Generation of 4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxides via a reaction of trifluoromethanesulfanylamide with 2-(2-alkynyl)benzenesulfonamide

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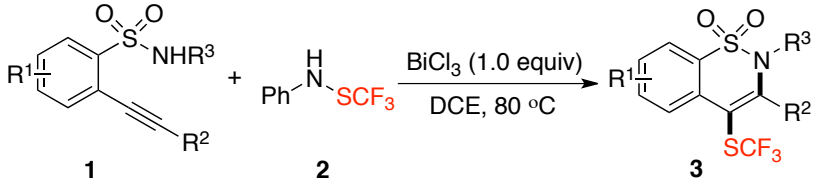
Supporting Information

1. General experimental methods (S2).
2. General experimental procedure and characterization data (S3-S12).
3. ^{19}F, ^{1}H and ^{13}C NMR spectra of compounds **3** and **4** (S13-S93).

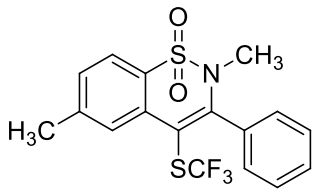
General experimental methods:

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.

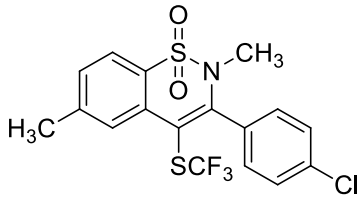
Synthesis of 4-((trifluoromethyl)thio)-2H-benzo[e][1,2]thiazine 1,1-dioxides via a reaction of trifluoromethanesulfanylamide with 2-(2-alkynyl)benzenesulfonamide



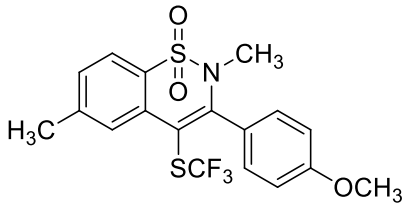
2-(2-Alkynyl)benzenesulfonamide **1** (0.2 mmol) was added to a solution of $BiCl_3$ (0.2 mmol) in DCE (2.0 mL) under N_2 atmosphere. Then trifluoromethanesulfanylamide **2** (0.6 mmol) was added. The mixture was stirred at 80 °C. After completion of reaction as indicated by TLC (~16 h), the mixture was purified by flash column chromatograph (EtOAc/*n*-hexane, 1:20) to give the desired product **3**. Excess trifluoromethanesulfanylamide **2** could be recycled.



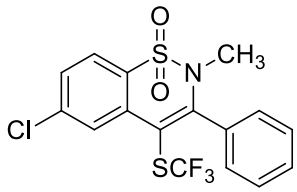
2,6-Dimethyl-3-phenyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3a**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.52-7.50 (m, 3H), 7.41-7.39 (m, 3H), 3.02 (s, 3H), 2.53 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 143.1, 134.3, 133.8, 130.3, 129.7, 129.5, 129.1, 128.8 (q, *J* = 312.8 Hz), 128.7, 127.5, 121.6, 104.6, 34.8, 21.9; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.17; HRMS (ESI) calcd for $C_{17}H_{15}F_3NO_2S_2^+$: 386.0491 [M + H^+], found: 386.0479.



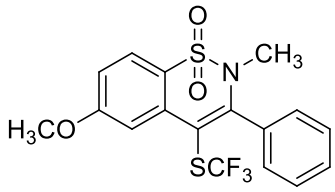
3-(4-Chlorophenyl)-2,6-dimethyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3b**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 3.02 (s, 4H), 2.53 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 143.2, 136.6, 134.0, 132.2, 131.1, 129.7, 129.2, 129.0, 128.6 (q, *J* = 310.3 Hz), 127.6, 121.7, 105.4, 34.9, 21.9; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.06; HRMS (ESI) calcd for $C_{17}H_{13}ClF_3NO_2S_2Na^+$: 441.9921 [M + Na^+], found: 441.9906.



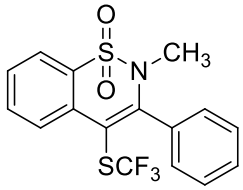
3-(4-Methoxyphenyl)-2,6-dimethyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazin e 1,1-dioxide (**3c**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.39-7.37 (m, 1H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 3.89 (s, 3H), 3.02 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 153.5, 142.9, 134.5, 131.5, 129.3, 129.1, 128.8 (q, *J* = 310.3 Hz), 127.6, 126.0, 121.6, 114.0, 104.4, 55.4, 35.1, 21.9; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.25; HRMS (ESI) calcd for $C_{18}H_{16}F_3NO_3S_2Na^+$: 438.0416 [M + Na^+], found: 438.0413.



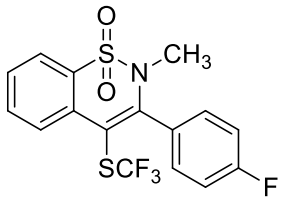
6-Chloro-2-methyl-3-phenyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3d**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 1.6 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.56-7.52 (m, 4H), 7.40-7.38 (m, 2H), 3.05 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.8, 138.9, 136.1, 133.4, 130.6, 129.6, 128.8, 128.7, 128.6 (q, *J* = 310.9 Hz), 127.8, 127.1, 123.2, 111.0, 103.7, 35.0; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.22; HRMS (ESI) calcd for $C_{16}H_{11}ClF_3NO_2S_2Na^+$: 427.9764 [M + Na^+], found: 427.9746.



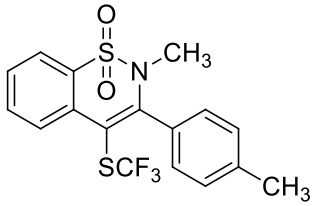
6-Methoxy-2-methyl-3-phenyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3e**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (d, *J* = 8.8 Hz, 1H), 7.66 (d, *J* = 1.6 Hz, 1H), 7.53-7.50 (m, 3H), 7.40-7.38 (m, 2H), 7.11-7.08 (m, 1H), 3.94 (s, 3H), 3.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6, 154.1, 136.4, 133.9, 130.3, 129.5, 128.8 (q, *J* = 300.7 Hz), 128.7, 123.7, 115.4, 111.1, 104.1, 55.8, 34.6; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.12; HRMS (ESI) calcd for $C_{17}H_{15}F_3NO_3S_2^+$: 402.0440 [M + H^+], found: 402.0425.



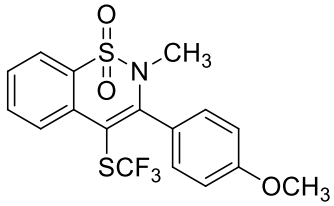
2-Methyl-3-phenyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3f**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 1H), 7.75-7.72 (m, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.53-7.50 (m, 3H), 7.42-7.40 (m, 2H), 3.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 134.3, 133.7, 1132.2, 131.5, 130.3, 129.7, 129.2 (q, *J* = 303.8 Hz), 128.7, 128.5, 127.4, 124.7, 121.6, 104.9, 34.9; 19F NMR (378 MHz, $CDCl_3$) δ -43.10; HRMS (ESI) calcd for $C_{16}H_{13}F_3NO_2S_2^+$: 372.0334 [M + H^+], found: 372.0329.



3-(4-Fluorophenyl)-2-methyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3g**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.76-7.72 (m, 1H), 7.62-7.59 (m, 1H), 7.44-7.40 (m, 2H), 7.21 (t, *J* = 8.4 Hz, 2H), 3.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7 (d, *J* = 250 Hz), 159.9, 152.4, 134.1, 132.3, 131.8 (d, *J* = 8.5 Hz), 131.6, 129.7, 128.7, 128.6 (q, *J* = 310.1 Hz), 127.5, 121.6, 115.9 (d, *J* = 22 Hz), 105.5, 35.0; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.07, -109.41; HRMS (ESI) calcd for $C_{16}H_{12}F_4NO_2S_2^+$: 390.0240 [M + H^+], found: 390.0242.

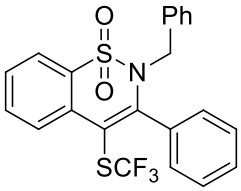


2-Methyl-3-(*p*-tolyl)-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3h**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.0 Hz, 1H), 7.95-7.93 (m, 2H), 7.74-7.70 (m, 1H), 7.60-7.58 (m, 1H), 7.33- (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H) 7.33-7.29 (m, 4H), 3.04 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 140.7, 134.4, 132.2, 131.5, 130.8, 129.4, 128.8 (q, *J* = 310.5 Hz), 128.4, 127.4, 121.5, 104.6, 35.0, 21.5; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.14; HRMS (ESI) calcd for $C_{17}H_{15}F_3NO_2S_2^+$: 386.0491 [M + H^+], found: 386.0482.

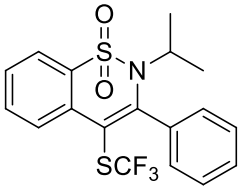


3-(4-Methoxyphenyl)-2-methyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3i**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 ((d, *J* = 8.4 Hz, 1H), 7.94-7.92 (m, 1H), 7.74-7.70 (m, 1H), 7.60-7.55 (m, 1H), 7.37-7.33 (m, 2H), 7.04-7.00 (m, 2H), 3.89 (s, 3H), 3.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2, 153.4, 134.5, 132.2,

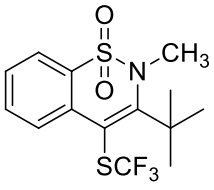
131.8, 131.5, 128.8 (q, J = 310.6 Hz), 128.4, 127.5, 125.8, 121.6, 114.0, 104.6, 55.4, 35.2. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42. HRMS (ESI) calcd for $C_{17}H_{14}F_3NO_2S_2Na^+$: 424.0259 [M + Na^+], found: 424.0243.



2-Benzyl-3-phenyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3j**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 8.0 Hz, 1H), 7.97 (d, J = 7.6 Hz, 1H), 7.71 (t, J = 8.0 Hz, 1H), 7.60 (t, J = 7.6 Hz, 1H), 7.49 (t, J = 7.2 Hz, 1H), 7.42 (t, J = 7.2 Hz, 2H), 7.25 (t, J = 7.2 Hz, 2H), 7.09 (t, J = 7.2 Hz, 1H), 7.02 (t, J = 7.2 Hz, 2H), 6.59 (d, J = 7.2 Hz, 2H), 4.73 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 135.5, 134.1, 133.2, 132.9, 132.2, 130.3, 128.8, 128.7 (q, J = 310.6 Hz), 128.3, 127.7, 127.3, 121.5, 108.0, 51.6, 29.7; 19F NMR (378 MHz, $CDCl_3$) δ -42.77; HRMS (ESI) calcd for $C_{22}H_{17}F_3NO_2S_2^+$: 448.0647 [M + H^+], found: 448.0623.

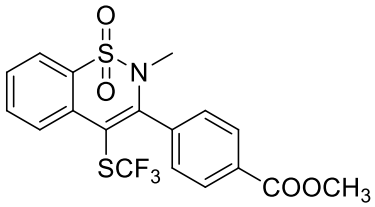


2-Isopropyl-3-phenyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3k**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 8.0 Hz, 1H), 7.93-7.91 (m, 1H), 7.74-7.70 (m, 1H), 7.61-7.57 (m, 1H), 7.55-7.48 (m, 5H), 3.91-3.84 (m, 1H), 1.13 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 134.8, 133.0, 131.9, 130.6, 130.4, 129.9, 129.1 (q, J = 304.2 Hz), 128.9, 128.2, 127.8, 121.5, 126.1, 109.4, 56.6, 25.8, 25.7; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.40; HRMS (ESI) calcd for $C_{18}H_{16}F_3NO_2S_2Na^+$: 422.0467 [M + Na^+], found: 422.0453.

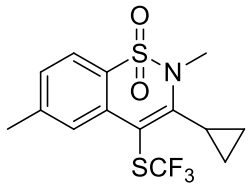


3-(*tert*-Butyl)-2-methyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3l**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.0 Hz, 1H), 7.85 (d, J =

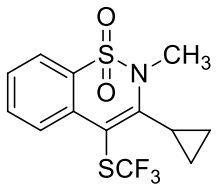
7.6 Hz, 1H), 7.70-7.66 (m, 1H), 7.52-7.48 (m, 1H), 3.03 (s, 3H), 1.50 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 135.5, 132.8, 130.6, 128.7, 128.6 (q, J = 309.3 Hz), 127.2, 123.8, 103.3, 40.2, 29.9, 29.7; ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.90; HRMS (ESI) calcd for $C_{14}H_{16}F_3NO_2S_2Na^+$: 374.0467 [M + Na^+], found: 374.0453.



Methyl-4-(2-methyl-1,1-dioxido-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazin-3-yl)benzoate (**3m**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (t, J = 8.4 Hz, 3H), 7.96-7.94 (m, 1H), 7.77-7.73 (m, 1H), 7.64-7.60 (m, 1H), 7.51 (d, J = 8.4 Hz, 2H), 3.97 (s, 3H), 3.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 152.2, 137.8, 133.9, 132.4, 131.8, 129.9, 129.0 (q, J = 310.2 Hz), 128.9, 127.4, 121.7, 105.7, 52.5, 34.9. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.97; HRMS (ESI) calcd for $C_{18}H_{14}F_3NO_2S_2$: 429.0316 [M^+], found: 429.0313.

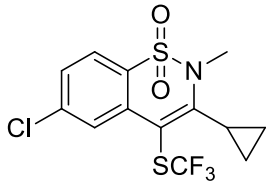


3-Cyclopropyl-2,6-dimethyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3n**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.35-7.33 (m, 1H), 3.07 (s, 3H), 2.50 (s, 3H), 2.26-2.22 (m, 1H), 1.22-1.18 (m, 2H), 1.10-1.06 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 143.2, 133.6, 129.4, 129.3 (q, J = 310.0 Hz), 129.2, 127.4, 122.9, 111.0, 35.7, 21.9, 15.0, 9.2. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.32; HRMS (ESI) calcd for $C_{14}H_{14}F_3NO_2S_2$: 349.0418 [M^+], found: 349.0417.

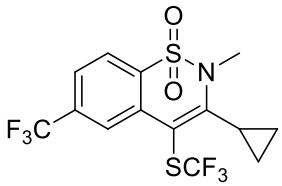


3-Cyclopropyl-2-methyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3o**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.0 Hz, 1H), 7.89-7.85

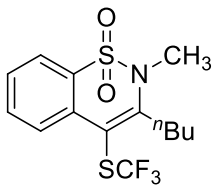
(m, 1H), 7.70-7.66 (m, 1H), 7.56-7.52 (m, 1H), 3.10 (s, 3H), 2.27-2.20 (m, 1H), 1.24-1.19 (m, 2H), 1.11-1.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 133.6, 132.4, 131.7, 129.2 (q, J = 310.2 Hz), 128.6, 127.2, 122.8, 111.0, 35.7, 29.7, 15.0, 9.3; ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.30; HRMS (ESI) calcd for $C_{13}H_{13}F_3NO_2S_2^+$: 336.0334 [M + H^+], found: 336.0319.



6-Chloro-3-cyclopropyl-2-methyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3p**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 1.6 Hz, 1H), 7.78 (d, J = 8.4 Hz, 1H), 7.51- 7.49 (m, 1H), 3.12 (s, 3H), 2.50-2.19 (m, 1H), 1.27-1.22 (m, 2H), 1.11-1.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 139.0, 135.5, 129.9, 129.1 (q, J = 310.3 Hz), 128.7, 127.0, 124.4, 109.8, 35.7, 15.3, 9.6. ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.32; HRMS (ESI) calcd for $C_{13}H_{11}F_3NO_2S_2$: 368.9872 [M^+], found: 368.9873.

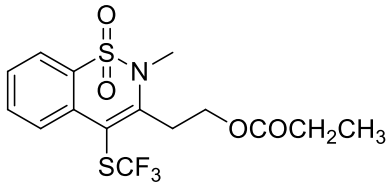


3-cyclopropyl-2-methyl-6-(trifluoromethyl)-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3q**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 3.17 (s, 3H), 2.26-2.19 (m, 1H), 1.30-1.26 (m, 2H), 1.13-1.08 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 134.6, 134.4 (q, J = 35.5 Hz), 129.0 (q, J = 310.7 Hz), 125.2, 125.1, 124.4, 124.3, 123.2 (q, J = 271.3 Hz), 35.7, 15.2, 9.8. ^{19}F NMR (378 MHz, $CDCl_3$) δ -41.37, -63.51; HRMS (ESI) calcd for $C_{14}H_{11}F_6NO_2S_2$: 403.0135 [M^+], found: 403.0139.

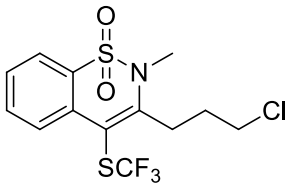


3-Butyl-2-methyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3r**):

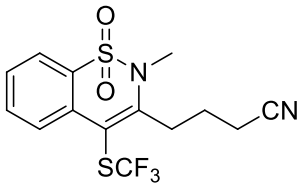
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 6.8 Hz, 1H), 7.69-7.65 (m, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 3.39 (s, 3H), 3.04-3.00 (m, 2H), 1.71-1.64 (m, 2H), 1.55-1.47 (m, 2H), 1.00 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 133.9, 132.1, 131.2, 129.0 (q, *J* = 310.7 Hz), 127.9, 127.0, 121.4, 104.0, 40.2, 29.9, 29.7; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.68; HRMS (ESI) calcd for $C_{14}H_{17}F_3NO_2S_2^+$: 352.0674 [M + H^+], found: 352.0647.



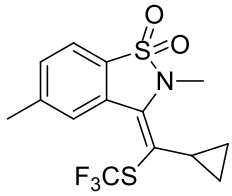
2-(2-Methyl-1,1-dioxido-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazin-3-yl)ethyl propionate (**3s**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.74-7.70 (m, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 4.48-4.37 (m, 2H), 3.33-3.24 (m, 2H), 3.03 (s, 3H), 2.33 (q, *J* = 7.6 Hz, 2H), 1.13 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 163.3, 133.3, 129.9, 128.8 (q, *J* = 310.6 Hz), 127.1, 1 124.5, 121.5, 109.4, 60.1, 33.1, 30.0, 27.3, 8.9. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.53; HRMS (ESI) calcd for $C_{15}H_{16}F_3NO_4S_2$: 395.0473 [M^+], found: 395.0475.



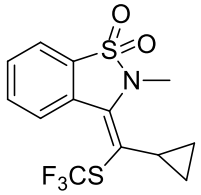
3-(3-Chloropropyl)-2-methyl-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazine 1,1-dioxide (**3t**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.0 Hz, 1H), 7.89-7.87 (m, 1H), 7.74-7.70 (m, 1H), 7.56-7.52 (m, 1H), 3.66-3.62 (m, 2H), 3.20-3.13 (m, 1H), 3.08-3.05 (m, 1H), 3.04 (s, 3H), 2.25-2.18 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 133.4, 129.0, 128.9 (q, *J* = 310.4 Hz), 127.1, 124.5, 122.0, 105.6, 43.7, 31.0, 30.1, 29.1. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.55; HRMS (ESI) calcd for $C_{13}H_{13}F_3NO_2S_2Cl$: 371.0028 [M^+], found: 371.0025.



4-(2-Methyl-1,1-dioxido-4-((trifluoromethyl)thio)-2*H*-benzo[*e*][1,2]thiazin-3-yl)butanenitrile (**3u**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.90-7.88 (m, 1H), 7.75-7.71 (m, 1H), 7.57-7.52 (m, 1H), 3.25-3.18 (m, 1H), 3.05 (s, 3H), 3.02-2.95 (m, 1H), 2.56-2.46 (m, 2H), 2.16-2.09 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 133.5, 133.3, 129.2, 128.8 (q, *J* = 309.6 Hz), 127.3, 124.7, 104.5, 32.1, 30.1, 22.4, 16.5. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.44; HRMS (ESI) calcd for $C_{14}H_{13}F_3NO_2S_2$: 362.0371 [M^+], found: 362.0368.

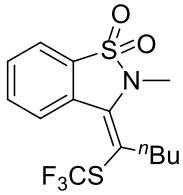


(*E*)-3-(Cyclopropyl((trifluoromethyl)thio)methylene)-2,5-dimethyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (**4a**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.26-7.24 (m, 1H), 2.96 (s, 3H), 2.79-2.74 (m, 1H), 2.48 (s, 3H), 1.29-1.24 (m, 1H), 1.19-1.13 (m, 1H), 1.06-1.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 144.3, 134.4, 129.3 (q, *J* = 310.0 Hz), 128.8, 127.2, 126.7, 124.4, 100.6, 30.2, 22.0, 14.2, 7.8, 7.7. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.98; HRMS (ESI) calcd for $C_{14}H_{14}F_3NO_2S_2$: 349.0418 [M^+], found: 349.0419.

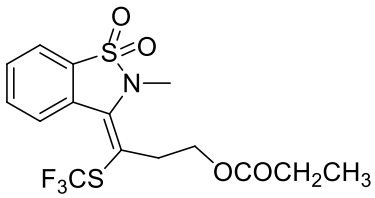


(E)-3-(Cyclopropyl((trifluoromethyl)thio)methylene)-2-methyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (**4b**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.0 Hz, 1H), 7.84-7.82 (m, 1H), 7.71-7.66 (m, 1H), 7.48-7.44 (m, 1H), 3.00 (s, 3H), 2.82-2.75 (m, 1H), 1.30-1.26 (m, 1H), 1.83-1.71 (m, 1H), 1.08-1.03 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 133.8, 134.5, 133.3, 129.0 (q, *J* = 310.0 Hz), 129.9, 128.0, 126.4, 124.4, 100.8, 30.1, 14.2, 8.0, 7.8; ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.96; HRMS (ESI)

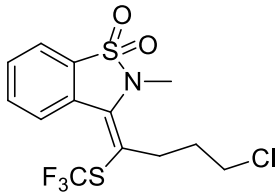
calcd for $C_{13}H_{13}F_3NO_2S_2^+$: 336.0334 [M + H^+], found: 336.0322.



(*E*)-2-Methyl-3-(1-((trifluoromethyl)thio)pentylidene)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (**4c**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.71-7.67 (m, 1H), 7.51 (t, *J* = 6.8 Hz, 1H), 3.03 (s, 3H), 2.92-2.89 (m, 2H), 1.75-1.67 (m, 2H), 1.49-1.38 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 133.8, 133.2, 130.1, 129.0 (q, *J* = 310.0 Hz), 128.6, 126.9, 102.7, 33.4, 30.1, 28.6, 22.3, 13.8. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.67; HRMS (ESI) calcd for $C_{14}H_{16}F_3NO_2S_2Na^+$: 374.0467 [M + Na^+], found: 374.0461.

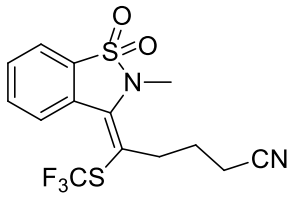


(*E*)-3-(2-Methyl-1,1-dioxidobenzo[*d*]isothiazol-3(2*H*)-ylidene)-3-((trifluoromethyl)thio)propyl propionate (**4d**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.0 Hz, 1H), 7.89-7.87 (m, 1H), 7.72-7.67 (m, 1H), 7.58-7.54 (m, 1H), 4.36 (t, *J* = 8.0 Hz, 2H), 3.47 (s, 3H), 3.39 (t, *J* = 7.2 Hz, 2H), 2.36 (t, *J* = 8.0 Hz, 2H), 1.14 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 150.8, 134.5, 132.2, 129.3 (q, *J* = 304.3 Hz), 128.5, 127.1, 121.1, 110.1, 61.2, 33.1, 31.7, 27.3, 8.9. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.51; HRMS (ESI) calcd for $C_{15}H_{16}F_3NO_4S_2$: 395.0473 [M^+], found: 395.0475.

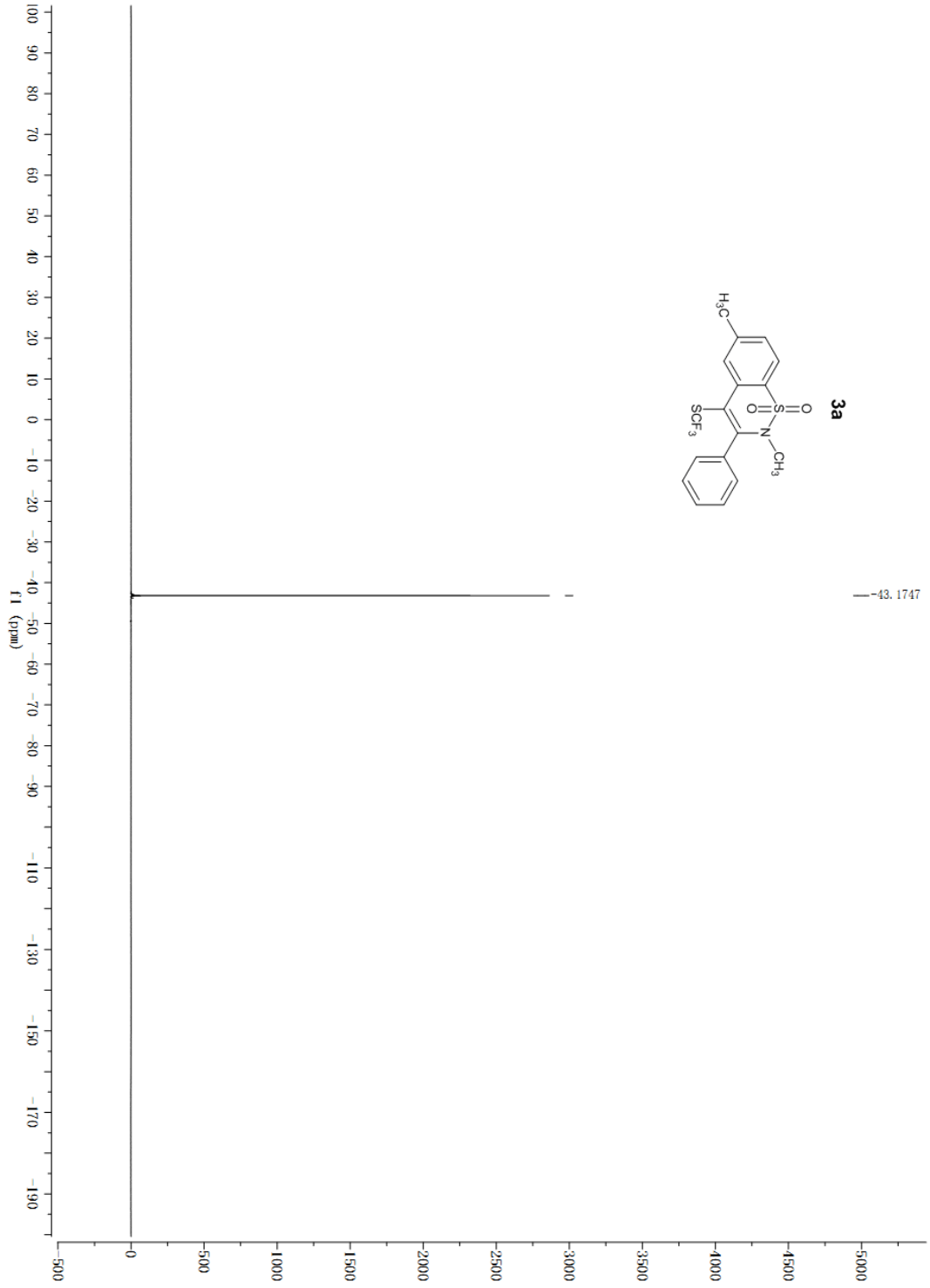


(*E*)-3-(4-Chloro-1-((trifluoromethyl)thio)butylidene)-2-methyl-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide (**4e**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.0 Hz, 1H), 7.88-7.86 (m, 1H), 7.70-7.66 (m, 1H), 7.56-7.52 (m, 1H), 3.70 (t, *J* = 6.0 Hz, 2H), 3.40 (s, 3H), 3.23-3.19 (m, 2H), 2.20-2.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 135.5, 128.9 (q, *J* = 310.0 Hz), 128.4, 127.2, 121.5, 109.9, 106.0, 44.0, 33.0,

30.0, 29.8. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.39; HRMS (ESI) calcd for $C_{14}H_{16}F_3NO_2S_2Na^+$: 371.0028 [$M^+$], found: 371.0030.



