Electronic Supplementary Material (ESI) for ChemComm.

A facile and general route to 3-((trifluoromethyl)thio)benzofurans and 3-((trifluoromethyl)thio)benzothiophenes

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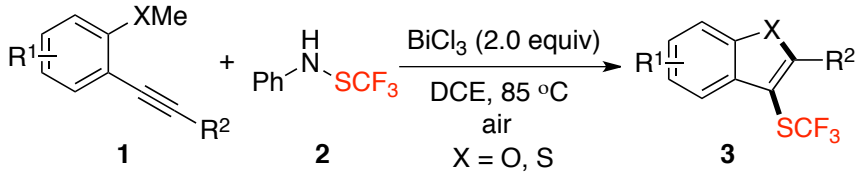
Supporting Information

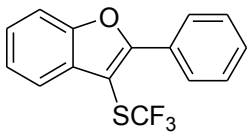
General Materials and Methods:

Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

General procedure for the synthesis of 3-((trifluoromethyl)thio)benzofurans and 3-((trifluoromethyl)thio)benzothiophenes.

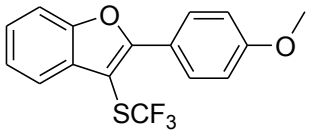


Trifluoromethanesulfanylamide **2** (0.22 mmol, 42.5 mg) was added to a solution of compound **1** (0.2 mmol) and $BiCl_3$ (0.4 mmol, 126.2 mg) in DCE (2.0 mL), and the solution was stirred at 85 °C for 12-16 hours. After completion of the reaction as indicated by TLC, the reaction mixture was filtered by silica gel and washed by CH_2Cl_2 (3 × 5.0 mL). The solution was concentrated in vacuo and the residue was purified by column chromatography on silica gel to provide the product **3**.



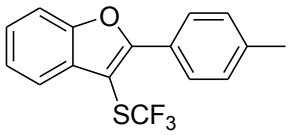
2-Phenyl-3-(trifluoromethylthio)benzofuran (**3a**)

White solid; mp: 74.8-76.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34–7.38 (m, 2H), 7.44–7.54 (m, 4H), 7.73–7.75 (m, 1H), 8.20 (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 97.5, 111.4, 120.2, 124.1, 125.7, 128.0, 128.7, 128.9, 129.4 (q, J = 309.4 Hz), 130.2, 130.9, 153.7, 160.1; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.43 (s); HRMS (EI) calcd for $C_{15}H_9F_3OS$: 294.0326 (M^+), found: 294.0348.



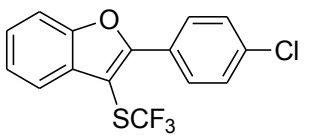
2-(4-Methoxyphenyl)-3-(trifluoromethylthio)benzofuran (**3b**)

White solid; mp: 85.6-86.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.92 (s, 3H), 7.06 (d, J = 8.9 Hz, 2H), 7.38–7.40 (m, 2H), 7.56–7.58 (m, 1H), 7.75–7.77 (m, 1H), 8.23 (d, J = 8.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 95.6, 111.2, 114.1, 119.9, 121.5, 123.9, 125.2, 129.4 (q, J = 309.7 Hz), 129.5, 131.1, 153.4, 160.2, 161.1; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.66 (s); HRMS (EI) calcd for $C_{16}H_{11}F_3O_2S$: 324.0432 (M^+), found: 324.0438.



2-*p*-Tolyl-3-(trifluoromethylthio)benzofuran (**3c**)

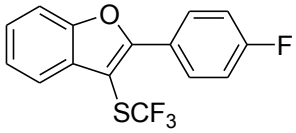
White solid; mp: 69.2-70.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 7.29 (d, J = 8.1 Hz, 2H), 7.32–7.37 (m, 2H), 7.51–7.54 (m, 1H), 7.71–7.73 (m, 1H), 8.10 (d, J = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 96.5, 111.2, 119.9, 123.9, 125.4, 126.0, 127.7, 129.28, 129.31 (q, J = 309.5 Hz), 140.4, 153.5, 160.3; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.54 (s); HRMS (EI) calcd for $C_{16}H_{11}F_3OS$: 308.0483 (M^+), found: 308.0495.



2-(4-Chlorophenyl)-3-(trifluoromethylthio)benzofuran (**3d**)

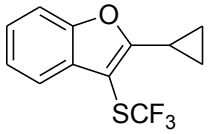
Yellow solid; mp: 73.8-74.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35–7.42 (m, 2H),

7.47 (dd, J_1 = 1.8 Hz, J_2 = 6.9 Hz, 2H), 7.53–7.55 (m, 1H), 7.73–7.75 (m, 1H), 8.23 (dd, J_1 = 1.8 Hz, J_2 = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 97.8, 111.3, 120.1, 124.1, 125.9, 127.2, 128.9, 129.0, 129.1 (q, J = 309.5 Hz), 130.6, 136.2, 153.5, 158.7; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.42 (s); HRMS (EI) calcd for $C_{15}H_8ClF_3OS$: 327.9936 (M^+), found: 327.9932.



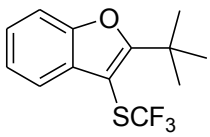
2-(4-Fluorophenyl)-3-(trifluoromethylthio)benzofuran (**3e**)

White solid; mp: 70.4-71.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (t, J = 8.4 Hz, 2H), 7.37–7.43 (m, 2H), 7.55–7.57 (m, 1H), 7.76 (d, J = 7.9 Hz, 1H), 8.23 (dd, J_1 = 5.5 Hz, J_2 = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 97.2, 111.4, 115.9 (d, $^2J_{CF}$ = 21.8 Hz), 120.2, 124.2, 125.1, 125.8, 129.3 (q, J = 309.8 Hz), 130.0 (d, $^3J_{CF}$ = 8.4 Hz), 130.8, 153.6, 159.1, 163.7 (d, $^1J_{CF}$ = 250.6 Hz); ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.50 (s), -109.63 (s); HRMS (EI) calcd for $C_{15}H_8F_4OS$: 312.0232 (M^+), found: 312.0242.



2-Cyclopropyl-3-(trifluoromethylthio)benzofuran (**3f**)

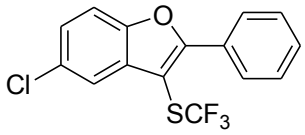
White solid; mp: 48.2-49.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.11–1.16 (m, 2H), 1.21–1.25 (m, 2H), 2.44–2.50 (m, 1H), 7.23–7.30 (m, 2H), 7.37 (d, J = 7.8 Hz, 1H), 7.58 (d, J = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 8.3, 8.6, 96.7, 111.0, 118.8, 123.7, 124.3, 129.4 (q, J = 309.2 Hz), 130.1, 153.2, 167.0; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.73 (s); HRMS (EI) calcd for $C_{12}H_9F_3OS$: 258.0326 (M^+), found: 258.0334.



2-*tert*-Butyl-3-(trifluoromethylthio)benzofuran (**3g**)

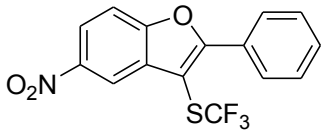
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.57 (s, 9H), 7.32–7.34 (m, 2H), 7.46–7.48 (m, 1H), 7.67–7.69 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.7, 31.9,

95.9, 111.0, 119.7, 123.5, 124.7, 129.2 (q, J = 309.4 Hz), 152.9, 171.3; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.94 (s); HRMS (EI) calcd for $C_{13}H_{13}F_3OS$: 274.0639 (M^+), found: 274.0648.



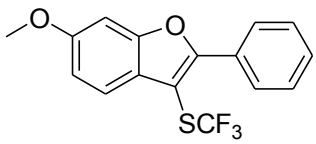
5-Chloro-2-phenyl-3-(trifluoromethylthio)benzofuran (**3i**)

White solid; mp: 98.8-99.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (dd, J_1 = 2.1 Hz, J_2 = 8.7 Hz, 1H), 7.45 (d, J = 8.7 Hz, 1H), 7.48–7.53 (m, 3H), 7.69 (d, J = 1.3 Hz, 1H), 8.18–8.20 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 97.0, 112.5, 119.8, 126.0, 127.9, 128.4, 128.7, 129.2 (q, J = 310.0 Hz), 130.0, 130.5, 132.3, 152.0, 161.4; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.38 (s); HRMS (EI) calcd for $C_{15}H_8ClF_3OS$: 327.9936 (M^+), found: 327.9948.



5-Nitro-2-phenyl-3-(trifluoromethylthio)benzofuran (**3j**)

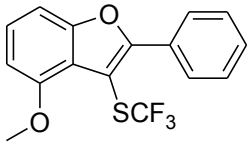
Yellow solid; mp: 95.4-96.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52–7.53 (m, 3H), 7.62 (d, J = 9.0 Hz, 1H), 8.19–8.21 (m, 2H), 8.10 (dd, J_1 = 2.1 Hz, J_2 = 9.0 Hz, 1H), 8.61 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 98.3, 112.0, 116.6, 121.4, 125.2, 128.0, 128.86, 128.93, 129.0 (q, J = 310.1 Hz), 131.2, 145.2, 156.2, 163.1; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.15 (s); HRMS (EI) calcd for $C_{15}H_8F_3NO_3S$: 339.0177 (M^+), found: 339.0185.



6-Methoxy-2-phenyl-3-(trifluoromethylthio)benzofuran (**3k**)

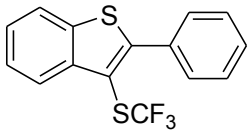
Yellow solid; mp: 119.6-120.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.96 (s, 3H), 7.49–7.516 (m, 3H), 7.56 (d, J = 8.6 Hz, 1H), 8.10 (dd, J_1 = 1.6 Hz, J_2 = 8.6 Hz, 1H), 8.19–8.21 (m, 2H), 8.44 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 52.2, 98.0, 111.3, 122.4, 126.6, 127.4, 127.9, 128.7, 129.1 (q, J = 310.2 Hz), 130.6, 130.9, 156.1, 161.4,

166.7; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.32 (s); HRMS (EI) calcd for $C_{16}H_{11}F_3O_2S$: 324.0432 (M^+), found: 324.0451.



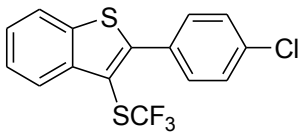
4-Methoxy-2-phenyl-3-(trifluoromethylthio)benzofuran (**3l**)

Yellow solid; mp: 109.4-110.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.97 (s, 3H), 6.76 (d, *J* = 8.0 Hz, 1H), 7.17 (d, *J* = 8.2 Hz, 1H), 7.29 (t, *J* = 8.2 Hz, 1H), 7.43–7.52 (m, 3H), 8.16–8.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.7, 96.6, 104.4, 105.0, 114.6, 119.4, 126.2, 128.1, 128.5, 129.3 (q, *J* = 309.3 Hz), 129.0, 129.9, 154.9, 155.0; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.68 (s); HRMS (EI) calcd for $C_{16}H_{11}F_3O_2S$: 324.0432 (M^+), found: 324.0426.



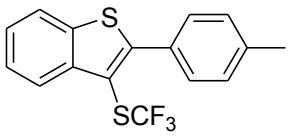
2-Phenyl-3-(trifluoromethylthio)benzo[*b*]thiophene (**3m**)

White solid; mp: 69.4-70.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.56 (m, 5H), 7.66–7.69 (m, 2H), 7.87 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 111.1, 122.1, 123.7, 125.47, 125.50, 128.5, 129.3, 129.2 (q, *J* = 309.8 Hz), 130.2, 132.6, 137.9, 141.3, 154.3; ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.92 (s); HRMS (EI) calcd for $C_{15}H_9F_3S_2$: 310.0098 (M^+), found: 310.0082.



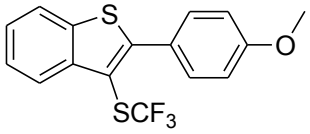
2-(4-Chlorophenyl)-3-(trifluoromethylthio)benzo[*b*]thiophene (**3n**)

Yellow solid; mp: 87.2-88.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43–7.47 (m, 3H), 7.50–7.54 (m, 1H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.07 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 103.2, 122.1, 123.7, 125.6, 125.7, 128.8, 129.1 (q, *J* = 309.8 Hz), 131.0, 131.4, 135.6, 137.8, 141.2, 152.7; ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.88 (s); HRMS (EI) calcd for $C_{15}H_8ClF_3S_2$: 343.9708 (M^+), found: 343.9702.



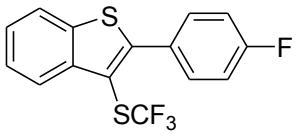
2-*p*-Tolyl-3-(trifluoromethylthio)benzo[*b*]thiophene (**3o**)

Yellow solid; mp: 89.4-90.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.45 (s, 3H), 7.31 (d, *J* = 7.1 Hz, 2H), 7.42–7.45 (m, 1H), 7.50–7.54 (m, 1H), 7.58 (d, *J* = 7.1 Hz, 2H), 7.85 (d, *J* = 7.8 Hz, 1H), 8.09 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 110.6, 122.1, 123.5, 125.35, 125.37, 129.20 (q, *J* = 309.7 Hz), 129.23, 129.7, 130.0, 137.8, 139.5, 141.4, 154.5; ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.89 (s); HRMS (EI) calcd for $C_{16}H_{11}F_3S_2$: 324.0254 (M^+), found: 324.0268.



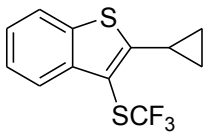
2-(4-Methoxyphenyl)-3-(trifluoromethylthio)benzo[*b*]thiophene (**3p**)

Yellow solid; mp: 110.0-111.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.87 (s, 3H), 6.99–7.03 (m, 2H), 7.39–7.43 (m, 1H), 7.48–7.52 (m, 1H), 7.60–7.63 (m, 2H), 7.83 (d, *J* = 7.9 Hz, 1H), 8.05 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.3, 110.1, 114.0, 122.0, 123.5, 124.9, 125.3, 125.4, 129.2 (q, *J* = 310.0 Hz), 131.4, 137.6, 141.4, 154.2, 160.5; ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.94 (s); HRMS (EI) calcd for $C_{16}H_{11}F_3OS_2$: 340.0203 (M^+), found: 340.0215.



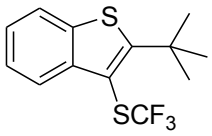
2-(4-Fluorophenyl)-3-(trifluoromethylthio)benzo[*b*]thiophene (**3q**)

White solid; mp: 65.5-66.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17–7.22 (m, 2H), 7.44–7.55 (m, 2H), 7.63–7.64 (m, 2H), 7.83–7.88 (m, 1H), 8.06–8.10 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 111.3, 115.7 (d, $^{2}J_{CF}$ = 21.8 Hz), 122.1, 123.7, 125.59, 125.62, 128.6, 129.1 (q, *J* = 309.3 Hz), 132.0 (d, $^{3}J_{CF}$ = 7.8 Hz), 137.8, 141.2, 153.0, 163.4 (d, $^{1}J_{CF}$ = 248.9 Hz); ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.92 (s), -111.85 (s); HRMS (EI) calcd for $C_{15}H_8F_4S_2$: 328.0004 (M^+), found: 328.0018.



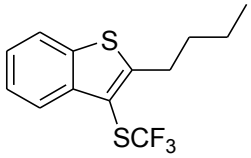
2-Cyclopropyl-3-(trifluoromethylthio)benzo[*b*]thiophene (**3r**)

White solid; mp: 46.1-47.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.93–0.97 (m, 2H), 1.24–1.29 (m, 2H), 2.73–2.80 (m, 1H), 7.30–7.34 (m, 1H), 7.41–7.45 (m, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.9, 12.2, 111.0, 122.0, 122.2, 124.6, 125.2, 128.9 (q, J = 310.2 Hz), 135.6, 141.3, 161.5; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.59 (s); HRMS (EI) calcd for $C_{12}H_9F_3S_2$: 274.0098 (M^+), found: 274.0082.



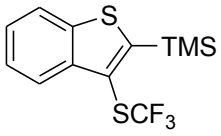
2-*tert*-Butyl-3-(trifluoromethylthio)benzo[*b*]thiophene (**3s**)

White solid; mp: 39.2-40.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.63 (s, 9H), 7.34–7.38 (m, 1H), 7.43–7.47 (m, 1H), 7.79 (d, J = 8.0 Hz, 1H), 8.00 (d, J = 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.7, 36.7, 109.3, 121.7, 122.7, 124.7, 124.9, 129.8 (q, J = 309.5 Hz), 135.7, 142.3, 166.3; ^{19}F NMR (378 MHz, $CDCl_3$) δ -40.91 (s); HRMS (EI) calcd for $C_{13}H_{13}F_3S_2$: 290.0411 (M^+), found: 290.0423.



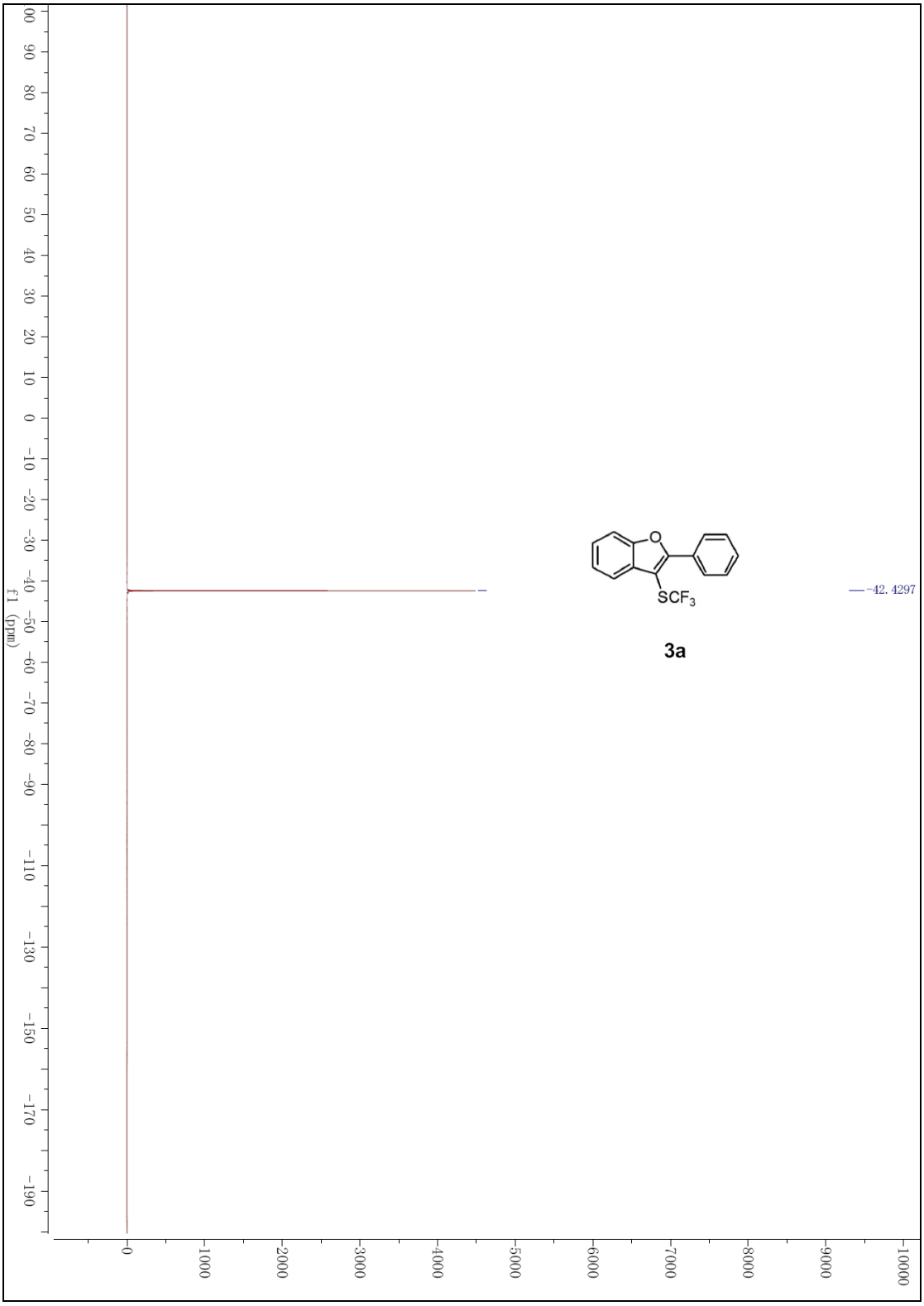
2-Butyl-3-(trifluoromethylthio)benzo[*b*]thiophene (**3t**)

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.97 (t, J = 7.1 Hz, 3H), 1.40–1.48 (m, 2H), 1.70–1.77 (m, 2H), 3.18 (t, J = 7.6 Hz, 2H), 7.35 (t, J = 7.4 Hz, 1H), 7.42–7.46 (m, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.95 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.8, 22.4, 29.4, 33.4, 111.1, 122.2, 122.7, 124.8, 125.1, 129.2 (q, J = 309.4 Hz), 137.3, 140.7, 158.4; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.59 (s); HRMS (EI) calcd for $C_{13}H_{13}F_3S_2$: 290.0411 (M^+), found: 290.0401.



Trimethyl(3-(trifluoromethylthio)benzo[*b*]thiophen-2-yl)silane (**3u**)

Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.50 (s, 9H), 7.43 (dd, J_1 = 0.8 Hz, J_2 = 8.0 Hz, 2H), 7.47–7.51 (m, 1H), 7.88 (d, J = 7.9 Hz, 1H), 8.06 (d, J = 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 0.1, 12.9, 122.2, 123.0, 124.3, 125.0, 125.1, 125.6, 125.8, 125.9 (q, J = 309.0 Hz); ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.57 (s); HRMS (EI) calcd for $C_{12}H_{13}F_3S_2Si$: 306.0180 (M^+), found: 306.0196.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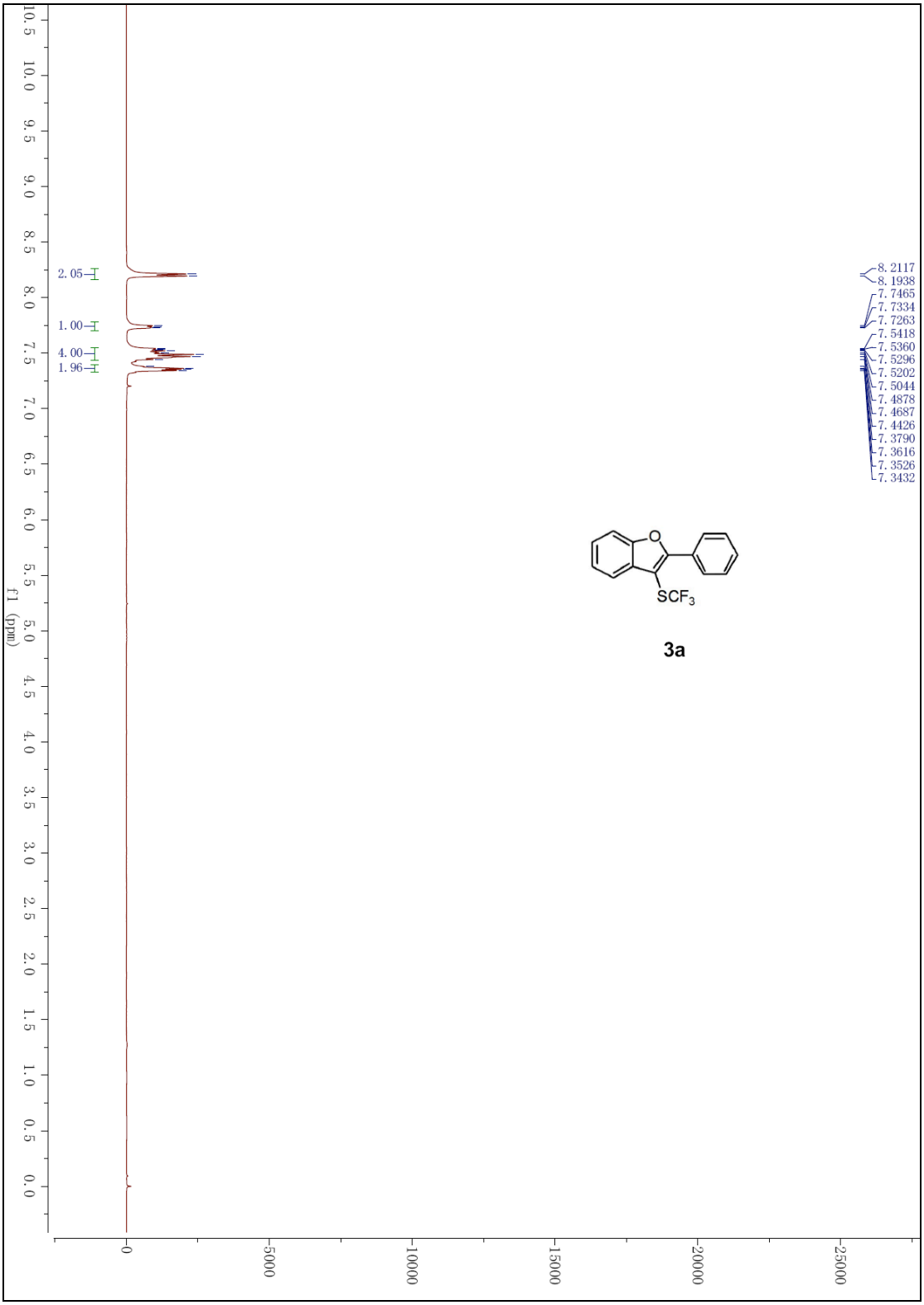
SCF3
3a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7.7465
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7.7263
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7.5296
7.5202
7.5044
7.4878
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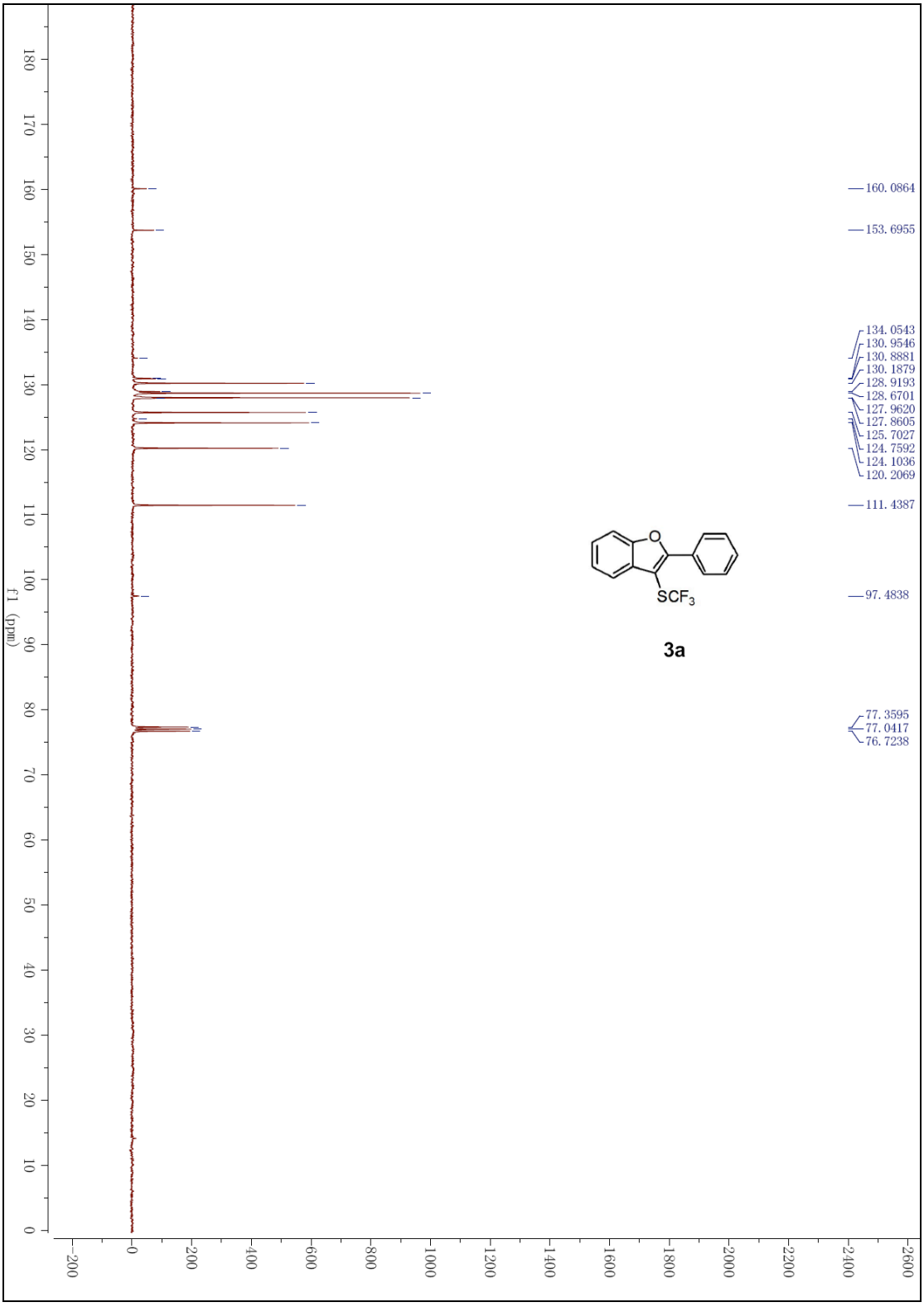
7.4426
7.3790
7.3616
7.3526
7.3432
SCF3
f1 (ppm)

