Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Copper-Catalyzed Trifluoromethylthiolation-Peroxidation of Alkenes and Allenes

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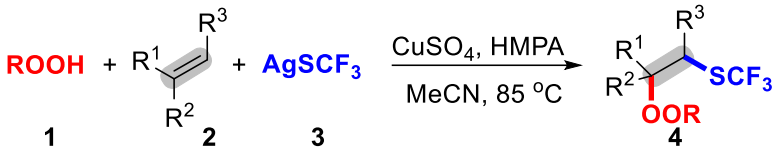
Contents

1. General information

^{1}H NMR spectra were recorded on Bruker 400 MHz and 600 MHz spectrometer and the chemical shifts were reported in parts per million (δ) relative to internal standard TMS (0 ppm) for $CDCl_3$. The peak patterns are indicated as follows: s, singlet; d, doublet; dd, doublet of doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, *J*, are reported in Hertz (Hz). ^{13}C NMR spectra were obtained at Bruker 100 MHz, 150 MHz and referenced to the internal solvent signals (central peak is 77.0 ppm in $CDCl_3$). ^{19}F NMR spectra were obtained at Bruker 376 MHz, 564 MHz. $CDCl_3$ was used as the NMR solvent. APEX II (Bruker Inc.) was used for ESI-MS and EI-MS. IR spectra were recorded by a Bruker Tensor 27 infrared spectrometer. Flash column chromatography was performed over silica gel 200-300. All reagents were weighed and handled in air at room temperature. All chemical reagents were purchased from Alfa, Acros, Aldrich, TCI, and J&K and used without further purification.

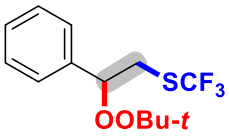
CAUTION: Mixing a metal salt and peroxide can cause explosion. See: D. G. Churchill, Chemical Structure and Accidental Explosion Risk in the Research Laboratory, *J. Chem. Edu.* 2006, **83**, 1798.

2. General procedure for synthesis of 4



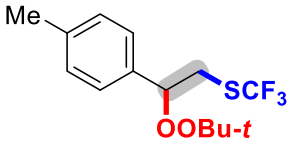
To a dry Schlenk tube were added $CuSO_4$ (0.1 mmol), $AgSCF_3$ **3** (1.0 mmol), $K_2S_2O_8$ (1.5 mmol)，HMPA (0.25 mmol), alkene **2** (0.5 mmol) and anhydrous MeCN (5.0 mL) under N_2 atmosphere at room temperature. Subsequently, **1a** (T-hydro, 70% in water, 2.5 mmol) was added to the mixture, and the resulting solution was stirred at 85 °C for 5 h. The resulting mixture and the solvent was evaporated under vacuum. The residue was purified by flash column chromatography on silica gel (eluent: ethylacetate/ petroleum ether) to give the trifluoromethylthiolation-peroxidation products **4**.

3. Characterization of 4



4a

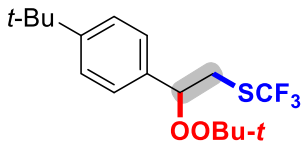
(2-(*tert*-Butylperoxy)-2-phenylethyl)(trifluoromethyl)sulfane (4a): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 66% yield (97mg); Colorless oil; IR (KBr): ν_{max} 2983, 2920, 1457, 1363, 1320, 1252, 1153, 1116, 1051, 871, 758, 697 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.31-7.37 (m, 5H), 5.10 (t, J = 6.4Hz, 1H), 3.44 (dd, J = 7.5Hz, J = 13.6Hz, 1H), 3.16 (dd, J = 5.9Hz, J = 13.6Hz, 1H), 1.24 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 138.1, 131.1 (q, J = 304.3 Hz), 128.7, 128.6, 127.0, 84.2, 81.1, 33.7, 26.3; ^{19}F NMR (564 MHz, $CDCl_3$) δ -41.78 (s, 3F); HRMS (ESI) calcd for $C_{13}H_{17}F_3O_2SNa$ (M+Na)+: 317.0794; found: 317.0797.



4b

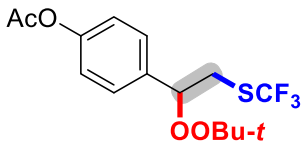
(2-**(*tert*-Butylperoxy)-2-(p-tolyl)ethyl)(trifluoromethyl)sulfane (4b):** Isolated by

flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 67% yield (103 mg); Colorless oil; IR (KBr): ν_{max} 2982, 2926, 1690, 1612, 1517, 1463, 1365, 1263, 1197, 1158, 1115, 1053, 1011, 872, 814, 755 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.23 (d, J = 7.8 Hz, 2H), 7.18 (d, J = 8.1 Hz, 2H), 5.06 (t, J = 6.8 Hz, 1H), 3.47 (dd, J = 7.2 Hz, J = 13.5 Hz, 1H), 3.15 (dd, J = 6.3 Hz, J = 13.5 Hz 1H), 2.35 (s, 3H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 134.8, 129.3, 129.1 (q, J = 290.0 Hz), 127.0, 84.1, 81.1, 33.6, 26.3, 21.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.77 (s, 3F); HRMS (ESI) calcd for $C_{14}H_{20}F_3O_2S$ (M+H)+: 309.1131; found: 309.1172.



4c

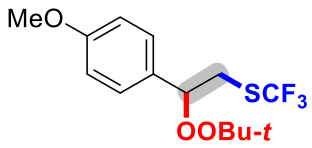
(2-(4-(*tert*-Butyl)phenyl)-2-(*tert*-butylperoxy)ethyl)(trifluoromethyl)sulfane (4c): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 73% yield (128 mg); white solid; IR (KBr): ν_{max} 2985, 2931, 1923, 1701, 1622, 1466, 1369, 1326, 1260, 1163, 1120, 1064, 1016, 841, 755 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, J = 8.3 Hz, 2H), 7.26 (d, J = 8.3 Hz, 2H), 5.08 (t, J = 6.6 Hz, 1H), 3.47 (dd, J = 7.4 Hz, J = 13.5 Hz, 1H), 3.17 (dd, J = 6.0 Hz, J = 13.5 Hz, 1H), 1.31 (s, 9H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 134.8, 129.2 (q, J = 304.2 Hz), 126.7, 125.5, 84.1, 81.1, 34.6, 33.7, 31.3, 26.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.83 (s, 3F); HRMS (ESI) calcd for $C_{17}H_{25}F_3O_2SNa$ (M+Na)+: 373.1420; found: 373.1406, $C_{17}H_{26}F_3O_2S$ (M+H)+: 351.1600; found: 351.1649.



4d

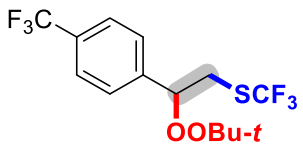
4-(1-(*tert*-Butylperoxy)-2-((trifluoromethyl)thio)ethyl)phenyl acetate (4d): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 70% yield (123 mg); white solid; IR (KBr): ν_{max} 2983, 2930, 1765, 1605, 1509, 1371, 1206, 1115, 1012, 913, 866, 755 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J

= 8.6 Hz, 2H), 7.10 (d, *J* = 8.6 Hz, 2H), 5.09 (dd, *J* = 6.0 Hz, *J* = 7.4 Hz, 1H), 3.40 (dd, *J* = 7.7 Hz, *J* = 13.8 Hz, 1H), 3.14 (dd, *J* = 5.8 Hz, *J* = 13.8 Hz, 1H), 2.29 (s, 3H), 2.14 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 150.8, 135.6, 130.5 (q, *J* = 305.4 Hz), 128.0, 121.7, 83.6, 81.2, 33.6, 26.3, 21.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.77 (s, 3F) ; HRMS (ESI) calcd for $C_{15}H_{19}F_3O_4SNa$ $(M+Na)^+$: 375.0848; found: 375.0851.



4e

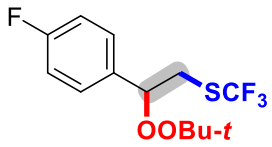
(2-(*tert*-Butylperoxy)-2-(4-methoxyphenyl)ethyl)(trifluoromethyl)sulfane (4e): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 60% yield (98 mg); Colorless oil; IR (KBr): ν_{max} 2980, 2926, 2844, 1680, 1605, 1513, 1460, 1368, 1310, 1255, 1146, 1031, 830, 755 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.7 Hz, 2H), 6.90 (d, *J* = 9.0 Hz, 2H), 5.04 (t, *J* = 6.8 Hz, 1H), 3.80 (s, 3H) , 3.49 (dd, *J* = 7.1 Hz, *J* = 13.5 Hz, 1H), 3.15 (dd, *J* = 6.6 Hz, *J* = 13.4 Hz, 1H), 1.24(s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 130.8, 130.0 (q, *J* = 304.0 Hz), 129.7, 128.4, 113.9, 83.9, 81.0, 55.2, 33.4, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.76 (s, 3F); HRMS (ESI) calcd for $C_{14}H_{20}F_3O_3S$ $(M+H)^+$: 325.1080; found: 325.0943.



4f

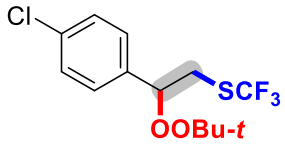
(2-(*tert*-Butylperoxy)-2-(4-(trifluoromethyl)phenyl)ethyl)(trifluoromethyl)sulfane (4f): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, Rf = 0. 6) in 71% yield (129 mg); Colorless oil; IR (KBr): ν_{max} 2969, 2870, 1690, 1609, 1468, 1403, 1364, 1263, 1200, 1153, 1116, 1011, 870, 832, 756 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.2 Hz , 2H), 7.48 (d, *J* = 8.1 Hz, 2H), 5.16 (dd, *J* = 5.8 Hz, *J* = 7.6 Hz, 1H), 3.45 (dd, *J* = 7.9 Hz, *J* = 14.0 Hz, 1H), 3.14 (dd, *J* = 5.5 Hz, *J*

= 14.0 Hz, 1H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, CDCl3) δ 142.5, 130.9 (q, J = 304.4 Hz), 127.2, 125.6, 125.5, 83.5, 81.5, 33.6, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.83 (s, 3F), -62.72 (s, 3F); HRMS (ESI) calcd for $C_{14}H_{16}F_6O_2SNa$ $(M+Na)^+$: 385.0667; found: 385.0621.



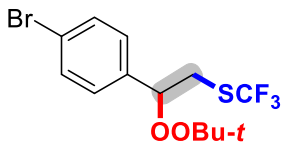
4g

(2-(*tert*-Butylperoxy)-2-(4-fluorophenyl)ethyl)(trifluoromethyl)sulfane (4g): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 79% yield (123 mg); Colorless oil; IR (KBr): ν_{max} 2983, 2926, 1694, 1605, 1511, 1485, 1364, 1309, 1283, 1193, 1054, 929, 871, 853, 756 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.30 (m, 2H), 7.08-7.03 (m, 2H), 5.07 (t, J = 6.8 Hz, 1H), 3.42 (dd, J = 7.4 Hz, J = 13.7 Hz, 1H), 3.13 (dd, J = 6.1 Hz, J = 13.7 Hz, 1H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 130.9 (q, J = 305.5 Hz), 128.8, 128.7, 115.6, 115.4, 83.5, 81.2, 33.6, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.76 (s, 3F), -112.98 (s, 1F); HRMS (ESI) calcd for $C_{13}H_{17}F_4O_2S$ $(M+H)^+$: 313.0880; found: 313.0817.



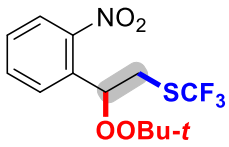
4h

(2-(*tert*-Butylperoxy)-2-(4-chlorophenyl)ethyl)(trifluoromethyl)sulfane (4h): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 74% yield (122 mg); Colorless oil; IR (KBr): ν_{max} 2983, 2928, 1693, 1595, 1522, 1458, 1365, 1255, 1156, 1117, 1053, 930, 868, 823, 756 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8.5 Hz, 2H), 7.28 (d, J = 8.5 Hz, 2H), 5.07 (t, J =6.4 Hz, 1H), 3.38 (dd, J = 7.6 Hz, J = 13.8 Hz, 1H), 3.11 (dd, J = 5.9 Hz, J = 13.8 Hz, 1H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 134.5, 130.9 (q, J = 304.5 Hz), 128.8, 128.3, 83.5, 81.3, 33.5, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.71 (s, 3F). HRMS (ESI) calcd for $C_{13}H_{16}ClF_3O_2SNa$ $(M+Na)^+$: 351.0404; found: 351.0495.



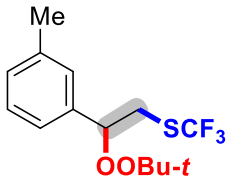
4i

(2-(4-Bromophenyl)-2-(*tert*-butylperoxy)ethyl)(trifluoromethyl)sulfane (4i): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 76% yield (142 mg); white solid; IR (KBr): ν_{max} 2982, 2926, 1693, 1604, 1461, 1369, 1320, 1254, 1154, 1116, 1053, 1010, 872, 757, 699 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, J = 8.4 Hz, 2H), 7.22 (d, J = 8.3 Hz, 2H), 5.06 (t, J = 6.4 Hz, 1H), 3.37 (dd, J = 7.6 Hz, J = 13.8 Hz, 1H), 3.11 (dd, J = 5.8 Hz, J = 13.8 Hz, 1H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 131.7, 130.9 (q, J = 304.3 Hz), 128.6, 122.7, 83.5, 81.2, 33.5, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.68 (s, 3F); HRMS (ESI) calcd for $C_{13}H_{16}BrF_3O_2SNa$ (M+Na)+: 394.9199; found: 394.9096.



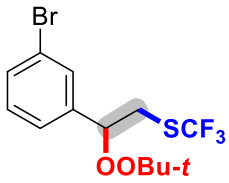
4j

(2-(*tert*-Butylperoxy)-2-(2-nitrophenyl)ethyl)(trifluoromethyl)sulfane (4j): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 63% yield (107 mg); Colorless oil; IR (KBr): ν_{max} 2982, 2927, 1579, 1529, 1466, 1398, 1353, 1304, 1253, 1110, 862, 792, 755 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.05-8.03 (m, 1H), 7.84-7.82 (m, 1H), 7.73-7.69 (m, 1H), 7.52-7.48 (m, 1H), 5.73 (dd, J = 3.3 Hz, J = 9.0 Hz, 1H), 3.55 (dd, J = 3.3 Hz, J = 14.0 Hz, 1H), 3.14 (dd, J = 9.0 Hz, J = 14.1 Hz, 1H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 135.2, 133.7, 130.7 (q, J = 304.6 Hz), 129.0, 128.7, 124.7, 81.8, 79.4, 33.5, 26.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.69 (s, 3F); HRMS (ESI) calcd for $C_{13}H_{16}F_3NO_4SNa$ $(M+Na)^+$: 362.0644; found: 362.0650.



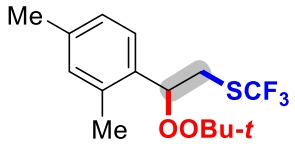
4k

(2-(*tert*-Butylperoxy)-2-(m-tolyl)ethyl)(trifluoromethyl)sulfane (4k): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 74% yield (114 mg); Colorless oil; IR (KBr): ν_{max} 2982, 2926, 1693, 1603, 1461, 1369, 1320, 1254, 1154, 1116, 1053, 1010, 872, 757, 699 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.28-7.23 (m, 1H), 7.16-7.14 (m, 3H), 5.06 (t, J = 6.6 Hz, 1H), 3.44 (dd, J = 7.5 Hz, J = 13.6 Hz, 1H), 3.15 (dd, J = 6.0 Hz, J = 13.8 Hz, 1H), 2.36 (s, 3H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 137.9, 131.0 (q, J = 304.1 Hz), 129.5, 128.5, 127.6, 124.1, 84.3, 81.2, 33.7, 26.3, 21.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.80 (s, 3F); HRMS (ESI) calcd for $C_{14}H_{20}F_3O_2S$ (M+H)+: 309.1131; found: 309.1172.



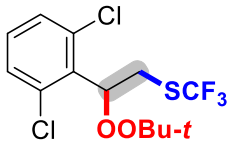
4l

(3-Bromophenyl)-2-(*tert*-butylperoxy)ethyl)(trifluoromethyl)sulfane (4l): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 72% yield (134 mg); Colorless oil; IR (KBr): ν_{max} 2982, 2928, 1697, 1573, 1473, 1425, 1395, 1369, 1252, 1198, 1159, 1116, 1058, 1011, 874, 790, 752, 687 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.49-7.46 (m, 2H), 7.29-7.22 (m, 2H), 5.05 (dd, J = 5.9 Hz, J = 7.6 Hz, 1H), 3.35 (dd, J = 7.8 Hz, J = 13.9 Hz, 1H), 3.11 (dd, J = 5.6 Hz, J = 13.9 Hz, 1H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 131.7, 130.8 (q, J = 305.8 Hz), 130.1, 129.9, 125.5, 122.6, 83.4, 81.4, 33.6, 26.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.69 (s, 3F); HRMS (ESI) calcd for $C_{13}H_{17}BrF_3O_2S$ $(M+H)^+$: 373.0079; found: 373.0151.



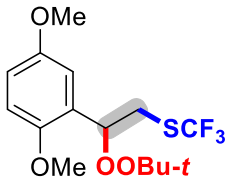
4m

(2-(*tert*-Butylperoxy)-2-(2,4-dimethylphenyl)ethyl)(trifluoromethyl)sulfane (4m): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 69% yield (111 mg); Colorless oil; IR (KBr): ν_{max} 2980, 2926, 1697, 1612, 1459, 1369, 1252, 1199, 1154, 1116, 1053, 1010, 862, 755 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.24 (d, J = 7.9 Hz, 1H), 7.04 (d, J = 7.9 Hz, 1H), 7.00 (s, 1H), 5.35 (t, J = 6.7 Hz, 1H), 3.41 (dd, J = 7.2 Hz, J = 13.4 Hz, 1H), 3.16 (dd, J = 5.2 Hz, J = 12.9 Hz, 1H), 2.35 (s, 3H), 2.30 (s, 3H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 135.7, 133.2, 131.4, 131.1 (q, J = 304.2 Hz), 127.0, 126.3, 81.0, 80.5, 33.1, 26.4, 21.0, 19.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.9 (s, 3F); HRMS (ESI) calcd for $C_{15}H_{22}F_3O_2S$ $(M+H)^+$: 323.1287; found: 323.1257.



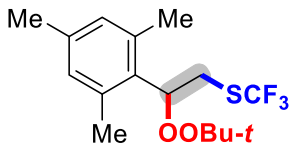
4n

(2-(*tert*-Butylperoxy)-2-(2,6-dichlorophenyl)ethyl)(trifluoromethyl)sulfane (4n): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 75% yield (136mg); Colorless oil; IR (KBr): ν_{max} 2986, 2912, 1612, 1458, 1386, 1250, 1188, 1154, 1012, 1053, 862, 766 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, J = 8.0 Hz, 2H), 7.18 (t, J = 8.0 Hz, 1H), 5.98 (dd, J = 6.6 Hz, J = 8.2 Hz, 1H), 3.73 (dd, J = 8.4 Hz, J = 14.2 Hz, 1H), 3.42 (dd, J = 6.4 Hz, J = 14.2 Hz, 1H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 132.9, 131.8, 130.8 (q, J = 304.2 Hz), 129.9, 129.4, 81.3, 81.0, 30.2, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.73 (s, 3F); HRMS (ESI) calcd for $C_{13}H_{15}Cl_2F_3O_2SNa$ $(M+Na)^+$: 385.0014; found: 385.0012, $C_{13}H_{16}Cl_2F_3O_2S$ $(M+H)^+$: 363.0195; found: 363.0136.



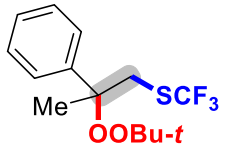
4o

(2-(*tert*-Butylperoxy)-2-(2,5-dimethoxyphenyl)ethyl)(trifluoromethyl)sulfane (4o): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, Rf = 0. 6) in 49% yield (86 mg); Colorless oil; IR (KBr): ν_{max} 2981, 2929, 1676, 1571, 1533, 1470, 1436, 1368, 1326, 1254, 1117, 1056, 1015, 930, 869, 774, 721 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 6.92 (s, 1H), 6.73 (s, 2H), 5.42 (dd, J = 4.4 Hz, J = 8.3 Hz, 1H), 3.72 (s, 3H), 3.71 (s, 3H), 3.28 (dd, J = 4.4 Hz, J = 13.7 Hz, 1H), 3.10 (dd, J = 8.3 Hz, J = 13.7 Hz, 1H), 1.20 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.6, 150.6, 131.1 (q, J = 304.1 Hz), 127.9, 113.6, 113.3, 111.5, 81.1, 78.6, 55.9, 55.7, 32.9, 26.4; ^{19}F NMR (564 MHz, $CDCl_3$) δ -41.89 (s, 3F); HRMS (ESI) calcd for $C_{15}H_{21}F_3O_4SNa$ $(M+Na)^+$: 377.1005; found: 377.1009, $C_{15}H_{22}F_3O_4S$ $(M+H)^+$: 355.1185; found: 355.1150.



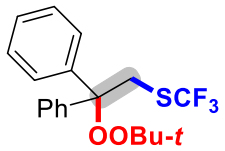
4p

(2-(*tert*-Butylperoxy)-2-mesitylethyl)(trifluoromethyl)sulfane (4p): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 72% yield (121 mg); white solid; IR (KBr): ν_{max} 2987, 2920, 2842, 1743, 1661, 1593, 1533, 1461, 1427, 1359, 1310, 1274, 1223, 1115, 1044, 943, 874, 805, 753 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 6.83 (s, 2H), 5.57 (t, J = 6.5 Hz, 1H), 3.60 (dd, J = 8.0 Hz, J = 13.6 Hz, 1H), 3.22 (dd, J = 6.3 Hz, J = 13.6 Hz, 1H), 2.40 (s, 6H), 2.25 (s, 3H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.9, 136.7, 131.1, 131.0 (q, J = 304.1 Hz), 130.2, 81.6, 80.8, 31.9, 26.4, 20.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.98 (s, 3F); HRMS (ESI) calcd for $C_{16}H_{23}F_3O_2SNa$ $(M+Na)^+$: 359.1263; found: 359.1269.



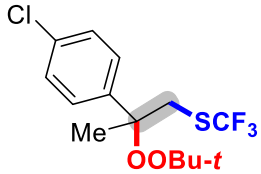
4q

(2-(*tert*-Butylperoxy)-2-phenylpropyl)(trifluoromethyl)sulfane (4q): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 84% yield (128 mg); Colorless oil; IR (KBr): ν_{max} 2984, 2928, 1451, 1370, 1191, 1115, 876, 758, 696 cm^{-1}; ^1H NMR (400 MHz, CDCl3) δ 7.43-7.26 (m, 5H), 3.50 (d, J = 12.7 Hz, 1H), 3.41 (d, J = 12.7 Hz, 1H), 1.69 (s, 3H), 1.26 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 131.3 (q, J = 305.2 Hz), 128.2, 127.6, 125.5, 82.1, 79.9, 38.8, 26.5, 24.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.90 (s, 3F); HRMS (ESI) calcd for $C_{14}H_{20}F_3O_2S$ $(M+H)^+$: 309.1131; found: 309.1170.



4r

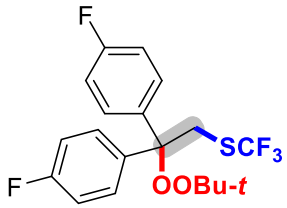
(2-(*tert*-Butylperoxy)-2,2-diphenylethyl)(trifluoromethyl)sulfane (4r): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 84% yield (155 mg); white solid; IR (KBr): ν_{max} 2983, 2930, 1663, 1600, 1495, 1388, 1365, 1277, 1244, 1150, 1119, 1030, 1003, 910, 876, 781, 755, 697 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.34-7.23 (m, 10H), 4.03 (s, 2H), 1.24 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.0, 131.3 (q, J = 304.0 Hz), 128.0, 127.7, 126.8, 85.2, 80.4, 37.5, 26.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -42.10 (s, 3F); HRMS (ESI) calcd for $C_{19}H_{21}F_3O_2SNa$ $(M+Na)^+$: 393.1107; found: 393.1105.



4s

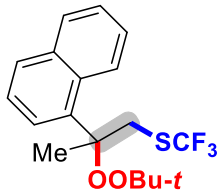
(2-(*tert*-Butylperoxy)-2-(4-chlorophenyl)propyl)(trifluoromethyl)sulfane (4s):

Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 80% yield (136 mg); white solid; IR (KBr): ν_{max} 2981, 2938, 2394, 2288, 1733, 1463, 1369, 1266, 1151, 1115, 1027, 847, 807, 755 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35-7.30 (m, 4H), 3.46 (d, J = 12.8 Hz, 1H), 3.37 (d, J = 12.8 Hz, 1H), 1.66 (s, 3H), 1.26 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.3, 133.5, 131.1 (q, J = 303.7 Hz), 128.4, 127.1, 81.9, 80.1, 38.6, 26.5, 24.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.91 (s, 3F); HRMS (ESI) calcd for $C_{14}H_{19}ClF_3O_2S$ $(M+H)^+$: 343.0941; found: 343.1085.



4t

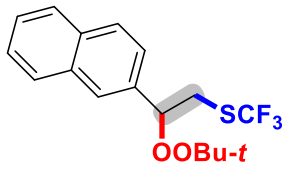
(2-(*tert*-Butylperoxy)-2,2-bis(4-fluorophenyl)ethyl)(trifluoromethyl)sulfane (4t): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 86% yield (175 mg); Colorless oil; IR (KBr): ν_{max} 2983, 1605, 1509, 1364, 1236, 1195, 1156, 1116, 1005, 878, 834, 753 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.30-7.27 (m, 4H), 7.03-6.98 (m, 4H), 3.96 (s, 2H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2 (d, J = 245.9 Hz), 137.7 (d, J = 2.6 Hz), 131.1 (q, J = 304.1 Hz), 128.7 (d, J = 8.1 Hz), 115.0 (d, J = 21.3 Hz), 84.7, 80.6, 37.7, 26.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -42.19 (s, 3F), -114.05 (s, 2F); HRMS (ESI) calcd for $C_{19}H_{19}F_5O_2SNa$ (M+Na)+: 429.0918; found: 429.0895.



4u

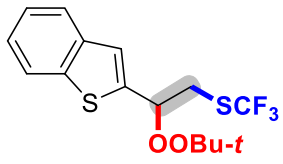
(2-(*tert*-Butylperoxy)-2-(naphthalen-1-yl)propyl)(trifluoromethyl)sulfane (4u): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 80% yield (143 mg); yellow solid; IR (KBr): ν_{max} 2983, 2929, 1511, 1460, 1370, 1254, 1115, 872, 807, 772 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.72 (d, J = 8.3

Hz,1H), 7.83 (d, *J* = 9.4 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.52-7.43 (m, 3H), 7.39 (t, *J* = 7.8 Hz, 1H), 3.97 (d, *J* = 12.6 Hz, 1H), 3.64 (d, *J* = 12.6 Hz, 1H), 1.97 (s, 3H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 137.6, 134.7, 131.3 (q, *J* = 303.9 Hz), 131.0, 129.5, 129.1, 126.4, 125.6, 125.3, 124.7, 124.6, 84.0, 79.9, 38.5, 26.7, 24.1; ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -41.68 (s, 3F); HRMS (ESI) calcd for $C_{17}H_{18}F_3O_2SNa$ $(M+Na)^+$: 359.1287; found: 359.1199.



4v

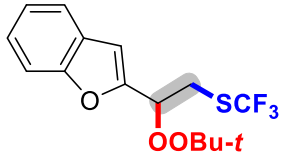
(2-(*tert*-Butylperoxy)-2-(naphthalen-2-yl)ethyl)(trifluoromethyl)sulfane (4v): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0.6) in 73% yield (126mg); white solid; IR (KBr): ν_{max} 2981, 2928, 1687, 1600, 1512, 1466, 1369, 1316, 1253, 1158, 1115, 1054, 953, 818, 752, 712 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.85-7.80 (m, 4H), 7.48-7.44 (m, 3H), 5.26 (t, *J* = 6.4 Hz, 1H), 3.52 (dd, *J* = 7.6 Hz, *J* = 13.6 Hz, 1H), 3.24 (dd, *J* = 5.9 Hz, *J* = 13.6 Hz, 1H), 1.26 (s, 9H); ^{13}C NMR (100 MHz,$CDCl_3$)*δ* 135.5, 133.5, 133.1, 131.0 (q, *J* = 304.2 Hz), 128.5, 128.1, 127.7, 126.5, 126.4, 126.3, 124.2, 84.4, 81.2, 33.6, 26.4; ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -41.62 (s, 3F); HRMS (ESI) calcd for $C_{17}H_{19}F_3O_2SNa$ $(M+Na)^+$: 367.0950; found: 367.0950.



4w

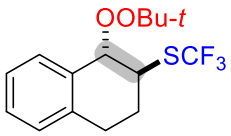
2-(1-(*tert*-Butylperoxy)-2-((trifluoromethyl)thio)ethyl)benzo[b]thiophene (4w): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 5:1, R_f = 0.6) in 54% yield (94 mg); white solid; IR (KBr):ν_{max} 2981, 2928, 1667, 1463, 1362, 1313, 1251, 1154, 1115, 1014, 865, 752 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.82-7.74 (m, 2H), 7.37-7.29 (m, 3H), 5.39 (t, *J* = 6.8 Hz, 1H), 3.60 (dd, *J* = 7.0 Hz, *J*

= 13.8 Hz, 1H), 3.29 (dd, *J* = 6.5 Hz, *J* = 13.8 Hz, 1H), 1.26 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$)δ 141.1, 139.8, 139.0, 130.9 (q, *J* = 304.5 Hz), 124.7, 124.4, 123.9, 123.2, 122.4, 81.5, 80.4, 33.5, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.59 (s, 3F); HRMS (ESI) calcd for $C_{15}H_{17}F_3O_2S_2Na$ (M+Na)+: 351.0695; found: 351.0681.



4x

2-(1-(*tert*-Butylperoxy)-2-((trifluoromethyl)thio)ethyl)benzofuran (4x): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 57% yield (98 mg); white solid; IR (KBr): ν_{max} 2982, 2928, 1669, 1614, 1453, 1364, 1313, 1253, 1156, 1116, 1006, 947, 871, 811, 750 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.32-7.28 (m, 1H), 7.25-7.23 (m, 1H), 6.8 (s, 1H), 5.24 (t, *J* = 7.0 Hz, 1H), 3.60 (dd, *J* = 7.0 Hz, *J* = 14.0 Hz, 1H), 3.40 (dd, *J* = 7.0 Hz, *J* = 14.0 Hz, 1H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 152.6, 130.8 (q, *J* = 304.5 Hz), 127.7, 124.8, 123.0, 121.4, 111.5, 106.8, 81.5, 78.1, 30.3, 26.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.62 (s, 3F); HRMS (ESI) calcd for $C_{15}H_{17}F_3O_3SNa$ $(M+Na)^+$: 357.0743; found: 357.0715.



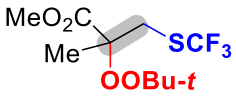
4y

***trans*:*cis* > 20:1**

(1-(*tert*-Butylperoxy)-1,2,3,4-tetrahydronaphthalen-2-yl)(trifluoromethyl)sulfane (4y): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 59% yield (94 mg), *trans*:*cis* > 20:1; Colorless oil; IR (KBr): ν_{max} 2981, 2928, 1694, 1606, 1455, 1394, 1364, 1323, 1251, 1197, 1110, 1007, 937, 876, 816, 758 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.12 (m, 4H), 5.03 (s, 1H), 4.36-4.34 (m, 1H), 2.95-2.78 (m, 2H), 2.57-2.50 (m, 1H), 2.09-2.05 (m, 1H), 1.30 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.3, 132.3, 131.3 (q, *J* = 304.5 Hz), 129.3, 129.2, 129.0,

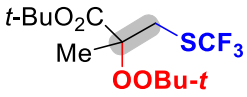
126.3, 81.8, 80.8, 40.9, 26.5, 24.5, 22.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.63 (s, 3F); HRMS (ESI) calcd for $C_{15}H_{19}F_3O_2SNa$ $(M+Na)^+$:343.0950; found: 343.0976.

4. Characterization of 4aa-4ha and 6



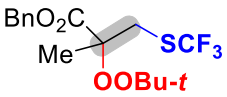
4aa

Methyl 2-(*tert*-butylperoxy)-2-methyl-3-((trifluoromethyl)thio)propanoate (4aa): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 53% yield (77 mg); Colorless oil; IR (KBr): ν_{max} 2984, 1746, 1454, 1368, 1308, 1266, 1194, 1116, 1022, 878, 810, 766 cm^{-1}; ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.70 (s, 3H), 3.53 (d, J = 13.5 Hz, 1H), 3.24 (d, J = 13.5 Hz, 1H), 1.42 (s, 3H), 1.14 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ171.9, 131.3 (q, J = 303.6 Hz), 82.3, 80.6, 52.3, 34.1, 26.3, 20.0; ^{19}F NMR (564 MHz, $CDCl_3$) δ -41.79 (s, 3F); HRMS (ESI) calcd for $C_{10}H_{17}F_3O_4SNa$ (M+Na)+: 313.0692; found: 313.0697.



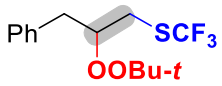
4ba

***tert*-Butyl 2-(*tert*-butylperoxy)-2-methyl-3-((trifluoromethyl)thio)propanoate (4ba):** Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 50% yield (83 mg); white solid; IR (KBr): ν_{max} 2981, 2938, 2394, 2288, 1733, 1463, 1369, 1166, 1151, 1115, 1027, 847, 807, 755 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.55 (d, J = 13.3 Hz, 1H), 3.28 (d, J = 13.3 Hz, 1H), 1.49 (s, 9H), 1.46 (s, 3H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 131.2 (q, J = 303.5 Hz), 82.4, 82.0, 80.2, 34.1, 27.8, 26.4, 20.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.91 (s, 3F); HRMS (ESI) calcd for $C_{13}H_{23}F_3O_4SNa$ $(M+Na)^+$: 355.1161; found: 355.1153.



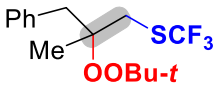
4ca

Benzyl 2-(*tert*-butylperoxy)-2-methyl-3-((trifluoromethyl)thio)propanoate (4ca): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 34% yield (63 mg); white solid; IR (KBr): ν_{max} 3033, 2980, 1742, 1457, 1373, 1300, 1258, 1111, 1028, 873, 805, 748, 696 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.30-7.26 (m, 5H), 5.14 (d, J = 4.8 Hz, 2H), 3.56 (d, J = 13.5 Hz, 1H), 3.24 (d, J = 13.5 Hz, 1H), 1.42 (s, 3H), 1.09 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 135.4, 131.0 (q, J = 303.8 Hz), 128.5, 128.3, 128.2, 82.3, 80.6, 67.1, 34.1, 26.3, 20.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.69 (s, 3F); HRMS (ESI) calcd for $C_{16}H_{21}F_3O_4SNa$ $(M+Na)^+$: 389.1005; found: 389.1000.



4da

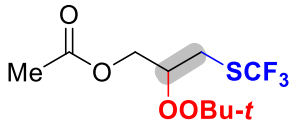
(2-(*tert*-Butylperoxy)-3-phenylpropyl)(trifluoromethyl)sulfane (4da): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 31% yield (48 mg); white solid; IR (KBr): ν_{max} 2977, 2924, 1745, 1644, 1458, 1365, 1251, 1193, 1152, 1116, 1030, 870, 749, 699 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.28-7.21 (m, 5H), 4.36-4.30 (m, 1H), 3.20-3.16 (m, 1H), 3.04-2.92 (m, 3H), 1.16 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.0, 129.5, 128.4, 126.7, 82.7, 80.9, 37.8, 31.6, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.54 (s, 3F); HRMS (ESI) calcd for $C_{14}H_{20}F_3O_2S$ $(M+H)^+$: 309.1131; found: 309.0923.



4ea

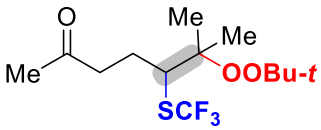
(2-(*tert*-Butylperoxy)-2-methyl-3-phenylpropyl)(trifluoromethyl)sulfane (4ea): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 42% yield (68 mg); white solid; IR (KBr): ν_{max} 2981, 2919, 2849, 2358, 1647, 1460, 1367, 1263, 1194, 1150, 1114, 934, 874, 805, 754, 701 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.29-7.23 (m, 5H), 3.21 (d, J = 12.6 Hz, 1H), 3.07 (d, J = 12.6 Hz, 1H), 3.05 (d, J = 13.8 Hz, 1H), 2.85 (d, J = 13.8 Hz, 1H), 1.24 (s, 9H), 1.21 (s, 3H) ;

^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 130.7, 129.4 (q, J = 307.2 Hz), 128.0, 126.6, 81.1, 79.6, 42.8, 37.1, 26.6, 21.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.7 (s, 3F); HRMS (ESI) calcd for $C_{15}H_{21}F_3O_2SNa$ $(M+Na)^+$: 345.1107; found: 345.1056.



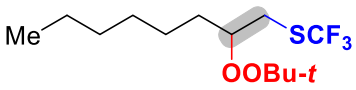
4fa

2-(*tert*-Butylperoxy)-3-((trifluoromethyl)thio)propyl acetate (4fa): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 43% yield (63 mg); Colorless oil; IR (KBr): ν_{max} 2981, 2929, 2359, 1748, 1462, 1371, 1283, 1155, 1116, 1042, 872, 755 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.28-4.17 (m, 3H), 3.13 (dd, J = 5.8 Hz, J = 13.6 Hz, 1H), 3.00 (dd, J = 5.1 Hz, J = 13.8 Hz, 1H), 2.02 (s, 3H), 1.17 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 130.8 (q, J = 304.2 Hz), 81.1, 79.6, 62.4, 28.9, 26.1, 20.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.8 (s, 3F); HRMS (ESI) calcd for $C_{10}H_{17}F_3O_4SNa$ (M+Na)+: 313.0692; found: 313.0692.



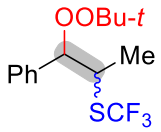
4ga

5-(*tert*-Butylperoxy)-6-methyl-6-((trifluoromethyl)thio)heptan-2-one (4ga): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 36% yield (57 mg); Colorless oil; IR (KBr): ν_{max} 2921, 2855, 2392, 2281, 1516, 1465, 1362, 1268, 1025, 904, 756 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.78-2.55 (m, 3H), 2.14 (s, 3H), 2.11-1.98 (m, 1H), 1.77-1.67 (m, 1H), 1.39 (s, 3H), 1.19 (s, 9H), 1.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 208.1, 80.0, 78.9, 48.1, 43.2, 29.8, 26.6, 25.4, 21.2, 18.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3 (s, 3F); HRMS (ESI) calcd for $C_{13}H_{24}F_3O_3S$ (M+H)+: 317.1393; found: 317.1365;317.1367.



4ha

(2-(*tert*-Butylperoxy)octyl)(trifluoromethyl)sulfane (4ha): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 36% yield (57 mg); Colorless oil; IR (KBr): ν_{max} 2928, 2862, 1752, 1644, 1462, 1370, 1334, 1250, 1152, 1117, 1029, 876, 755 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 4.19-4.08 (m, 1H), 3.21 (dd, J = 5.1 Hz, J = 13.3 Hz, 1H), 3.04 (dd, J = 5.8 Hz, J = 13.3 Hz, 1H), 1.64-1.56 (m, 2H), 1.33-1.29 (m, 8H), 1.24 (s, 9H), 0.89 (t, J = 6.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.2 (q, J = 303.7 Hz), 81.7, 80.4, 32.3, 31.7, 29.2, 26.4, 25.5, 25.2, 22.6, 14.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.9 (s, 3F); HRMS (ESI) calcd for $C_{13}H_{26}F_3O_2S$ $(M+H)^+$: 303.1600; found: 303.1454.

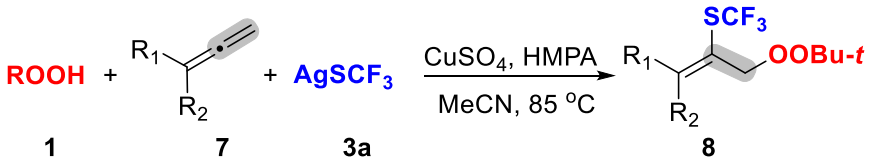


6

dr=2:1

(1-(*tert*-Butylperoxy)-1-phenylpropan-2-yl)(trifluoromethyl)sulfane (5): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 63% yield (97 mg), *dr*=2:1; Colorless oil; IR (KBr): ν_{max} 2983, 2359, 1457, 1369, 1266, 1193, 1115, 1022, 755, 701 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.43-7.33 (m, 10H), 5.26 (d, J = 3.1 Hz, 1H), 5.07 (d, J = 5.4 Hz, 1H), 3.90-3.84 (m, 1H), 3.71-3.65 (m, 1H), 1.39 (d, J = 7.2 Hz, 3H), 1.38 (d, J = 7.0 Hz, 3H), 1.32 (s, 9H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 136.5, 131.3 (q, J = 304.6 Hz), 128.3, 128.2, 128.1, 128.0, 127.6, 126.7, 87.0, 86.9, 81.2, 81.0, 45.0, 43.0, 26.4, 26.3, 17.7, 16.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.57 (s, 3F), -40.57 (s, 3F); HRMS (ESI) calcd for $C_{14}H_{20}F_3O_2S$ $(M+H)^+$: 309.1131; found: 309.1171.

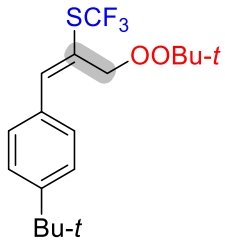
5. General procedure for synthesis of 8



1 7 3a 8

To a dry Schlenk tube were added $CuSO_4$ (0.1 mmol), $AgSCF_3$ **3** (1.0 mmol), $K_2S_2O_8$ (1.5 mmol), HMPA (0.25 mmol), allenes **7** (0.5 mmol) and anhydrous MeCN (5.0 mL) under N_2 atmosphere at room temperature. Subsequently, **1** (T-hydro, 70% in water, 2.5 mmol) was added to the mixture, and the resulting solution was stirred at 85 °C for 5 h. The resulting mixture and the solvent was evaporated under vacuum. The residue was purified by flash column chromatography on silica gel (eluent: ethylacetate/ petroleum ether) to give the trifluoromethylthiolation-peroxidation products **8**.

6. Characterization of 8



8a

E/*Z*=11:1

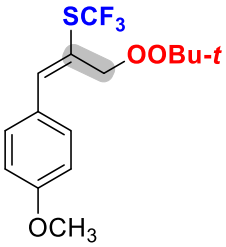
(1-(4-(*tert*-Butyl)phenyl)-3-(*tert*-butylperoxy)prop-1-en-2-yl)(trifluoromethyl)sulfane (8a): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 48% yield (87 mg), *E*/*Z*=11:1; Colorless oil; IR (KBr): ν_{max} 2978, 1603, 1510, 1462, 1362, 1265, 1117, 1028, 913, 828, 754 cm^{-1};

E-isomer ^1H NMR (400 MHz, $CDCl_3$) δ 7.46-7.36 (m, 5H), 4.79 (s, 2H), 1.33 (s, 9H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 150.2, 131.9, 130.0 (q, J = 307.3 Hz), 129.0, 125.6, 121.8, 80.9, 74.3, 34.8, 31.2, 26.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -42.12 (s, 3F);

Z-isomer ^1H NMR (400 MHz, $CDCl_3$) 4.71 (s, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ

-39.27 (s, 3F);

HRMS (ESI) calcd for $C_{18}H_{26}F_3O_2S$ $(M+H)^+$: 363.1600; found: 363.1604.



8b

E/*Z*=1.3:1

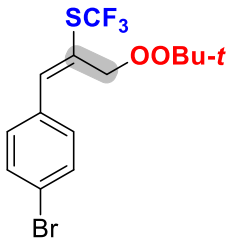
(3-(*tert*-Butylperoxy)-1-(4-methoxyphenyl)prop-1-en-2-yl)(trifluoromethyl)sulfane (8b): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 50% yield (84 mg), *E*/*Z*=1.3:1; Colorless oil; IR (KBr): ν_{max} 2976, 2926, 1606, 1512, 1462, 1368, 1295, 1258, 1117, 1031, 877, 830, 754 cm^{-1};

E-isomer ^1H NMR (400 MHz, $CDCl_3$) δ 4.72 (s, 2H), 1.21 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -42.29 (s, 3F);

Z-isomer ^1H NMR (400 MHz, $CDCl_3$) δ 4.63 (s, 2H), 1.20 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.58 (s, 3F);

Overlap ^1H NMR (400 MHz, $CDCl_3$) δ 7.58-6.82 (m, 10H), 3.76 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 160.2, 150.2, 143.9, 131.6, 130.9, 127.4, 127.1, 120.0, 118.0, 114.0, 113.7, 80.9, 80.8, 80.0, 74.5, 55.3, 55.2, 26.4;

HRMS (ESI) calcd for $C_{15}H_{19}F_3O_3SNa$ $(M+Na)^+$: 359.0899; found: 359.0902.



8c

E/*Z*=2:1

(1-(4-Bromophenyl)-3-(*tert*-butylperoxy)prop-1-en-2-yl)(trifluoromethyl)sulfane (8c): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1,

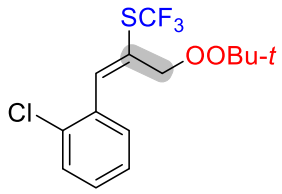
R_f = 0. 6) in 44% yield (84mg); Colorless oil; IR (KBr): ν_{max} 2977, 2923, 2855, 1644, 1480, 1363, 1265, 1117, 1013, 912, 877, 814, 752, 662 cm^{-1};

E-isomer ^1H NMR (400 MHz, $CDCl_3$) δ 4.72 (s, 2H), 1.26 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.76 (s, 3F);

Z-isomer ^1H NMR (400 MHz, $CDCl_3$) δ 4.71 (s, 2H), 1.28 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.13 (s, 3F) ;

Overlap ^1H NMR (400 MHz, $CDCl_3$) δ 7.55-7.28 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 142.0, 133.5, 131.8, 131.5, 131.2, 130.6, 124. 0, 123.50, 122.2, 81.0, 80.9, 79.1, 73.9, 26.3;

HRMS (ESI) calcd for $C_{14}H_{17}BrF_3O_2S$ $(M+H)^+$: 385.0079; found: 385.0107.



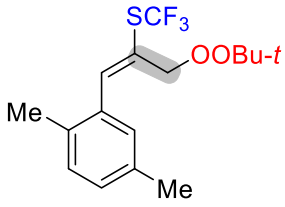
8d
E/*Z*=5:1

(3-(*tert*-Butylperoxy)-1-(2-chlorophenyl)prop-1-en-2-yl)(trifluoromethyl)sulfane (8d): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 53% yield (91 mg), *E*/*Z*=5:1; Colorless oil; IR (KBr): ν_{max} 2970, 2928, 1692, 1611, 1458, 1365, 1258, 1119, 1026, 877, 825, 753 cm^{-1};

E-isomer ^1H NMR (400 MHz, $CDCl_3$) δ 7.54-7.28 (m, 5H), 4.65 (s, 2H), 1.23 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 133.8, 133.2, 130.4, 130.2, 129.9 (q, *J* = 306.3 Hz), 129.6, 126.7, 125.5, 80.9, 73.7, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.53 (s, 3F);

Z-isomer ^1H NMR (400 MHz, $CDCl_3$) δ 4.77 (s, 2H), 1.24 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.02 (s, 3F);

HRMS (ESI) calcd for $C_{14}H_{17}ClF_3O_2S$ $(M+H)^+$: 341.0584; found: 341.0509.



8e

E/*Z*=5:1

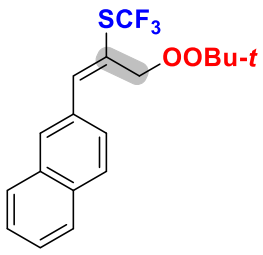
(3-(*tert*-Butylperoxy)-1-(2,5-dimethylphenyl)prop-1-en-2-yl)(trifluoromethyl)sulfane (8e): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 52% yield (87 mg), *E*/*Z*=5:1; Colorless oil; IR (KBr): ν_{max} 2977, 2927, 1467, 1365, 1266, 1120, 912, 875, 754 cm^{-1};

E-isomer ^1H NMR (400 MHz, $CDCl_3$) δ 4.65 (s, 2H), 2.32 (s, 3H), 2.24 (s, 3H), 1.23 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -42.14 (s, 3F);

Z-isomer ^1H NMR (400 MHz, $CDCl_3$) δ 4 .74 (s, 2H), 2.42 (s, 3H), 2.22 (s, 3H), 1.28 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.22 (s, 3F);

Overlap ^1H NMR (400 MHz, $CDCl_3$) δ 7.50- 7.01 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 139.0, 136.4, 131.2, 130.9, 128.7, 127.7 (q, J = 304.8 Hz), 126.5, 123.1, 80.7, 73.9, 26.3, 21.1, 19.6;

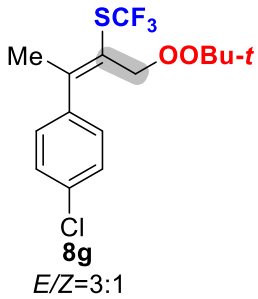
HRMS (ESI) calcd for $C_{16}H_{21}F_3O_2SNa$ $(M+Na)^+$: 357.1107; found: 357.1183.



8f

(3-(*tert*-Butylperoxy)-1-(naphthalen-2-yl)prop-1-en-2-yl)(trifluoromethyl)sulfane (8f): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 50% yield (89 mg); Colorless oil; IR (KBr): ν_{max} 2923, 2855, 2358, 1118, 913, 746, 662 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.90-7.87 (m, 3H), 7.67 (s, 1H), 7.57-7.53 (m, 3H), 4.88 (s, 2H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 133.3, 133.0, 132.2, 128.9, 128.4, 128.3, 127.7 ,127.0, 126.6, 126.2,

123.3, 80.9, 74.2, 26.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.83 (s, 3F); HRMS (ESI) calcd for $C_{18}H_{20}F_3O_2S$ $(M+H)^+$: 357.1131; found: 357.1207.



8g

E/*Z*=3:1

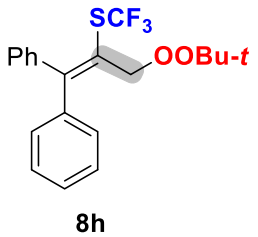
(1-(*tert*-Butylperoxy)-3-(4-chlorophenyl)but-2-en-2-yl)(trifluoromethyl)sulfane (8g): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 48% yield (84 mg), *E*/*Z*=3:1; Colorless oil; IR (KBr): ν_{max} 2980, 2930, 1725, 1602, 1486, 1366, 1258, 1112, 1014, 876, 829, 755 cm^{-1};

E-isomer ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.45 (s, 2H), 2.40 (s, 3H), 1.18 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ-41.02 (s, 3F);

Z-isomer ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.86 (s, 2H), 2.28 (s, 3H), 1.29 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -40.90 (s, 3F);

Overlap ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.32 (m, 4H), 7.17 (d, J = 8.4 Hz, 2H), 7.08 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.2, 139.3, 134.1, 128.7, 128.6, 128.4, 126.4, 118.9, 80.7, 76.1, 75.2, 29.7, 26.4, 26.3, 25.3, 23.5;

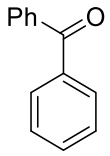
HRMS (ESI) calcd for $C_{15}H_{19}ClF_3O_2S$ $(M+H)^+$: 355.0741; found: 335.0697.



8h

(3-(*tert*-Butylperoxy)-1,1-diphenylprop-1-en-2-yl)(trifluoromethyl)sulfane (8h): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 55% yield (105 mg); Colorless oil; IR (KBr): ν_{max} 2979, 2930, 1587, 1484, 1450, 1360, 1250, 1191, 1125, 1093, 1020, 975, 917, 876, 755 cm^{-1}; ^{1}H NMR (400 MHz,

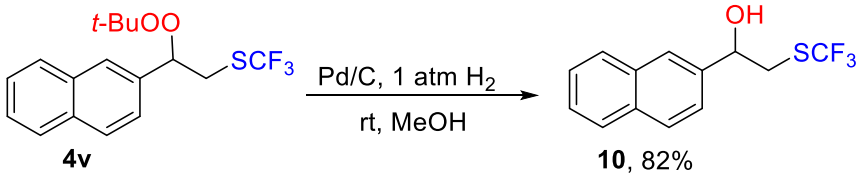
$CDCl_3$) δ 7.34-7.28 (m, 6H), 7.22-7.17 (m, 4H), 4.70 (s, 2H), 1.21 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 141.1, 140.1, 129.1, 128.9, 128.4, 128.2, 128.1, 128.0, 120.5, 80.7, 75.3, 26.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -40.09 (s, 3F); HRMS (ESI) calcd for $C_{20}H_{22}F_3O_2S$ $(M+H)^+$: 383.1287; found: 383.1290.



9

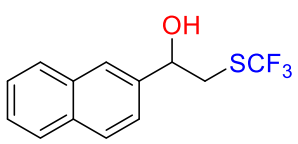
Benzophenone (9):[1] Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 4) in 27% yield (25 mg); white solid; ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 7.1 Hz, 4H), 7.57 (t, J = 7.4 Hz, 2H), 7.46 (t, J = 7.6 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 137.4, 132.2, 129.9, 128.1.

7. Transformation of trifluoromethylthio-peroxide compounds



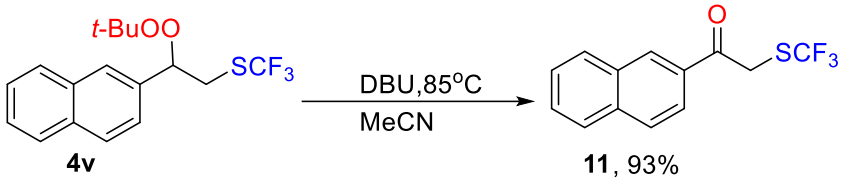
4v **10**, 82%

To a solution of peroxide **4v** (0.2 mmol) dissolved in anhydrous MeOH (2.0 mL), Pd/C (10% w/w on activated charcoal, 0.02 mmol, 10 mol%) was added. The mixture was stirred under 1 atmosphere of hydrogen (balloon) for 5 h at room temperature. Then the mixture was filtered through a pad of Celite using $CHCl_3$ / MeOH 1:1 as eluent. The solvent was removed under reduced pressure. The residue was purified by flash column chromatography on silica gel (eluent: ethylacetate/ petroleum ether) to give the alcohol **10**.



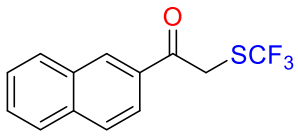
10

1-(Naphthalen-2-yl)-2-((trifluoromethyl)thio)ethan-1-ol (10): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 3) in 82% yield (45 mg); Colorless oil; IR (KBr): ν_{max} 2979, 2927, 2859, 1770, 1700, 1466, 1371, 1264, 1209, 1120, 1021, 861, 815, 764 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.87-7.82 (m, 4H), 7.52-744 (m, 3H), 5.08-5.05 (m, 1H), 3.29 (dd, J = 4.2 Hz, J = 13.9 Hz, 1H), 3.21 (dd, J = 8.9 Hz, J = 13.9 Hz, 1H), 2.60 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 133.3, 133.1, 130.9 (q, J = 304.2 Hz), 128.7, 128.0, 127.7, 126.5, 126.4, 124.9, 123.3, 72.8, 38.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -40.81 (s, 3F); HRMS (ESI) calcd for $C_{13}H_{12}F_3OS$ $(M+H)^+$: 273.0555; found: 273.0455.



4v **11**, 93%

To a dry Schlenk tube were added DBU (0.04 mmol), the peroxide **4v** (0.2 mmol) and anhydrous MeCN (2.0 mL) under N_2 atmosphere at room temperature. Subsequently, the resulting solution was stirred at room temperature for 5 h. The solvent was evaporated under vacuum and the residue was purified by flash column chromatography on silica gel (eluent: ethylacetate/ petroleum ether) to give the carbonyls **11**.

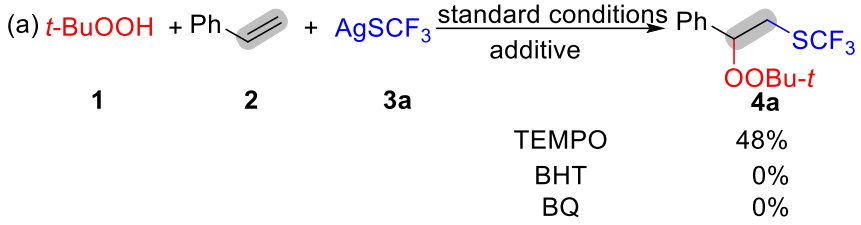


11

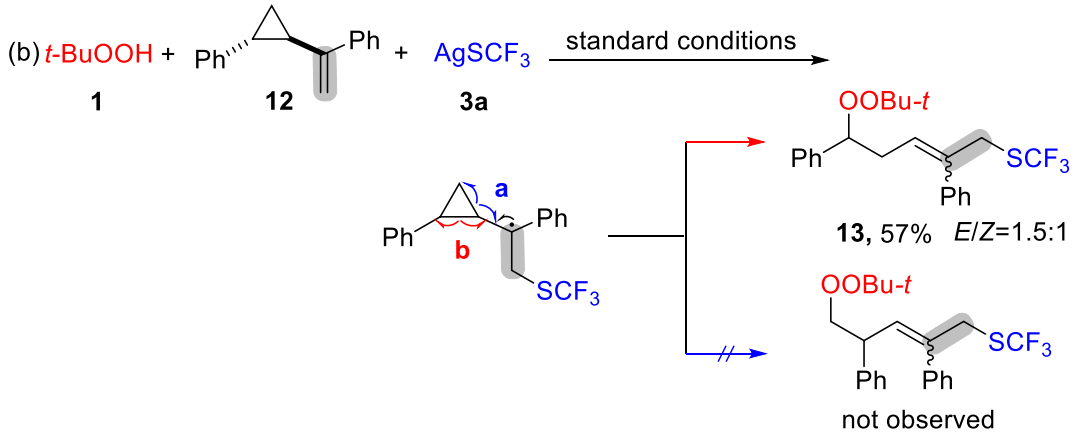
1-(Naphthalen-2-yl)-2-((trifluoromethyl)thio)ethan-1-one (11): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 10:1, R_f = 0. 4) in 93% yield (50 mg); Colorless oil; IR (KBr): ν_{max} 2923, 2358, 1680, 1393, 1362, 1269, 1141, 855, 818, 753 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.99-7.87 (m, 4H), 7.66-7.56 (m, 2H), 4.64 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 135.9, 132.3, 131.9, 130.4, 129.6, 129.2, 128.9, 127.9, 127.2, 123.5, 38.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.30 (s, 3F); HRMS (ESI) calcd for $C_{13}H_9F_3OSNa$ $(M+Na)^+$: 293.0218;

found: 293.0212.

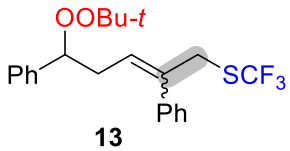
8. Mechanistic studies



To a dry Schlenk tube were added $CuSO_4$ (0.1 mmol), $AgSCF_3$ **3** (1.0 mmol), $K_2S_2O_8$ (1.5 mmol), HMPA (0.25 mmol), alkene **2a** (0.5 mmol), TEMPO (1.5 mmol, 3 equiv)/BHT/BQ and anhydrous MeCN (5.0 mL) under N_2 atmosphere at room temperature. Subsequently, **1a** (T-hydro, 70% in water, 2.5 mmol) was added to the mixture, and the resulting solution was stirred at 85 °C for 5 h. The resulting mixture and the solvent was evaporated under vacuum. The formation of **5a** was determined by ^1H NMR and **5a** was observed in 48%, 0%, 0% yield.



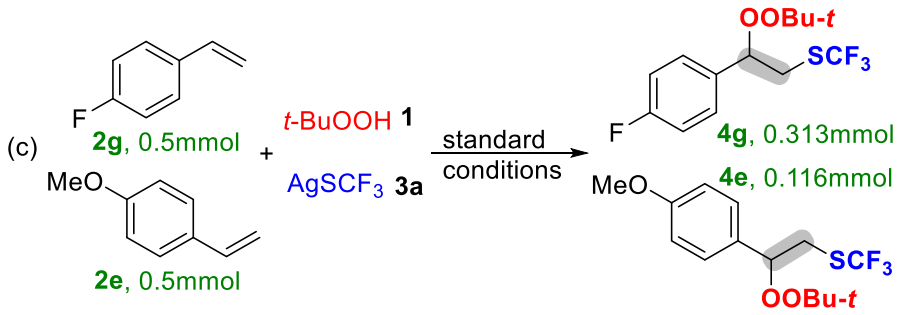
To a dry Schlenk tube were added $CuSO_4$ (0.1 mmol), $AgSCF_3$ **3** (1.0 mmol), $K_2S_2O_8$ (1.5 mmol), HMPA (0.25 mmol), alkene **12** (0.5 mmol) and anhydrous MeCN (5.0 mL) under N_2 atmosphere at room temperature. Subsequently, **1a** (T-hydro, 70% in water, 2.5 mmol) was added to the mixture, and the resulting solution was stirred at 85 °C for 5 h. The resulting mixture and the solvent was evaporated under vacuum. The formation of **13** was isolated in 57% yield.



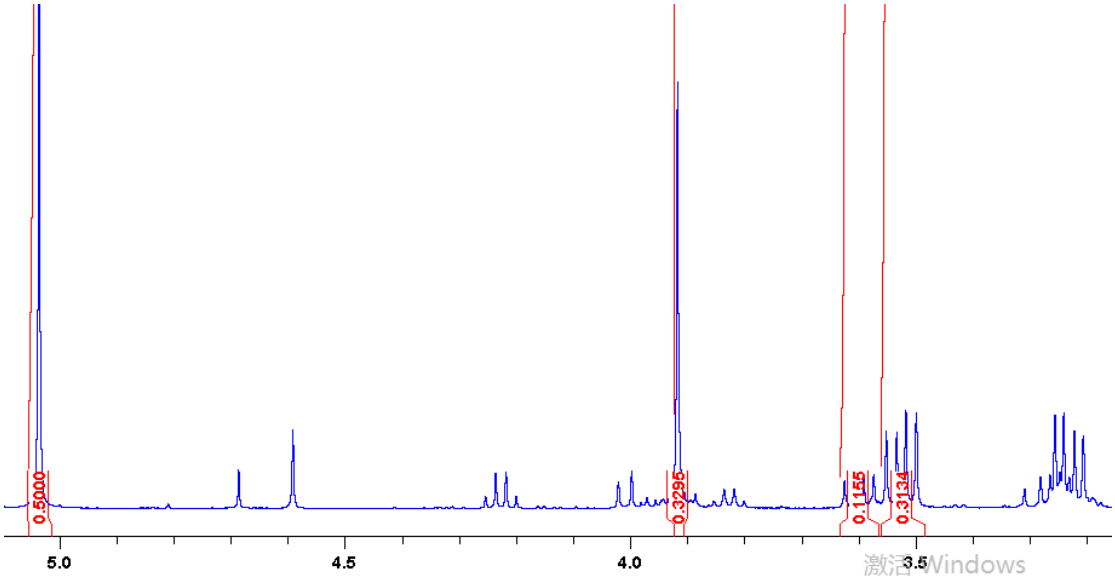
13

E/*Z*=1.5:1

(5-(*tert*-Butylperoxy)-2,5-diphenylpent-2-en-1-yl)(trifluoromethyl)sulfane (13): Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 57% yield (117 mg); Colorless oil; IR (KBr): ν_{max} 2974, 2923, 2858, 1688, 1595, 1455, 1364, 1267, 1193, 1115, 1020, 877, 766, 700 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36-7.03 (m, 20H), 5.90 (t, J = 7.6 Hz, 1H), 5.78 (t, J = 7.4 Hz, 1H), 4.99 (t, J = 6.6 Hz, 1H), 4.85 (t, J = 6.7 Hz, 1H), 3.93 (s, 2H), 3.77 (s, 2H), 2.97-2.90 (m, 1H), 2.75-2.68 (m, 1H), 2.63-2.56 (m, 1H), 2.42-2.35 (m, 1H), 1.24 (s, 9H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 140.3, 137.9, 136.7, 134.6, 129.4, 128.6, 128.5, 128.3, 128.2, 128.0, 127.8, 127.7, 127.6, 126.9, 85.2, 85.0, 80.5, 80.4, 38.5, 34.8, 34.5, 29.7, 29.4, 26.5 ; ^{19}F NMR (376 MHz, $CDCl_3$) δ -41.04 (s, 3F), -41.87 (s, 3F); HRMS (ESI) calcd for $C_{22}H_{26}F_3O_2S$ $(M+H)^+$: 411.1600; found: 411.1512.



To a dry Schlenk tube were added $CuSO_4$ (0.10 mmol), $AgSCF_3$ **3** (2.0 mmol), $K_2S_2O_8$ (1.5 mmol), HMPA (0.5mmol), alkene **2g** (0.5 mmol) and **2e** (0.5 mmol) and anhydrous MeCN (10.0 mL) under N_2 atmosphere at room temperature. Subsequently, **1a** (T-hydro, 70% in water, 5.0mmol) was added to the mixture, and the resulting solution was stirred at 80 ^oC for 5 h. The resulting mixture and the solvent was evaporated under vacuum. The ratio between the electron-deficient product **4g** and electron-rich trifluoromethylthiolation-peroxidation product **4e** was approximately 2.7 : 1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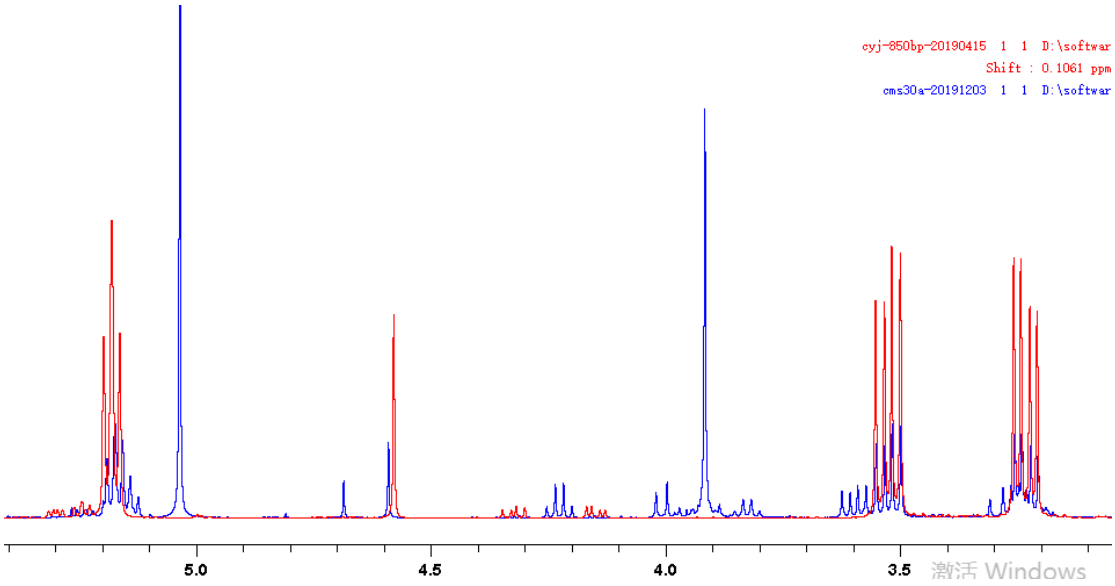
0.3296
0.1155
0.3134
5.0
4.5
4.0
3.5
激活 Windows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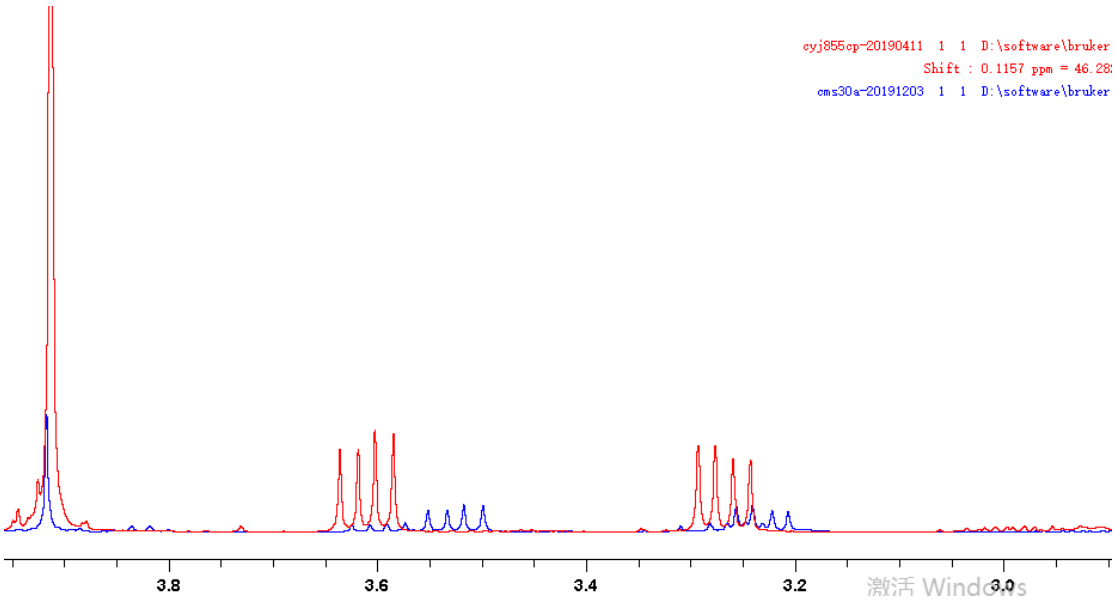
Shift : 0.1061 ppm
cms30a-20191203 1 1 D:\softwar
5.0
4.5
4.0
3.5
激活 Windows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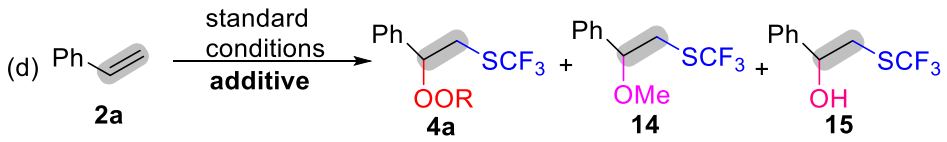
cms30a-20191203 1 1 D:\software\bruker
3.8
3.6
3.4
3.2
3.0
激活 Windows



To a dry Schlenk tube were added $CuSO_4$ (0.10 mmol), $AgSCF_3$ **3** (2.0 mmol), $K_2S_2O_8$ (1.5 mmol), HMPA (0.5mmol), alkene**,** additive and anhydrous MeCN (10.0 mL) under N_2 atmosphere at room temperature. Subsequently, **1a** (T-hydro, 70% in water, 5.0mmol) was added to the mixture, and the resulting solution was stirred at 80 ^oC for 5 h. The resulting mixture and the solvent was evaporated under vacuum. The formation of **4a** was determined by ^1H NMR.

entry	additive	4a	**14**	**15**(%)
1	none	75	/	/
2	MeOH, 1 equiv	69	0	/
3	MeOH, 10 equiv	66	0	/
4	H_20, 1 equiv	68	/	0
5	H_20, 10 equiv	70	/	0
6	H_20, 0.5ml	67	/	0

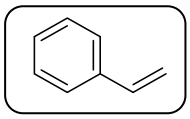
DFT calculation

Computational Methods

The geometries of all stationary points were optimized using the M06-2X density functional method[2] with the 6-31G (d) basis set[3] for all atoms. Vibrational frequency analyses at the same level of theory were performed on all optimized structures to characterize stationary points as local minima or transition states. Transition states were verified to have one imaginary vibrational frequency and were connected to the appropriate reactant and product by optimizations along the reaction coordinate. Solvation effects were calculated at the same level of theory as in the optimizations by performing single point calculations using the SMD solvation model method.[4] The solvents for reaction is acetonitrile. A larger basis set, 6-311G (d, p), was utilized for singlepoint energy calculations on stationary points. The solution-phase Gibbs free energy was determined by adding the solvation single-point energy and the gas-phase

thermal correction to the Gibbs free energy obtained from the vibrational frequencies. The solution-phase Gibbs free energy was determined by adding the solvation single-point energy and the gas-phase thermal correction to the Gibbs free energy obtained from the vibrational frequencies. Unless otherwise specified, the solution-phase Gibbs free energy was used in the present discussions. The Gaussian 09 suite of programs[5] was used for all calculations.

Cartesian Coordinates of Optimized Stationary Points



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C	1.88711797	1.18572457	0.00000000
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H	1.74106633	1.18342212	-2.16074639
H	-0.75408048	1.18330600	-2.16242647
H	-2.00256489	1.18682177	-0.00293421
C	3.42711771	1.18583660	0.00088786
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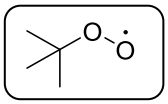
H	3.88313621	1.18702353	1.00000124
H	5.24265092	1.18463653	-1.11363807

H	3.68836606	1.18339271	-2.11338466



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H	-6.46416686	-0.91572772	-0.94038700
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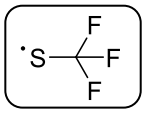
H	-4.97369586	1.79511228	1.19124900
H	-6.46436486	2.82737928	1.21597100
O	-6.17340211	1.71323728	-1.17619368
O	-6.62473267	1.08553770	-2.24609740



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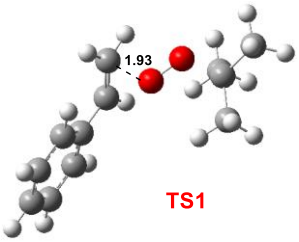
F	-0.90096993	-1.45635126	0.00000000



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C	0.84068504	-0.38391431	-0.63567483
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C	1.25863004	1.99369569	-0.63567283
C	-0.11382696	2.23161669	-0.63566983
C	-1.01829696	1.16339569	-0.63566783
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H	1.21181904	-1.40637531	-0.63567383
H	1.94410404	2.83643969	-0.63567483
H	-0.48127796	3.25469769	-0.63566883
H	-2.08838096	1.35321969	-0.63567083
C	3.20375604	0.36758969	-0.63567083
C	4.37573418	1.36703899	-0.63566854
H	3.43499504	-0.69789631	-0.63565983
H	5.21362949	0.93416975	-1.14109476
H	4.07984174	2.26367636	-1.13904623

C	5.88054399	2.92124933	3.50315280
C	6.62721901	2.01566851	2.52969107
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H	4.85914598	2.56310491	3.66082287
H	6.39768036	2.92640655	4.46846451
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H	7.15398442	-0.07200695	2.23700698
H	7.19769672	0.47632319	3.92462064
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H	8.63826218	2.54978828	3.08158355
H	8.50107013	1.91391057	1.43115836
H	7.96029568	3.57025731	1.79859746
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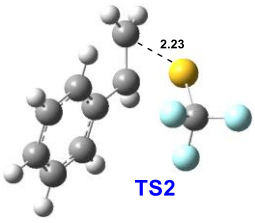
O	4.66623627	1.65769366	1.25728307



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H	1.35242500	0.16304700	2.34936400
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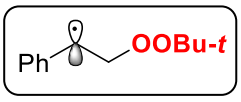
F	-2.89151600	-1.43732600	-0.19817700
F	-0.97209300	-1.35061300	-1.09800200



C	-0.20636354	1.18740410	1.20639121
C	1.18879599	1.18670129	1.20729748
C	1.88711797	1.18572457	0.00000000
C	1.19024831	1.18425127	-1.20896114

C	-0.20457651	1.18447495	-1.20978894
C	-0.90296129	1.18644794	-0.00203702
H	-0.75674048	1.18862412	2.15835054
H	1.73768599	1.18823267	2.16016642
H	1.74106633	1.18342212	-2.16074639
H	-0.75408048	1.18330600	-2.16242647
H	-2.00256489	1.18682177	-0.00293421
C	3.42711771	1.18583660	0.00088786
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O	5.33993569	2.18714088	-1.10507286
O	5.82052833	2.64859088	-2.24458794
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H	7.00939331	3.52798465	-0.03941844
H	8.50376872	4.13666318	-0.86320480

H	7.73430354	0.83481700	-2.55717525
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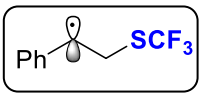
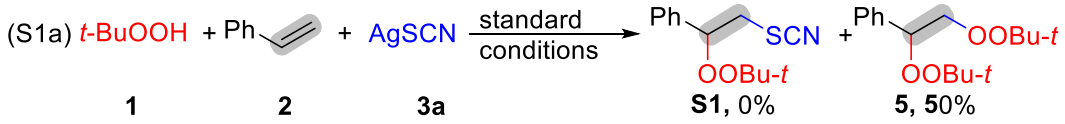
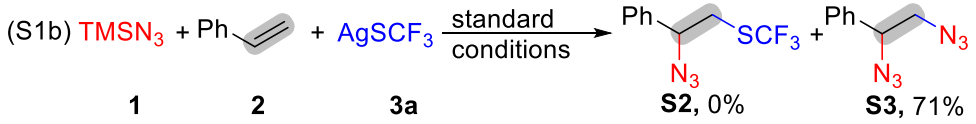


C	-3.87973300	1.24803800	-0.25788700
C	-2.56968000	1.34280000	0.18753200
C	-1.76884700	0.17968700	0.38997200
C	-2.36908500	-1.08278300	0.11089800
C	-3.68137500	-1.16512800	-0.33704100
C	-4.44806000	-0.00648300	-0.52478400
H	-4.46648300	2.15164600	-0.40213400
H	-2.13273300	2.31735100	0.39193700
H	-1.79920100	-1.99693100	0.24680100
H	-4.11555000	-2.14001500	-0.54401400
H	-5.47403900	-0.07976300	-0.87442100
C	-0.43647000	0.33466200	0.85546700
C	0.53173400	-0.75313000	1.10452100
H	-0.07440000	1.34931600	0.99720100
H	1.20708800	-0.52117800	1.93111100

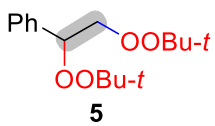
H	0.06873000	-1.72185200	1.30469600
C	2.81872500	0.24875100	-0.21375600
S	1.66234300	-1.13686600	-0.37092000
F	3.45639900	0.27053300	0.97558700
F	3.75257500	0.13218600	-1.17660500
F	2.23611900	1.45870200	-0.35520300

9. Further application





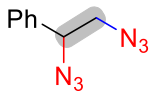
To explore the application of the radical coupling strategy for alkene three-component difunctionalization of other radical systems, two experiments were carried out. To our disappointment, when styrene (**2a**) was used as a template by treatment with AgSCN instead of $AgSCF_3$ under the above system, the bisperoxidation product **5** [6] was isolated with a moderate yield of 50% with no desired β-thiocyanated peroxides **S1** detected. Besides, $TMSN_3$, $AgSCF_3$ and styrene failed to give the desired trifluoromethylthiolation-azidation product **S2**. Interestingly, 1,2-diazide **S3** were isolated in 71%.[7] We hypothesized that the reactivity of azidyl radical ($\cdot N_3$) is much higher than that of SCF3 radical under our reaction conditions and thus overwhelms the reaction with $AgSCF_3$.



5

(1,2-Bis(*tert*-butylperoxy)ethyl)benzene (5):[6] Isolated by flash column

chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 50% yield (71 mg); Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.30 (m, 5H), 5.22 (dd, J = 4.0 Hz, J = 7.8 Hz, 1H), 4.24 (dd, J = 7.8 Hz, J = 11.6 Hz, 1H), 4.09 (dd, J = 4.0 Hz, J = 11.6 Hz, 1H), 1.26 (s, 9H), 1.25 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 128.2, 127.9, 127.0, 83.3, 80.6, 80.4, 76.8, 26.3, 26.2.

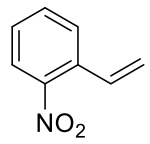
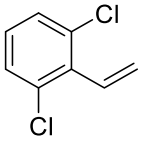
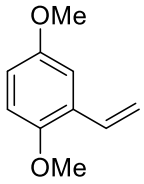
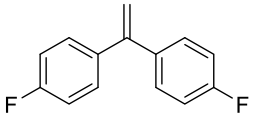
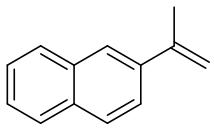
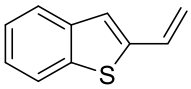


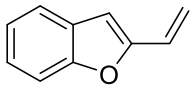
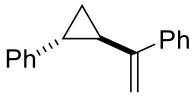
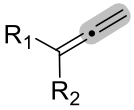
S3

(1,2-Diazidoethyl)benzene (S3):[7] Isolated by flash column chromatography (petroleum ether/ethyl acetate = 20:1, R_f = 0. 6) in 71% yield (67 mg); Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.32 (m, 5H), 4.67 (dd, J = 4.9 Hz, J = 8.2 Hz,1H), 3.49 (dd, J = 8.3 Hz, J = 12.8 Hz, 1H), 3.42 (dd, J = 4.9 Hz, J = 12.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 129.1, 129.0, 127.0, 65.6, 56.0.

10. General procedure for synthesis of olefins

Table S1 These substrates were prepared according to the reported literatures.

	[8]		[9]
	[10]		[11]
	[12]		[13]

	[14]		[15]
	[16]		

11. References:

[1] T. Wang and N. Jiao. TEMPO-catalyzed Aerobic Oxygenation and Nitrogenation of Olefins via C═C Double-Bond Cleavage. *J, Am. Chem. Soc.* 2013, **135**, 11692.

[2] Y. Zhao and D. G. Truhlar. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* 2008, **120**, 215.

[3] P. C. Hariharan and J. A. Pople. The Influence of Polarization Functions on Molecular Orbital Hydrogenation Energies. *Theor. Chim. Acta.* 1973, **28**, 213.

[4] A. V. Marenich, C. J. Cramer and D. G. Truhlar. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B.* 2009, **113**, 6378.

[5] M. J. Frisch, G.W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B.

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[6] A. O. Terent'ev, M. Y. Sharipov, I. B. Krylov, D. V. Gaidarenko and G. I. Nikishin, Manganese triacetate as an efficient catalyst for bisperoxidation of styrenes. *Org. Biomol. Chem*. 2015, **13**, 1439.

[7] diazidation of alkenes, see: (a) S.-J. Shen, C.-L. Zhu, D.-F. Lu and H. Xu, Iron-Catalyzed Direct Olefin Diazidation via Peroxyester Activation Promoted by Nitrogen-Based Ligands. *ACS Catal*., 2018, **8**, 4473; (b) H. Zhou, W. Jian, B. Qian, C. Ye, D. Li, J. Zhou, H. Bao, Copper-Catalyzed Ligand-Free Diazidation of Olefins with $TMSN_3$ in CH_3CN or in H_2O. *Org. Lett.* 2017, **19**, 6120. (c) Y.-A. Yuan, D.-F. Lu, Y.-R. Chen and H. Xu, Iron‐Catalyzed Direct Diazidation for a Broad Range of Olefins. *Angew. Chem., Int. Ed.*, 2016, **55**, 534; (d) M.-Z. Lu, C.-Q. Wang and T.-P. Loh, Copper-Catalyzed Vicinal Oxyazidation and Diazidation of Styrenes under Mild Conditions: Access to Alkyl Azides. *Org. Lett*., 2015, **17**, 6110; (e) Z.-M. Chen, Z. Zhang, Y.-Q. Tu, M.-H. Xu, F.-M. Zhang, C.-C. Li and S.-H. Wang, A Mn(iii)/TEMPO-co-mediated tandem azidation–1,2-carbon migration reaction of allylic silyl ethers. *Chem. Commun*., 2014, **50**, 10805.

[8] L. Yang, L. Shi, Q. Xing, K.-W. Huang, C. Xia, F. Li. Enabling CO Insertion into o-Nitrostyrenes beyond Reduction for Selective Access to Indolin-2-one and Dihydroquinolin-2-one Derivatives. *ACS Catal.* 2018, **8**, 10340.

[9] A. Gonzalez-de-Castro, J.l. Xiao., Green and Efficient: Iron-Catalyzed Selective Oxidation of Olefins to Carbonyls with O_2. *J. Am. Chem. Soc.* 2015, **137**, 8206.

[10]. M. D. Greenhalgh, S. P. Thomas, Iron-Catalyzed, Highly Regioselective Synthesis of α-Aryl Carboxylic Acids from Styrene Derivatives and CO_2. *J. Am. Chem. Soc.* 2012, **134**, 11900.

[11] C. Chatalova-Sazepin, Q. Wang, G. M. Sammis, J. Zhu. Copper‐Catalyzed Intermolecular Carboetherification of Unactivated Alkenes by Alkyl Nitriles and Alcohols. *Angew. Chem. Int. Ed.*, 2015, **54**, 5443. For spectroscopic data, see: H. Namai, H. Ikeda, N. Kato, K. Mizuno. Substituent Effects on the Energies of the Electronic Transitions of Geminally Diphenyl-Substituted Trimethylenemethane (TMM) Radical Cations. Experimental and Theoretical Evidence for a Twisted Molecular and Localized Electronic Structure. *J. Phys. Chem. A.*, 2007, **111**, 4436.