(*E*)-5-(2-Methyl-1,1-dioxidobenzo[*d*]isothiazol-3(2*H*)-ylidene)-5-((trifluoromethyl)thio)pentanenitrile (**4f**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.0 Hz, 1H), 7.92-7.90 (m, 1H), 7.76-7.72 (m, 1H), 7.62-7.58 (m, 1H), 3.87 (s, 3H), 3.23 (t, *J* = 7.2 Hz, 2H), 2.58 (t, *J* = 8.0 Hz, 2H), 2.15-2.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 132.4, 131.9 128.9, 128.8 (q, *J* = 310.1 Hz), 127.5, 121.7, 118.9, 105.8, 33.4, 30.9, 23.6, 16.5. ^{19}F NMR (378 MHz, $CDCl_3$) δ -42.07; HRMS (ESI) calcd for $C_{14}H_{13}F_3NO_2S_2$: 362.0371 [M^+], found: 362.0368.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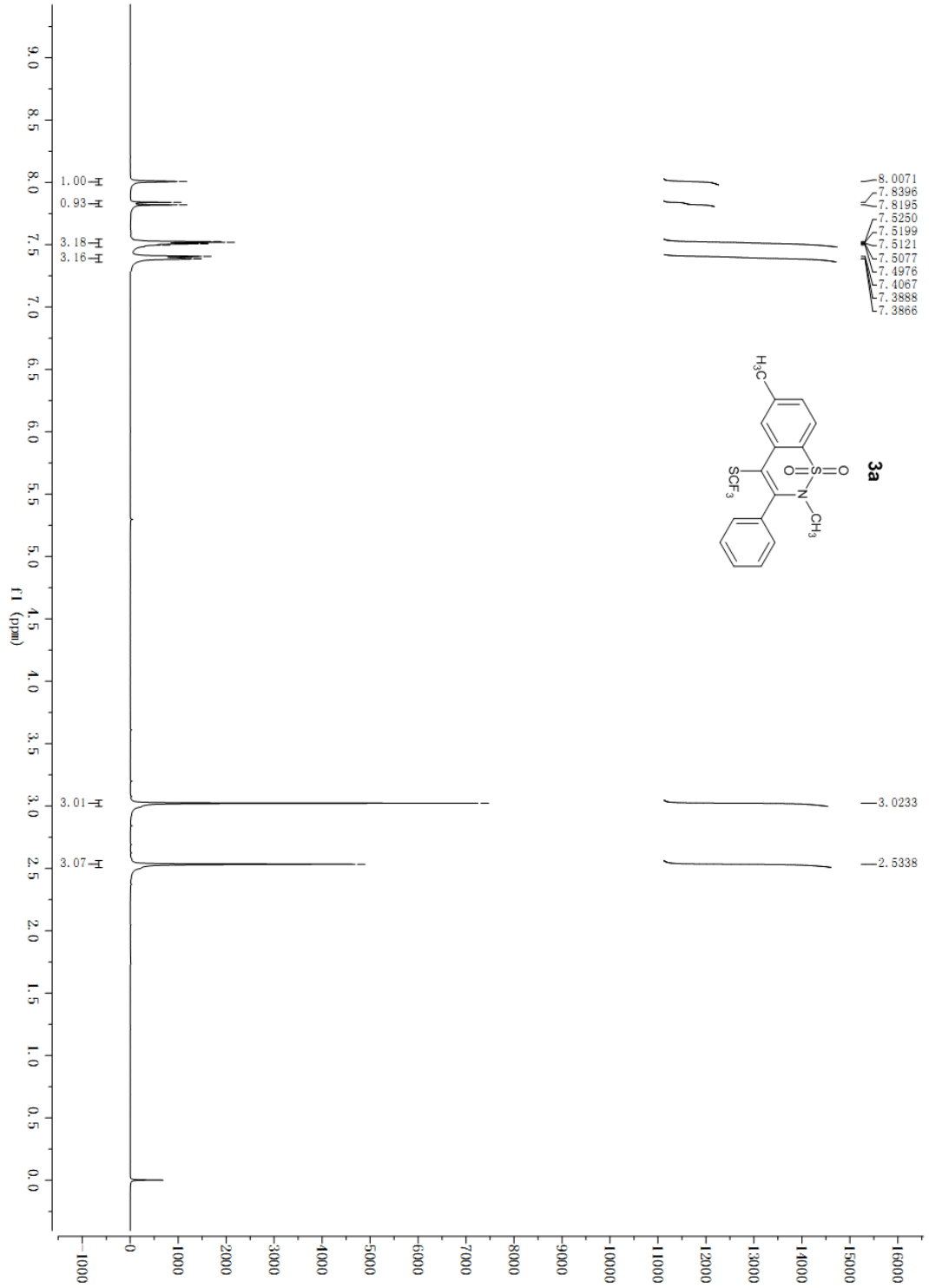
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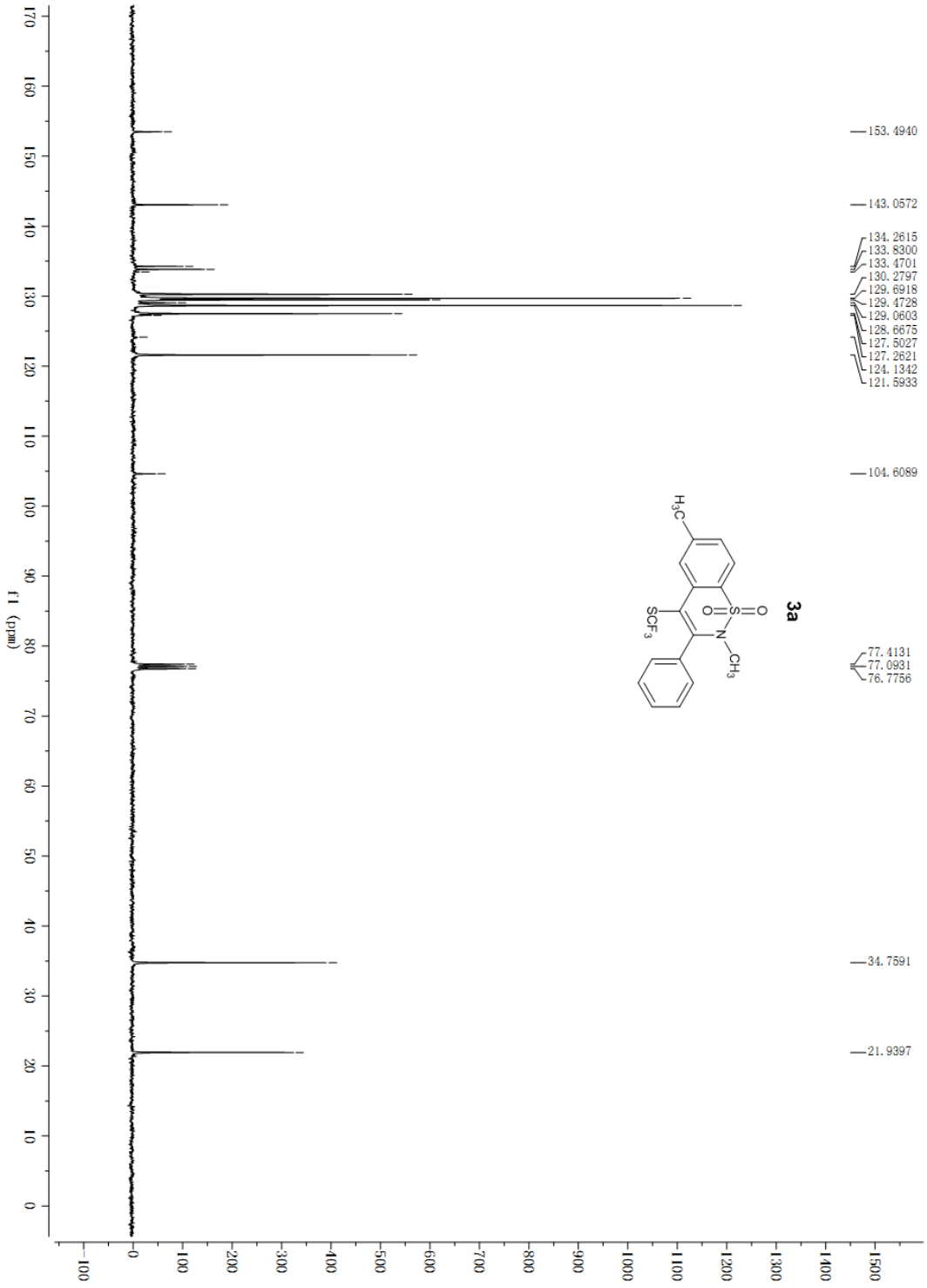
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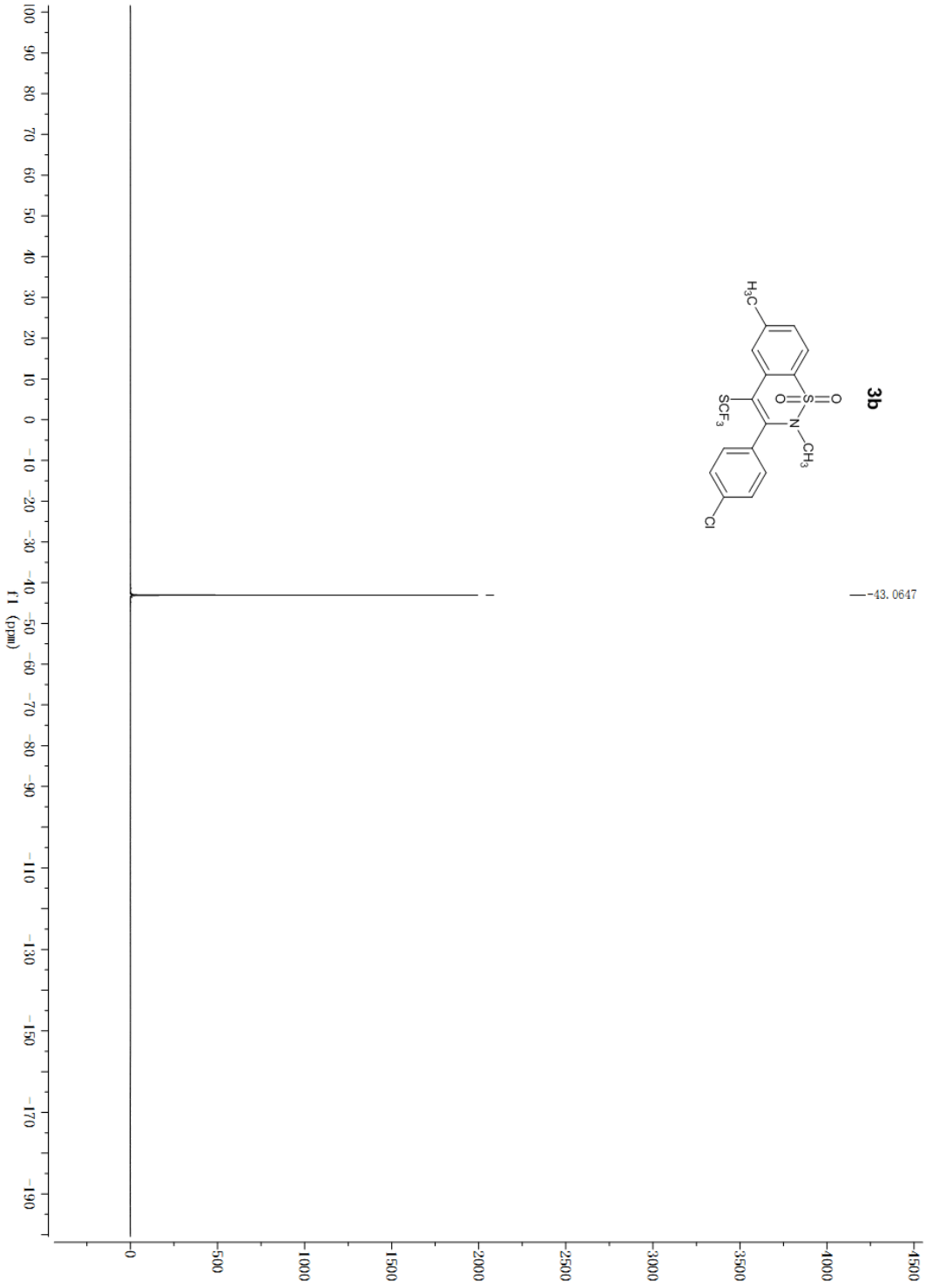
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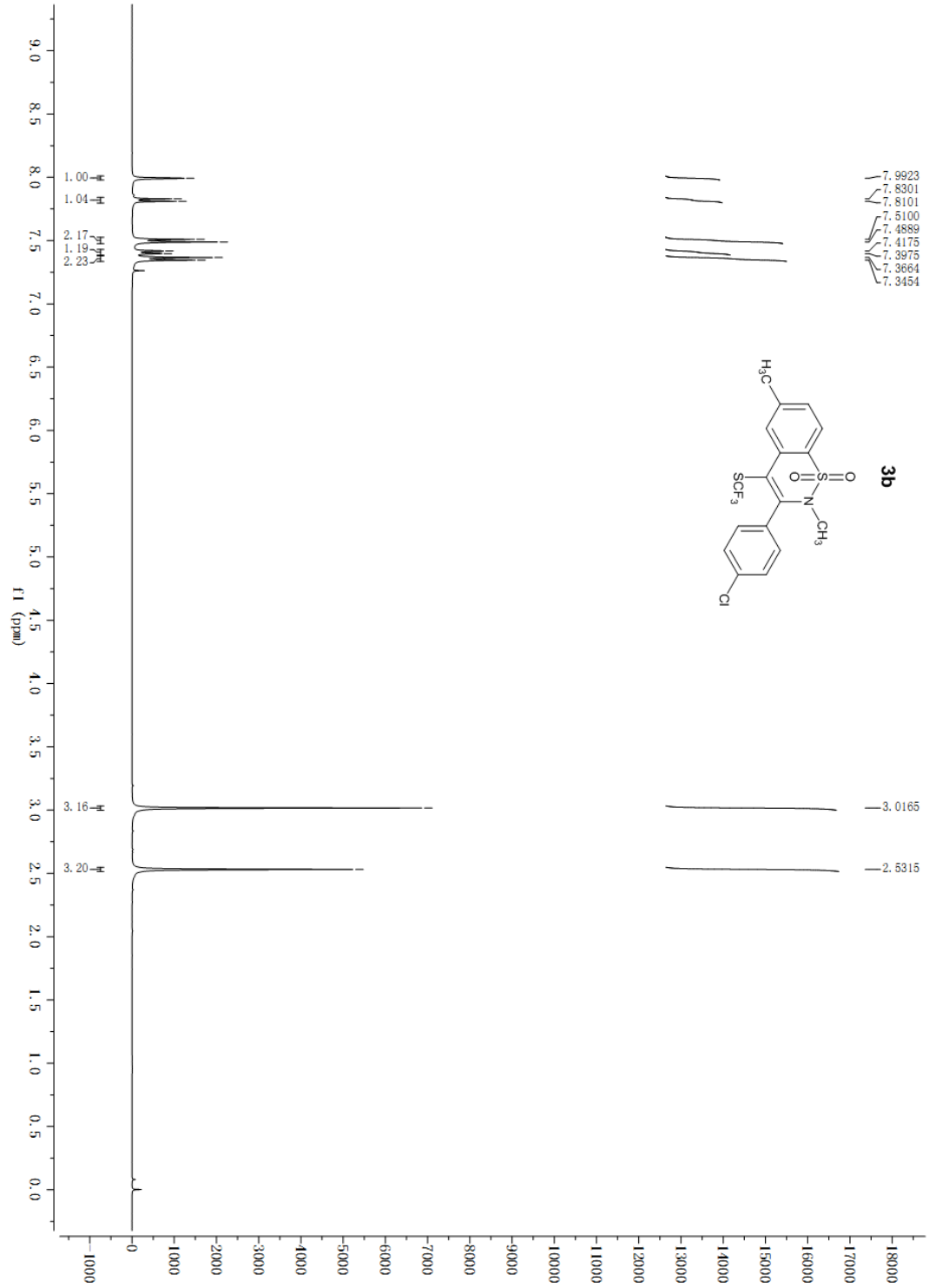
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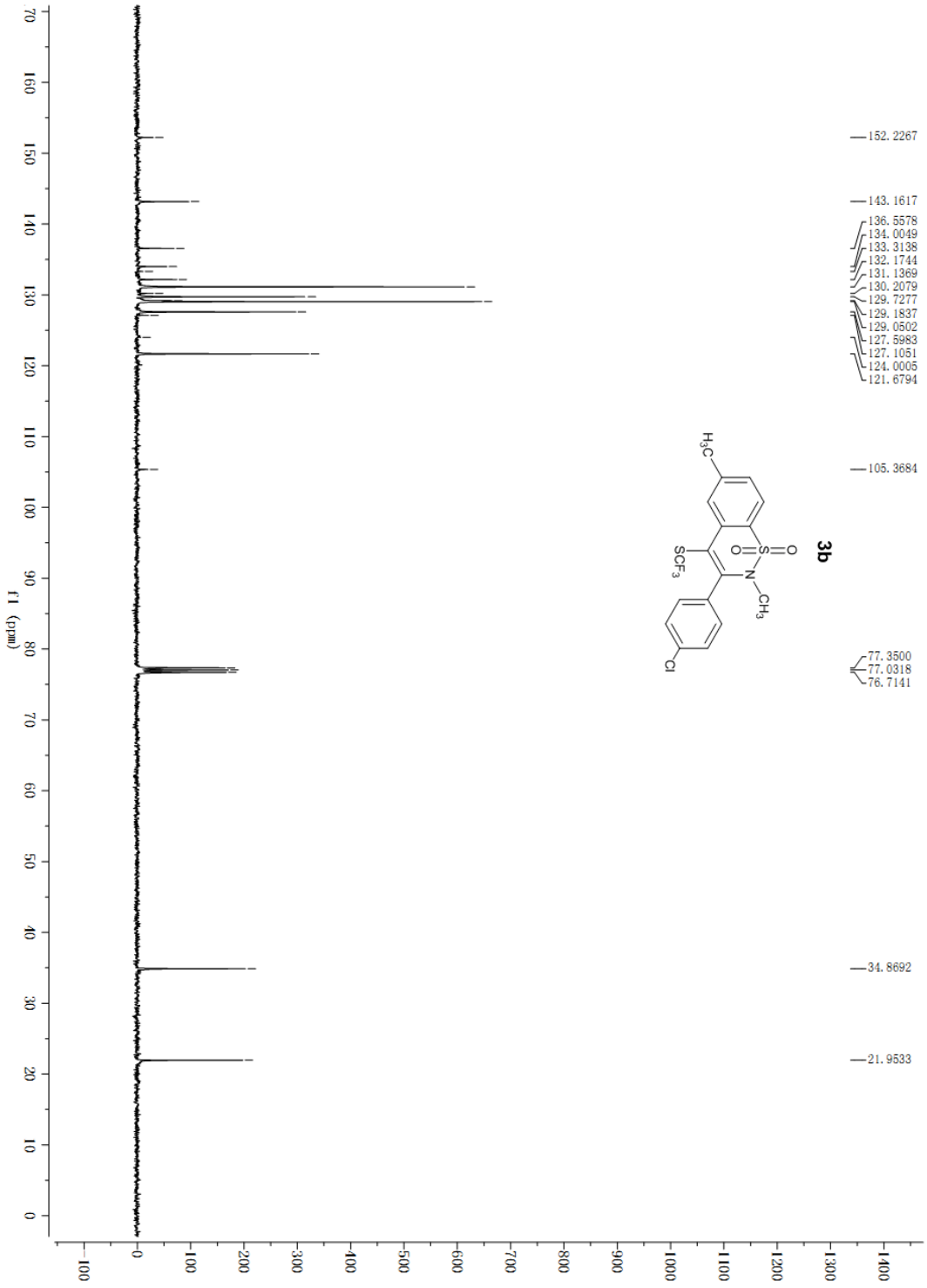
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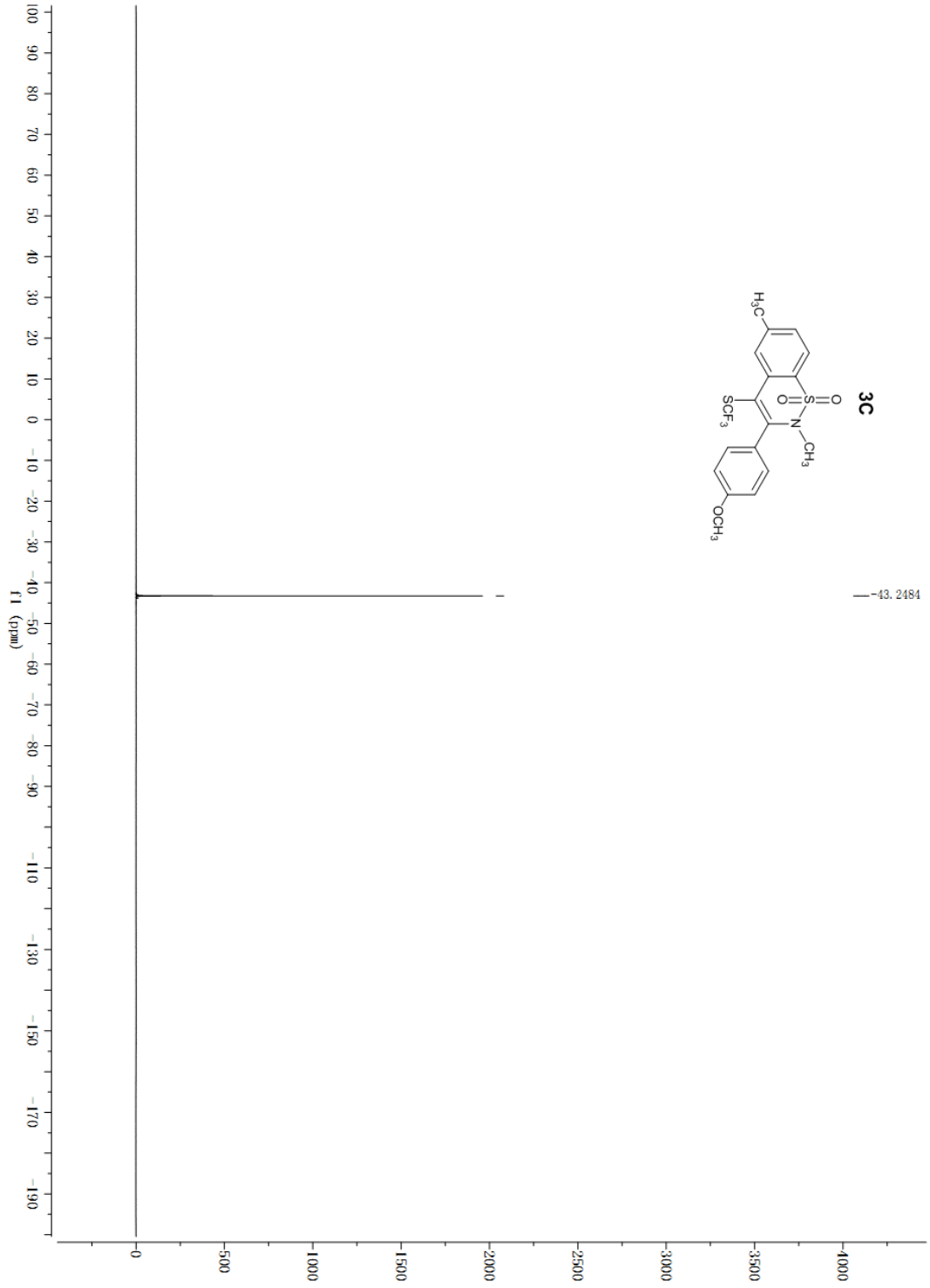
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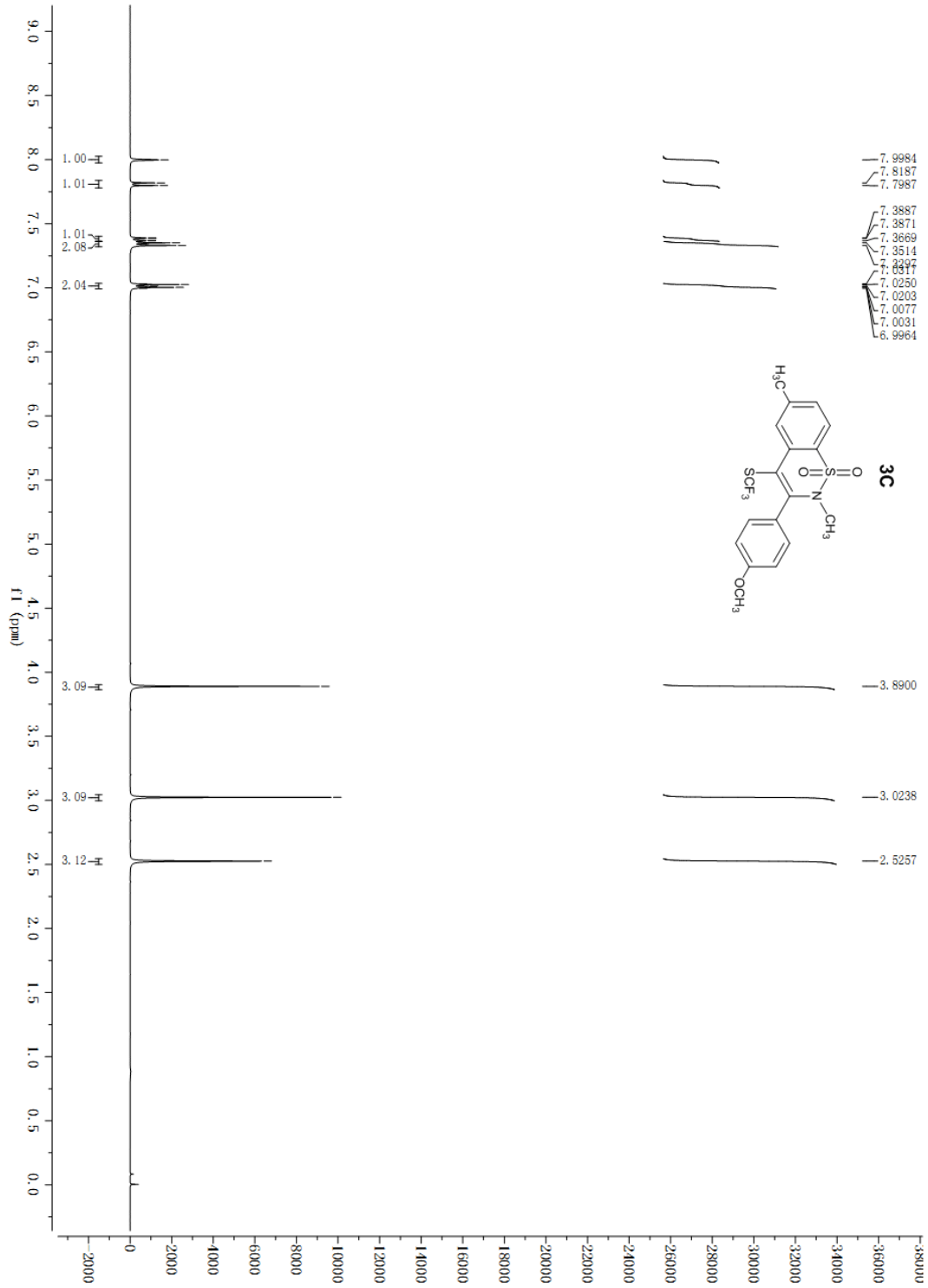
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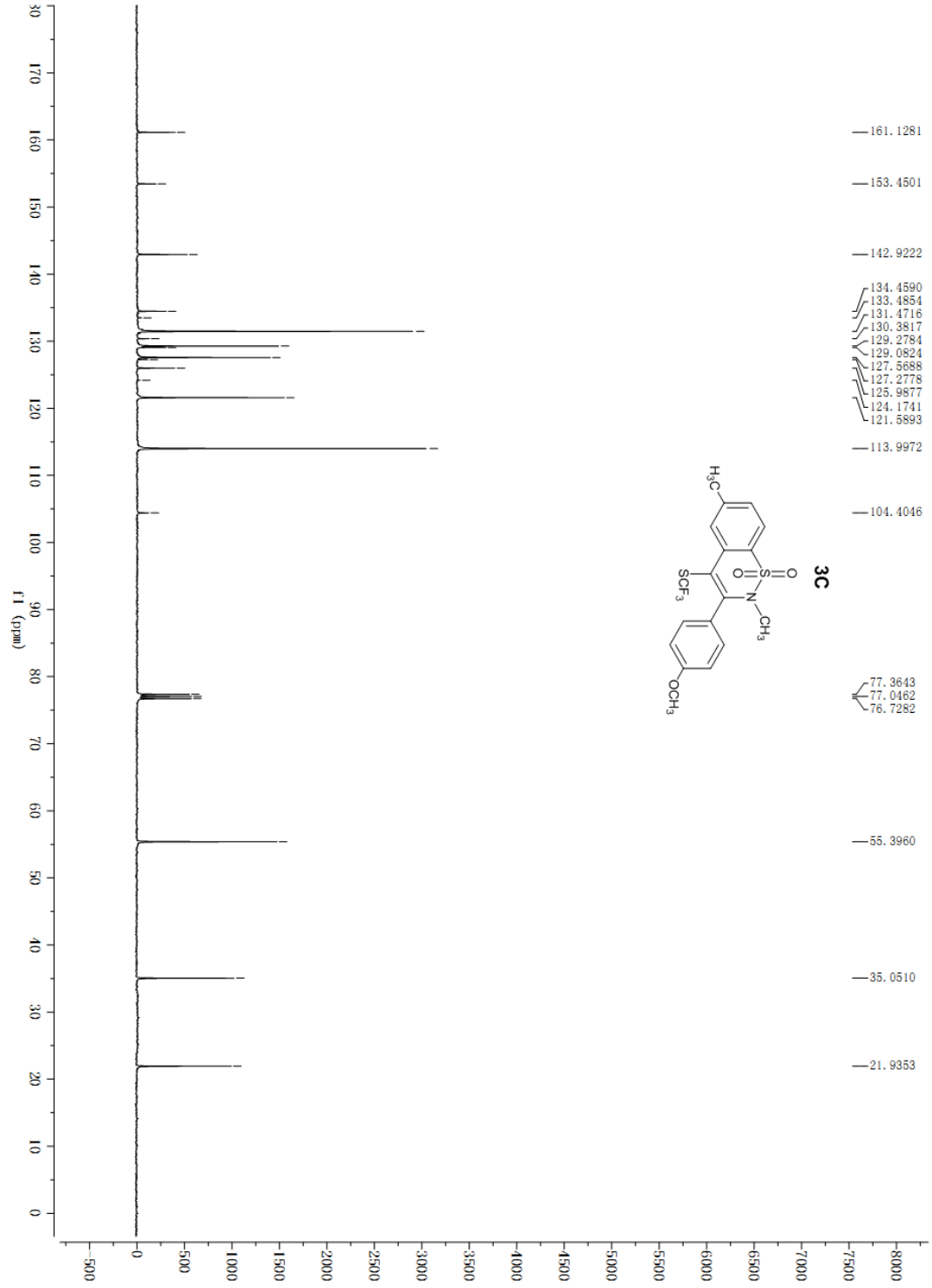
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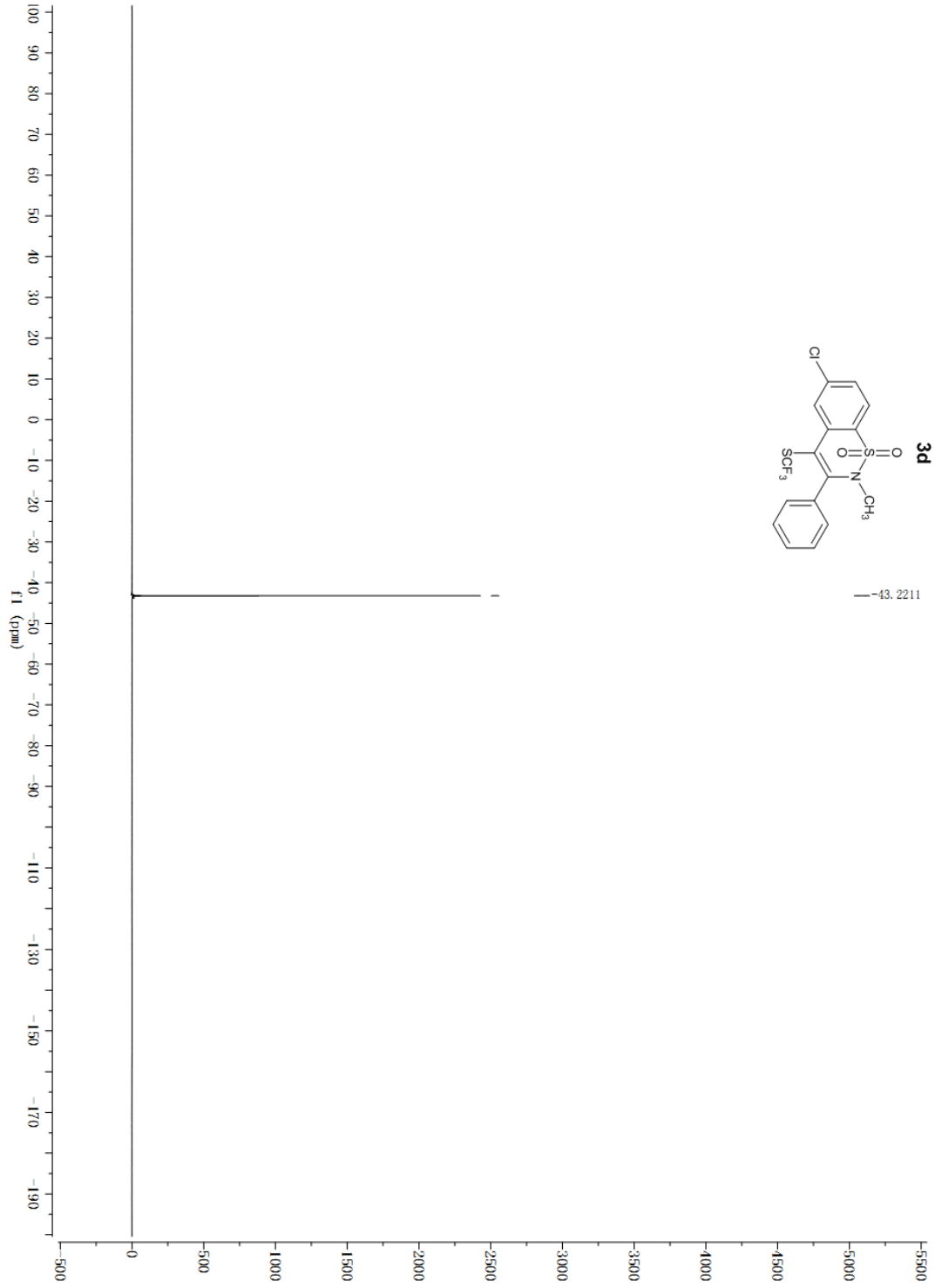
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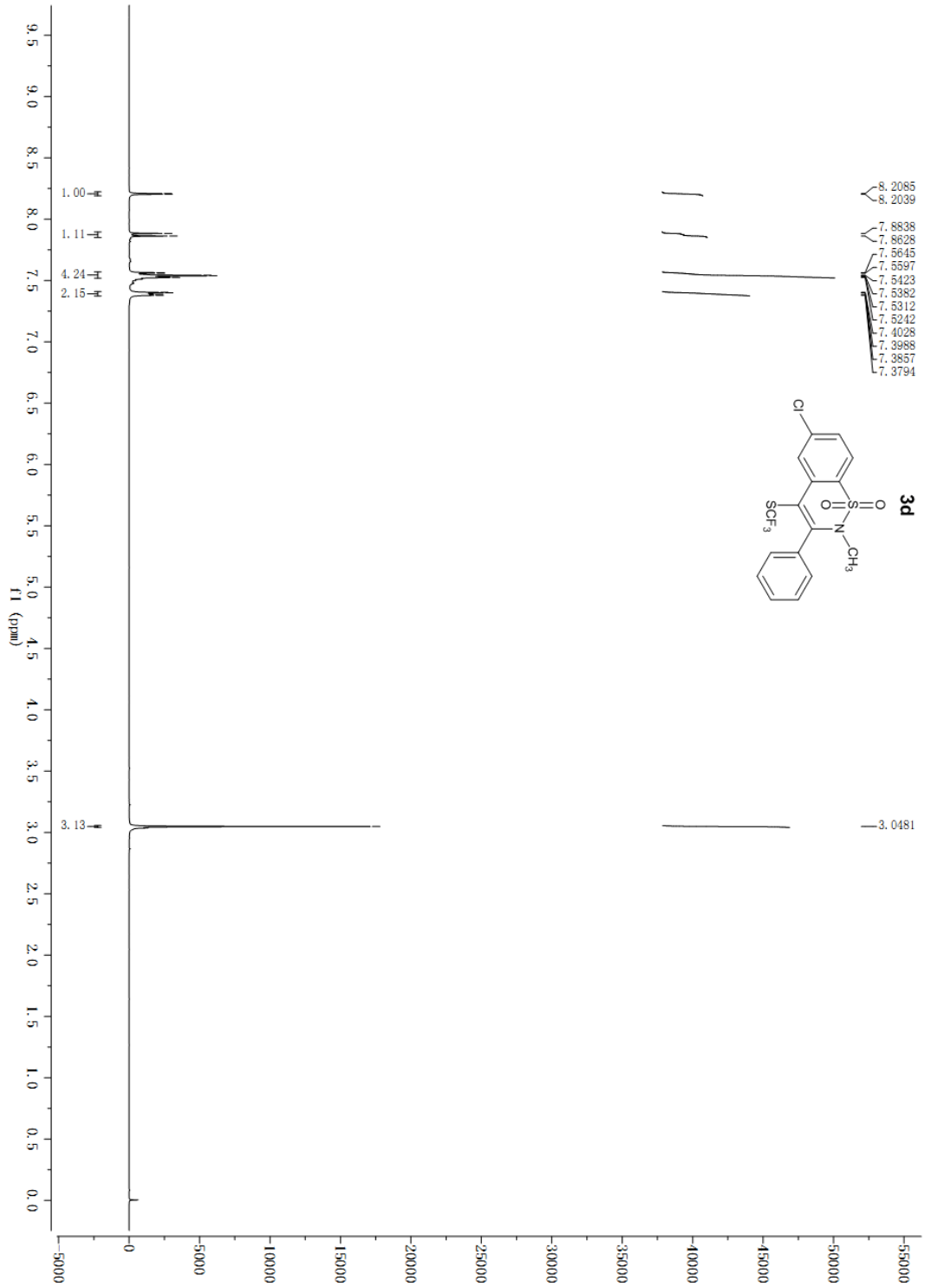
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Cl
SCF3
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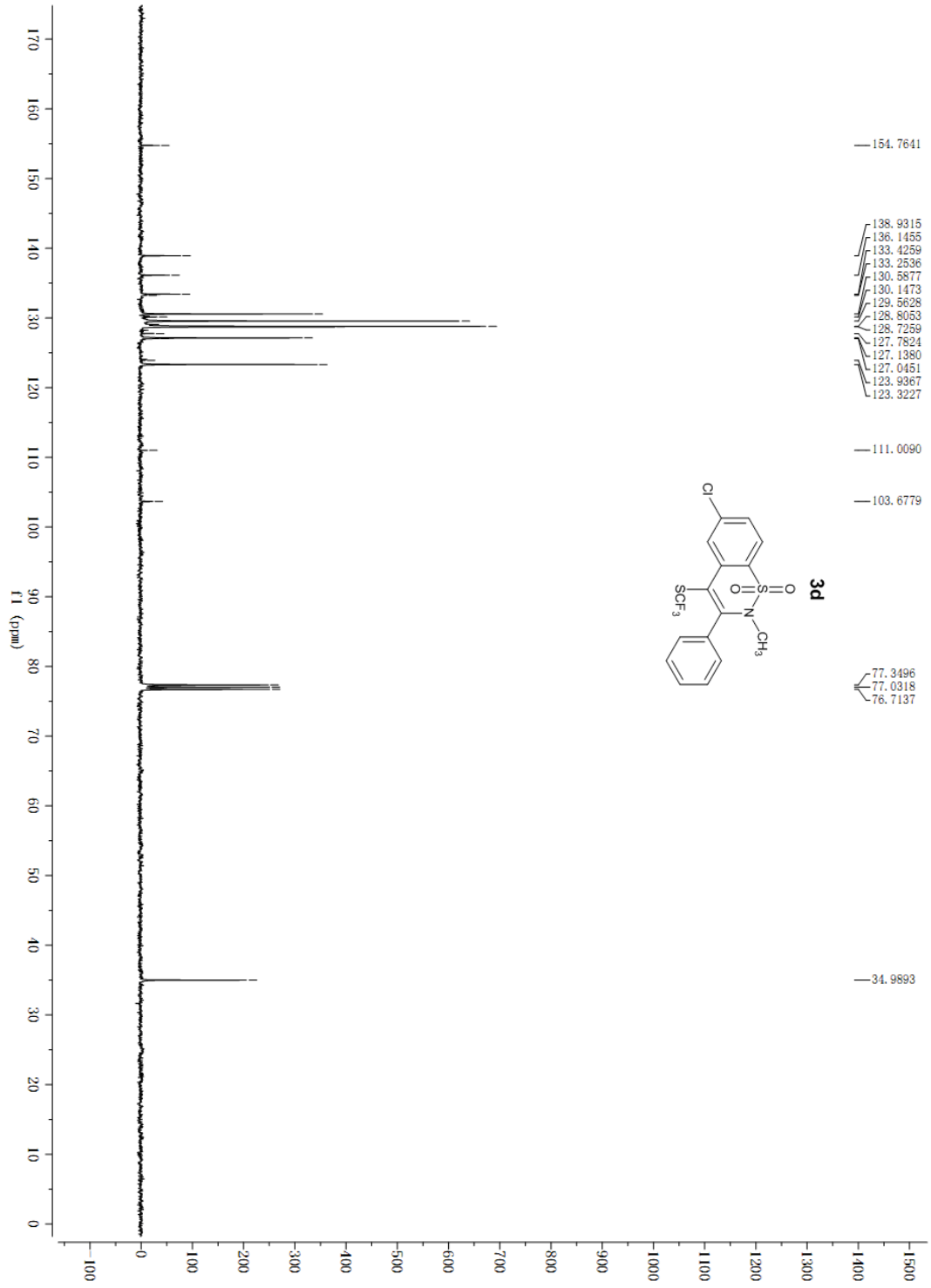
3d
f1 (ppm)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130.1473
129.5628
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128.7259
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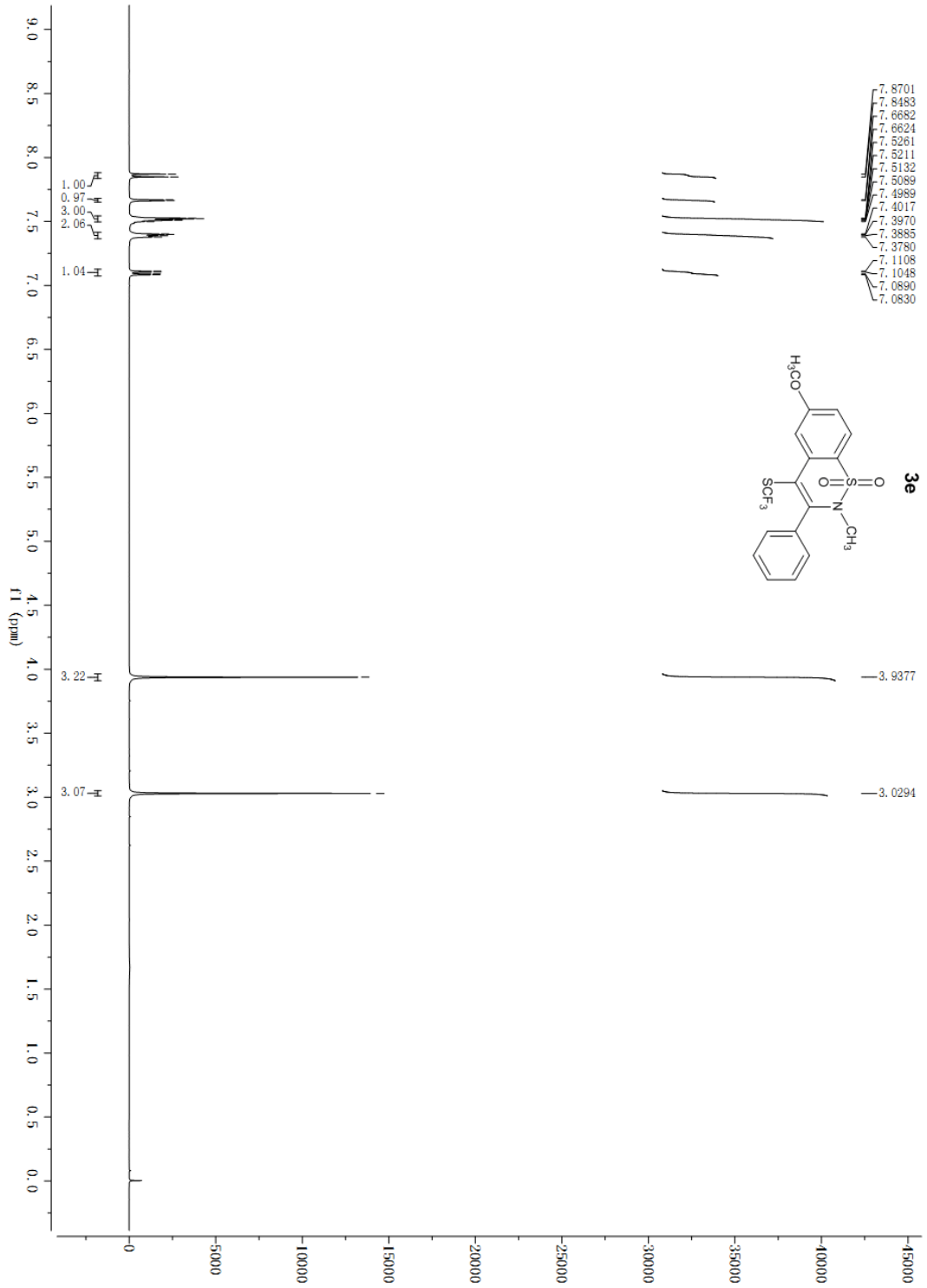
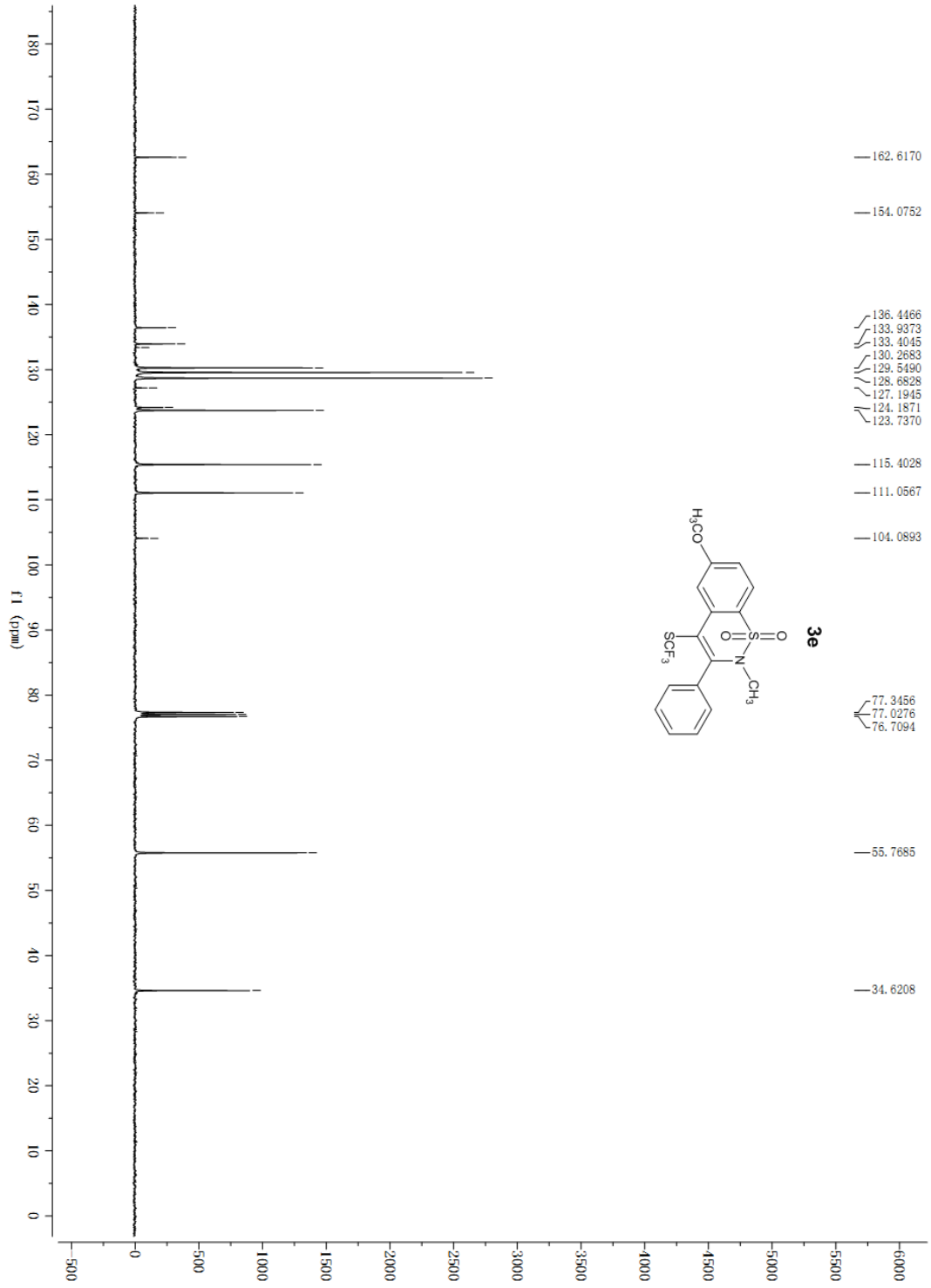
127.1380
127.0451
123.9367
123.3227
111.0090
103.6779
77.3496
77.0318
76.7137
34.9893
3d
Cl
SCF3
CH3
f1 (ppm)


3e
-43.1170
f1 (ppm)


7.8701
7.8483
7.6682
7.6624
7.5261
7.5211
7.5132
7.5089
7.4989
7.4017
7.3970
7.3885
7.3780
7.1108
7.1048
7.0890
7.0830
1.00
0.97
3.00
2.06
1.04
3.22
3.07
3.9377
3.0294
H3CO
SCF3
CH3
3e
f1 (ppm)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136.4466
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133.4045
130.2683
129.5490
128.6828
127.1945
124.1871
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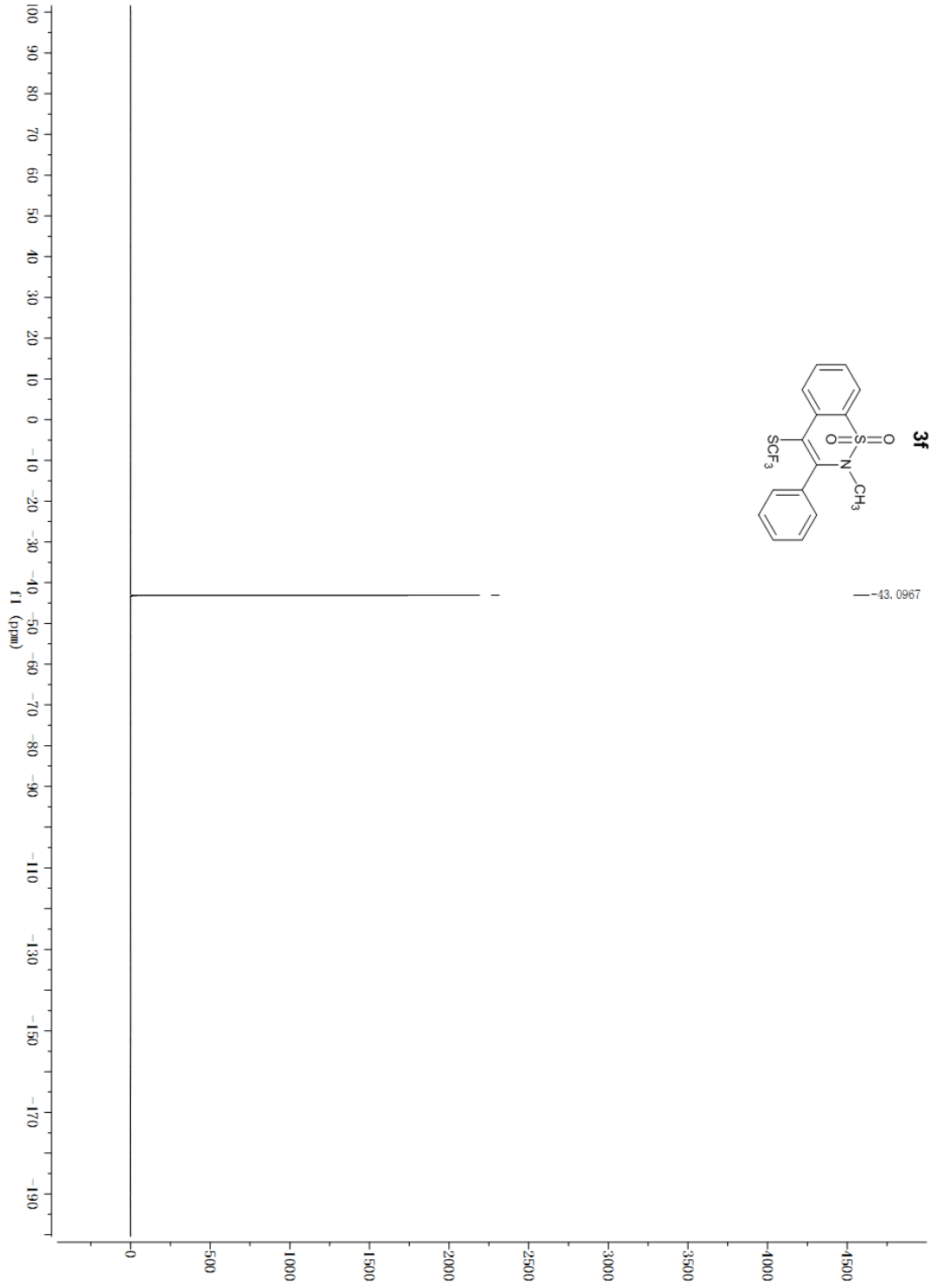
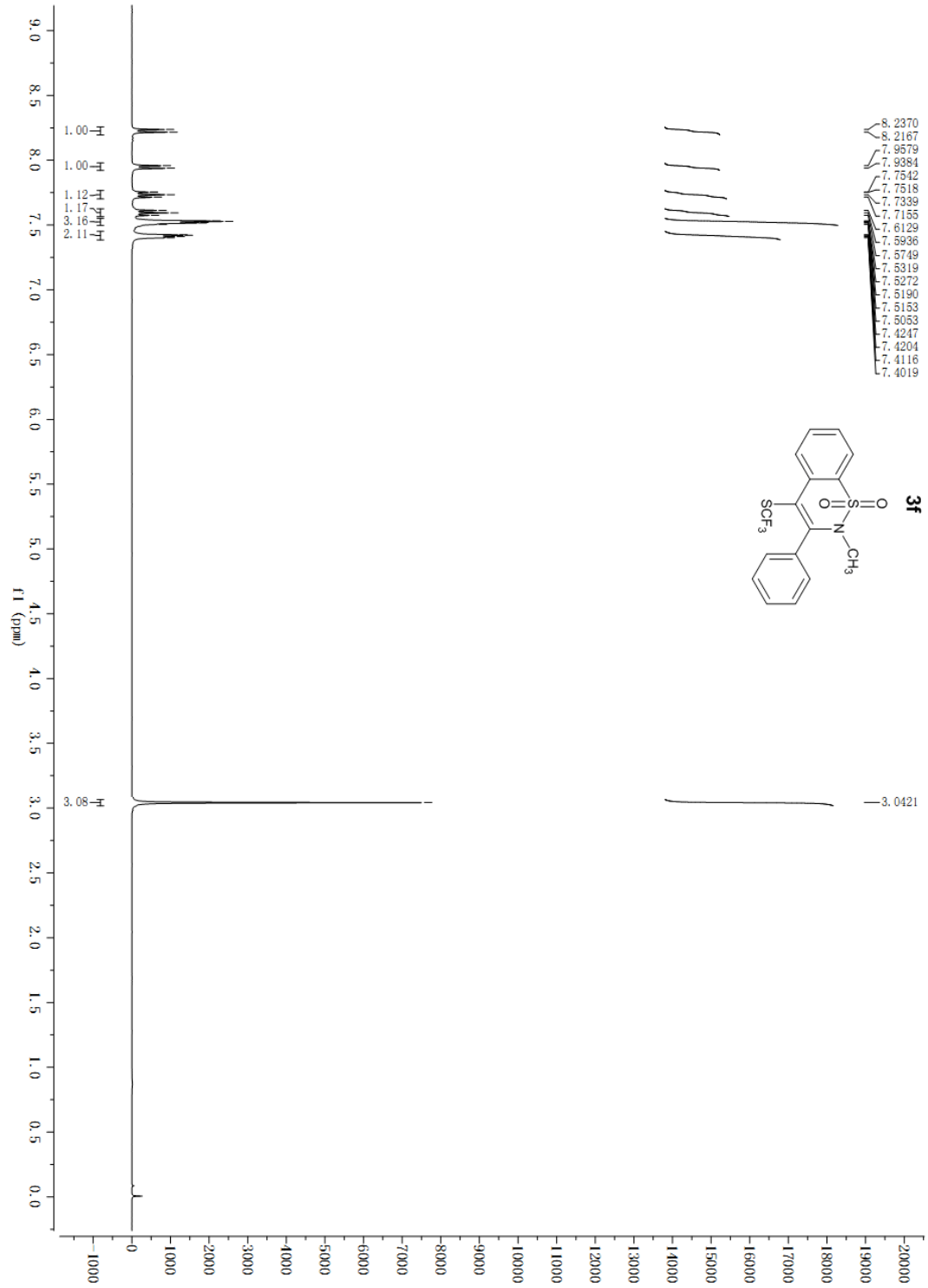
115.4028
111.0567
104.0893
77.3456
77.0276
76.7094
55.7685
34.6208
f1 (ppm)
H3CO
SCF3
CH3
3e