3a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134.0543
130.9546
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128.9193
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127.9620
127.8605
125.7027
124.7592
124.1036
120.2069
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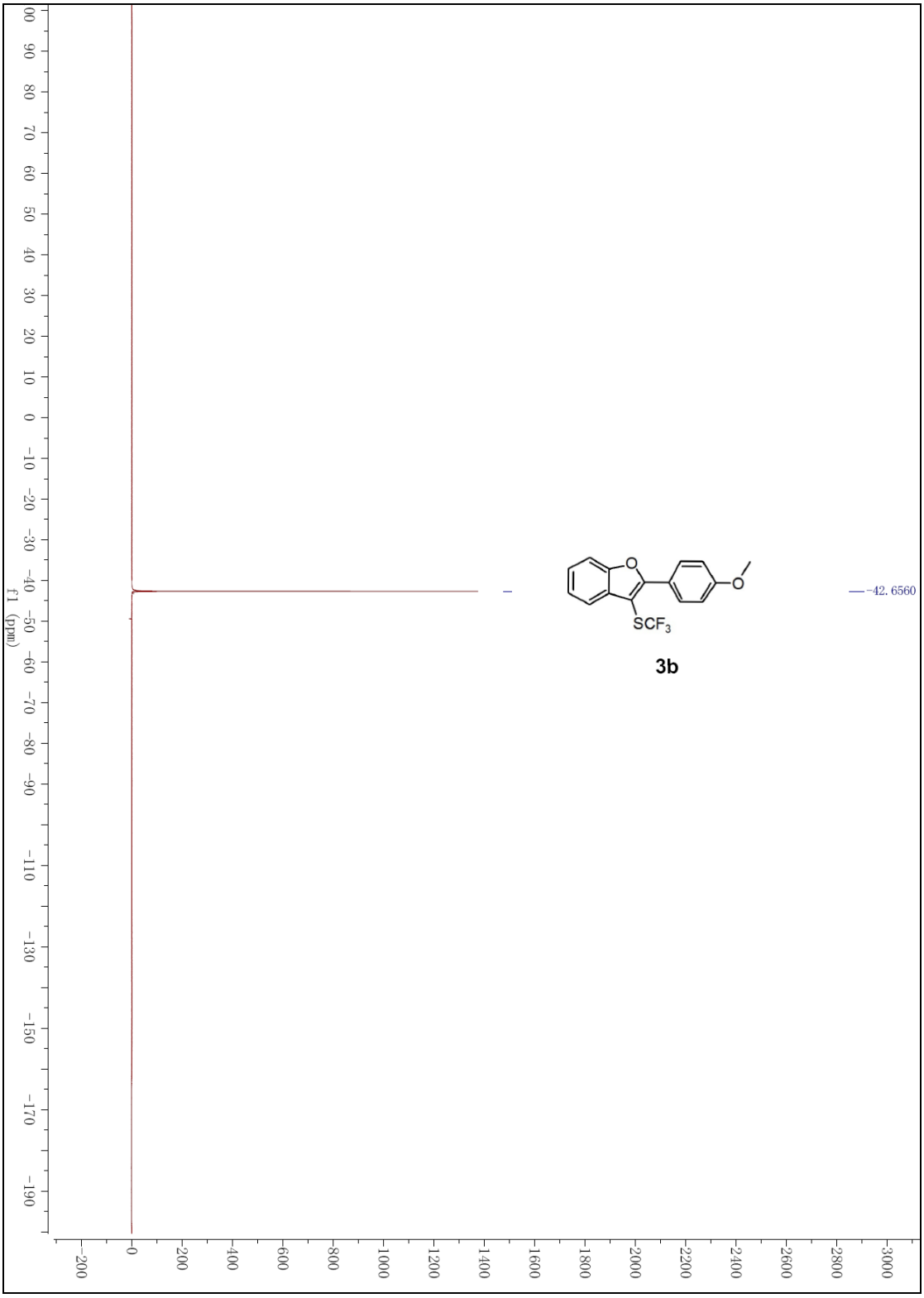
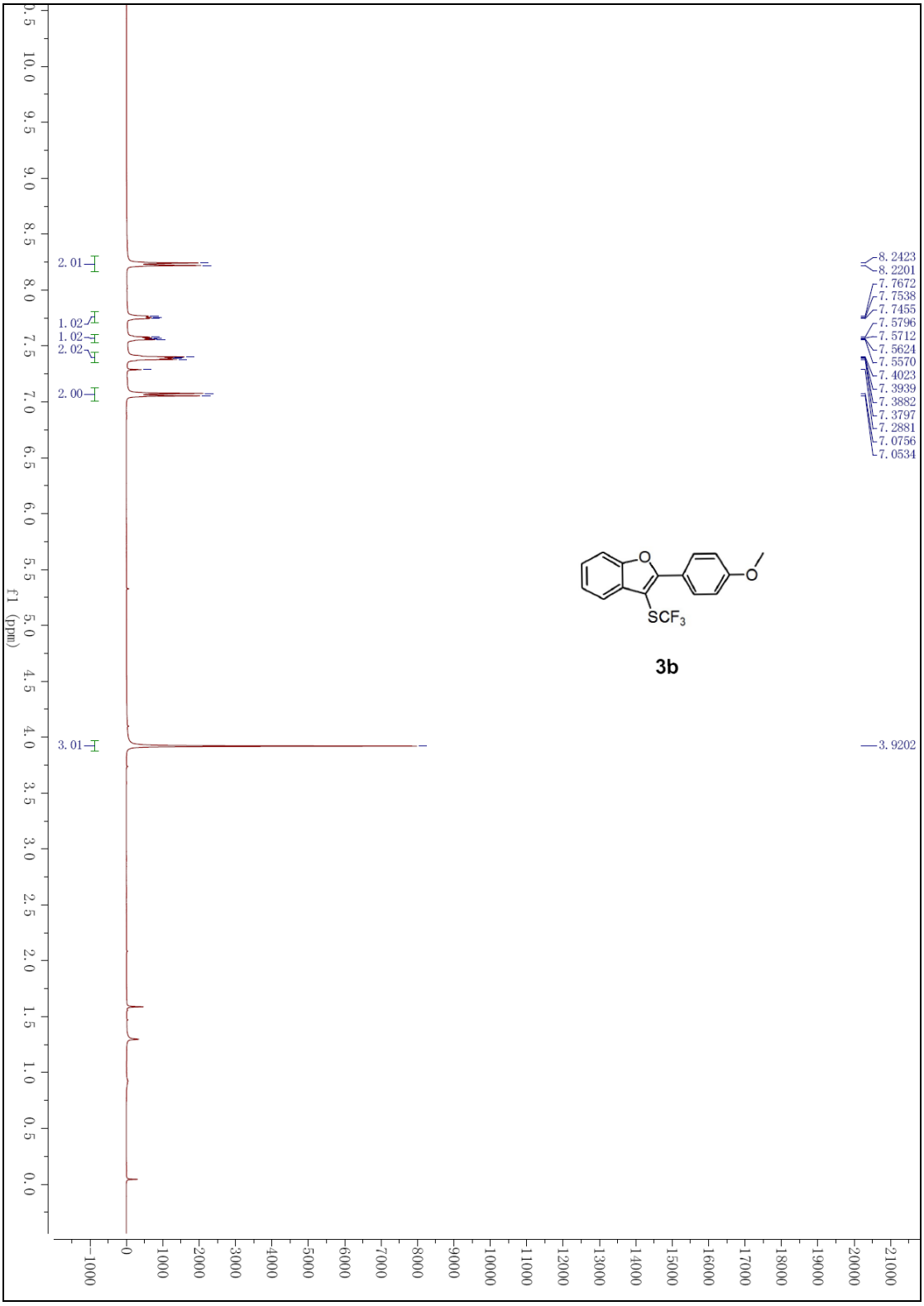
97.4838
77.3595
77.0417
76.7238
SCF3
3a
f1 (ppm)


-42.6560
SCF3
3b
f1 (ppm)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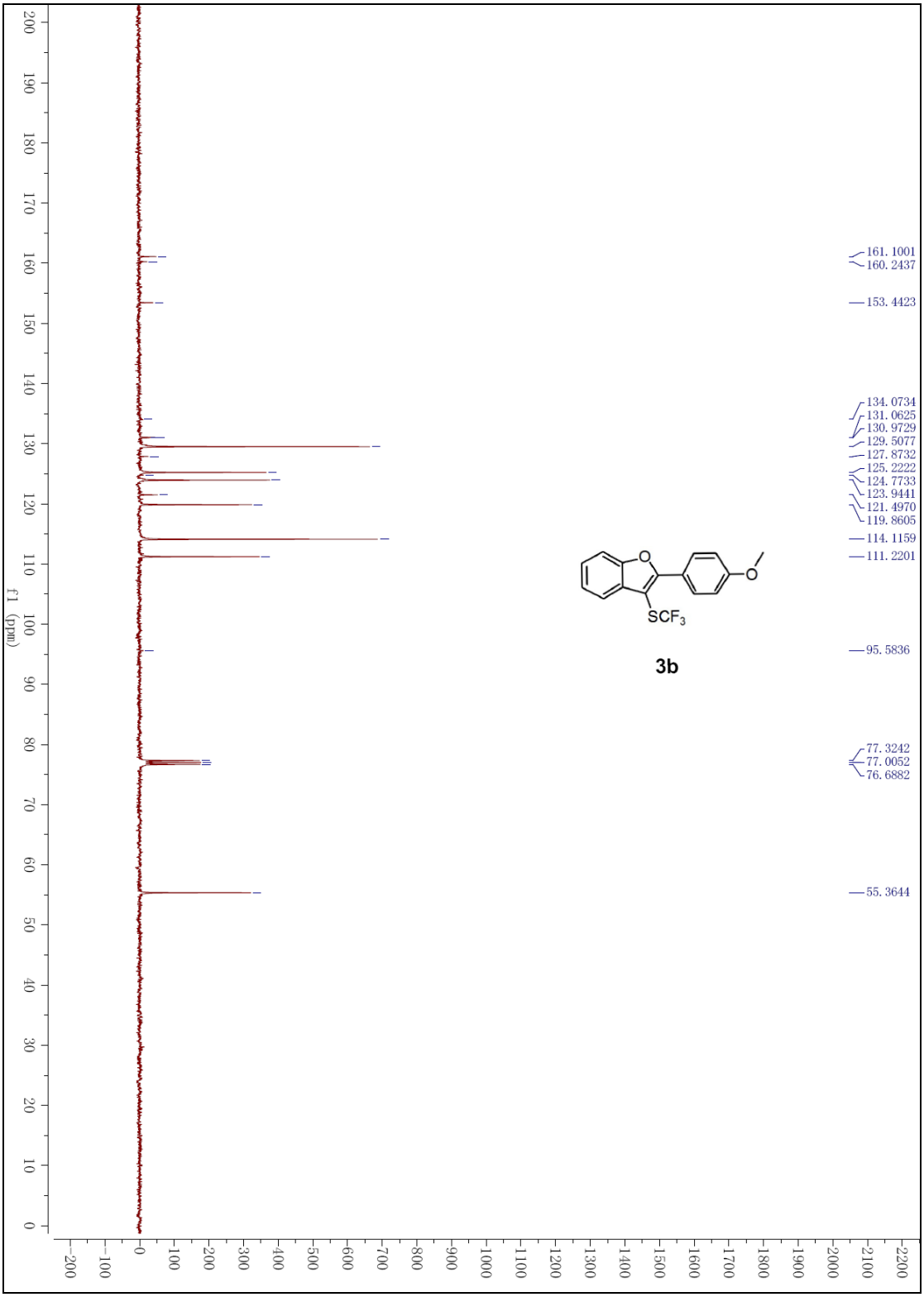
7.7672
7.7538
7.7455
7.5796
7.5712
7.5624
7.5570
7.4023
7.3939
7.3882
7.3797
7.2881
7.0756
7.0534
3.9202
2.01
1.02
1.02
2.02
2.00
3.01
f1 (ppm)
SCF3
3b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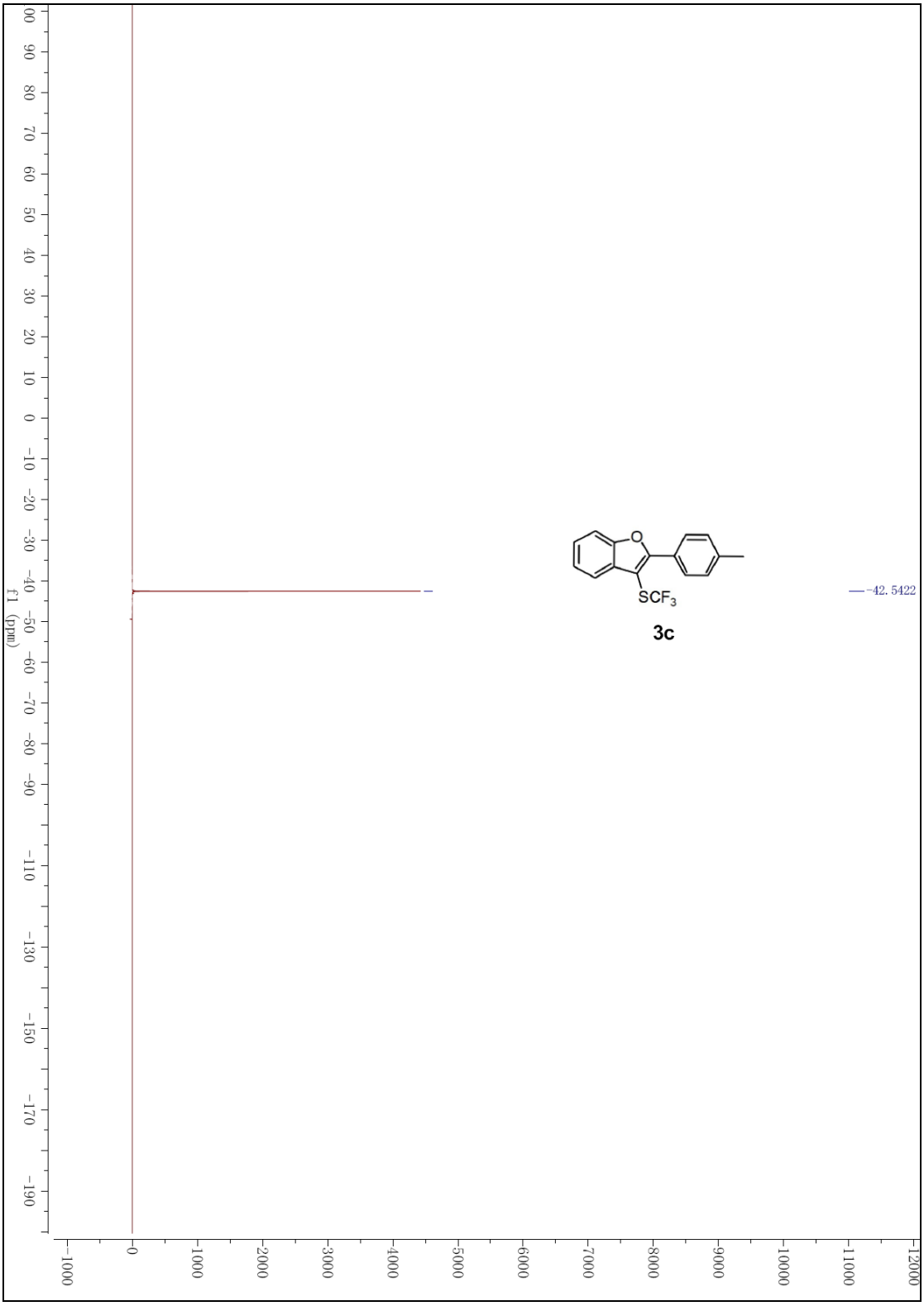
153.4423
134.0734
131.0625
130.9729
129.5077
127.8732
125.2222
124.7733
123.9441
121.4970
119.8605
114.1159
111.2201
95.5836
77.3242
77.0052
76.6882
55.3644
SCF3
3b
f1 (ppm)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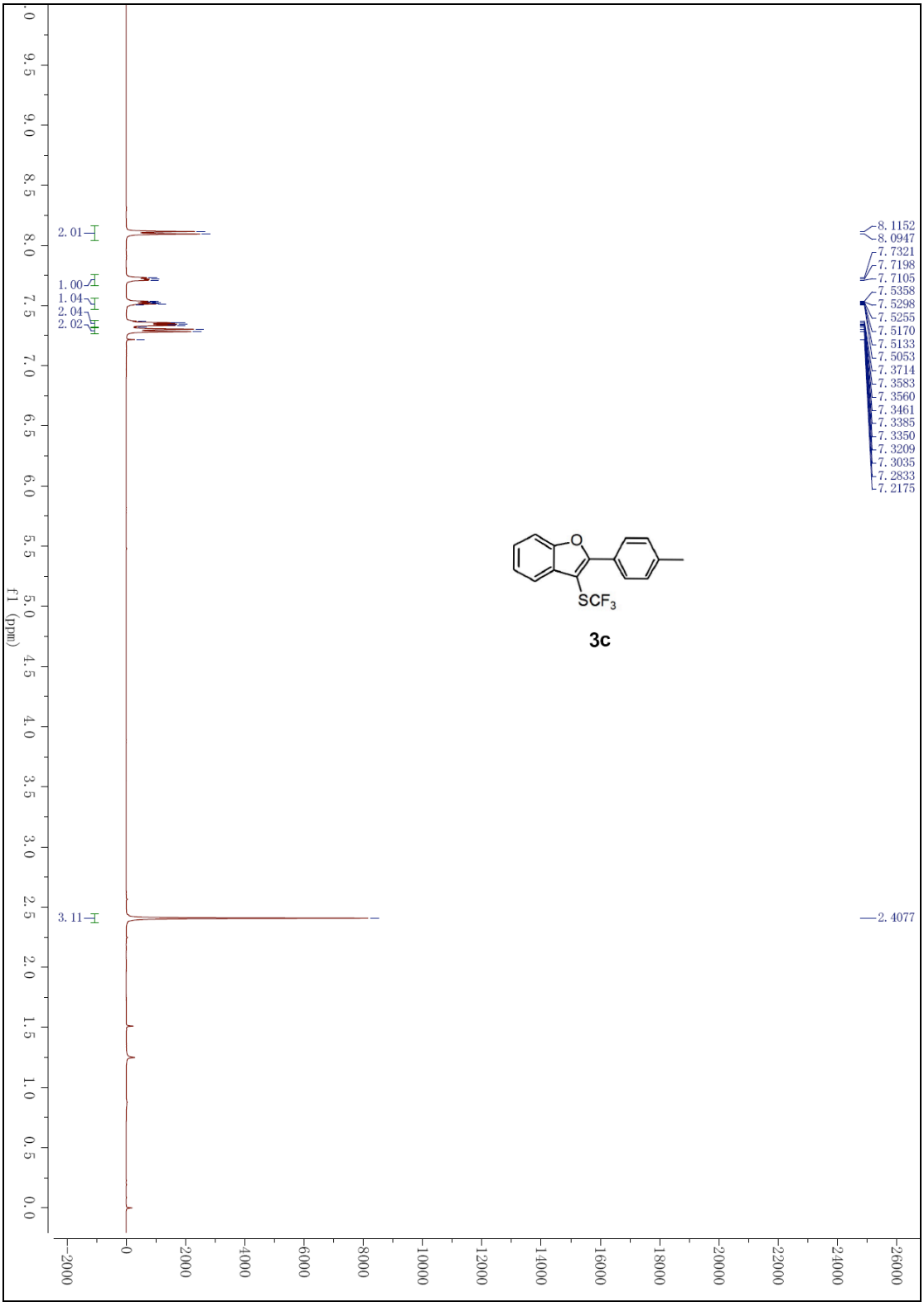
3c
f1 (ppm)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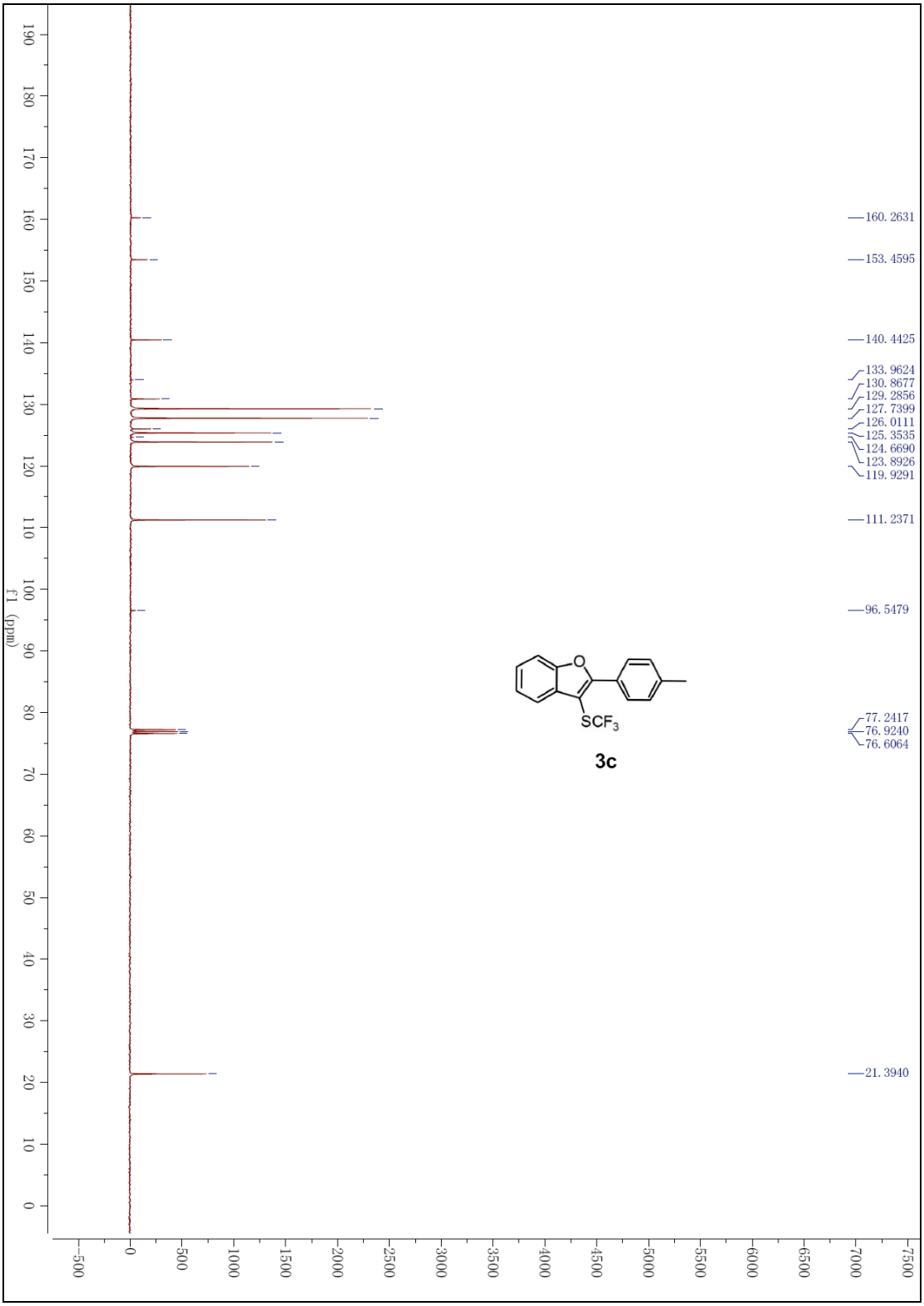
1.00
1.04
2.04
2.02
3.11
8.1152
8.0947
7.7321
7.7198
7.7105
7.5358
7.5298
7.5255
7.5170
7.5133
7.5053
7.3714
7.3583
7.3560
7.3461
7.3385
7.3350
7.3209
7.3035
7.2833
7.2175
2.4077
O
SCF3
f1 (ppm)

3c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129.2856
127.7399
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123.8926
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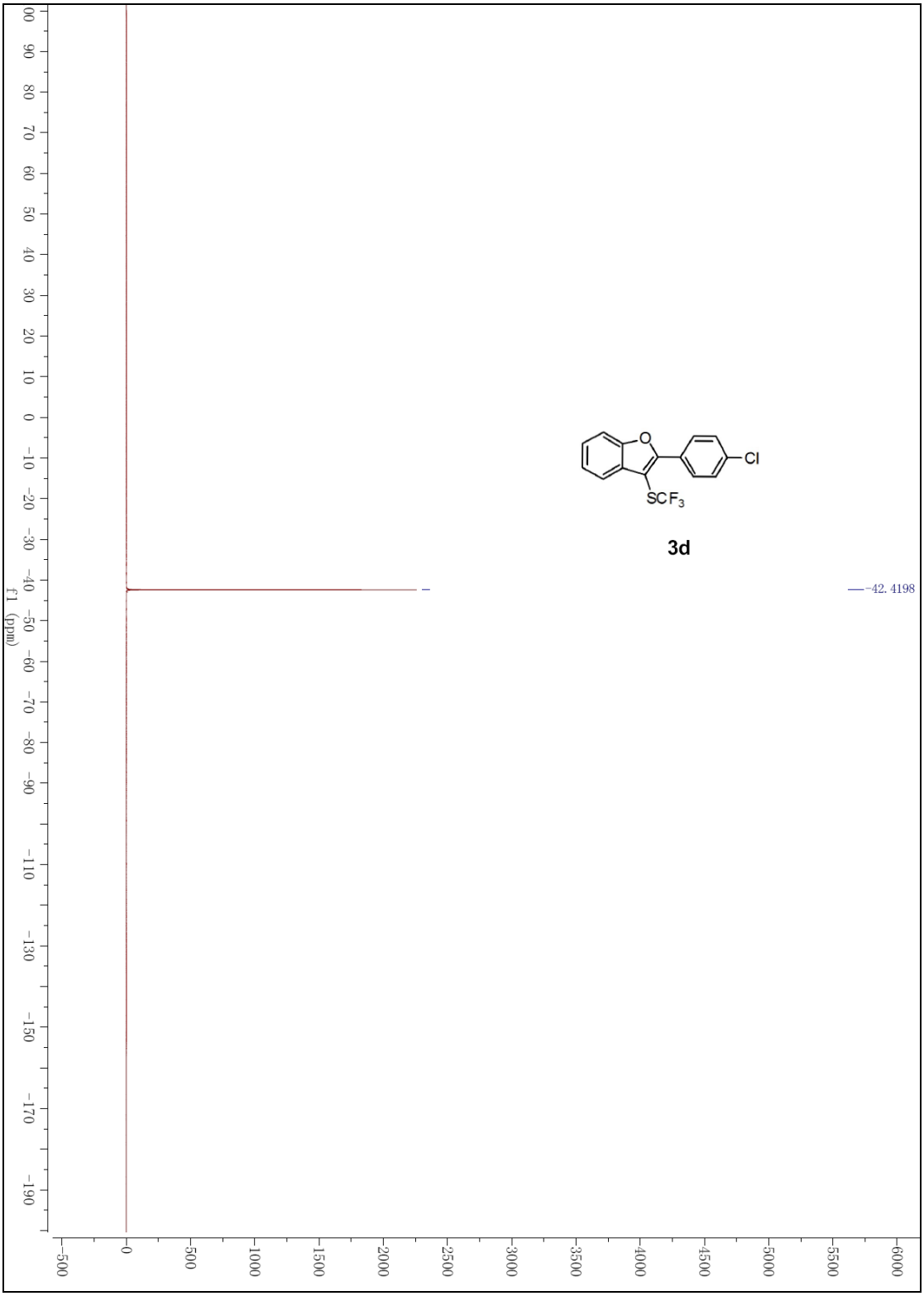
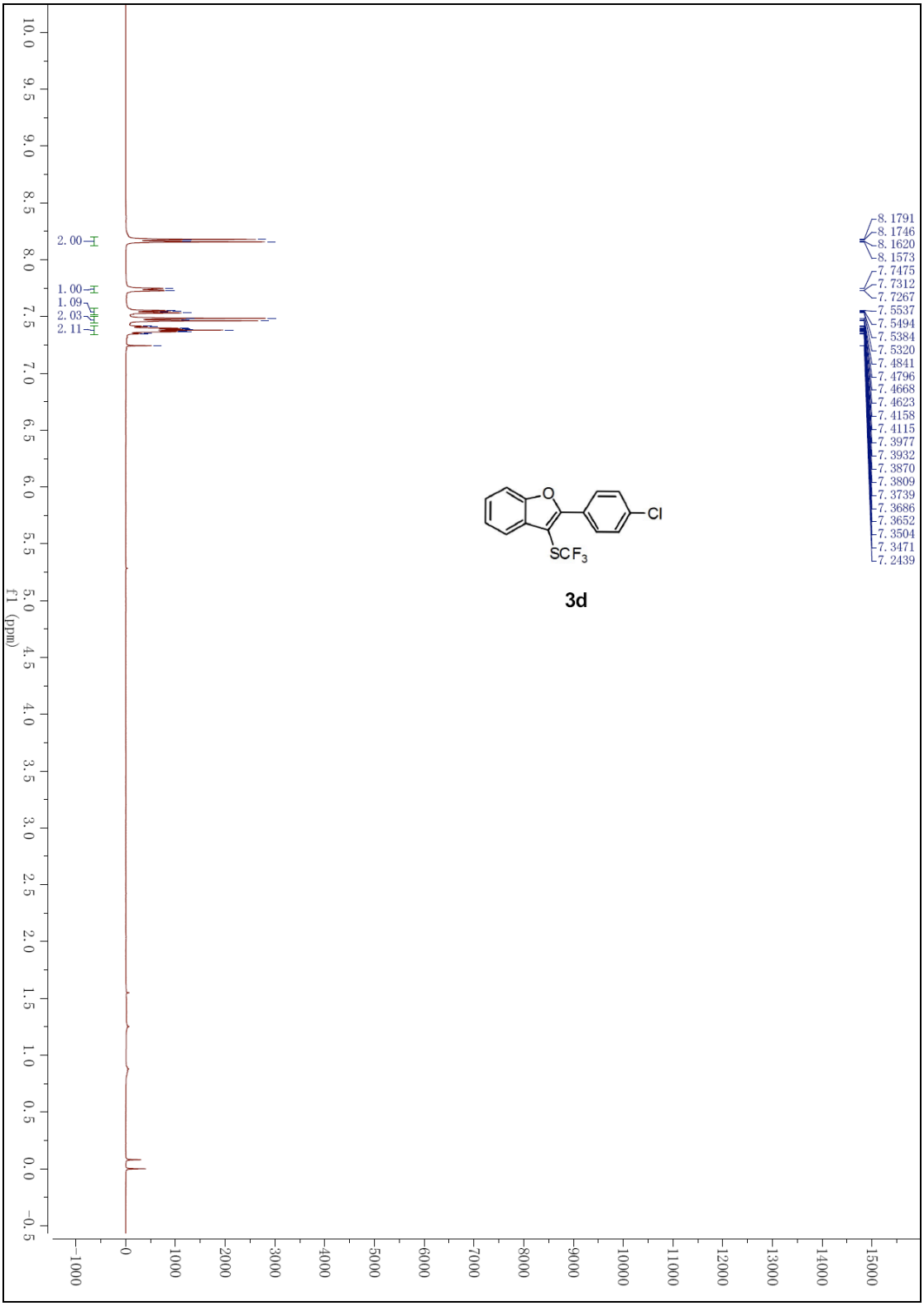
76.9240
76.6064
21.3940
f1 (ppm)
SCF3
3c


O
Cl
SCF3
3d
−42.4198
f1 (ppm)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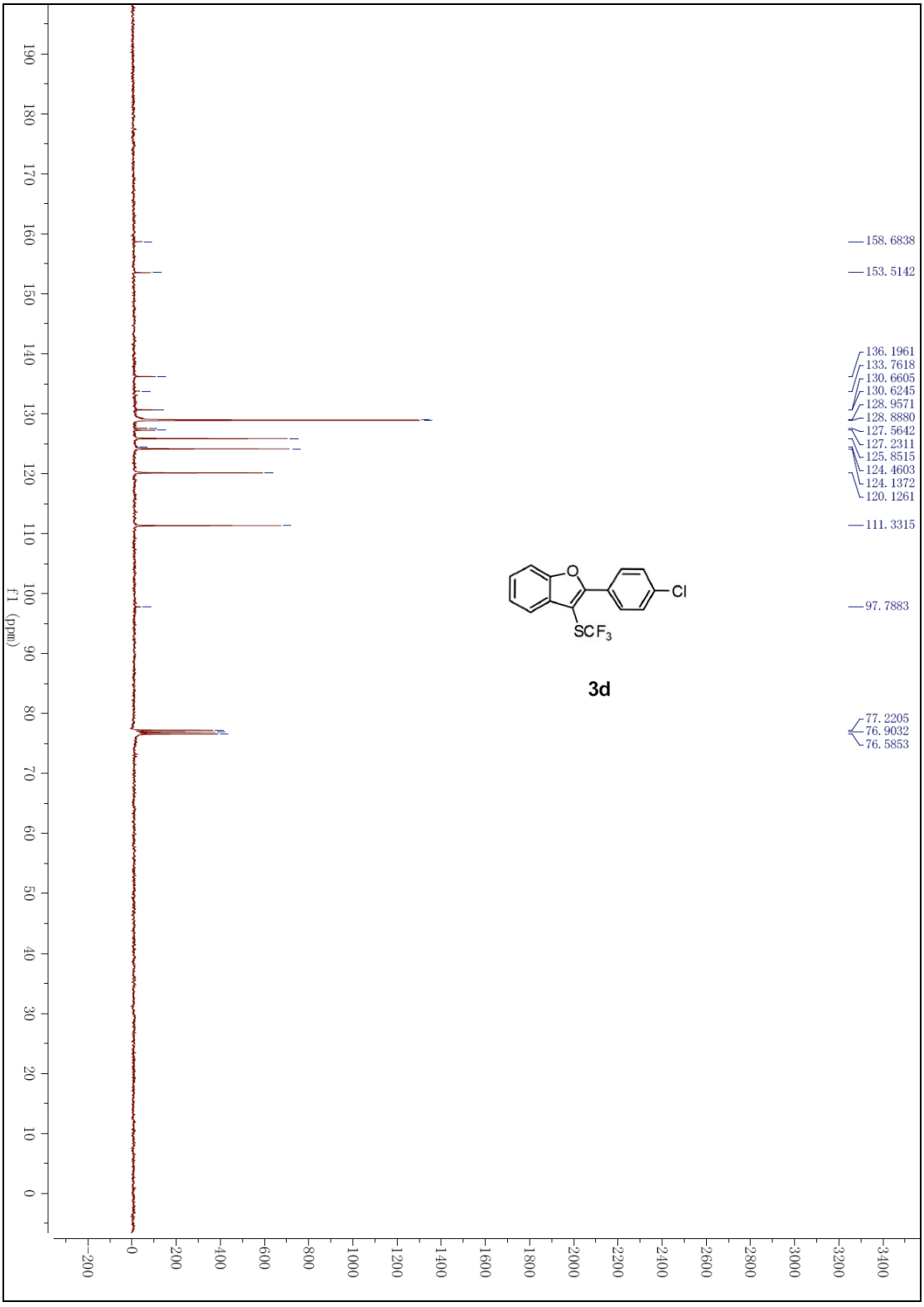
8.1620
8.1573
7.7475
7.7312
7.7267
7.5537
7.5494
7.5384
7.5320
7.4841
7.4796
7.4668
7.4623
7.4158
7.4115
7.3977
7.3932
7.3870
7.3809
7.3739
7.3686
7.3652
7.3504
7.3471
7.2439
2.00
1.00
1.09
2.03
2.11
O
Cl
SCF3
f1 (ppm)