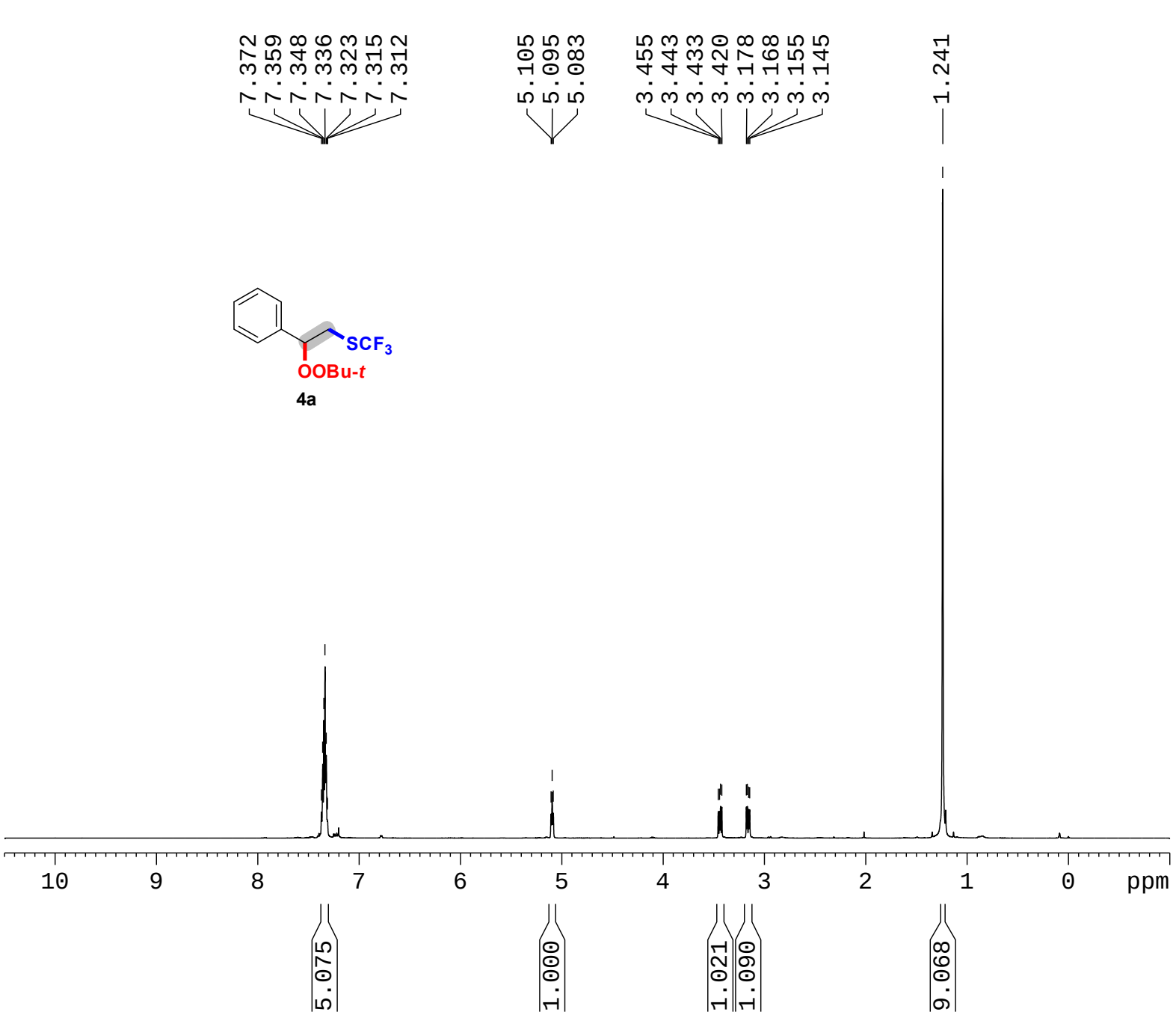
[12] J.-H. Li, Wu, L.-B. Gong, Y.-Z. Xia, R.-J. Song, Y.-X. Xie, J.-H. Li, Nickel‐Catalyzed Kumada Reaction of Tosylalkanes with Grignard Reagents to Produce Alkenes and Modified Arylketones. *Angew. Chem., Int, Ed.* 2012, **51**, 9909.

[13] F. Cong, Y. Wei，P. Tang, Combining photoredox and silver catalysis for azidotrifluoromethoxylation of styrenes. *Chem. Commun.*, 2018, **54**, 4473.

[14] H. Seo, A. Liu, T. F. Jamison. Direct β-Selective Hydrocarboxylation of Styrenes with CO2 Enabled by Continuous Flow Photoredox Catalysis. *J. Am. Chem. Soc.* 2017, **139**, 13969−13972.

[15] C. Chen, X. Shen, J. Chen, X. Hong, Z. Lu, Iron-Catalyzed Hydroboration of Vinylcyclopropanes. *Org. Lett.* 2017, **19**, 5422.

[16] Z. Zhao, Lanne Racicot, G. K. Murphy, Fluorinative Rearrangements of Substituted Phenylallenes Mediated by (Difluoroiodo)toluene: Synthesis of α‐(Difluoromethyl)styrenes. *Angew. Chem. Int. Ed.* 2017, **56**, 11620.



BRUKER

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TE	295.6 K
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TD0	1
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SSB	0
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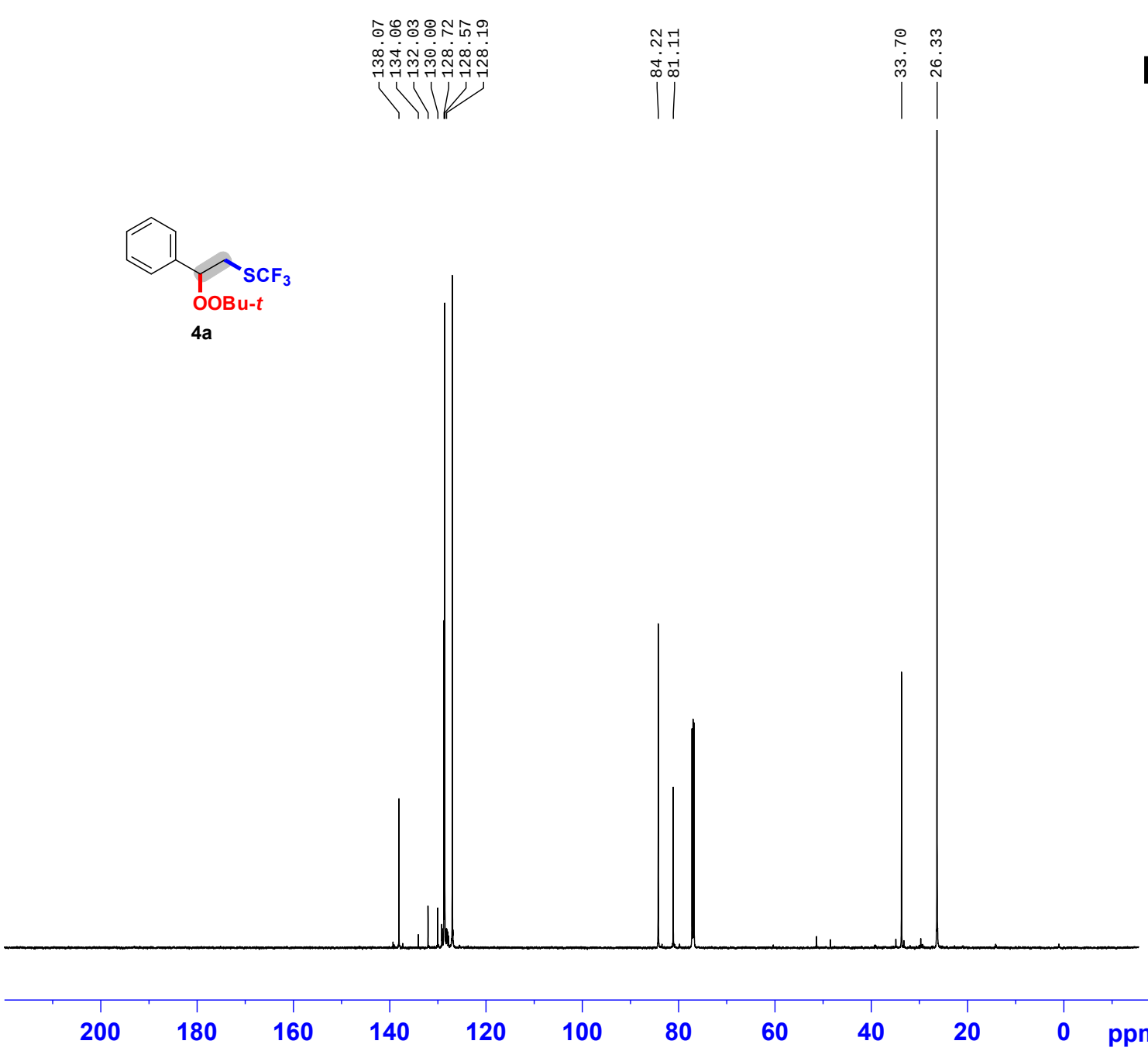
GB	0
PC	1.00

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TD0                      1

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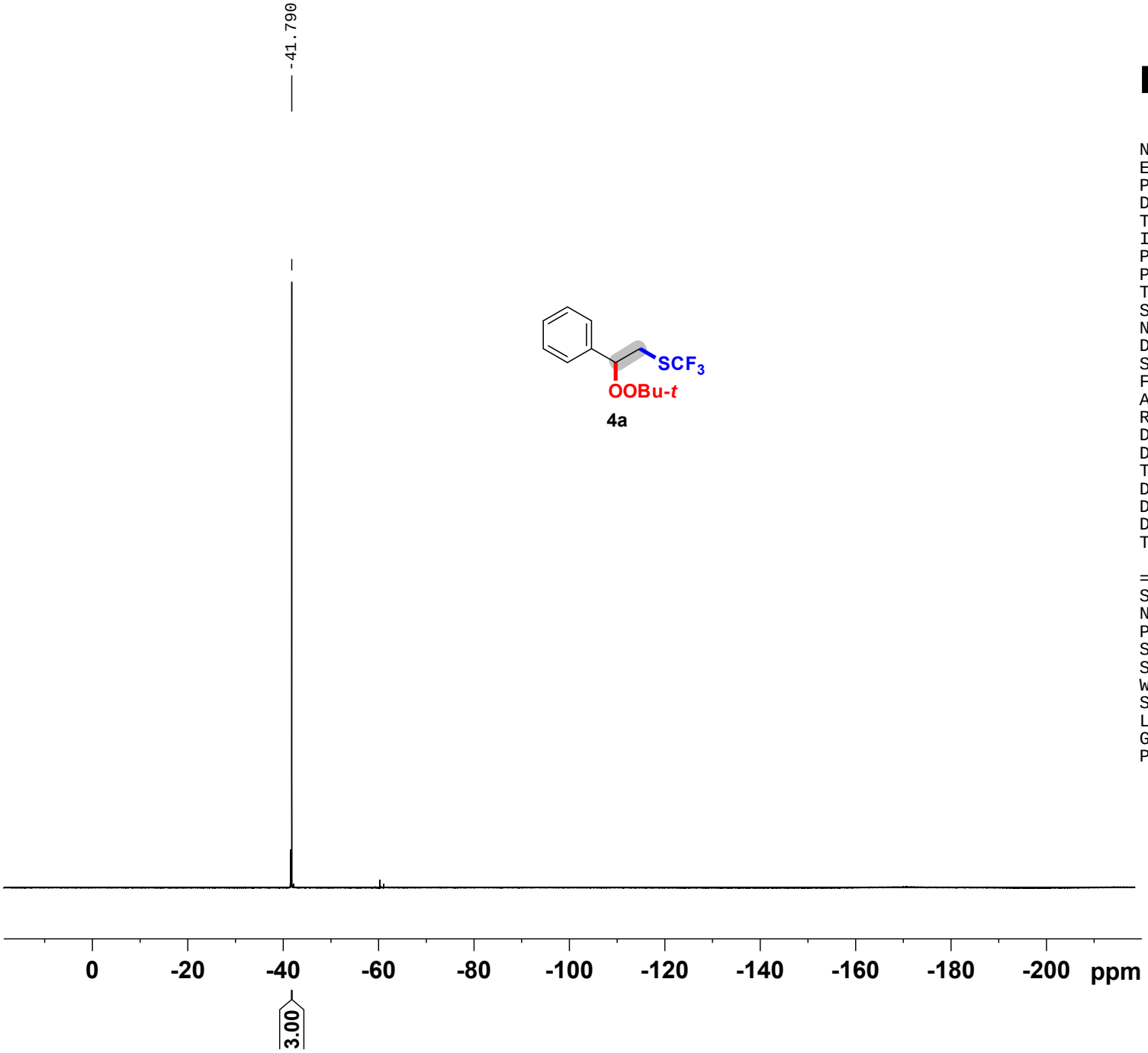


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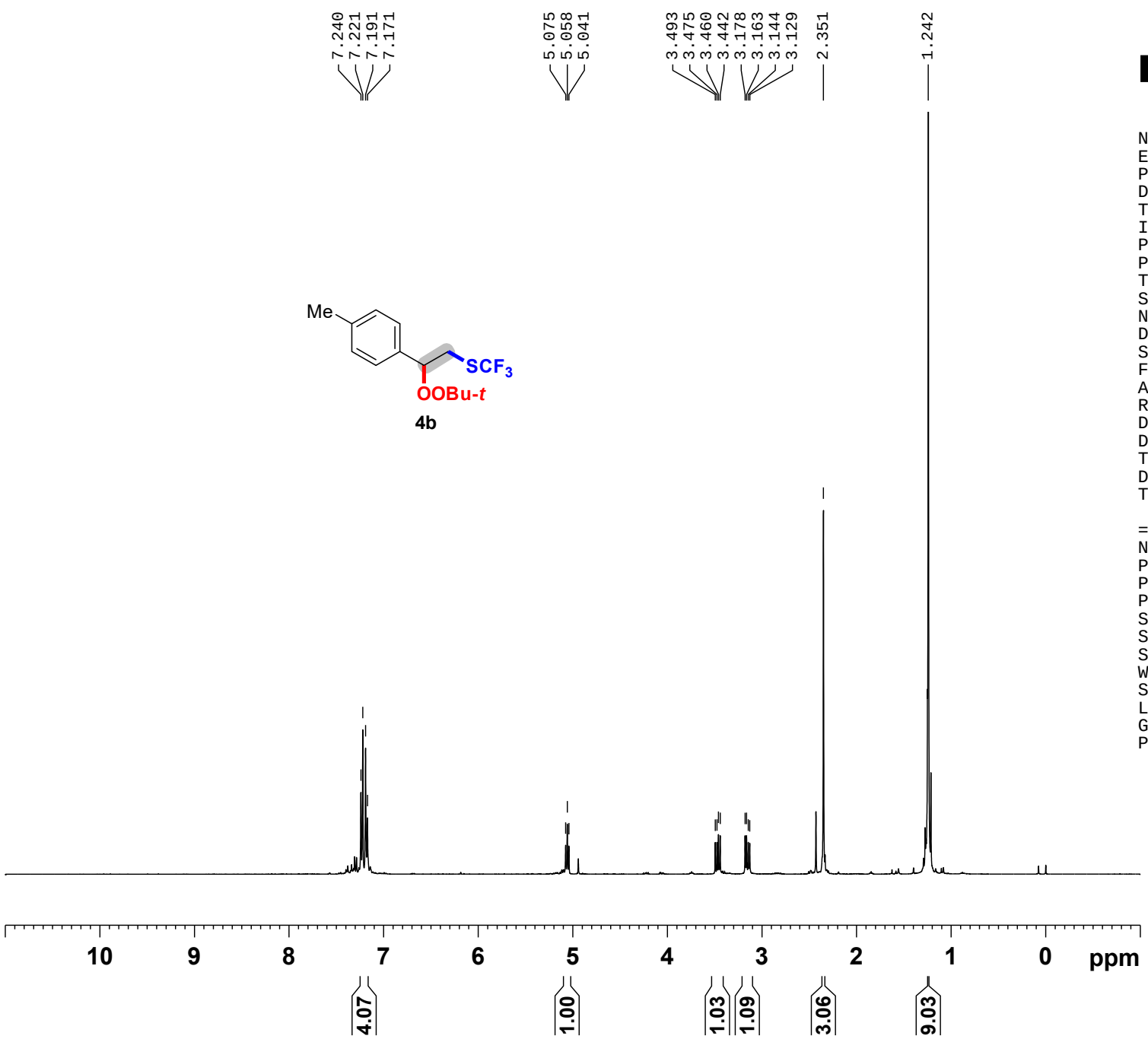


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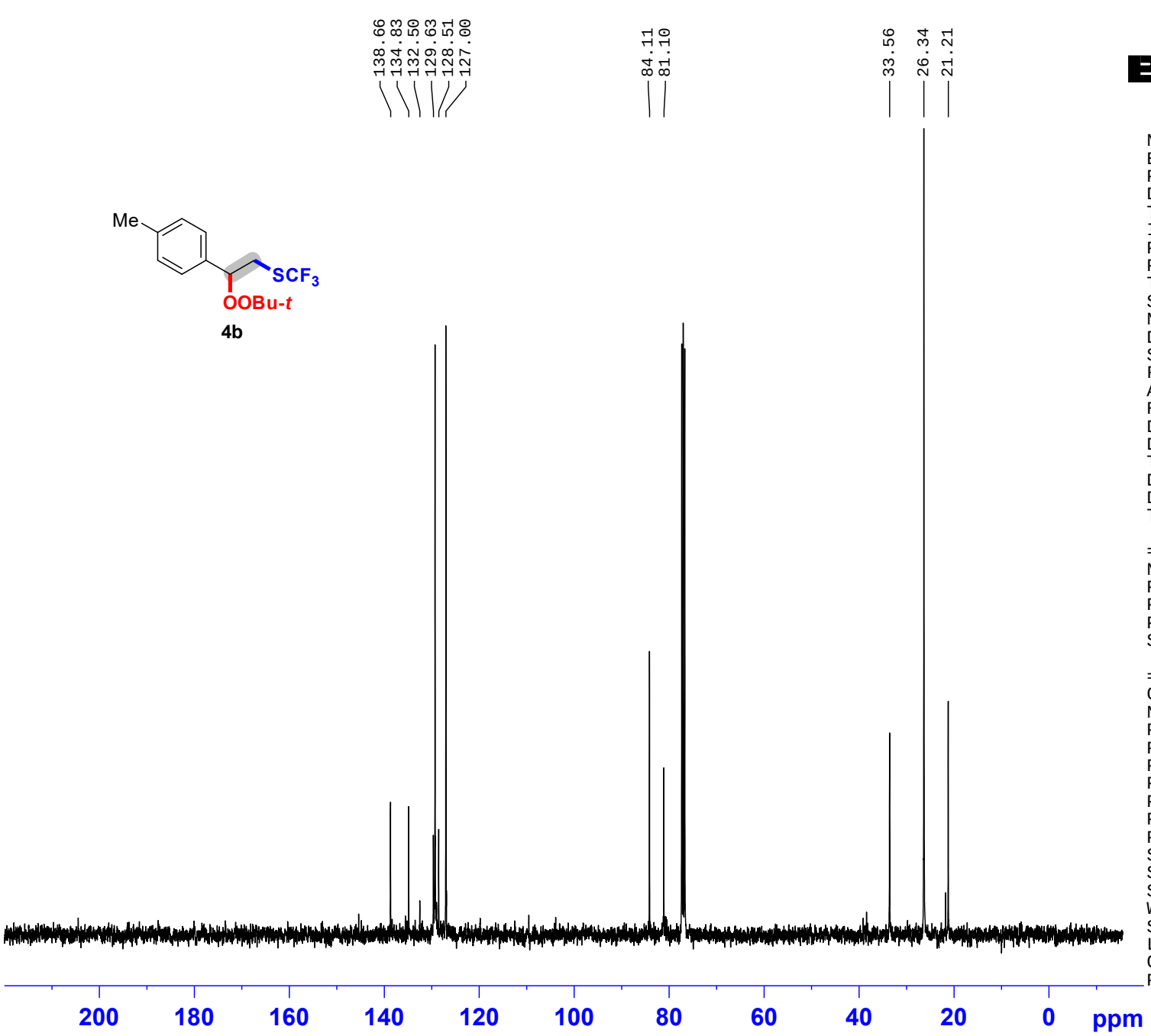


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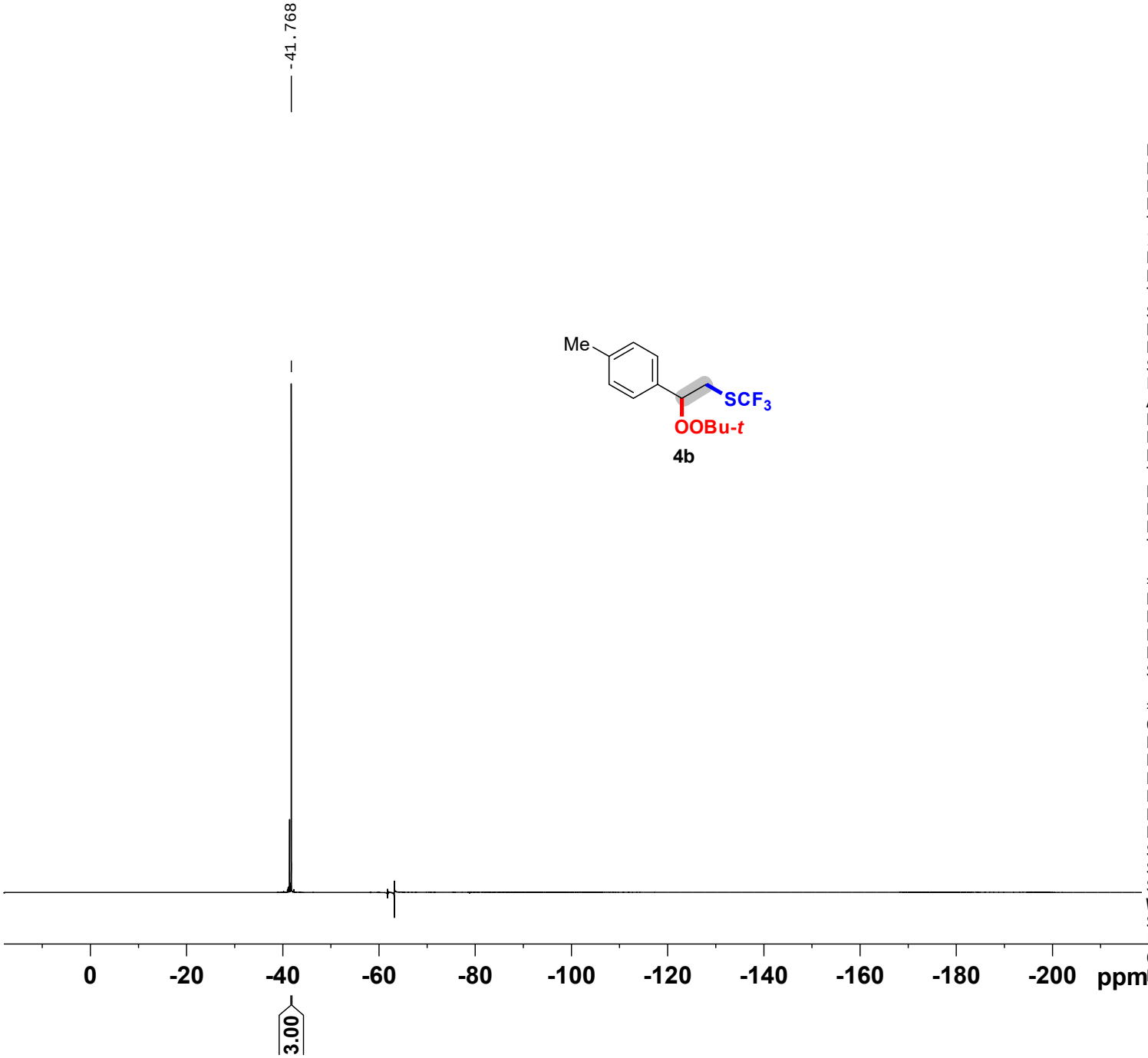


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TD0                      1

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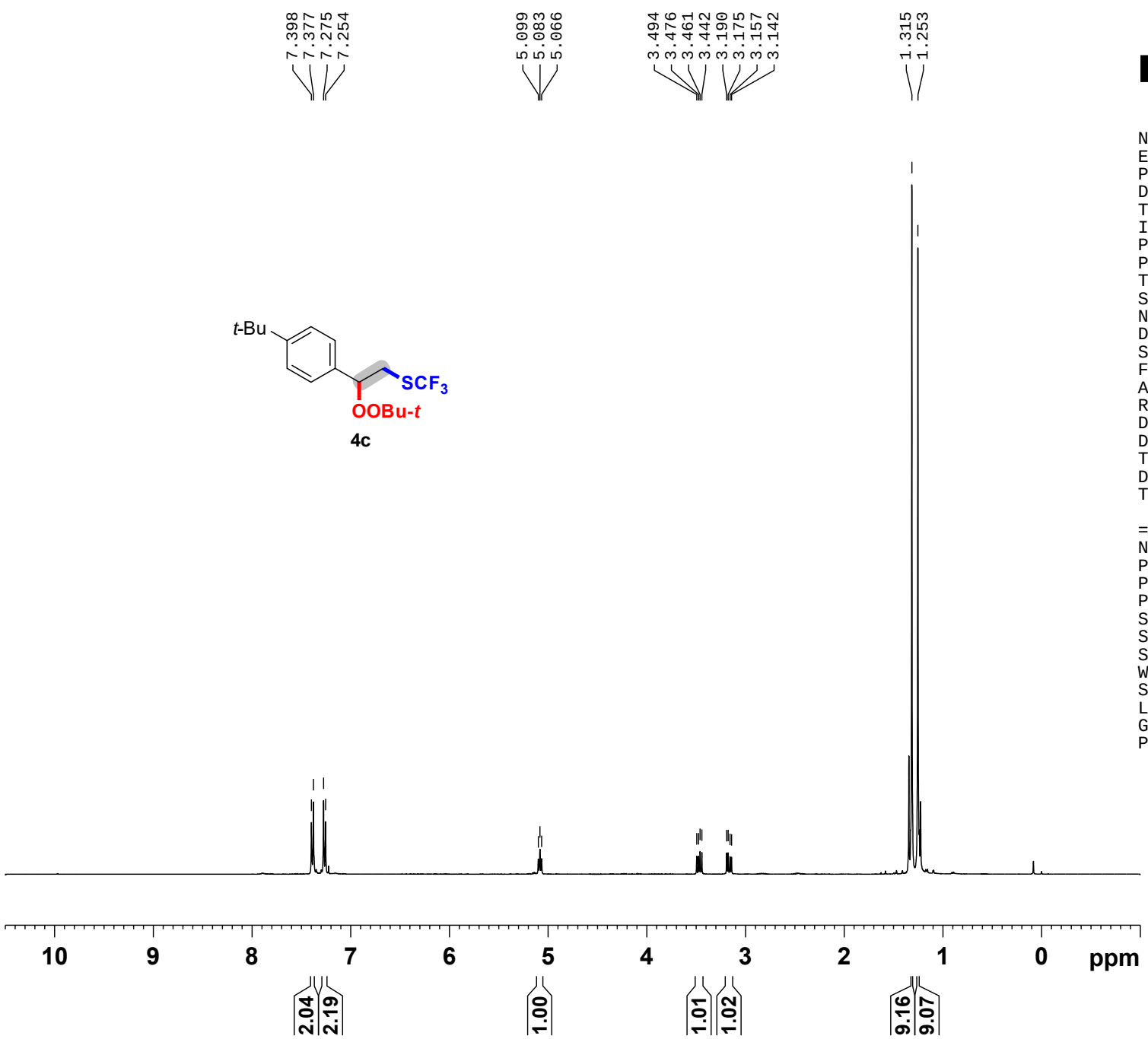


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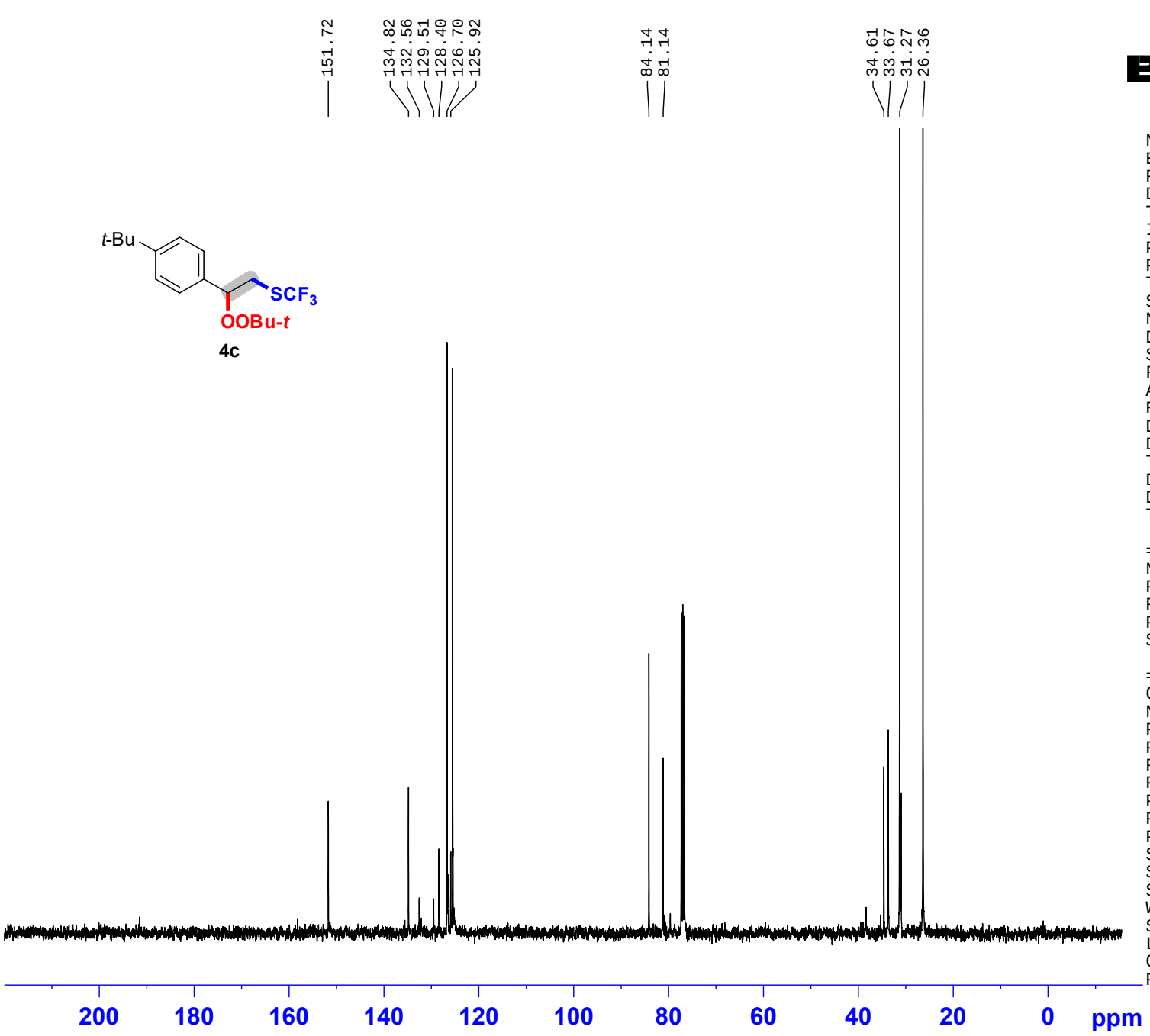
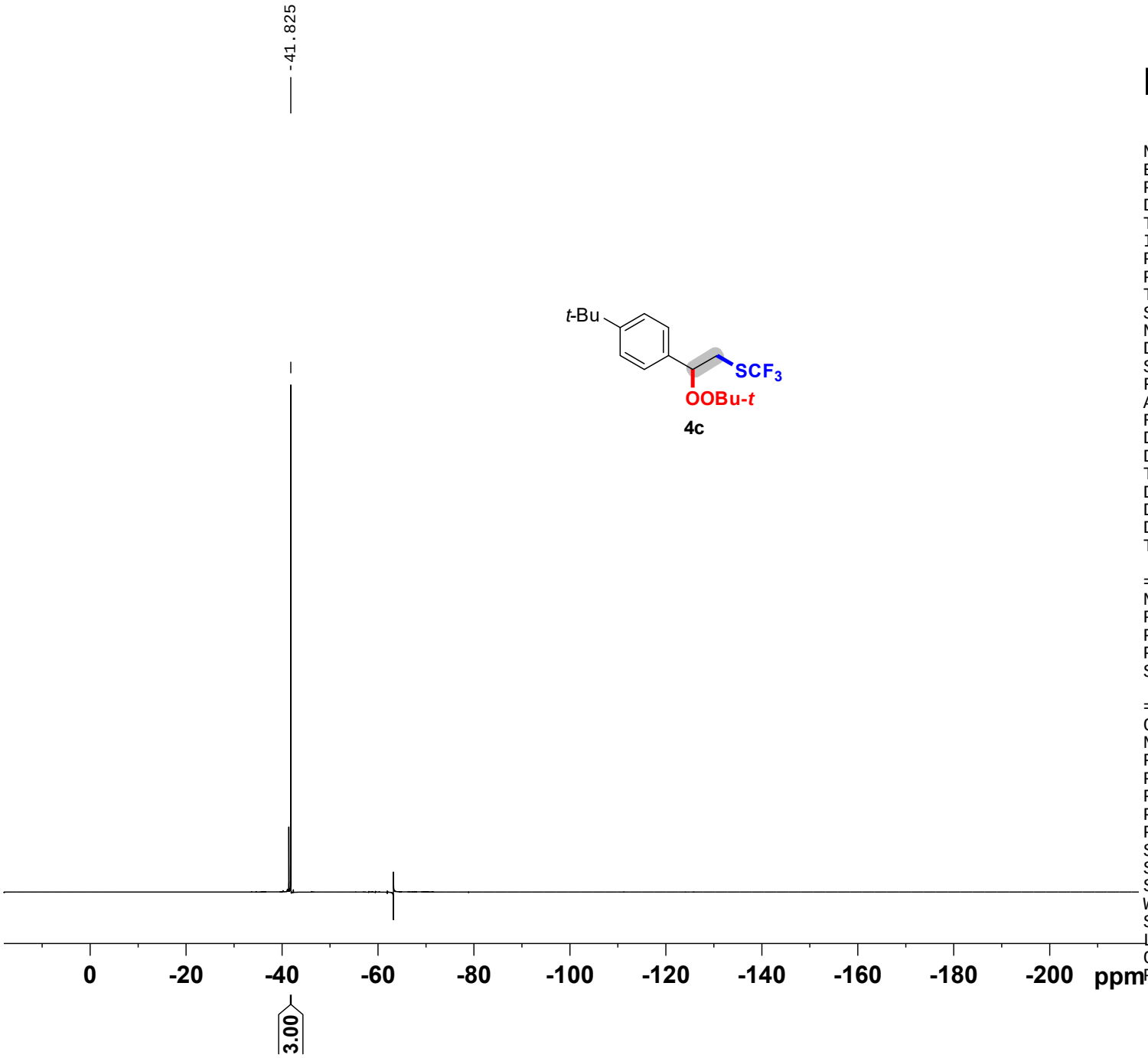
SFO1           400.1326008 MHz
SI                     32768
SF             400.1300247 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```




```
NAME      cyj855bp-20190403
EXPNO                    2
PROCNO                   1
Date_             20190402
Time                 22.46
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       48
DS                        4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                      181
DW                   19.800 usec
DE                    6.50 usec
TE                   294.6 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       3

======== CHANNEL f1 ========
NUC1                    13C
P1                   15.00 usec
PL1                   2.00 dB
PL1W            55.31277084 W
SFO1           100.6238364 MHz

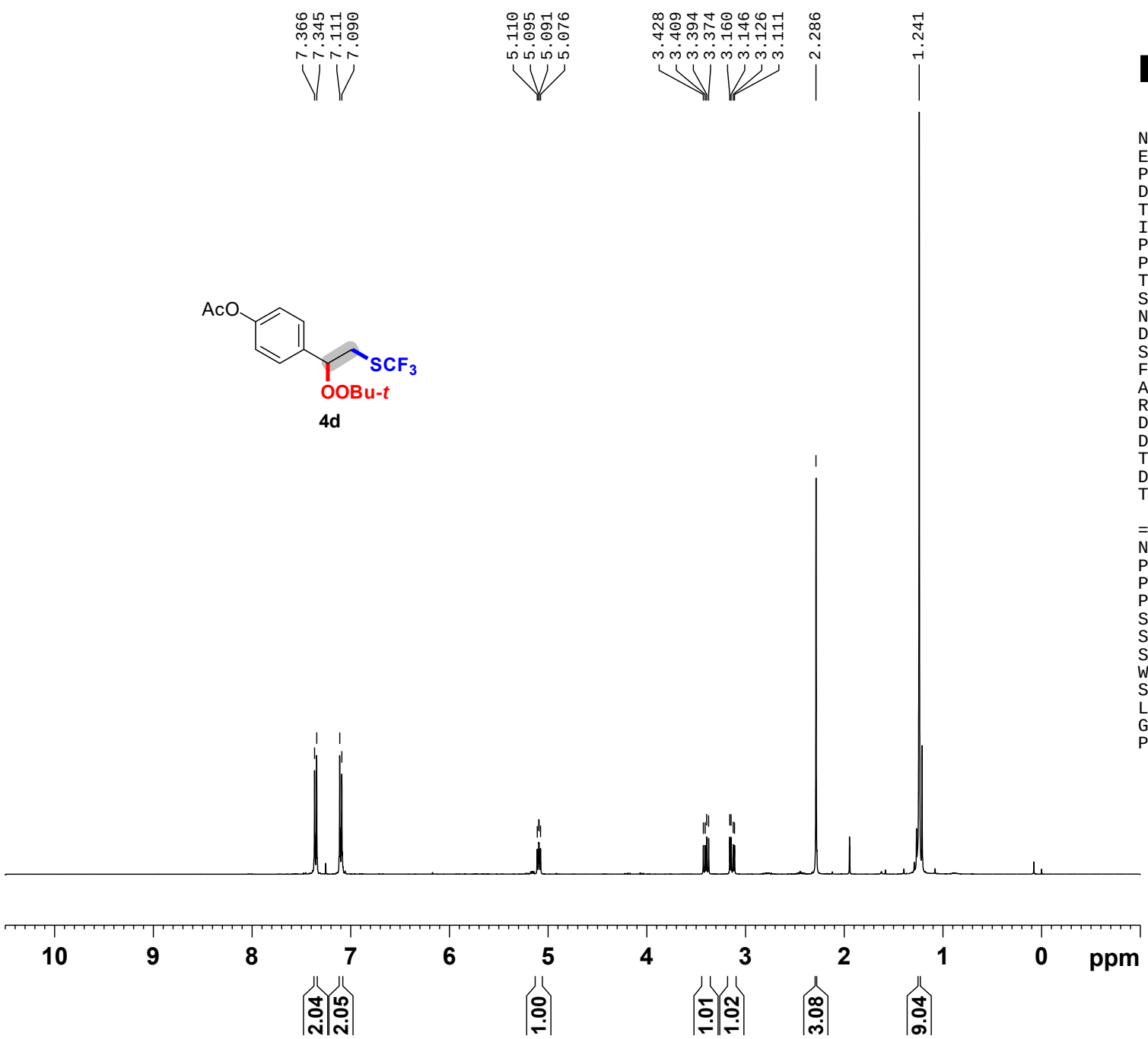
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
PL13W            0.38087484 W
SFO2           400.1316005 MHz
SI                    32768
SF             100.6127734 MHz
WDW                      EM
SSB                       0
LB                    3.00 Hz
GB                        0
PC                     1.40
```




```
NAME      cyj-855bp-20190402
EXPNO                      3
PROCNO                     1
Date_               20190402
Time                   22.51
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES                 0.681196 Hz
AQ                     0.7340532 sec
RG                       812
DW                       5.600 usec
DE                       6.50 usec
TE                     293.7 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

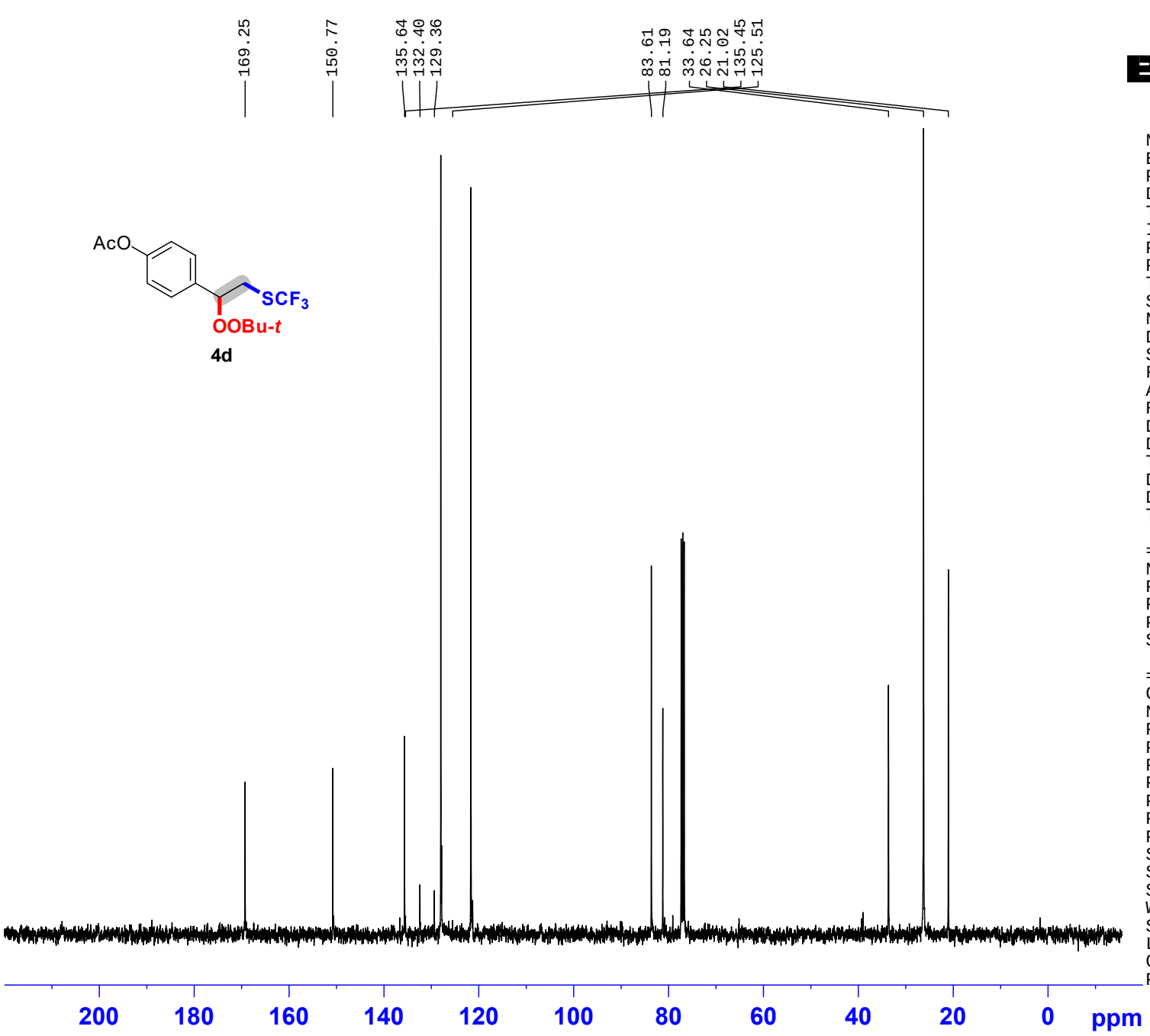
======== CHANNEL f1 ========
NUC1                      19F
P1                       14.20 usec
PL1                      -2.00 dB
PL1W              20.42289734 W
SFO1              376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                    80.00 usec
PL2                      -1.00 dB
PL12                     16.72 dB
PL2W              17.01305389 W
PL12W              0.28759566 W
SFO2              400.1316005 MHz
SI                     65536
SF                376.4983660 MHz
WDW                       EM
SSB                        0
LB                       3.00 Hz
GB                         0
PC                       1.00
```




```
NAME      cyj855dp-20190328
EXPNO                    1
PROCNO                   1
Date_             20190328
Time                 20.27
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                      57
DW                  78.200 usec
DE                   6.50 usec
TE                  292.3 K
D1              1.00000000 sec
TD0                      1

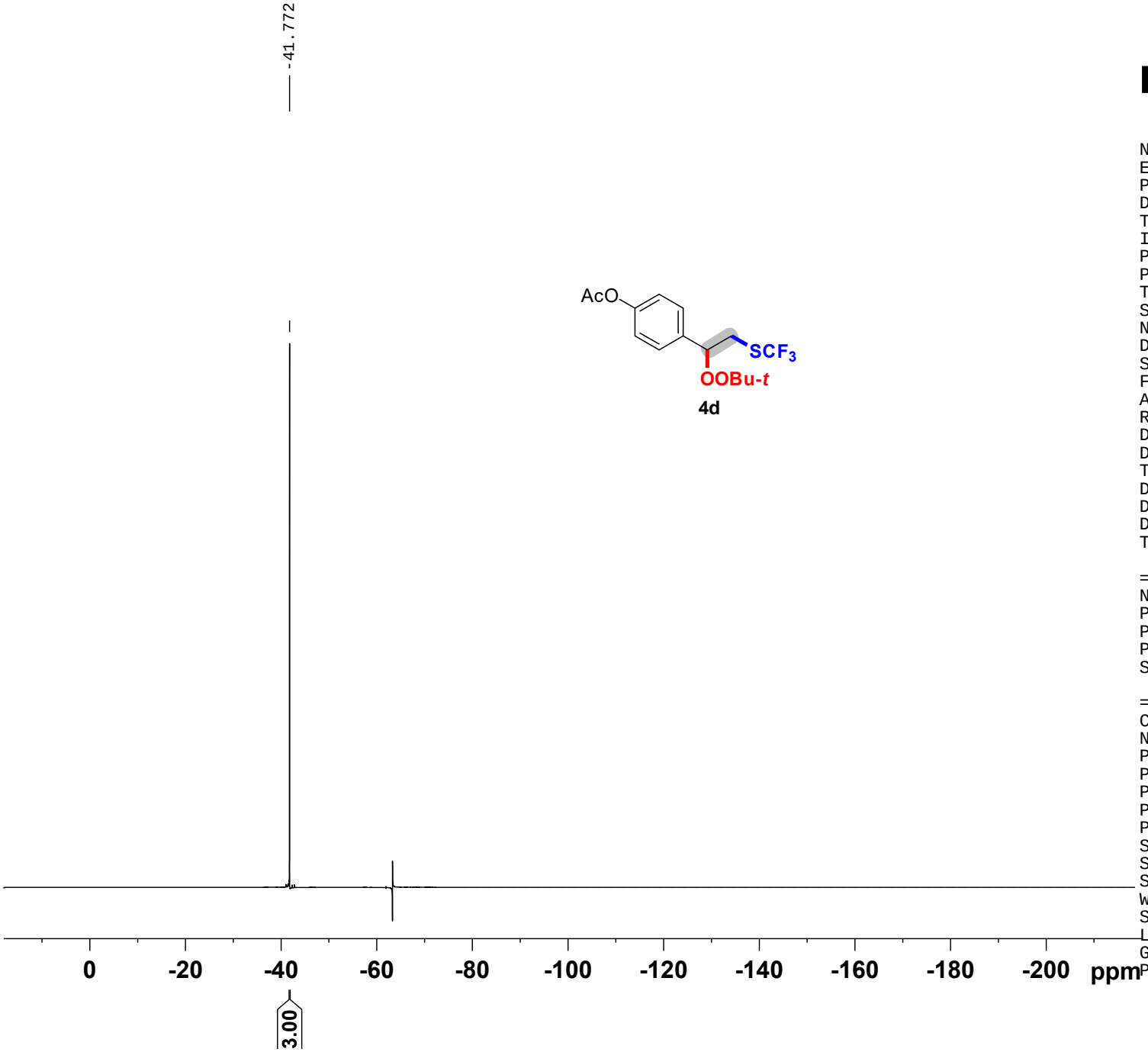
======== CHANNEL f1 ========
NUC1                    1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300130 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                  1.00
```




```
NAME      cyj855dp-20190328
EXPNO                    2
PROCNO                   1
Date_             20190328
Time                 20.31
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      40
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  293.5 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

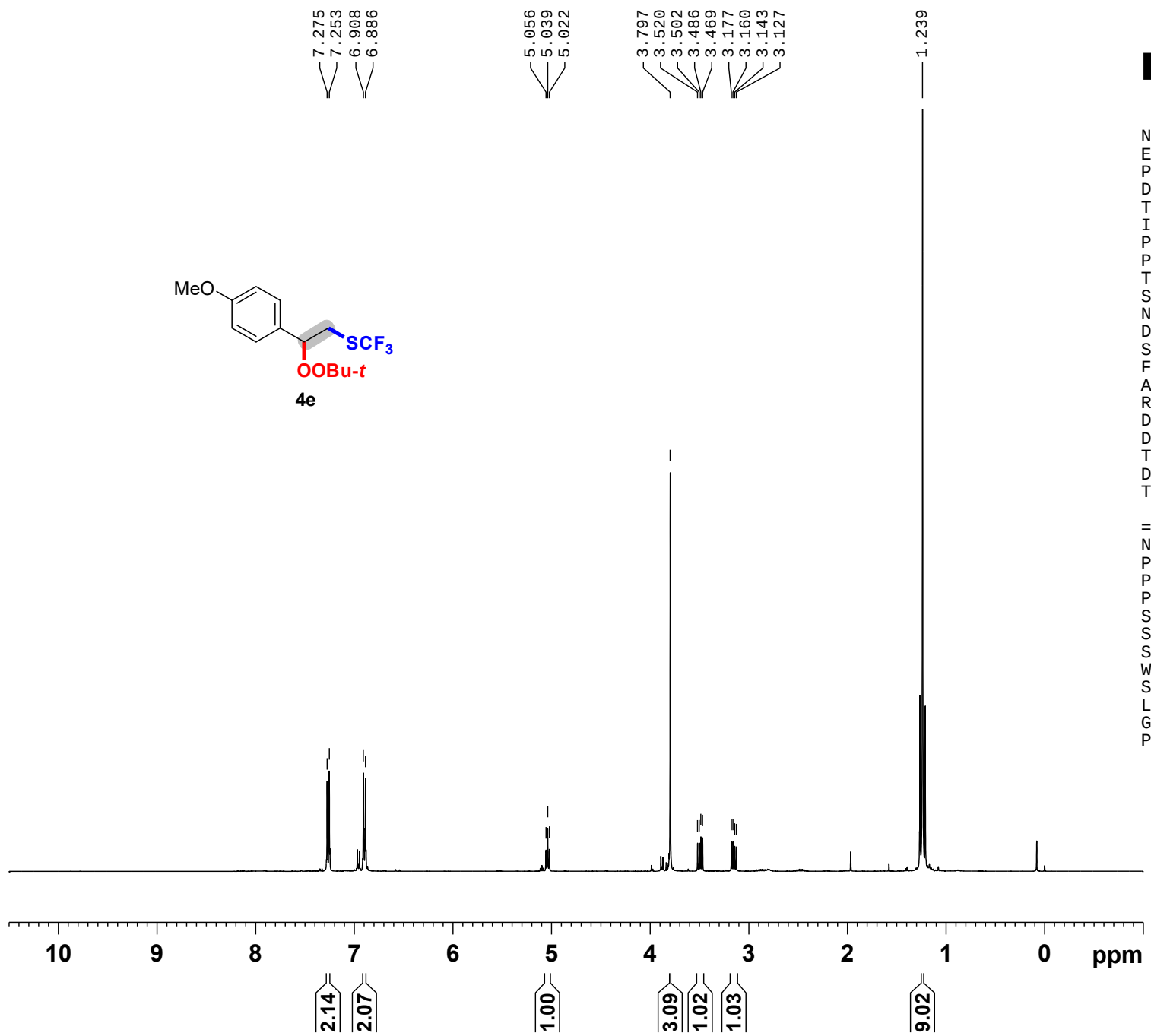
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127774 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyj855dp-20190328
EXPNO                    3
PROCNO                   1
Date_             20190328
Time                 20.36
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       32
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                      812
DW                    5.600 usec
DE                     6.50 usec
TE                    292.7 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                      1

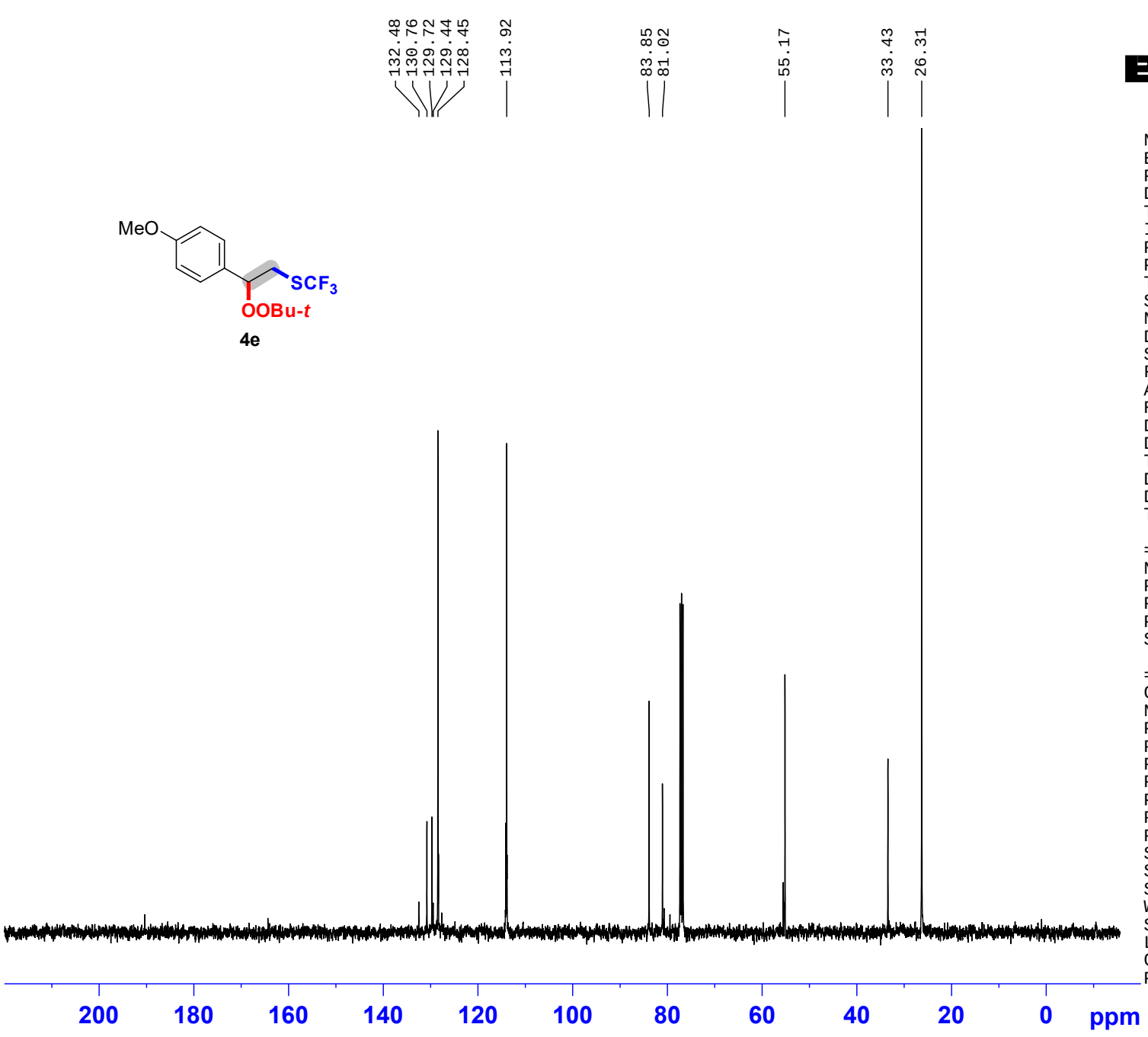
======== CHANNEL f1 ========
NUC1                    19F
P1                    14.20 usec
PL1                   -2.00 dB
PL1W           20.42289734 W
SFO1           376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  16.72 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
SFO2           400.1316005 MHz
SI                    65536
SF             376.4983660 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.00
```




```
NAME      cyj855cp-20190411
EXPNO                    1
PROCNO                   1
Date_             20190411
Time                 9.09
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6393.862 Hz
FIDRES           0.195125 Hz
AQ               2.5625076 sec
RG                     64
DW                 78.200 usec
DE                  6.50 usec
TE                 293.3 K
D1              1.00000000 sec
TD0                     1

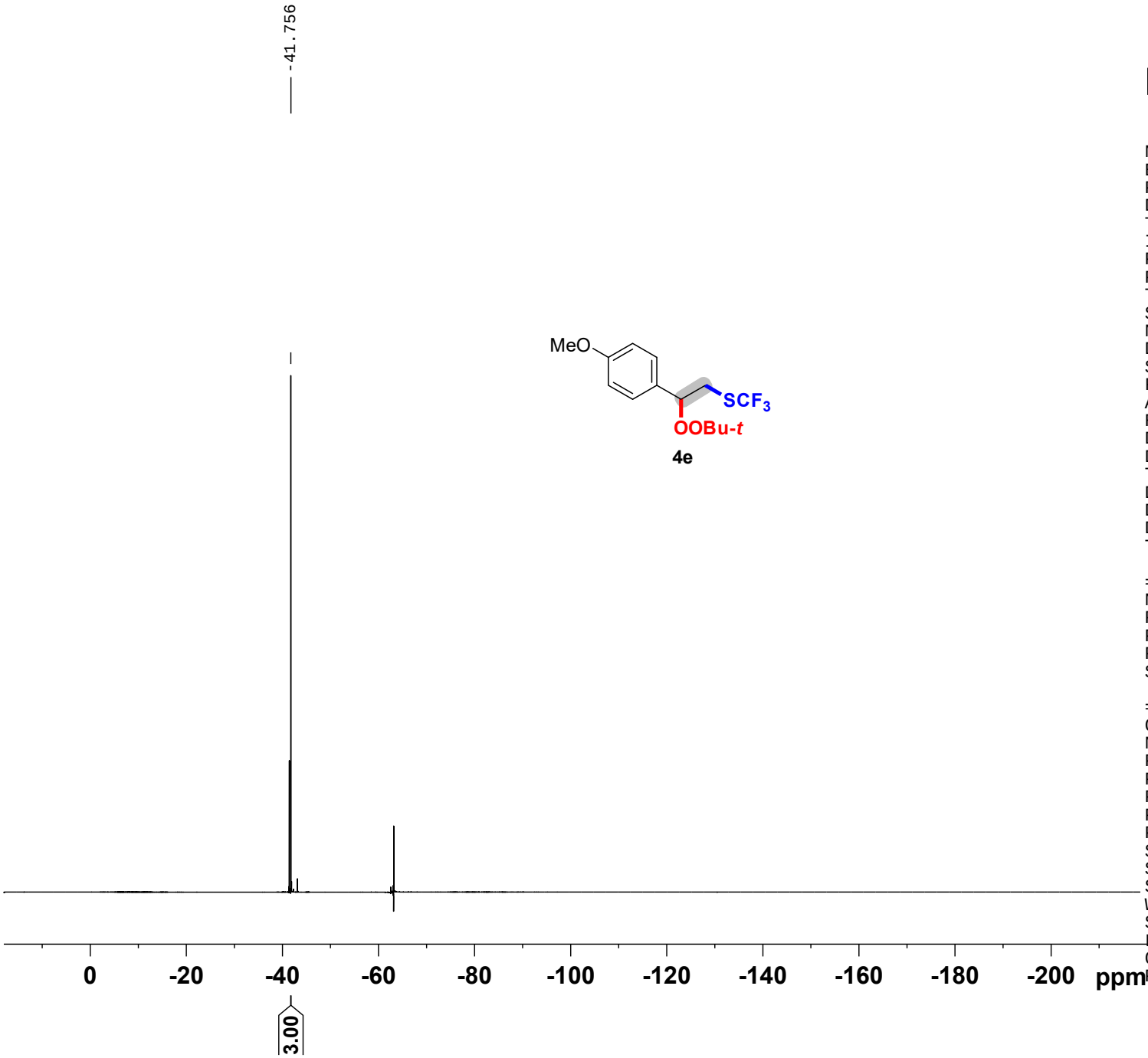
======== CHANNEL f1 ========
NUC1                   1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                  32768
SF           400.1300153 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                  1.00
```




```
NAME      cyj855cp-20190411
EXPNO                     2
PROCNO                    1
Date_              20190411
Time                  9.13
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       40
DS                        4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                      181
DW                   19.800 usec
DE                    6.50 usec
TE                   294.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       3

======== CHANNEL f1 ========
NUC1                    13C
P1                   15.00 usec
PL1                   2.00 dB
PL1W            55.31277084 W
SFO1            100.6238364 MHz

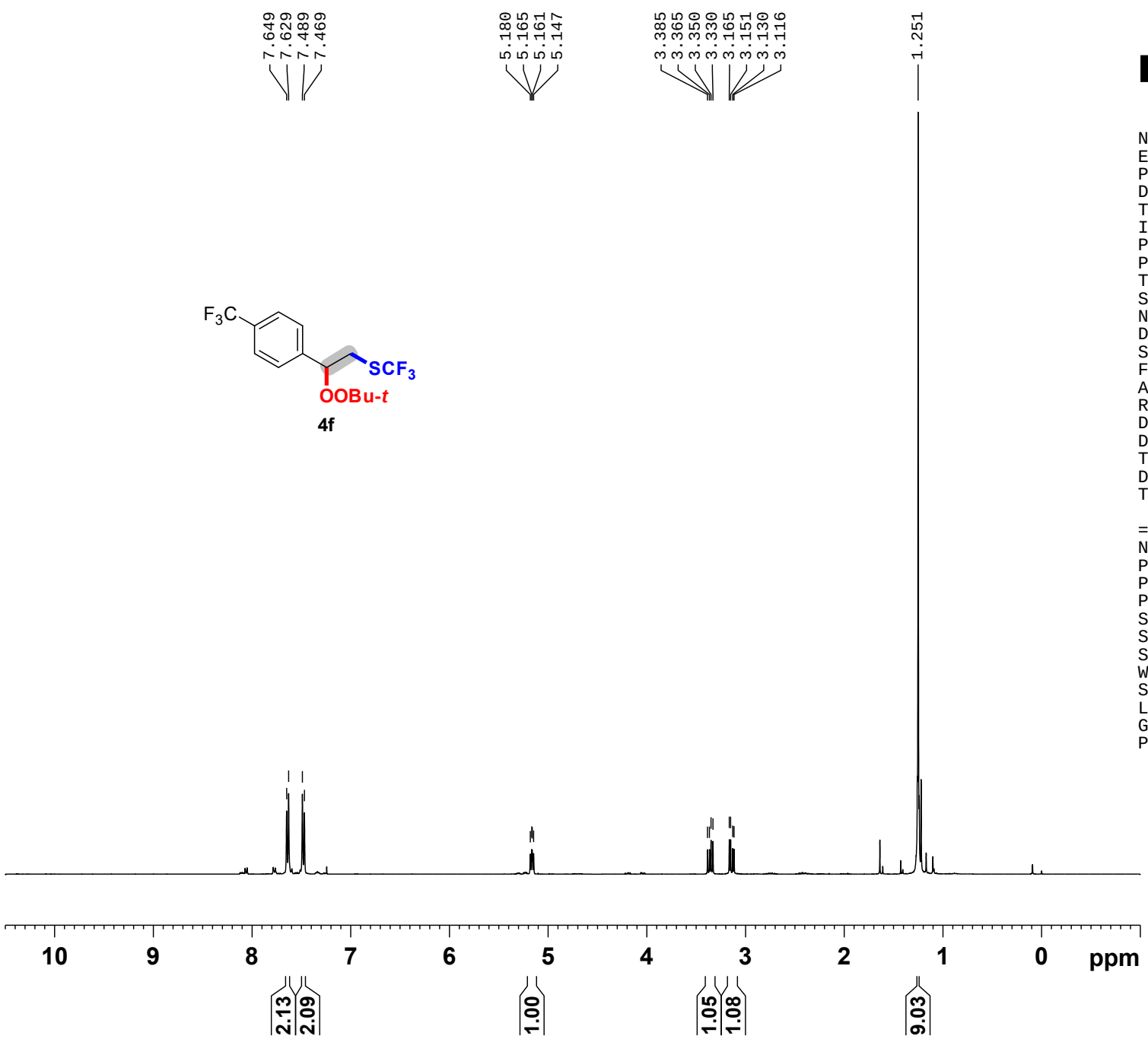
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
PL13W            0.38087484 W
SFO2            400.1316005 MHz
SI                    32768
SF              100.6127750 MHz
WDW                      EM
SSB                       0
LB                    3.00 Hz
GB                        0
PC                     1.40
```




```
NAME      cyj855cp-20190411
EXPNO                    3
PROCNO                   1
Date_             20190411
Time                 9.17
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT             CDCl3
NS                     64
DS                      4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                    2050
DW                   5.600 usec
DE                   6.50 usec
TE                  293.7 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                     4

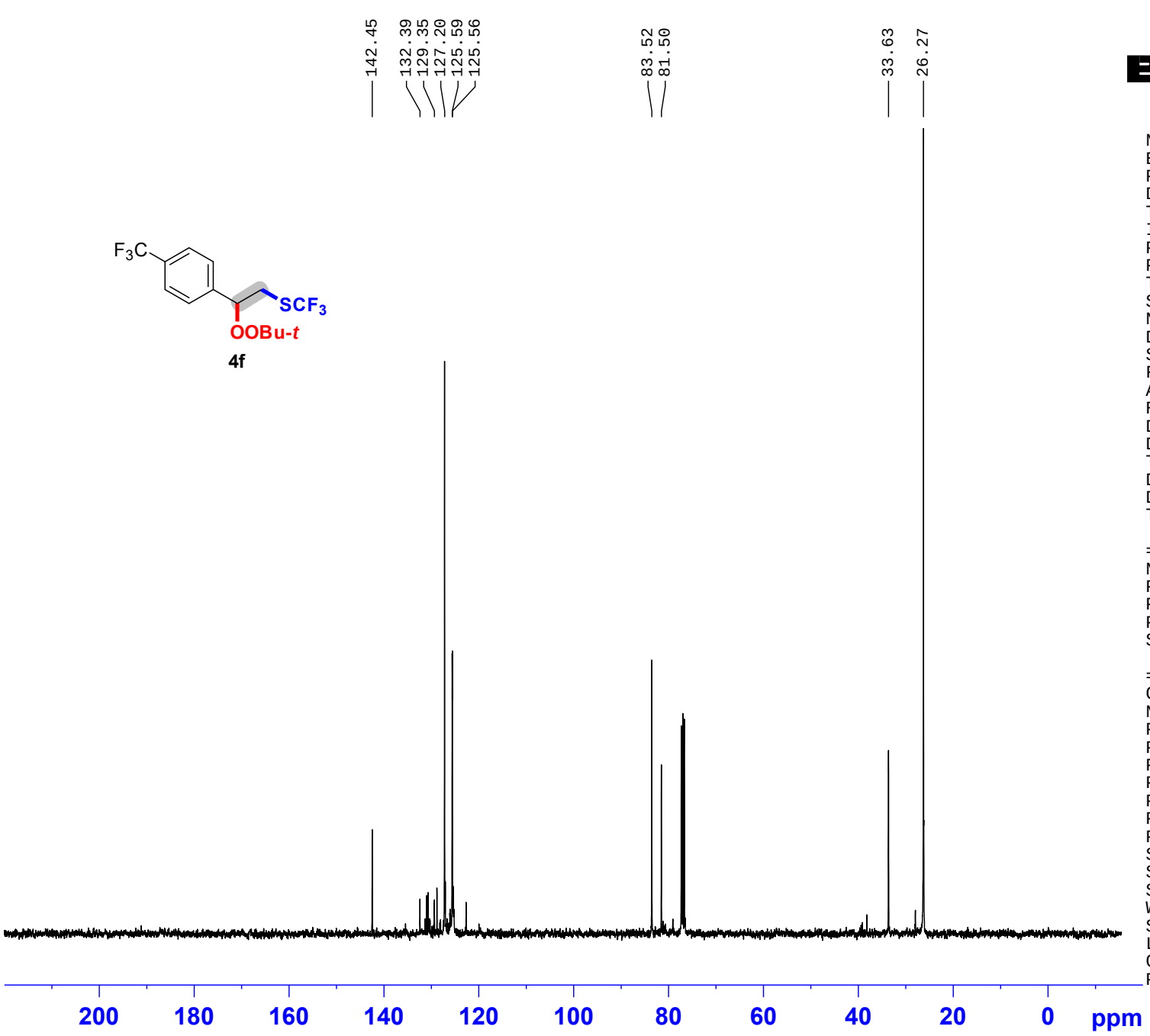
======== CHANNEL f1 ========
NUC1                   19F
P1                   14.20 usec
PL1                  -2.00 dB
PL1W          20.42289734 W
SFO1          376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
SFO2          400.1316005 MHz
SI                  65536
SF            376.4983660 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cyj862ap-20190411
EXPNO                    1
PROCNO                   1
Date_             20190411
Time                 8.34
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                      57
DW                  78.200 usec
DE                   6.50 usec
TE                  293.1 K
D1              1.00000000 sec
TD0                      1

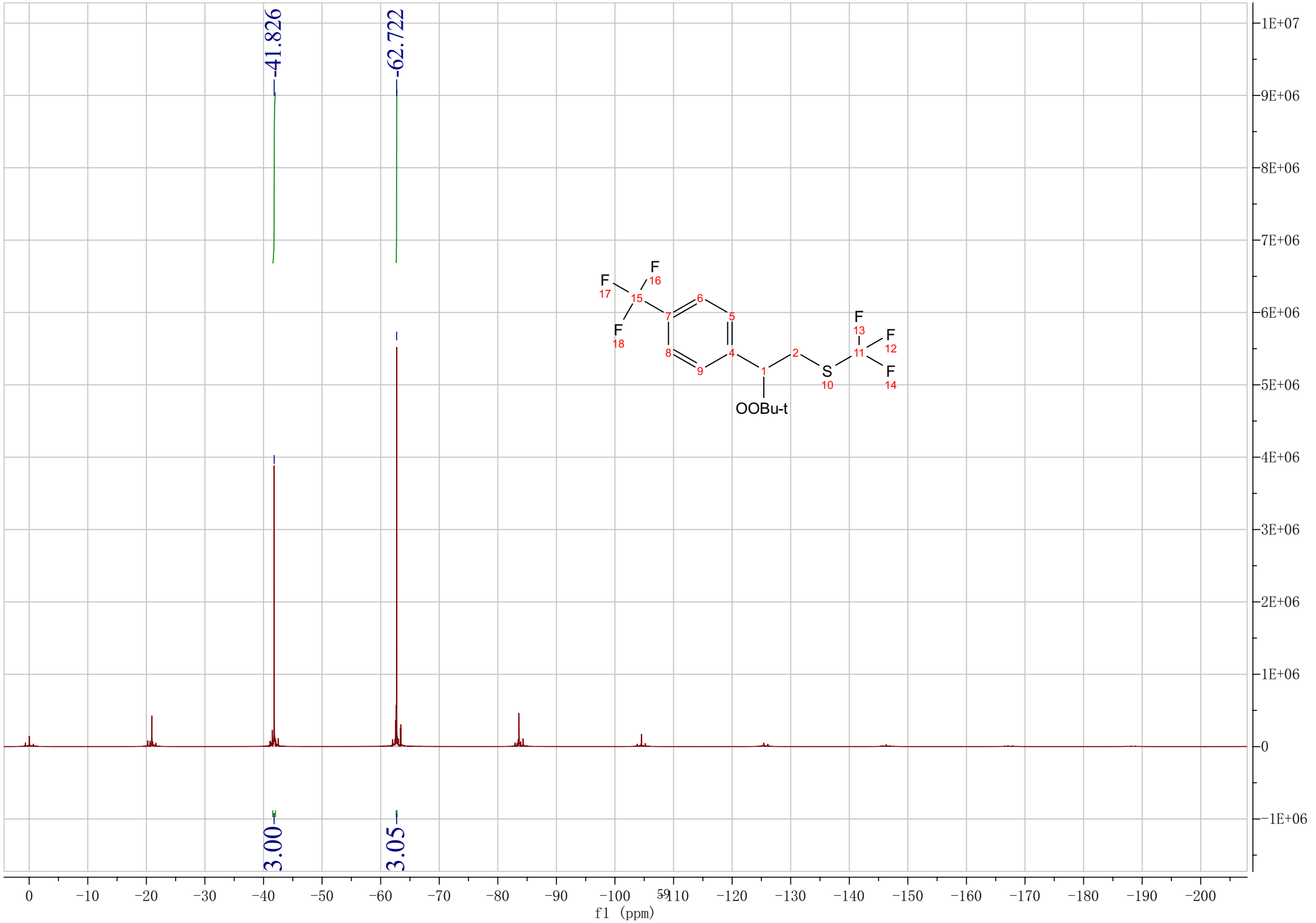
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300171 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                   1.00
```

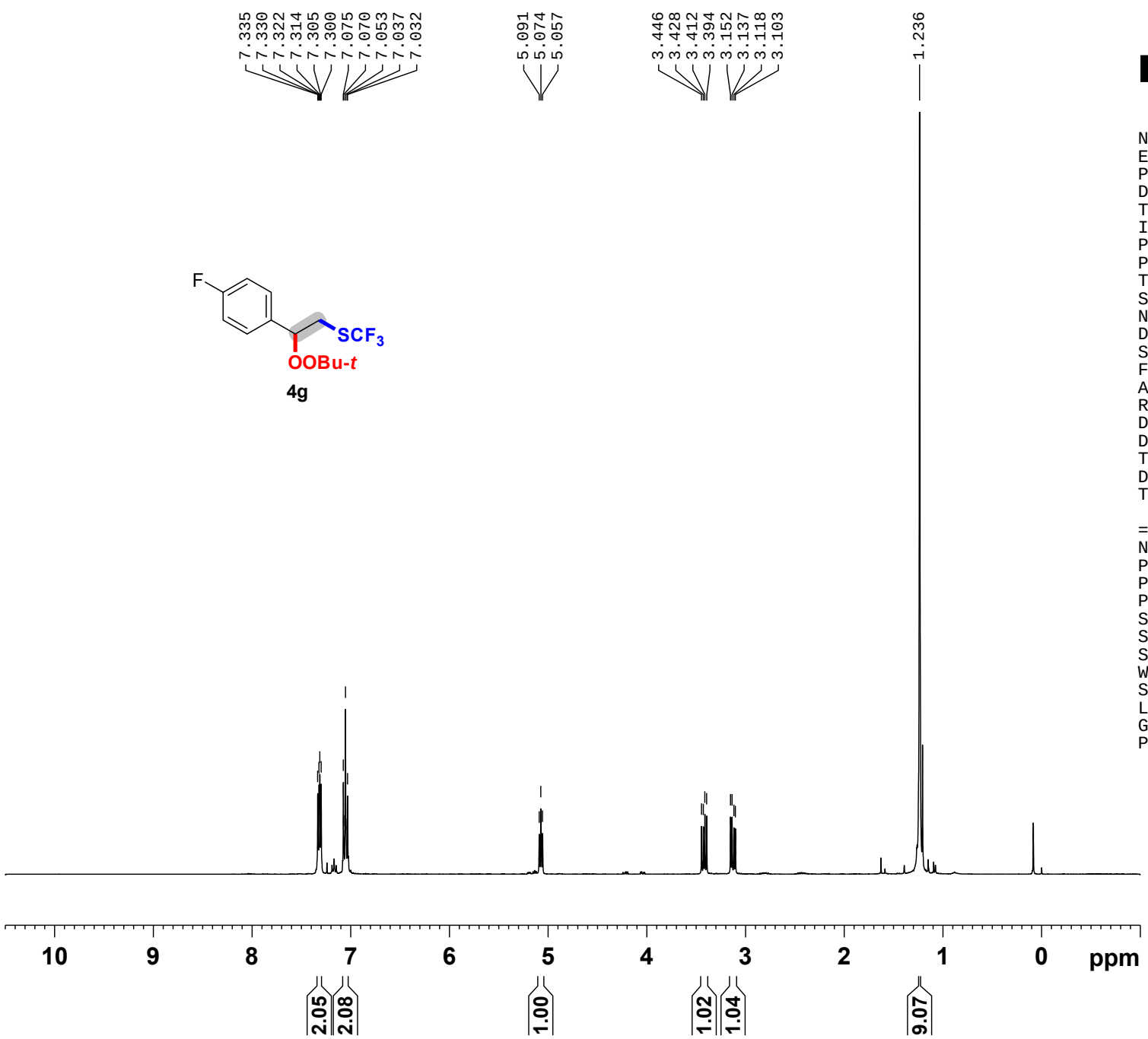



```
NAME      cyj862ap-20190410
EXPNO                    2
PROCNO                   1
Date_             20190411
Time                  8.40
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       64
DS                        4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                      181
DW                   19.800 usec
DE                    6.50 usec
TE                   294.7 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       3

======== CHANNEL f1 ========
NUC1                    13C
P1                   15.00 usec
PL1                   2.00 dB
PL1W           55.31277084 W
SFO1           100.6238364 MHz

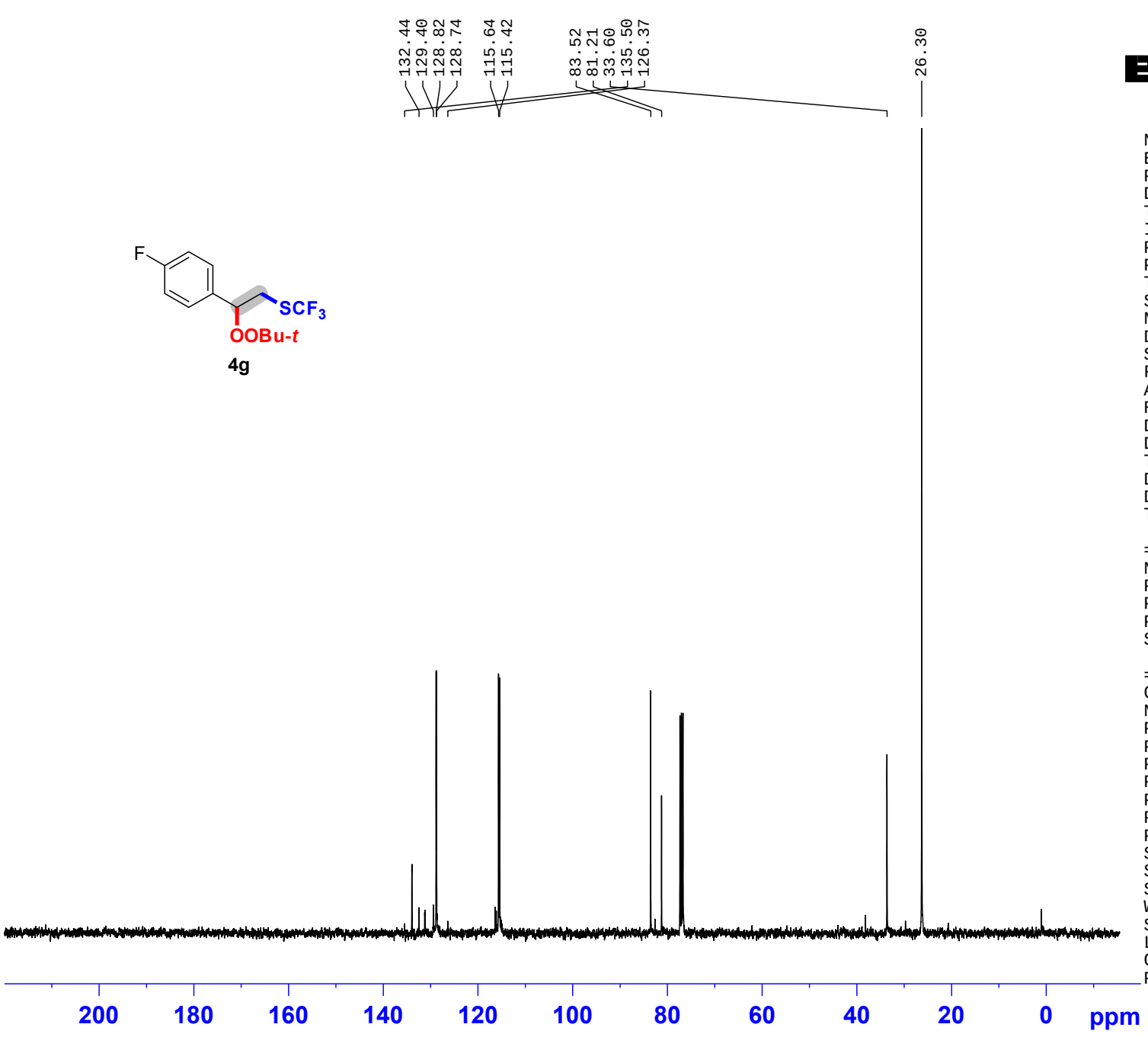
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
PL13W           0.38087484 W
SFO2           400.1316005 MHz
SI                    32768
SF             100.6127674 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```


-41.826
-62.722
3.00
3.05
F
16
F
17
15
6
7
5
F
18
F
13
F
12
8
4
2
11
9
1
S
10
F
14
OOBu-t
1E+07
9E+06
8E+06
7E+06
6E+06
5E+06
4E+06
3E+06
2E+06
1E+06
0
-1E+06
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)




```
NAME      cyj-850bp-20190415
EXPNO                      1
PROCNO                     1
Date_               20190415
Time                   17.08
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6393.862 Hz
FIDRES              0.195125 Hz
AQ                2.5625076 sec
RG                      40.3
DW                    78.200 usec
DE                     6.50 usec
TE                    296.3 K
D1                1.00000000 sec
TD0                        1

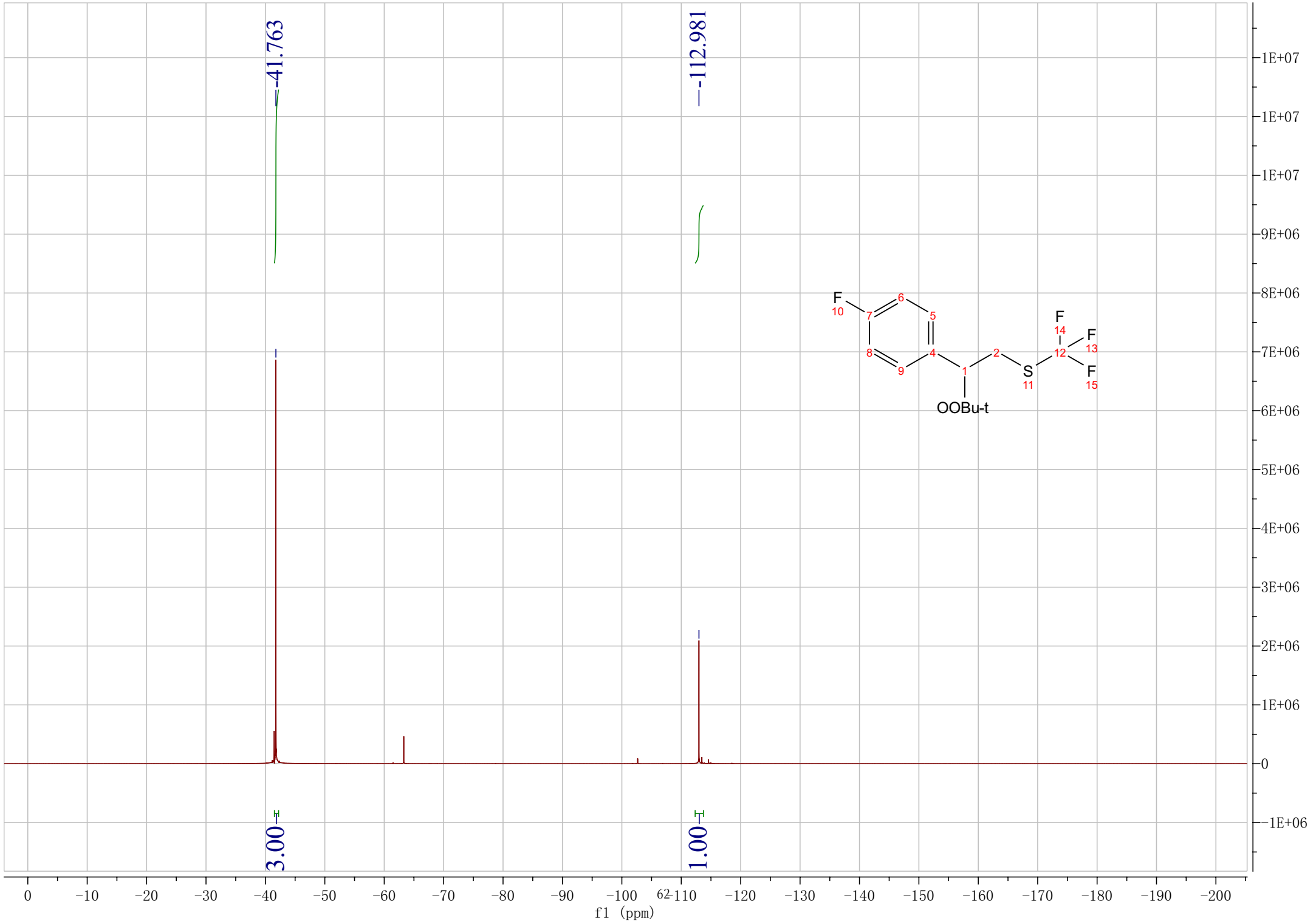
======== CHANNEL f1 ========
NUC1                      1H
P1                     10.40 usec
PL1                    -1.00 dB
PL1W           17.01305389 W
SFO1           400.1326008 MHz
SI                     32768
SF             400.1300180 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```