3f
SCF3
O
S
O
N
CH3
-43.0967
f1 (ppm)
100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190
0 500 1000 1500 2000 2500 3000 3500 4000 4500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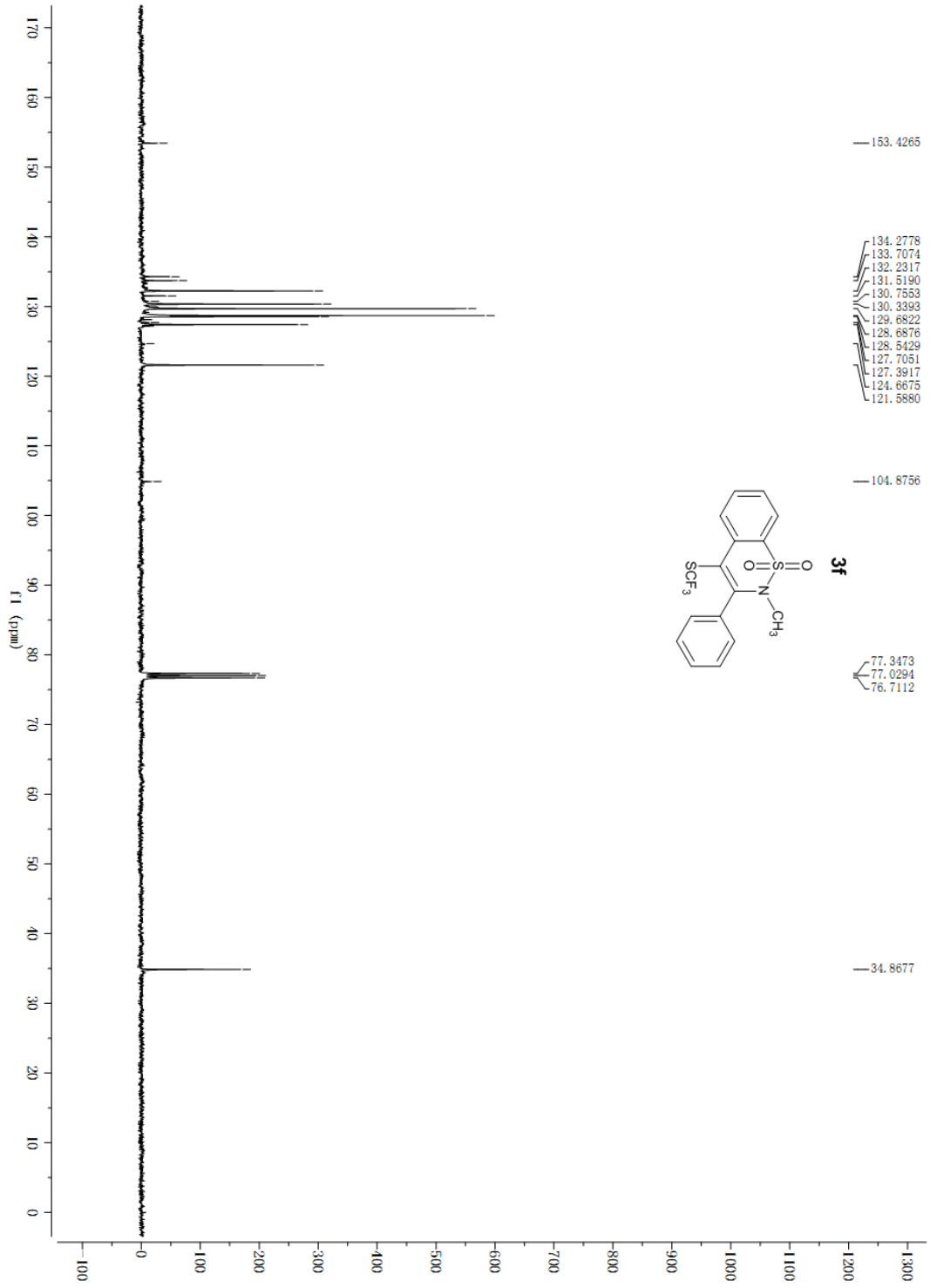
7.9579
7.9384
7.7542
7.7518
7.7339
7.7155
7.6129
7.5936
7.5749
7.5319
7.5272
7.5190
7.5153
7.5053
7.4247
7.4204
7.4116
7.4019
1.00
1.00
1.12
1.17
3.16
2.11
3.08
3.0421
3f
SCF3
CH3
f1 (ppm)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133.7074
132.2317
131.5190
130.7553
130.3393
129.6822
128.6876
128.5429
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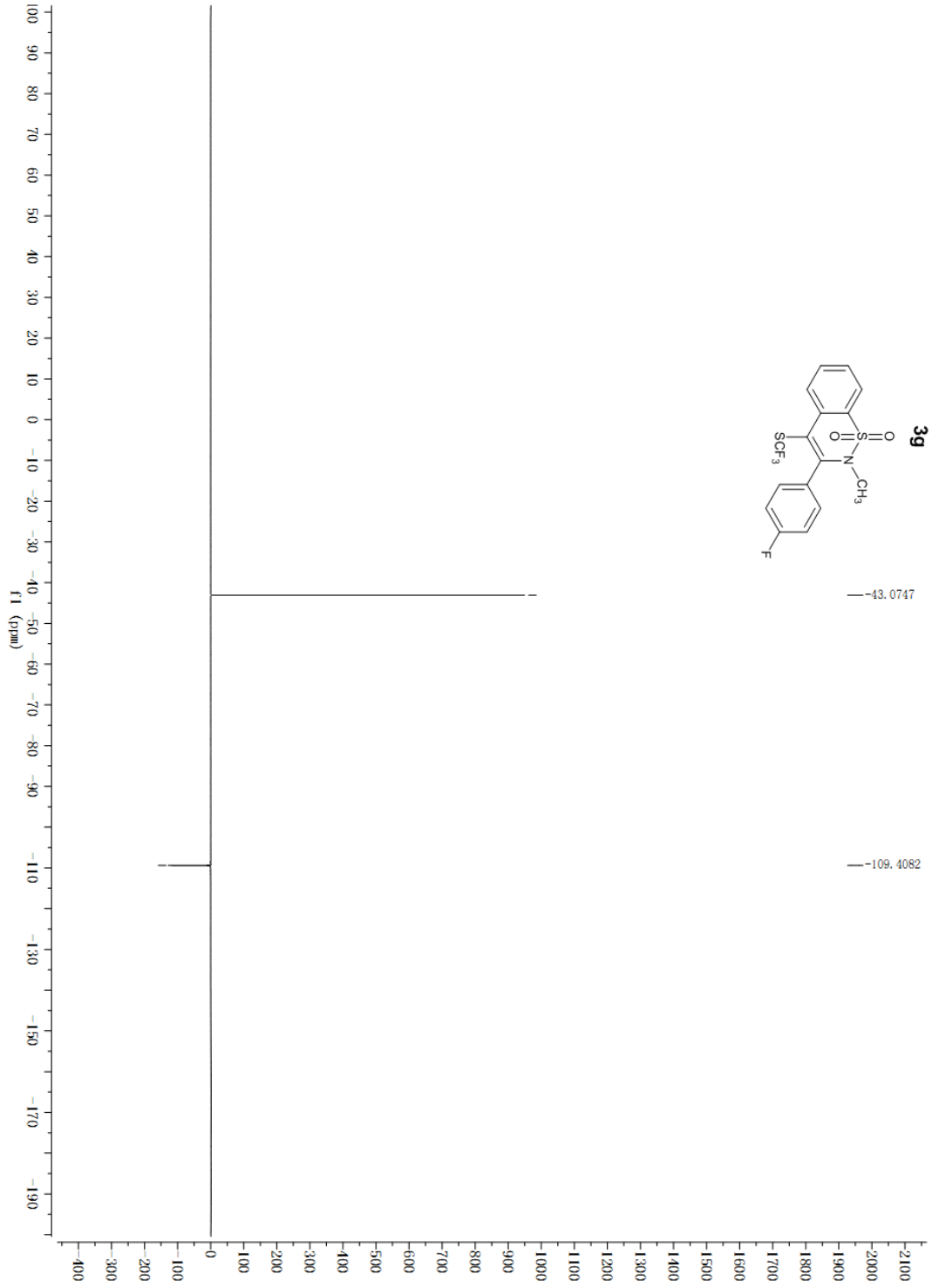
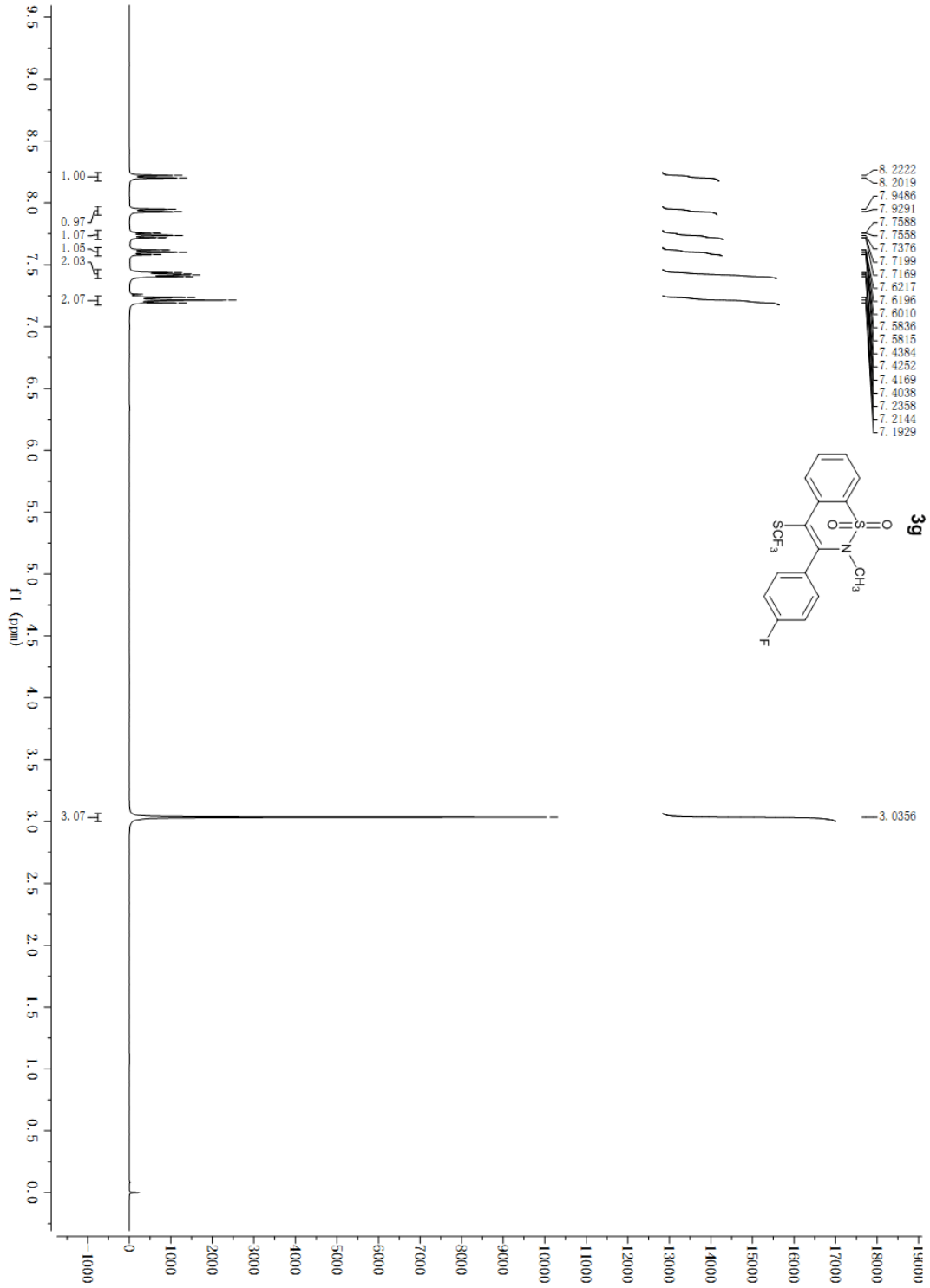
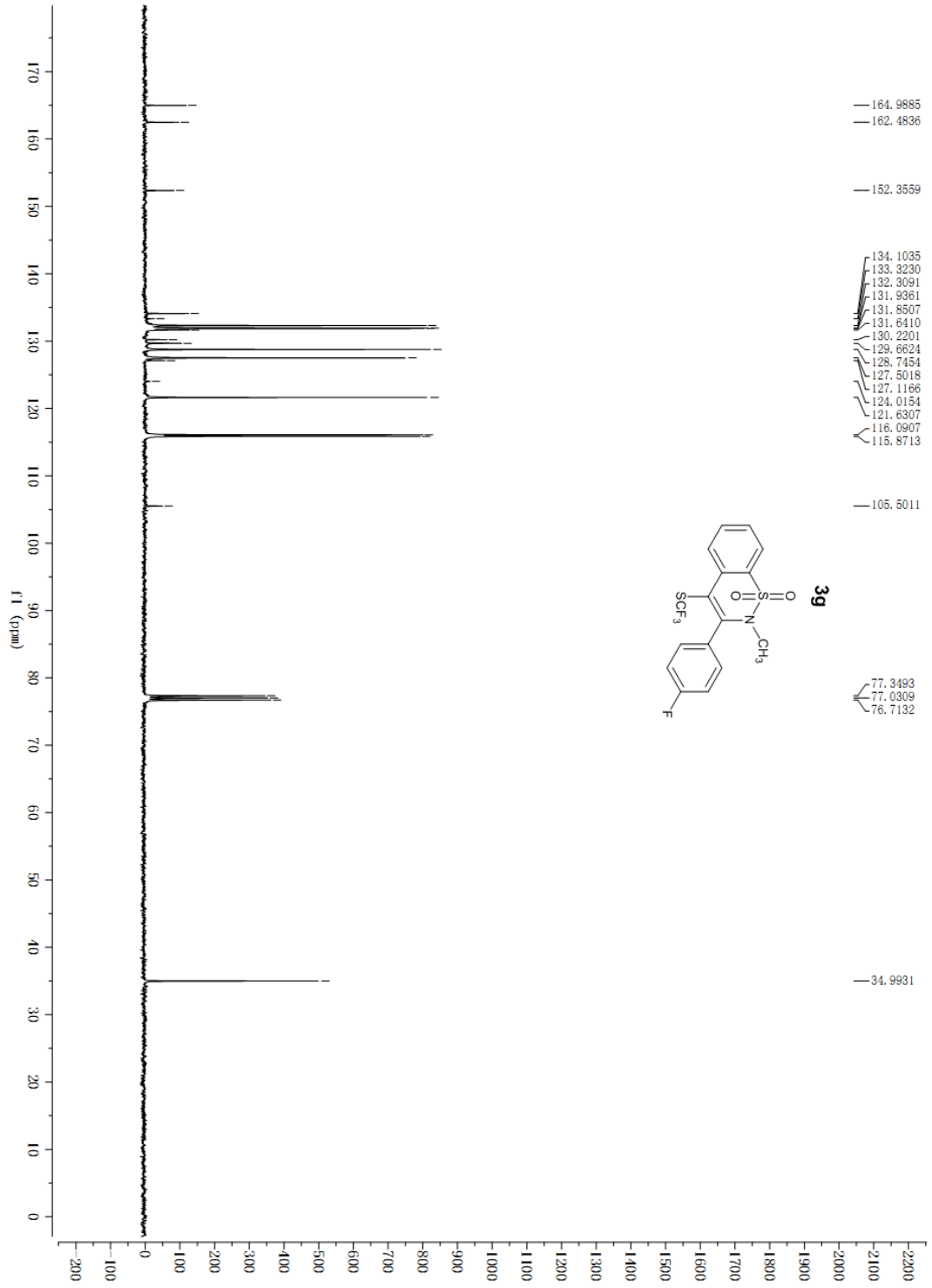
127.3917
124.6675
121.5880
104.8756
77.3473
77.0294
76.7112
34.8677
f1 (ppm)
SCF3
CH3
3f


3g
-43.0747
-109.4082
f1 (ppm)


8.2222
8.2019
7.9486
7.9291
7.7588
7.7558
7.7376
7.7199
7.7169
7.6217
7.6196
7.6010
7.5836
7.5815
7.4384
7.4252
7.4169
7.4038
7.2358
7.2144
7.1929
1.00
0.97
1.07
1.05
2.03
2.07
3.07
3.0356
3g
SCF3
CH3
F
f1 (ppm)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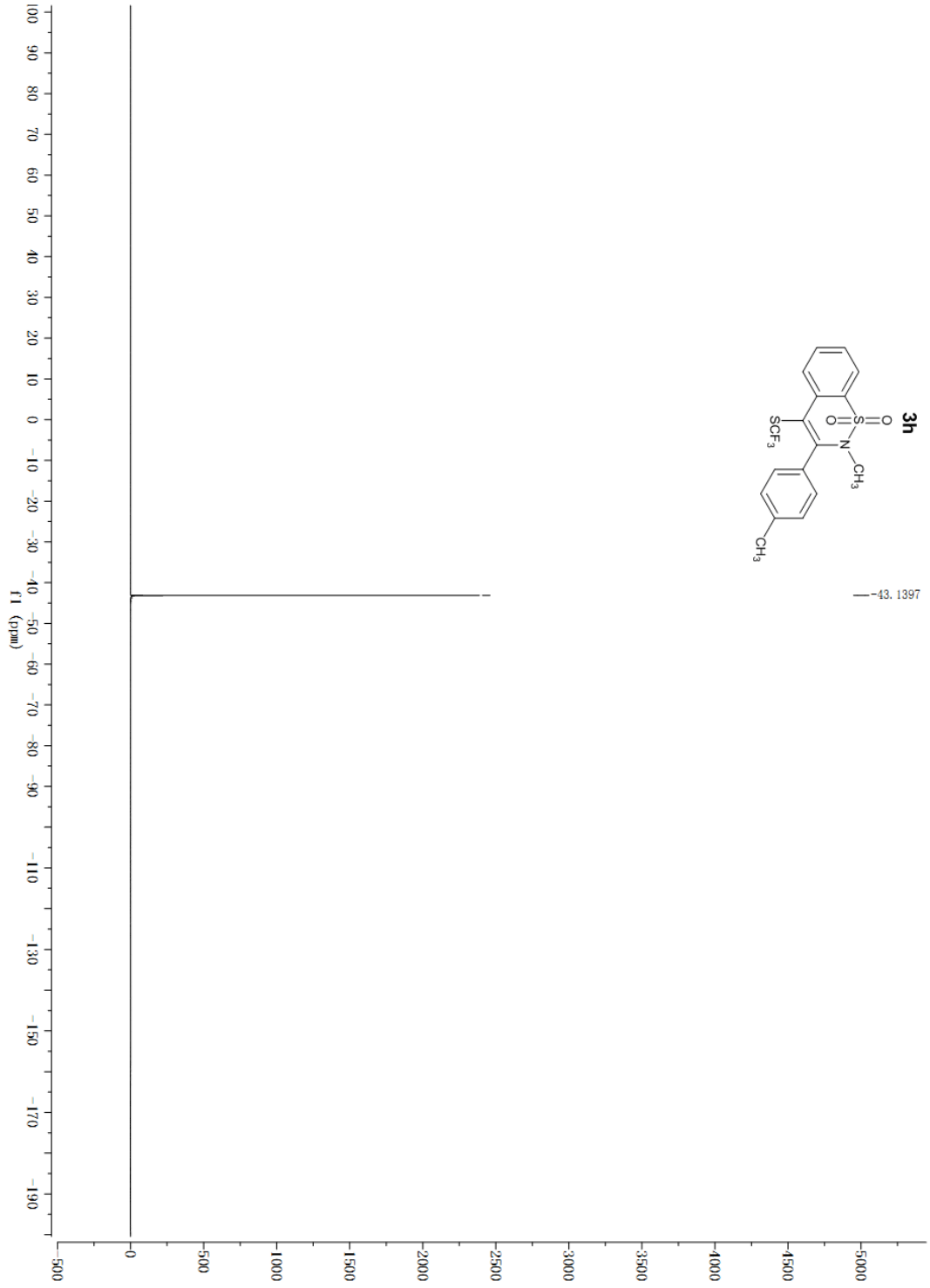
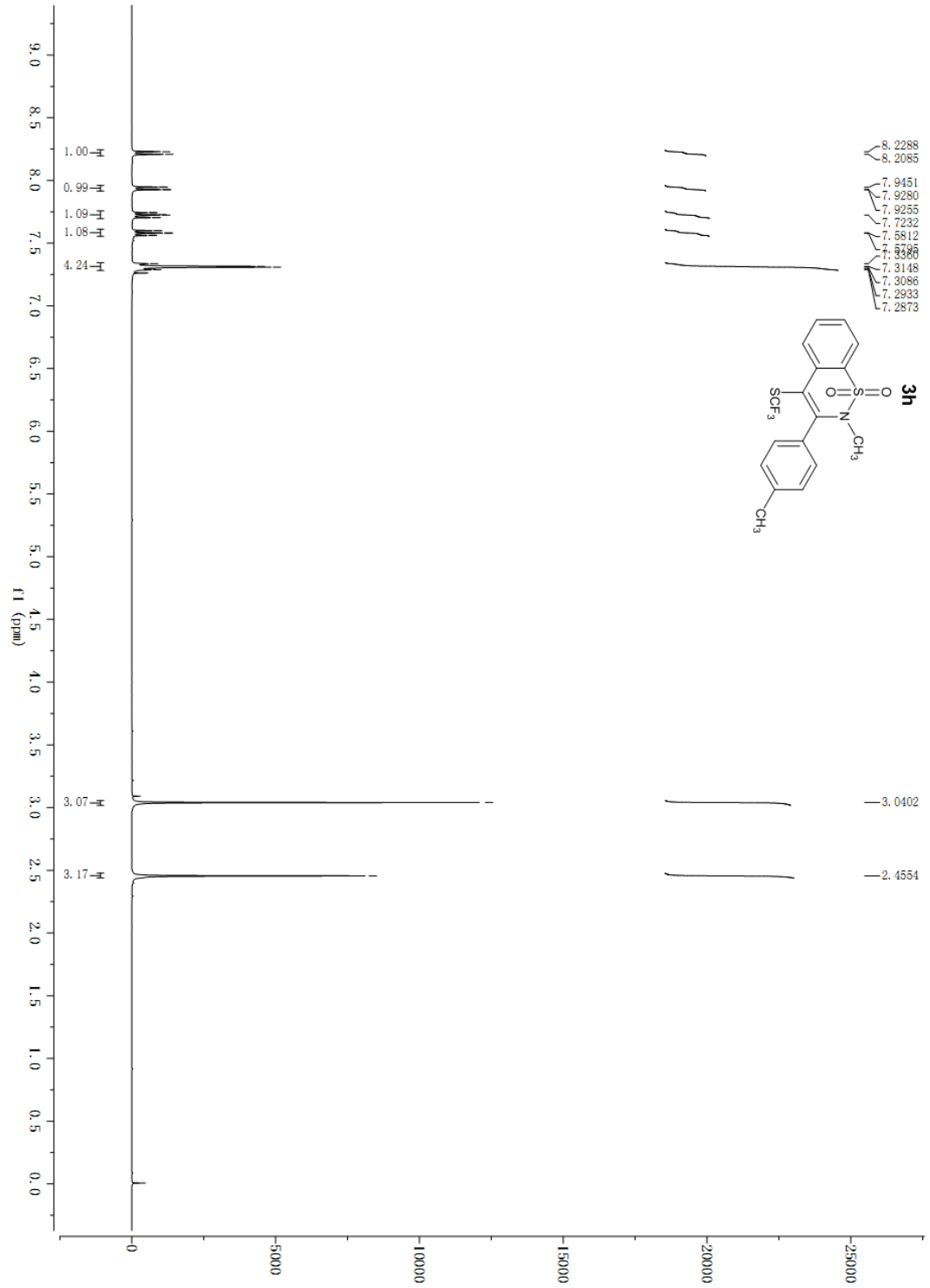
162.4836
152.3559
134.1035
133.3230
132.3091
131.9361
131.8507
131.6410
130.2201
129.6624
128.7454
127.5018
127.1166
124.0154
121.6307
116.0907
115.8713
105.5011
77.3493
77.0309
76.7132
34.9931
f1 (ppm)
3g


3h
SCF3
CH3
CH3
-43.1397
f1 (ppm)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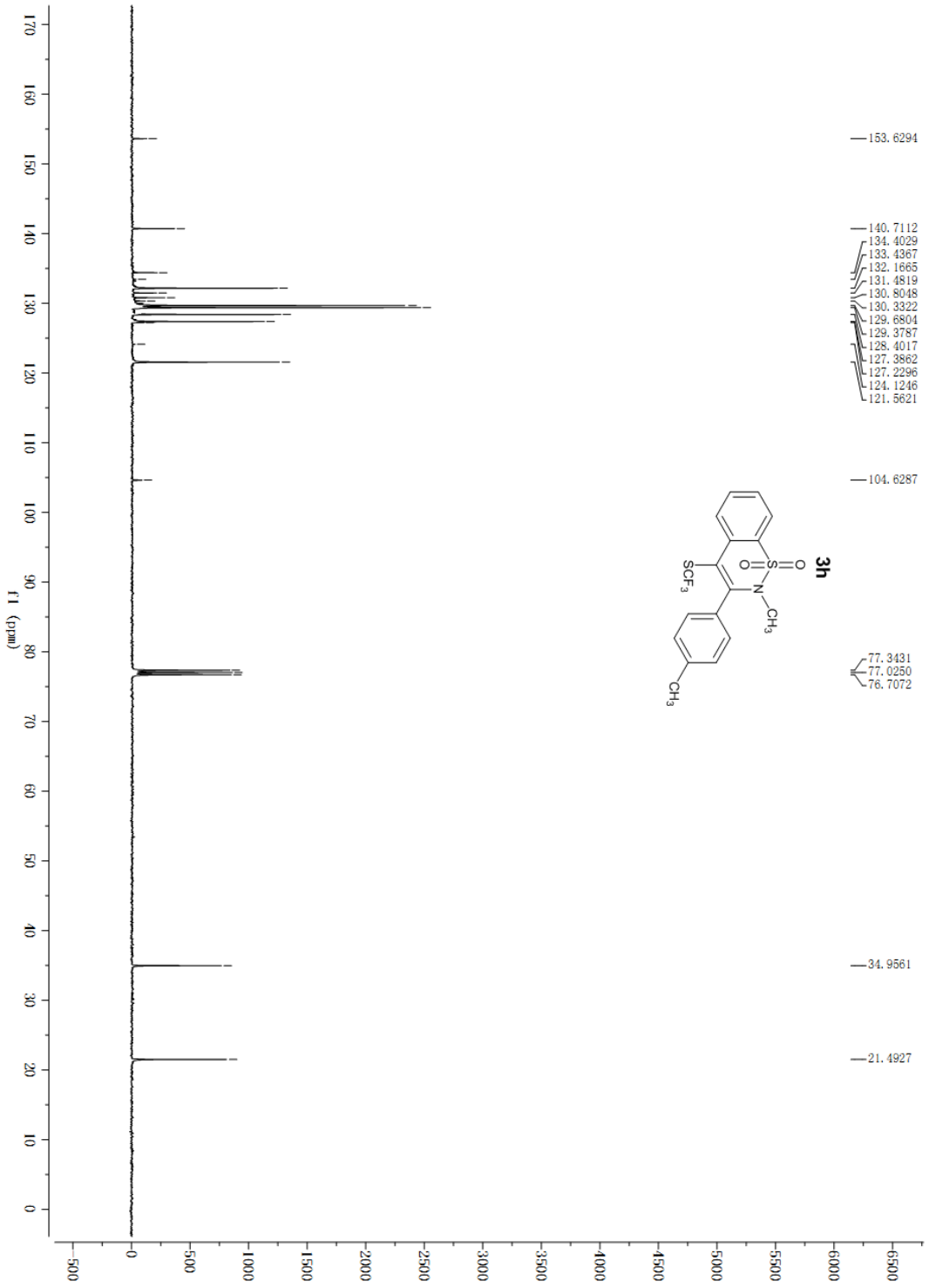
8.2085
7.9451
7.9280
7.9255
7.7232
7.5812
7.3360
7.3148
7.3086
7.2933
7.2873
1.00
0.99
1.09
1.08
4.24
3.07
3.17
3.0402
2.4554
3h
SCF3
CH3
CH3
f1 (ppm)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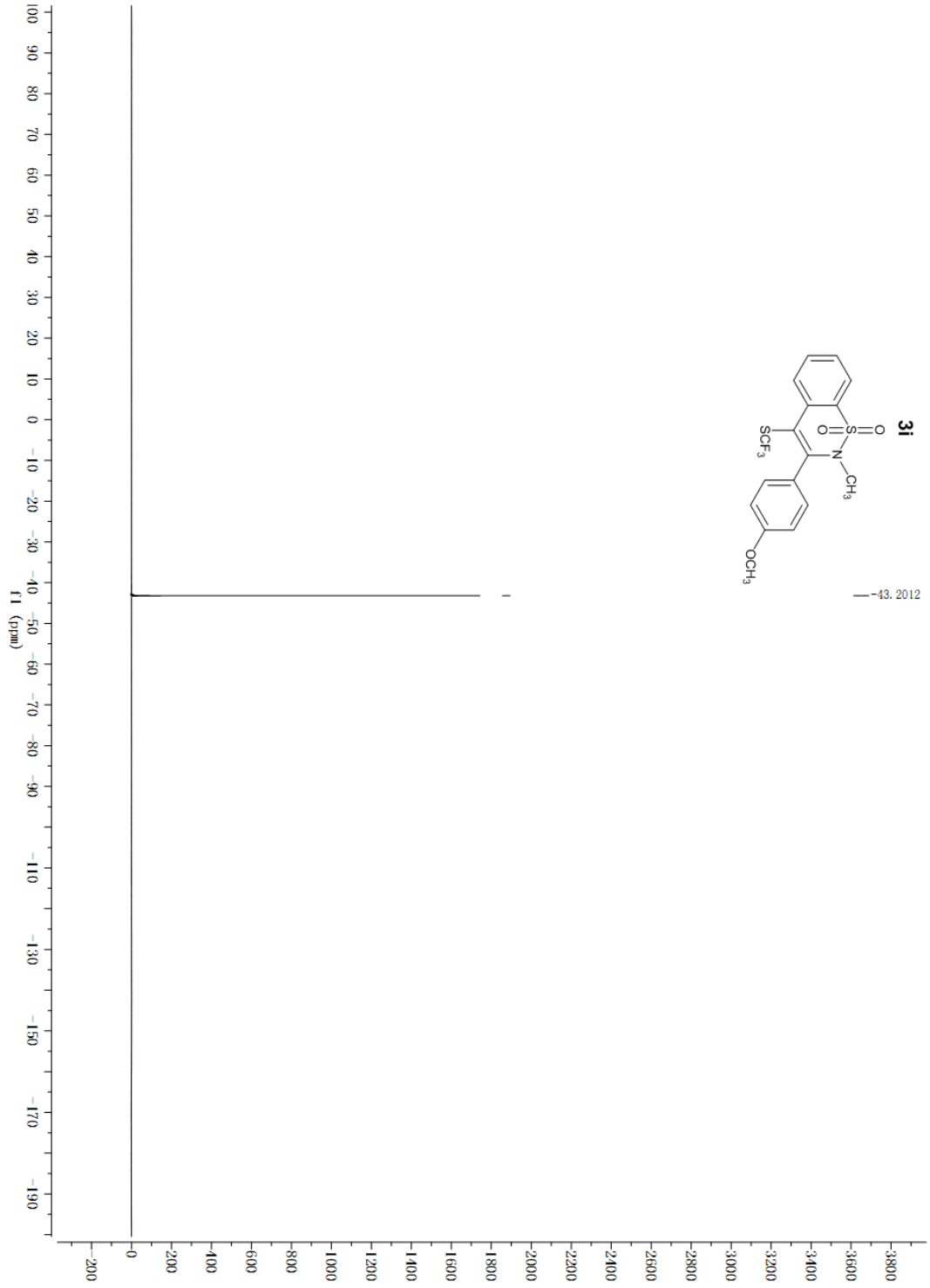
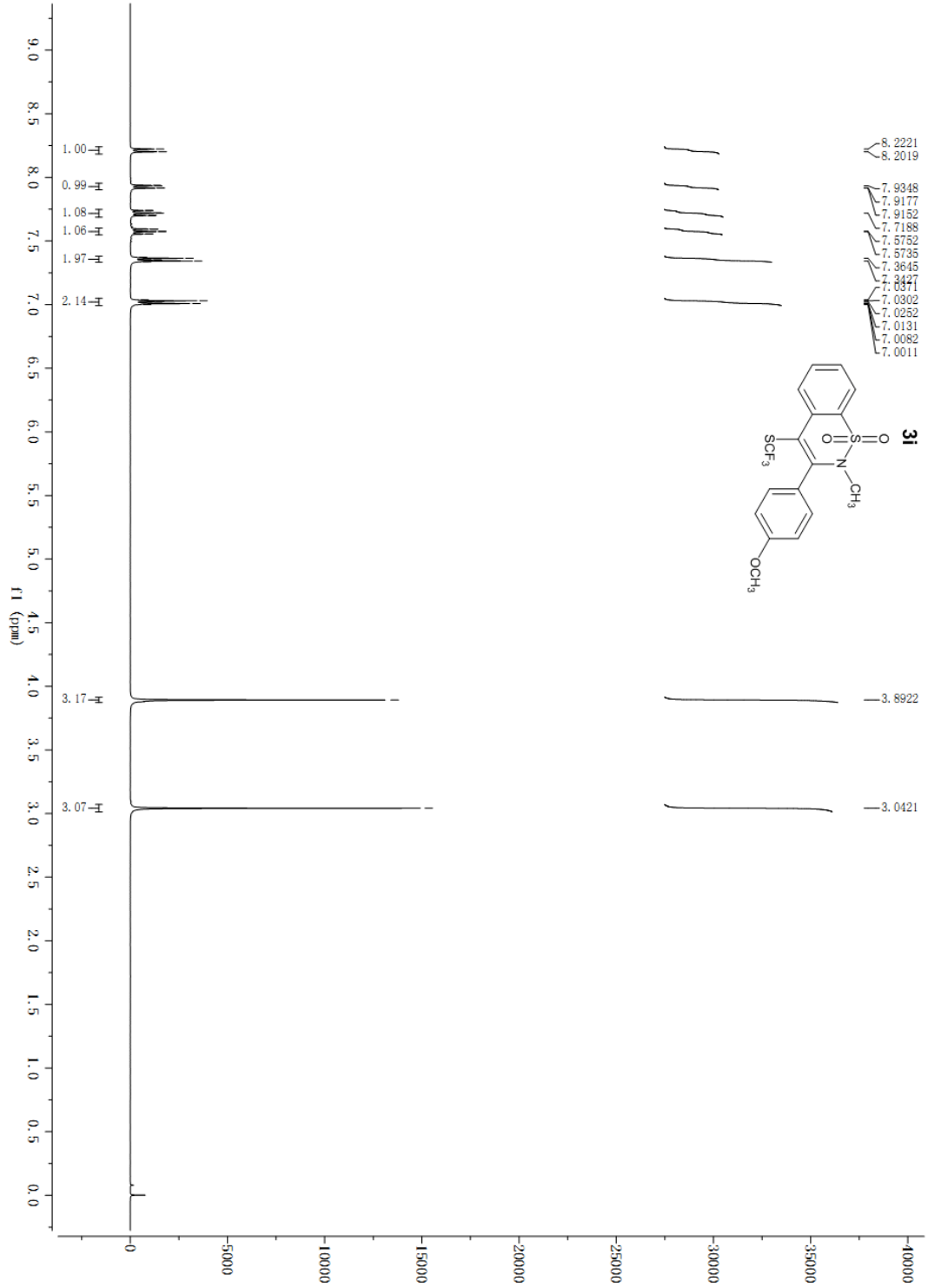
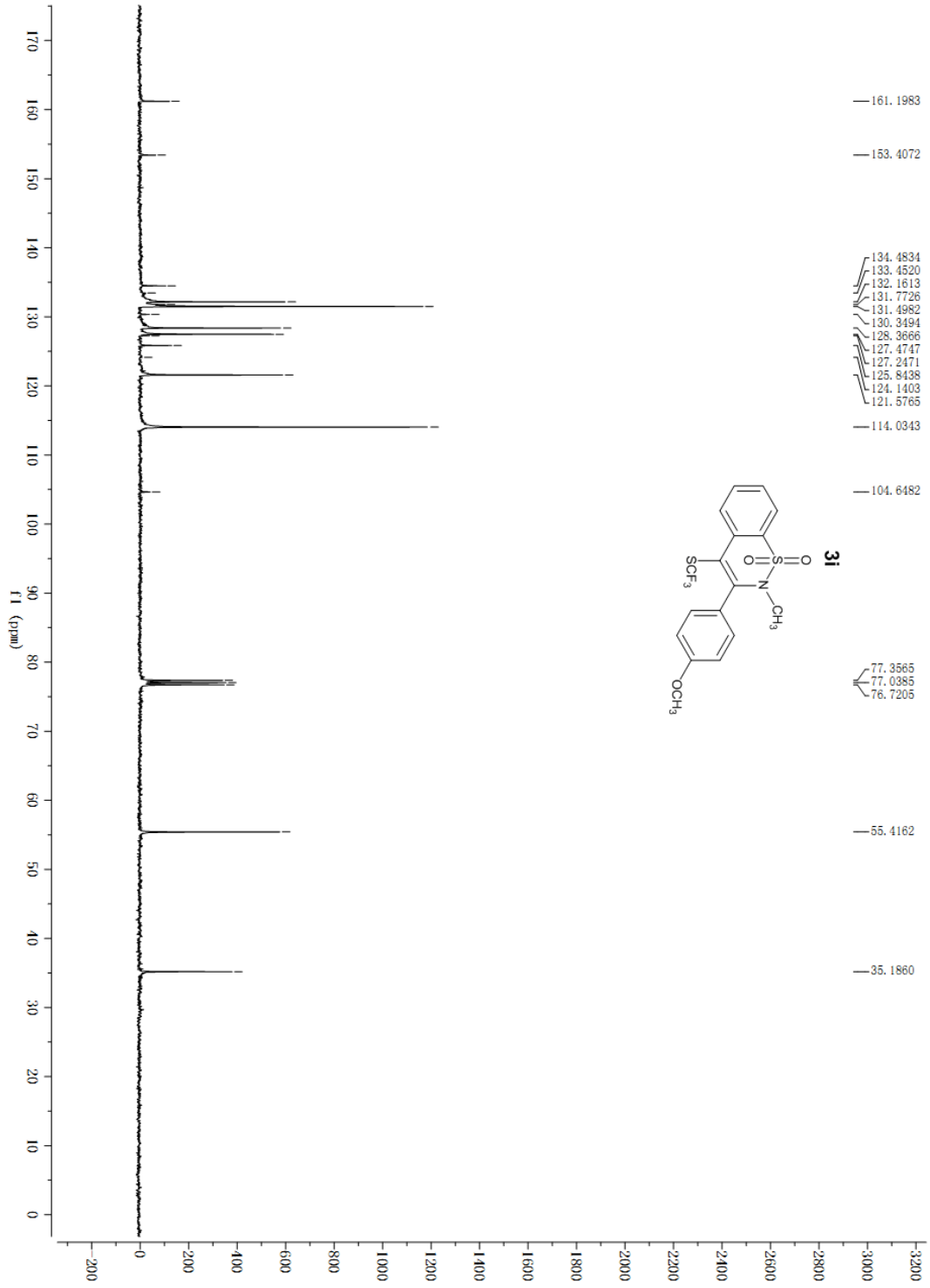
134.4029
133.4367
132.1665
131.4819
130.8048
130.3322
129.6804
129.3787
128.4017
127.3862
127.2296
124.1246
121.5621
104.6287
77.3431
77.0250
76.7072
34.9561
21.4927
3h
SCF3
CH3
CH3
f1 (ppm)


3i
-43.2012
f1 (ppm)


