Electronic Supplementary Material (ESI) for Chemical Communications

Synthesis of 3-((trifluoromethyl)thio)indoles via a reaction of 2-alkynylaniline with trifluoromethanesulfanylamide

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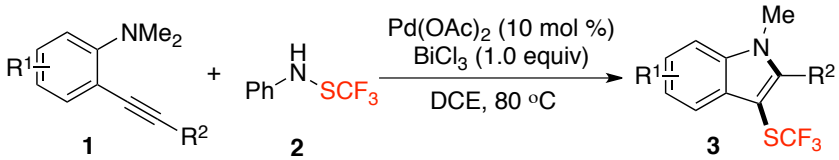
Supporting Information

1. General experimental methods (S2).
2. General experimental procedure and characterization data (S2-S8).
3. ^{19}F, ^{1}H, and ^{13}C NMR spectra of compounds **3** (S9-S56).

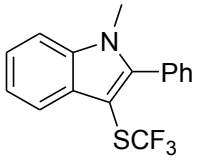
General experimental methods:

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.

General procedure for the synthesis of 3-((trifluoromethyl)thio)indoles via a palladium-catalyzed reaction of 2-alkynylaniline with trifluoromethanesulfanylamide in the presence of bismuth chloride.

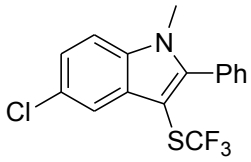


Trifluoromethanesulfanylamide (116.0 mg, 0.6 mmol) was added to a solution of 2-alkynylaniline **1** (0.2 mmol), $Pd(OAc)_2$ (0.02 mmol, 4.5 mg), and $BiCl_3$ (0.2 mmol, 63.1 mg) in DCE (2.0 mL) under N_2 atmosphere. The mixture was stirred at 80 °C for 12-16 hours. After completion of the reaction as indicated by TLC, the reaction mixture was filtered through a thin layer of silica gel and washed by CH_2Cl_2 (3 × 5.0 mL). The residue was concentrated in vacuo and purified by column chromatography on silica gel (eluted with PE/EA = 200:1) to provide the product **3**.



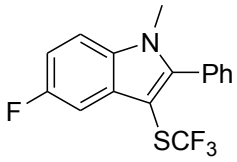
1-Methyl-2-phenyl-3-(trifluoromethylthio)-1*H*-indole (**3a**)

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.66 (s, 3H), 7.28–7.36 (m, 2H), 7.39–7.43 (m, 3H), 7.50–7.53 (m, 3H), 7.83 (d, J = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.7, 92.7, 110.1, 119.6, 121.7, 123.2, 128.5, 129.3, 129.8 (q, J = 309.5 Hz), 129.9, 130.3, 130.9, 137.2, 148.2; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.44 (s); HRMS (ESI) calcd for $C_{16}H_{13}F_3NS$: 308.0715 ($M + H^+$), found: 308.0695.



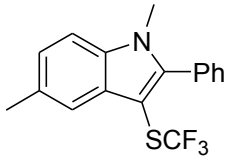
5-Chloro-1-methyl-2-phenyl-3-(trifluoromethylthio)-1*H*-indole (**3b**)

Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.66 (s, 3H), 7.30–7.32 (m, 2H), 7.42–7.43 (m, 2H), 7.53–7.54 (m, 3H), 7.80 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.8, 92.4, 111.1, 119.0, 123.5, 127.6, 128.5, 129.3, 129.4, 129.5 (q, J = 309.6 Hz), 130.7, 131.3, 135.5, 149.2; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.38 (s); HRMS (ESI) calcd for $C_{16}H_{12}ClF_3NS$: 342.0326 ($M + H^+$), found: 342.0310.



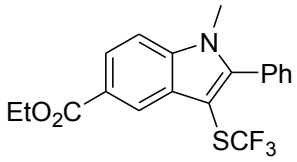
5-Fluoro-1-methyl-2-phenyl-3-(trifluoromethylthio)-1*H*-indole (**3c**)

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.64 (s, 3H), 7.04–7.09 (m, 1H), 7.29–7.32 (m, 1H), 7. 40–7.42 (m, 2H), 7.47–7.53 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.8, 92.7, 104.7 (d, $^{2}J_{CF}$ = 24.5 Hz), 110.9, 111.0, 111.6 (d, $^{2}J_{CF}$ = 26.3 Hz), 128.4, 129.4, 129.5, 129.6 (q, J = 309.6 Hz), 130.7, 133.6, 149.5, 159.2 (d, $^{1}J_{CF}$ = 236.3 Hz); ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.44 (s); HRMS (ESI) calcd for $C_{16}H_{12}F_4NS$: 326.0627 ($M + H^+$), found: 326.0621.



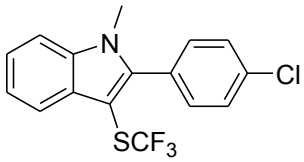
1,5-Dimethyl-2-phenyl-3-(trifluoromethylthio)-1*H*-indole (**3d**)

Brown solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.53 (s, 3H), 3.65 (s, 3H), 7.18 (d, J = 8.2 Hz, 1H), 7.30 (d, J = 8.3 Hz, 1H), 7.42–7.44 (m, 2H), 7.51–7.53 (m, 3H), 7.63 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.6, 31.7, 92.0, 109.7, 119.2, 124.8, 128.4, 129.2, 129.8 (q, J = 309.8 Hz), 130.0, 130.5, 130.9, 131.2, 135.6, 148.0; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.49 (s); HRMS (ESI) calcd for $C_{17}H_{15}F_3NS$: 322.0872 ($M + H^+$), found: 322.0867.



Ethyl 1-methyl-2-phenyl-3-(trifluoromethylthio)-1*H*-indole-5-carboxylate (**3e**)

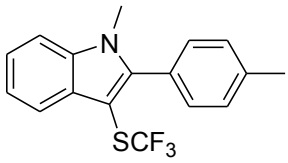
Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.42 (t, J = 7.0 Hz, 3H), 3.64 (s, 3H), 4.41 (q, J = 7.0 Hz, 2H), 7.37 (d, J = 8.6 Hz, 1H), 7.41–7.50 (m, 5H), 8.03 (d, J = 8.5 Hz, 1H), 8.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.4, 31.9, 60.9, 94.2, 109.8, 122.1, 124.1, 124.5, 128.5, 129.2, 129.5, 129.5 (q, J = 309.5 Hz), 129.8, 130.7, 139.6, 149.6, 167.3; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.19 (s); HRMS (ESI) calcd for $C_{19}H_{17}F_3NO_2S$: 380.0927 ($M + H^+$), found: 380.0934.



1,5-Dimethyl-2-phenyl-3-(trifluoromethylthio)-1*H*-indole (**3f**)

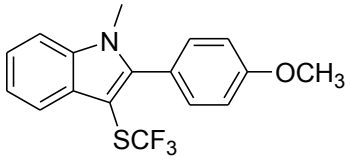
Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.67 (s, 3H), 7.31–7.35 (m, 1H), 7.35–7.40 (m, 3H), 7.41–7.43 (m, 1H), 7.50–7.54 (m, 2H), 7.85 (d, J = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.7, 93.1, 110.0, 119.6, 121.8, 123.4, 128.8, 129.6 (q, J = 309.6 Hz), 130.1, 132.1, 132.5, 135.6, 137.2, 146.7; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.39 (s); HRMS (ESI) calcd for $C_{16}H_{12}ClF_3NS$: 342.0326 ($M + H^+$), found:

342.0324.



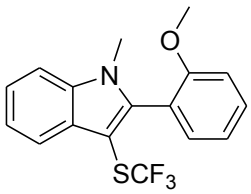
1-Methyl-2-p-tolyl-3-(trifluoromethylthio)-1*H*-indole (**3g**)

Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.48 (s, 3H), 3.66 (s, 3H), 7.31–7.38 (m, 6H), 7.40–7.42 (m, 1H), 7.88 (d, J = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 31.6, 92.5, 110.0, 119.5, 121.6, 123.1, 126.8, 129.2, 129.8 (q, J = 309.5 Hz), 130.3, 130.7, 137.2, 139.3, 148.3; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.35 (s); HRMS (ESI) calcd for $C_{17}H_{15}F_3NS$: 322.0872 ($M + H^+$), found: 322.0885.



2-(4-Methoxyphenyl)-1-methyl-3-(trifluoromethylthio)-1*H*-indole (**3h**)

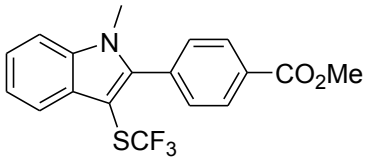
Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.64 (s, 3H), 3.87 (s, 3H), 7.02–7.04 (m, 2H), 7.27–7.39 (m, 5H), 7.82 (d, J = 7.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.6, 55.3, 92.4, 109.9, 113.9, 119.5, 121.6, 123.0, 129.7 (q, J = 309.6 Hz), 130.2, 130.6, 132.1, 137.1, 148.1, 160.3; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.43 (s); HRMS (ESI) calcd for $C_{17}H_{15}F_3NOS$: 338.0821 ($M + H^+$), found: 338.0816.



2-(2-Methoxyphenyl)-1-methyl-3-(trifluoromethylthio)-1*H*-indole (**3i**)

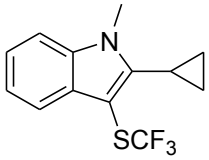
Brown solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.59 (s, 3H), 3.77 (s, 3H), 7.05 (d, J = 8.4 Hz, 1H), 7.12 (t, J = 7.4 Hz, 1H), 7.28–7.36 (m, 3H), 7.42 (d, J = 7.9 Hz, 1H), 7.49–7.54 (m, 1H), 7.85 (d, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.2, 55.5, 92.7, 109.9, 111.0, 119.5, 120.5, 121.3, 122.8, 124.8, 129.7 (q, J = 309.4 Hz),

130.3, 131.3, 133.0, 137.1, 145.6, 158.1; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.48 (s); HRMS (ESI) calcd for $C_{17}H_{15}F_3NOS$: 338.0821 ($M + H^+$), found: 338.0796..



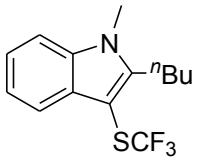
Methyl 4-(1-methyl-3-(trifluoromethylthio)-1*H*-indol-2-yl)benzoate (**3j**)

Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.66 (s, 3H), 3.96 (s, 3H), 7.30–7.42 (m, 3H), 7.52 (d, J = 8.0 Hz, 2H), 7.85 (d, J = 7.5 Hz, 1H), 8.19 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.8, 52.4, 93.3, 110.1, 119.7, 121.9, 123.6, 129.5 (q, J = 309.5 Hz), 129.6, 130.1, 130.8, 130.9, 143.3, 137.3, 148.2, 166.6; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.33 (s); HRMS (ESI) calcd for $C_{18}H_{15}F_3NO_2S$: 366.0770 ($M + H^+$), found: 366.0765.