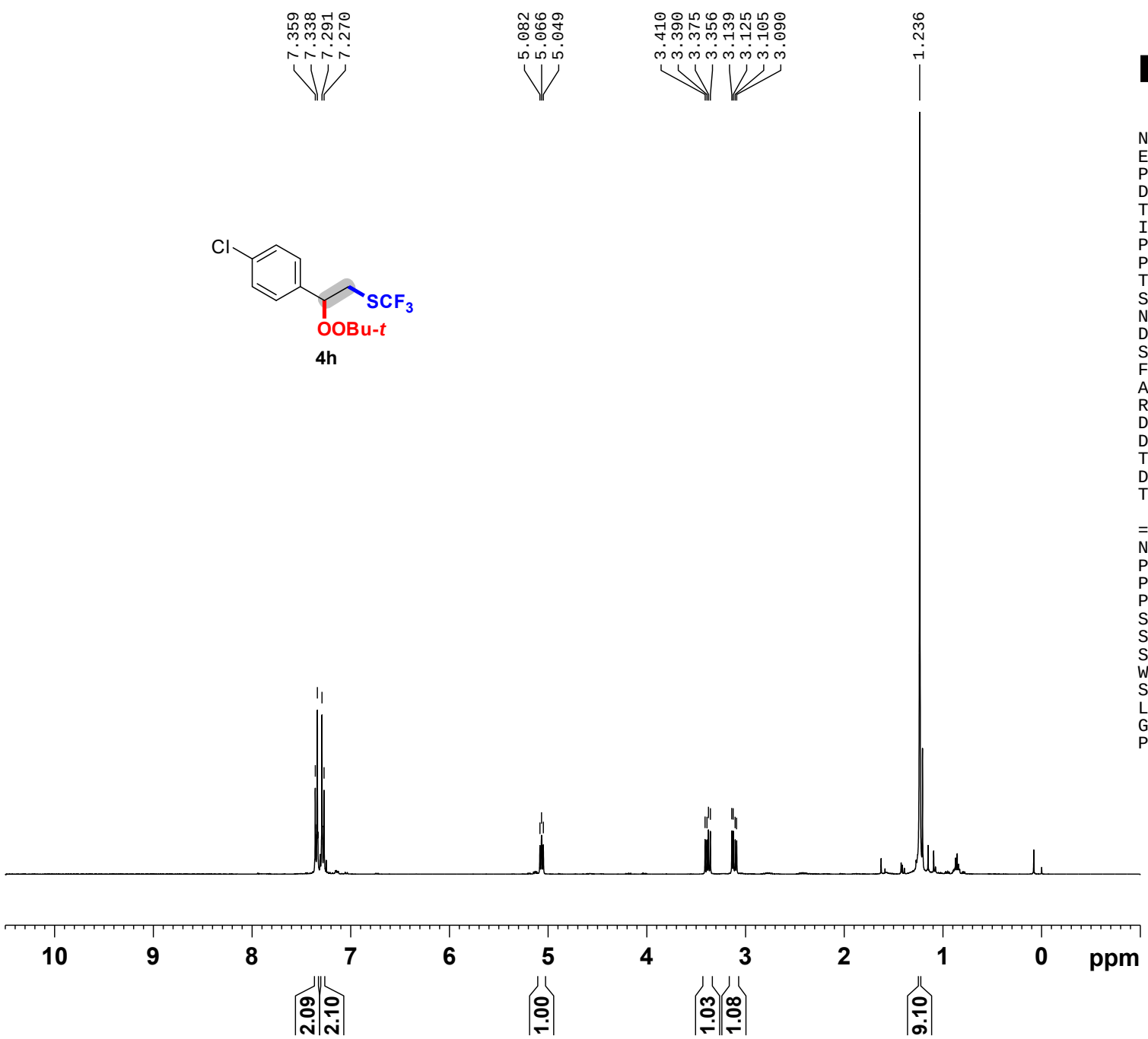



```
NAME      cyj-850bp-20190415
EXPNO                      2
PROCNO                     1
Date_               20190415
Time                   17.12
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         40
DS                          4
SWH                 25252.525 Hz
FIDRES                0.385323 Hz
AQ                  1.2976629 sec
RG                        181
DW                     19.800 usec
DE                      6.50 usec
TE                     297.5 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         3

======== CHANNEL f1 ========
NUC1                      13C
P1                     15.00 usec
PL1                     2.00 dB
PL1W               55.31277084 W
SFO1               100.6238364 MHz

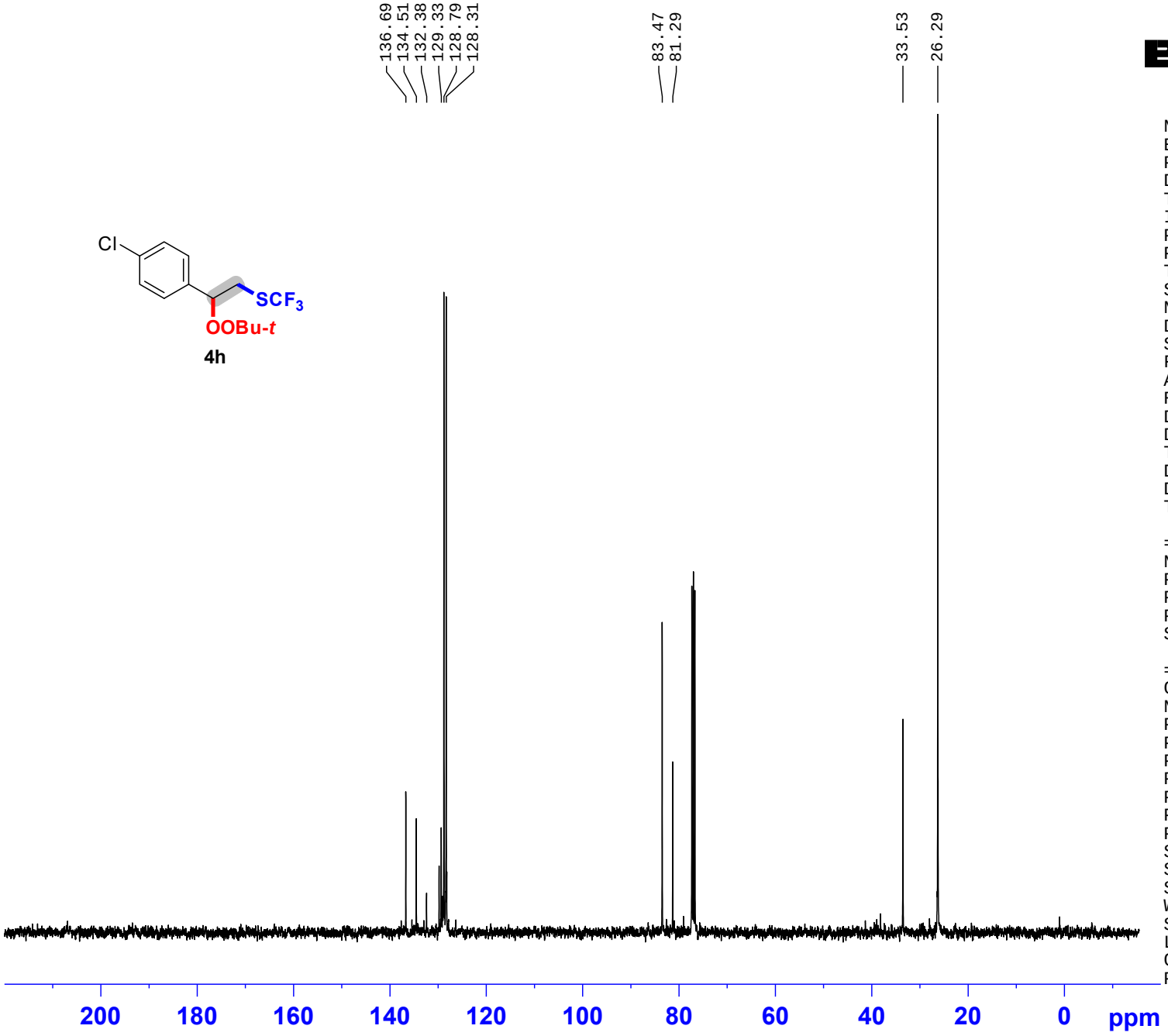
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL13                   15.50 dB
PL2W               17.01305389 W
PL12W               0.28759566 W
PL13W               0.38087484 W
SFO2               400.1316005 MHz
SI                      32768
SF                 100.6127701 MHz
WDW                        EM
SSB                         0
LB                      3.00 Hz
GB                          0
PC                      1.40
```


-41.763
-112.981
3.00
1.00
F
10
6
7
5
8
4
9
1
2
S
11
12
F
14
F
13
F
15
OOBu-t
1E+07
1E+07
1E+07
9E+06
8E+06
7E+06
6E+06
5E+06
4E+06
3E+06
2E+06
1E+06
0
-1E+06
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)




```
NAME      cyj850cp-20190328
EXPNO                    1
PROCNO                   1
Date_             20190328
Time                19.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6393.862 Hz
FIDRES           0.195125 Hz
AQ               2.5625076 sec
RG                     64
DW                 78.200 usec
DE                  6.50 usec
TE                 292.3 K
D1              1.00000000 sec
TD0                     1

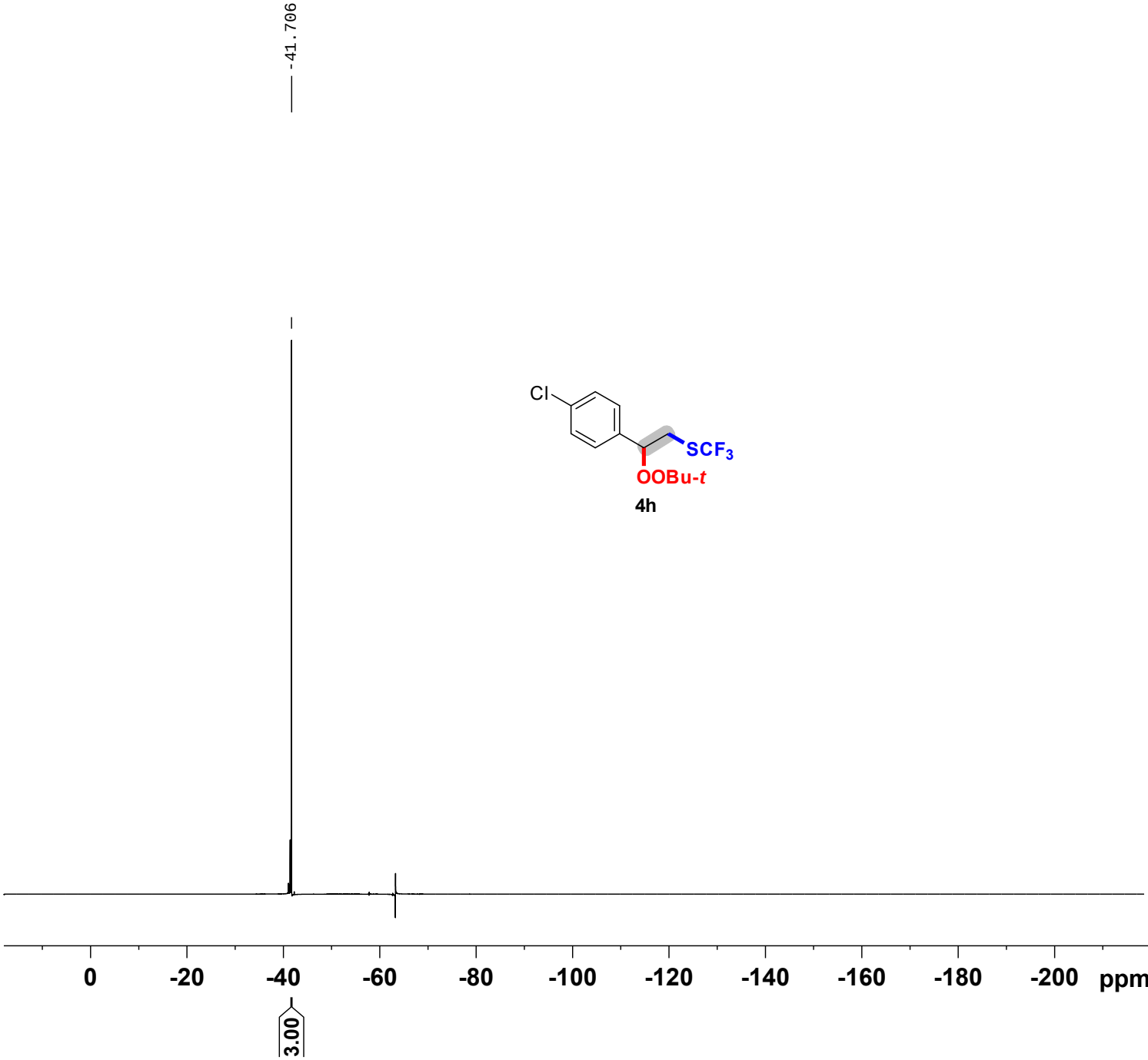
======== CHANNEL f1 ========
NUC1                   1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                  32768
SF           400.1300152 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                  1.00
```




```
NAME      cyj850cp-20190328
EXPNO                    2
PROCNO                   1
Date_             20190328
Time                19.35
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      72
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  293.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

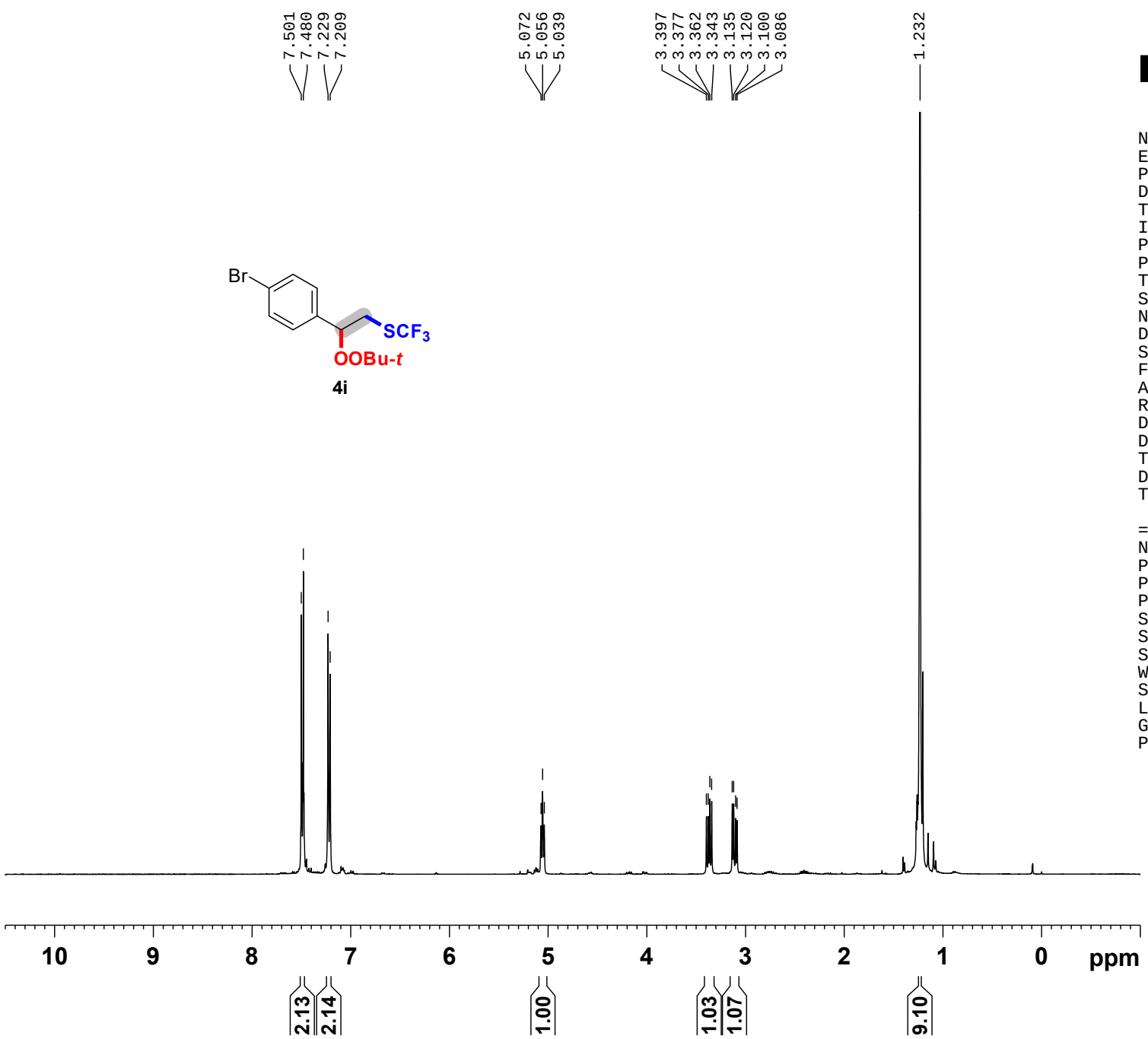
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127727 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyj850cp-20190328
EXPNO                     3
PROCNO                    1
Date_              20190328
Time                  19.43
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       32
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                      812
DW                    5.600 usec
DE                    6.50 usec
TE                   292.7 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       1

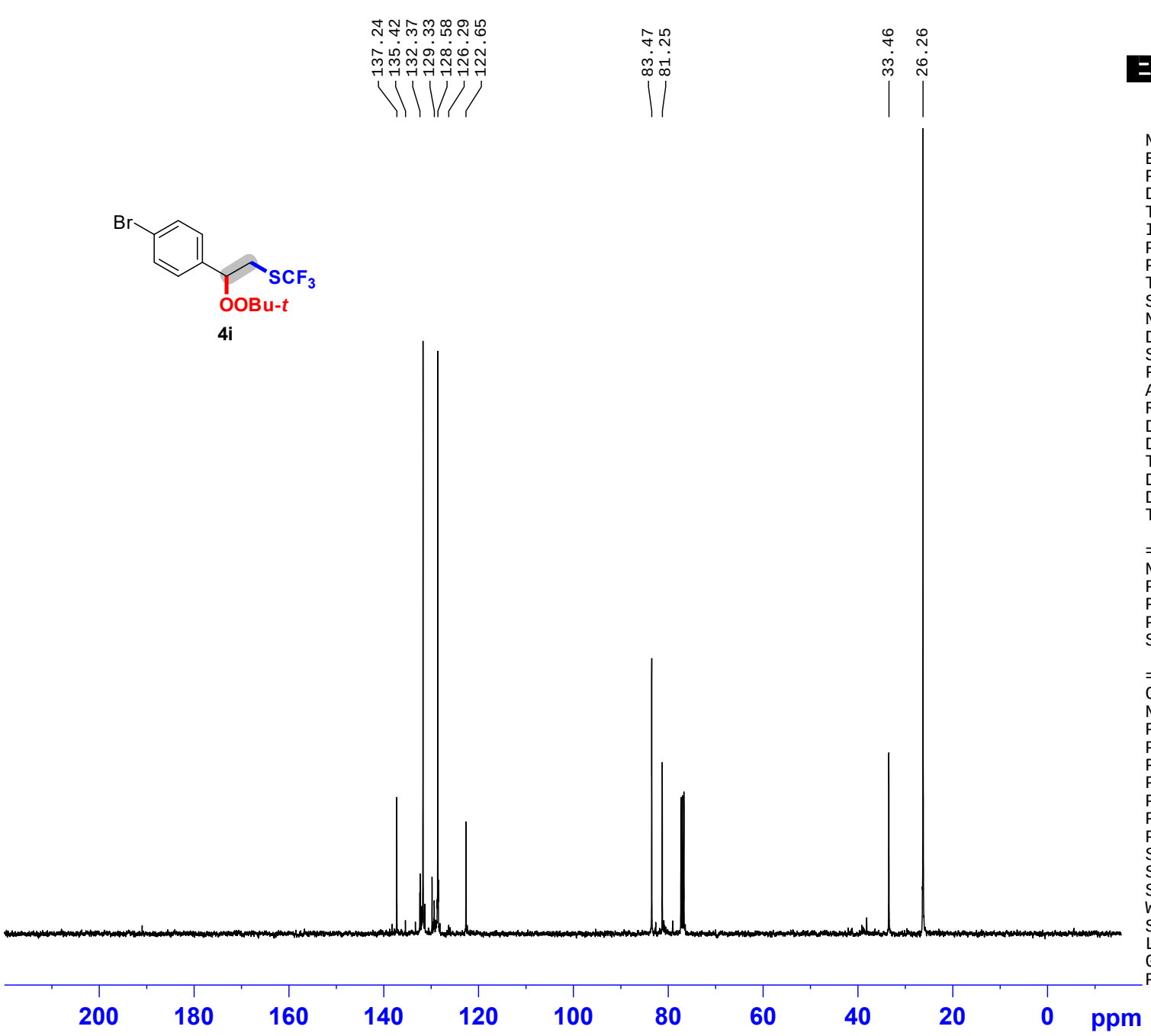
======== CHANNEL f1 ========
NUC1                     19F
P1                    14.20 usec
PL1                   -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                    65536
SF              376.4983660 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.00
```




```
NAME      cyj856cp-20190411
EXPNO                    1
PROCNO                   1
Date_             20190411
Time                 8.52
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6393.862 Hz
FIDRES           0.195125 Hz
AQ               2.5625076 sec
RG                     36
DW                 78.200 usec
DE                  6.50 usec
TE                 293.2 K
D1              1.00000000 sec
TD0                     1

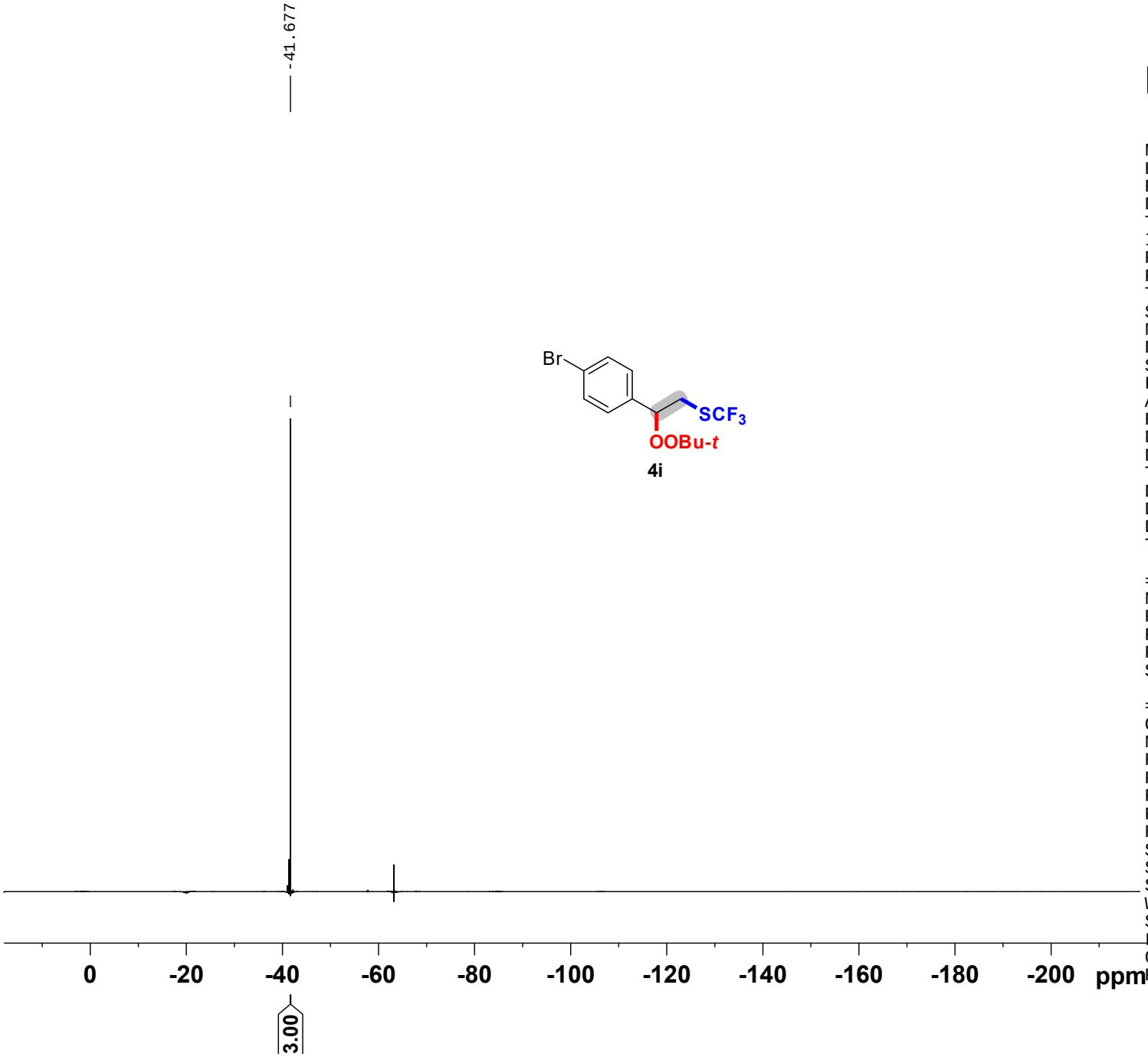
======== CHANNEL f1 ========
NUC1                   1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                  32768
SF           400.1300218 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                  1.00
```




```
NAME      cyj856cp-20190411
EXPNO                    2
PROCNO                   1
Date_             20190411
Time                 8.58
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      64
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  294.7 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

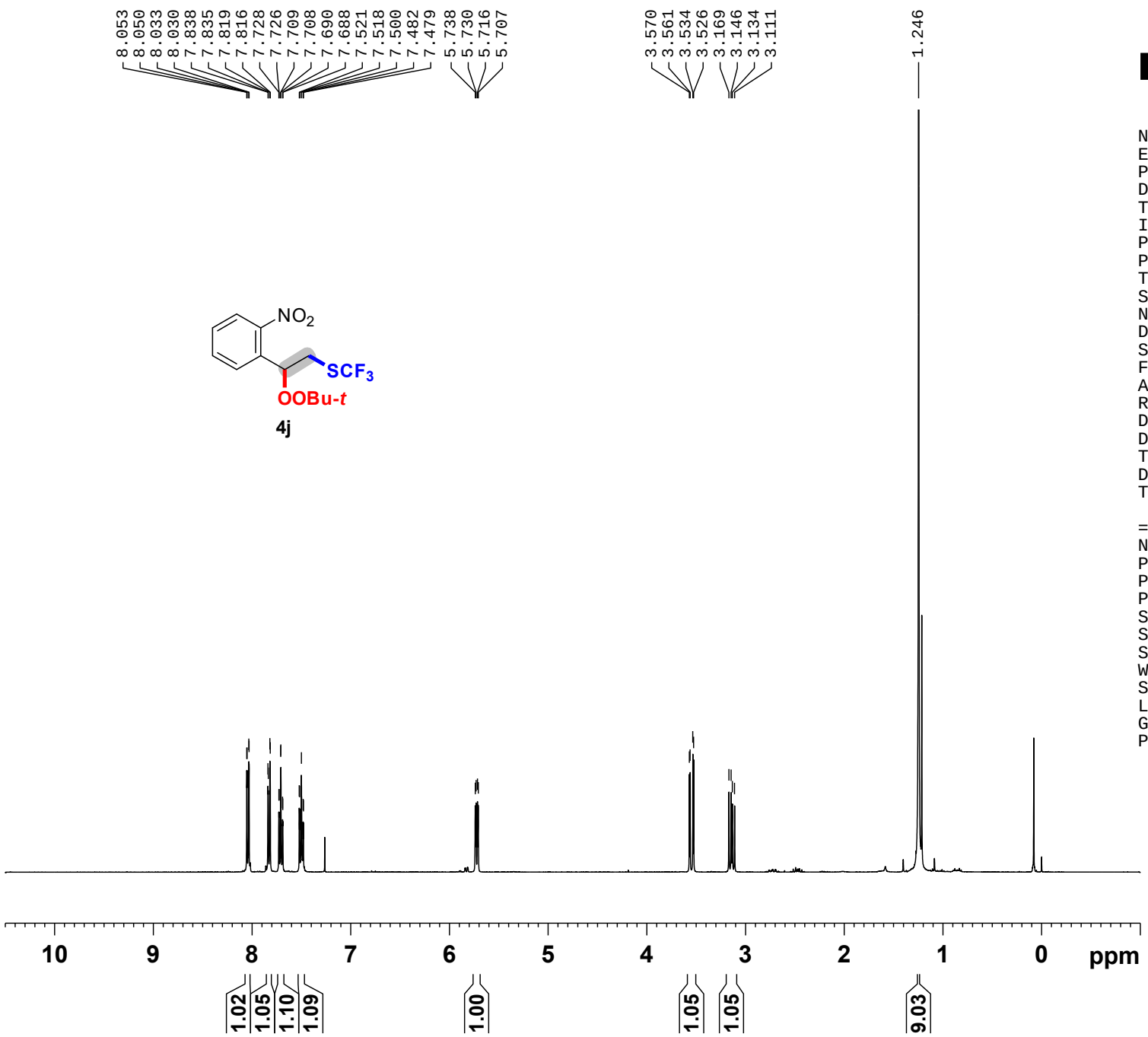
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127762 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyj856cp-20190411
EXPNO                    3
PROCNO                   1
Date_             20190411
Time                 9.02
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT             CDCl3
NS                     64
DS                      4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                    2050
DW                   5.600 usec
DE                   6.50 usec
TE                  293.6 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                     4

======== CHANNEL f1 ========
NUC1                   19F
P1                   14.20 usec
PL1                  -2.00 dB
PL1W          20.42289734 W
SFO1          376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
SFO2          400.1316005 MHz
SI                  65536
SF            376.4983660 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

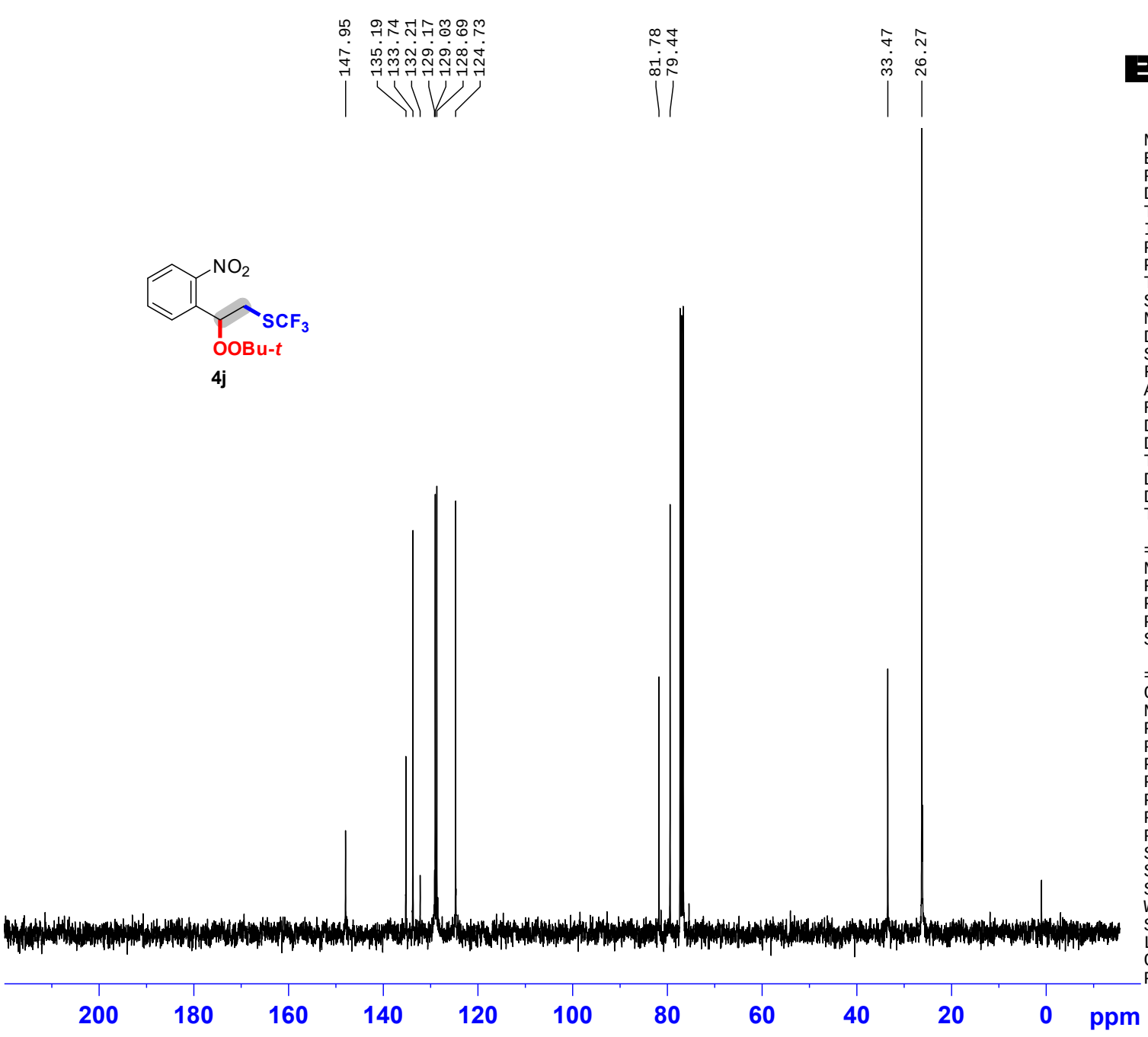


BRUKER

NAME	cyj845ap-20190329
EXPNO	1
PROCNO	1
Date_	20190329
Time	9.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	90.5
DW	78.200 usec
DE	6.50 usec
TE	294.7 K
D1	1.00000000 sec
TD0	1

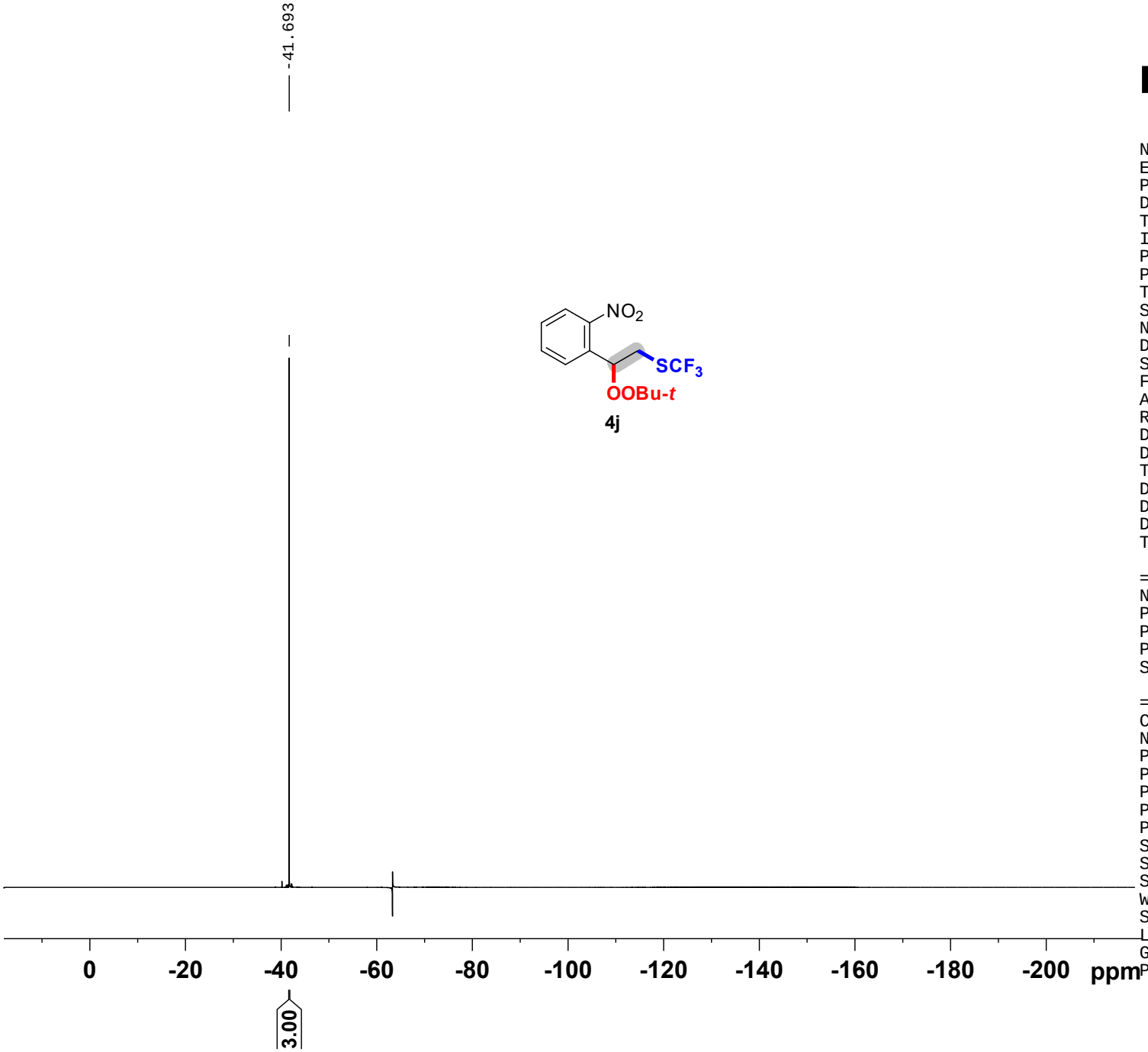
======== CHANNEL f1 ========

NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300091 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

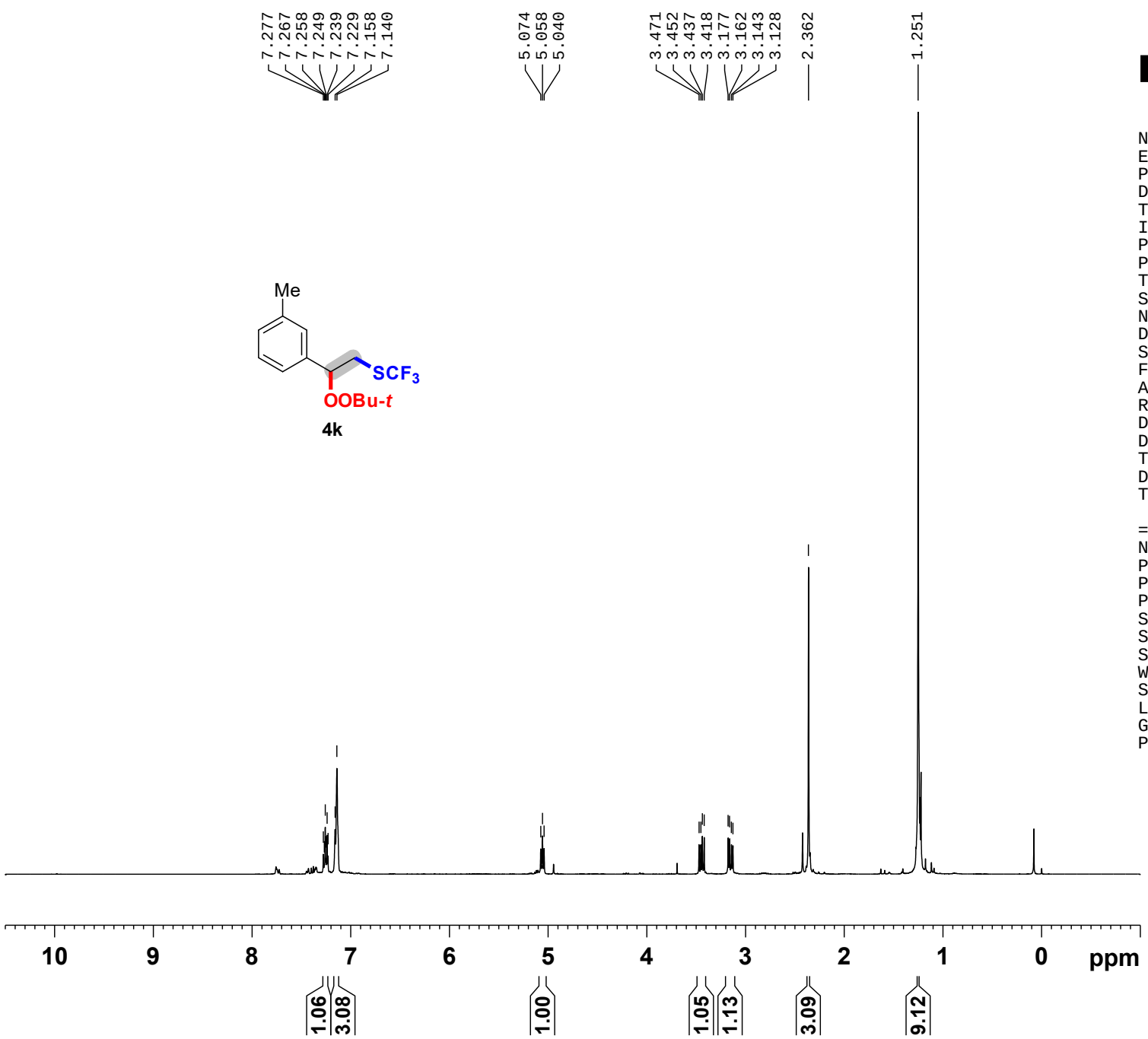
NAME	cyj-845ap-20190329
EXPNO	2
PROCNO	1
Date_	20190329
Time	9.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	40
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	181
DW	19.800 usec
DE	6.50 usec
TE	295.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	13C
P1	15.00 usec
PL1	2.00 dB
PL1W	55.31277084 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	16.72 dB
PL13	15.50 dB
PL2W	17.01305389 W
PL12W	0.28759566 W
PL13W	0.38087484 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127723 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40




```
NAME      cyj-845ap-20190329
EXPNO                      3
PROCNO                     1
Date_               20190329
Time                    9.53
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES             0.681196 Hz
AQ                 0.7340532 sec
RG                       812
DW                     5.600 usec
DE                     6.50 usec
TE                     295.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

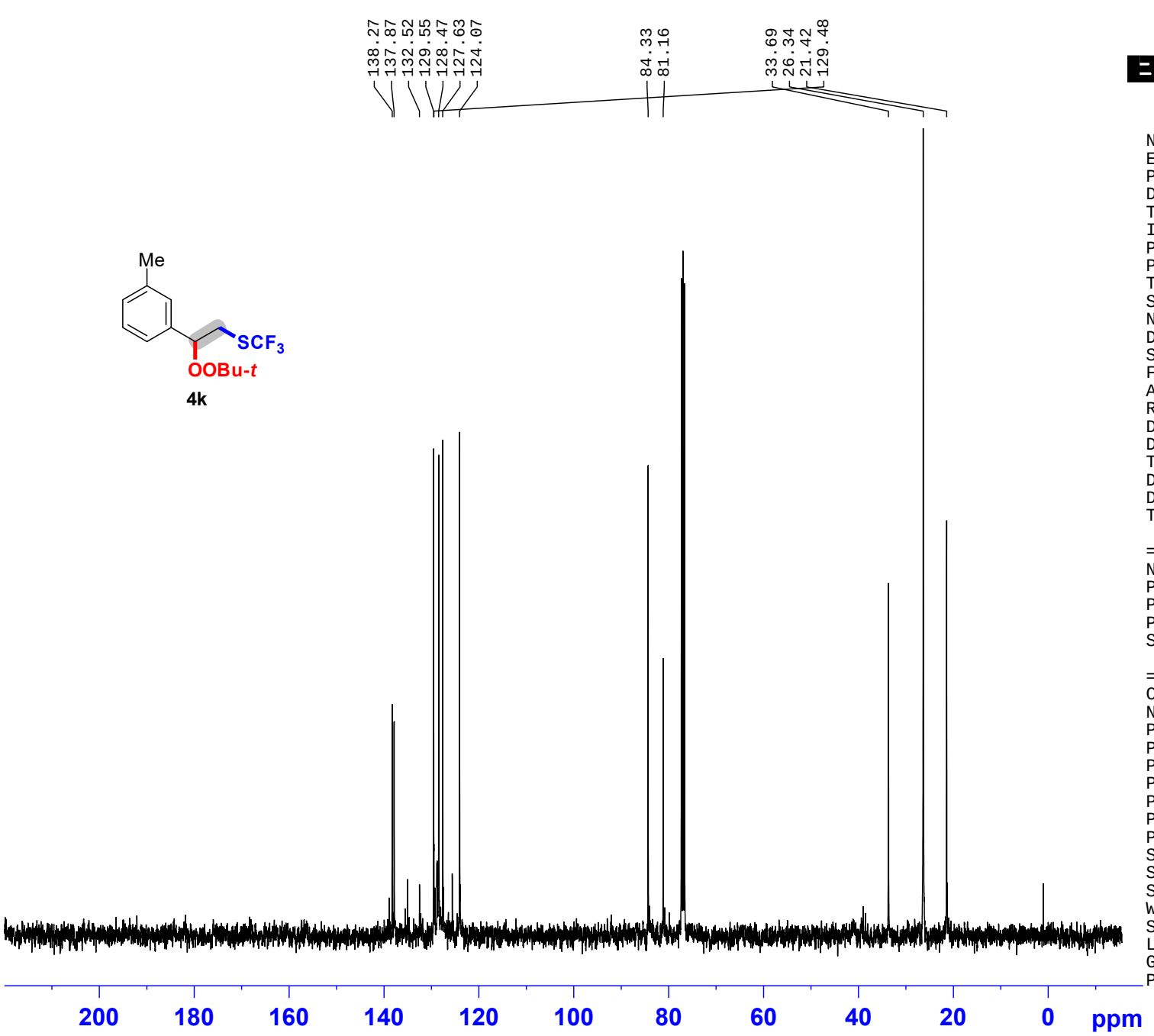
======== CHANNEL f1 ========
NUC1                      19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                     65536
SF              376.4983660 MHz
WDW                       EM
SSB                        0
LB                      3.00 Hz
GB                         0
PC                      1.00
```




```
NAME      cyj856bp-20190328
EXPNO                    1
PROCNO                   1
Date_             20190328
Time                 20.42
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                      57
DW                  78.200 usec
DE                   6.50 usec
TE                  292.3 K
D1             1.00000000 sec
TD0                      1

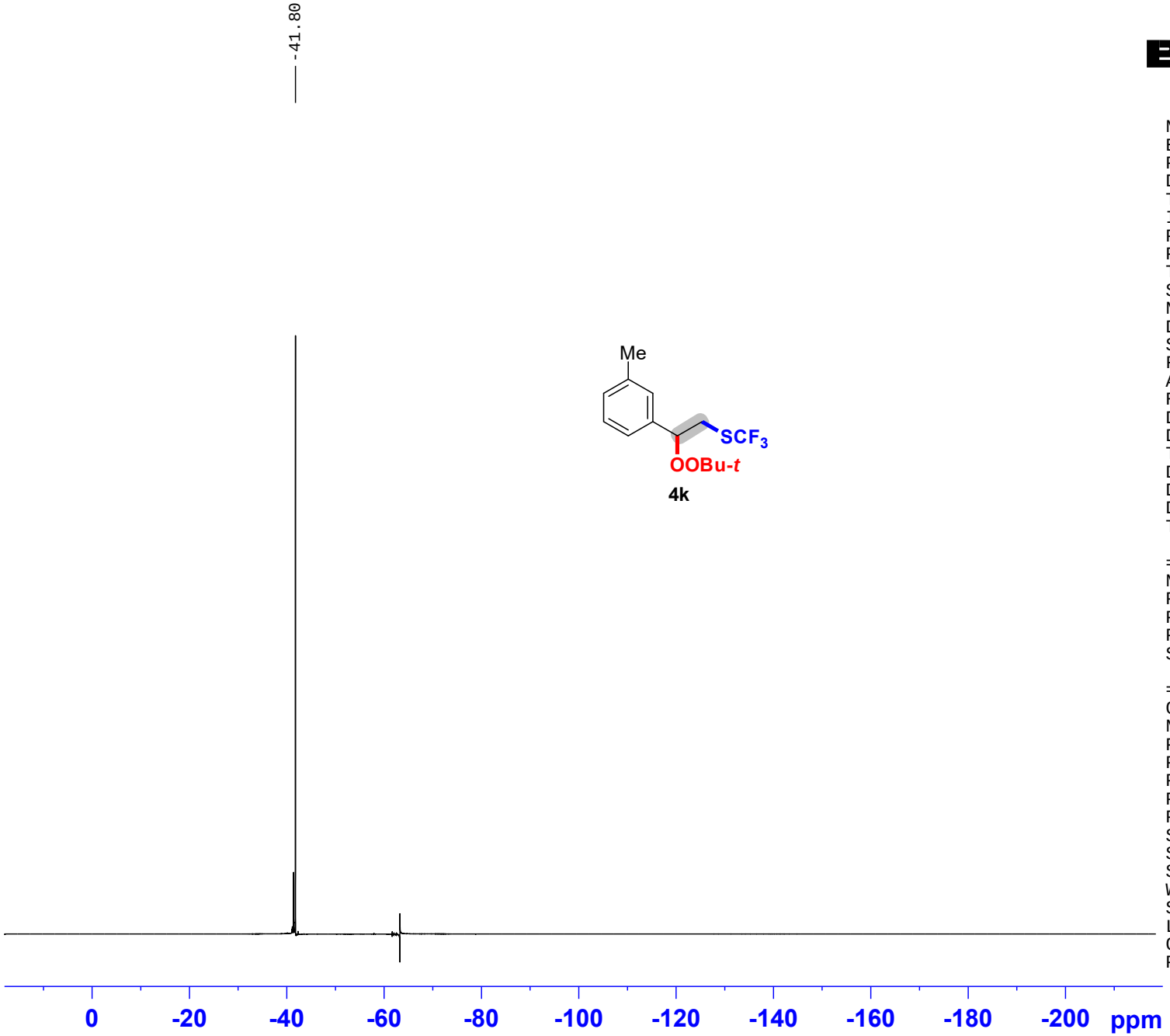
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300226 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                   1.00
```




```
NAME      cyj856bp-20190328
EXPNO                    2
PROCNO                   1
Date_             20190328
Time                 20.47
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      64
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  293.6 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

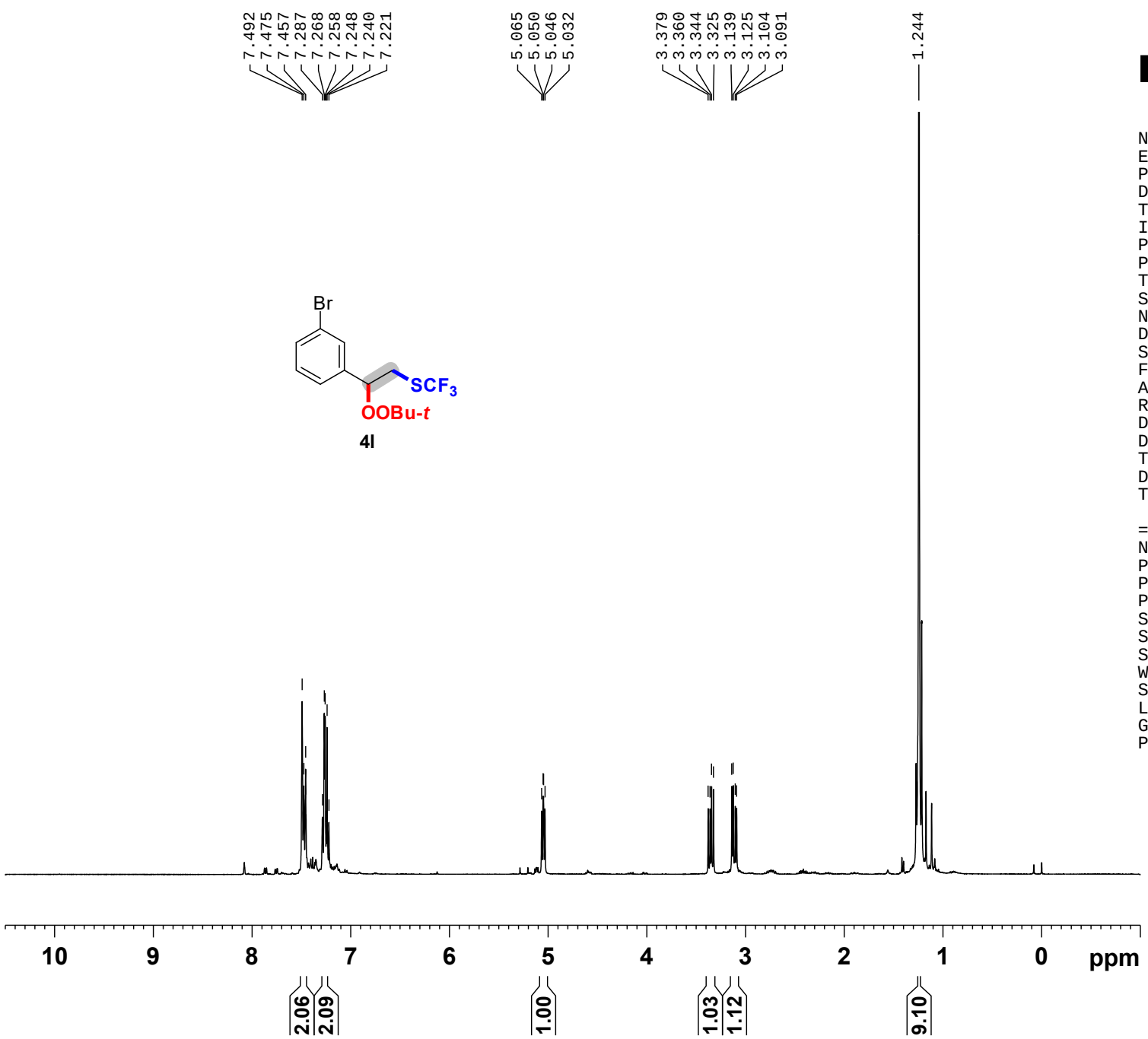
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127742 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyj856bp-20190328
EXPNO                     3
PROCNO                    1
Date_              20190328
Time                  20.52
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       32
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                      812
DW                    5.600 usec
DE                     6.50 usec
TE                    292.8 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                    65536
SF              376.4983660 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.00
```

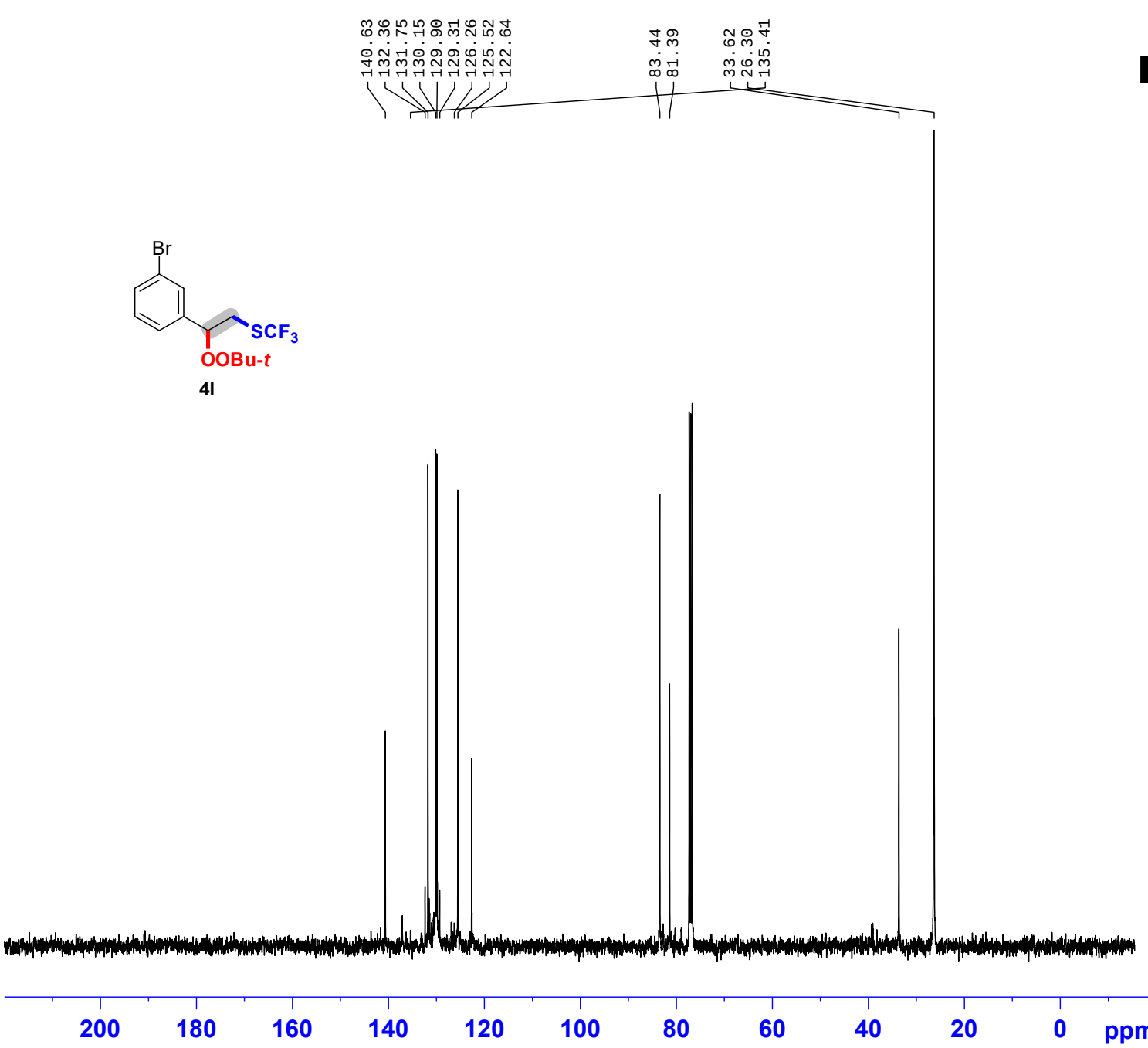


BRUKER

NAME	cyj856dp-20190328
EXPNO	1
PROCNO	1
Date_	20190328
Time	20.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	57
DW	78.200 usec
DE	6.50 usec
TE	292.3 K
D1	1.00000000 sec
TD0	1

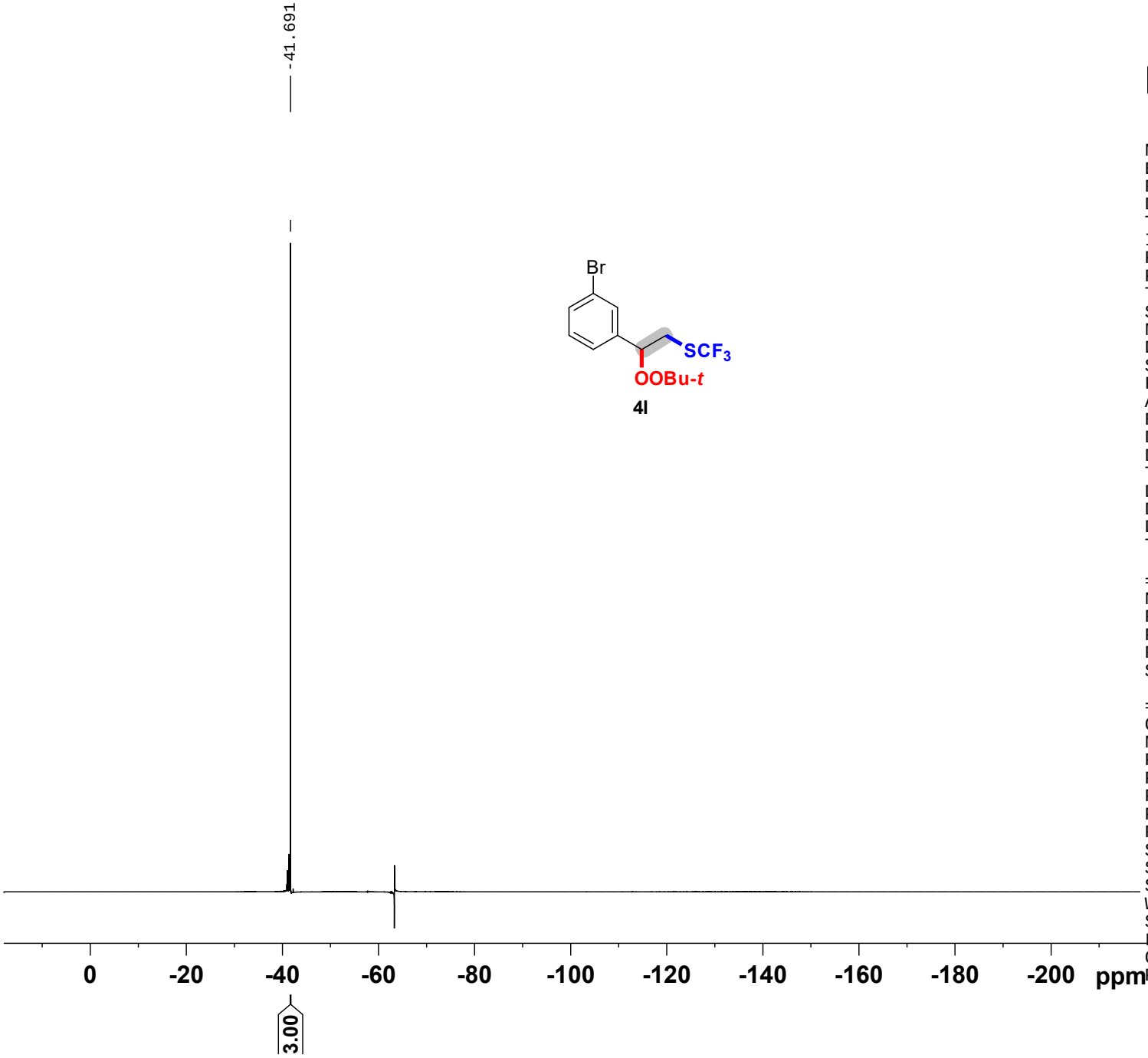
======== CHANNEL f1 ========

NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300154 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

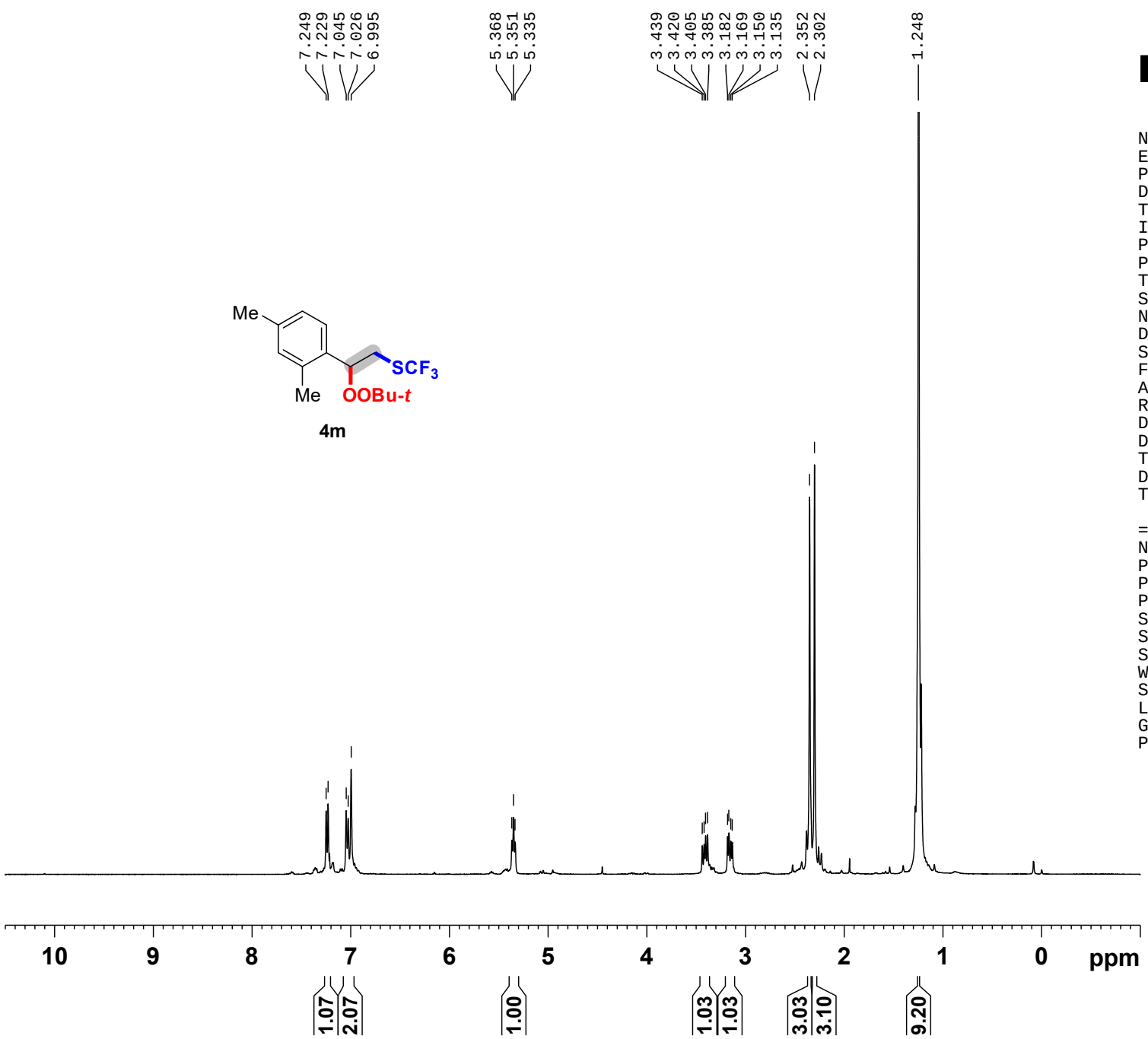
NAME	cyj856dp-20190328
EXPNO	2
PROCNO	1
Date_	20190328
Time	21.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	72
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	181
DW	19.800 usec
DE	6.50 usec
TE	293.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	13C
P1	15.00 usec
PL1	2.00 dB
PL1W	55.31277084 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	16.72 dB
PL13	15.50 dB
PL2W	17.01305389 W
PL12W	0.28759566 W
PL13W	0.38087484 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127739 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40




```
NAME      cyj856dp-20190328
EXPNO                    3
PROCNO                   1
Date_             20190328
Time                 21.09
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      32
DS                       4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                     812
DW                 5.600 usec
DE                 6.50 usec
TE                 292.7 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                      1

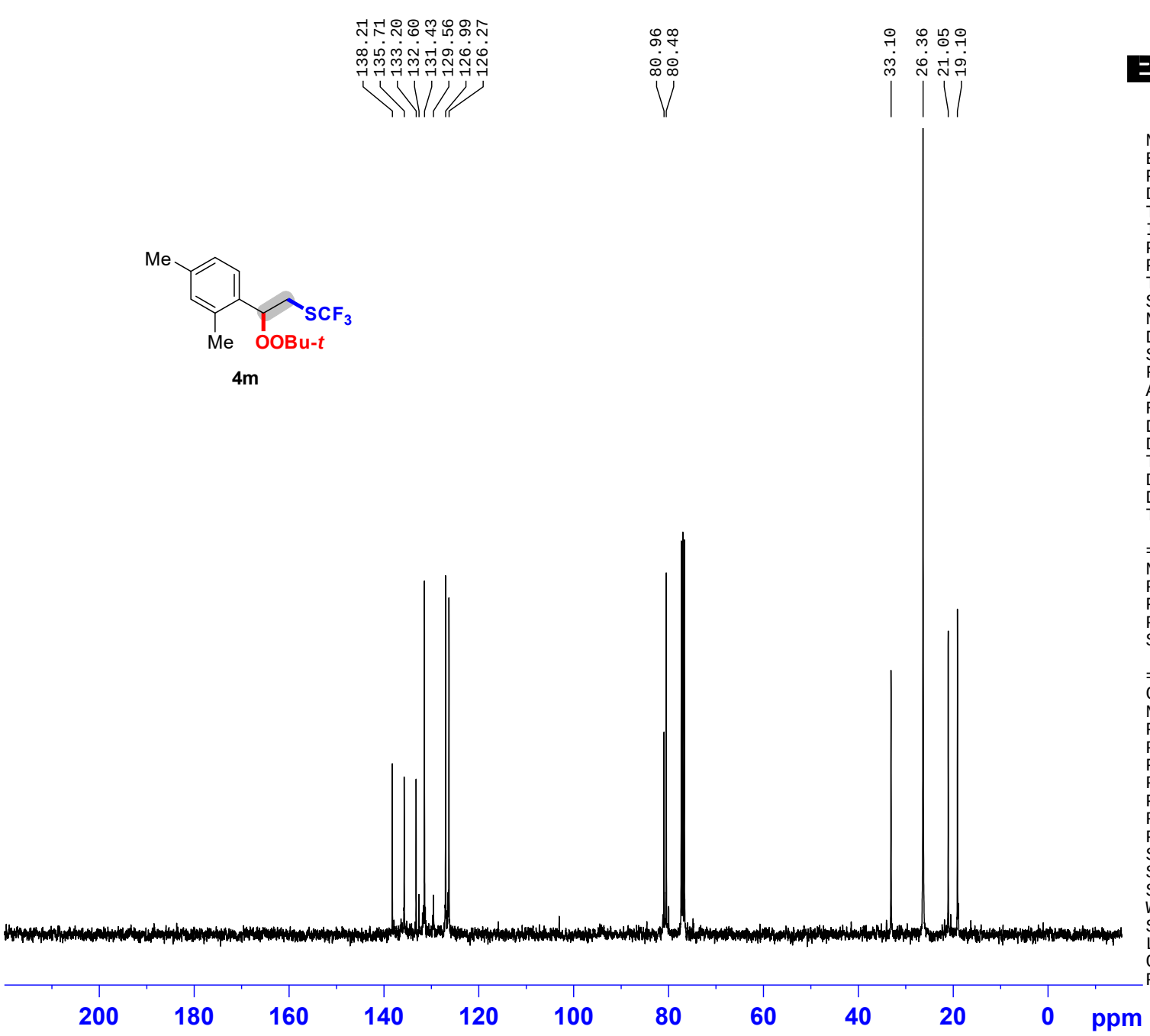
======== CHANNEL f1 ========
NUC1                   19F
P1                 14.20 usec
PL1                -2.00 dB
PL1W         20.42289734 W
SFO1         376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
SFO2         400.1316005 MHz
SI                 65536
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.00
```




```
NAME      cyj859ap-20190328
EXPNO                    1
PROCNO                   1
Date_             20190328
Time                 18.29
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                    45.2
DW                  78.200 usec
DE                   6.50 usec
TE                  292.3 K
D1             1.00000000 sec
TD0                      1

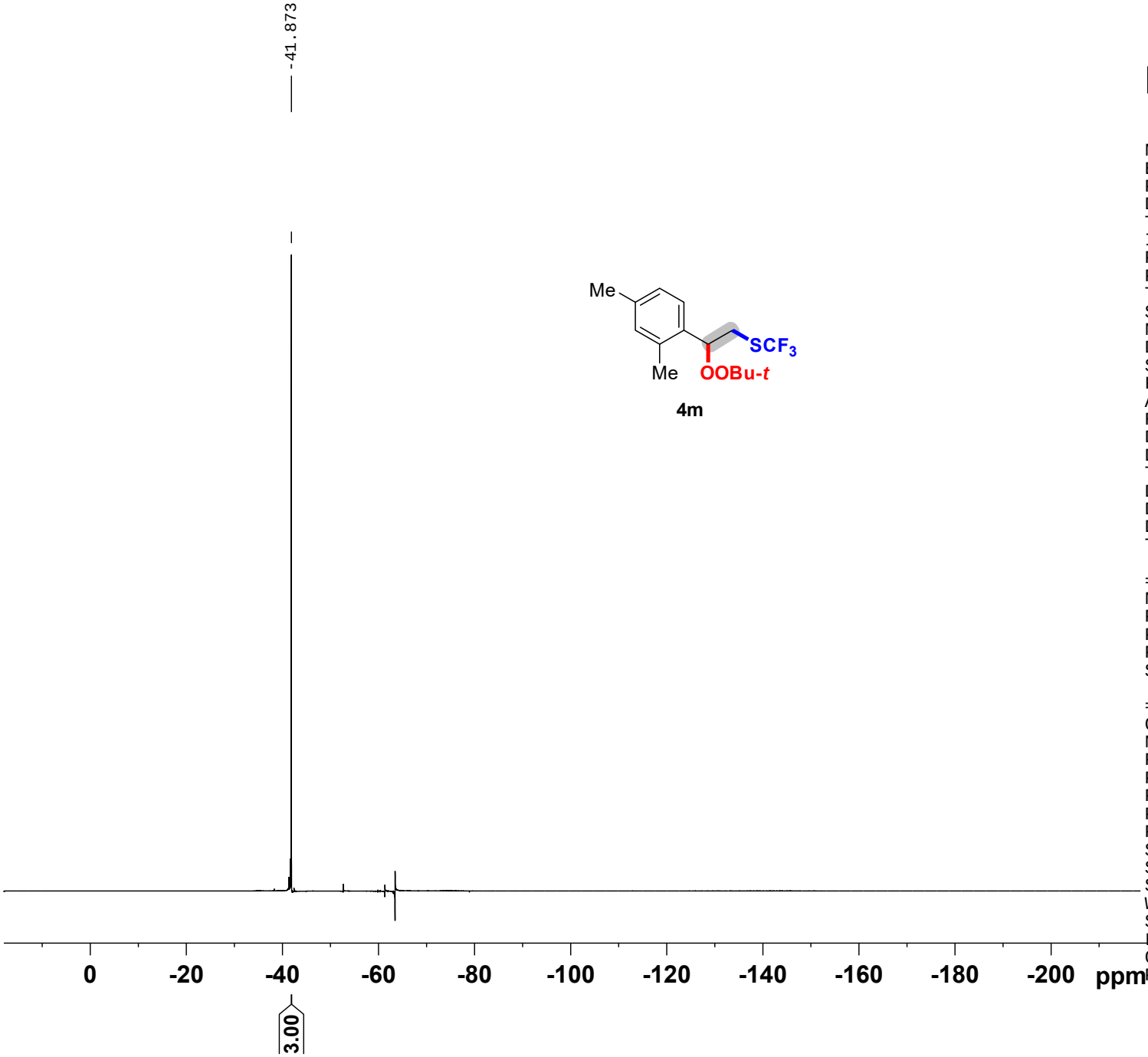
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300293 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                   1.00
```




```
NAME      cyj859ap-20190328
EXPNO                    2
PROCNO                   1
Date_             20190328
Time                 18.33
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       80
DS                        4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                      181
DW                   19.800 usec
DE                    6.50 usec
TE                   293.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       3

======== CHANNEL f1 ========
NUC1                    13C
P1                   15.00 usec
PL1                   2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