8.2221
8.2019
7.9348
7.9177
7.9152
7.7188
7.5752
7.5735
7.3645
7.3427
7.0371
7.0302
7.0252
7.0131
7.0082
7.0011
1.00
0.99
1.08
1.06
1.97
2.14
3.17
3.07
3.8922
3.0421
3i
SCF3
OCH3
CH3
f1 (ppm)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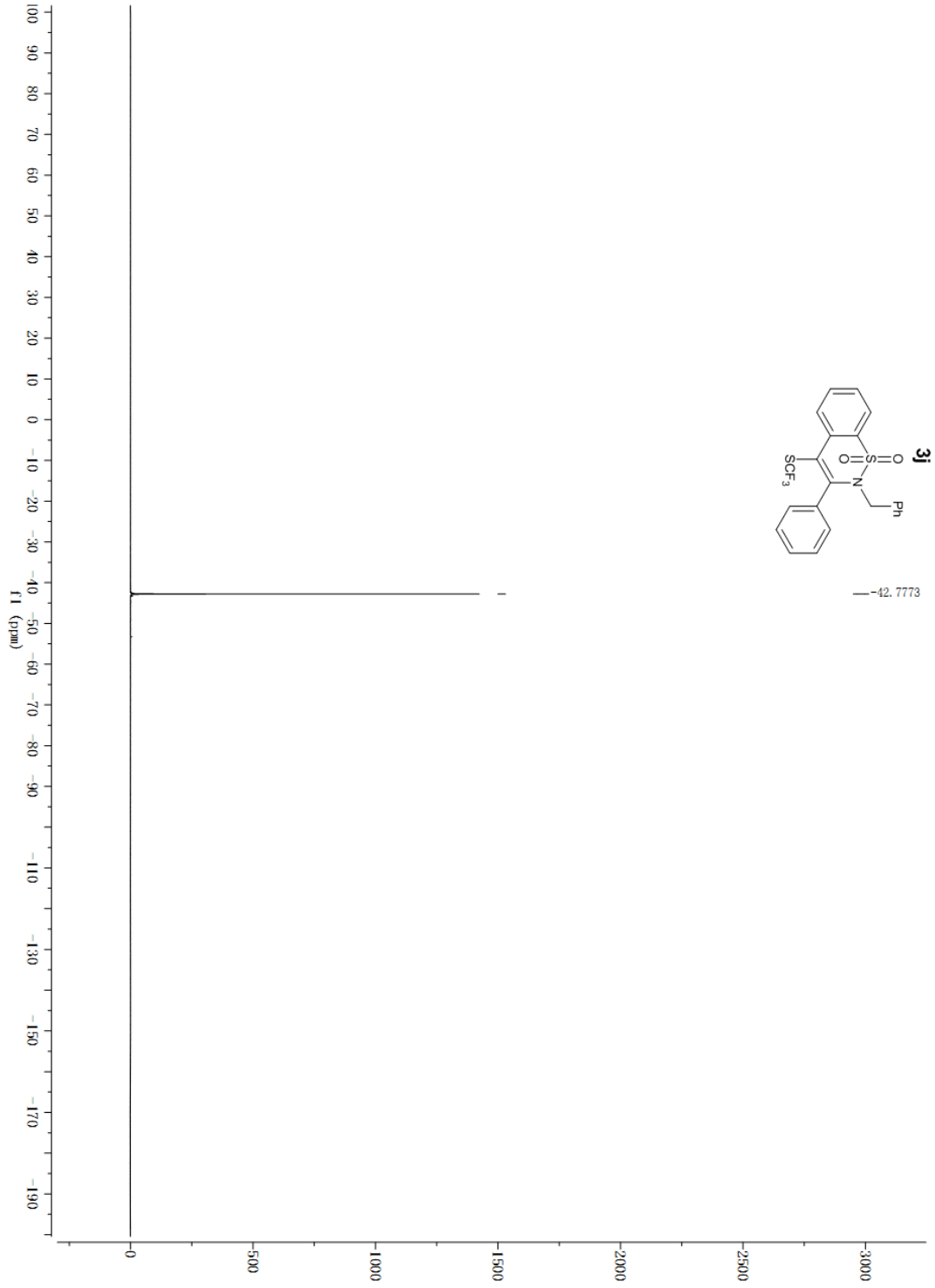
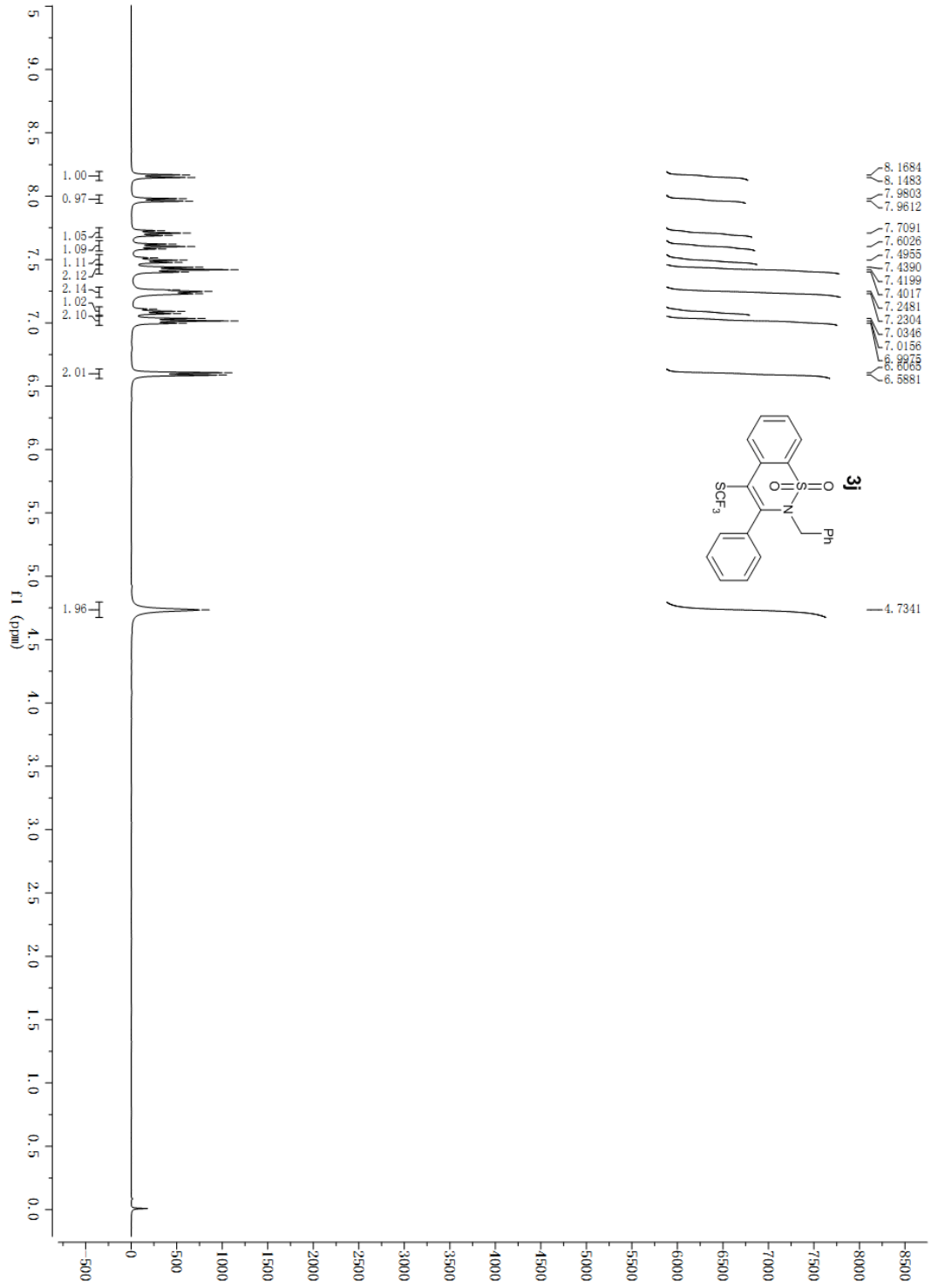
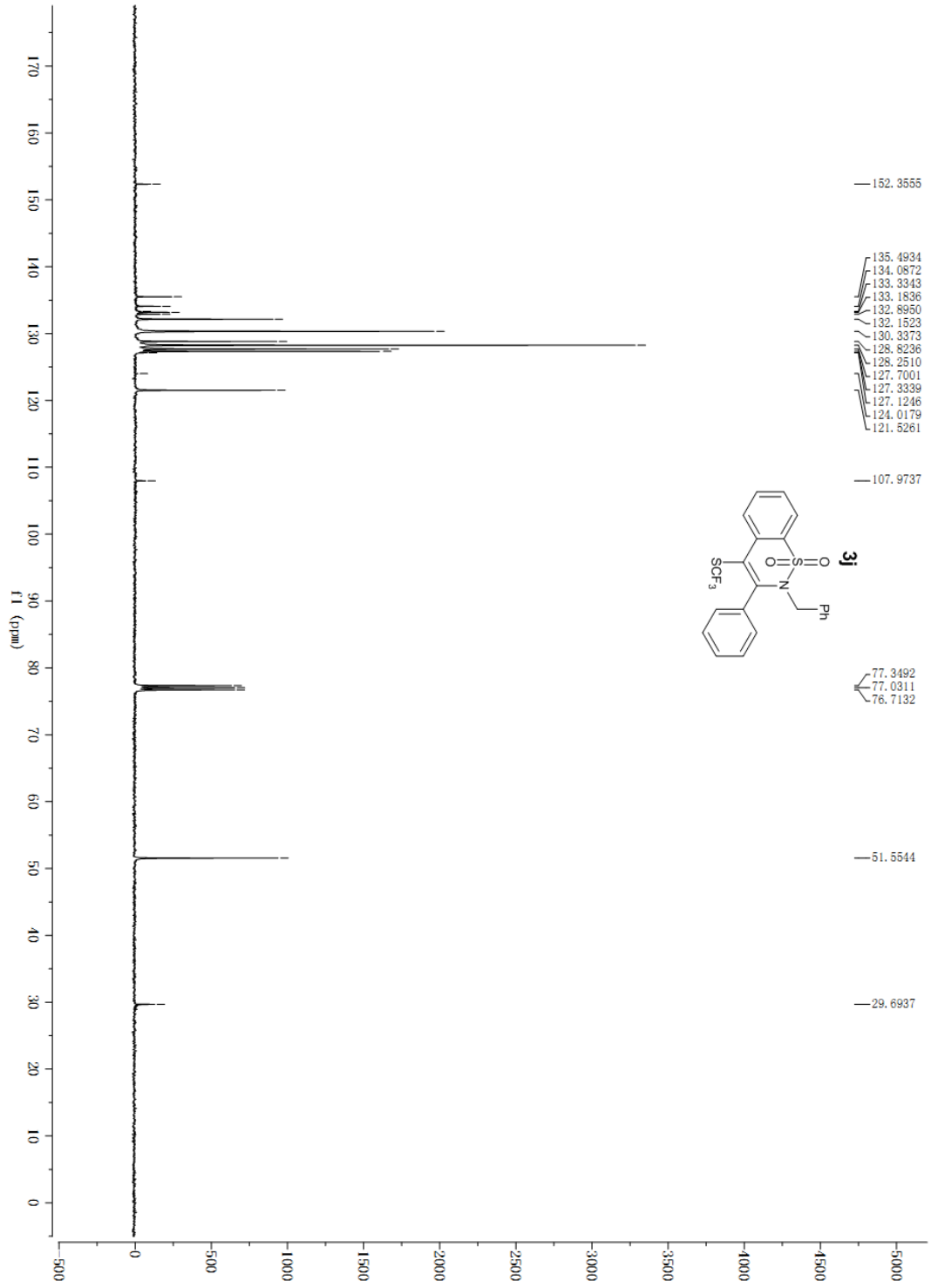
134.4834
133.4520
132.1613
131.7726
131.4982
130.3494
128.3666
127.4747
127.2471
125.8438
124.1403
121.5765
114.0343
104.6482
77.3565
77.0385
76.7205
55.4162
35.1860
3i
SCF3
OCH3
CH3
f1 (ppm)


3j
SCF3
Ph
-42.7773
f1 (ppm)


8.1684
8.1483
7.9803
7.9612
7.7091
7.6026
7.4955
7.4390
7.4199
7.4017
7.2481
7.2304
7.0346
7.0156
6.6068
6.5881
4.7341
1.00
0.97
1.05
1.09
1.11
2.12
2.14
1.02
2.10
2.01
1.96
3j
SCF3
Ph
f1 (ppm)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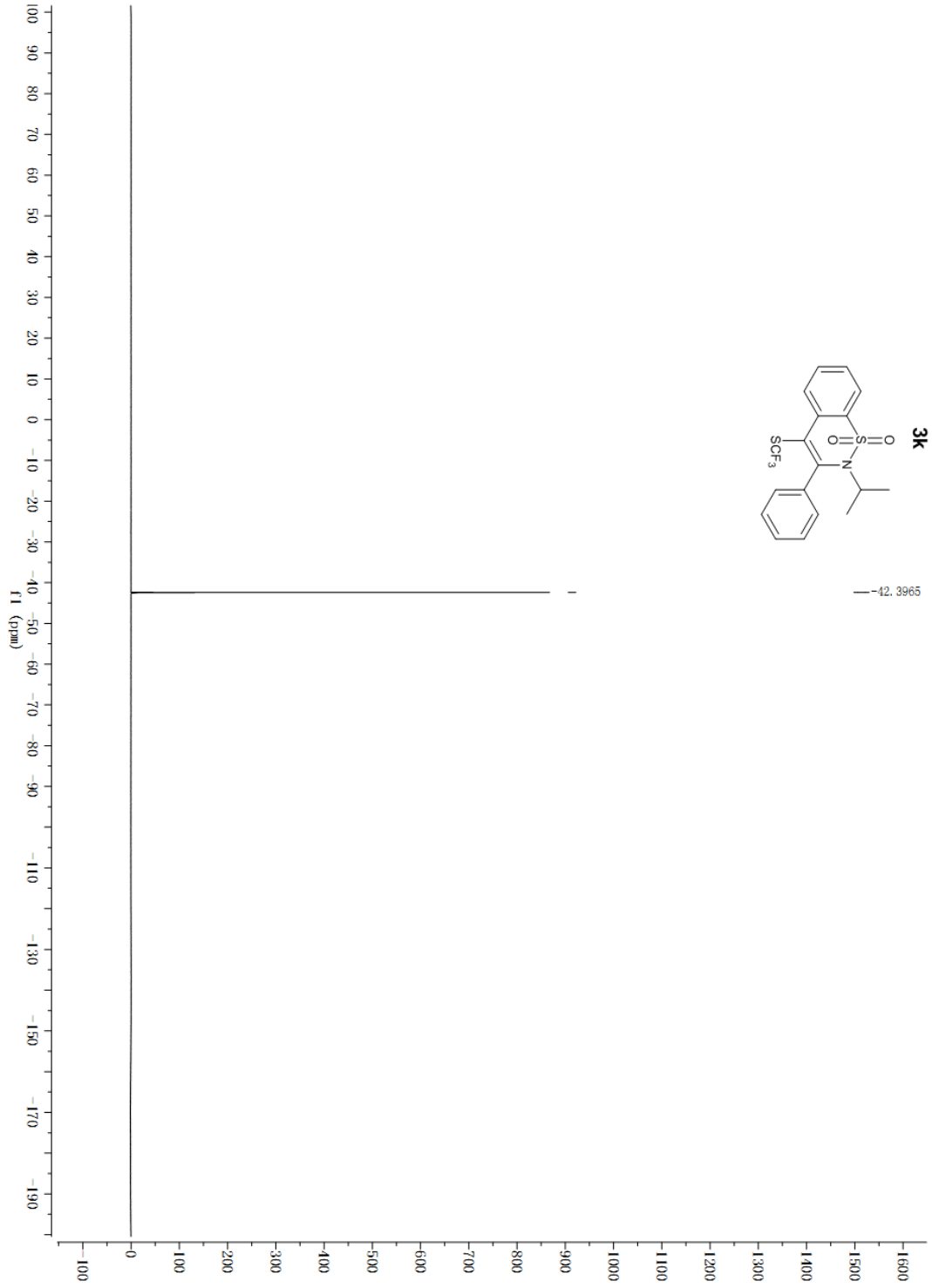
134.0872
133.3343
133.1836
132.8950
132.1523
130.3373
128.8236
128.2510
127.7001
127.3339
127.1246
124.0179
121.5261
107.9737
77.3492
77.0311
76.7132
51.5544
29.6937
3j
SCF3
O
S
O
N
Ph
f1 (ppm)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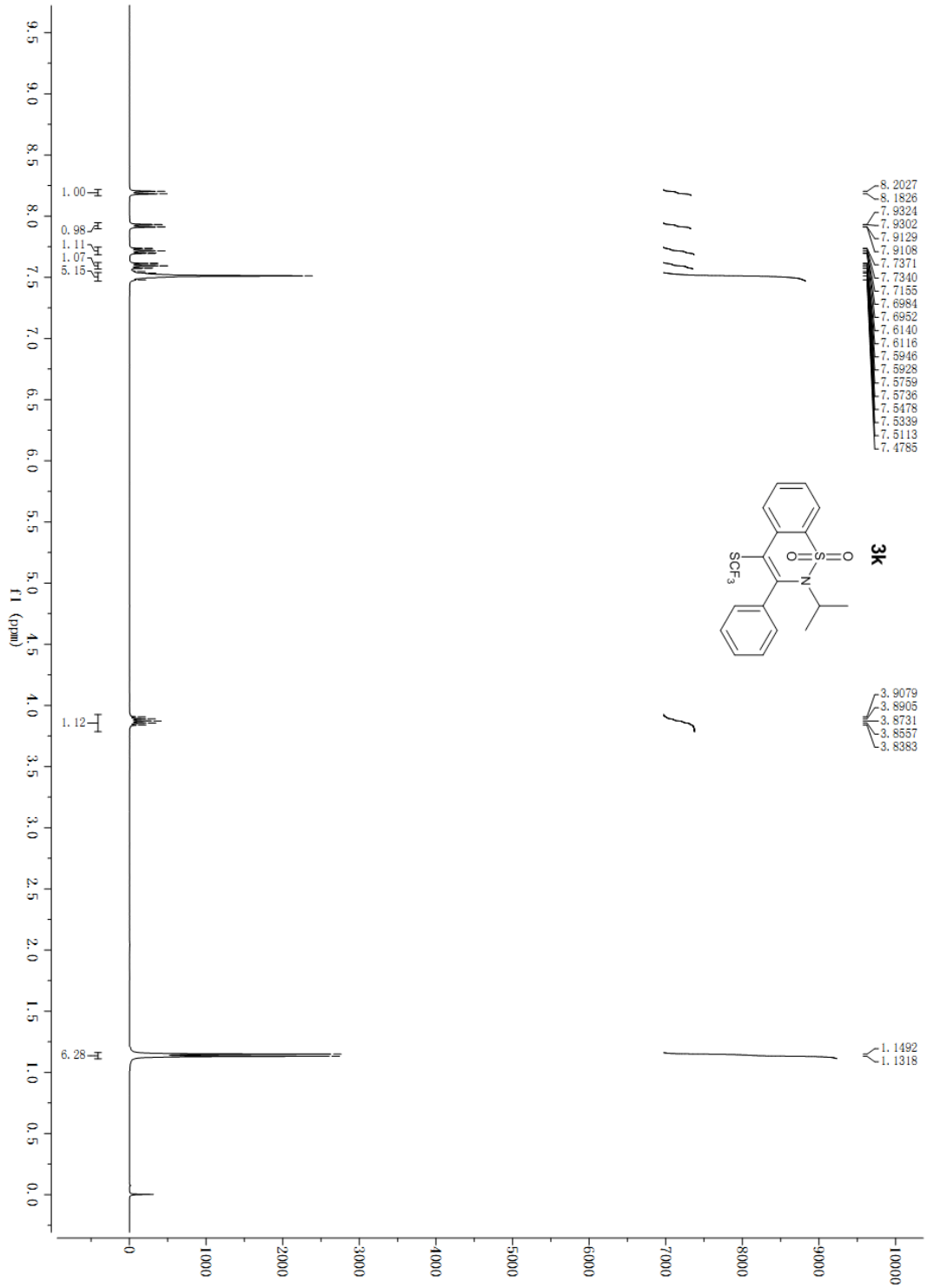
O
S
O
N
-42.3965
f1 (ppm)


f1 (ppm)
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0.98
1.11
1.07
5.15
1.12
6.28
8.2027
8.1826
7.9324
7.9302
7.9129
7.9108
7.7371
7.7340
7.7155
7.6984
7.6952
7.6140
7.6116
7.5946
7.5928
7.5759
7.5736
7.5478
7.5339
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3k
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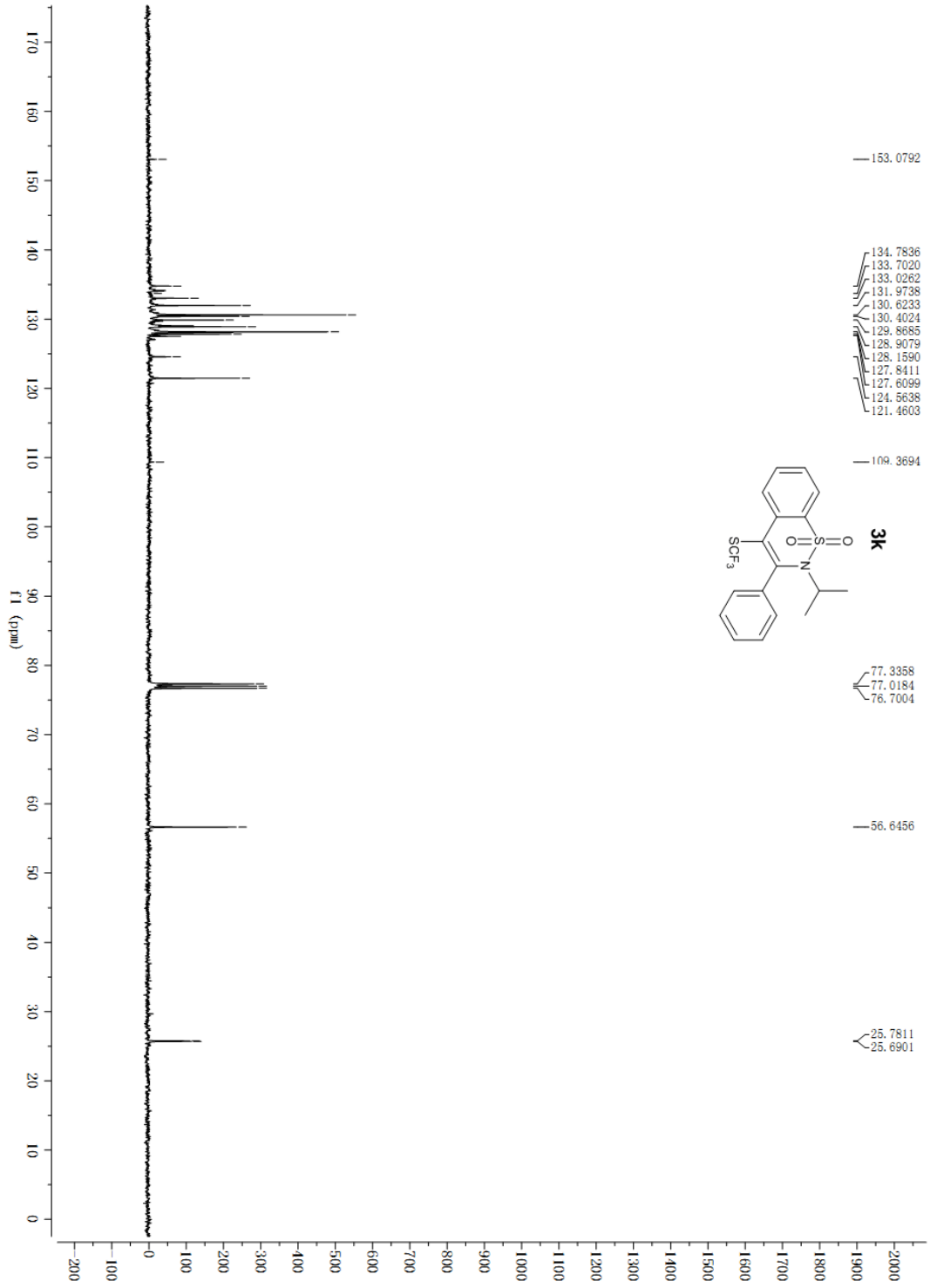
3.8557
3.8383
1.1492
1.1318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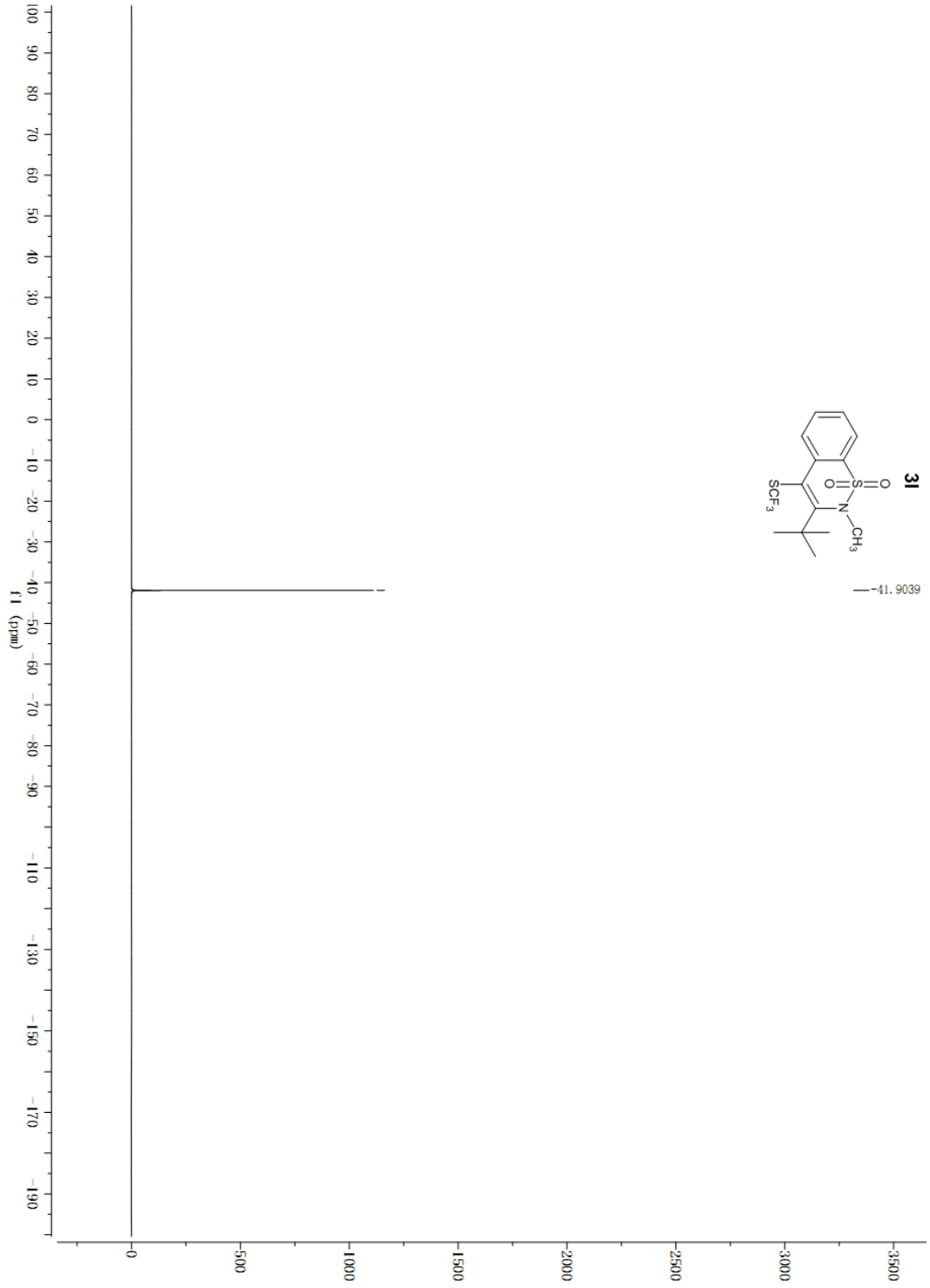
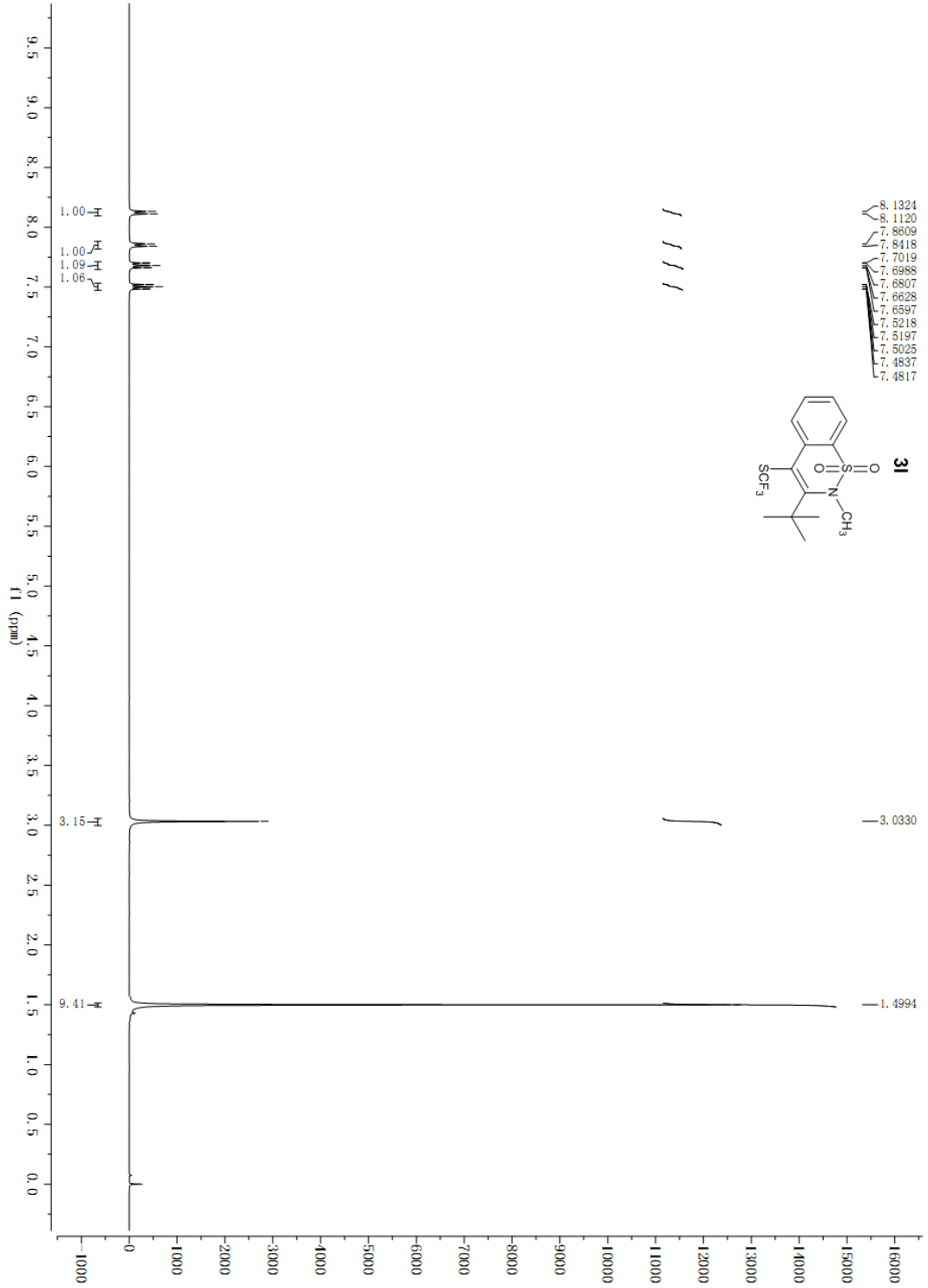
128.9079
128.1590
127.8411
127.6099
124.5638
121.4603
109.3694
77.3358
77.0184
76.7004
56.6456
25.7811
25.6901
f1 (ppm)
3k
SCF3
S
O
O
N


3l
SCF3
O
S
O
N
CH3
-41.9039
f1 (ppm)
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
0
500
1000
1500
2000
2500
3000
3500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7.8609
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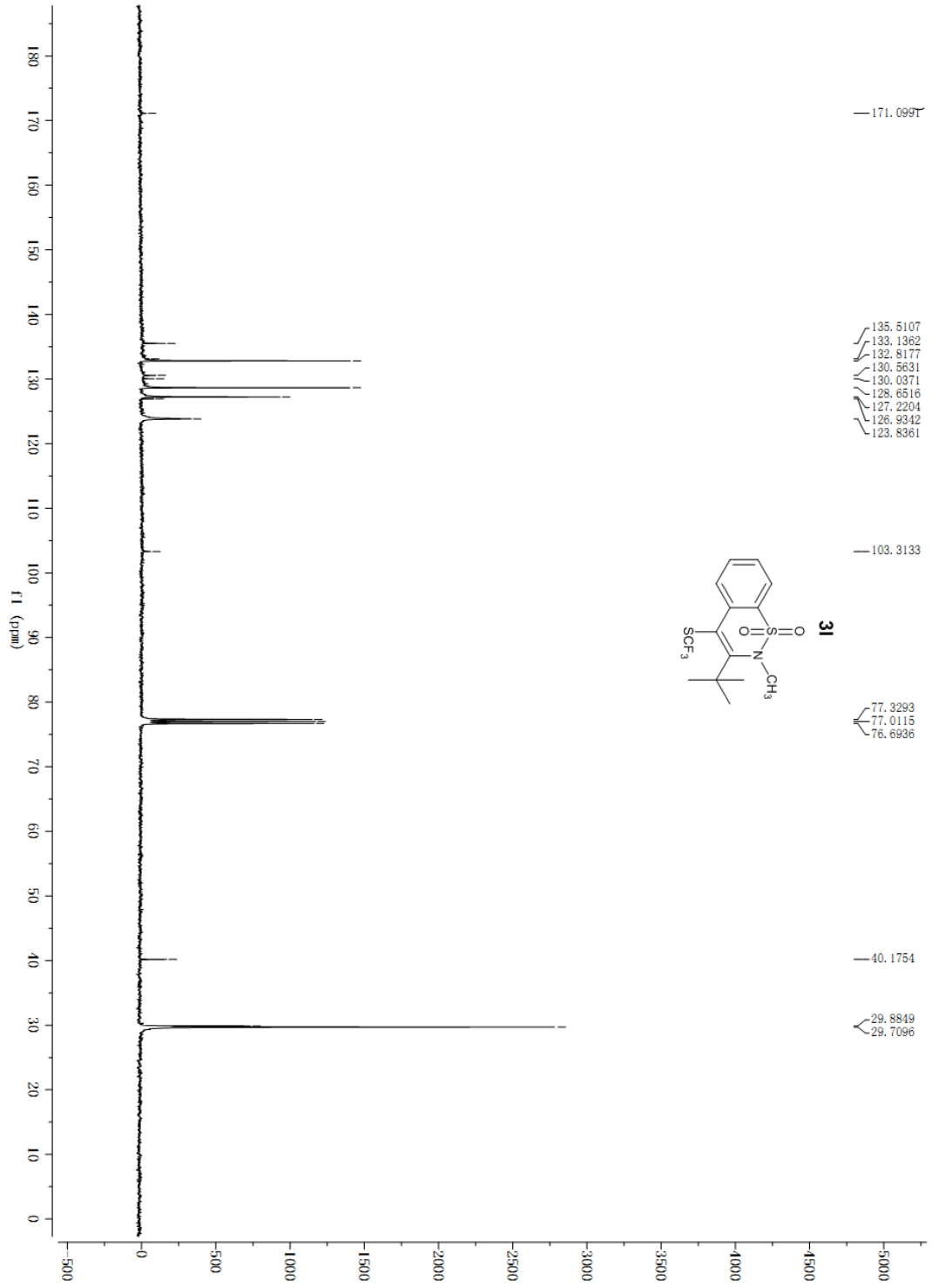
7.7019
7.6988
7.6807
7.6628
7.6597
7.5218
7.5197
7.5025
7.4837
7.4817
31
1.00H
1.00H
1.09H
1.06H
3.15H
9.41H
3.0330
1.4994
f1 (ppm)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128.6516
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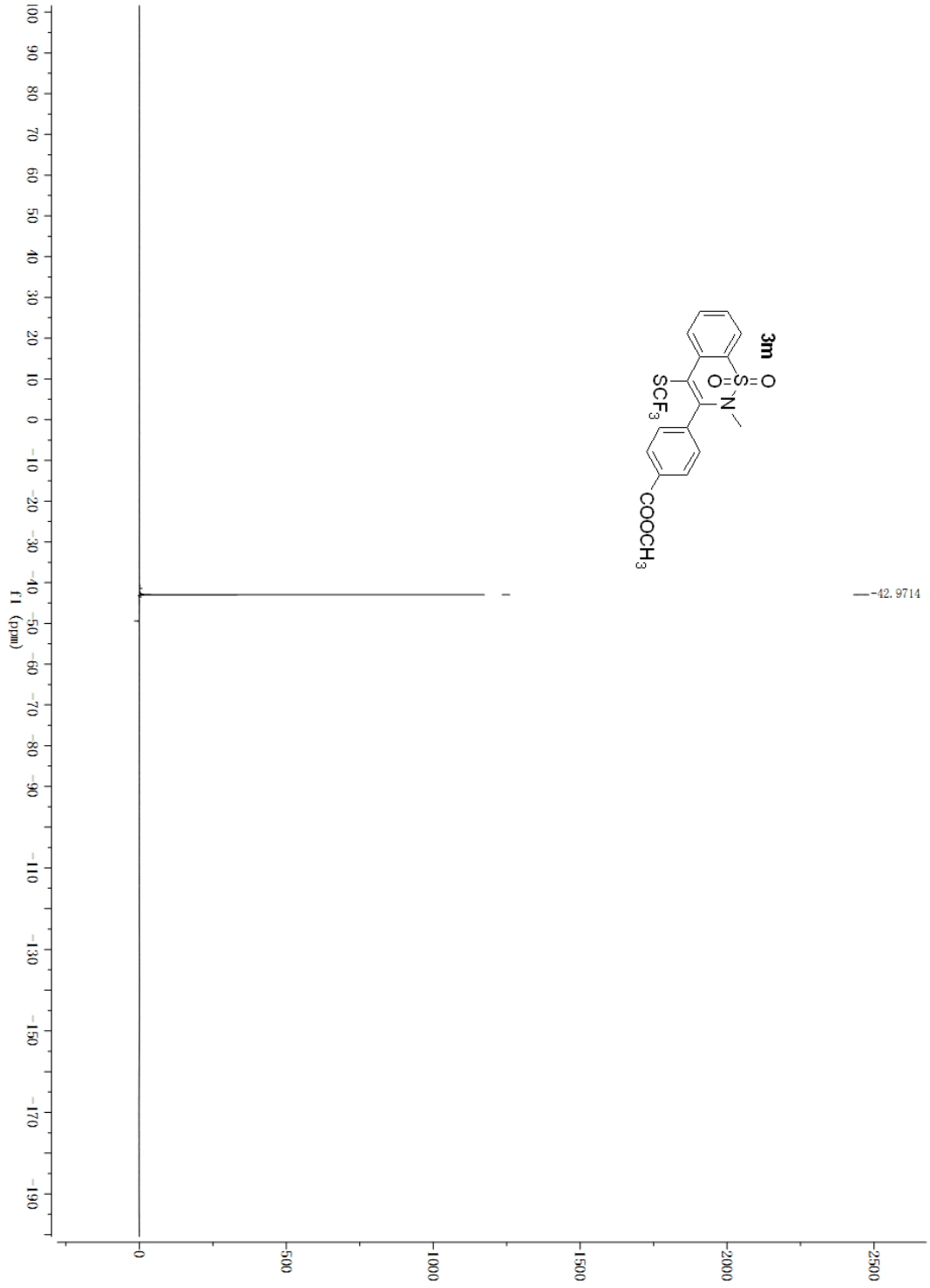
123.8361
103.3133
77.3293
77.0115
76.6936
40.1754
29.8849
29.7096
3l
SCF3
O
S
O
N
CH3
f1 (ppm)


3m
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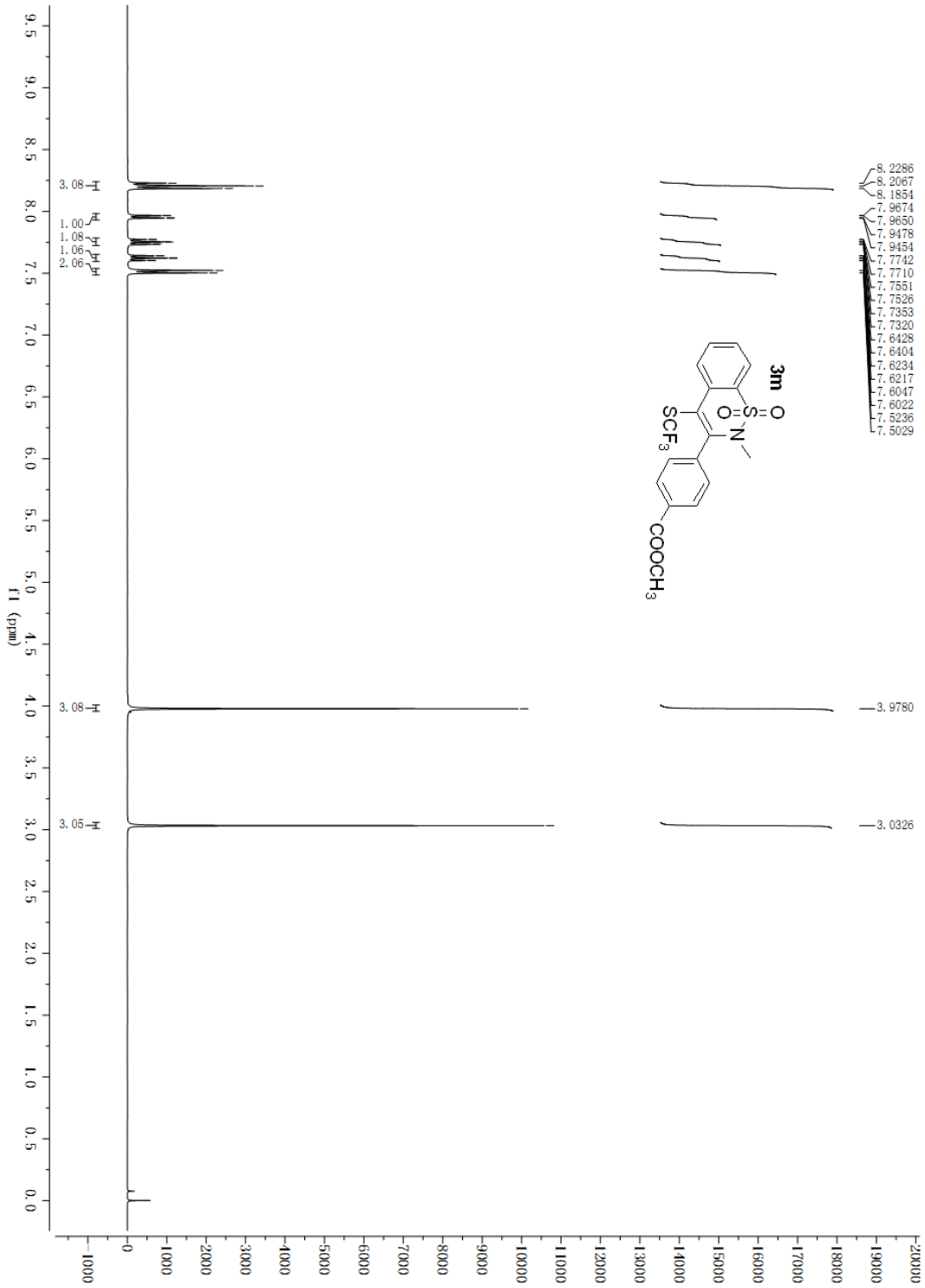
COOCH3
-42.9714
f1 (ppm)


