (5), 252 (8), 196 (20), 181 (30), 153 (30), 119 (17), 105 (76), 77 (52); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3008 (m), 2931 (m), 1611 (s), 1512 (s), 1257 (s), 1170 (s); **HRMS** (FAB) for **$C_{23}H_{20}NO_3$**, **$[M+H]^+$** (358.1443) found: 358.1448.

5-(furan-2-yl)-4-(4-methoxyphenyl)-2-phenyloxazole (1bh):



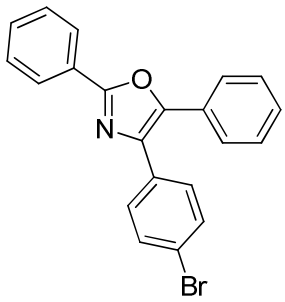
Brown soild; R_f 0.3 (ethyl acetate/hexanes: 1/20); mp.: 83.4-84.6 °C; **^{1}H-NMR** (500 MHz, $CDCl_3$, 25 °C) *δ*/ppm: 8.14 (dd, 2H, *J* = 8.0 Hz, 1.9 Hz), 7.85 (d, 2H,*J* = 8.8 Hz), 7.52-7.50 (m, 1H), 7.49-7.46 (m, 3H), 6.98 (d, 2H, *J* = 8.8 Hz), 6.74 (d, 1H, *J* = 3.3 Hz), 6.52 (dd, 1H, *J* = 3.3 Hz, 1.7 Hz), 3.85(s, 3H); **^{13}C-NMR** (125 MHz, $CDCl_3$, 25 °C) *δ*/ppm: 159.9, 159.7, 144.1, 142.7, 137.0, 136.9, 130.4, 129.3, 128.7, 127.1, 126.5, 124.2, 113.8, 111.5, 108.9, 55.3; **MS** (70 eV, EI) *m/z* (%): 317 $[M]^+$ (77), 171 (2), 156 (46), 128 (55), 95 (100), 77 (39); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3069 (w), 2931 (w), 1609 (m), 1490 (m), 1255 (s), 1028 (s); **HRMS** (ESI) for **$C_{20}H_{16}NO_3$**, **$[M+H]^+$** (318.1130) found: 318.1123.

2-(furan-2-yl)-4-(4-methoxyphenyl)-5-phenyloxazole (1'bh):



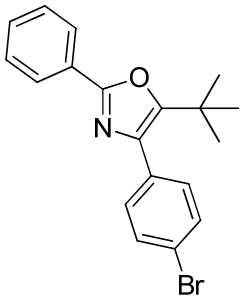
Brown soild; R_f 0.15 (ethyl acetate/hexanes: 1/20); mp.: 86.5 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) *δ*/ppm: 7.58 (td, 4H, *J* = 6.5 Hz, 1.4 Hz), 7.51 (d, 1H, *J* = 1.8 Hz), 7.32-7.22 (m, 3H), 7.03 (dd, 1H, *J* = 3.4 Hz, 0.5 Hz), 6.85 (d, 2H, *J* = 8.8 Hz), 6.49 (dd, 1H, *J*= 3.3 Hz, 1.7 Hz), 3.77 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) *δ*/ppm: 159.8, 152.9, 144.4, 143.0, 136.3, 129.5, 128.8, 128.7, 128.5, 126.5, 124.5, 114.1, 111.9, 111.6, 55.3; **MS** (70 eV, EI) *m/z* (%): 317 $[M]^+$ (100), 375 (11), 181 (9), 157 (17), 128 (21), 77 (15); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3099 (w), 2916 (m), 1615 (m), 1512 (m), 1246 (s), 1177 (s); **HRMS** (FAB) for **$C_{20}H_{16}NO_3$**, **$[M+H]^+$** (318.1130) found: 318.1125.

4-(4-bromophenyl)-2,5-diphenyloxazole (1ca):



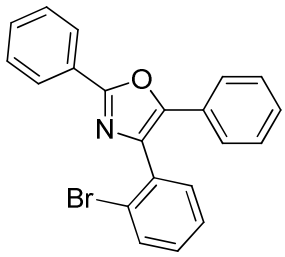
White solid; R_f 0.29 (ethyl acetate/hexanes: 1/20); mp.: 132.8-133.8 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.13 (dd, 2H, J = 7.7 Hz, 2.7 Hz), 7.63 (d, 2H, J = 8.0 Hz), 7.60 (d, 2H, J = 8.4 Hz), 7.51 (d, 2H, J = 8.4 Hz), 7.48-7.43 (m, 3H), 7.41-7.33 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.3, 145.8, 135.6, 131.7, 131.5, 130.4, 129.6, 128.8, 128.7, 128.6, 127.2, 126.7, 126.4, 122.2; **MS** (70 eV, EI) *m/z* (%): 377 $[M+2]^+$ (27), 183 $[M]^+$ (31), 295 (5), 167 (14), 165 (46), 105 (100), 77 (74); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 1637 (w), 1489 (m), 1399 (m), 1070 (m); **HRMS** (MALDI) for **$C_{21}H_{15}BrNO$**, **$[M+H]^+$** (376.0337) found: 376.0349.

4-(4-bromophenyl)-5-(*tert*-butyl)-2-phenyloxazole (1ce):



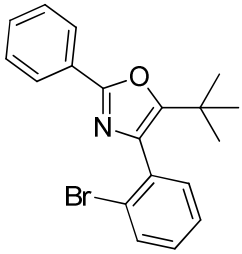
White solid; R_f 0.21 (ethyl acetate/hexanes: 1/20); mp.: 119.3-119.5 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.05 (dd, 2H, J = 8.0 Hz, 2.0 Hz), 7.53 (d, 2H, J = 8.2 Hz), 7.46-7.41 (m, 3H), 7.35 (d, 2H, J = 8.2 Hz), 1.32 (s, 9H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 158.4, 154.7, 134.1, 133.1, 131.8, 131.1, 130.0, 128.6, 127.5, 126.1, 122.1, 32.8, 29.8; **MS** (70 eV, EI) *m/z* (%): 357 $[M+2]^+$ (42), 355 $[M]^+$ (62), 342 (100), 340 (91), 261 (10), 190 (2), 167 (19), 157 (11), 115 (24), 105 (50), 89 (44), 57 (25); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3084 (w), 2959 (s), 1618 (m), 1486 (s), 1323 (m), 1067 (s), 690 (s); **HRMS** (FAB) for **$C_{19}H_{19}BrNO$**, **$[M+H]^+$** (356.0650) found: 356.0646.

4-(2-bromophenyl)-2,5-diphenyloxazole (1da):



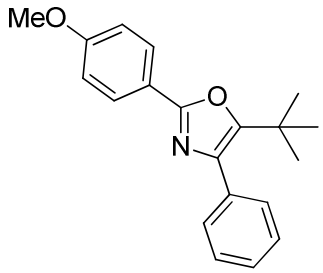
White solid; R_f 0.28 (ethyl acetate/hexanes: 1/20); mp.: 98.7-99.5 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.19-8.17 (m, 2H), 7.73 (d, 1H, J = 8.0 Hz), 7.54-7.48 (m, 6H), 7.43 (t, 1H, J = 7.5 Hz), 7.35-7.28 (m, 4H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 159.7, 146.5, 135.8, 134.2, 133.3, 132.1, 130.5, 130.3, 128.8, 128.7, 128.4, 128.3, 127.8, 127.3, 126.5, 125.1, 124.4; **MS** (70 eV, EI) *m/z* (%): 377 $[M+2]^+$ (14), 375 $[M]^+$ (16), 165 (64), 105 (98), 77 (100); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 2927 (m), 1630 (m), 1454 (m), 1248 (m), 1025 (m), 688 (s); **HRMS** (MALDI) for **$C_{21}H_{15}BrNO$**, **$[M+H]^+$** (376.0337) found: 376.0343.

4-(2-bromophenyl)-5-(*tert*-butyl)-2-phenyloxazole (1de):



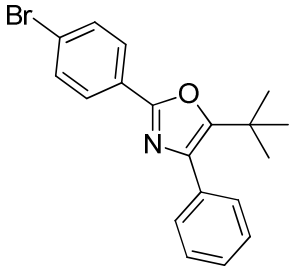
Colorless oil; R_f 0.34 (ethyl acetate/hexanes: 1/20); **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.08-8.06 (m, 2H), 7.64 (dd, 1H, J = 8.0 Hz, 1.0 Hz), 7.47-7.41 (m, 3H), 7.40 (dd, 1H, J = 7.5 Hz, 1.8 Hz), 7.34 (td, 1H, J = 7.4 Hz, 1.2 Hz), 7.27-7.21 (m, 1H), 1.26 (s, 9H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 158.6, 155.0, 135.5, 133.7, 132.6, 132.5, 130.0, 129.9, 128.6, 127.7, 126.9, 126.2, 125.5, 32.7, 29.2; **MS** (70 eV, EI) *m/z* (%): 357 $[M+2]^+$ (43), 355 $[M]^+$ (64), 342 (86), 340 (100), 261 (18), 246 (5), 190 (5), 183 (8), 158 (17), 156 (14), 130 (33), 105 (98), 77 (61); **IR** (CH_2Cl_2) $\tilde{\nu}$ (cm^{-1}): 3045 (m), 2923 (s), 1603 (w), 1487 (s), 1368 (m), 1113 (m); **HRMS** (FAB) for **$C_{19}H_{19}BrNO$**, **$[M+H]^+$** (356.0650) found: 356.0641.

5-(*tert*-butyl)-2-(4-methoxyphenyl)-4-phenyloxazole (1ee):



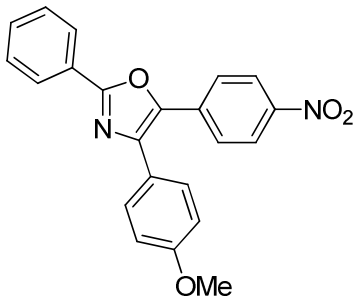
White solid; R_f 0.17 (ethyl acetate/hexanes: 1/20); mp.: 93.8-94.8 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.99 (d, 2H, J = 8.8 Hz), 7.47 (dd, 2H, J = 8.0 Hz, 1.5 Hz), 7.40-7.32 (m, 3H), 6.95 (d, 2H, J = 8.8 Hz), 3.84 (s, 3H), 1.31 (s, 9H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 161.0, 159.2, 153.8, 134.9, 134.3, 130.1, 127.9, 127.8, 127.7, 120.6, 114.0, 55.3, 32.7, 29.9; **MS** (70 eV, EI) *m/z* (%): 307 $[M]^+$ (33), 292 (100), 264 (1), 135 (29), 115 (9), 89 (14), 57 (10); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3076 (w), 2974 (m), 1614 (s), 1503 (s), 1463 (m), 1254 (s), 1020 (m); **HRMS** (MALDI) for **$C_{20}H_{22}NO_2$**, **$[M+H]^+$** (308.1650) found: 308.1663.

2-(4-bromophenyl)-5-(*tert*-butyl)-4-phenyloxazole (1fe):



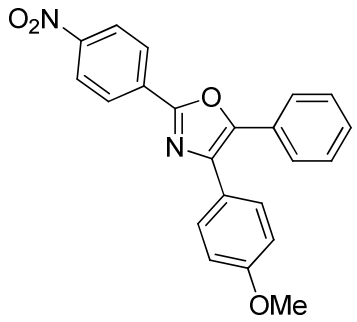
White solid; R_f 0.3 (ethyl acetate/hexanes: 1/20); mp.: 66.6 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.91 (d, 2H, J = 8.5 Hz), 7.56 (d, 2H, J = 8.4 Hz), 7.46 (d, 2H, J = 7.8 Hz), 7.42-7.33 (m, 3H), 1.31 (s, 9H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 157.3, 154.8, 135.4, 133.9, 131.8, 130.0, 128.0, 127.9, 127.5, 126.6, 124.2, 32.7, 29.8; **MS** (70 eV, EI) *m/z* (%): 357 $[M+2]^+$ (70), 355 $[M]^+$ (53), 342 (100), 340 (91), 261 (22), 190 (2), 183 (35), 155 (8), 115 (13), 89 (33); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3046 (w), 2967 (m), 1629 (m), 1491 (w), 1478 (m), 1340 (m), 1112 (m), 703 (s); **HRMS** (MALDI) for **$C_{19}H_{19}BrNO$**, **$[M+H]^+$** (356.0650) found: 356.0661.

4-(4-methoxyphenyl)-5-(4-nitrophenyl)-2-phenyloxazole (1bc):



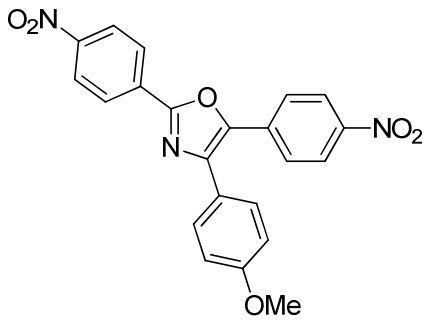
Yellow solid; R_f 0.18 (ethyl acetate/hexanes: 1/50); mp.: 184.6-185.1 °C; **^{1}H-NMR** (500 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.21 (d, 2H, J = 8.9 Hz), 8.18-8.16 (m, 2H), 7.83 (d, 2H, J = 9.0 Hz), 7.62 (d, 2H, J = 8.8 Hz), 7.52-7.50 (m, 3H), 6.99 (d, 2H, J = 8.8 Hz), 3.88 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 161.3, 160.4, 146.8, 142.7, 140.2, 135.1, 131.0, 129.8, 128.9, 126.8, 126.7, 126.0, 124.1, 124.1, 114.4, 55.4; **MS** (70 eV, EI) *m/z* (%): 372 $[M]^+$ (52), 359 (11), 327 (25), 298 (11), 267 (55), 240 (23), 134 (41), 98 (100); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3046 (w), 2930 (w), 1601 (m), 1543 (m), 1514 (m), 1336 (s), 1254 (m), 1107 (m); **HRMS** (MALDI) for **$C_{22}H_{17}N_2O_4$**, **$[M+H]^+$** (373.1188) found: 373.1198.

4-(4-methoxyphenyl)-2-(4-nitrophenyl)-5-phenyloxazole (1'bc):



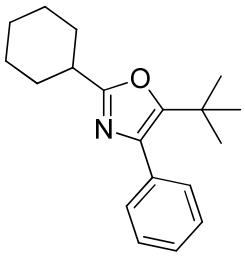
Yellow soild; R_f 0.2 (ethyl acetate/hexanes: 1/50); mp.: 175.4-176.4 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.34 (d, 2H, J = 9.1 Hz), 8.31 (d, 2H, J = 9.1 Hz), 7.69 (dd, 2H, J = 8.2 Hz, 1.3 Hz), 7.65 (d, 2H, J = 8.7 Hz), 7.44-7.36 (m, 3H), 6.96 (d, 2H, J = 8.7 Hz), 3.87 (s, 3H); **MS** (70 eV, EI) *m/z* (%): 372 $[M]^+$ (100), 298 (5), 195 (5), 181 (19), 152 (21), 119 (6), 105 (39), 77 (39); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (w), 2931 (w), 1600 (m), 1542 (m), 1512 (s), 1333 (s), 1253 (m), 1105 (m); **HRMS** (FAB) for **$C_{22}H_{17}N_2O_4$**, **$[M+H]^+$** (373.1188) found: 373.1188.

4-(4-methoxyphenyl)-2,5-bis(4-nitrophenyl)oxazole (9bc):



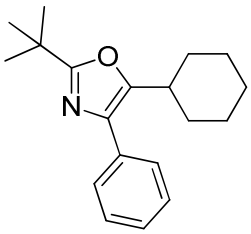
Yellow soild; R_f 0.13 (ethyl acetate/hexanes: 1/20); mp.: 264.5-265.1 °C; **^{1}H-NMR** (500 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.40 (d, 2H, J = 8.9 Hz), 8.36 (d, 2H, J = 9.0 Hz), 8.28 (d, 2H, J = 8.9 Hz), 7.90 (d, 2H, J = 8.8 Hz), 7.65 (d, 2H, J = 8.8 Hz), 7.04 (d, 2H, J = 8.8 Hz), 3.92 (s, 3H); **^{13}C-NMR** (125 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.6, 159.0, 149.0, 147.3, 144.1, 140.8, 134.5, 132.2, 129.7, 127.4, 126.5, 124.3, 124.2, 123.4, 114.6, 55.4; **MS** (70 eV, EI) *m/z* (%): 417 $[M]^+$ (100), 371 (9), 343 (4), 194 (11), 152 (42), 119 (17), 76 (31); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3107 (w), 2916 (w), 1611 (m), 1554 (m), 1512 (s), 1341 (s), 1250 (m), 1109 (m); **HRMS** (FAB) for **$C_{22}H_{16}N_3O_6$**, **$[M+H]^+$** (418.1039) found: 418.1037.

2-(*tert*-butyl)-5-cyclohexyl-4-phenyloxazole (1ge):



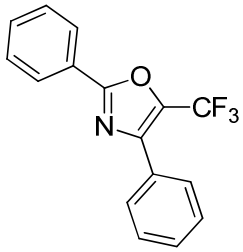
Colorlesssolid; R_f 0.24 (ethyl acetate/hexanes: 1/20); mp.: 38.5 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.39 (dd, 2H, J = 7.4 Hz, 1.6 Hz), 7.35-7.29 (m, 3H), 2.77 (tt, 1H, J = 11.4 Hz, 3.6 Hz), 2.09 (dd, 1H, J = 13.0 Hz, 2.7 Hz), 1.81 (dt, 2H, J = 12.9 Hz, 3.5 Hz), 1.71-1.68 (m, 1H), 1.60 (qd, 2H, J = 12.1 Hz, 3.0 Hz), 1.41-1.25 (m, 3H), 1.23 (s, 9H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 164.6, 153.2, 134.4, 133.0, 130.2, 127.7, 127.6, 37.4, 32.5, 30.6, 29.8, 25.8, 25.7; **MS** (70 eV, EI) *m/z* (%): 283 $[M]^+$ (61), 268 (95), 228 (28), 215 (100), 212 (8), 186 (11), 158 (15), 143 (9), 131 (16), 115 (14), 91 (21), 89 (23), 77 (14), 57 (30), 55 (71); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3069 (w), 2931 (s), 2855 (m), 1592 (w), 1566 (m), 1440 (m), 1101 (m), 697 (m); **HRMS** (EI) for **$C_{19}H_{25}NO$**, **$[M]^+$** (283.1936) found: 283.1938.

5-(*tert*-butyl)-2-cyclohexyl-4-phenyloxazole (1'ge):



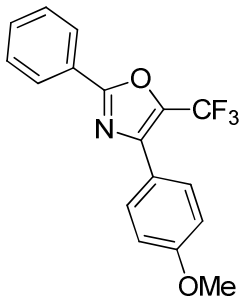
Colorlesssolid; R_f 0.39 (ethyl acetate/hexanes: 1/20); mp.: 58.3 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.59 (d, 2H, J = 7.2 Hz), 7.39 (t, 2H, J = 7.7 Hz), 7.27 (t, 1H, J = 7.7 Hz), 2.93 (tt, 1H, J = 11.7 Hz, 6.4 Hz), 1.89-1.78 (m, 4H), 1.74-1.55 (m, 3H), 1.40 (s, 9H), 1.38-1.28 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 168.6, 151.0, 133.0, 132.5, 128.5, 127.3, 127.0, 35.5, 33.6, 31.4, 28.6, 26.2, 25.8; **MS** (70 eV, EI) *m/z* (%): 283 $[M]^+$ (83), 268 (31), 254 (3), 240 (31), 226 (19), 212 (9), 184 (4), 172 (6), 157 (15), 129 (10), 115 (17), 104 (8), 89 (17), 83 (30), 69 (17), 57 (55), 55 (100); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3053 (m), 2969 (m), 2924 (s), 2847 (m), 1600 (w), 1497 (w), 1444 (m), 1162 (m); **HRMS** (EI) for **$C_{19}H_{25}NO$**, **$[M]^+$** (283.1936) found: 283.1938.

2,4-diphenyl-5-(trifluoromethyl)oxazole (1ak):



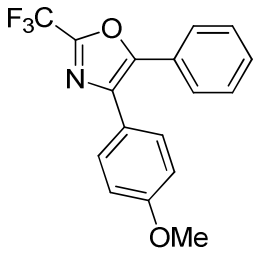
White solid; R_f0.50 (ethyl acetate/hexanes: 1/20); mp.: 49.8-50.6 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.15 (dd, 2H, J = 7.8 Hz, 1.7 Hz), 7.77 (dd, 2H, J = 8.0 Hz, 1.6 Hz), 7.56-7.49 (m, 3H), 7.49-7.42 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 161.7, 142.5 (quart, J = 2.5 Hz), 133.5 (quart, J = 42.6 Hz), 131.6, 129.6, 129.4, 128.9, 128.6, 128.5 (quart, J = 1.6 Hz), 127.1, 126.1, 119.8 (quart, J = 267.9 Hz); **MS** (70 eV, EI) *m/z* (%): 289 $[M]^+$ (100), 270 (6), 220 (67), 192 (60), 165 (21), 108 (10), 103 (36), 89 (85), 63 (45); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3061 (w), 1608 (m), 1497 (m), 1448 (m), 1383 (s), 1204 (s); **HRMS** (ESI) for **$C_{16}H_{11}F_3NO$**, **$[M+H]^+$** (290.0793) found: 290.0779.

4-(4-methoxyphenyl)-2-phenyl-5-(trifluoromethyl)oxazole (1bk):



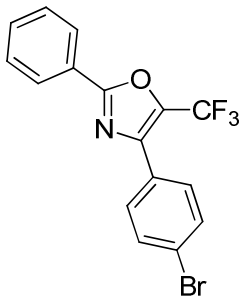
White solid; R_f0.14 (ethyl acetate/hexanes: 1/20); mp.: 69.7-70.7 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.14 (dd, 2H, J = 7.9 Hz, 1.5 Hz), 7.73 (d, 2H, J = 8.8 Hz), 7.54-7.47 (m, 3H), 6.99 (d, 2H, J = 8.7 Hz), 3.86 (s, 3H); **^{13}C-NMR** (125 MHz, $CDCl_3$, 25 °C) δ/ppm: 161.5, 160.6, 142.3 (quart, J = 2.6 Hz), 132.7 (quart, J = 42.6 Hz), 131.5, 129.9 (quart, J = 1.8 Hz), 128.9, 127.1, 126.1, 121.8, 120.0 (quart, J = 267.6 Hz), 114.1, 55.3; **MS** (70 eV, EI) *m/z* (%): 319 $[M]^+$ (100), 301 (5), 251 (5), 223 (18), 189 (35), 145 (8), 119 (10), 76 (5); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3061 (w), 2926 (w), 1624 (m), 1509 (w), 1390 (m), 1307 (w), 1110 (m); **HRMS** (MALDI) for **$C_{17}H_{13}F_3NO_2$**, **$[M+H]^+$** (320.0898) found: 320.0910.

4-(4-methoxyphenyl)-5-phenyl-2-(trifluoromethyl)oxazole (1'bk):



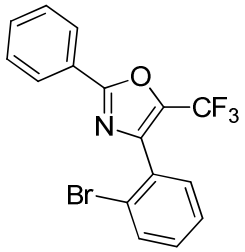
White solid; R_f0.25 (ethyl acetate/hexanes: 1/20); mp.: 105.9-106.4 °C;**H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.14 (dd, 2H, J = 7.7 Hz, 1.8 Hz), 7.73 (d, 2H, J = 8.8 Hz), 7.57-7.45 (m, 3H), 7.00 (d, 2H, J = 8.8 Hz), 3.86 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.1, 149.0 (quart, J = 43.8 Hz), 147.2, 135.9, 129.6, 129.4, 128.9, 127.5, 127.0, 123.1, 116.7 (quart, J = 270.7 Hz), 114.2, 55.3; **MS** (70 eV, EI) *m/z* (%): 319 $[M]^+$ (100), 276 (86), 229 (12), 223 (39), 182 (14), 153 (41), 119 (5), 105 (15), 77 (17); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3008 (w), 2924 (m), 1615 (w), 1512 (m), 1448 (m), 13352 (m), 1150 (s); **HRMS** (FAB) for **$C_{17}H_{12}F_3NO_2$**, **$[M]^+$** (319.0820) found: 319.0828.

4-(4-bromophenyl)-2-phenyl-5-(trifluoromethyl)oxazole (1ck):



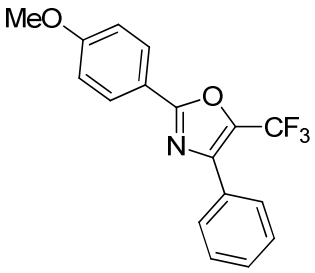
White solid; R_f0.58 (ethyl acetate/hexanes: 1/20); mp.: 66.2-67.2 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.13 (dd, 2H, J = 7.7 Hz, 1.3 Hz), 7.65 (d, 2H, J = 8.6 Hz), 7.61 (d, 2H, J = 8.6 Hz), 7.55-7.48 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 161.8, 141.4 (quart, J = 2.4 Hz), 133.7 (quart, J = 42.9 Hz), 131.9, 131.8, 130.0 (quart, J = 1.6 Hz), 129.0, 128.3, 127.1, 125.9, 124.0, 119.7 (quart, J = 268.1 Hz); **MS** (70 eV, EI) *m/z* (%): 369 $[M+2]^+$ (73), 367 $[M]^+$ (91), 300 (9), 288 (26), 260 (32), 219 (6), 191 (30), 157 (45), 137 (20), 103 (54), 89 (81), 69 (100); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3061 (w), 1608 (m), 1490 (s), 1379 (s), 1204 (s), 1105 (s), 686 (m); **HRMS** (FAB) for **$C_{16}H_{10}BrF_3NO$**, **$[M+H]^+$** (367.9898) found: 367.9892.

4-(2-bromophenyl)-2-phenyl-5-(trifluoromethyl)oxazole (1dk):



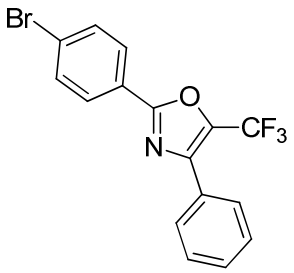
Colorless oil; R_f0.48 (ethyl acetate/hexanes: 1/20); **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.15 (d, 2H, J = 8.0 Hz), 7.70 (d, 1H, J = 8.0 Hz), 7.55-7.49 (m, 3H), 7.45-7.40 (m, 2H), 7.33 (td, 1H, J = 7.4 Hz, 2.6 Hz); **^{13}C-NMR** (125 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.1, 141.5 (quart, J = 2.3 Hz), 135.3 (quart, J = 42.5 Hz), 133.1, 131.8, 131.6, 131.1, 130.9, 129.0, 127.24, 127.2, 125.9, 123.6, 119.2 (quart, J = 268.2 Hz); **MS** (70 eV, EI) *m/z* (%): 369 $[M+2]^+$ (62), 367 $[M]^+$ (77), 298 (6), 288 (100), 287 (86), 270 (24), 219 (12), 191 (35), 157 (35), 144 (39), 137 (19), 89 (14), 77 (8); **IR** (CH_2Cl_2) $\tilde{\nu}$ (cm^{-1}): 3045 (w), 1606 (m), 1484 (m), 1387 (s), 1197 (s); **HRMS** (FAB) for **$C_{16}H_{10}BrF_3NO$**, **$[M+H]^+$** (367.9898) found: 367.9899.

2-(4-methoxyphenyl)-4-phenyl-5-(trifluoromethyl)oxazole (1ek):



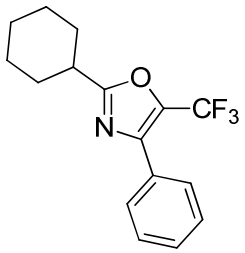
White solid; R_f0.50 (ethyl acetate/hexanes: 1/20); mp.: 73.5-74.1 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.07 (d, 2H, J = 8.9 Hz), 7.76 (dd, 2H, J = 7.9 Hz, 1.3 Hz), 7.48-7.40 (m, 3H), 6.98 (d, 2H, J = 8.9 Hz), 3.84 (s, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 162.3, 161.8, 142.3 (quart, J = 2.4 Hz), 132.9 (quart, J = 42.6 Hz), 129.5, 129.4, 128.9, 128.5, 128.4 (quart, J = 1.8 Hz), 119.9 (quart, J= 267.7 Hz), 118.7, 114.3, 55.4; **MS** (70 eV, EI) *m/z* (%): 319 $[M]^+$ (100), 250 (27), 222 (64), 186 (9), 133 (33), 89 (83), 63 (28); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3015 (w), 2840 (w), 1615 (s), 1501 (s), 1375 (s), 1253 (s), 1116 (s); **HRMS** (ESI) for **$C_{17}H_{13}F_3NO_2$**, **$[M+H]^+$** (320.0898) found: 320.0887.

2-(4-bromophenyl)-4-phenyl-5-(trifluoromethyl)oxazole (1fk):



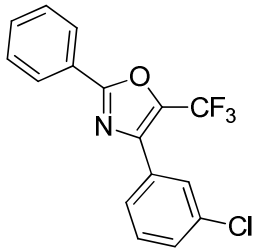
White solid; R_f0.38 (ethyl acetate/hexanes: 1/20); mp.: 61.1-61.7 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.04 (d, 2H, J = 8.6 Hz), 7.79 (dd, 2H, J = 7.9 Hz, 2.0 Hz), 7.68 (d, 2H, J = 8.6 Hz), 7.54-7.47 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.8, 142.6 (quart, J = 2.5 Hz), 133.7 (quart, J = 42.9Hz), 132.3, 129.7, 128.6, 128.5, 128.4 (quart, J = 1.5 Hz), 128.0, 126.4, 124.9, 119.7 (quart, J = 268.0 Hz); **MS** (70 eV, EI) *m/z* (%): 369 $[M+2]^+$ (43), 367 $[M]^+$ (53), 300 (52), 298 (62), 270 (35), 260 (17), 219 (25), 214 (41), 191 (62), 183 (100), 181 (48), 165 (35), 158 (18), 102 (27), 89 (38), 69 (31); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3046 (w), 1604 (s), 1501 (m), 1379 (s), 1204 (s), 1120 (s), 682 (m); **HRMS** (FAB) for **$C_{16}H_{10}BrF_3NO$**, **$[M+H]^+$** (367.9898) found: 367.9894.

2-cyclohexyl-4-phenyl-5-(trifluoromethyl)oxazole (1gk):



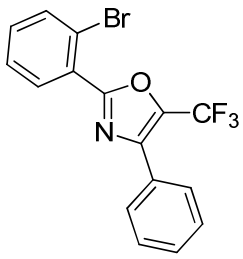
Colorless oil; R_f0.60 (ethyl acetate/hexanes: 1/20); **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.68 (dd, 2H, J = 8.0 Hz, 1.8 Hz), 7.46-7.37 (m, 3H), 2.89 (tt, 1H, J = 11.4 Hz, 7.3 Hz), 2.13 (dd, 2H, J = 13.2 Hz, 2.2 Hz), 1.86 (dt, 2H, J = 13.1 Hz, 3.7 Hz), 1.75-1.71 (m, 1H), 1.68-1.59 (m, 2H), 1.46-1.26 (m, 3H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 168.7, 141.0 (quart, J = 2.6 Hz), 133.0 (quart, J = 42.5 Hz), 129.5, 129.3, 128.5, 128.4 (quart, J = 1.8 Hz), 119.8 (quart, J = 267.7 Hz), 37.5, 30.4, 25.6, 25.5; **MS** (70 eV, EI) *m/z* (%): 295 $[M]^+$ (17), 276 (10), 240 (29), 227 (78), 212 (9), 198 (26), 184 (5), 170 (17), 115 (21), 104 (12), 89 (39), 69 (20), 55 (100); **IR** (CH_2Cl_2) $\tilde{\nu}$ (cm^{-1}): 3047 (m), 2934 (s), 1597 (m), 1496 (w), 1389 (m), 1134 (s); **HRMS** (EI) for **$C_{16}H_{16}F_3NO$**, **$[M]^+$** (295.1184) found: 295.1185.

4-(3-chlorophenyl)-2-phenyl-5-(trifluoromethyl)oxazole (1hk):

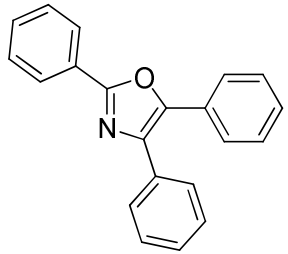


White solid; R_f0.40 (ethyl acetate/hexanes: 1/20); mp.: 51.2-51.8 °C; **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.14 (d, 2H, J = 7.0 Hz), 7.81 (s, 1H), 7.64 (d, 1H, J = 6.8 Hz), 7.58-7.47 (m, 3H), 7.45-7.37 (m, 2H); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 161.9, 141.1 (quart, J = 2.4 Hz), 134.7, 134.0 (quart, J = 43.0 Hz), 131.8, 131.1, 129.8, 129.7, 129.0, 128.6 (quart, J = 1.5 Hz), 127.1, 126.6 (quart, J = 2.0 Hz), 125.8, 119.6 (q, J = 268.2 Hz); **MS** (20 eV, EI) *m/z* (%): 325 $[M+2]^+$ (33), 323 $[M]^+$ (100), 288 (26), 254 (55), 226 (39), 191 (28), 157 (18), 123 (51), 89 (16), 63 (7); **IR** (KBr) $\tilde{\nu}$ (cm^{-1}): 3061 (w), 1608 (w), 1493 (w), 1383 (s), 1280 (m), 1200 (s), 686 (s); **HRMS** (FAB) for **$C_{16}H_{10}ClF_3NO$**, **$[M+H]^+$** (324.0403) found: 324.0402.

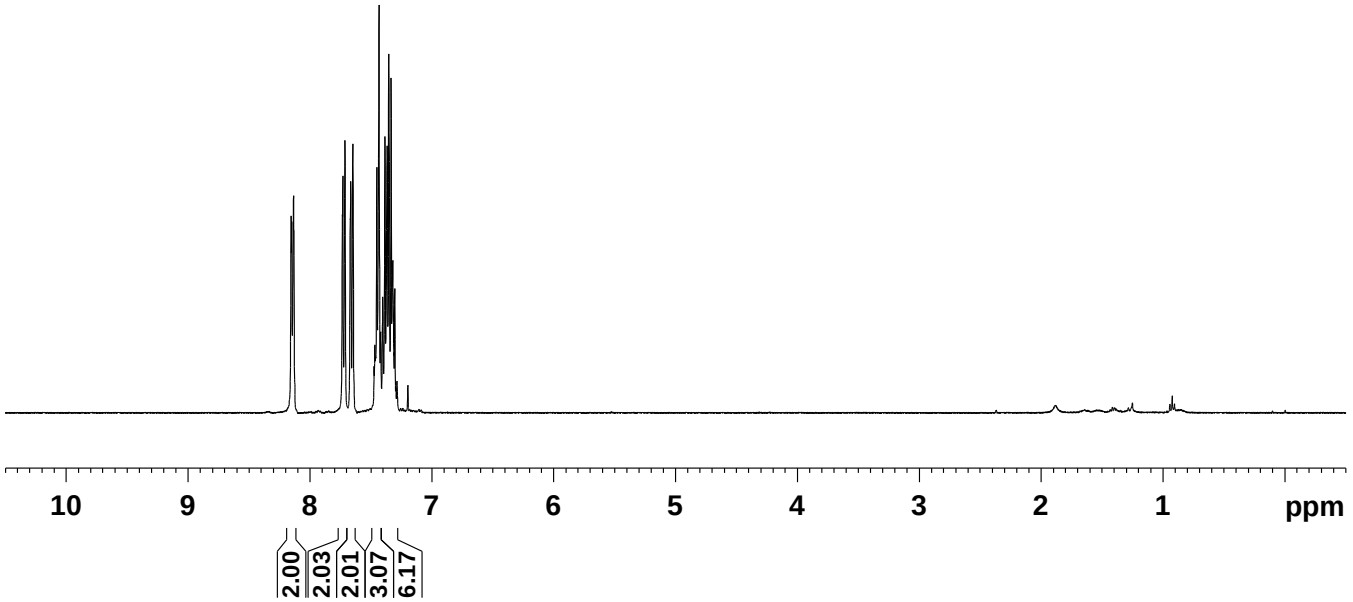
2-(2-bromophenyl)-4-phenyl-5-(trifluoromethyl)oxazole (1ik):



Colorless oil; R_f0.35 (ethyl acetate/hexanes: 1/20); **^{1}H-NMR** (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.02 (dd, 1H, J = 7.8 Hz, 1.5 Hz), 7.80 (d, 2H, J = 6.6 Hz), 7.73 (d, 1H, J = 8.0 Hz), 7.49-7.39 (m, 4H), 7.33 (td, 1H, J = 7.7 Hz, 1.6 Hz); **^{13}C-NMR** (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 160.2, 142.1 (quart, J = 2.8 Hz), 134.7, 133.9 (quart, J = 42.9 Hz), 132.2, 131.7, 129.6, 129.1, 128.6, 128.5 (quart, J = 1.4 Hz), 127.4, 127.0, 121.6, 119.7 (quart, J = 268.3 Hz); **MS** (70 eV, EI) *m/z* (%): 369 $[M+2]^+$ (100), 367 $[M]^+$ (96), 350 (5), 298 (39), 288 (29), 272 (21), 219 (23), 214 (66), 191 (48), 183 (44), 158 (19), 108 (30), 89 (85), 63 (29); **IR** (CH_2Cl_2) $\tilde{\nu}$ (cm^{-1}): 3047 (w), 1597 (s), 1493 (s), 1445 (s), 1389 (s), 1200 (s); **HRMS** (EI) for **$C_{16}H_9BrF_3NO$**, **$[M]^+$** (366.9820) found: 366.9816.



1aa



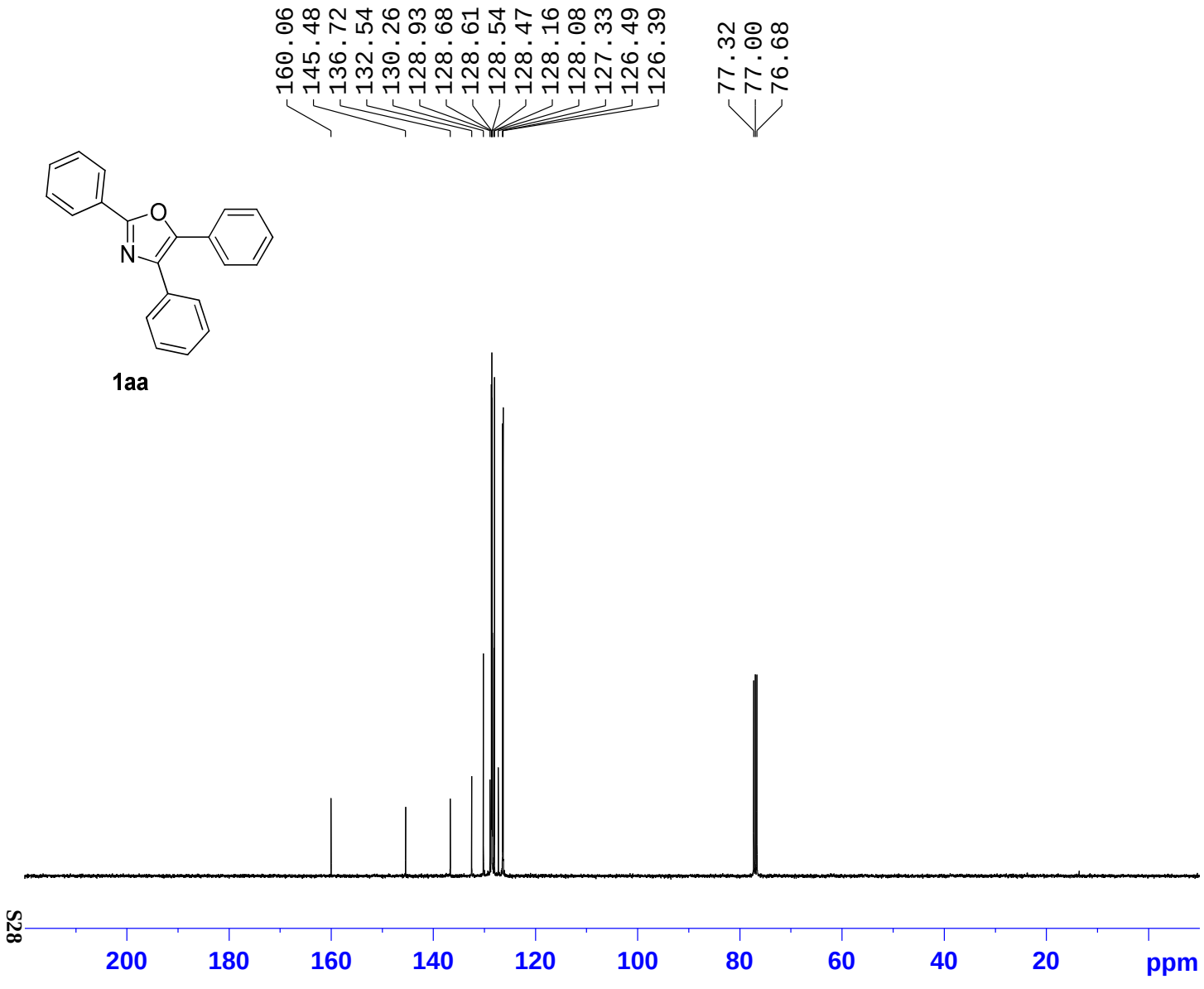

```
Current Data Parameters
NAME                  mina071
EXPNO                       5
PROCNO                      1

F2 - Acquisition Parameters
Date_                20121014
Time                    19.01
INSTRUM                 spect
PROBHD   5 mm BBO BB-1H
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          0
SWH                  7246.377 Hz
FIDRES               0.221142 Hz
AQ                   2.2611110 sec
RG                          4
DW                     69.000 usec
DE                      6.50 usec
TE                     299.3 K
D1                2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.90 usec
PL1                     3.00 dB
SFO1             400.1324008 MHz

F2 - Processing parameters
SI                      16384
SF               400.1300331 MHz
WDW                        EM
SSB          0
LB           0 Hz
GB           0
PC                      1.00
```

IV. ^{1}H NMR, ^{13}C NMR and X-ray of the substrates




```
Current Data Parameters
NAME                  mina071
EXPNO                       7
PROCNO                      1

F2 - Acquisition Parameters
Date_                20121014
Time                    19.07
INSTRUM                 spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                        455
DS                          0
SWH                 24038.461 Hz
FIDRES               0.733596 Hz
AQ                   0.6816452 sec
RG                      9195.2
DW                      20.800 usec
DE                       6.50 usec
TE                      299.4 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.40 usec
PL1                      7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                   90.00 usec
PL2                      3.00 dB
PL12                    20.70 dB
PL13                    23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF                100.6127819 MHz
WDW                        EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.00
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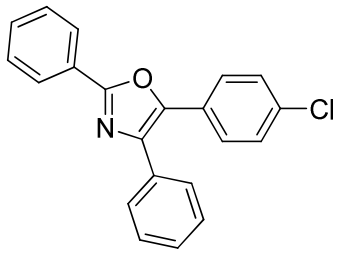
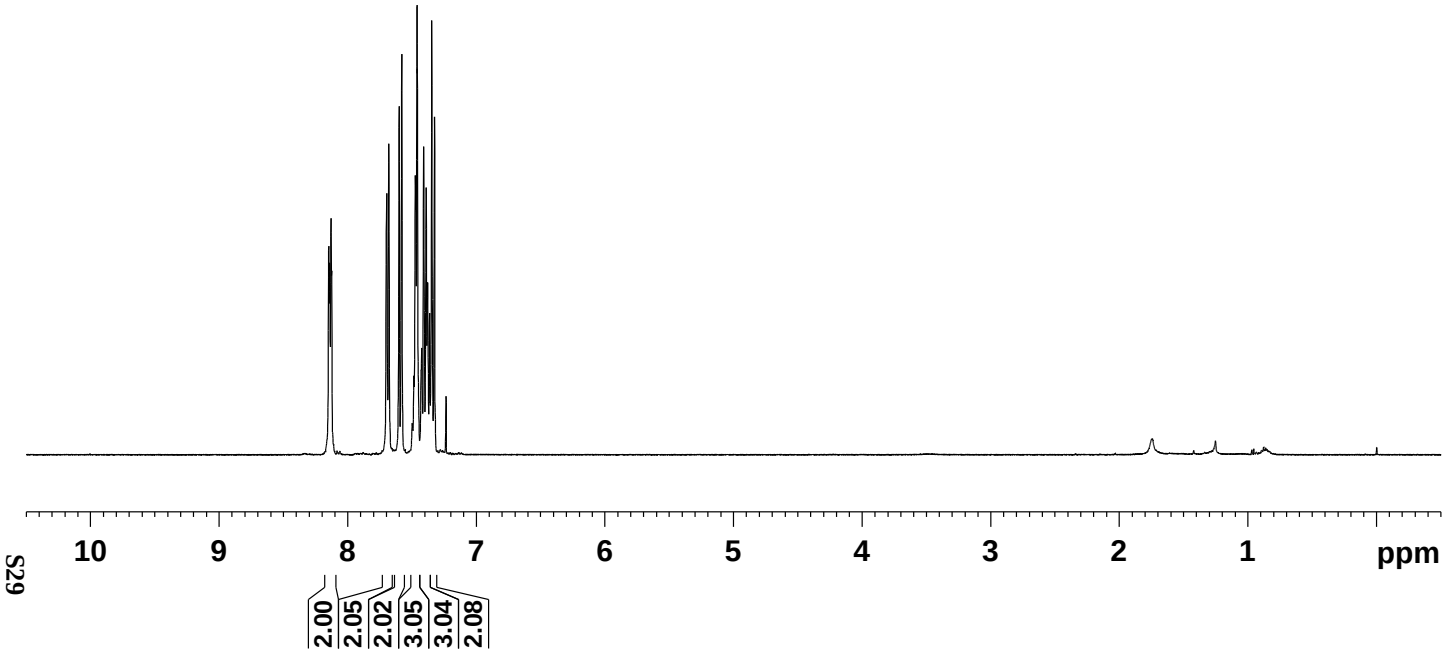


1ab

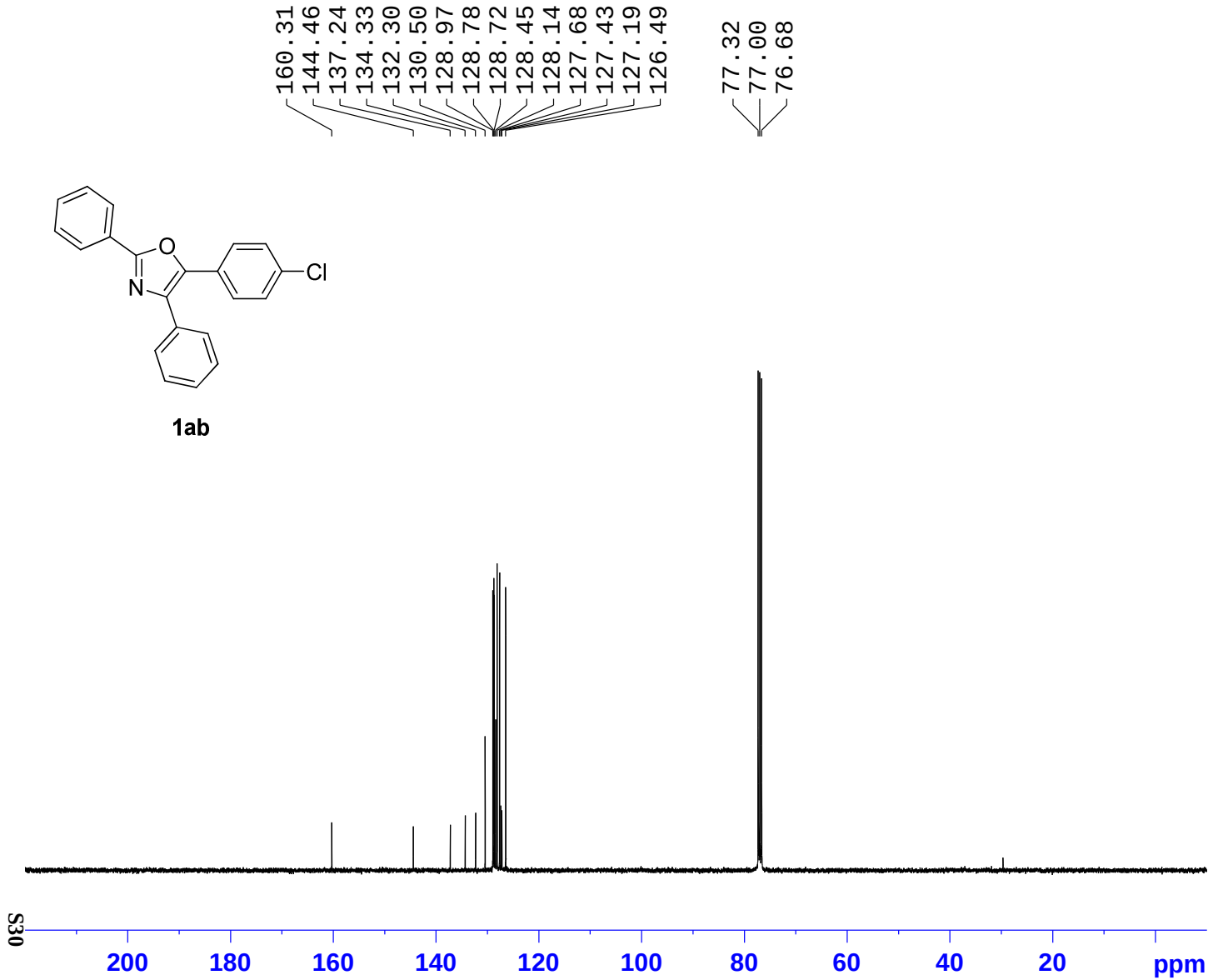