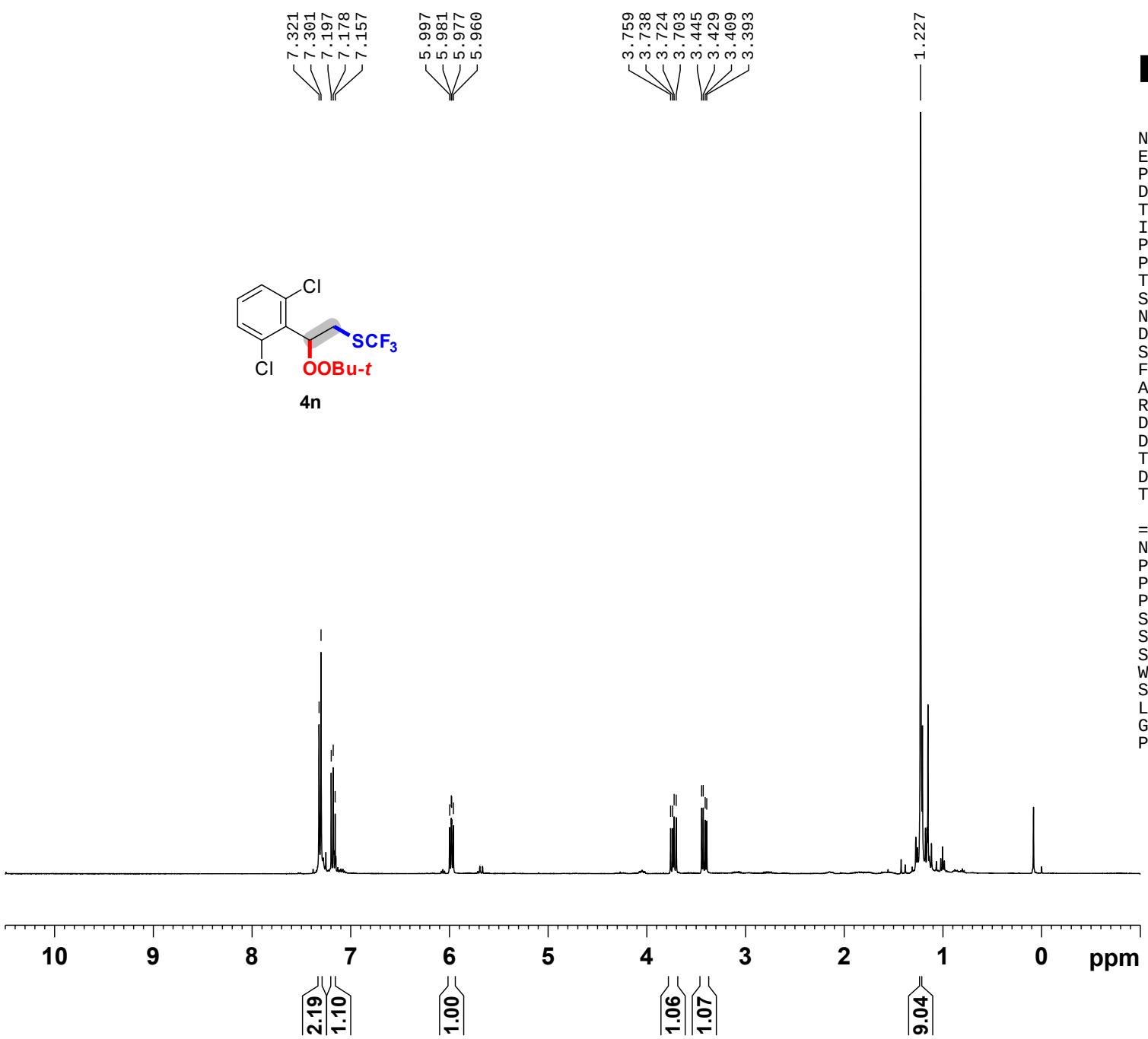
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                    32768
SF            100.6127753 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```




```
NAME      cyj859ap-20190328
EXPNO                    3
PROCNO                   1
Date_             20190328
Time                 18.41
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      32
DS                       4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                     812
DW                 5.600 usec
DE                 6.50 usec
TE                 292.8 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0                      1

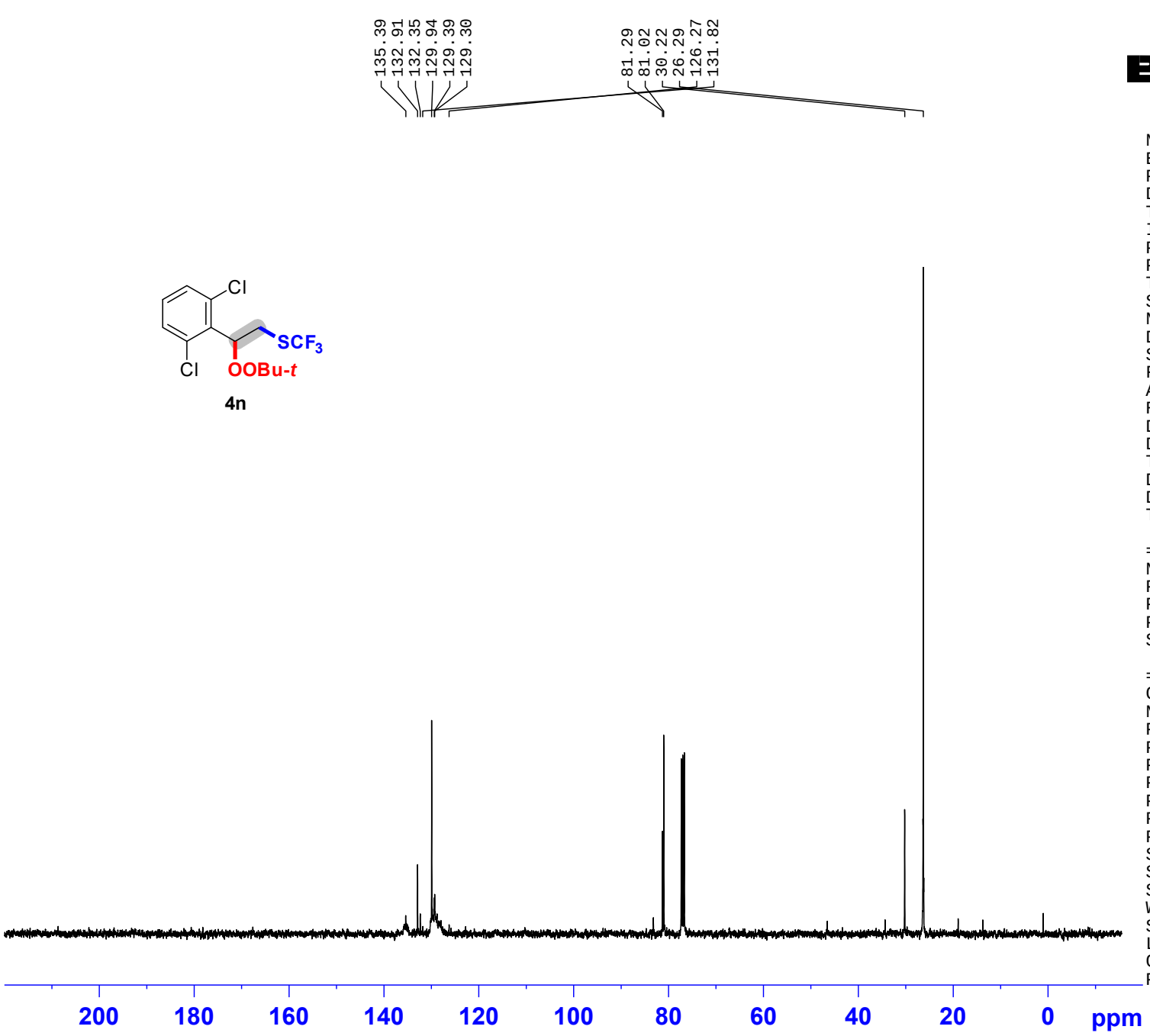
======== CHANNEL f1 ========
NUC1                    19F
P1                  14.20 usec
PL1                 -2.00 dB
PL1W         20.42289734 W
SFO1         376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
SFO2         400.1316005 MHz
SI                  65536
SF           376.4983660 MHz
WDW                    EM
SSB                     0
LB                  3.00 Hz
GB                      0
PC                  1.00
```




```
NAME      cyj845cp-20190328
EXPNO                    1
PROCNO                   1
Date_             20190328
Time                 19.53
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                      64
DW                  78.200 usec
DE                   6.50 usec
TE                  292.2 K
D1             1.00000000 sec
TD0                      1

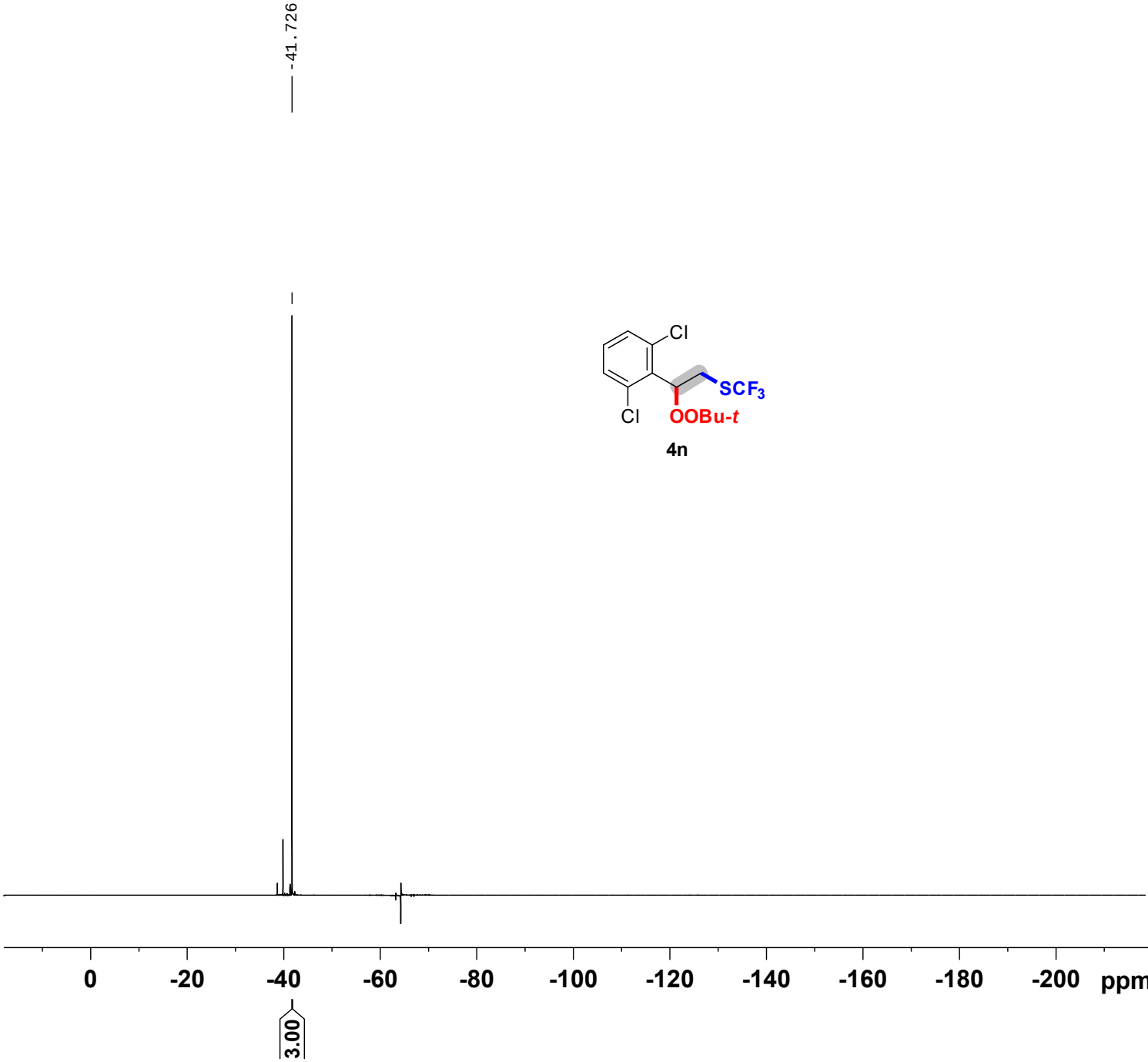
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300138 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                   1.00
```




```
NAME      cyj845cp-20190328
EXPNO                    2
PROCNO                   1
Date_             20190328
Time                19.57
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      40
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  293.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

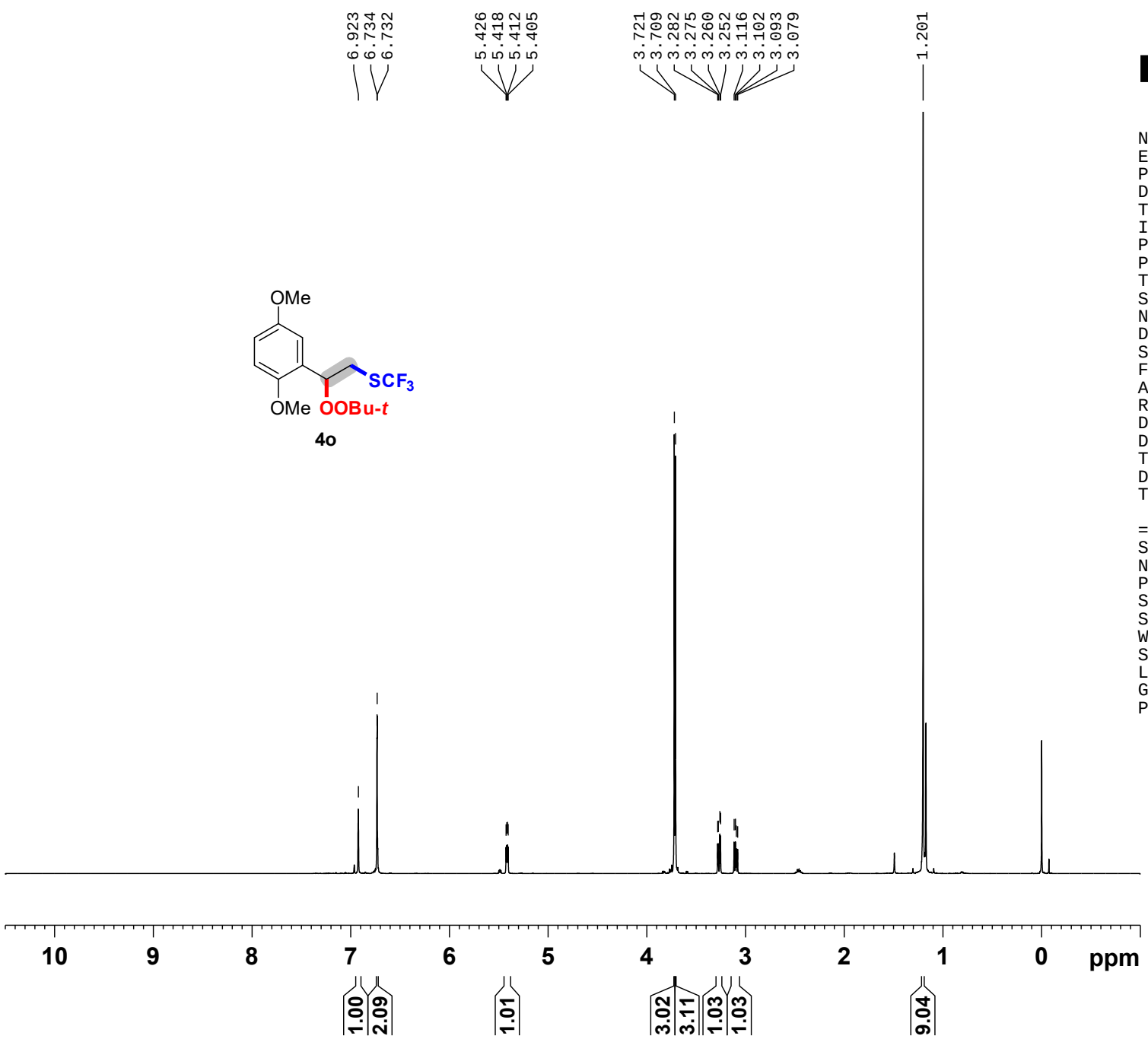
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127726 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyj845cp-20190328
EXPNO                     3
PROCNO                    1
Date_              20190328
Time                  20.20
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       32
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                      812
DW                    5.600 usec
DE                    6.50 usec
TE                   292.6 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       1

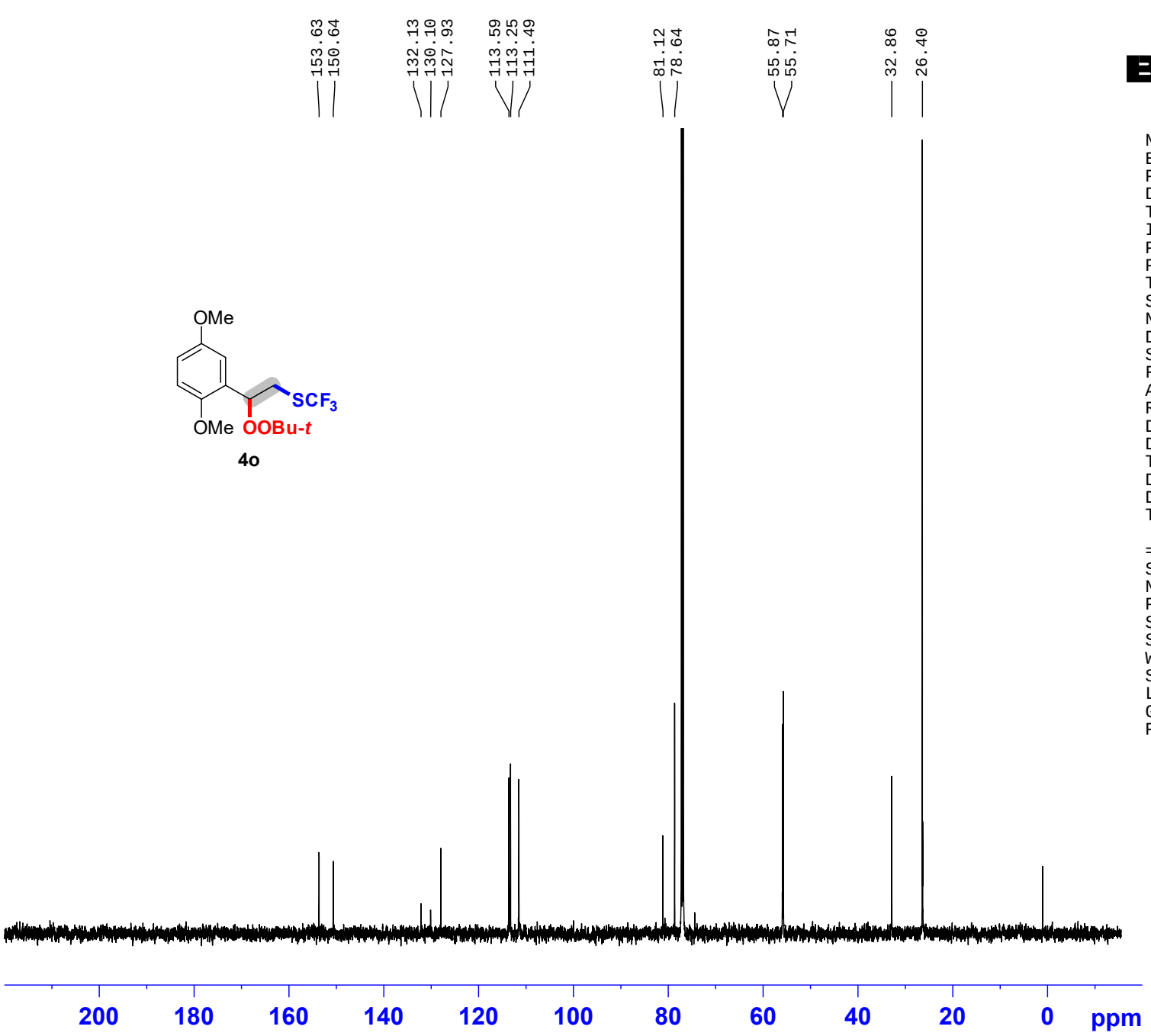
======== CHANNEL f1 ========
NUC1                     19F
P1                    14.20 usec
PL1                   -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                    65536
SF              376.4983660 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.00
```



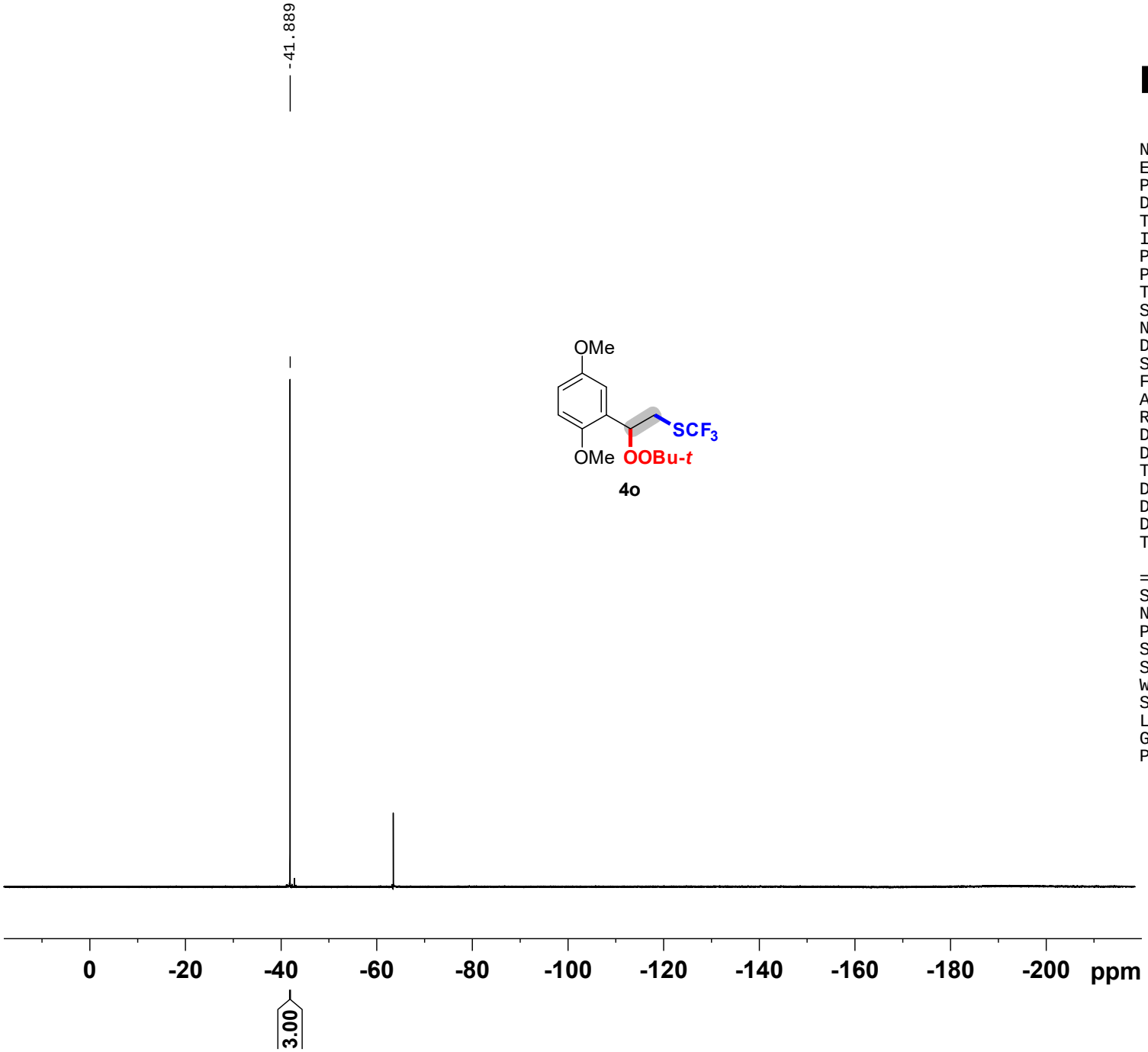

```
NAME                CYJ845dp
EXPNO                      1
PROCNO                     1
Date_               20190311
Time                   13.45
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                9615.385 Hz
FIDRES             0.146719 Hz
AQ                 3.4079220 sec
RG                    50.85
DW                   52.000 usec
DE                    6.50 usec
TE                   297.4 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            600.1739011 MHz
NUC1                    1H
P1                    9.77 usec
SI                    65536
SF              600.1700628 MHz
WDW                     EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



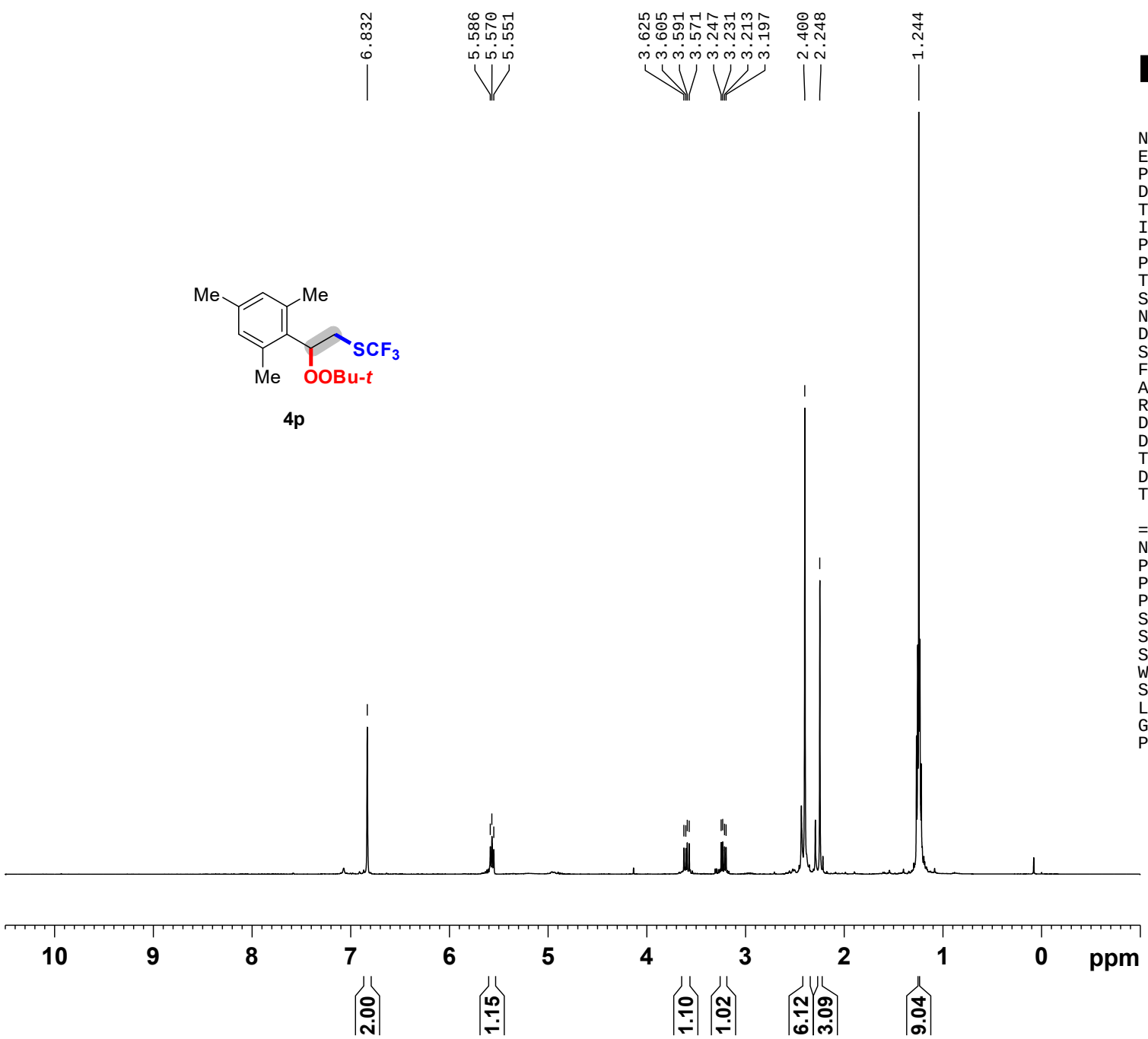

```
NAME              CYJ845dp
EXPNO                    2
PROCNO                   1
Date_             20190311
Time                 13.48
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     64
DS                      4
SWH              37878.789 Hz
FIDRES           0.577984 Hz
AQ               0.8651252 sec
RG                  190.02
DW                  13.200 usec
DE                   6.50 usec
TE                  297.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          150.9294669 MHz
NUC1                    13C
P1                  11.90 usec
SI                  32768
SF            150.9128697 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```



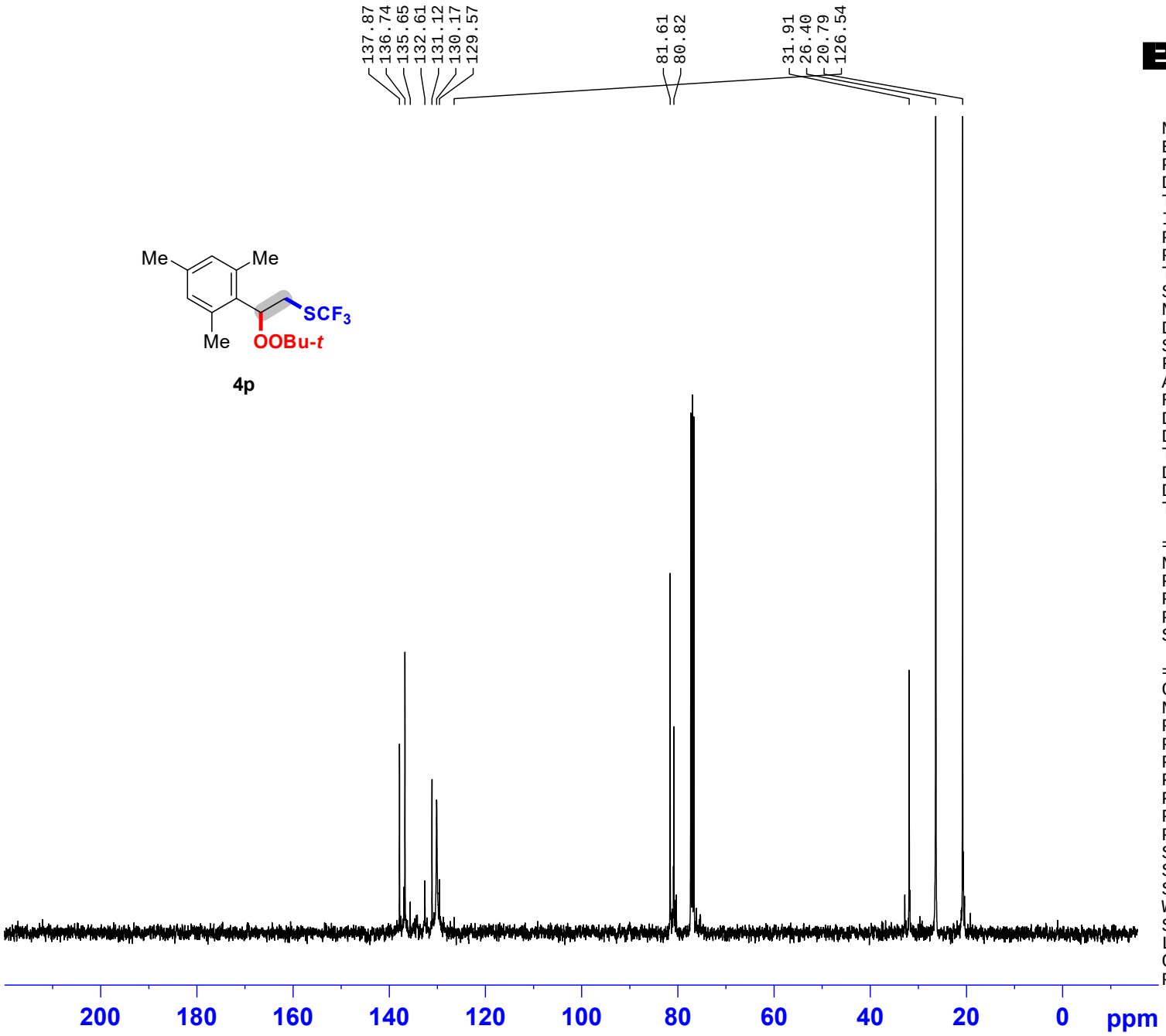

```
NAME              CYJ845dp
EXPNO                    3
PROCNO                   1
Date_             20190311
Time                 13.52
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG       zgfhigqn.2
TD                  131072
SOLVENT               CDCl3
NS                       40
DS                        4
SWH              133928.578 Hz
FIDRES             1.021794 Hz
AQ                 0.4893855 sec
RG                     15.49
DW                     3.733 usec
DE                      6.50 usec
TE                     297.5 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             564.6675534 MHz
NUC1                     19F
P1                     11.90 usec
SI                     65536
SF               564.7240258 MHz
WDW                       EM
SSB                        0
LB                      3.00 Hz
GB                         0
PC                      1.00
```




```
NAME      cyj-855ap-20190326
EXPNO                      1
PROCNO                     1
Date_               20190326
Time                   10.19
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6393.862 Hz
FIDRES              0.195125 Hz
AQ                  2.5625076 sec
RG                      50.8
DW                     78.200 usec
DE                      6.50 usec
TE                     292.7 K
D1                 1.00000000 sec
TD0                        1

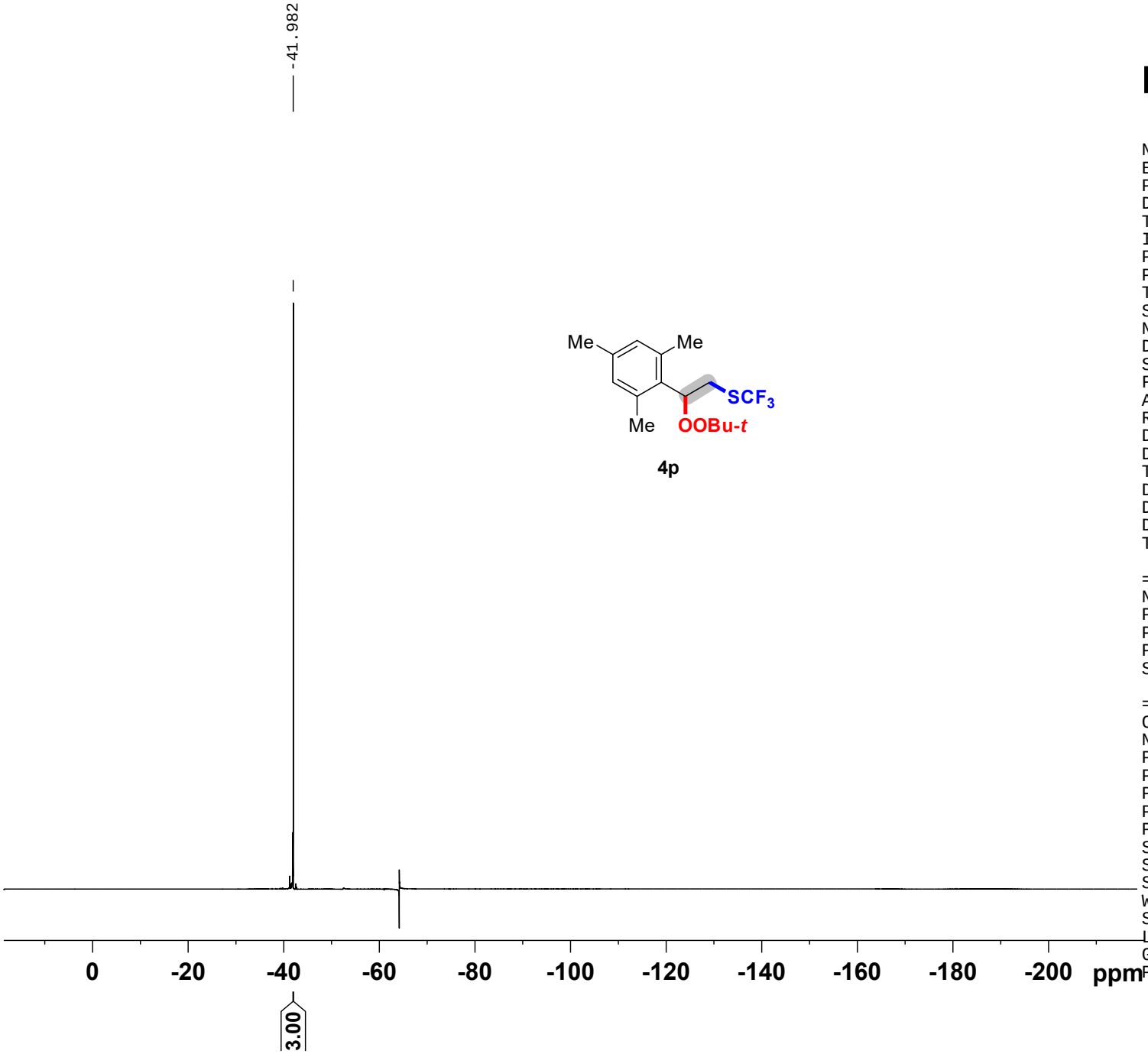
======== CHANNEL f1 ========
NUC1                      1H
P1                     10.40 usec
PL1                    -1.00 dB
PL1W            17.01305389 W
SFO1            400.1326008 MHz
SI                     32768
SF              400.1300262 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```




```
NAME      cyj-855ap-20190326
EXPNO                      2
PROCNO                     1
Date_               20190326
Time                   10.26
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         96
DS                          4
SWH                 25252.525 Hz
FIDRES                0.385323 Hz
AQ                    1.2976629 sec
RG                        181
DW                       19.800 usec
DE                        6.50 usec
TE                       294.4 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         3

======== CHANNEL f1 ========
NUC1                      13C
P1                       15.00 usec
PL1                       2.00 dB
PL1W               55.31277084 W
SFO1               100.6238364 MHz

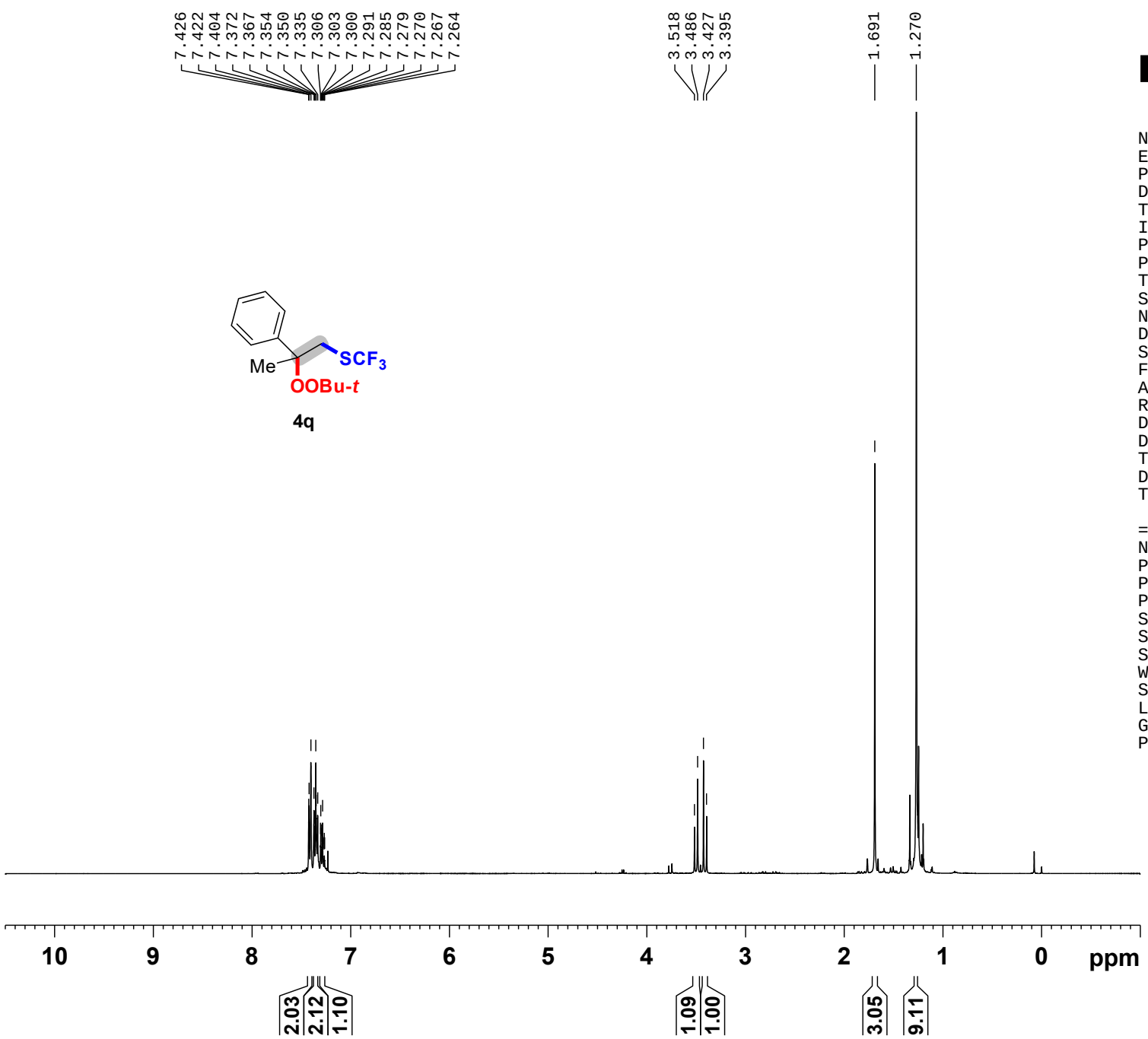
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                      -1.00 dB
PL12                     16.72 dB
PL13                     15.50 dB
PL2W               17.01305389 W
PL12W               0.28759566 W
PL13W               0.38087484 W
SFO2               400.1316005 MHz
SI                        32768
SF                 100.6127742 MHz
WDW                          EM
SSB                           0
LB                        3.00 Hz
GB                            0
PC                        1.40
```




```
NAME      cyj-855ap-20190326
EXPNO                      3
PROCNO                     1
Date_               20190326
Time                   10.31
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES             0.681196 Hz
AQ                 0.7340532 sec
RG                       812
DW                     5.600 usec
DE                     6.50 usec
TE                     293.4 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

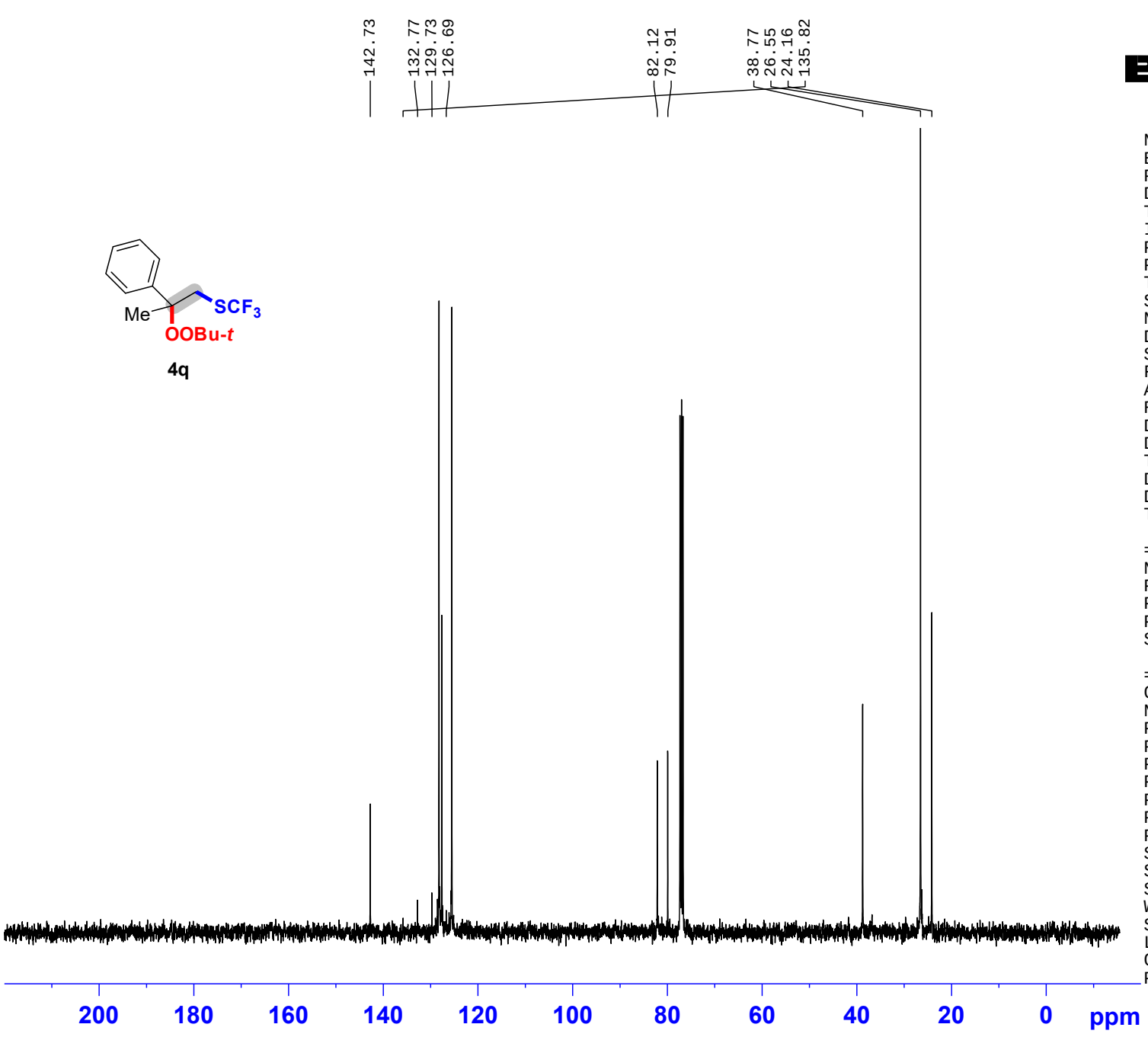
======== CHANNEL f1 ========
NUC1                      19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                     65536
SF              376.4983660 MHz
WDW                       EM
SSB                        0
LB                      3.00 Hz
GB                         0
PC                      1.00
```




```
NAME      cyj862bp-20190411
EXPNO                    1
PROCNO                   1
Date_             20190411
Time                 8.17
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6393.862 Hz
FIDRES           0.195125 Hz
AQ             2.5625076 sec
RG                     57
DW                78.200 usec
DE                 6.50 usec
TE                292.9 K
D1           1.00000000 sec
TD0                     1

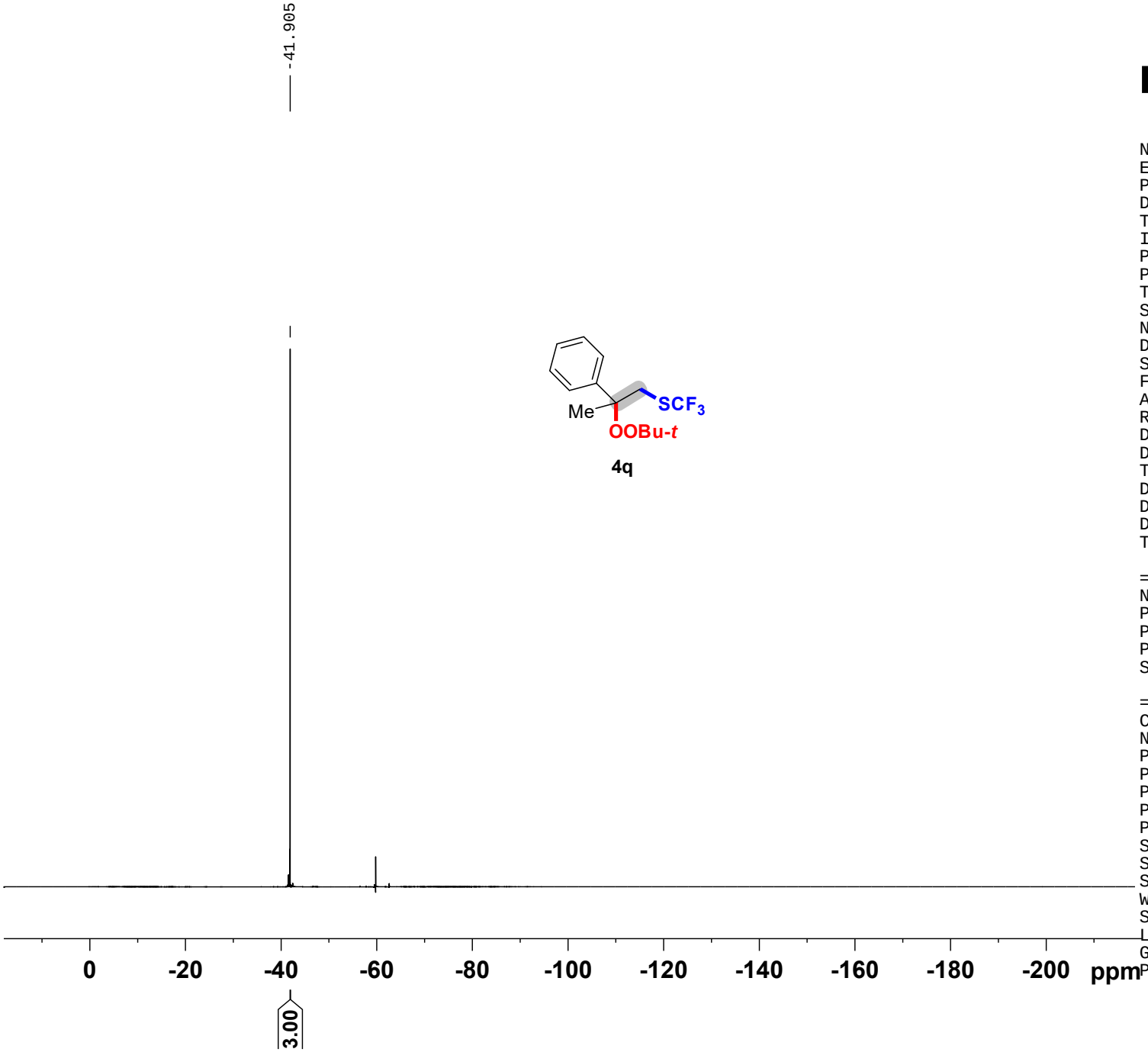
======== CHANNEL f1 ========
NUC1                   1H
P1                 10.40 usec
PL1                -1.00 dB
PL1W        17.01305389 W
SFO1        400.1326008 MHz
SI                  32768
SF          400.1300218 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```




```
NAME      cyj862bp-20190410
EXPNO                    2
PROCNO                   1
Date_             20190411
Time                 8.22
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      64
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  294.4 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

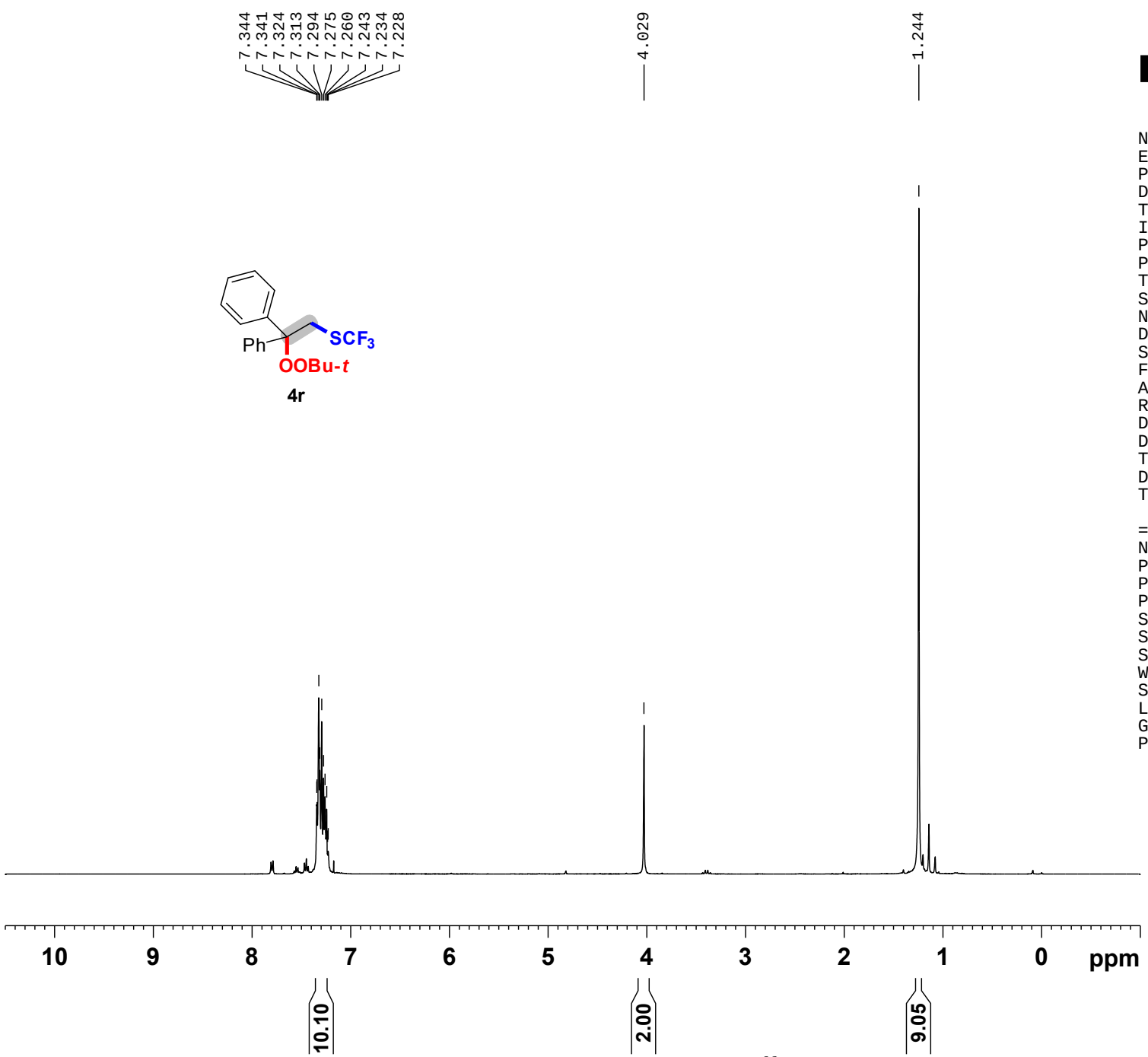
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127727 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyj862bp-20190411
EXPNO                    3
PROCNO                   1
Date_             20190411
Time                 8.27
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     64
DS                      4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                    2050
DW                   5.600 usec
DE                   6.50 usec
TE                  293.5 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                     4

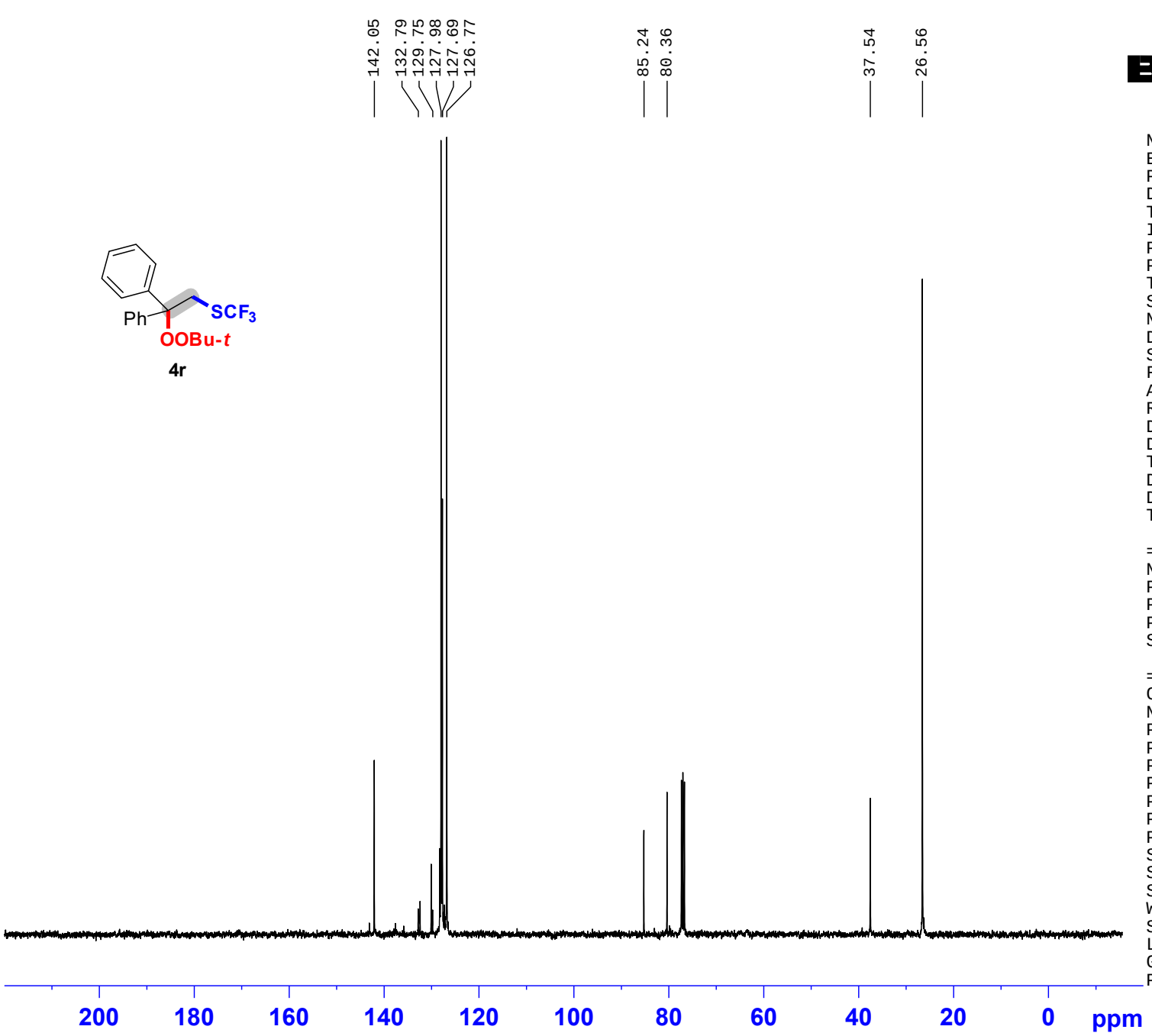
======== CHANNEL f1 ========
NUC1                   19F
P1                   14.20 usec
PL1                  -2.00 dB
PL1W          20.42289734 W
SFO1          376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
SFO2          400.1316005 MHz
SI                  65536
SF            376.4983660 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cyj862cp-20190410
EXPNO                    1
PROCNO                   1
Date_             20190410
Time                 23.31
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ              2.5625076 sec
RG                    45.2
DW                  78.200 usec
DE                   6.50 usec
TE                  293.5 K
D1             1.00000000 sec
TD0                      1

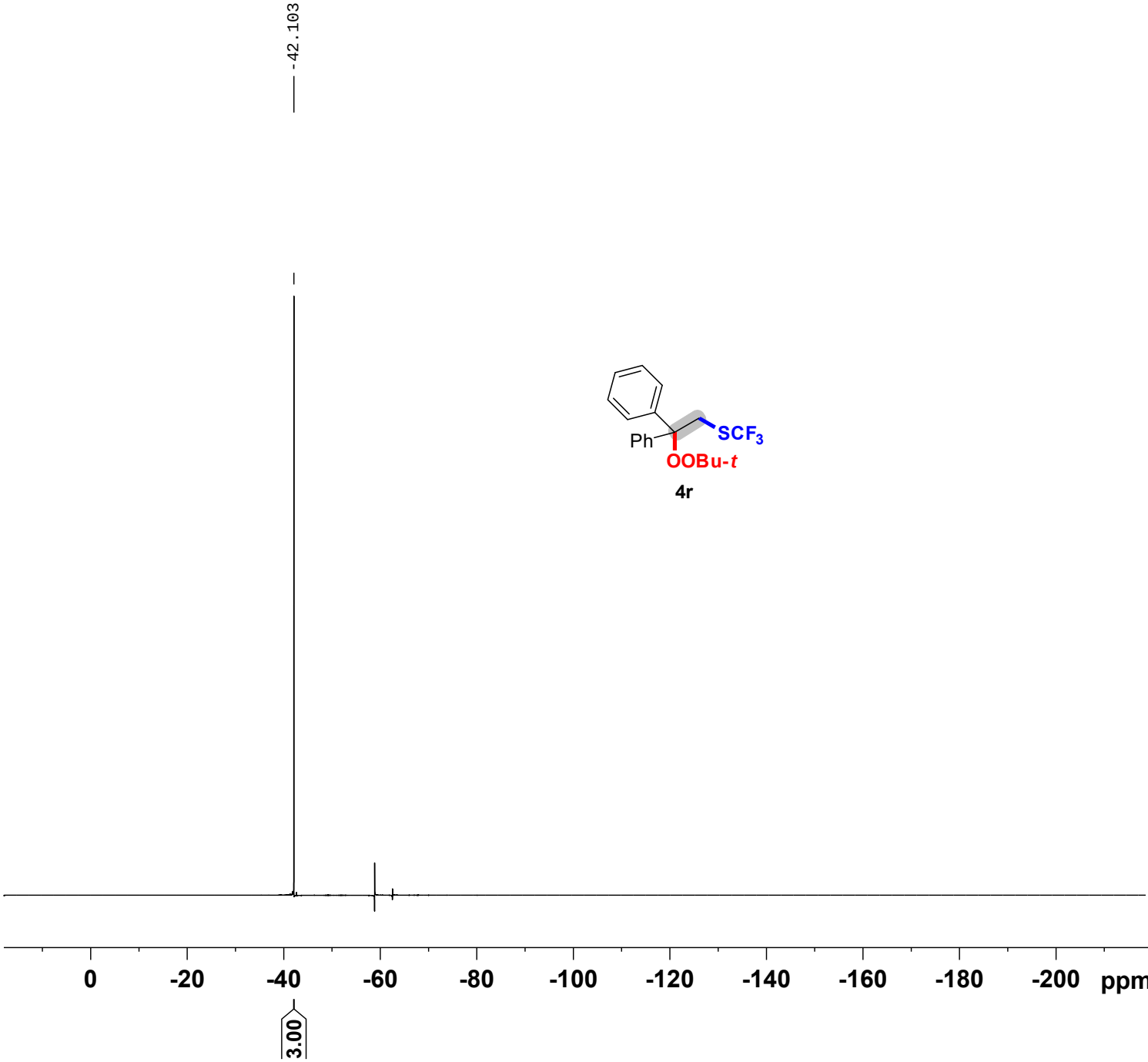
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                   32768
SF           400.1300453 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cyj862cp-20190410
EXPNO                    2
PROCNO                   1
Date_             20190410
Time                 23.36
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      56
DS                       4
SWH              25252.525 Hz
FIDRES            0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  294.5 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

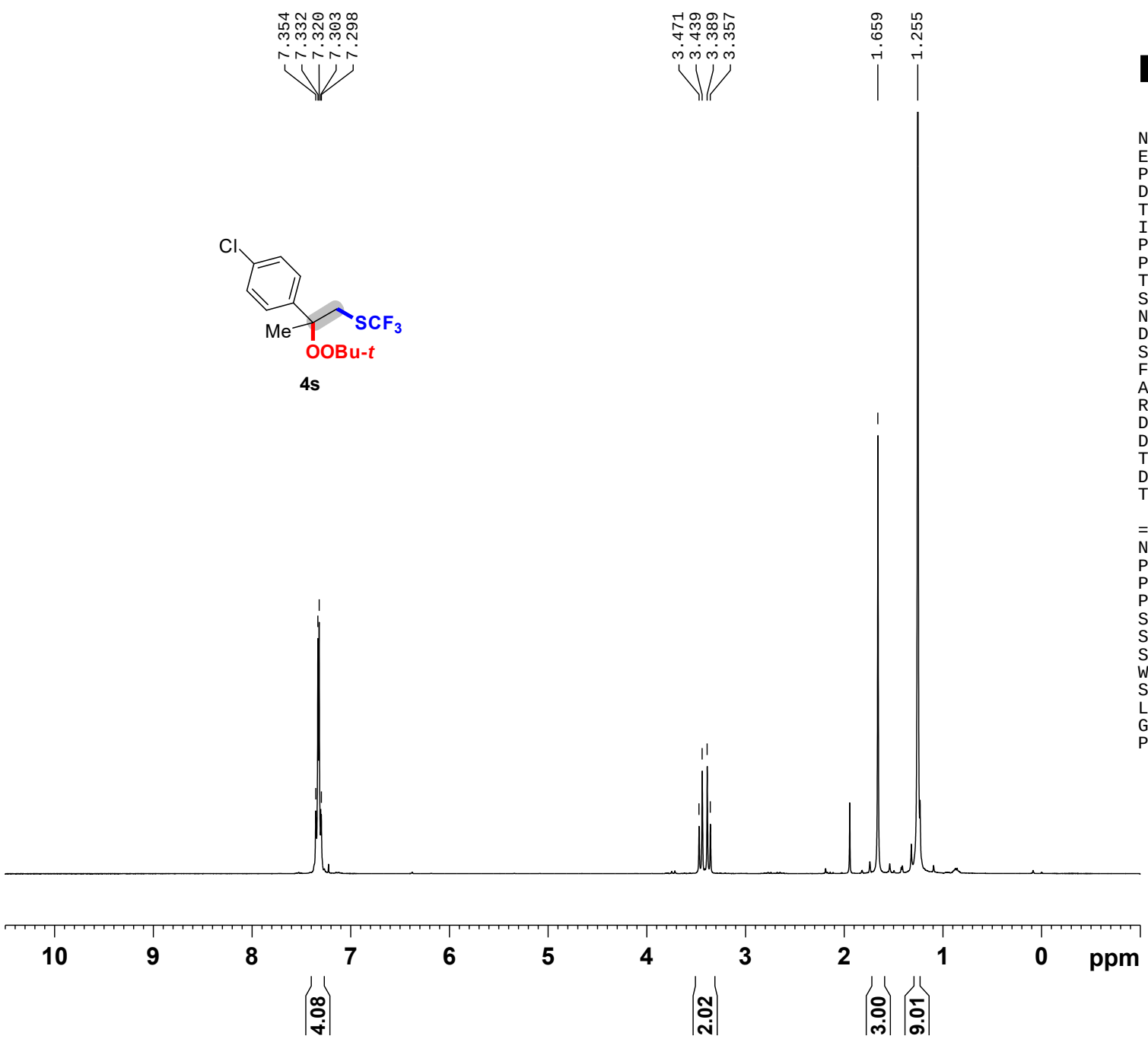
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127789 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyj862cp-20190410
EXPNO                    3
PROCNO                   1
Date_             20190410
Time                 23.42
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      64
DS                       4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                     645
DW                   5.600 usec
DE                   6.50 usec
TE                  293.8 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                      4

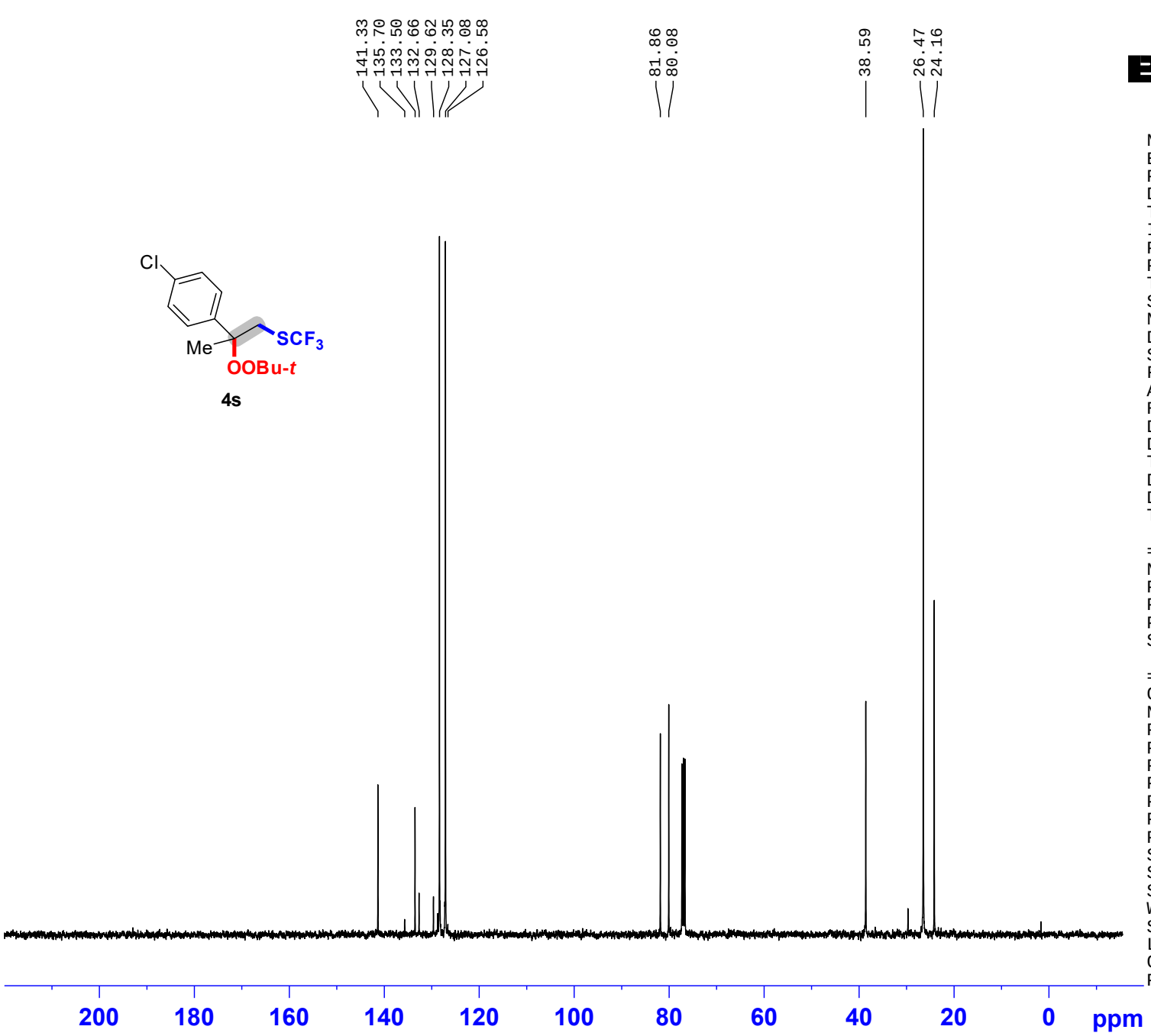
======== CHANNEL f1 ========
NUC1                   19F
P1                   14.20 usec
PL1                  -2.00 dB
PL1W          20.42289734 W
SFO1          376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
SFO2          400.1316005 MHz
SI                   65536
SF            376.4983660 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cms12p-20190725
EXPNO                   1
PROCNO                  1
Date_            20040408
Time                8.21
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             6393.862 Hz
FIDRES          0.195125 Hz
AQ             2.5625076 sec
RG                  28.5
DW                78.200 usec
DE                 6.50 usec
TE                296.4 K
D1           1.00000000 sec
TD0                    1

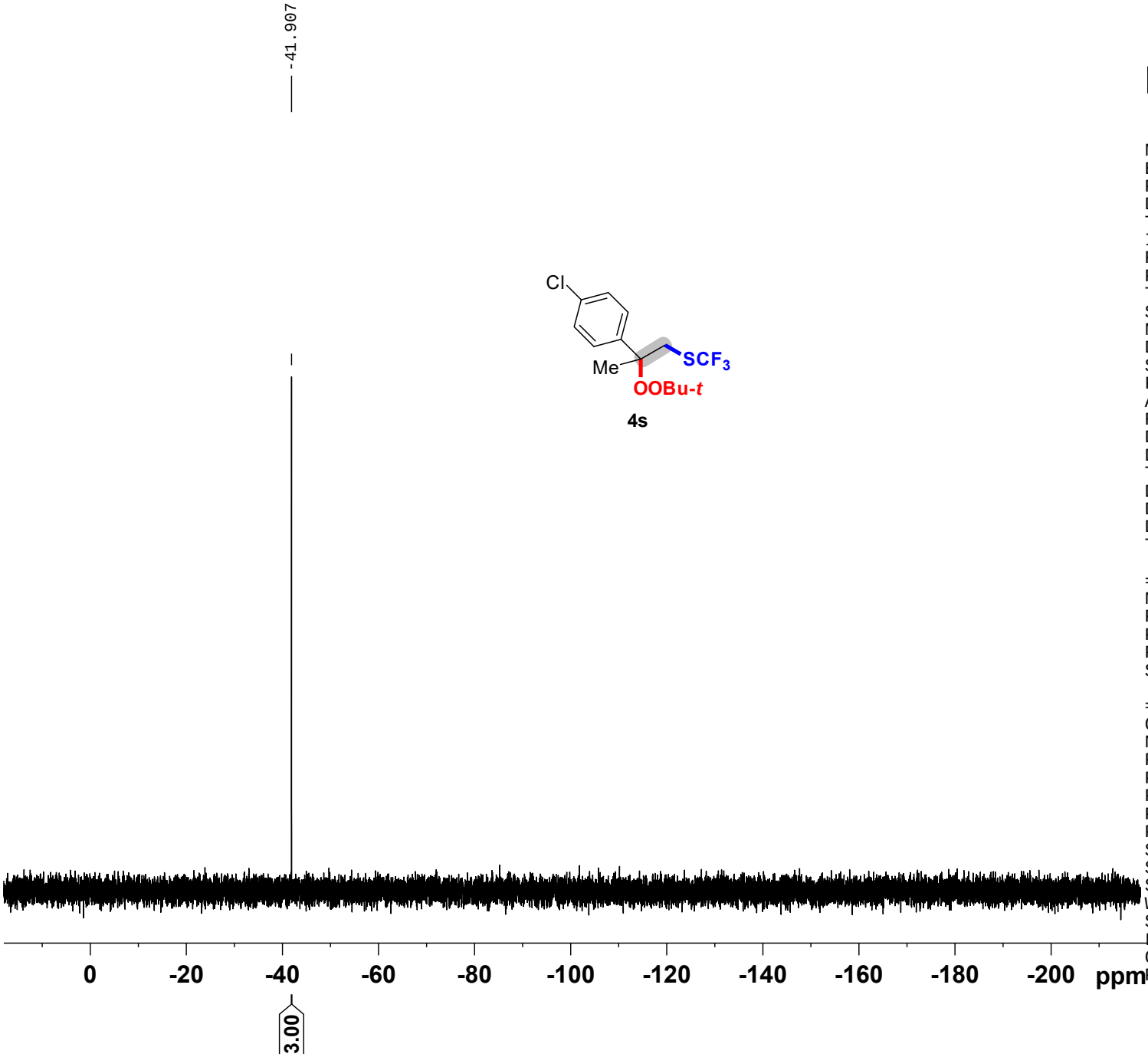
======== CHANNEL f1 ========
NUC1                   1H
P1                 10.40 usec
PL1                -1.00 dB
PL1W        17.01305389 W
SFO1        400.1326008 MHz
SI                 32768
SF          400.1300255 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```




```
NAME      cms12p-20190725
EXPNO                   2
PROCNO                  1
Date_            20040408
Time                 8.28
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    64
DS                     4
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976629 sec
RG                  2050
DW                19.800 usec
DE                 6.50 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    3

======== CHANNEL f1 ========
NUC1                  13C
P1                 15.00 usec
PL1                 2.00 dB
PL1W         55.31277084 W
SFO1         100.6238364 MHz

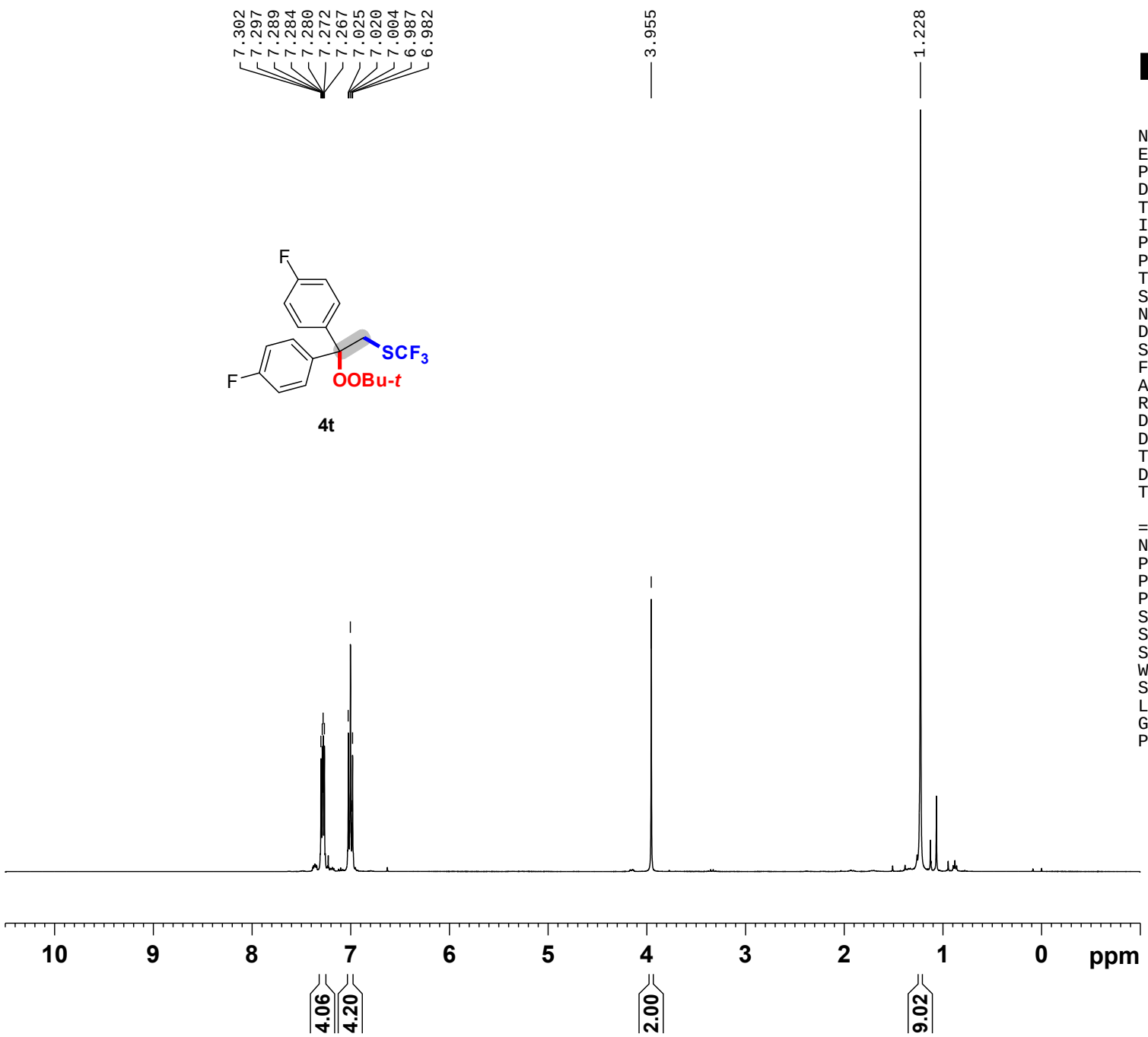
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL13               15.50 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
PL13W         0.38087484 W
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127723 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.40
```




```
NAME      cms12p-20190725
EXPNO                   3
PROCNO                  1
Date_            20040408
Time                 8.35
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     32
DS                      4
SWH             89285.711 Hz
FIDRES          0.681196 Hz
AQ              0.7340532 sec
RG                    812
DW                5.600 usec
DE                6.50 usec
TE                297.0 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                     1

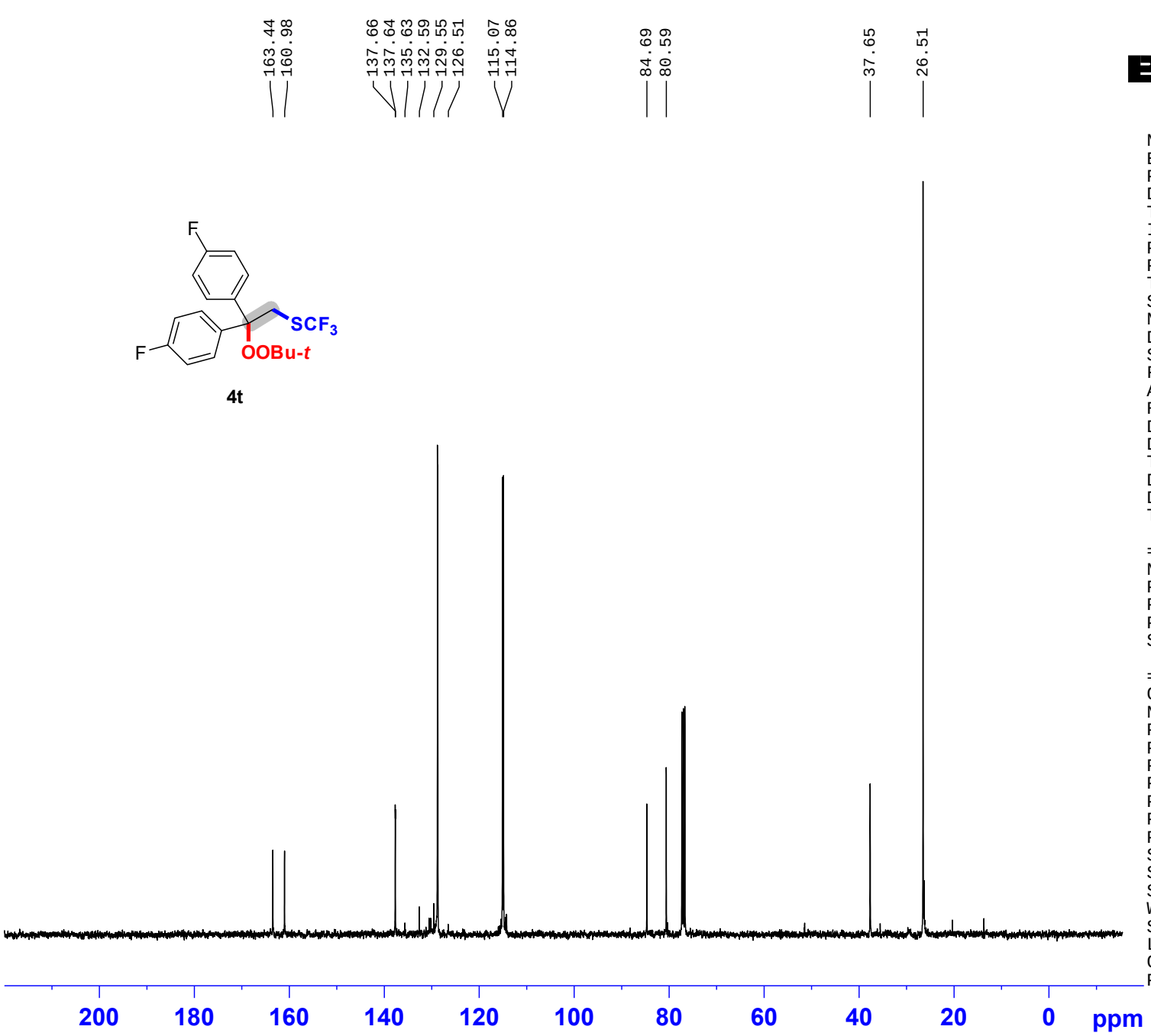
======== CHANNEL f1 ========
NUC1                   19F
P1                 14.20 usec
PL1                -2.00 dB
PL1W         20.42289734 W
SFO1         376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
SFO2         400.1316005 MHz
SI                 65536
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.00
```




```
NAME      cyj876bp-20190410
EXPNO                    1
PROCNO                   1
Date_             20190410
Time                 20.31
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                      57
DW                  78.200 usec
DE                   6.50 usec
TE                  293.4 K
D1              1.00000000 sec
TD0                      1

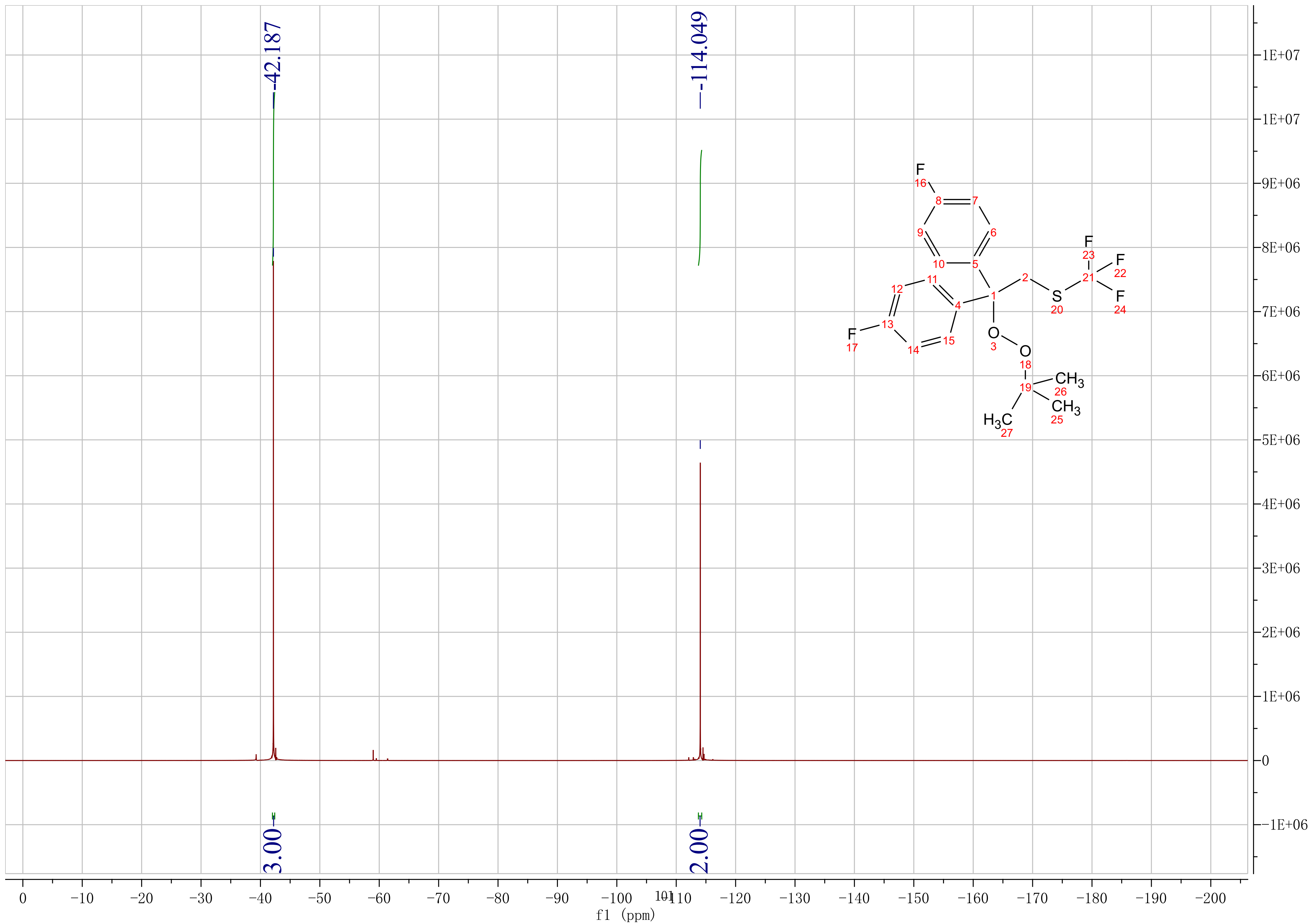
======== CHANNEL f1 ========
NUC1                    1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                   32768
SF           400.1300229 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                  1.00
```

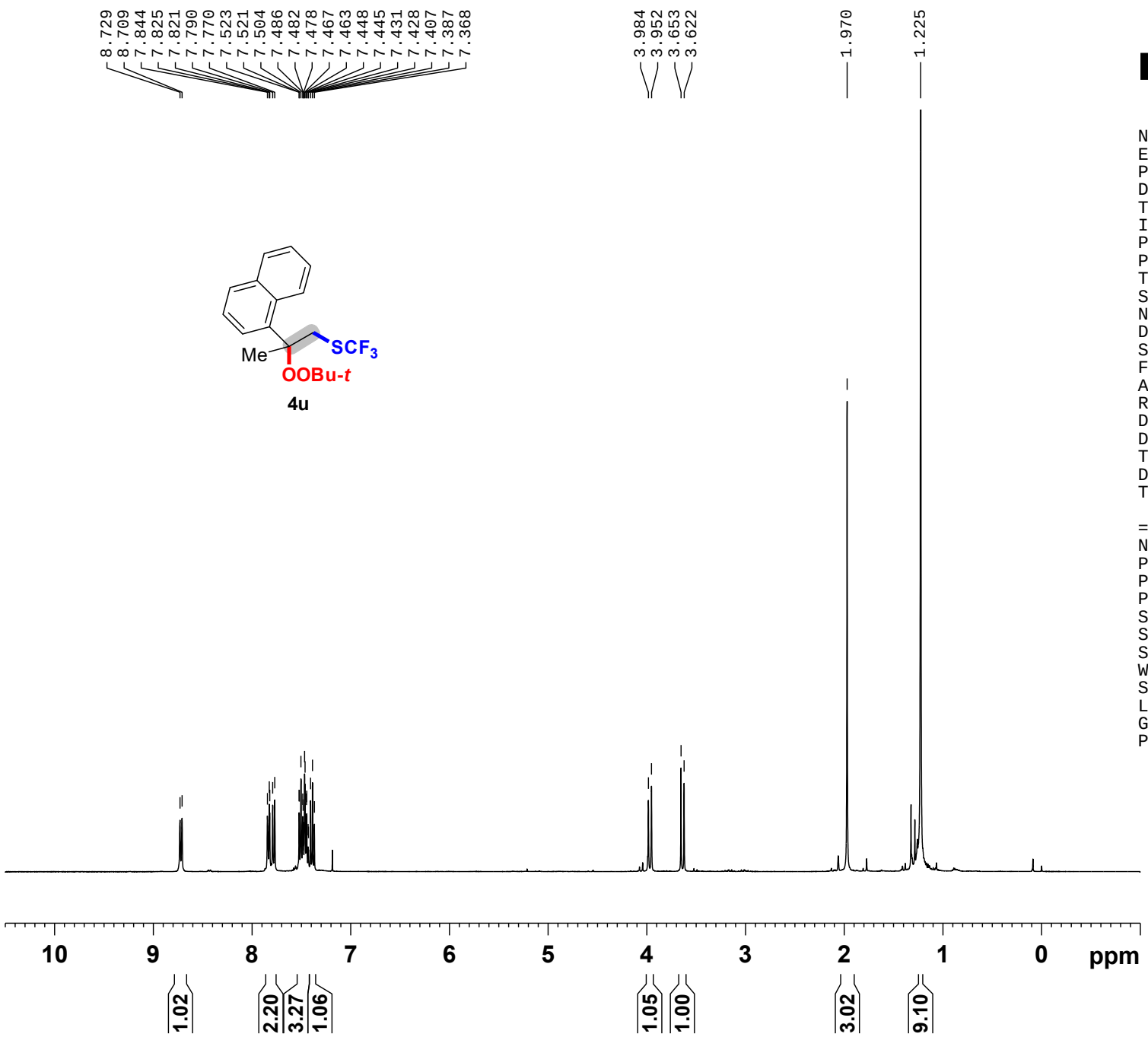



```
NAME      cyj876bp-20190410
EXPNO                    2
PROCNO                   1
Date_             20190410
Time                 20.39
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      88
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  295.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

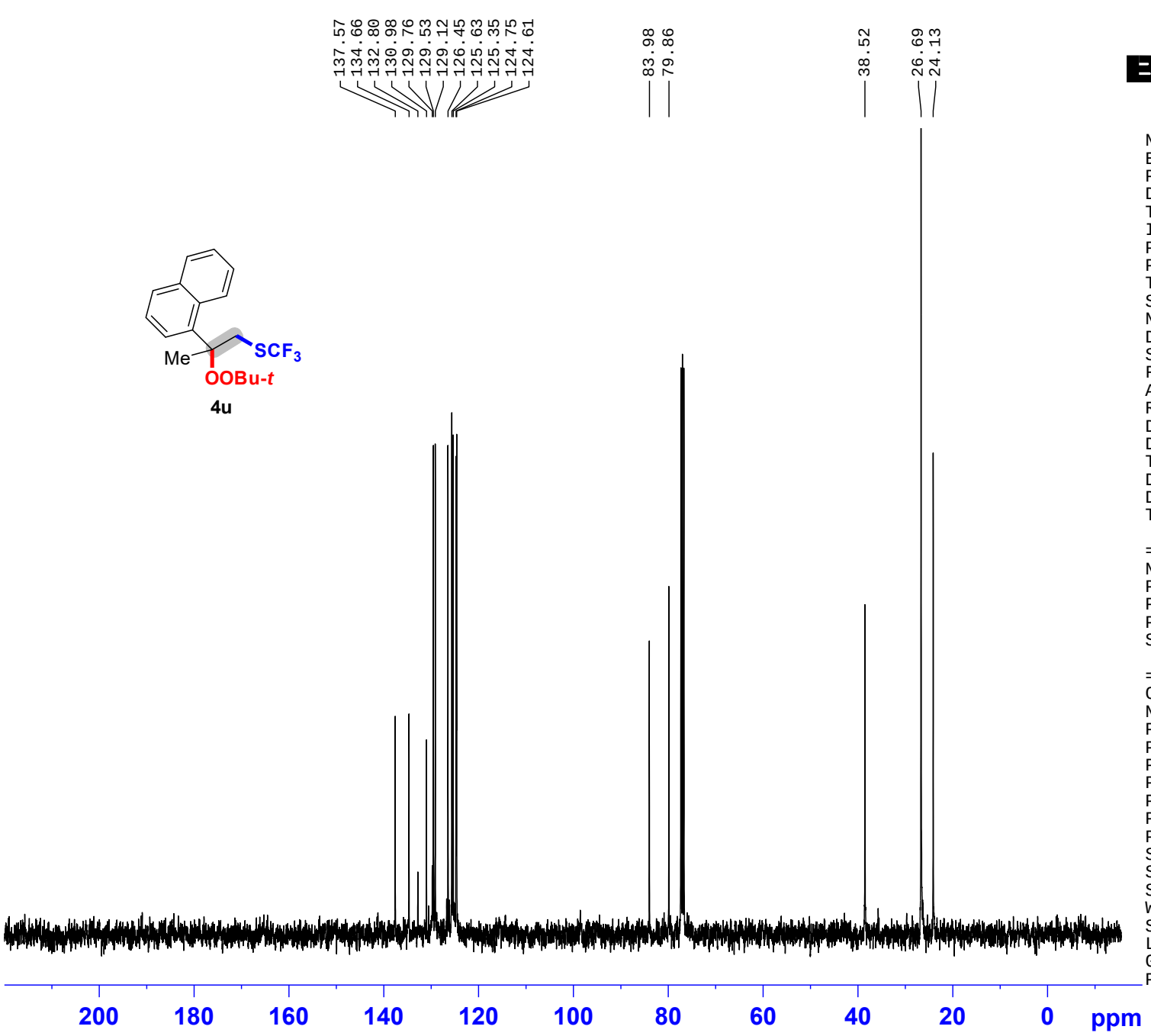
======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127714 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```