3m
SCF3
COOCH3
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8.2067
8.1854
7.9674
7.9650
7.9478
7.9454
7.7742
7.7710
7.7551
7.7526
7.7353
7.7320
7.6428
7.6404
7.6234
7.6217
7.6047
7.6022
7.5236
7.5029
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3.0326
3.08
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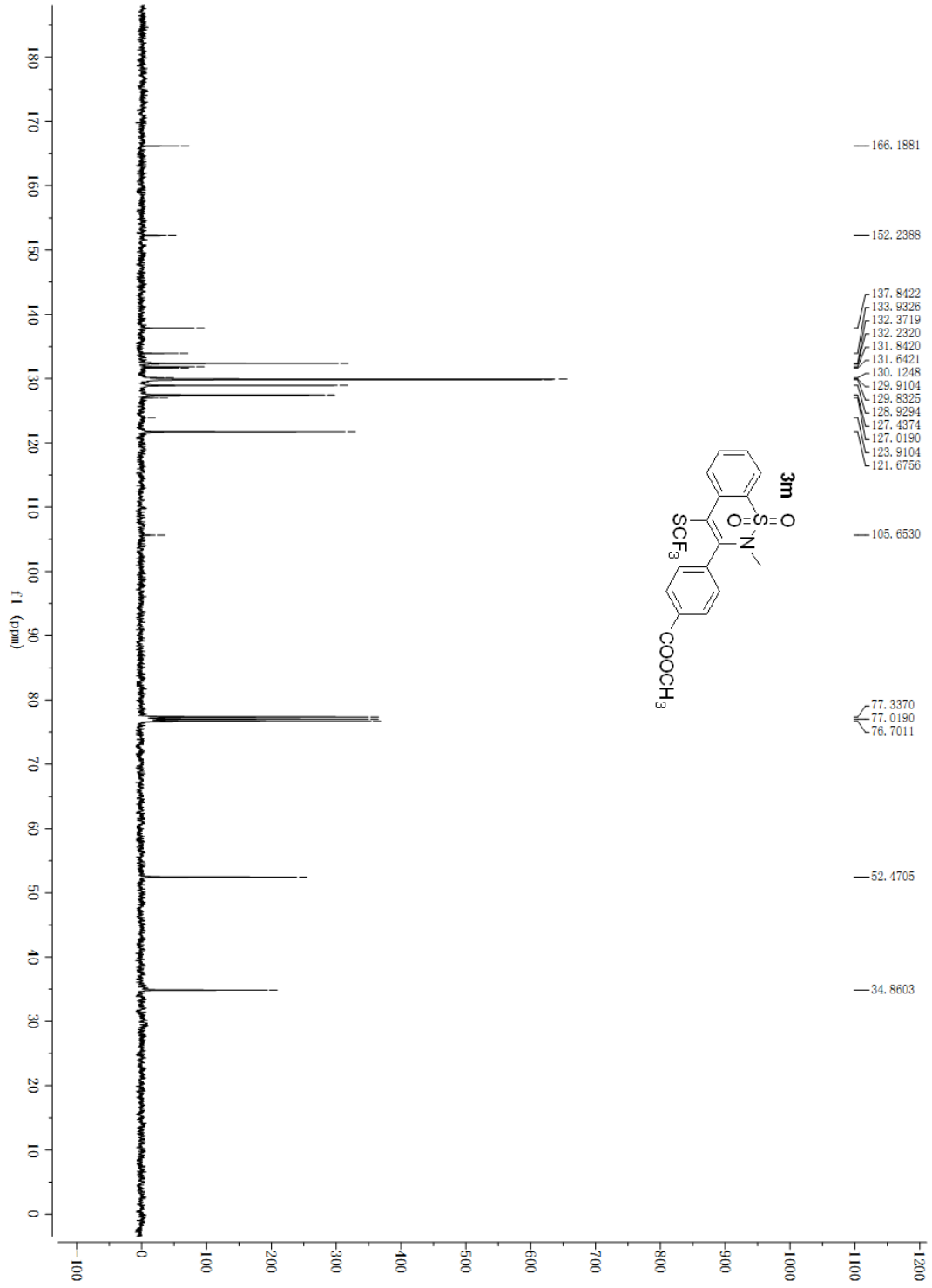
1.08
1.06
2.06
3.08
3.05
f1 (ppm)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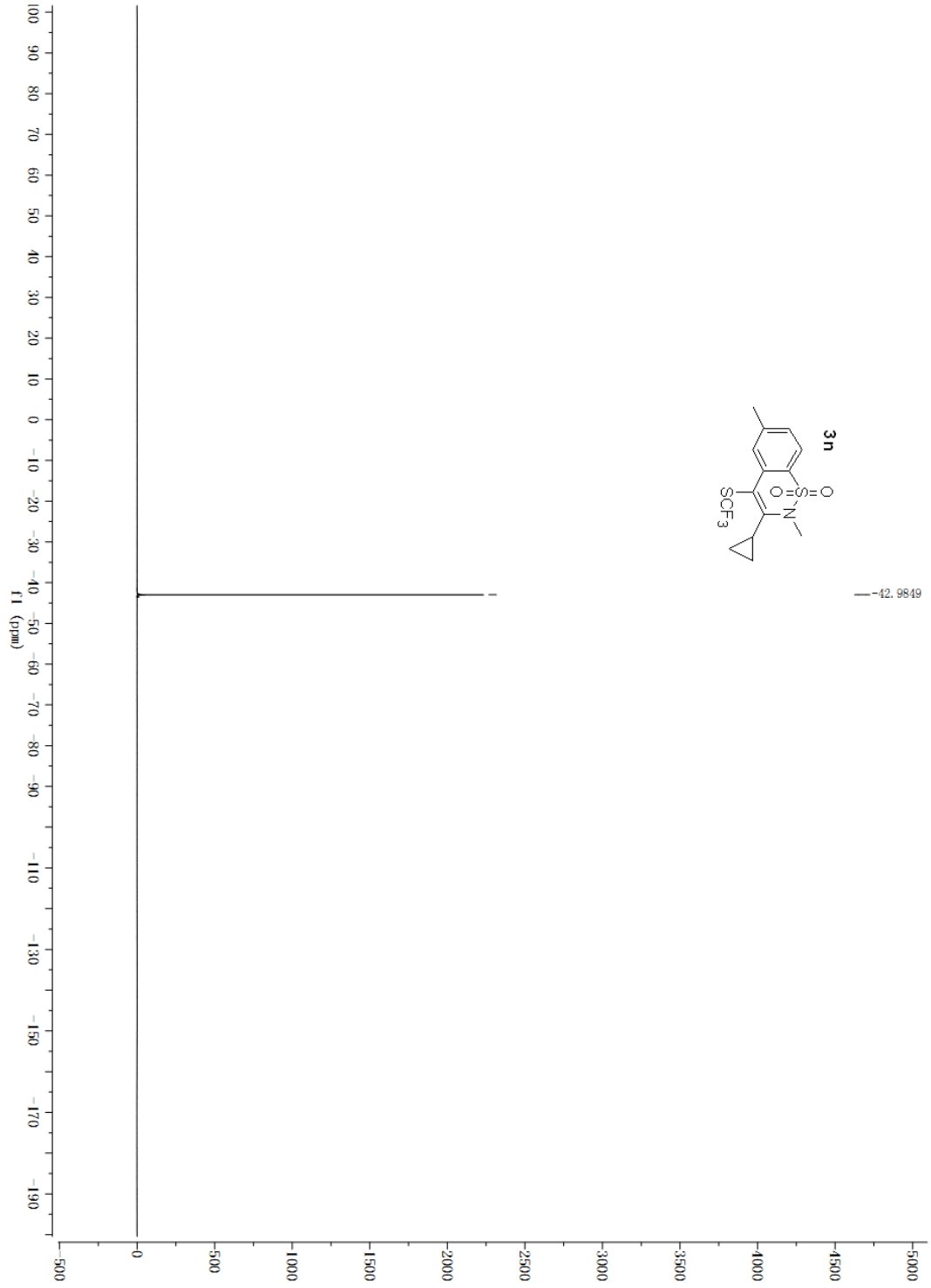
129.8325
128.9294
127.4374
127.0190
123.9104
121.6756
105.6530
77.3370
77.0190
76.7011
52.4705
34.8603
3m
SCF3
COOCH3
f1 (ppm)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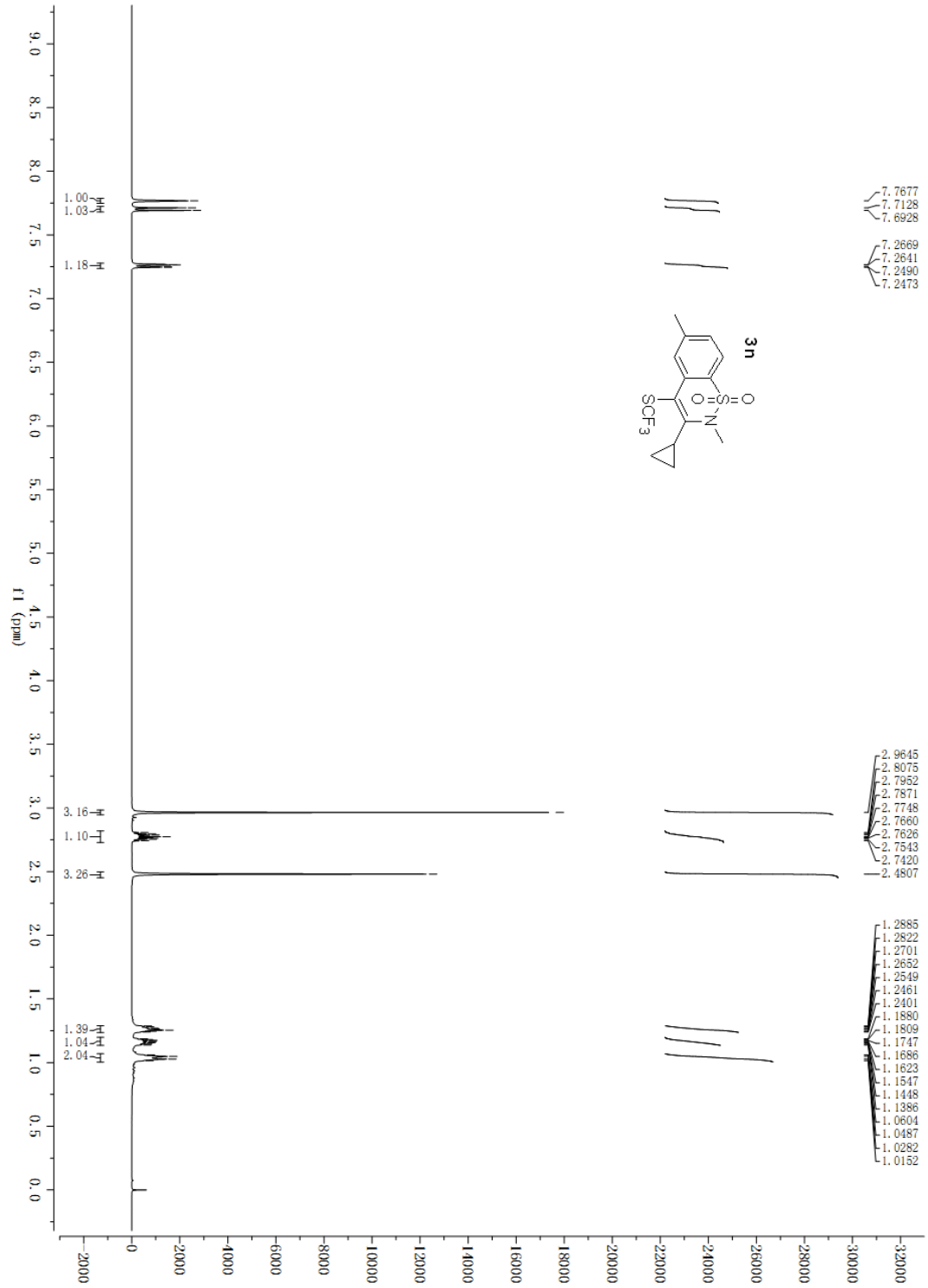
SCF3
-42.9849
f1 (ppm)


3n
SCF3
f1 (ppm)
1.00
1.03
1.18
3.16
1.10
3.26
1.39
1.04
2.04
7.7677
7.7128
7.6928
7.2669
7.2641
7.2490
7.2473
2.9645
2.8075
2.7952
2.7871
2.7748
2.7660
2.7626
2.7543
2.7420
2.4807
1.2885
1.2822
1.2701
1.2652
1.2549
1.2461
1.2401
1.1880
1.1809
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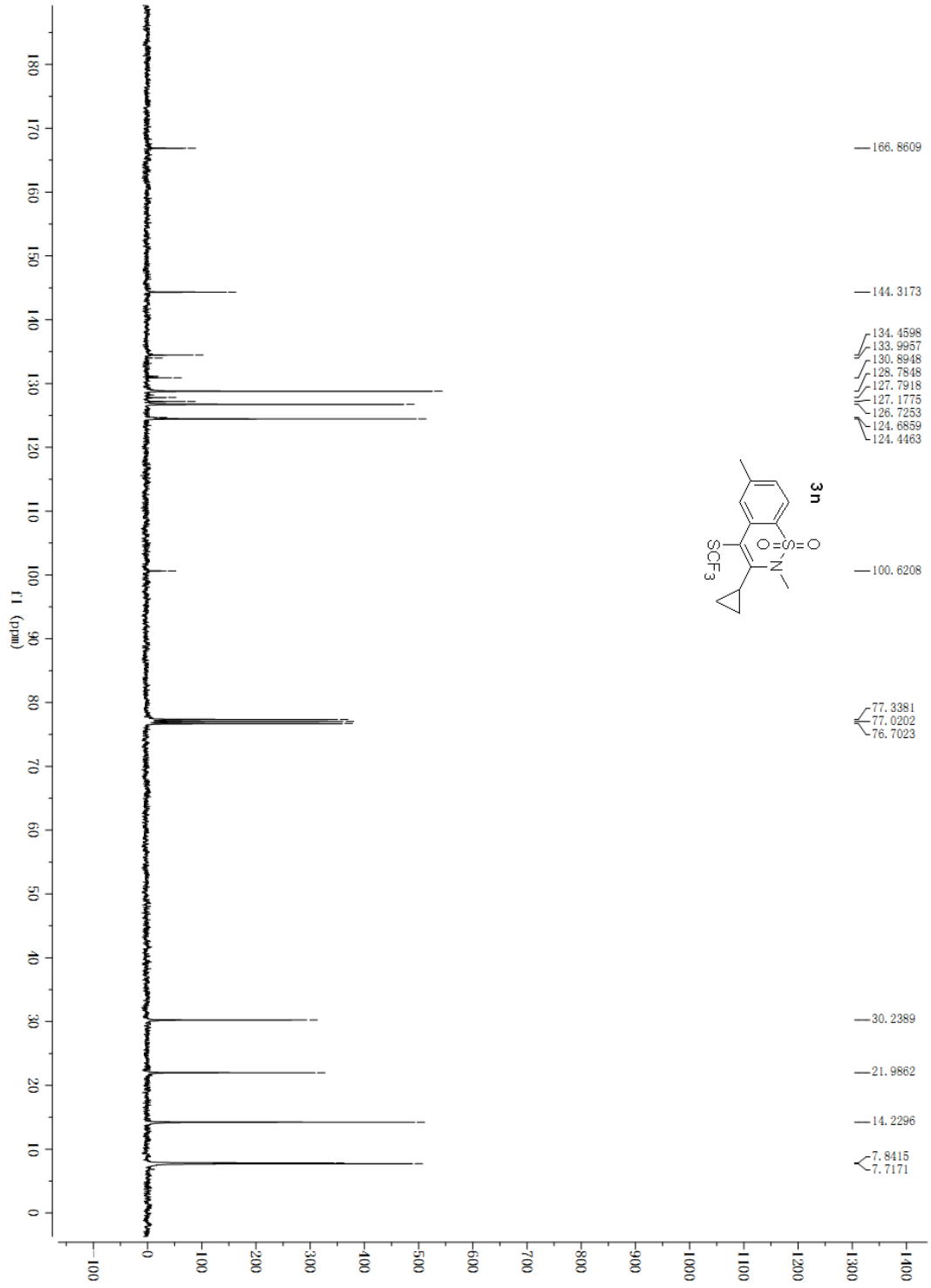
1.0282
1.0152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100.6208
77.3381
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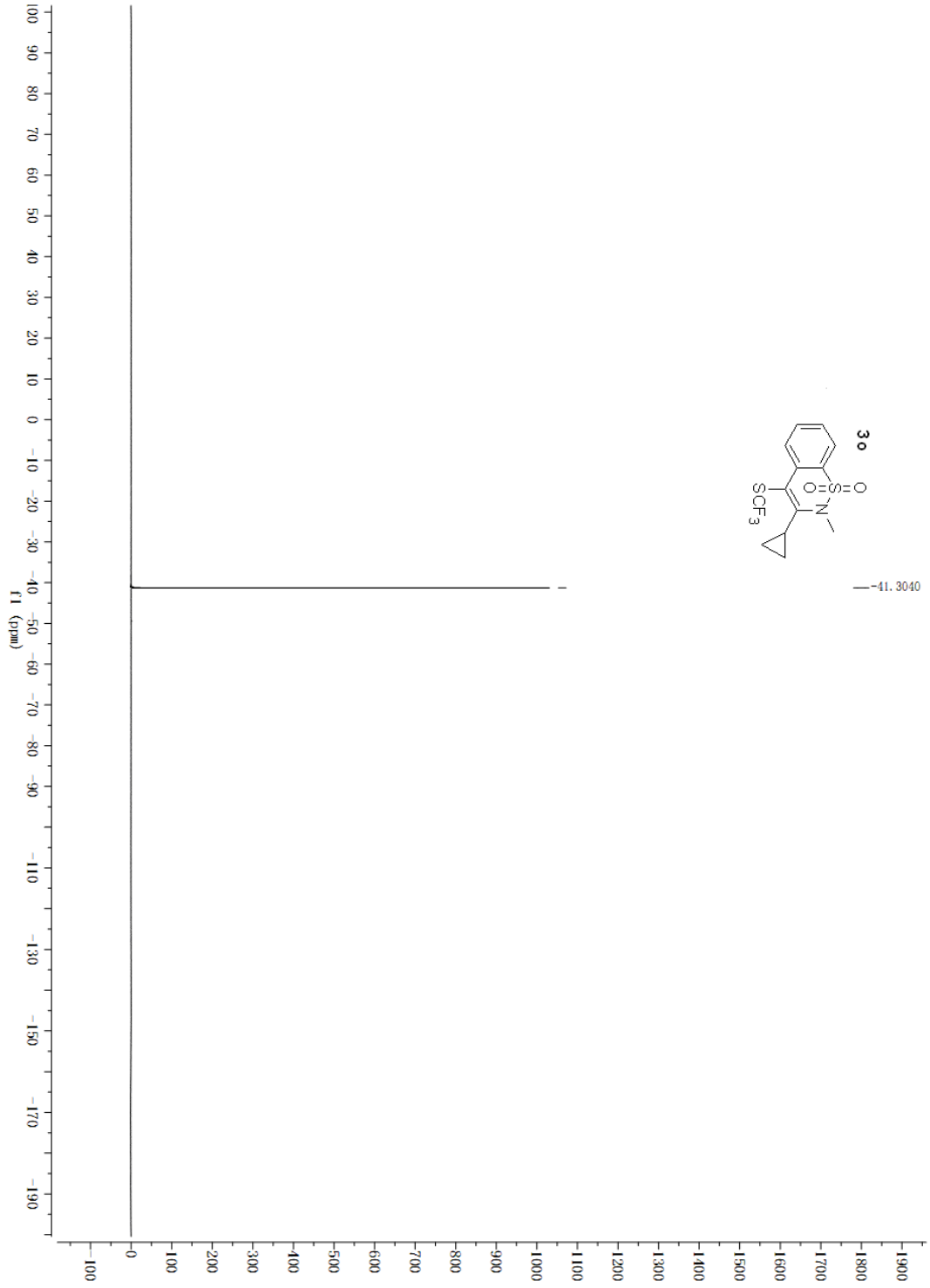
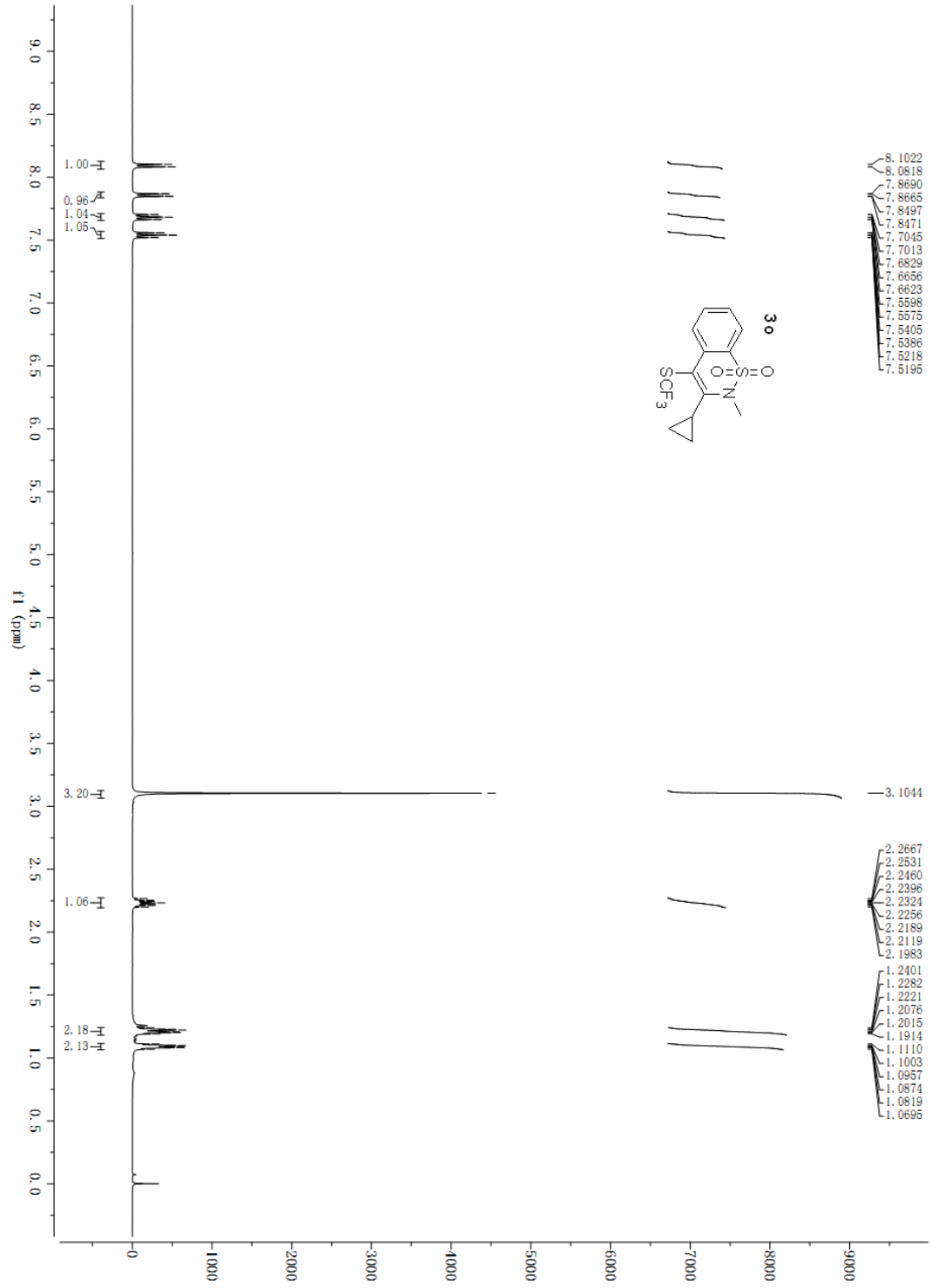
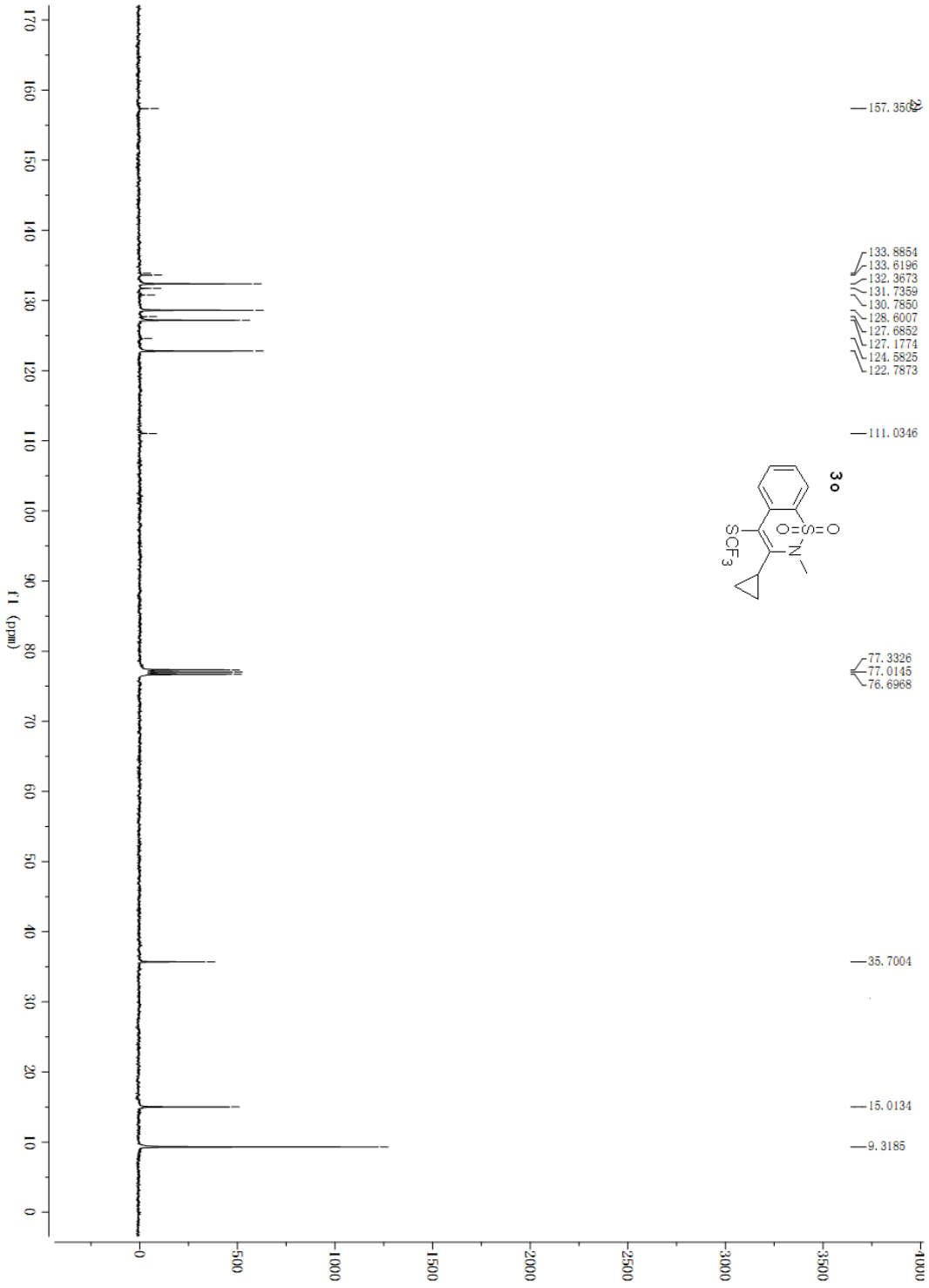
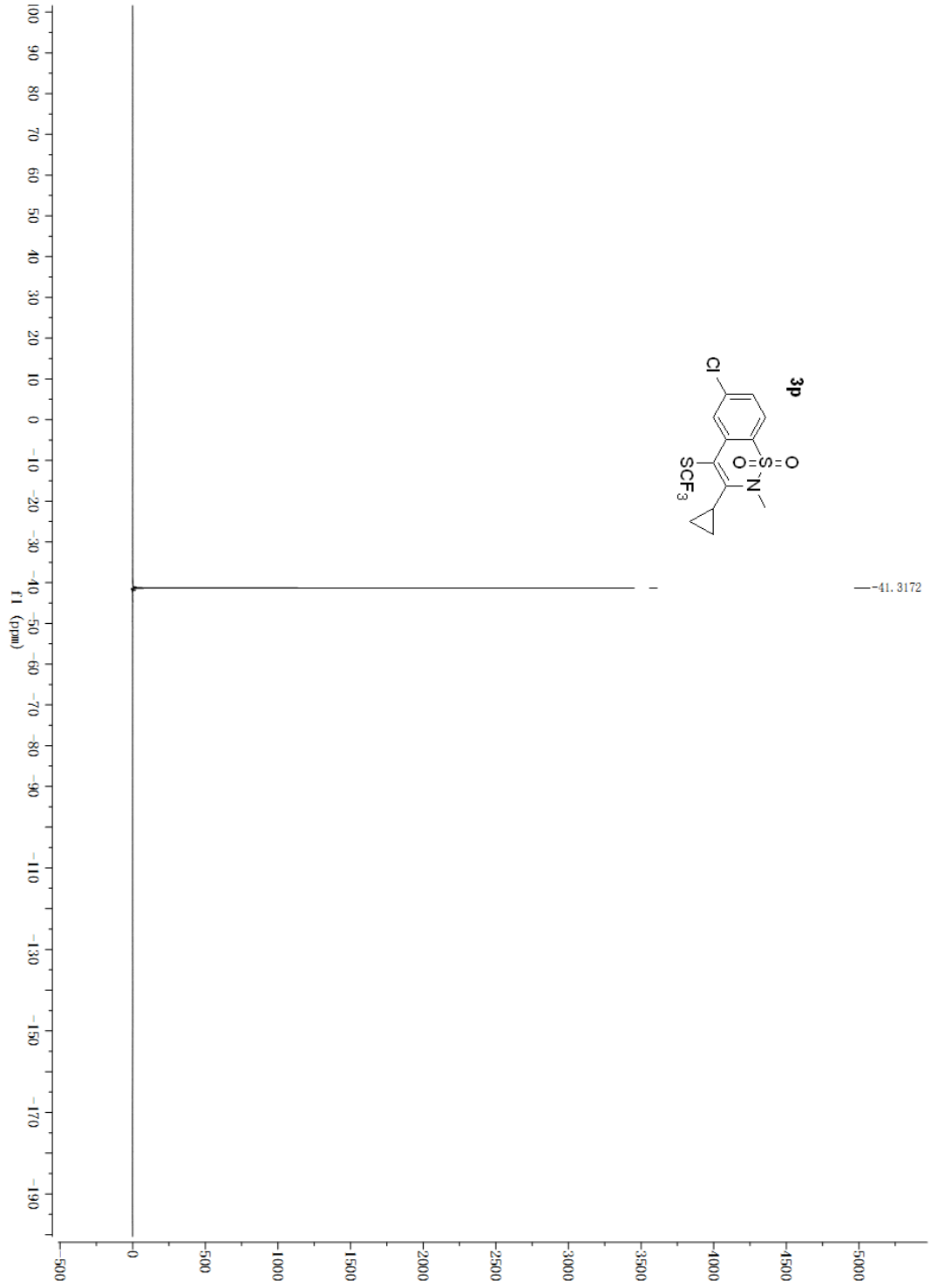
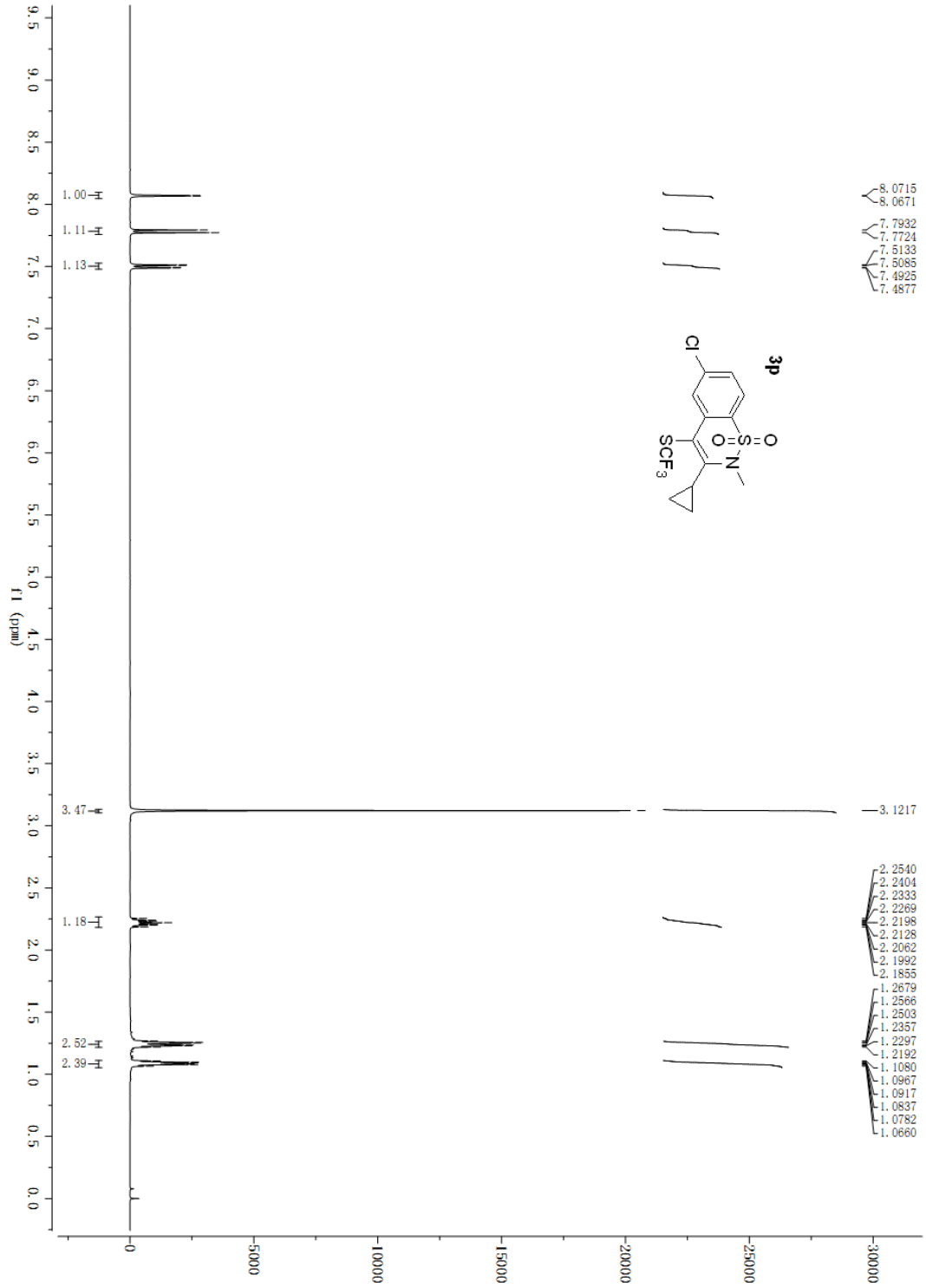
7.7171
3n
SCF3
f1 (ppm)

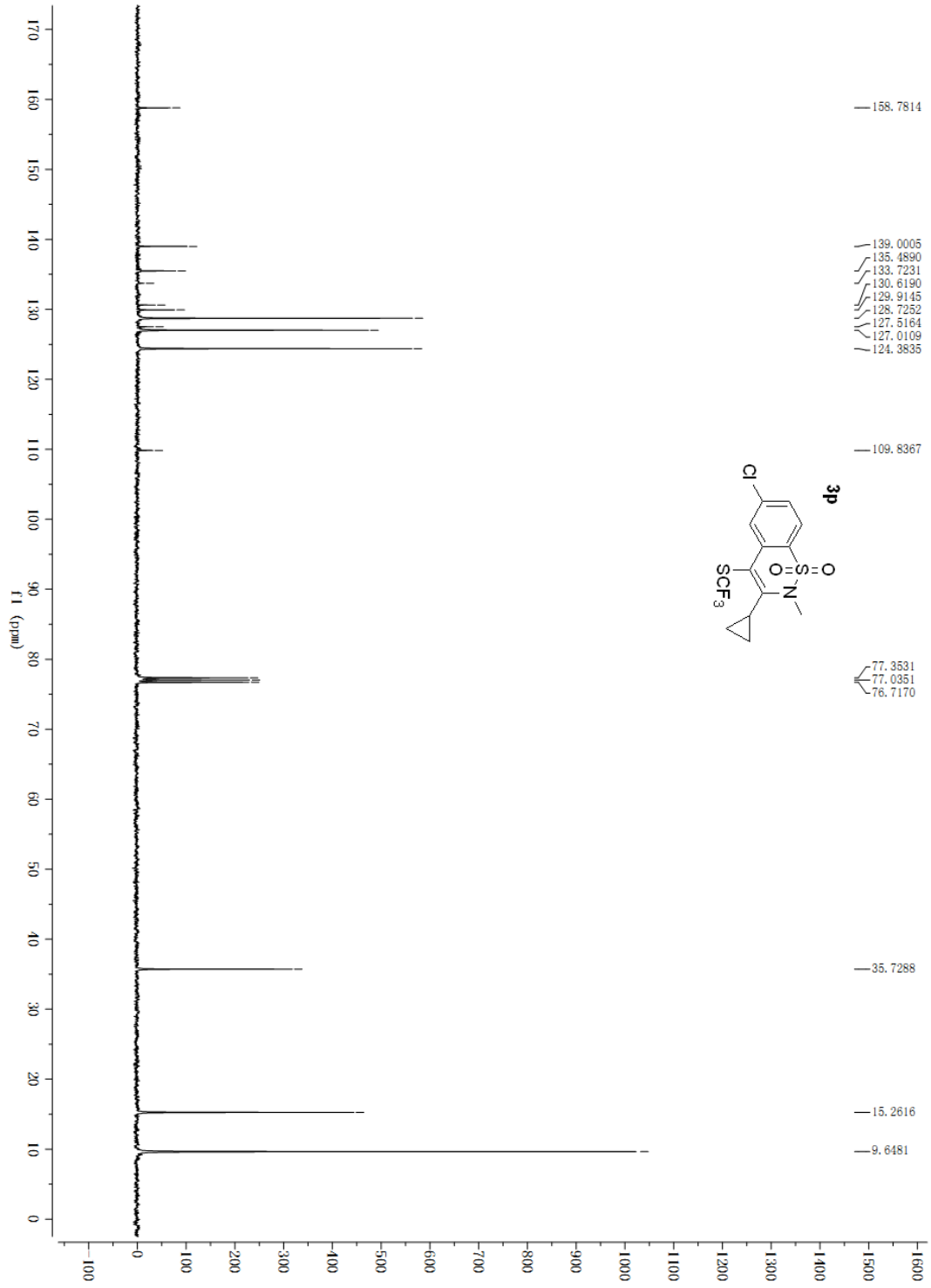

3o
SCF3
-41.3040
f1 (ppm)


3o
SCF3
1.00
0.96
1.04
1.05
3.20
1.06
2.18
2.13
8.1022
8.0818
7.8690
7.8665
7.8497
7.8471
7.7045
7.7013
7.6829
7.6656
7.6623
7.5598
7.5575
7.5405
7.5386
7.5218
7.5195
3.1044
2.2667
2.2531
2.2460
2.2396
2.2324
2.2256
2.2189
2.2119
2.1983
1.2401
1.2282
1.2221
1.2076
1.2015
1.1914
1.1110
1.1003
1.0957
1.0874
1.0819
1.0695
f1 (ppm)


157.3502
133.8854
133.6196
132.3673
131.7359
130.7850
128.6007
127.6852
127.1774
124.5825
122.7873
111.0346
77.3326
77.0145
76.6968
35.7004
15.0134
9.3185
3o
SCF3
O=S=O
N
f1 (ppm)
0
500
1000
1500
2000
2500
3000
3500
4000


3p
Cl
SCF3
O
S
O
N
-41.3172
f1 (ppm)