2-Cyclopropyl-1-methyl-3-(trifluoromethylthio)-1*H*-indole (**3k**)

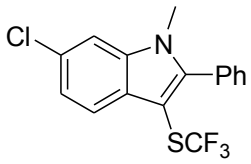
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.01–1.05 (m, 2H), 1.13–1.18 (m, 2H), 1.82–1.89 (m, 1H), 3.84 (s, 3H), 7.20–7.31 (m, 3H), 7.73 (d, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 6.4, 6.8, 30.4, 92.0, 109.2, 119.0, 121.1, 122.6, 129.8 (q, J = 309.1 Hz), 130.2, 136.6, 147.4; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.68 (s); HRMS (ESI) calcd for $C_{13}H_{13}F_3NS$: 272.0715 ($M + H^+$), found: 272.0718.



2-*n*-Butyl-1-methyl-3-(trifluoromethylthio)-1*H*-indole (**3l**)

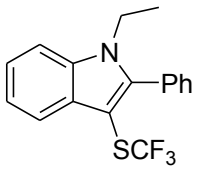
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.96 (t, J = 7.2 Hz, 3H), 1.39–1.48 (m, 2H), 1.55–1.61 (m, 2H), 2.97 (t, J = 8.0 Hz, 2H), 3.73 (s, 3H), 7.19–7.26 (m, 2H), 7.29–7.31 (m, 1H), 7.70–7.72 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.8, 22.7,

24.6, 31.6, 90.9, 109.3, 118.9, 121.2, 122.3, 129.7 (q, J = 309.5 Hz), 130.2, 137.0, 149.2; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.99 (s); HRMS (ESI) calcd for $C_{14}H_{17}F_3NS$: 288.1028 ($M + H^+$), found: 288.1033.



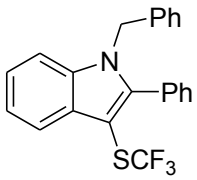
6-Chloro-1-methyl-2-phenyl-3-(trifluoromethylthio)-1*H*-indole (**3n**)

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (s, 3H), 7.27 (dd, J_1 = 8.5 Hz, J_2 = 1.8 Hz, 1H), 7.41–7.43 (m, 3H), 7.52–7.54 (m, 3H), 7.74 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.7, 93.1, 110.1, 120.6, 122.3, 128.5, 128.7, 129.1, 129.4, 129.5 (q, J = 309.7 Hz), 130.7, 137.5, 148.7; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.34 (s); HRMS (ESI) calcd for $C_{16}H_{13}ClF_3NS$: 342.0326 ($M + H^+$), found: 342.0357.



1-Ethyl-2-phenyl-3-(trifluoromethylthio)-1*H*-indole (**3o**)

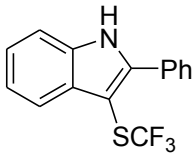
White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.29 (t, J = 7.2 Hz, 3H), 4.10 (q, J = 7.2 Hz, 2H), 7.28–7.36 (m, 2H), 7.40–7.44 (m, 3H), 7.50–7.53 (m, 3H), 7.86 (d, J = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 15.3, 39.6, 93.0, 119.7, 121.5, 123.0, 128.4, 129.2, 129.6 (q, J = 309.6 Hz), 130.1, 130.4, 130.7, 135.9, 147.7; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.43 (s); HRMS (ESI) calcd for $C_{17}H_{15}F_3NS$: 322.0872 ($M + H^+$), found: 322.0891.



1-Benzyl-2-phenyl-3-(trifluoromethylthio)-1*H*-indole (**3p**)

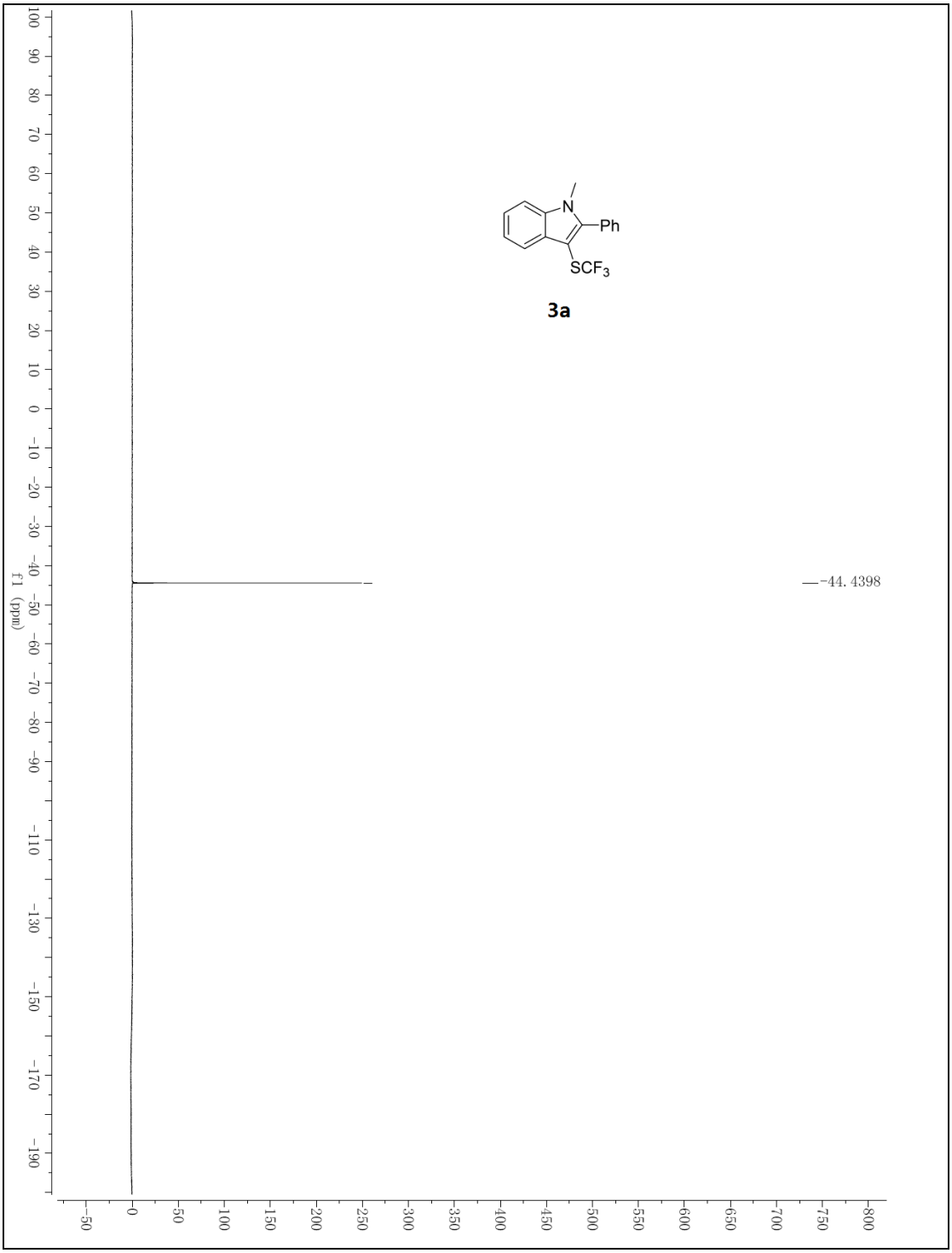
White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.28 (s, 2H), 6.91–6.93 (m, 2H),

7.22–7.27 (m, 5H), 7.28–7.32 (m, 1H), 7.35–7.37 (m, 2H), 7.41–7.47 (m, 3H), 7.88 (d, J = 7.8 Hz, 1H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 48.4, 110.9, 119.7, 121.8, 123.3, 126.0, 127.5, 128.3, 128.5, 128.8, 128.9 (q, J = 306.1 Hz), 129.3, 129.7, 130.4, 130.7, 137.0, 148.3; ^{19}F NMR (378 MHz, $CDCl_3$) δ -44.24 (s); HRMS (ESI) calcd for $C_{22}H_{17}F_3NS$: 384.1028 ($M + H^+$), found: 384.1016.



2-Phenyl-3-(trifluoromethylthio)-1*H*-indole (**3q**)