-42.187
-114.049
3.00
2.00
f1 (ppm)
F
16
8
7
9
6
10
5
F
23
F
22
21
2
11
12
1
S
20
F
24
4
F
17
13
O
3
15
14
O
18
CH_3
26
19
CH_3
25
H_3C
27

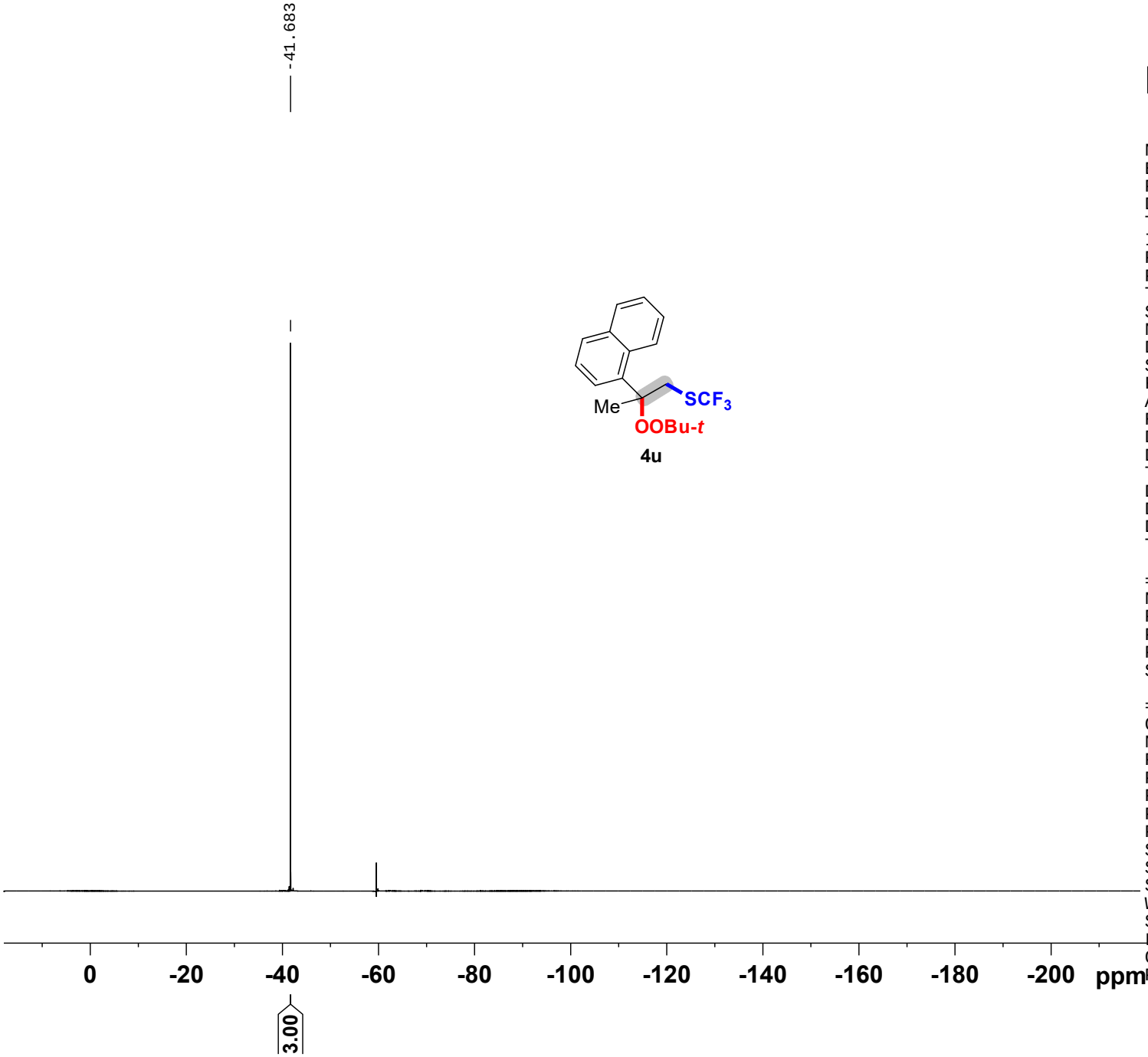


NAME	cyj876ap-20190410
EXPNO	1
PROCNO	1
Date_	20190410
Time	20.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	57
DW	78.200 usec
DE	6.50 usec
TE	293.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

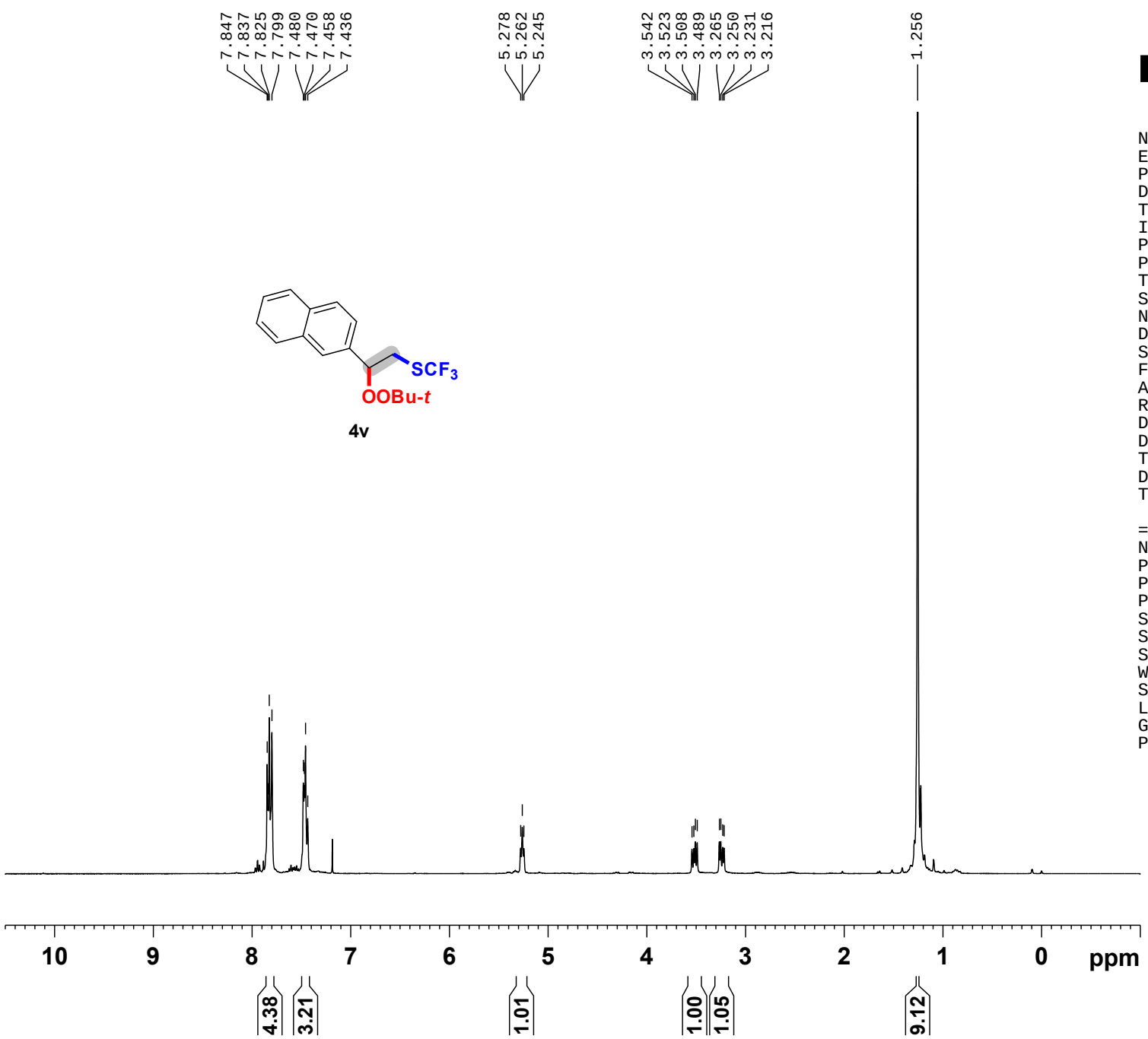
NAME	cyj876ap-20190410
EXPNO	2
PROCNO	1
Date_	20190410
Time	20.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	181
DW	19.800 usec
DE	6.50 usec
TE	294.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	13C
P1	15.00 usec
PL1	2.00 dB
PL1W	55.31277084 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	16.72 dB
PL13	15.50 dB
PL2W	17.01305389 W
PL12W	0.28759566 W
PL13W	0.38087484 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127766 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40




```
NAME      cyj876ap-20190410
EXPNO                    3
PROCNO                   1
Date_             20190410
Time                 21.01
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       64
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                     2050
DW                    5.600 usec
DE                    6.50 usec
TE                   293.8 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       4

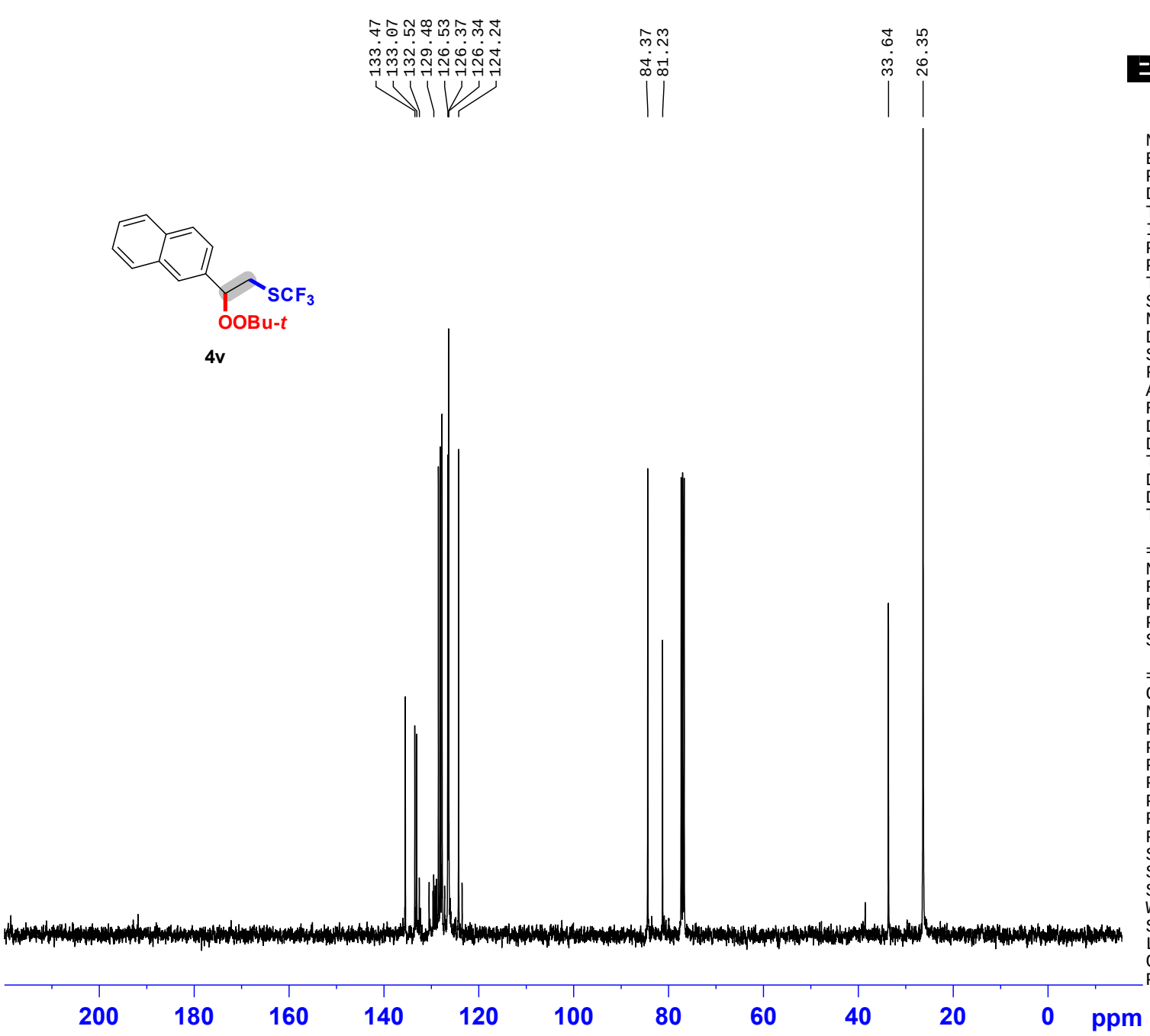
======== CHANNEL f1 ========
NUC1                    19F
P1                    14.20 usec
PL1                   -2.00 dB
PL1W           20.42289734 W
SFO1           376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   -1.00 dB
PL12                  16.72 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
SFO2           400.1316005 MHz
SI                   65536
SF             376.4983660 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



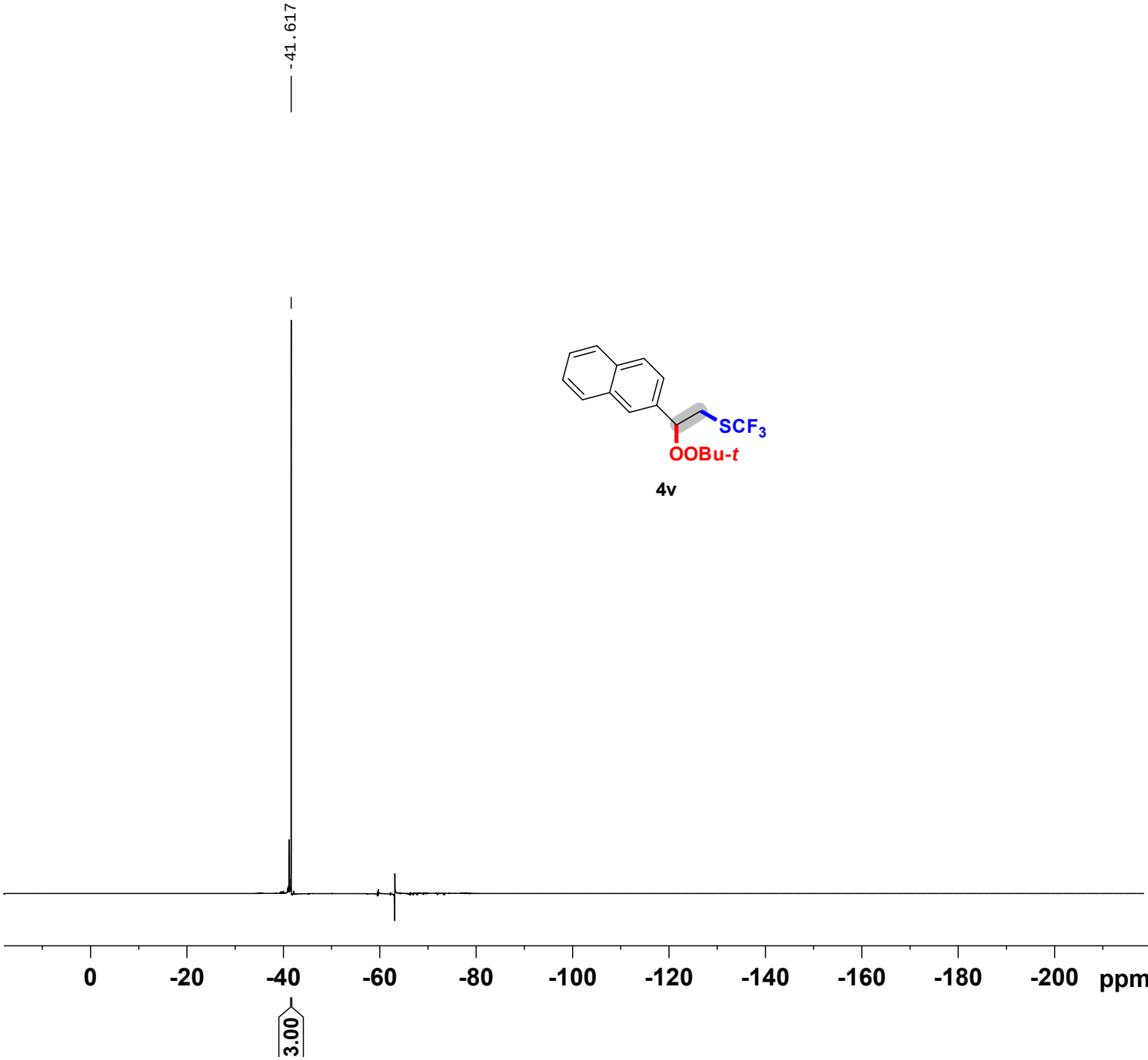
BRUKER

NAME	cyj859bp-20190328
EXPNO	1
PROCNO	1
Date_	20190328
Time	18.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	50.8
DW	78.200 usec
DE	6.50 usec
TE	292.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300398 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

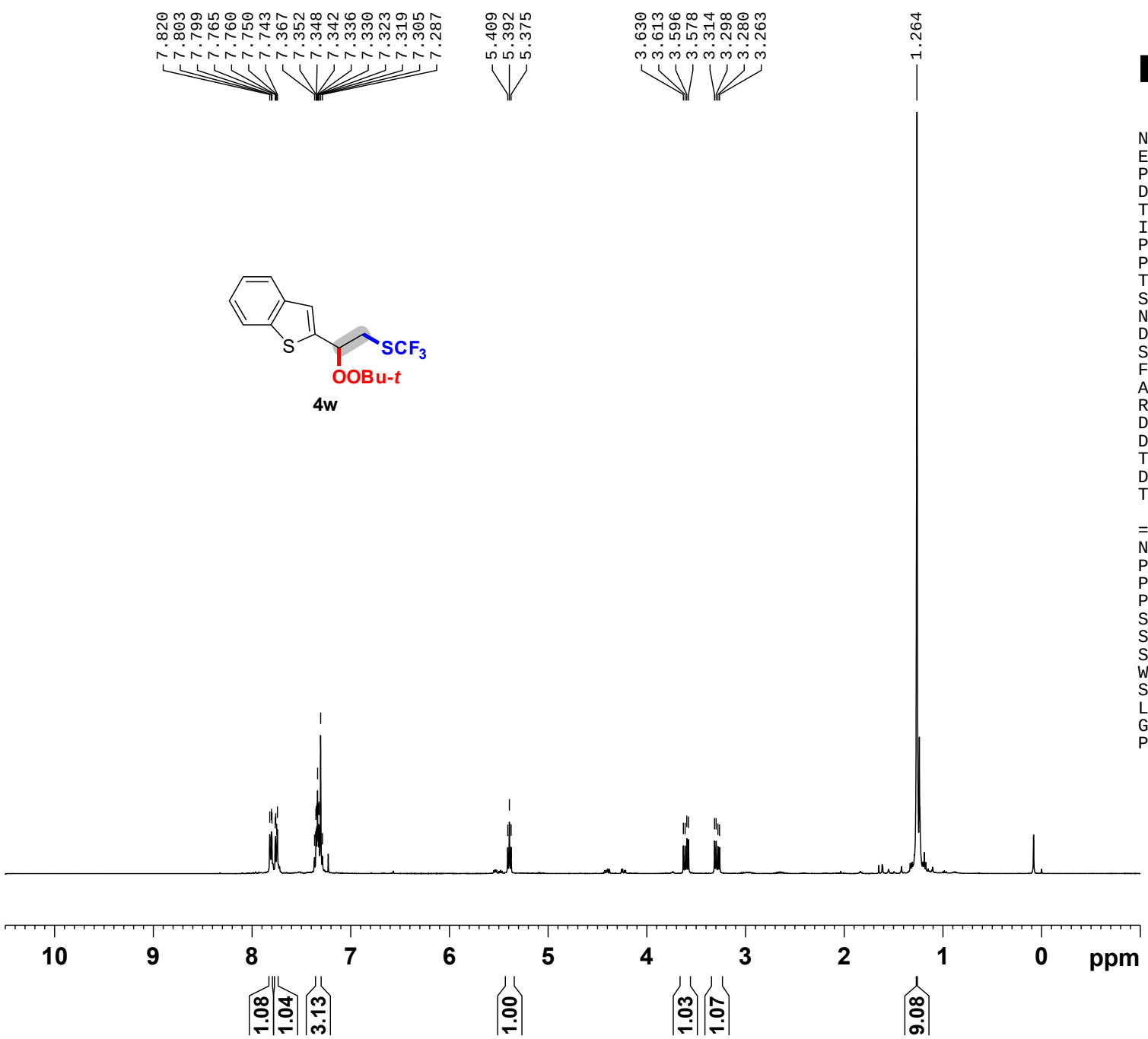
NAME	cyj859bp-20190328
EXPNO	2
PROCNO	1
Date_	20190328
Time	18.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	181
DW	19.800 usec
DE	6.50 usec
TE	293.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	13C
P1	15.00 usec
PL1	2.00 dB
PL1W	55.31277084 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	16.72 dB
PL13	15.50 dB
PL2W	17.01305389 W
PL12W	0.28759566 W
PL13W	0.38087484 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127789 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40




```
NAME      cyj859bp-20190328
EXPNO                    3
PROCNO                   1
Date_             20190328
Time                 18.23
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       32
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                      812
DW                    5.600 usec
DE                    6.50 usec
TE                   292.8 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                      1

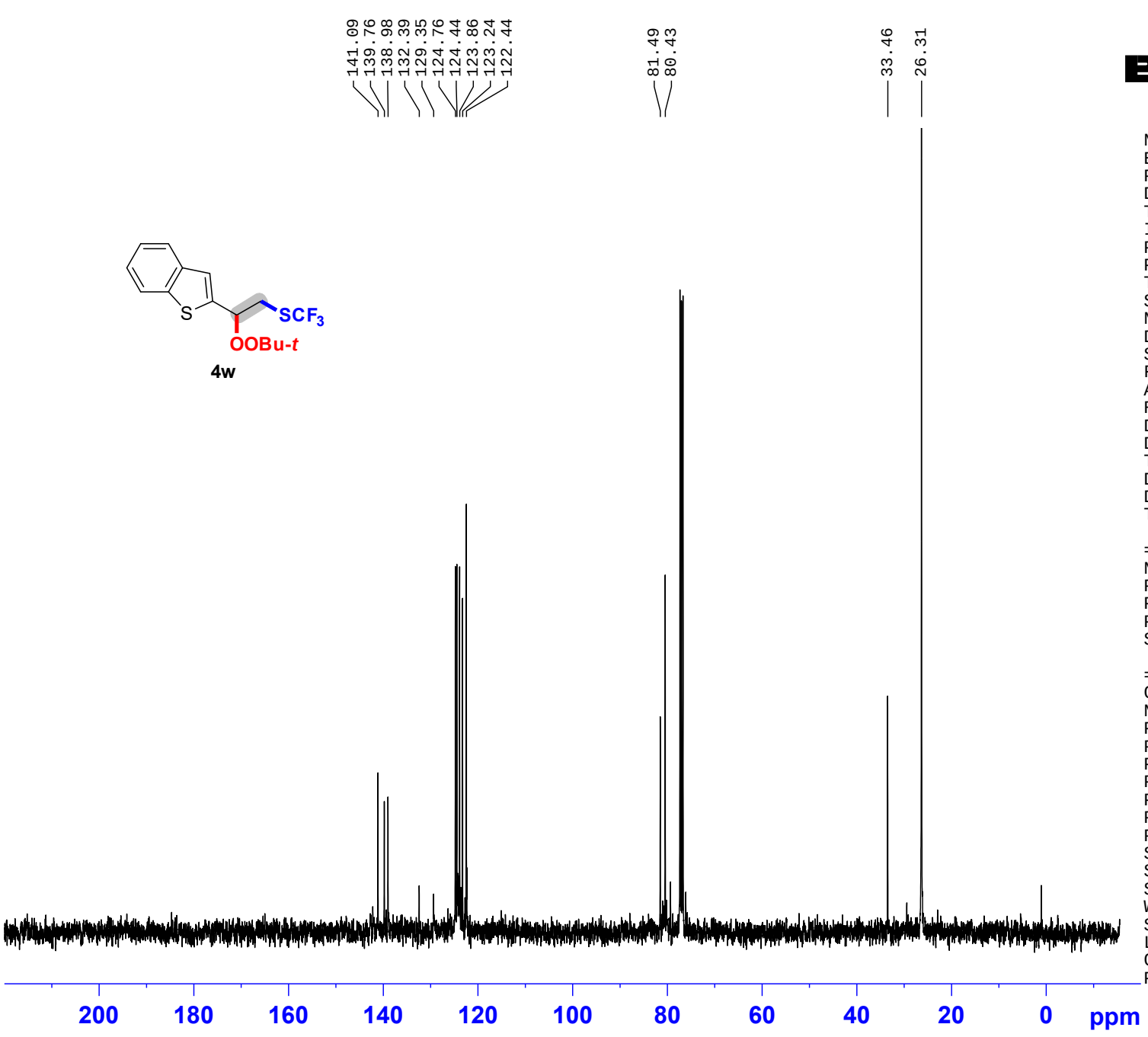
======== CHANNEL f1 ========
NUC1                    19F
P1                    14.20 usec
PL1                   -2.00 dB
PL1W           20.42289734 W
SFO1           376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  16.72 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
SFO2           400.1316005 MHz
SI                    65536
SF             376.4983660 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.00
```



BRUKER

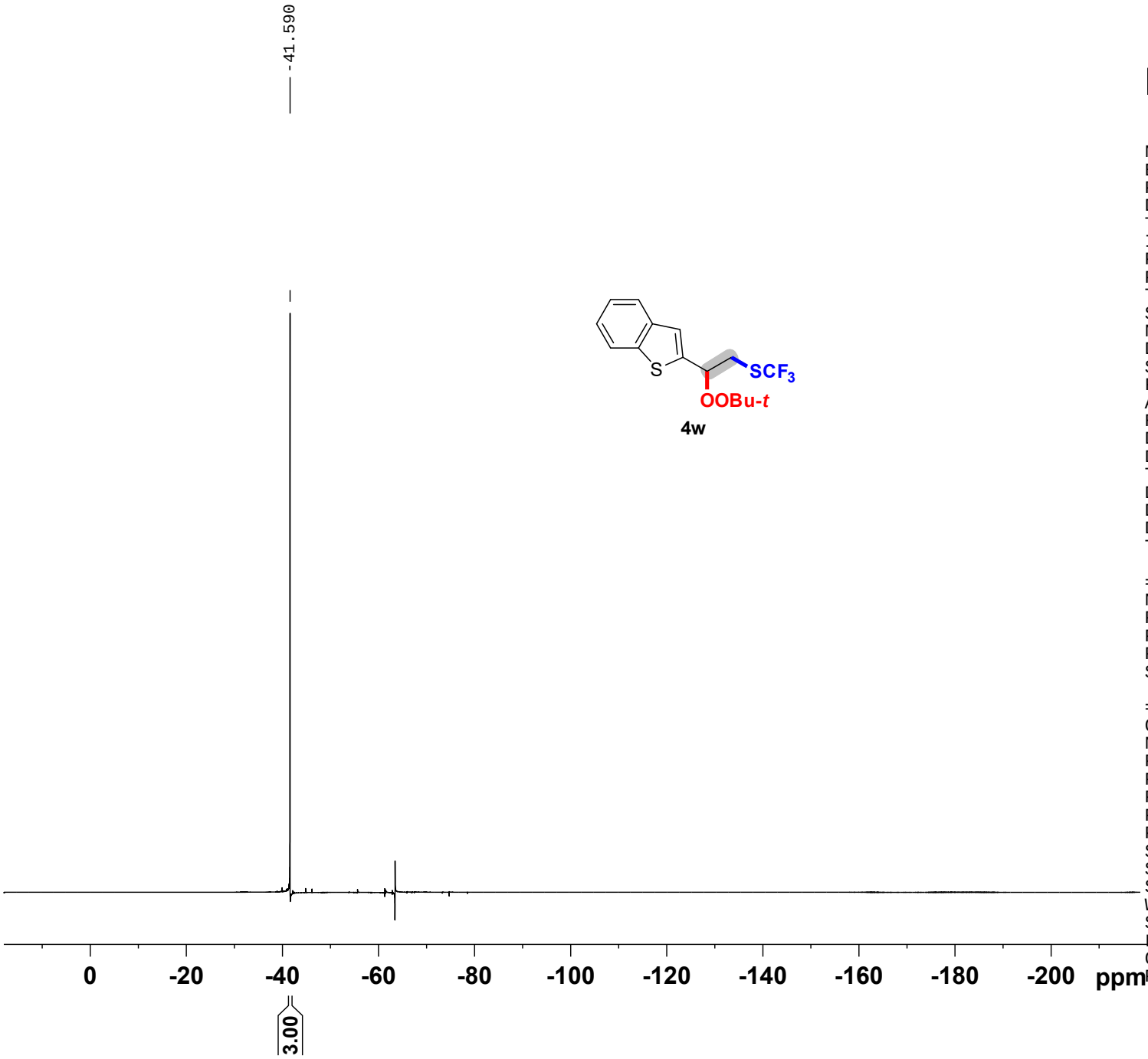
NAME	cyj898bp-20190430
EXPNO	1
PROCNO	1
Date_	20040113
Time	11.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	80.6
DW	78.200 usec
DE	6.50 usec
TE	293.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300233 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME      cyj898bp-20190430
EXPNO                    2
PROCNO                   1
Date_             20040113
Time                 12.03
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      56
DS                       4
SWH              25252.525 Hz
FIDRES            0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  294.4 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W           55.31277084 W
SFO1           100.6238364 MHz

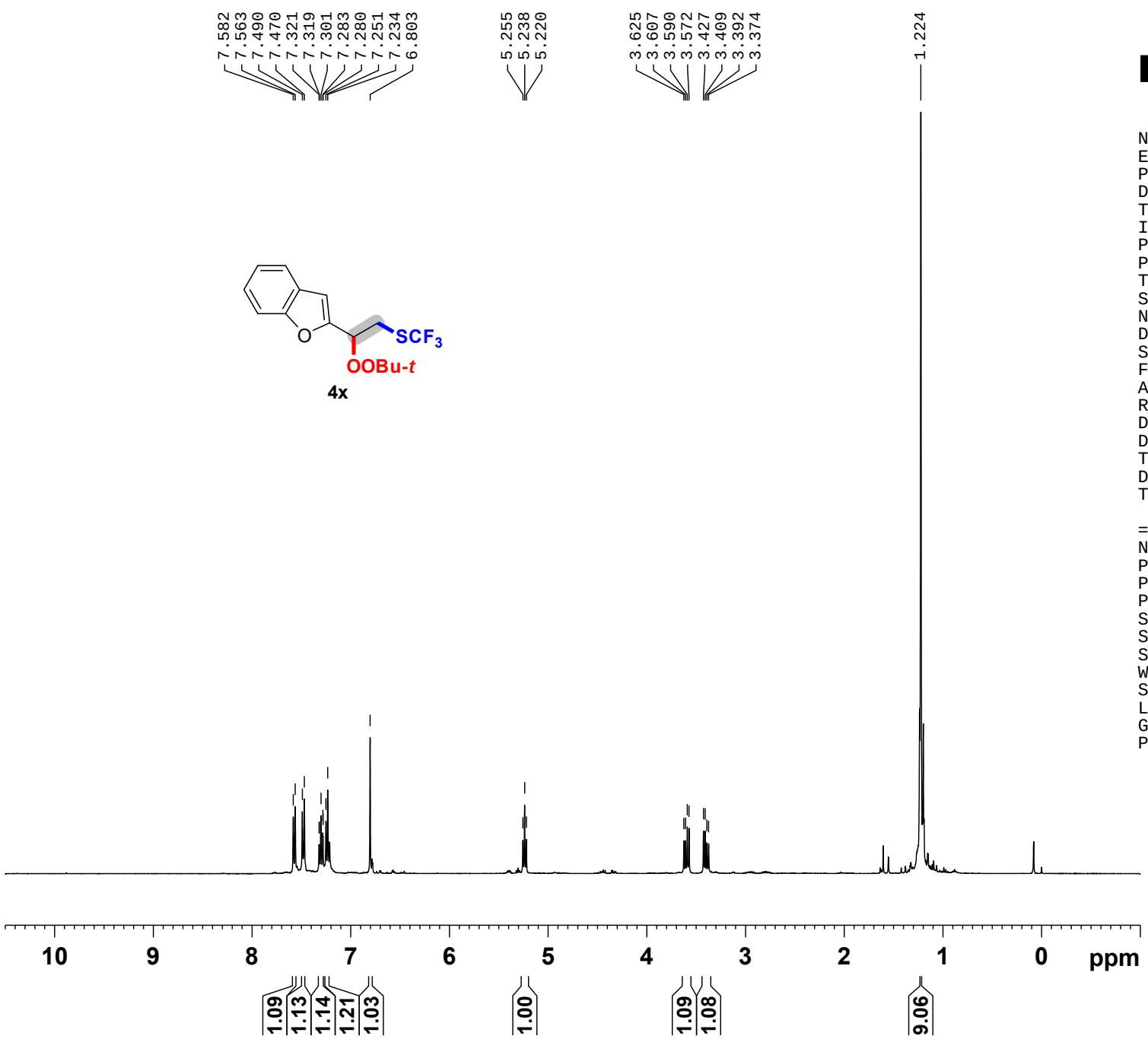
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
PL13W           0.38087484 W
SFO2           400.1316005 MHz
SI                   32768
SF             100.6127755 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyj-898bp-20190516
EXPNO                      3
PROCNO                     1
Date_               20040129
Time                    0.09
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES             0.681196 Hz
AQ                 0.7340532 sec
RG                       812
DW                     5.600 usec
DE                     6.50 usec
TE                     297.9 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

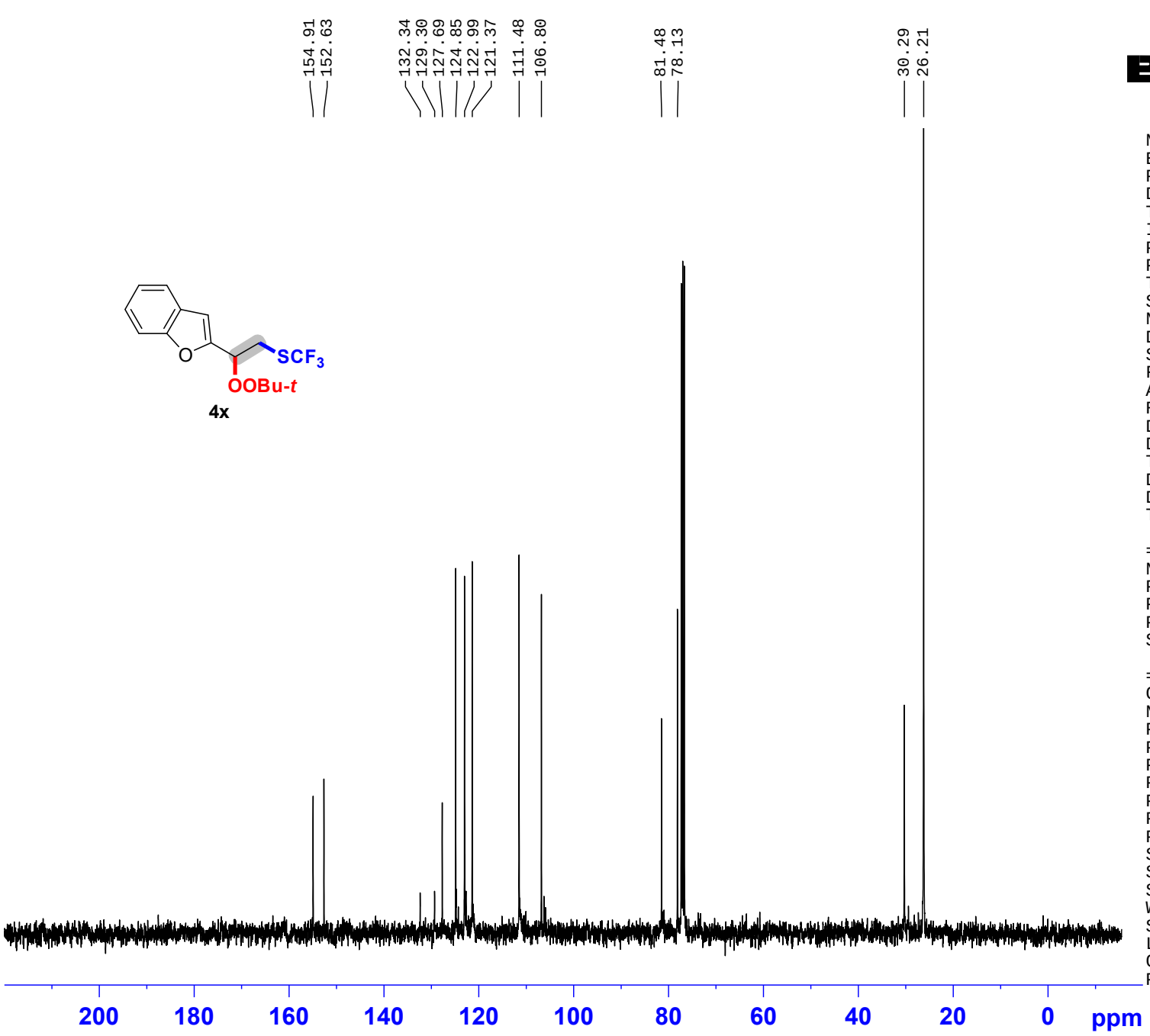
======== CHANNEL f1 ========
NUC1                      19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                     65536
SF              376.4983660 MHz
WDW                       EM
SSB                        0
LB                      3.00 Hz
GB                         0
PC                      1.00
```




```
NAME      cyj898cp-20190430
EXPNO                    1
PROCNO                   1
Date_             20040113
Time                 12.16
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                    80.6
DW                  78.200 usec
DE                   6.50 usec
TE                  293.0 K
D1             1.00000000 sec
TD0                      1

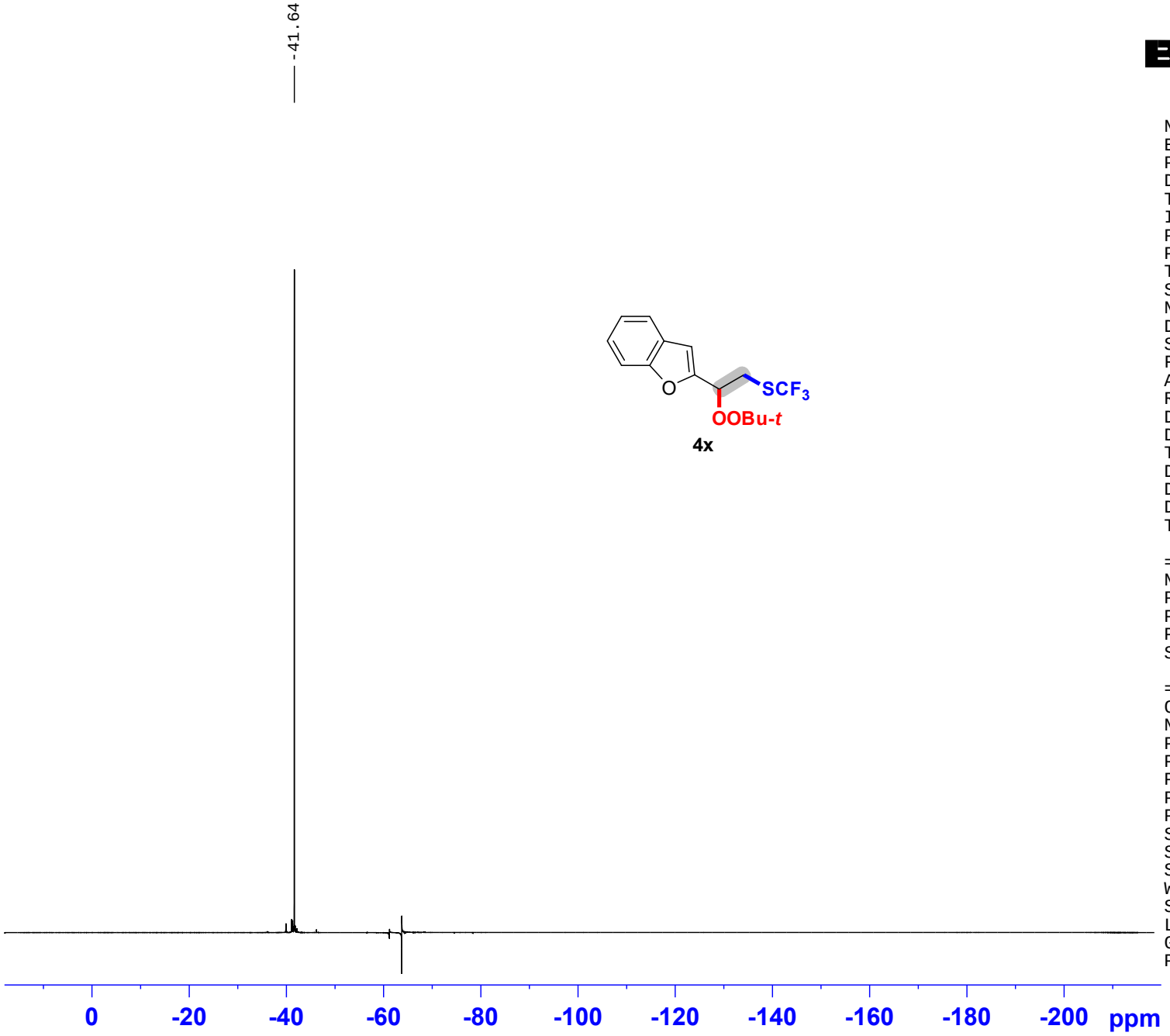
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300206 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




```
NAME      cyj898cp-20190430
EXPNO                    2
PROCNO                   1
Date_             20040113
Time                 12.22
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    80
DS                     4
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976629 sec
RG                   181
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    3

======== CHANNEL f1 ========
NUC1                  13C
P1                 15.00 usec
PL1                 2.00 dB
PL1W        55.31277084 W
SFO1        100.6238364 MHz

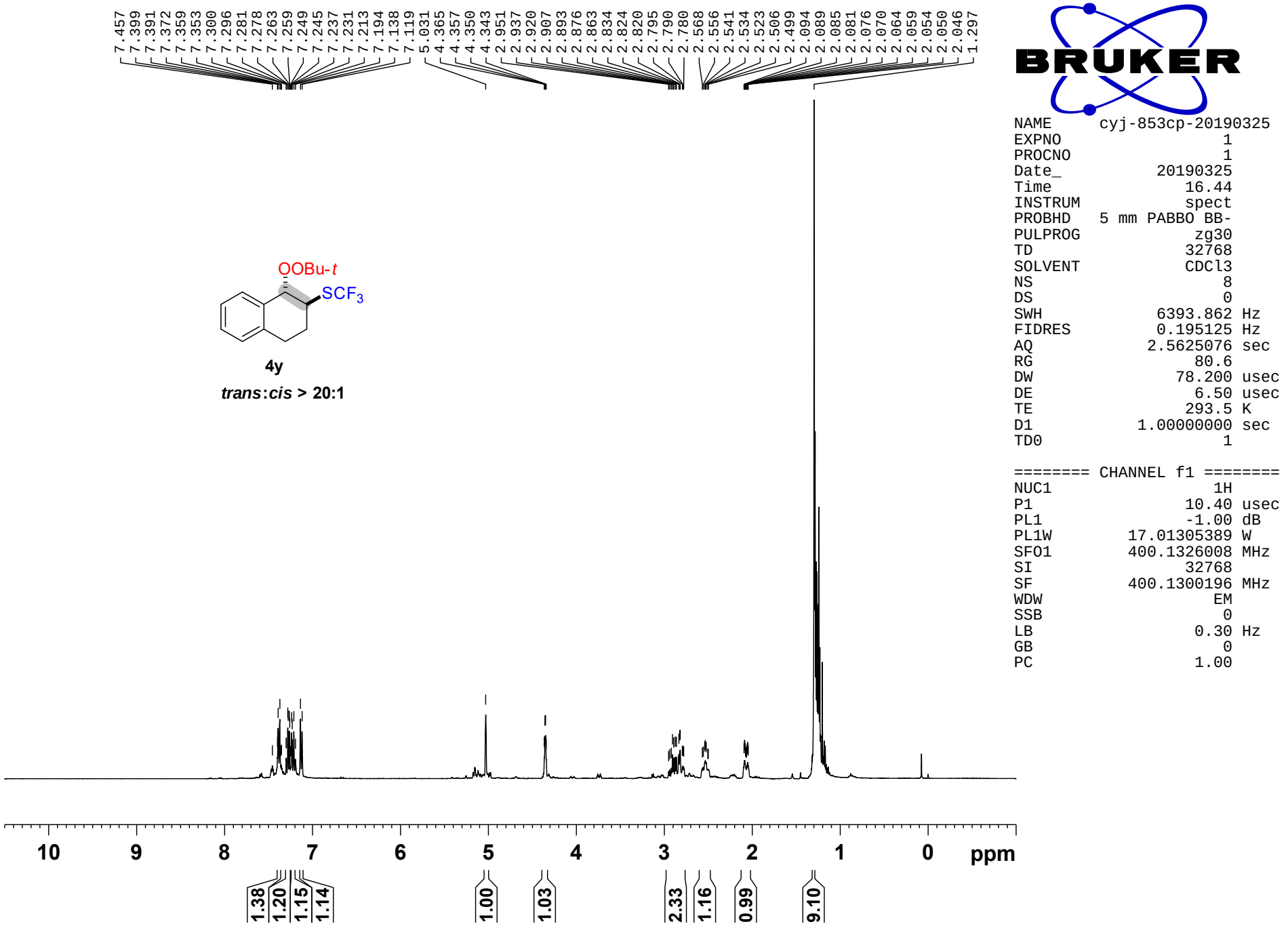
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL13               15.50 dB
PL2W        17.01305389 W
PL12W        0.28759566 W
PL13W        0.38087484 W
SFO2        400.1316005 MHz
SI                 32768
SF          100.6127737 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                  1.40
```




```
NAME      cyj-898cp-20190515
EXPNO                      3
PROCNO                     1
Date_               20040128
Time                    0.16
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES             0.681196 Hz
AQ                 0.7340532 sec
RG                       812
DW                     5.600 usec
DE                     6.50 usec
TE                     297.4 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

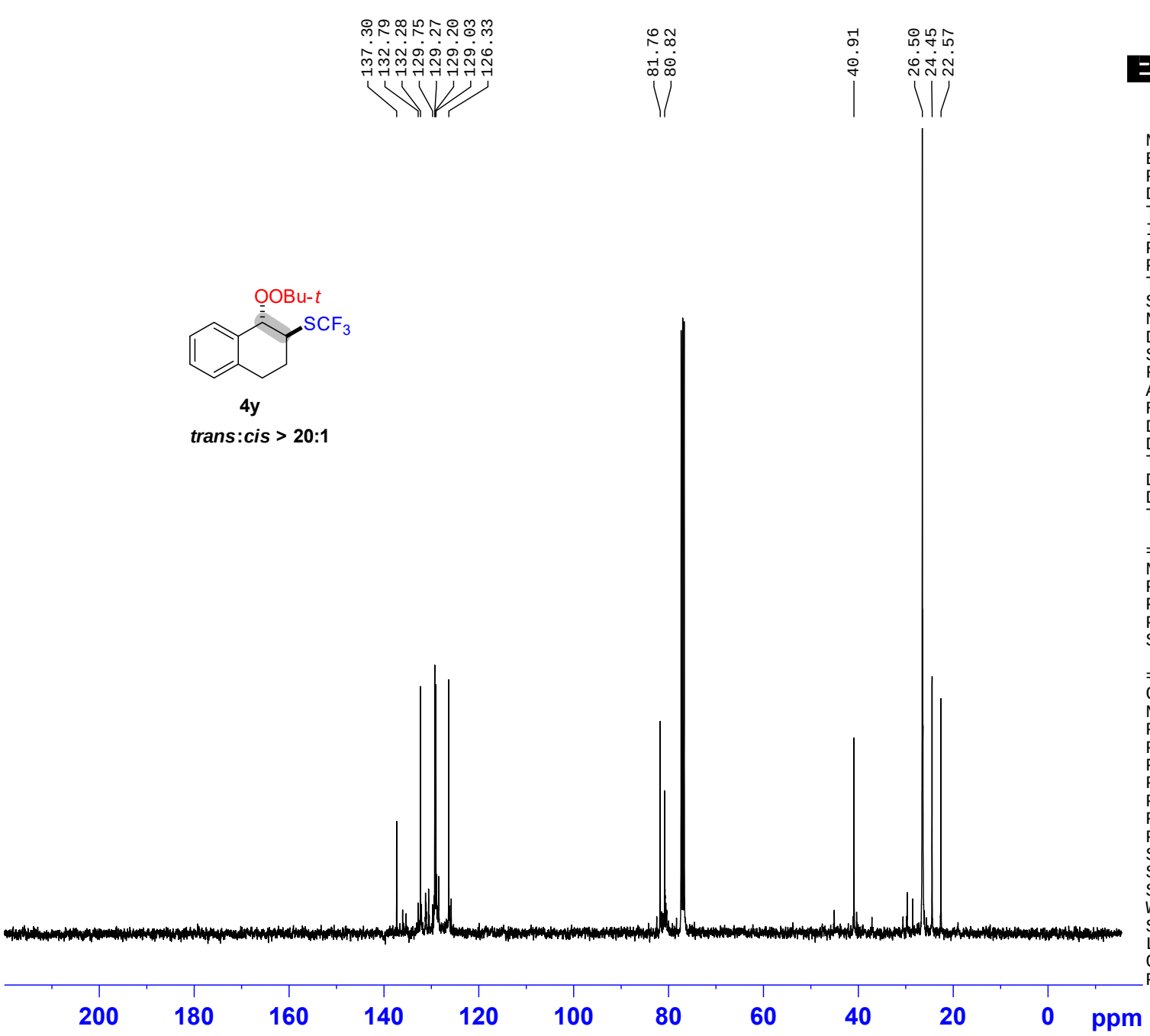
======== CHANNEL f1 ========
NUC1                     19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                       65536
SF              376.4983660 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.00
```




```
NAME      cyj-853cp-20190325
EXPNO                      1
PROCNO                     1
Date_               20190325
Time                   16.44
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                 6393.862 Hz
FIDRES              0.195125 Hz
AQ                2.5625076 sec
RG                      80.6
DW                    78.200 usec
DE                     6.50 usec
TE                    293.5 K
D1                1.00000000 sec
TD0                        1

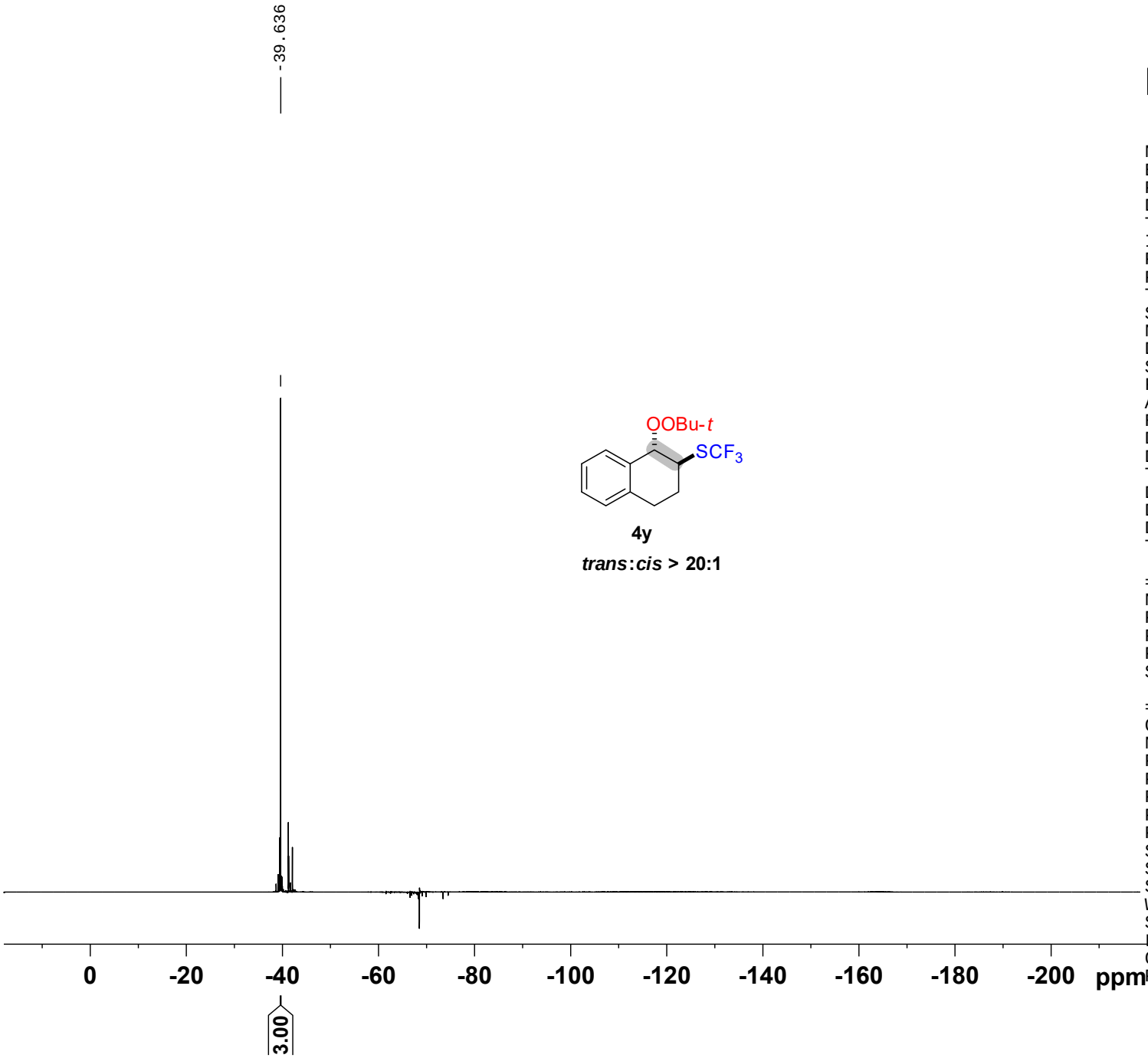
======== CHANNEL f1 ========
NUC1                      1H
P1                     10.40 usec
PL1                    -1.00 dB
PL1W            17.01305389 W
SFO1            400.1326008 MHz
SI                     32768
SF              400.1300196 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```




```
NAME      cyj-853cp-20190325
EXPNO                      2
PROCNO                     1
Date_               20190325
Time                   16.59
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        232
DS                          4
SWH                 25252.525 Hz
FIDRES                0.385323 Hz
AQ                  1.2976629 sec
RG                        181
DW                     19.800 usec
DE                      6.50 usec
TE                     295.3 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         3

======== CHANNEL f1 ========
NUC1                      13C
P1                     15.00 usec
PL1                     2.00 dB
PL1W               55.31277084 W
SFO1               100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL13                   15.50 dB
PL2W               17.01305389 W
PL12W               0.28759566 W
PL13W               0.38087484 W
SFO2               400.1316005 MHz
SI                      32768
SF                 100.6127727 MHz
WDW                        EM
SSB                         0
LB                     3.00 Hz
GB                          0
PC                     1.40
```



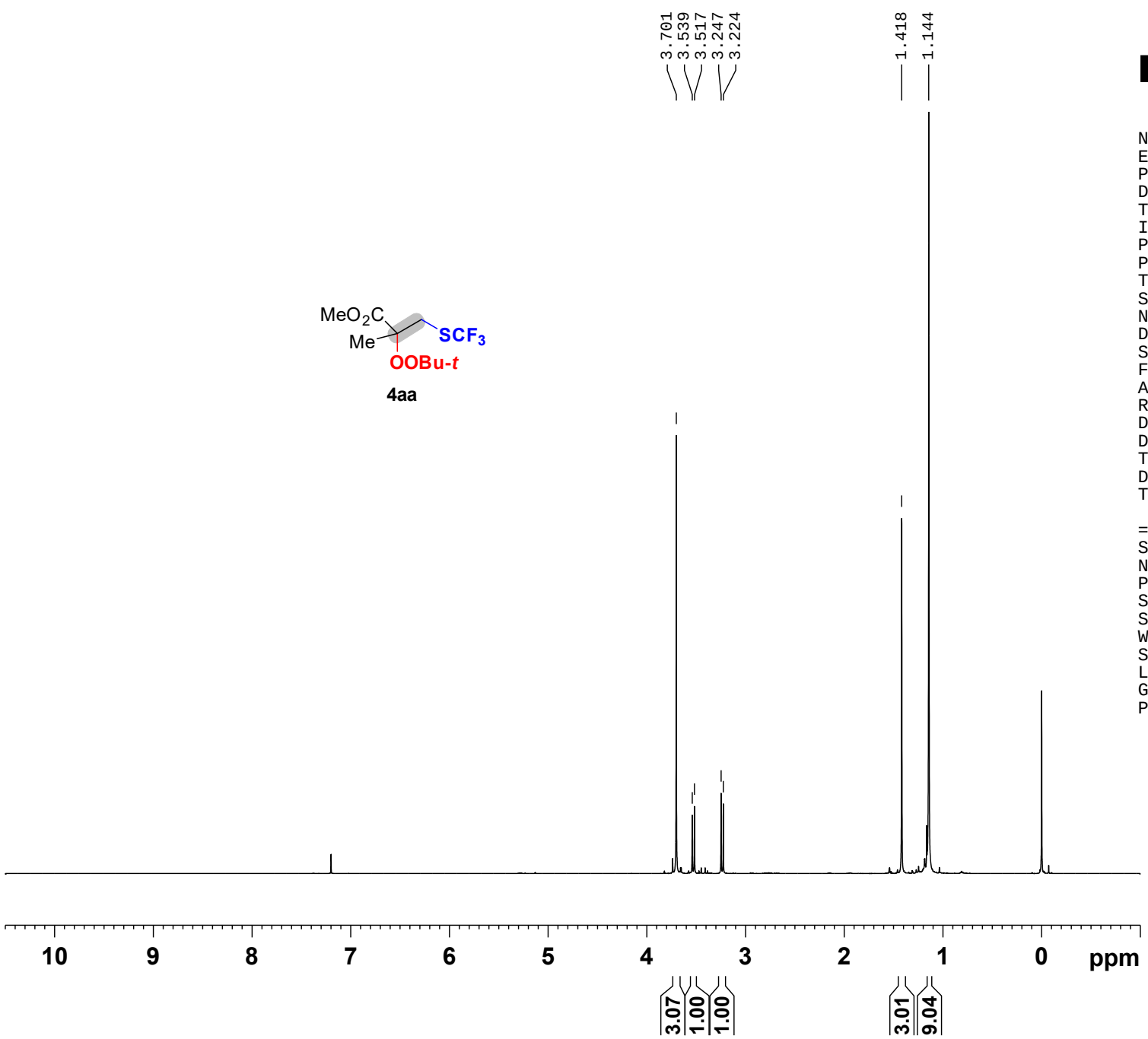
4y

***trans*:*cis* > 20:1**

```
NAME      cyj-853cp-20190325
EXPNO                      3
PROCNO                     1
Date_               20190325
Time                   17.03
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES             0.681196 Hz
AQ                 0.7340532 sec
RG                       812
DW                     5.600 usec
DE                     6.50 usec
TE                     294.2 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

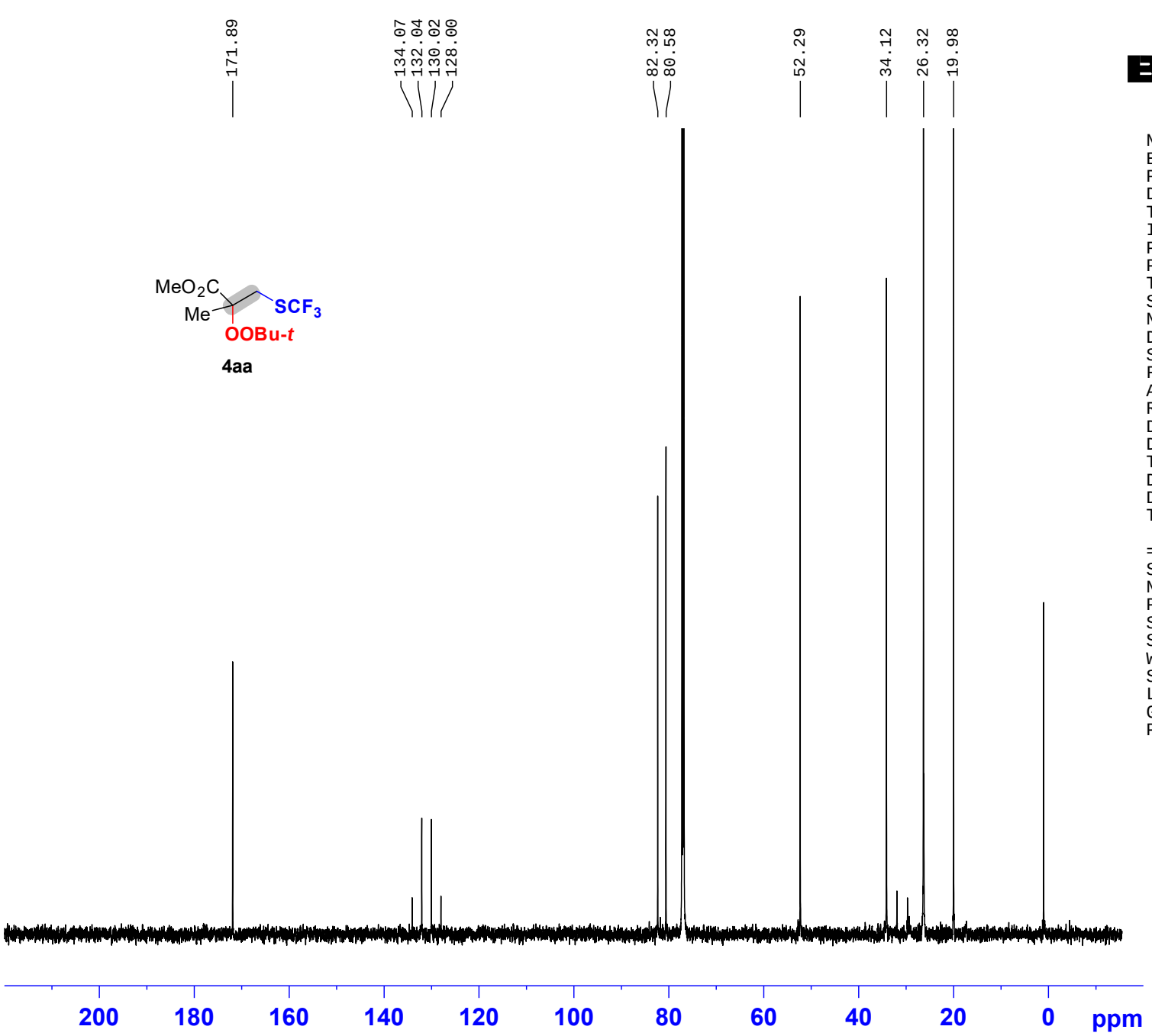
======== CHANNEL f1 ========
NUC1                      19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                     65536
SF              376.4983660 MHz
WDW                       EM
SSB                        0
LB                      3.00 Hz
GB                         0
PC                      1.00
```



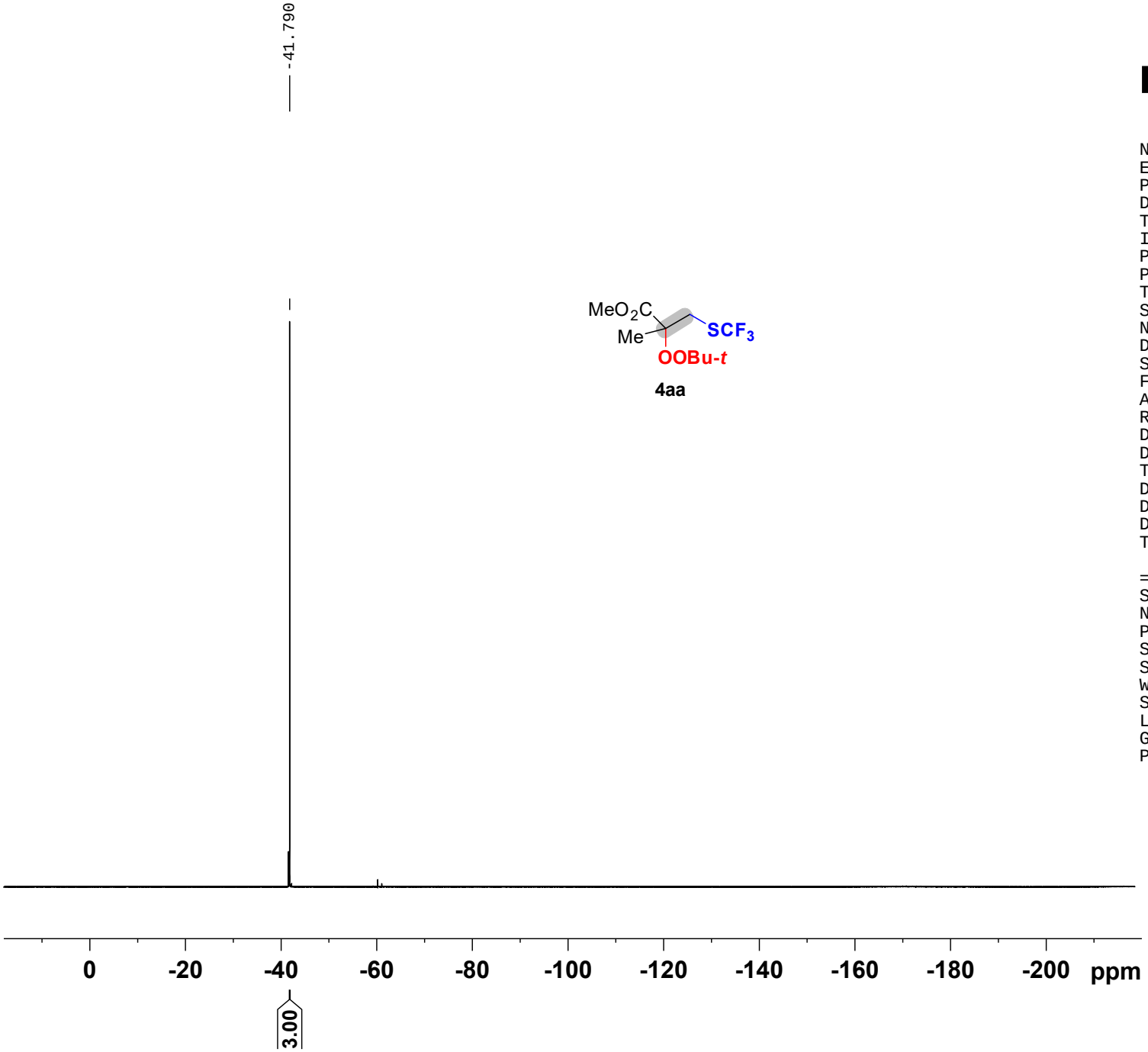

```
NAME                CYJm3p
EXPNO                    1
PROCNO                   1
Date_             20190314
Time                 13.01
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               9615.385 Hz
FIDRES            0.146719 Hz
AQ                3.4079220 sec
RG                    38.1
DW                  52.000 usec
DE                   6.50 usec
TE                  295.5 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            600.1739011 MHz
NUC1                    1H
P1                    9.77 usec
SI                   65536
SF              600.1700525 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



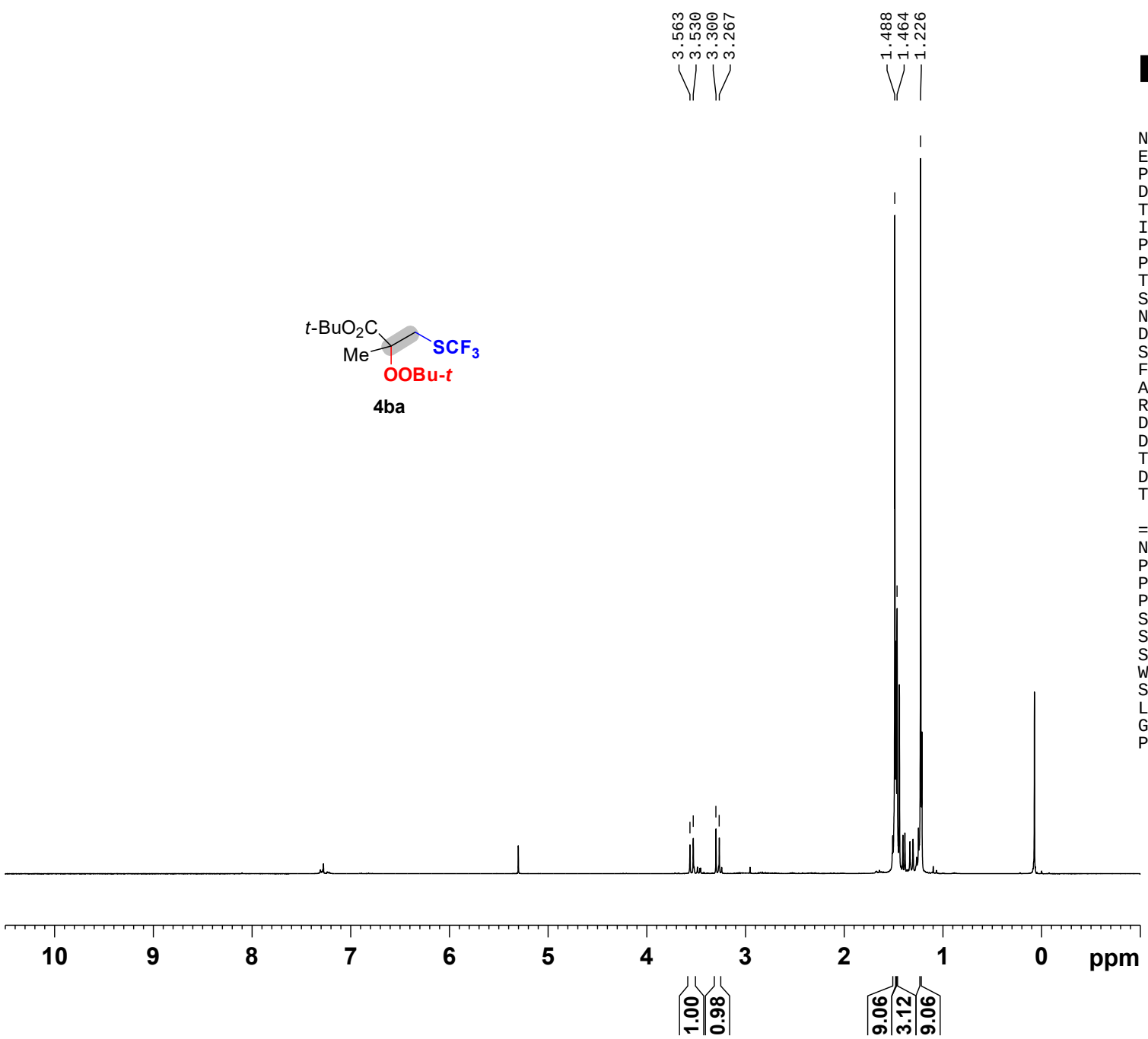

```
NAME                CYJm3p
EXPNO                    2
PROCNO                   1
Date_             20190314
Time                 13.18
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     320
DS                       4
SWH              37878.789 Hz
FIDRES           0.577984 Hz
AQ               0.8651252 sec
RG                  190.02
DW                  13.200 usec
DE                   6.50 usec
TE                  296.3 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          150.9294669 MHz
NUC1                    13C
P1                  11.90 usec
SI                   32768
SF            150.9128674 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```



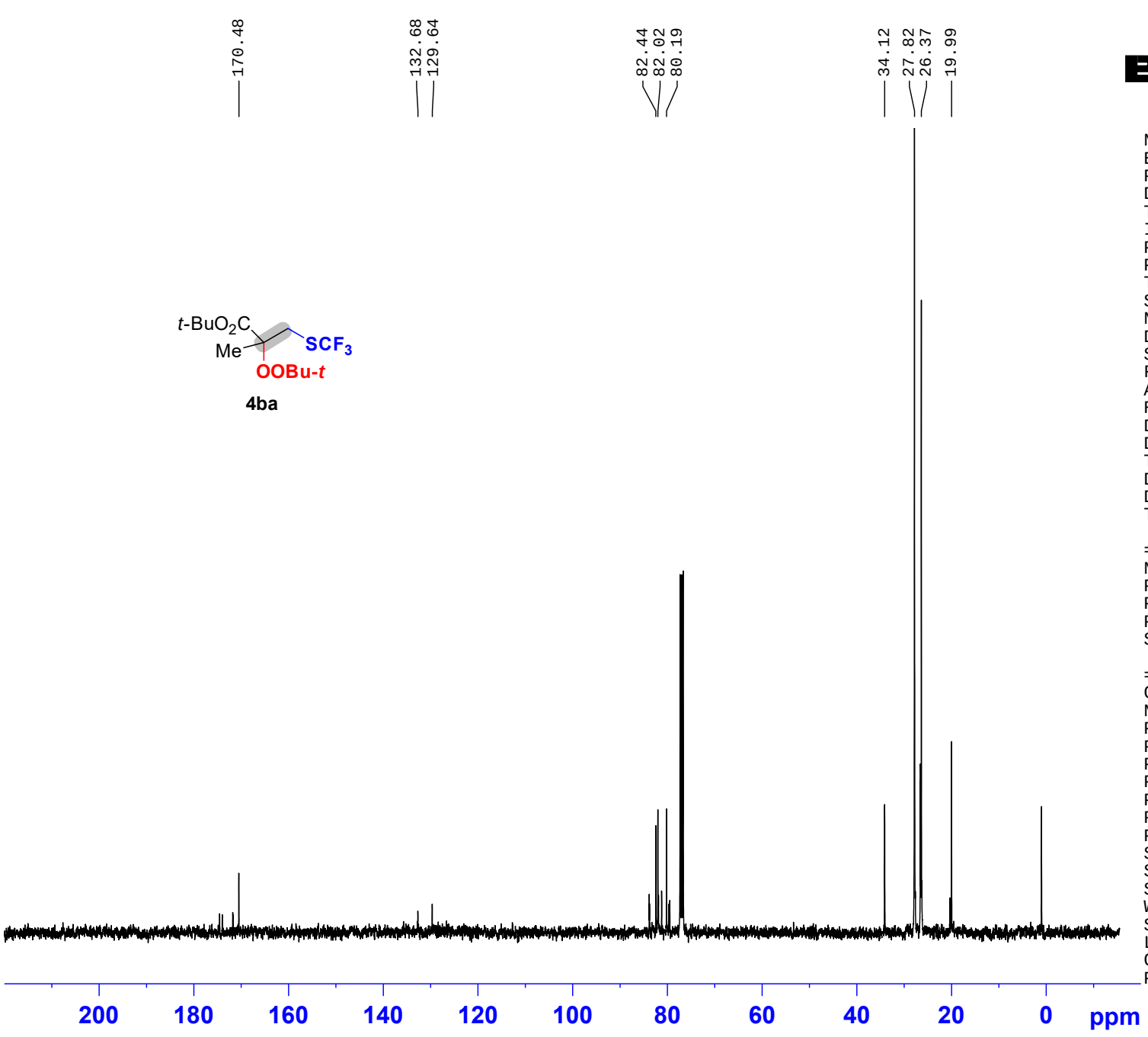

```
NAME                CYJm3p
EXPNO                    3
PROCNO                   1
Date_             20190314
Time                 13.21
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG       zgfhigqn.2
TD                  131072
SOLVENT               CDCl3
NS                       64
DS                        4
SWH              133928.578 Hz
FIDRES             1.021794 Hz
AQ                 0.4893855 sec
RG                       14
DW                    3.733 usec
DE                    6.50 usec
TE                   296.0 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             564.6675534 MHz
NUC1                    19F
P1                    11.90 usec
SI                    65536
SF               564.7240258 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.00
```




```
NAME      cyjm12p-20190410
EXPNO                    1
PROCNO                   1
Date_             20190410
Time                 21.29
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                      57
DW                  78.200 usec
DE                   6.50 usec
TE                  293.5 K
D1              1.00000000 sec
TD0                      1

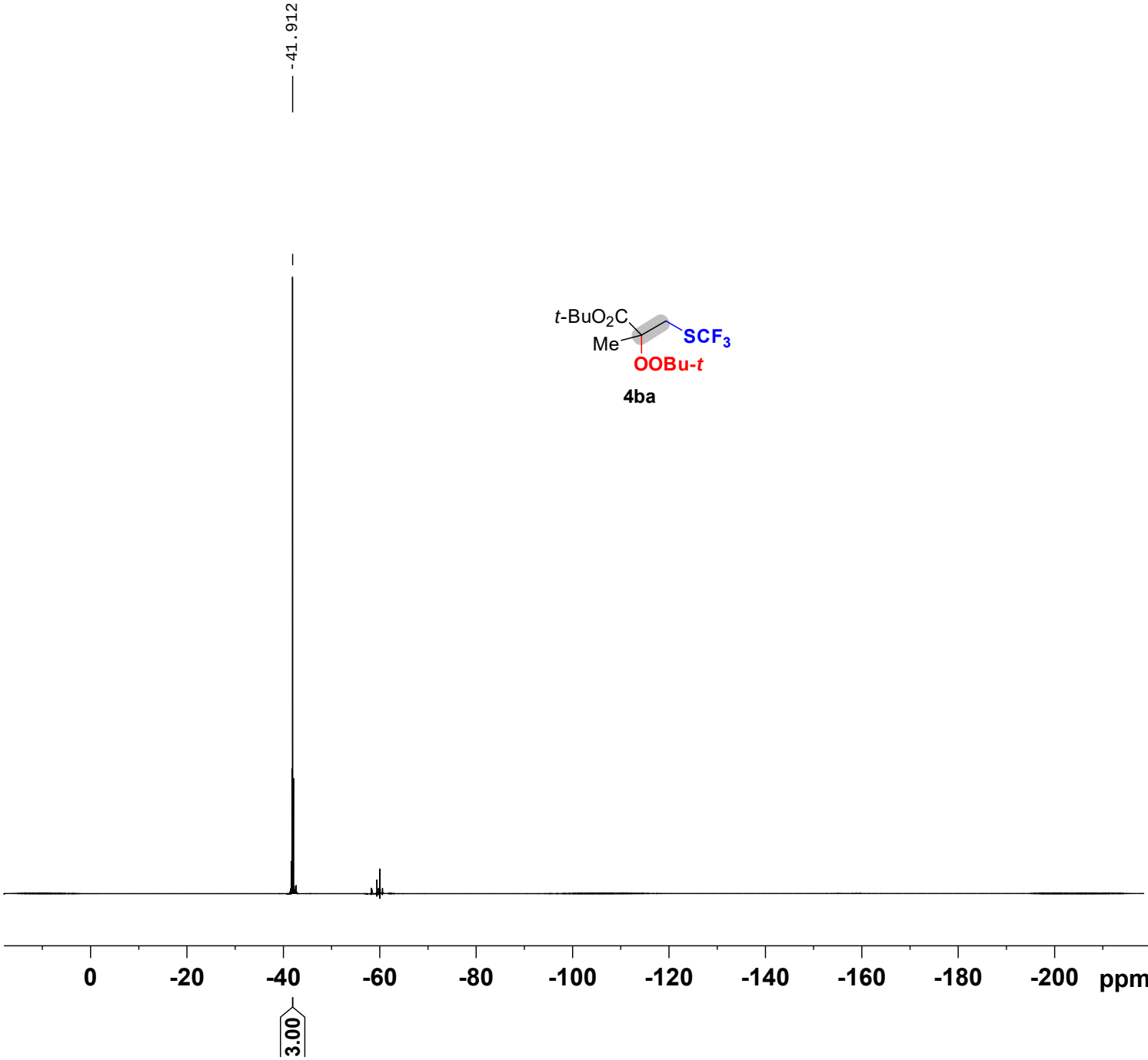
======== CHANNEL f1 ========
NUC1                    1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300039 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                  1.00
```




```
NAME      cyjm12p-20190410
EXPNO                    2
PROCNO                   1
Date_             20190410
Time                 21.33
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      72
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  294.1 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

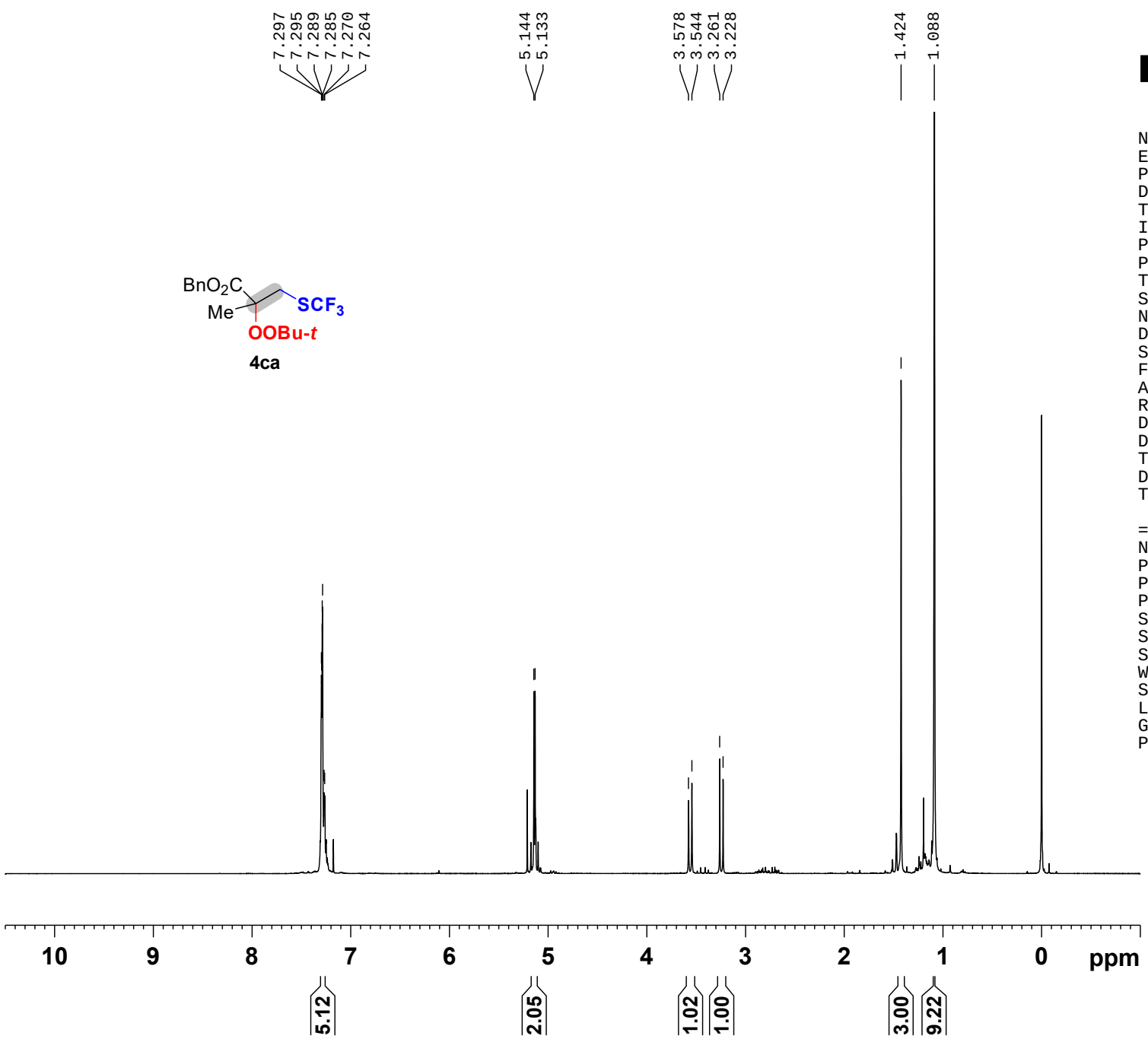
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127698 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyjm12p-20190410
EXPNO                    3
PROCNO                   1
Date_             20190410
Time                 21.40
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      64
DS                       4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                    2050
DW                   5.600 usec
DE                   6.50 usec
TE                  293.8 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                      4

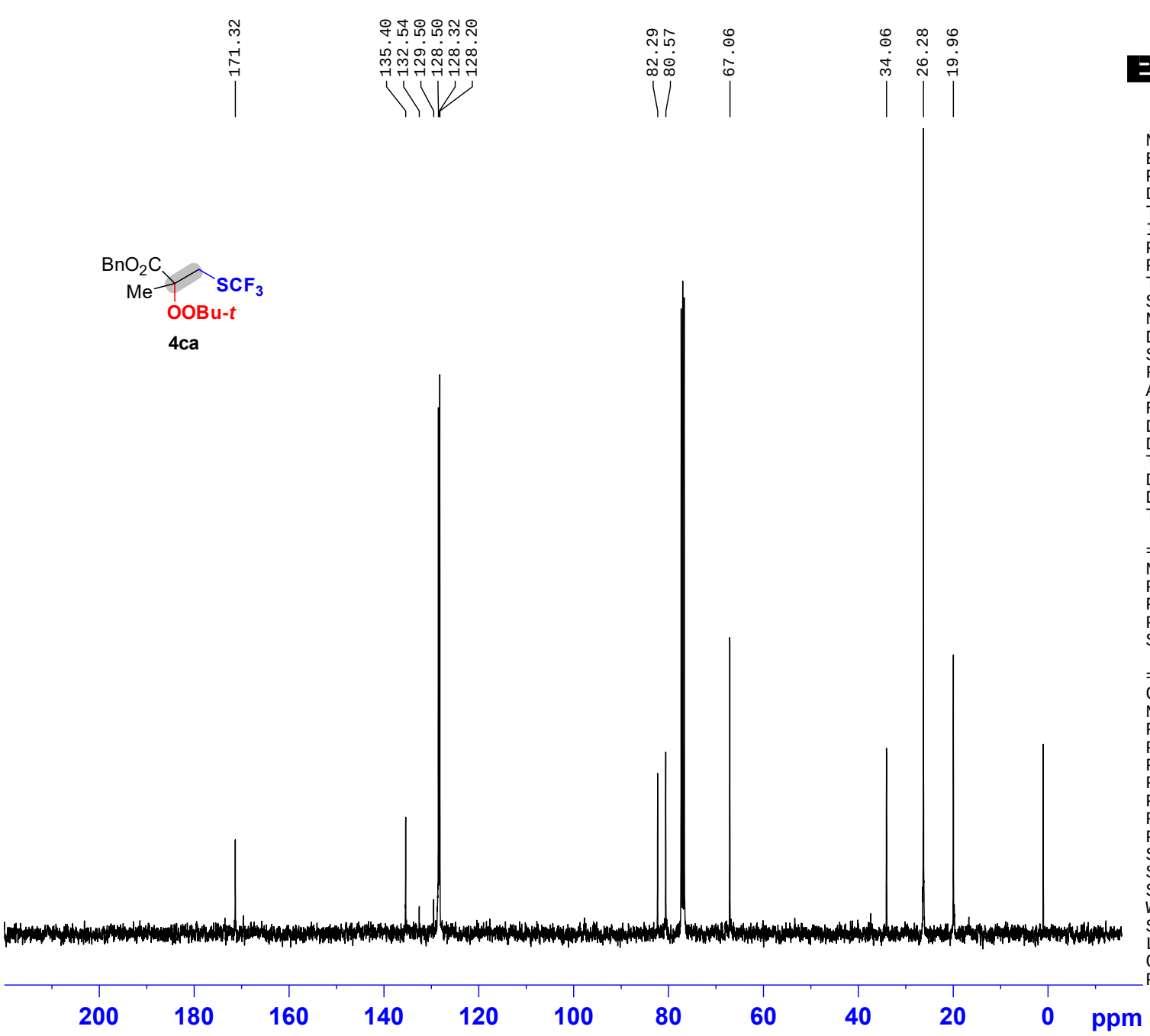
======== CHANNEL f1 ========
NUC1                   19F
P1                   14.20 usec
PL1                  -2.00 dB
PL1W          20.42289734 W
SFO1          376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
SFO2          400.1316005 MHz
SI                  65536
SF            376.4983660 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cyjm11p-20190410
EXPNO                    1
PROCNO                   1
Date_             20190410
Time                 21.08
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                    90.5
DW                  78.200 usec
DE                   6.50 usec
TE                  293.4 K
D1             1.00000000 sec
TD0                      1

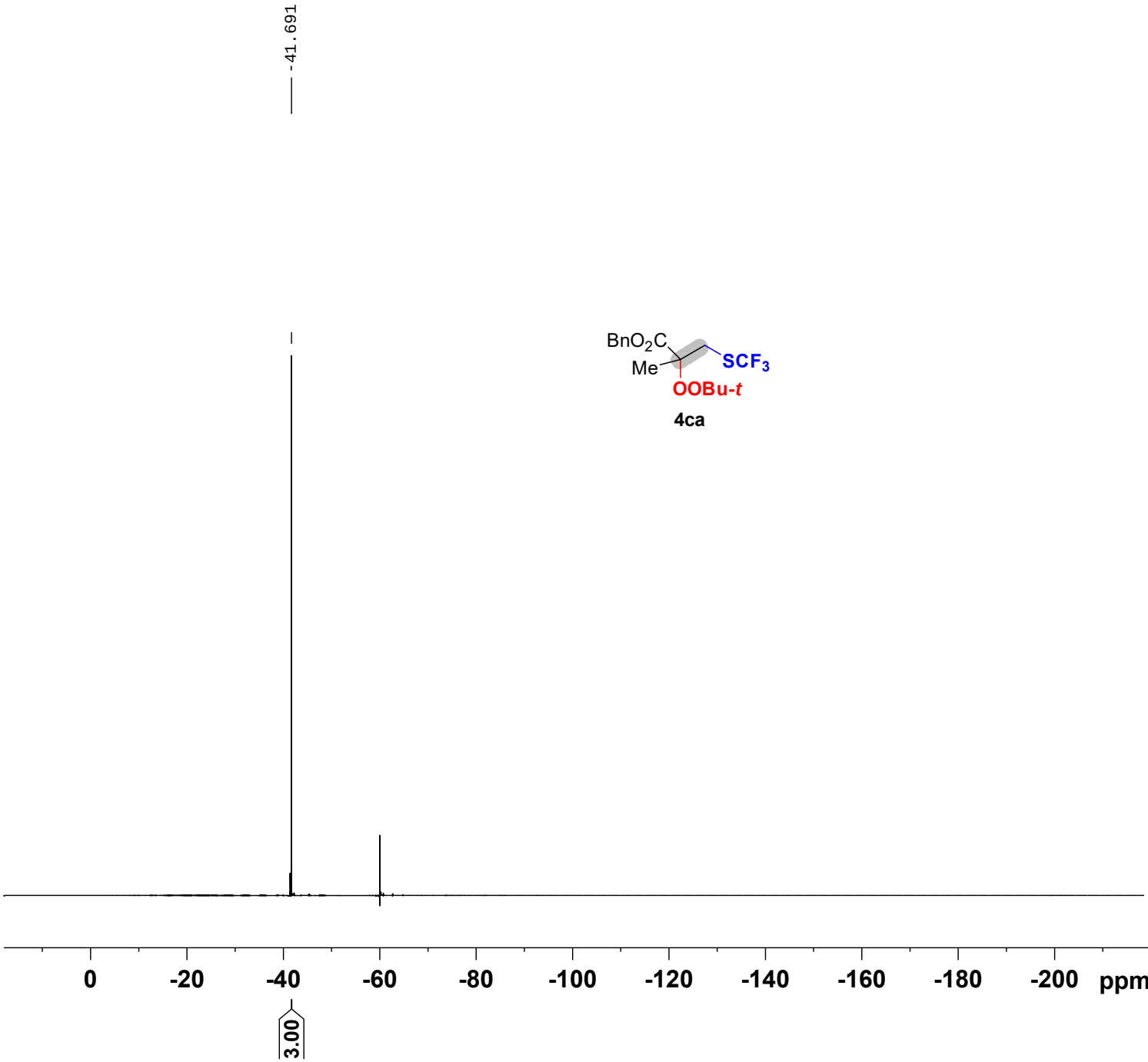
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300442 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