3p
Cl
SCF3
O
S
N
f1 (ppm)
1.00
1.11
1.13
3.47
1.18
2.52
2.39
8.0715
8.0671
7.7932
7.7724
7.5133
7.5085
7.4925
7.4877
3.1217
2.2540
2.2404
2.2333
2.2269
2.2198
2.2128
2.2062
2.1992
2.1855
1.2679
1.2566
1.2503
1.2357
1.2297
1.2192
1.1080
1.0967
1.0917
1.0837
1.0782
1.0660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135.4890
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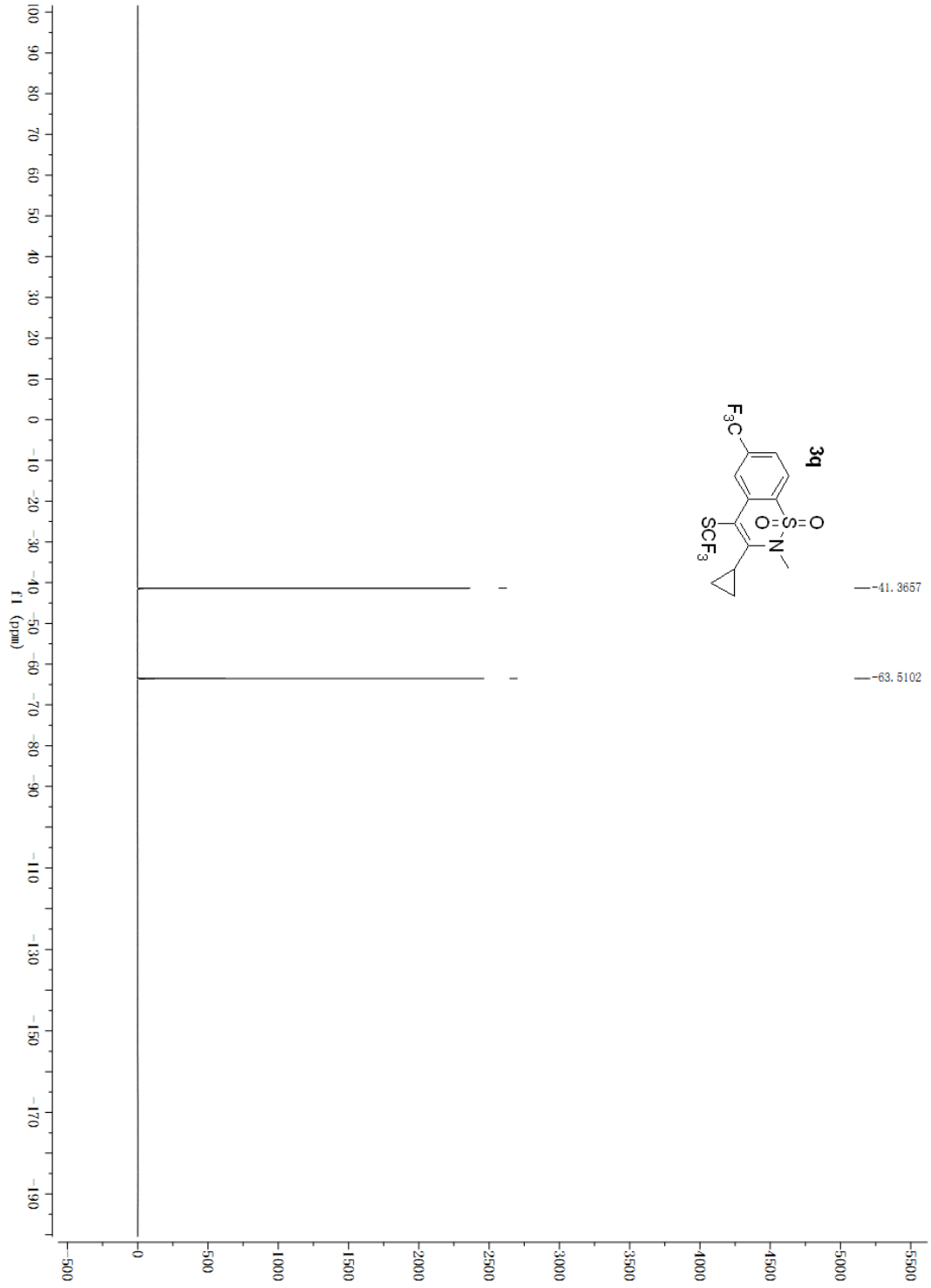
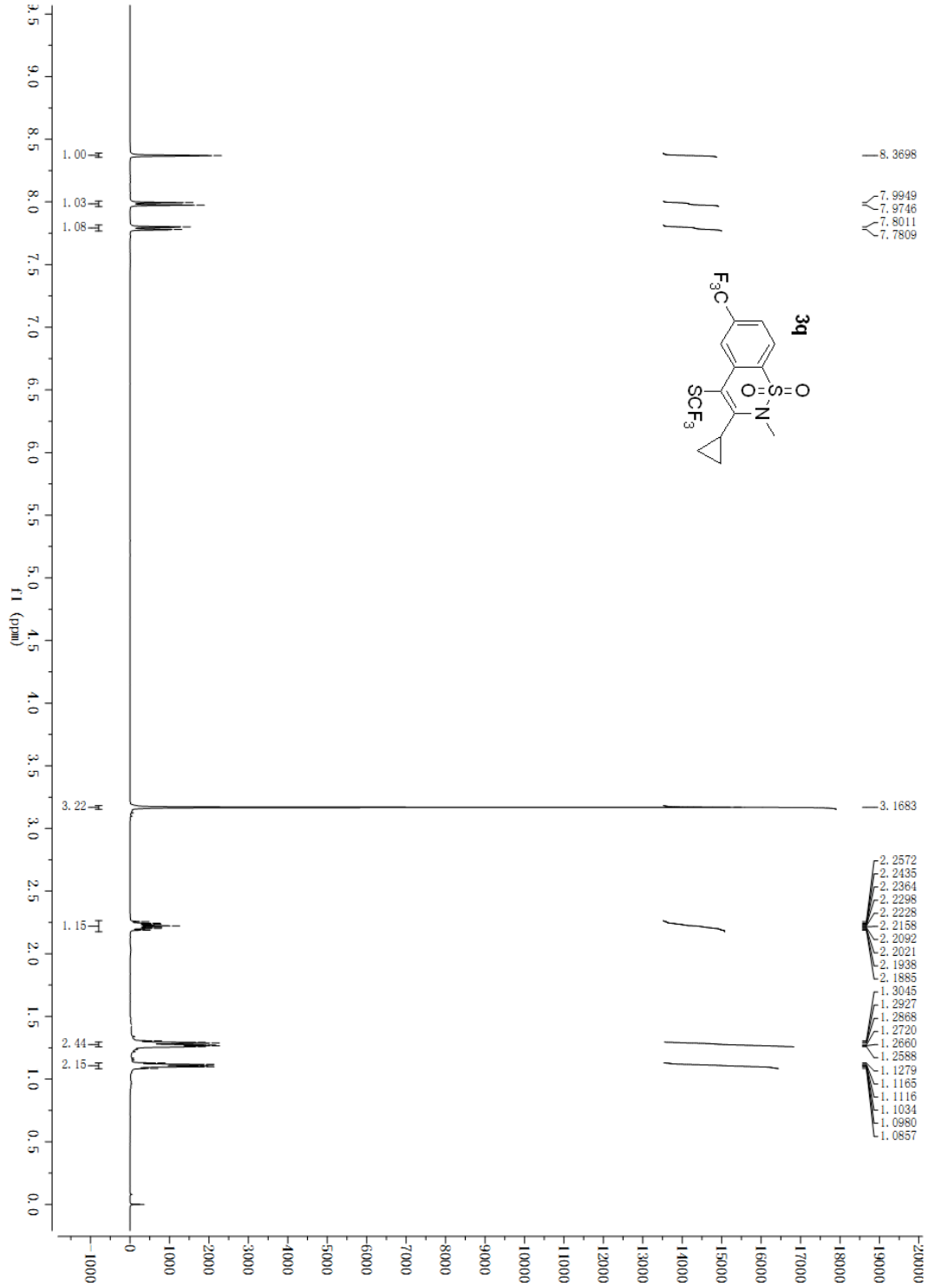
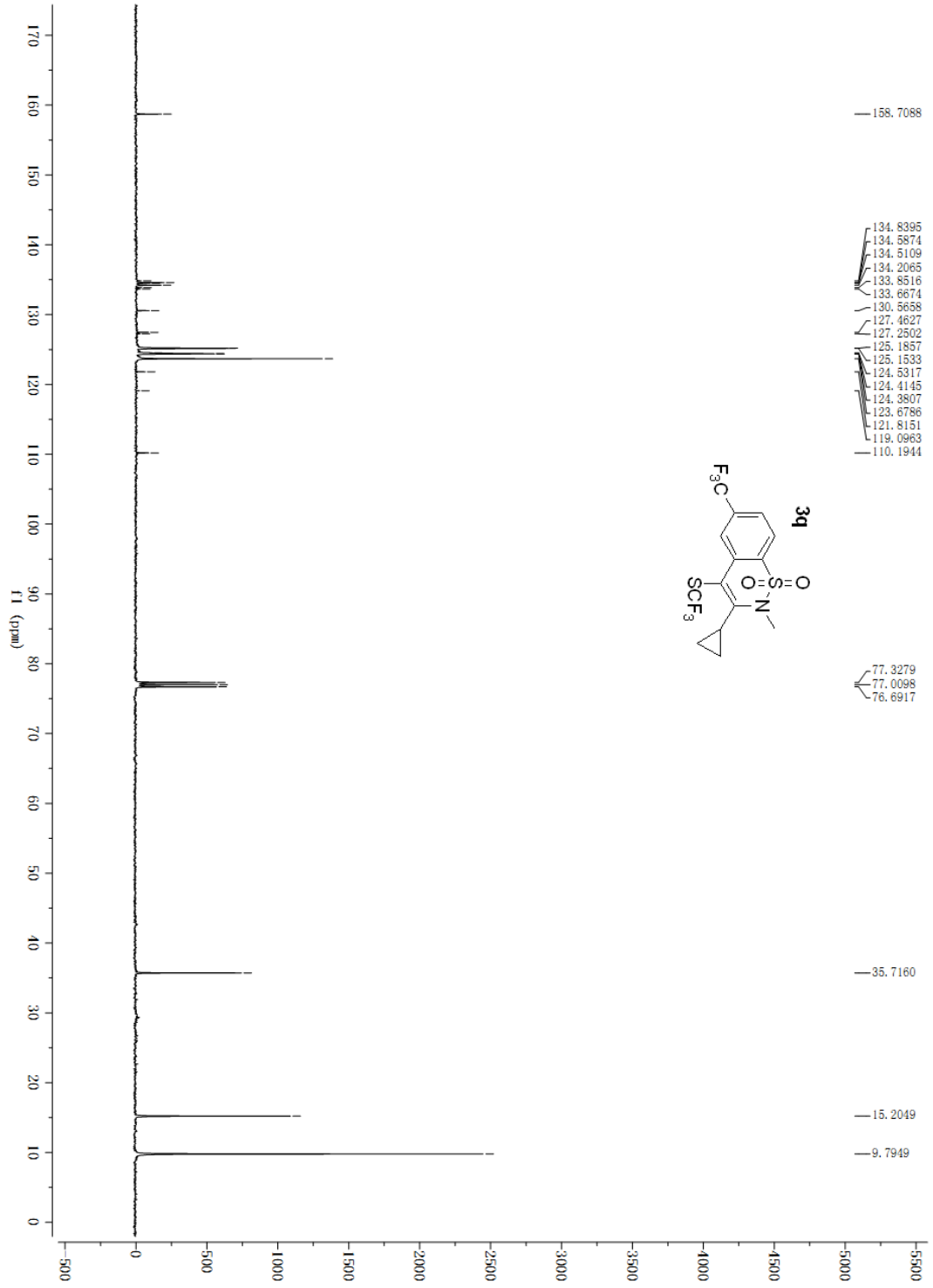
130.6190
129.9145
128.7252
127.5164
127.0109
124.3835
109.8367
77.3531
77.0351
76.7170
35.7288
15.2616
9.6481
3p
Cl
SCF3
O
S
O
N
f1 (ppm)


3q
F3C
SCF3
O
S
O
N
-41.3657
-63.5102
f1 (ppm)


3q
F3C
SCF3
O
S
O
N
1.00
1.03
1.08
3.22
1.15
2.44
2.15
8.3698
7.9949
7.9746
7.8011
7.7809
3.1683
2.2572
2.2435
2.2364
2.2298
2.2228
2.2158
2.2092
2.2021
2.1938
2.1885
1.3045
1.2927
1.2868
1.2720
1.2660
1.2588
1.1279
1.1165
1.1116
1.1034
1.0980
1.0857
f1 (ppm)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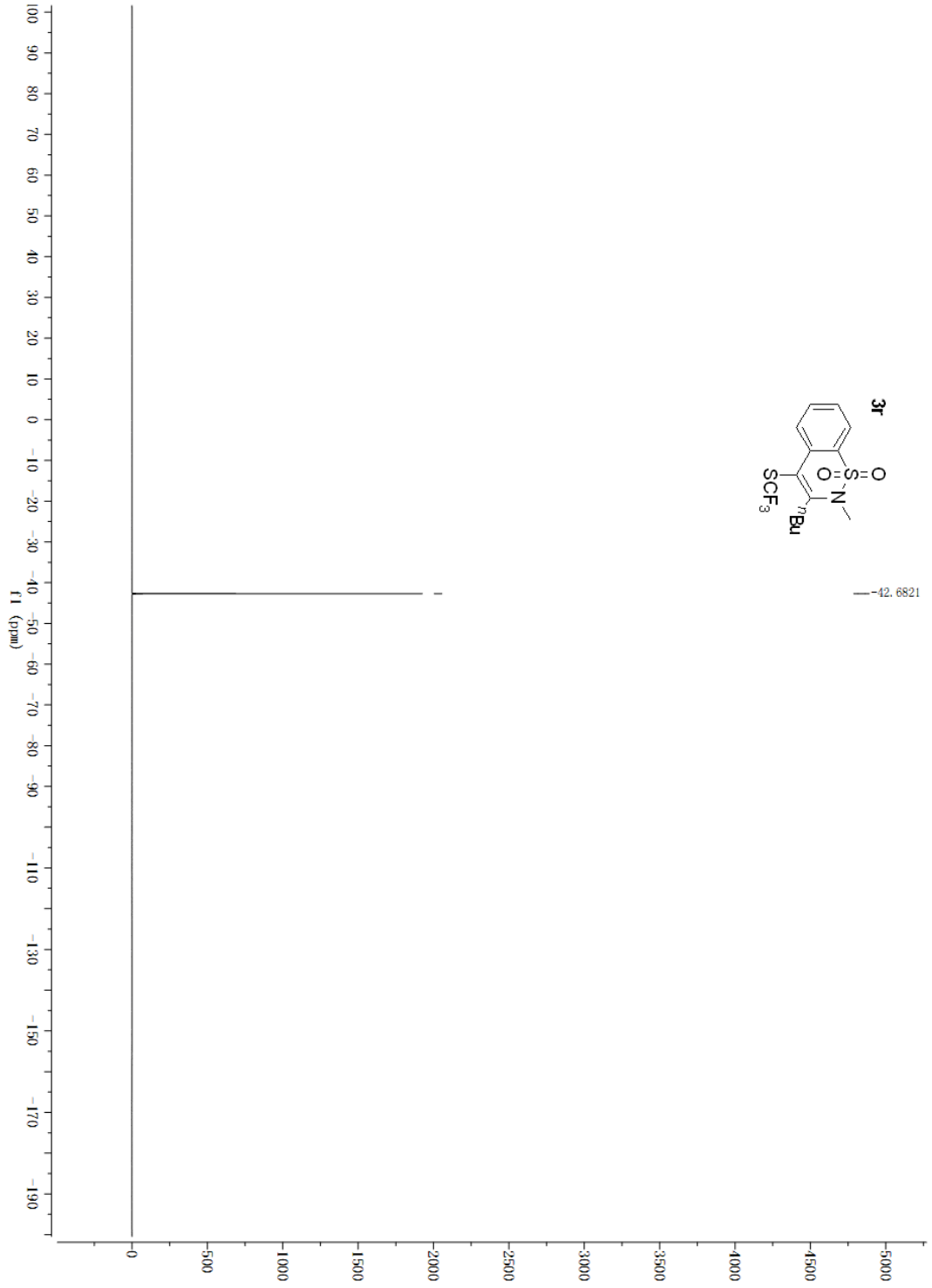
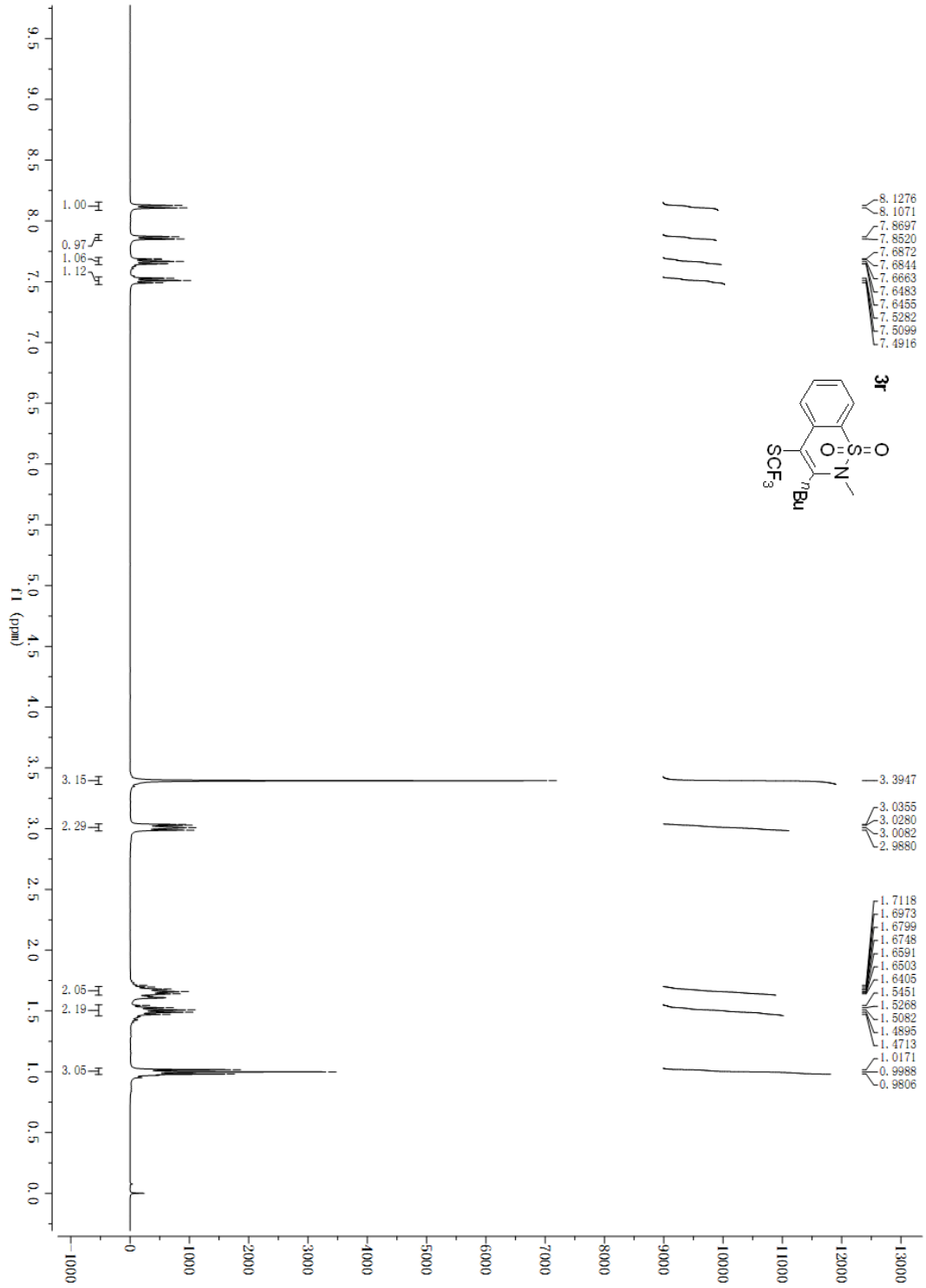
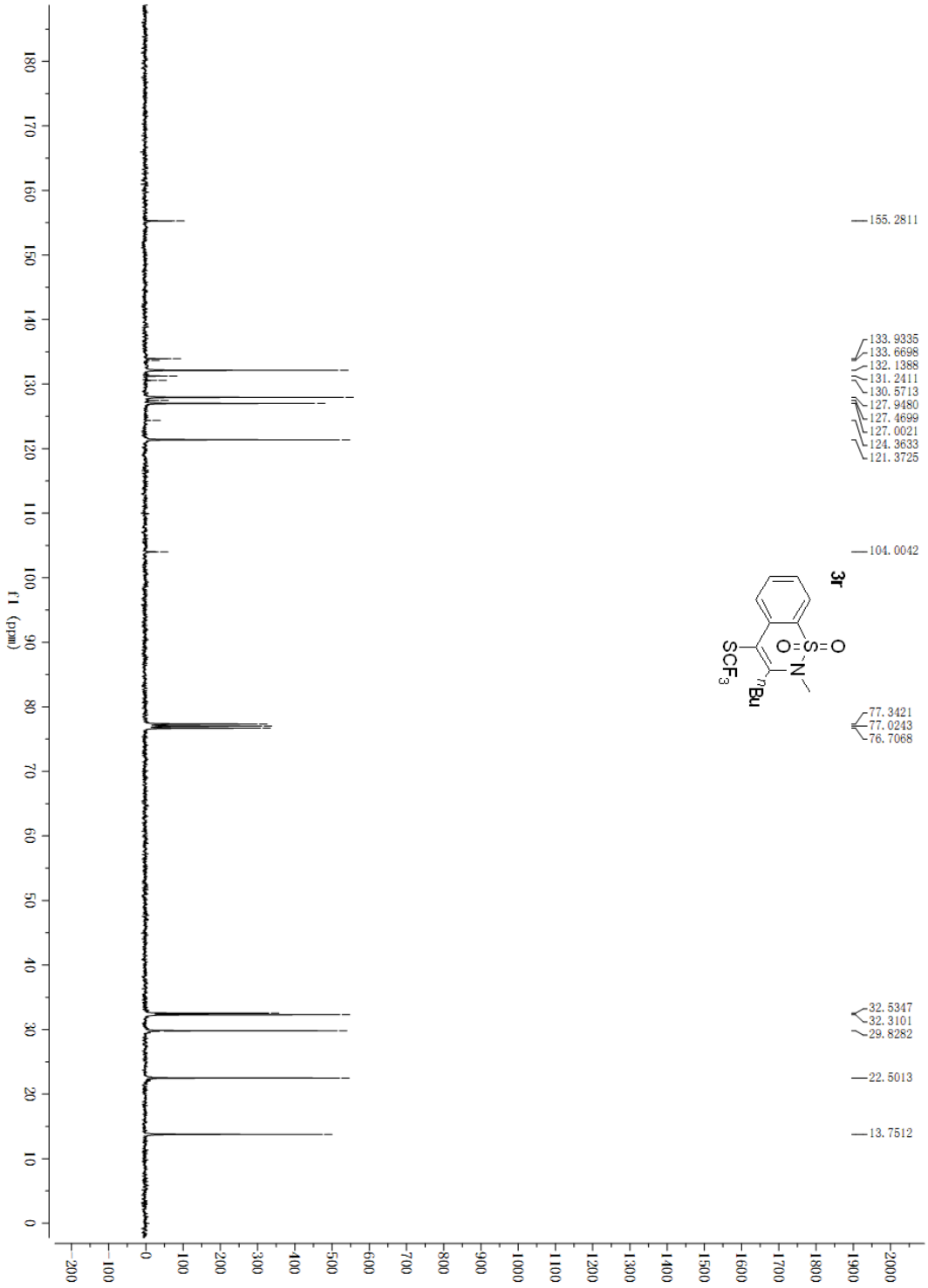
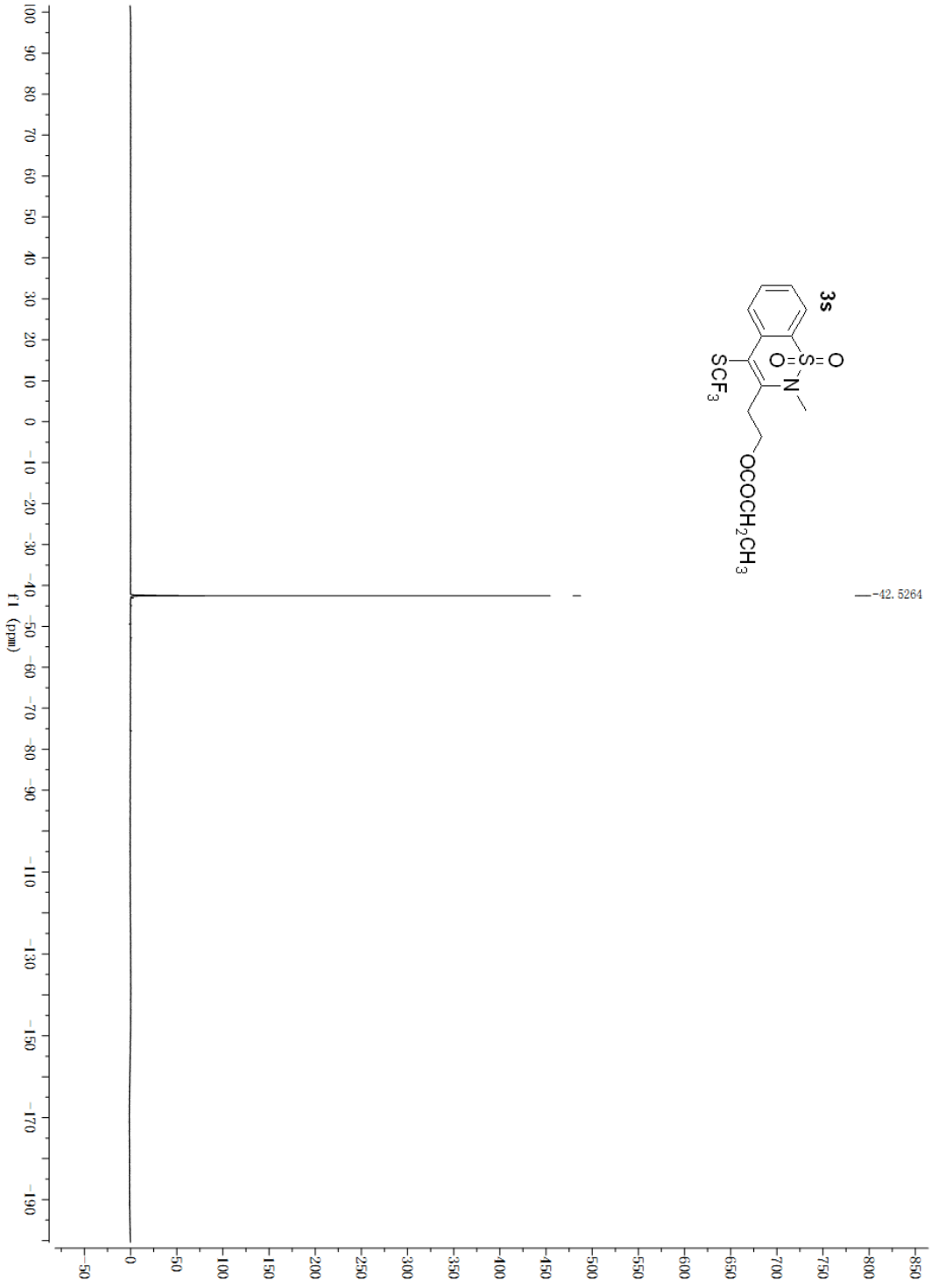
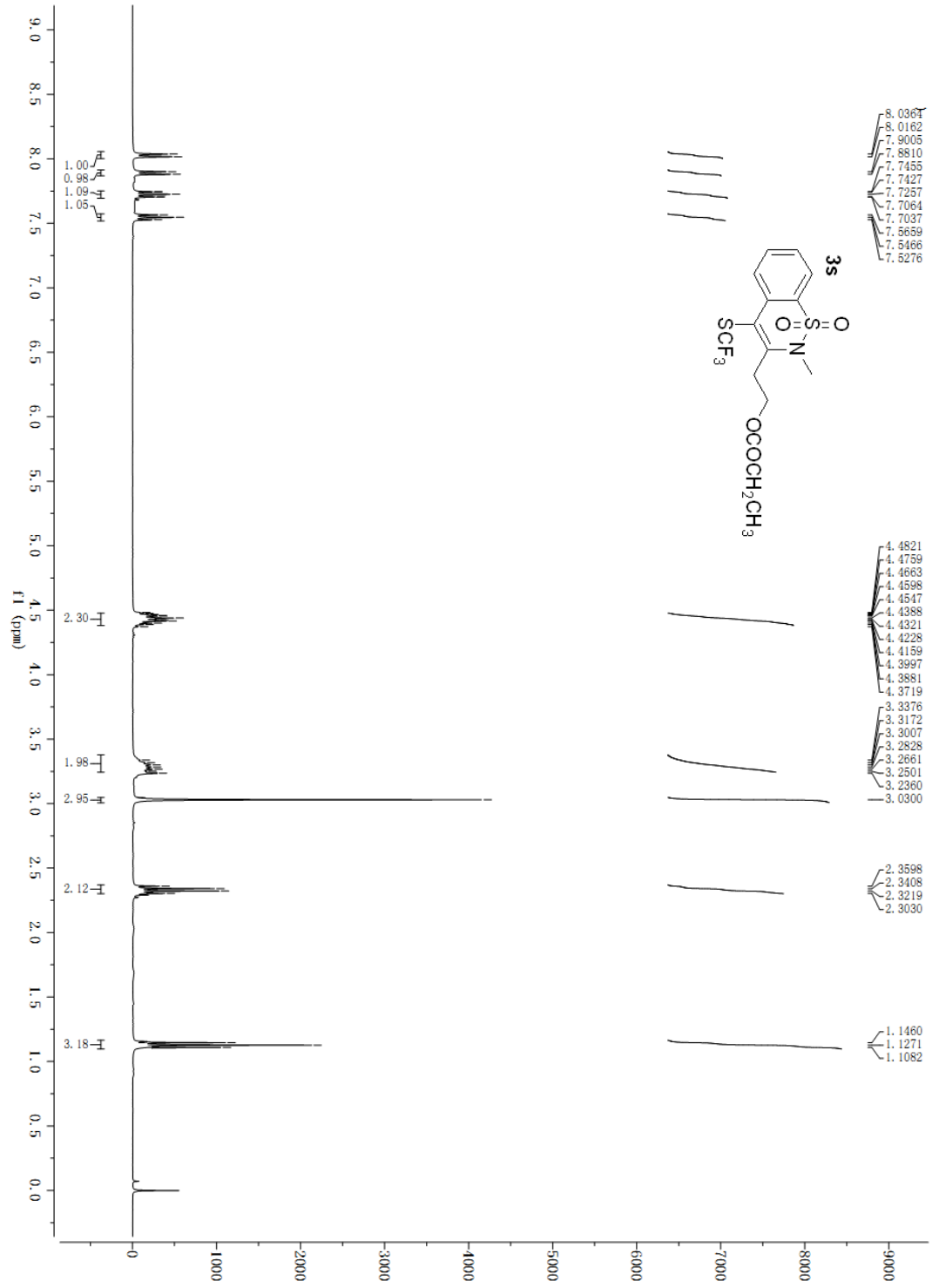
134.8395
134.5874
134.5109
134.2065
133.8516
133.6674
130.5658
127.4627
127.2502
125.1857
125.1533
124.5317
124.4145
124.3807
123.6786
121.8151
119.0963
110.1944
77.3279
77.0098
76.6917
35.7160
15.2049
9.7949
3q
F3C
SCF3
O
S
N
f1 (ppm)

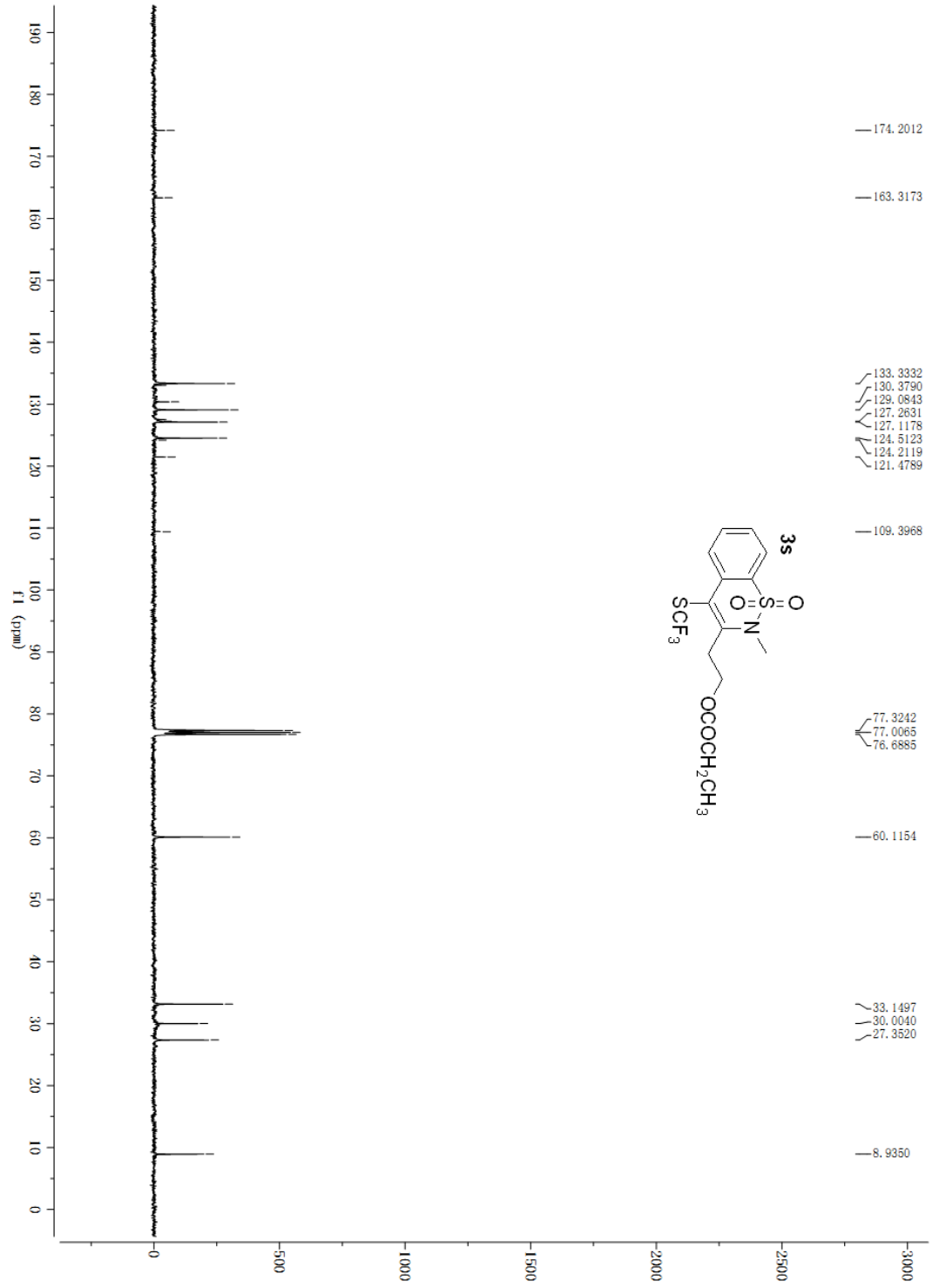

3r
SCF3
nBu
-42.6821
f1 (ppm)

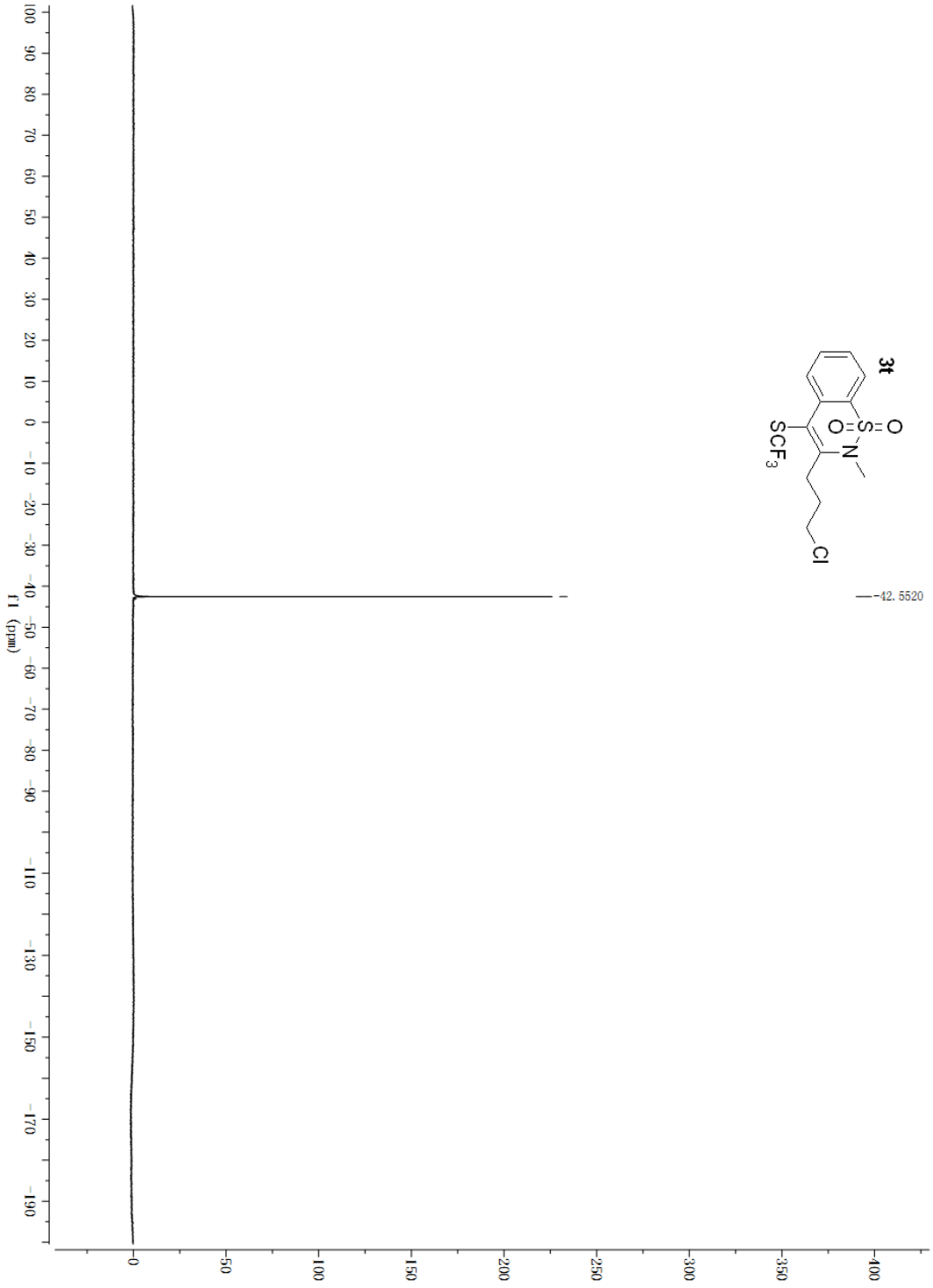

3r
SCF3
nBu
O=S=O
N
f1 (ppm)
1.00
0.97
1.06
1.12
3.15
2.29
2.05
2.19
3.05
8.1276
8.1071
7.8697
7.8520
7.6872
7.6844
7.6663
7.6483
7.6455
7.5282
7.5099
7.4916
3.3947
3.0355
3.0280
3.0082
2.9880
1.7118
1.6973
1.6799
1.6748
1.6591
1.6503
1.6405
1.5451
1.5268
1.5082
1.4895
1.4713
1.0171
0.9988
0.9806

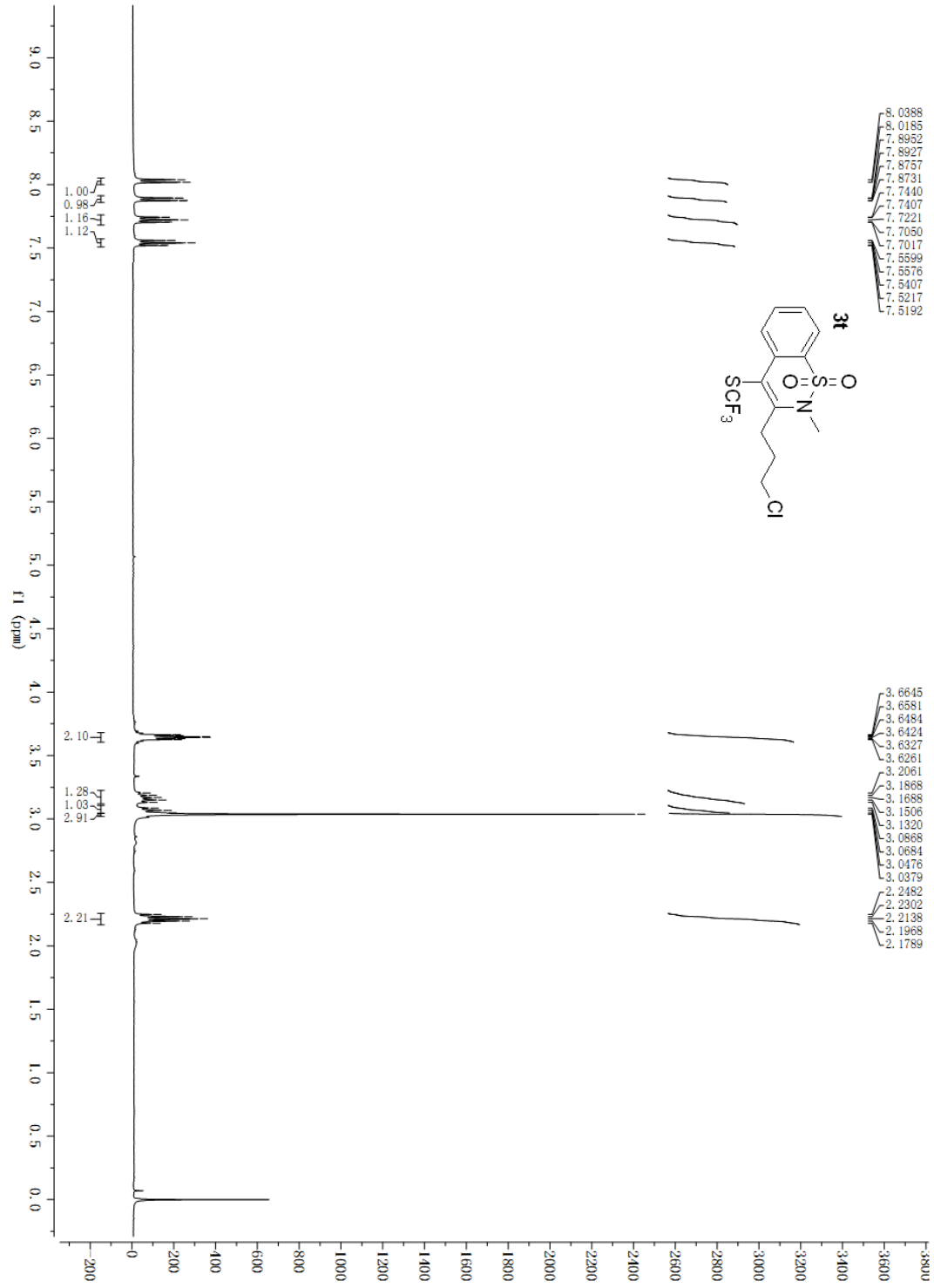

155.2811
133.9335
133.6698
132.1388
131.2411
130.5713
127.9480
127.4699
127.0021
124.3633
121.3725
104.0042
77.3421
77.0243
76.7068
32.5347
32.3101
29.8282
22.5013
13.7512
3r
f1 (ppm)

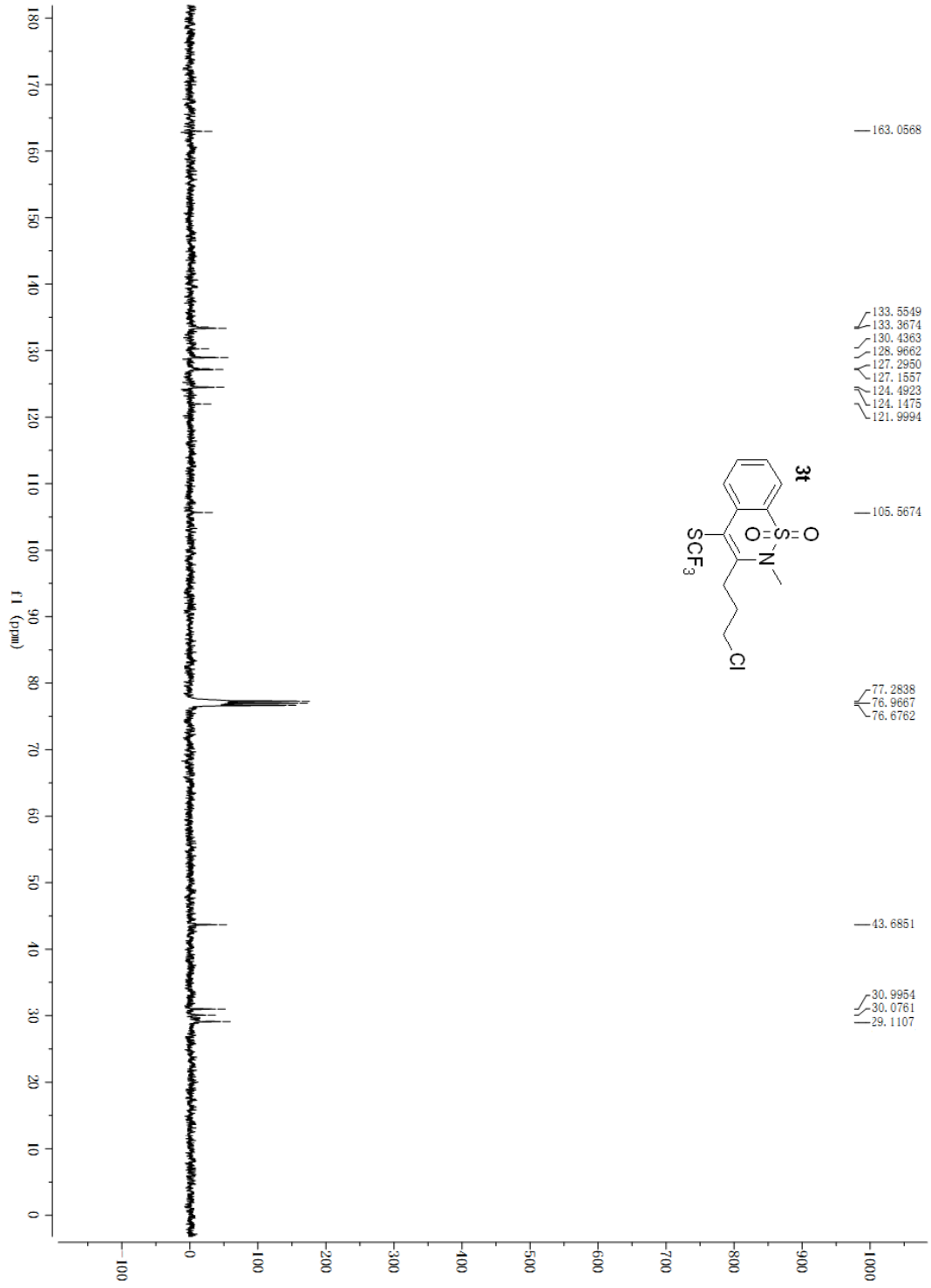

3s
SCF3
OCOCH2CH3
-42.5264
f1 (ppm)