```
Current Data Parameters
NAME            mina070
EXPNO                 6
PROCNO                1

F2 - Acquisition Parameters
Date_          20121012
Time              21.24
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    4
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 90.5
DW               69.000 usec
DE                 6.50 usec
TE                299.3 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300186 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



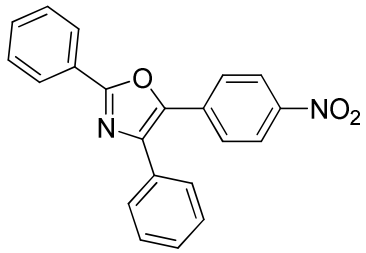

```
Current Data Parameters
NAME                  mina070
EXPNO                      11
PROCNO                      1

F2 - Acquisition Parameters
Date_               20121020
Time                    0.20
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                       1333
DS                          0
SWH                 24038.461 Hz
FIDRES               0.733596 Hz
AQ                   0.6816452 sec
RG                      9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     299.1 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

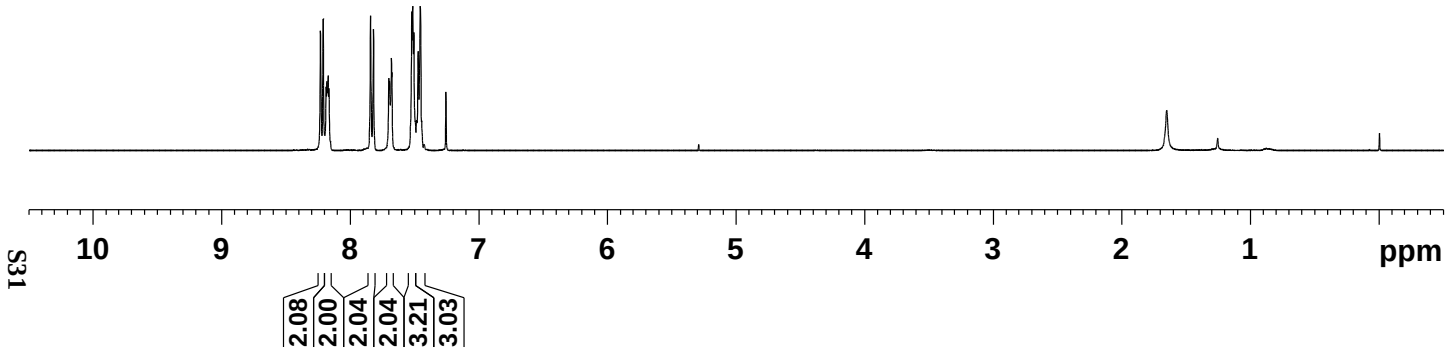
======== CHANNEL f1 ========
NUC1                      13C
P1                      9.40 usec
PL1                     7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  90.00 usec
PL2                     3.00 dB
PL12                   20.70 dB
PL13                   23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF               100.6127717 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.00
```



1ac



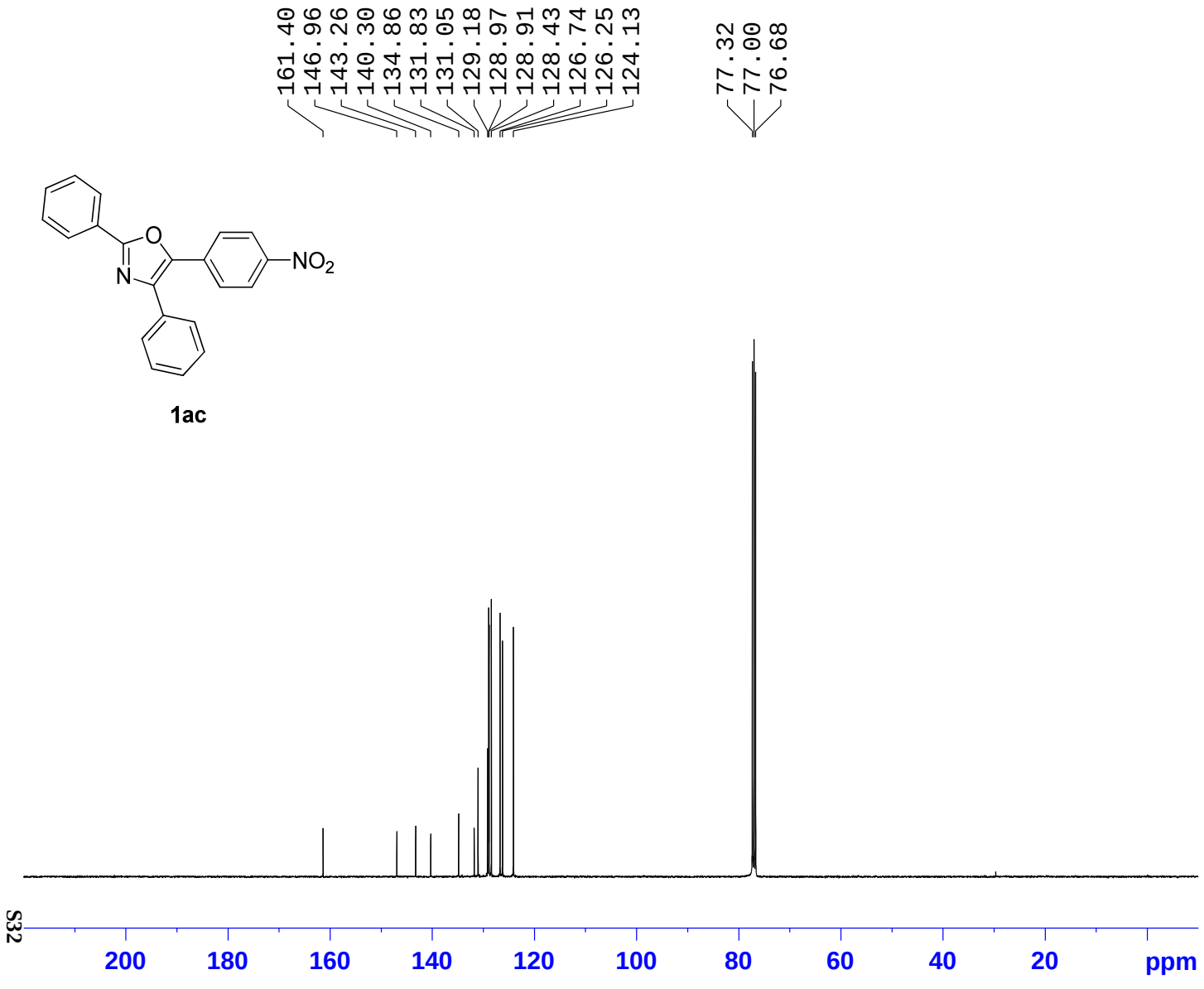
S31

```
Current Data Parameters
NAME            mina052
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20120905
Time              18.20
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  181
DW               69.000 usec
DE                6.50 usec
TE                298.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.70 usec
PL1                4.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300000 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



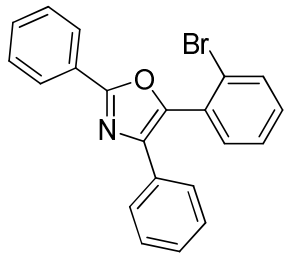

```
Current Data Parameters
NAME                  mina052
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_               20120911
Time                   23.16
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                       9913
DS                          0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     299.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

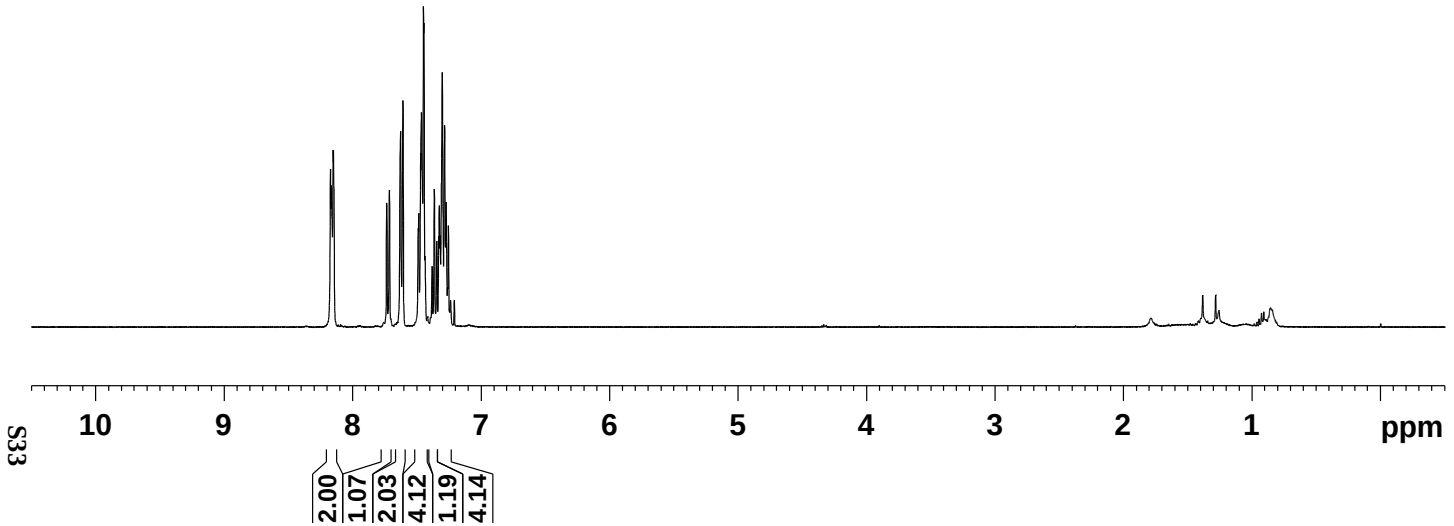
======== CHANNEL f1 ========
NUC1                      13C
P1                      8.90 usec
PL1                     7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  90.00 usec
PL2                     3.80 dB
PL12                   21.60 dB
PL13                   24.60 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF               100.6127716 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.00
```



1ad

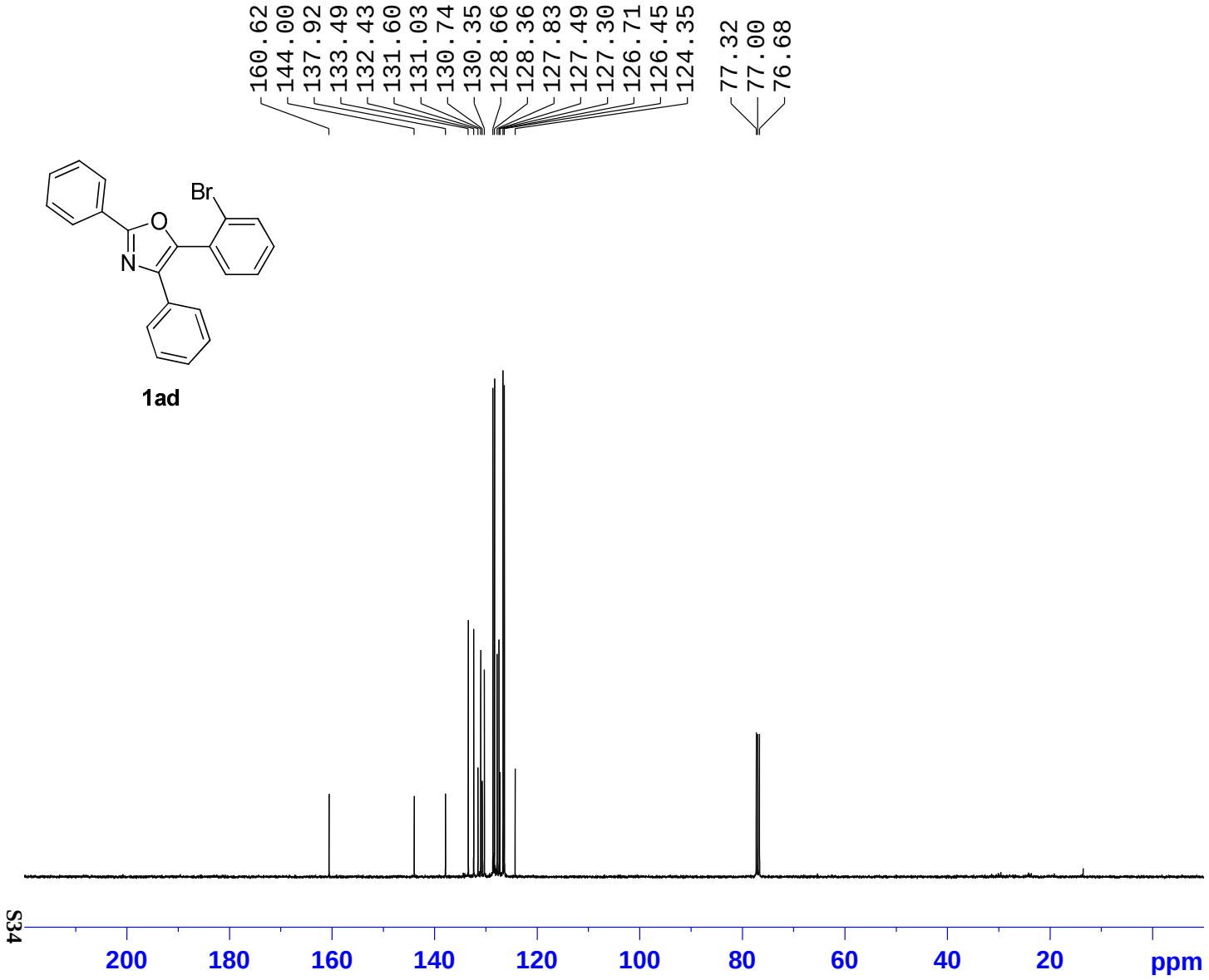



```
Current Data Parameters
NAME            mina072
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20121014
Time              18.42
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                    4
DW               69.000 usec
DE                6.50 usec
TE                299.5 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300282 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



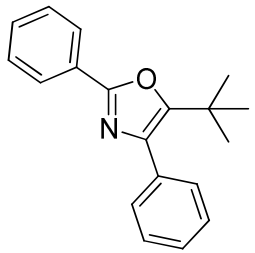

```
Current Data Parameters
NAME                 mina072
EXPNO                      9
PROCNO                     1

F2 - Acquisition Parameters
Date_               20121015
Time                   12.36
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                        317
DS                          0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     299.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

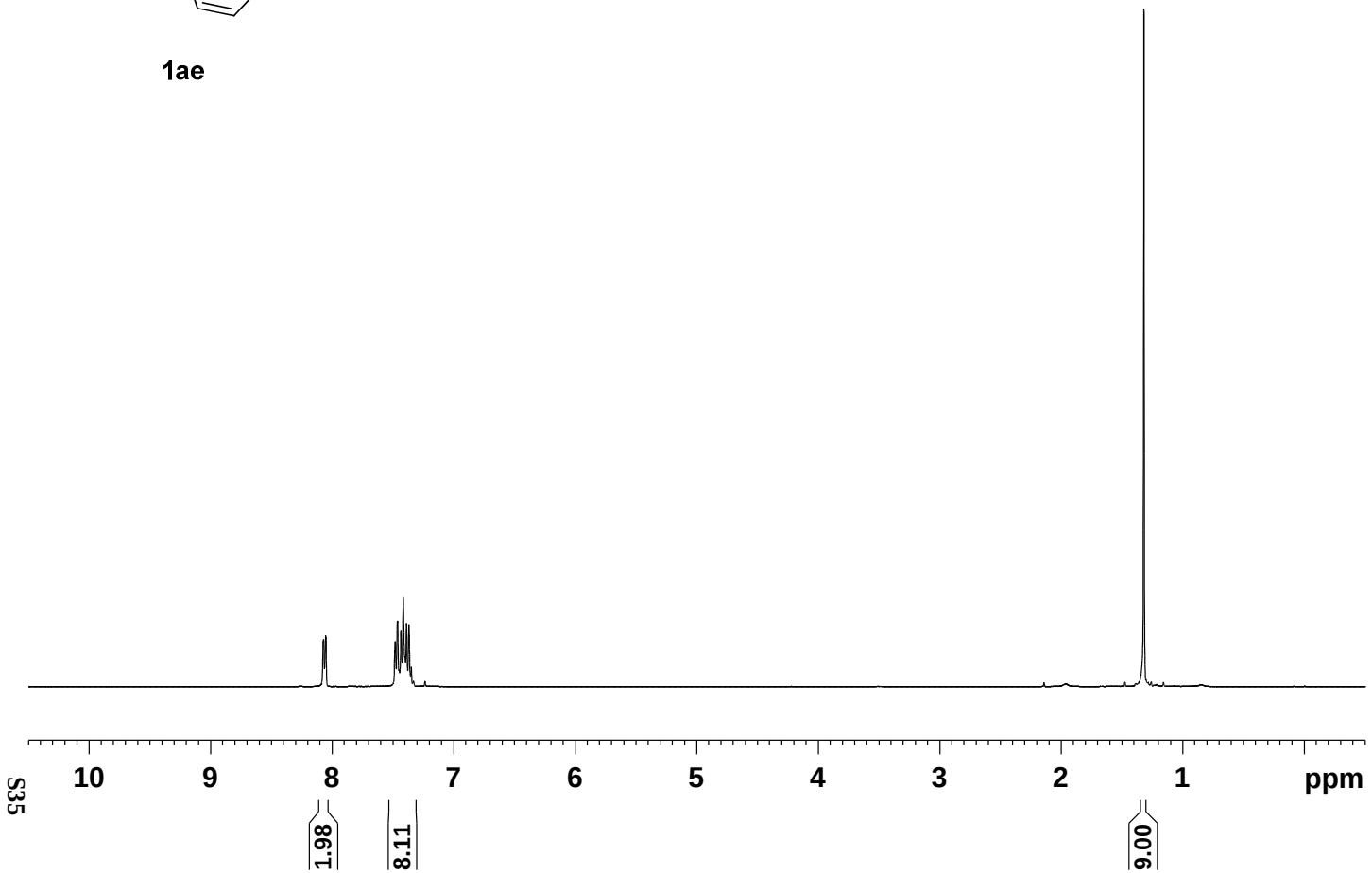
======== CHANNEL f1 ========
NUC1                      13C
P1                       9.40 usec
PL1                      7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                   90.00 usec
PL2                      3.00 dB
PL12                    20.70 dB
PL13                    23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF               100.6127902 MHz
WDW                        EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.00
```



1ae

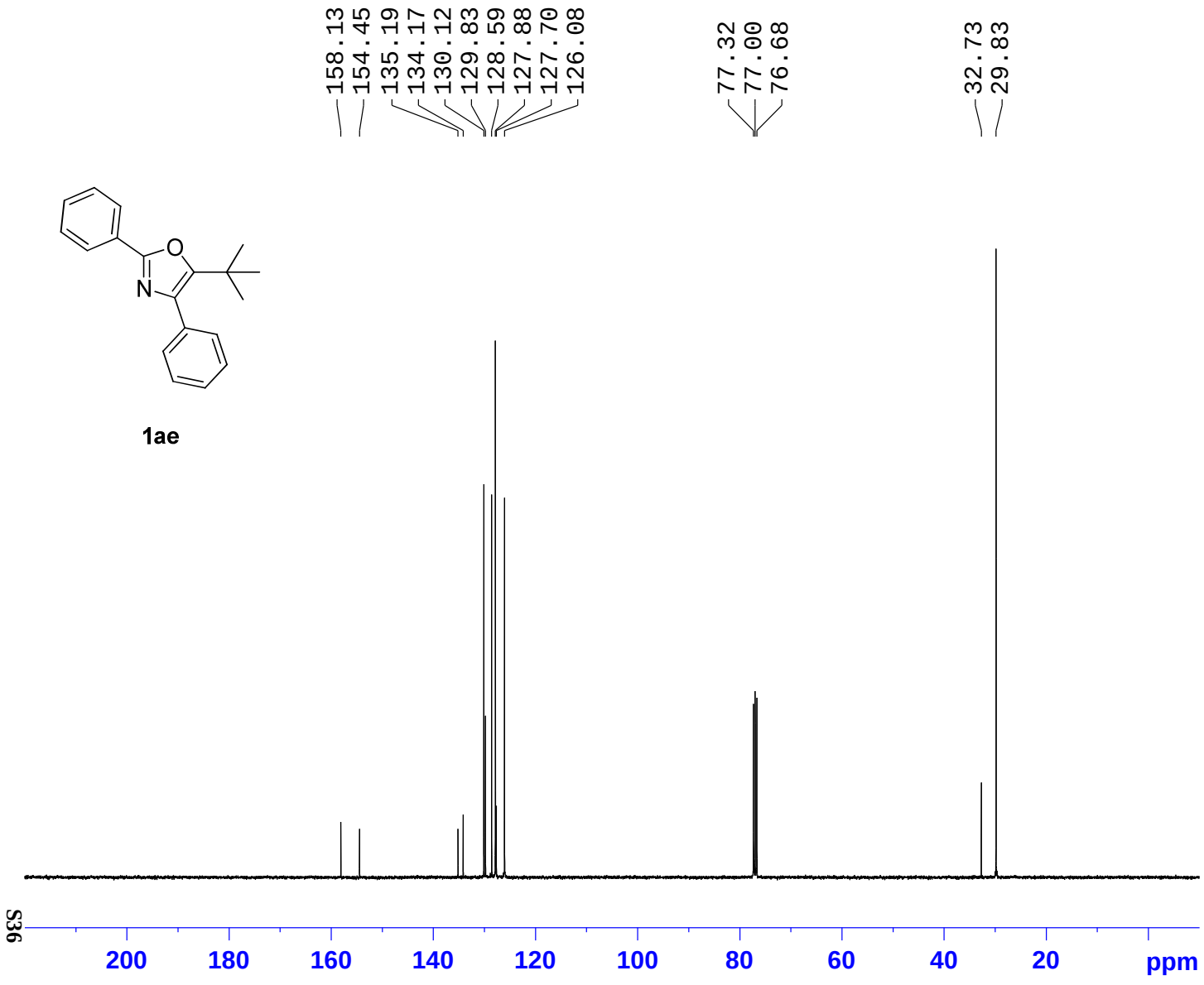



```
Current Data Parameters
NAME            mina054
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20121024
Time              22.34
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 35.9
DW                69.000 usec
DE                 6.50 usec
TE                298.4 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300189 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



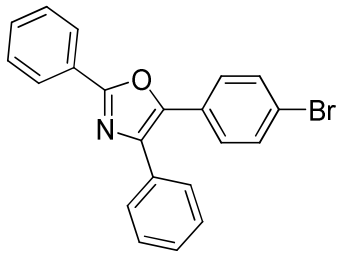

```
Current Data Parameters
NAME                 mina054
EXPNO                      9
PROCNO                     1

F2 - Acquisition Parameters
Date_              20121024
Time                  22.36
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      500
DS                        0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                0.6816452 sec
RG                   9195.2
DW                   20.800 usec
DE                    6.50 usec
TE                   298.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

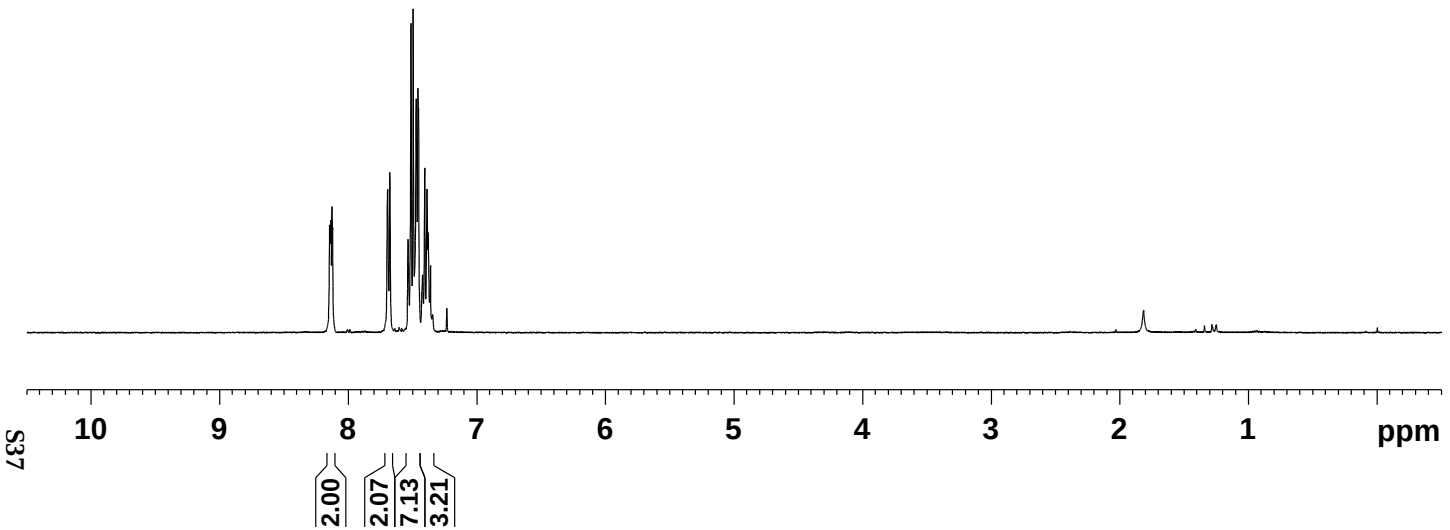
======== CHANNEL f1 ========
NUC1                    13C
P1                    9.40 usec
PL1                   7.00 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   3.00 dB
PL12                 20.70 dB
PL13                 23.70 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6127775 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```



1af

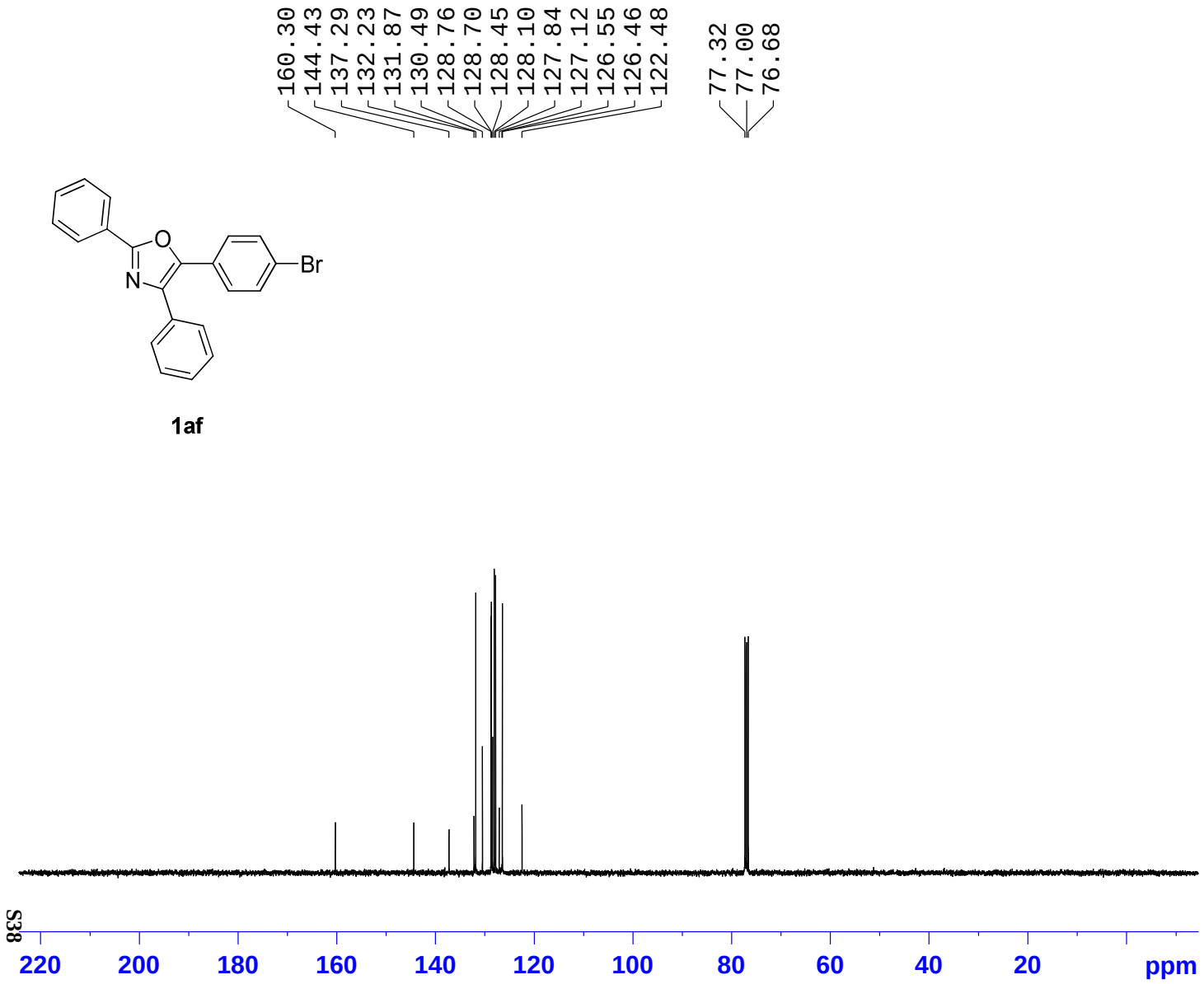



```
Current Data Parameters
NAME            mina051
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20120905
Time              18.24
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 90.5
DW                69.000 usec
DE                 6.50 usec
TE                298.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.70 usec
PL1                4.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300188 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



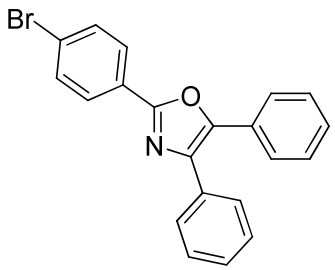

```
Current Data Parameters
NAME            mina051
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20120905
Time              18.30
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  206
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG               9195.2
DW                20.800 usec
DE                 6.50 usec
TE                298.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

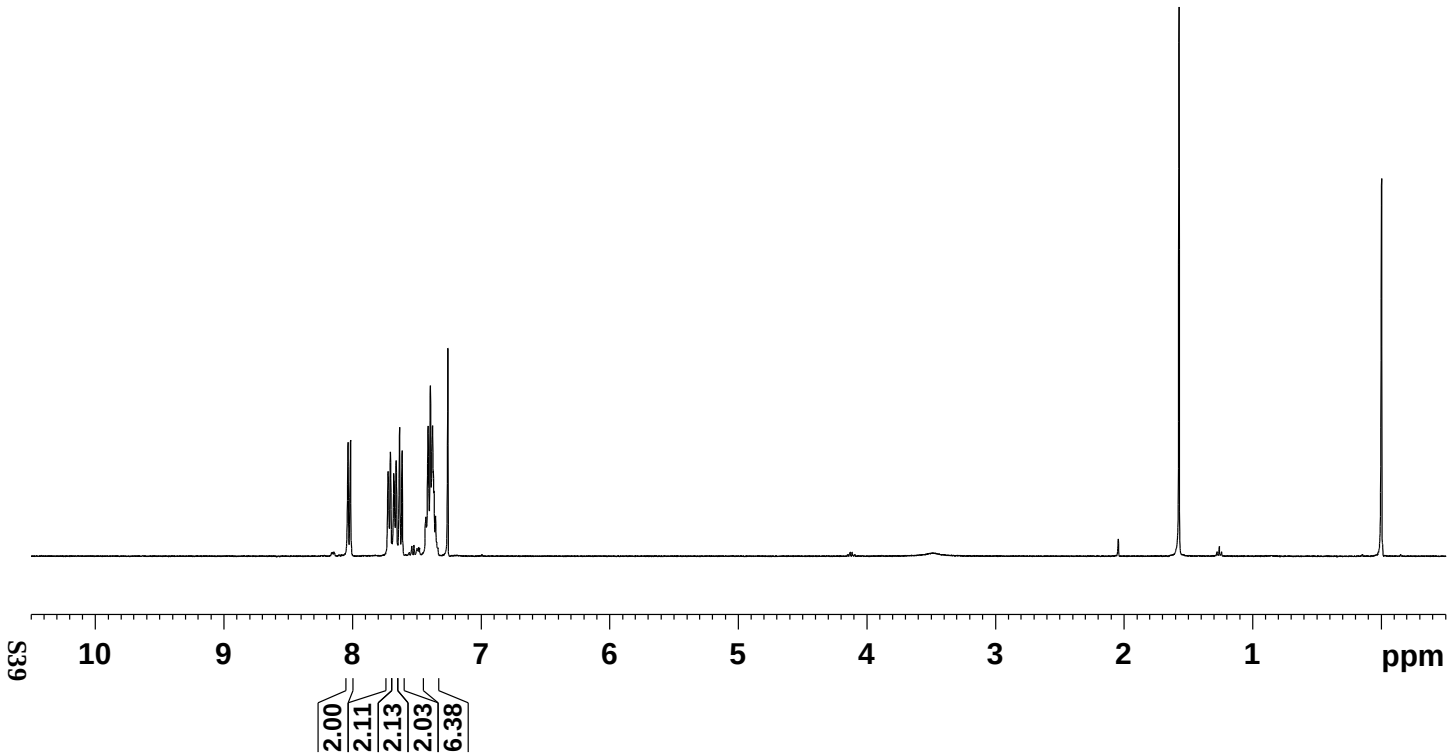
======== CHANNEL f1 ========
NUC1                13C
P1                 8.90 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2              90.00 usec
PL2                 3.80 dB
PL12               21.60 dB
PL13               24.60 dB
SFO2        400.1316005 MHz

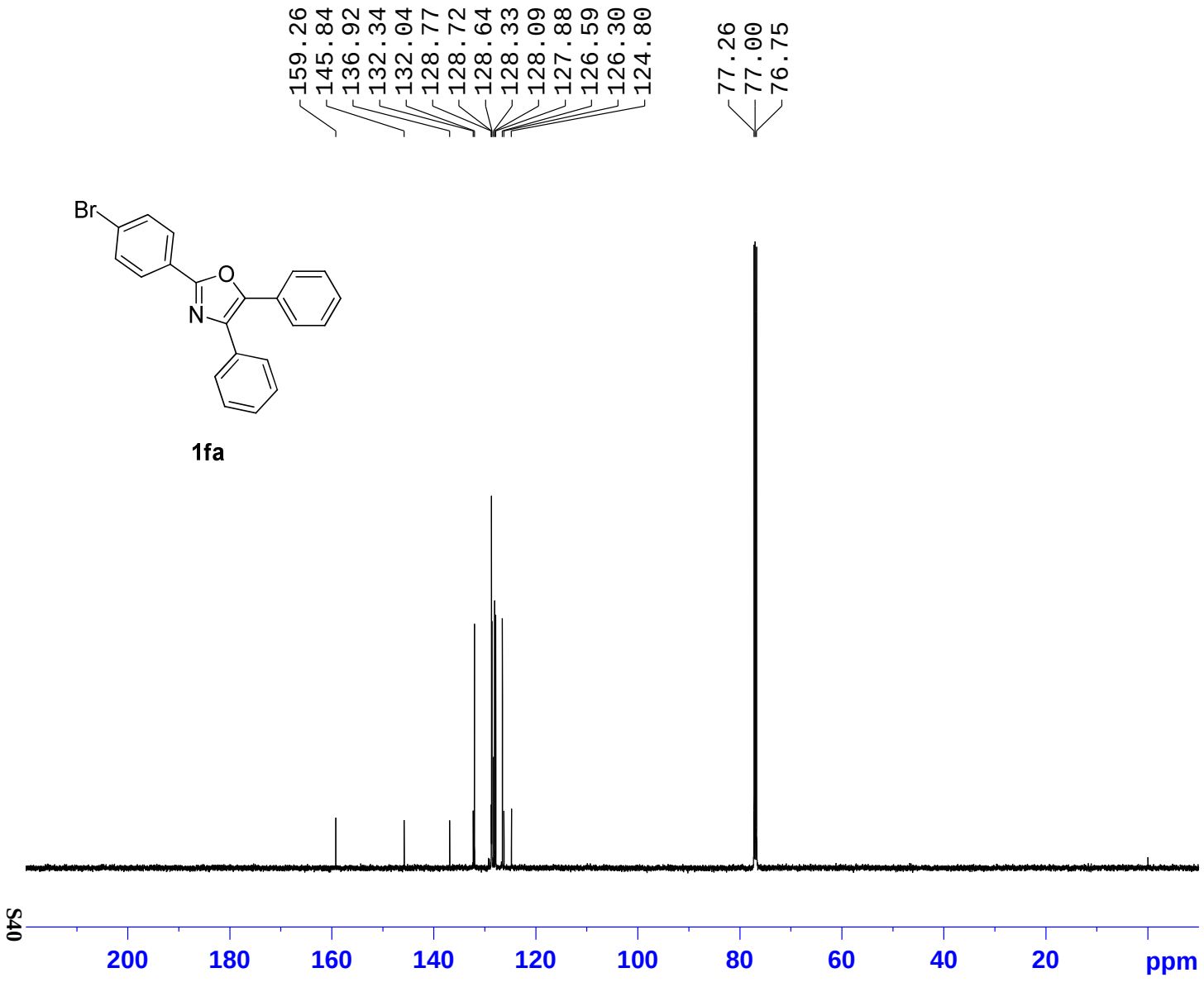
F2 - Processing parameters
SI                 32768
SF          100.6127767 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.00
```



1fa



NAME	mina084
EXPNO	6
PROCNO	1
Date_	20121113
Time	18.43
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	7246.377 Hz
FIDRES	0.221142 Hz
AQ	2.2611110 sec
RG	322.5
DW	69.000 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	11.90 usec
PL1	3.00 dB
SFO1	400.1324008 MHz
SI	16384
SF	400.1300092 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



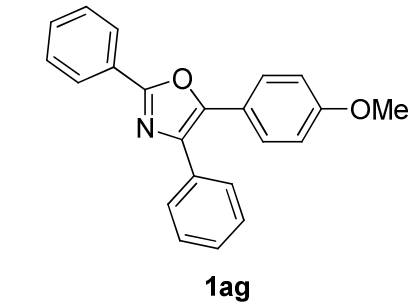

```
Current Data Parameters
NAME            mina084
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20121124
Time              14.01
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  667
DS                    0
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912410 sec
RG               9195.2
DW               16.650 usec
DE                6.50 usec
TE                297.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

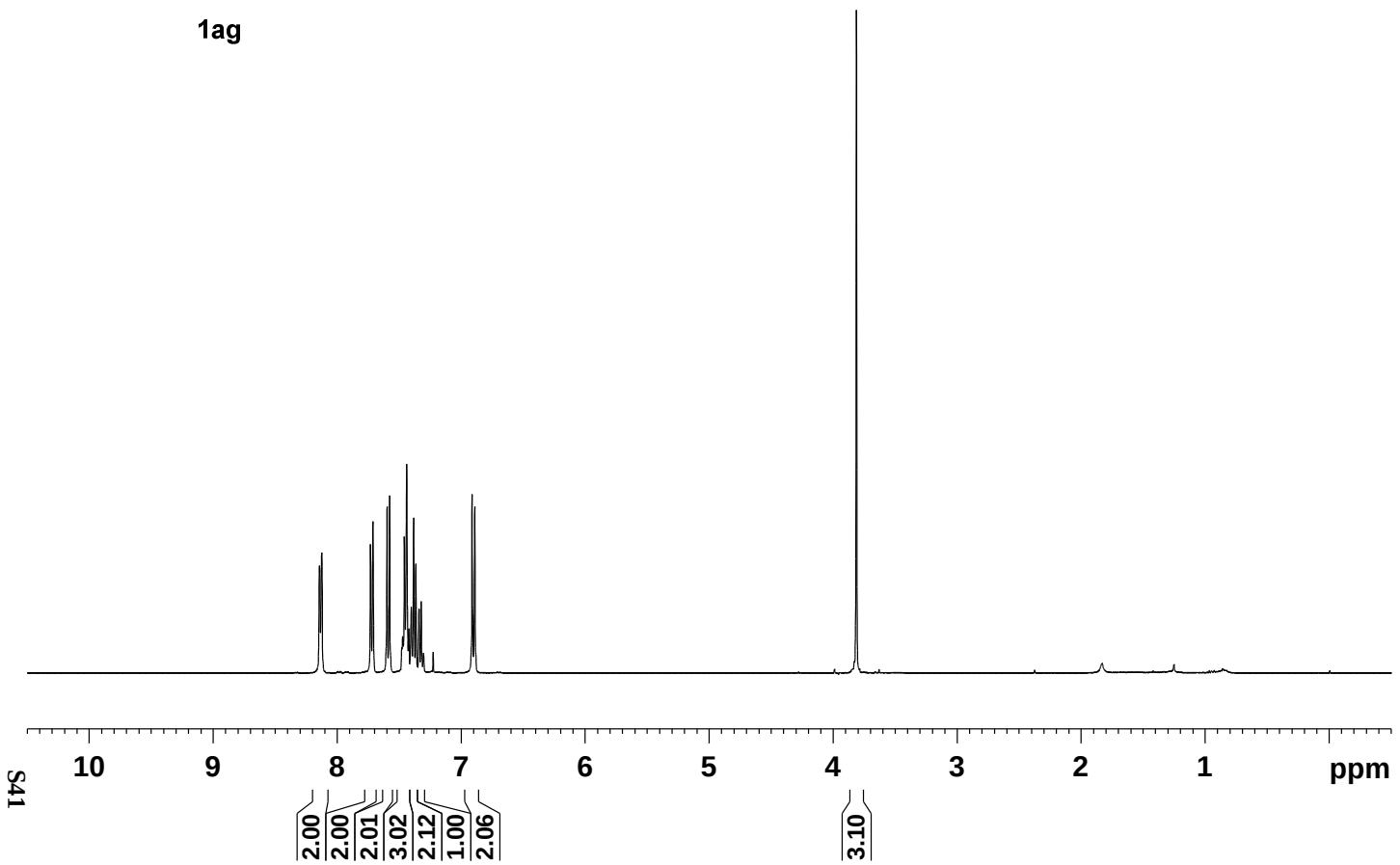
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                6.50 dB
SFO1        125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -0.60 dB
PL12              15.20 dB
PL13              18.20 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                65536
SF          125.7577927 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```



1ag



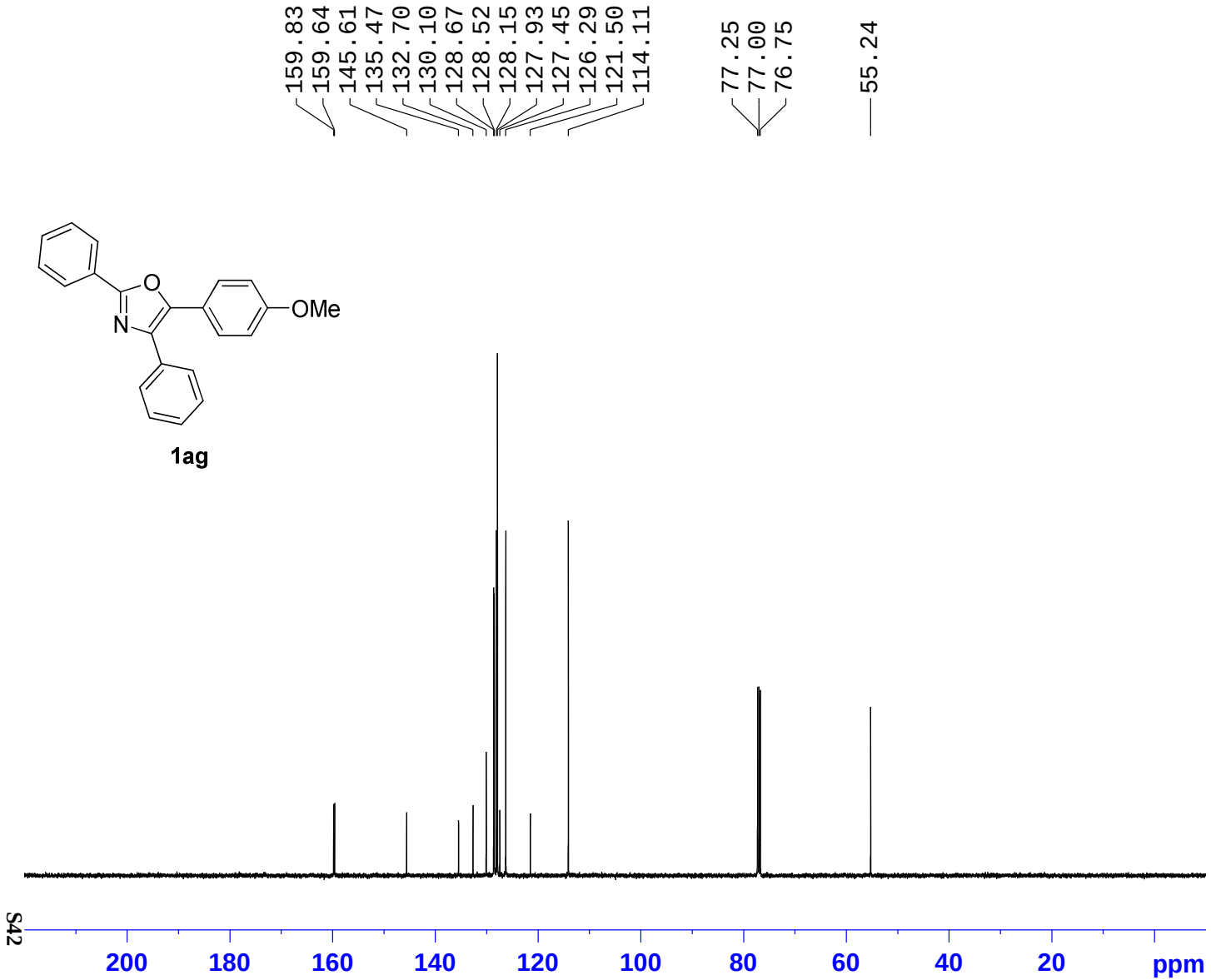
S41

```
Current Data Parameters
NAME            mina069
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20121011
Time              10.50
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                   64
DW               69.000 usec
DE                6.50 usec
TE               299.3 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300228 MHz
WDW                  EM
SSB      0
LB       0 Hz
GB       0
PC                 1.00
```