3d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125.8515
124.4603
124.1372
120.1261
111.3315
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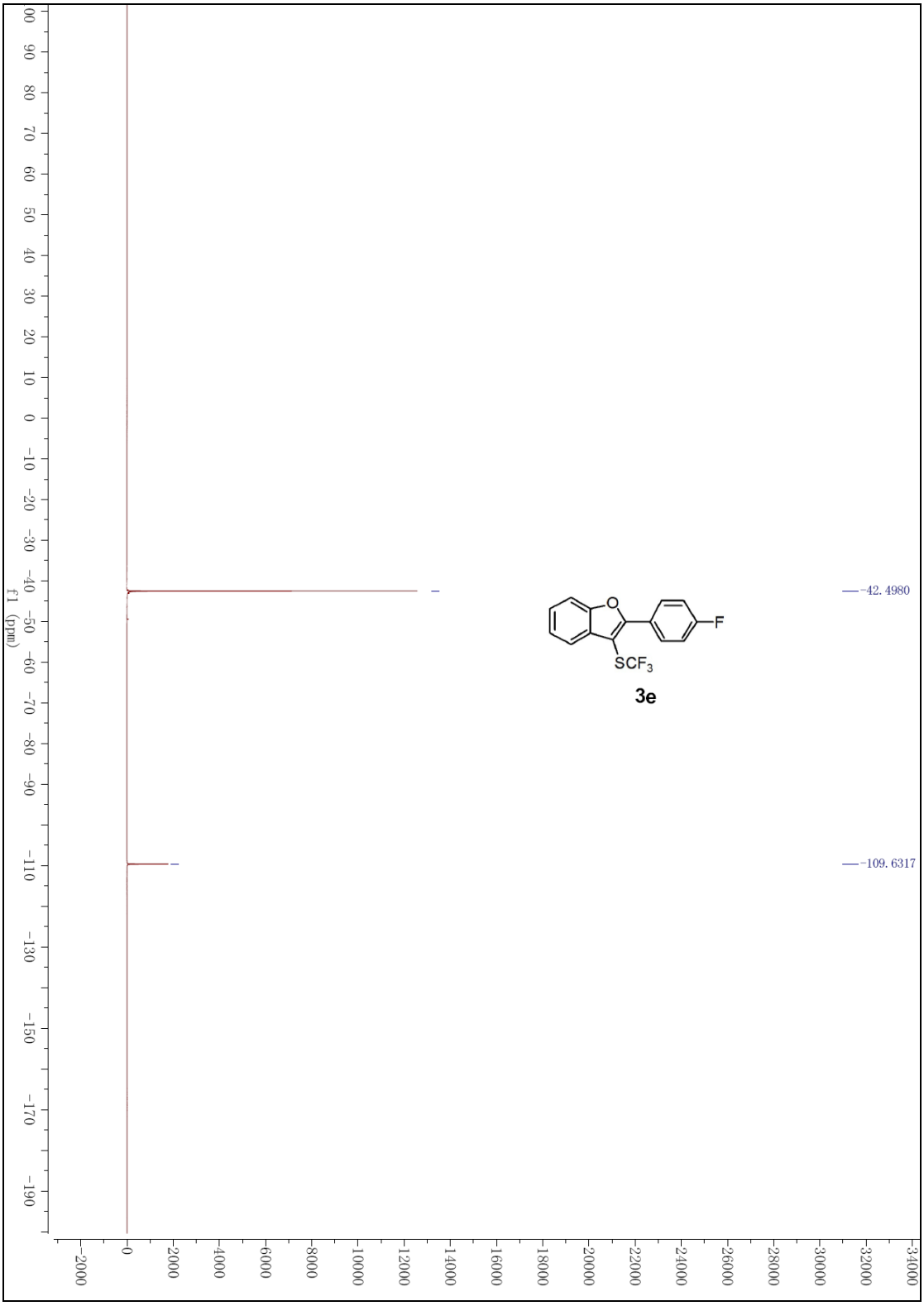
77.2205
76.9032
76.5853
f1 (ppm)
Cl
SCF3
3d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-109.6317
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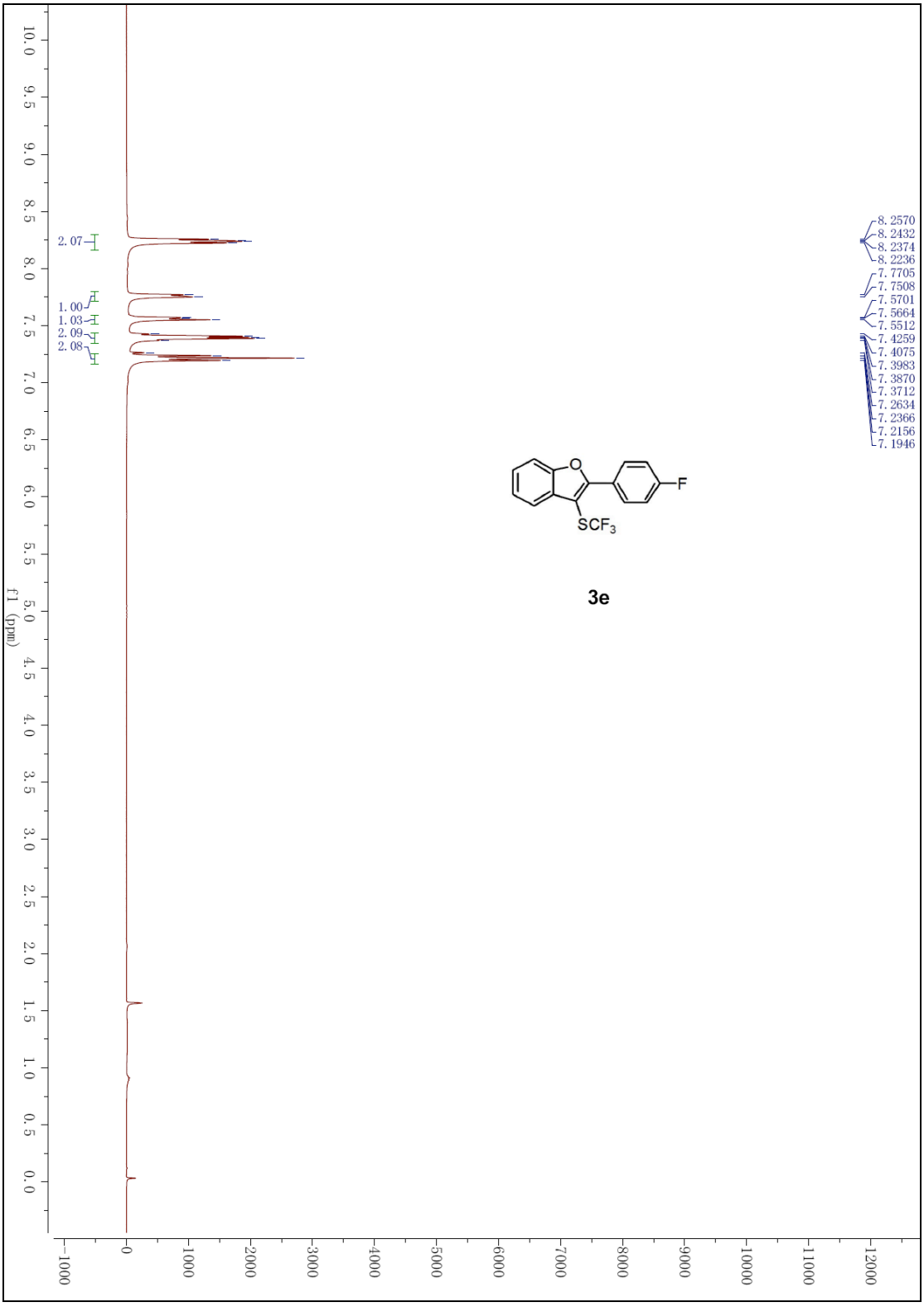
SCF3
3e
f1 (ppm)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8.2236
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7.7508
7.5701
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7.5512
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7.4075
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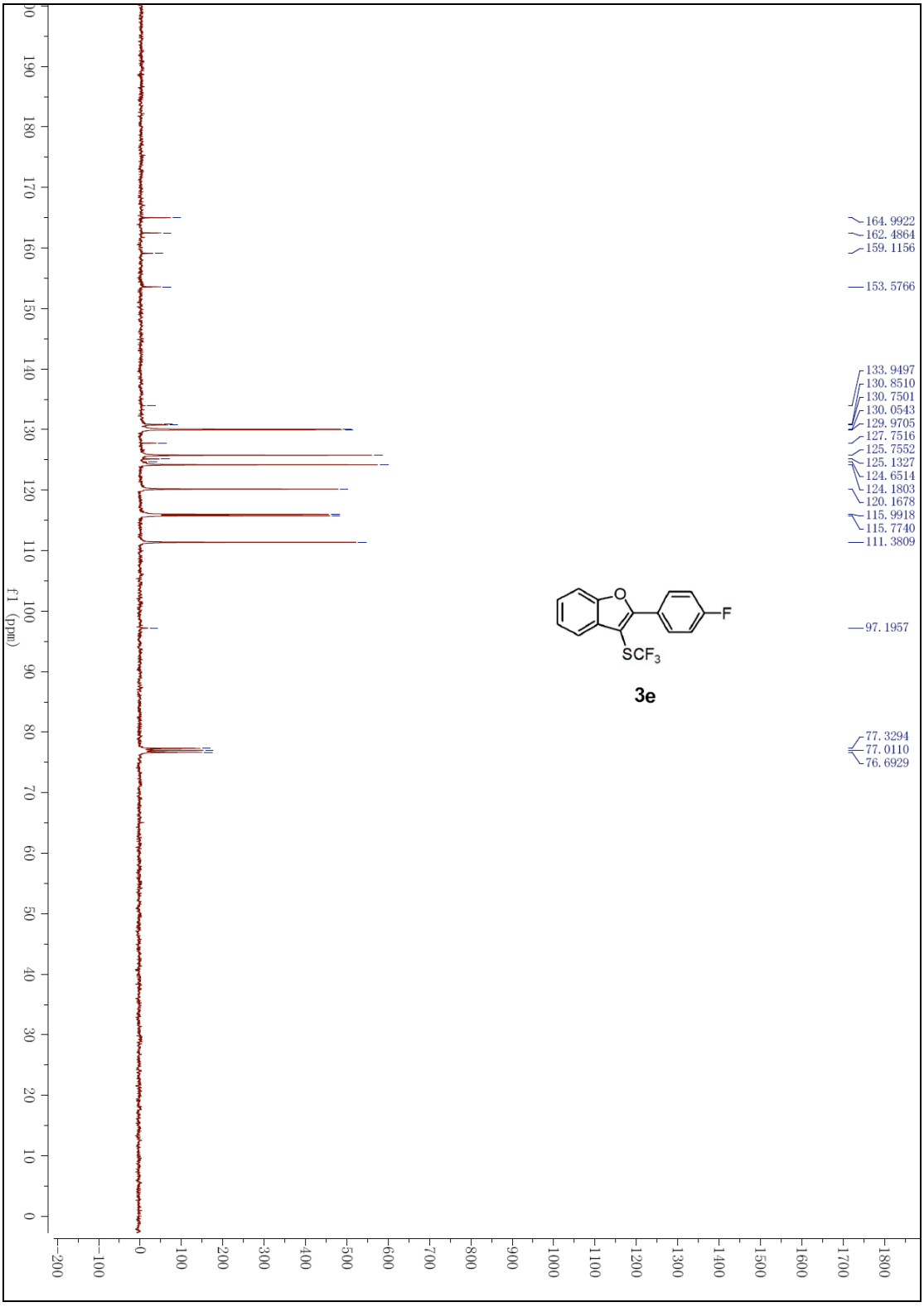
7.3870
7.3712
7.2634
7.2366
7.2156
7.1946
2.07
1.00
1.03
2.09
2.08
F
SCF3
f1 (ppm)

3e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133.9497
130.8510
130.7501
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127.7516
125.7552
125.1327
124.6514
124.1803
120.1678
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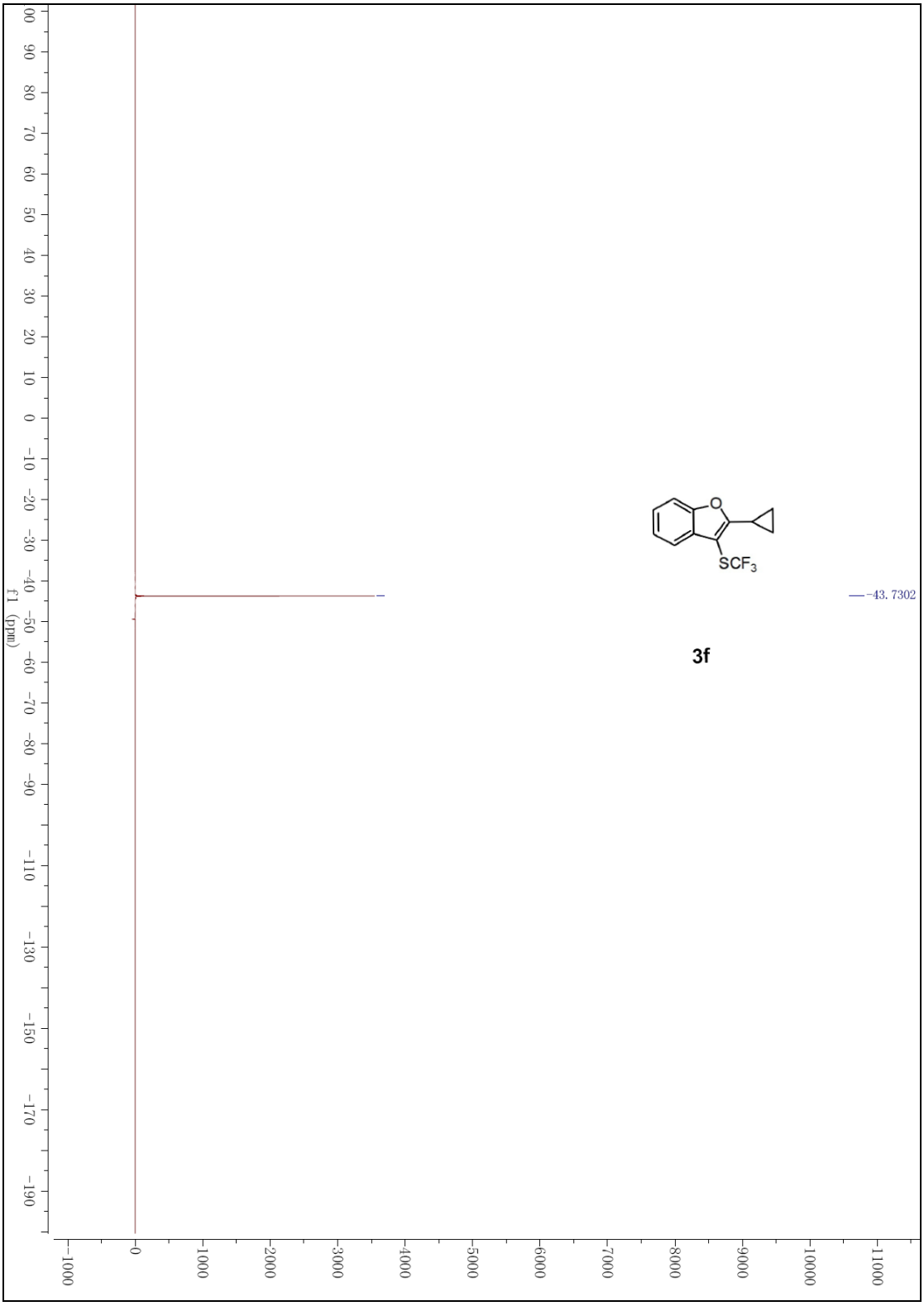
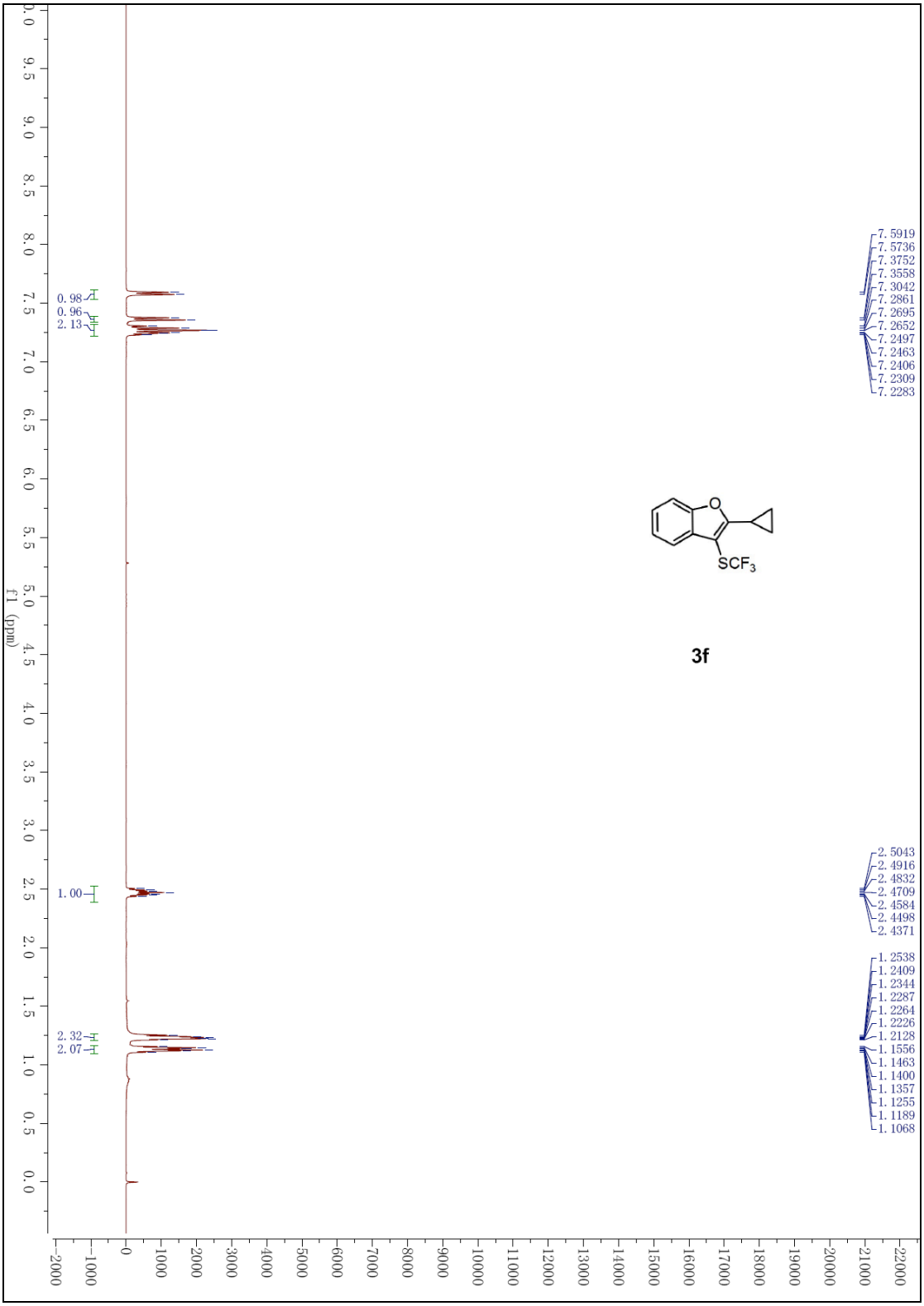
97.1957
77.3294
77.0110
76.6929
F
SCF3
f1 (ppm)

3e


-43.7302
f1 (ppm)
3f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7.3558
7.3042
7.2861
7.2695
7.2652
7.2497
7.2463
7.2406
7.2309
7.2283
0.98
0.96
2.13
1.00
2.32
2.07
2.5043
2.4916
2.4832
2.4709
2.4584
2.4498
2.4371
1.2538
1.2409
1.2344
1.2287
1.2264
1.2226
1.2128
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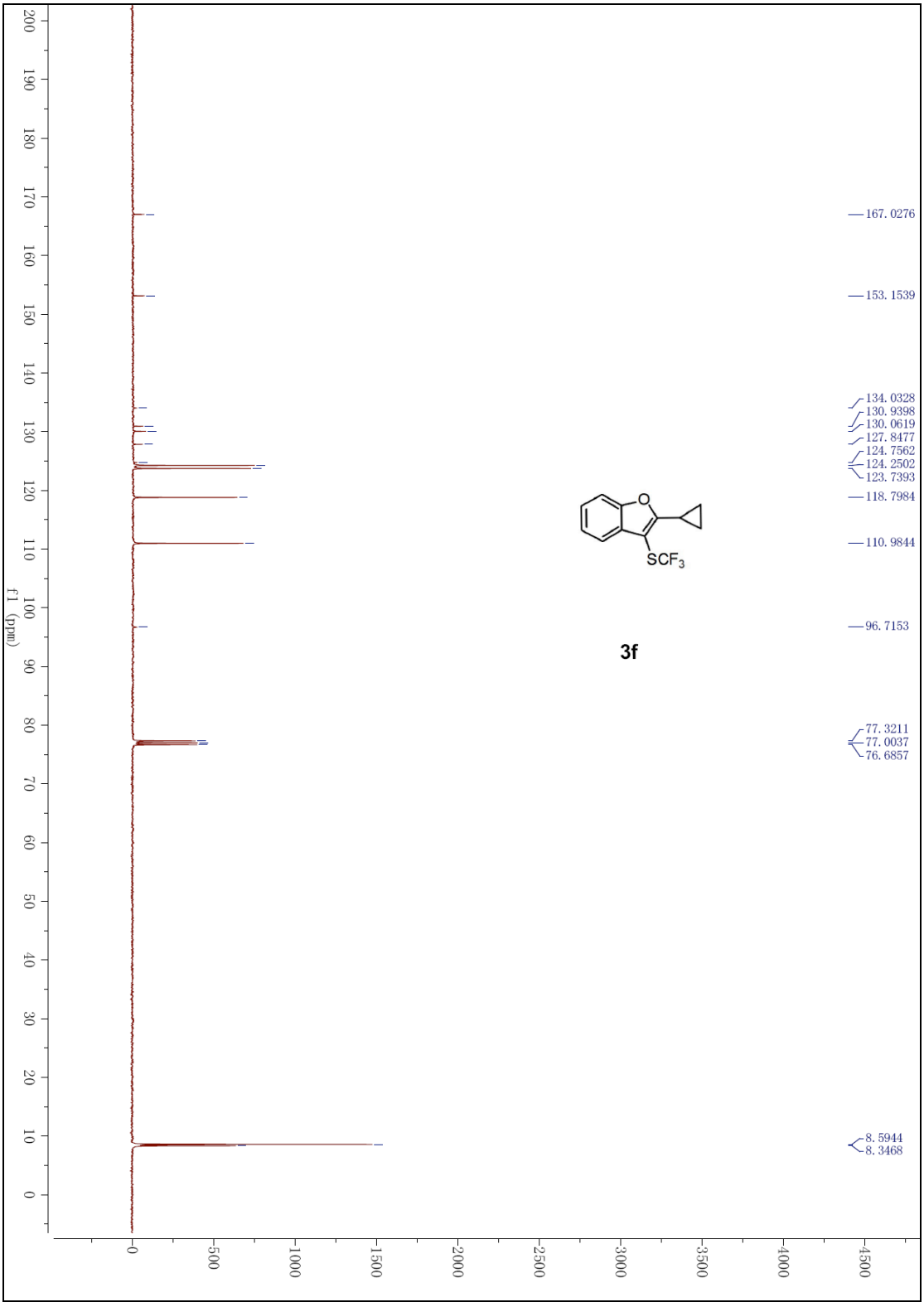
1.1357
1.1255
1.1189
1.1068
SCF3
f1 (ppm)

3f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130.0619
127.8477
124.7562
124.2502
123.7393
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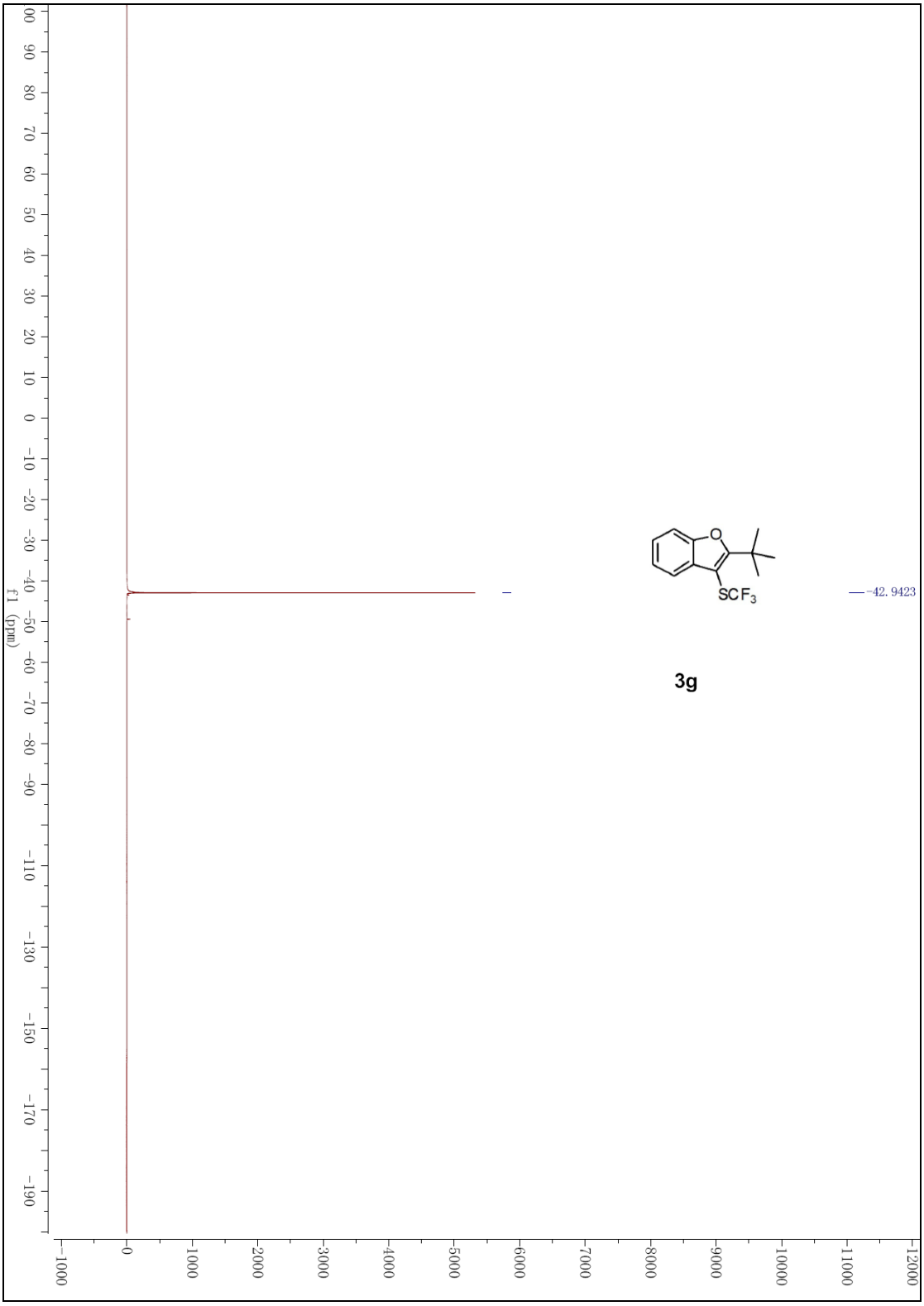
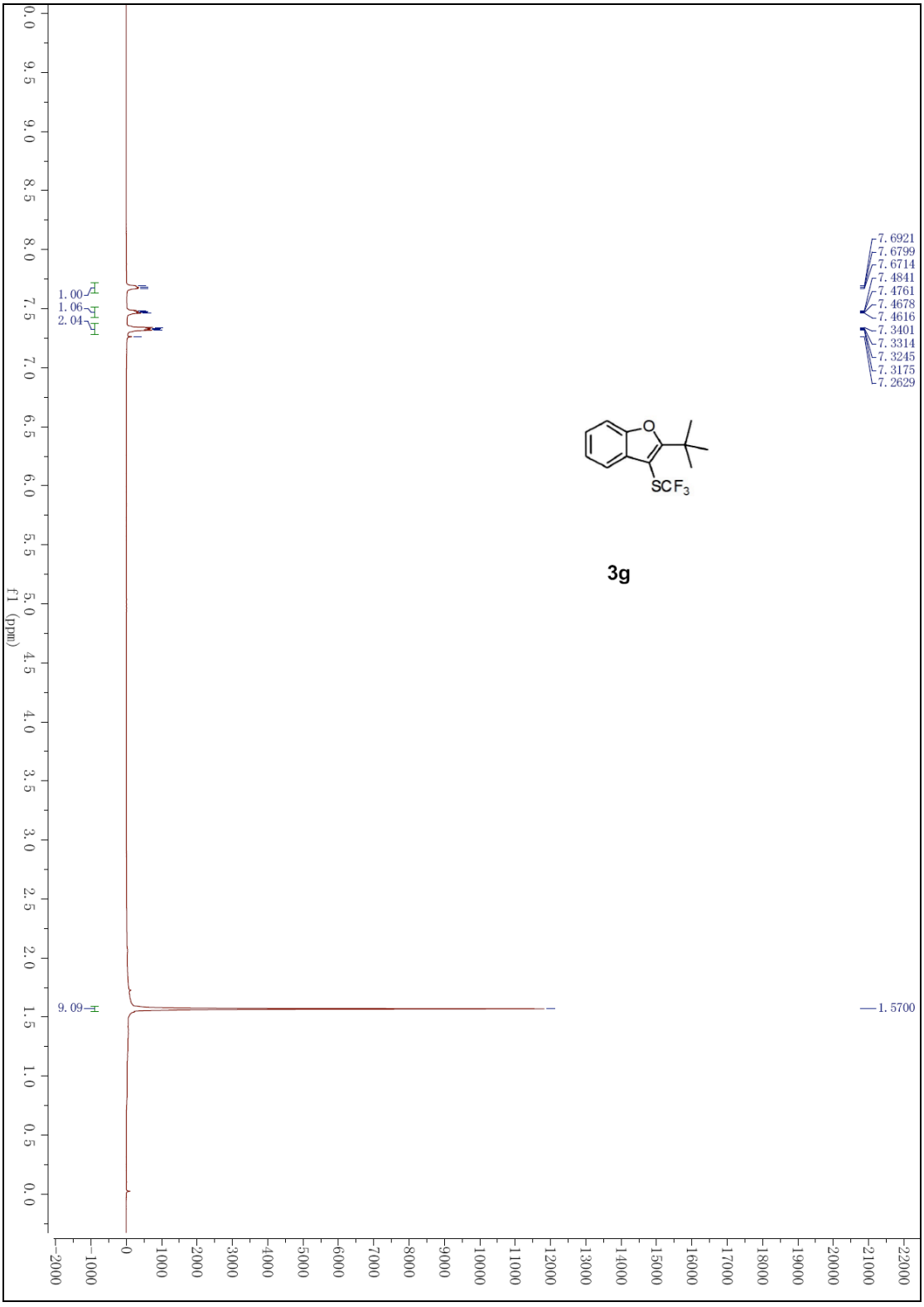
8.5944
8.3468
SCF3
3f
f1 (ppm)