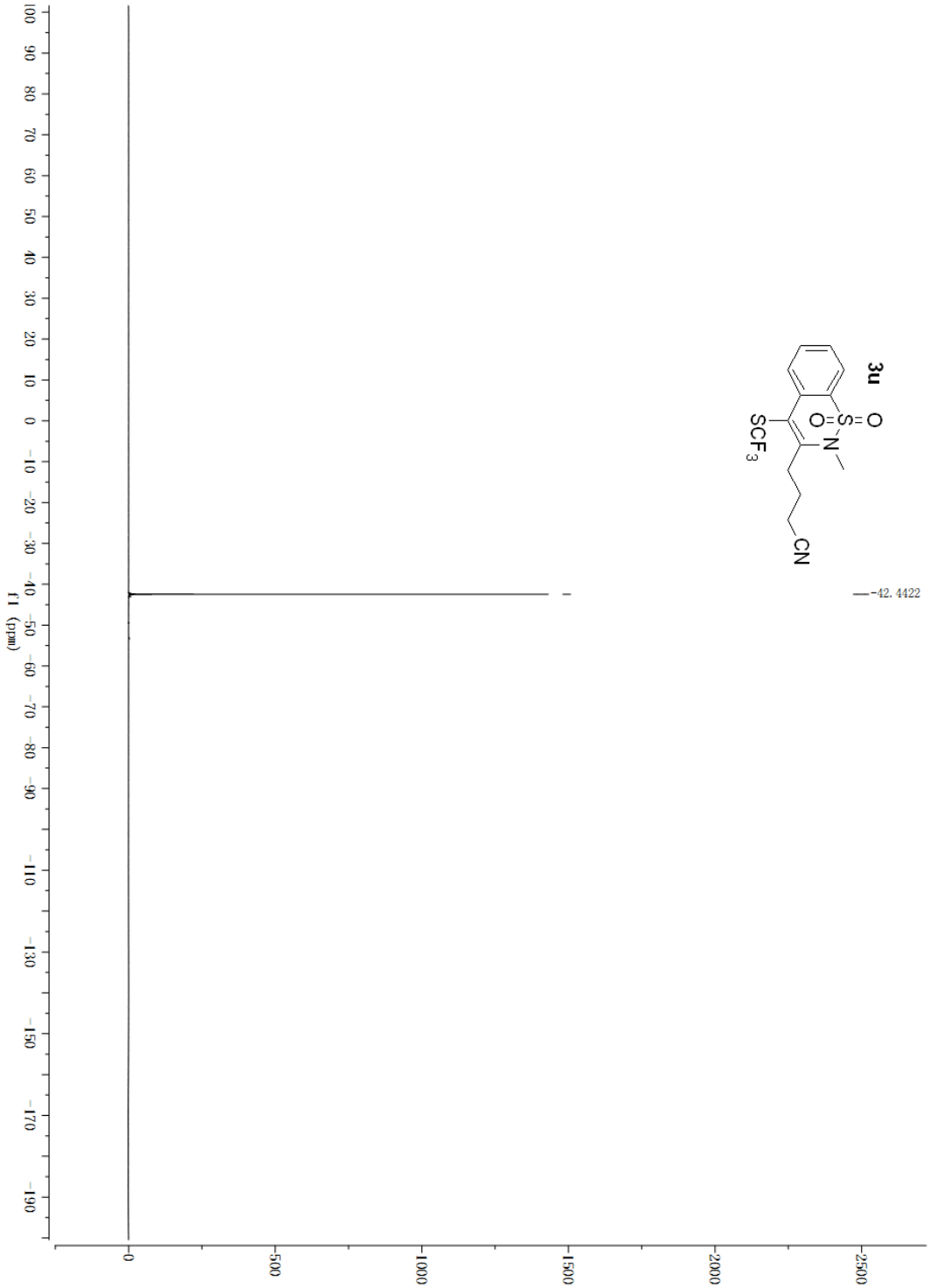

3s
SCF3
OCOCH2CH3
f1 (ppm)
1.00
0.98
1.09
1.05
2.30
1.98
2.95
2.12
3.18
8.0361
8.0162
7.9005
7.8810
7.7455
7.7427
7.7257
7.7064
7.7037
7.5659
7.5466
7.5276
4.4821
4.4759
4.4663
4.4598
4.4547
4.4388
4.4321
4.4228
4.4159
4.3997
4.3881
4.3719
3.3376
3.3172
3.3007
3.2828
3.2661
3.2501
3.2360
3.0300
2.3598
2.3408
2.3219
2.3030
1.1460
1.1271
1.1082

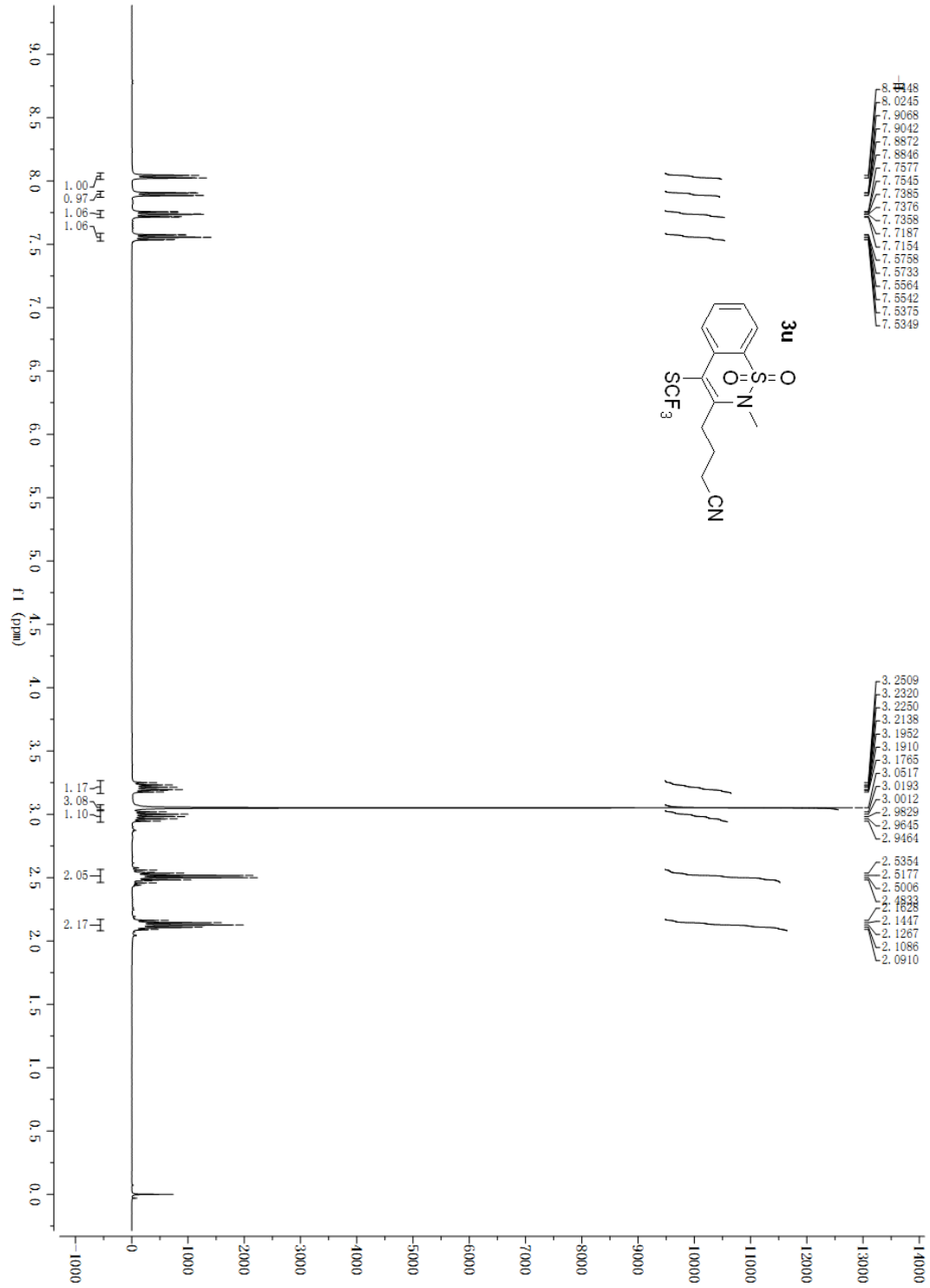

174.2012
163.3173
133.3332
130.3790
129.0843
127.2631
127.1178
124.5123
124.2119
121.4789
109.3968
77.3242
77.0065
76.6885
60.1154
33.1497
30.0040
27.3520
8.9350
3s
SCF3
OCOCH2CH3
f1 (ppm)

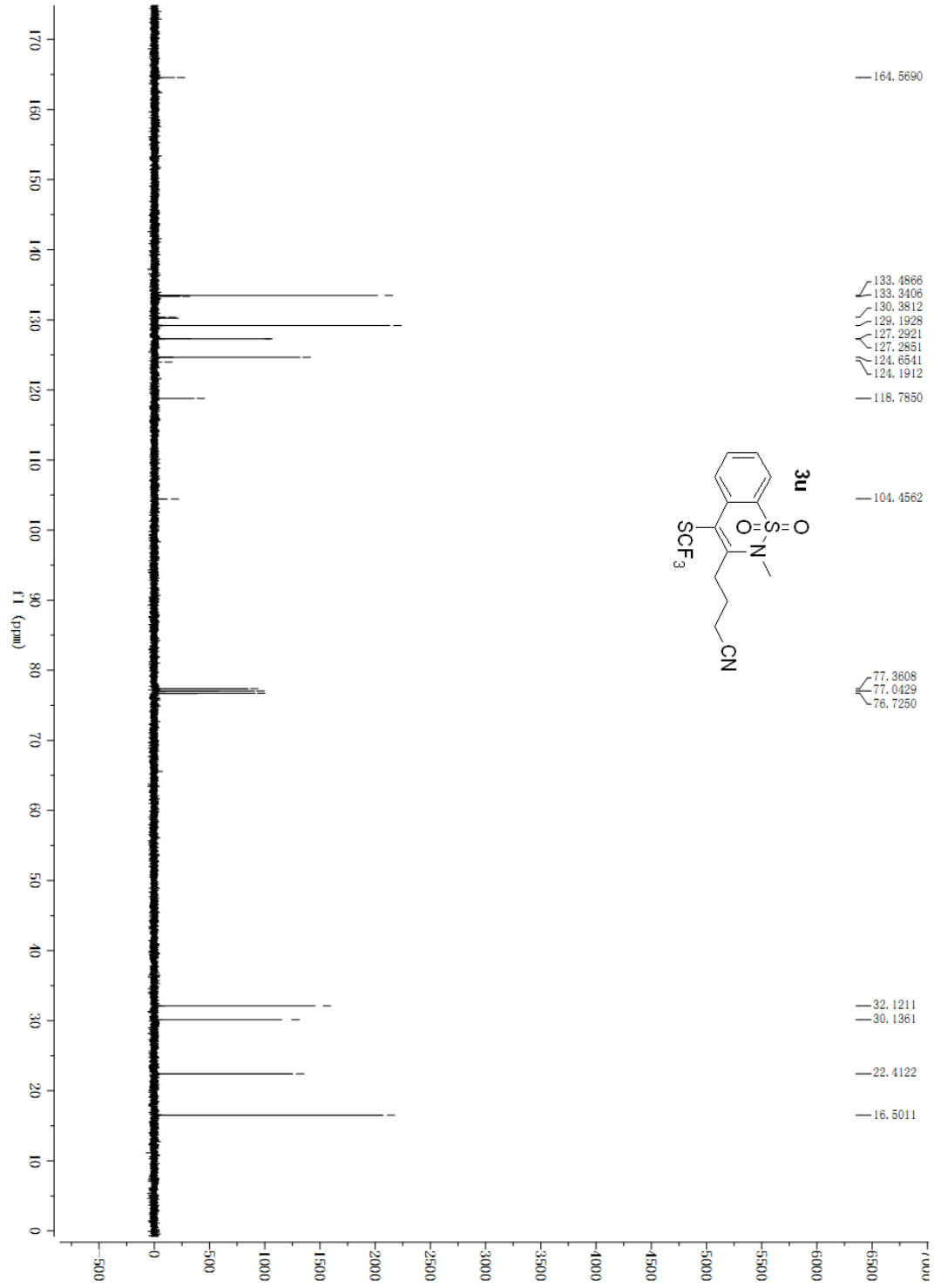

3t
O
S
O
N
SCF3
Cl
-42.5520
f1 (ppm)
100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190
0 50 100 150 200 250 300 350 400


3t
SCF3
Cl
f1 (ppm)
1.00
0.98
1.16
1.12
2.10
1.28
1.03
2.91
2.21
8.0388
8.0185
7.8952
7.8927
7.8757
7.8731
7.7440
7.7407
7.7221
7.7050
7.7017
7.5599
7.5576
7.5407
7.5217
7.5192
3.6645
3.6581
3.6484
3.6424
3.6327
3.6261
3.2061
3.1868
3.1688
3.1506
3.1320
3.0868
3.0684
3.0476
3.0379
2.2482
2.2302
2.2138
2.1968
2.1789


163.0568
133.5549
133.3674
130.4363
128.9662
127.2950
127.1557
124.4923
124.1475
121.9994
105.5674
77.2838
76.9667
76.6762
43.6851
30.9954
30.0761
29.1107
3t
SCF3
Cl
f1 (ppm)


3u
O
S
O
N
SCF3
CN
-42.4422
f1 (ppm)
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
0
500
1000
1500
2000
2500


3u
SCF3
CN
f1 (ppm)


164.5690
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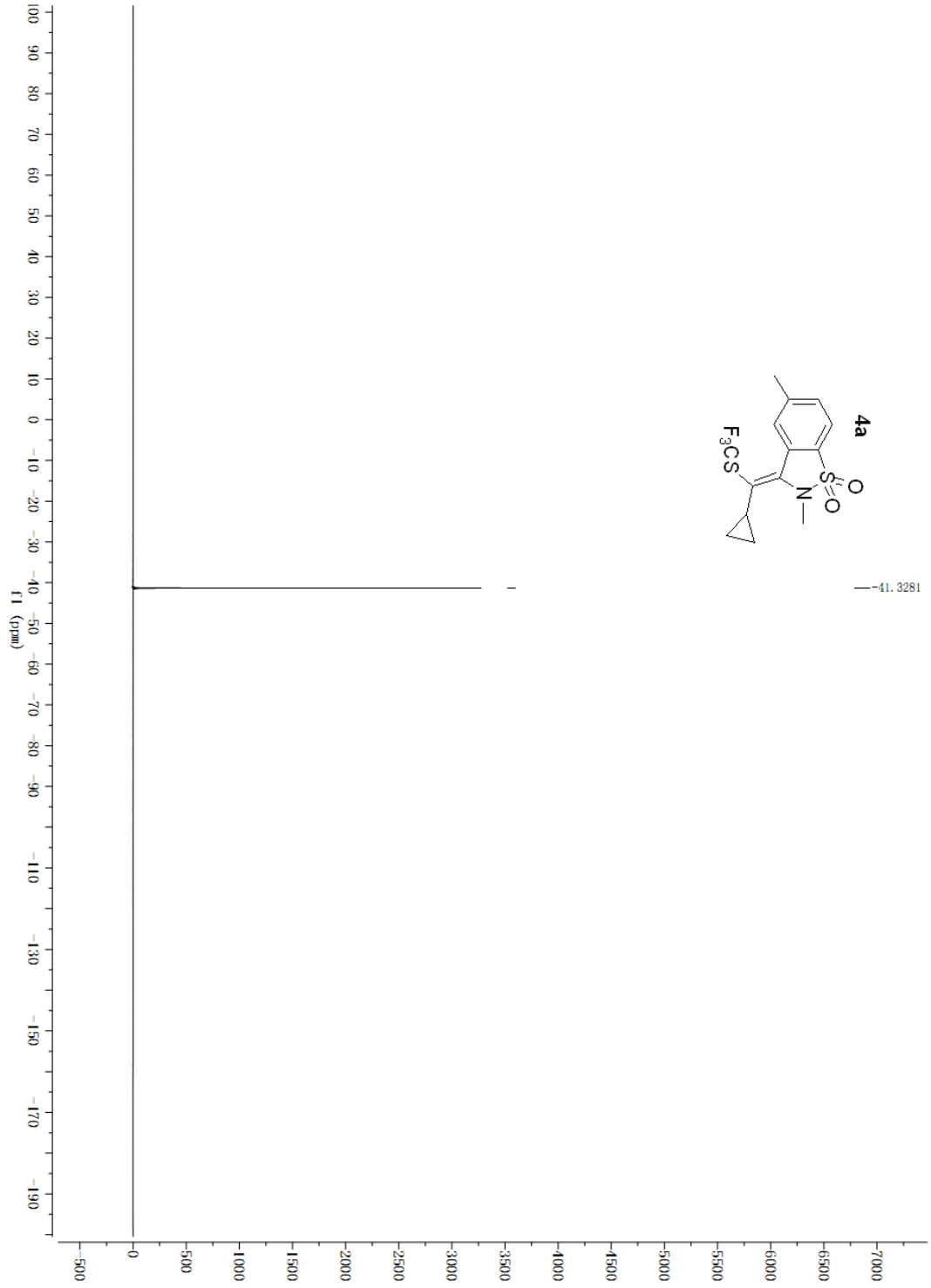
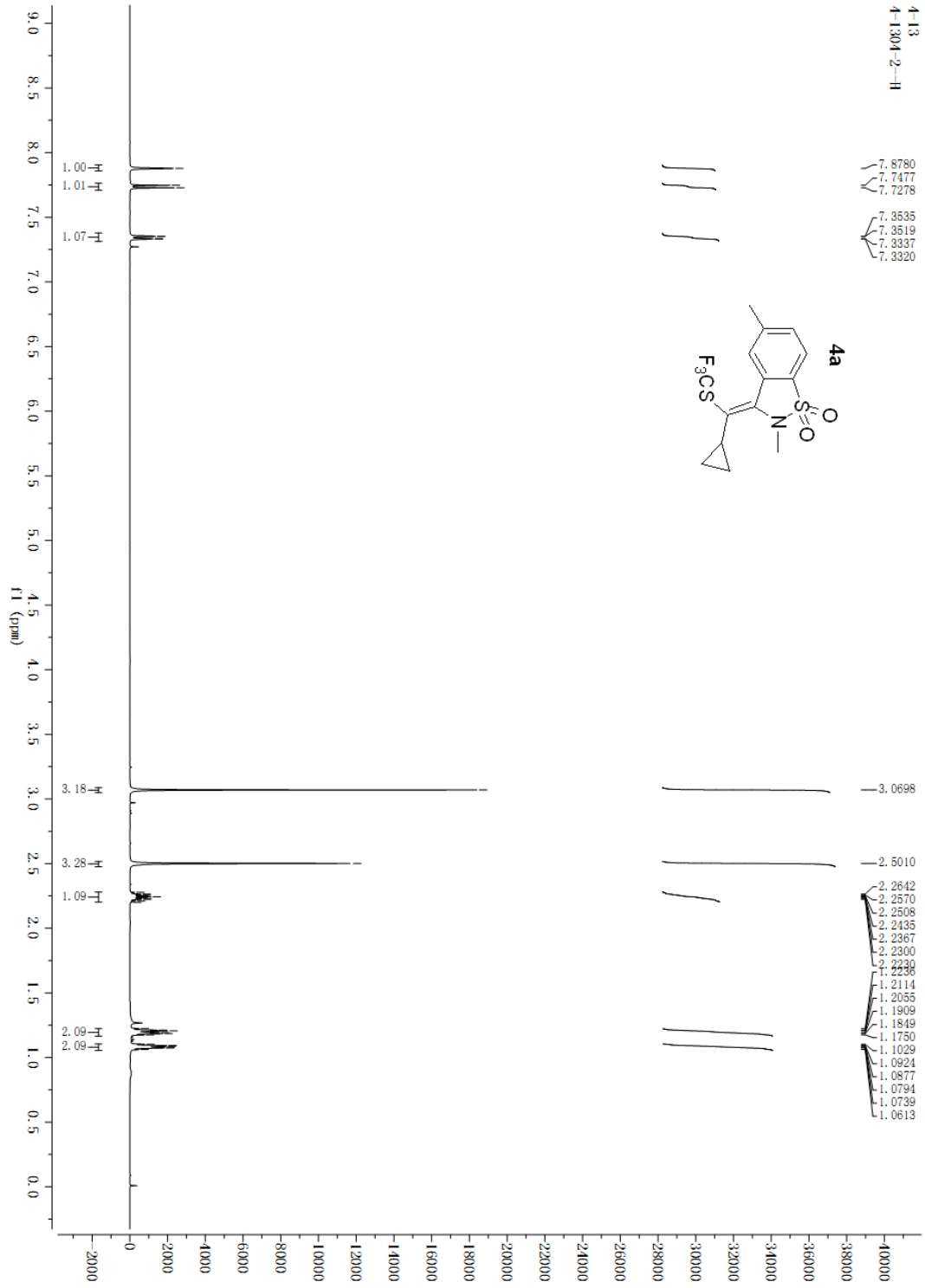
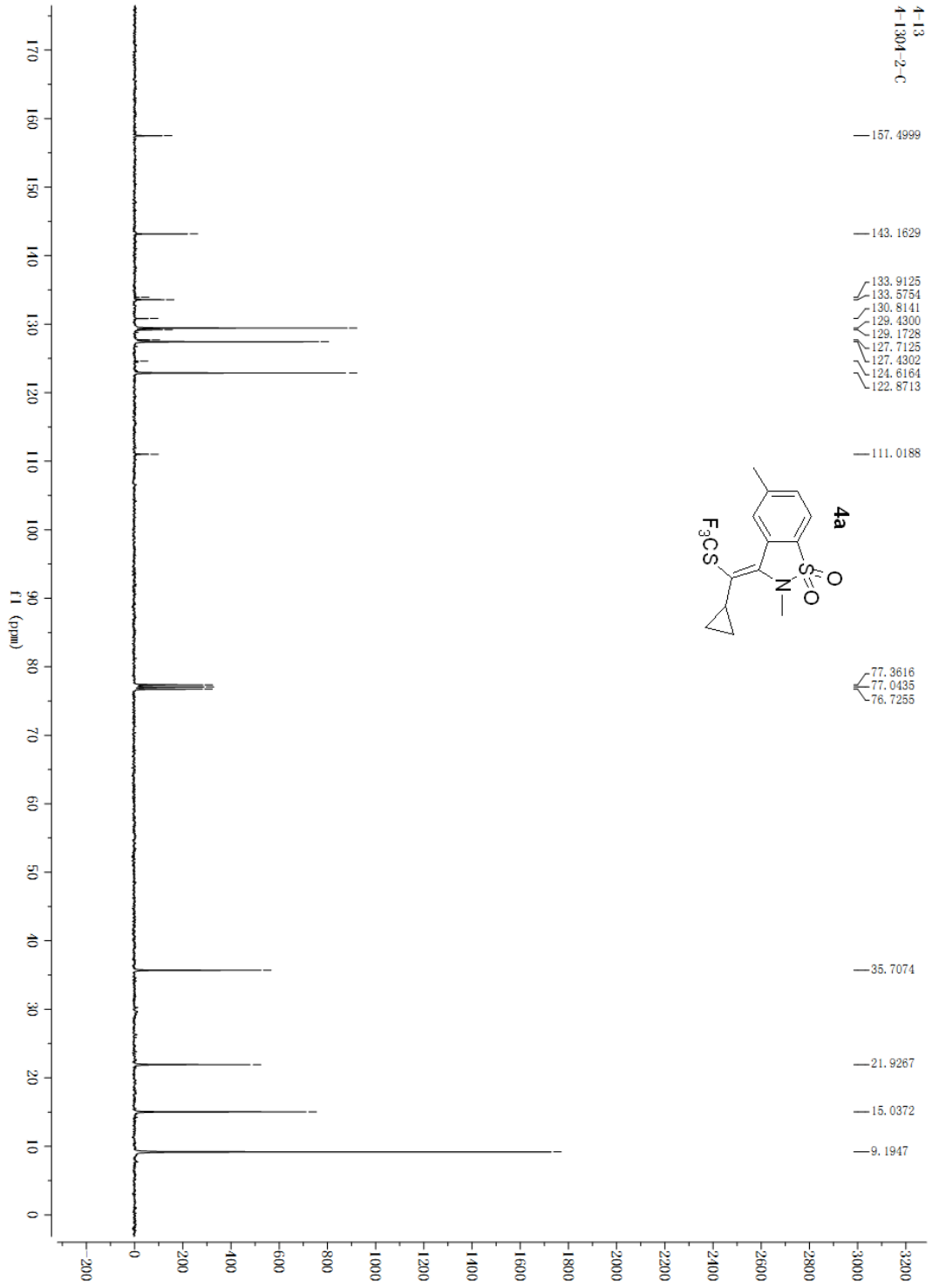
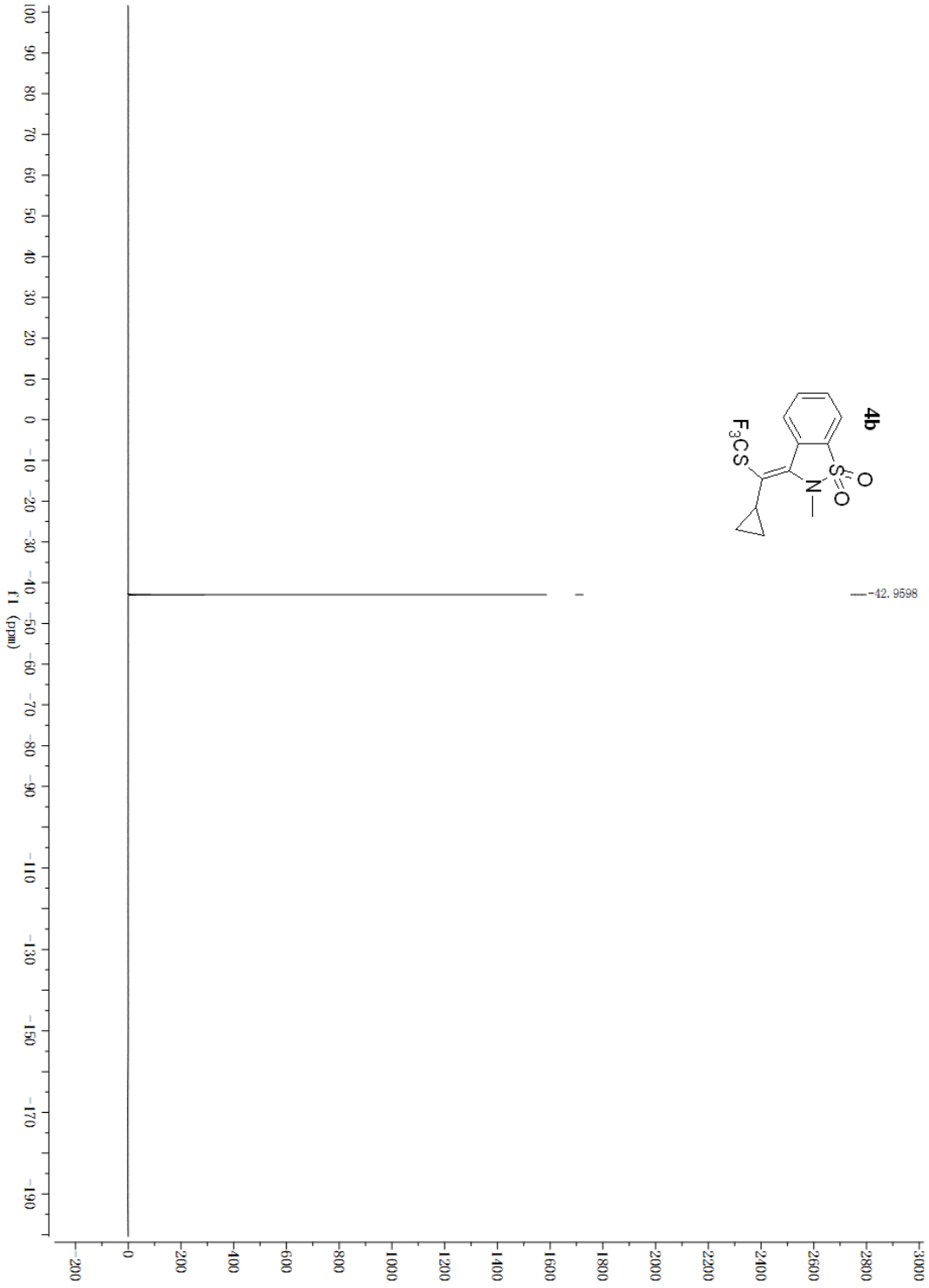
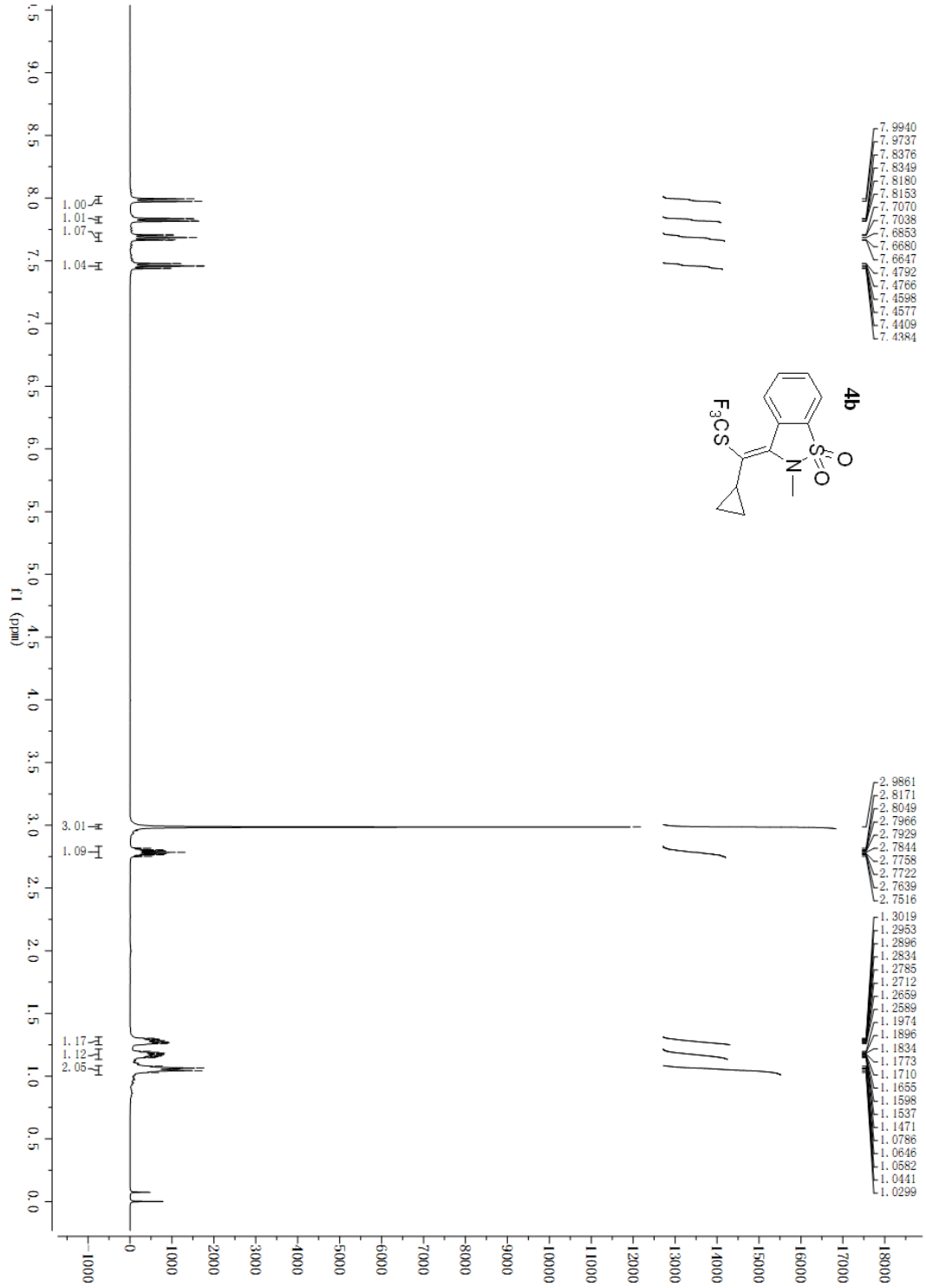
133.3406
130.3812
129.1928
127.2921
127.2851
124.6541
124.1912
118.7850
104.4562
77.3608
77.0429
76.7250
32.1211
30.1361
22.4122
16.5011
3u
SCF3
O
S
O
N
CN
f1 (ppm)

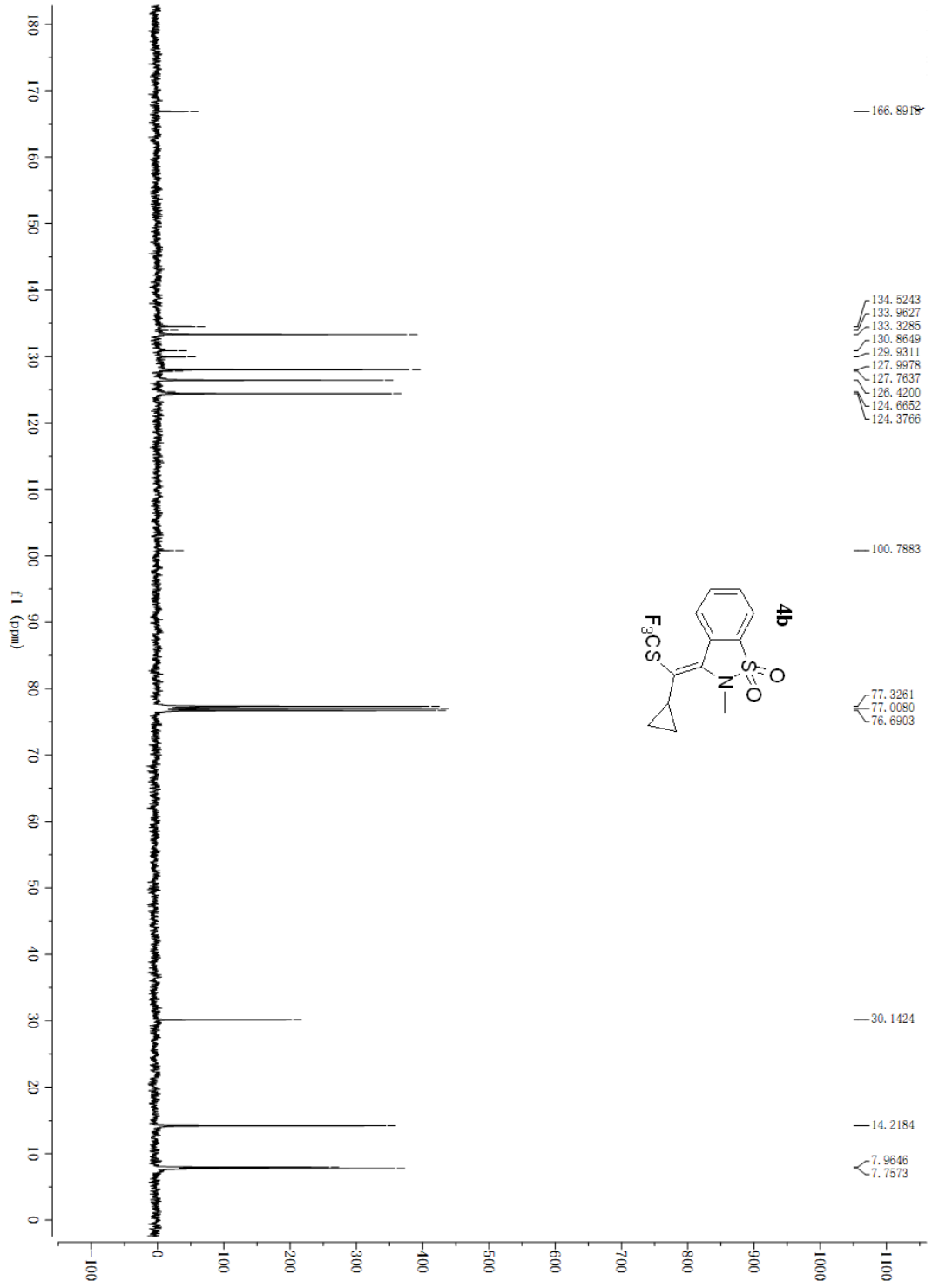

4a
F3CS
O
S
O
N
-41.3281
f1 (ppm)

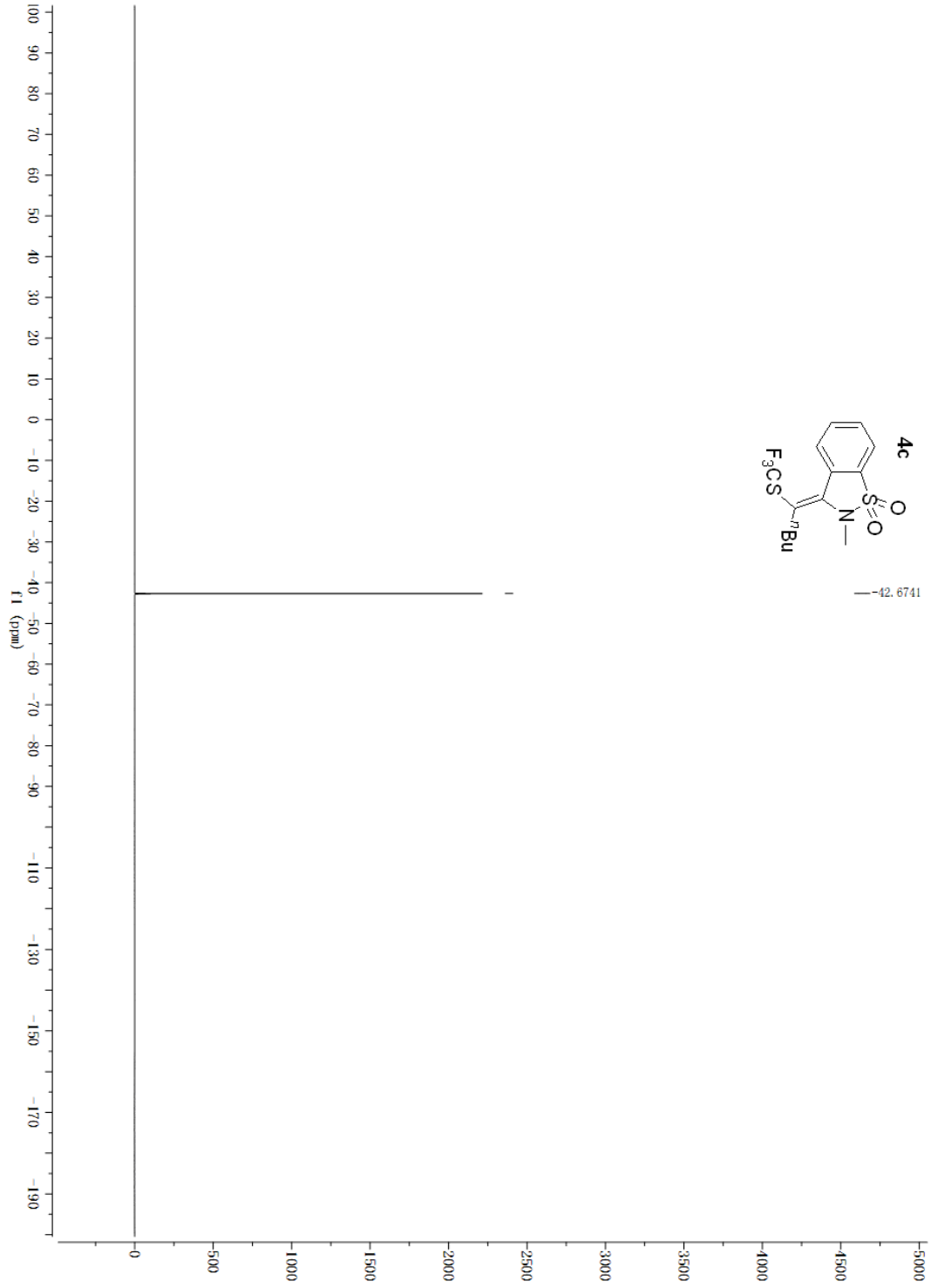

4-13
4-1304-2-H
4a
F3CS
O
S
O
N
7.8780
7.7477
7.7278
7.3535
7.3519
7.3337
7.3320
3.0698
2.5010
2.2642
2.2570
2.2508
2.2435
2.2367
2.2300
2.2230
2.2236
2.2114
2.2055
2.1909
2.1849
2.1750
2.1029
2.0924
2.0877
2.0794
2.0739
2.0613
1.00
1.01
1.07
3.18
3.28
1.09
2.09
2.09
f1 (ppm)

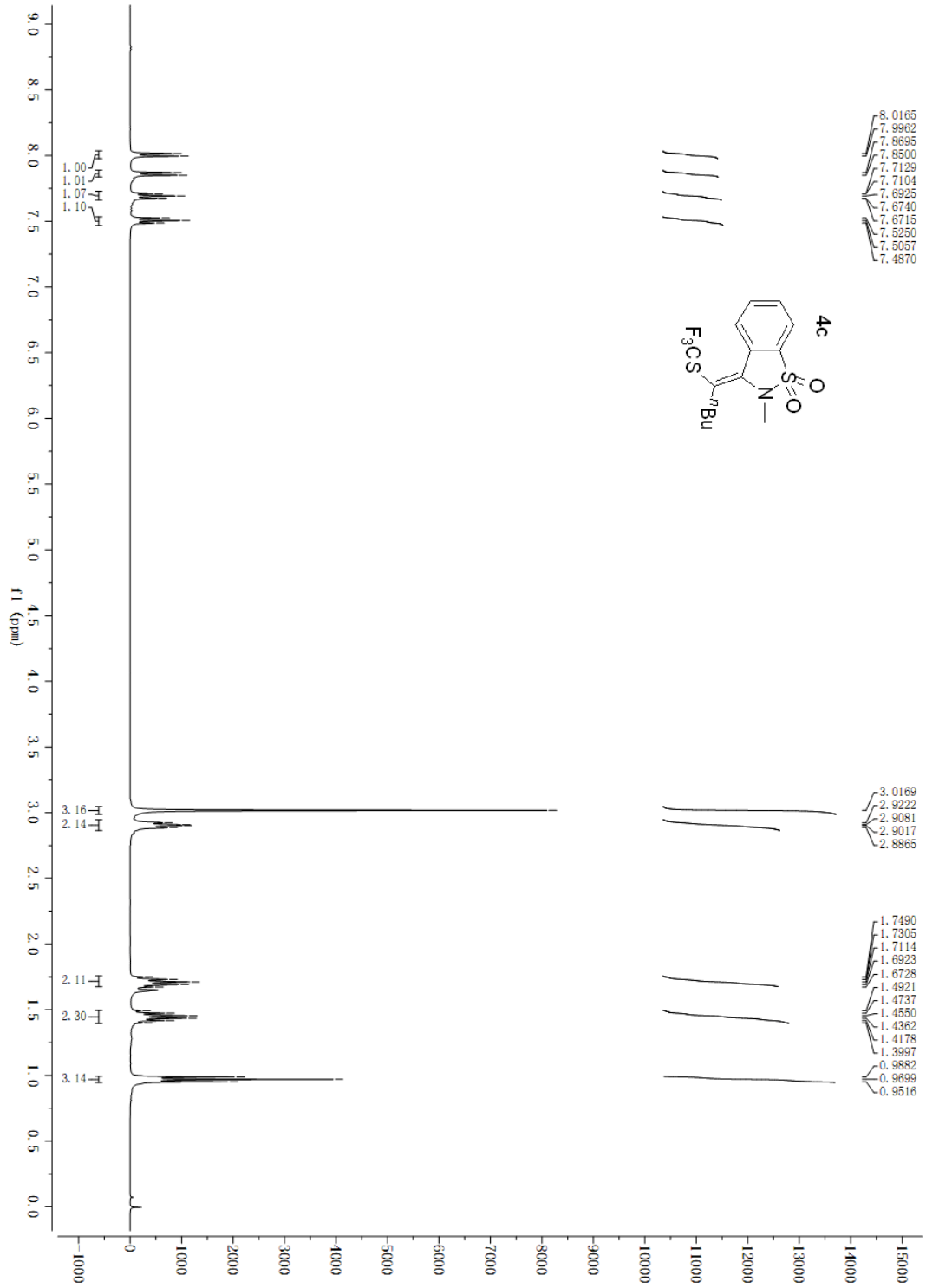

4-13
4-1304-2-C
157.4999
143.1629
133.9125
133.5754
130.8141
129.4300
129.1728
127.7125
127.4302
124.6164
122.8713
111.0188
77.3616
77.0435
76.7255
35.7074
21.9267
15.0372
9.1947
4a
F3CS
O
S
O
N
f1 (ppm)