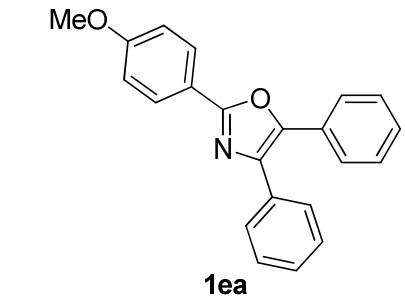

```
Current Data Parameters
NAME                  mina069
EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_                20121012
Time                    21.22
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         199
DS                           0
SWH                30030.029 Hz
FIDRES              0.458222 Hz
AQ                  1.0912410 sec
RG                     9195.2
DW                     16.650 usec
DE                      6.50 usec
TE                     295.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

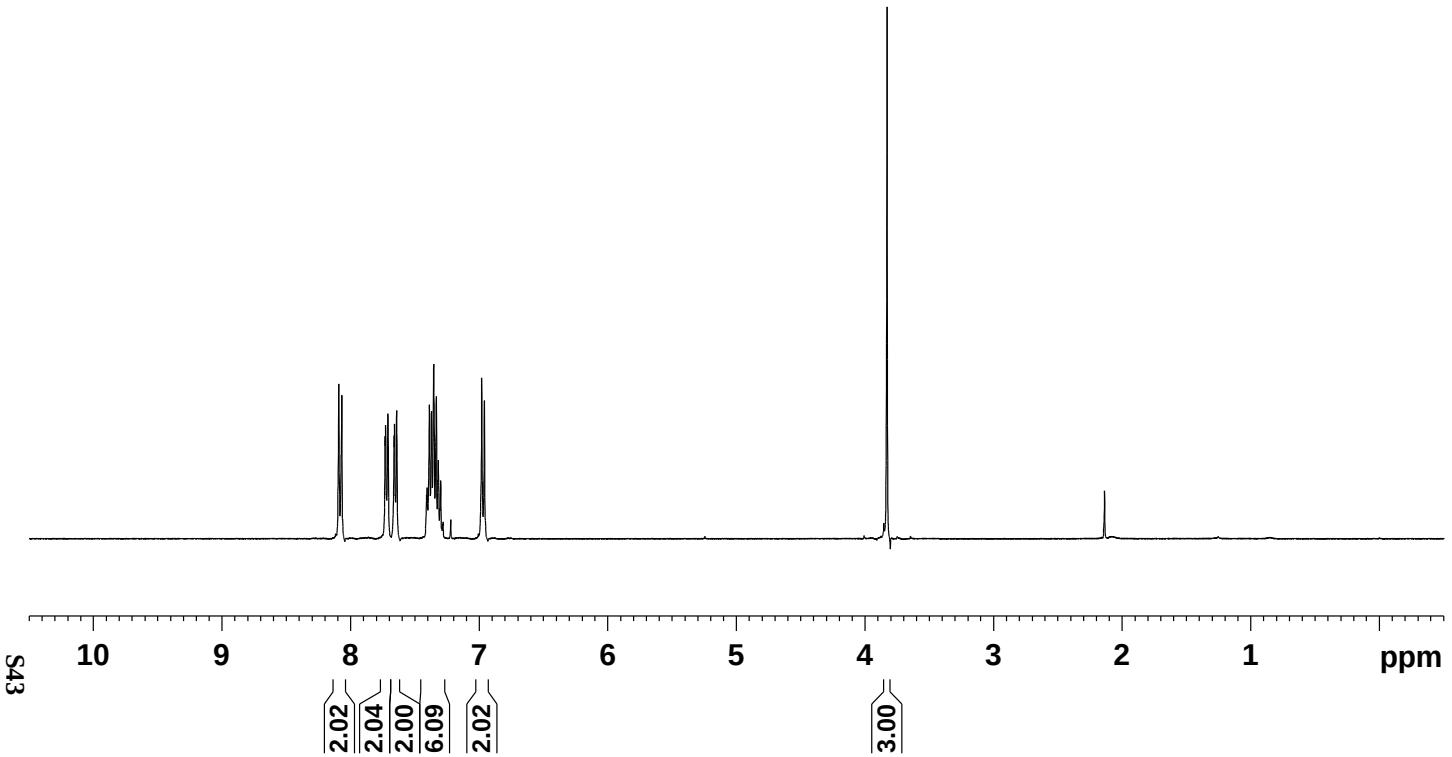
======== CHANNEL f1 ========
NUC1                       13C
P1                      10.00 usec
PL1                      6.50 dB
SFO1             125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   90.00 usec
PL2                     -0.60 dB
PL12                    15.20 dB
PL13                    18.20 dB
SFO2             500.1320005 MHz

F2 - Processing parameters
SI                       65536
SF                125.7578019 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.00
```



1ea



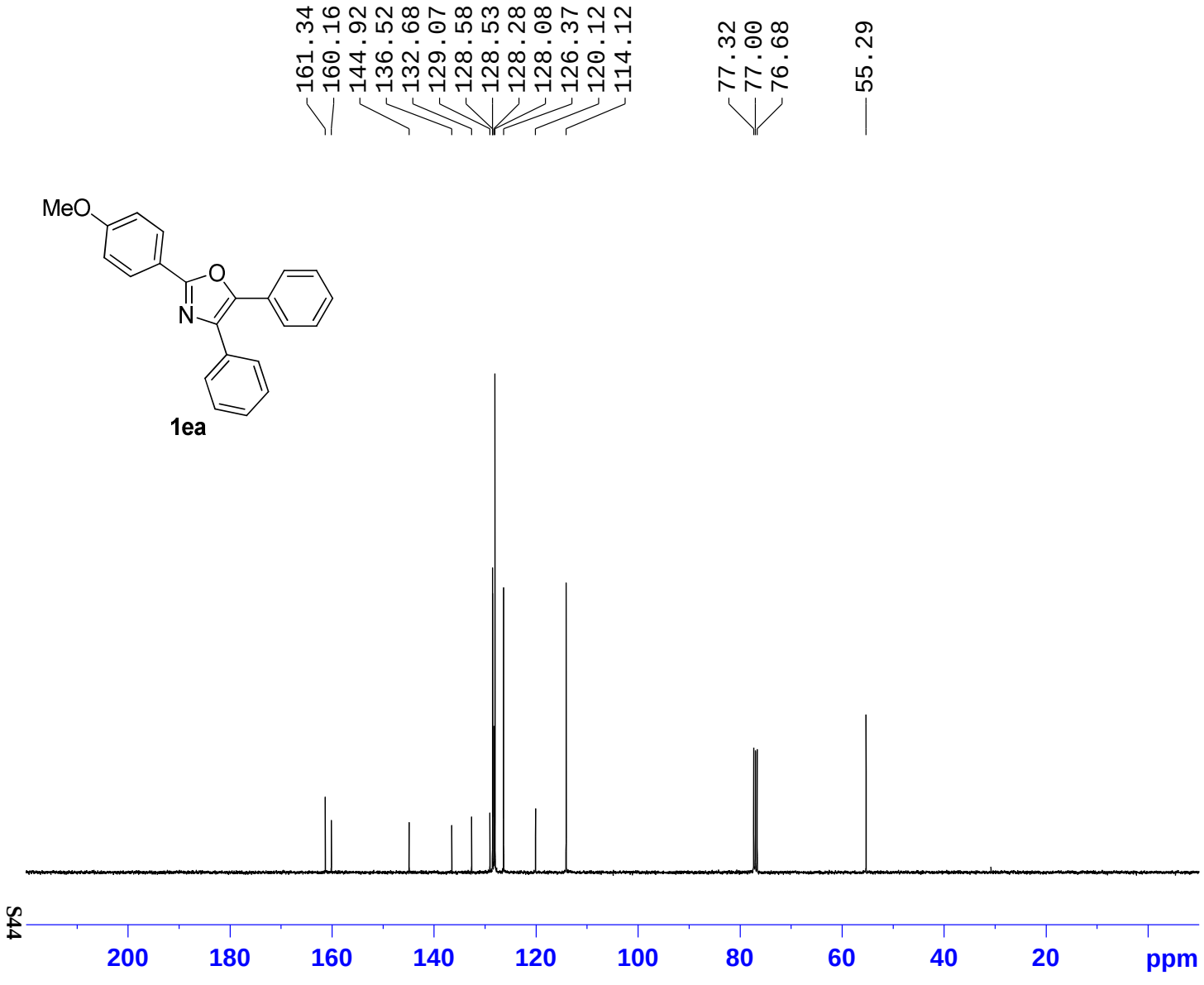
S43

```
Current Data Parameters
NAME            mina080
EXPNO                21
PROCNO                1

F2 - Acquisition Parameters
Date_          20121204
Time              20.35
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    1
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                   57
DW               69.000 usec
DE                6.50 usec
TE                299.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300246 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



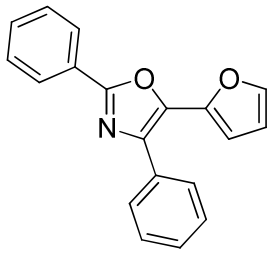

```
Current Data Parameters
NAME                 mina080
EXPNO                     20
PROCNO                     1

F2 - Acquisition Parameters
Date_              20121204
Time                  20.13
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      350
DS                        0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                0.6816452 sec
RG                   9195.2
DW                   20.800 usec
DE                    6.50 usec
TE                   299.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.40 usec
PL1                   7.00 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   3.00 dB
PL12                 20.70 dB
PL13                 23.70 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127797 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```



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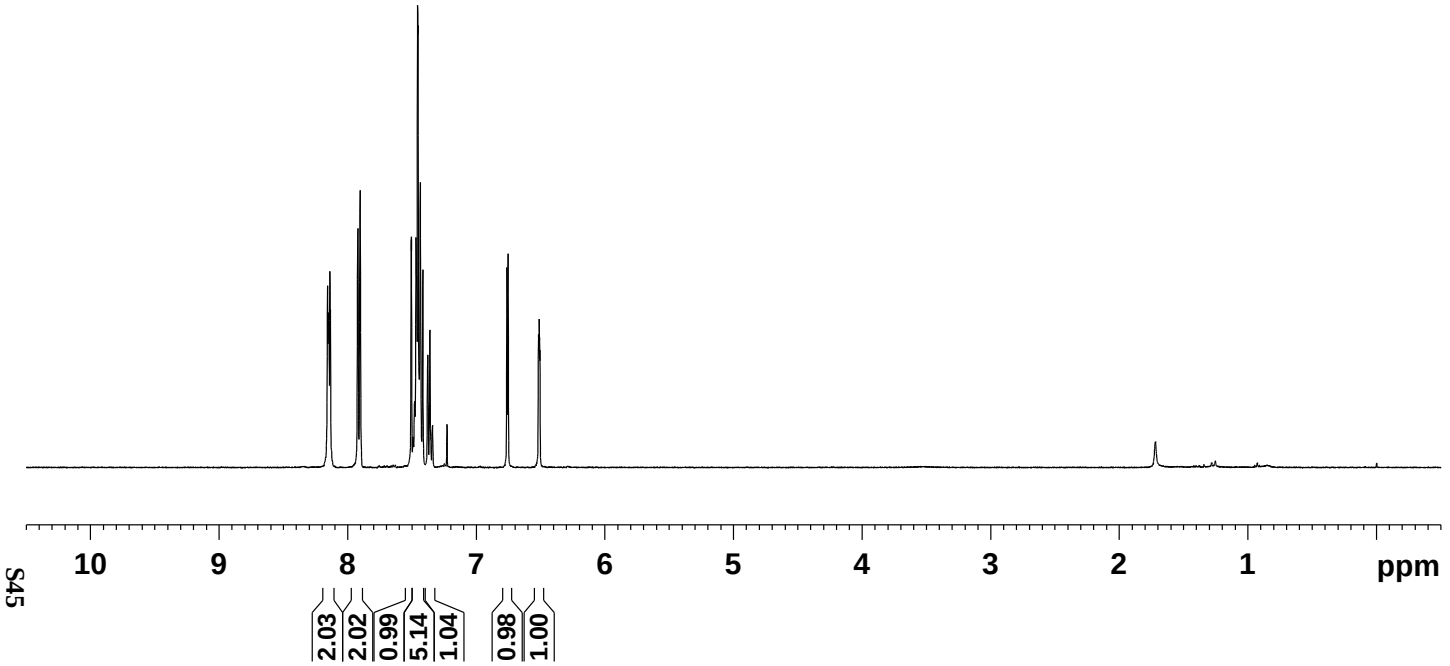
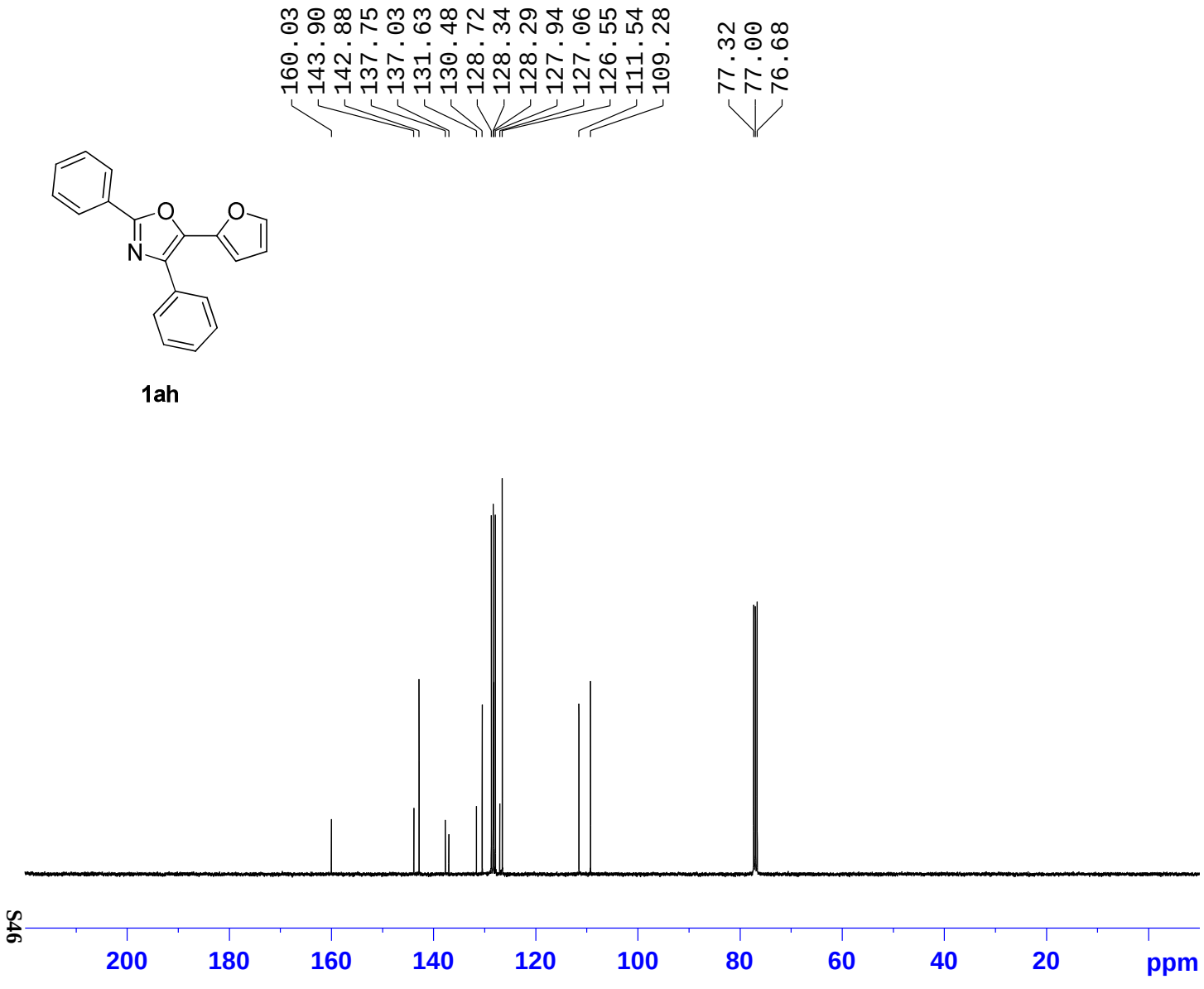



```
Current Data Parameters
NAME            mina073
EXPNO                13
PROCNO                1

F2 - Acquisition Parameters
Date_          20121016
Time              22.30
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                    4
DW               69.000 usec
DE                6.50 usec
TE               299.6 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300220 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



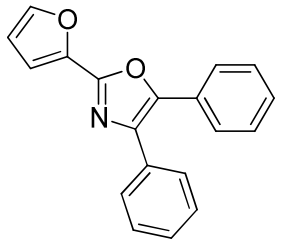

```
Current Data Parameters
NAME                 mina073
EXPNO                     12
PROCNO                     1

F2 - Acquisition Parameters
Date_              20121016
Time                   22.21
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                     32768
SOLVENT                CDCl3
NS                       577
DS                         0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                    9195.2
DW                    20.800 usec
DE                     6.50 usec
TE                     299.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      9.40 usec
PL1                     7.00 dB
SFO1            100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                  90.00 usec
PL2                     3.00 dB
PL12                   20.70 dB
PL13                   23.70 dB
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF              100.6127760 MHz
WDW                       EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.00
```



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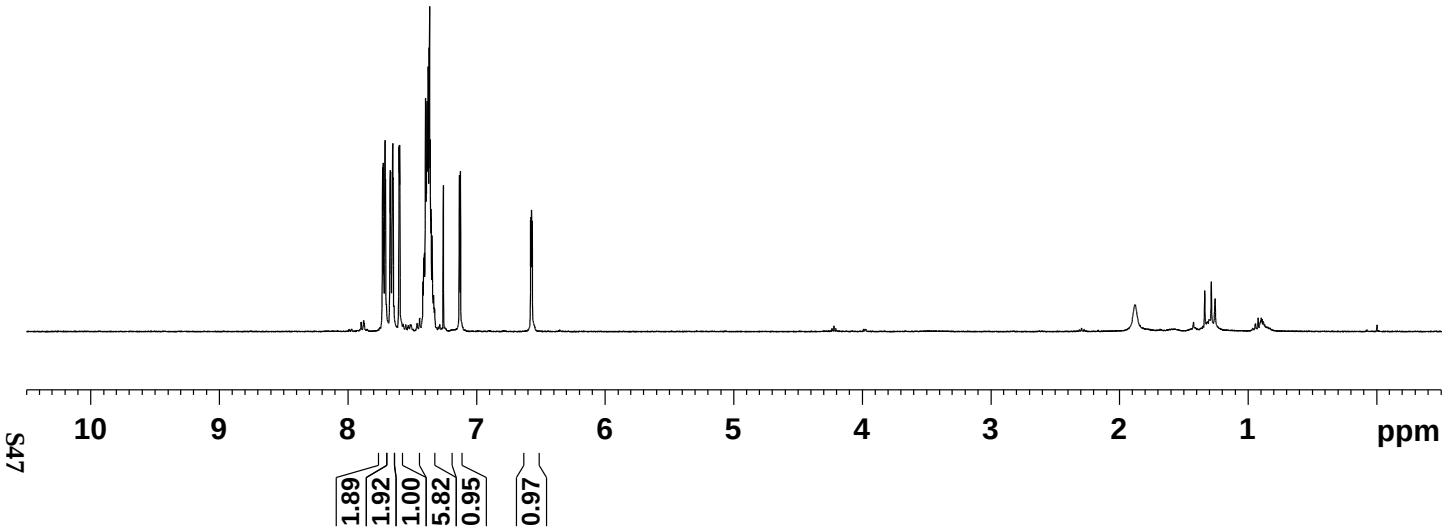
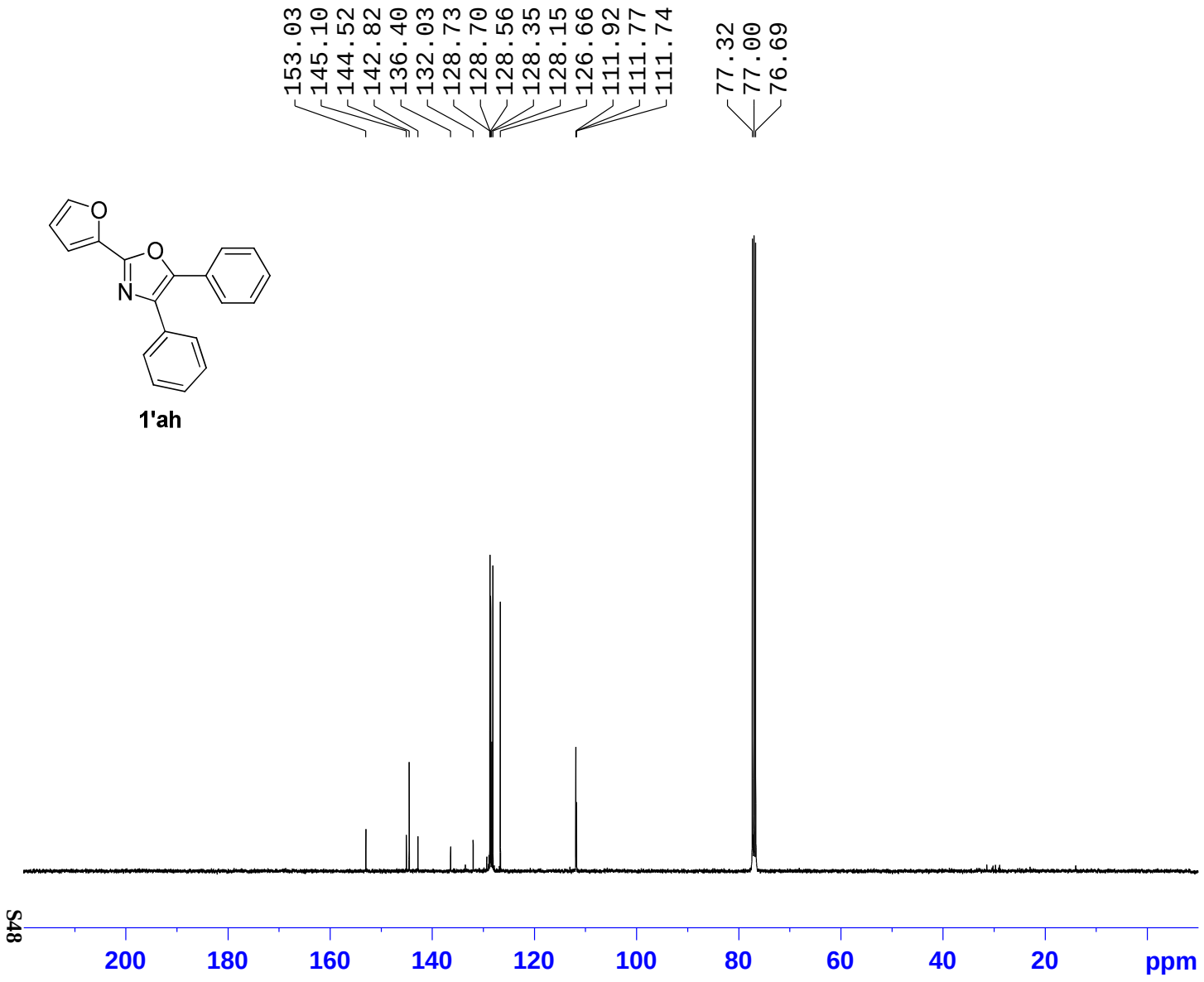



```
Current Data Parameters
NAME            mina073
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20130130
Time              11.22
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  181
DW               69.000 usec
DE                6.50 usec
TE                298.1 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300105 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



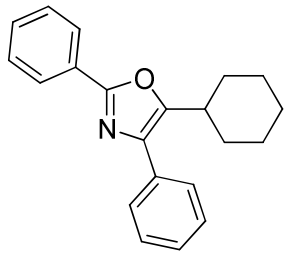

```
Current Data Parameters
NAME                  mina073
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_                20130130
Time                    17.49
INSTRUM                 spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                       4500
DS                          0
SWH                 24038.461 Hz
FIDRES               0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     298.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.40 usec
PL1                     7.00 dB
SFO1              100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  90.00 usec
PL2                     3.00 dB
PL12                   20.70 dB
PL13                   23.70 dB
SFO2              400.1316005 MHz

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



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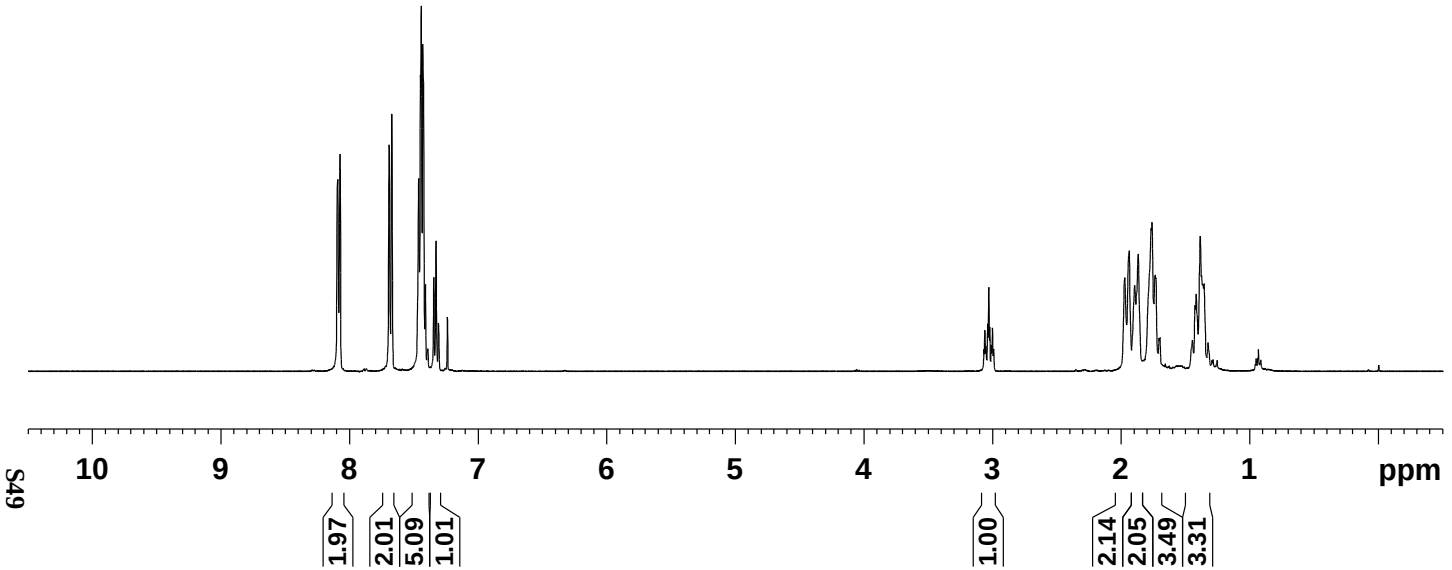
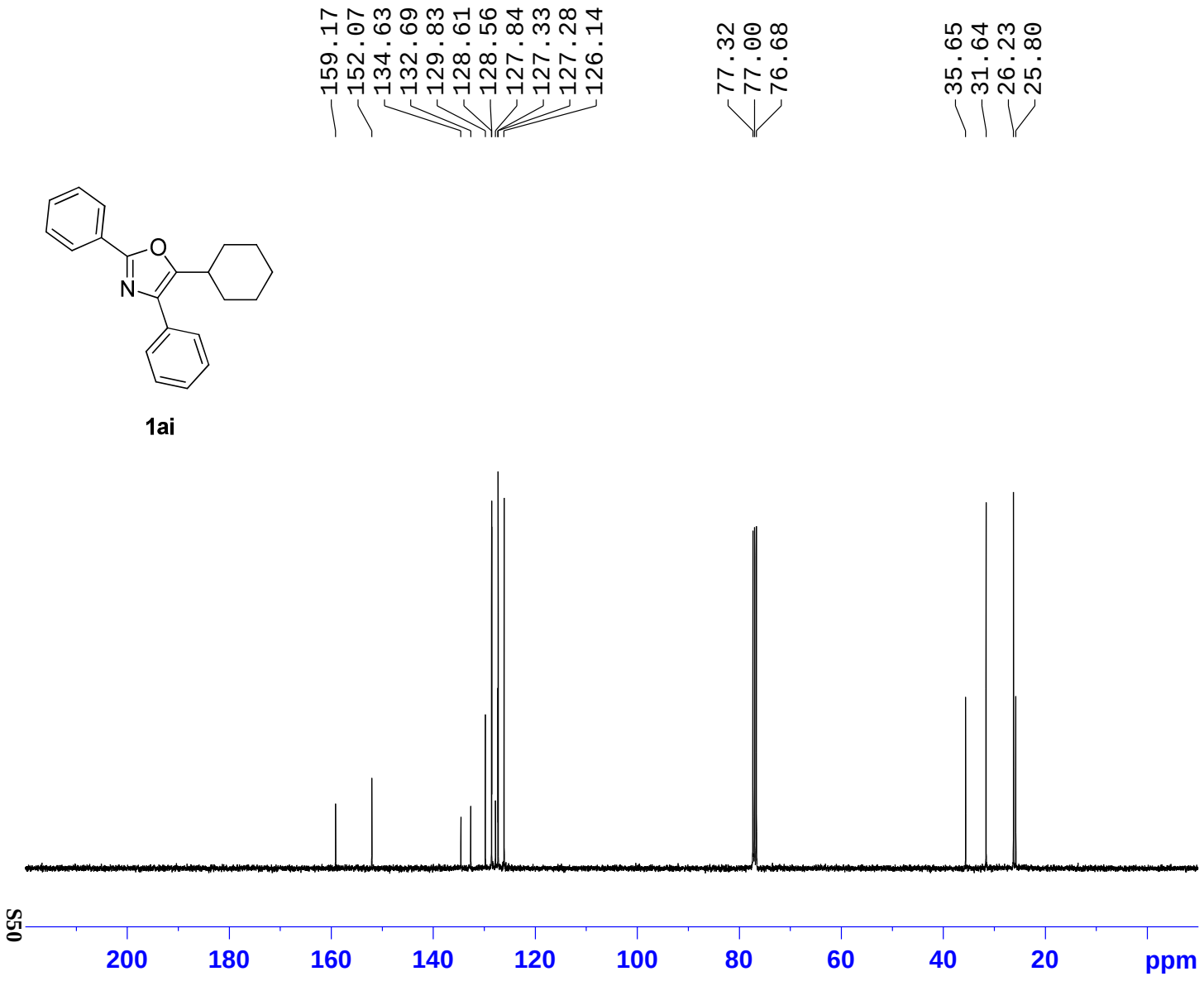



```
Current Data Parameters
NAME            mina064
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20121018
Time              19.07
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 71.8
DW               69.000 usec
DE                6.50 usec
TE                298.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300180 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



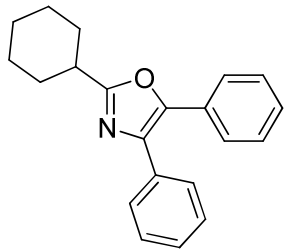

```
Current Data Parameters
NAME                  mina064
EXPNO                       9
PROCNO                      1

F2 - Acquisition Parameters
Date_                20121018
Time                    19.28
INSTRUM                 spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                        453
DS                          0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                 0.6816452 sec
RG                    9195.2
DW                    20.800 usec
DE                     6.50 usec
TE                     298.6 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.40 usec
PL1                      7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                   90.00 usec
PL2                      3.00 dB
PL12                    20.70 dB
PL13                    23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127753 MHz
WDW                          EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.00
```



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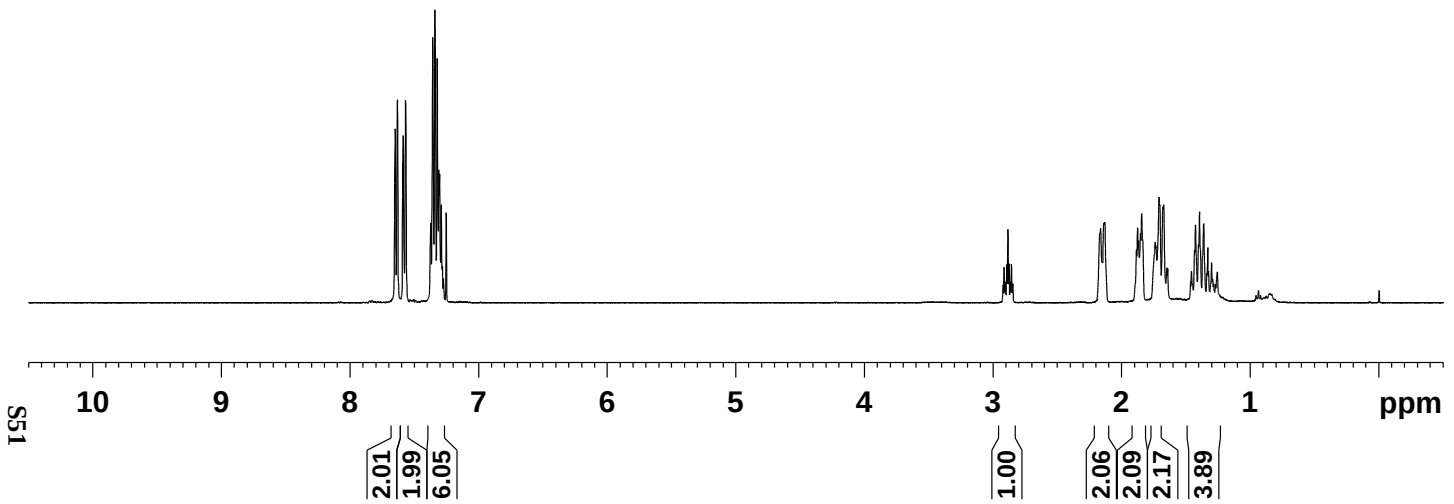
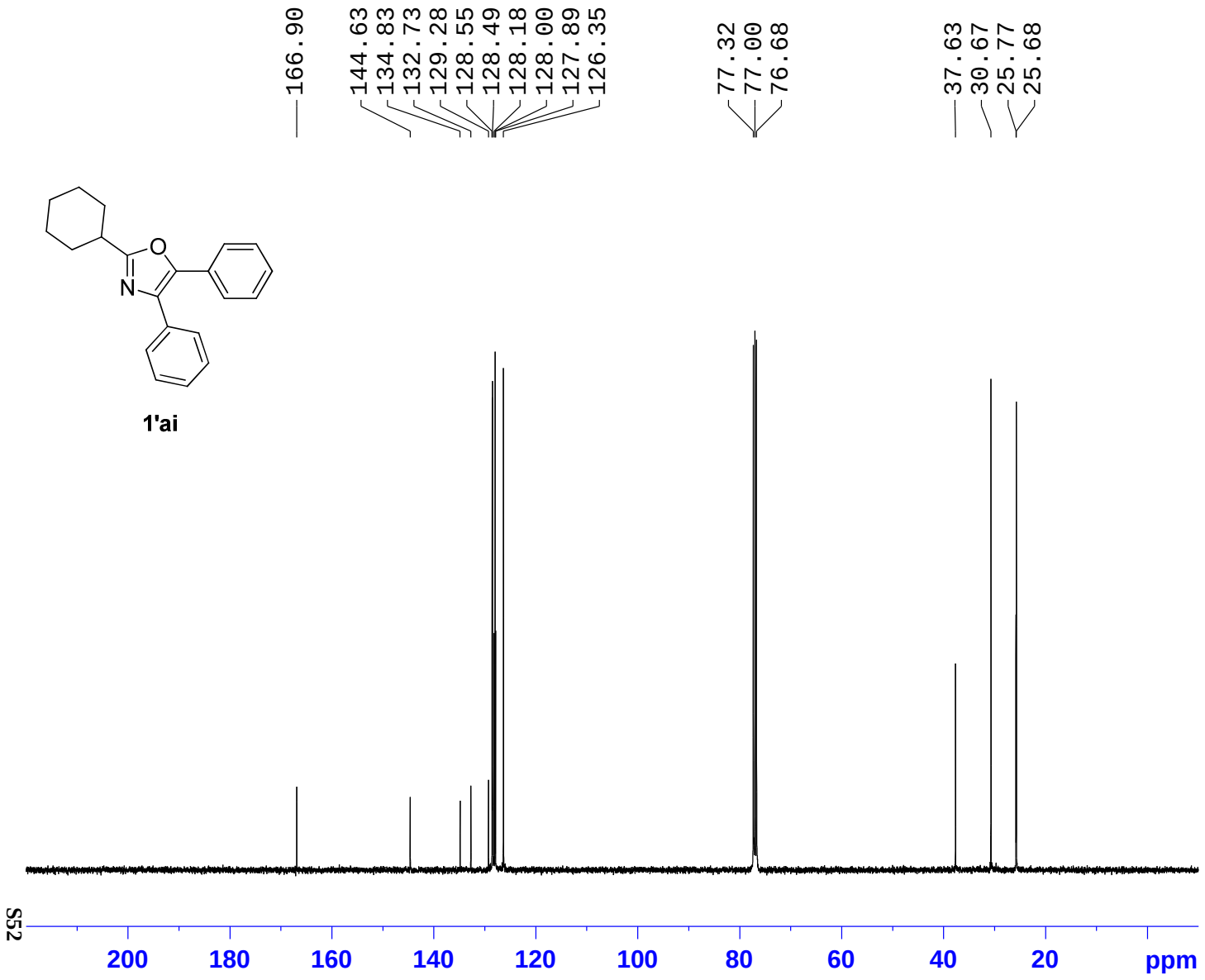



```
Current Data Parameters
NAME            mina064
EXPNO                 6
PROCNO                1

F2 - Acquisition Parameters
Date_          20121018
Time              19.12
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  128
DW               69.000 usec
DE                6.50 usec
TE                298.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300122 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



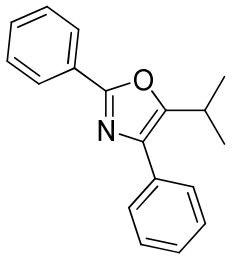

```
Current Data Parameters
NAME                 mina186
EXPNO                      7
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130316
Time                   15.12
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                       2301
DS                          0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

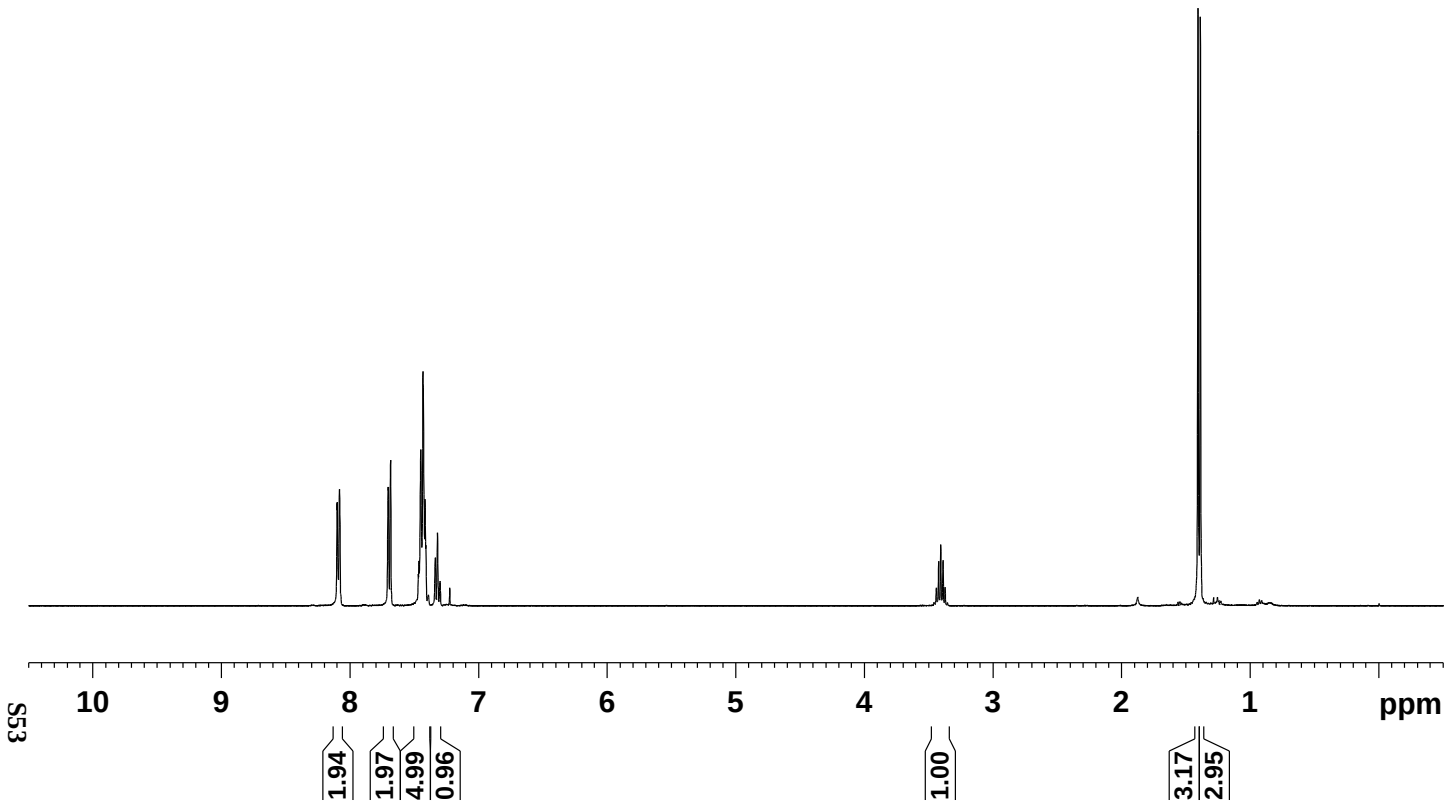
======== CHANNEL f1 ========
NUC1                      13C
P1                       9.40 usec
PL1                      7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                   90.00 usec
PL2                      3.00 dB
PL12                    20.70 dB
PL13                    23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF               100.6127730 MHz
WDW                        EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.00
```



1aj



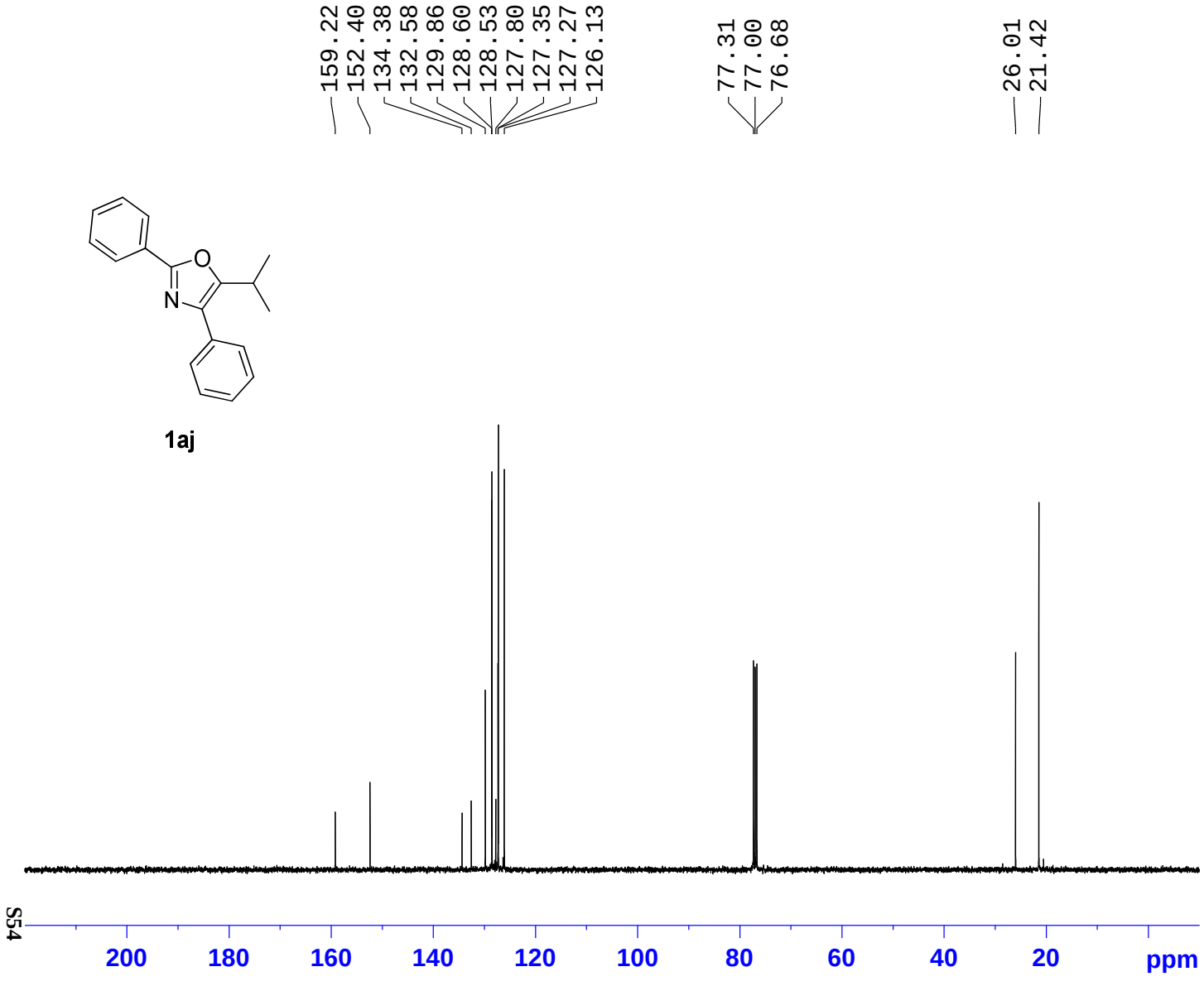
S53

```
Current Data Parameters
NAME            mina056
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20121018
Time              12.15
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                    4
DW               69.000 usec
DE                6.50 usec
TE                298.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300233 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



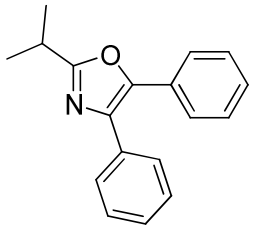

```
Current Data Parameters
NAME                  mina056
EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_               20121017
Time                   21.00
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                        203
DS                          0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     299.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

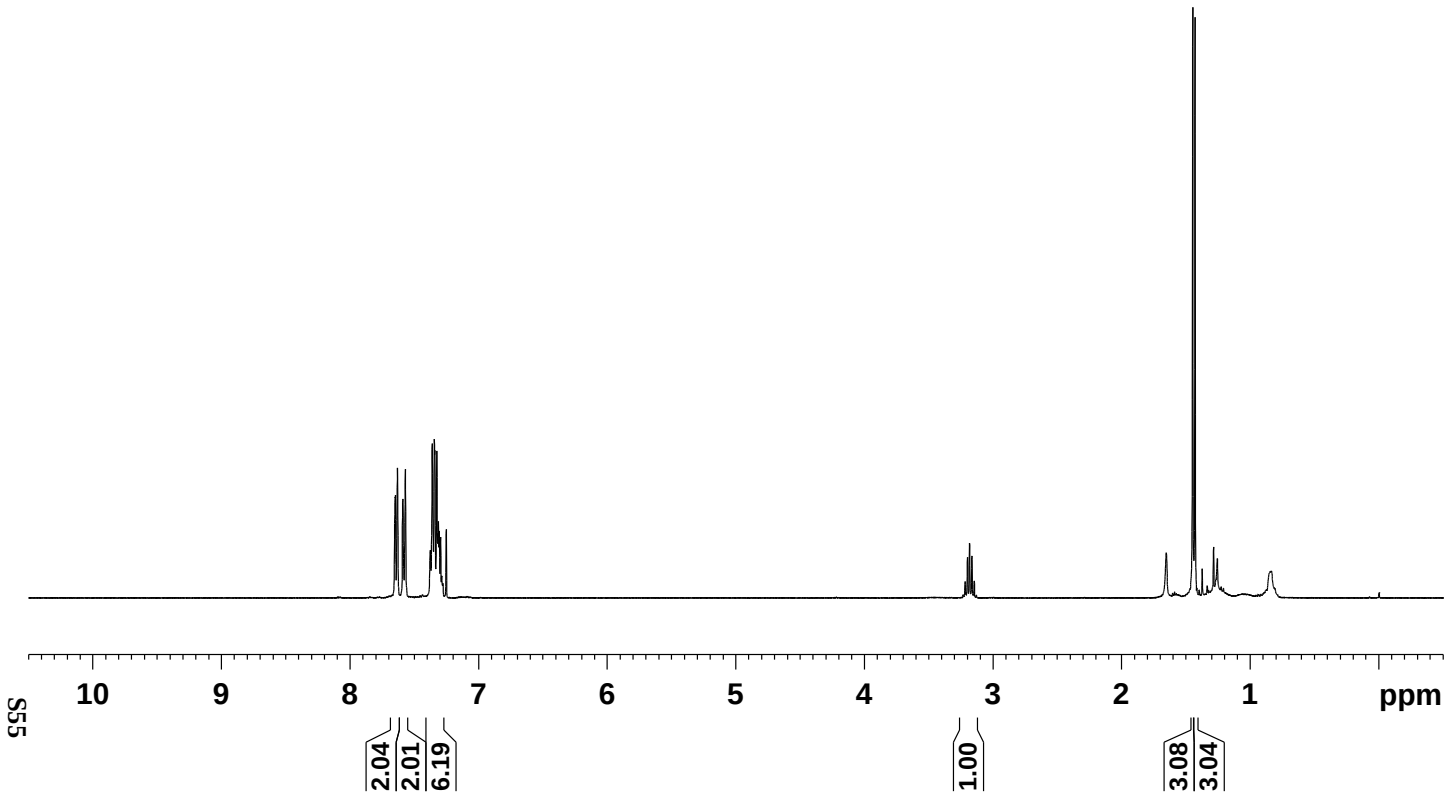
======== CHANNEL f1 ========
NUC1                      13C
P1                       9.40 usec
PL1                      7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                   90.00 usec
PL2                      3.00 dB
PL12                    20.70 dB
PL13                    23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF               100.6127775 MHz
WDW                        EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.00
```