```
NAME      cyjm11p-20190410
EXPNO                    2
PROCNO                   1
Date_             20190410
Time                 21.12
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     104
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                19.800 usec
DE                 6.50 usec
TE                 294.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

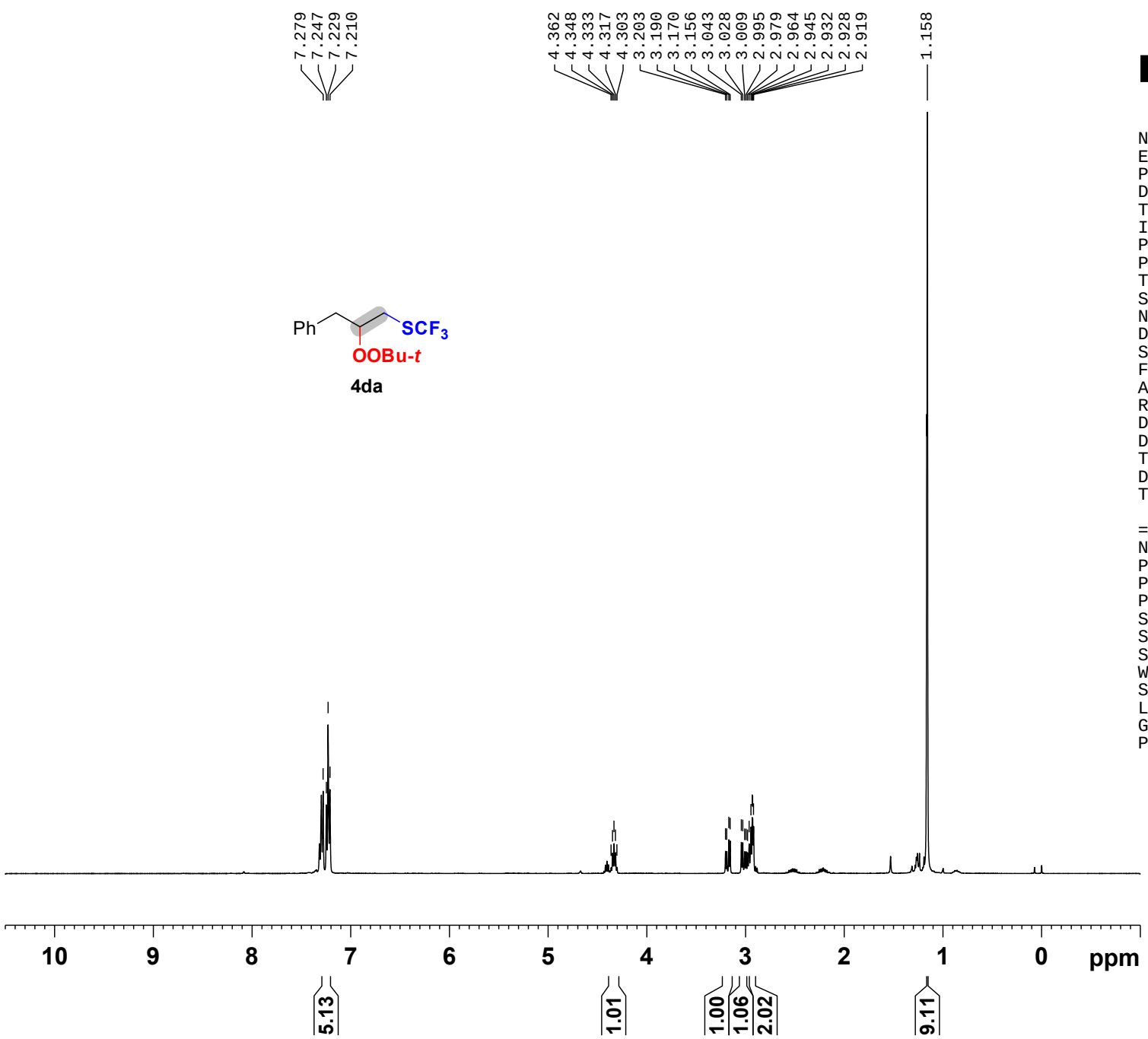
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127728 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```




```
NAME      cyjm11p-20190410
EXPNO                    3
PROCNO                   1
Date_             20190410
Time                 21.22
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      64
DS                       4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                    2050
DW                   5.600 usec
DE                   6.50 usec
TE                  293.8 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                      4

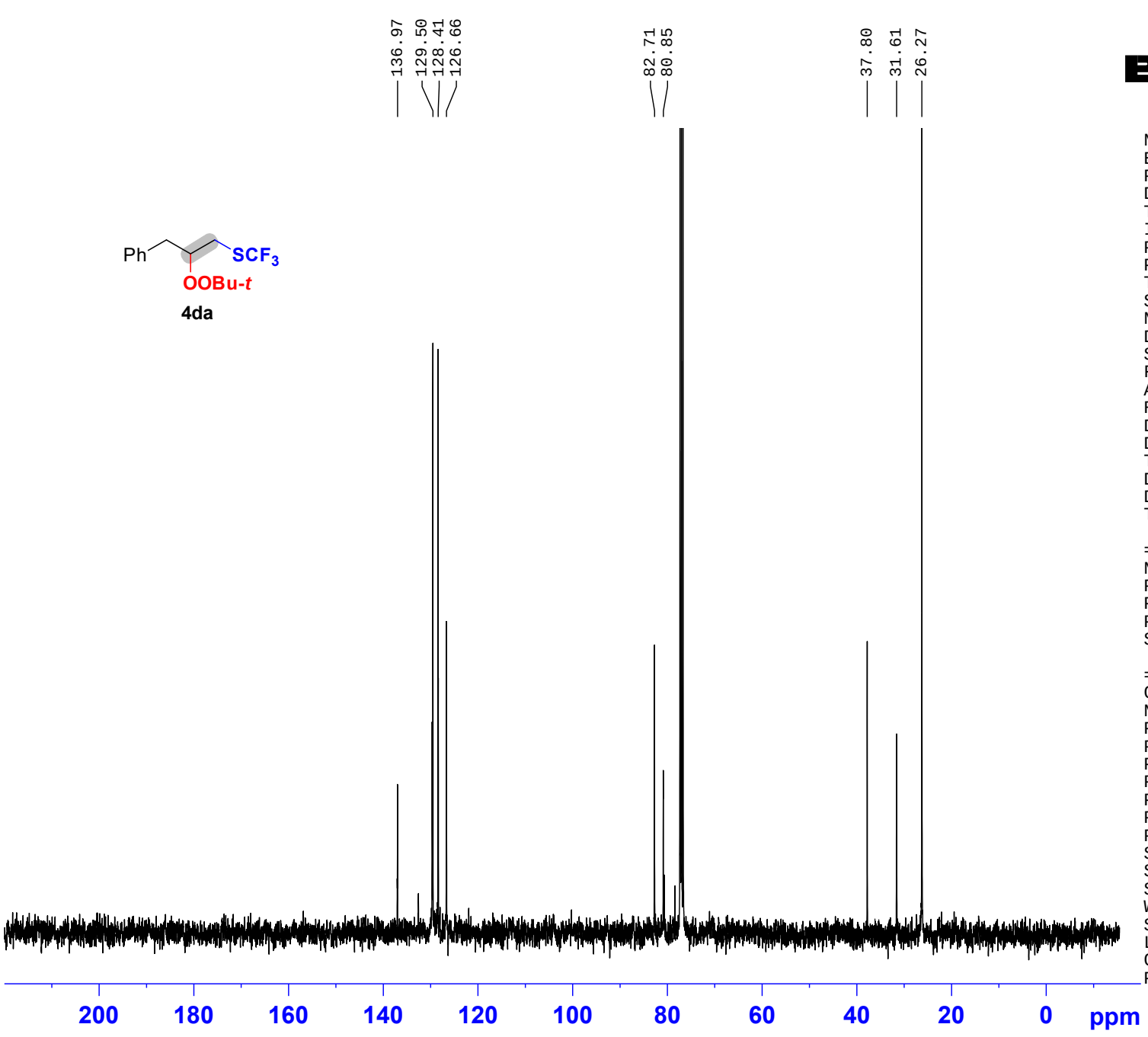
======== CHANNEL f1 ========
NUC1                    19F
P1                   14.20 usec
PL1                  -2.00 dB
PL1W          20.42289734 W
SFO1          376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
SFO2          400.1316005 MHz
SI                   65536
SF            376.4983660 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




```
NAME      cyjm8p-20190516
EXPNO                   1
PROCNO                  1
Date_            20040129
Time                10.20
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6393.862 Hz
FIDRES           0.195125 Hz
AQ               2.5625076 sec
RG                    144
DW                 78.200 usec
DE                  6.50 usec
TE                 299.6 K
D1              1.00000000 sec
TD0                     1

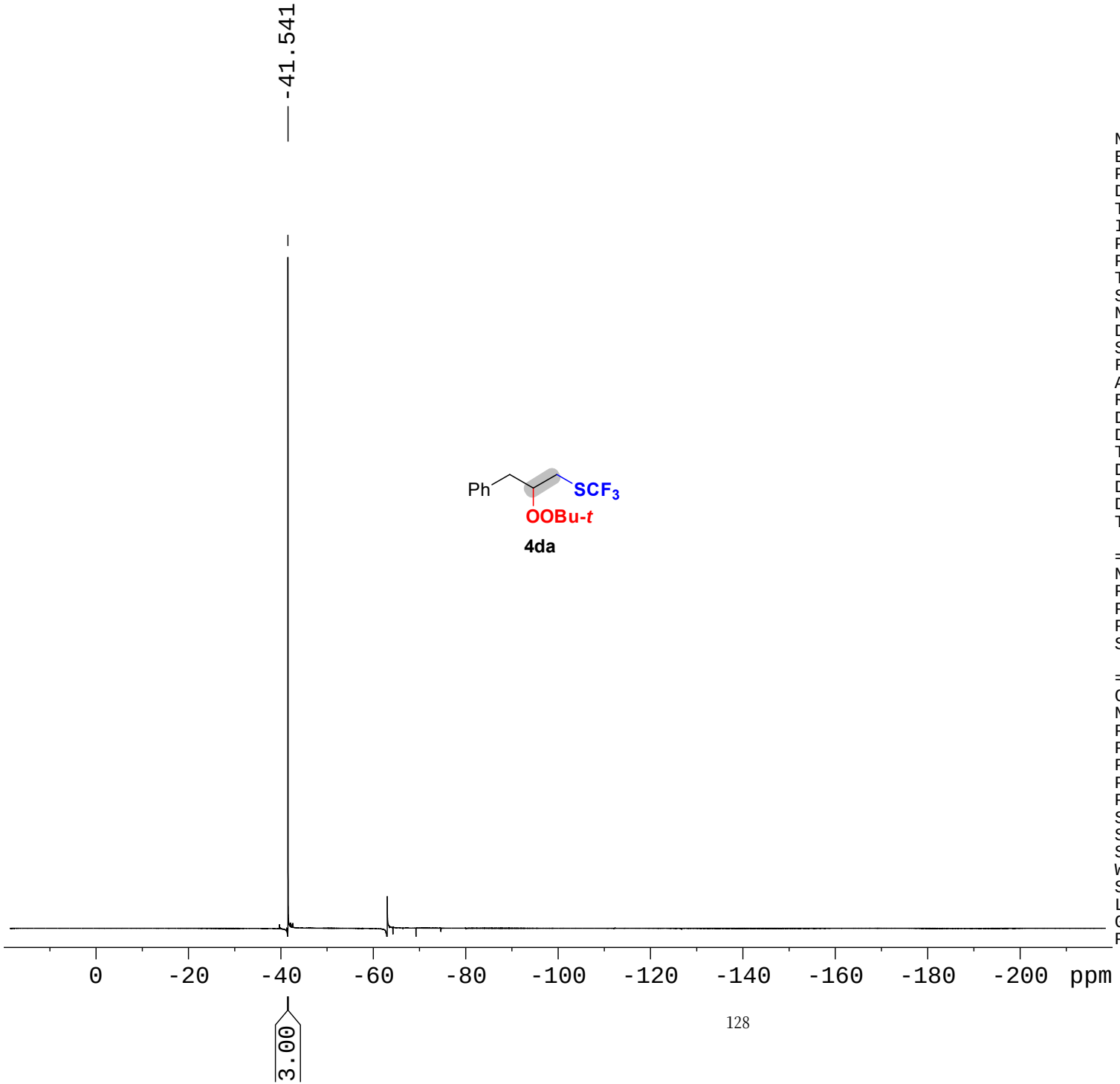
======== CHANNEL f1 ========
NUC1                   1H
P1                 10.40 usec
PL1                -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                  32768
SF           400.1300160 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```




```
NAME      cyjm8p-20190516
EXPNO                   2
PROCNO                  1
Date_            20040129
Time                10.27
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   120
DS                     4
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976629 sec
RG                  2050
DW                19.800 usec
DE                 6.50 usec
TE                300.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    3

======== CHANNEL f1 ========
NUC1                  13C
P1                 15.00 usec
PL1                 2.00 dB
PL1W         55.31277084 W
SFO1        100.6238364 MHz

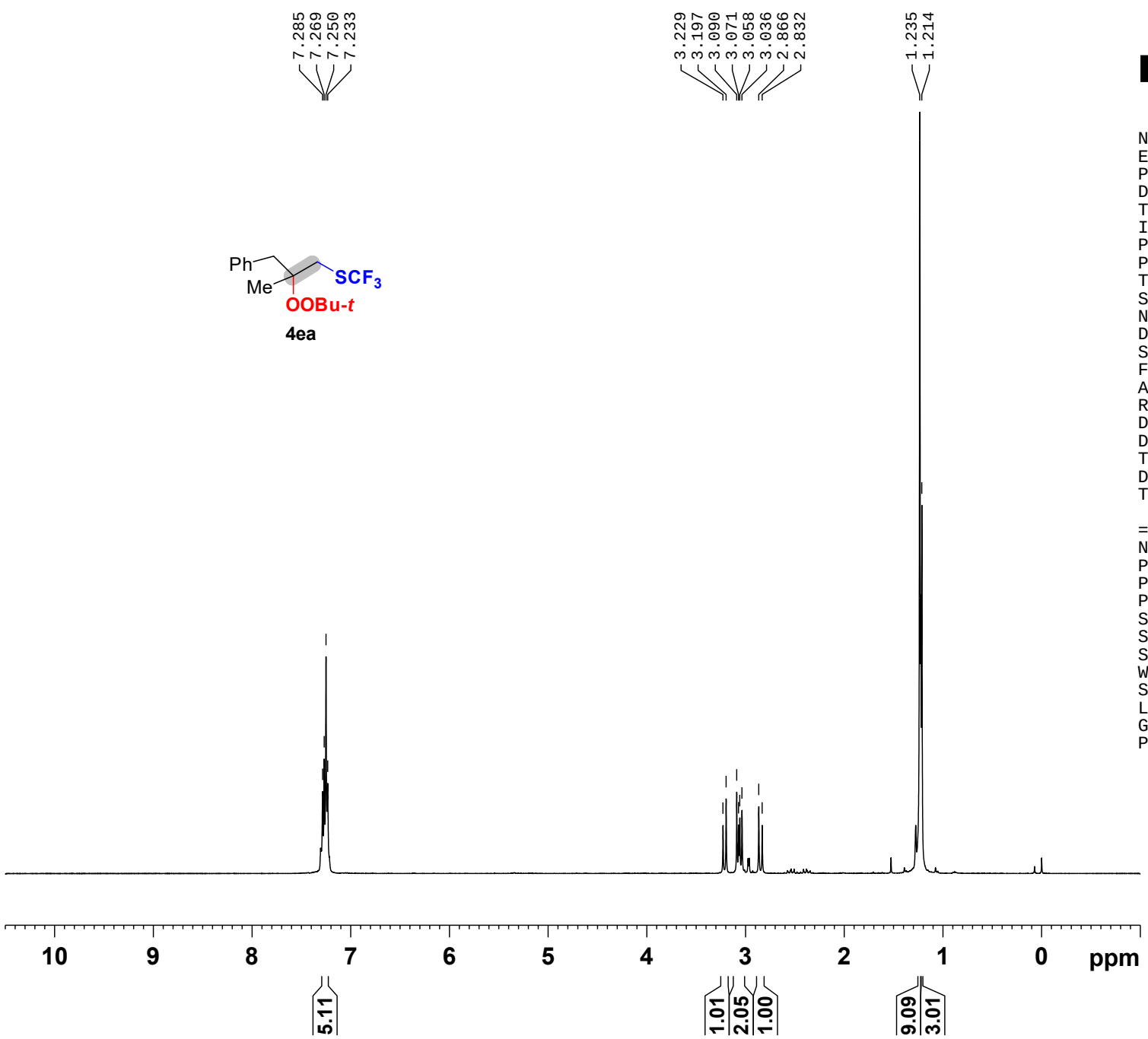
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL13               15.50 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
PL13W         0.38087484 W
SFO2        400.1316005 MHz
SI                 32768
SF          100.6127697 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                  1.40
```




```
NAME      cyjm8p-20190516
EXPNO                  3
PROCNO                 1
Date_           20040129
Time               10.34
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG         zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     32
DS                      4
SWH             89285.711 Hz
FIDRES          0.681196 Hz
AQ              0.7340532 sec
RG                    812
DW                  5.600 usec
DE                  6.50 usec
TE                  300.0 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                    1

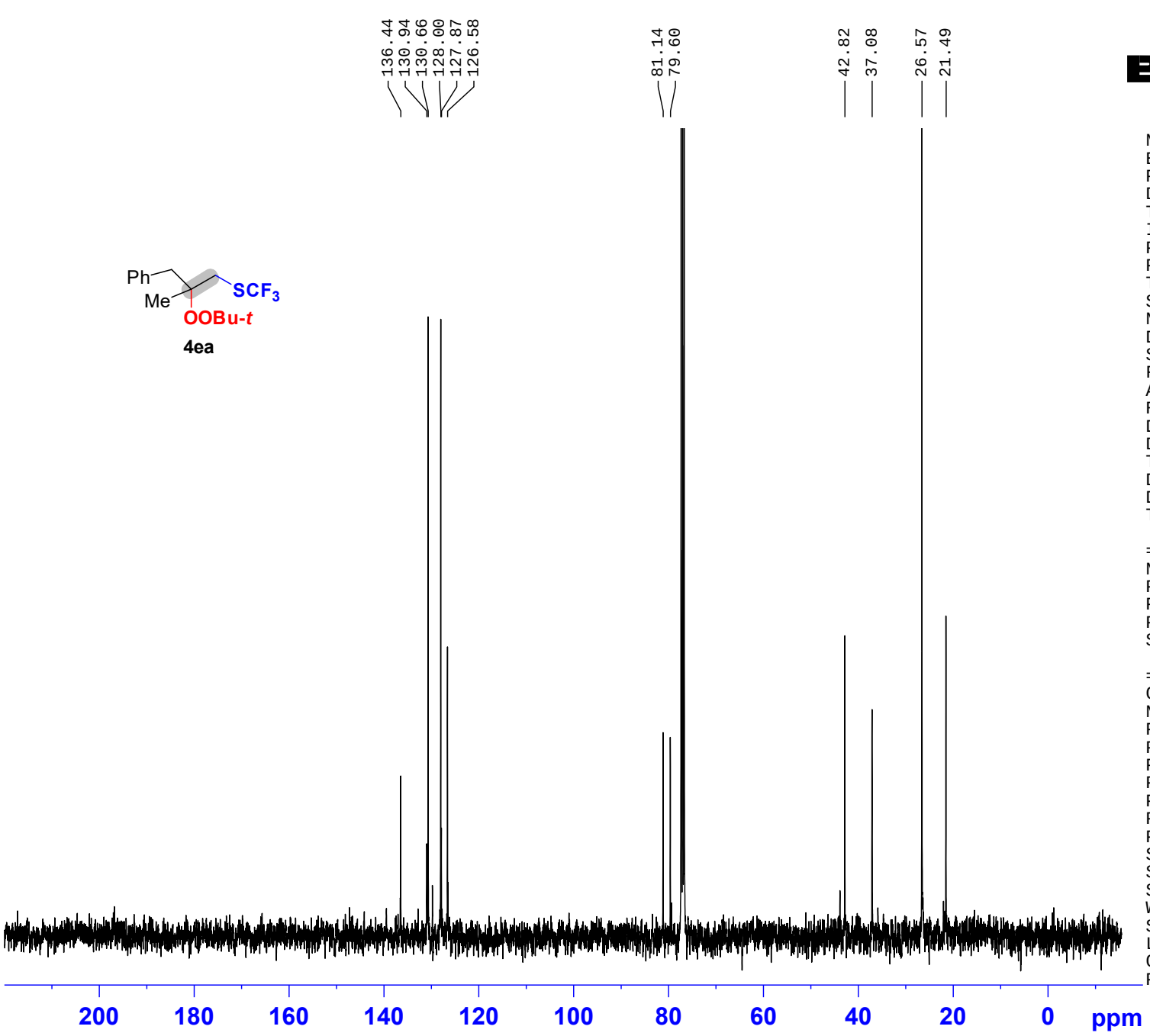
======== CHANNEL f1 ========
NUC1                  19F
P1                 14.20 usec
PL1                -2.00 dB
PL1W         20.42289734 W
SFO1         376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
SFO2         400.1316005 MHz
SI                 65536
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.00
```




```
NAME      cyj818cp-20181224
EXPNO                     1
PROCNO                    1
Date_              20181224
Time                   9.07
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                6393.862 Hz
FIDRES             0.195125 Hz
AQ                 2.5625076 sec
RG                      128
DW                   78.200 usec
DE                    6.50 usec
TE                   295.4 K
D1                1.00000000 sec
TD0                       1

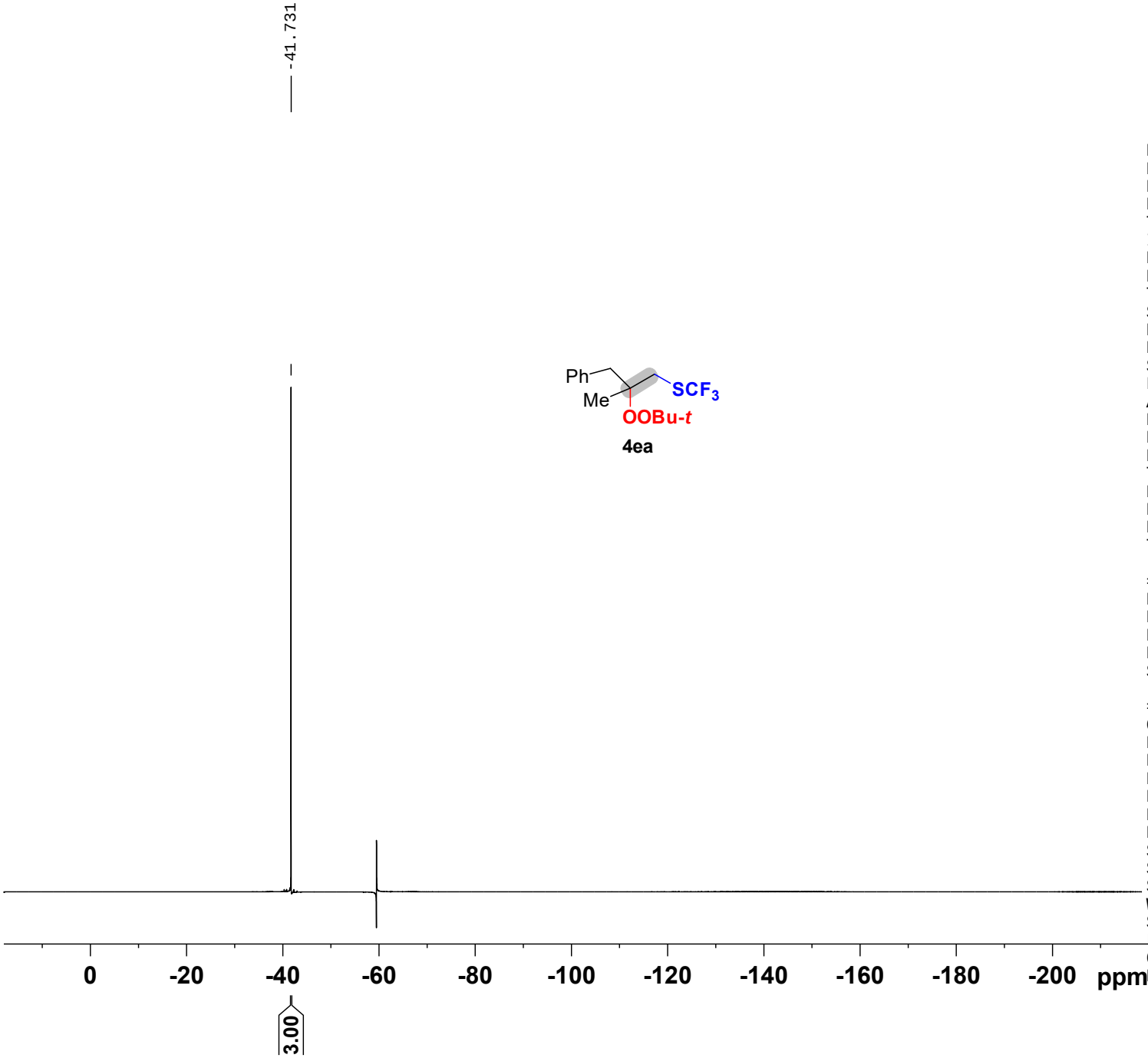
======== CHANNEL f1 ========
NUC1                      1H
P1                     10.40 usec
PL1                    -1.00 dB
PL1W           17.01305389 W
SFO1           400.1326008 MHz
SI                    32768
SF             400.1300153 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```




```
NAME      cyj818cp-20181224
EXPNO                     2
PROCNO                    1
Date_              20181224
Time                   9.11
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      168
DS                        4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                      181
DW                   19.800 usec
DE                    6.50 usec
TE                   296.6 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       3

======== CHANNEL f1 ========
NUC1                    13C
P1                   15.00 usec
PL1                   2.00 dB
PL1W            55.31277084 W
SFO1           100.6238364 MHz

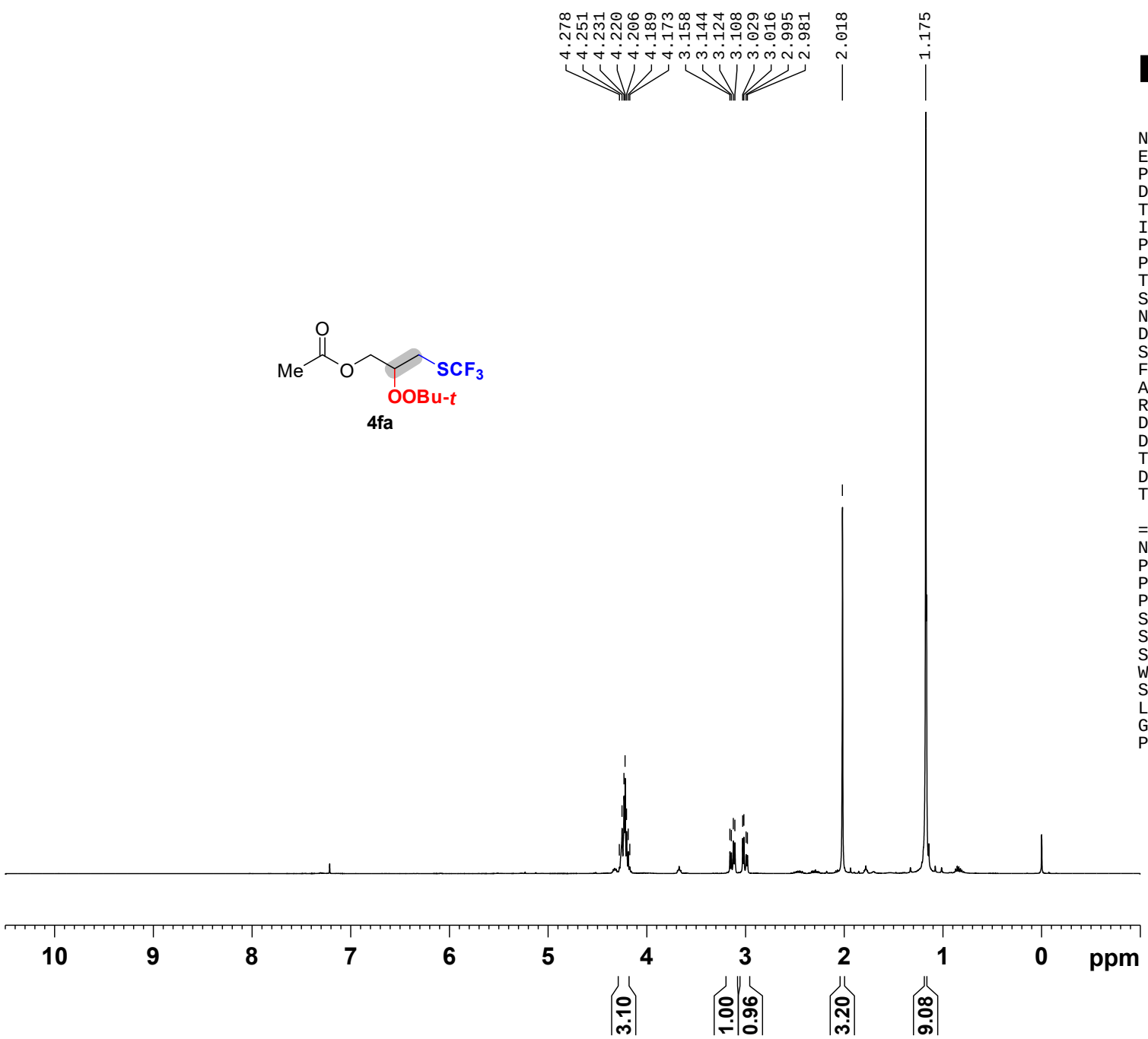
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
PL13W            0.38087484 W
SFO2           400.1316005 MHz
SI                    32768
SF             100.6127709 MHz
WDW                      EM
SSB                       0
LB                    3.00 Hz
GB                        0
PC                     1.40
```




```
NAME      cyj818cp-20190328
EXPNO                     3
PROCNO                    1
Date_              20190328
Time                  20.14
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       32
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                      812
DW                    5.600 usec
DE                     6.50 usec
TE                    292.7 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       1

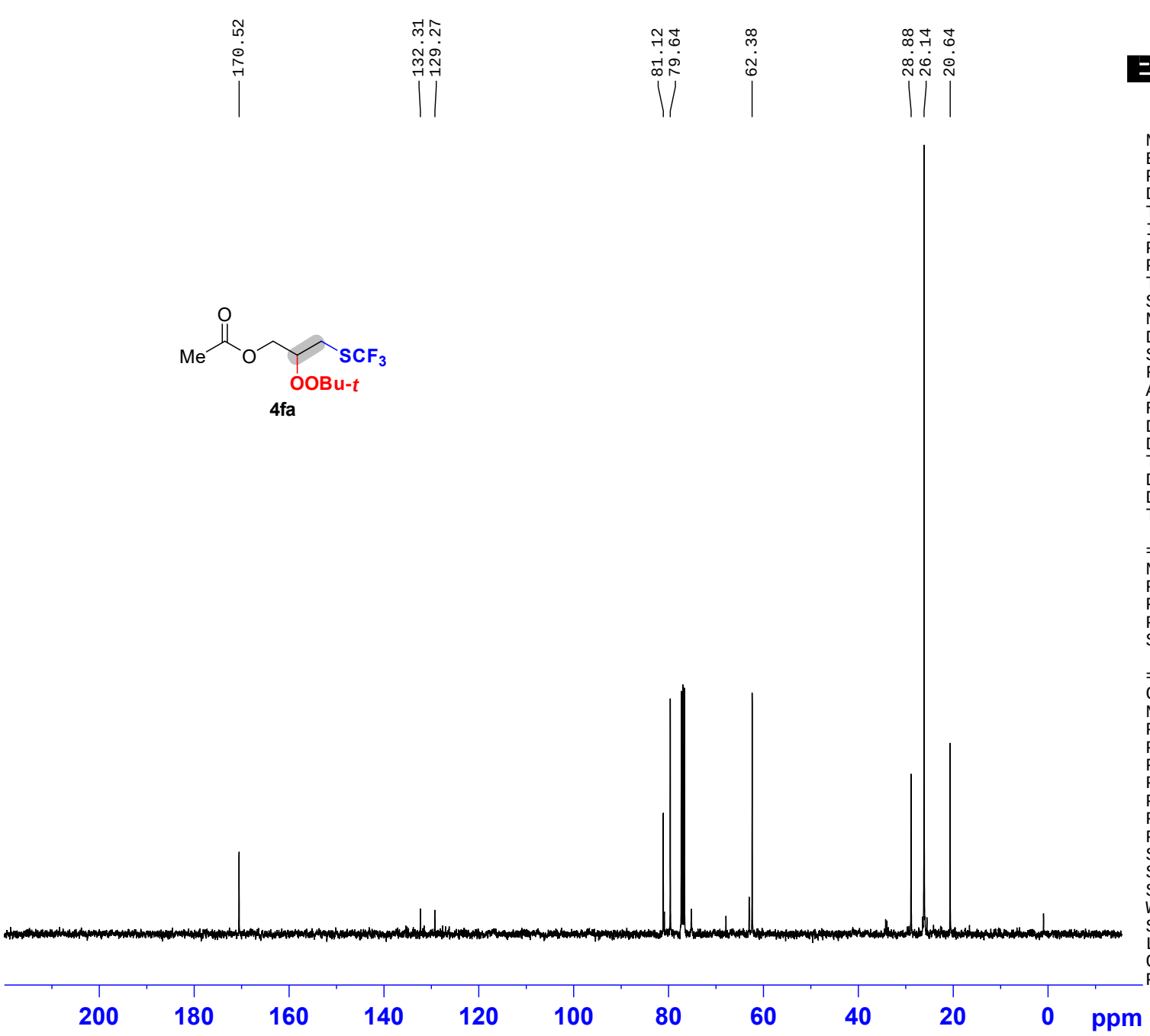
======== CHANNEL f1 ========
NUC1                     19F
P1                    14.20 usec
PL1                   -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                    65536
SF              376.4983660 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.00
```




```
NAME      cyjm9p-20190328
EXPNO                   1
PROCNO                  1
Date_            20190328
Time                19.12
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6393.862 Hz
FIDRES           0.195125 Hz
AQ               2.5625076 sec
RG                     64
DW                 78.200 usec
DE                  6.50 usec
TE                 292.3 K
D1              1.00000000 sec
TD0                     1

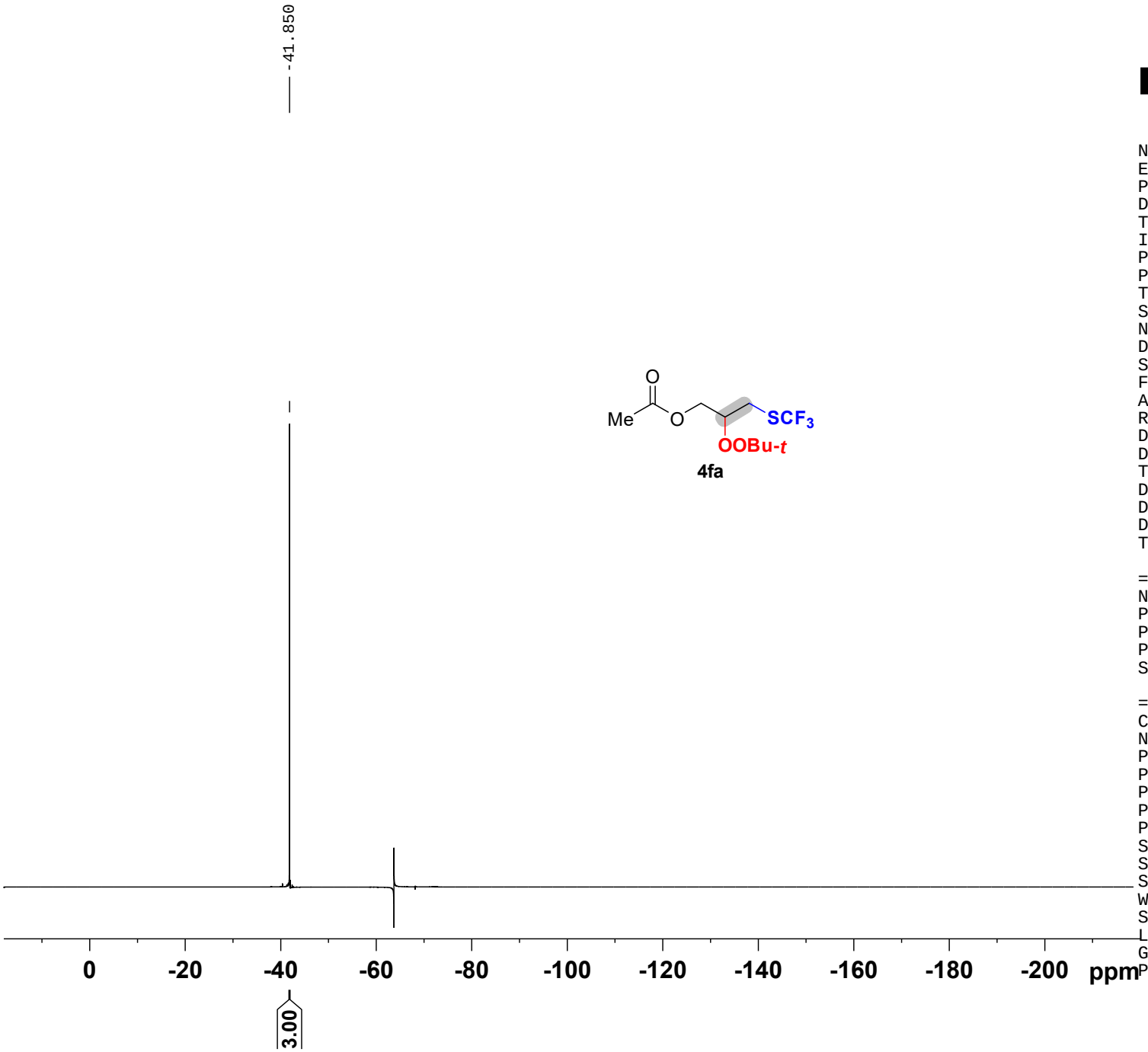
======== CHANNEL f1 ========
NUC1                   1H
P1                 10.40 usec
PL1                -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                  32768
SF           400.1300288 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```




```
NAME      cyjm9p-20190328
EXPNO                   2
PROCNO                  1
Date_            20190328
Time                19.17
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    72
DS                     4
SWH            25252.525 Hz
FIDRES           0.385323 Hz
AQ             1.2976629 sec
RG                   181
DW                19.800 usec
DE                 6.50 usec
TE                293.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    3

======== CHANNEL f1 ========
NUC1                  13C
P1                 15.00 usec
PL1                 2.00 dB
PL1W         55.31277084 W
SFO1        100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL13               15.50 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
PL13W         0.38087484 W
SFO2        400.1316005 MHz
SI                 32768
SF          100.6127722 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                  1.40
```

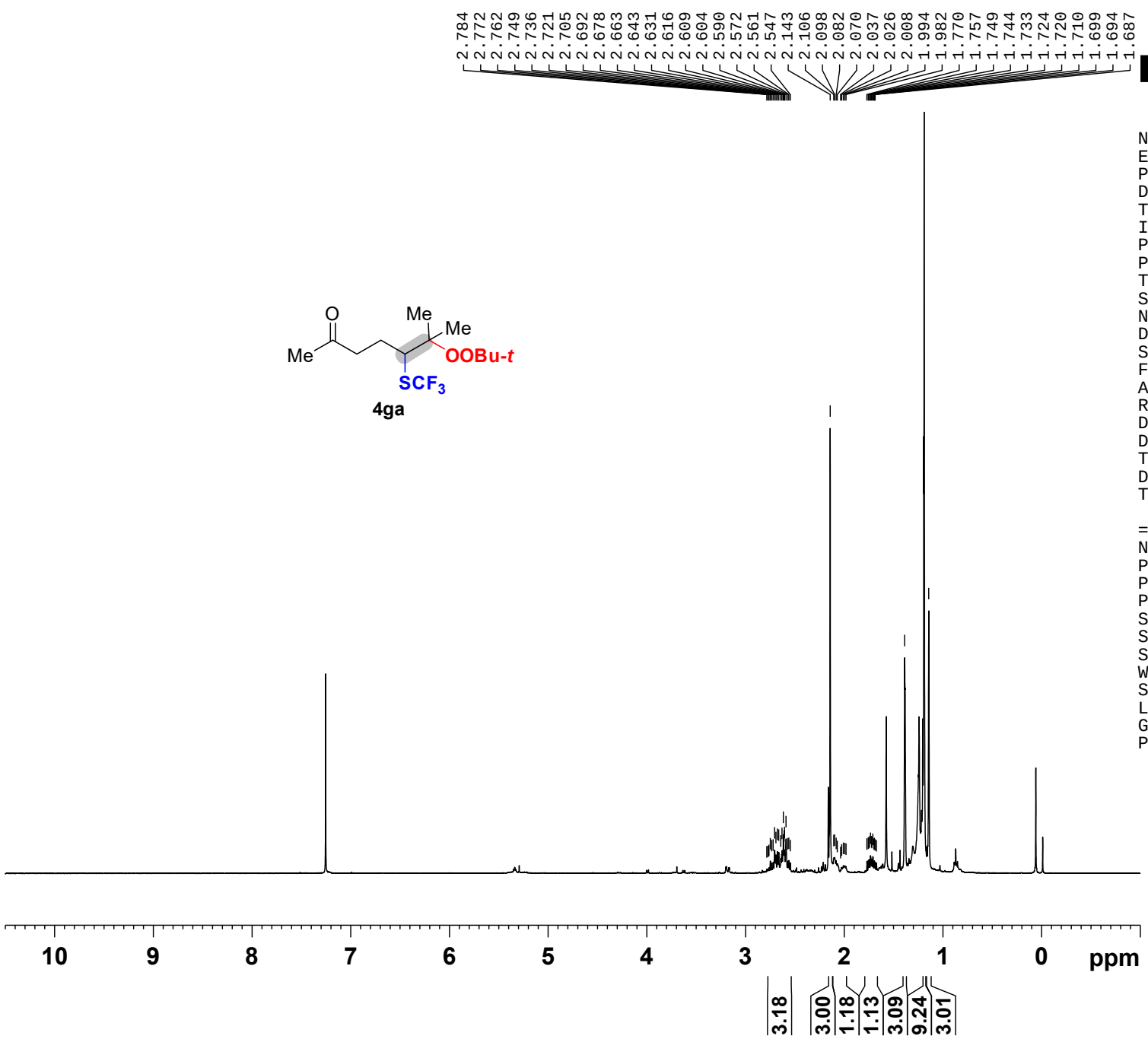


4fa

```
NAME      cyjm9p-20190328
EXPNO                   3
PROCNO                  1
Date_            20190328
Time                19.23
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     32
DS                      4
SWH             89285.711 Hz
FIDRES              0.681196 Hz
AQ                0.7340532 sec
RG                    812
DW                  5.600 usec
DE                  6.50 usec
TE                  292.8 K
D1              1.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   19F
P1                  14.20 usec
PL1                 -2.00 dB
PL1W          20.42289734 W
SFO1          376.4607164 MHz

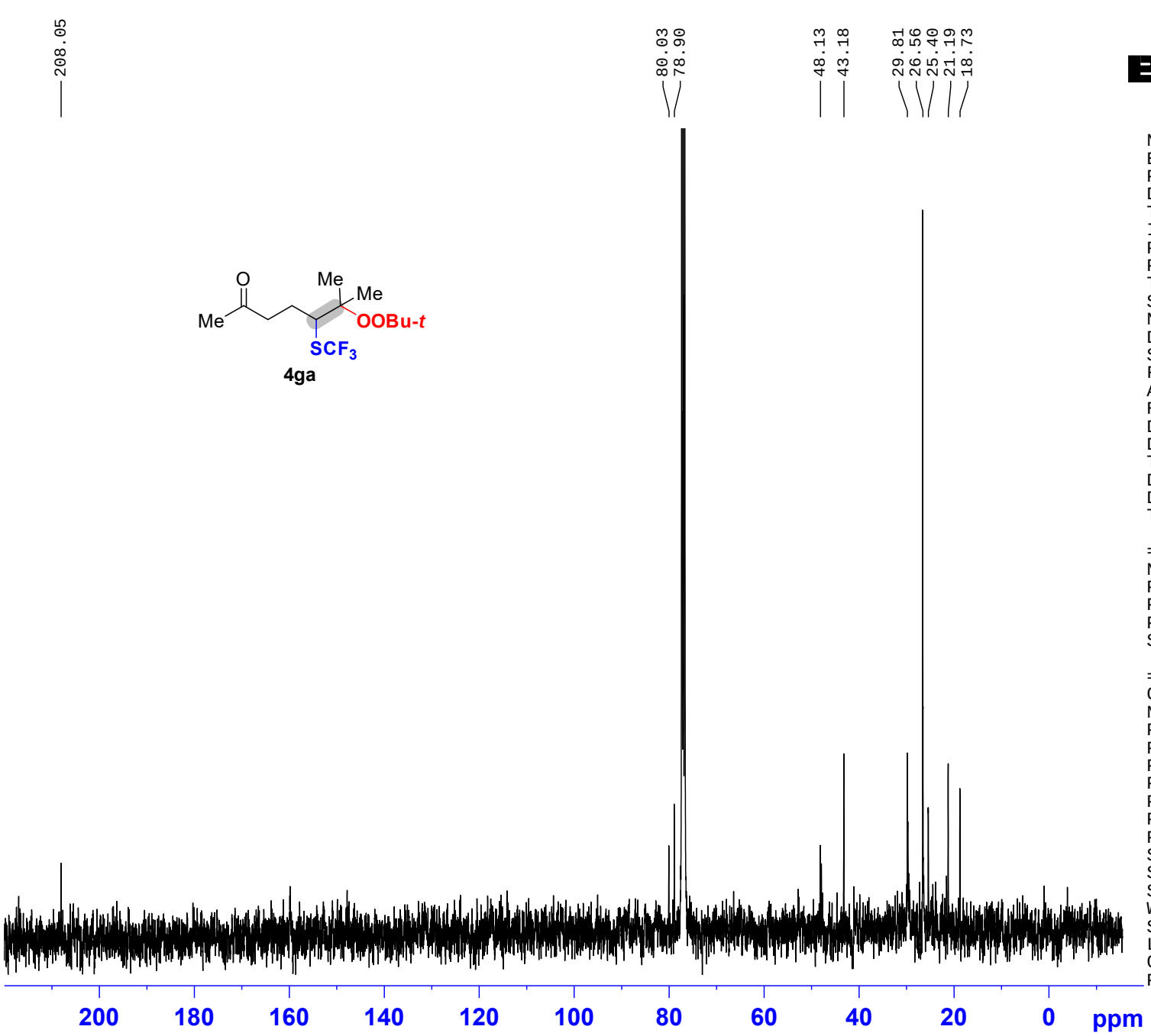
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
SFO2          400.1316005 MHz
SI                  65536
SF            376.4983660 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.00
```



BRUKER

```
NAME      cyj-m10p-20190321
EXPNO                    1
PROCNO                   1
Date_             20190321
Time                 10.21
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ              2.5625076 sec
RG                     287
DW                  78.200 usec
DE                   6.50 usec
TE                  294.2 K
D1             1.00000000 sec
TD0                      1

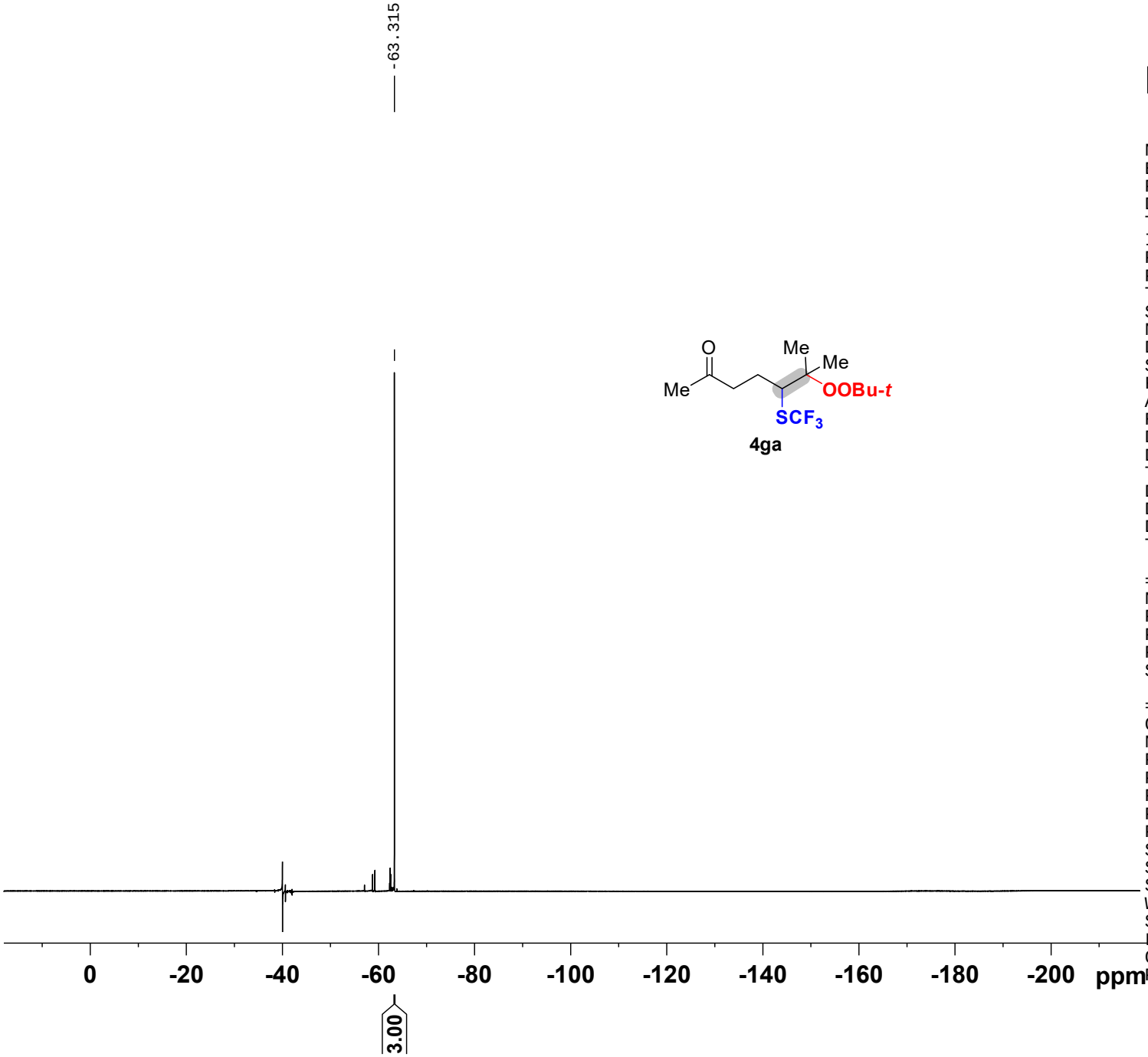
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300128 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```




```
NAME      cyj-m10p-20190321
EXPNO                    2
PROCNO                   1
Date_             20190321
Time                 10.25
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     360
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  295.6 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL13                15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                  32768
SF            100.6127709 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```

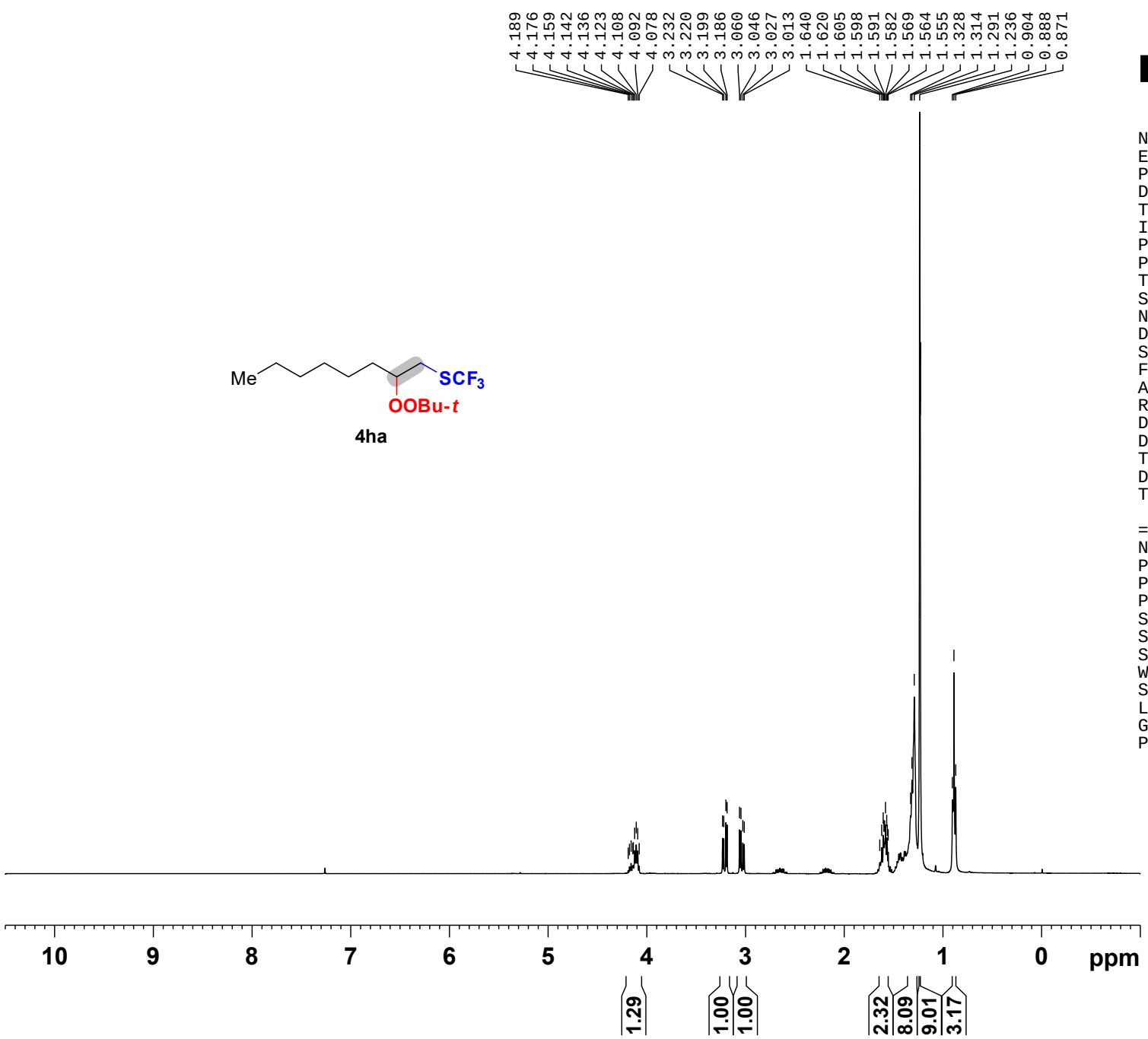


4ga

```
NAME      cyj-m10p-20190321
EXPNO                    3
PROCNO                   1
Date_             20190321
Time                 10.47
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       32
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                      812
DW                    5.600 usec
DE                    6.50 usec
TE                    294.9 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    19F
P1                    14.20 usec
PL1                   -2.00 dB
PL1W           20.42289734 W
SFO1           376.4607164 MHz

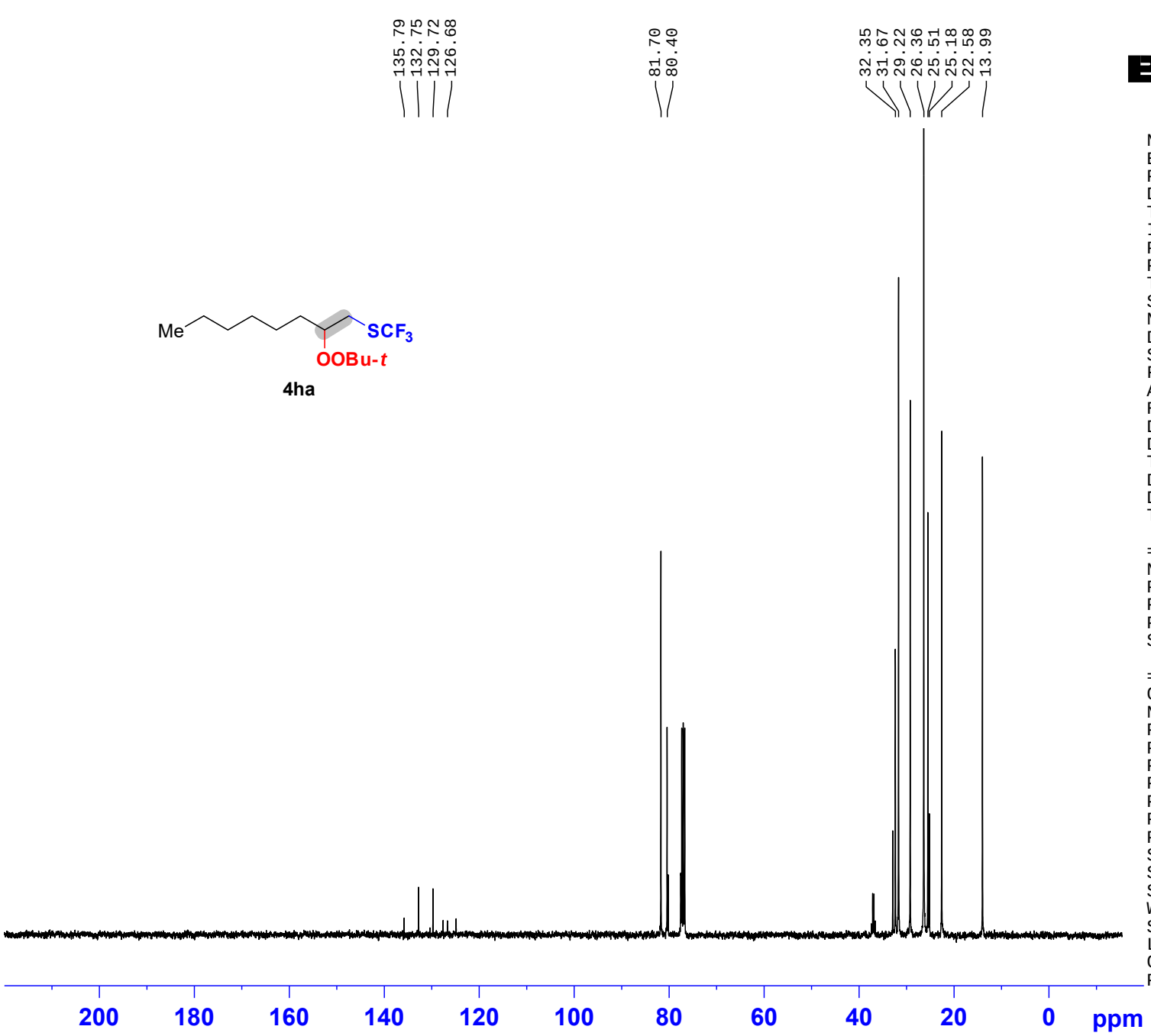
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  16.72 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
SFO2           400.1316005 MHz
SI                    65536
SF             376.4983660 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.00
```



BRUKER

```
NAME      cyjm4p2-20190415
EXPNO                    1
PROCNO                   1
Date_             20190415
Time                 21.24
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                    28.5
DW                  78.200 usec
DE                   6.50 usec
TE                  296.7 K
D1              1.00000000 sec
TD0                      1

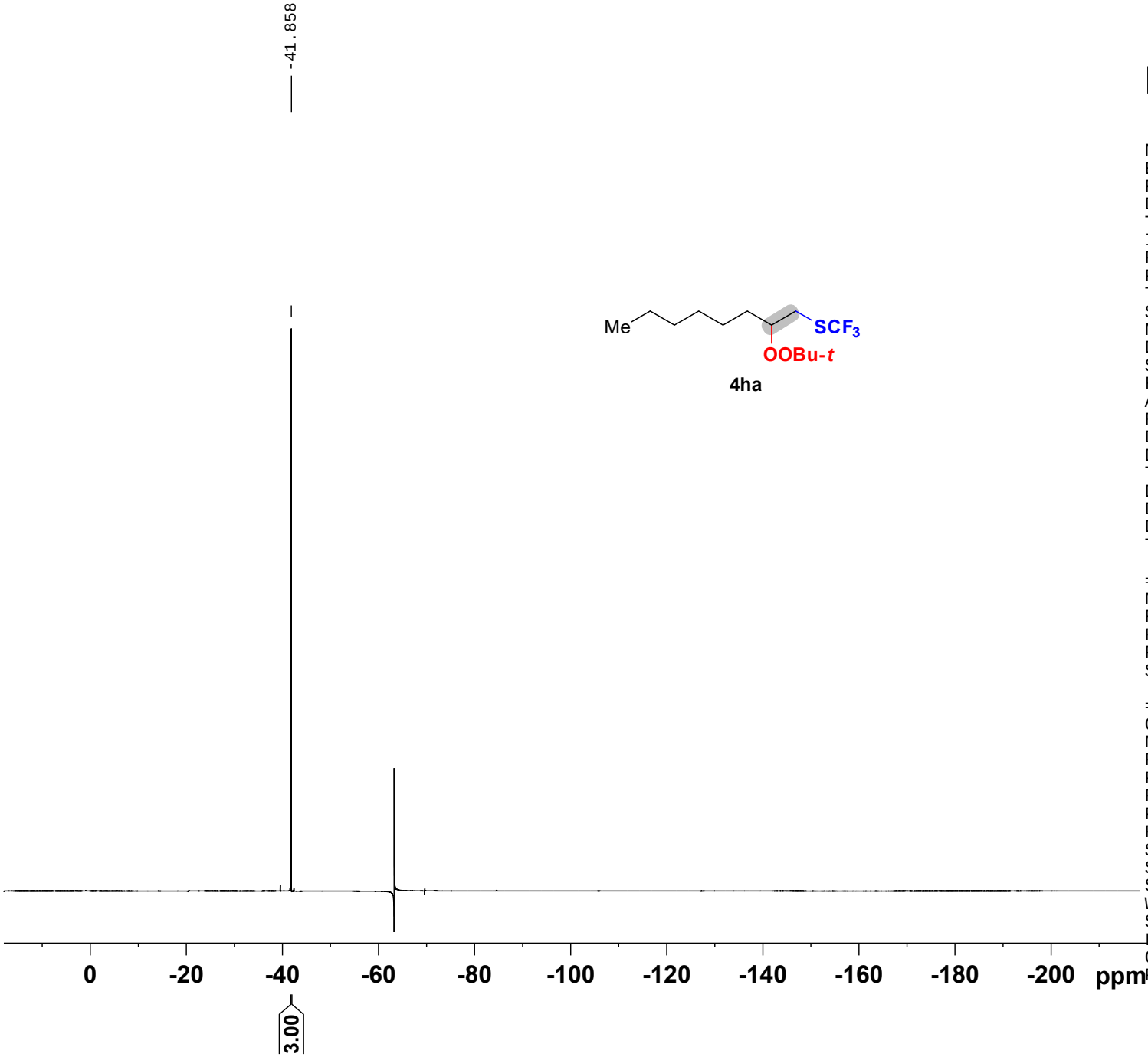
======== CHANNEL f1 ========
NUC1                    1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300105 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cyjm4p-20190415
EXPNO                   2
PROCNO                  1
Date_            20190415
Time                20.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     96
DS                      4
SWH             25252.525 Hz
FIDRES          0.385323 Hz
AQ              1.2976629 sec
RG                    181
DW                19.800 usec
DE                 6.50 usec
TE                 298.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     3

======== CHANNEL f1 ========
NUC1                  13C
P1                 15.00 usec
PL1                 2.00 dB
PL1W         55.31277084 W
SFO1         100.6238364 MHz

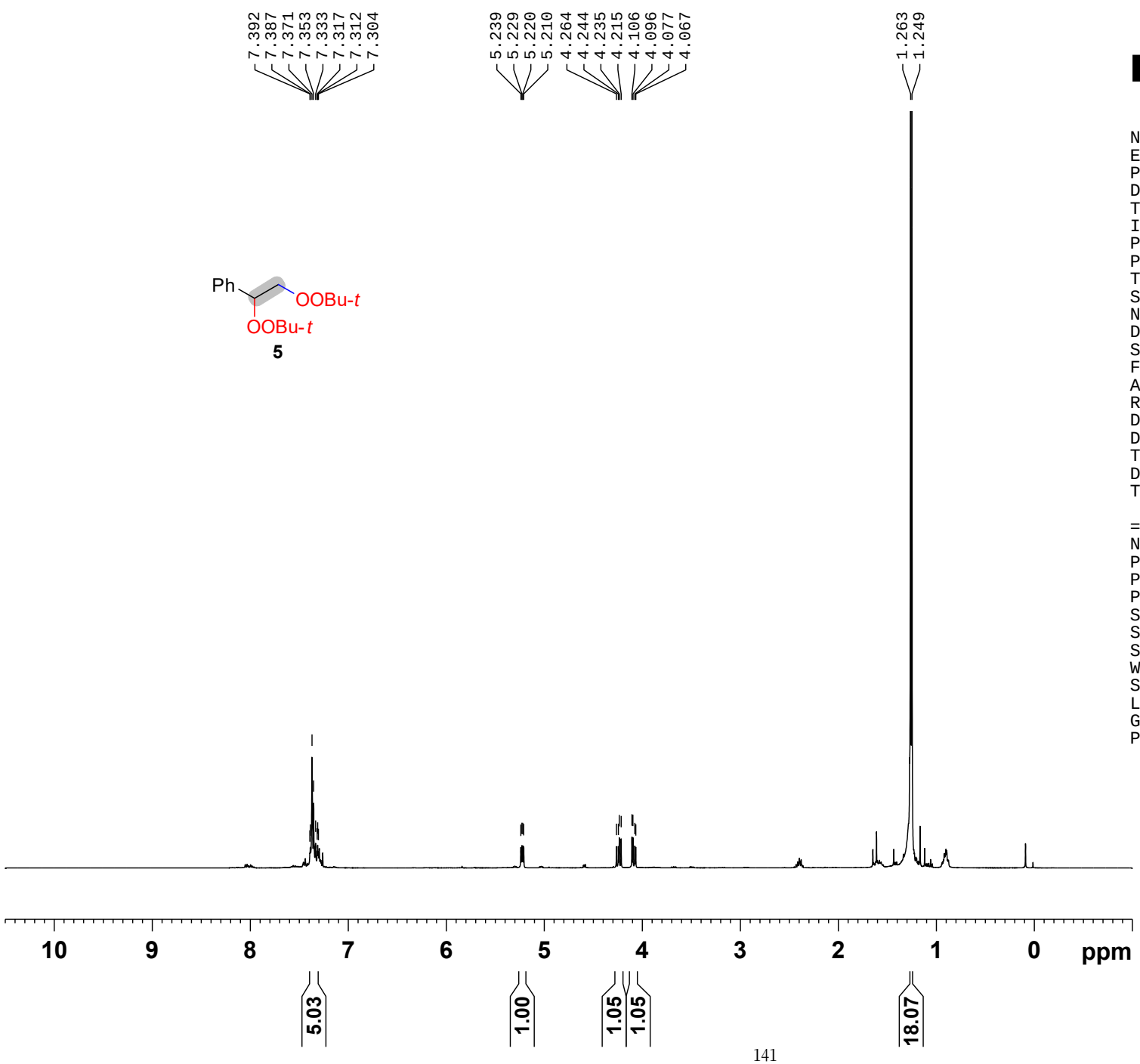
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL13               15.50 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
PL13W         0.38087484 W
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127635 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.40
```




```
NAME      cyjm4p-20190415
EXPNO                   3
PROCNO                  1
Date_            20190415
Time                20.36
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     64
DS                      4
SWH             89285.711 Hz
FIDRES          0.681196 Hz
AQ              0.7340532 sec
RG                   2050
DW                5.600 usec
DE                6.50 usec
TE                297.0 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                     4

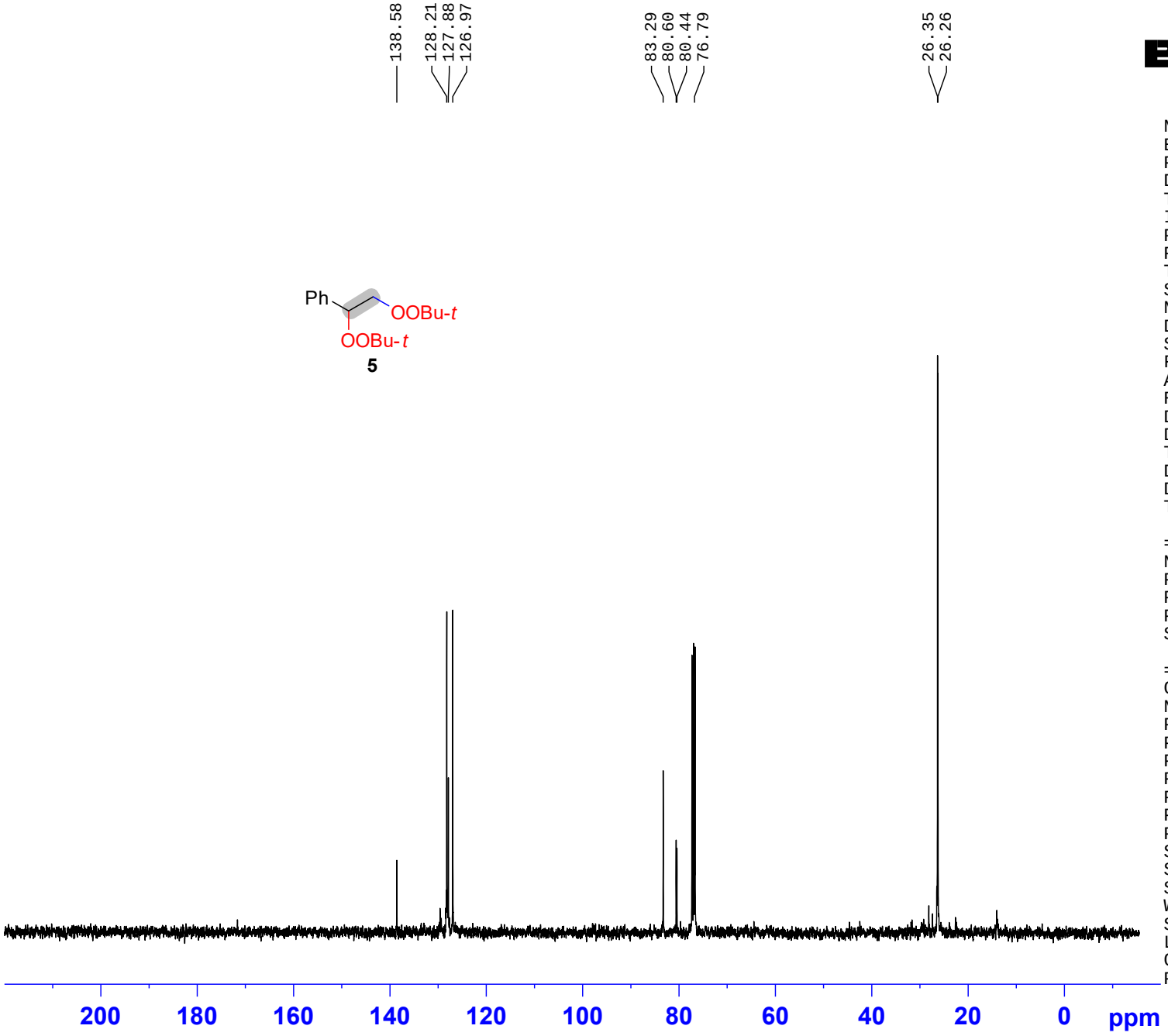
======== CHANNEL f1 ========
NUC1                   19F
P1                  14.20 usec
PL1                 -2.00 dB
PL1W         20.42289734 W
SFO1         376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.72 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
SFO2         400.1316005 MHz
SI                  65536
SF           376.4983660 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cms27ap1-20191126
EXPNO                    1
PROCNO                   1
Date_             20191126
Time                 16.28
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                      64
DW                  78.200 usec
DE                   6.50 usec
TE                  295.8 K
D1              1.00000000 sec
TD0                      1

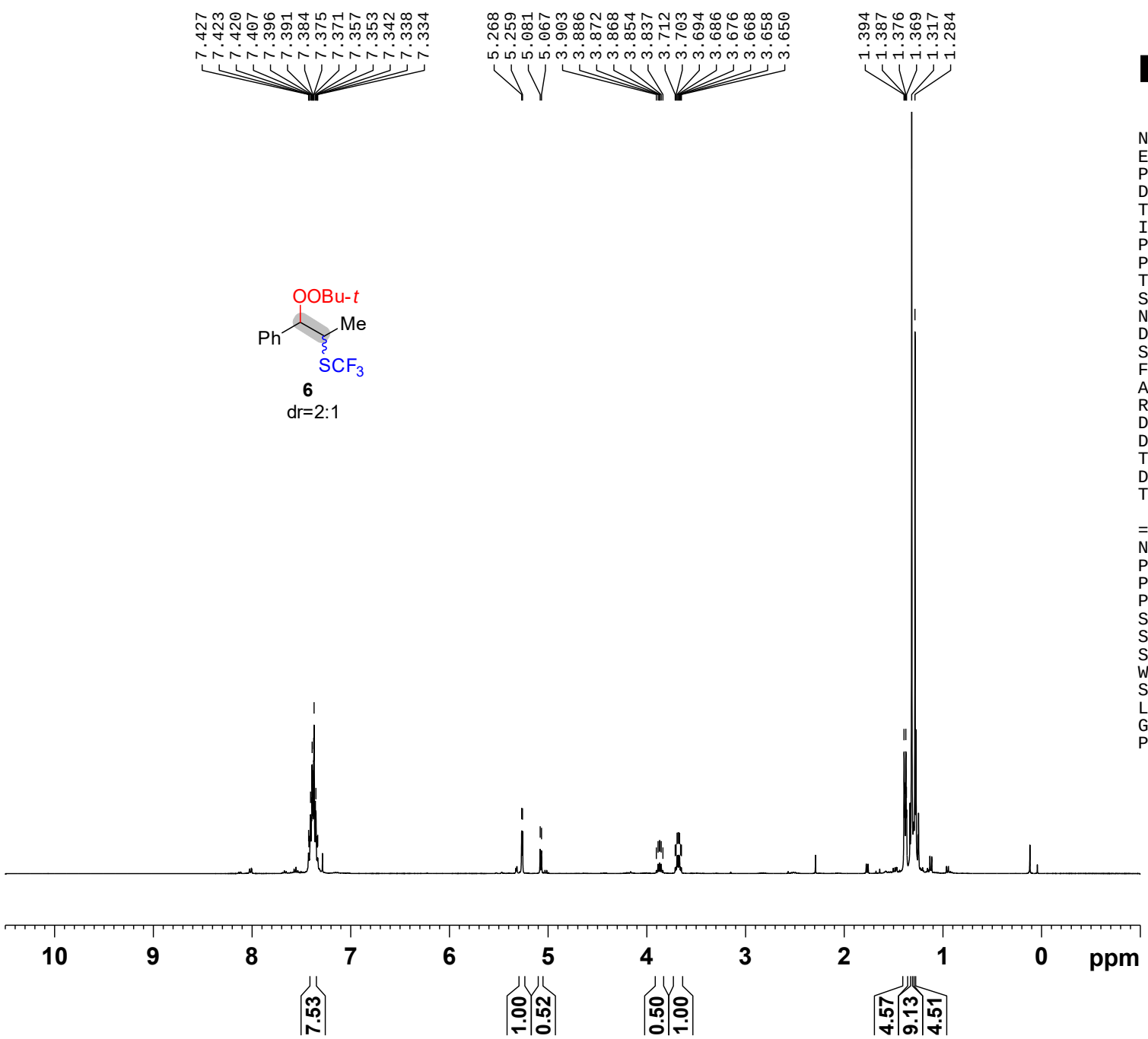
======== CHANNEL f1 ========
NUC1                    1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300092 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                  1.00
```




```
NAME      cms27ap1-20191129
EXPNO                    2
PROCNO                   1
Date_             20191128
Time                 9.37
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      40
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                    2050
DW                  19.800 usec
DE                   6.50 usec
TE                  296.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

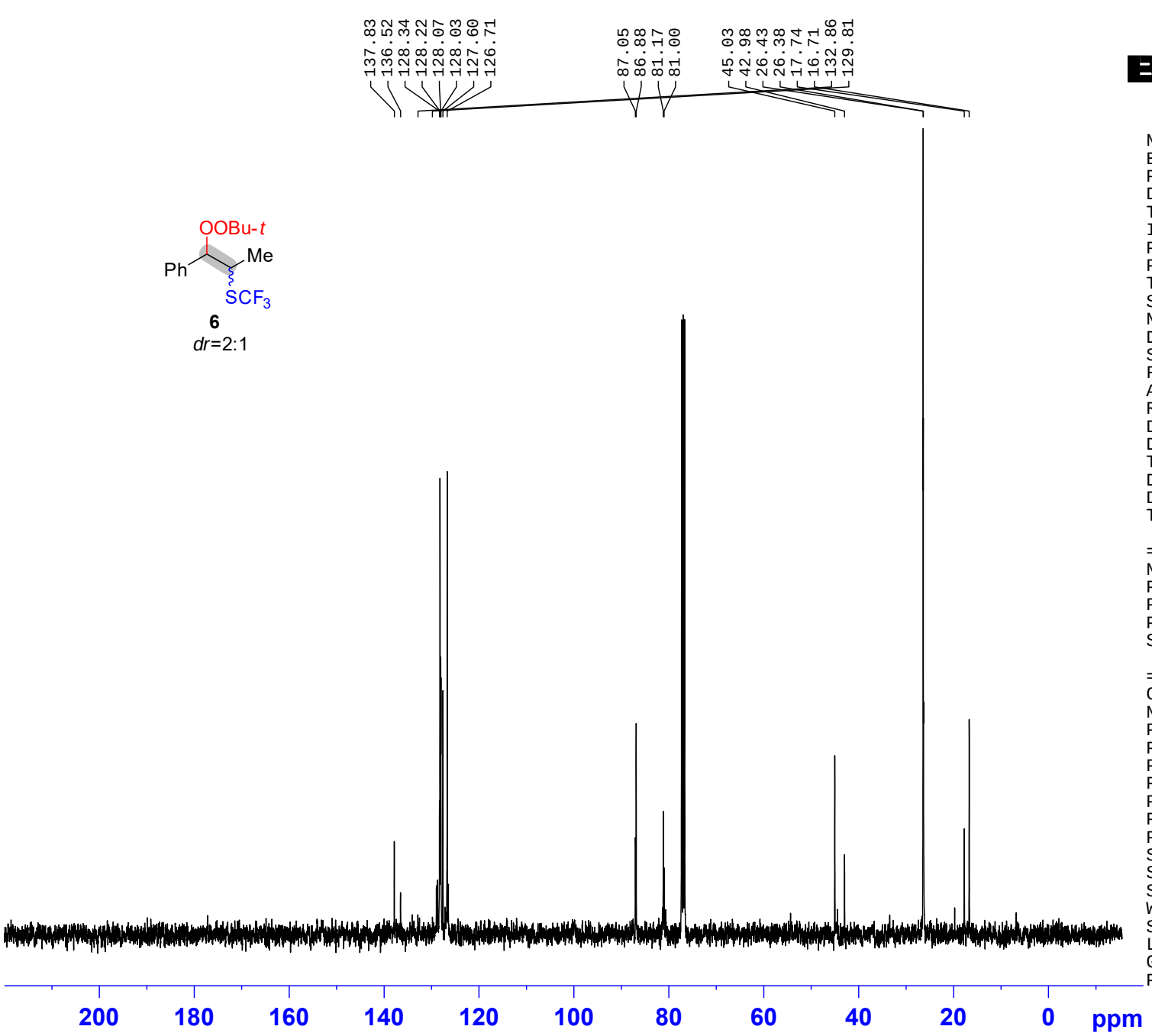
======== CHANNEL f1 ========
NUC1                   13C
P1                   15.00 usec
PL1                   2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                   32768
SF            100.6127742 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```