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29–7.33 (m, 2H), 7.40–7.42 (m, 1H), 7.45–7.53 (m, 3H), 7.75–7.77 (m, 2H), 7.85–7.87 (m, 1H), 8.58 (b, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 92.4, 111.3, 119.8, 121.8, 123.7, 128.7, 128.9, 129.3, 129.8 (q, J = 309.8 Hz), 130.7, 131.5, 135.3, 144.4; ^{19}F NMR (378 MHz, $CDCl_3$) δ -43.82 (s).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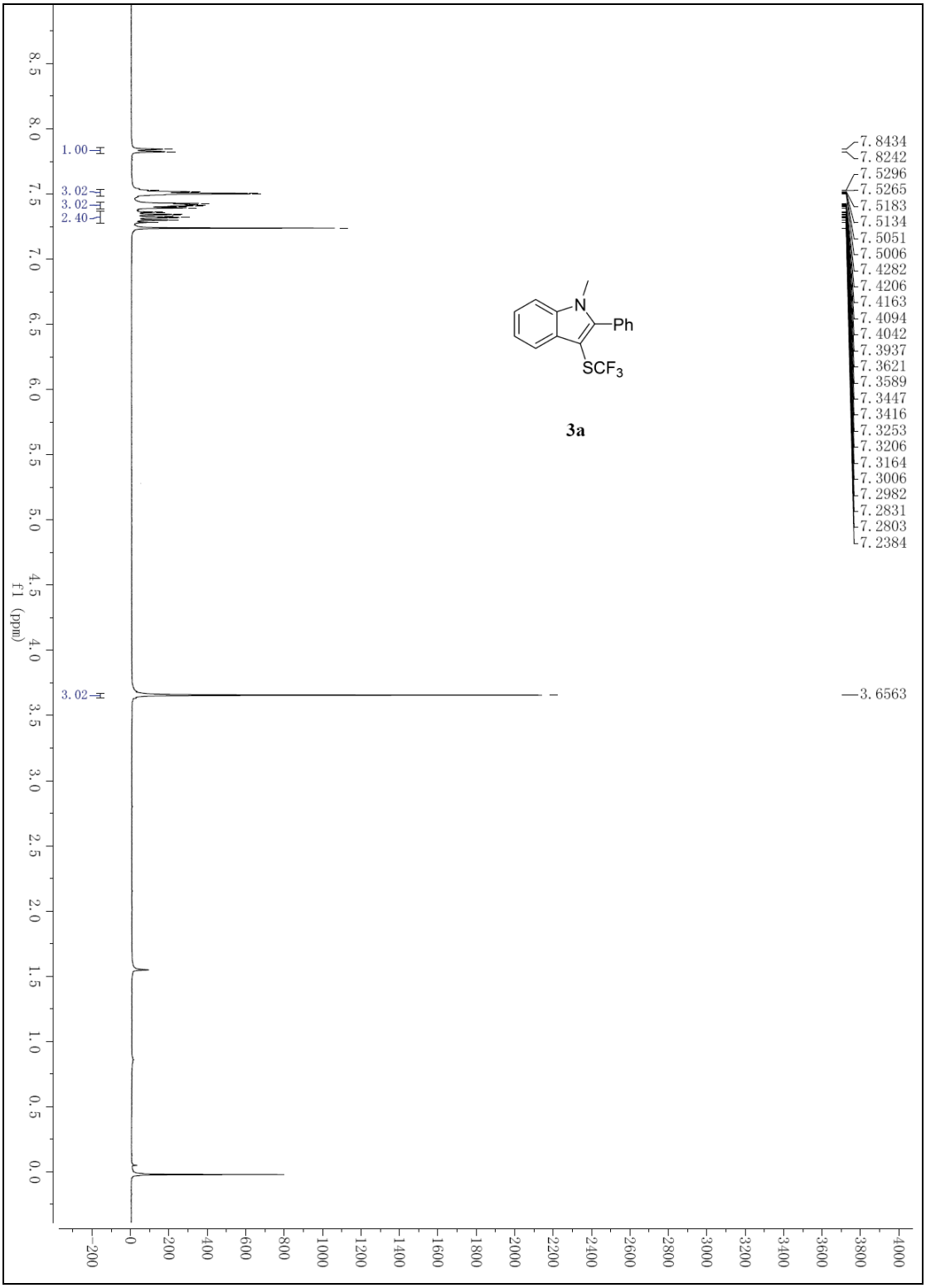
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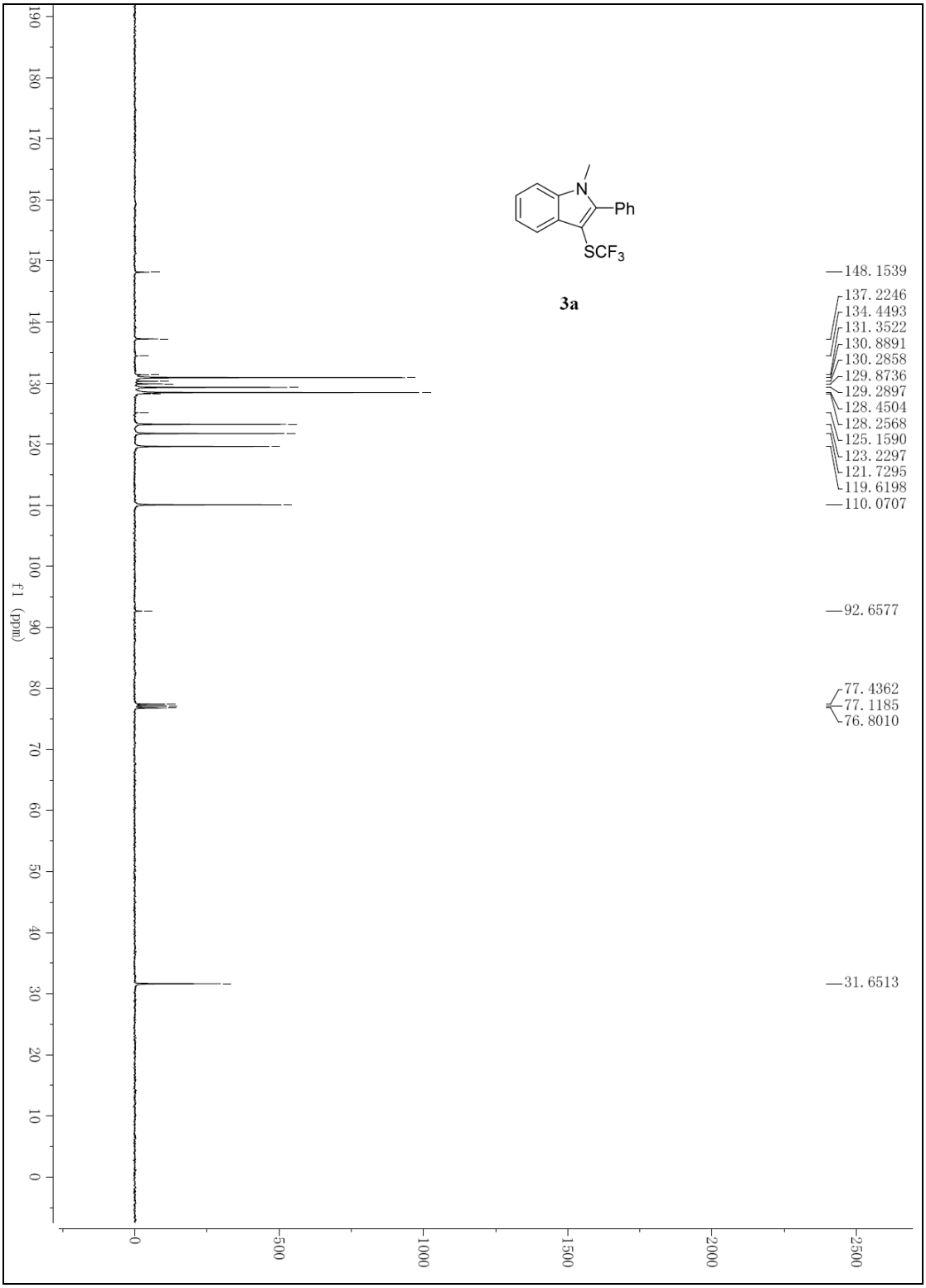
N
Ph
SCF3