1'aj

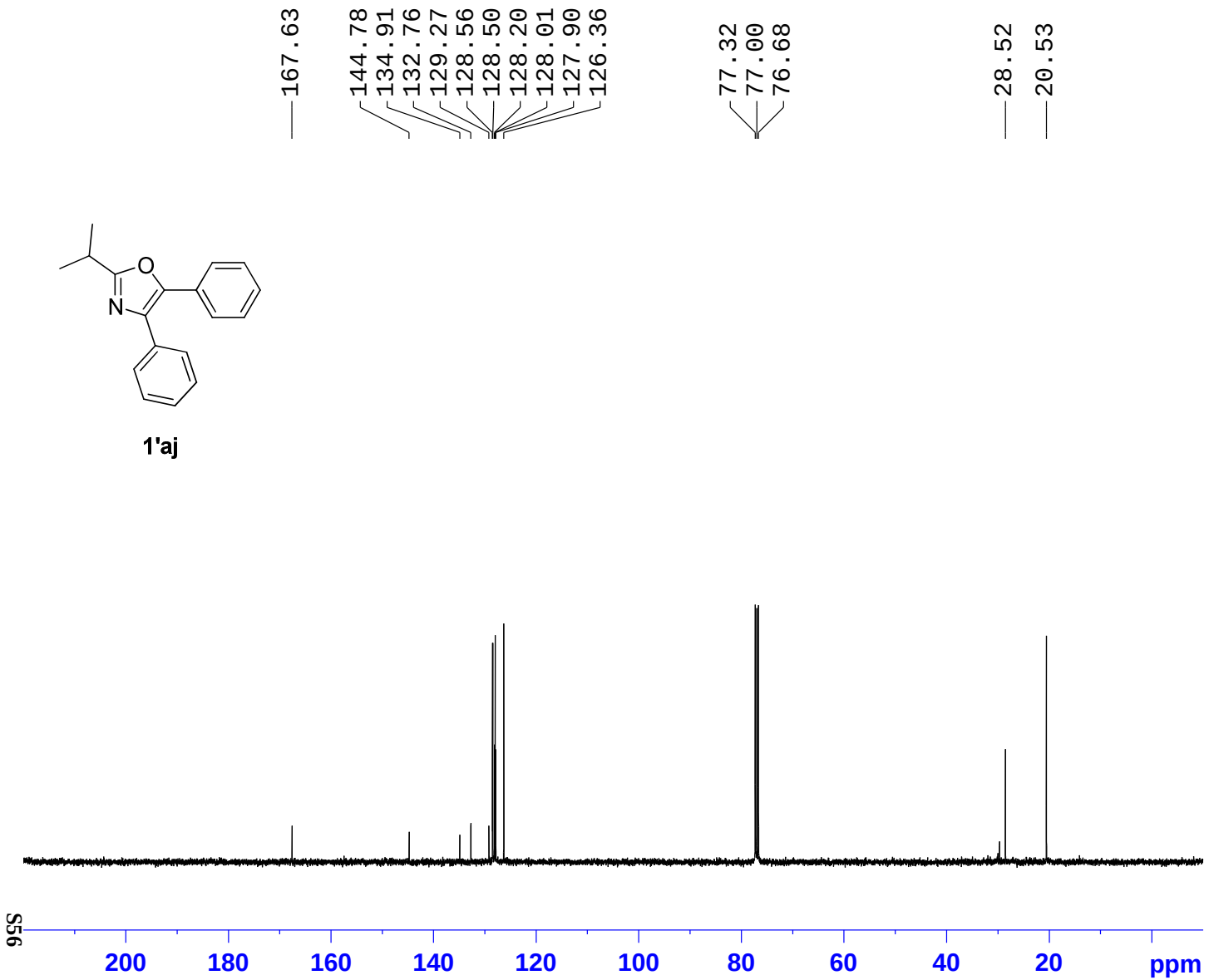



```
Current Data Parameters
NAME            mina056
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20121018
Time              12.12
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                161.3
DW               69.000 usec
DE                6.50 usec
TE                298.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300114 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



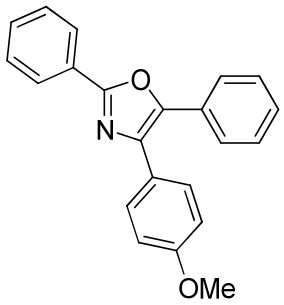

```
Current Data Parameters
NAME                 mina056
EXPNO                     10
PROCNO                     1

F2 - Acquisition Parameters
Date_              20121020
Time                  13.35
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      200
DS                        0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                0.6816452 sec
RG                   9195.2
DW                  20.800 usec
DE                   6.50 usec
TE                  298.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

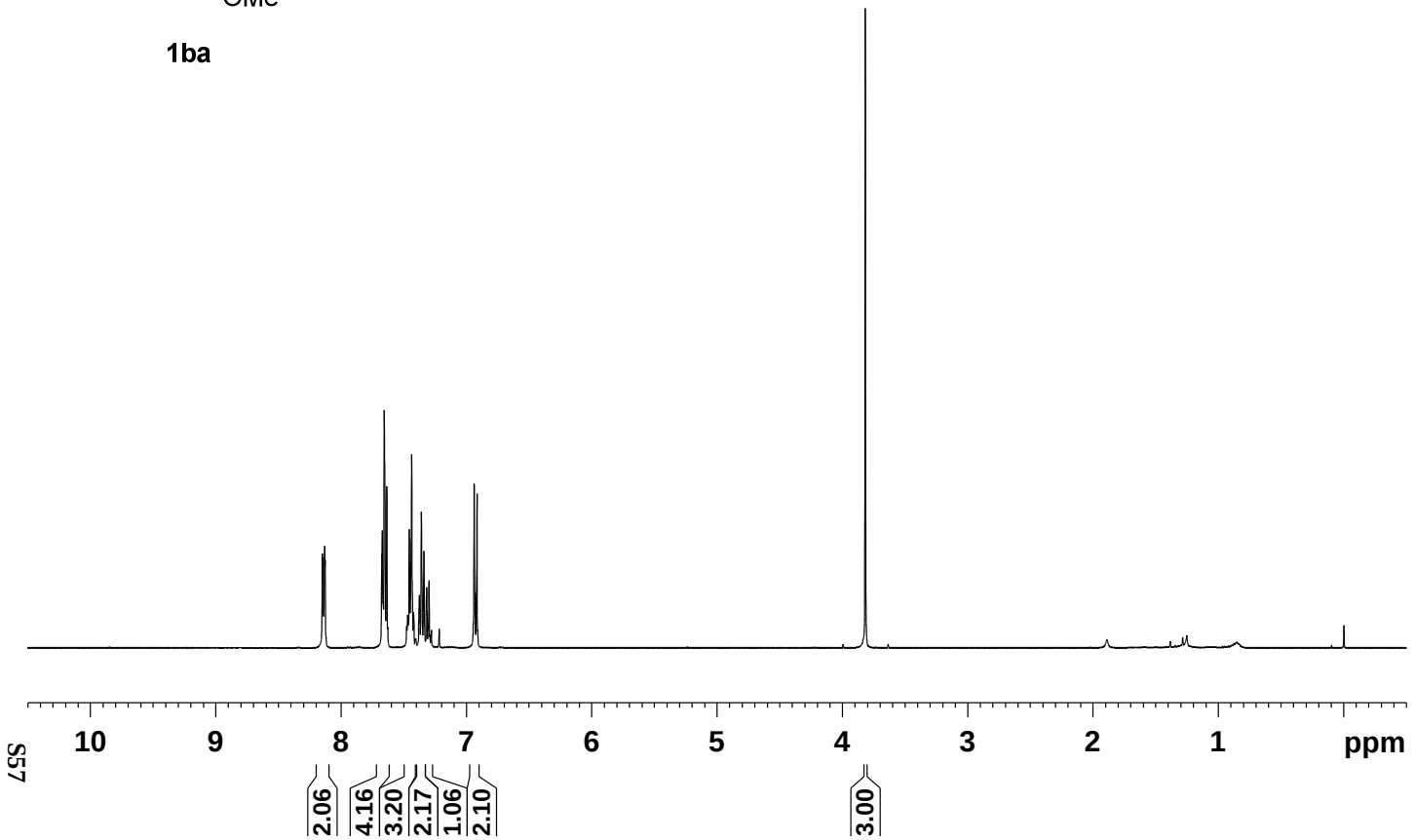
======== CHANNEL f1 ========
NUC1                    13C
P1                    9.40 usec
PL1                   7.00 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                   3.00 dB
PL12                 20.70 dB
PL13                 23.70 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127731 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```



1ba

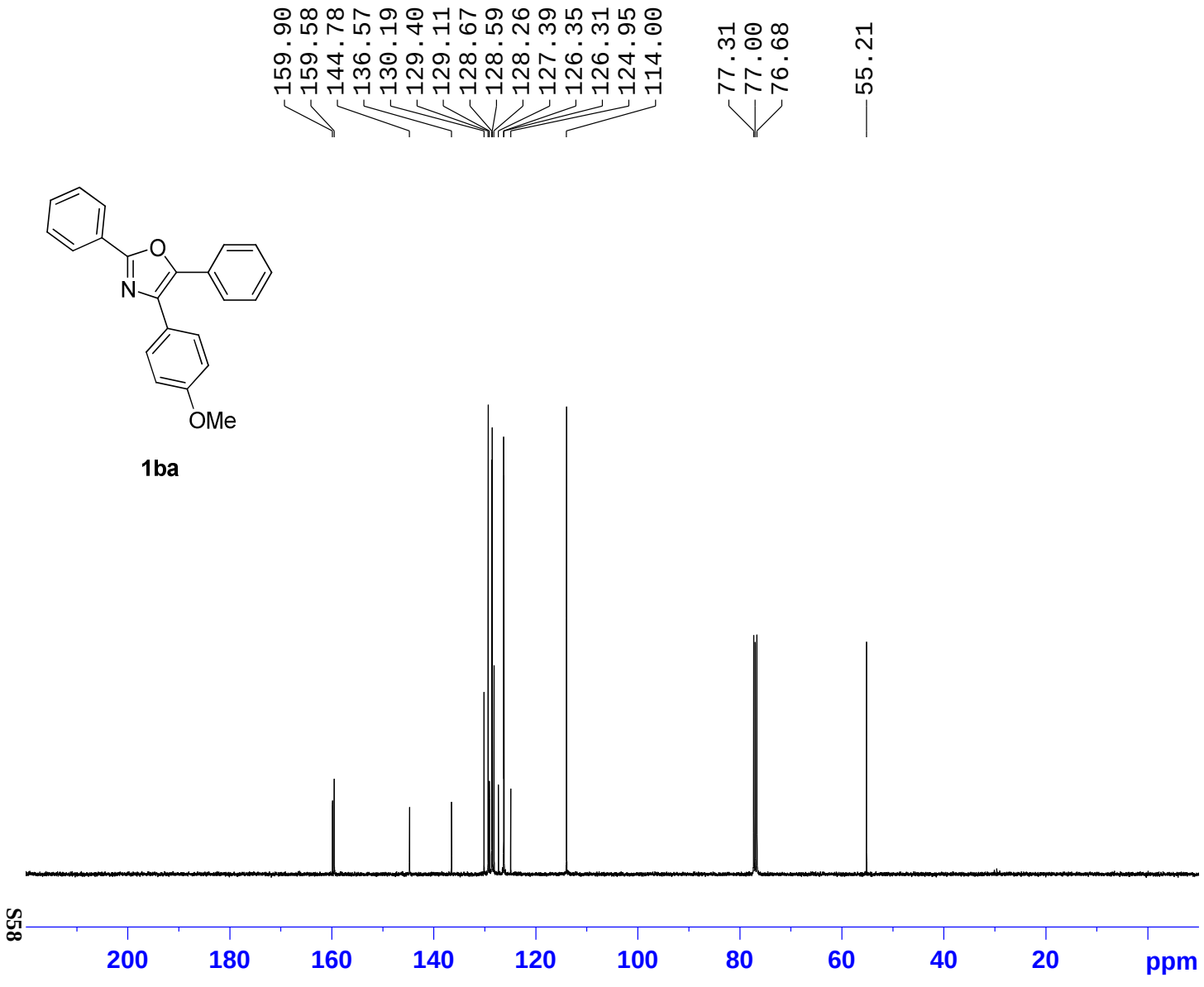



```
Current Data Parameters
NAME            mina086
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20121106
Time              20.28
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 40.3
DW               69.000 usec
DE                6.50 usec
TE               298.9 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300259 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



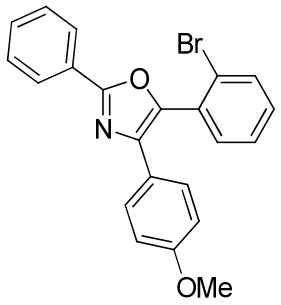

```
Current Data Parameters
NAME                 mina086
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_               20121106
Time                   20.04
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                     32768
SOLVENT                CDCl3
NS                       400
DS                         0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     299.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

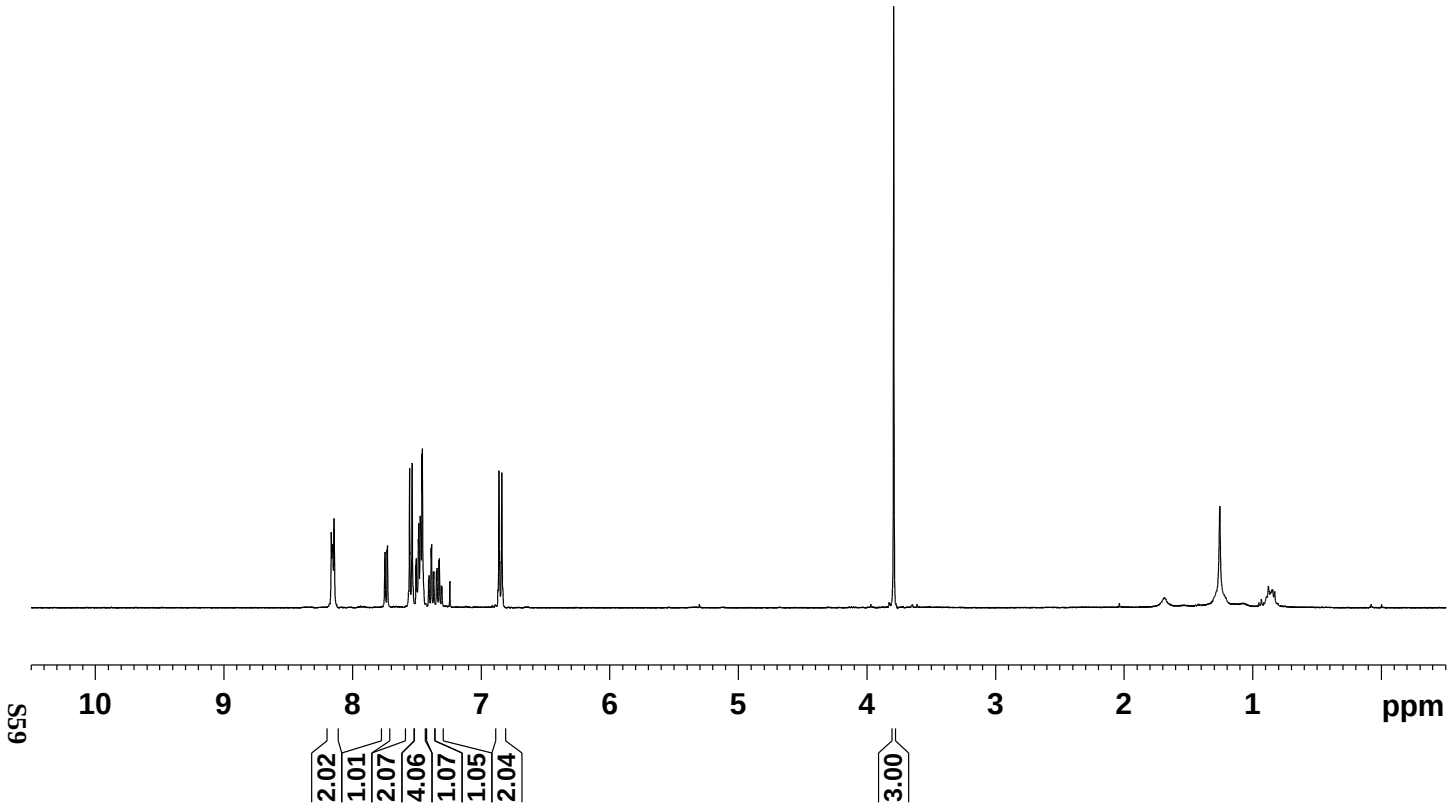
======== CHANNEL f1 ========
NUC1                     13C
P1                      9.40 usec
PL1                     7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                  90.00 usec
PL2                     3.00 dB
PL12                   20.70 dB
PL13                   23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF               100.6127803 MHz
WDW                       EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.00
```



1bd

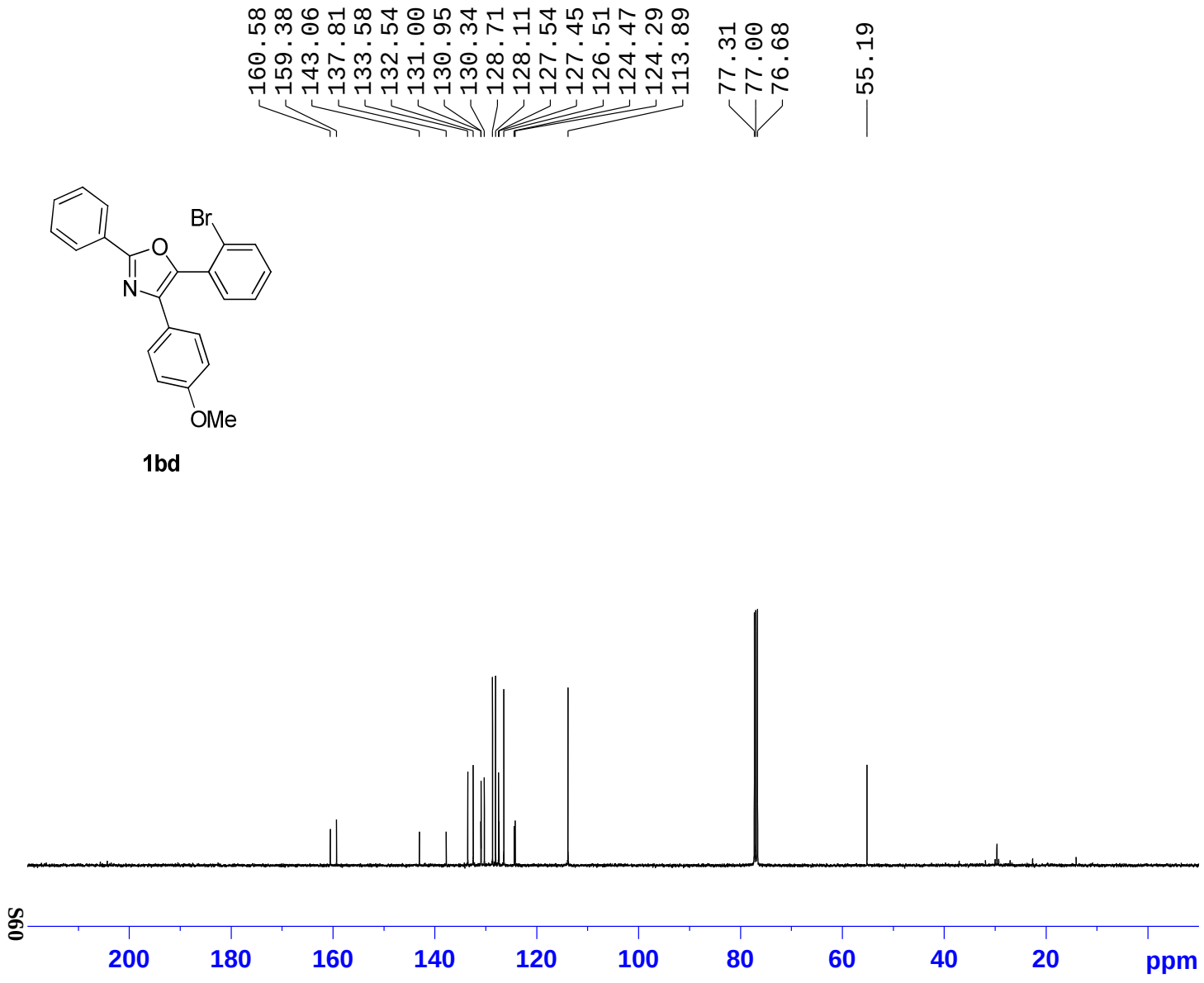



```
Current Data Parameters
NAME            mina028
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20120903
Time              20.03
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  114
DW               69.000 usec
DE                6.50 usec
TE                299.1 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.70 usec
PL1                4.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300144 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



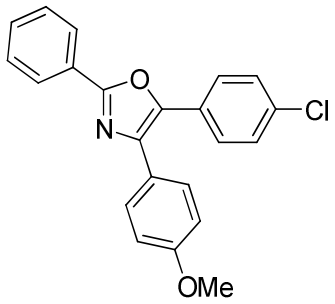

```
Current Data Parameters
NAME            mina028
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20120908
Time              17.27
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  731
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG               9195.2
DW                20.800 usec
DE                 6.50 usec
TE                299.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

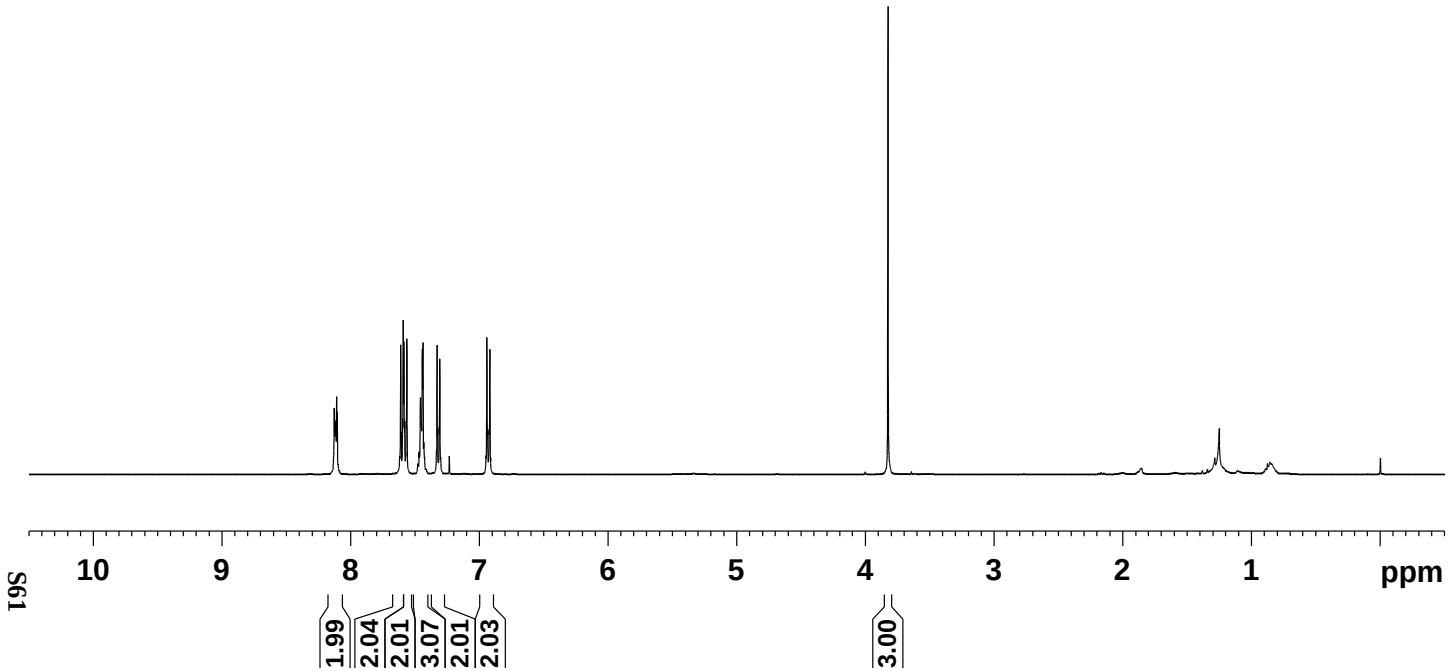
======== CHANNEL f1 ========
NUC1                13C
P1                 8.90 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2                3.80 dB
PL12               21.60 dB
PL13               24.60 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127740 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.00
```



1bb

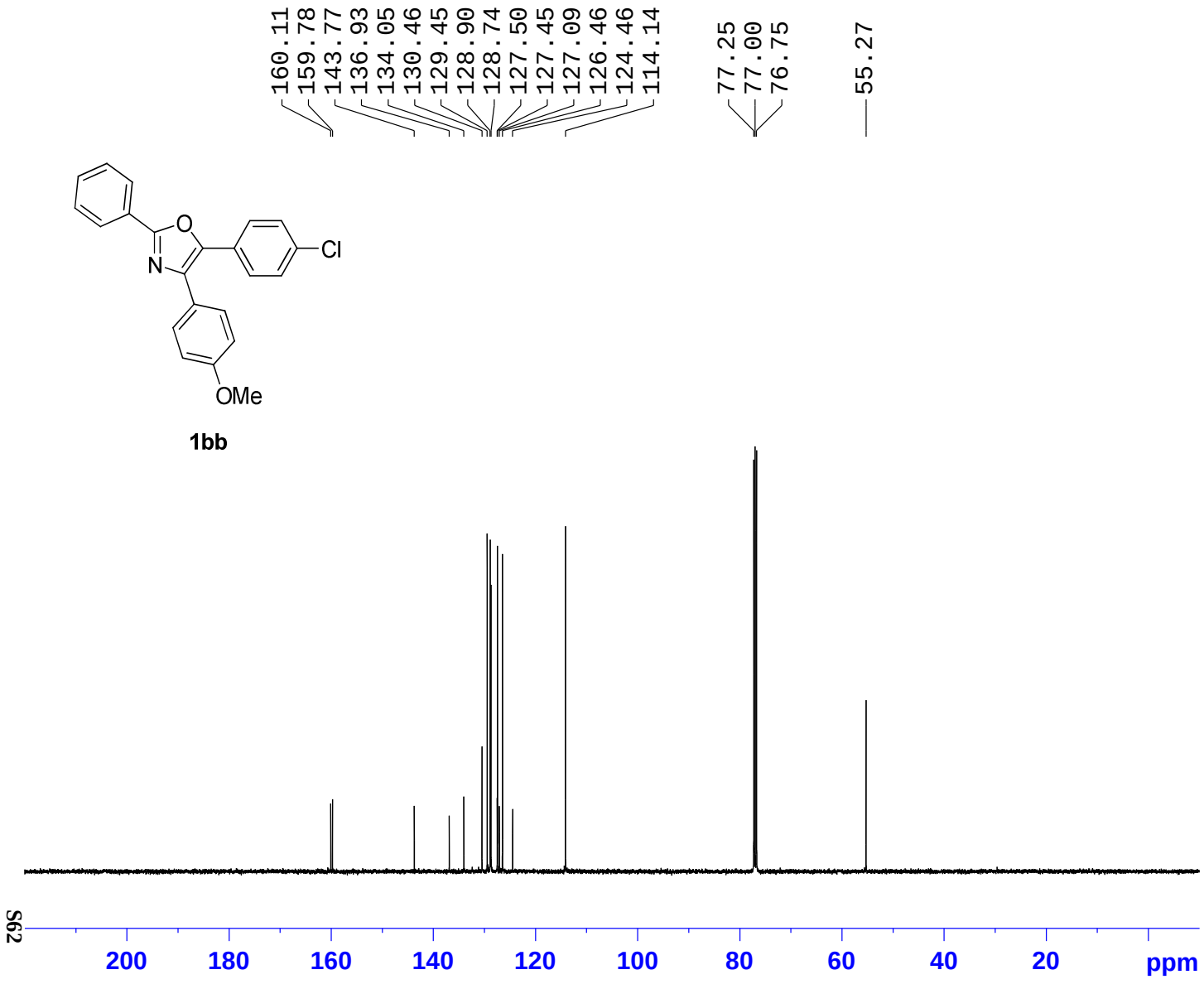



```
Current Data Parameters
NAME            mina091
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20121119
Time              20.47
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 40.3
DW               69.000 usec
DE                6.50 usec
TE               299.1 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300202 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



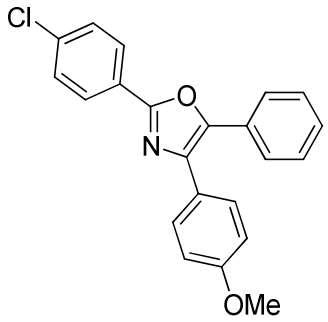

```
Current Data Parameters
NAME                 mina065
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20120927
Time                  19.34
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      298
DS                        0
SWH              30030.029 Hz
FIDRES            0.458222 Hz
AQ               1.0912410 sec
RG                     8192
DW                  16.650 usec
DE                   6.50 usec
TE                   295.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

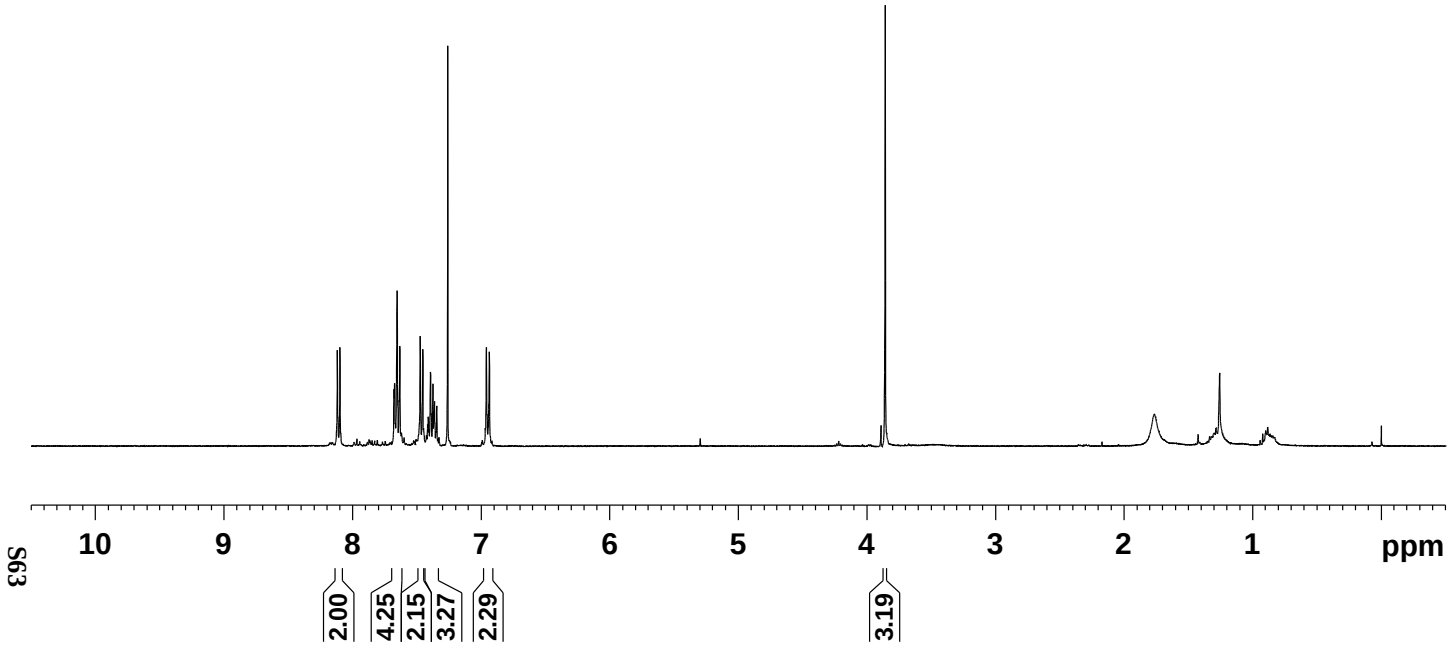
======== CHANNEL f1 ========
NUC1                    13C
P1                   10.50 usec
PL1                   7.00 dB
SFO1          125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -0.60 dB
PL12                 15.00 dB
PL13                 18.00 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                    65536
SF            125.7577985 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```



1'bb



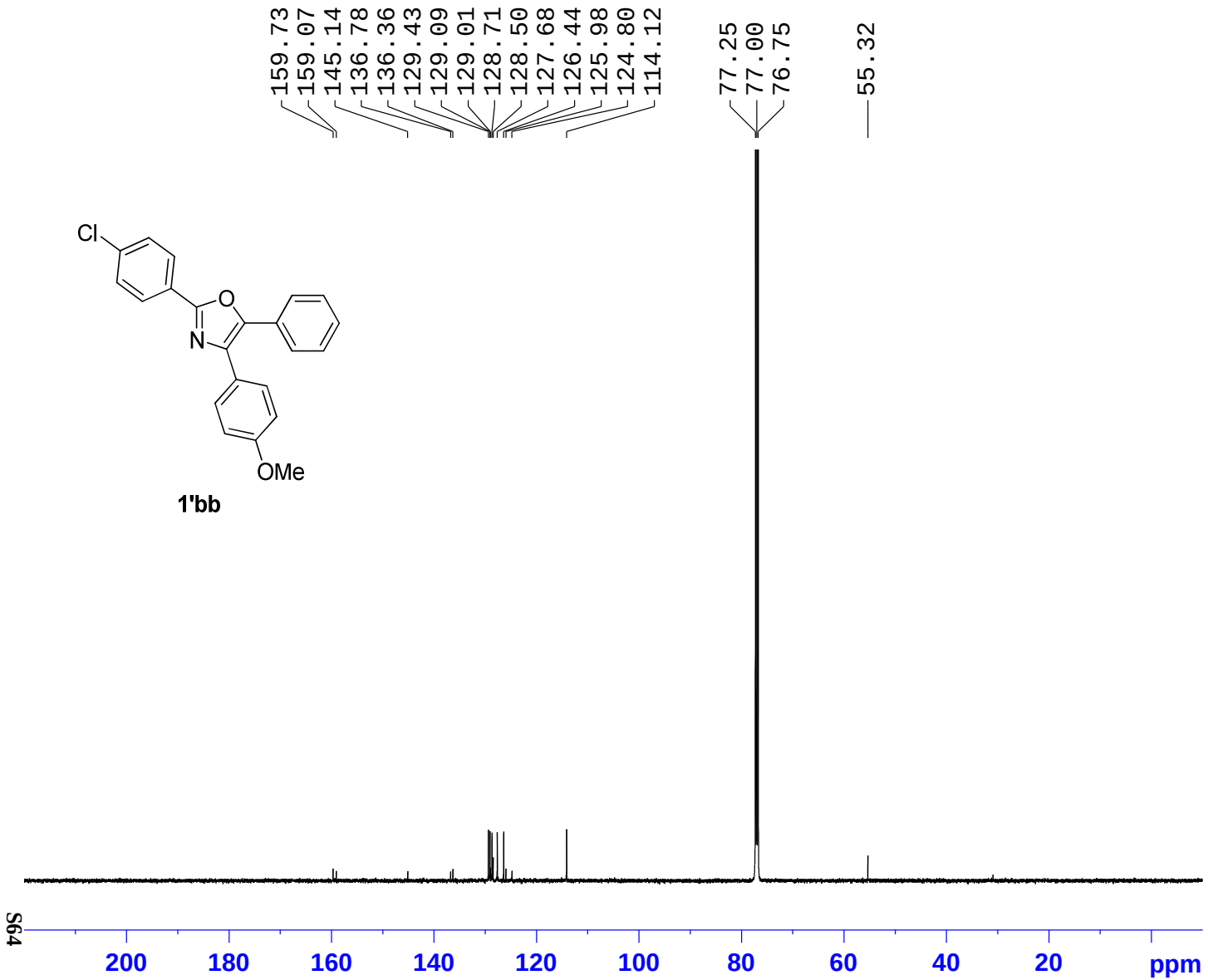
S63

```
Current Data Parameters
NAME            mina091
EXPNO                16
PROCNO                1

F2 - Acquisition Parameters
Date_          20130130
Time              11.15
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  362
DW               69.000 usec
DE                6.50 usec
TE                298.1 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

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



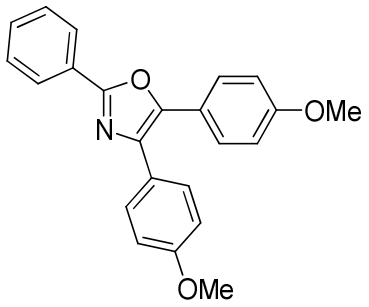

```
Current Data Parameters
NAME                 mina091
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_               20121207
Time                   23.49
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                     11220
DS                         0
SWH                30030.029 Hz
FIDRES              0.458222 Hz
AQ                  1.0912410 sec
RG                     9195.2
DW                    16.650 usec
DE                     6.50 usec
TE                     294.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

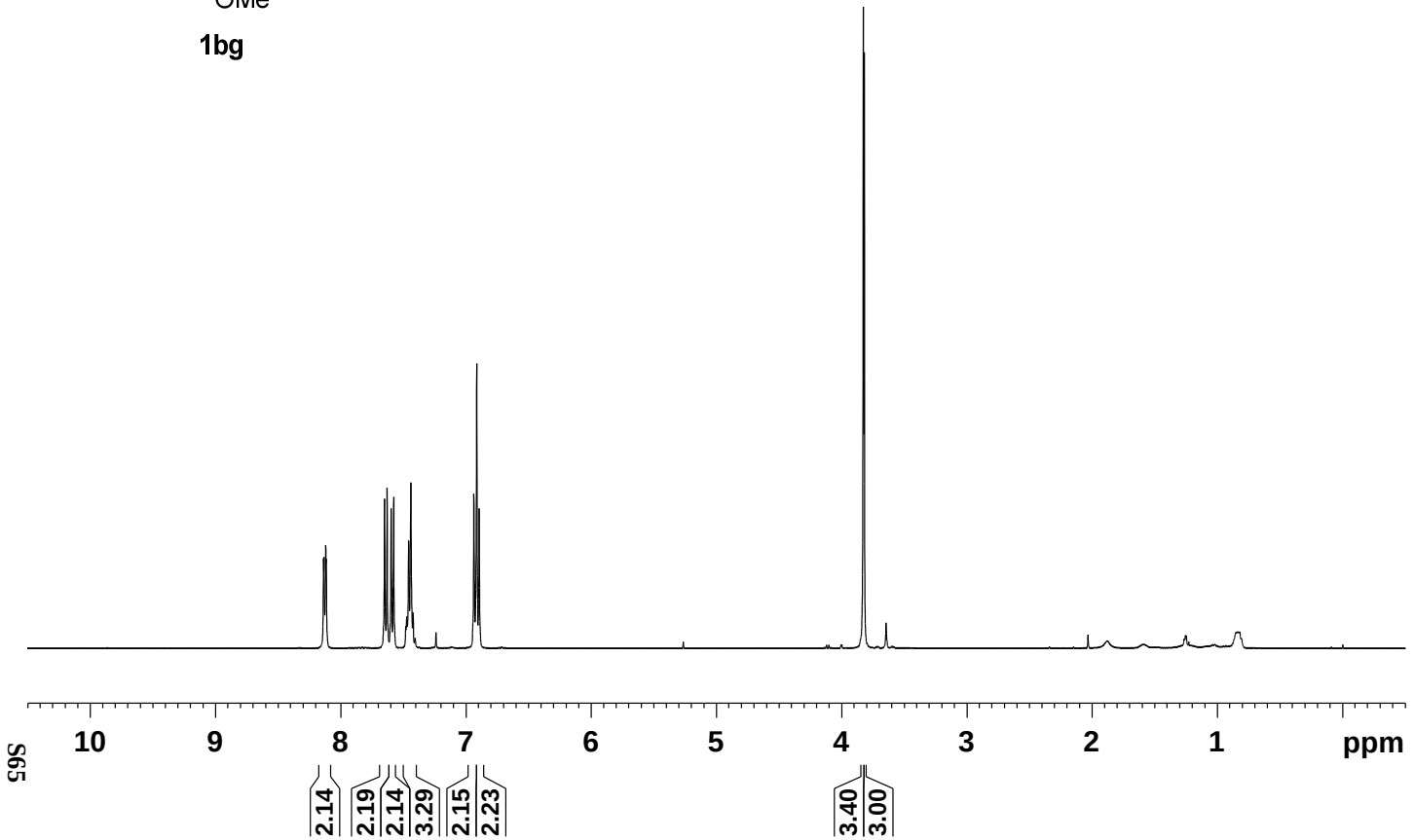
======== CHANNEL f1 ========
NUC1                     13C
P1                    10.00 usec
PL1                    6.50 dB
SFO1             125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 90.00 usec
PL2                   -0.60 dB
PL12                  15.20 dB
PL13                  18.20 dB
SFO2             500.1320005 MHz

F2 - Processing parameters
SI                     65536
SF               125.7577890 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.00
```



1bg

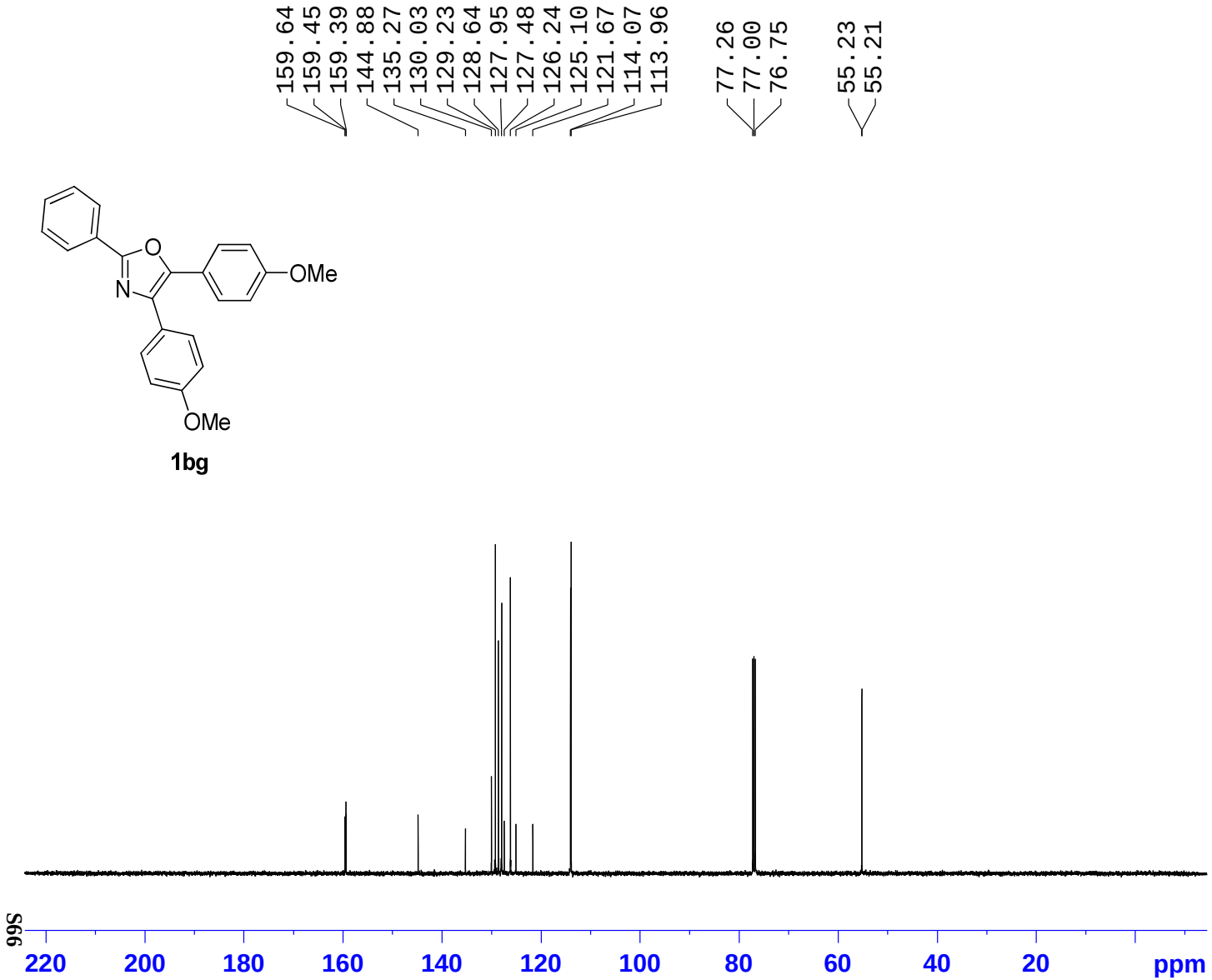



```
Current Data Parameters
NAME            mina025
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20120901
Time              15.31
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                   64
DW               69.000 usec
DE                6.50 usec
TE                299.1 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.70 usec
PL1                4.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300167 MHz
WDW                  EM
SSB      0
LB       0 Hz
GB       0
PC                1.00
```



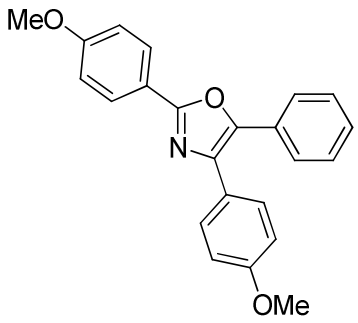

```
Current Data Parameters
NAME                 mina092
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130129
Time                   21.09
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        120
DS                          0
SWH                30030.029 Hz
FIDRES              0.458222 Hz
AQ                  1.0912410 sec
RG                     9195.2
DW                    16.650 usec
DE                     6.50 usec
TE                     294.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

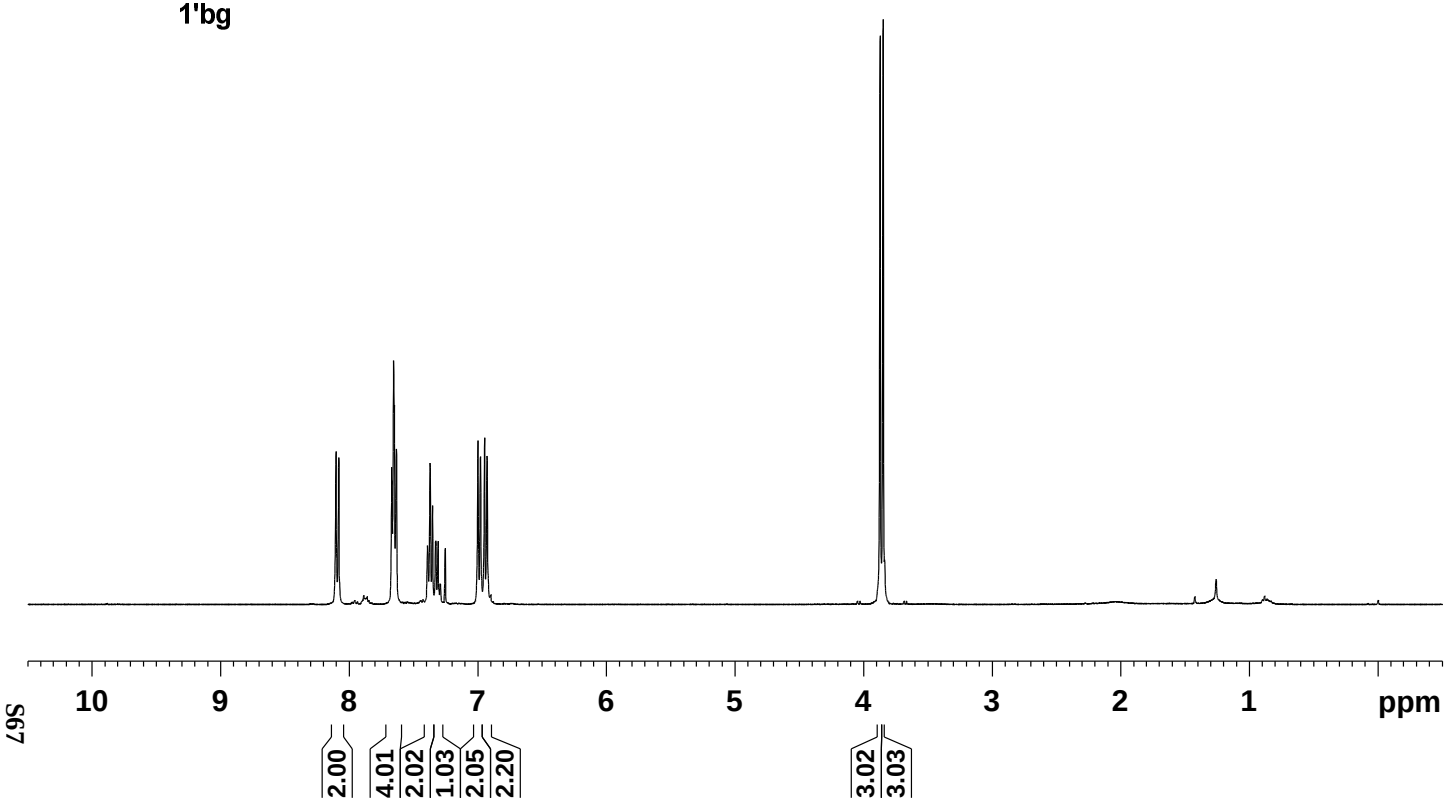
======== CHANNEL f1 ========
NUC1                      13C
P1                     10.00 usec
PL1                     6.50 dB
SFO1             125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  90.00 usec
PL2                    -0.60 dB
PL12                   15.20 dB
PL13                   18.20 dB
SFO2             500.1320005 MHz