```
NAME      cyj876cp-20190410
EXPNO                    1
PROCNO                   1
Date_             20190410
Time                 20.13
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                    90.5
DW                  78.200 usec
DE                   6.50 usec
TE                  293.4 K
D1             1.00000000 sec
TD0                      1

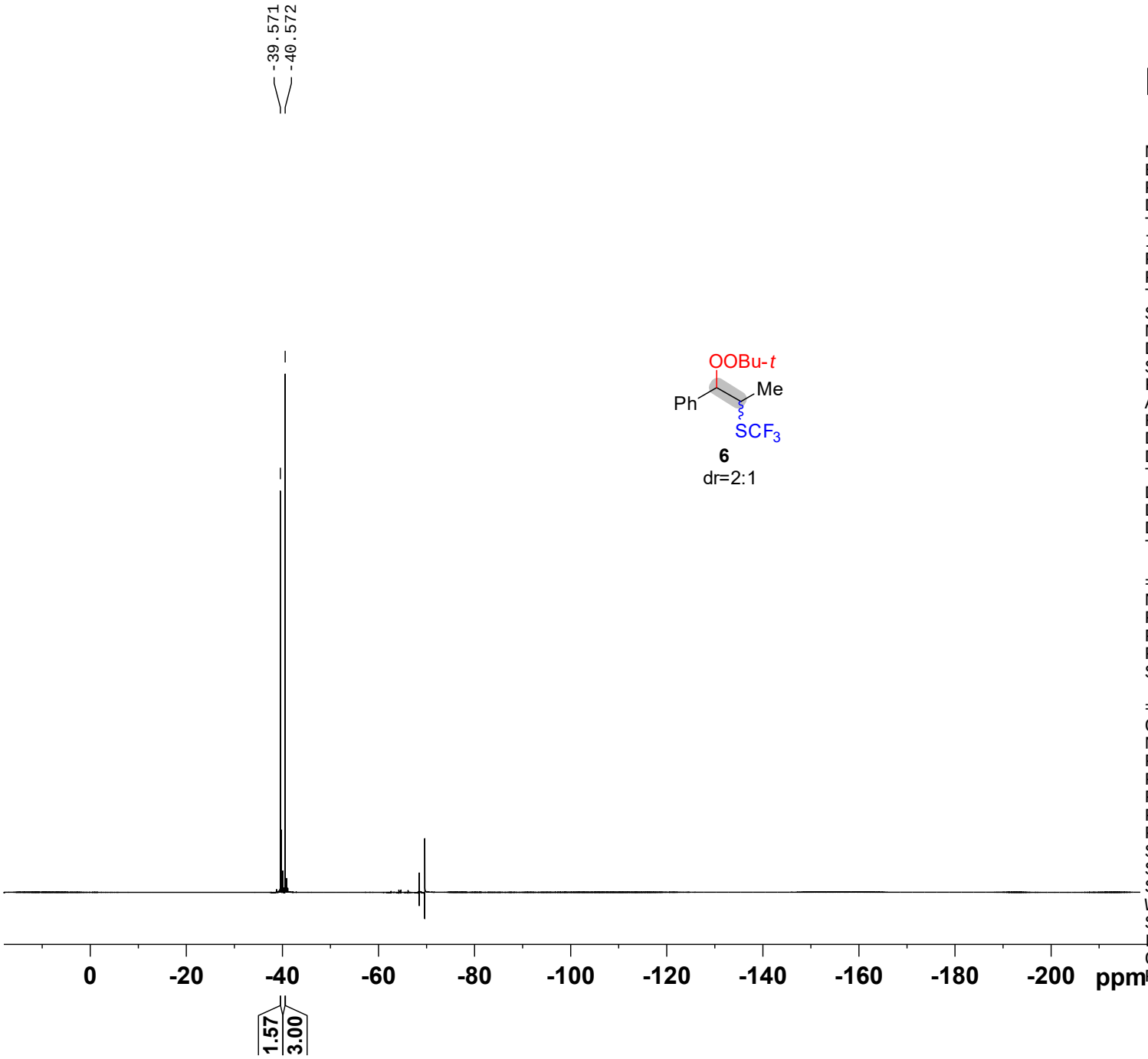
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                   1.00
```




```
NAME      cyj876cp-20190410
EXPNO                    2
PROCNO                   1
Date_             20190410
Time                 20.18
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       64
DS                        4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                      181
DW                   19.800 usec
DE                    6.50 usec
TE                   294.6 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       3

======== CHANNEL f1 ========
NUC1                    13C
P1                   15.00 usec
PL1                   2.00 dB
PL1W            55.31277084 W
SFO1            100.6238364 MHz

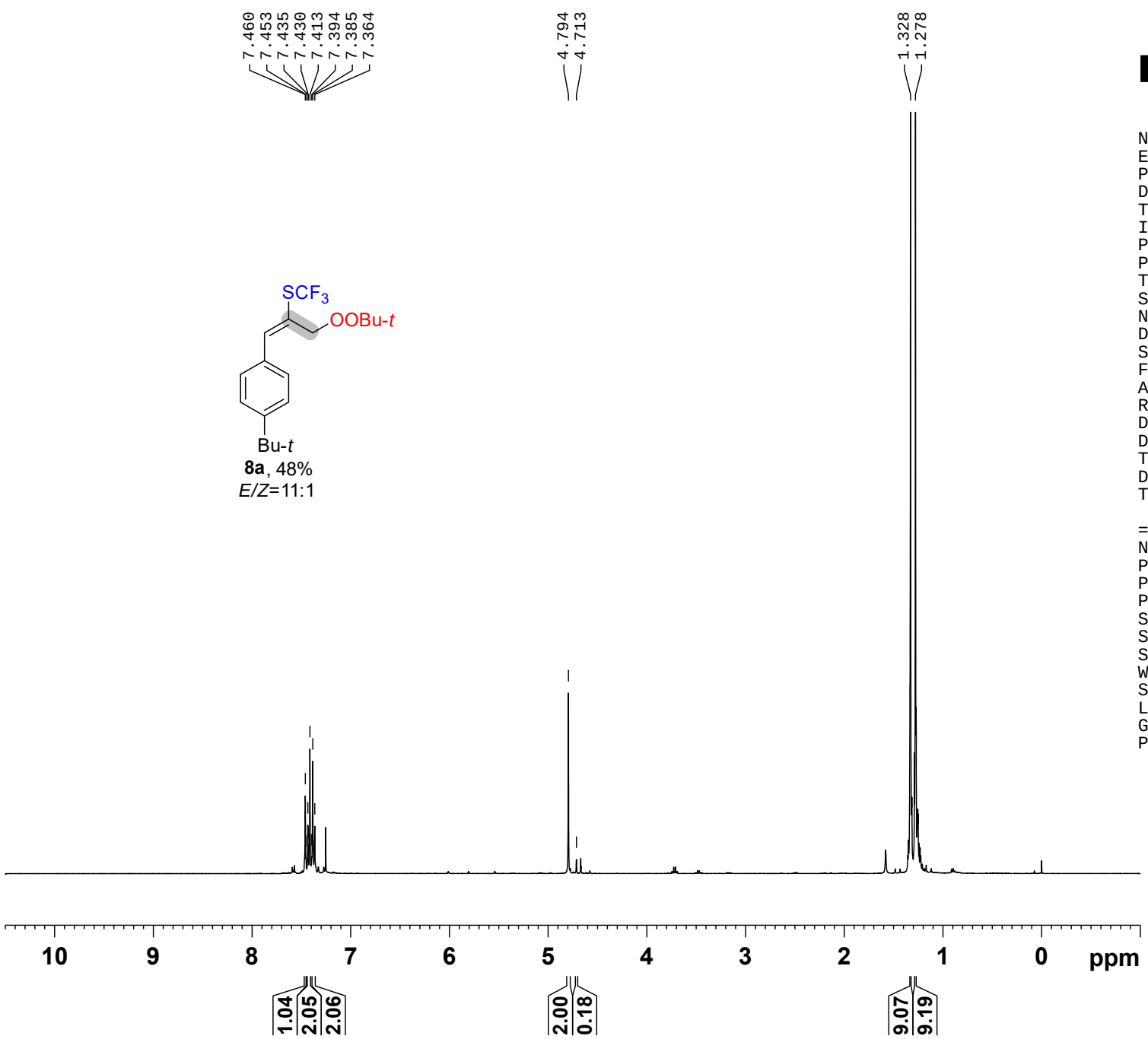
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
PL13W            0.38087484 W
SFO2            400.1316005 MHz
SI                    32768
SF              100.6127723 MHz
WDW                      EM
SSB                       0
LB                    3.00 Hz
GB                        0
PC                     1.40
```




```
NAME      cyj876cp-20190410
EXPNO                    3
PROCNO                   1
Date_             20190410
Time                 20.23
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      64
DS                       4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                    2050
DW                   5.600 usec
DE                   6.50 usec
TE                  293.8 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                      4

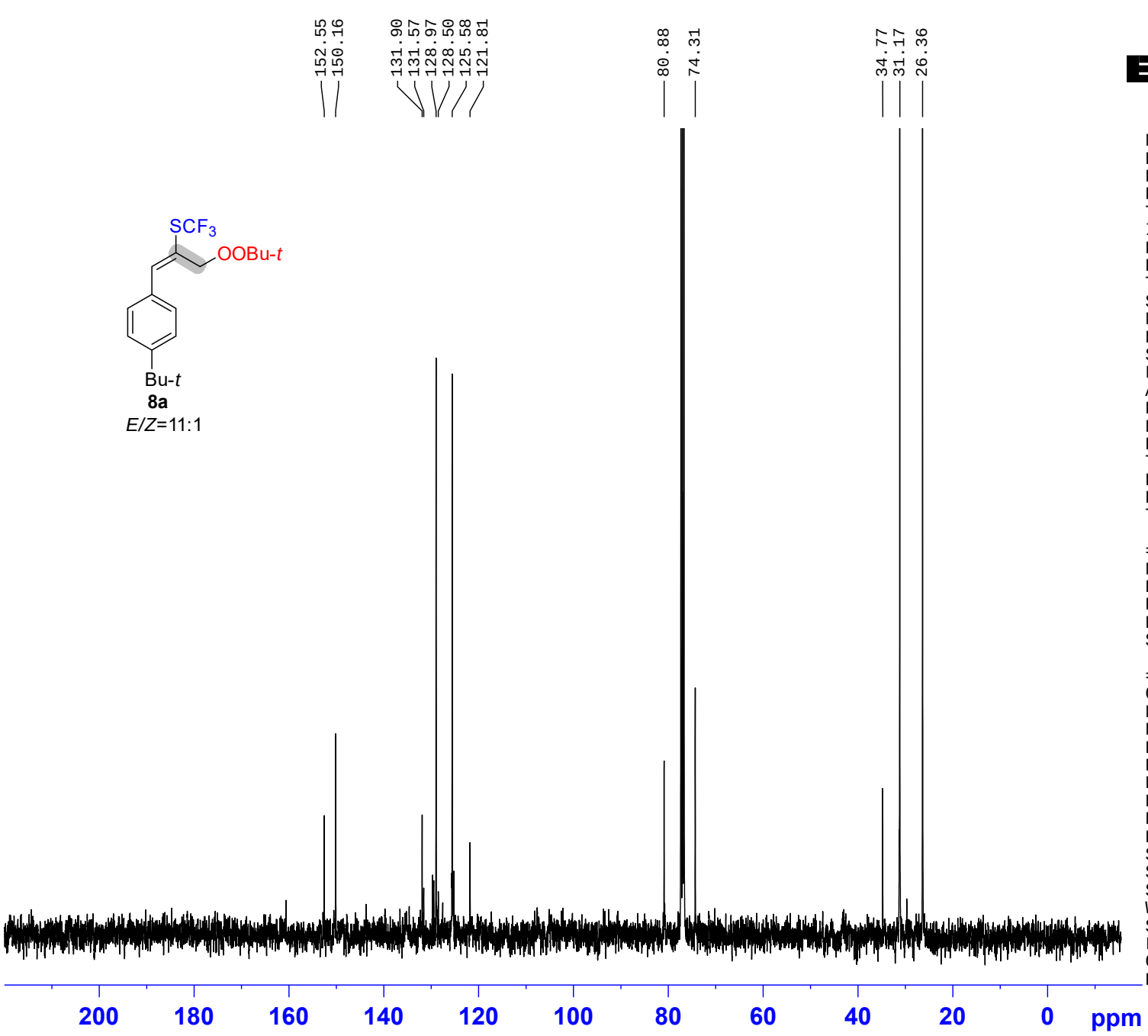
======== CHANNEL f1 ========
NUC1                   19F
P1                   14.20 usec
PL1                  -2.00 dB
PL1W          20.42289734 W
SFO1          376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
SFO2          400.1316005 MHz
SI                  65536
SF            376.4983660 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cyj960ap-20190712
EXPNO                    1
PROCNO                   1
Date_             20040325
Time                 23.18
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ              2.5625076 sec
RG                    80.6
DW                  78.200 usec
DE                   6.50 usec
TE                  295.3 K
D1             1.00000000 sec
TD0                      1

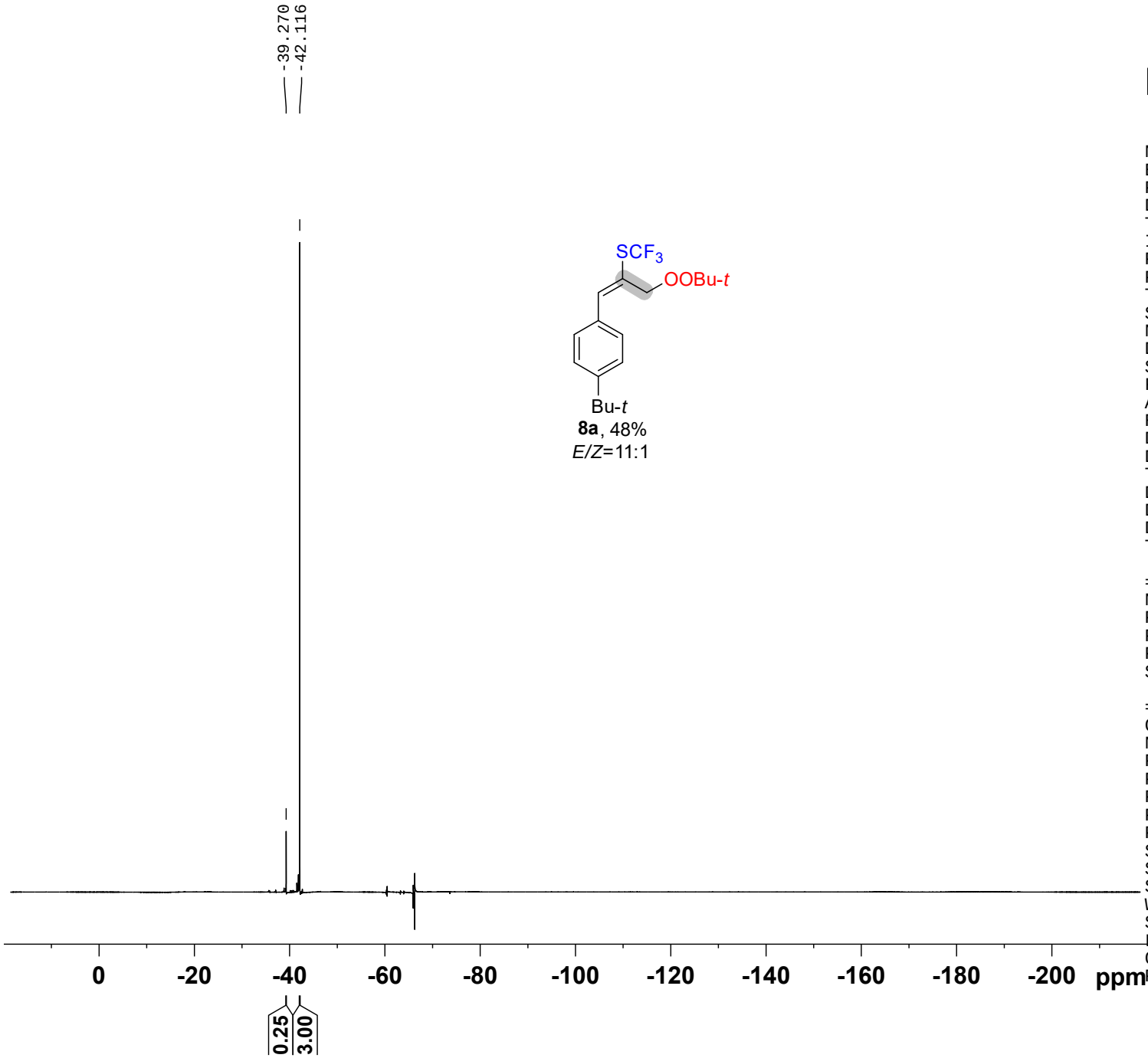
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                   32768
SF           400.1300136 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cyj960ap-20190712
EXPNO                     2
PROCNO                    1
Date_              20040325
Time                  23.24
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       80
DS                        4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                     2050
DW                   19.800 usec
DE                    6.50 usec
TE                   296.8 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       3

======== CHANNEL f1 ========
NUC1                    13C
P1                    15.00 usec
PL1                    2.00 dB
PL1W            55.31277084 W
SFO1            100.6238364 MHz

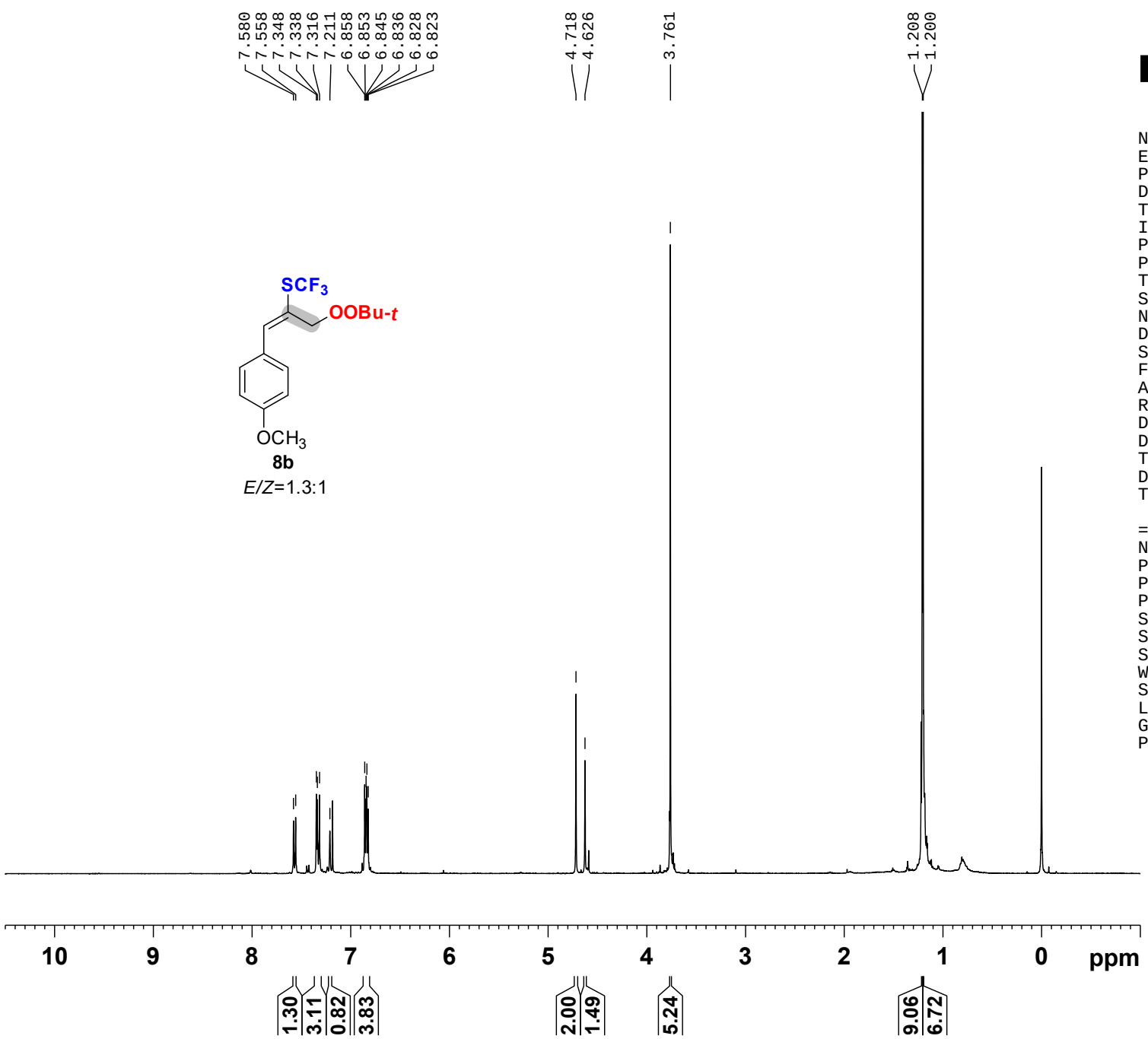
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  16.72 dB
PL13                  15.50 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
PL13W            0.38087484 W
SFO2            400.1316005 MHz
SI                    32768
SF              100.6127711 MHz
WDW                      EM
SSB                       0
LB                    3.00 Hz
GB                        0
PC                    1.40
```




```
NAME      cyj960p-20190712
EXPNO                    3
PROCNO                   1
Date_             20040325
Time                 23.29
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT              CDCl3
NS                      32
DS                       4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                     812
DW                 5.600 usec
DE                 6.50 usec
TE                 295.8 K
D1              1.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                      1

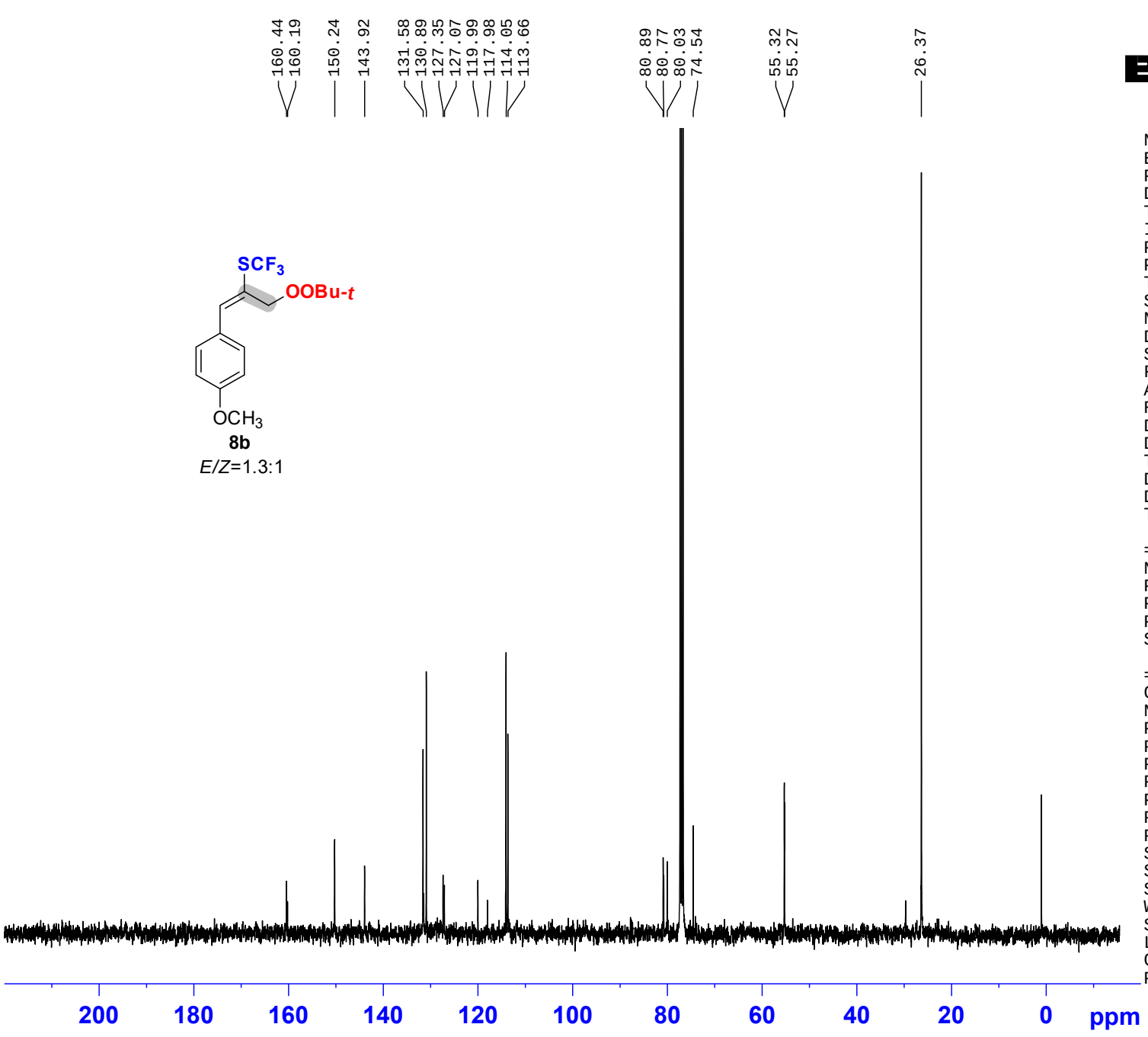
======== CHANNEL f1 ========
NUC1                   19F
P1                 14.20 usec
PL1                -2.00 dB
PL1W         20.42289734 W
SFO1         376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
SFO2         400.1316005 MHz
SI                 65536
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.00
```




```
NAME      cms17p-20191202
EXPNO                   1
PROCNO                  1
Date_            20191202
Time                16.40
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6393.862 Hz
FIDRES           0.195125 Hz
AQ             2.5625076 sec
RG                    144
DW                 78.200 usec
DE                  6.50 usec
TE                 295.7 K
D1           1.00000000 sec
TD0                     1

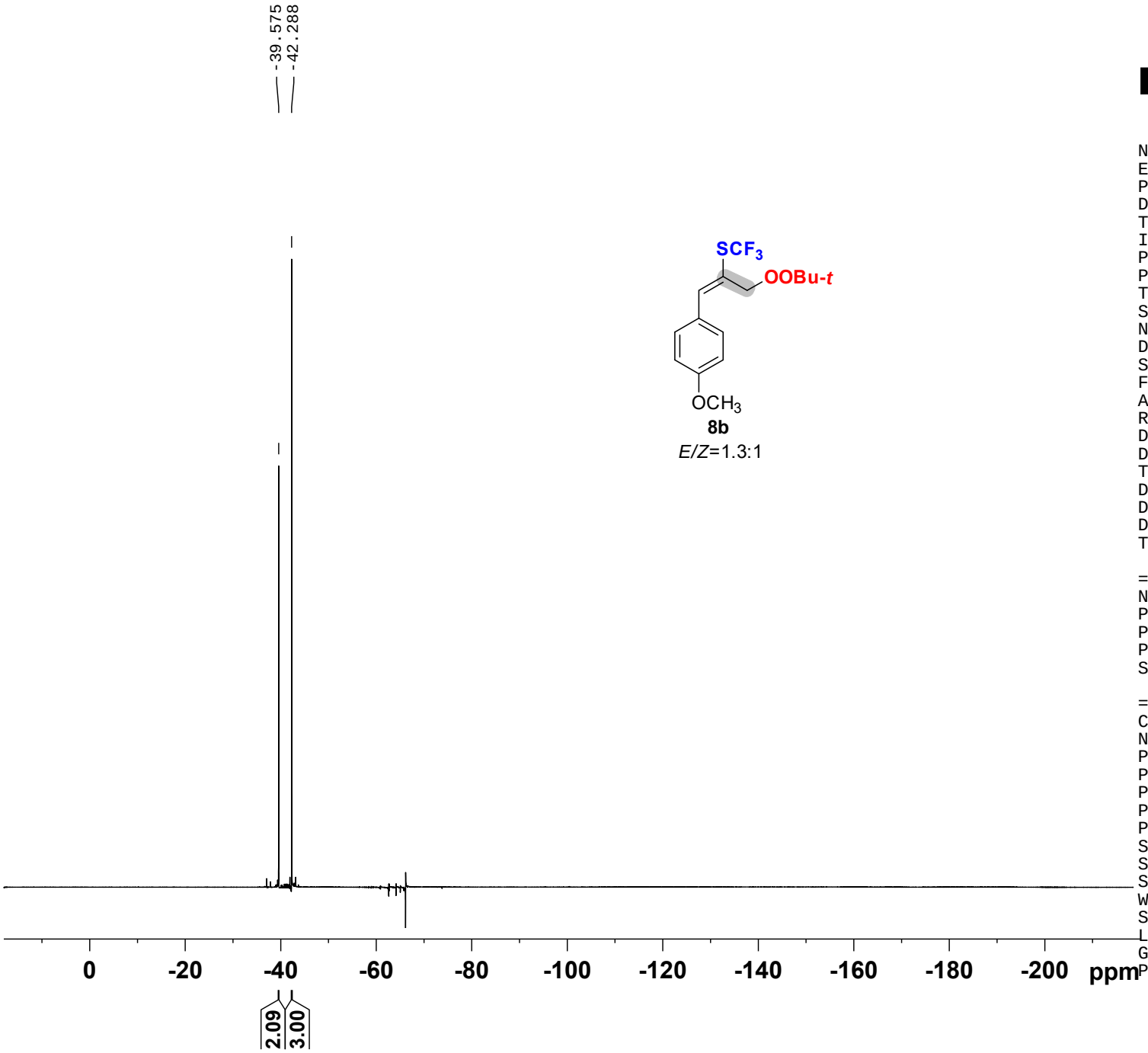
======== CHANNEL f1 ========
NUC1                   1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                  32768
SF           400.1300400 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                  1.00
```




```
NAME      cms17p-20191202
EXPNO                   2
PROCNO                  1
Date_            20191202
Time                17.19
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   184
DS                     4
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976629 sec
RG                  1030
DW                19.800 usec
DE                 6.50 usec
TE                297.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    3

======== CHANNEL f1 ========
NUC1                  13C
P1                 15.00 usec
PL1                 2.00 dB
PL1W         55.31277084 W
SFO1         100.6238364 MHz

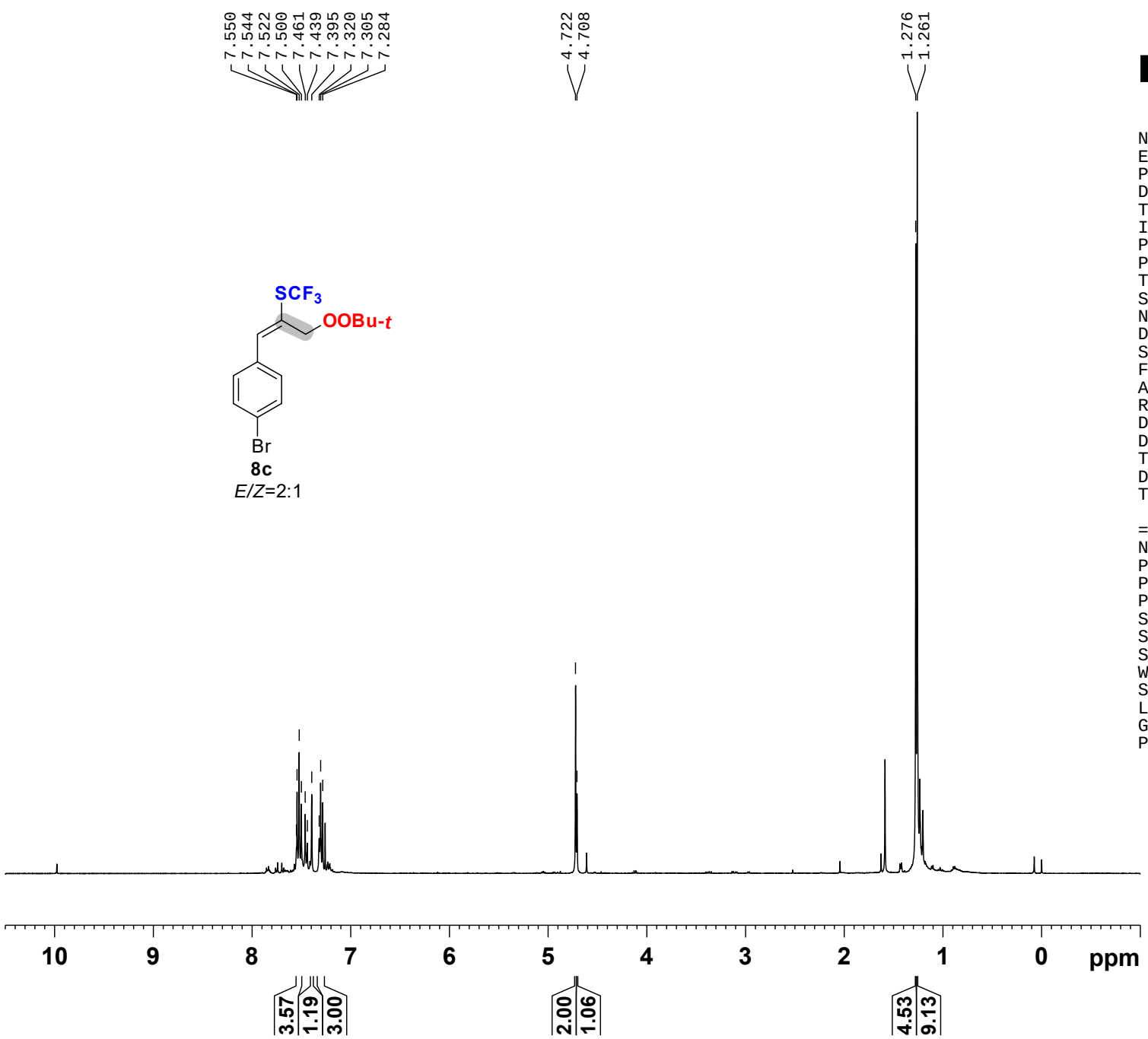
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL13               15.50 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
PL13W         0.38087484 W
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127706 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.40
```




```
NAME      cms17p-20191202
EXPNO                   3
PROCNO                  1
Date_            20191202
Time                17.31
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     32
DS                      4
SWH             89285.711 Hz
FIDRES          0.681196 Hz
AQ              0.7340532 sec
RG                    812
DW                5.600 usec
DE                6.50 usec
TE                296.3 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                     1

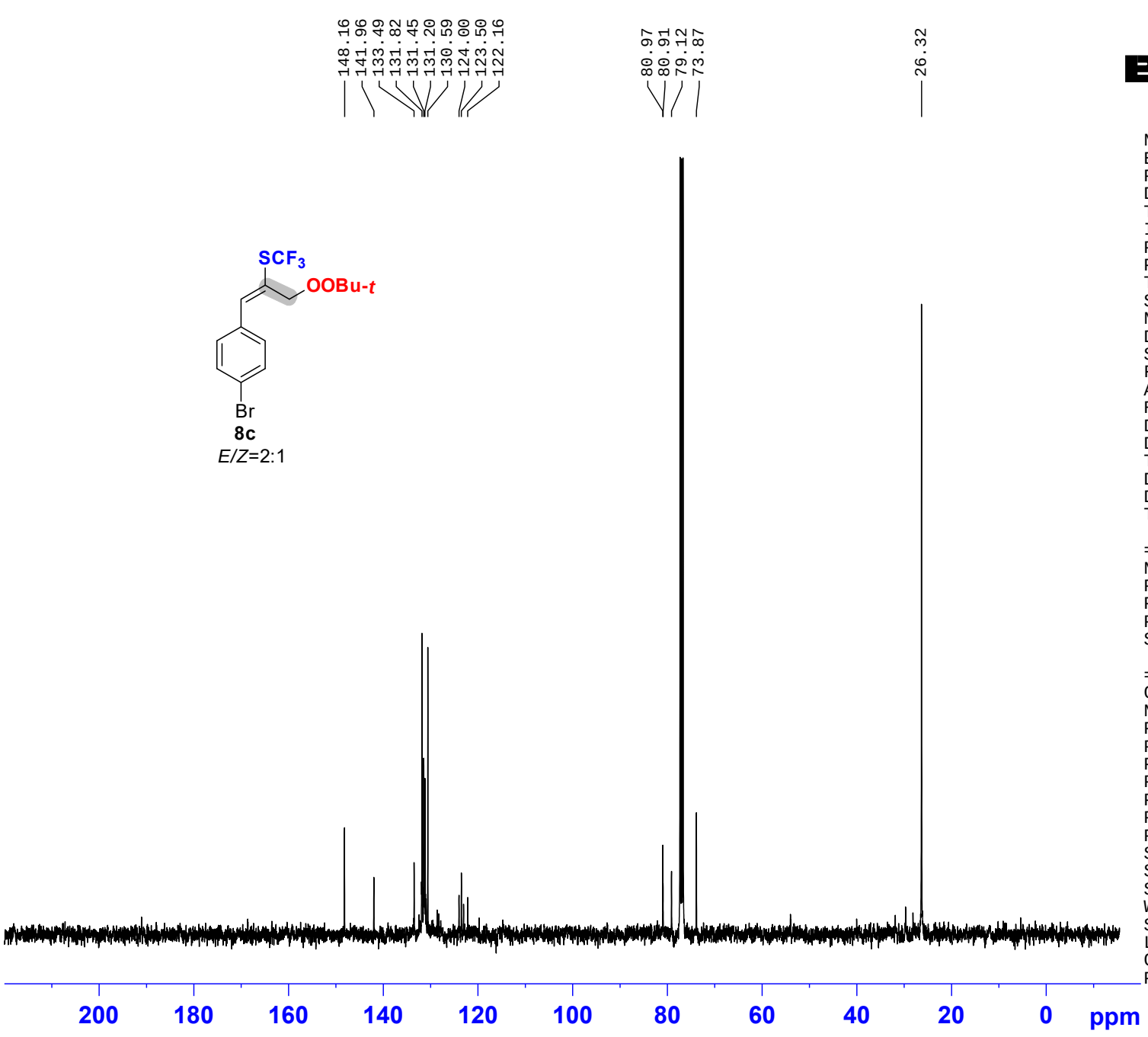
======== CHANNEL f1 ========
NUC1                   19F
P1                 14.20 usec
PL1                -2.00 dB
PL1W         20.42289734 W
SFO1         376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
SFO2         400.1316005 MHz
SI                 65536
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.00
```




```
NAME      cyj954ap01-20190705
EXPNO                       1
PROCNO                      1
Date_              20040319
Time                    8.03
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                          8
DS                          0
SWH                6393.862 Hz
FIDRES             0.195125 Hz
AQ                 2.5625076 sec
RG                        128
DW                   78.200 usec
DE                    6.50 usec
TE                   296.0 K
D1                 1.00000000 sec
TD0                         1

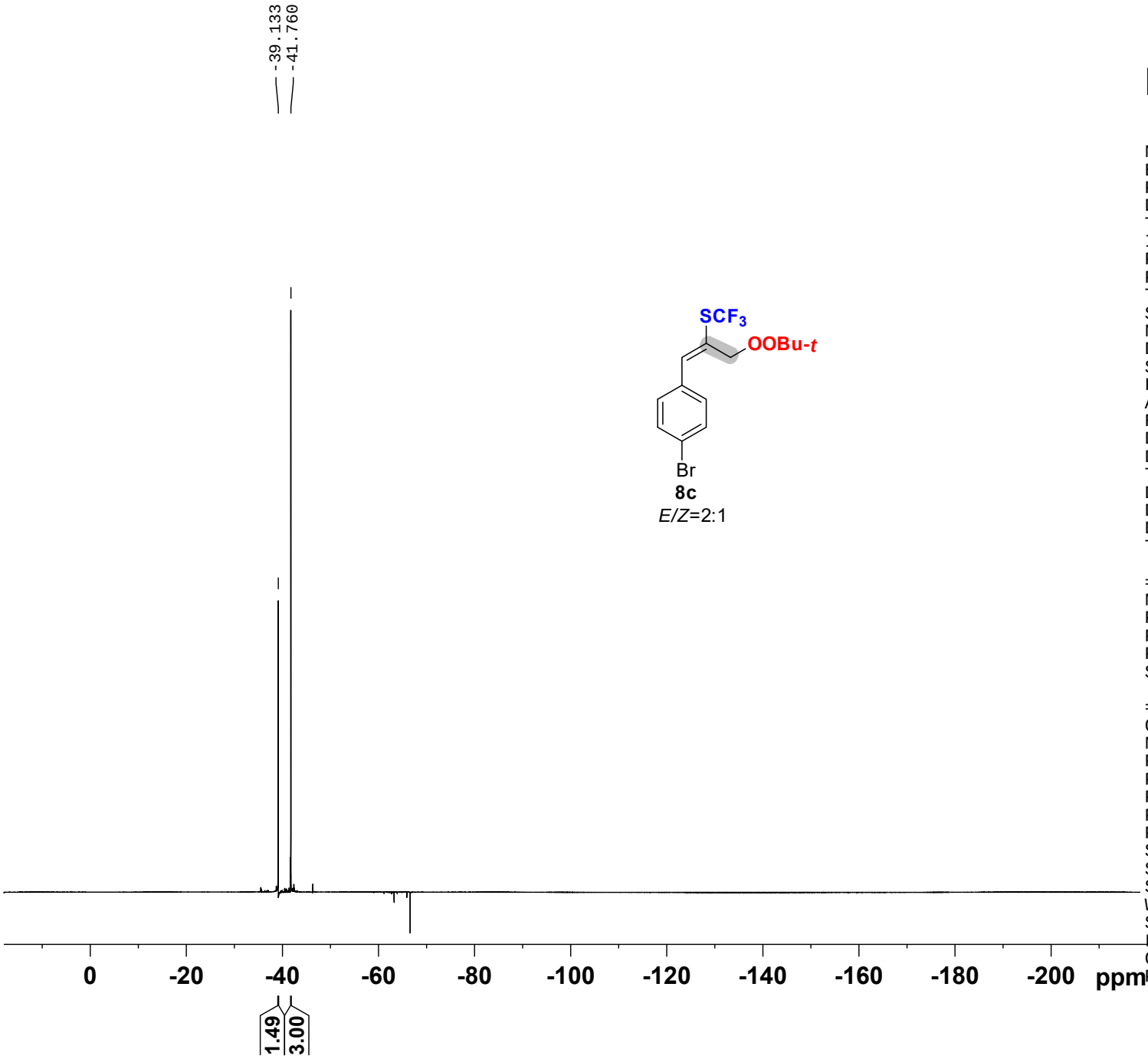
======== CHANNEL f1 ========
NUC1                       1H
P1                      10.40 usec
PL1                     -1.00 dB
PL1W            17.01305389 W
SFO1            400.1326008 MHz
SI                     32768
SF              400.1300113 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
PC                      1.00
```




```
NAME      cyj954ap1-20190705
EXPNO                      2
PROCNO                     1
Date_               20040319
Time                    8.09
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        120
DS                          4
SWH                 25252.525 Hz
FIDRES                0.385323 Hz
AQ                    1.2976629 sec
RG                         2050
DW                       19.800 usec
DE                        6.50 usec
TE                       297.3 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         3

======== CHANNEL f1 ========
NUC1                       13C
P1                       15.00 usec
PL1                       2.00 dB
PL1W               55.31277084 W
SFO1               100.6238364 MHz

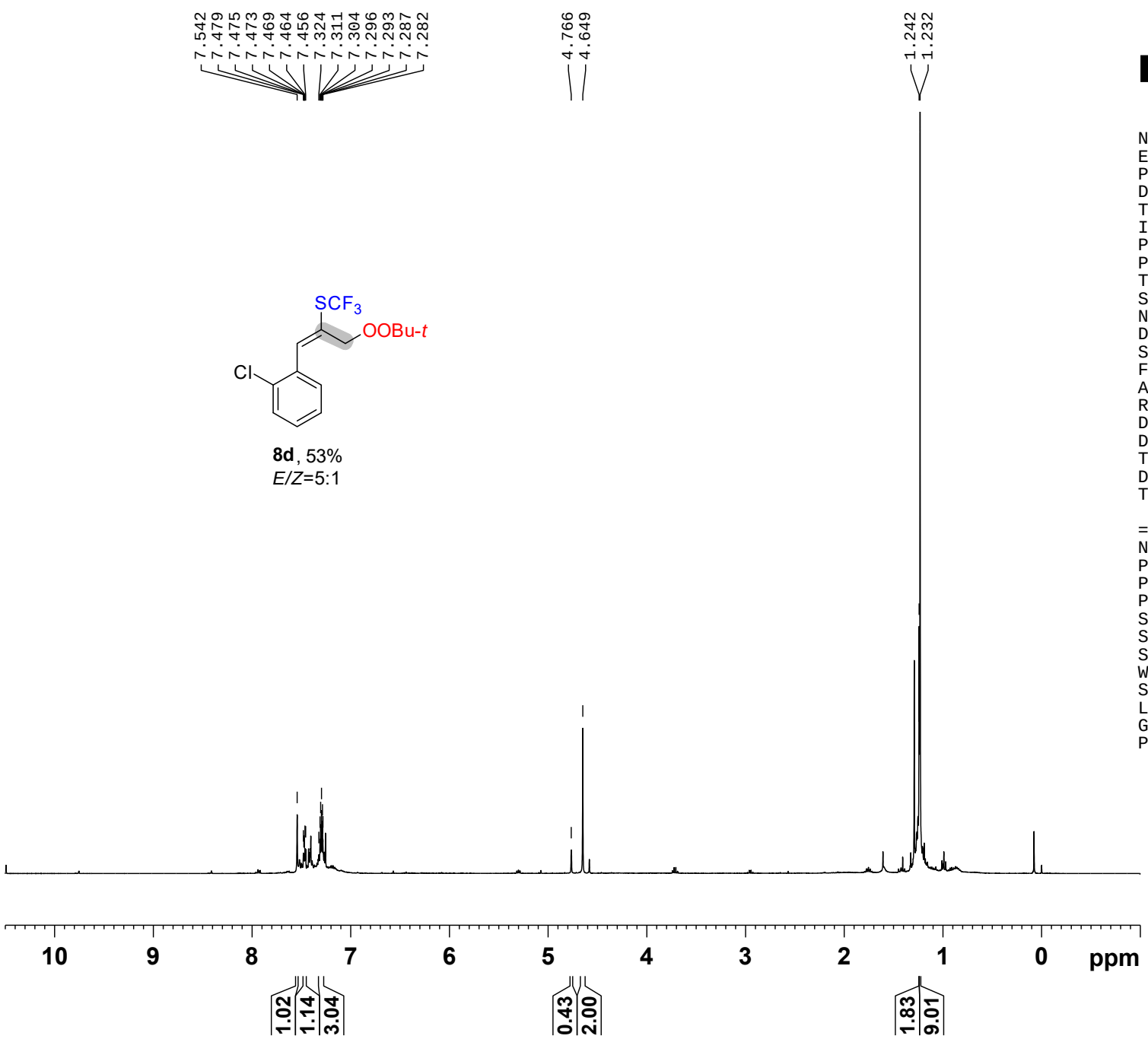
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                      -1.00 dB
PL12                     16.72 dB
PL13                     15.50 dB
PL2W               17.01305389 W
PL12W               0.28759566 W
PL13W               0.38087484 W
SFO2               400.1316005 MHz
SI                       32768
SF                 100.6127715 MHz
WDW                         EM
SSB                          0
LB                        3.00 Hz
GB                           0
PC                        1.40
```




```
NAME      cyj954ap1-20190705
EXPNO                      3
PROCNO                     1
Date_               20040319
Time                    8.18
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES             0.681196 Hz
AQ                 0.7340532 sec
RG                       812
DW                     5.600 usec
DE                     6.50 usec
TE                     296.5 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

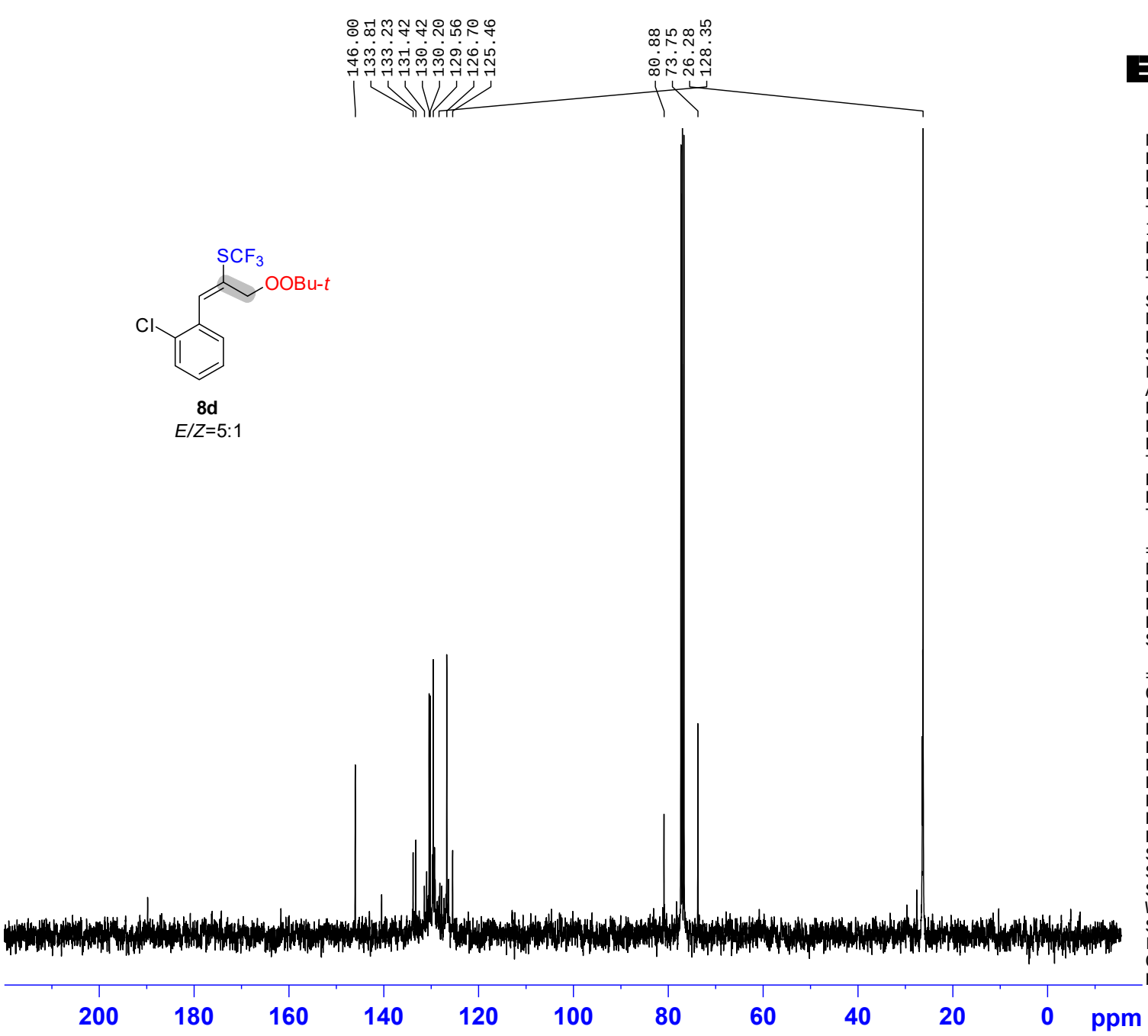
======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                     65536
SF              376.4983660 MHz
WDW                       EM
SSB                        0
LB                      3.00 Hz
GB                         0
PC                      1.00
```



8d, 53%
E/*Z*=5:1

```
NAME      cyj960bp-20190712
EXPNO                    1
PROCNO                   1
Date_             20040325
Time                 23.35
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                    80.6
DW                  78.200 usec
DE                   6.50 usec
TE                  295.3 K
D1             1.00000000 sec
TD0                      1

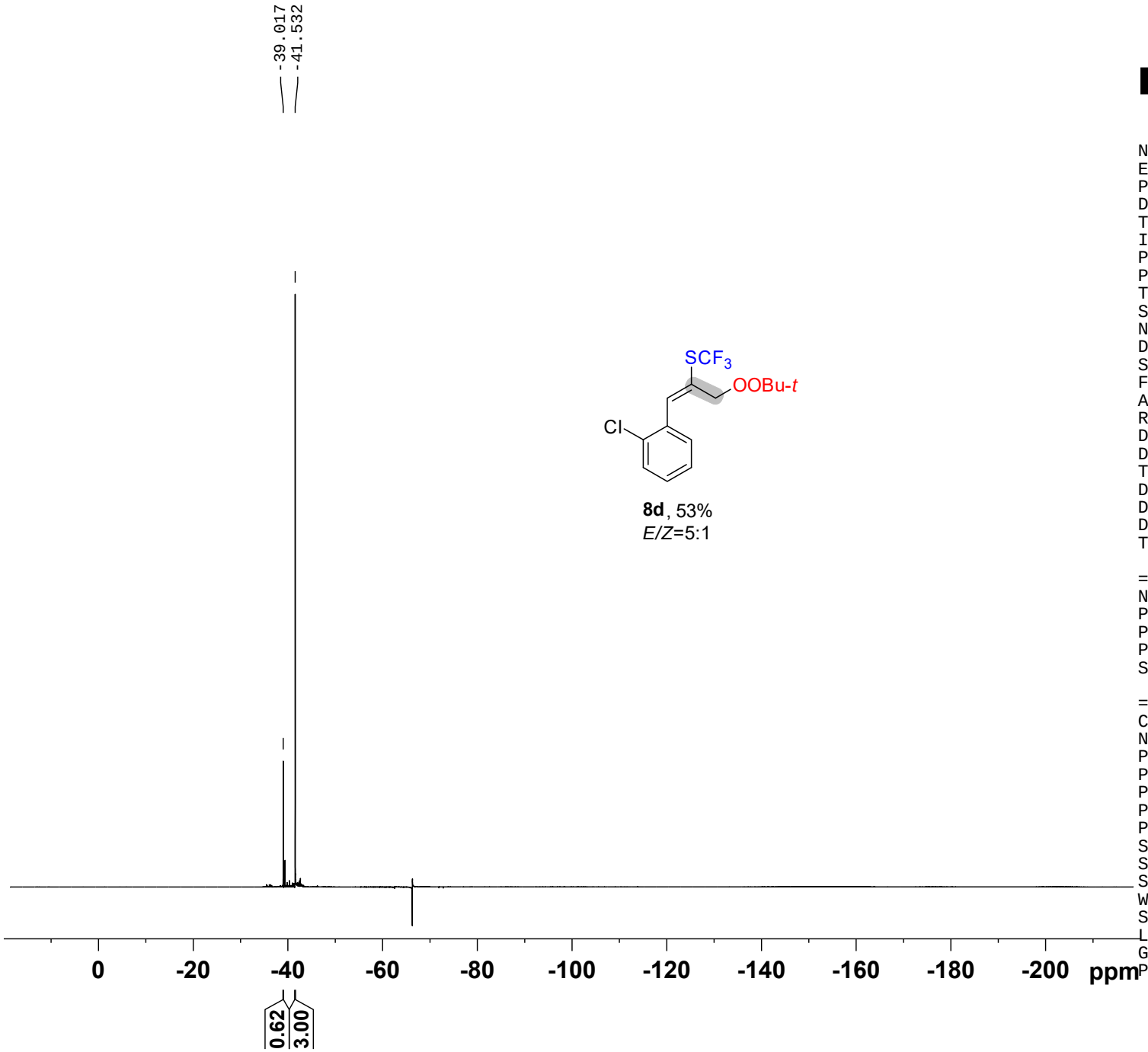
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300124 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                   1.00
```




```
NAME      cyj960bp-20190712
EXPNO                    2
PROCNO                   1
Date_             20040325
Time                 23.41
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       64
DS                        4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                     2050
DW                   19.800 usec
DE                    6.50 usec
TE                   296.8 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       3

======== CHANNEL f1 ========
NUC1                    13C
P1                    15.00 usec
PL1                    2.00 dB
PL1W           55.31277084 W
SFO1           100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
PL13W           0.38087484 W
SFO2           400.1316005 MHz
SI                    32768
SF             100.6127719 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```

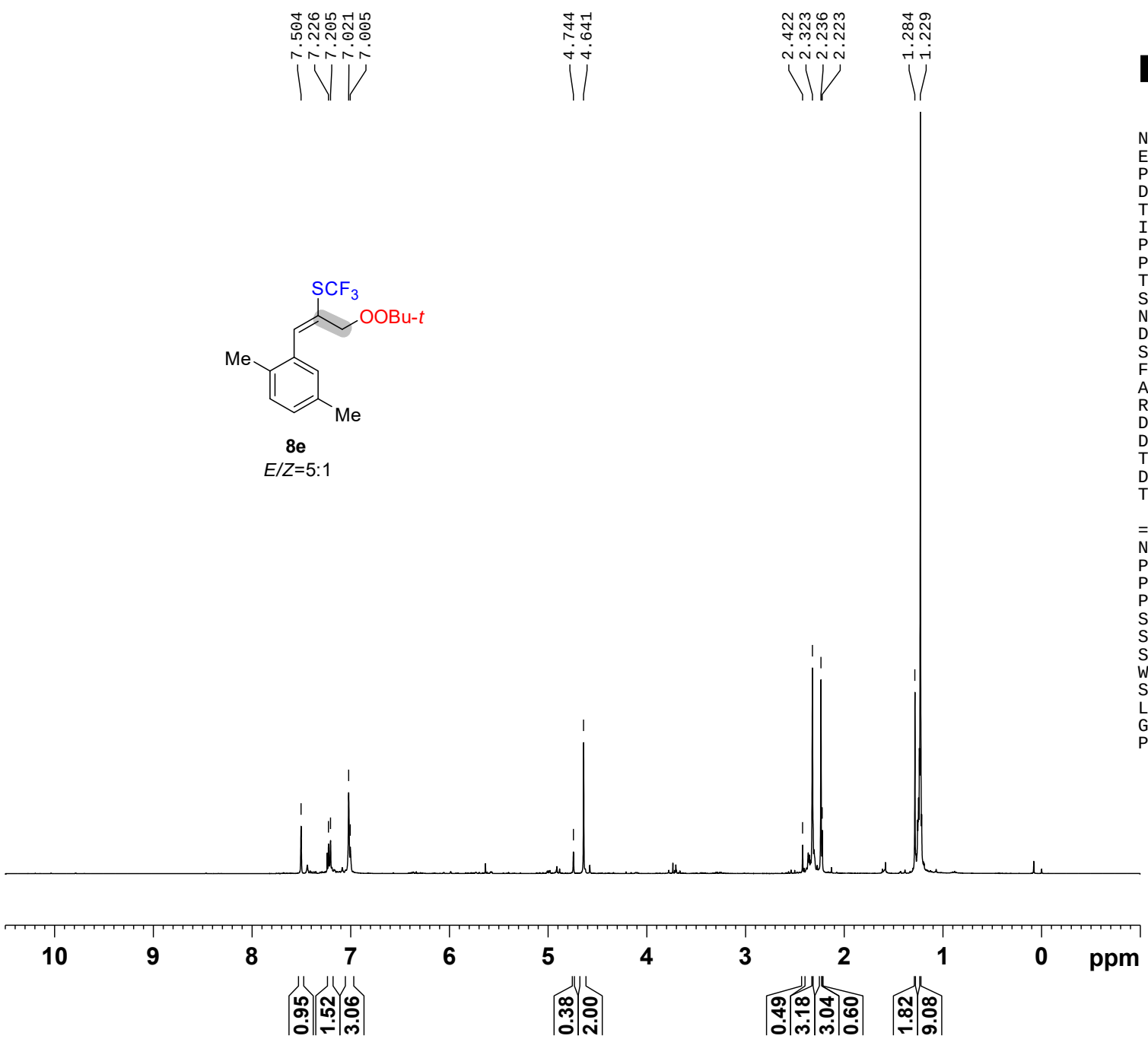


8d, 53%
E/*Z*=5:1

```
NAME      cyj960bp-20190712
EXPNO                     3
PROCNO                    1
Date_              20040325
Time                  23.45
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       32
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                      812
DW                    5.600 usec
DE                    6.50 usec
TE                    295.8 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       1

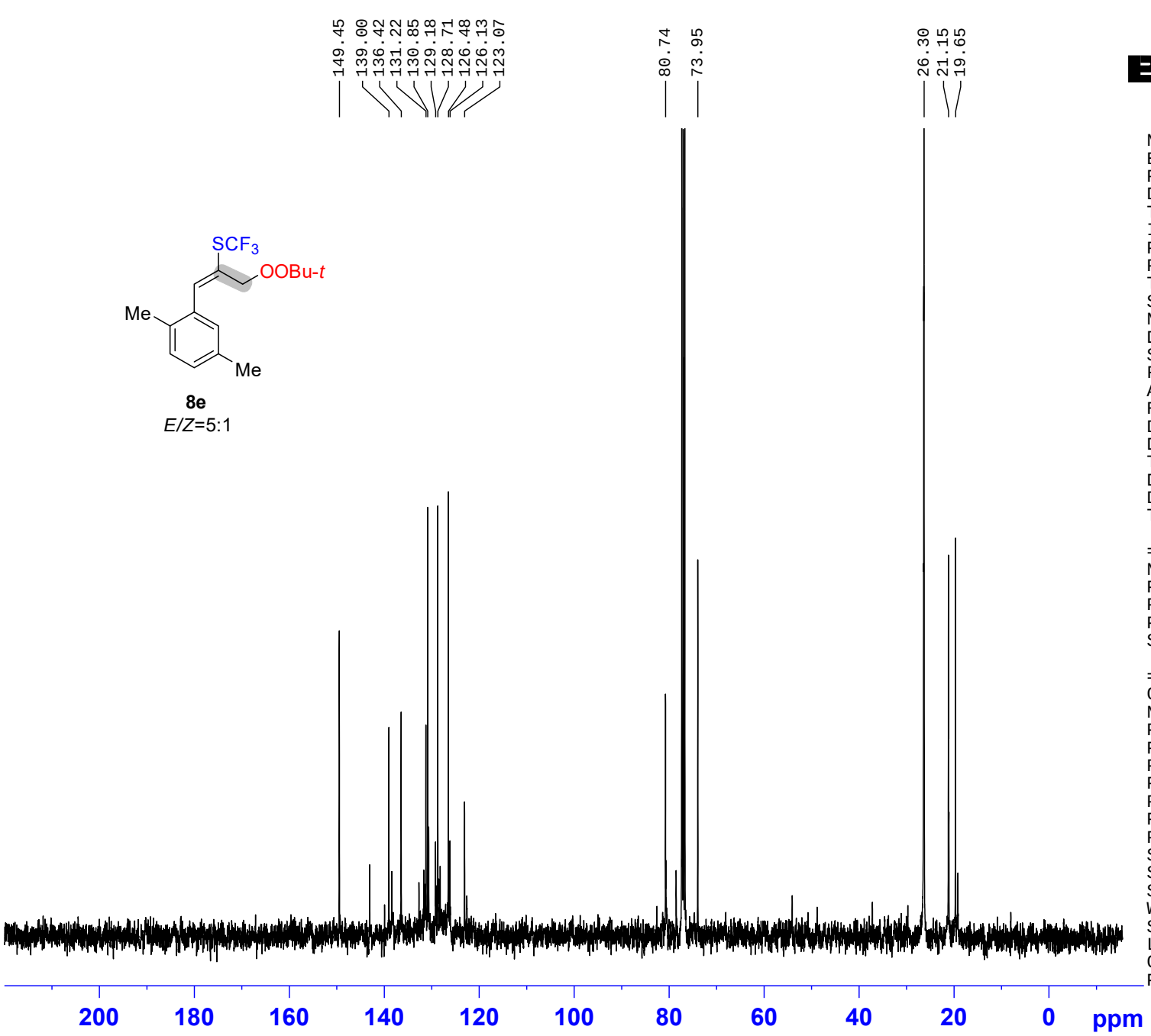
======== CHANNEL f1 ========
NUC1                     19F
P1                    14.20 usec
PL1                   -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -1.00 dB
PL12                  16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                    65536
SF              376.4983660 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.00
```




```
NAME      cyj960cp-20190712
EXPNO                    1
PROCNO                   1
Date_             20040325
Time                 23.51
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                      32
DW                  78.200 usec
DE                   6.50 usec
TE                  295.4 K
D1               1.00000000 sec
TD0                      1

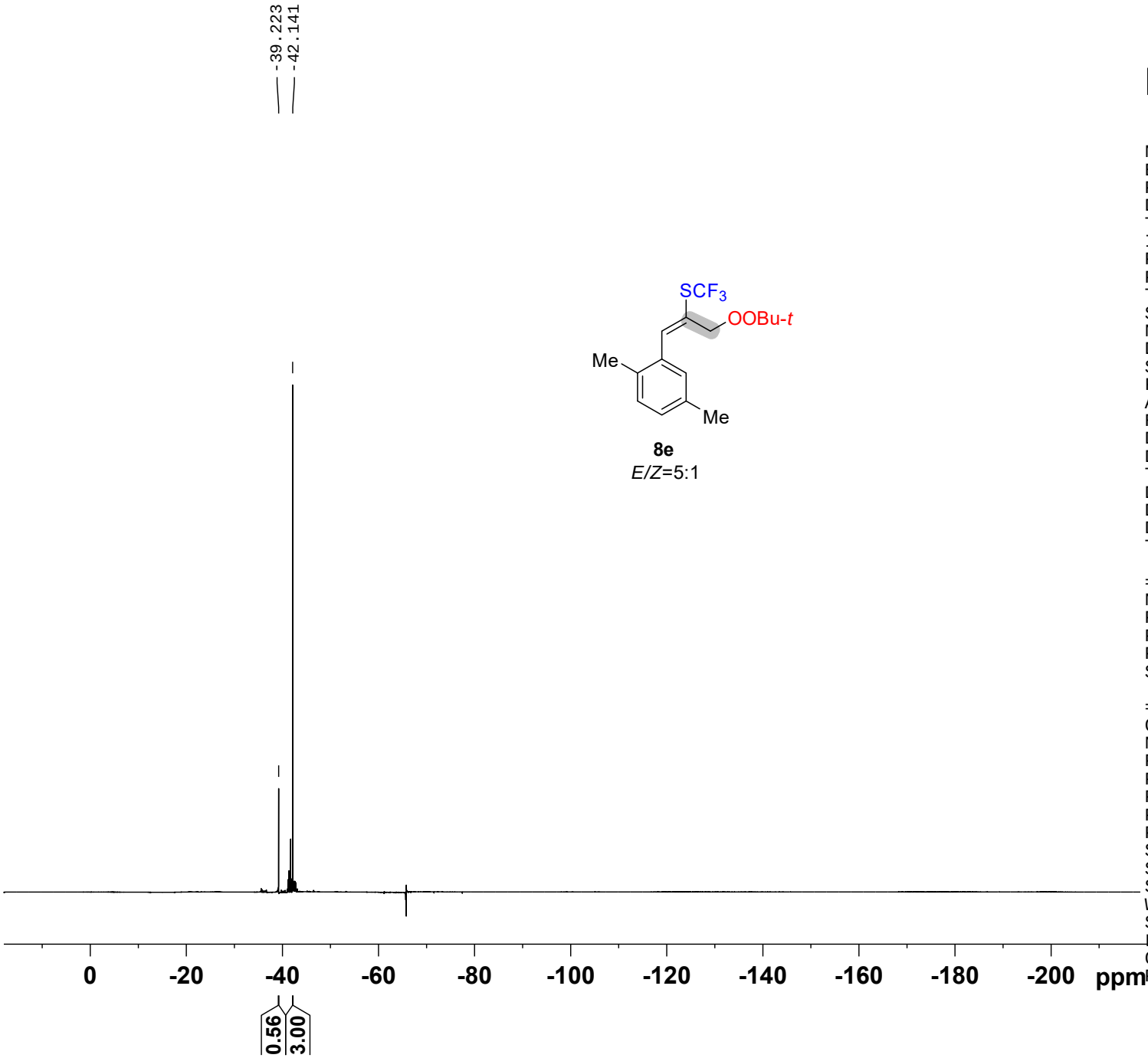
======== CHANNEL f1 ========
NUC1                    1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300192 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                  1.00
```




```
NAME      cyj960cp-20190712
EXPNO                    2
PROCNO                   1
Date_             20040325
Time                 23.58
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    80
DS                     4
SWH            25252.525 Hz
FIDRES          0.385323 Hz
AQ             1.2976629 sec
RG                  2050
DW                19.800 usec
DE                 6.50 usec
TE                296.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    3

======== CHANNEL f1 ========
NUC1                  13C
P1                 15.00 usec
PL1                 2.00 dB
PL1W         55.31277084 W
SFO1        100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL13               15.50 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
PL13W         0.38087484 W
SFO2        400.1316005 MHz
SI                 32768
SF          100.6127724 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.40
```



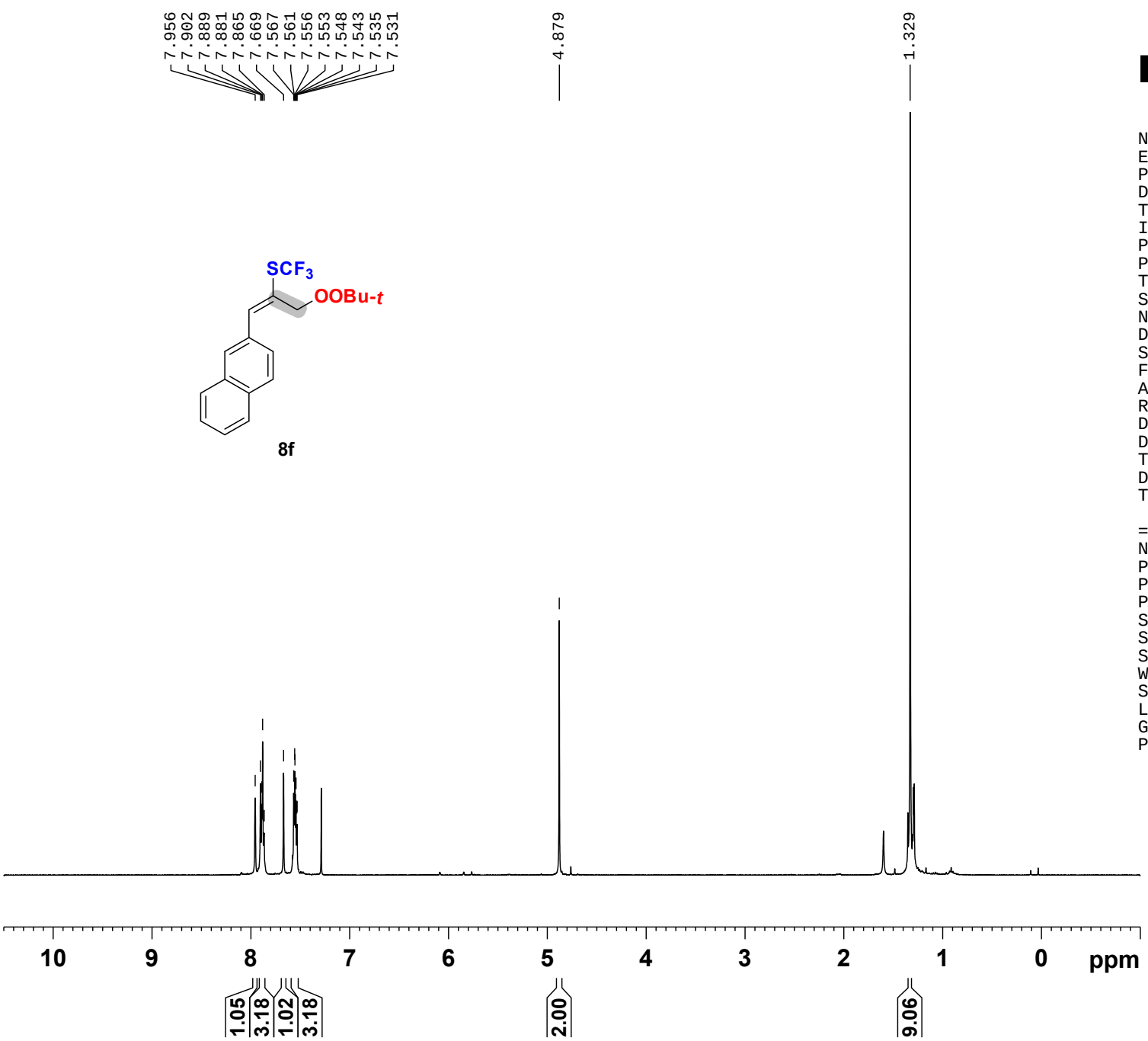
8e

E/*Z*=5:1

```
NAME      cyj960cp-20190712
EXPNO                     3
PROCNO                    1
Date_              20040326
Time                   0.03
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       32
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                      812
DW                  5.600 usec
DE                  6.50 usec
TE                  295.8 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       1

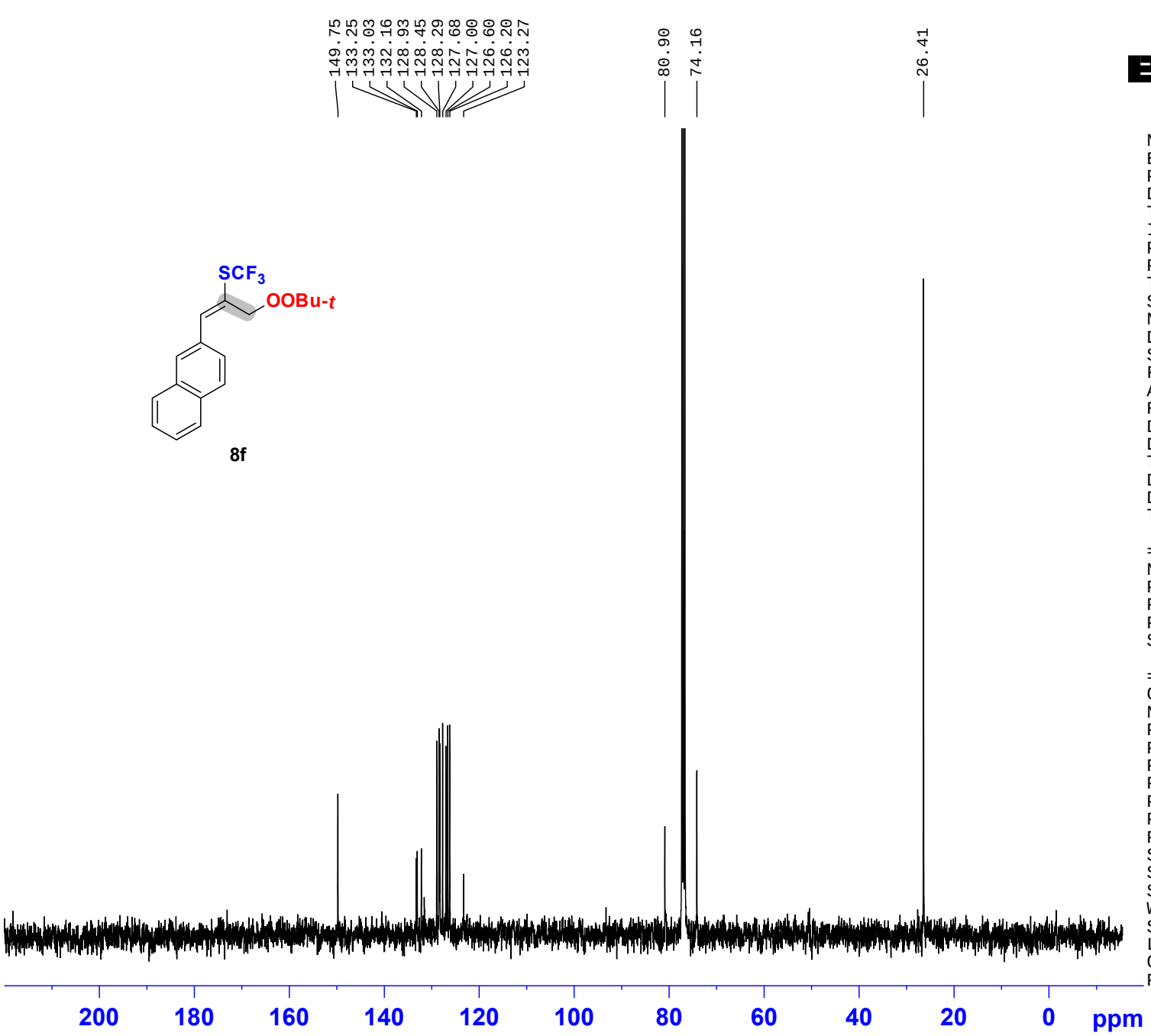
======== CHANNEL f1 ========
NUC1                     19F
P1                   14.20 usec
PL1                  -2.00 dB
PL1W           20.42289734 W
SFO1           376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
SFO2           400.1316005 MHz
SI                    65536
SF             376.4983660 MHz
WDW                      EM
SSB                       0
LB                     3.00 Hz
GB                        0
PC                     1.00
```




```
NAME      cyj946cp-20190627
EXPNO                    1
PROCNO                   1
Date_             20040311
Time                  7.20
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES            0.195125 Hz
AQ               2.5625076 sec
RG                     256
DW                  78.200 usec
DE                   6.50 usec
TE                  295.1 K
D1             1.00000000 sec
TD0                      1

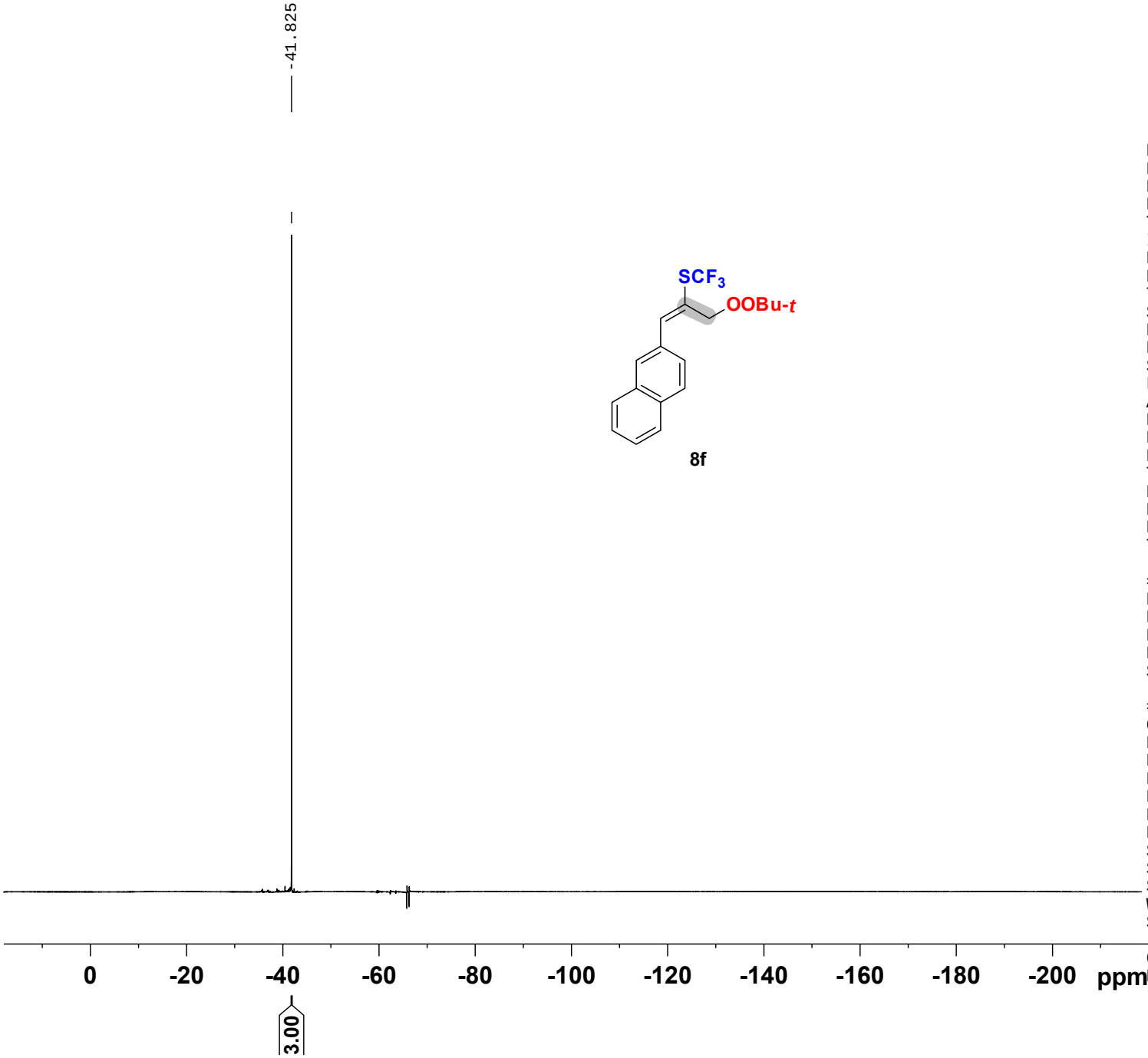
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.40 usec
PL1                  -1.00 dB
PL1W          17.01305389 W
SFO1          400.1326008 MHz
SI                   32768
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                   1.00
```




```
NAME      cyj946cp-20190627
EXPNO                    2
PROCNO                   1
Date_             20040311
Time                  7.26
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      136
DS                        4
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976629 sec
RG                     2050
DW                   19.800 usec
DE                    6.50 usec
TE                   296.6 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       3

======== CHANNEL f1 ========
NUC1                    13C
P1                    15.00 usec
PL1                    2.00 dB
PL1W            55.31277084 W
SFO1            100.6238364 MHz

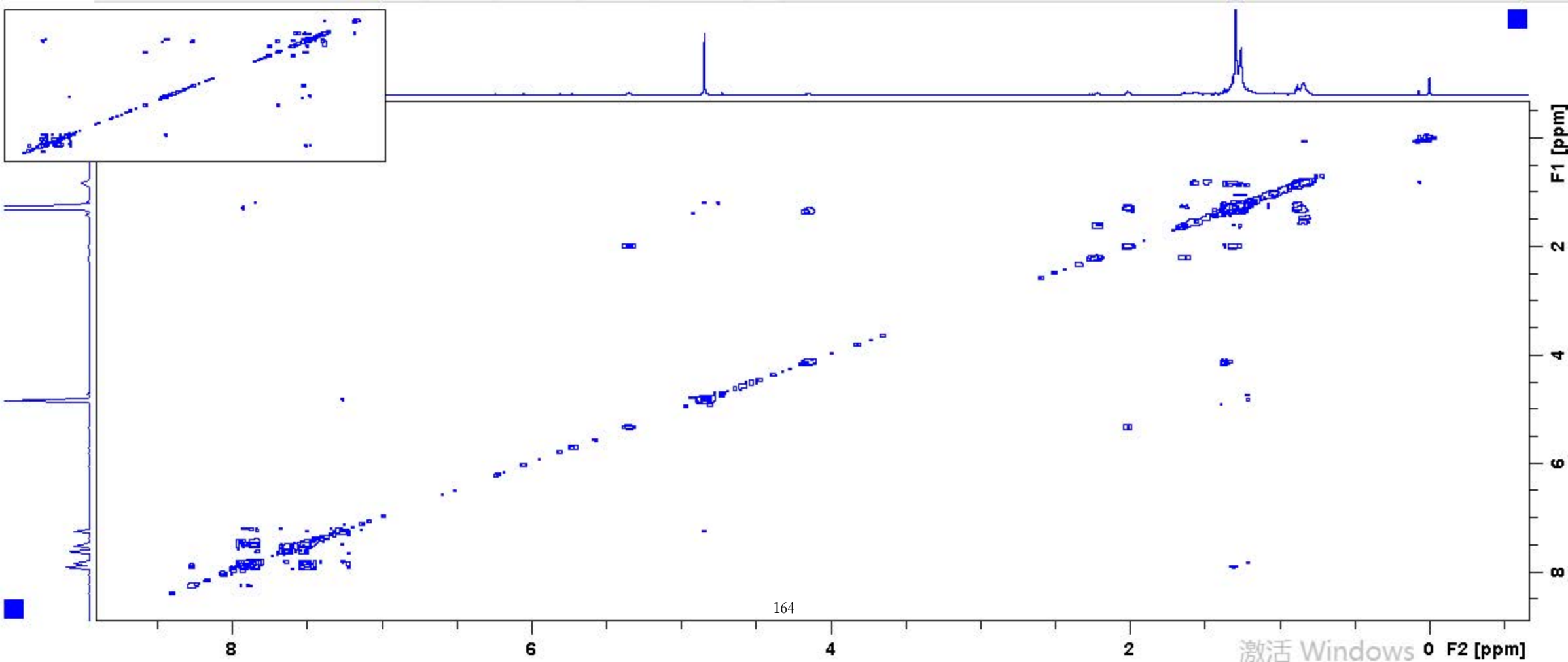
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
PL13W            0.38087484 W
SFO2            400.1316005 MHz
SI                    32768
SF              100.6127715 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```

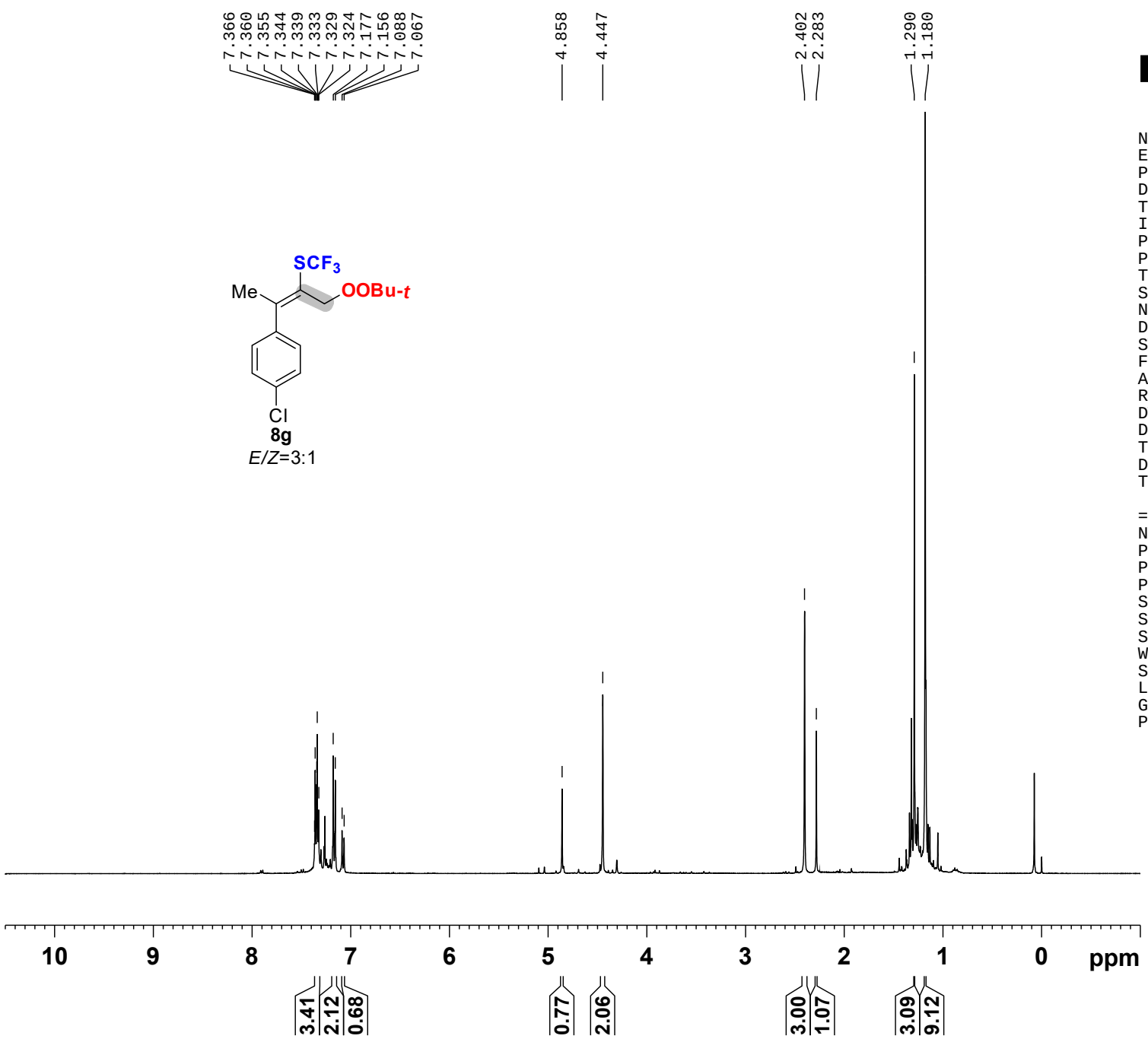