f1 (ppm)
SCF3
-42.9423
3g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7.4616
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7.3314
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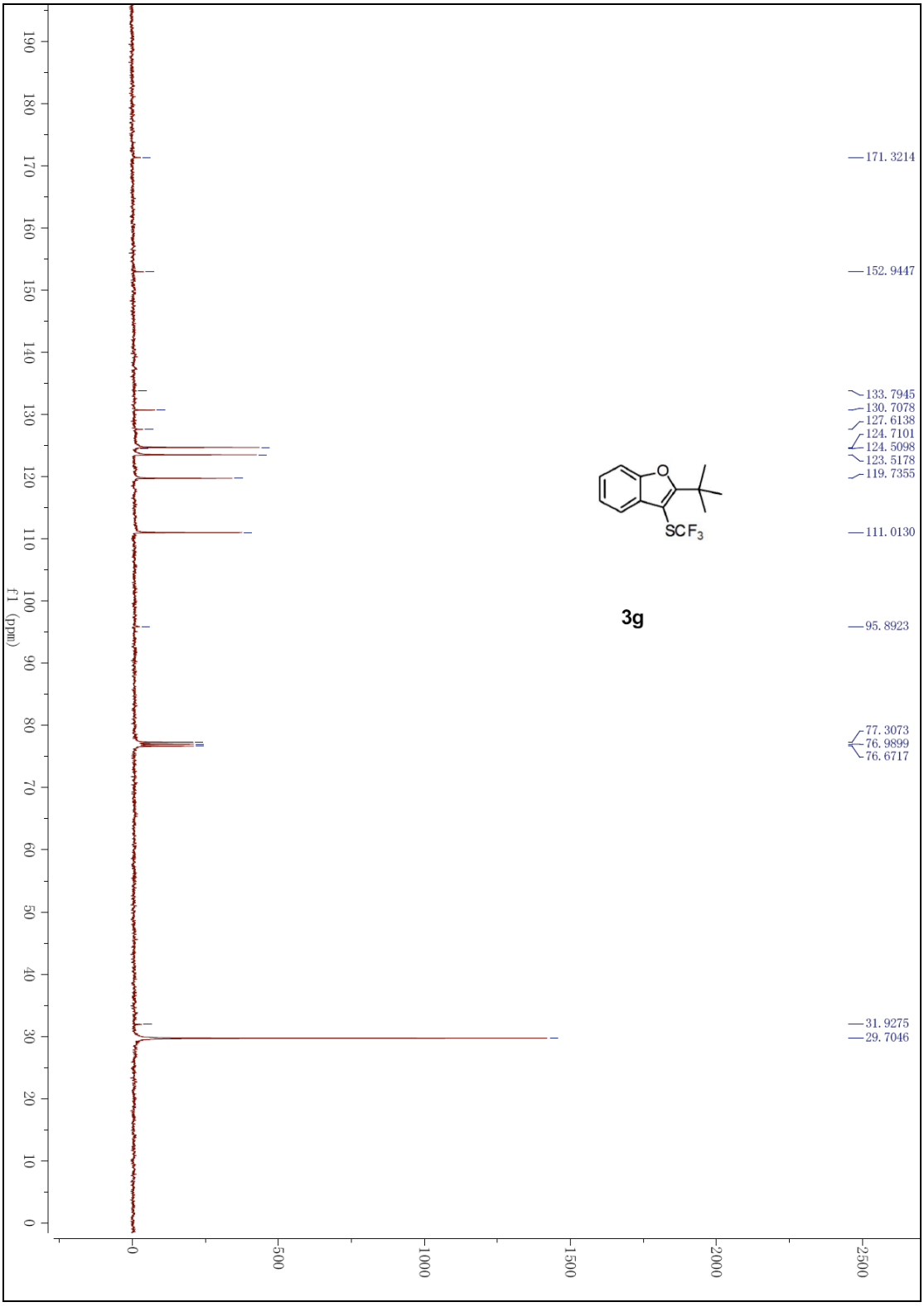
1.06
2.04
9.09
1.5700
SCF3
3g
f1 (ppm)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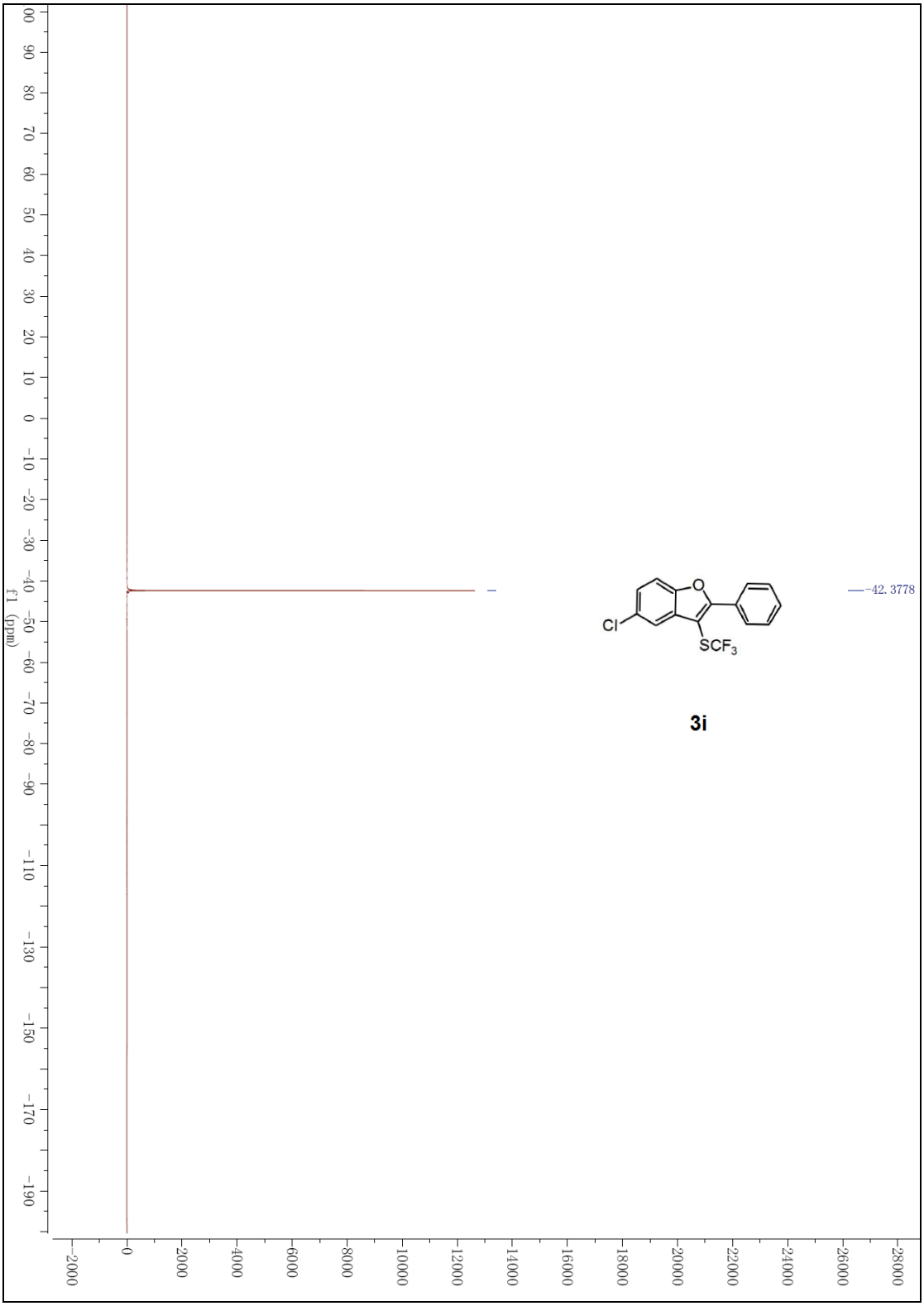
SCF3
3g
f1 (ppm)


−42.3778
Cl
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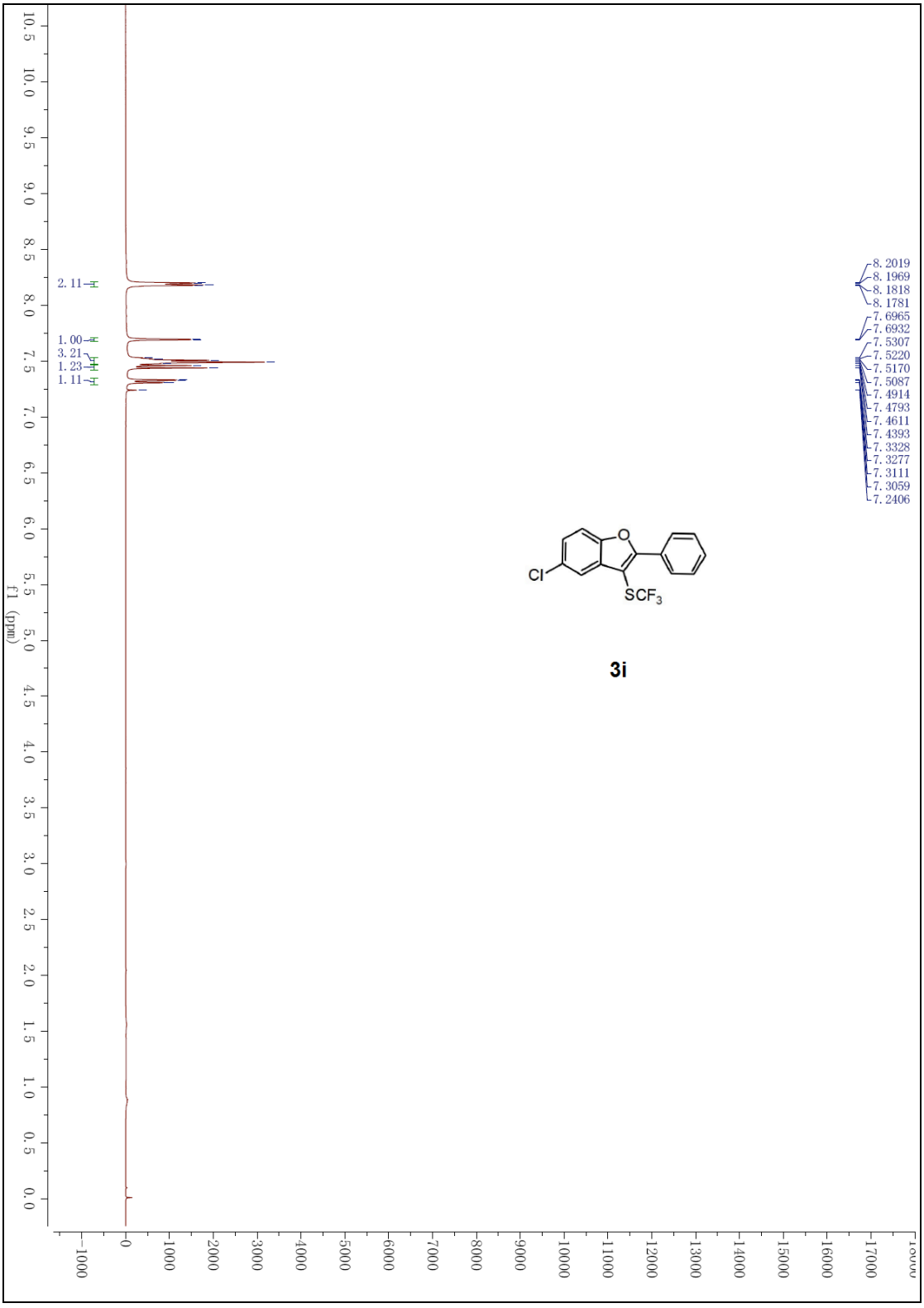
f1 (ppm)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7.3328
7.3277
7.3111
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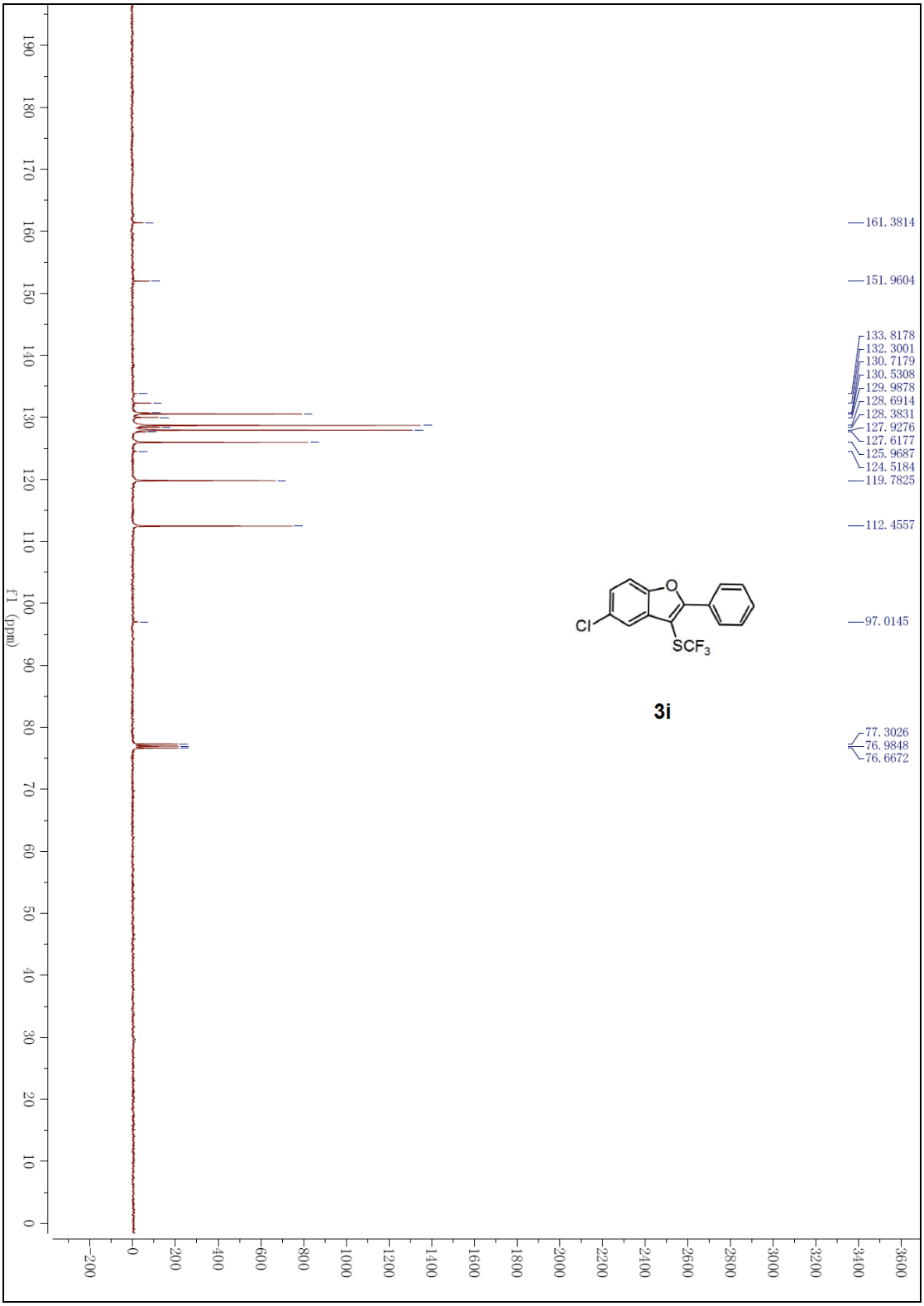
3.21
1.23
1.11
Cl
O
SCF3
f1 (ppm)

3i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127.6177
125.9687
124.5184
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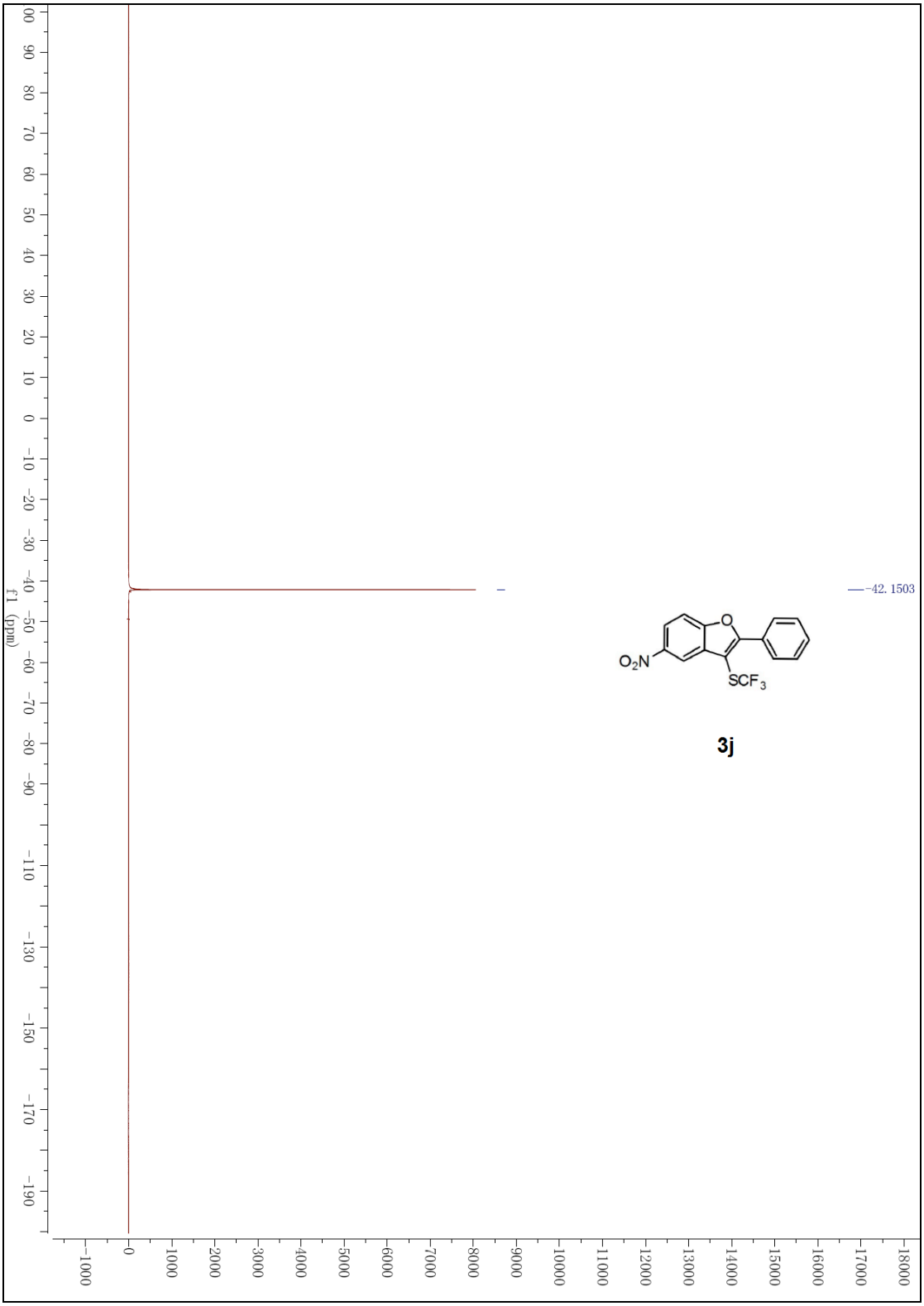
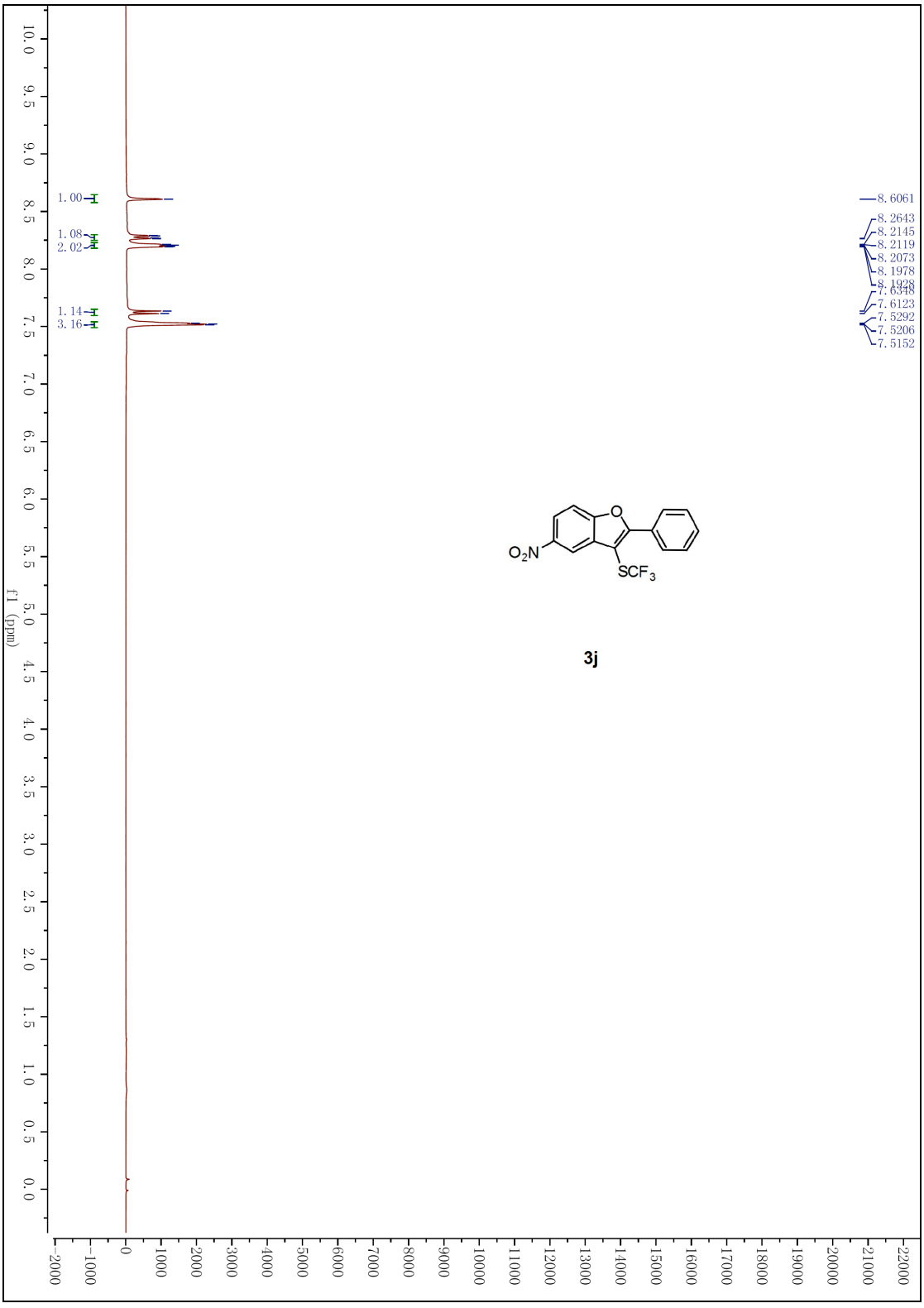
97.0145
77.3026
76.9848
76.6672
Cl
O
SCF3
f1 (ppm)

3i



3j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3.16
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8.2643
8.2145
8.2119
8.2073
8.1978
8.1928
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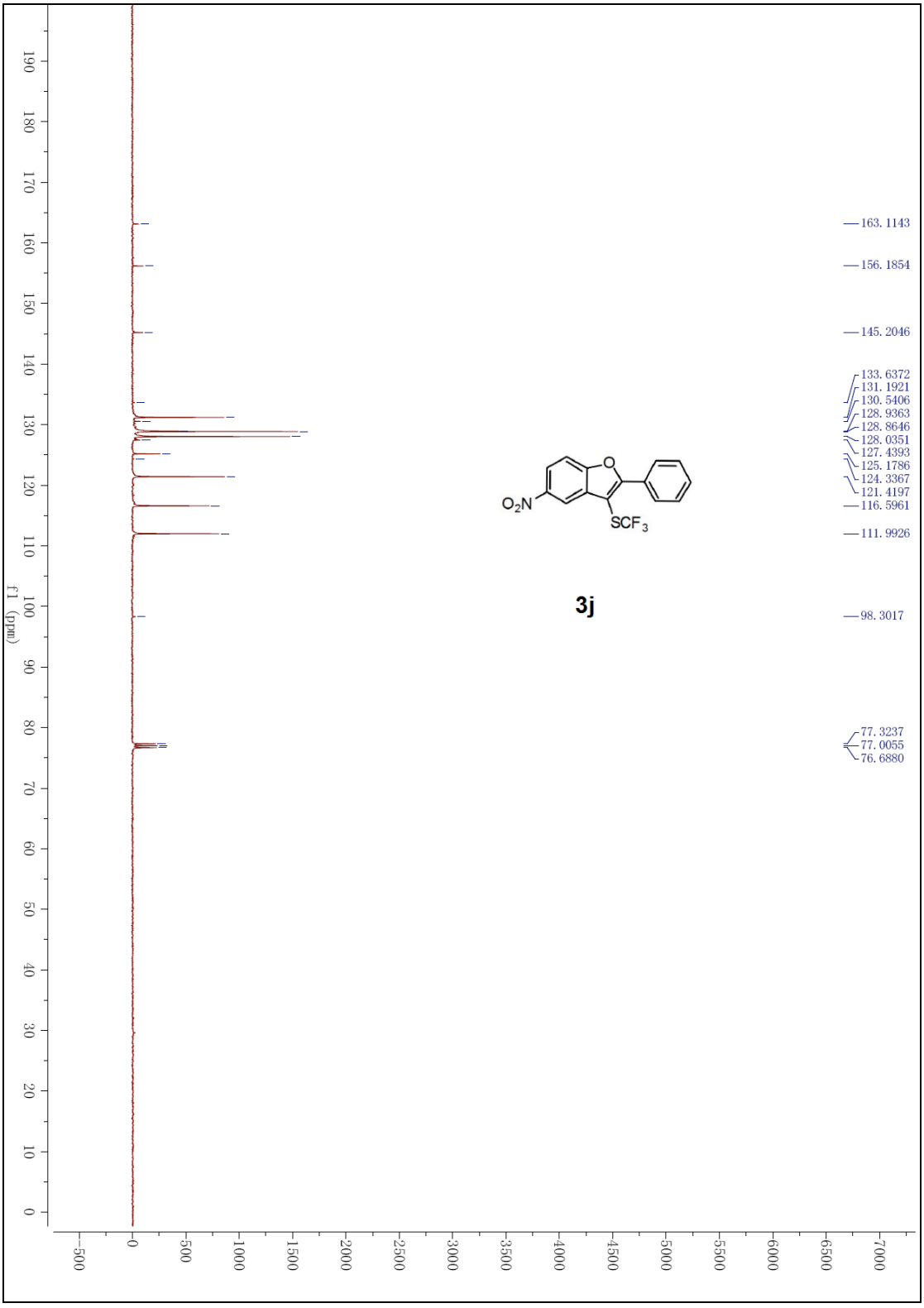
7.6123
7.5292
7.5206
7.5152
O2N
SCF3
f1 (ppm)

3j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124.3367
121.4197
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77.0055
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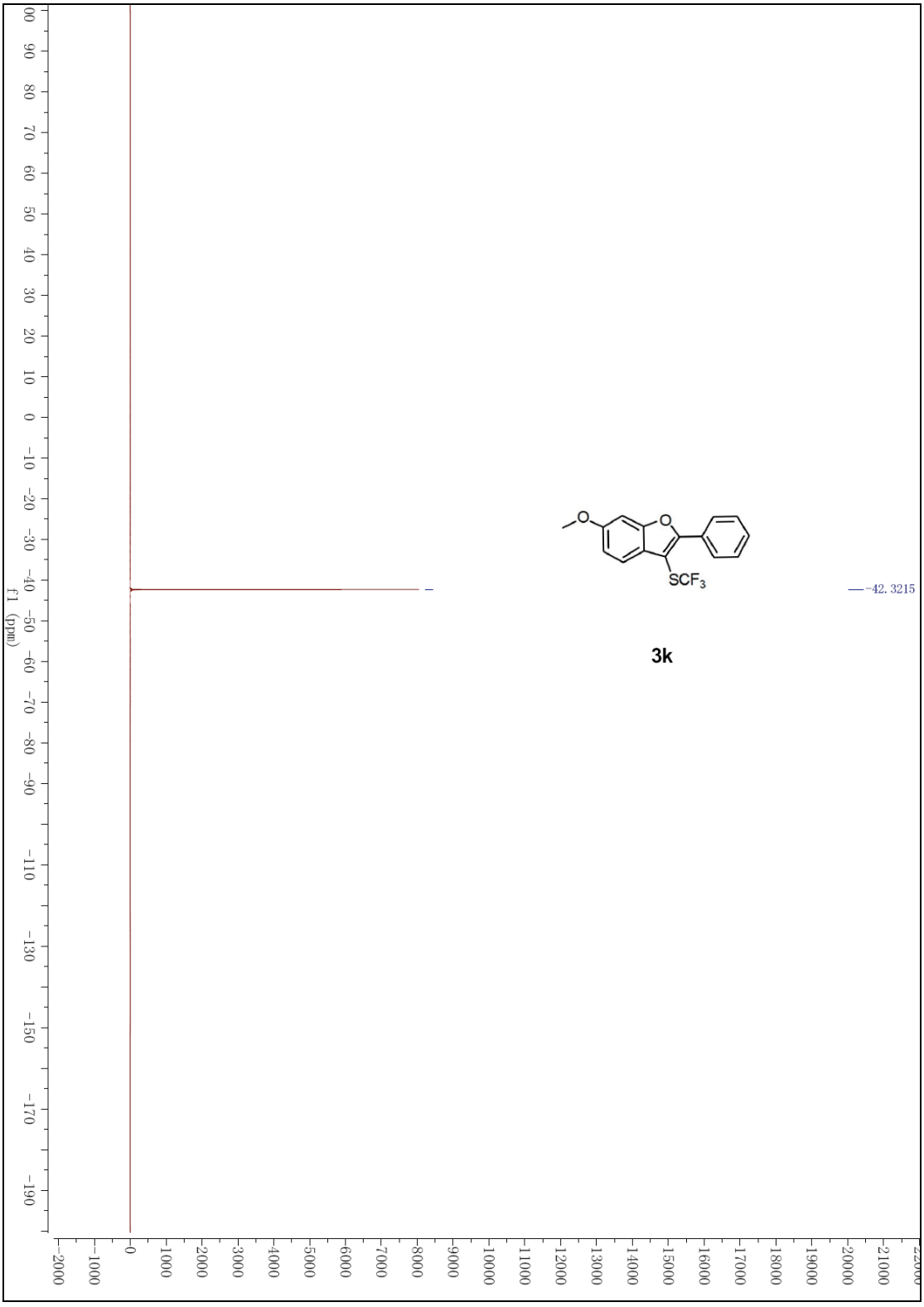
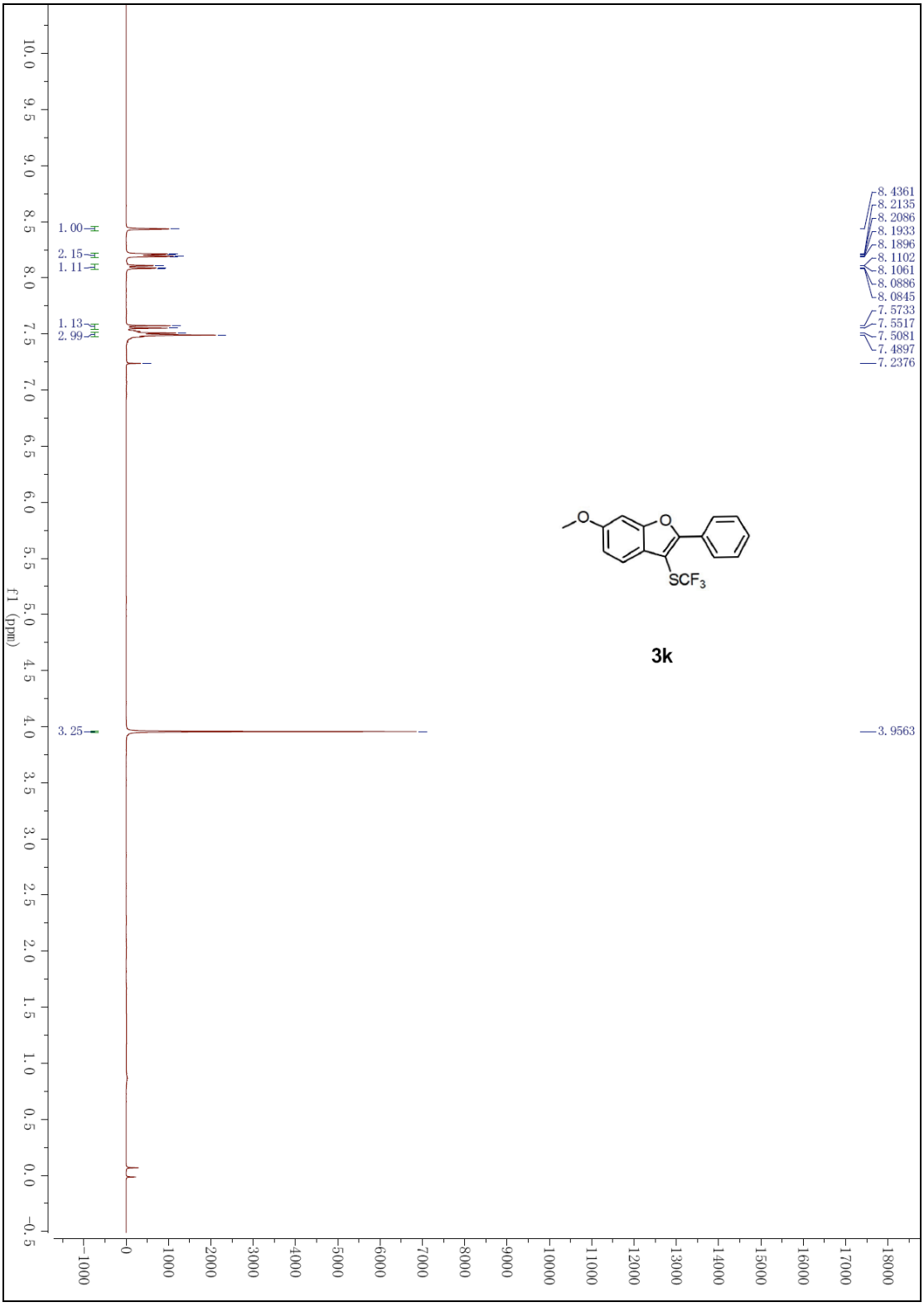
O2N
SCF3
3j
f1 (ppm)