F2 - Processing parameters
SI                      65536
SF               125.7578028 MHz
WDW                        EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.00
```



1'bg



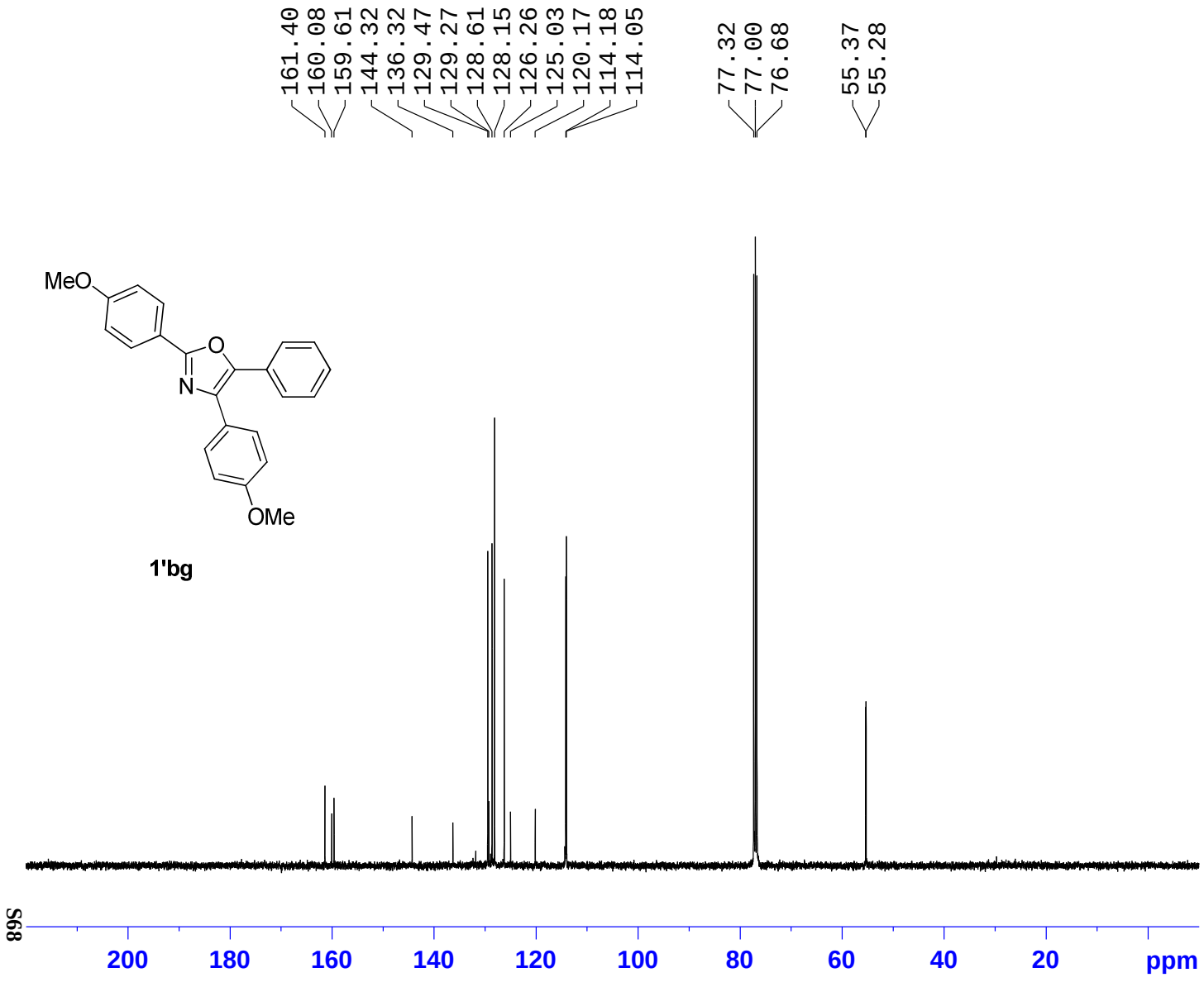
S67

```
Current Data Parameters
NAME            mina025
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20130226
Time              17.56
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  114
DW               69.000 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300122 MHz
WDW                  EM
SSB      0
LB       0 Hz
GB       0
PC                 1.00
```



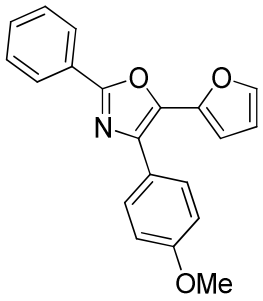

```
Current Data Parameters
NAME            mina025
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20130227
Time               7.24
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 1163
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG               9195.2
DW                20.800 usec
DE                 6.50 usec
TE                300.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

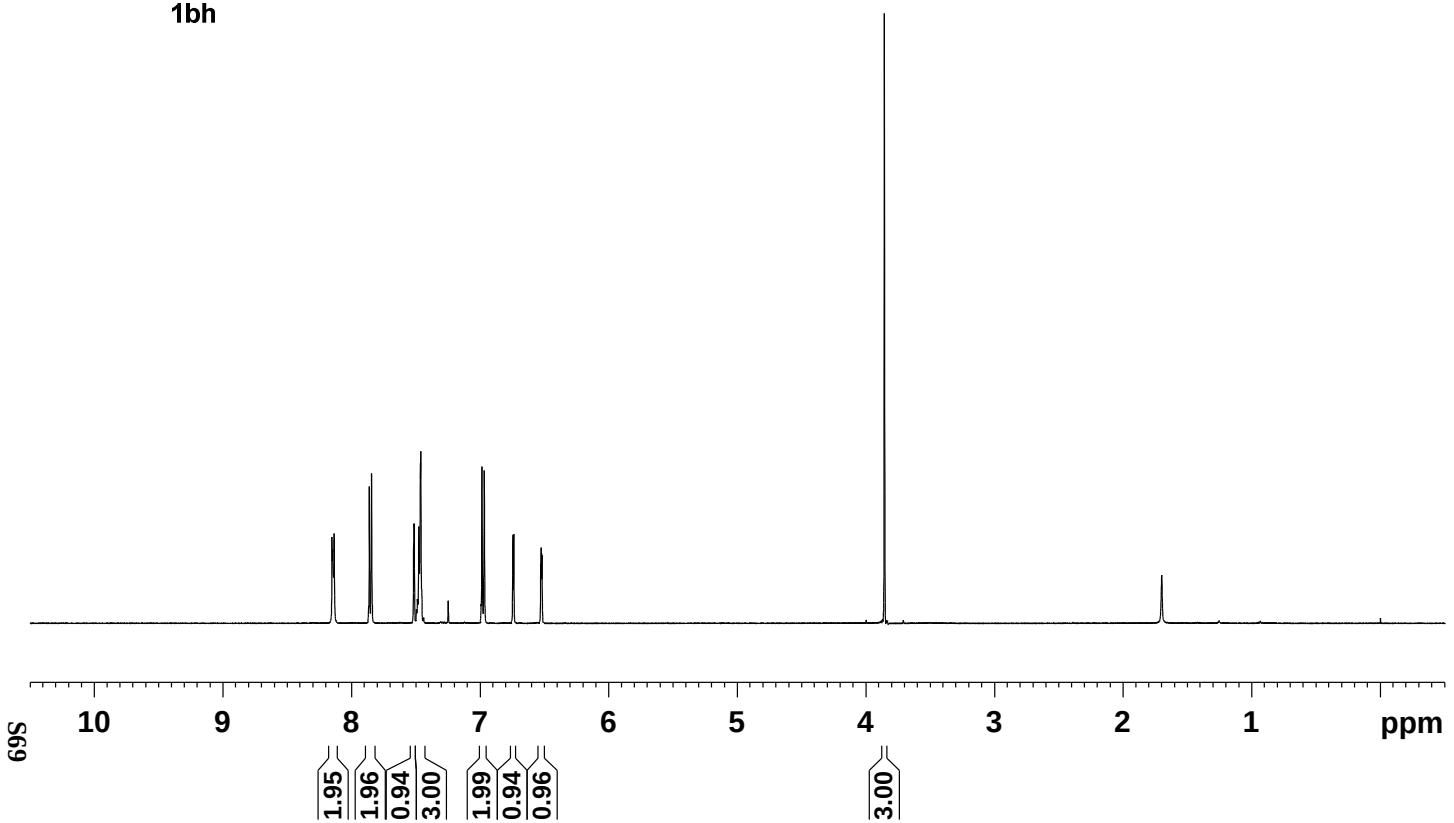
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.40 usec
PL1                 7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12                20.70 dB
PL13                23.70 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127716 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.00
```



1bh

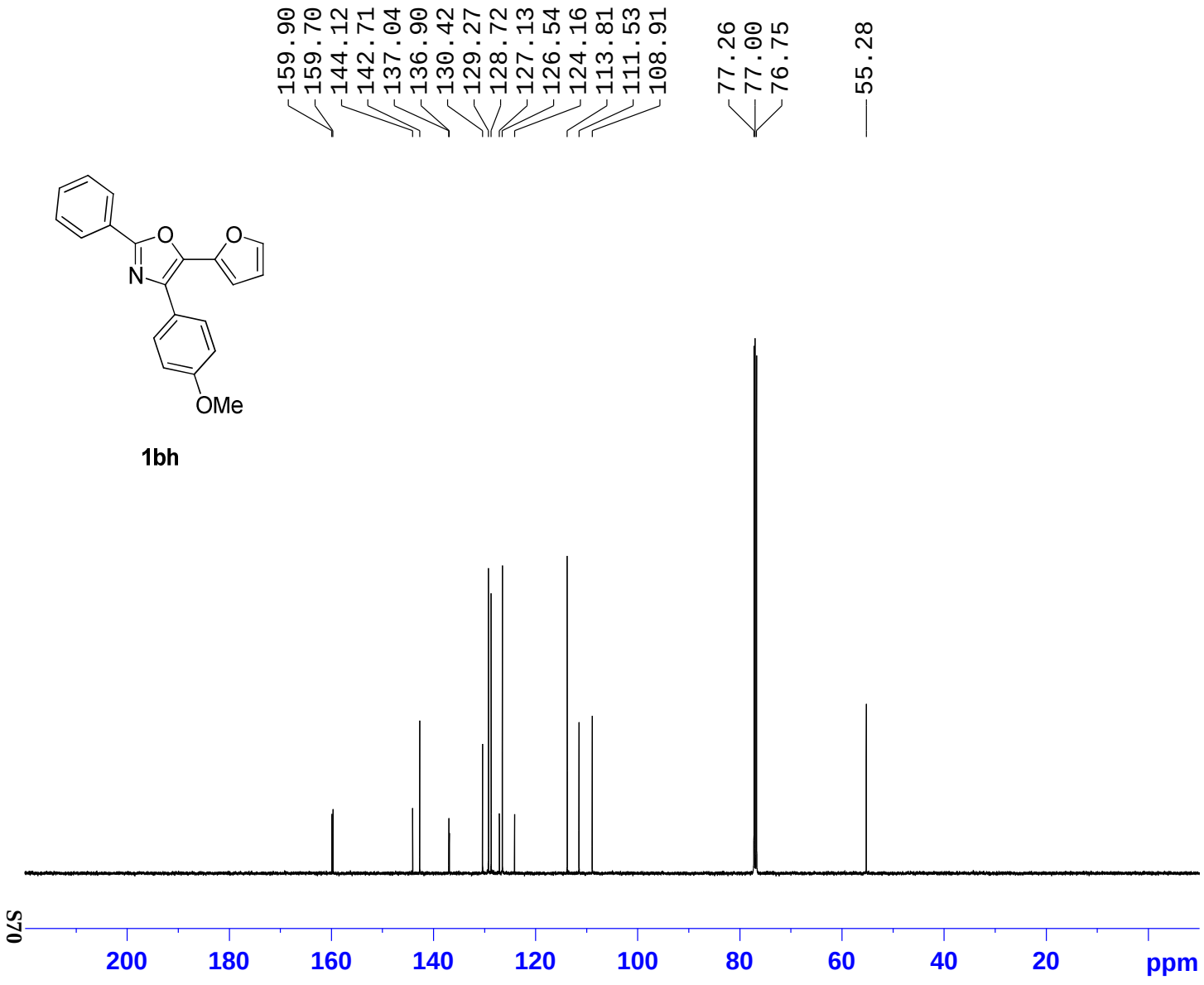



```
Current Data Parameters
NAME            mina045
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20120901
Time              15.19
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    4
DS                    0
SWH            9057.971 Hz
FIDRES         0.276427 Hz
AQ             1.8088988 sec
RG                  114
DW                55.200 usec
DE                 6.50 usec
TE                294.8 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1      0 dB
SFO1        500.1330008 MHz

F2 - Processing parameters
SI                16384
SF          500.1300184 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



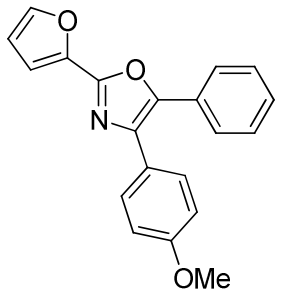

```
Current Data Parameters
NAME                  mina045
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20120901
Time                   15.21
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        747
DS                          0
SWH                30030.029 Hz
FIDRES              0.458222 Hz
AQ                  1.0912410 sec
RG                     9195.2
DW                     16.650 usec
DE                      6.50 usec
TE                     295.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                     10.50 usec
PL1                     7.00 dB
SFO1             125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  90.00 usec
PL2                    -0.60 dB
PL12                   15.00 dB
PL13                   18.00 dB
SFO2             500.1320005 MHz

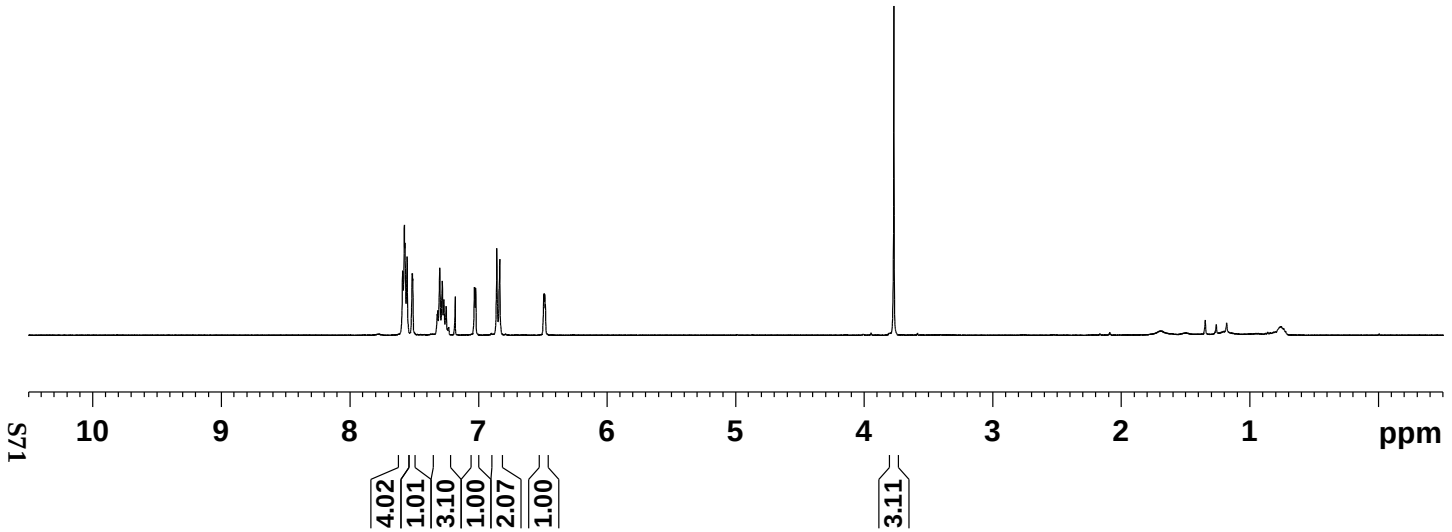
F2 - Processing parameters
SI                      65536
SF               125.7577949 MHz
WDW                        EM
SSB           0
LB                      1.00 Hz
GB            0
PC                      1.00
```

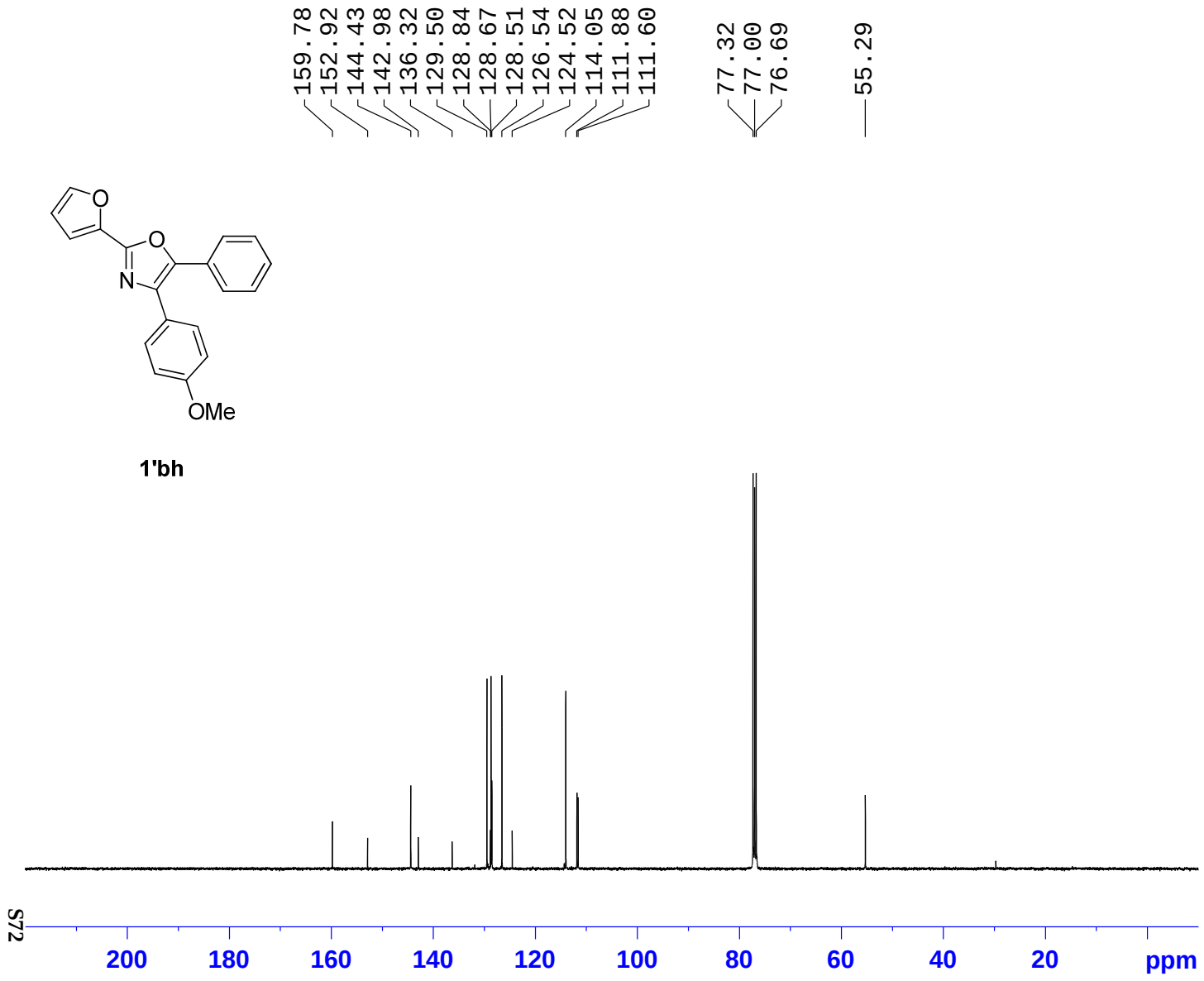


1'bh

```
NAME            mina093
EXPNO                 6
PROCNO                1
Date_          20121127
Time               8.15
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                161.3
DW               69.000 usec
DE                6.50 usec
TE                299.4 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz
SI                16384
SF          400.1300406 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```





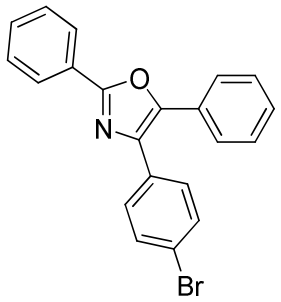

```
Current Data Parameters
NAME                 mina093
EXPNO                     13
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130131
Time                   0.12
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     4000
DS                        0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6816452 sec
RG                    9195.2
DW                   20.800 usec
DE                    6.50 usec
TE                   299.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

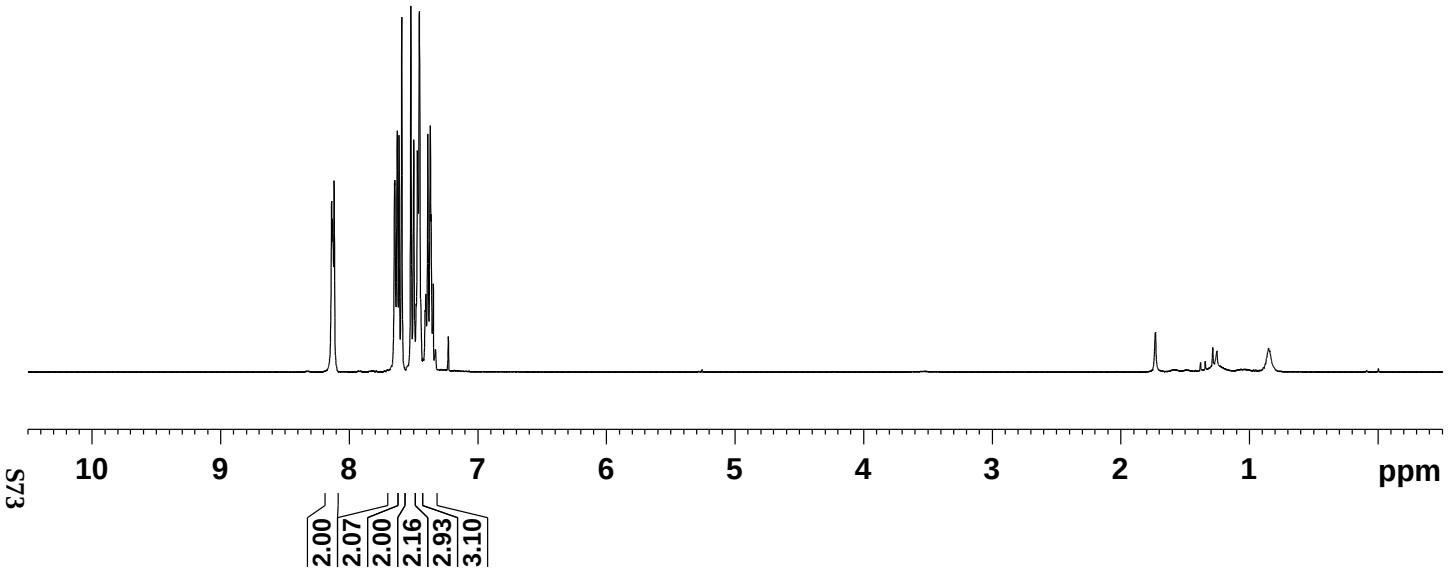
======== CHANNEL f1 ========
NUC1                    13C
P1                    10.50 usec
PL1                    7.00 dB
SFO1           100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -0.60 dB
PL12                 15.00 dB
PL13                 18.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6127679 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```



1ca

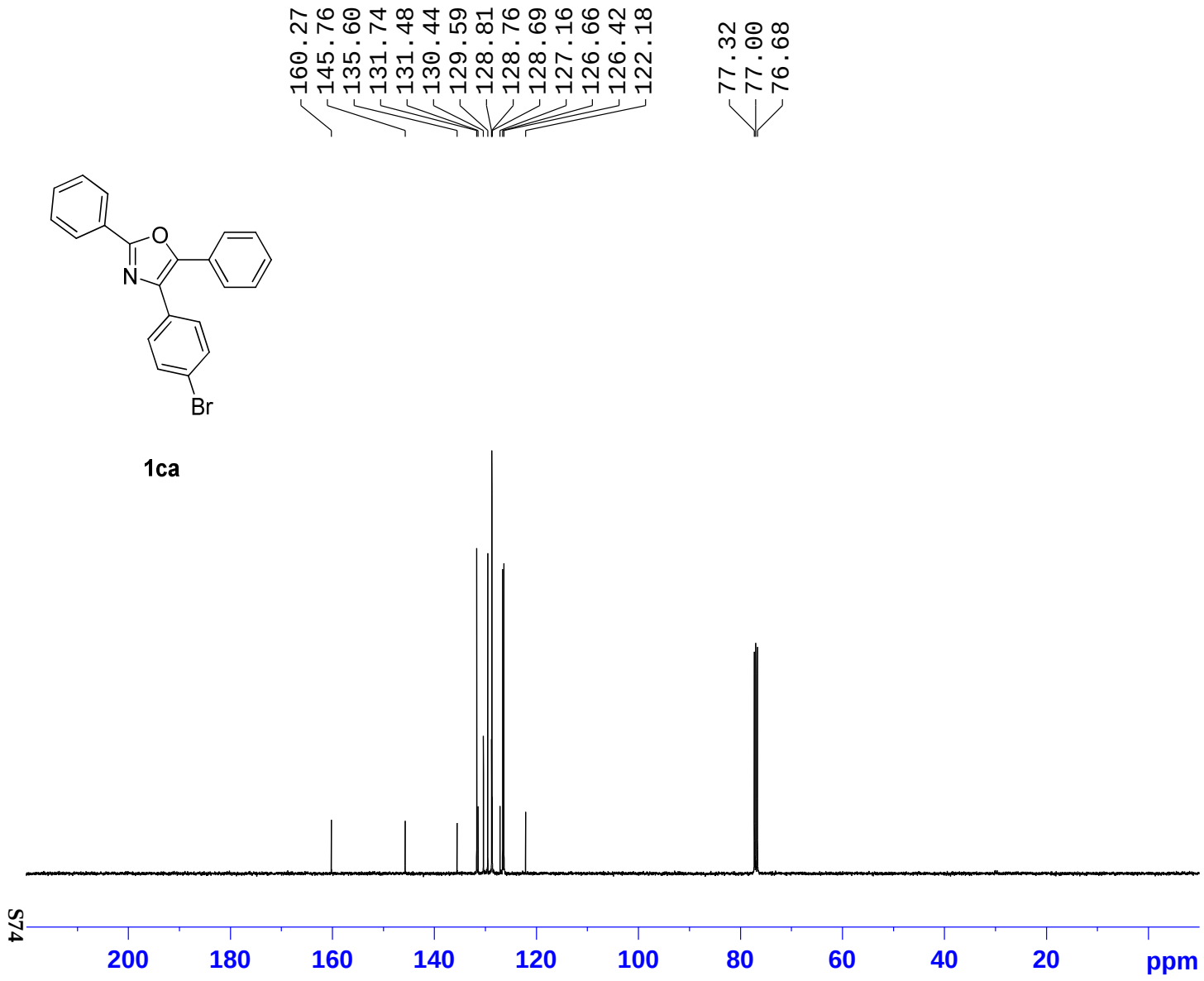



```
Current Data Parameters
NAME            mina075
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20121102
Time               7.15
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 71.8
DW               69.000 usec
DE                 6.50 usec
TE                299.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300211 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



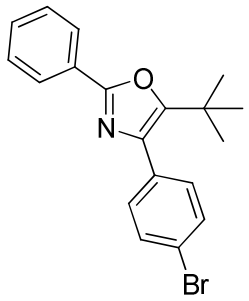

```
Current Data Parameters
NAME                  mina075
EXPNO                      10
PROCNO                      1

F2 - Acquisition Parameters
Date_               20121102
Time                    7.17
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                        550
DS                          0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     299.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

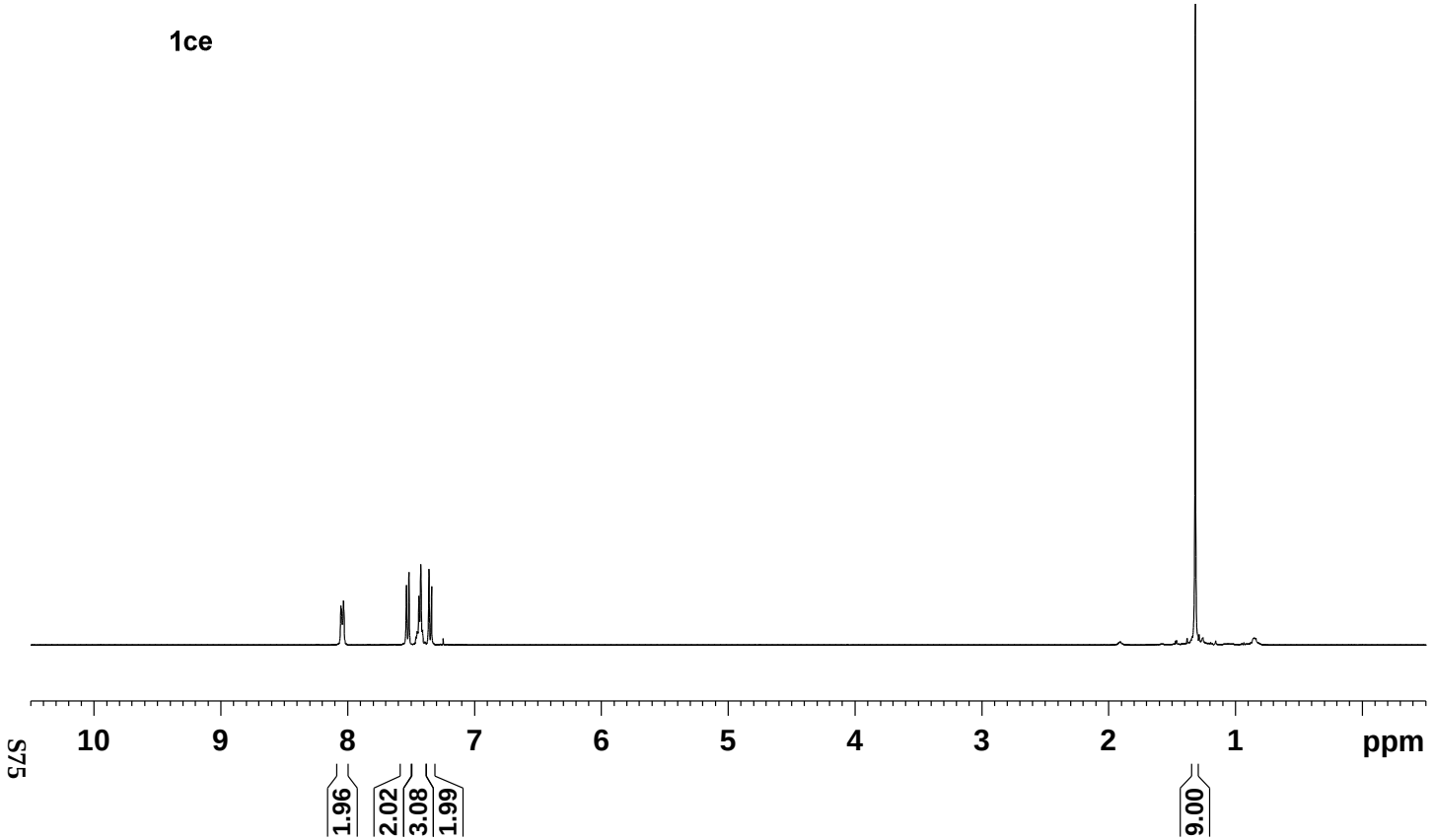
======== CHANNEL f1 ========
NUC1                      13C
P1                       9.40 usec
PL1                      7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                   90.00 usec
PL2                      3.00 dB
PL12                    20.70 dB
PL13                    23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF               100.6127767 MHz
WDW                        EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.00
```



1ce

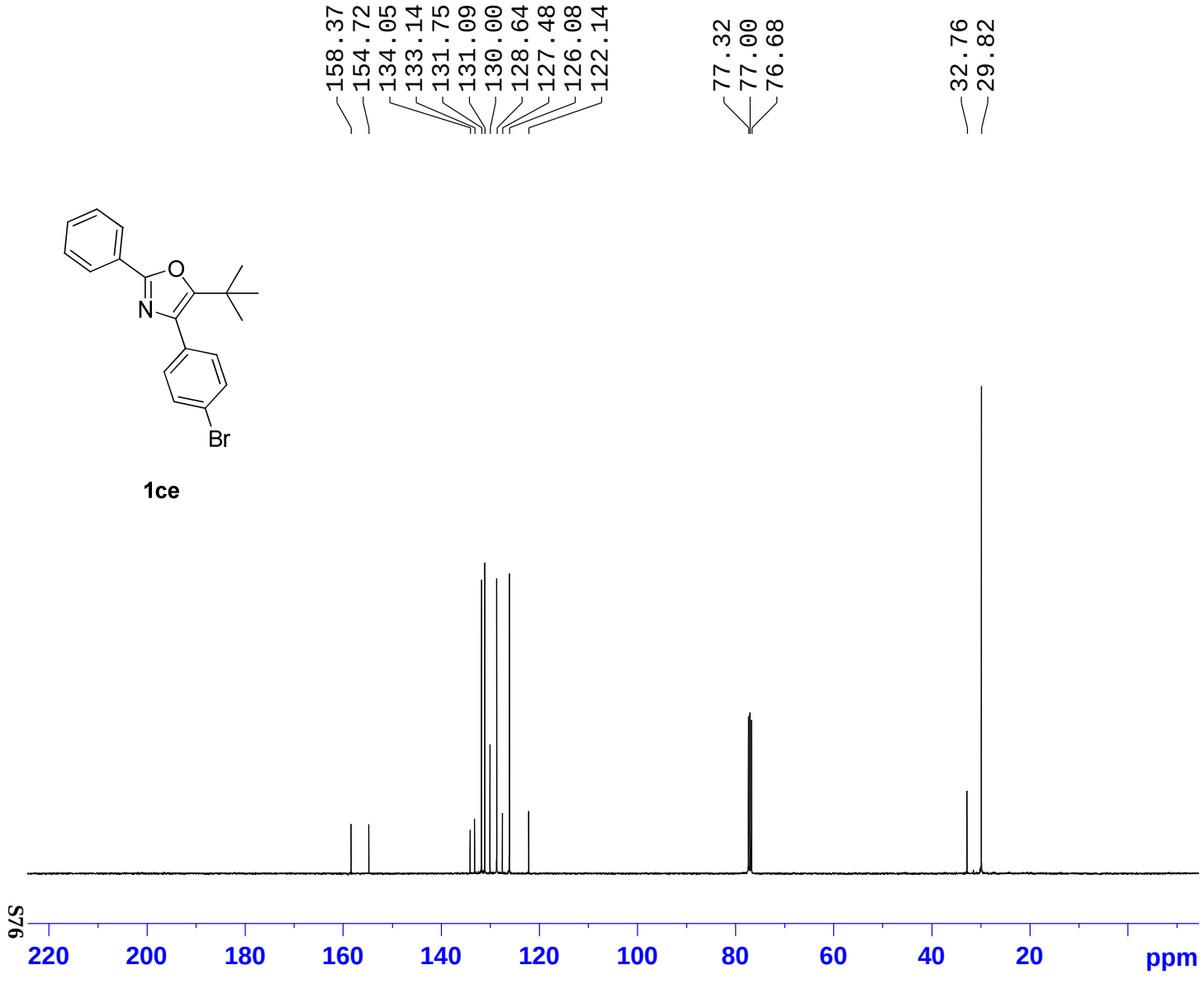



```
Current Data Parameters
NAME            mina076
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20121026
Time              18.31
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 45.3
DW               69.000 usec
DE                6.50 usec
TE                298.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300141 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



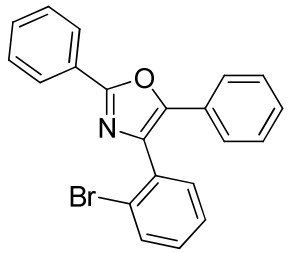

```
Current Data Parameters
NAME                 mina076
EXPNO                      8
PROCNO                     1

F2 - Acquisition Parameters
Date_               20121026
Time                   18.37
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      1000
DS                         0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     298.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

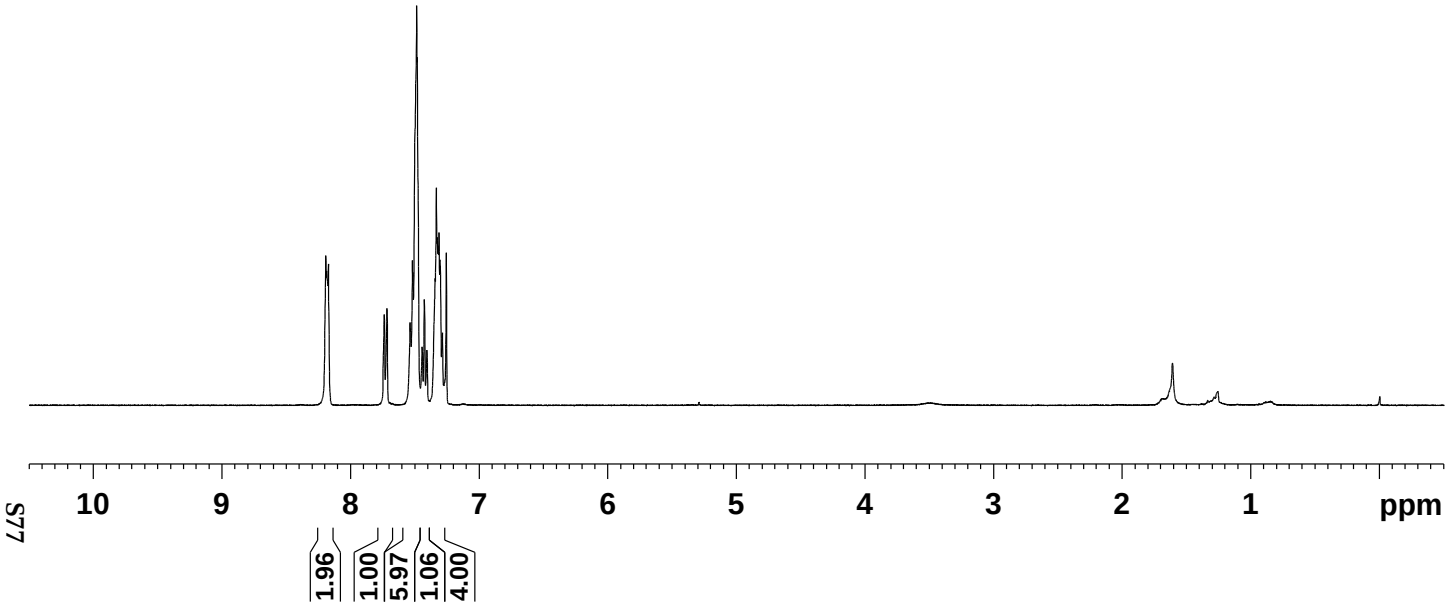
======== CHANNEL f1 ========
NUC1                     13C
P1                      9.40 usec
PL1                     7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                  90.00 usec
PL2                     3.00 dB
PL12                   20.70 dB
PL13                   23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF               100.6127690 MHz
WDW                       EM
SSB      0
LB                      1.00 Hz
GB       0
PC                      1.00
```



1da

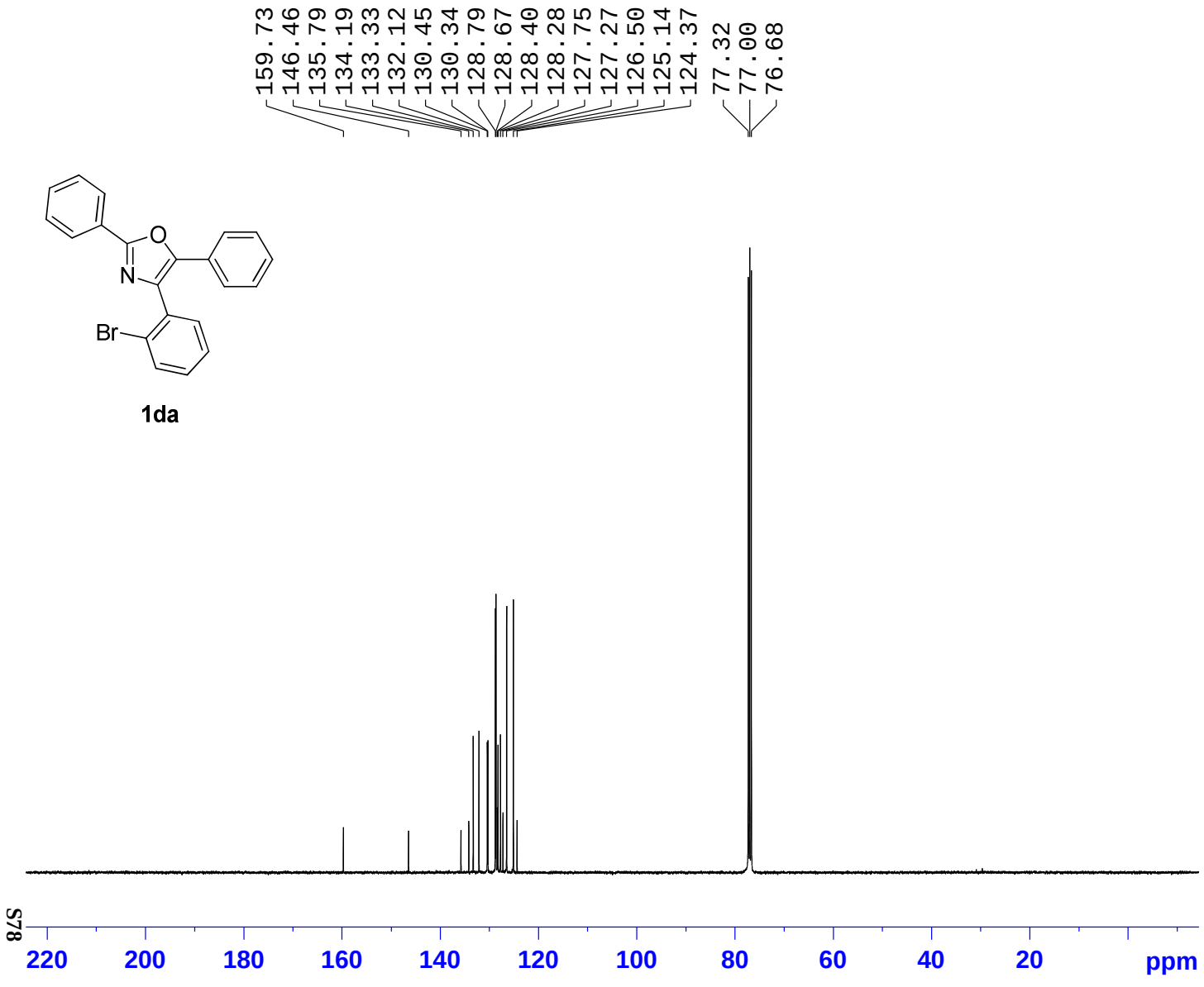



```
Current Data Parameters
NAME            mina088
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20121207
Time              22.59
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  256
DW               69.000 usec
DE                6.50 usec
TE                298.5 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300109 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



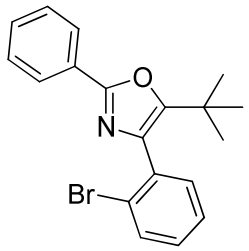

```
Current Data Parameters
NAME            mina088
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20121207
Time              23.01
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                11976
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG               9195.2
DW                20.800 usec
DE                 6.50 usec
TE                298.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

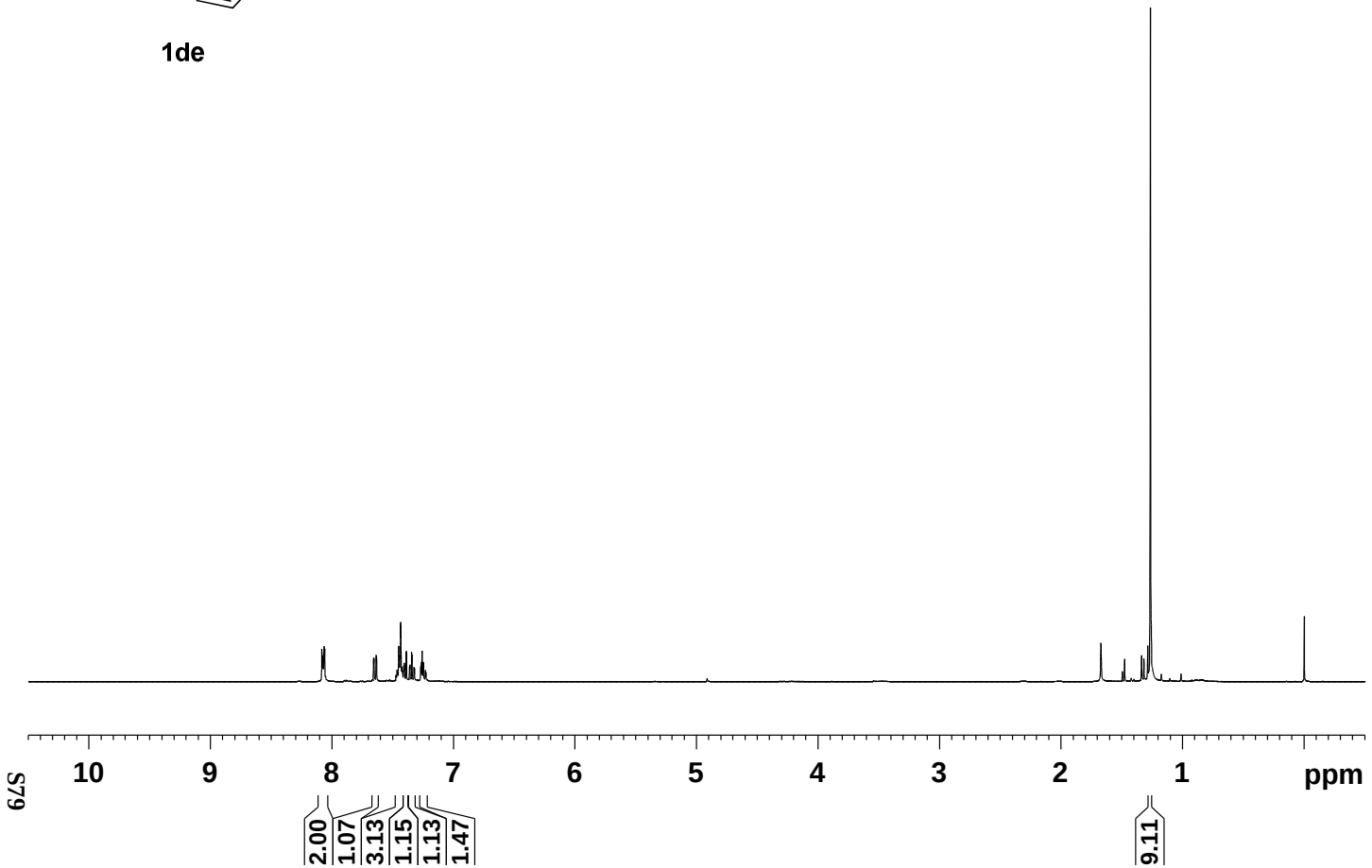
======== CHANNEL f1 ========
NUC1                13C
P1                 9.40 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             90.00 usec
PL2                3.00 dB
PL12               20.70 dB
PL13               23.70 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127716 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.00
```



1de

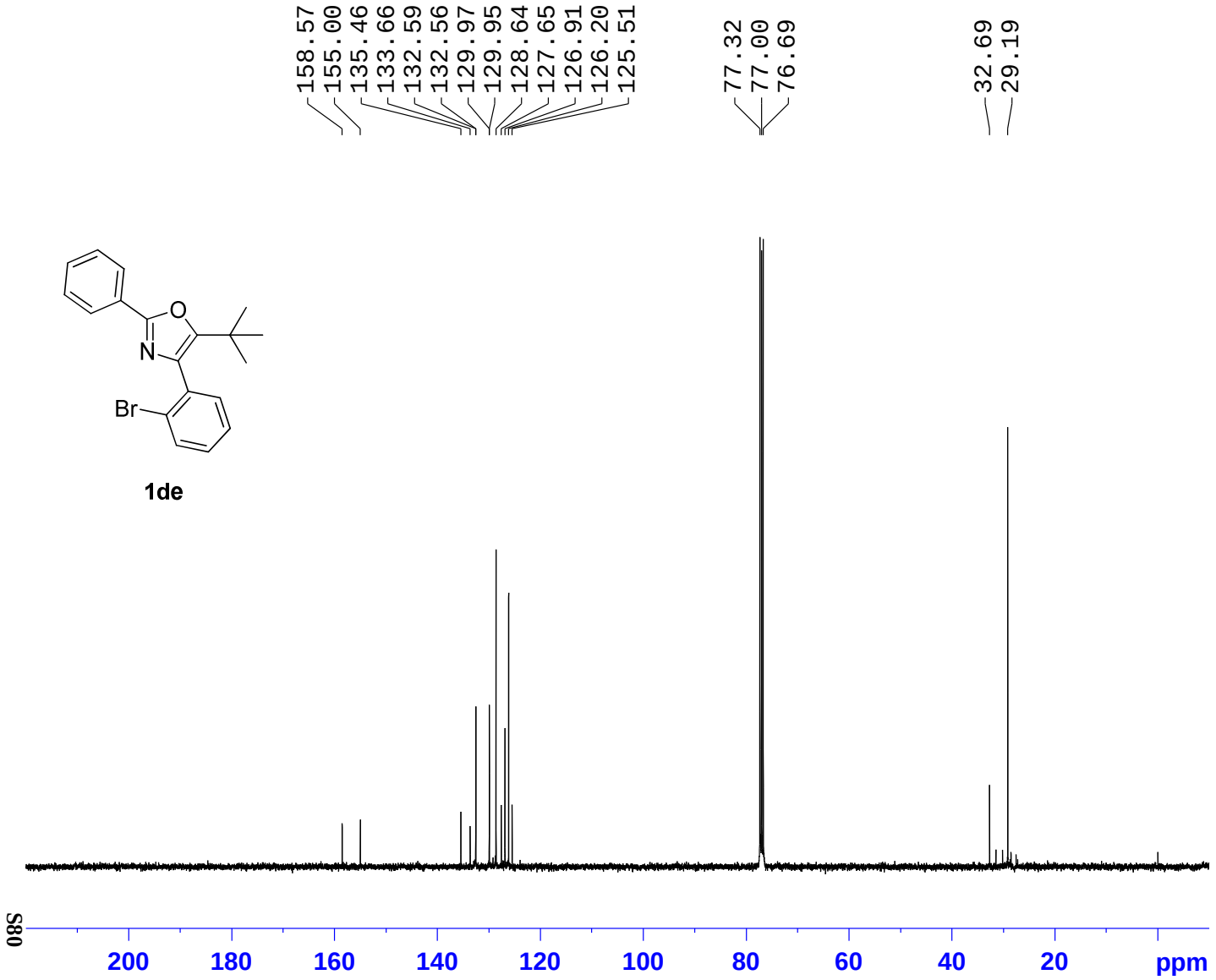