3a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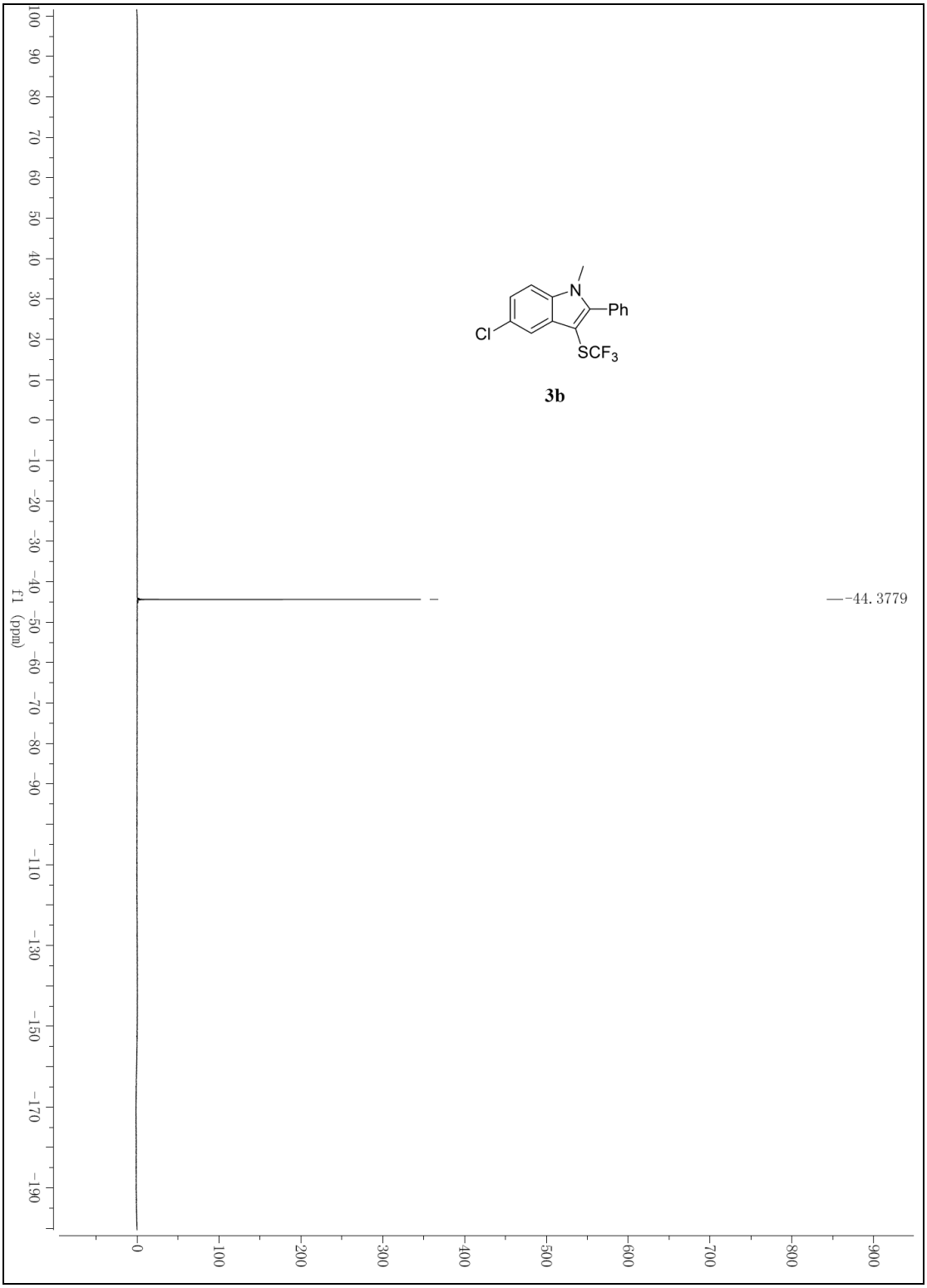
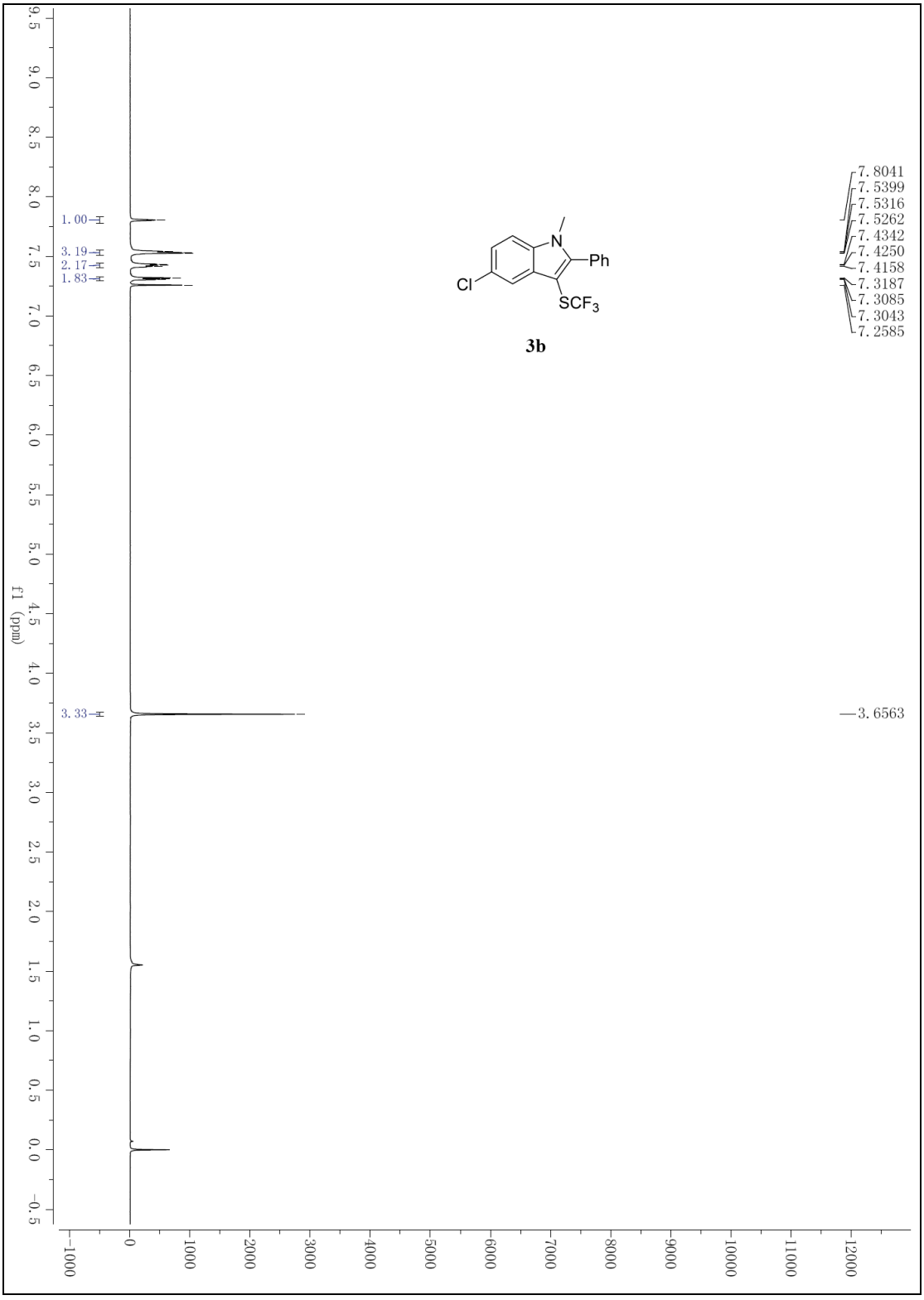
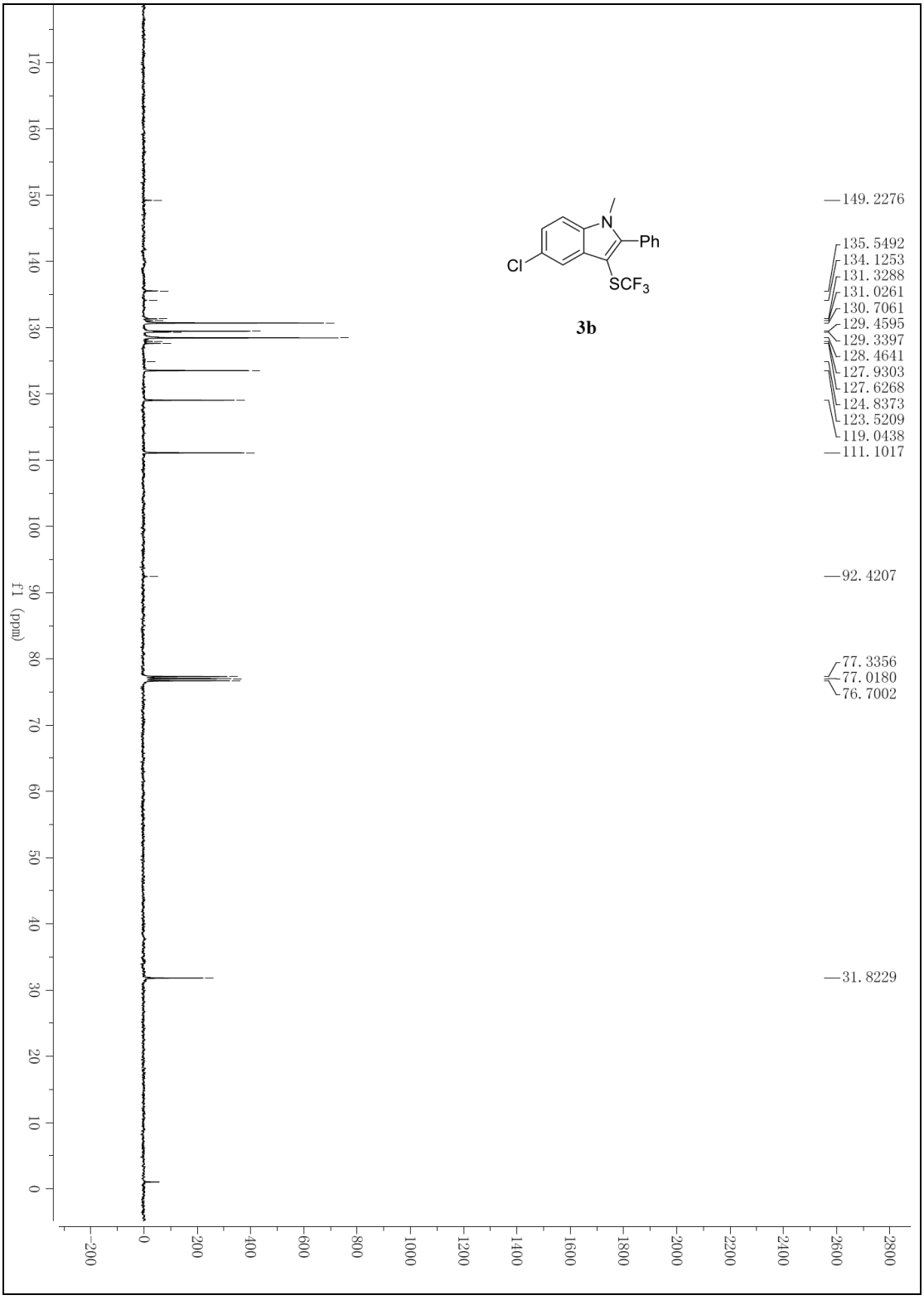
92.6577
77.4362
77.1185
76.8010
31.6513
f1 (ppm)