```
NAME      cyj946cp-20190627
EXPNO                    3
PROCNO                   1
Date_             20040311
Time                  7.35
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                 131072
SOLVENT             CDCl3
NS                     32
DS                      4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                     812
DW                 5.600 usec
DE                 6.50 usec
TE                 295.8 K
D1              1.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   19F
P1                 14.20 usec
PL1                -2.00 dB
PL1W         20.42289734 W
SFO1         376.4607164 MHz

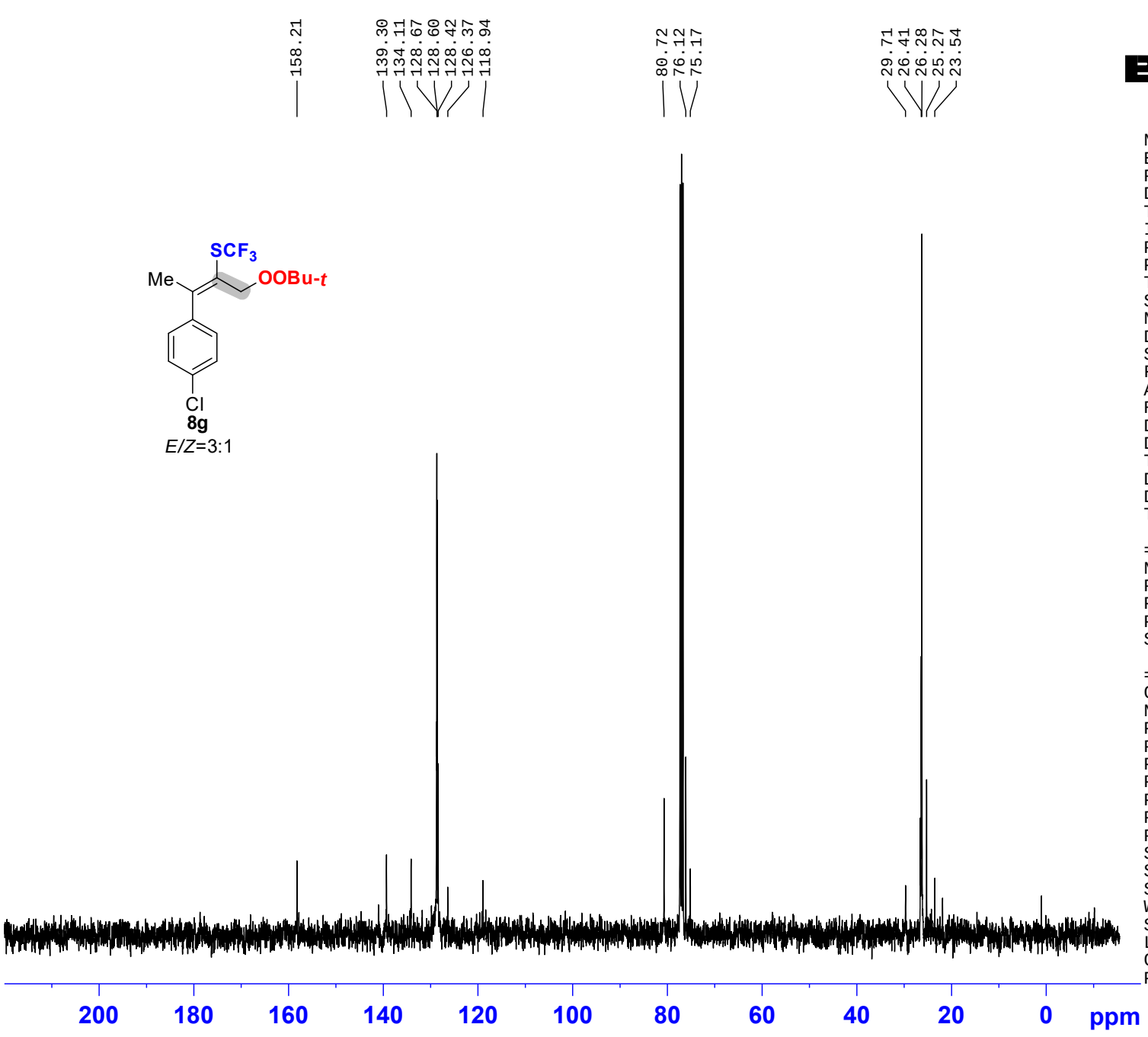
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.72 dB
PL2W         17.01305389 W
PL12W         0.28759566 W
SFO2         400.1316005 MHz
SI                 65536
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.00
```





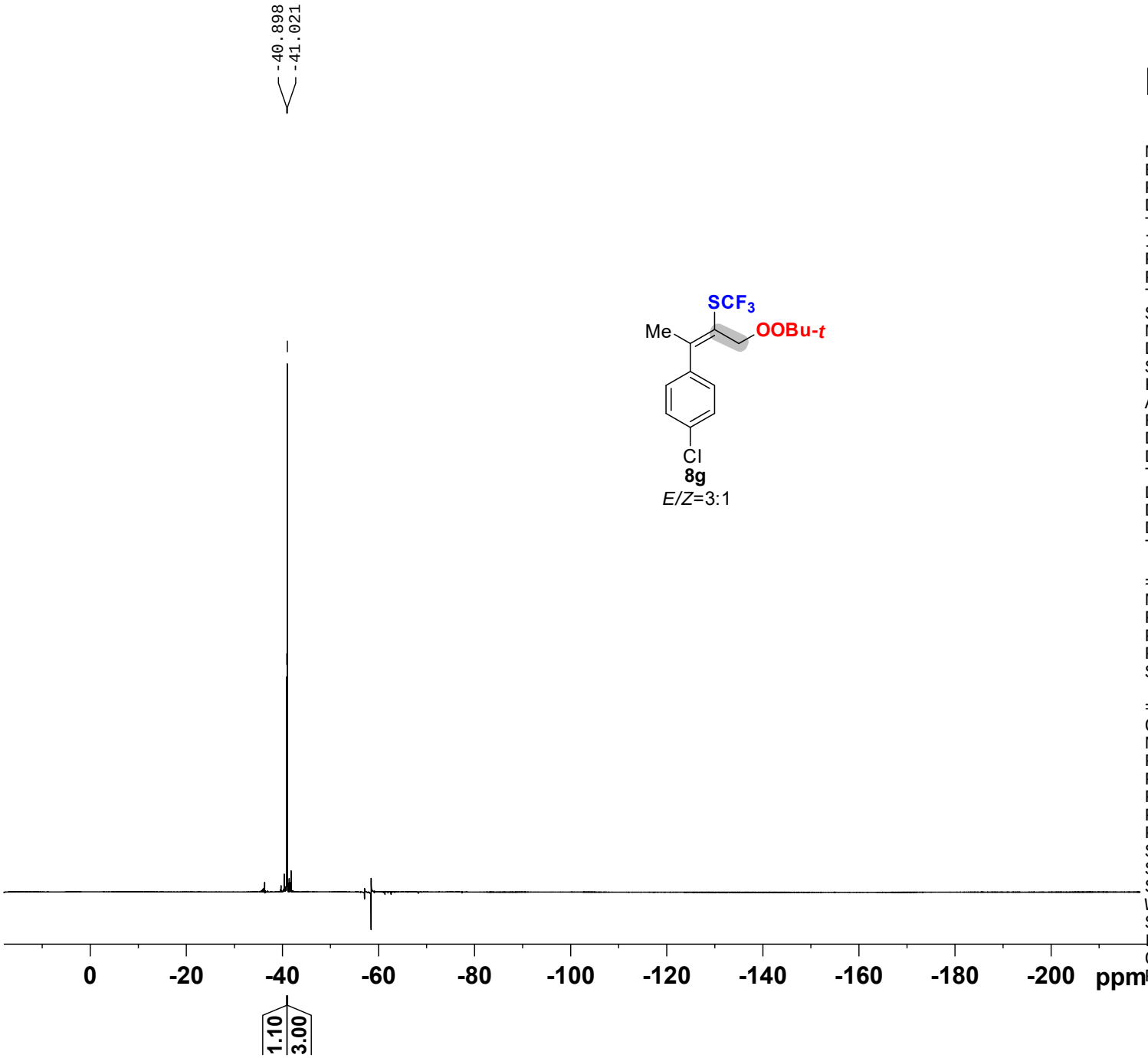

```
NAME      cyj953bp1-2-20190705
EXPNO                        1
PROCNO                       1
Date_             20040318
Time                    23.35
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                          8
DS                          0
SWH                  6393.862 Hz
FIDRES               0.195125 Hz
AQ                   2.5625076 sec
RG                        128
DW                      78.200 usec
DE                       6.50 usec
TE                      295.8 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                        1H
P1                      10.40 usec
PL1                     -1.00 dB
PL1W               17.01305389 W
SFO1               400.1326008 MHz
SI                      32768
SF                 400.1300103 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```



BRUKER

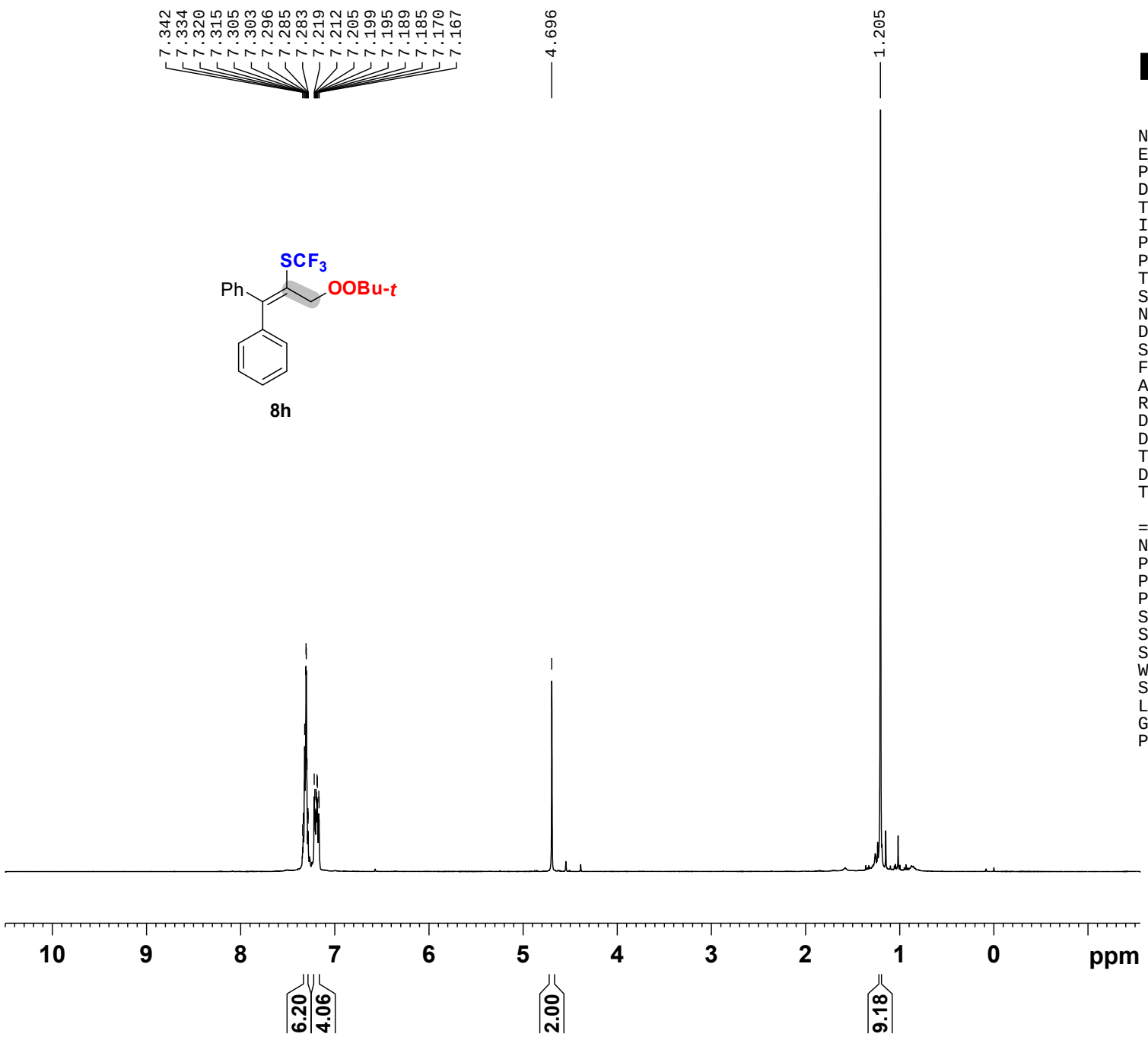
NAME	cyj953bp1-20190705
EXPNO	2
PROCNO	1
Date_	20040318
Time	23.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	2050
DW	19.800 usec
DE	6.50 usec
TE	297.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	13C
P1	15.00 usec
PL1	2.00 dB
PL1W	55.31277084 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	16.72 dB
PL13	15.50 dB
PL2W	17.01305389 W
PL12W	0.28759566 W
PL13W	0.38087484 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40




```
NAME      cyj953bp1-20190705
EXPNO                      3
PROCNO                     1
Date_               20040318
Time                   23.47
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES             0.681196 Hz
AQ                 0.7340532 sec
RG                       812
DW                     5.600 usec
DE                     6.50 usec
TE                     296.3 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

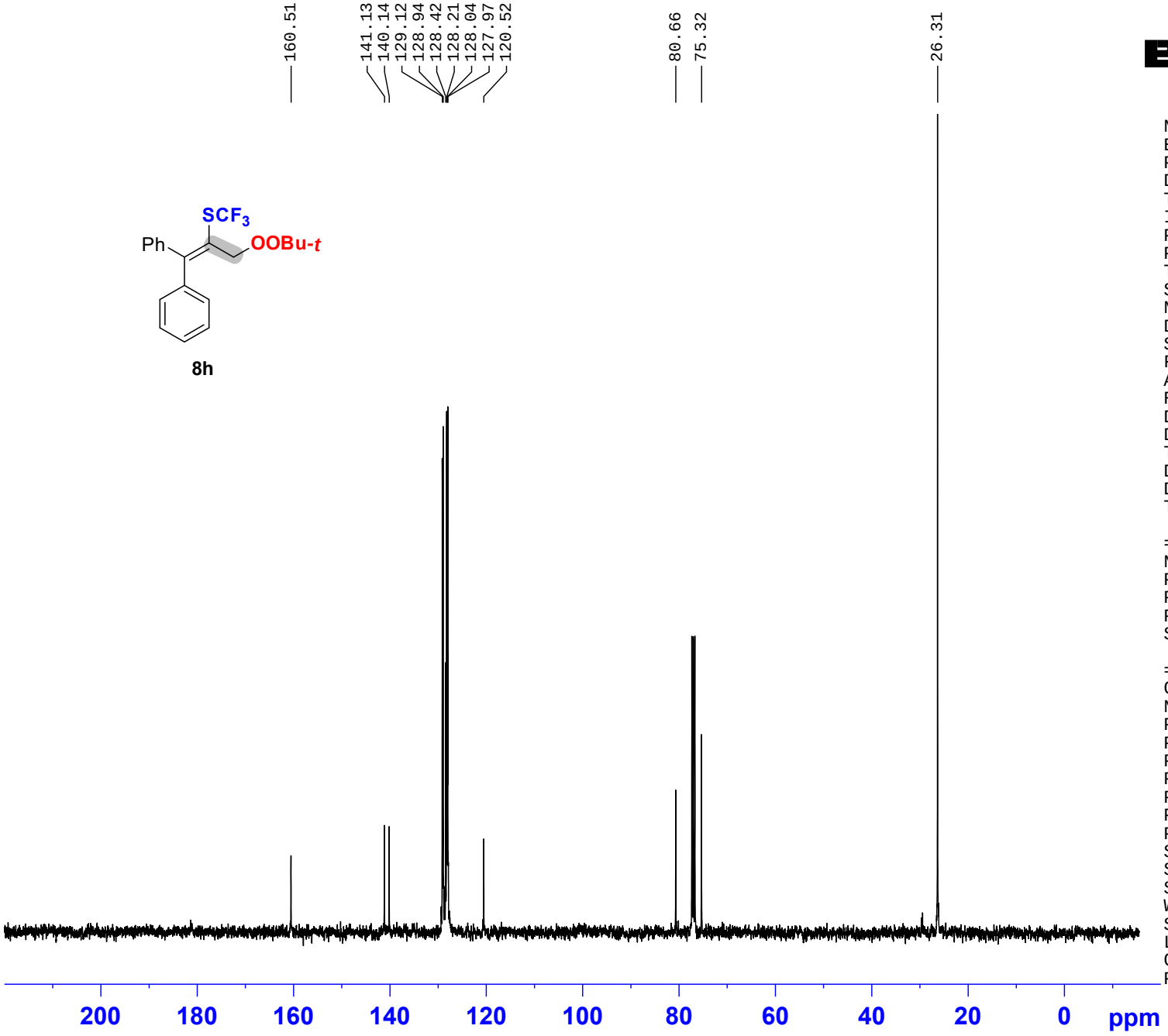
======== CHANNEL f1 ========
NUC1                      19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                     65536
SF              376.4983660 MHz
WDW                       EM
SSB                        0
LB                      3.00 Hz
GB                         0
PC                      1.00
```



BRUKER

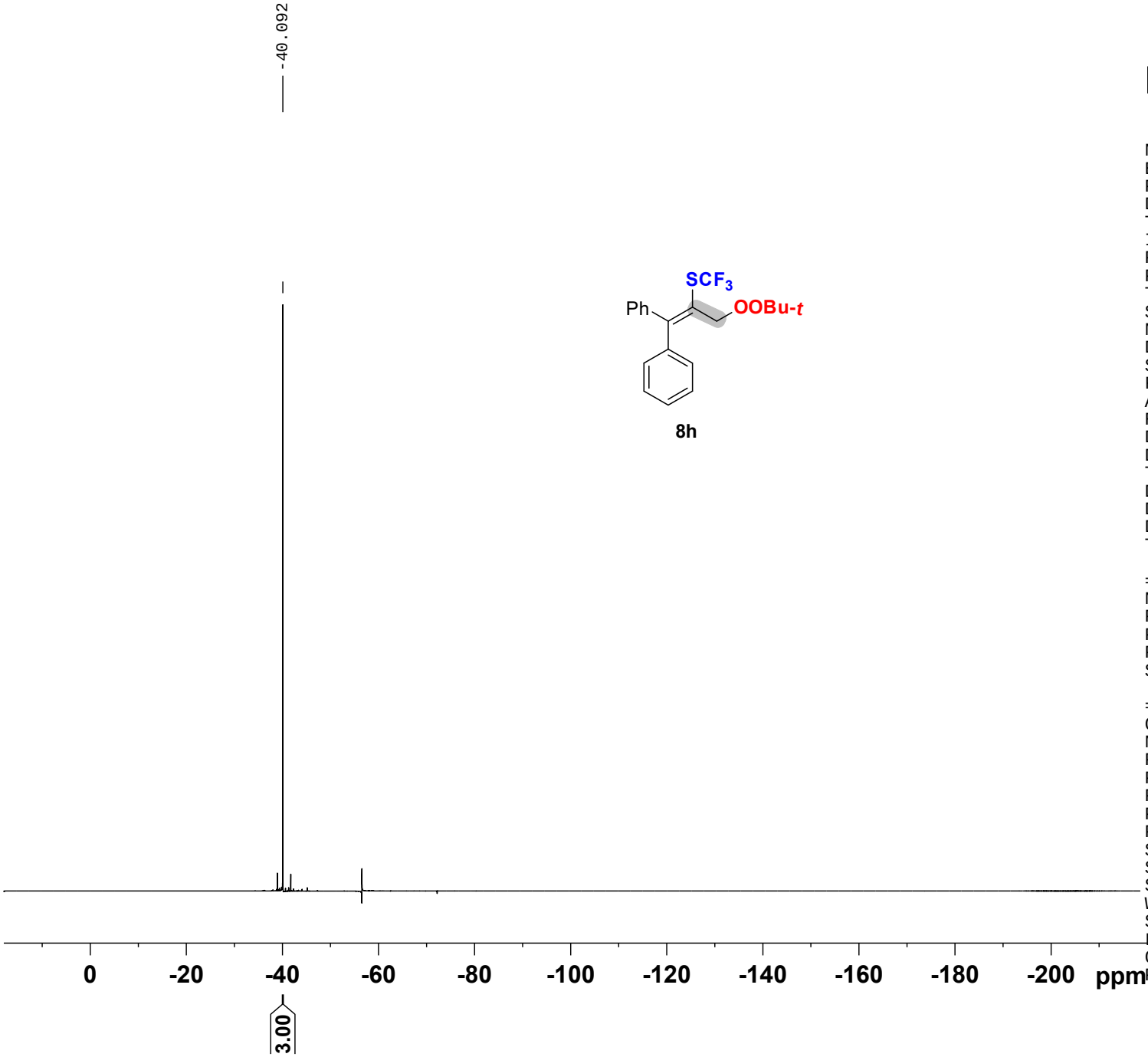
NAME	cyj957bp2-20190710
EXPNO	1
PROCNO	1
Date_	20040324
Time	0.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	32
DW	78.200 usec
DE	6.50 usec
TE	295.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300263 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME      cyj957bp2-20190710
EXPNO                      2
PROCNO                     1
Date_               20040324
Time                    0.21
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         48
DS                          4
SWH                 25252.525 Hz
FIDRES                0.385323 Hz
AQ                  1.2976629 sec
RG                       2050
DW                     19.800 usec
DE                      6.50 usec
TE                     296.3 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         3

======== CHANNEL f1 ========
NUC1                      13C
P1                     15.00 usec
PL1                     2.00 dB
PL1W             55.31277084 W
SFO1             100.6238364 MHz

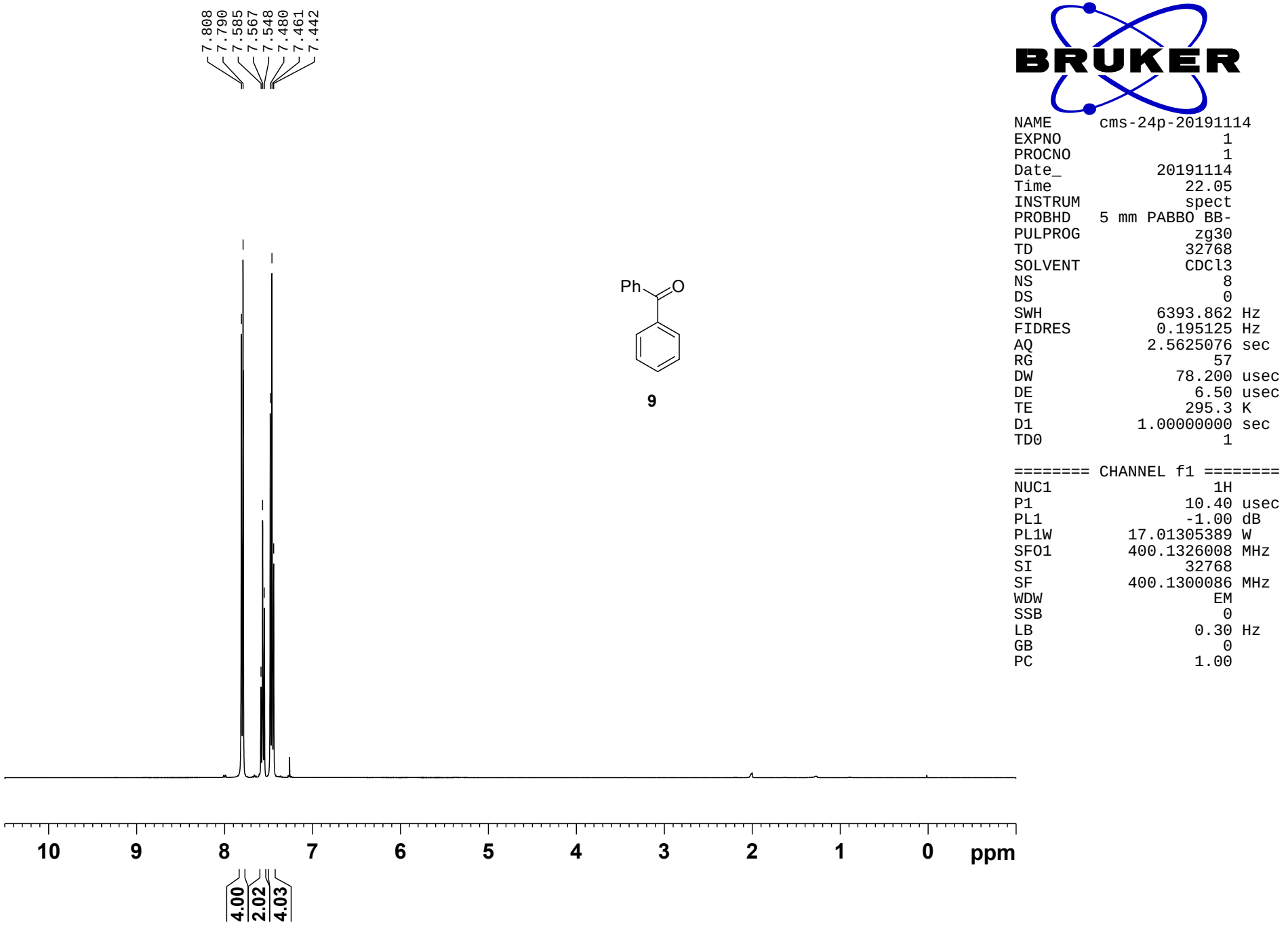
======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL13                   15.50 dB
PL2W             17.01305389 W
PL12W             0.28759566 W
PL13W             0.38087484 W
SFO2             400.1316005 MHz
SI                      32768
SF               100.6127754 MHz
WDW                        EM
SSB                         0
LB                      3.00 Hz
GB                          0
PC                      1.40
```




```
NAME      cyj957bp2-20190710
EXPNO                      3
PROCNO                     1
Date_               20040324
Time                    0.31
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES             0.681196 Hz
AQ                 0.7340532 sec
RG                       812
DW                     5.600 usec
DE                     6.50 usec
TE                     295.5 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W            20.42289734 W
SFO1            376.4607164 MHz

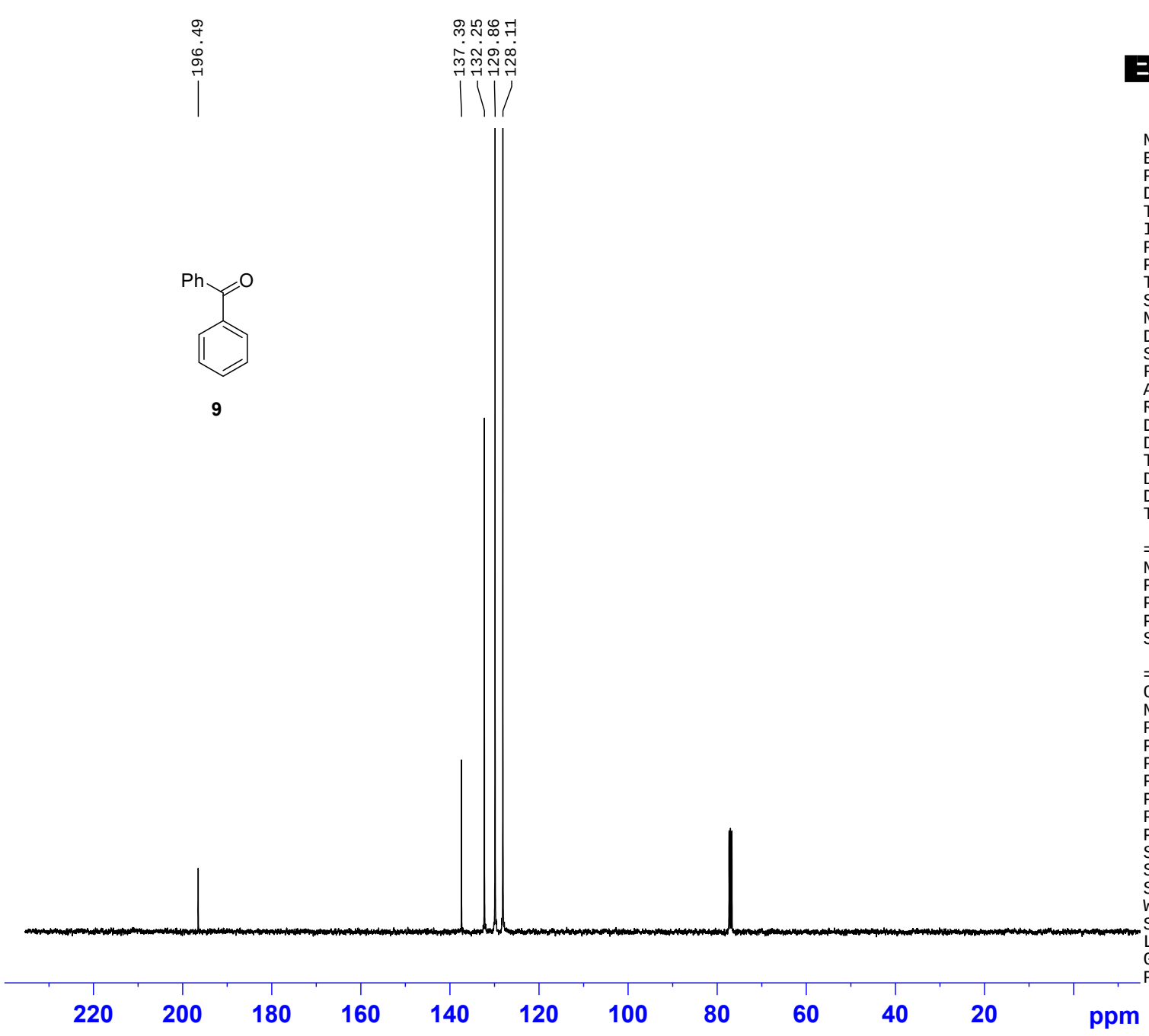
======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W            17.01305389 W
PL12W            0.28759566 W
SFO2            400.1316005 MHz
SI                     65536
SF              376.4983660 MHz
WDW                       EM
SSB                        0
LB                      3.00 Hz
GB                         0
PC                      1.00
```



9

```
NAME      cms-24p-20191114
EXPNO                    1
PROCNO                   1
Date_             20191114
Time                 22.05
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               6393.862 Hz
FIDRES           0.195125 Hz
AQ              2.5625076 sec
RG                      57
DW                  78.200 usec
DE                   6.50 usec
TE                  295.3 K
D1             1.00000000 sec
TD0                      1

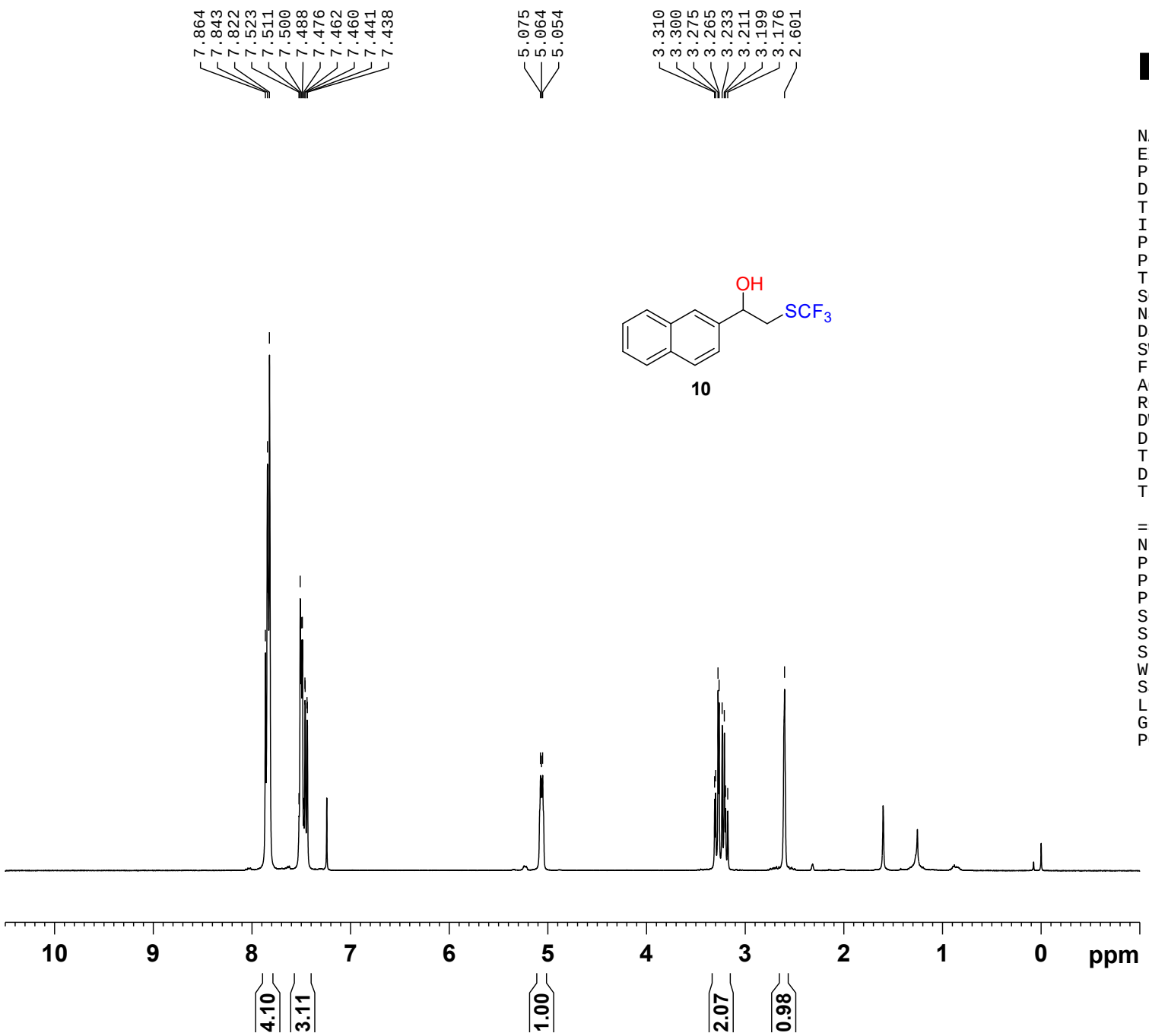
======== CHANNEL f1 ========
NUC1                    1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                   32768
SF           400.1300086 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



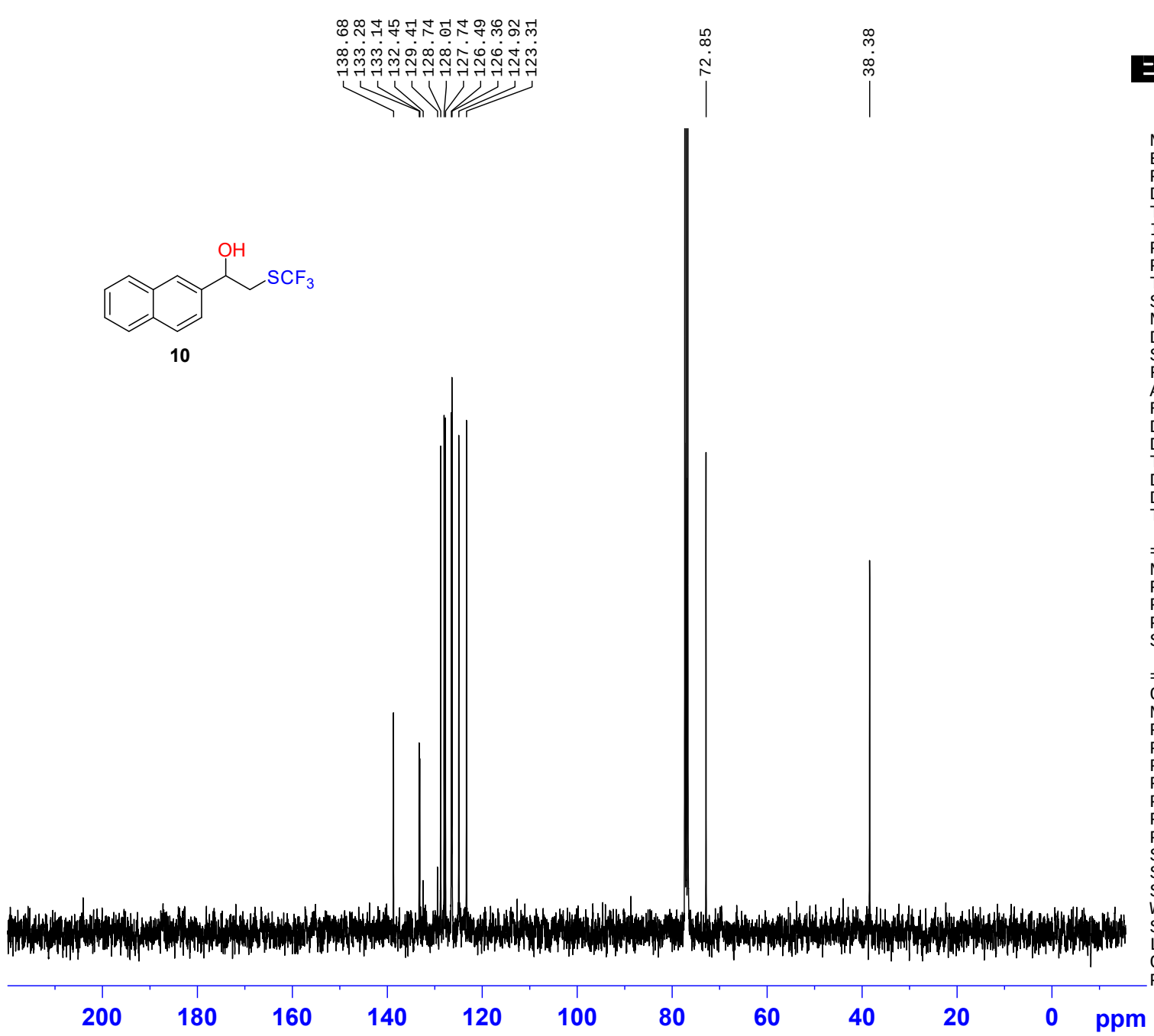

```
NAME      cms-24p-20191114
EXPNO                    2
PROCNO                   1
Date_             20191114
Time                 22.09
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      24
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                    2050
DW                  19.800 usec
DE                   6.50 usec
TE                  296.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                   15.00 usec
PL1                   2.00 dB
PL1W          55.31277084 W
SFO1          100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
PL13W          0.38087484 W
SFO2          400.1316005 MHz
SI                    32768
SF            100.6127904 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.40
```

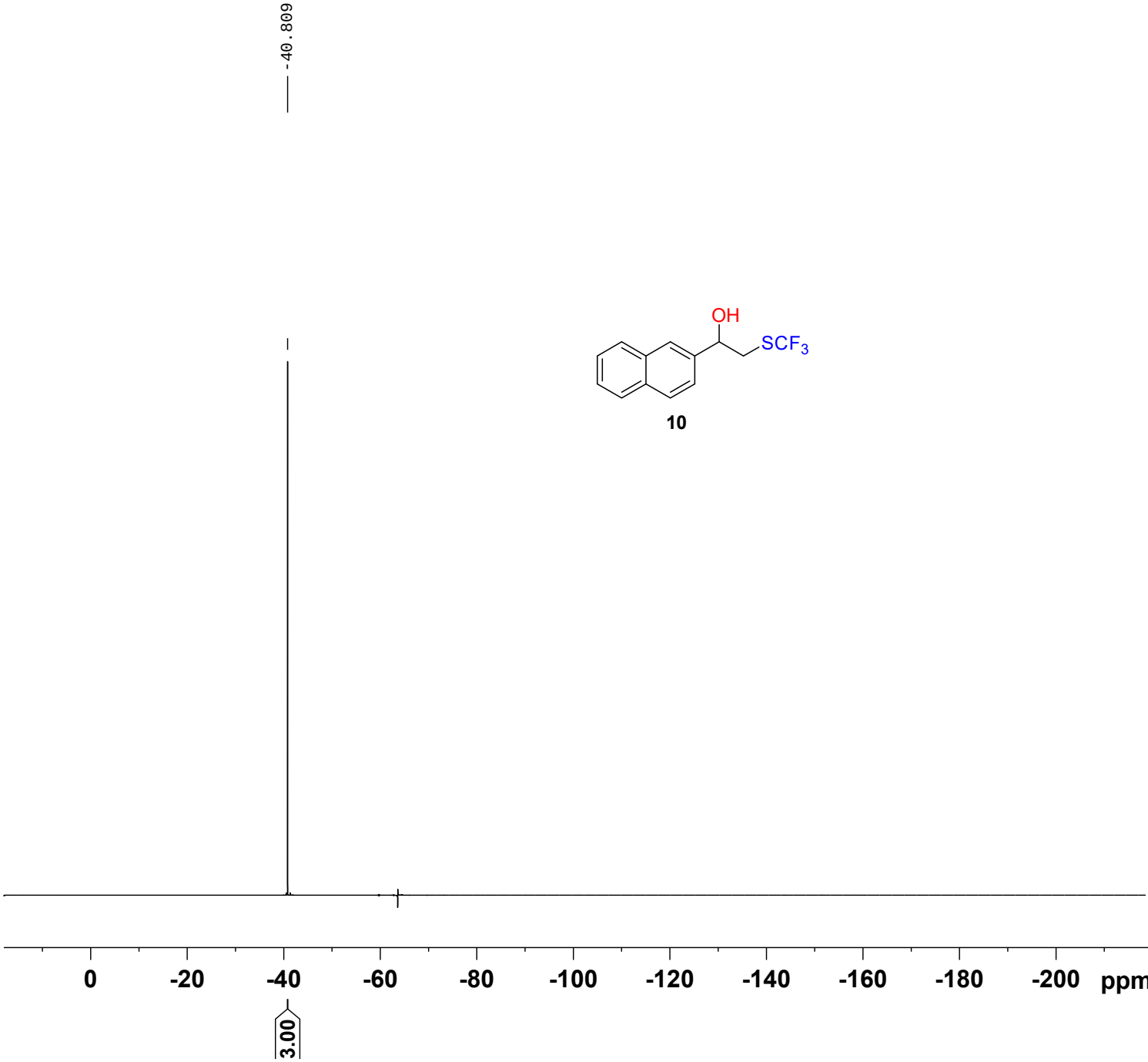


NAME	cyj-m16p-20190425
EXPNO	1
PROCNO	1
Date_	20040107
Time	23.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	161
DW	78.200 usec
DE	6.50 usec
TE	293.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300178 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

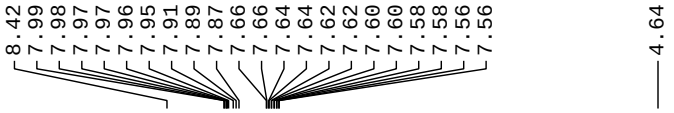
NAME	cyjm16p-20180425
EXPNO	2
PROCNO	1
Date_	20040107
Time	23.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	88
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	181
DW	19.800 usec
DE	6.50 usec
TE	294.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	3
======== CHANNEL f1 ========	
NUC1	13C
P1	15.00 usec
PL1	2.00 dB
PL1W	55.31277084 W
SFO1	100.6238364 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	16.72 dB
PL13	15.50 dB
PL2W	17.01305389 W
PL12W	0.28759566 W
PL13W	0.38087484 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127747 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

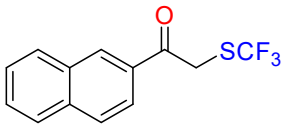



```
NAME      cyj-m16p-20190425
EXPNO                    3
PROCNO                   1
Date_             20040107
Time                 23.59
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgfhigqn
TD                  131072
SOLVENT               CDCl3
NS                       64
DS                        4
SWH               89285.711 Hz
FIDRES             0.681196 Hz
AQ                0.7340532 sec
RG                     2050
DW                    5.600 usec
DE                    6.50 usec
TE                   293.9 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                       4

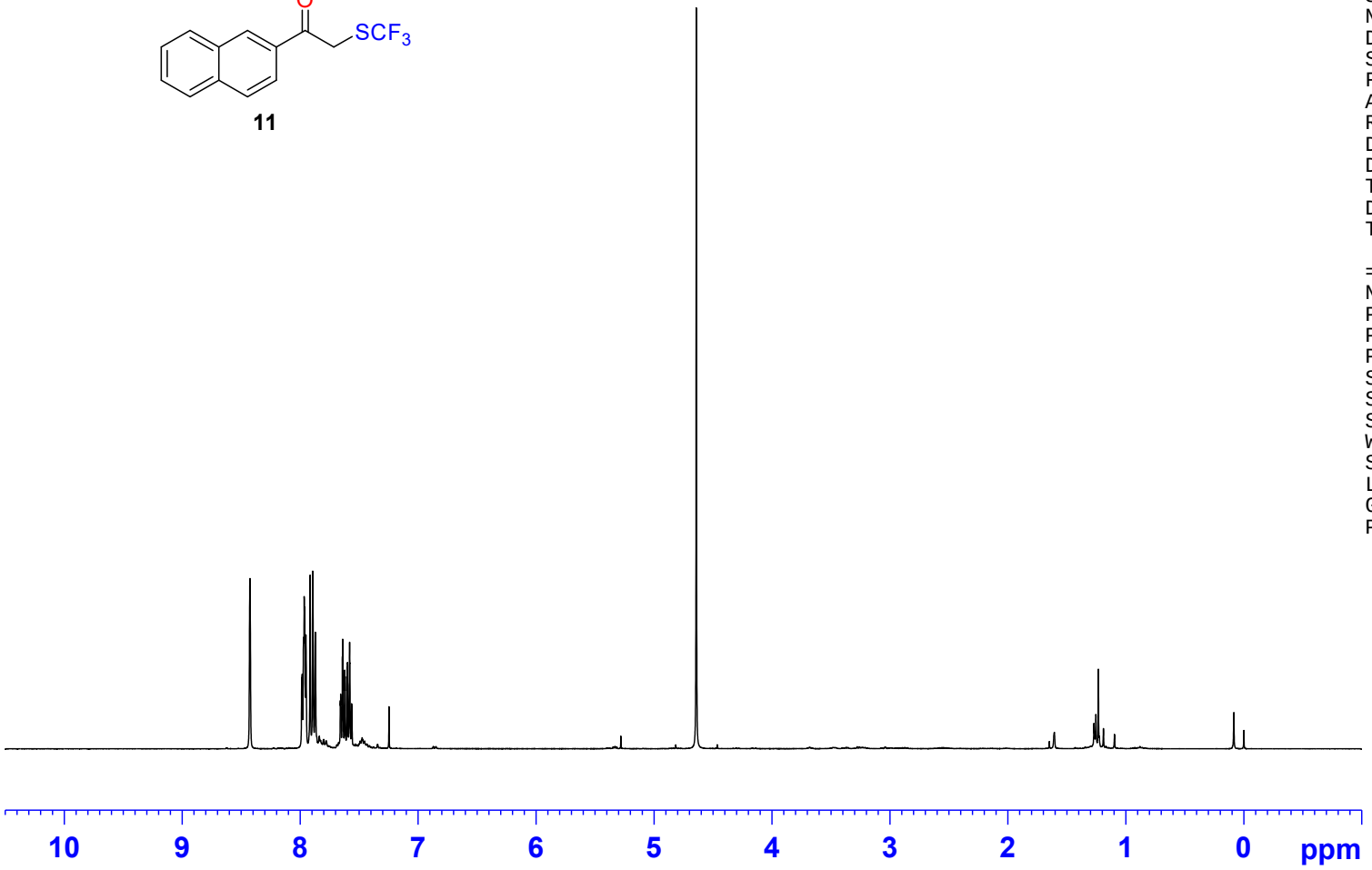
======== CHANNEL f1 ========
NUC1                    19F
P1                    14.20 usec
PL1                   -2.00 dB
PL1W           20.42289734 W
SFO1           376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
SFO2           400.1316005 MHz
SI                   65536
SF             376.4983660 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

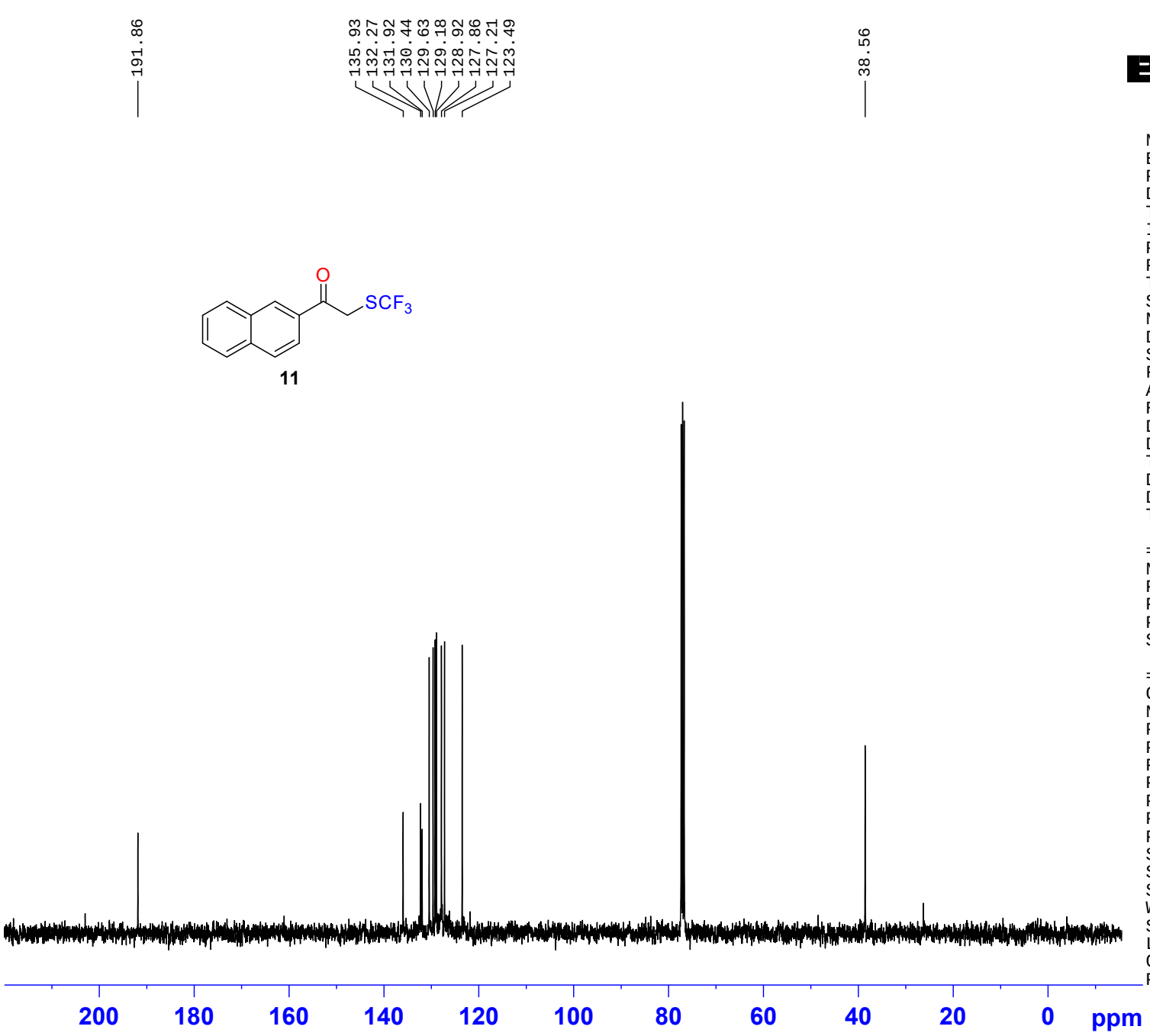




11



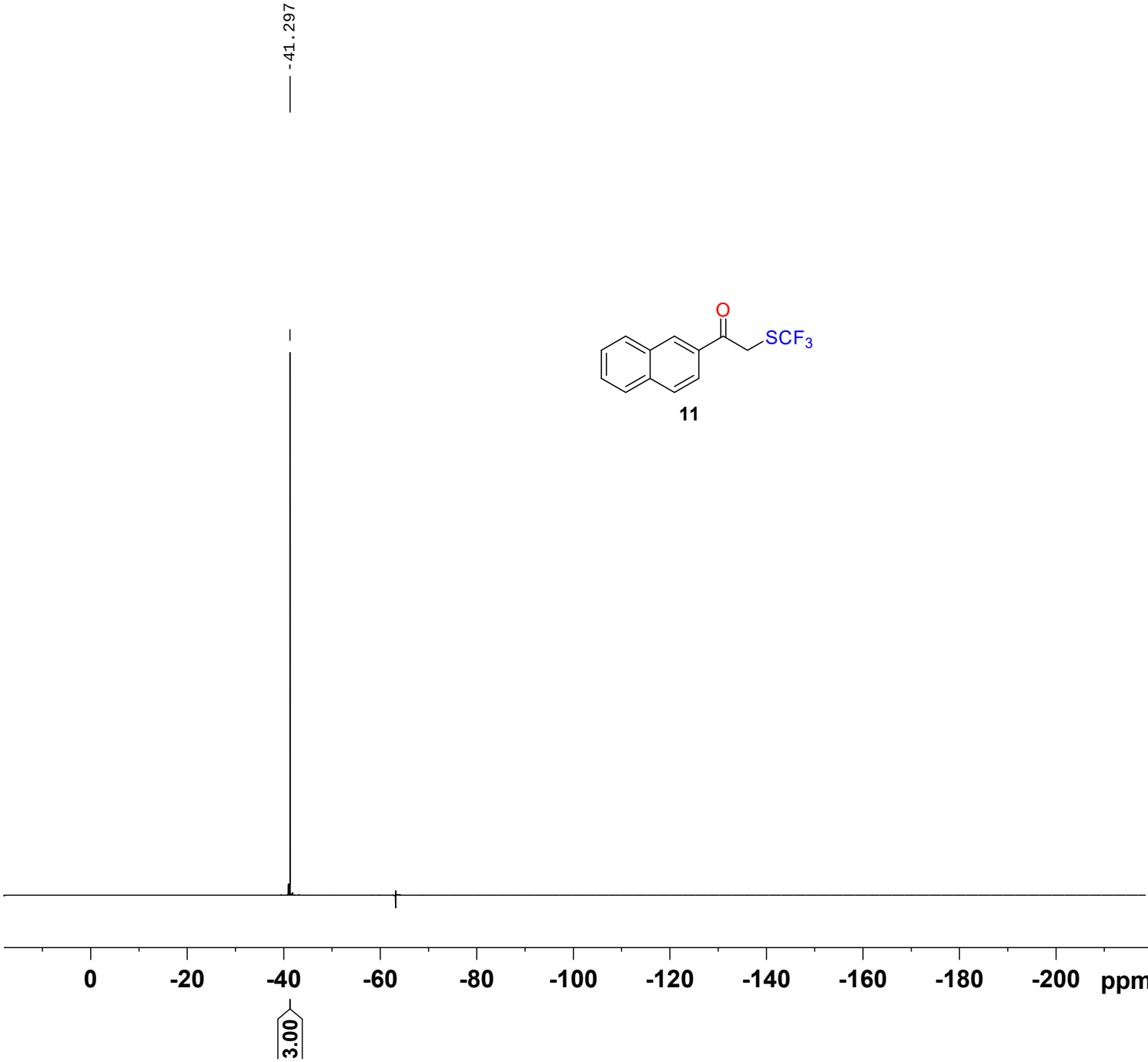
NAME	cyj-m13p-20190421
EXPNO	1
PROCNO	1
Date_	20040104
Time	1.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6393.862 Hz
FIDRES	0.195125 Hz
AQ	2.5625076 sec
RG	128
DW	78.200 usec
DE	6.50 usec
TE	292.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.40 usec
PL1	-1.00 dB
PL1W	17.01305389 W
SFO1	400.1326008 MHz
SI	32768
SF	400.1300160 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME      cyjm13p-20180421
EXPNO                    2
PROCNO                   1
Date_             20040104
Time                 1.58
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    40
DS                     4
SWH            25252.525 Hz
FIDRES           0.385323 Hz
AQ             1.2976629 sec
RG                   181
DW                19.800 usec
DE                 6.50 usec
TE                294.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    3

======== CHANNEL f1 ========
NUC1                 13C
P1                15.00 usec
PL1                2.00 dB
PL1W        55.31277084 W
SFO1        100.6238364 MHz

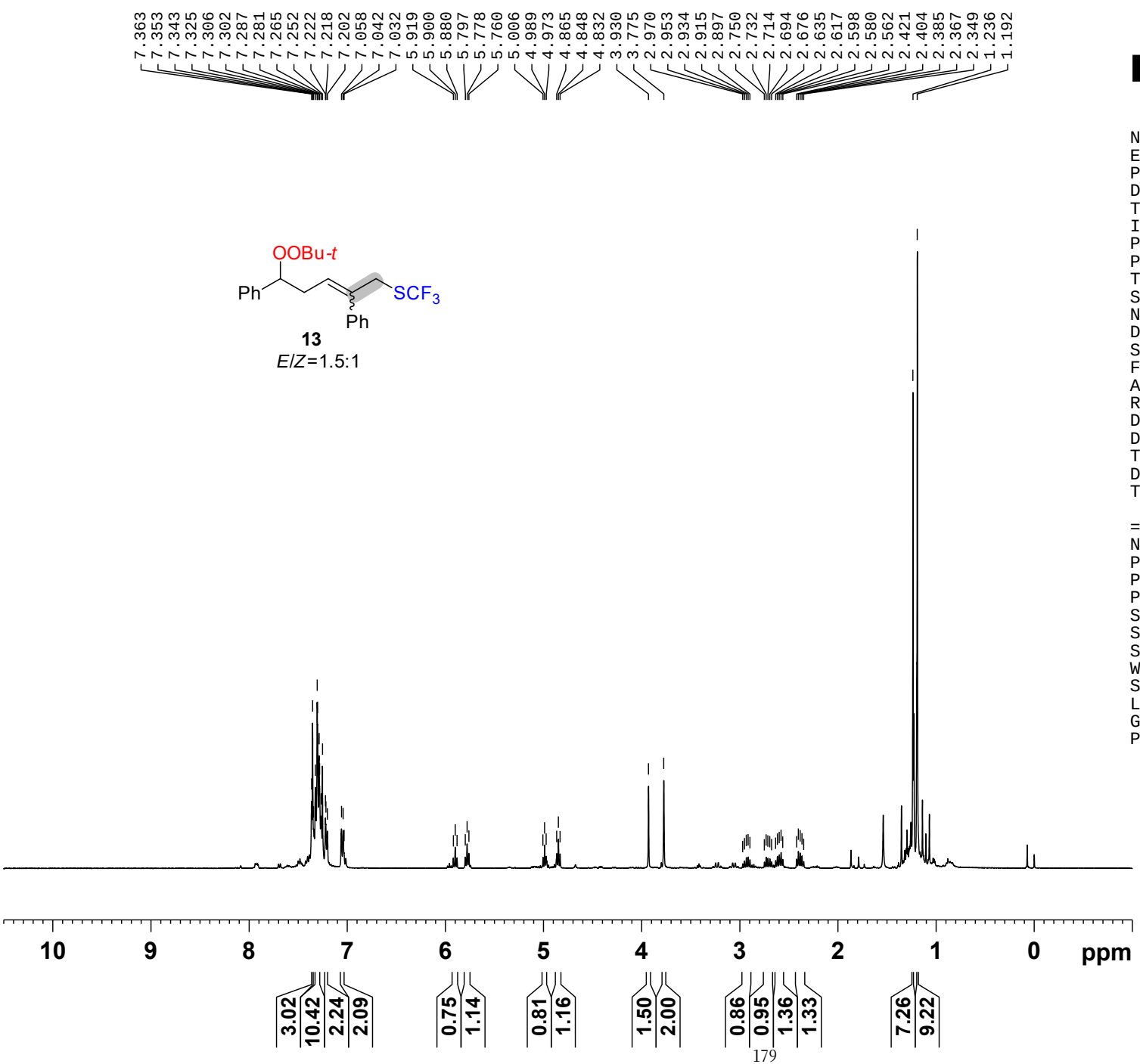
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              16.72 dB
PL13              15.50 dB
PL2W        17.01305389 W
PL12W        0.28759566 W
PL13W        0.38087484 W
SFO2        400.1316005 MHz
SI                32768
SF          100.6127758 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.40
```




```
NAME      cyj-m13p-20190421
EXPNO                    3
PROCNO                   1
Date_             20040104
Time                 2.02
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     64
DS                      4
SWH              89285.711 Hz
FIDRES           0.681196 Hz
AQ               0.7340532 sec
RG                    2050
DW                   5.600 usec
DE                   6.50 usec
TE                  293.0 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                     4

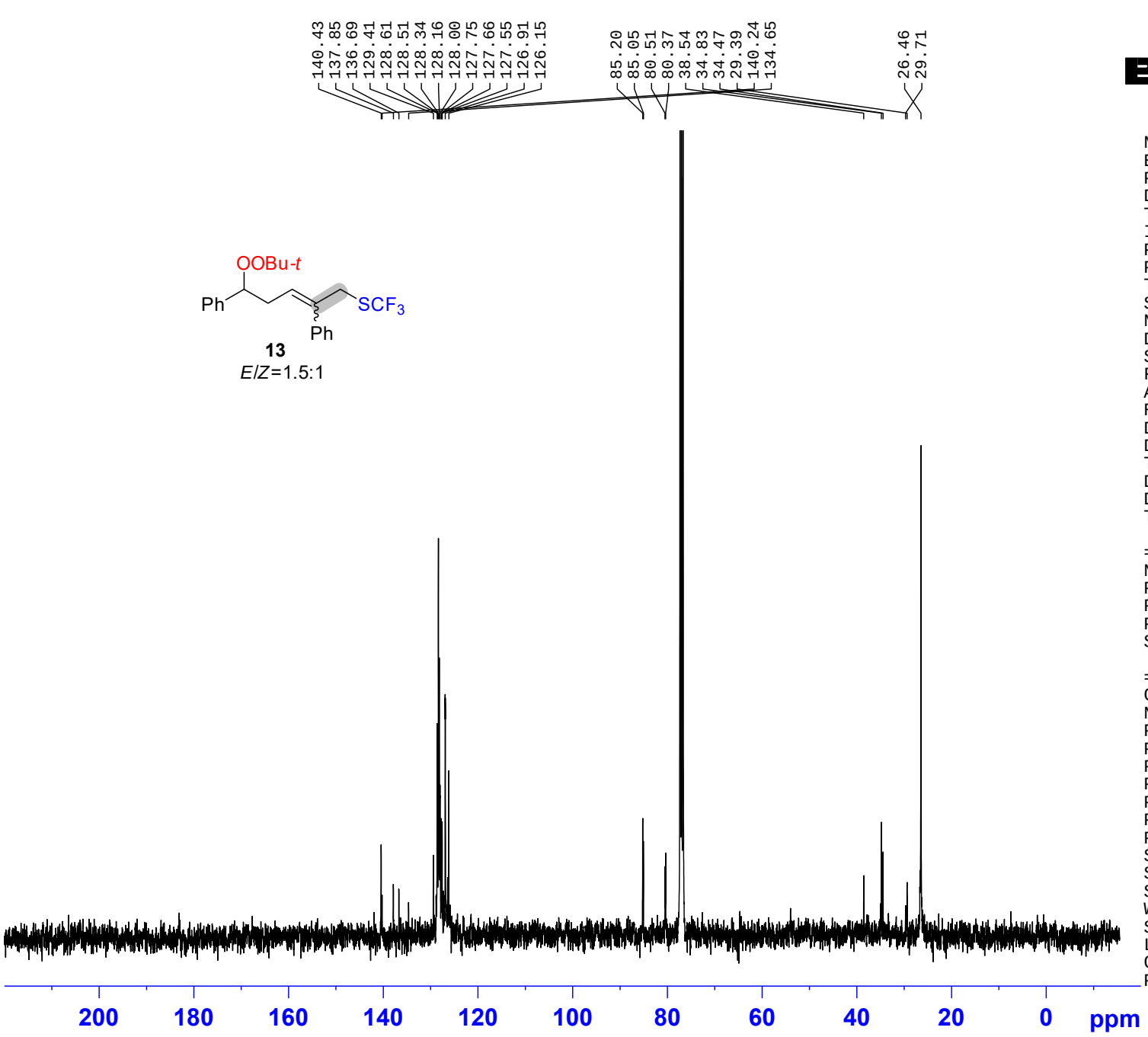
======== CHANNEL f1 ========
NUC1                   19F
P1                   14.20 usec
PL1                  -2.00 dB
PL1W          20.42289734 W
SFO1          376.4607164 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL2W          17.01305389 W
PL12W          0.28759566 W
SFO2          400.1316005 MHz
SI                  65536
SF            376.4983660 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
NAME      cyj890bp1-20190510
EXPNO                      1
PROCNO                     1
Date_               20040123
Time                    8.20
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         0
SWH                6393.862 Hz
FIDRES             0.195125 Hz
AQ                 2.5625076 sec
RG                       203
DW                    78.200 usec
DE                     6.50 usec
TE                    297.5 K
D1                 1.00000000 sec
TD0                        1

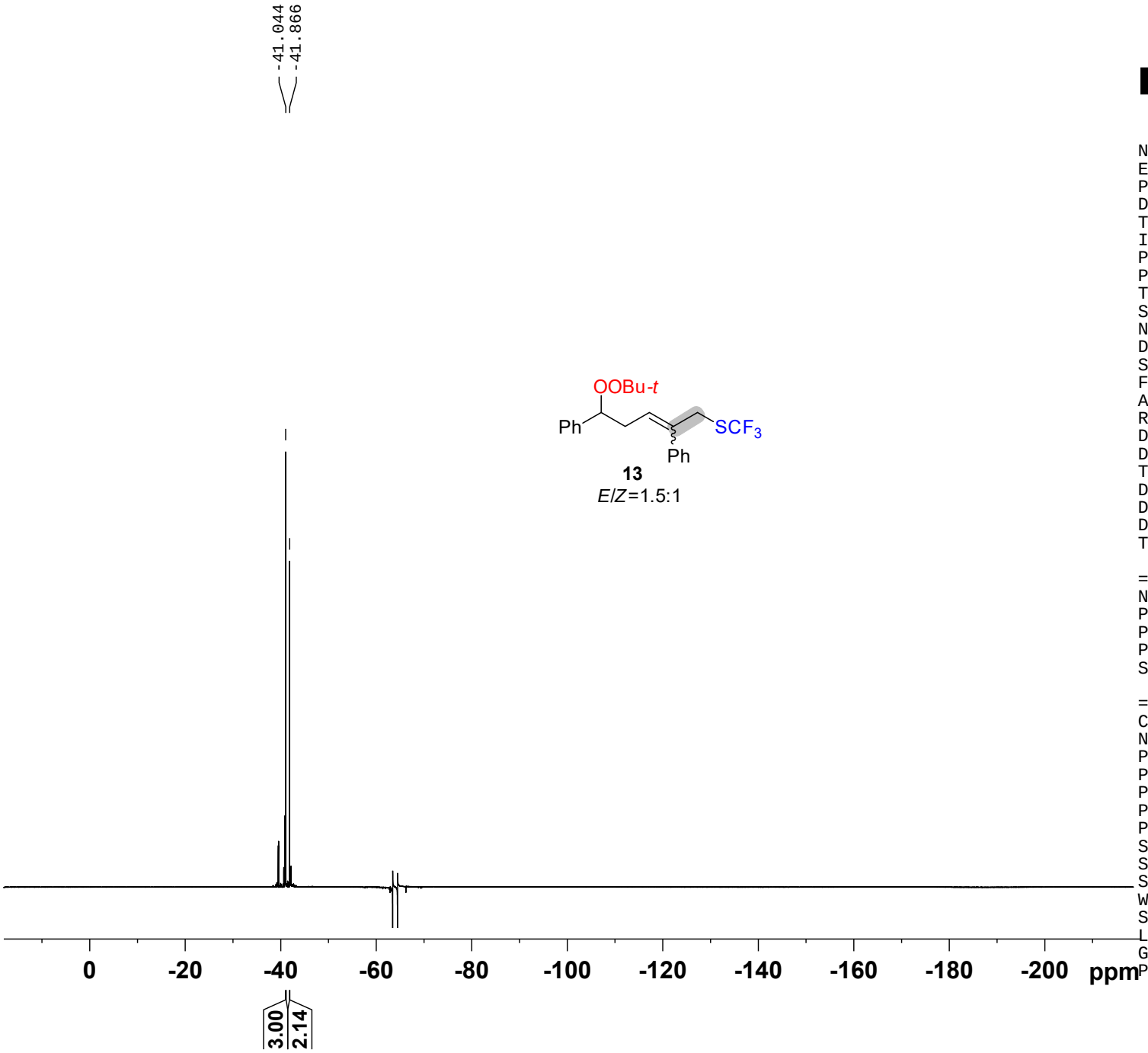
======== CHANNEL f1 ========
NUC1                      1H
P1                     10.40 usec
PL1                    -1.00 dB
PL1W            17.01305389 W
SFO1            400.1326008 MHz
SI                     32768
SF              400.1300139 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```




```
NAME      cyj890bp1-20190510
EXPNO                      2
PROCNO                     1
Date_               20040123
Time                    8.28
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        448
DS                          4
SWH                 25252.525 Hz
FIDRES                0.385323 Hz
AQ                    1.2976629 sec
RG                         1030
DW                       19.800 usec
DE                        6.50 usec
TE                       299.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         3

======== CHANNEL f1 ========
NUC1                       13C
P1                       15.00 usec
PL1                       2.00 dB
PL1W               55.31277084 W
SFO1               100.6238364 MHz

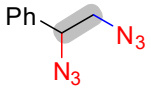
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                      -1.00 dB
PL12                     16.72 dB
PL13                     15.50 dB
PL2W               17.01305389 W
PL12W               0.28759566 W
PL13W               0.38087484 W
SFO2               400.1316005 MHz
SI                       32768
SF                 100.6127690 MHz
WDW                         EM
SSB                          0
LB                        3.00 Hz
GB                           0
PC                        1.40
```




```
NAME      cyj890bp1-201905010
EXPNO                       3
PROCNO                      1
Date_            20040123
Time                    8.54
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgfhigqn
TD                    131072
SOLVENT                CDCl3
NS                        32
DS                         4
SWH                89285.711 Hz
FIDRES             0.681196 Hz
AQ                 0.7340532 sec
RG                       812
DW                     5.600 usec
DE                     6.50 usec
TE                     298.3 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      19F
P1                     14.20 usec
PL1                    -2.00 dB
PL1W             20.42289734 W
SFO1             376.4607164 MHz

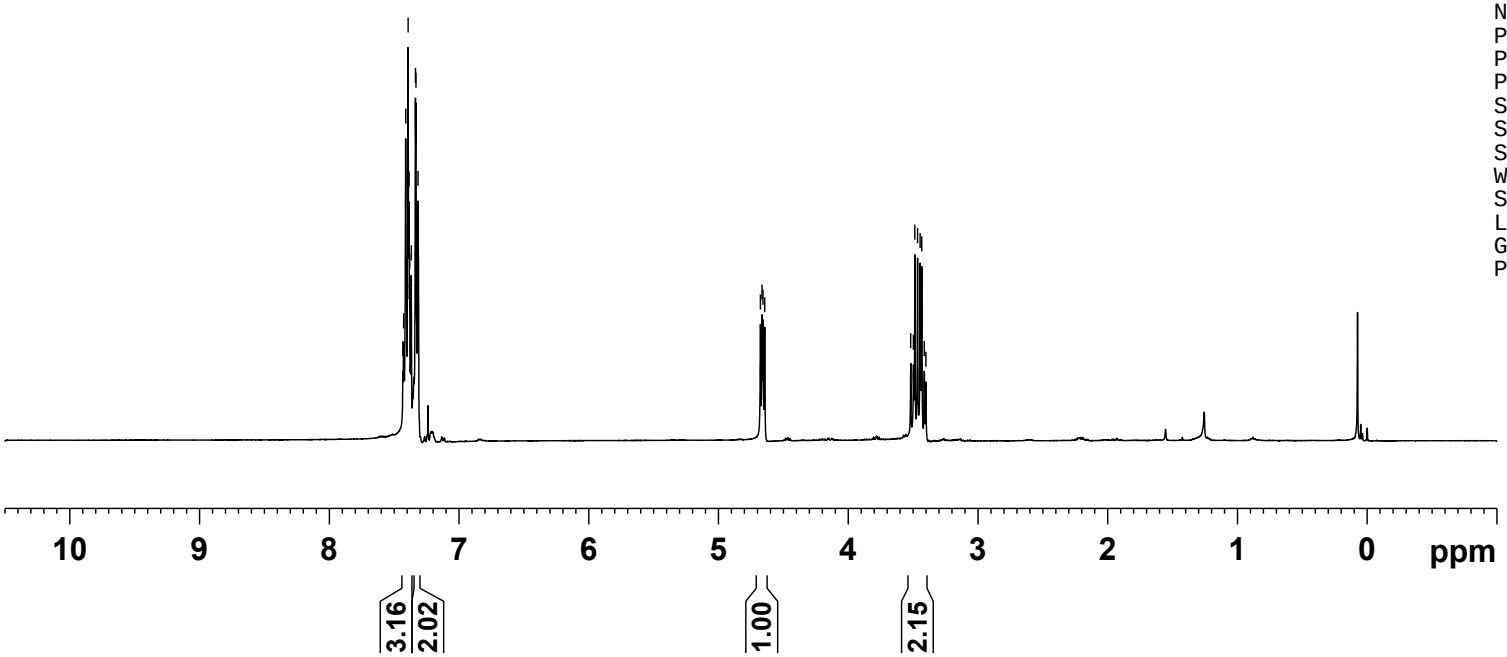
======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -1.00 dB
PL12                   16.72 dB
PL2W             17.01305389 W
PL12W             0.28759566 W
SFO2             400.1316005 MHz
SI                     65536
SF               376.4983660 MHz
WDW                       EM
SSB                        0
LB                      3.00 Hz
GB                         0
PC                      1.00
```

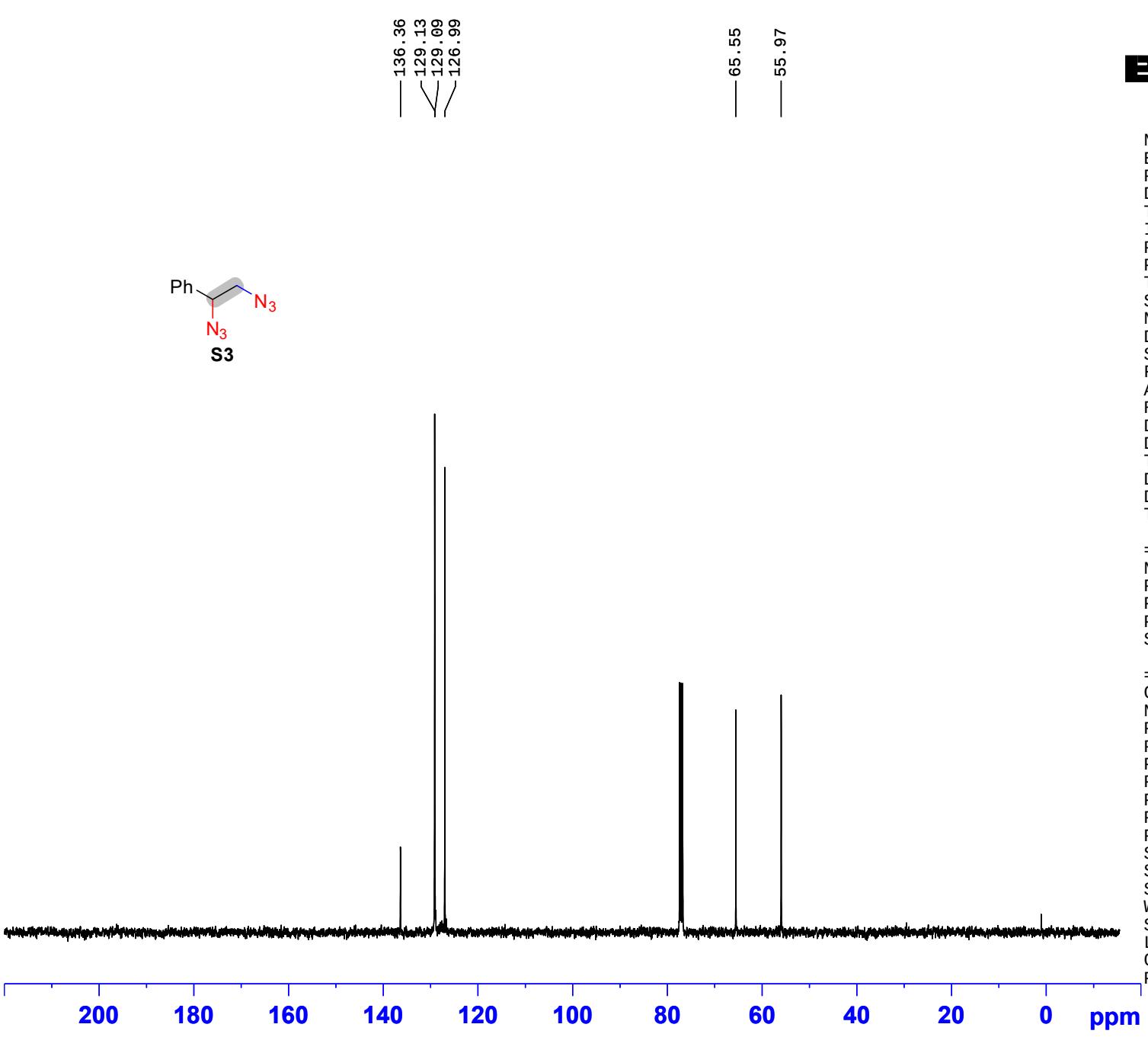


S3

```
NAME      cyj877bp-20190409
EXPNO                    1
PROCNO                   1
Date_             20190409
Time                 9.44
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH              6393.862 Hz
FIDRES           0.195125 Hz
AQ               2.5625076 sec
RG                    144
DW                 78.200 usec
DE                  6.50 usec
TE                 293.8 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.40 usec
PL1                 -1.00 dB
PL1W         17.01305389 W
SFO1         400.1326008 MHz
SI                  32768
SF           400.1300192 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                  1.00
```






```
NAME      cyj877bp-20190409
EXPNO                    2
PROCNO                   1
Date_             20190409
Time                 9.50
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      56
DS                       4
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976629 sec
RG                     181
DW                  19.800 usec
DE                   6.50 usec
TE                  295.1 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      3

======== CHANNEL f1 ========
NUC1                   13C
P1                  15.00 usec
PL1                  2.00 dB
PL1W           55.31277084 W
SFO1           100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -1.00 dB
PL12                 16.72 dB
PL13                 15.50 dB
PL2W           17.01305389 W
PL12W           0.28759566 W
PL13W           0.38087484 W
SFO2           400.1316005 MHz
SI                   32768
SF             100.6127690 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.40
```