```
Current Data Parameters
NAME            mina089
EXPNO                 8
PROCNO                1

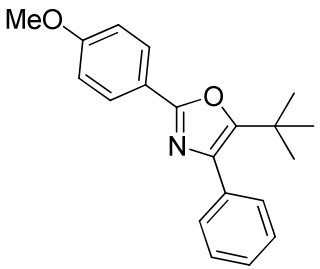
F2 - Acquisition Parameters
Date_          20130110
Time              13.33
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES         0.221142 Hz
AQ             2.2611110 sec
RG                  114
DW                69.000 usec
DE                 6.50 usec
TE                296.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

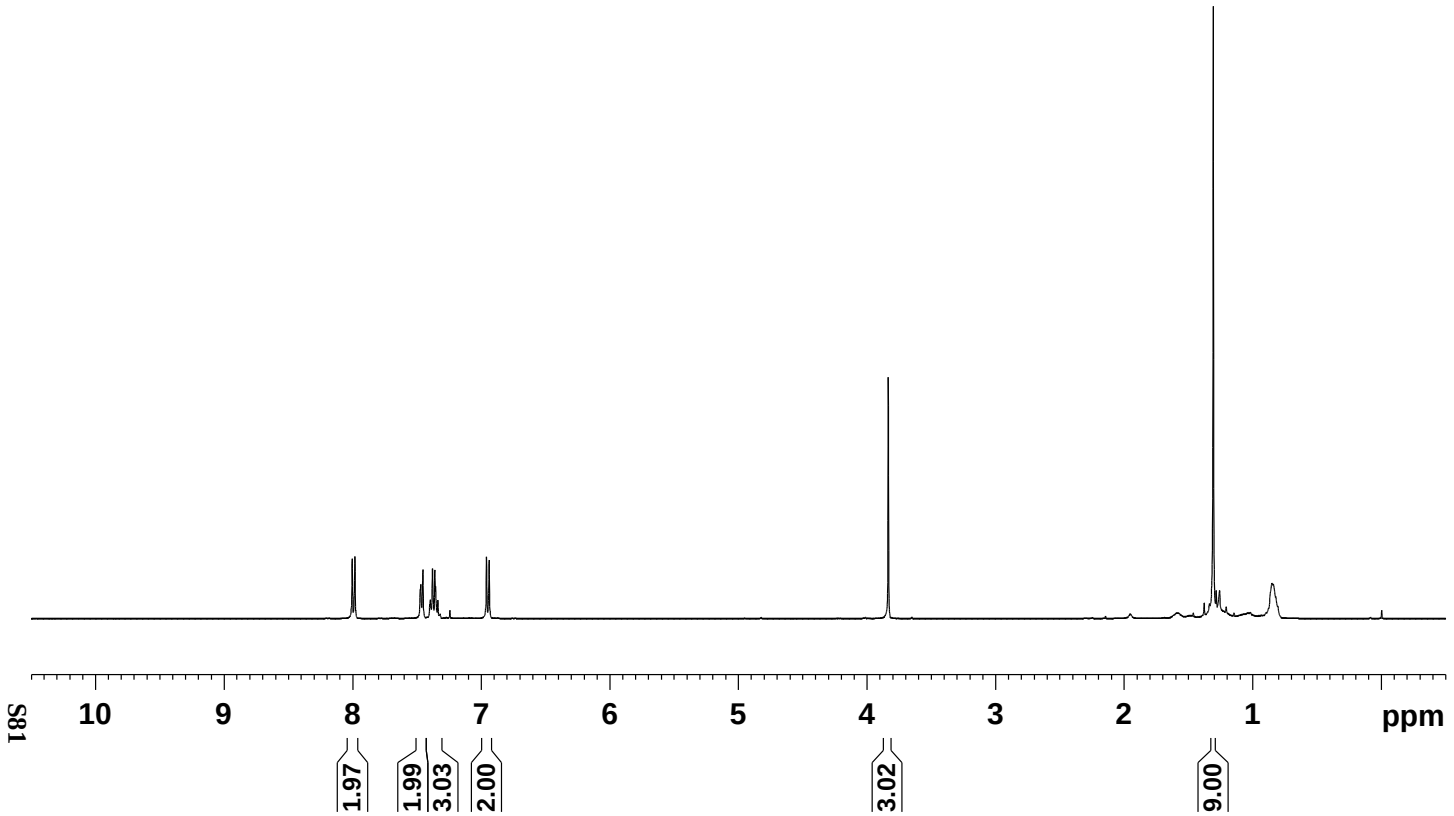
F2 - Processing parameters
SI                16384
SF          400.1300100 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



NAME	mina089
EXPNO	11
PROCNO	1
Date_	20130110
Time	22.18
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	1038
DS	0
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	0.6816452 sec
RG	9195.2
DW	20.800 usec
DE	6.50 usec
TE	296.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.40 usec
PL1	7.00 dB
SFO1	100.6233325 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	3.00 dB
PL12	20.70 dB
PL13	23.70 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127716 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

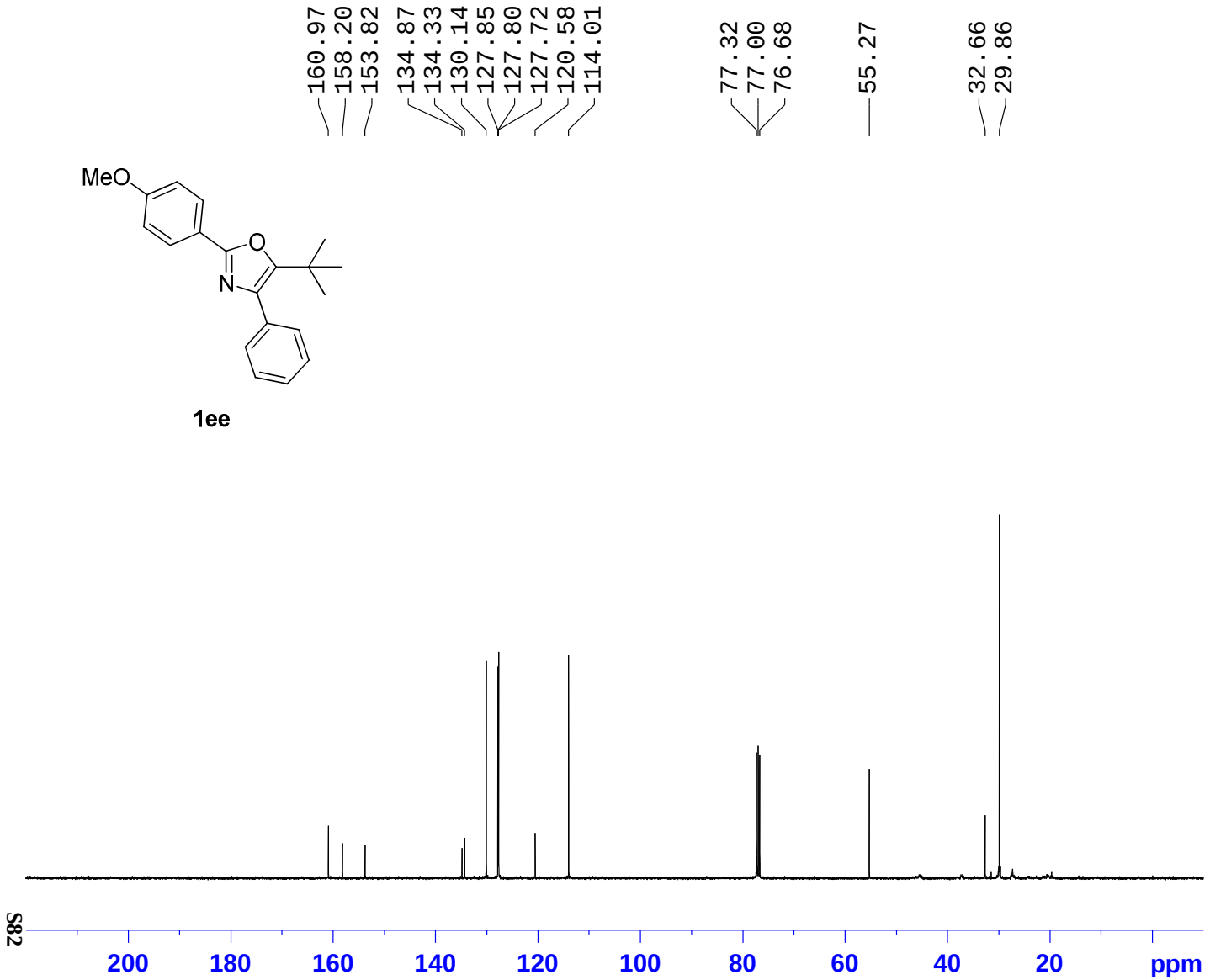


1ee

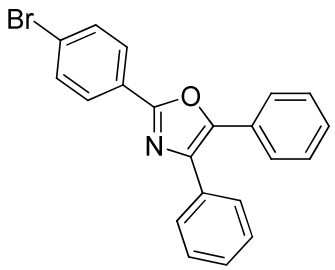



```
NAME            mina081
EXPNO                 5
PROCNO                1
Date_          20121103
Time              18.06
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 35.9
DW                69.000 usec
DE                 6.50 usec
TE                298.6 K
D1           2.00000000 sec
TD0                   1

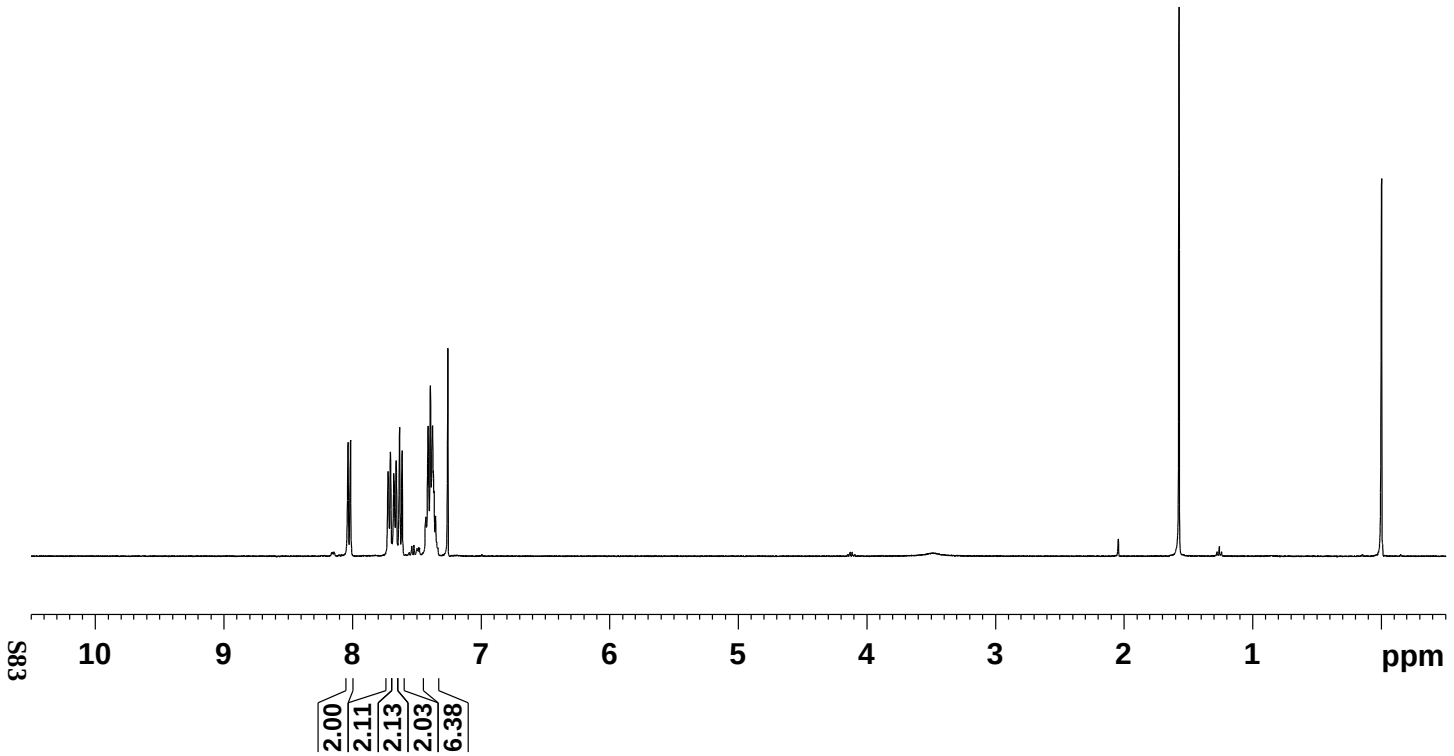
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.90 usec
PL1                 3.00 dB
SFO1        400.1324008 MHz
SI                 16384
SF          400.1300154 MHz
WDW                   EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```



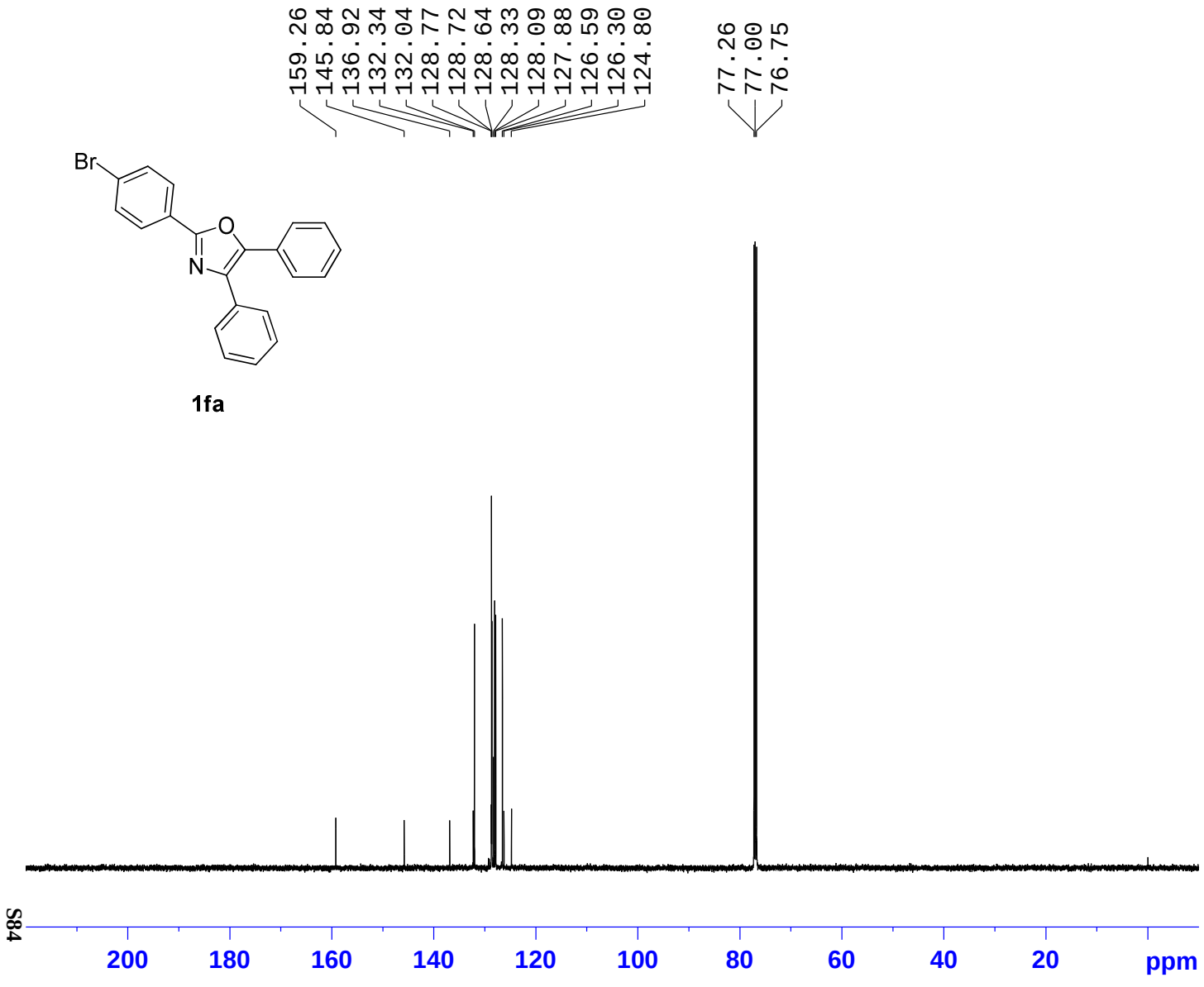
NAME	mina081
EXPNO	6
PROCNO	1
Date_	20121103
Time	18.14
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	400
DS	0
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	0.6816452 sec
RG	9195.2
DW	20.800 usec
DE	6.50 usec
TE	298.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.40 usec
PL1	7.00 dB
SFO1	100.6233325 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	3.00 dB
PL12	20.70 dB
PL13	23.70 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127760 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00



1fa



NAME	mina084
EXPNO	6
PROCNO	1
Date_	20121113
Time	18.43
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	7246.377 Hz
FIDRES	0.221142 Hz
AQ	2.2611110 sec
RG	322.5
DW	69.000 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	11.90 usec
PL1	3.00 dB
SFO1	400.1324008 MHz
SI	16384
SF	400.1300092 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



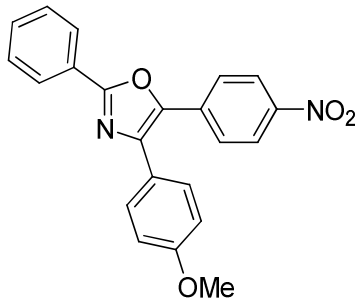

```
Current Data Parameters
NAME            mina084
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20121124
Time              14.01
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  667
DS                    0
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912410 sec
RG               9195.2
DW              16.650 usec
DE               6.50 usec
TE              297.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

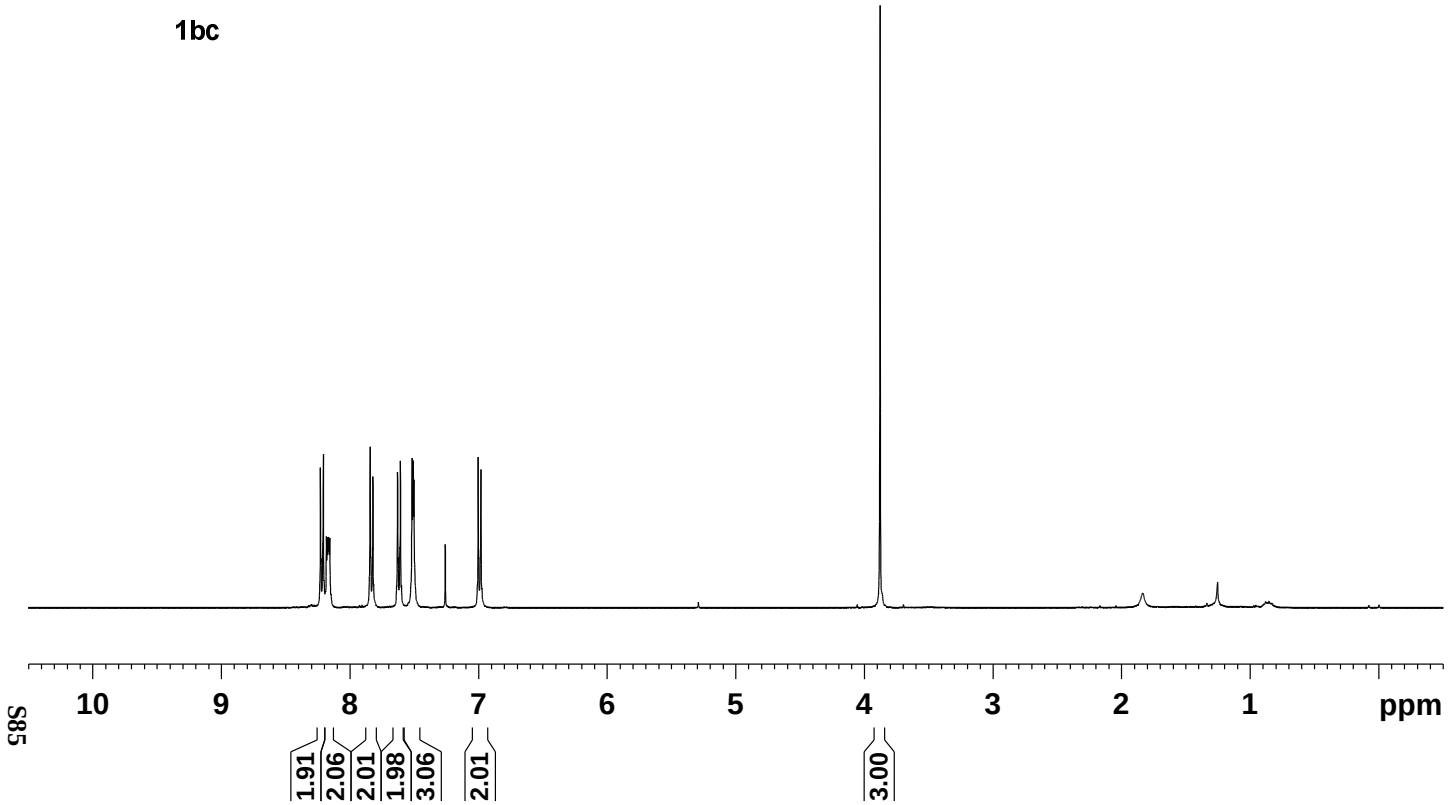
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                6.50 dB
SFO1        125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -0.60 dB
PL12              15.20 dB
PL13              18.20 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                65536
SF          125.7577927 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.00
```



1bc

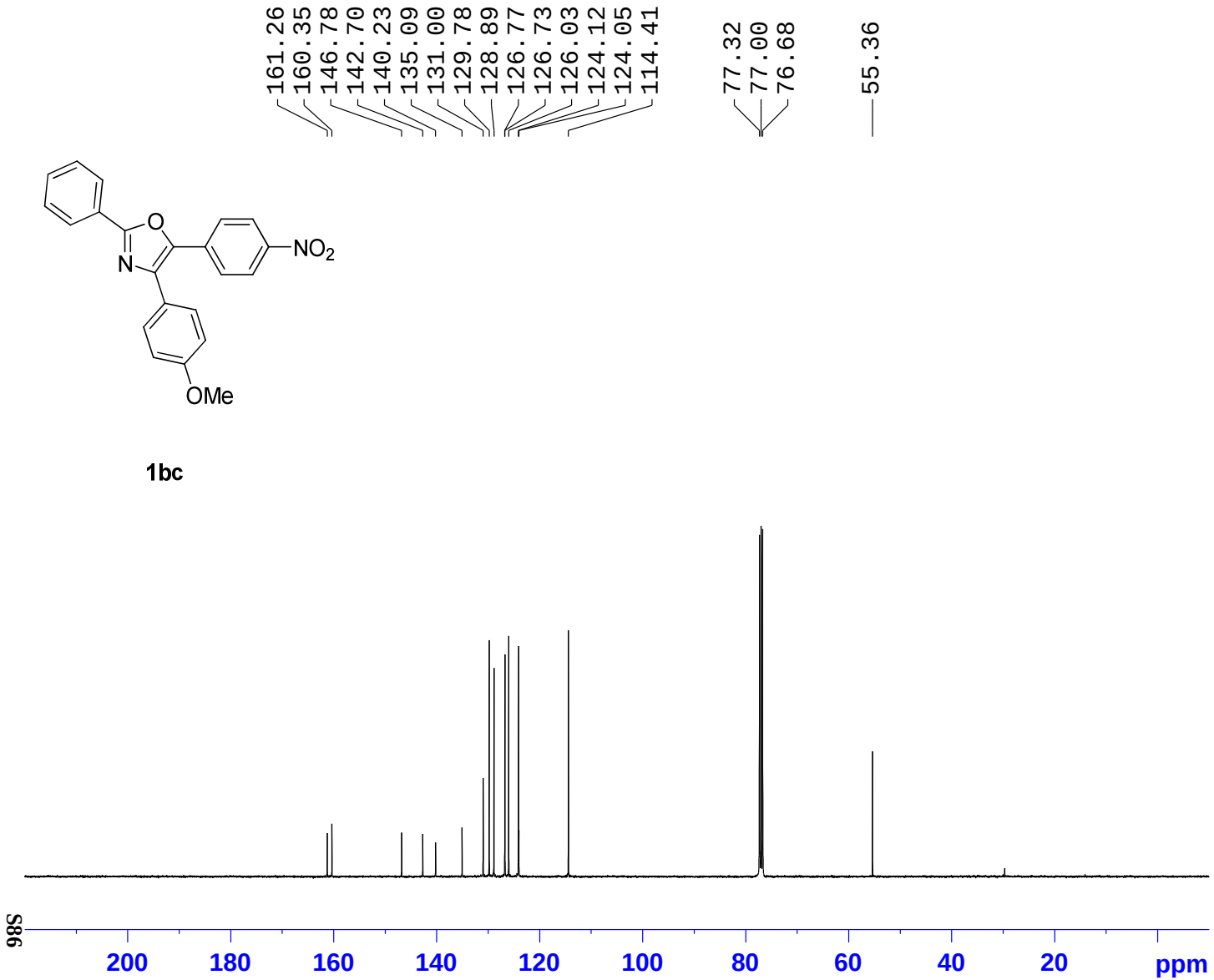



```
Current Data Parameters
NAME            mina027
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20130124
Time              12.02
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                161.3
DW               69.000 usec
DE                6.50 usec
TE                298.1 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300096 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



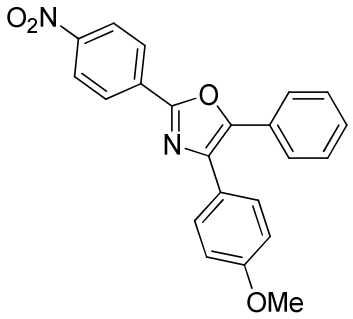

```
Current Data Parameters
NAME                 mina027
EXPNO                      9
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130126
Time                 23.55
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                   10000
DS                       0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6816452 sec
RG                   9195.2
DW                  20.800 usec
DE                   6.50 usec
TE                  298.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.40 usec
PL1                  7.00 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                  3.00 dB
PL12                20.70 dB
PL13                23.70 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127716 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.00
```



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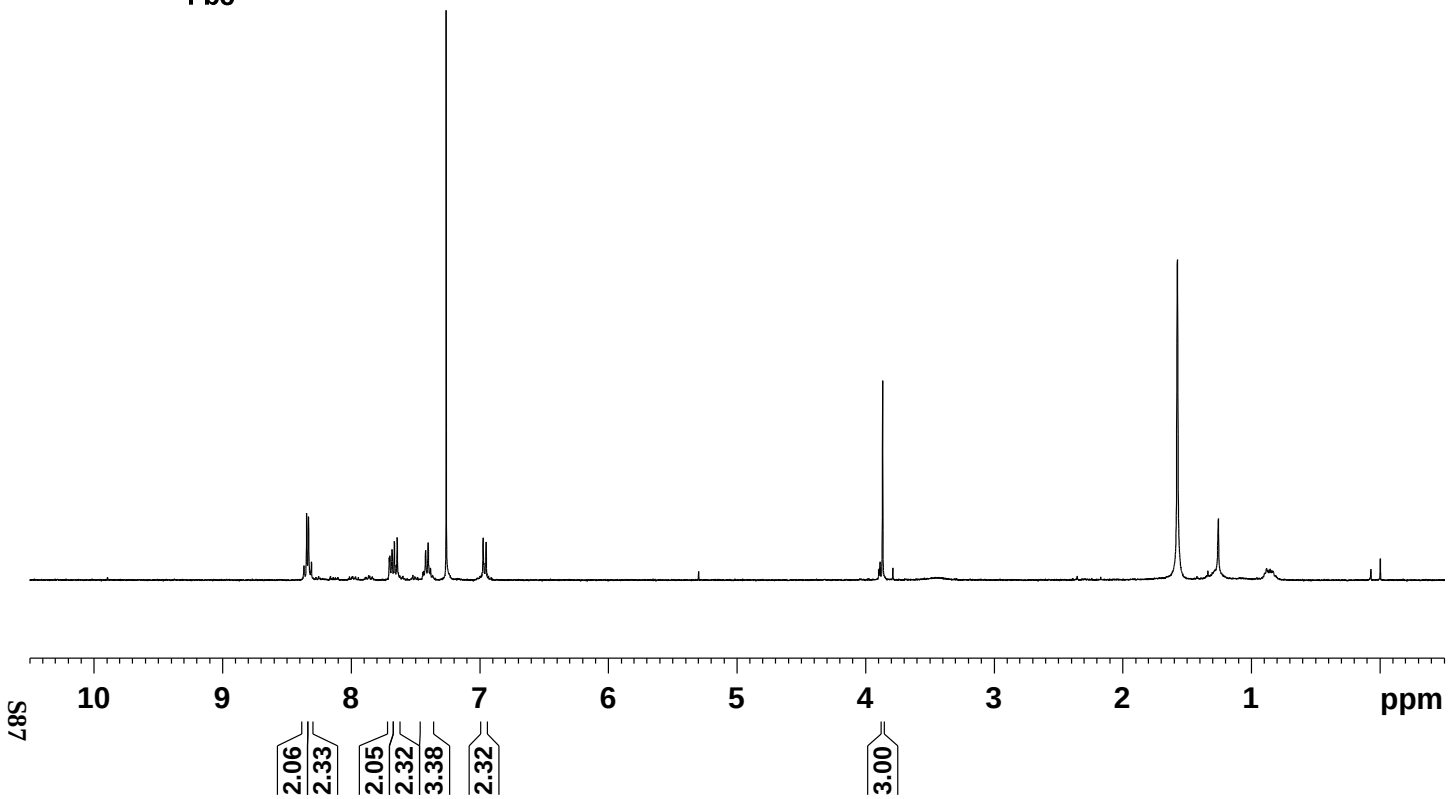
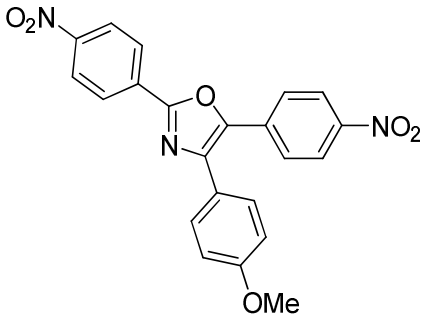



```
Current Data Parameters
NAME                  mina027
EXPNO                       5
PROCNO                      1

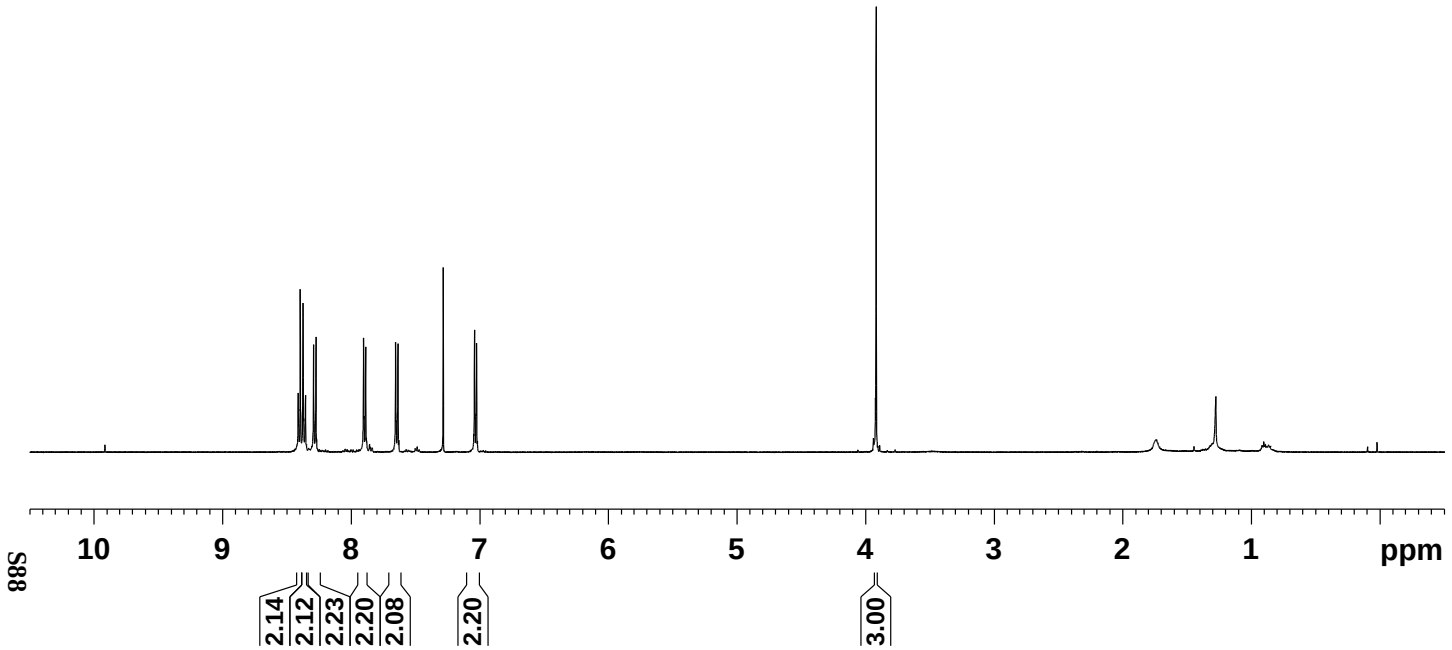
F2 - Acquisition Parameters
Date_               20130123
Time                   23.56
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 7246.377 Hz
FIDRES              0.221142 Hz
AQ                  2.2611110 sec
RG                       362
DW                    69.000 usec
DE                     6.50 usec
TE                    299.3 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.90 usec
PL1                     3.00 dB
SFO1             400.1324008 MHz

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



9bc

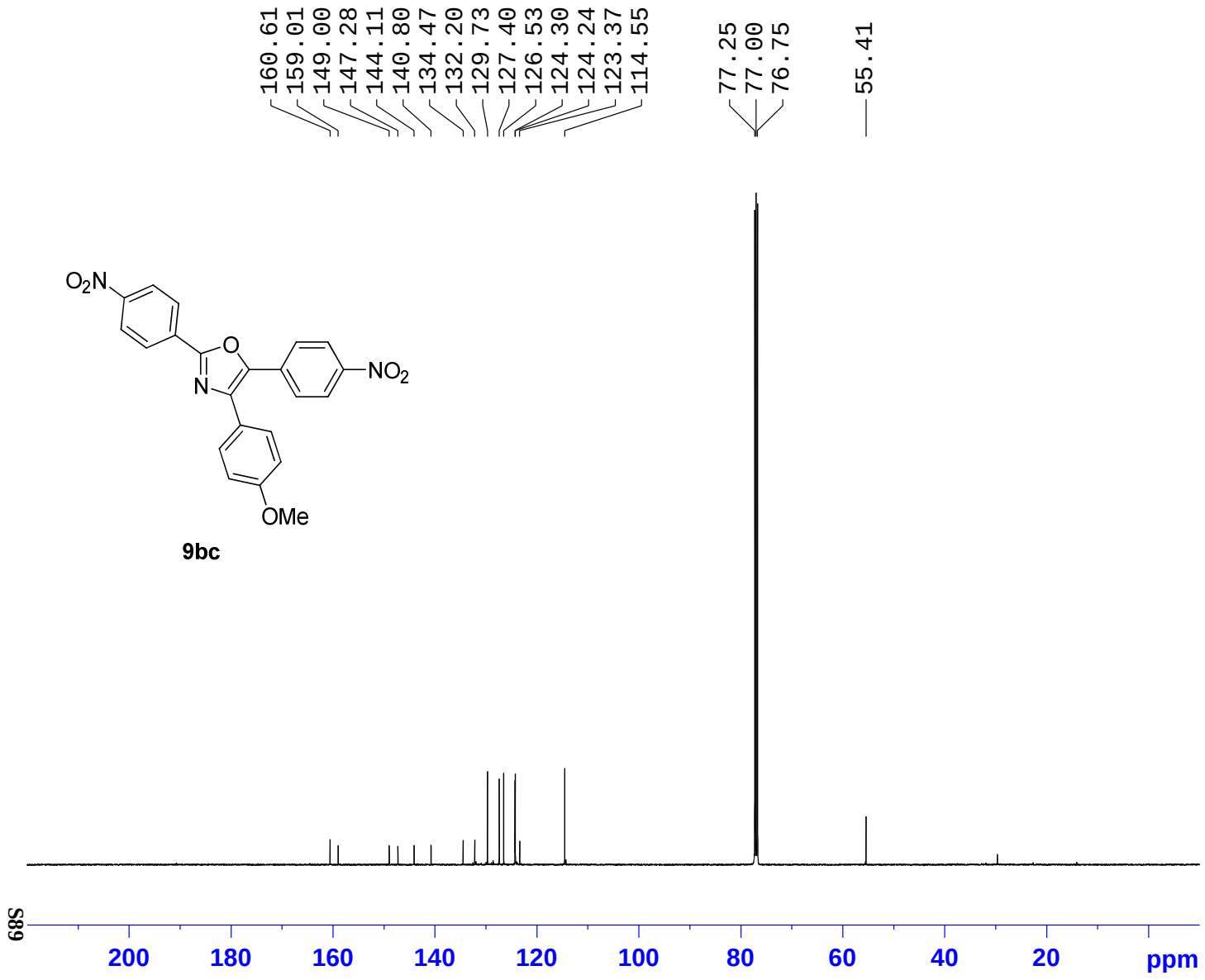



```
Current Data Parameters
NAME            mina027
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20130130
Time              21.39
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            9057.971 Hz
FIDRES         0.276427 Hz
AQ             1.8088988 sec
RG                  362
DW                55.200 usec
DE                 6.50 usec
TE                294.1 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.20 usec
PL1               -0.60 dB
SFO1        500.1330008 MHz

F2 - Processing parameters
SI                16384
SF          500.1300000 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



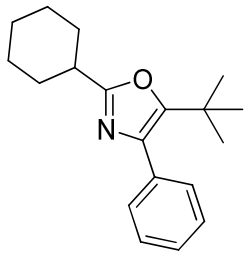

```
Current Data Parameters
NAME            mina027
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20130130
Time              21.42
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                11951
DS                    0
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912410 sec
RG               9195.2
DW               16.650 usec
DE                6.50 usec
TE                294.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                6.50 dB
SFO1        125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -0.60 dB
PL12              15.20 dB
PL13              18.20 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                65536
SF          125.7577908 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.00
```



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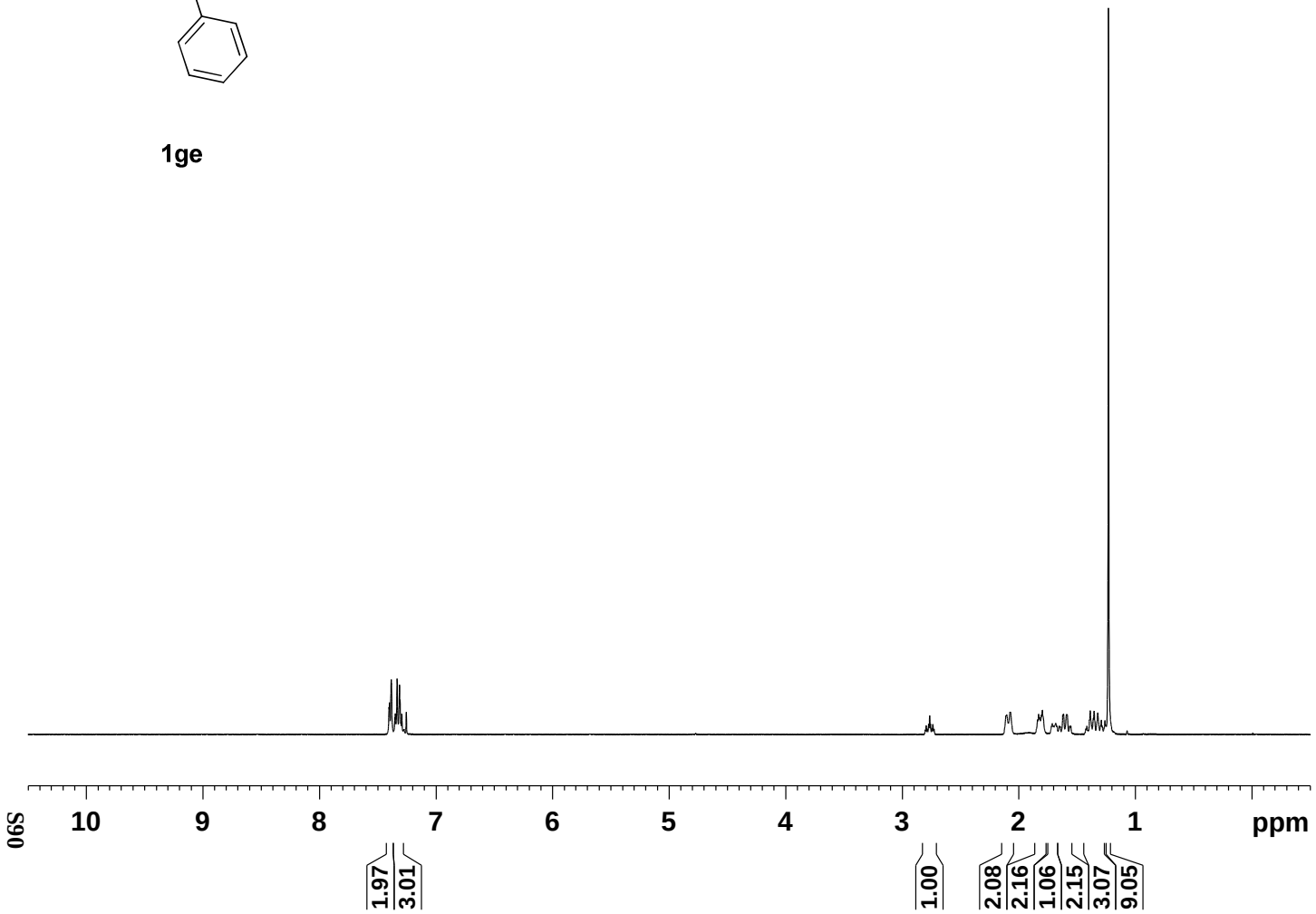
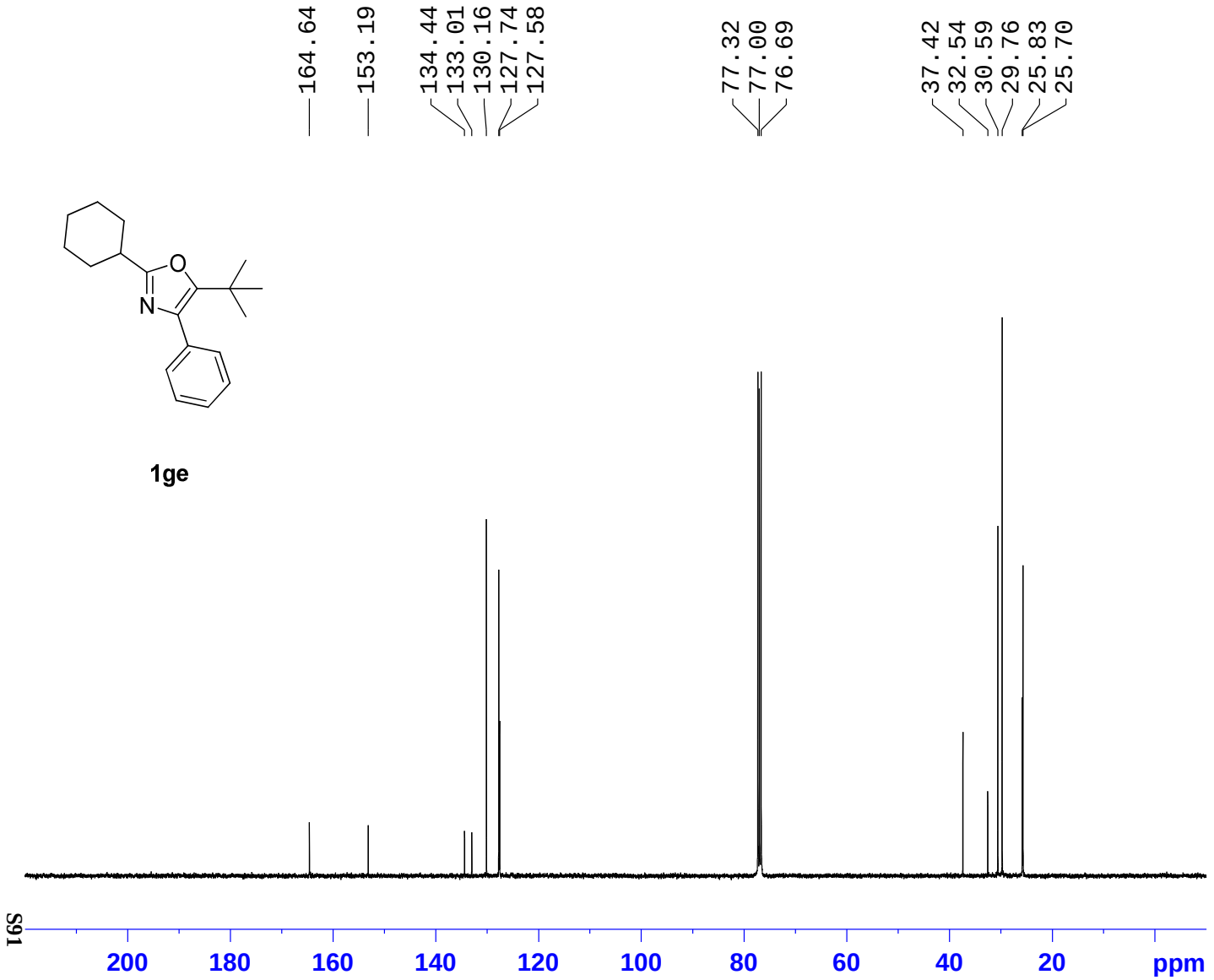


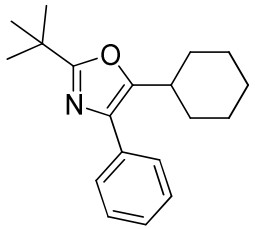
NAME	mina187
EXPNO	6
PROCNO	1
Date_	20130315
Time	10.51
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	7246.377 Hz
FIDRES	0.221142 Hz
AQ	2.2611110 sec
RG	114
DW	69.000 usec
DE	6.50 usec
TE	300.4 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	11.90 usec
PL1	3.00 dB
SFO1	400.1324008 MHz
SI	16384
SF	400.1300118 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