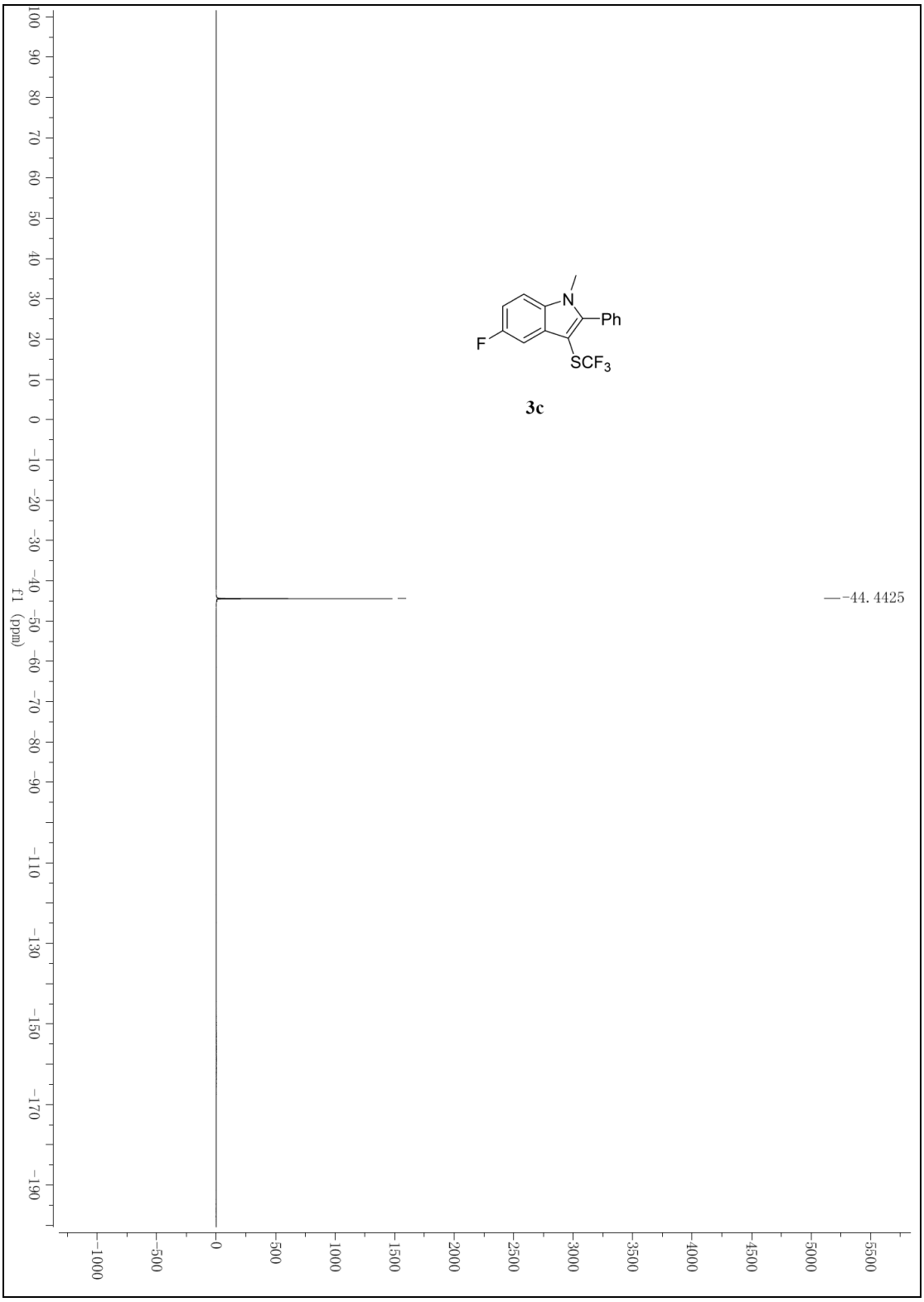

N
Ph
Cl
SCF3
3b
f1 (ppm)
-44.3779

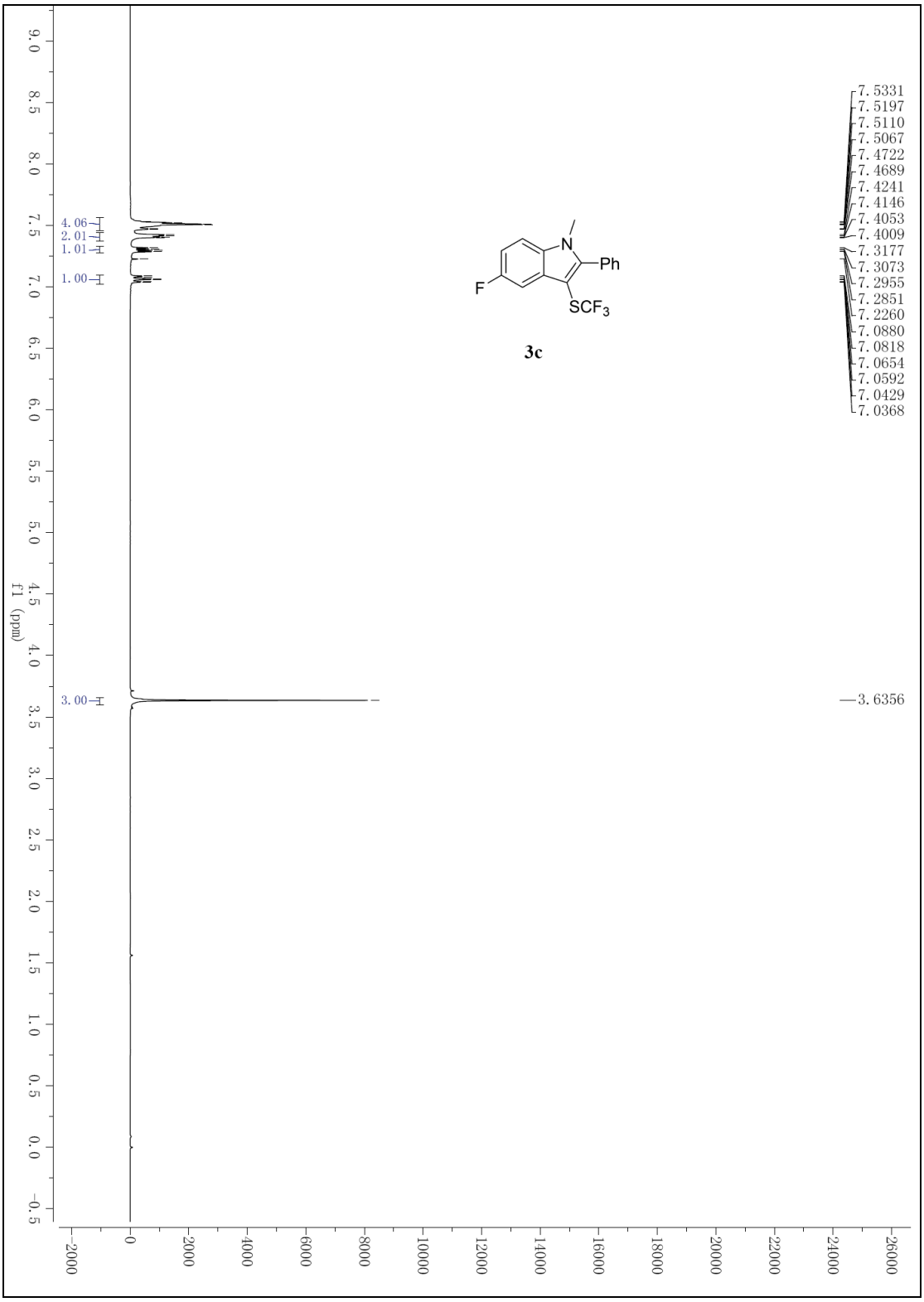

1.00
3.19
2.17
1.83
3.33
7.8041
7.5399
7.5316
7.5262
7.4342
7.4250
7.4158
7.3187
7.3085
7.3043
7.2585
3.6563
Cl
N
Ph
SCF3
f1 (ppm)

3b

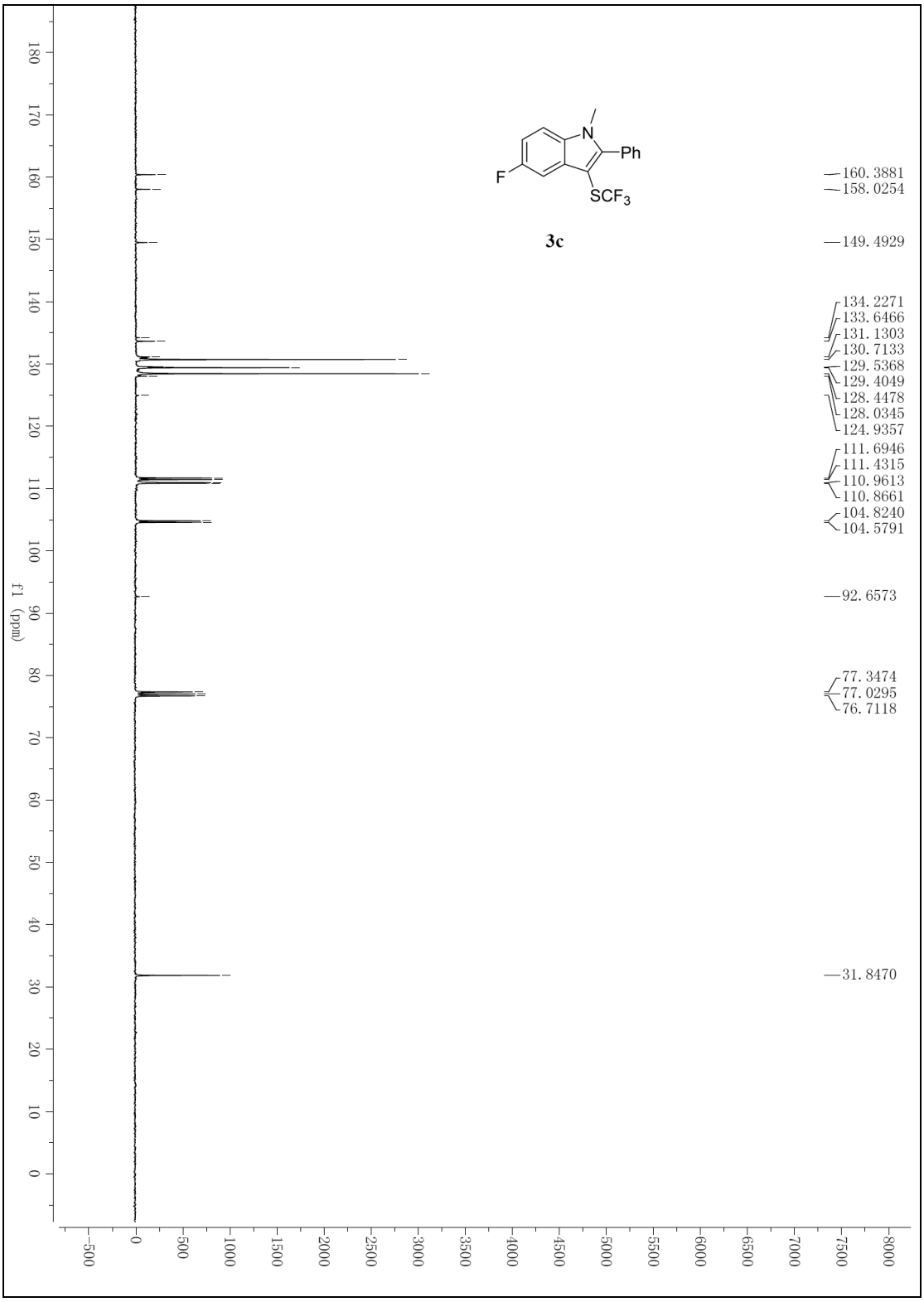

149.2276
135.5492
134.1253
131.3288
131.0261
130.7061
129.4595
129.3397
128.4641
127.9303
127.6268
124.8373
123.5209
119.0438
111.1017
92.4207
77.3356
77.0180
76.7002
31.8229
f1 (ppm)
Cl
N
Ph
SCF3