3k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8.1933
8.1896
8.1102
8.1061
8.0886
8.0845
7.5733
7.5517
7.5081
7.4897
7.2376
3.9563
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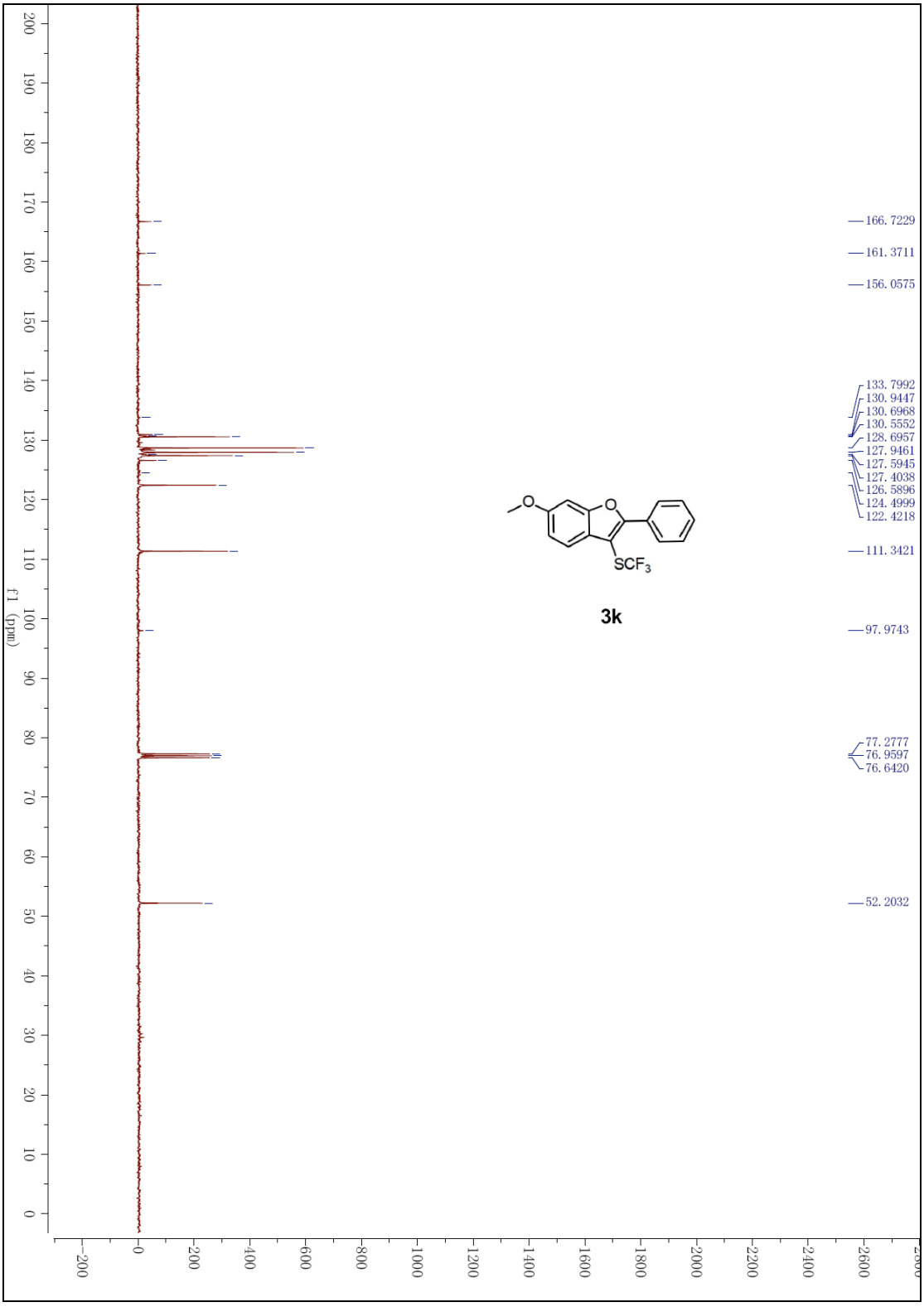
2.15
1.11
1.13
2.99
3.25
O
O
SCF3
f1 (ppm)

3k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156.0575
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130.9447
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127.9461
127.5945
127.4038
126.5896
124.4999
122.4218
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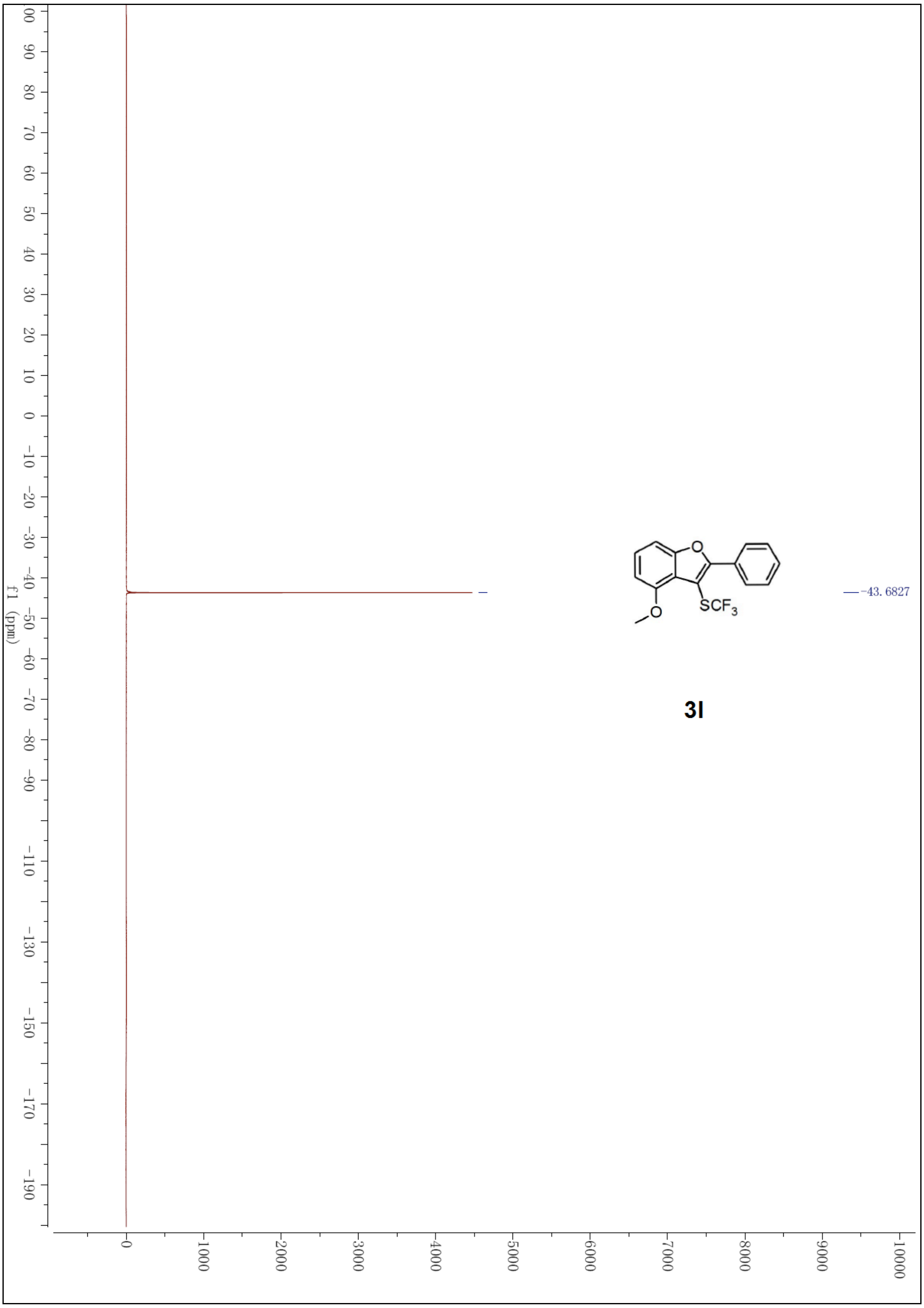
77.2777
76.9597
76.6420
52.2032
SCF3
3k
f1 (ppm)



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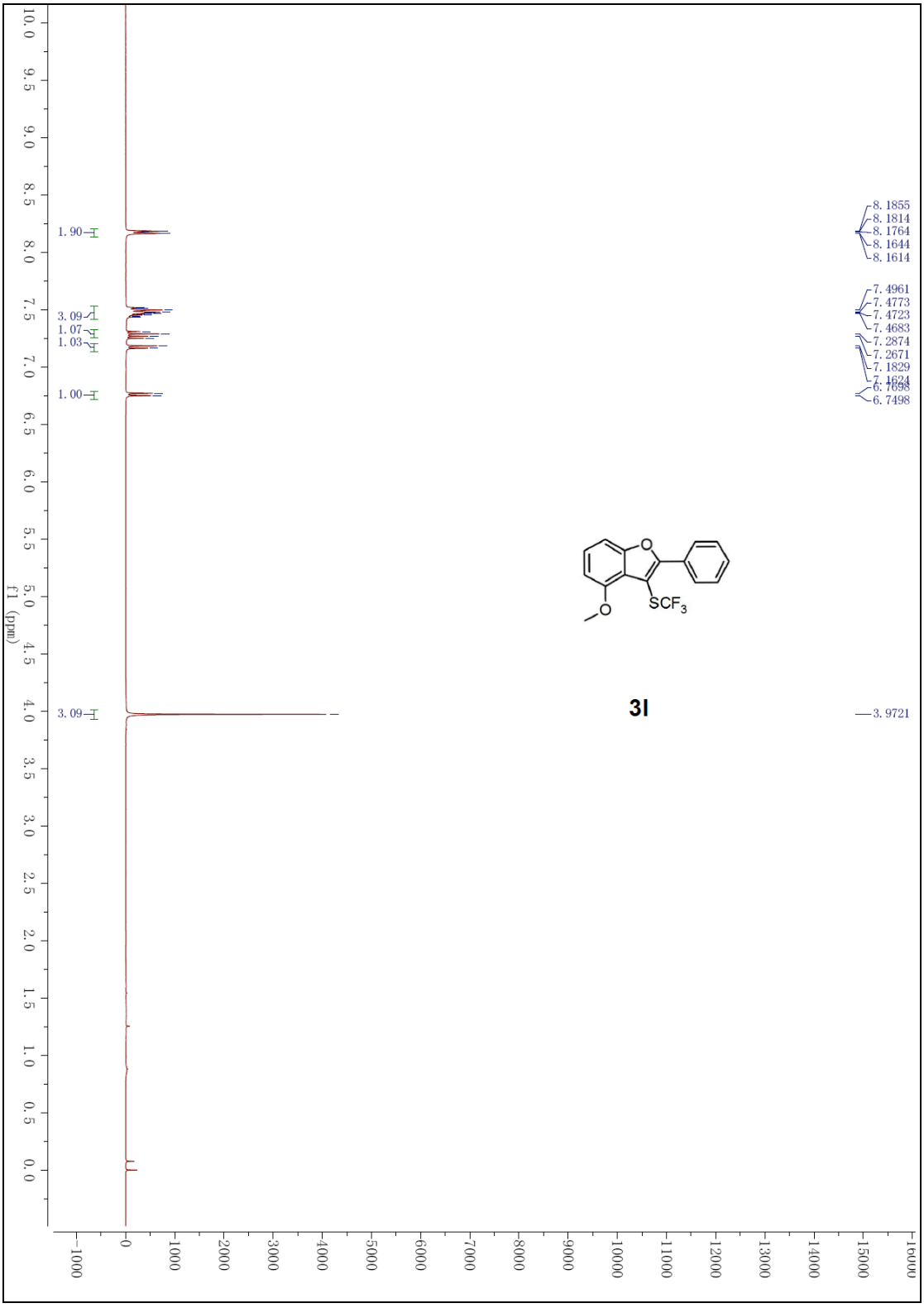
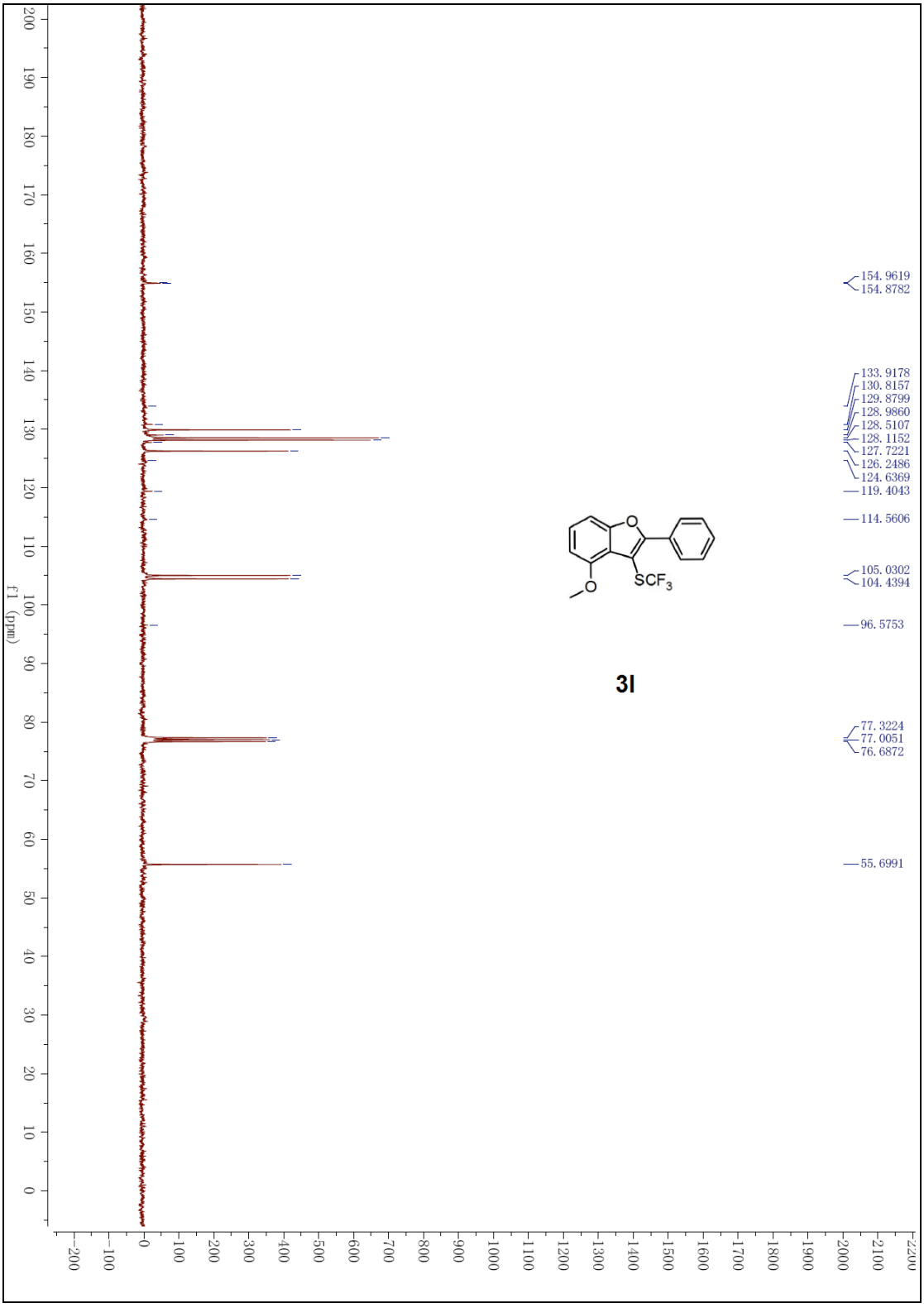
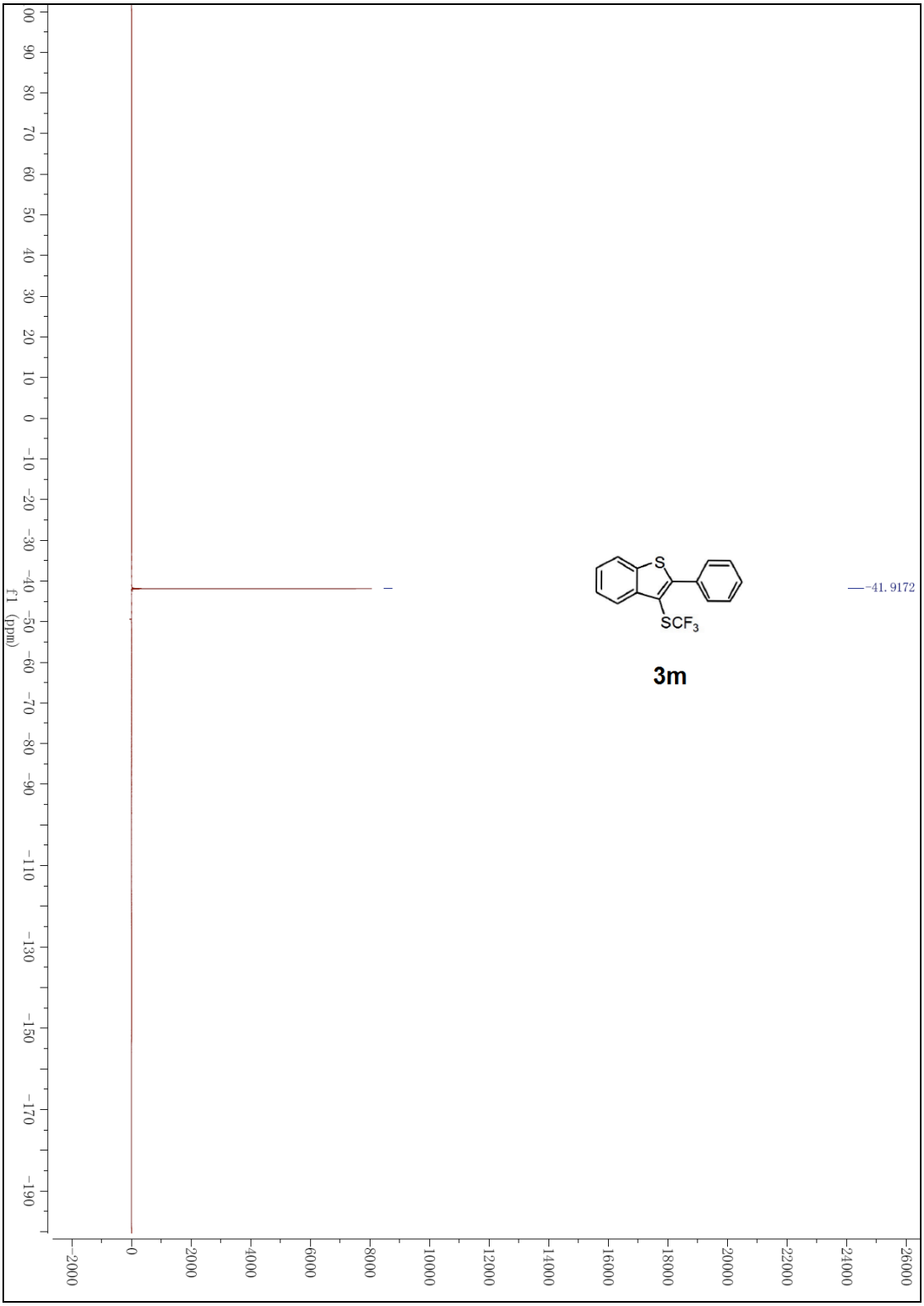
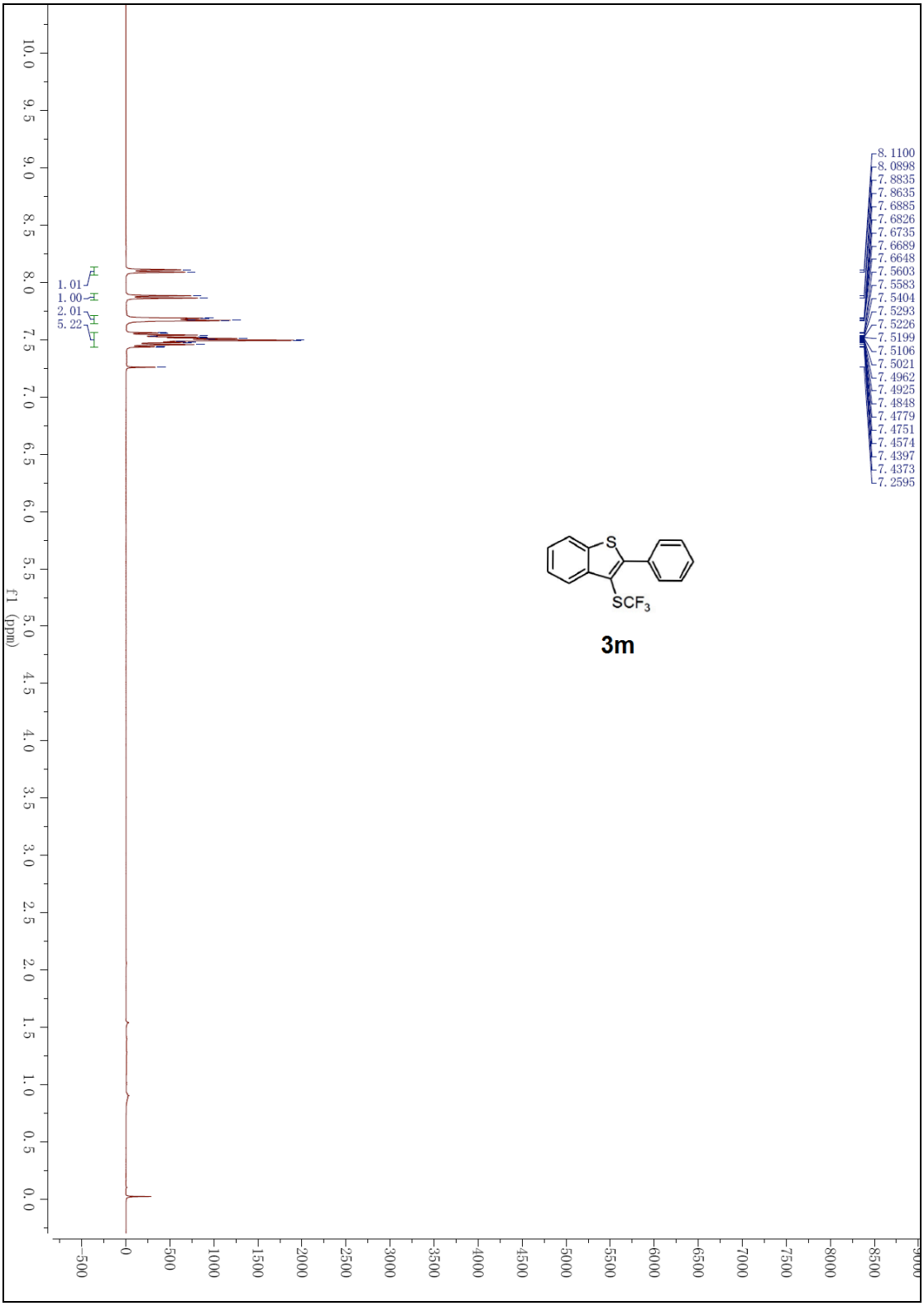
f1 (ppm)
O
SCF3
3l

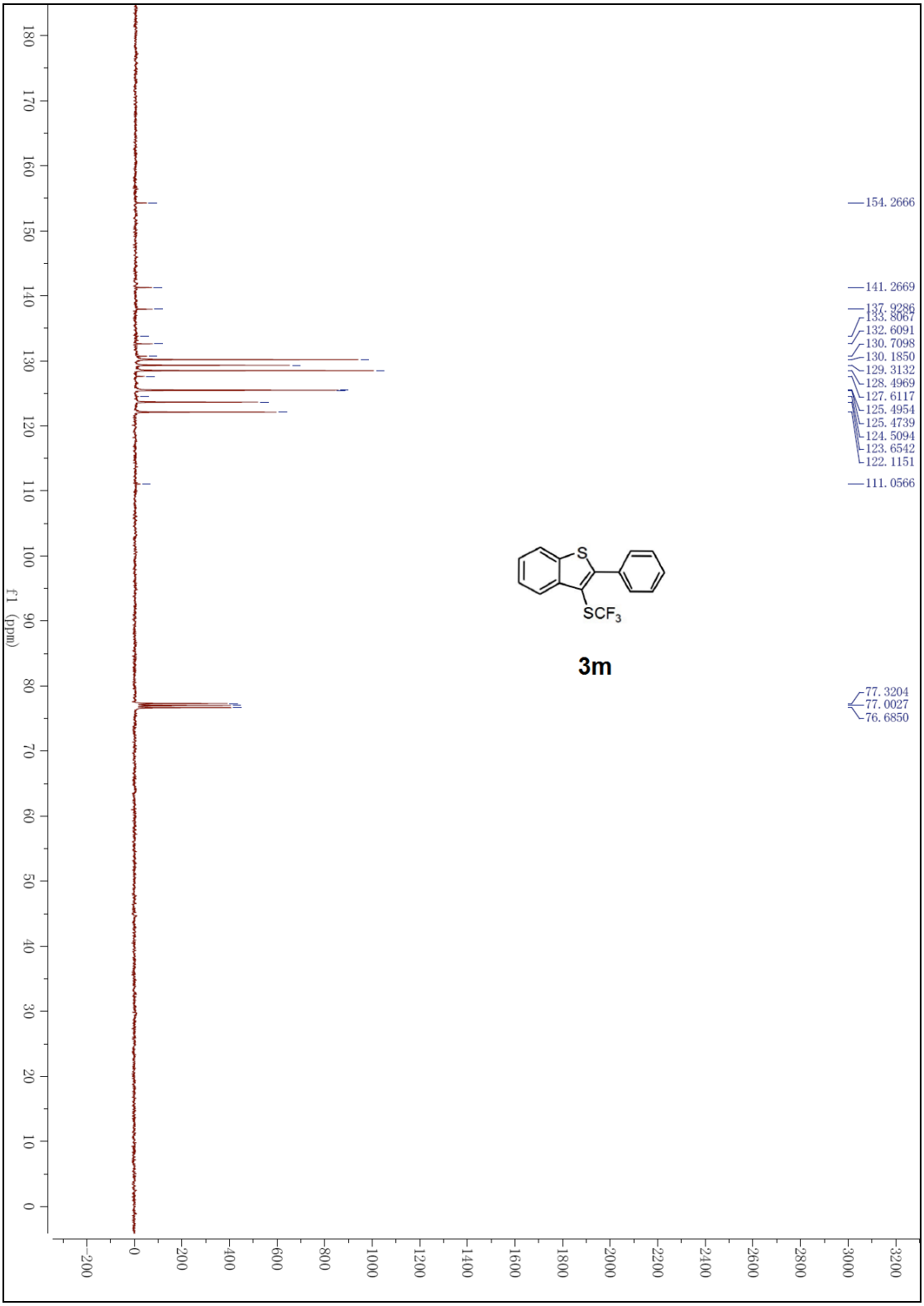

8.1855
8.1814
8.1764
8.1644
8.1614
7.4961
7.4773
7.4723
7.4683
7.2874
7.2671
7.1829
7.1624
6.7698
6.7498
3.9721
1.90
3.09
1.07
1.03
1.00
3.09
SCF3
O
O
3I
f1 (ppm)