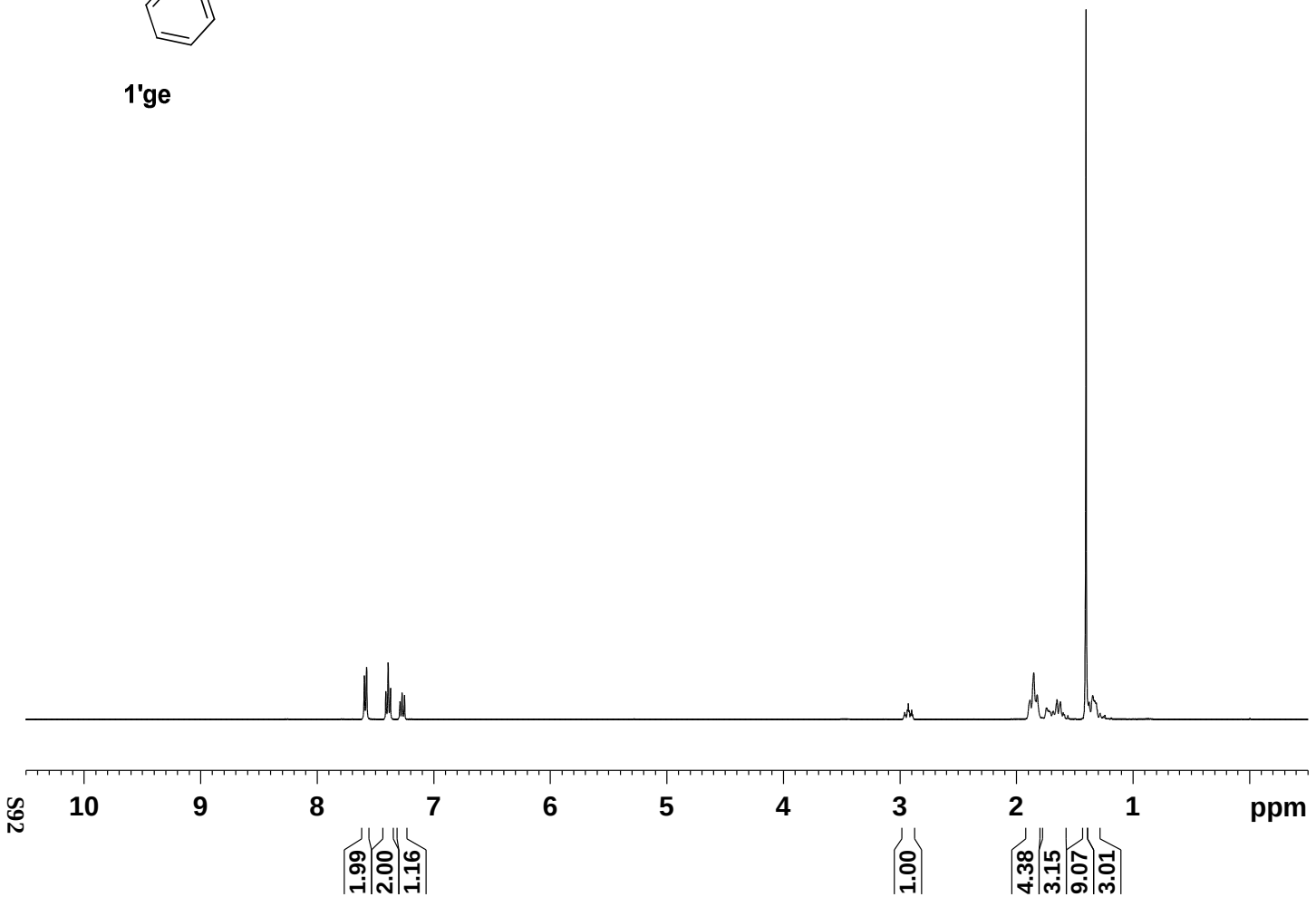

```
NAME            mina187
EXPNO                14
PROCNO                1
Date_          20130316
Time               8.36
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 1842
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG               9195.2
DW                20.800 usec
DE                 6.50 usec
TE                298.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 9.40 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

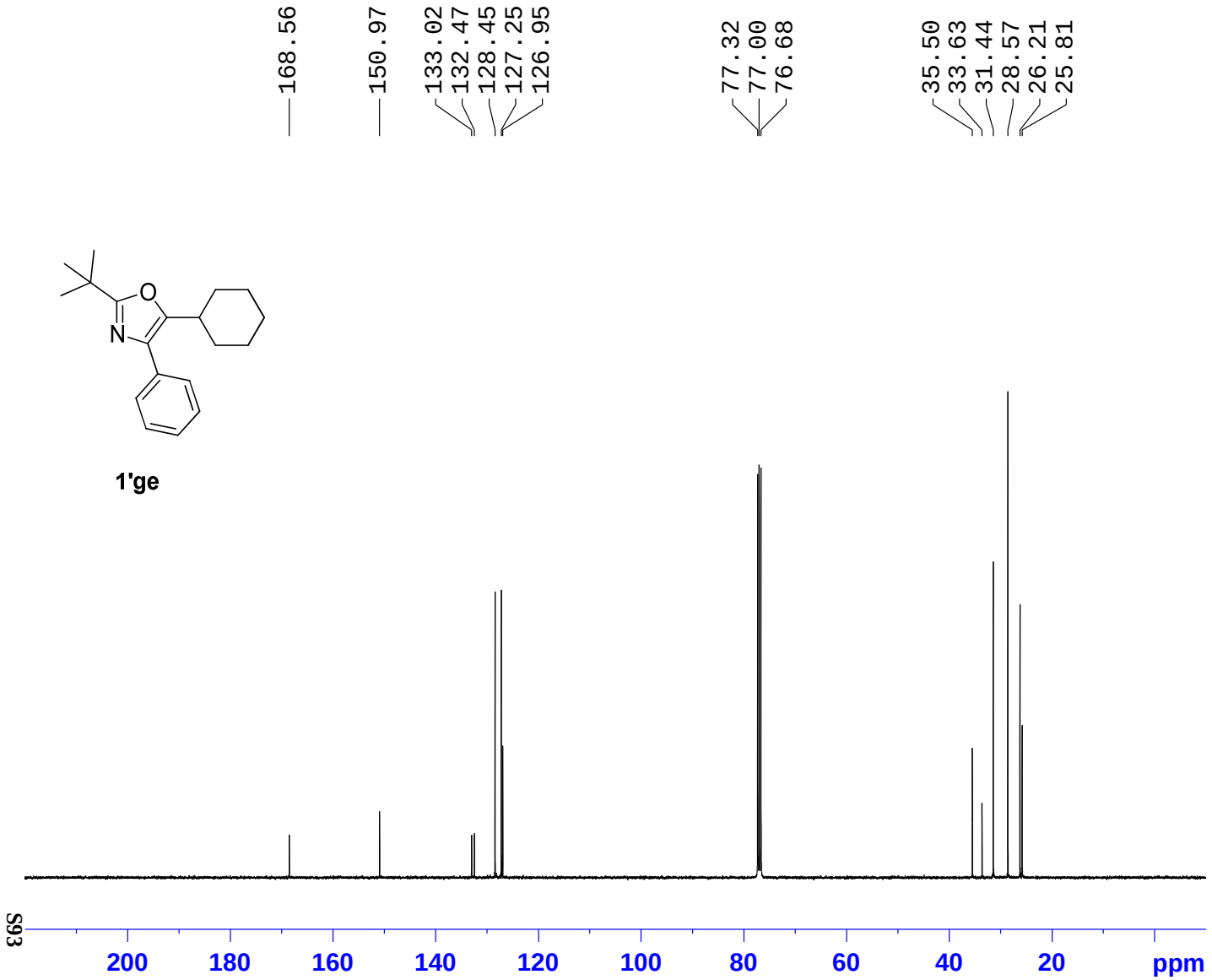
======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            90.00 usec
PL2                3.00 dB
PL12              20.70 dB
PL13              23.70 dB
SFO2        400.1316005 MHz
SI                32768
SF          100.6127709 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.00
```



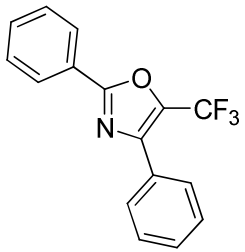
1'ge



NAME	mina187
EXPNO	8
PROCNO	1
Date_	20130318
Time	9.38
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	7246.377 Hz
FIDRES	0.221142 Hz
AQ	2.2611110 sec
RG	71.8
DW	69.000 usec
DE	6.50 usec
TE	299.3 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	11.90 usec
PL1	3.00 dB
SFO1	400.1324008 MHz
SI	16384
SF	400.1300127 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	mina187
EXPNO	9
PROCNO	1
Date_	20130318
Time	12.55
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	2386
DS	0
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	0.6816452 sec
RG	9195.2
DW	20.800 usec
DE	6.50 usec
TE	299.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.40 usec
PL1	7.00 dB
SFO1	100.6233325 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	3.00 dB
PL12	20.70 dB
PL13	23.70 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127716 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00



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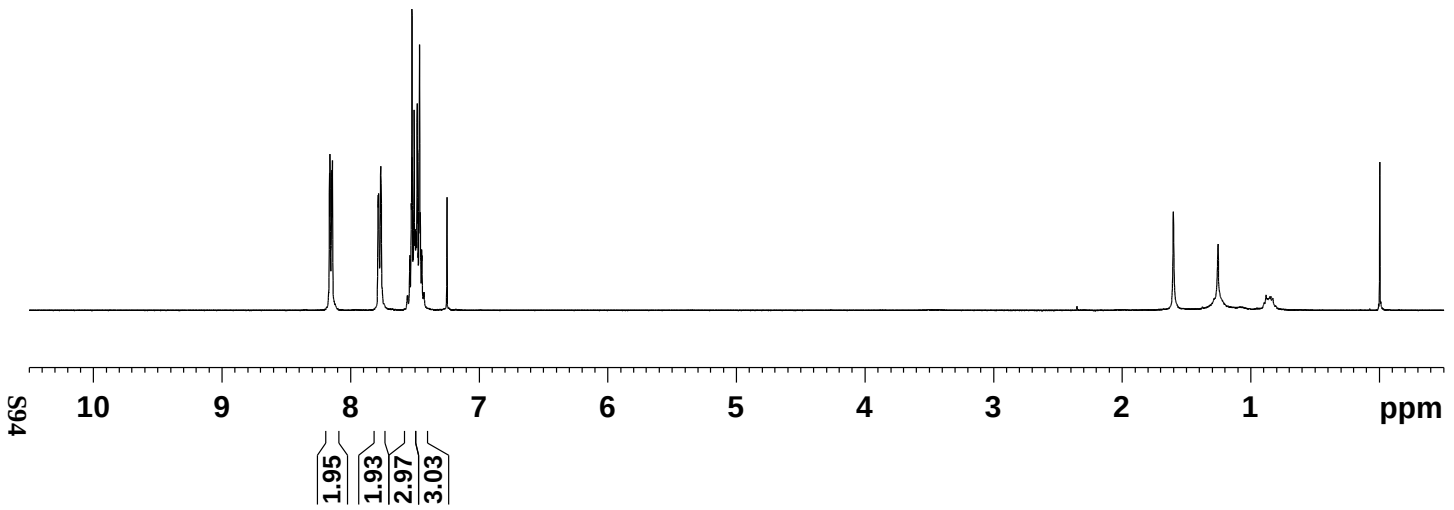
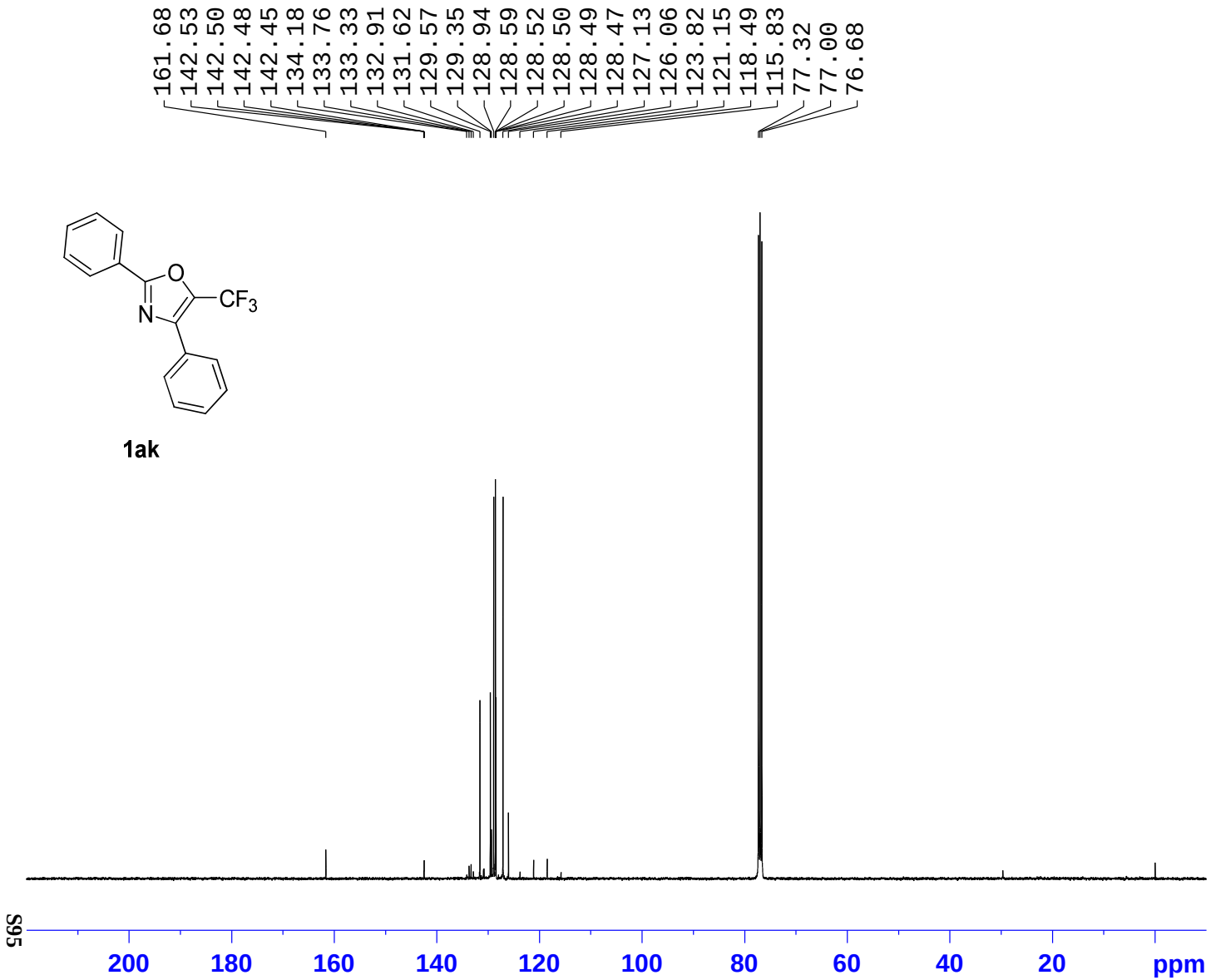


NAME	mina151	
EXPNO	2	
PROCNO	1	
Date_	20130109	
Time	18.47	
INSTRUM	spect	
PROBHD	5 mm BBO BB-1H	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	16	
DS	0	
SWH	7246.377	Hz
FIDRES	0.221142	Hz
AQ	2.2611110	sec
RG	128	
DW	69.000	usec
DE	6.50	usec
TE	295.7	K
D1	2.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	11.90	usec
PL1	3.00	dB
SFO1	400.1324008	MHz
SI	16384	
SF	400.1300127	MHz
WDW	EM	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	



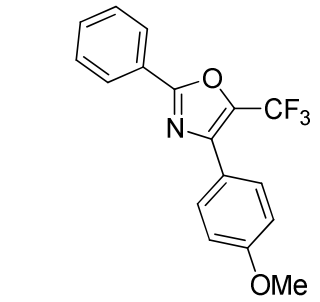

```
Current Data Parameters
NAME            mina152
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20130113
Time              20.04
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                14928
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG               9195.2
DW                20.800 usec
DE                 6.50 usec
TE                299.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.40 usec
PL1                 7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12                20.70 dB
PL13                23.70 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127694 MHz
WDW                  EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.00
```



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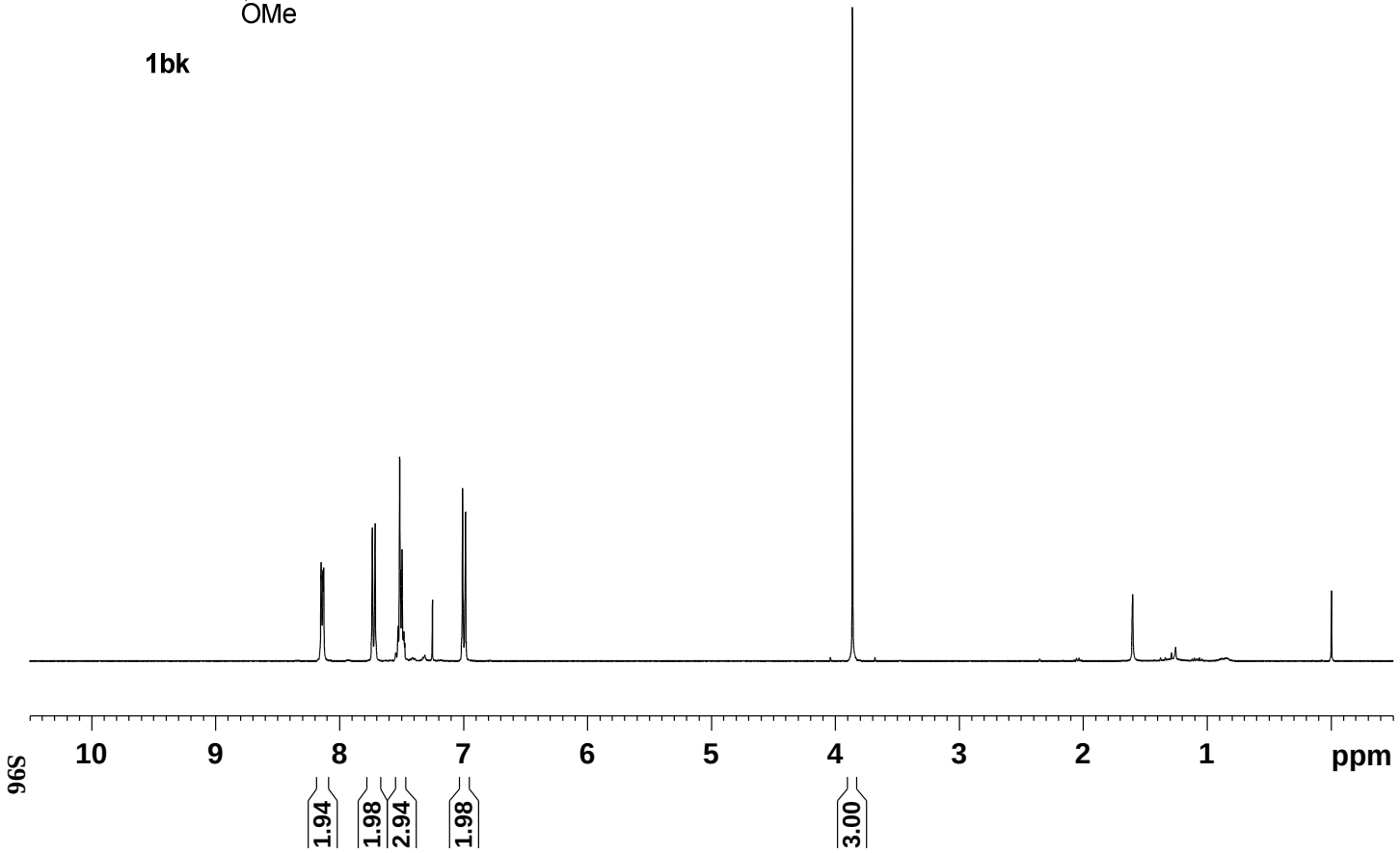
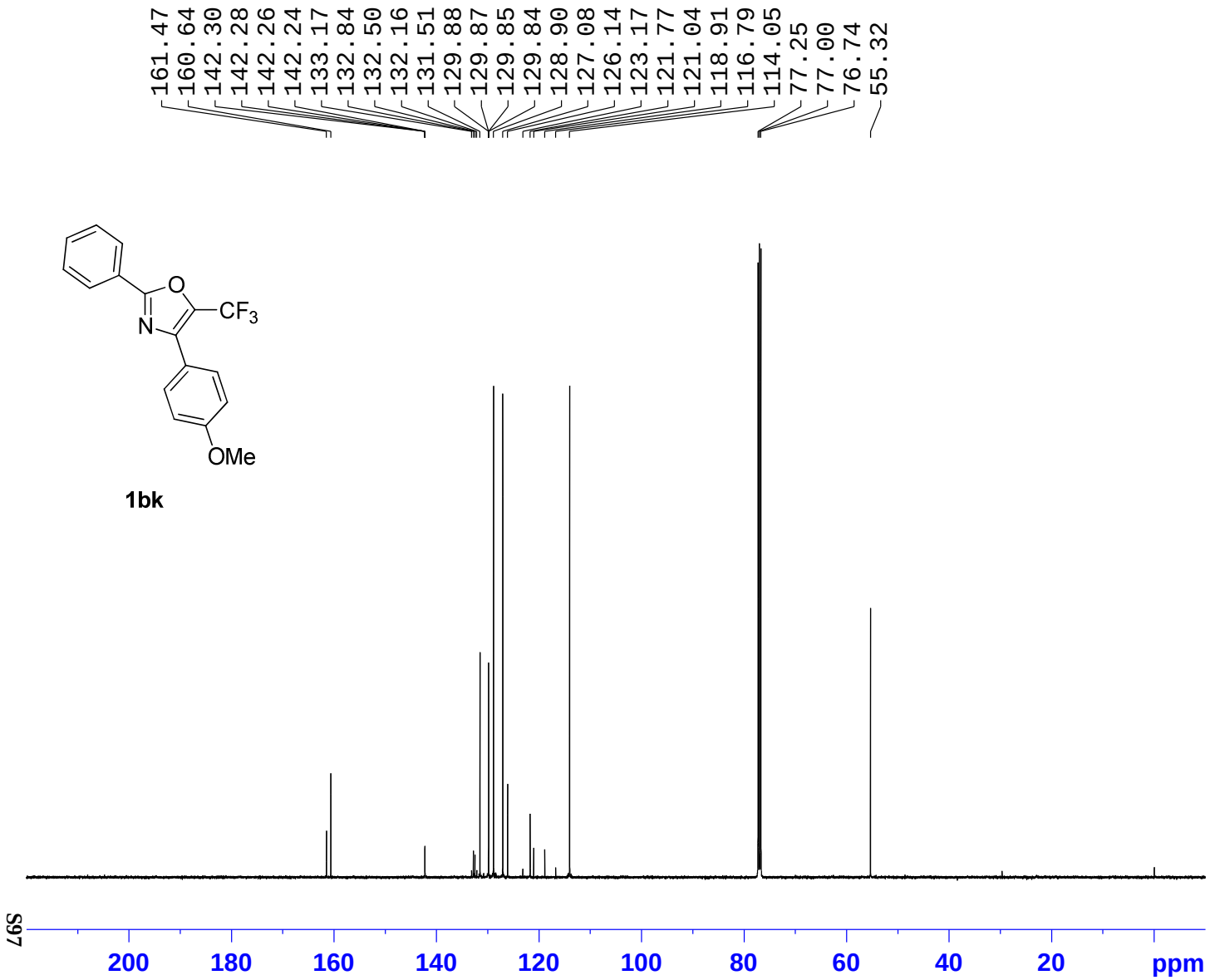



```
Current Data Parameters
NAME            mina141
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20121224
Time              17.07
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  181
DW               69.000 usec
DE                6.50 usec
TE                298.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300122 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



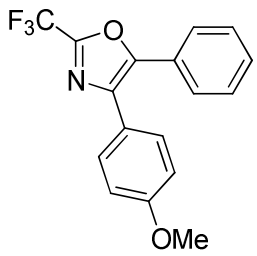

```
Current Data Parameters
NAME            mina141
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20121225
Time              19.17
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2780
DS                    0
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912410 sec
RG               9195.2
DW               16.650 usec
DE                6.50 usec
TE                300.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

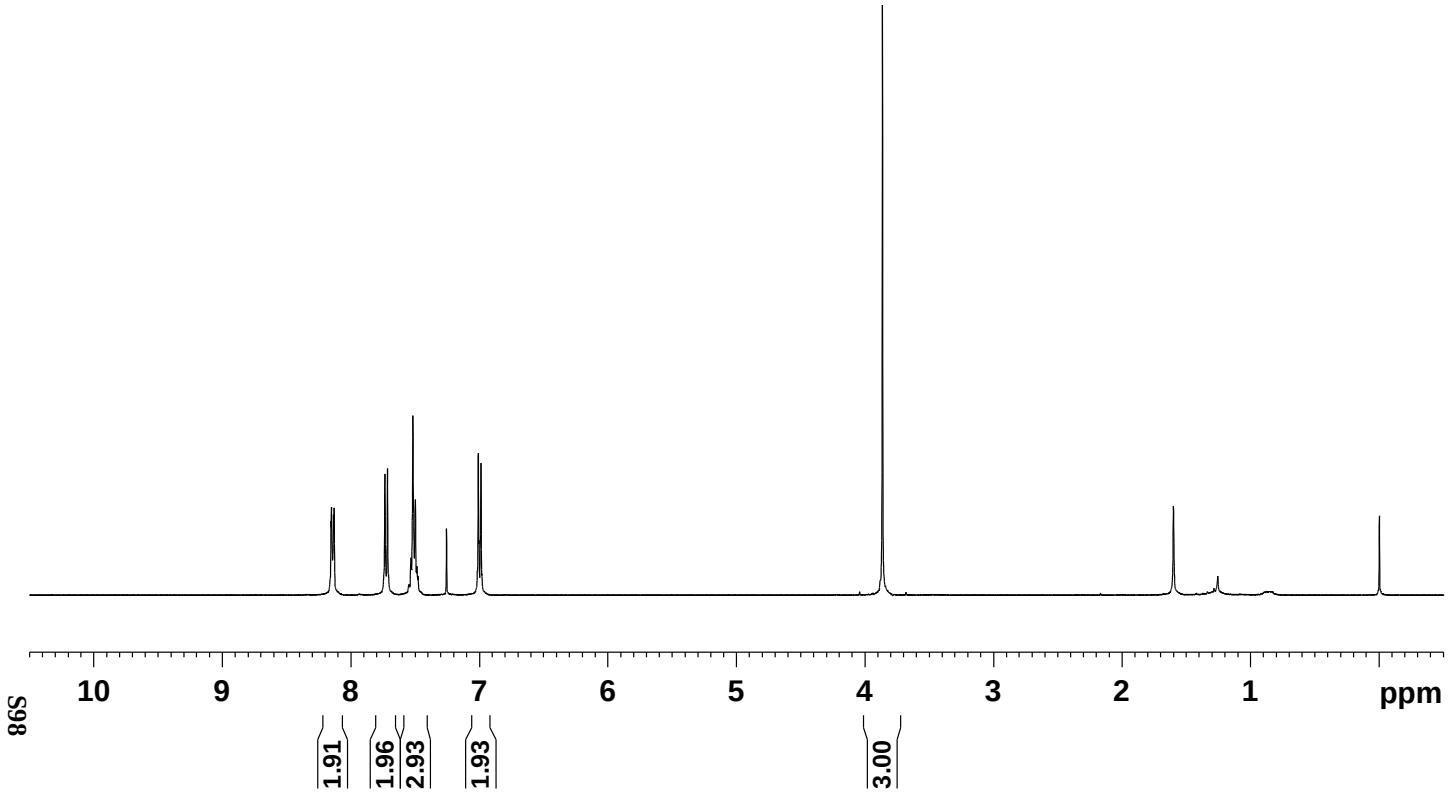
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                6.50 dB
SFO1        125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -0.60 dB
PL12              15.20 dB
PL13              18.20 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                65536
SF          125.7577922 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.00
```



1'bk



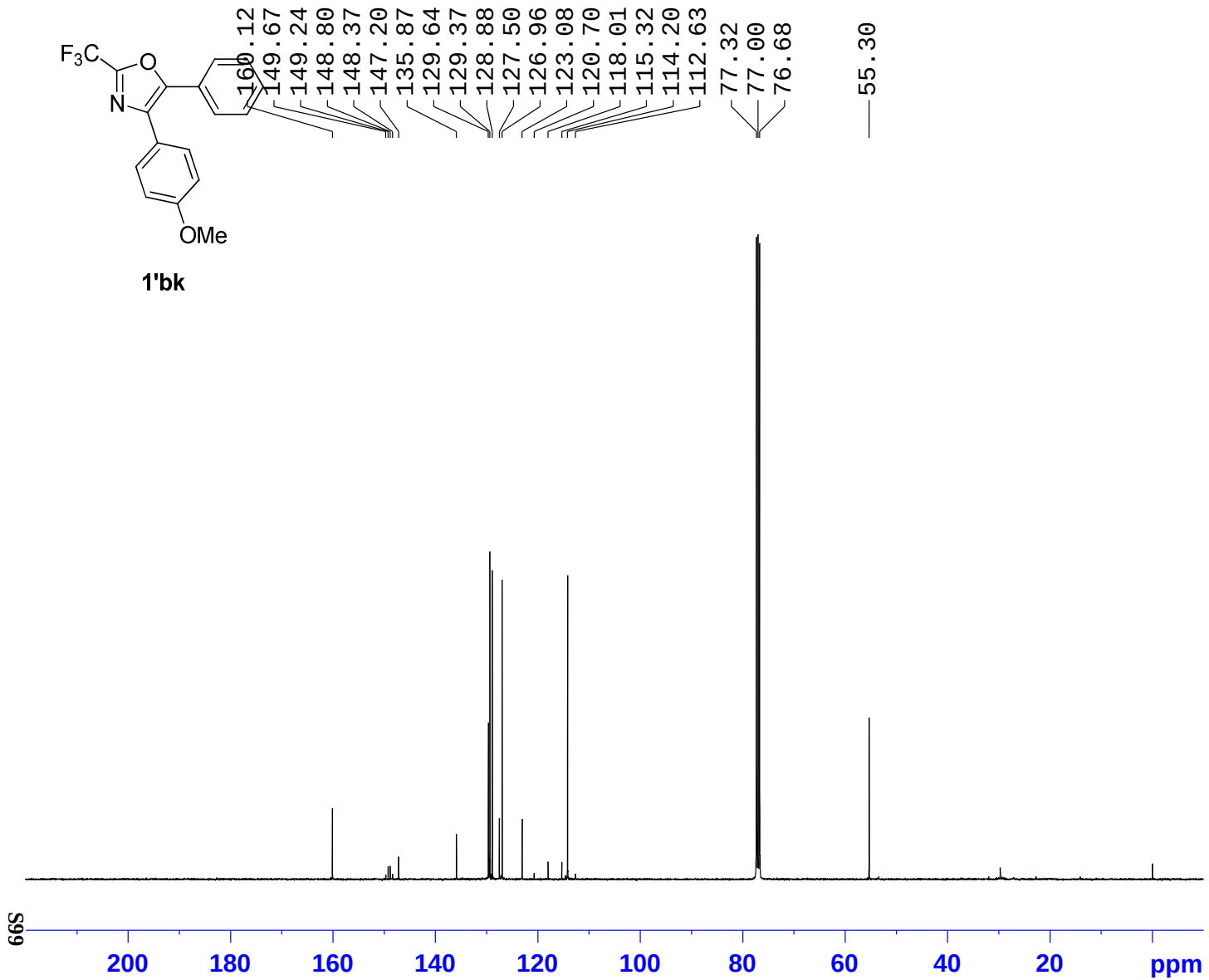
S98

```
Current Data Parameters
NAME            mina145
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20121229
Time              15.57
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  181
DW               69.000 usec
DE                6.50 usec
TE                297.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300114 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



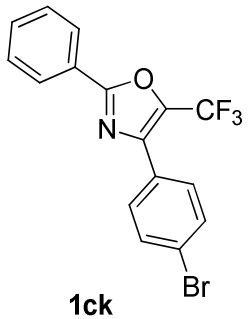

```
Current Data Parameters
NAME                  mina145
EXPNO                       5
PROCNO                      1

F2 - Acquisition Parameters
Date_                20121230
Time                    21.25
INSTRUM                  spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                      14130
DS                          0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     298.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.40 usec
PL1                      7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                   90.00 usec
PL2                      3.00 dB
PL12                    20.70 dB
PL13                    23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF               100.6127701 MHz
WDW                        EM
SSB           0
LB                       1.00 Hz
GB            0
PC                       1.00
```



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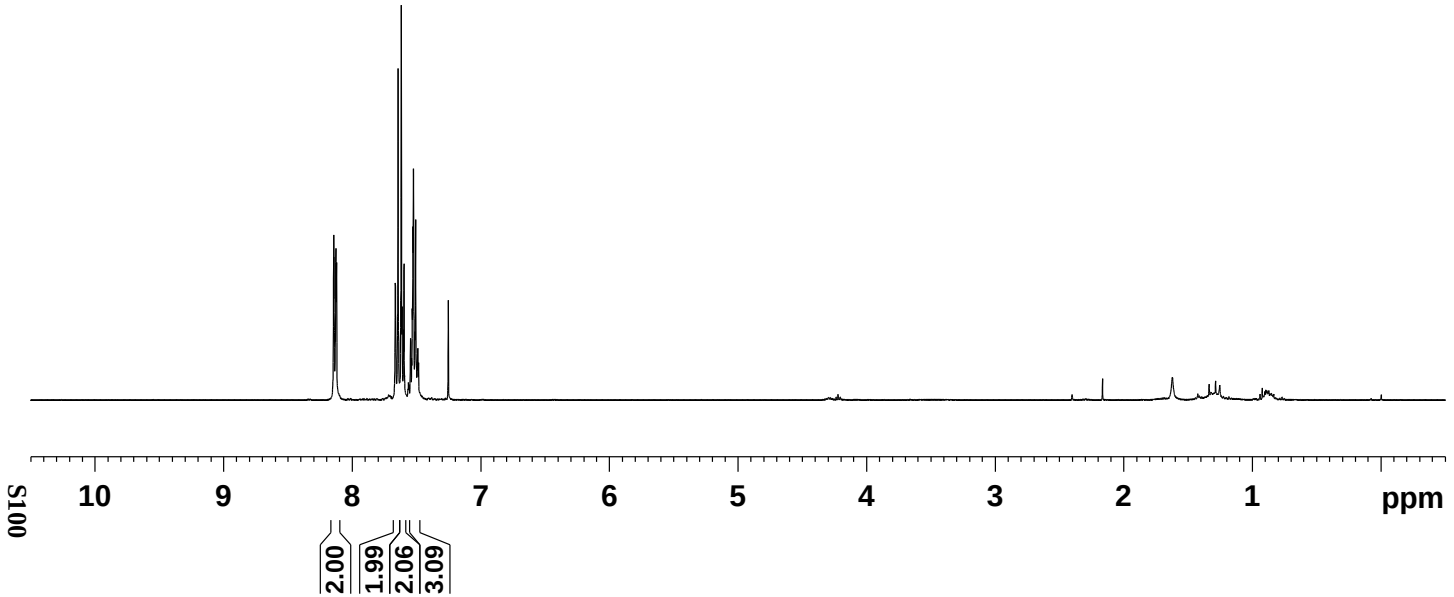
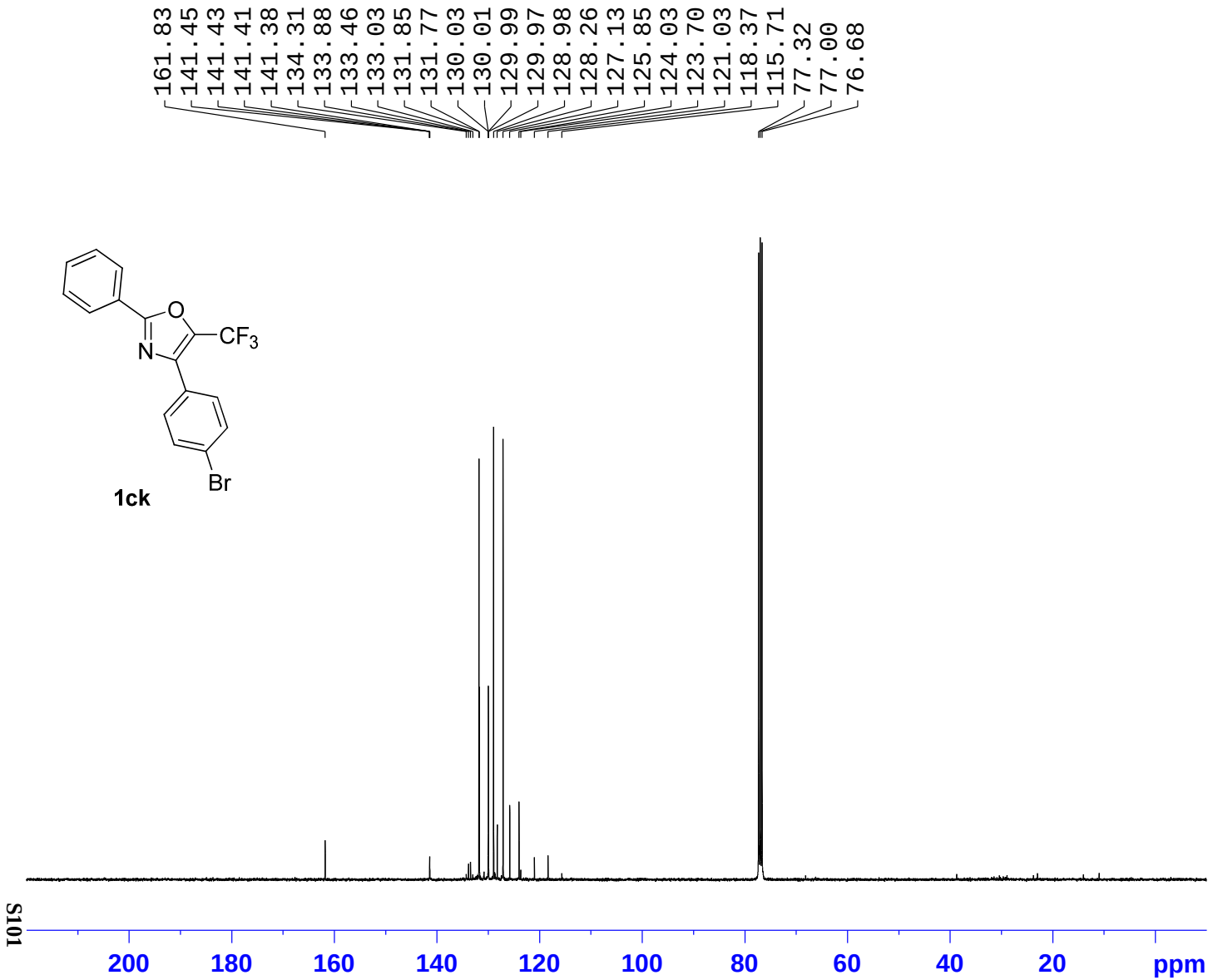



```
Current Data Parameters
NAME            mina155
EXPNO                13
PROCNO                1

F2 - Acquisition Parameters
Date_          20130124
Time               0.02
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  181
DW               69.000 usec
DE                6.50 usec
TE                298.8 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300118 MHz
WDW                  EM
SSB      0
LB       0 Hz
GB       0
PC                 1.00
```



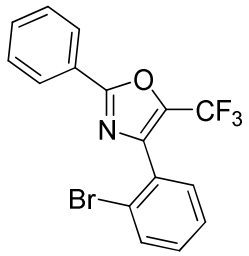

```
Current Data Parameters
NAME                  mina155
EXPNO                      14
PROCNO                      1

F2 - Acquisition Parameters
Date_                20130123
Time                     6.38
INSTRUM                 spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                       8185
DS                          0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     299.8 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

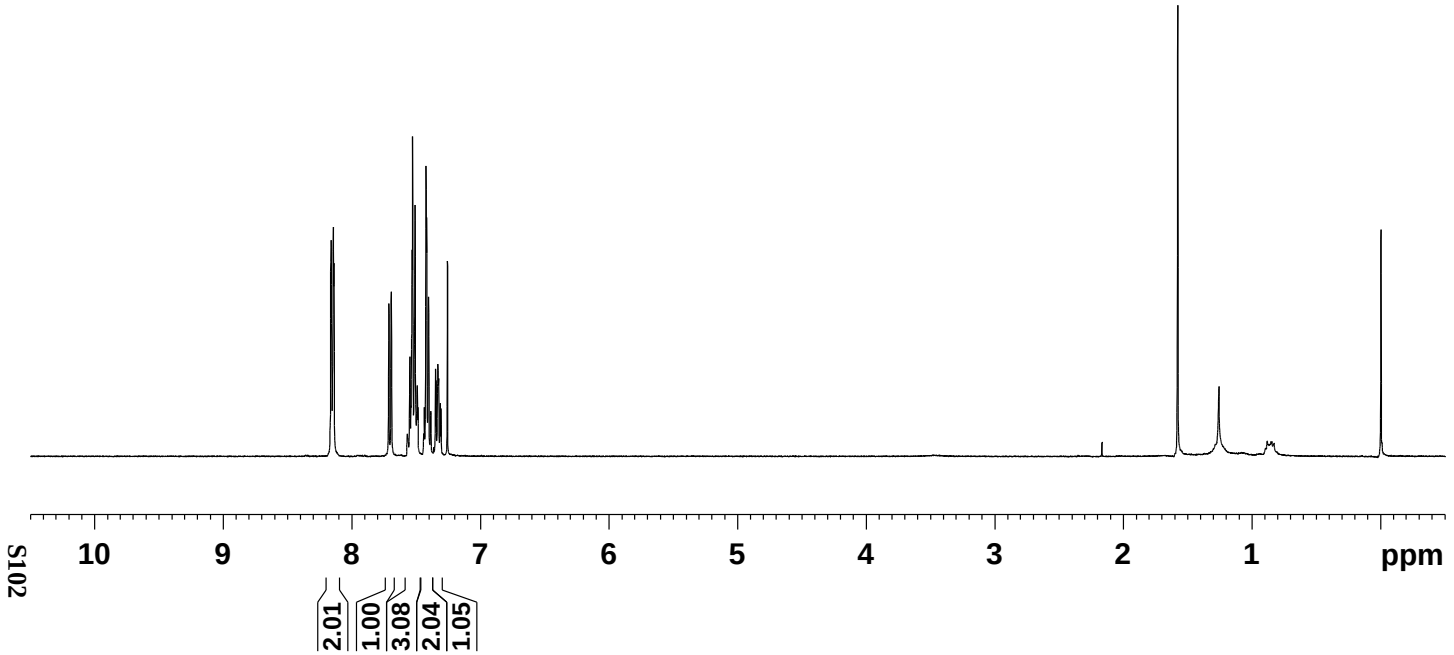
======== CHANNEL f1 ========
NUC1                      13C
P1                       9.40 usec
PL1                      7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                   90.00 usec
PL2                      3.00 dB
PL12                    20.70 dB
PL13                    23.70 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF               100.6127701 MHz
WDW                        EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.00
```



1dk

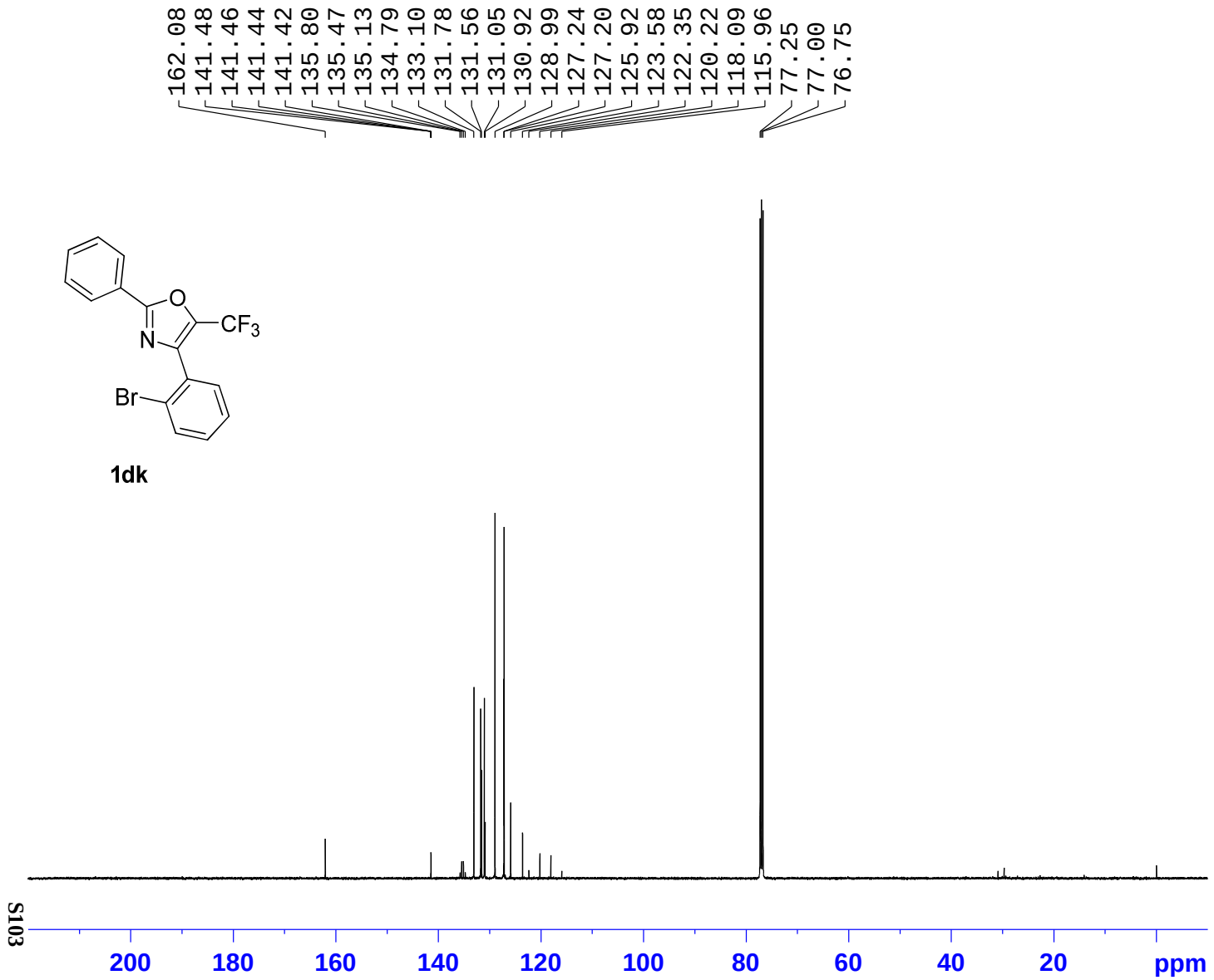



```
Current Data Parameters
NAME            mina160
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20130116
Time              13.29
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                228.1
DW               69.000 usec
DE                6.50 usec
TE                299.1 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300105 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



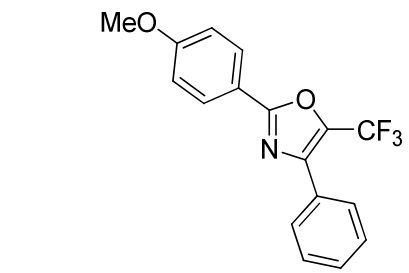

```
Current Data Parameters
NAME            mina159
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20130117
Time              22.45
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 9992
DS                    0
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912410 sec
RG               9195.2
DW               16.650 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