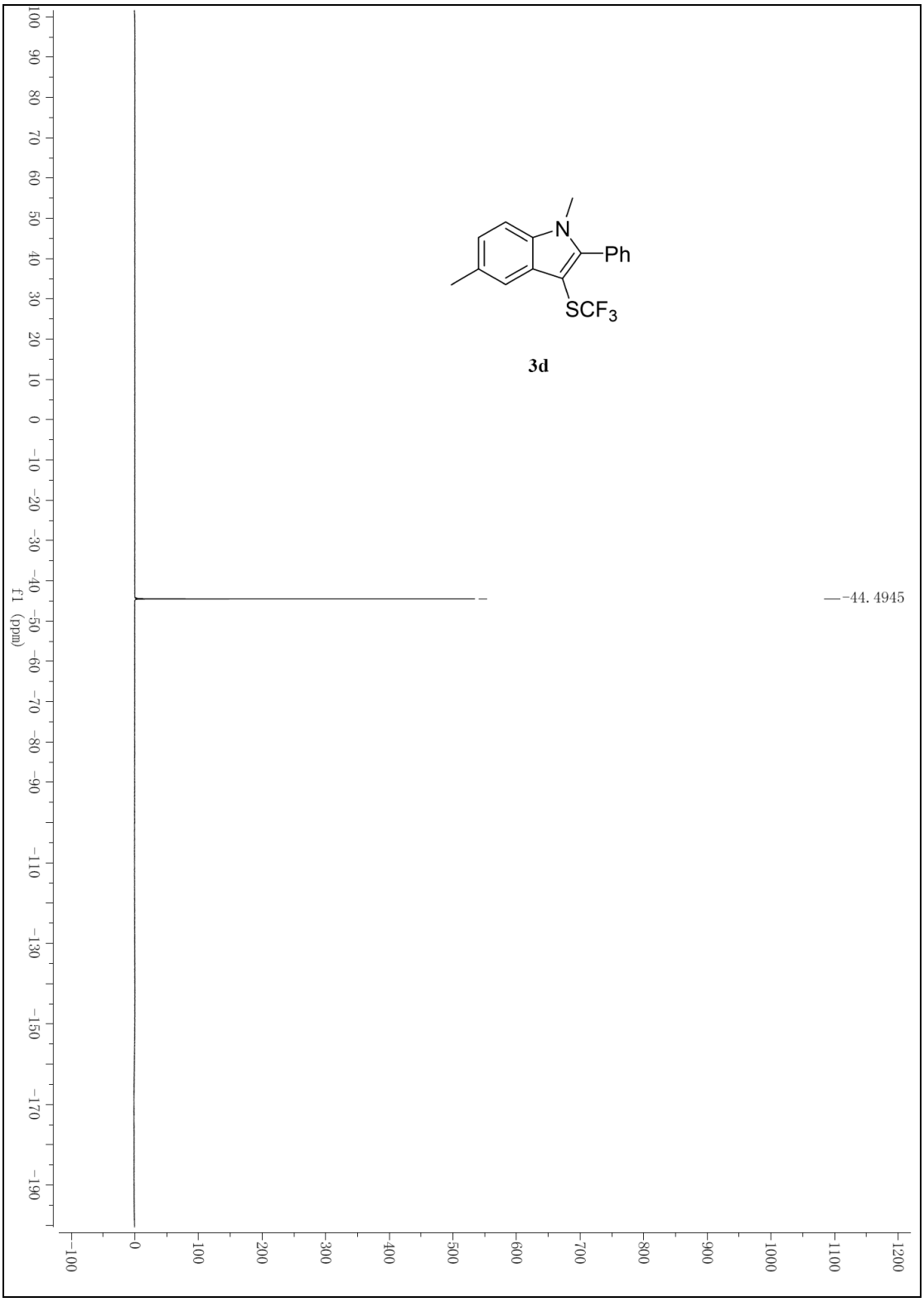
3b

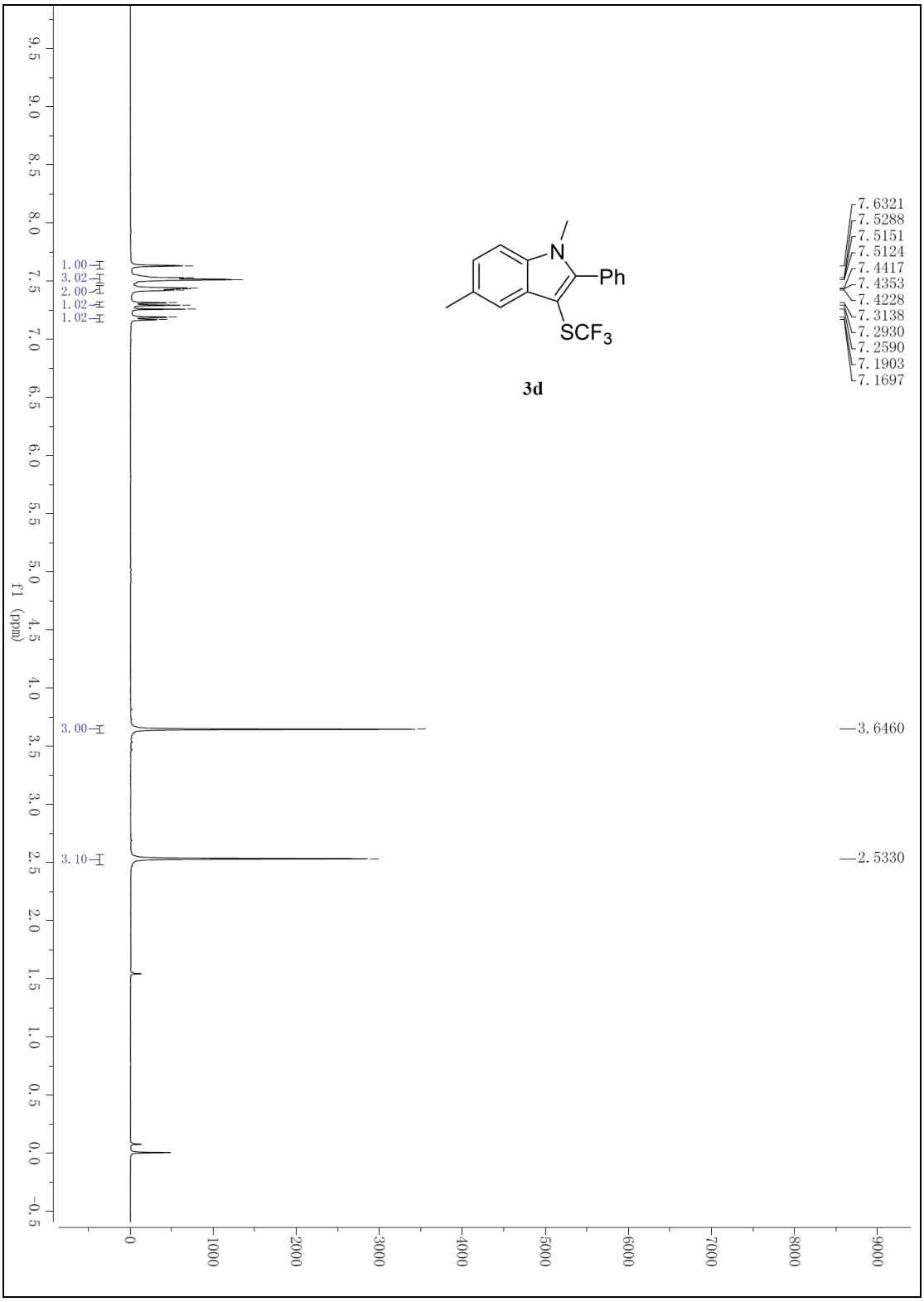

N
Ph
F
SCF3
3c
f1 (ppm)
−44.4425


7.5331
7.5197
7.5110
7.5067
7.4722
7.4689
7.4241
7.4146
7.4053
7.4009
7.3177
7.3073
7.2955
7.2851
7.2260
7.0880
7.0818
7.0654
7.0592
7.0429
7.0368
4.06
2.01
1.01
1.00
3.00
3.6356
f1 (ppm)
N
Ph
F
SCF3

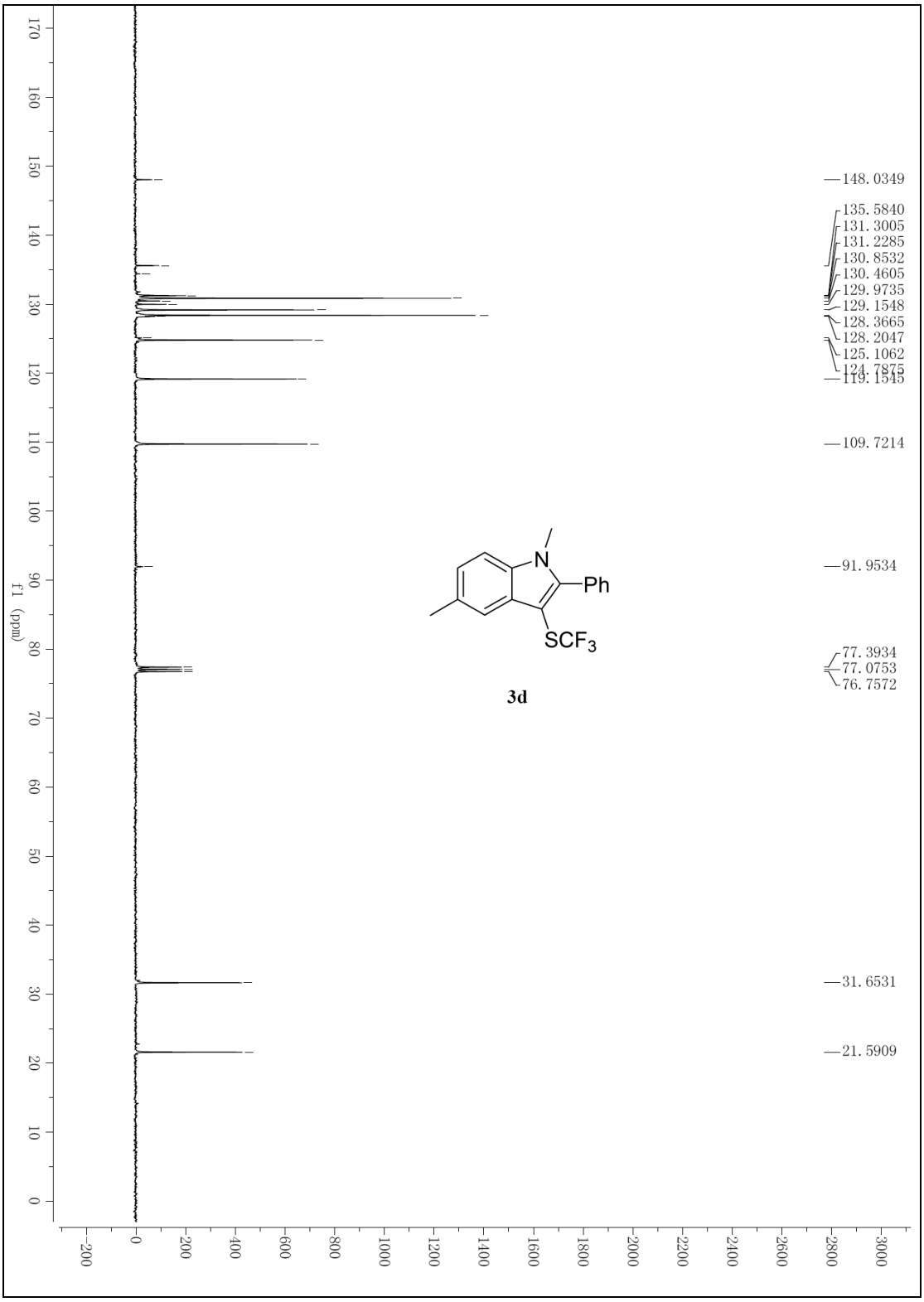
3c


N
Ph
F
SCF3
3c
160.3881
158.0254
149.4929
134.2271
133.6466
131.1303
130.7133
129.5368
129.4049
128.4478
128.0345
124.9357
111.6946
111.4315
110.9613
110.8661
104.8240
104.5791
92.6573
77.3474
77.0295
76.7118
31.8470
f1 (ppm)