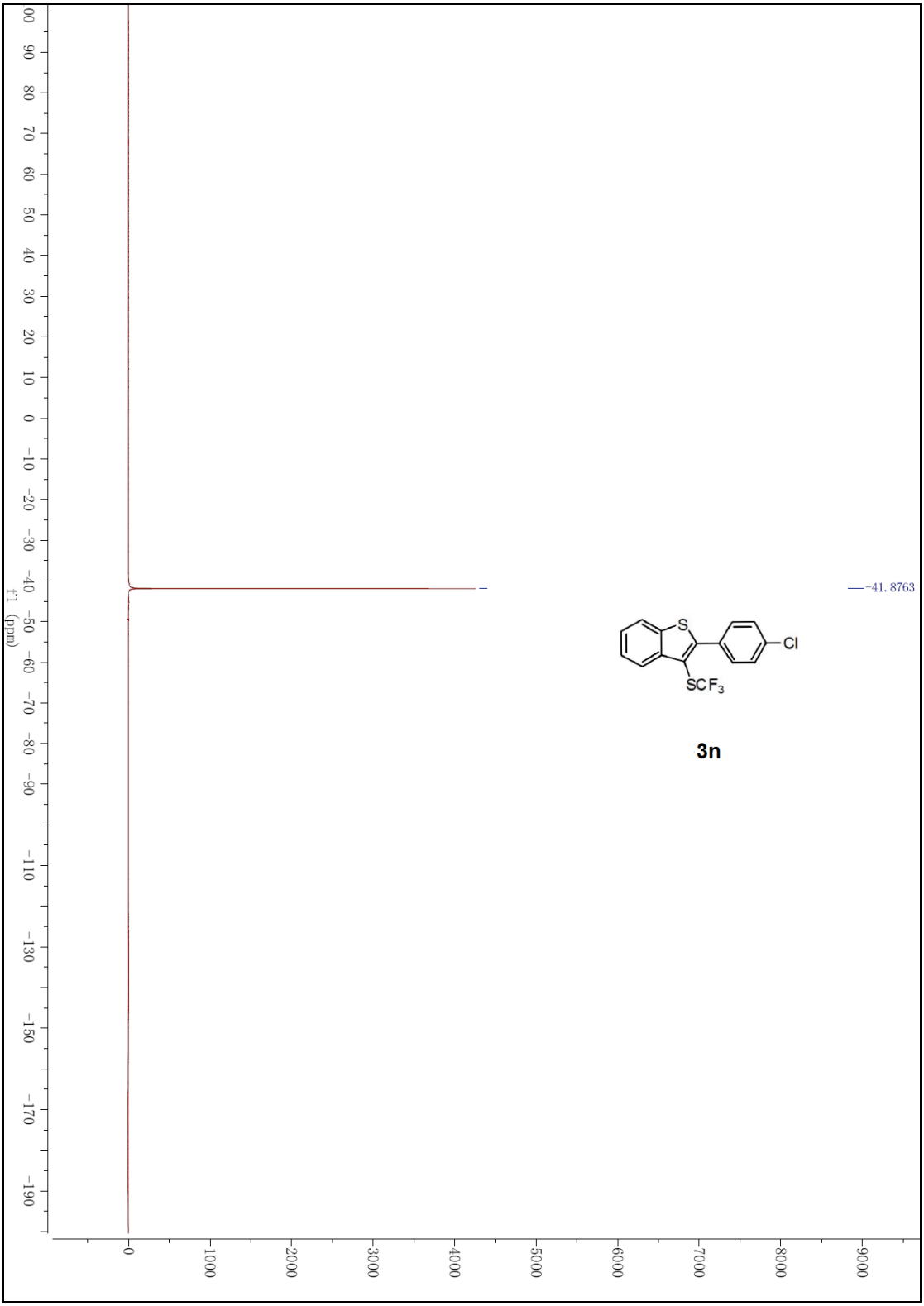

154.9619
154.8782
133.9178
130.8157
129.8799
128.9860
128.5107
128.1152
127.7221
126.2486
124.6369
119.4043
114.5606
105.0302
104.4394
96.5753
77.3224
77.0051
76.6872
55.6991
SCF3
O
O
3l
f1 (ppm)

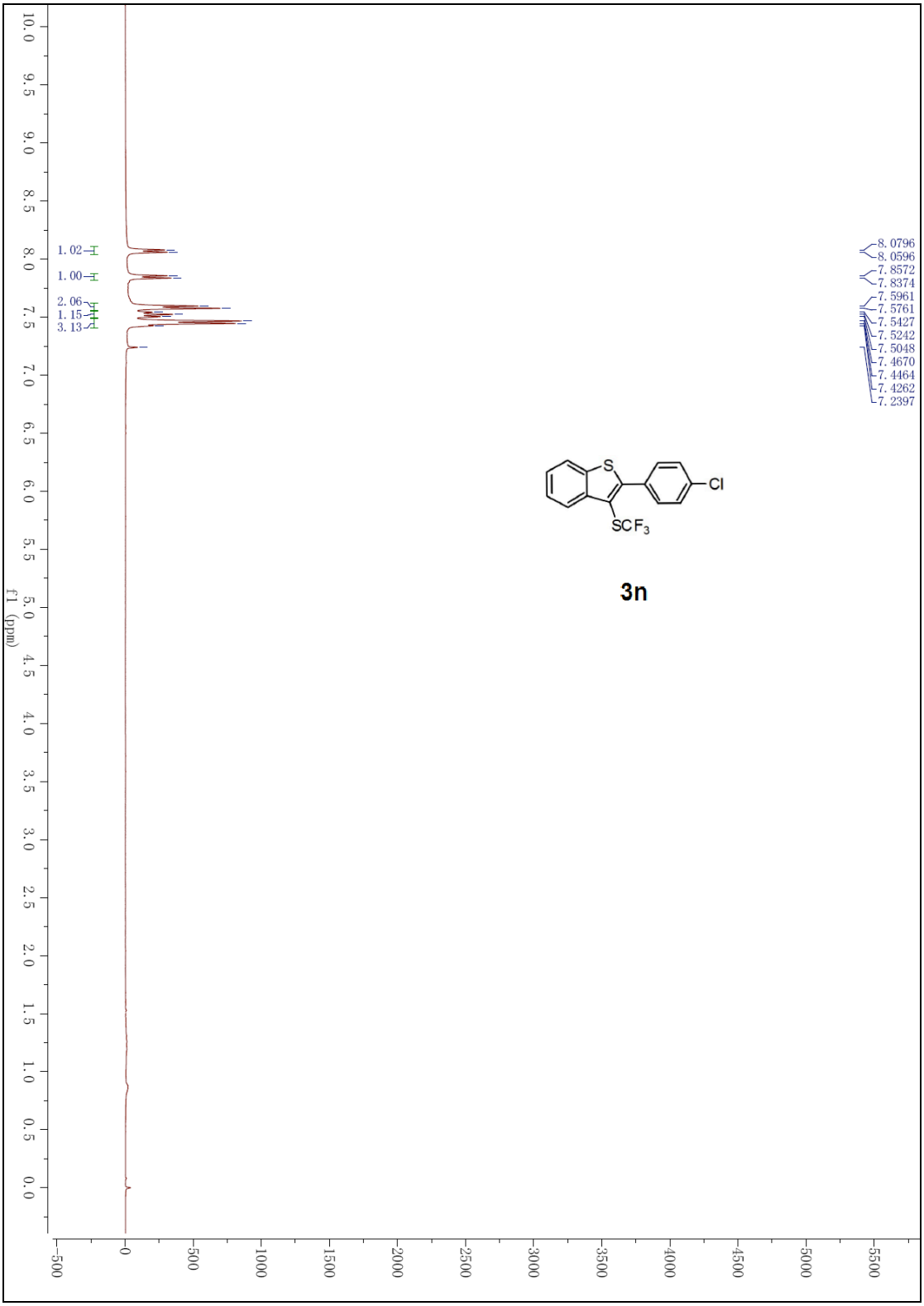

f1 (ppm)
-41.9172
S
SCF3
3m


8.1100
8.0898
7.8835
7.8635
7.6885
7.6826
7.6735
7.6689
7.6648
7.5603
7.5583
7.5404
7.5293
7.5226
7.5199
7.5106
7.5021
7.4962
7.4925
7.4848
7.4779
7.4751
7.4574
7.4397
7.4373
7.2595
1.01
1.00
2.01
5.22
S
SCF3
f1 (ppm)

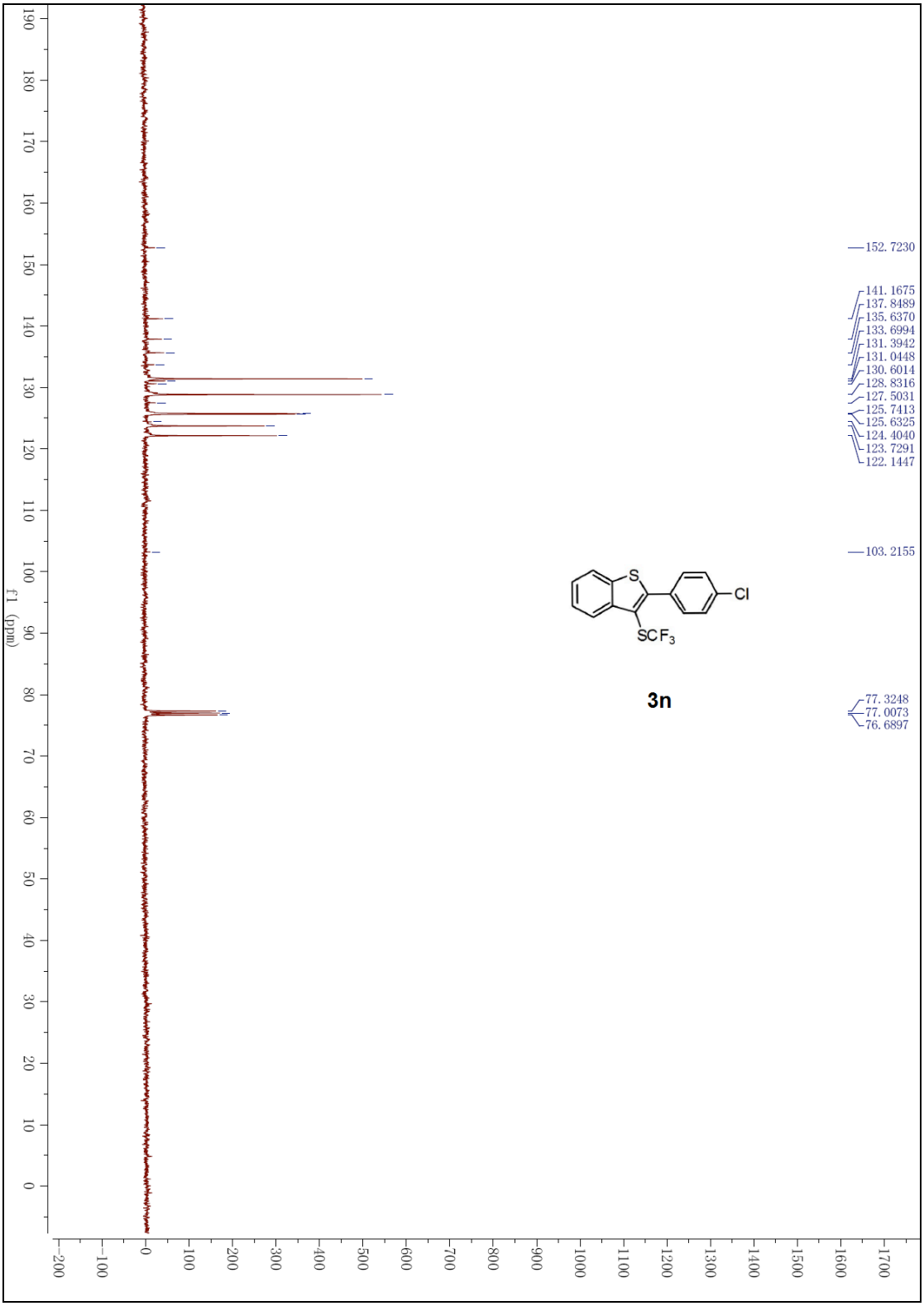
3m


154.2666
141.2669
137.9286
133.8067
132.6091
130.7098
130.1850
129.3132
128.4969
127.6117
125.4954
125.4739
124.5094
123.6542
122.1151
111.0566
77.3204
77.0027
76.6850
S
SCF3
3m
f1 (ppm)


−41.8763
S
Cl
SCF3
3n
f1 (ppm)


1.02
1.00
2.06
1.15
3.13
8.0796
8.0596
7.8572
7.8374
7.5961
7.5761
7.5427
7.5242
7.5048
7.4670
7.4464
7.4262
7.2397
S
Cl
SCF3
f1 (ppm)

3n


152.7230
141.1675
137.8489
135.6370
133.6994
131.3942
131.0448
130.6014
128.8316
127.5031
125.7413
125.6325
124.4040
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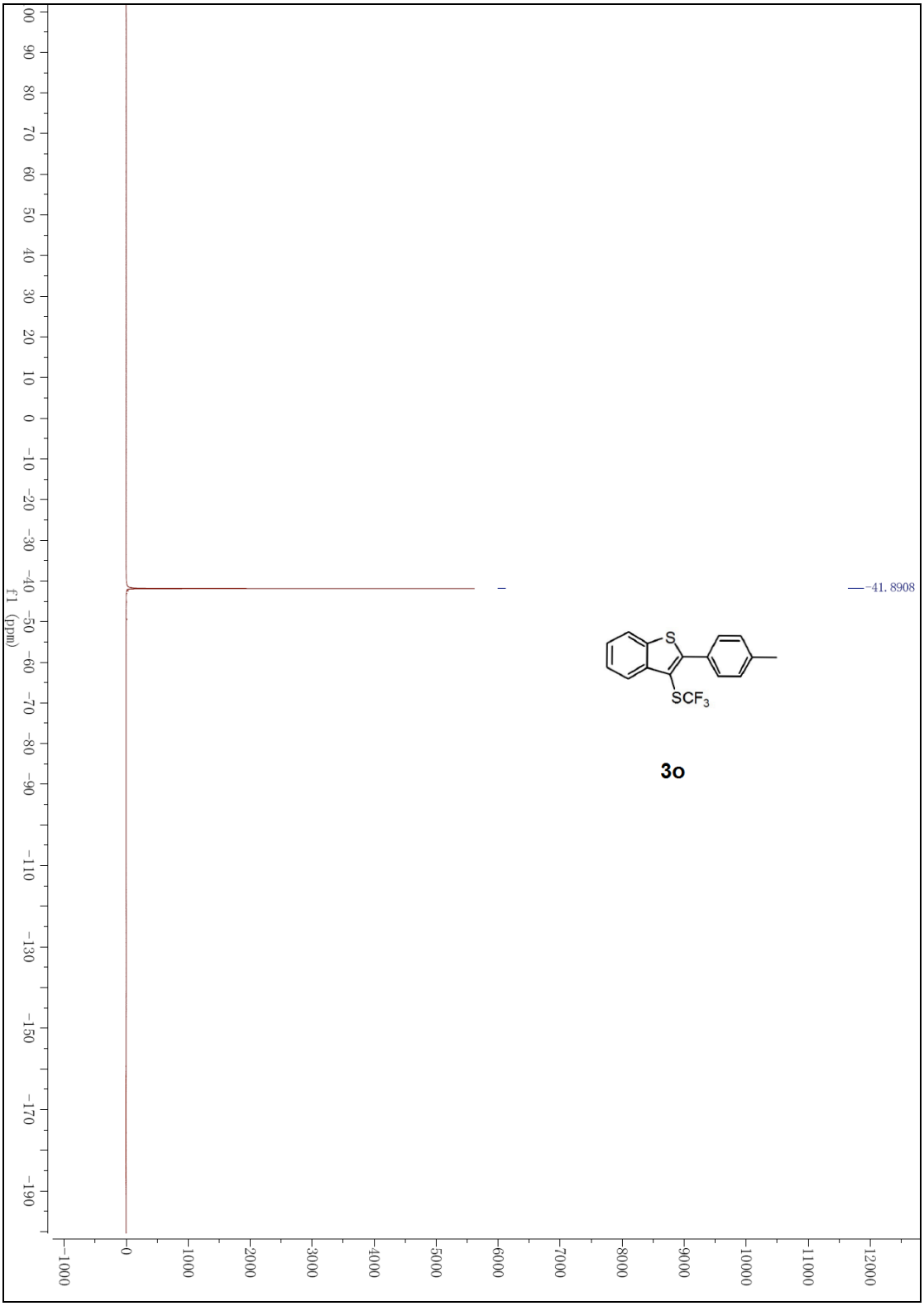
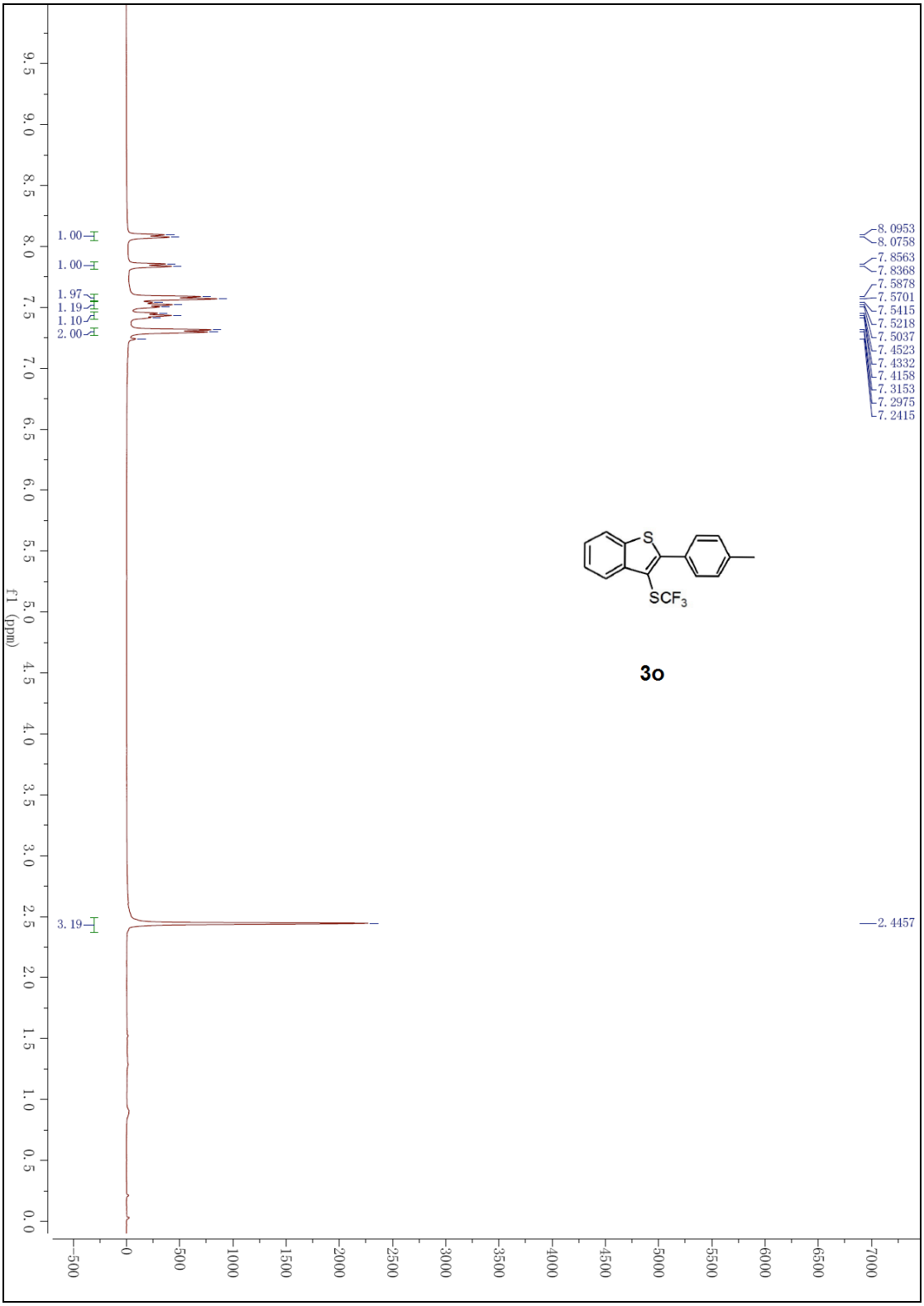
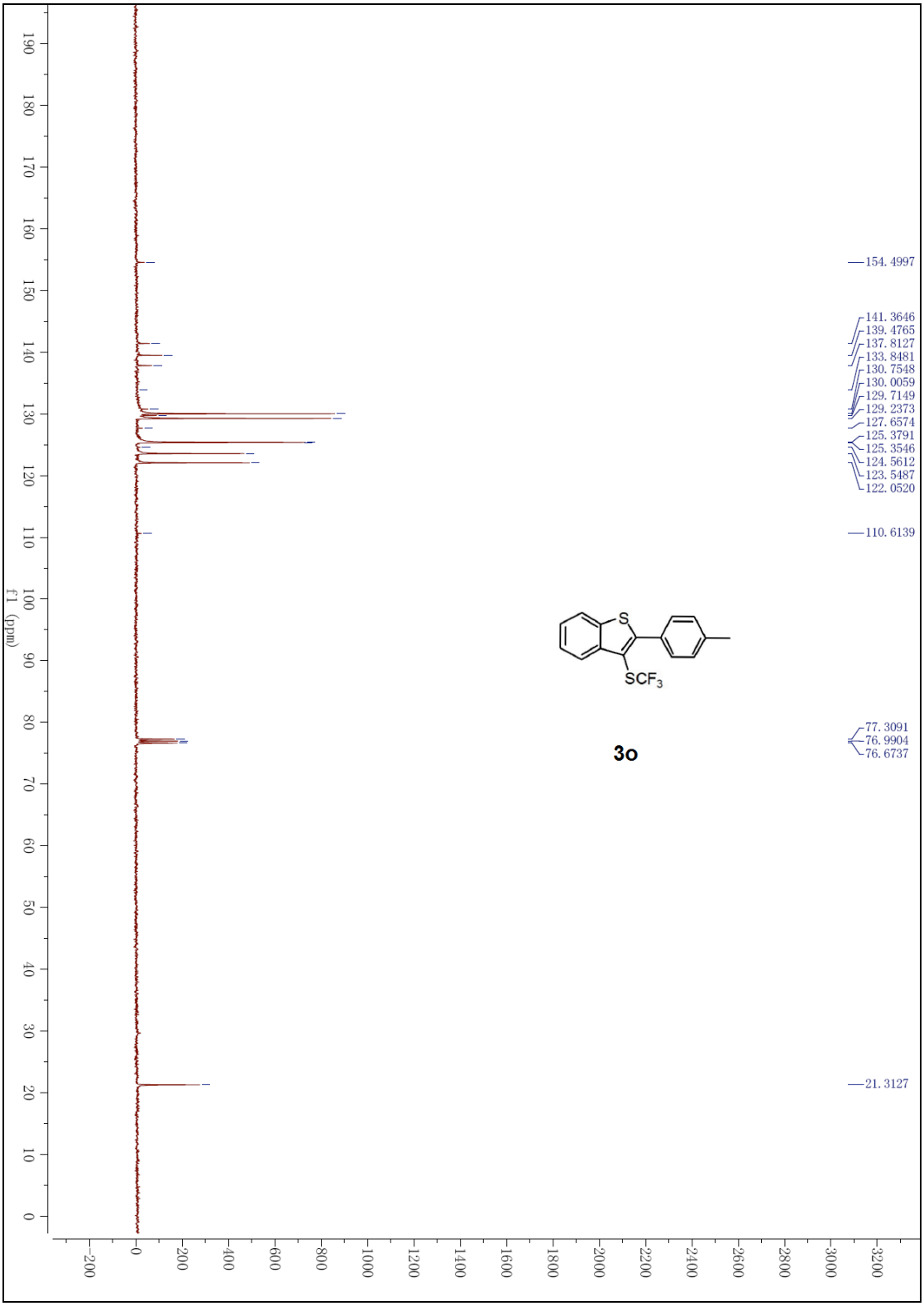
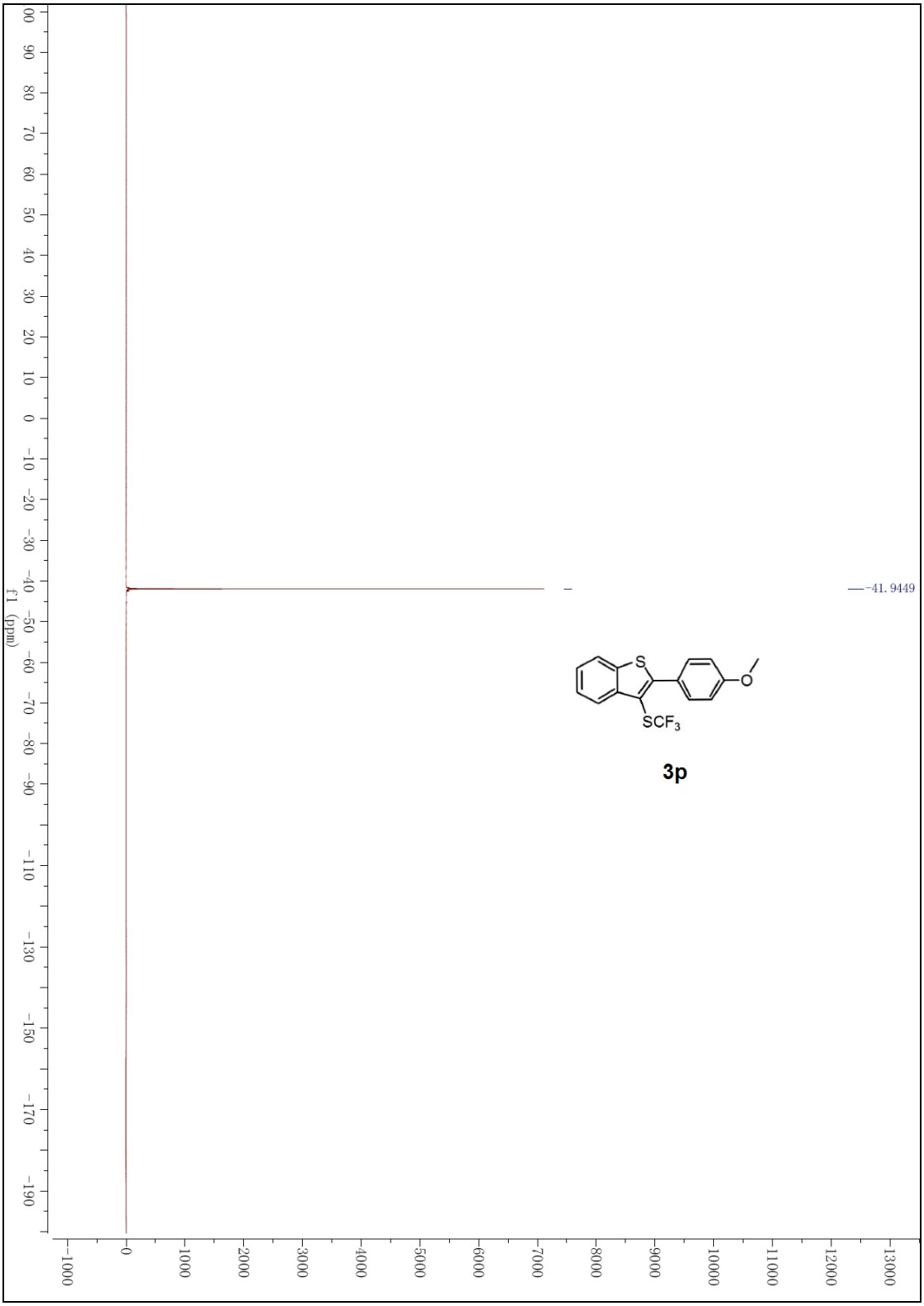
76.6897
S
Cl
SCF3
3n
f1 (ppm)

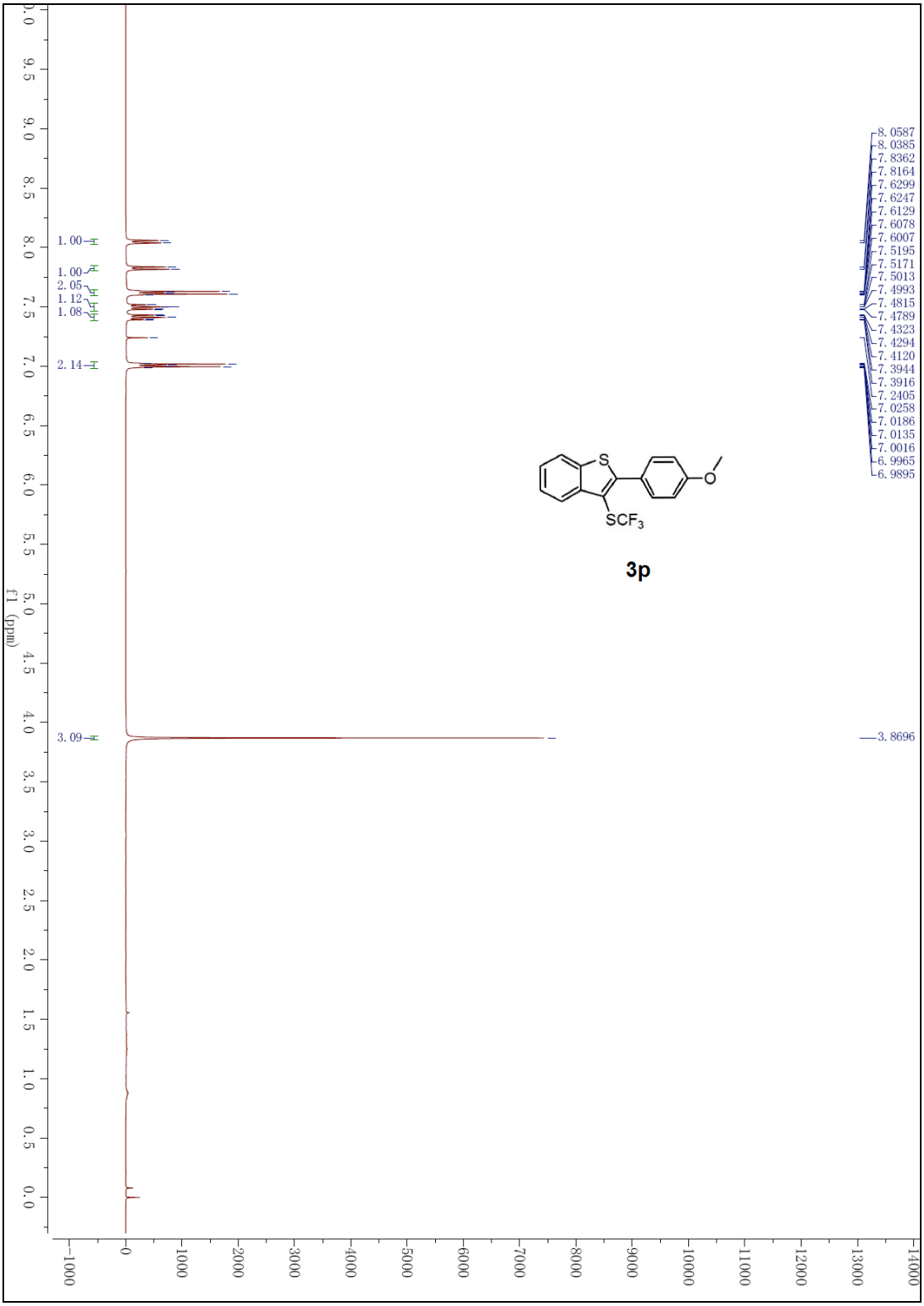

f1 (ppm)
−41.8908
S
SCF3
3o


1.00
1.00
1.97
1.19
1.10
2.00
3.19
8.0953
8.0758
7.8563
7.8368
7.5878
7.5701
7.5415
7.5218
7.5037
7.4523
7.4332
7.4158
7.3153
7.2975
7.2415
2.4457
S
SCF3
f1 (ppm)

3o


154.4997
141.3646
139.4765
137.8127
133.8481
130.7548
130.0059
129.7149
129.2373
127.6574
125.3791
125.3546
124.5612
123.5487
122.0520
110.6139
77.3091
76.9904
76.6737
21.3127
f1 (ppm)
S
SCF3
3o