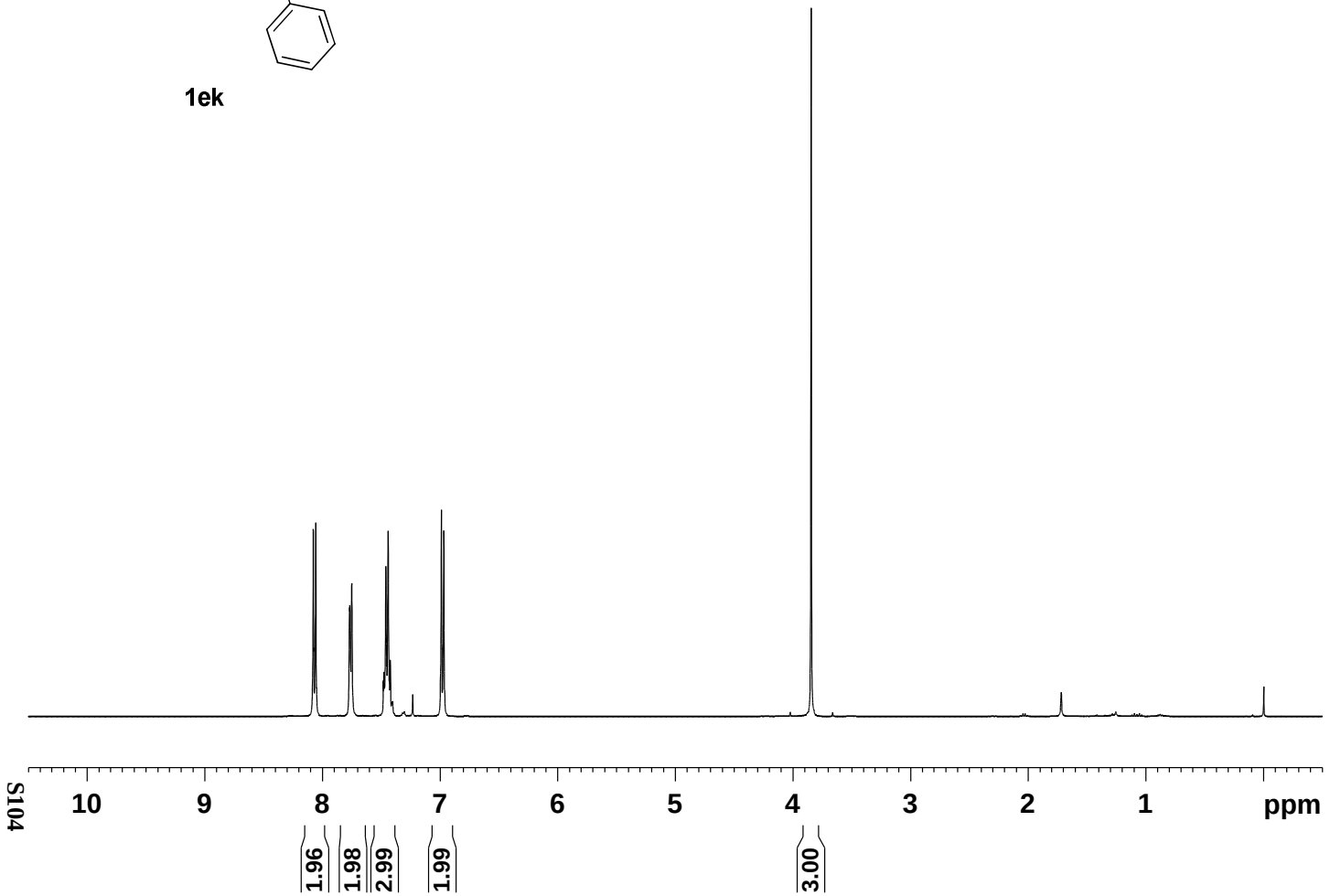
======== CHANNEL f1 ========
NUC1                 13C
P1                10.50 usec
PL1                7.00 dB
SFO1        125.7709931 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -0.60 dB
PL12              15.00 dB
PL13              18.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                65536
SF          125.7577899 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.00
```

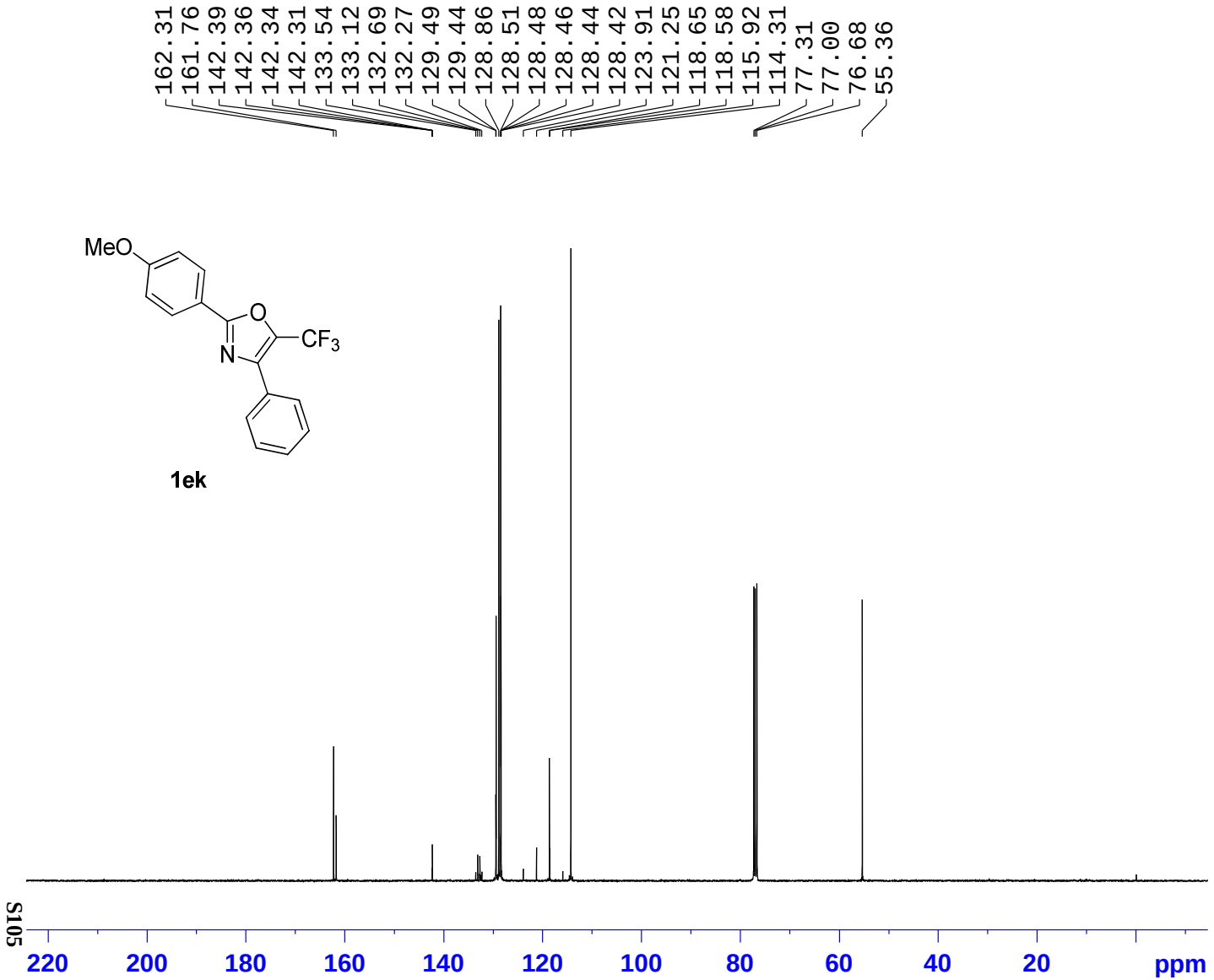


1ek




```
NAME            mina153
EXPNO                 2
PROCNO                1
Date_          20130101
Time              20.18
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                 71.8
DW               69.000 usec
DE                6.50 usec
TE                296.8 K
D1           2.00000000 sec
TD0                   1

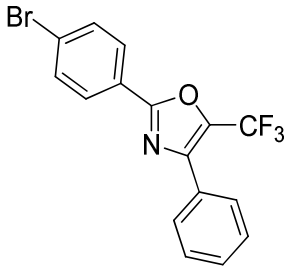
======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz
SI                 16384
SF          400.1300202 MHz
WDW                   EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```



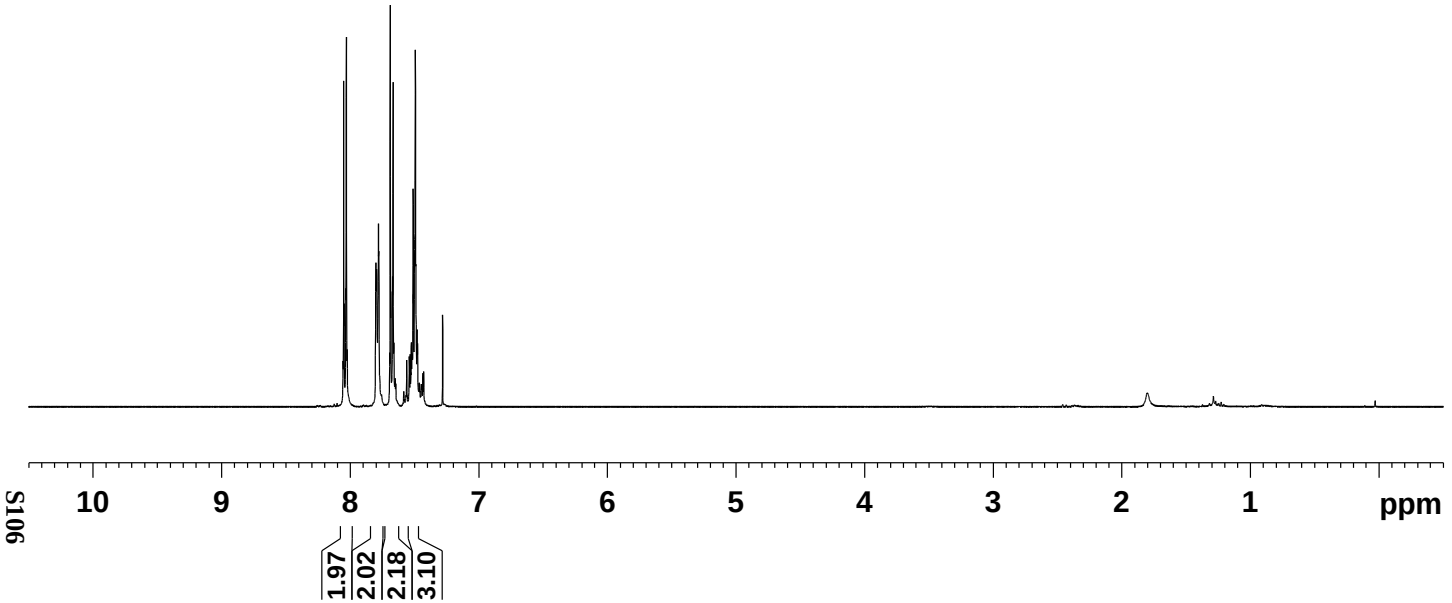

```
NAME            mina153
EXPNO                 3
PROCNO                1
Date_          20130101
Time              20.20
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 2436
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG               9195.2
DW                20.800 usec
DE                 6.50 usec
TE                296.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 9.40 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12               20.70 dB
PL13               23.70 dB
SFO2        400.1316005 MHz
SI                32768
SF          100.6127745 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.00
```



1fk

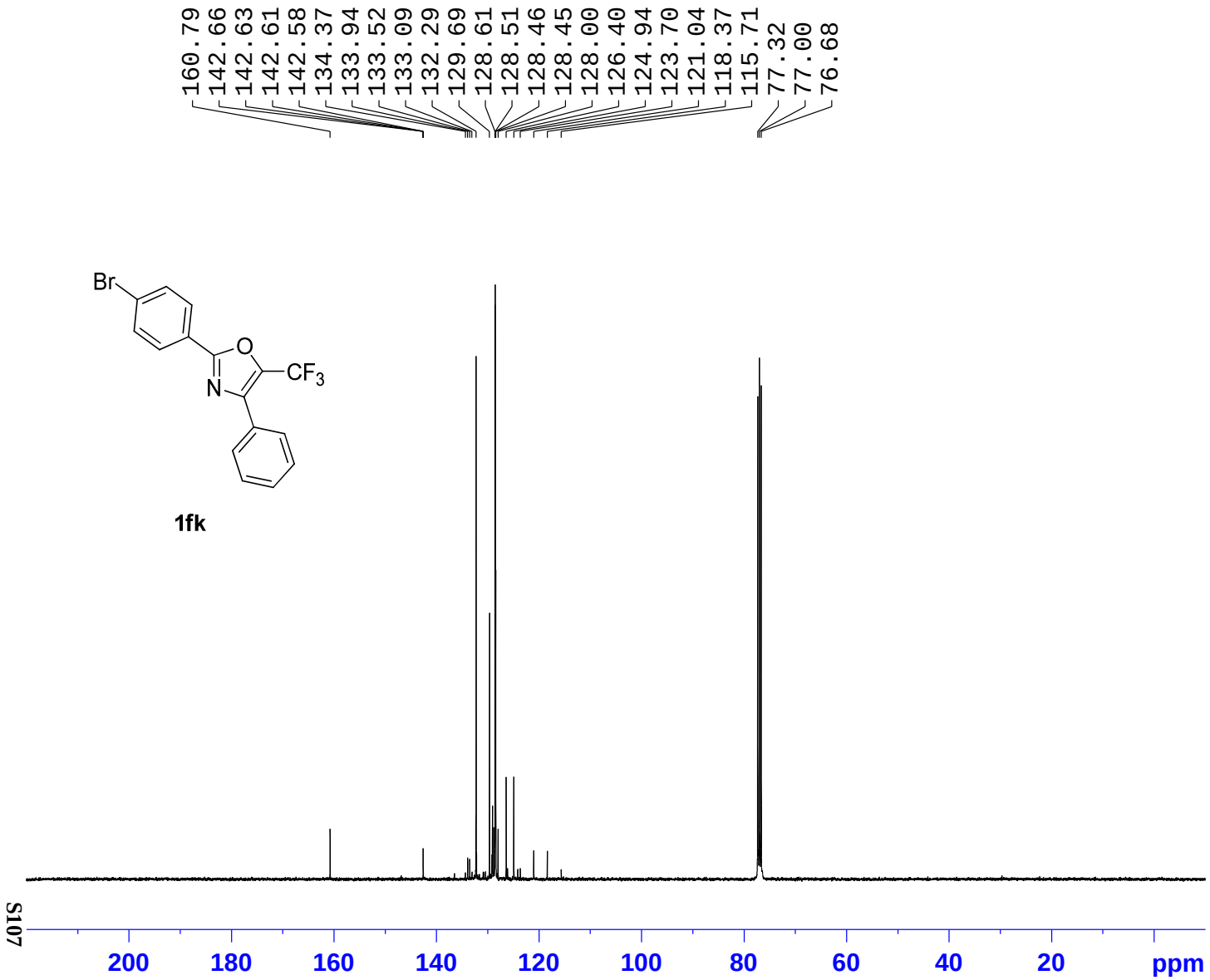



```
Current Data Parameters
NAME            mina157
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20130126
Time              11.51
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                161.3
DW               69.000 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300000 MHz
WDW                  EM
SSB      0
LB       0 Hz
GB       0
PC                 1.00
```



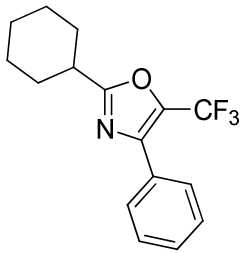

```
Current Data Parameters
NAME            mina157
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20130131
Time               3.18
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 6199
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG               9195.2
DW                20.800 usec
DE                 6.50 usec
TE                299.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

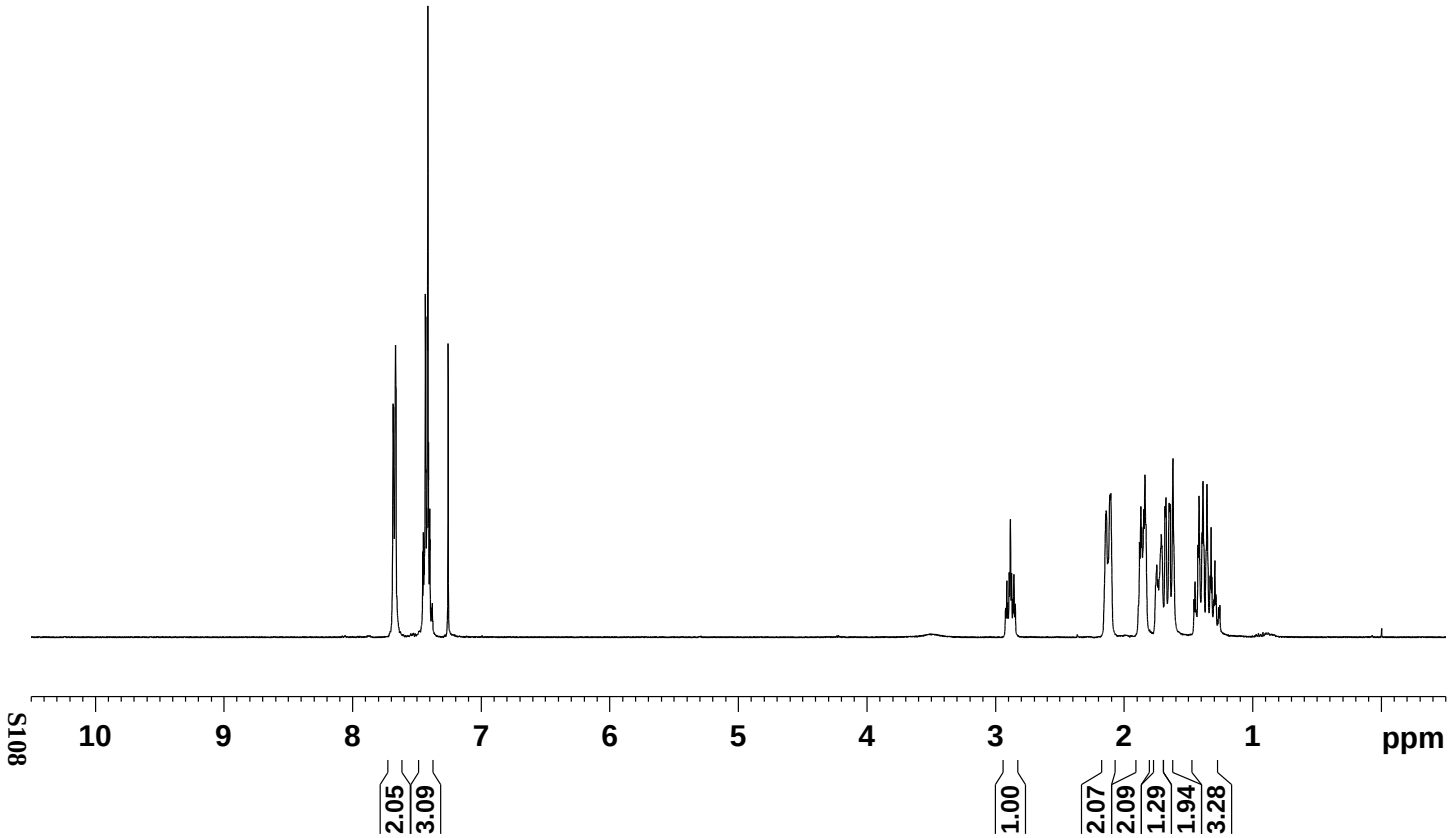
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.40 usec
PL1                 7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                 3.00 dB
PL12                20.70 dB
PL13                23.70 dB
SFO2        400.1316005 MHz

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

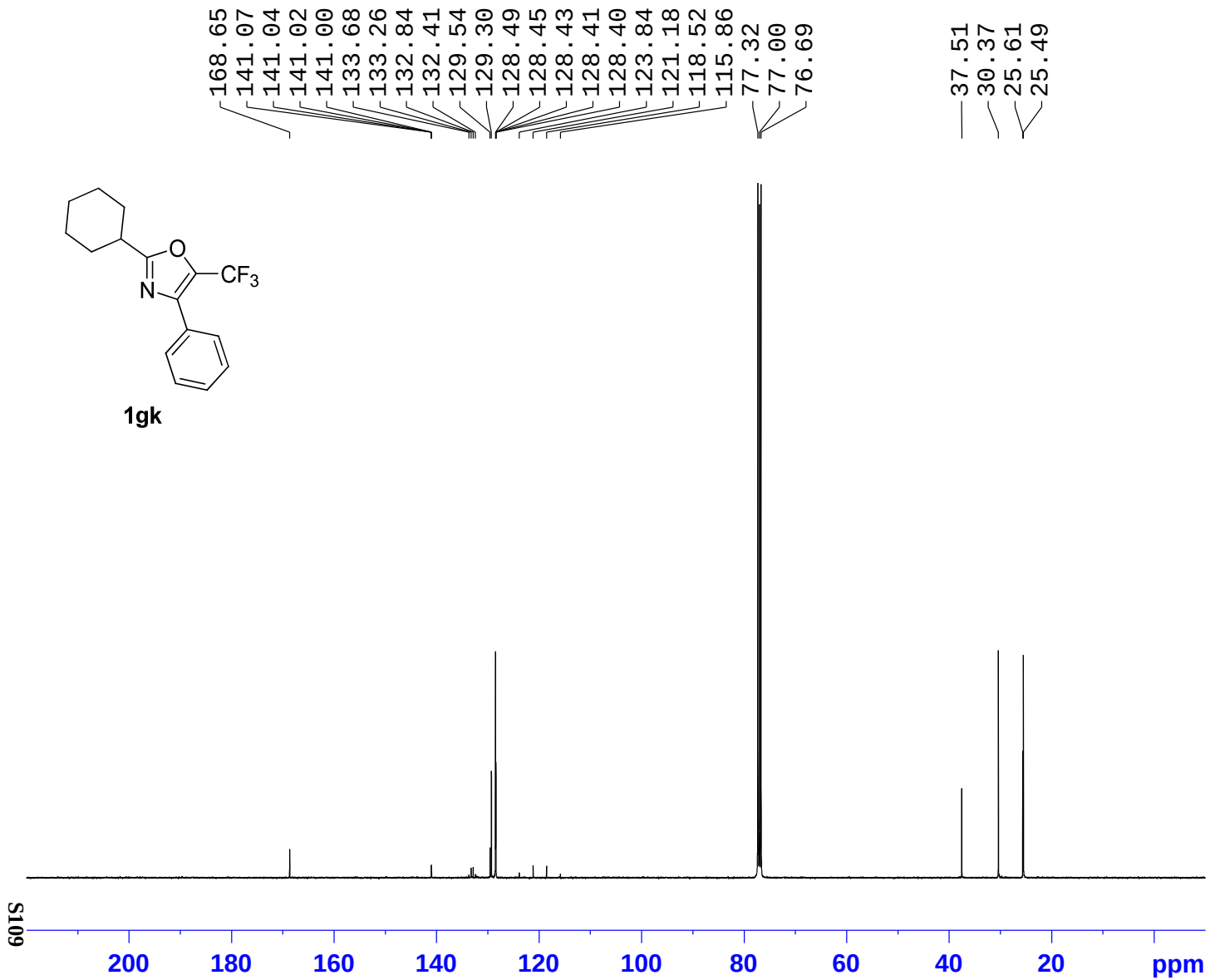


1gk




```
NAME            mina193
EXPNO                 7
PROCNO                1
Date_          20130326
Time              20.37
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  181
DW               69.000 usec
DE                6.50 usec
TE               299.7 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz
SI                16384
SF          400.1300105 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```



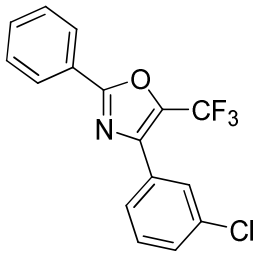

```
Current Data Parameters
NAME                 mina193
EXPNO                      9
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130329
Time                   23.19
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                     32768
SOLVENT                CDCl3
NS                     24265
DS                         0
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6816452 sec
RG                     9195.2
DW                     20.800 usec
DE                      6.50 usec
TE                     299.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

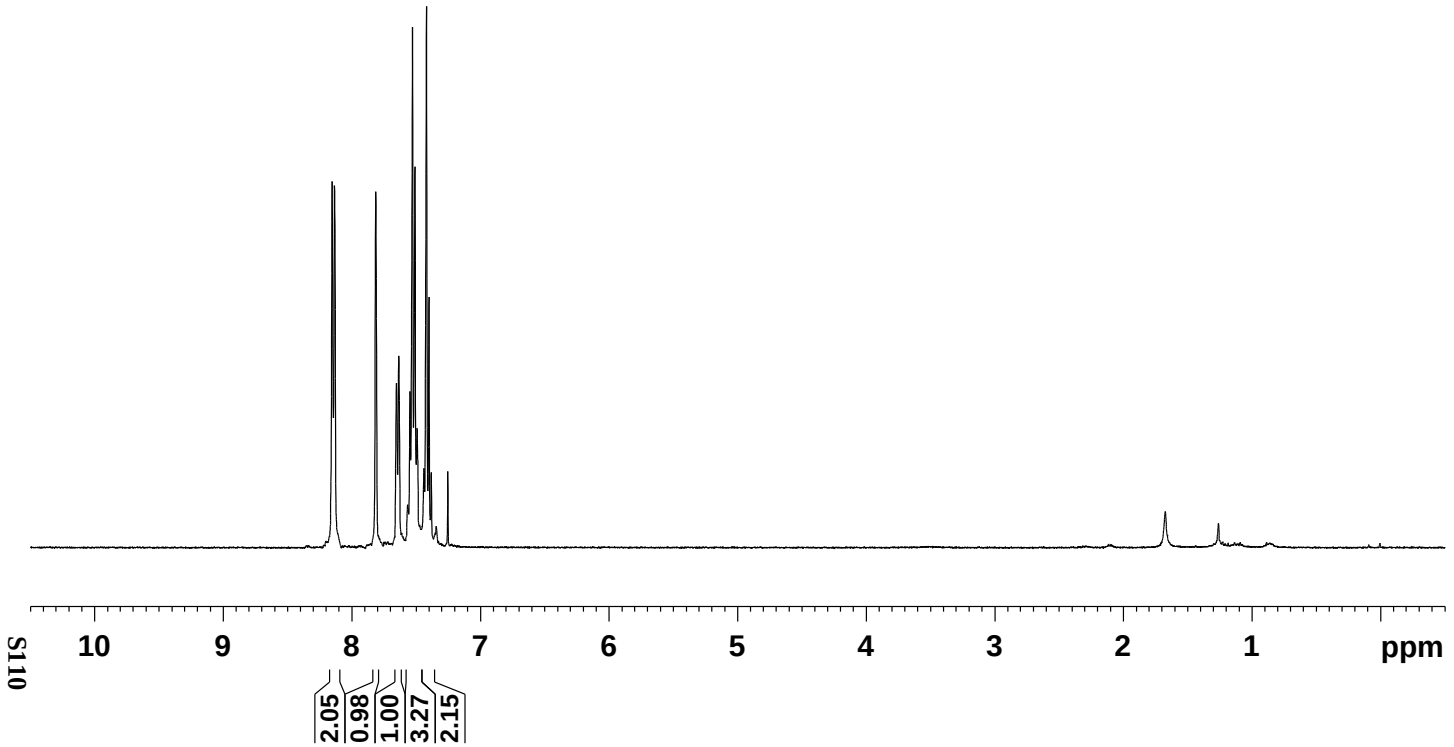
======== CHANNEL f1 ========
NUC1                     13C
P1                      9.40 usec
PL1                     7.00 dB
SFO1             100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                  90.00 usec
PL2                     3.00 dB
PL12                   20.70 dB
PL13                   23.70 dB
SFO2             400.1316005 MHz

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



1hk

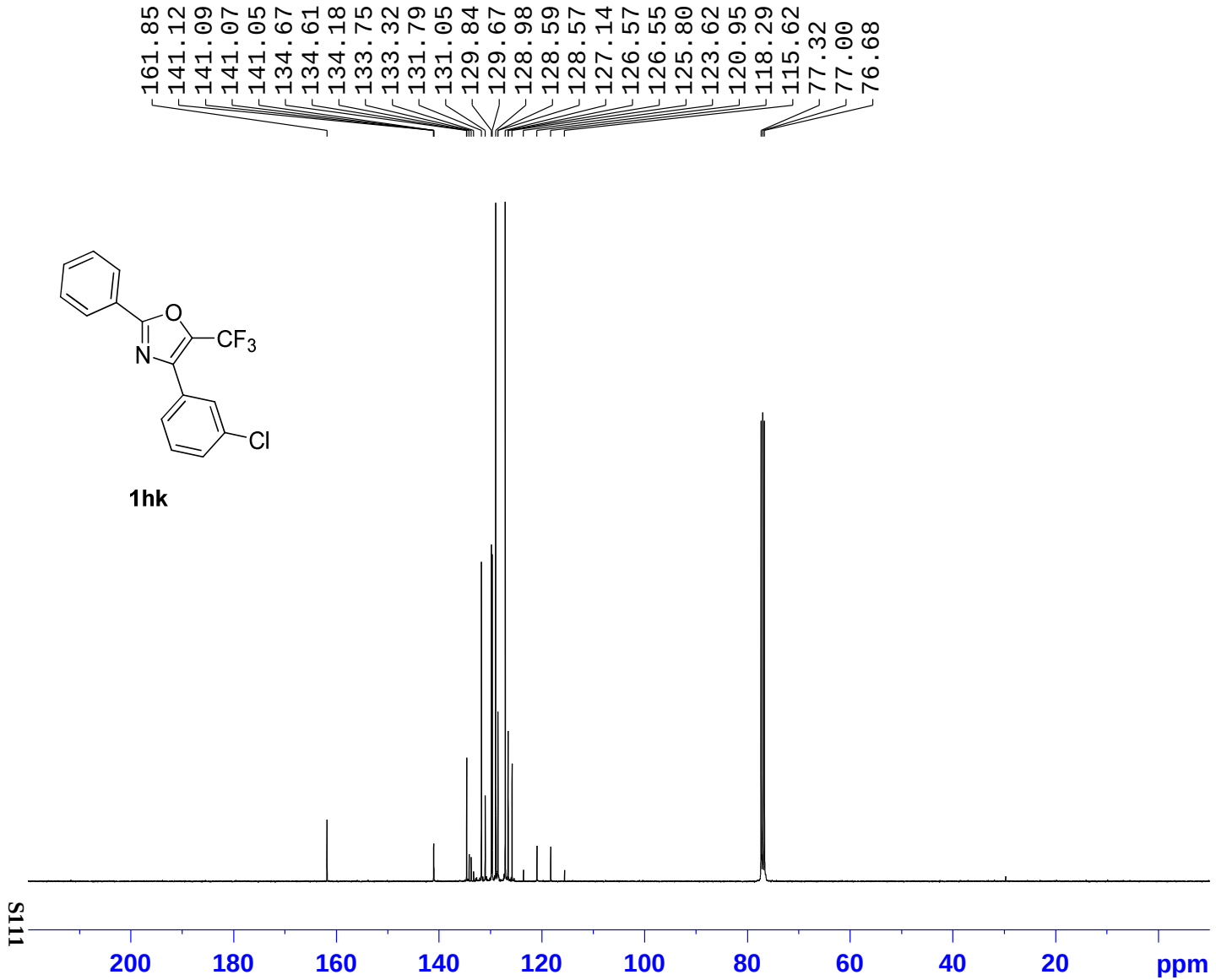



```
Current Data Parameters
NAME            mina172
EXPNO                 3
PROCNO                1

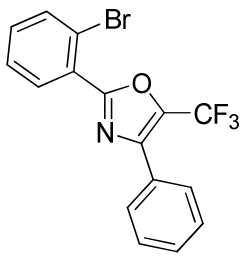
F2 - Acquisition Parameters
Date_          20130224
Time              21.31
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    1
DS                    0
SWH            7246.377 Hz
FIDRES        0.221142 Hz
AQ            2.2611110 sec
RG                  114
DW               69.000 usec
DE                6.50 usec
TE                298.5 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

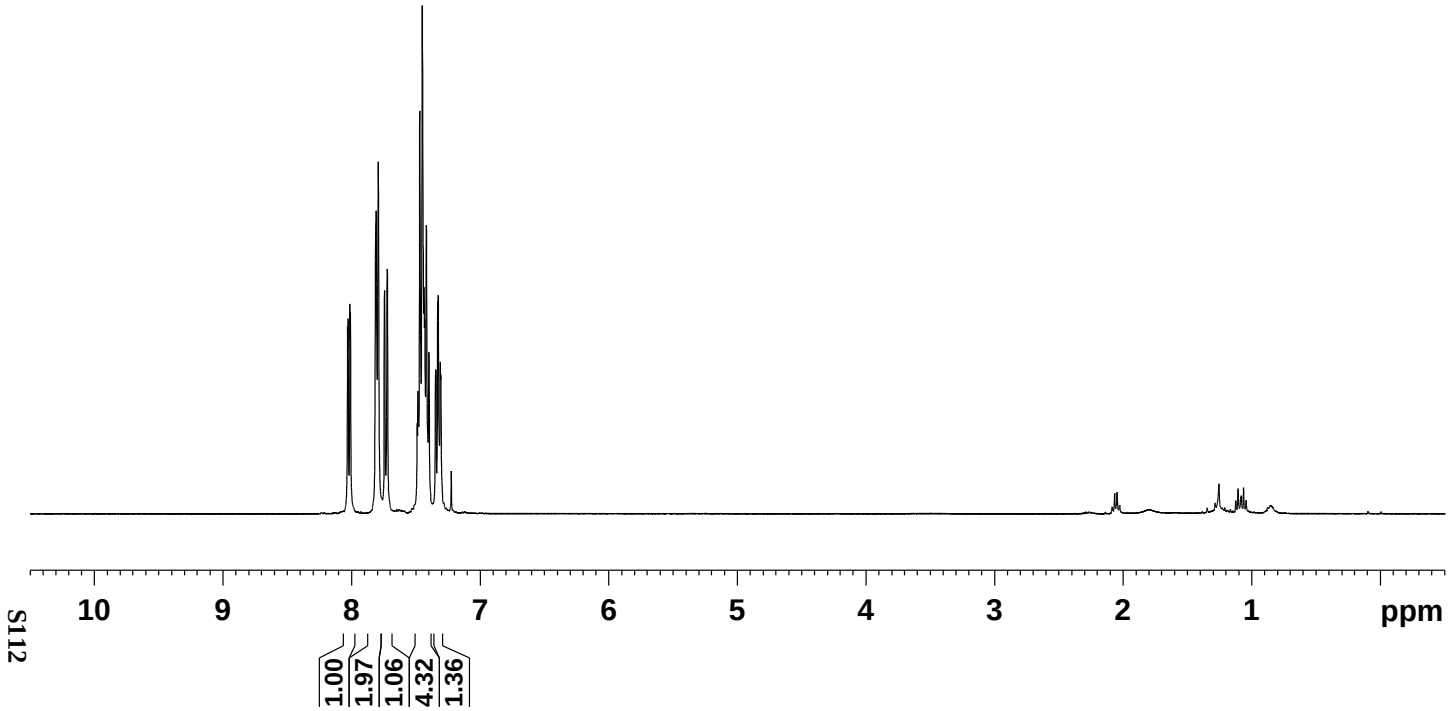
F2 - Processing parameters
SI                16384
SF          400.1300118 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



NAME	mina172
EXPNO	4
PROCNO	1
Date_	20130222
Time	12.05
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	18516
DS	0
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	0.6816452 sec
RG	9195.2
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.40 usec
PL1	7.00 dB
SFO1	100.6233325 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	3.00 dB
PL12	20.70 dB
PL13	23.70 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127708 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00



1ik



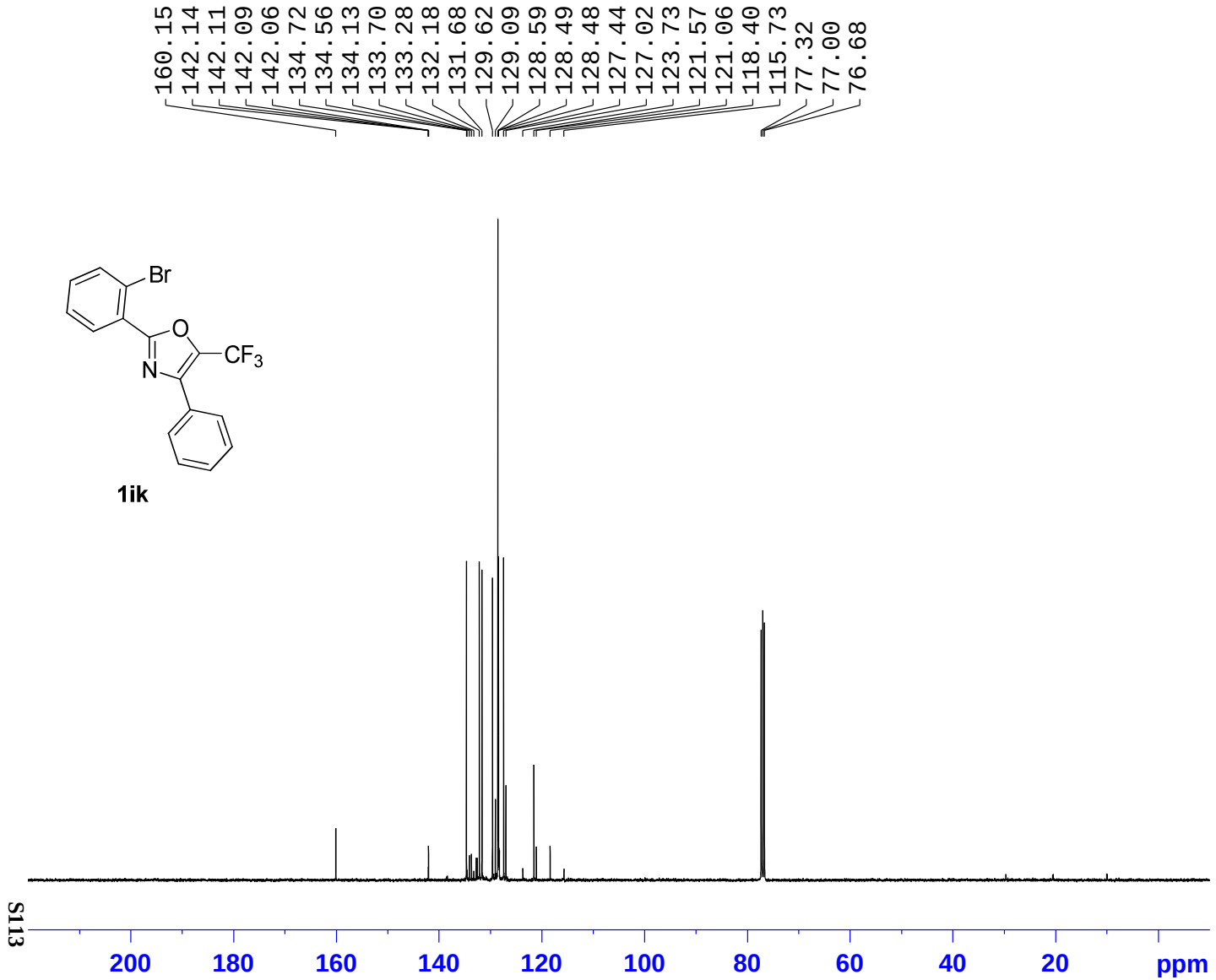
S112

```
Current Data Parameters
NAME            mina183
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20130313
Time               9.01
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ             2.2611110 sec
RG                    57
DW                69.000 usec
DE                 6.50 usec
TE                300.8 K
D1           2.00000000 sec
TD0                   1

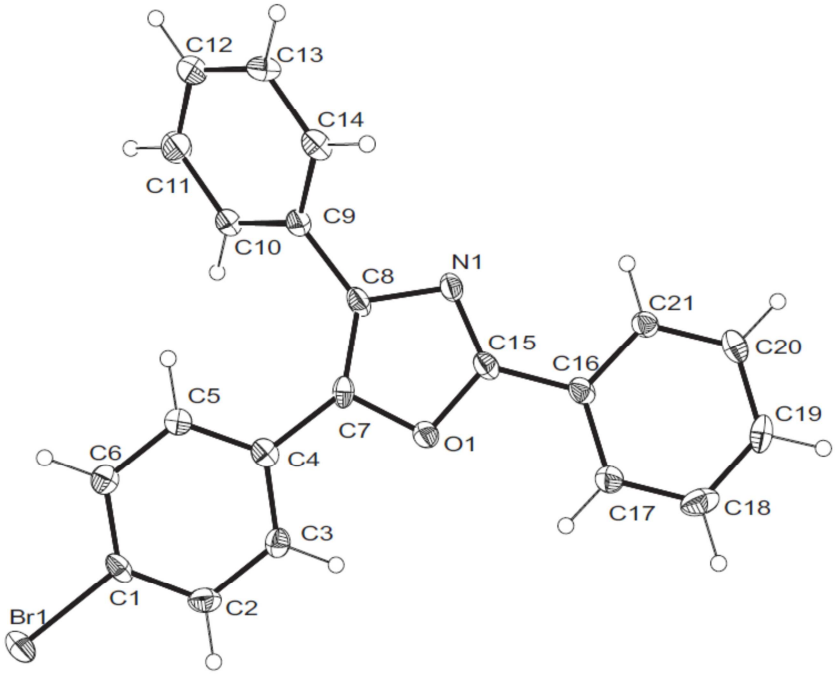
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.90 usec
PL1                 3.00 dB
SFO1         400.1324008 MHz

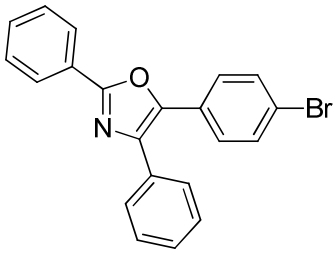
F2 - Processing parameters
SI                 16384
SF          400.1300233 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```



NAME	mina183
EXPNO	6
PROCNO	1
Date_	20130313
Time	17.59
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	1333
DS	0
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	0.6816452 sec
RG	9195.2
DW	20.800 usec
DE	6.50 usec
TE	300.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.40 usec
PL1	7.00 dB
SFO1	100.6233325 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	3.00 dB
PL12	20.70 dB
PL13	23.70 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6127753 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

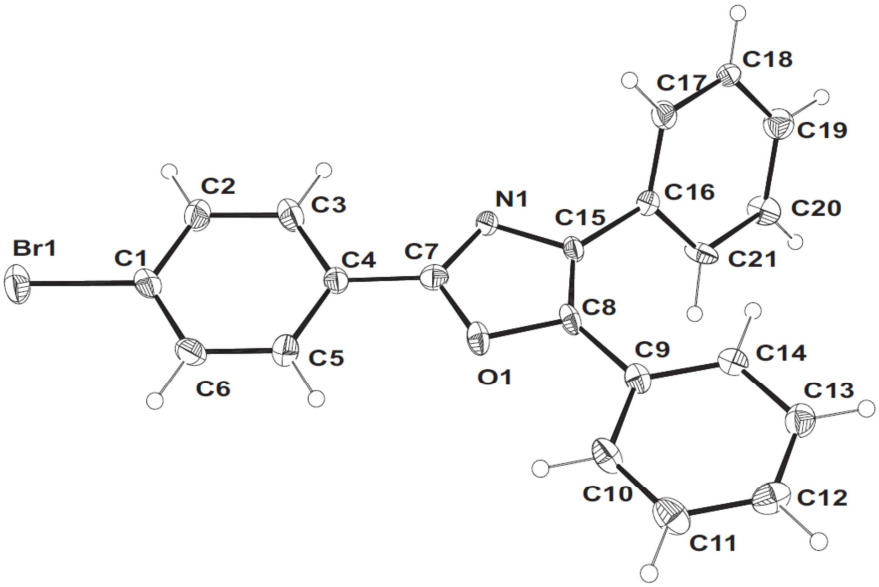
X-ray structure of **1af**. (CCDC-940035)

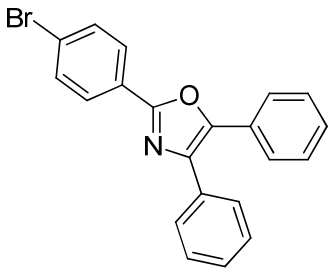




1af

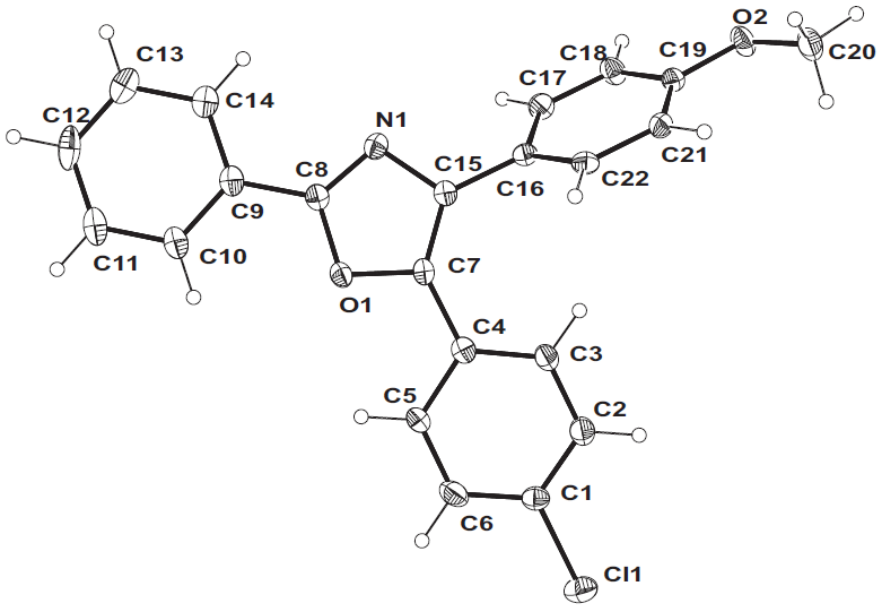
X-ray structure of **1'af**. (CCDC-940036)

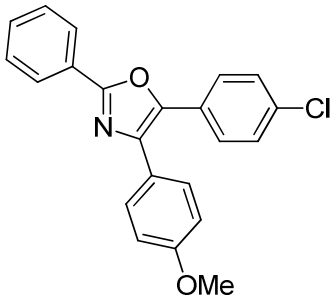




1'af

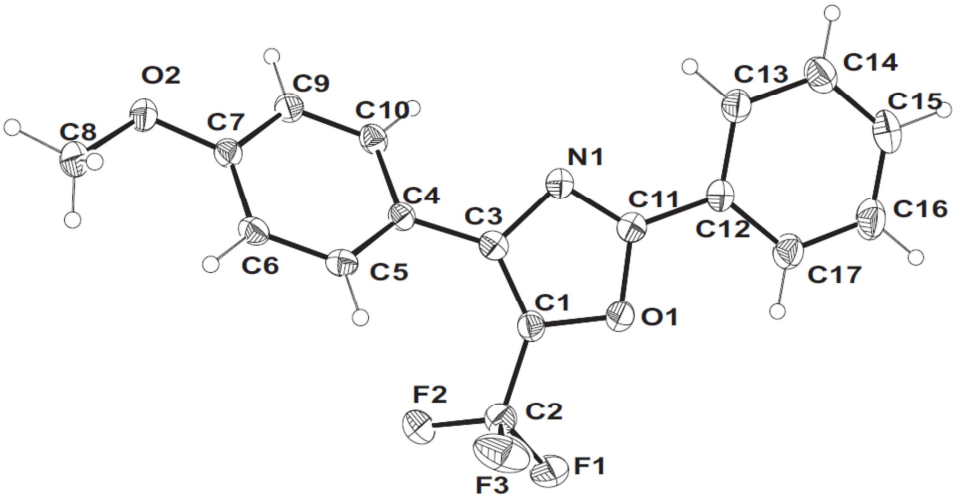
X-ray structure of **1bb**. (CCDC-940039)

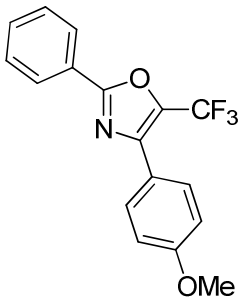




1bb

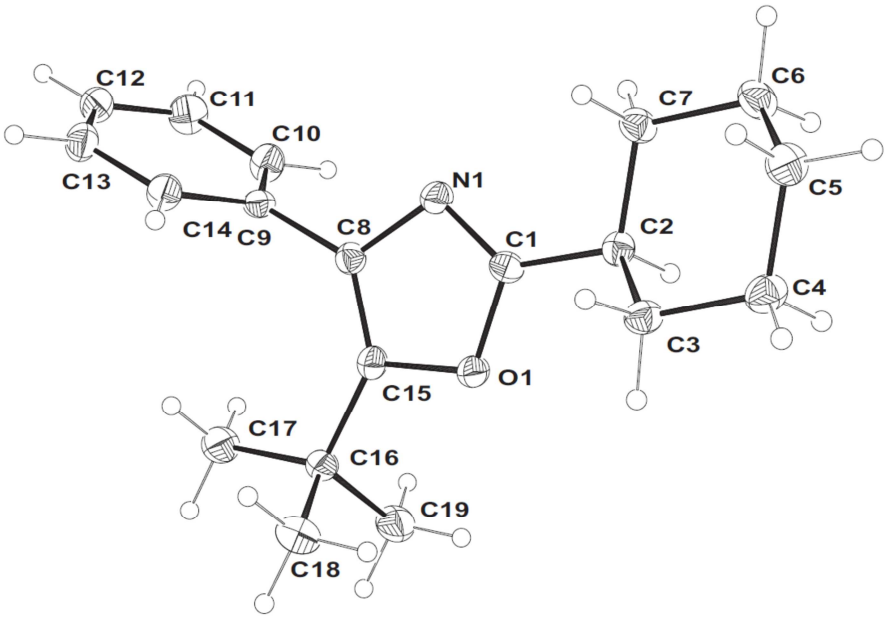
X-ray structure of **1bk**. (CCDC-940038)

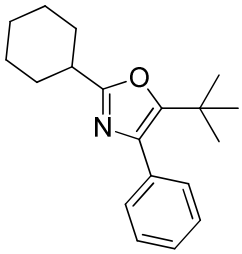




1bk

X-ray structure of **1ge**. (CCDC-940042)





1ge