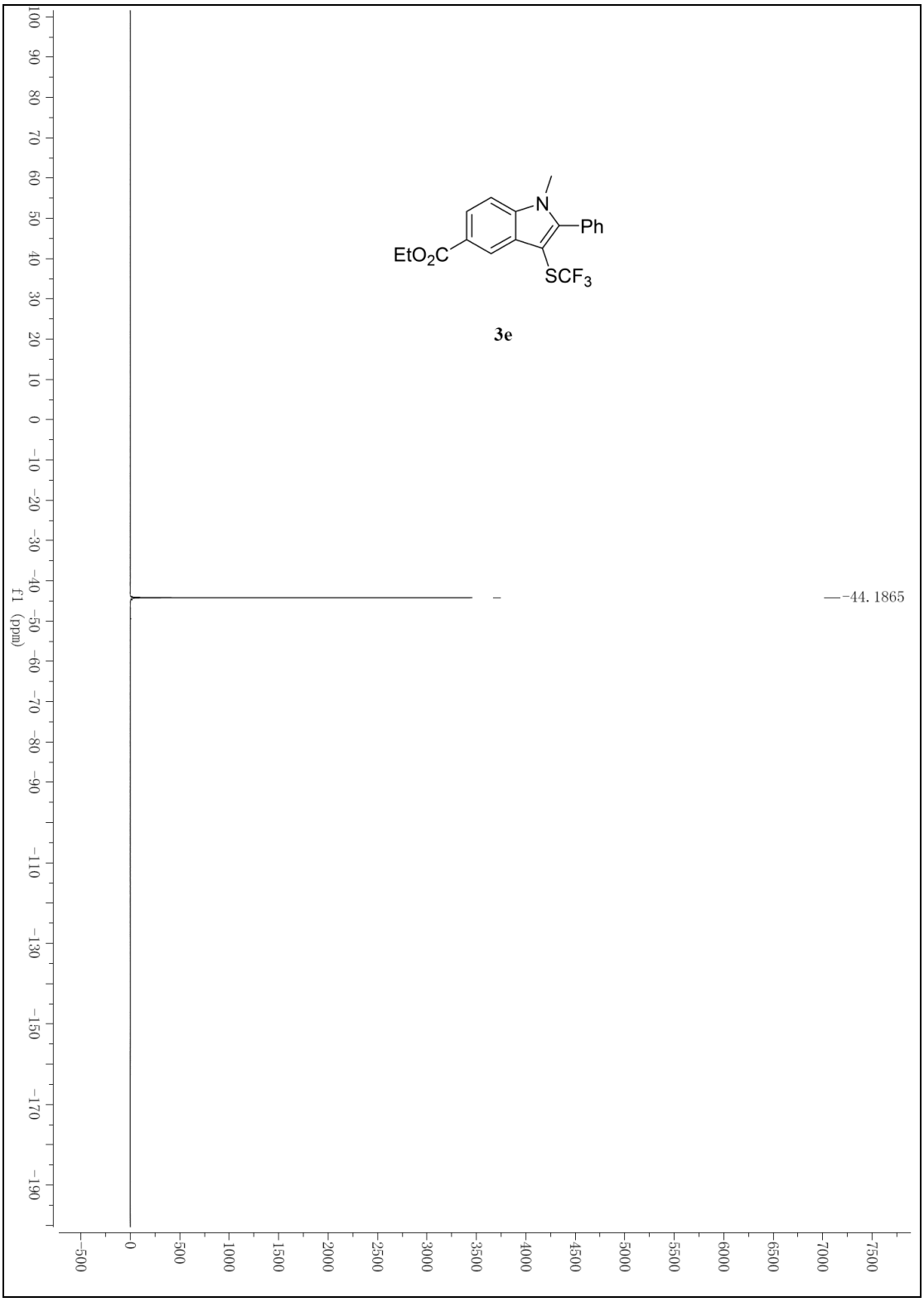

N
Ph
SCF3
3d
f1 (ppm)
-44.4945

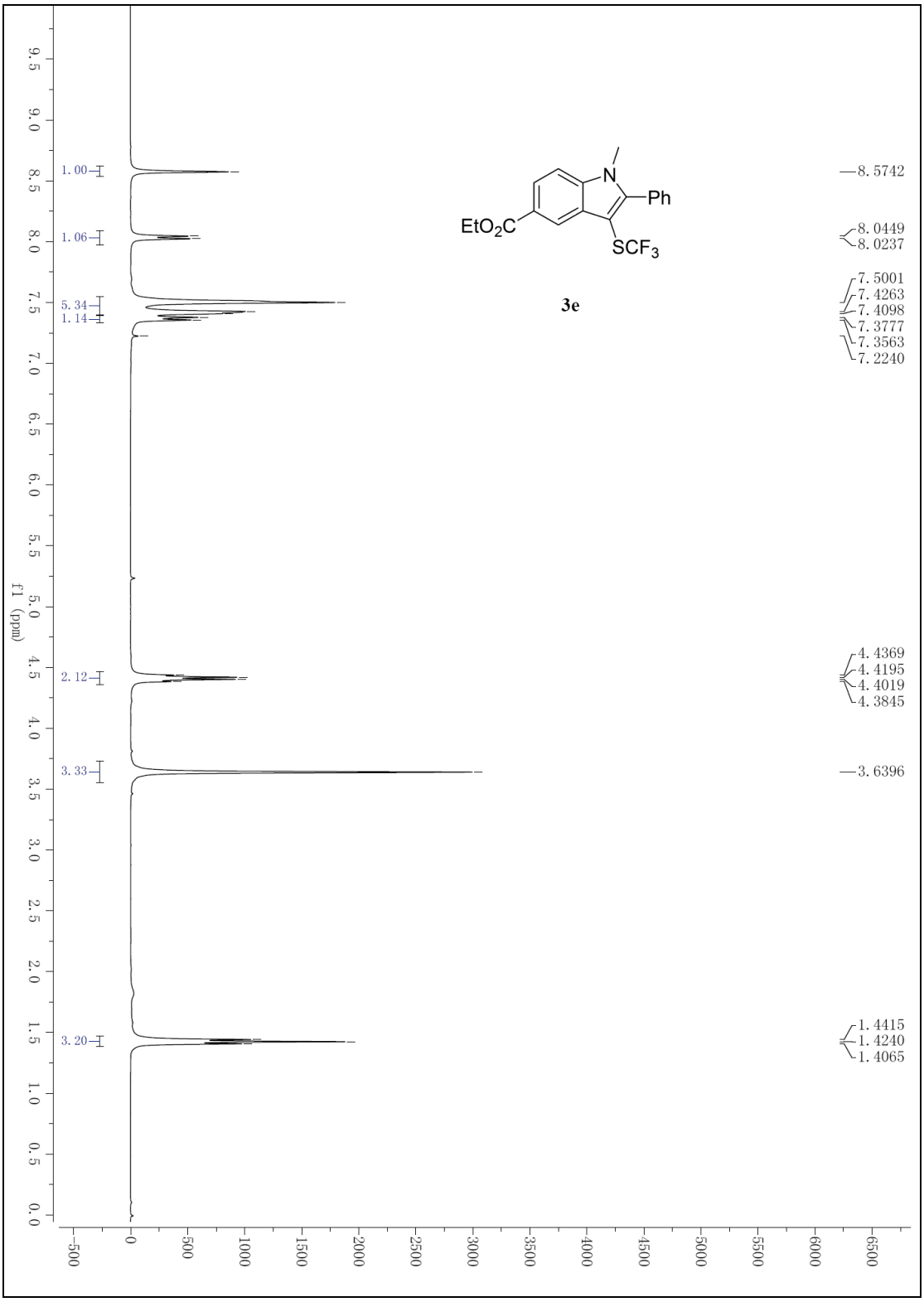

7.6321
7.5288
7.5151
7.5124
7.4417
7.4353
7.4228
7.3138
7.2930
7.2590
7.1903
7.1697
1.00—H
3.02—H
2.00—H
1.02—H
1.02—H
3.00—H
3.10—H
3.6460
2.5330
f1 (ppm)
N
Ph
SCF3