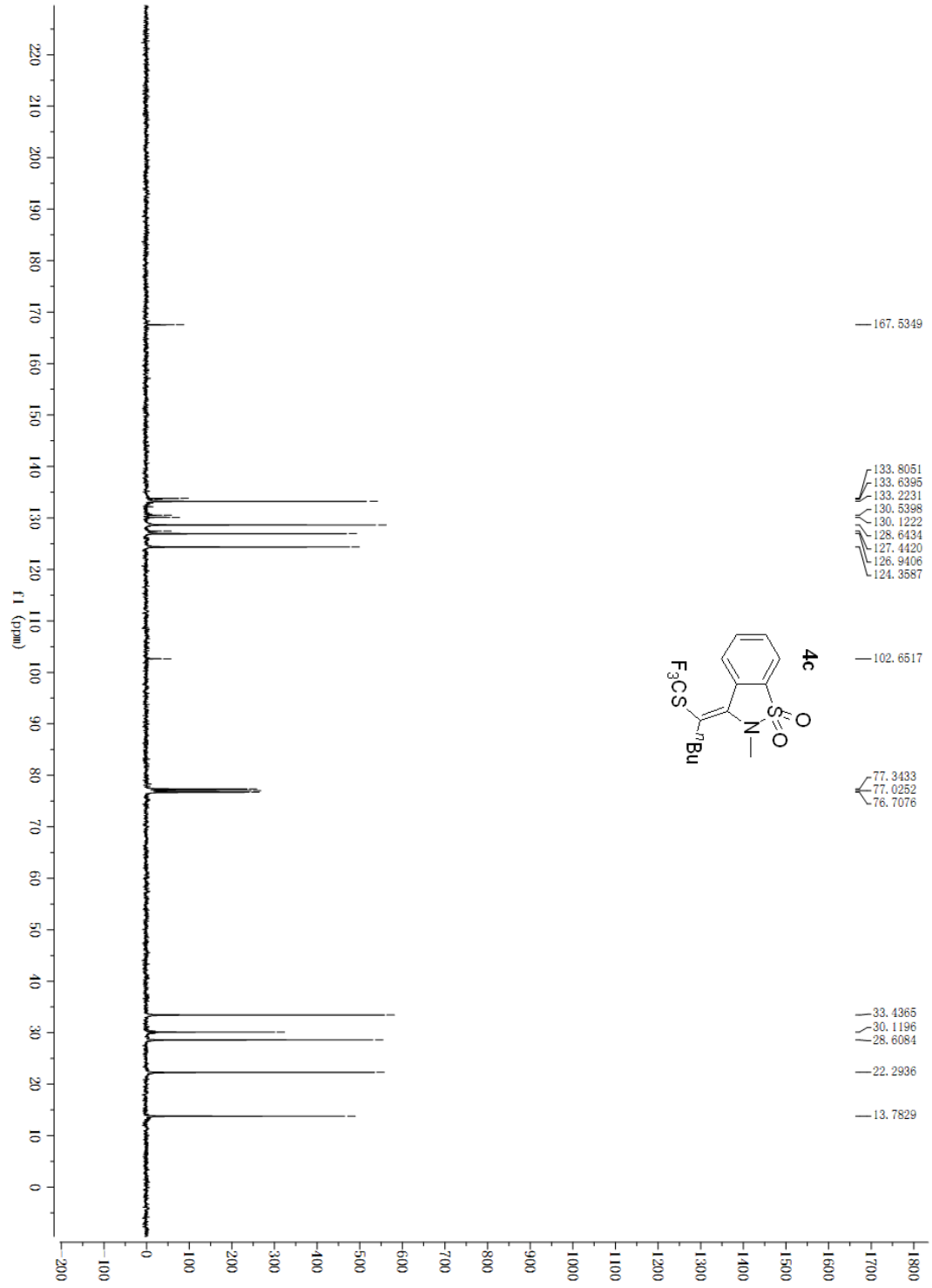

4b
F3CS
O
S
O
N
-42.9598
f1 (ppm)

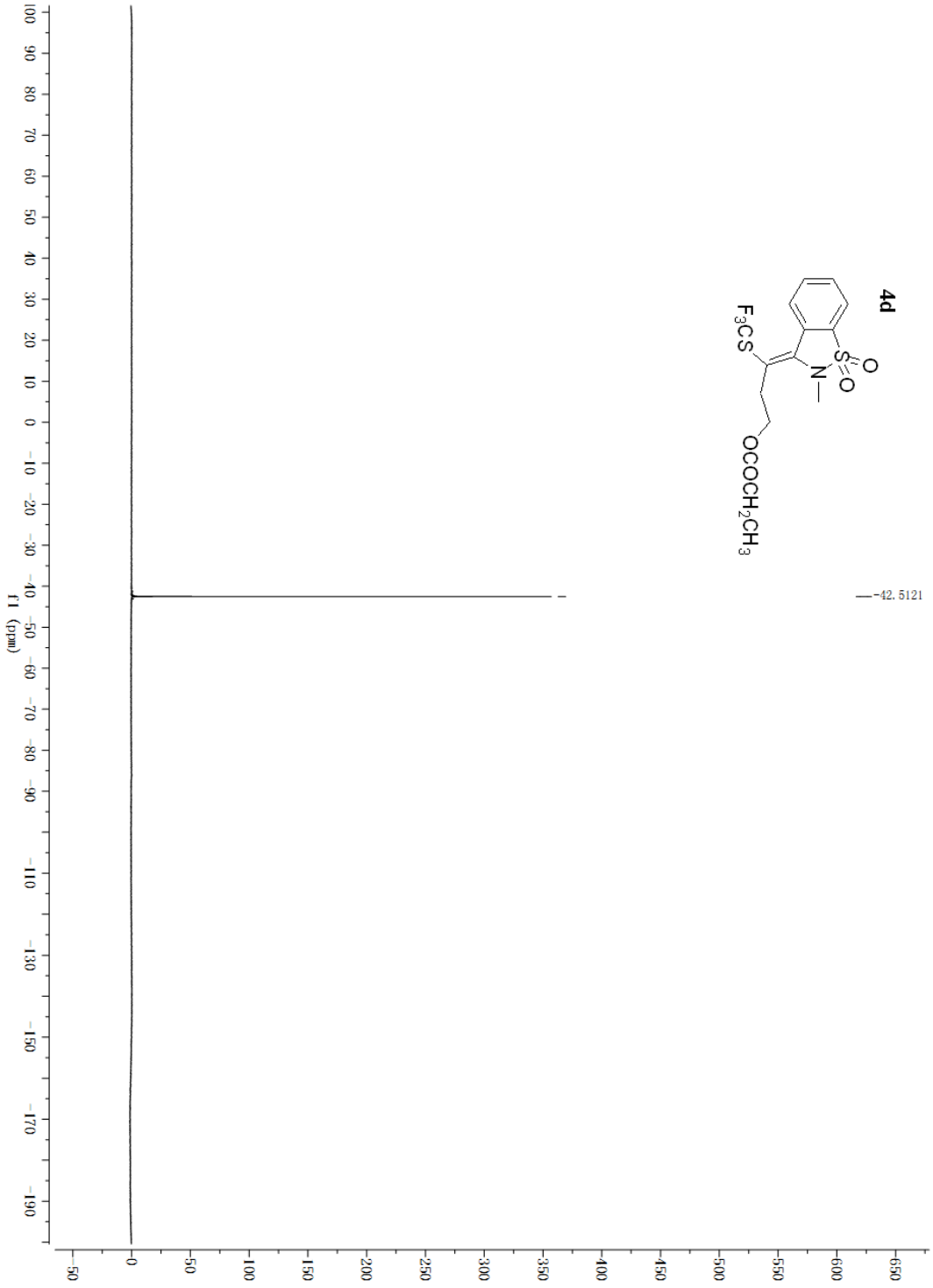

4b
F3CS
O
S
O
N
f1 (ppm)
1.00
1.01
1.07
1.04
3.01
1.09
1.17
1.12
2.05
7.9940
7.9737
7.8376
7.8349
7.8180
7.8153
7.7070
7.7038
7.6853
7.6680
7.6647
7.4792
7.4766
7.4598
7.4577
7.4409
7.4384
2.9861
2.8171
2.8049
2.7966
2.7929
2.7844
2.7758
2.7722
2.7639
2.7516
1.3019
1.2953
1.2896
1.2834
1.2785
1.2712
1.2659
1.2589
1.1974
1.1896
1.1834
1.1773
1.1710
1.1655
1.1598
1.1537
1.1471
1.0786
1.0646
1.0582
1.0441
1.0299

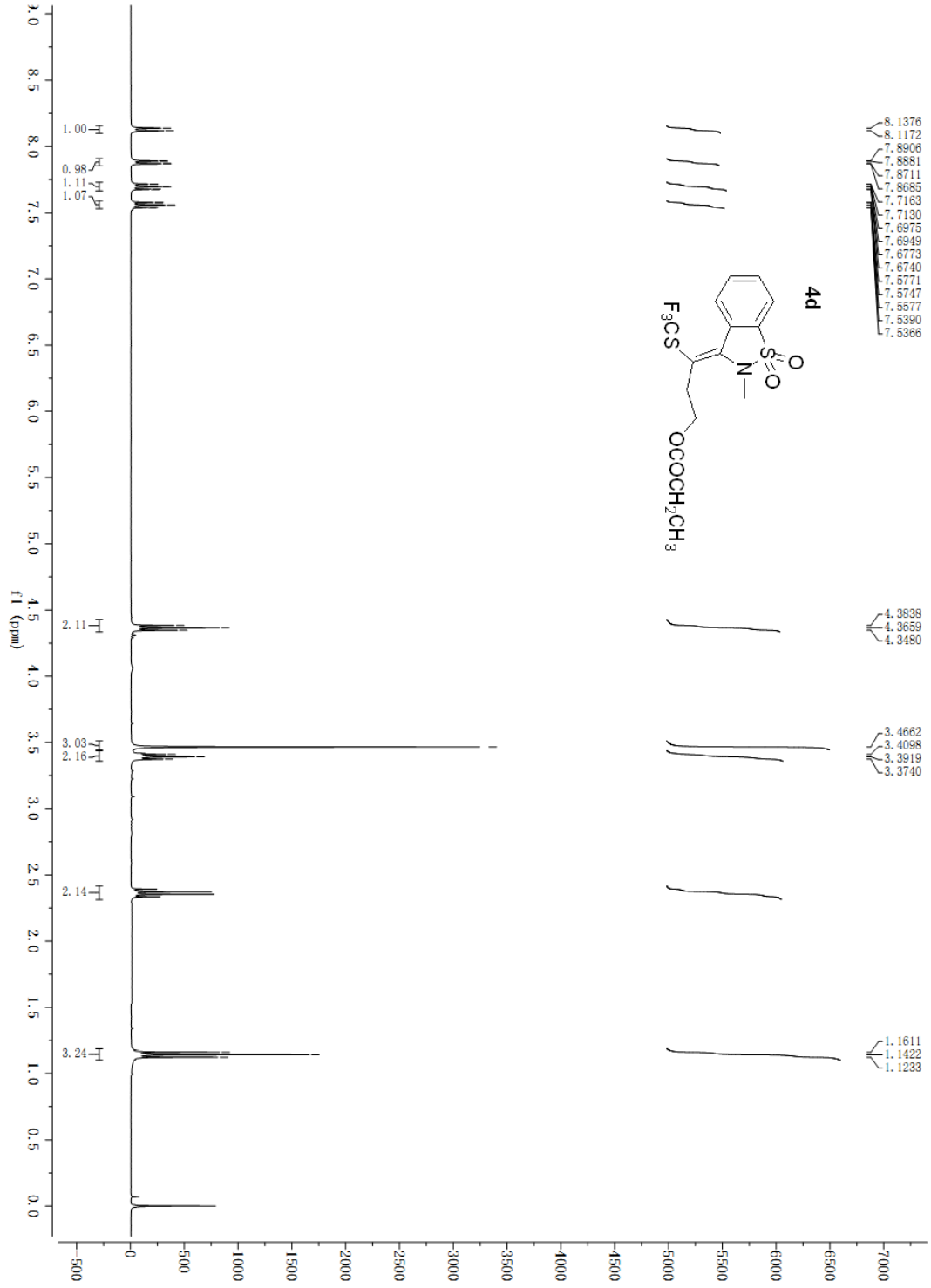

166.8918
134.5243
133.9627
133.3285
130.8649
129.9311
127.9978
127.7637
126.4200
124.6652
124.3766
100.7883
77.3261
77.0080
76.6903
30.1424
14.2184
7.9646
7.7573
4b
F3CS
O
S
N
O
f1 (ppm)

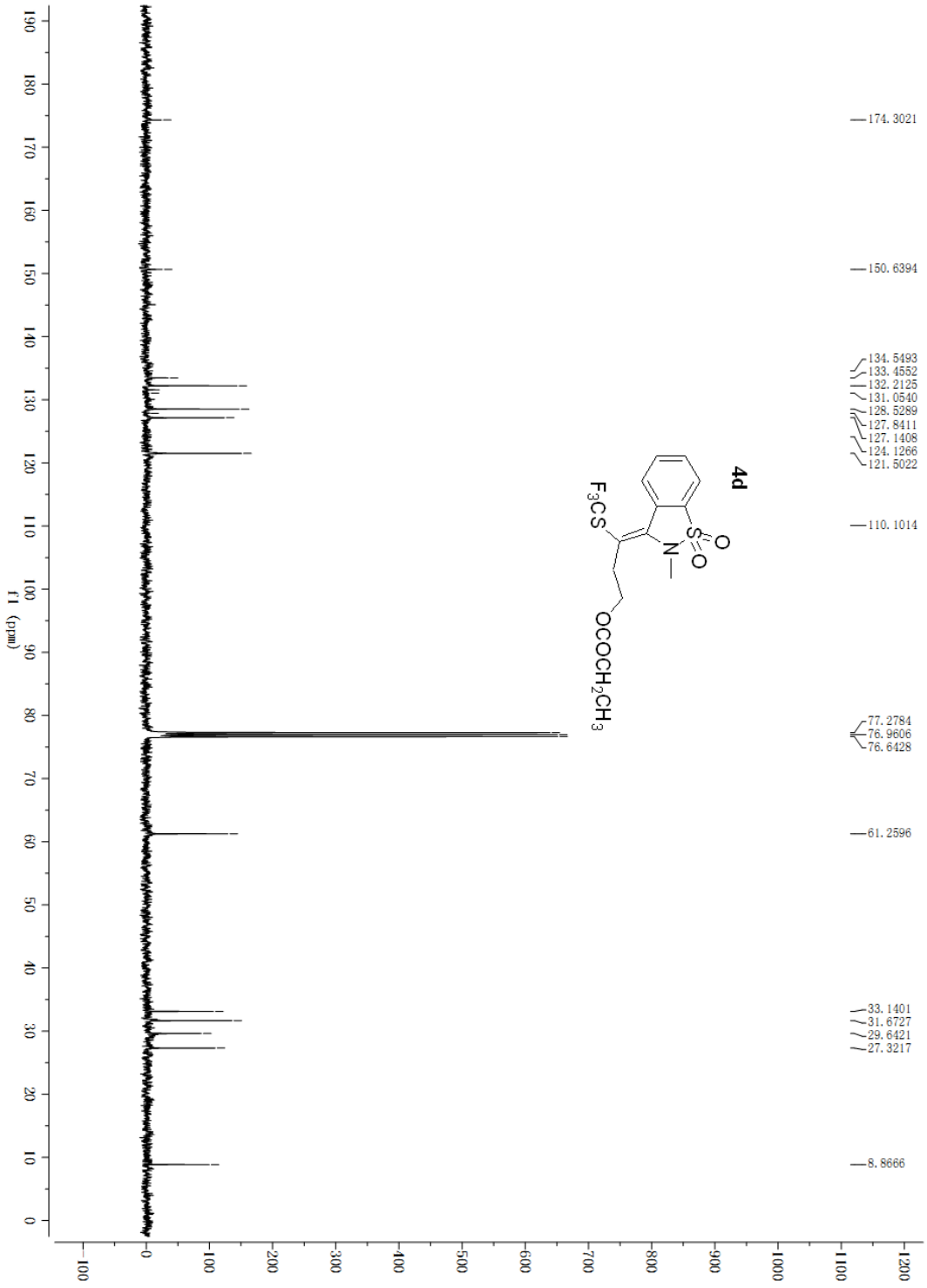

4c
F3CS
nBu
O
S
O
N
—42.6741
f1 (ppm)


4c
F3CS
nBu
O
S
O
N
8.0165
7.9962
7.8695
7.8500
7.7129
7.7104
7.6925
7.6740
7.6715
7.5250
7.5057
7.4870
3.0169
2.9222
2.9081
2.9017
2.8865
1.7490
1.7305
1.7114
1.6923
1.6728
1.4921
1.4737
1.4550
1.4362
1.4178
1.3997
0.9882
0.9699
0.9516
1.00
1.01
1.07
1.10
3.16
2.14
2.11
2.30
3.14
f1 (ppm)


167.5349
133.8051
133.6395
133.2231
130.5398
130.1222
128.6434
127.4420
126.9406
124.3587
102.6517
77.3433
77.0252
76.7076
33.4365
30.1196
28.6084
22.2936
13.7829
4c
F3CS
nBu
O
S
O
N
f1 (ppm)


4d
F3CS
OCOCH2CH3
-42.5121
f1 (ppm)


4d
F3CS
OCOCH2CH3
8.1376
8.1172
7.8906
7.8881
7.8711
7.8685
7.7163
7.7130
7.6975
7.6949
7.6773
7.6740
7.5771
7.5747
7.5577
7.5390
7.5366
4.3838
4.3659
4.3480
3.4662
3.4098
3.3919
3.3740
1.1611
1.1422
1.1233
1.00
0.98
1.11
1.07
2.11
3.03
2.16
2.14
3.24
f1 (ppm)


4d
F3CS
OCOCH2CH3
174.3021
150.6394
134.5493
133.4552
132.2125
131.0540
128.5289
127.8411
127.1408
124.1266
121.5022
110.1014
77.2784
76.9606
76.6428
61.2596
33.1401
31.6727
29.6421
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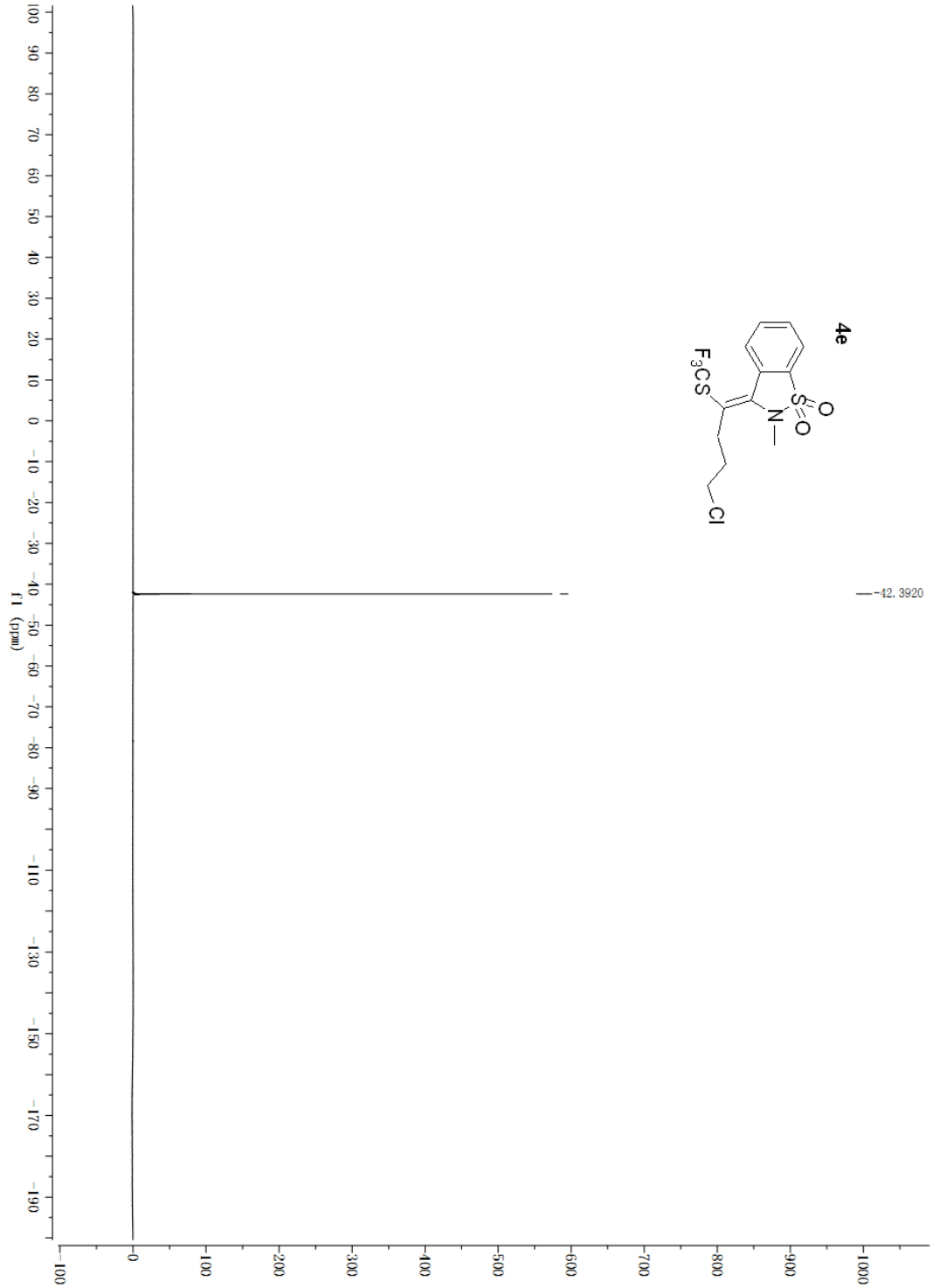
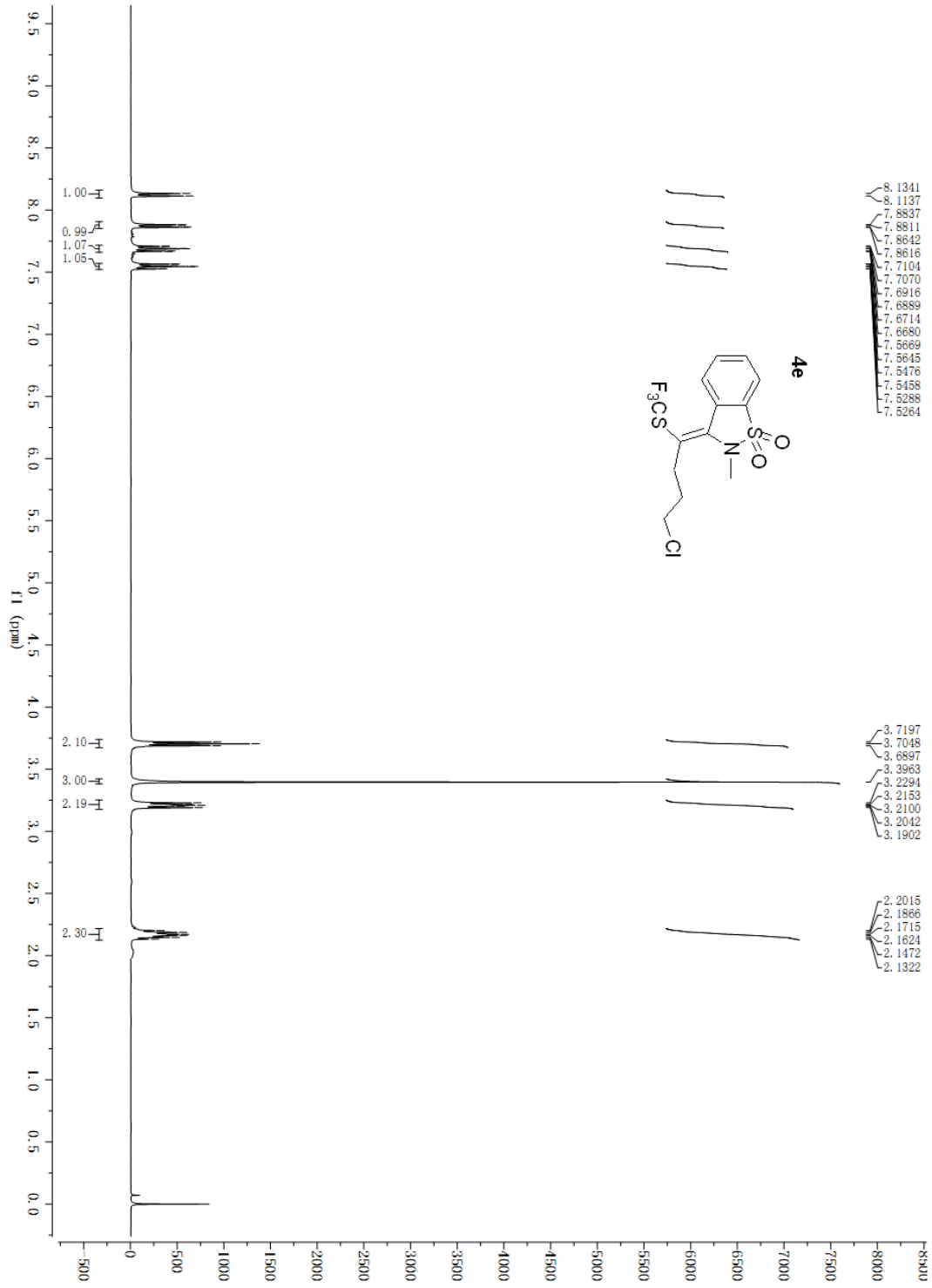
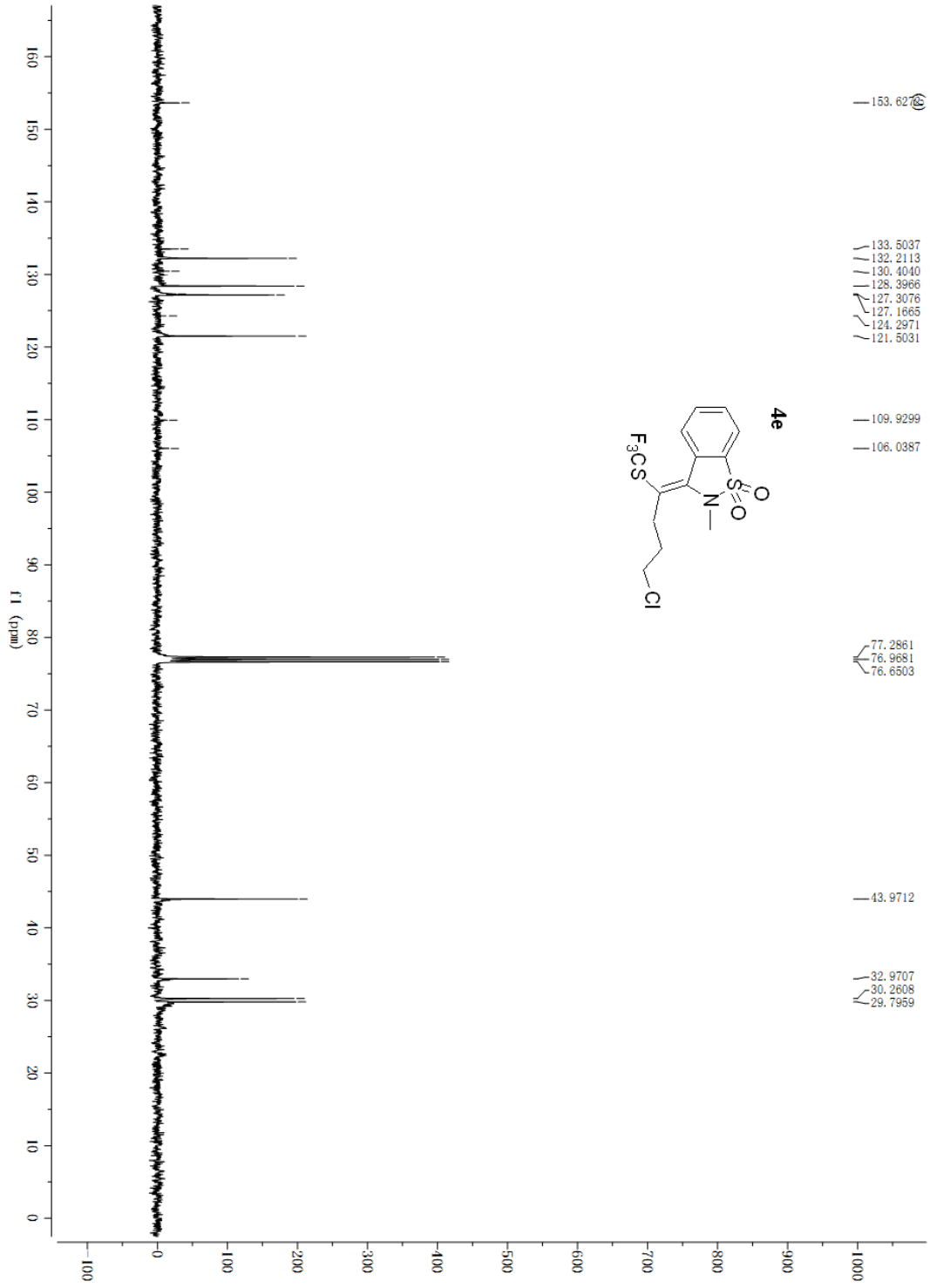
8.8666
f1 (ppm)


4e
F3CS
O
S
O
N
Cl
-42.3920
f1 (ppm)


4e
F3CS
O
S
O
N
Cl
1.00
0.99
1.07
1.05
2.10
3.00
2.19
2.30
8.1341
8.1137
7.8837
7.8811
7.8642
7.8616
7.7104
7.7070
7.6916
7.6889
7.6714
7.6680
7.5669
7.5645
7.5476
7.5458
7.5288
7.5264
3.7197
3.7048
3.6897
3.3963
3.2294
3.2153
3.2100
3.2042
3.1902
2.2015
2.1866
2.1715
2.1624
2.1472
2.1322
f1 (ppm)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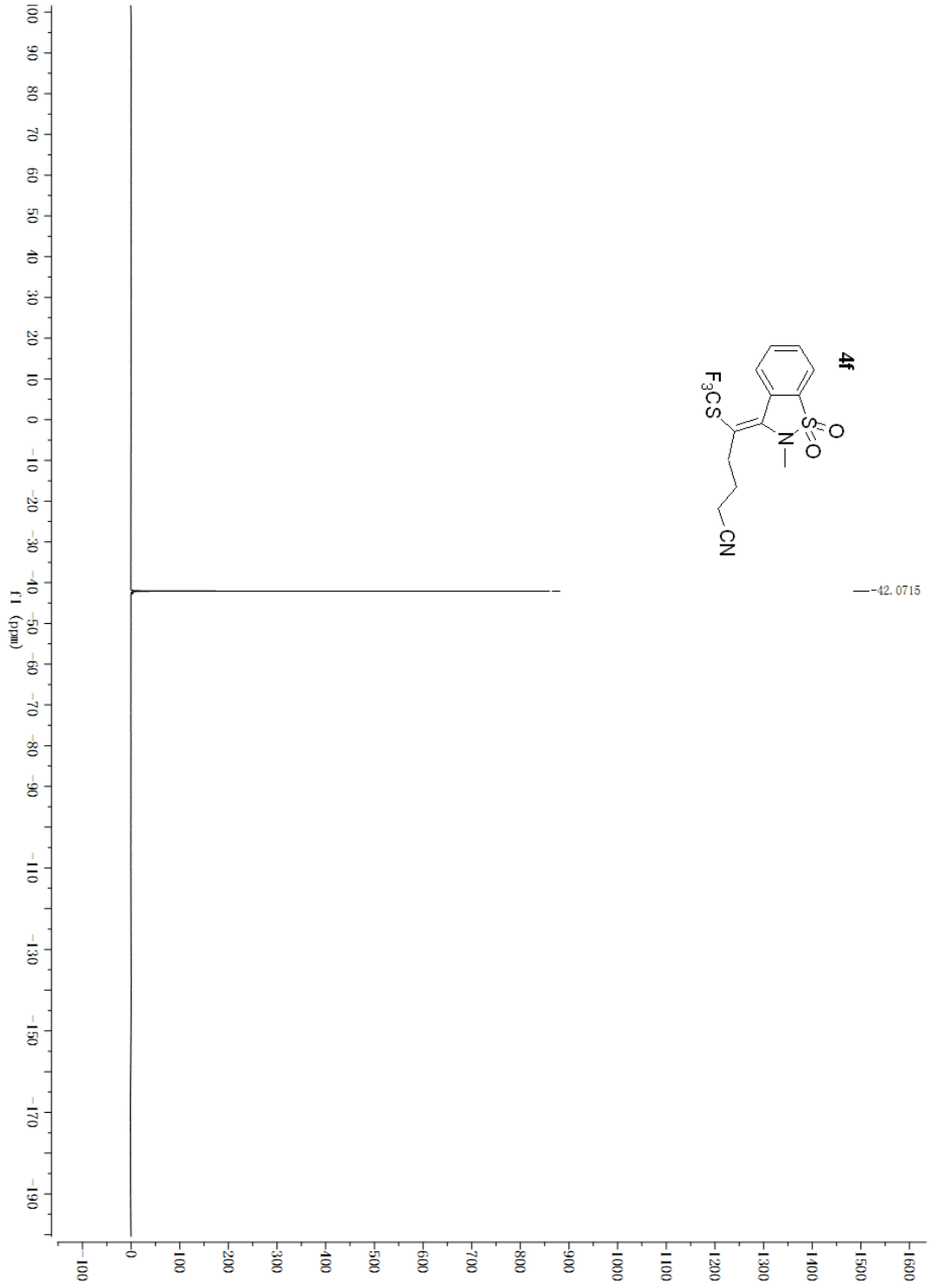
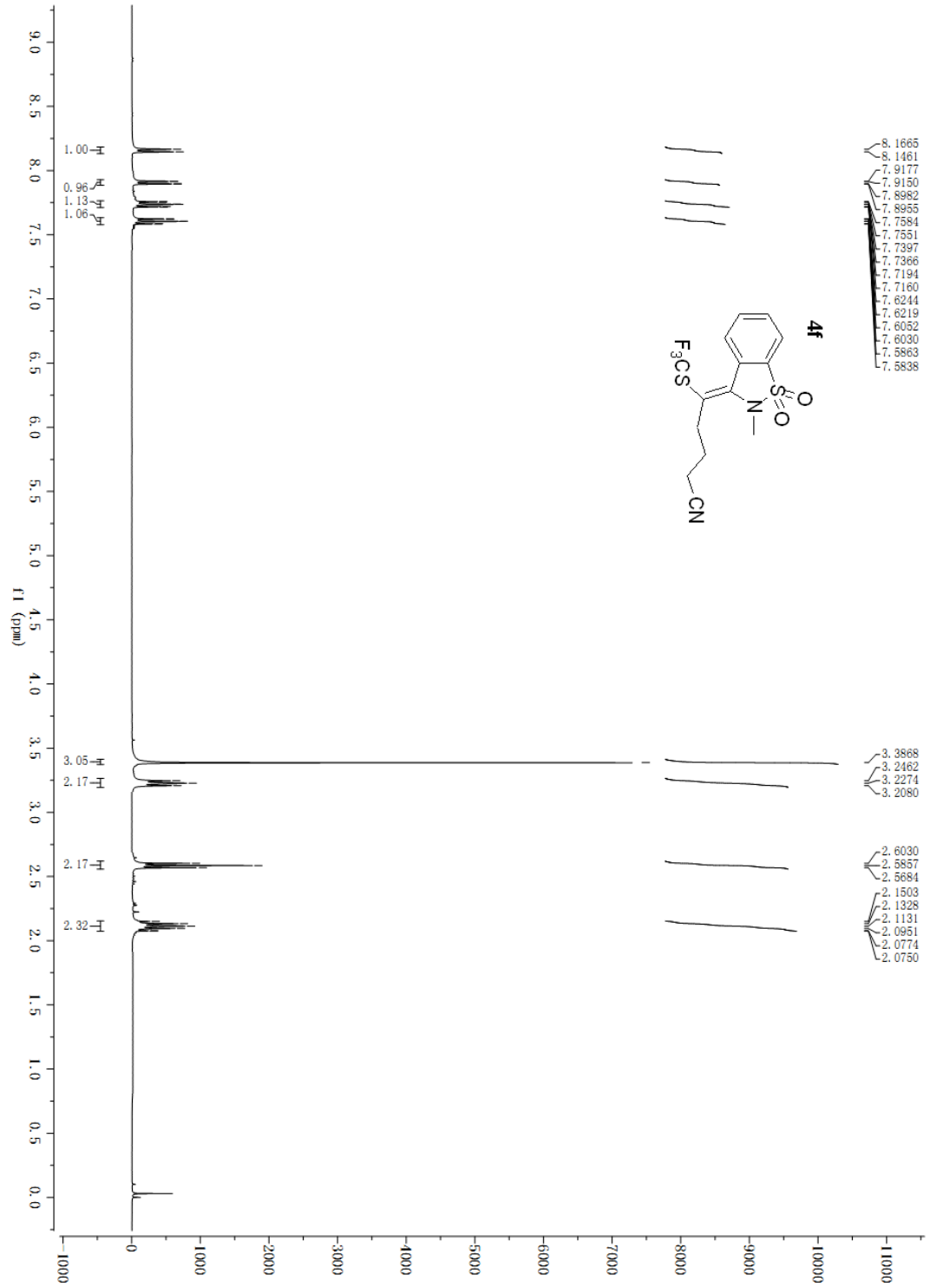
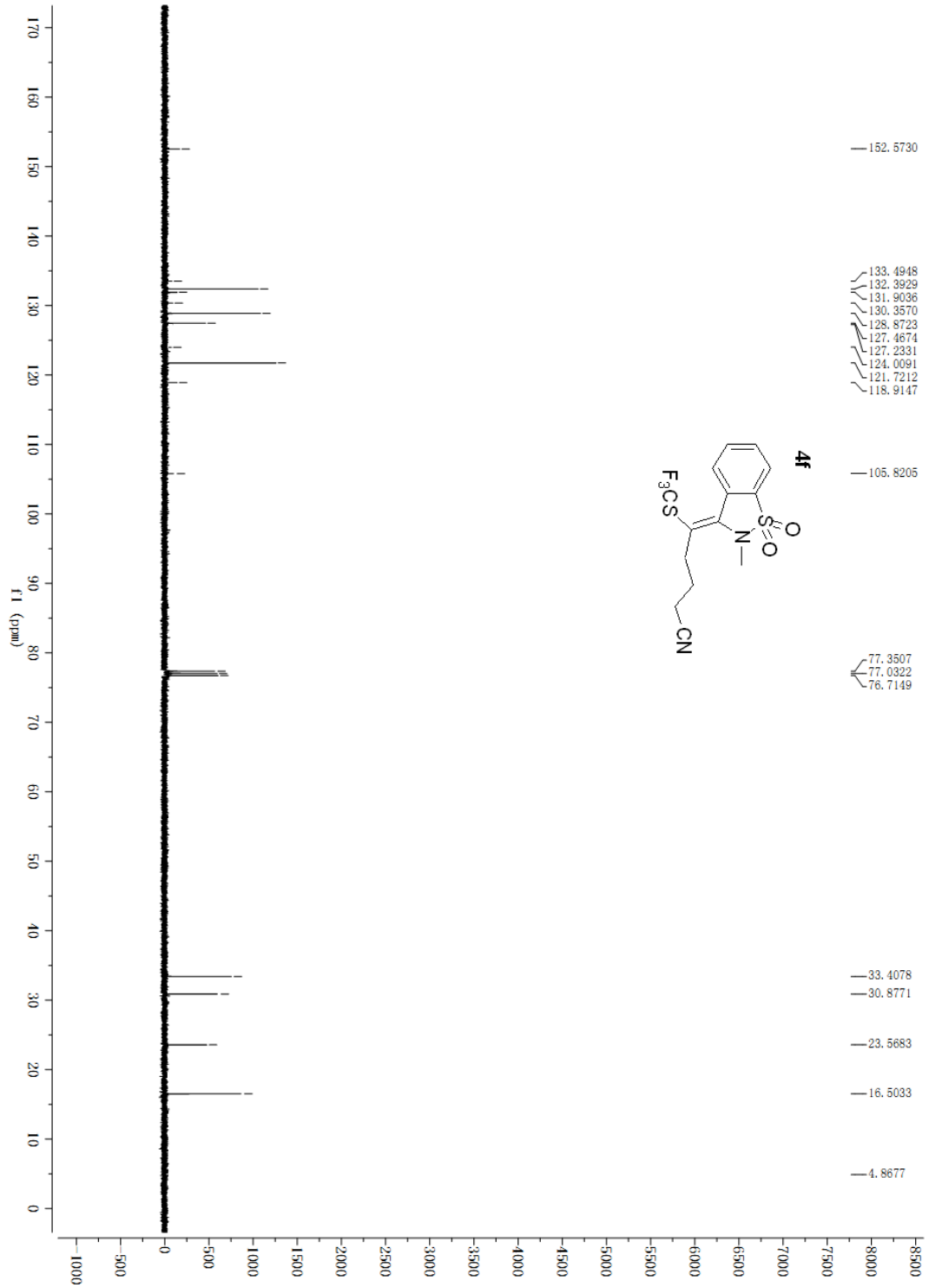
133.5037
132.2113
130.4040
128.3966
127.3076
127.1665
124.2971
121.5031
109.9299
106.0387
77.2861
76.9681
76.6503
43.9712
32.9707
30.2608
29.7959
4e
F3CS
S
O
O
N
Cl
f1 (ppm)


4f
F3CS
O
S
O
N
CN
-42.0715
f1 (ppm)


4f
F3CS
O
S
O
N
CN
8.1665
8.1461
7.9177
7.9150
7.8982
7.8955
7.7584
7.7551
7.7397
7.7366
7.7194
7.7160
7.6244
7.6219
7.6052
7.6030
7.5863
7.5838
3.3868
3.2462
3.2274
3.2080
2.6030
2.5857
2.5684
2.1503
2.1328
2.1131
2.0951
2.0774
2.0750
1.00
0.96
1.13
1.06
3.05
2.17
2.17
2.32
f1 (ppm)


f1 (ppm)
152.5730
133.4948
132.3929
131.9036
130.3570
128.8723
127.4674
127.2331
124.0091
121.7212
118.9147
105.8205
77.3507
77.0322
76.7149
33.4078
30.8771
23.5683
16.5033
4.8677
4f
F3CS
S
O
O
N
CN