-41.9449
S
O
SCF3
3p
f1 (ppm)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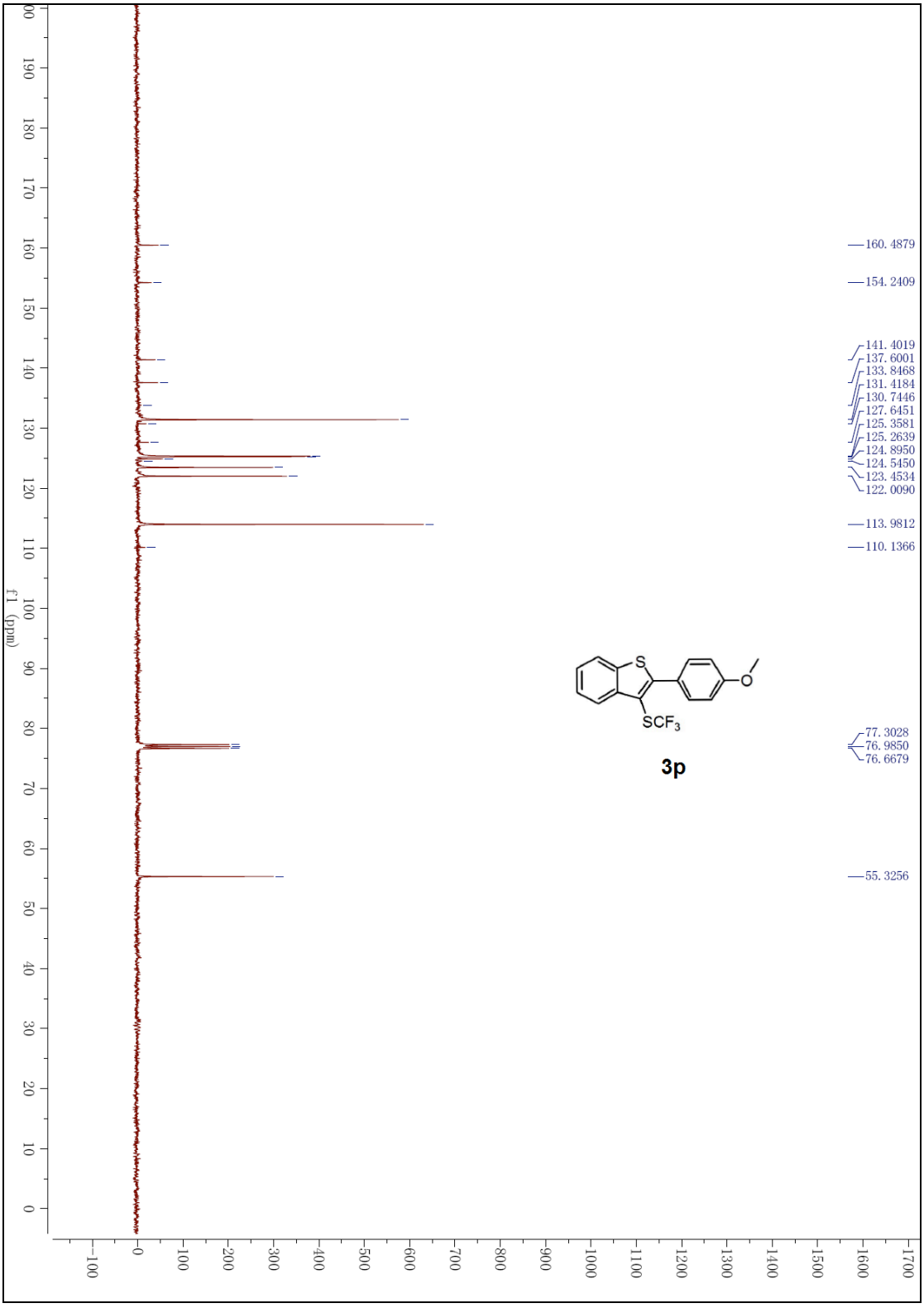
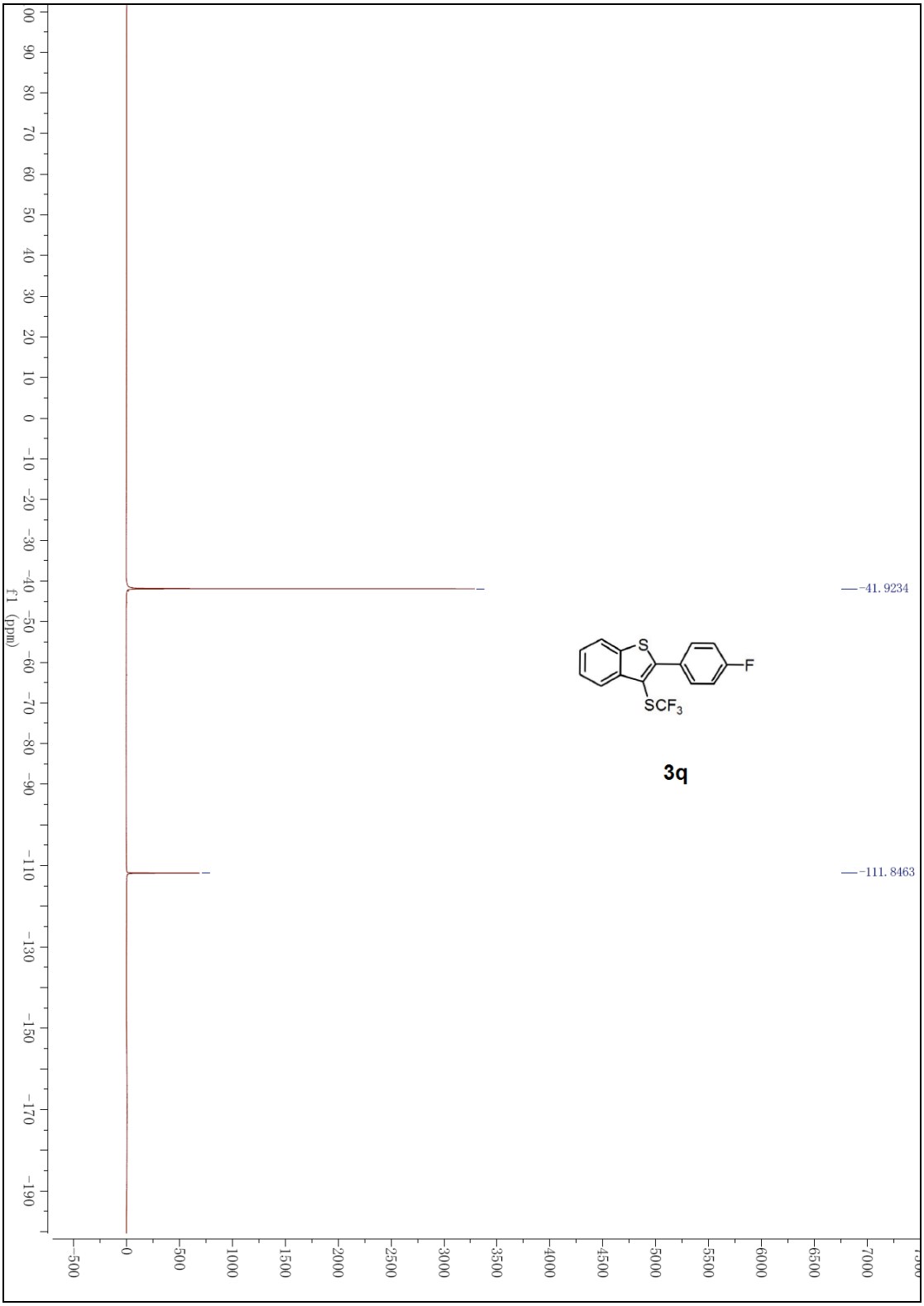
8.0385
7.8362
7.8164
7.6299
7.6247
7.6129
7.6078
7.6007
7.5195
7.5171
7.5013
7.4993
7.4815
7.4789
7.4323
7.4294
7.4120
7.3944
7.3916
7.2405
7.0258
7.0186
7.0135
7.0016
6.9965
6.9895
3.8696
1.00
1.00
2.05
1.12
1.08
2.14
3.09
S
O
SCF3
f1 (ppm)

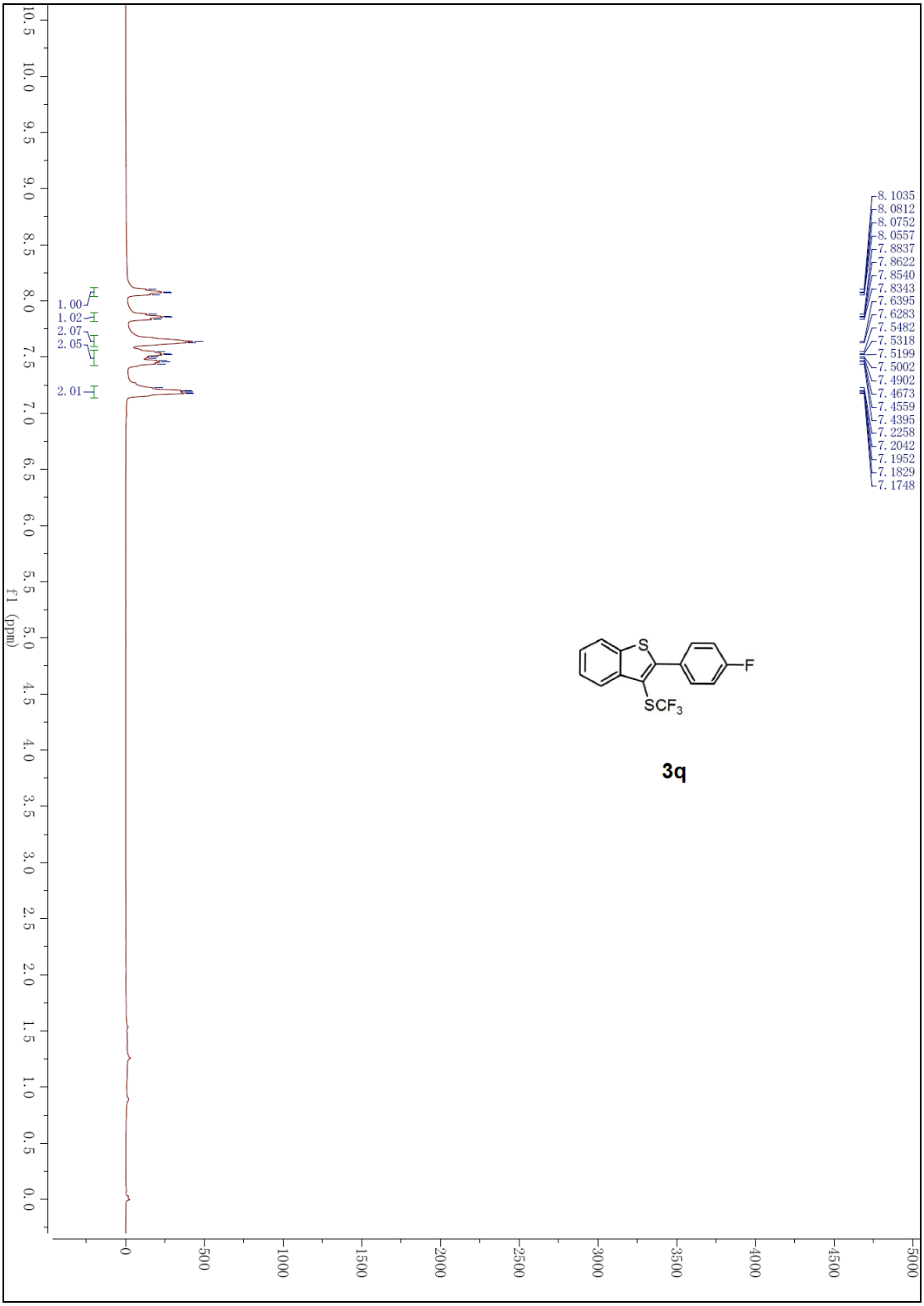
3p


160.4879
154.2409
141.4019
137.6001
133.8468
131.4184
130.7446
127.6451
125.3581
125.2639
124.8950
124.5450
123.4534
122.0090
113.9812
110.1366
77.3028
76.9850
76.6679
55.3256
f1 (ppm)
S
O
SCF3

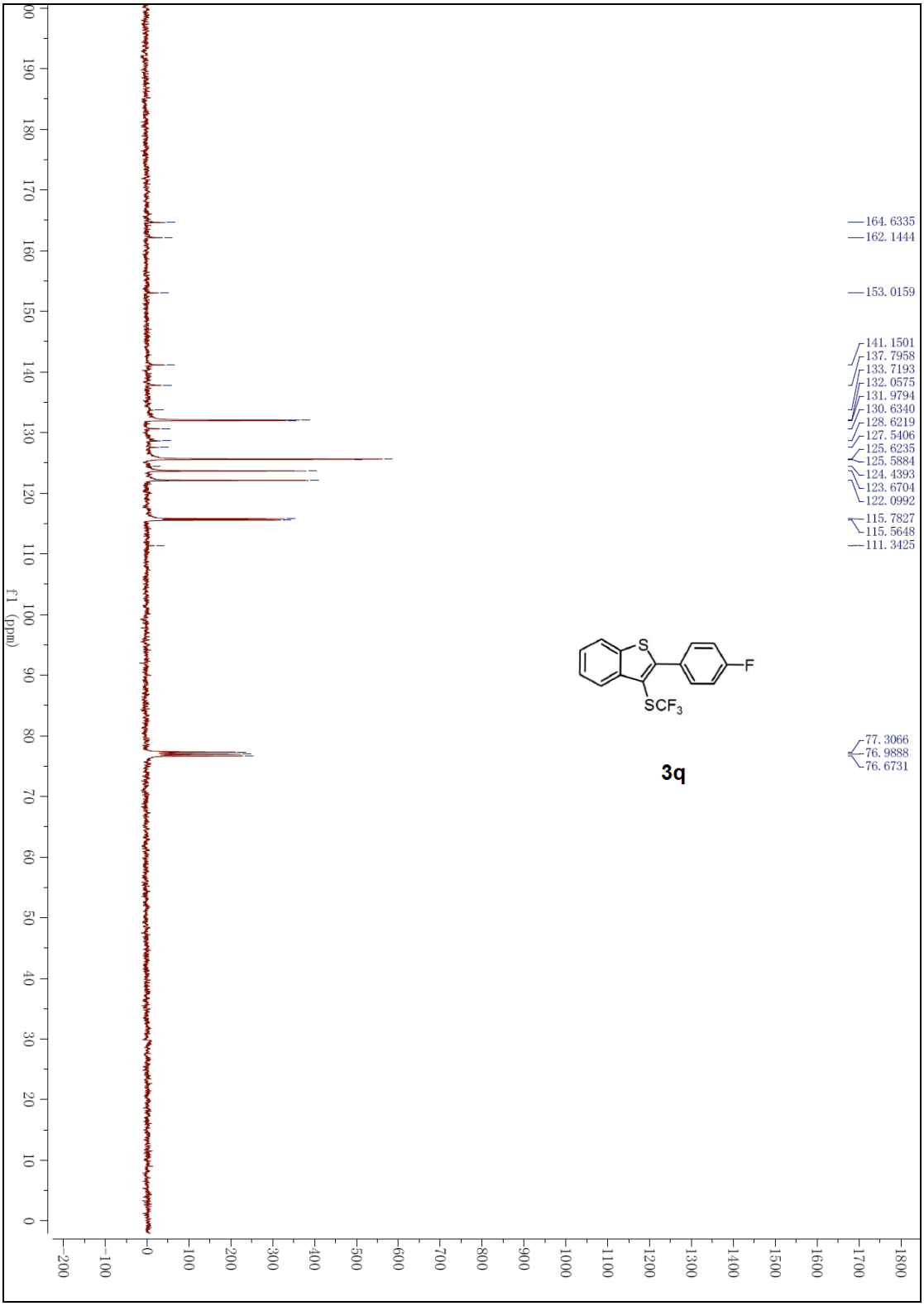
3p

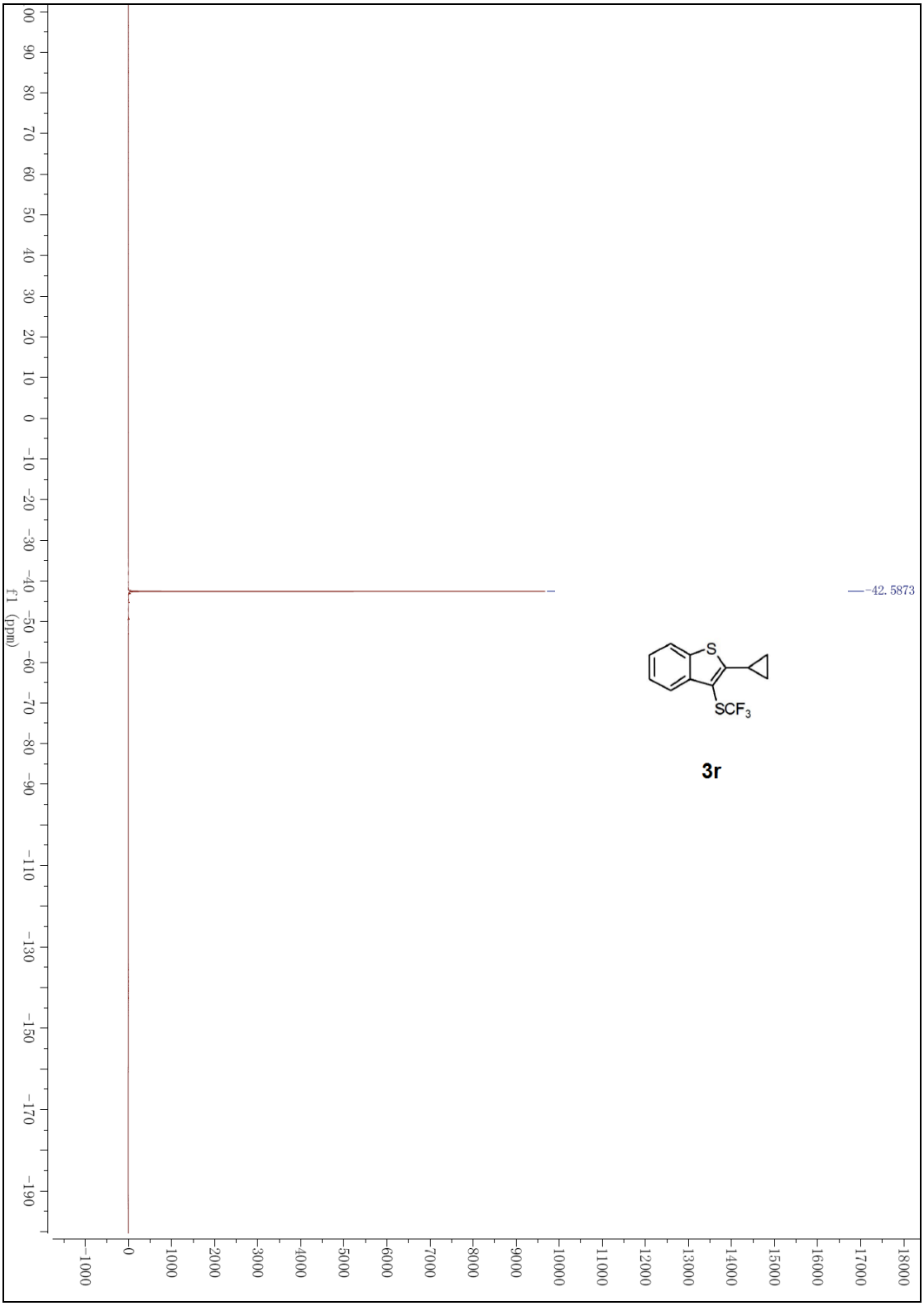


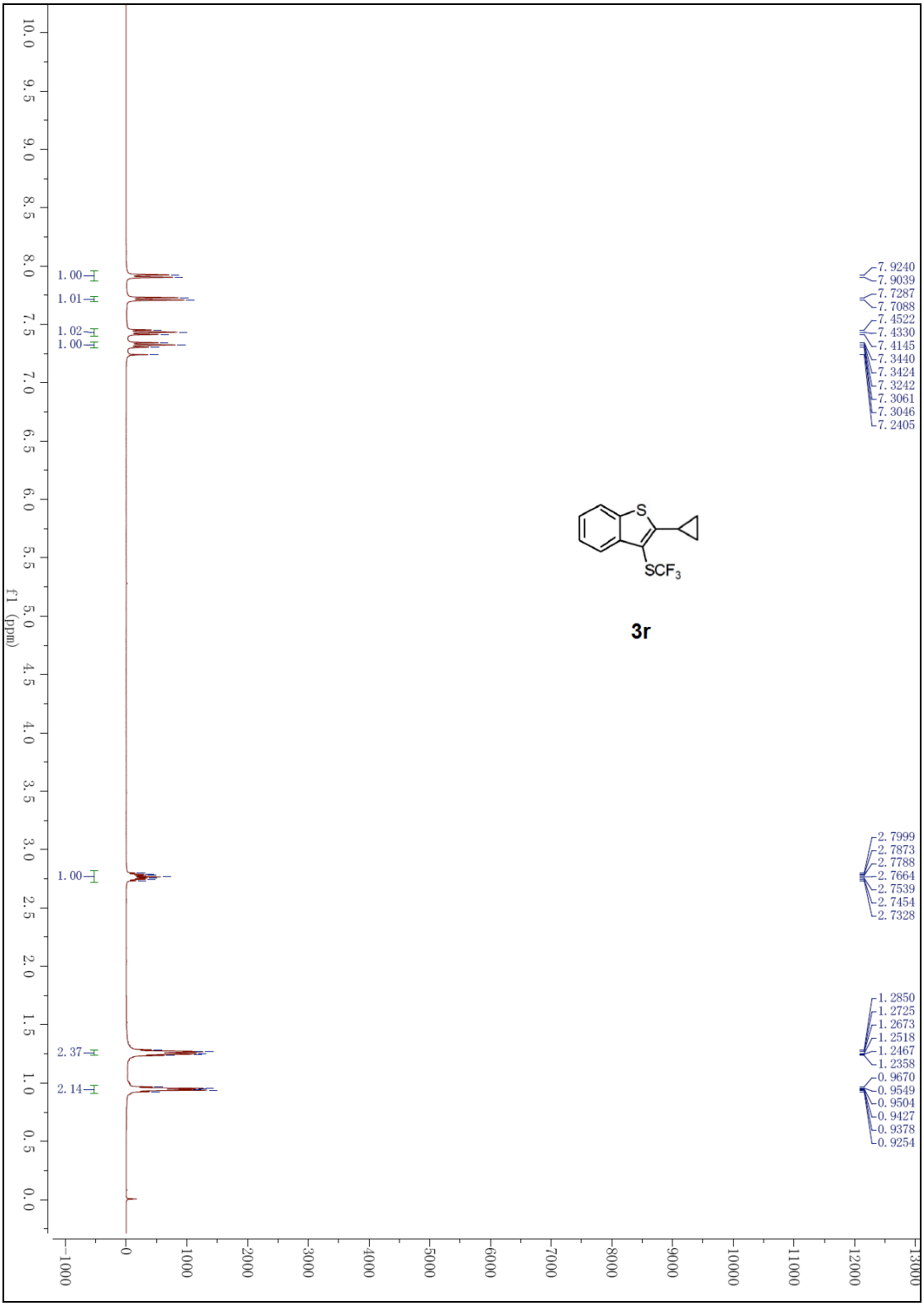
3q

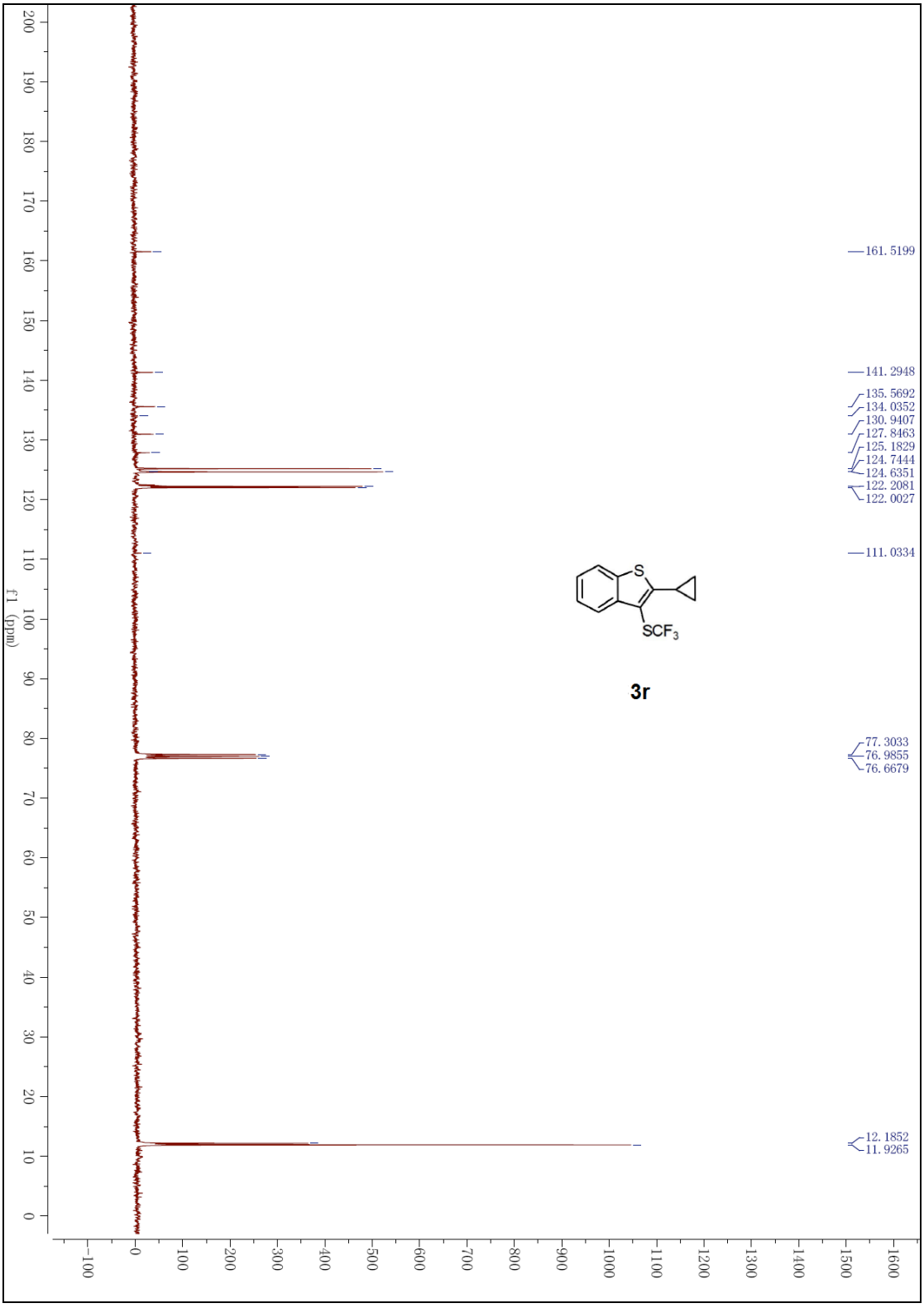

8.1035
8.0812
8.0752
8.0557
7.8837
7.8622
7.8540
7.8343
7.6395
7.6283
7.5482
7.5318
7.5199
7.5002
7.4902
7.4673
7.4559
7.4395
7.2258
7.2042
7.1952
7.1829
7.1748
1.00
1.02
2.07
2.05
2.01
S
F
SCF3
f1 (ppm)

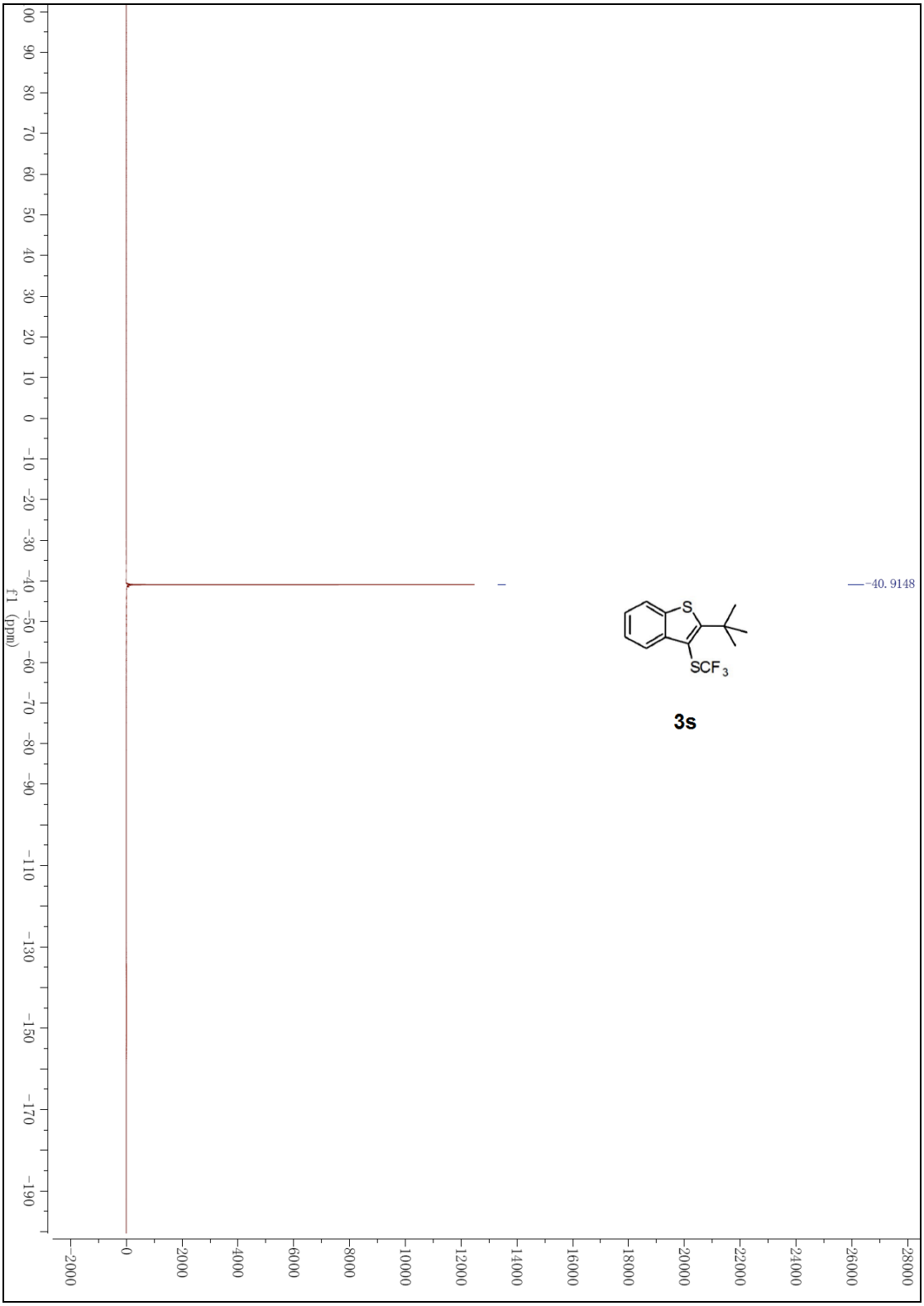
3q

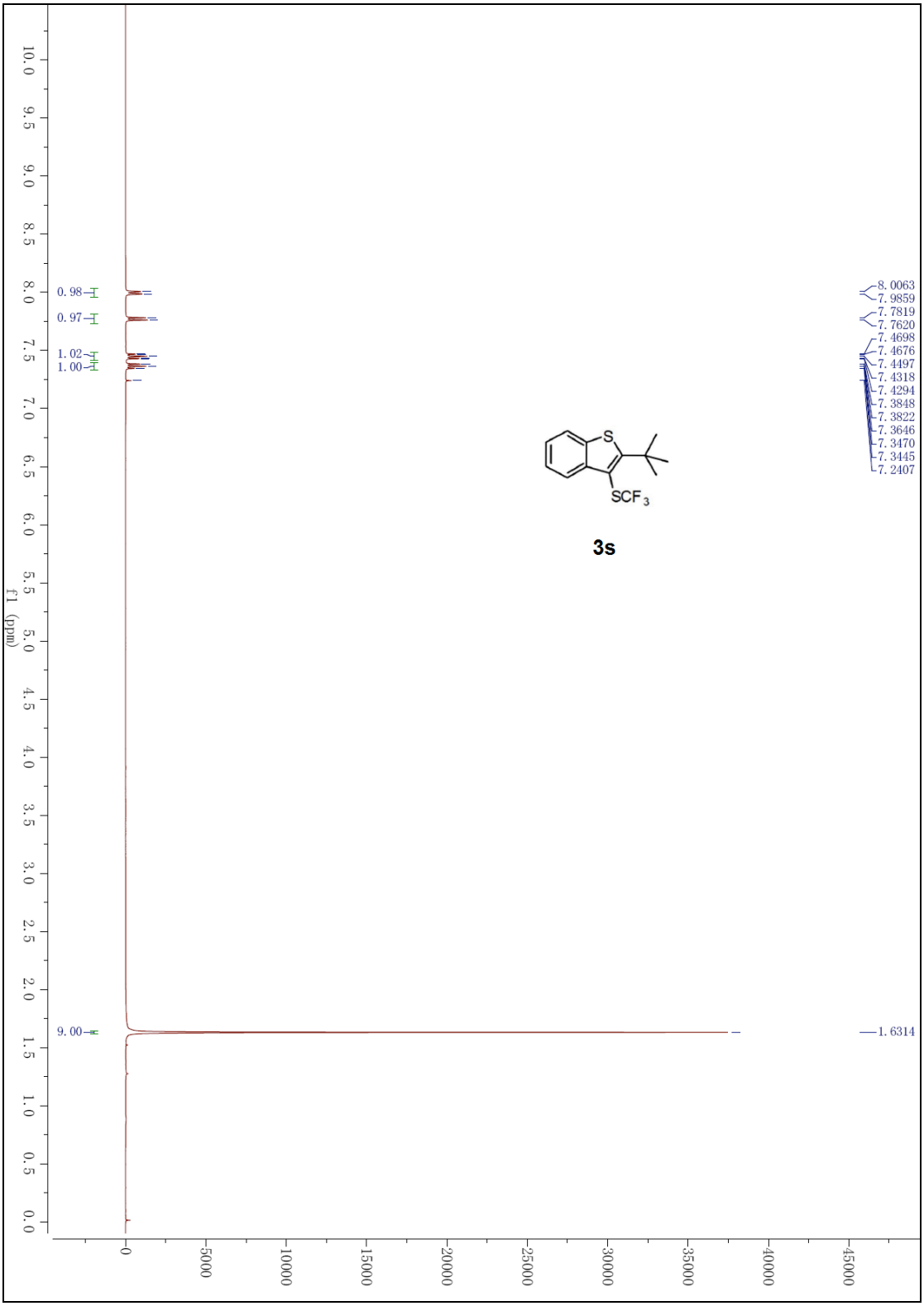

164.6335
162.1444
153.0159
141.1501
137.7958
133.7193
132.0575
131.9794
130.6340
128.6219
127.5406
125.6235
125.5884
124.4393
123.6704
122.0992
115.7827
115.5648
111.3425
77.3066
76.9888
76.6731
S
F
SCF3
3q
f1 (ppm)


-42.5873
f1 (ppm)
S
SCF3
3r


7.9240
7.9039
7.7287
7.7088
7.4522
7.4330
7.4145
7.3440
7.3424
7.3242
7.3061
7.3046
7.2405
2.7999
2.7873
2.7788
2.7664
2.7539
2.7454
2.7328
1.2850
1.2725
1.2673
1.2518
1.2467
1.2358
0.9670
0.9549
0.9504
0.9427
0.9378
0.9254
1.00
1.01
1.02
1.00
1.00
2.37
2.14
S
SCF3
3r
f1 (ppm)


161.5199
141.2948
135.5692
134.0352
130.9407
127.8463
125.1829
124.7444
124.6351
122.2081
122.0027
111.0334
77.3033
76.9855
76.6679
12.1852
11.9265
S
SCF3
3r
f1 (ppm)


−40.9148
S
SCF3
3s
f1 (ppm)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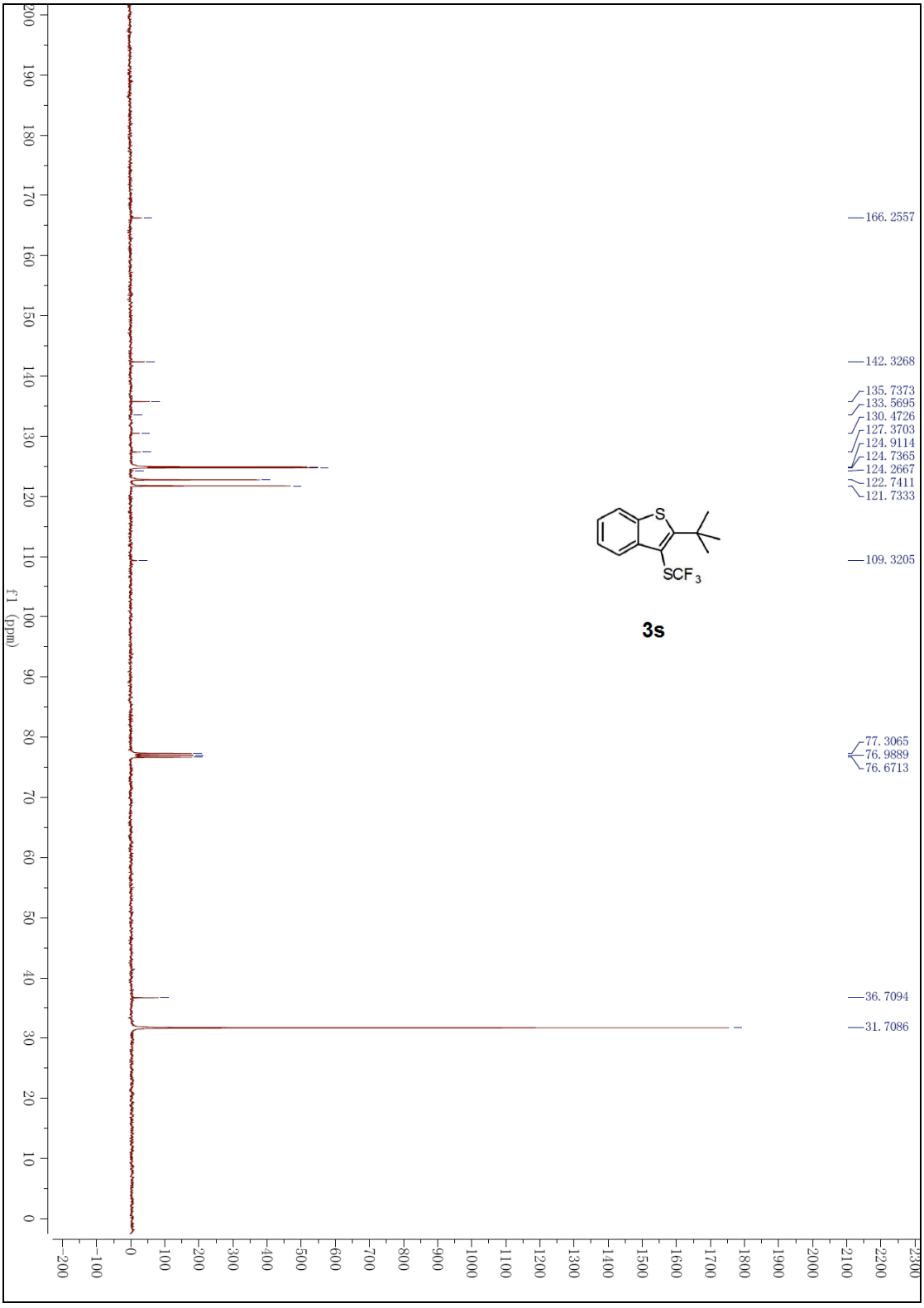
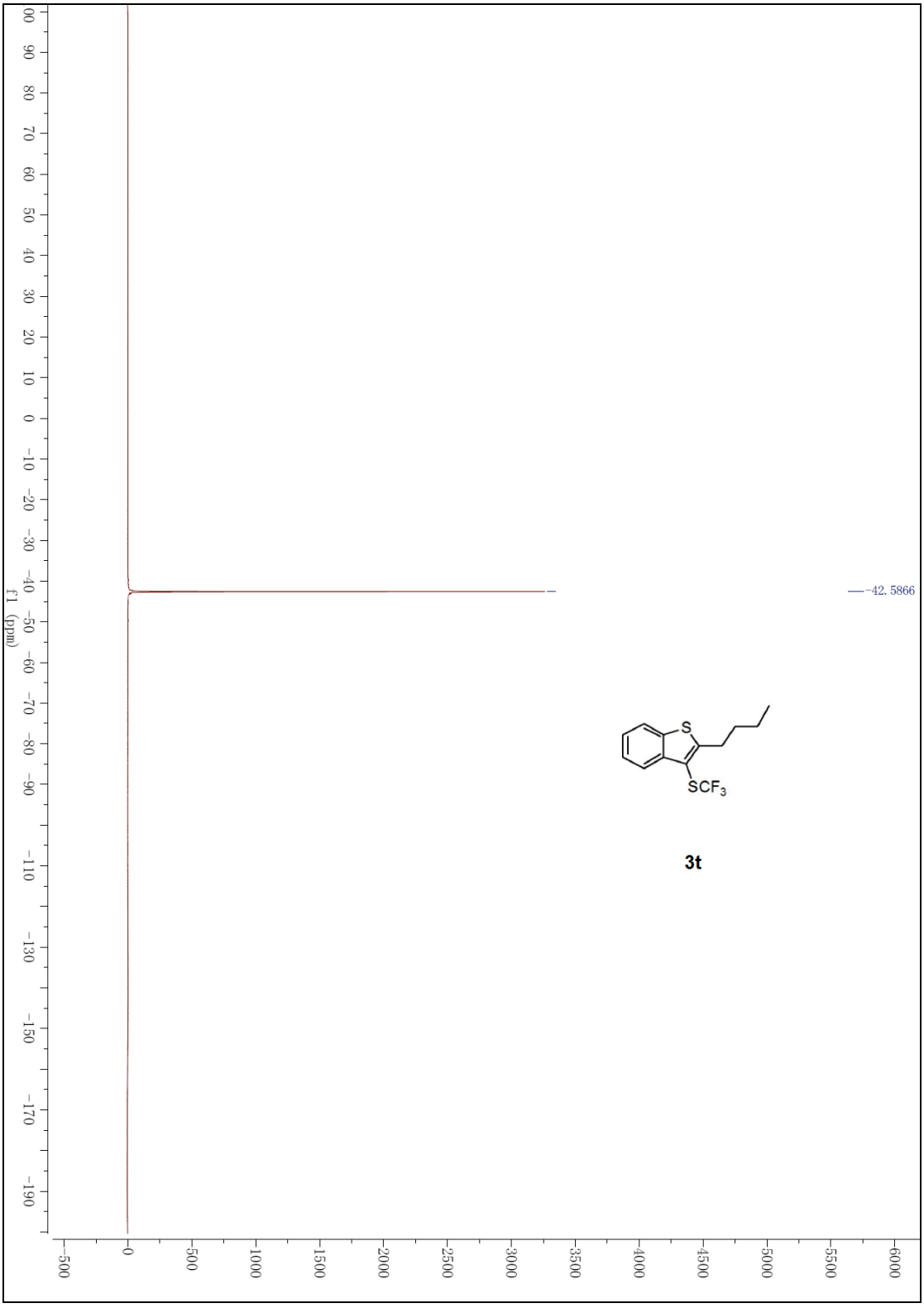
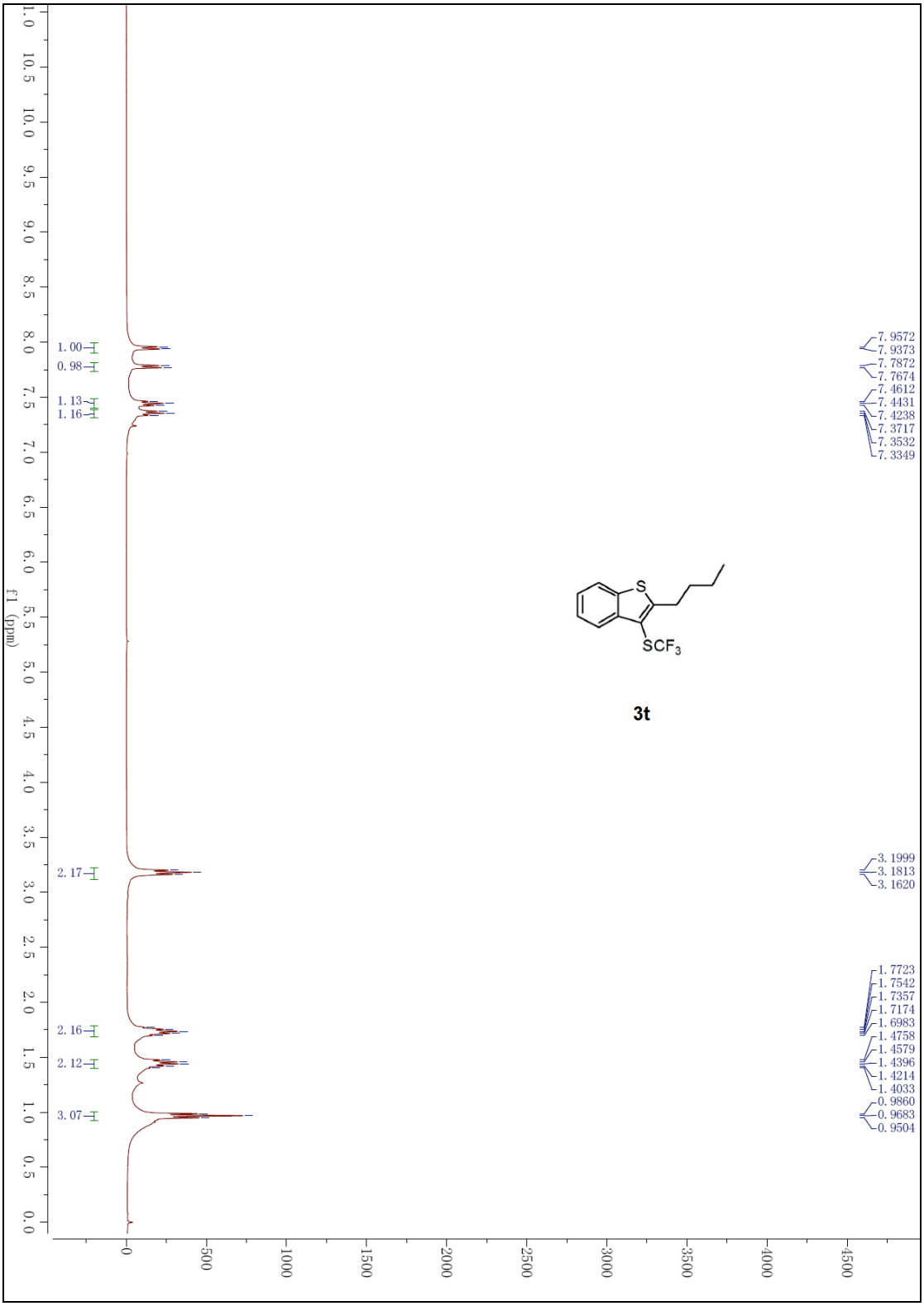
7.7819
7.7620
7.4698
7.4676
7.4497
7.4318
7.4294
7.3848
7.3822
7.3646
7.3470
7.3445
7.2407
0.98
0.97
1.02
1.00
9.00
1.6314
S
SCF3
3s
f1 (ppm)


166.2557
142.3268
135.7373
133.5695
130.4726
127.3703
124.9114
124.7365
124.2667
122.7411
121.7333
109.3205
77.3065
76.9889
76.6713
36.7094
31.7086
S
SCF3
3s
f1 (ppm)


-42.5866
S
SCF3
3t
f1 (ppm)


f1 (ppm)
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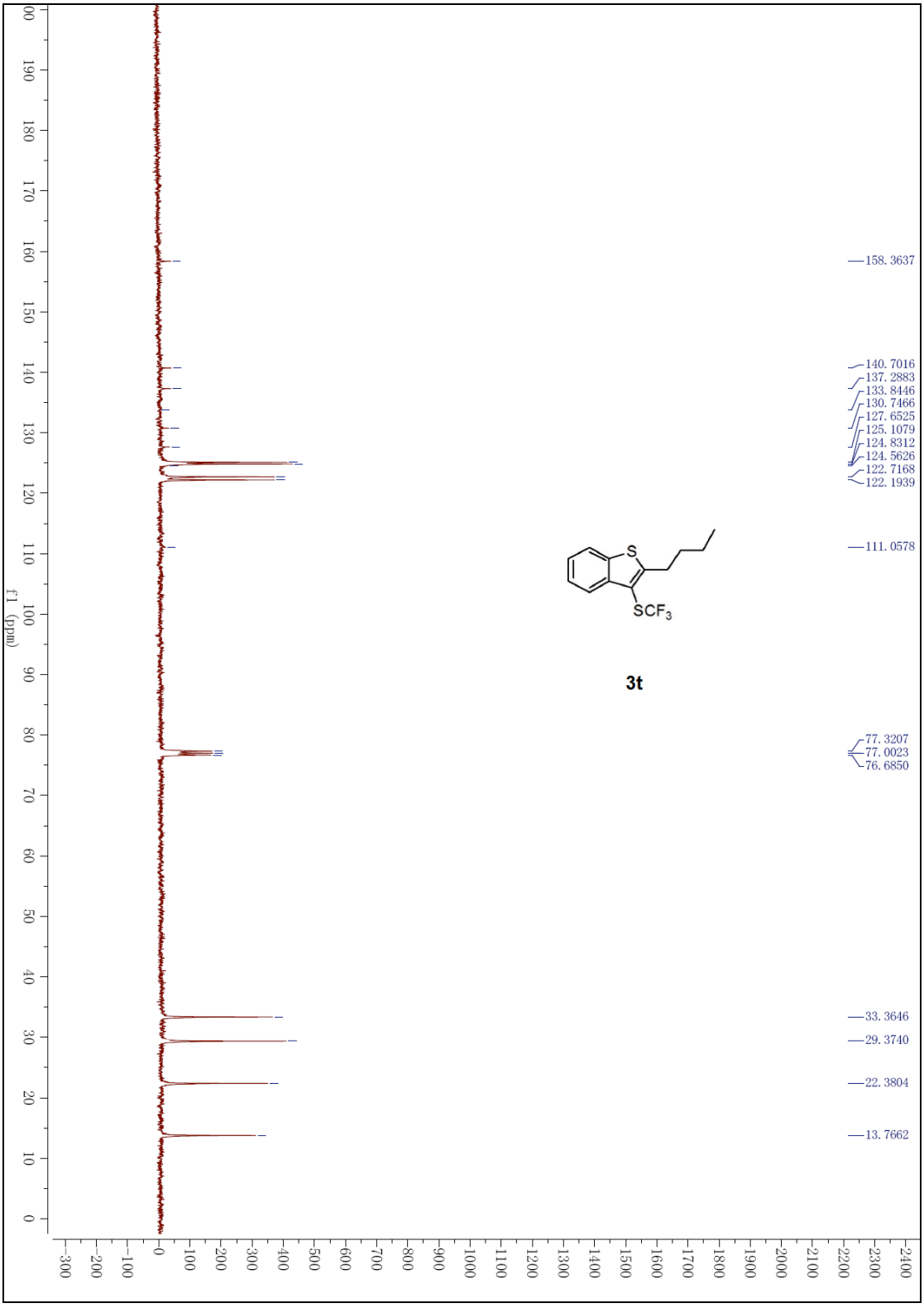
0.98
1.13
1.16
2.17
2.16
2.12
3.07
7.9572
7.9373
7.7872
7.7674
7.4612
7.4431
7.4238
7.3717
7.3532
7.3349
3.1999
3.1813
3.1620
1.7723
1.7542
1.7357
1.7174
1.6983
1.4758
1.4579
1.4396
1.4214
1.4033
0.9860
0.9683
0.9504
S
SCF3

3t


158.3637
140.7016
137.2883
133.8446
130.7466
127.6525
125.1079
124.8312
124.5626
122.7168
122.1939
111.0578
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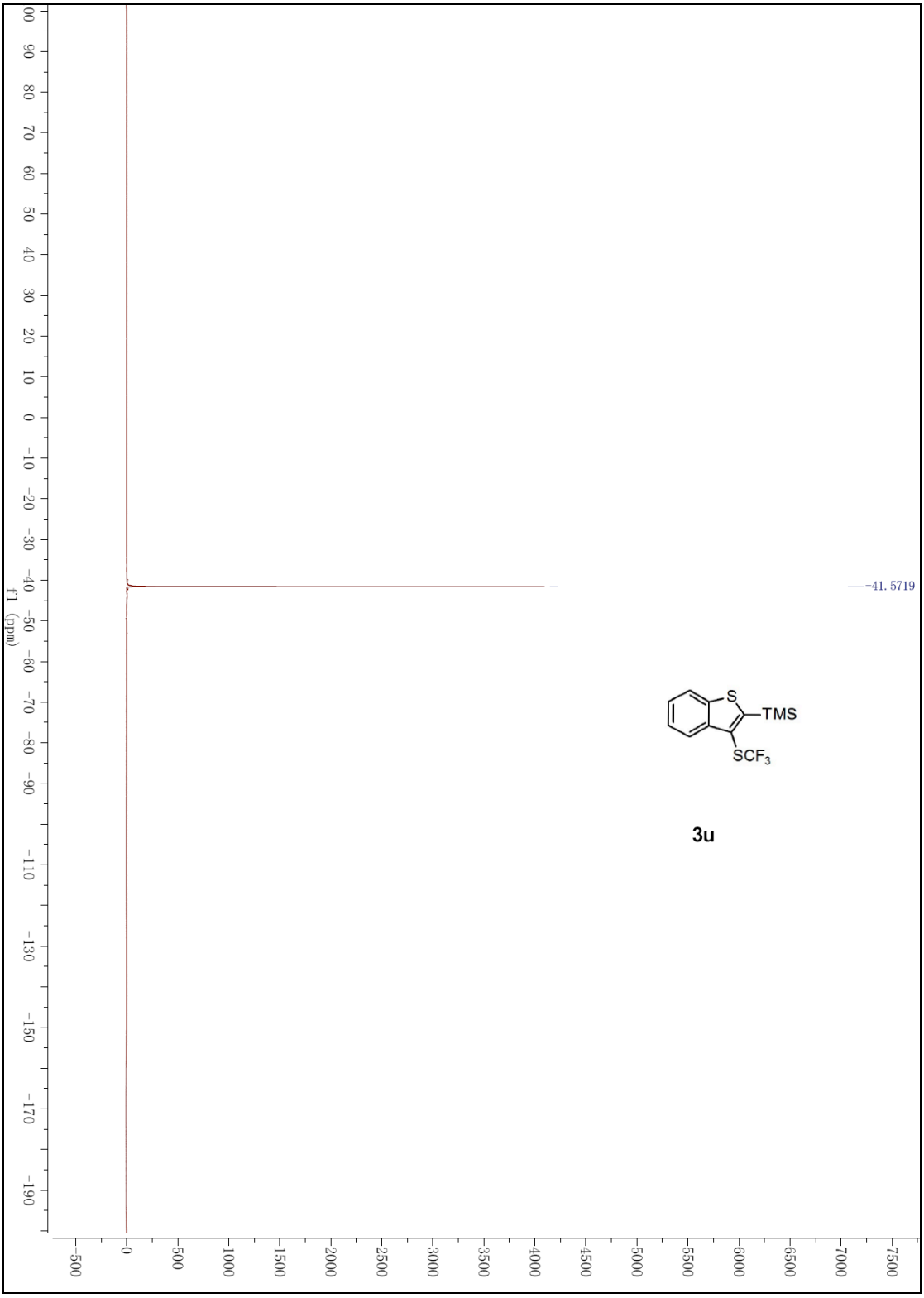
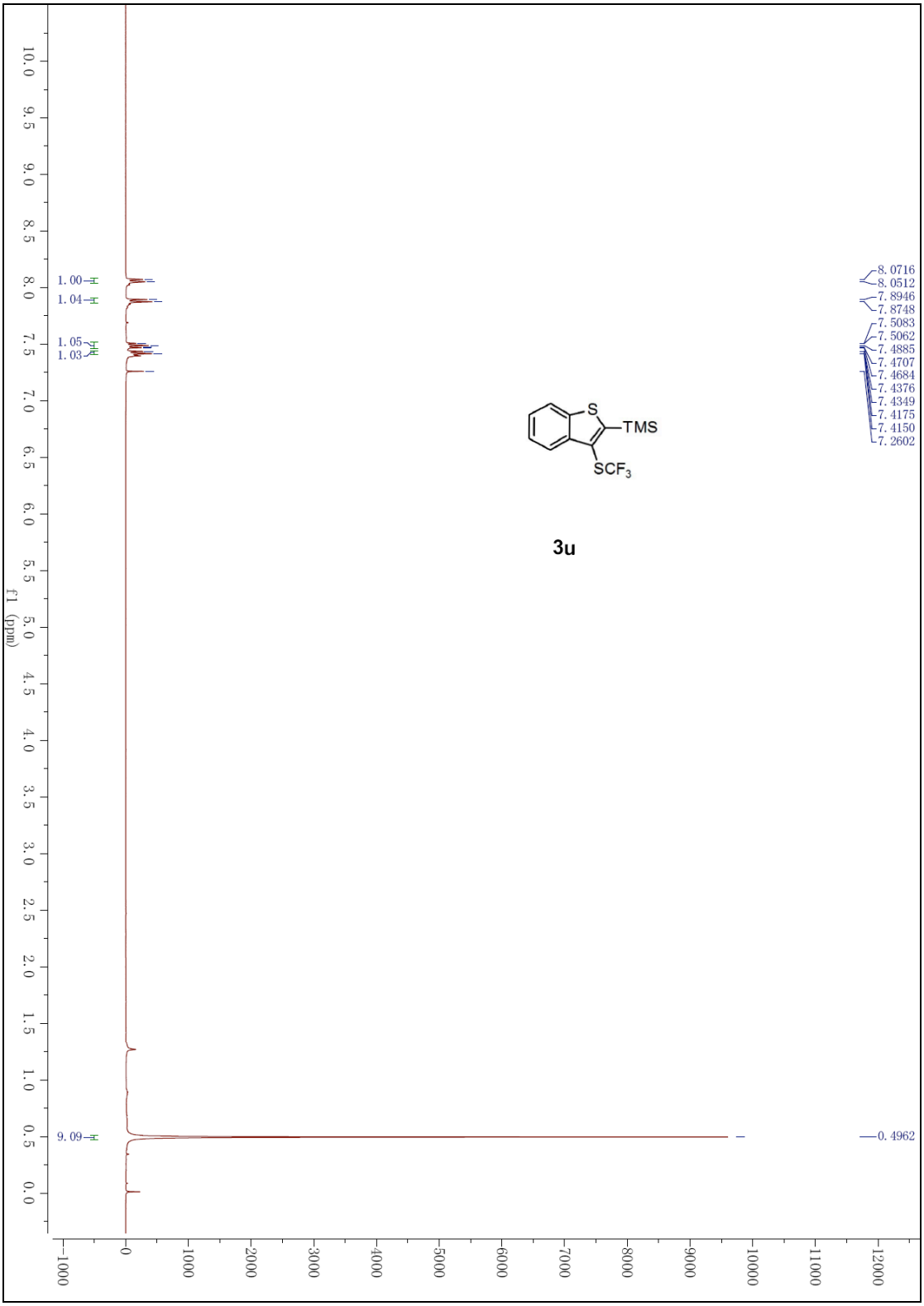
13.7662
S
SCF3
3t
f1 (ppm)


−41.5719
S
TMS
SCF3
3u
f1 (ppm)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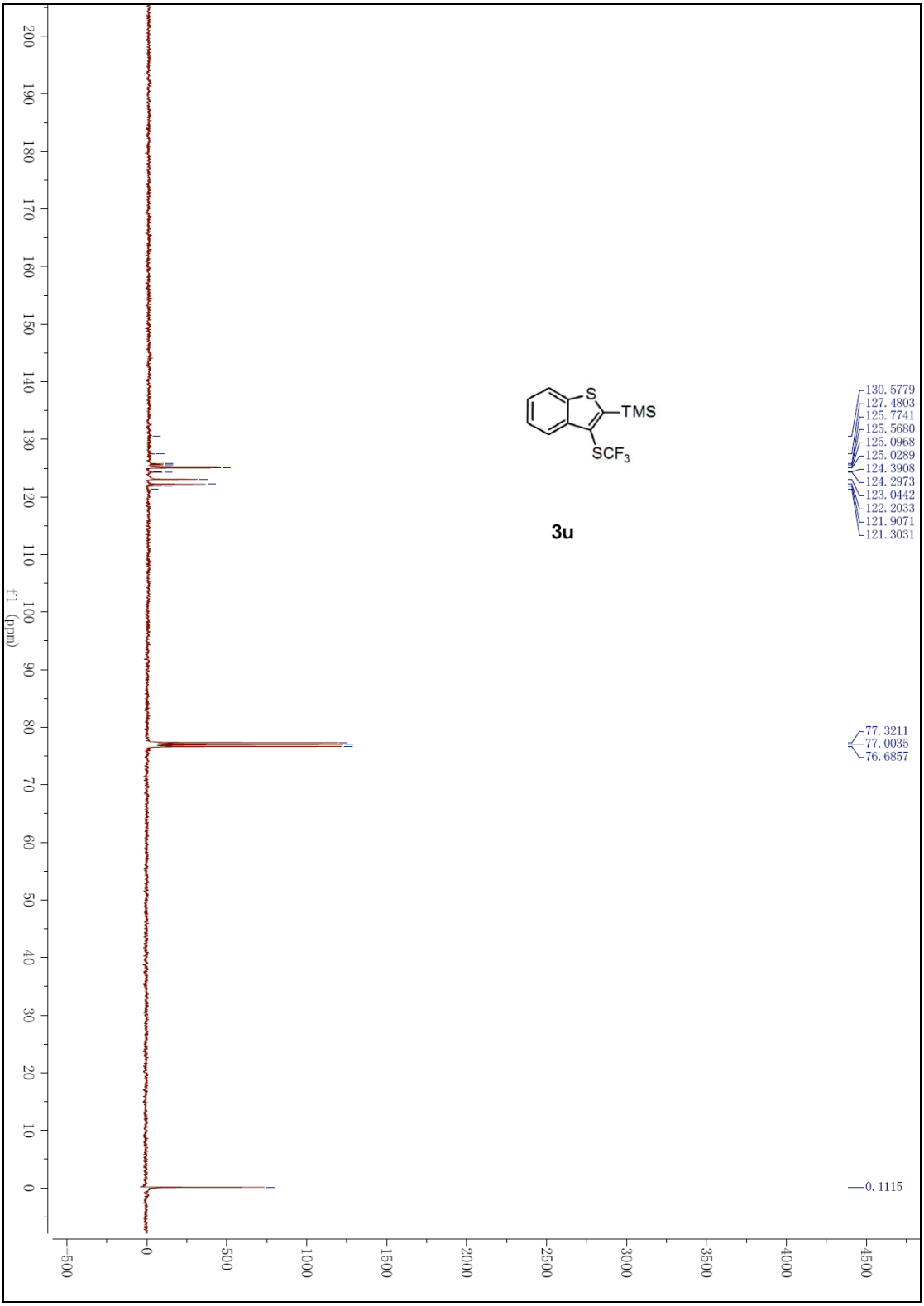
8.0512
7.8946
7.8748
7.5083
7.5062
7.4885
7.4707
7.4684
7.4376
7.4349
7.4175
7.4150
7.2602
1.00
1.04
1.05
1.03
9.09
0.4962
S
TMS
SCF3
3u
f1 (ppm)


S
TMS
SCF3
3u
130.5779
127.4803
125.7741
125.5680
125.0968
125.0289
124.3908
124.2973
123.0442
122.2033
121.9071
121.3031
77.3211
77.0035
76.6857
0.1115
f1 (ppm)