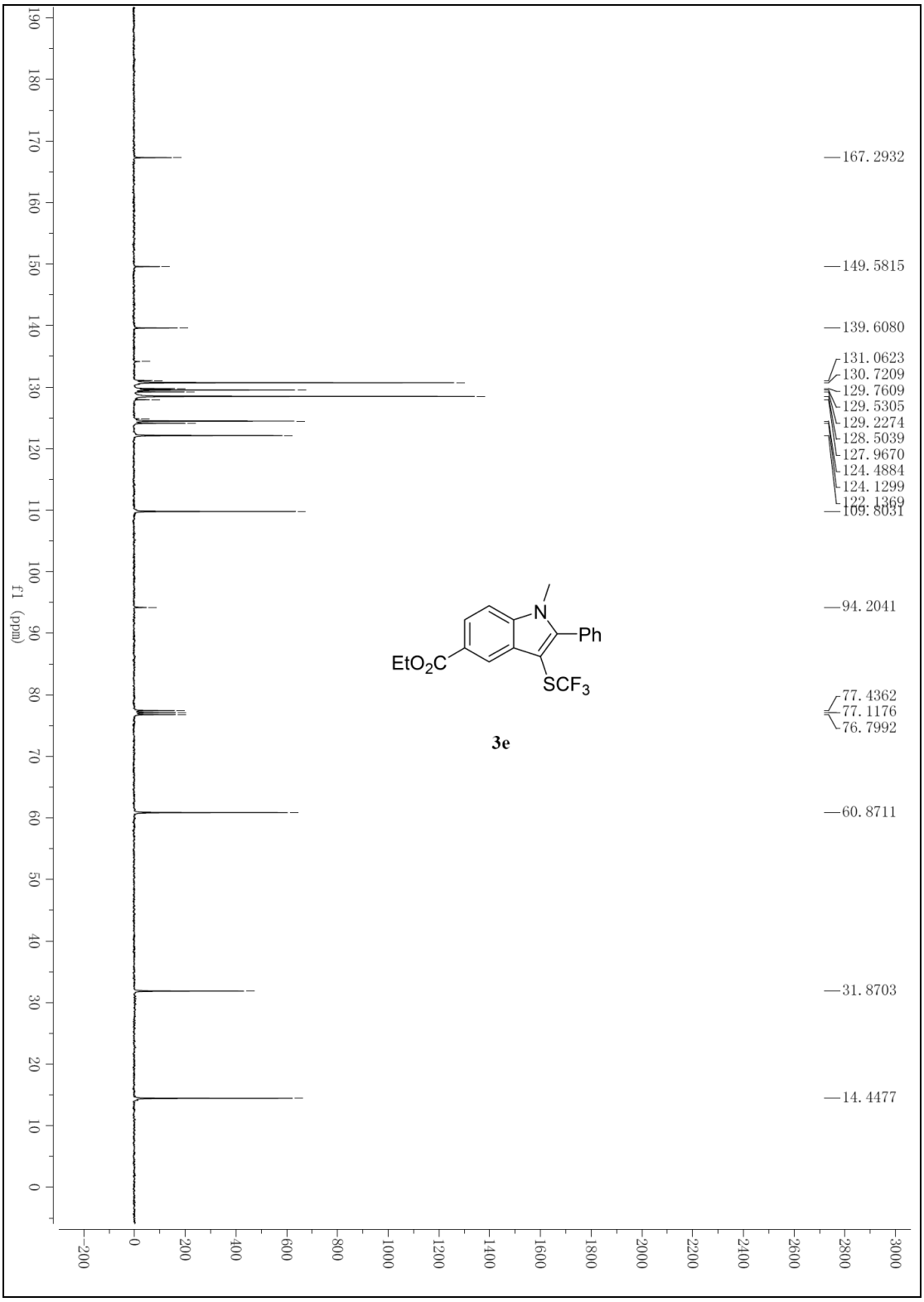
3d


148.0349
135.5840
131.3005
131.2285
130.8532
130.4605
129.9735
129.1548
128.3665
128.2047
125.1062
124.7875
119.1545
109.7214
91.9534
77.3934
77.0753
76.7572
31.6531
21.5909
f1 (ppm)
N
Ph
SCF3

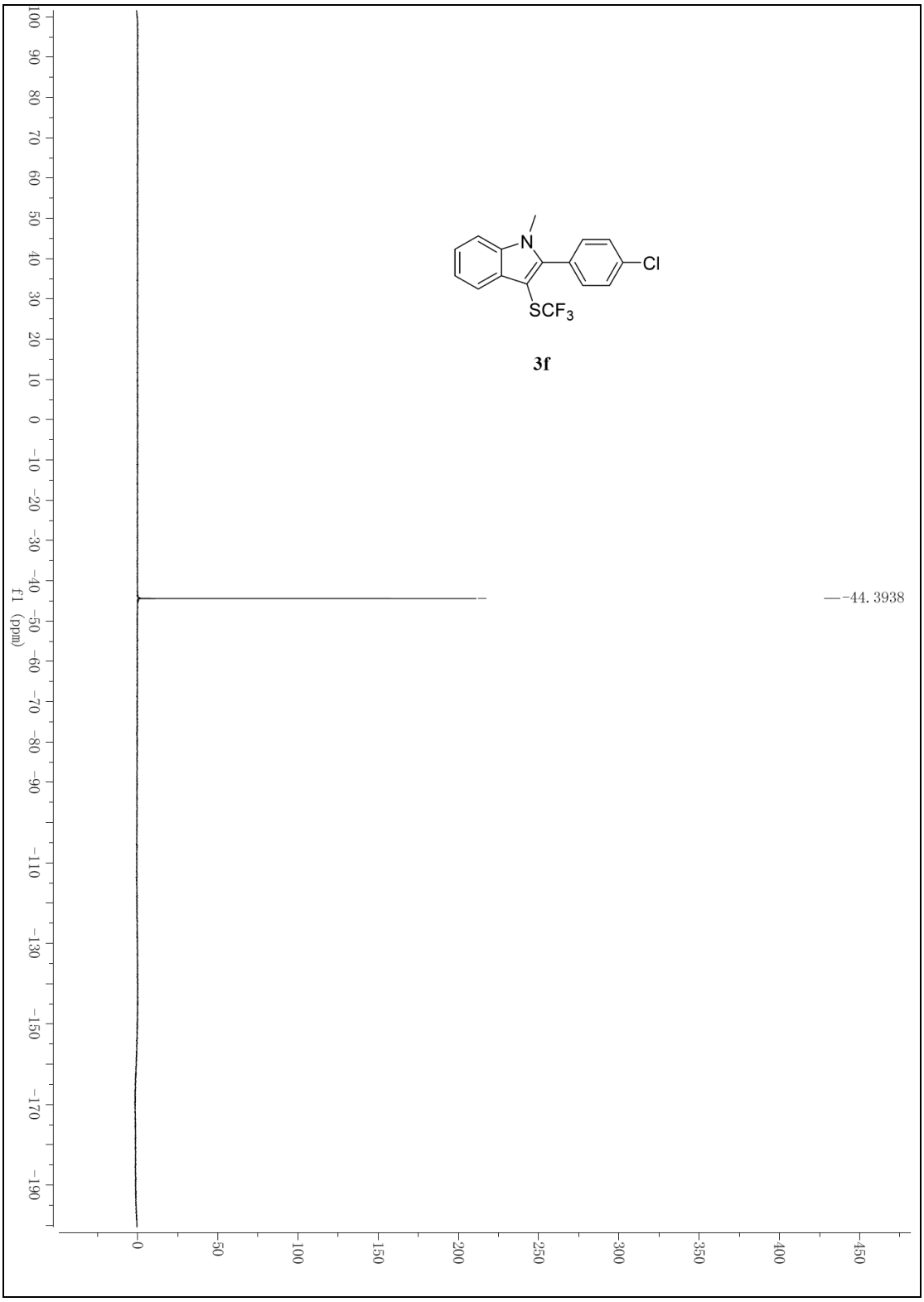
3d

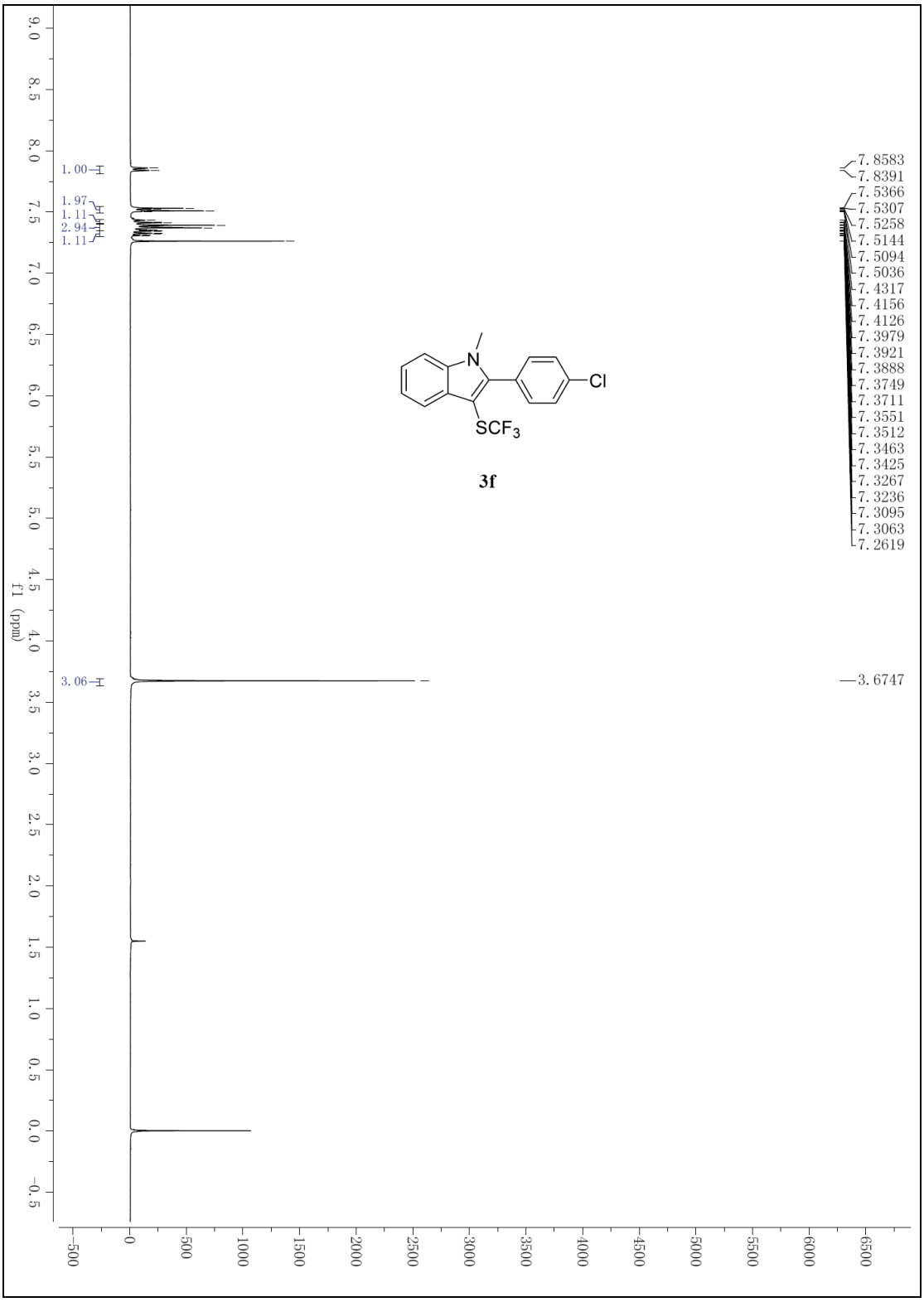

N
Ph
EtO2C
SCF3
3e
f1 (ppm)
-44.1865


f1 (ppm)
1.00
1.06
5.34
1.14
2.12
3.33
3.20
N
Ph
EtO2C
SCF3
3e
8.5742
8.0449
8.0237
7.5001
7.4263
7.4098
7.3777
7.3563
7.2240
4.4369
4.4195
4.4019
4.3845
3.6396
1.4415
1.4240
1.4065


167.2932
149.5815
139.6080
131.0623
130.7209
129.7609
129.5305
129.2274
128.5039
127.9670
124.4884
124.1299
122.1369
109.8031
94.2041
77.4362
77.1176
76.7992
60.8711
31.8703
14.4477
f1 (ppm)
N
Ph
EtO2C
SCF3

3e


N
Cl
SCF3
3f
f1 (ppm)
-44.3938


1.00
1.97
1.11
2.94
1.11
3.06
7.8583
7.8391
7.5366
7.5307
7.5258
7.5144
7.5094
7.5036
7.4317
7.4156
7.4126
7.3979
7.3921
7.3888
7.3749
7.3711
7.3551
7.3512
7.3463
7.3425
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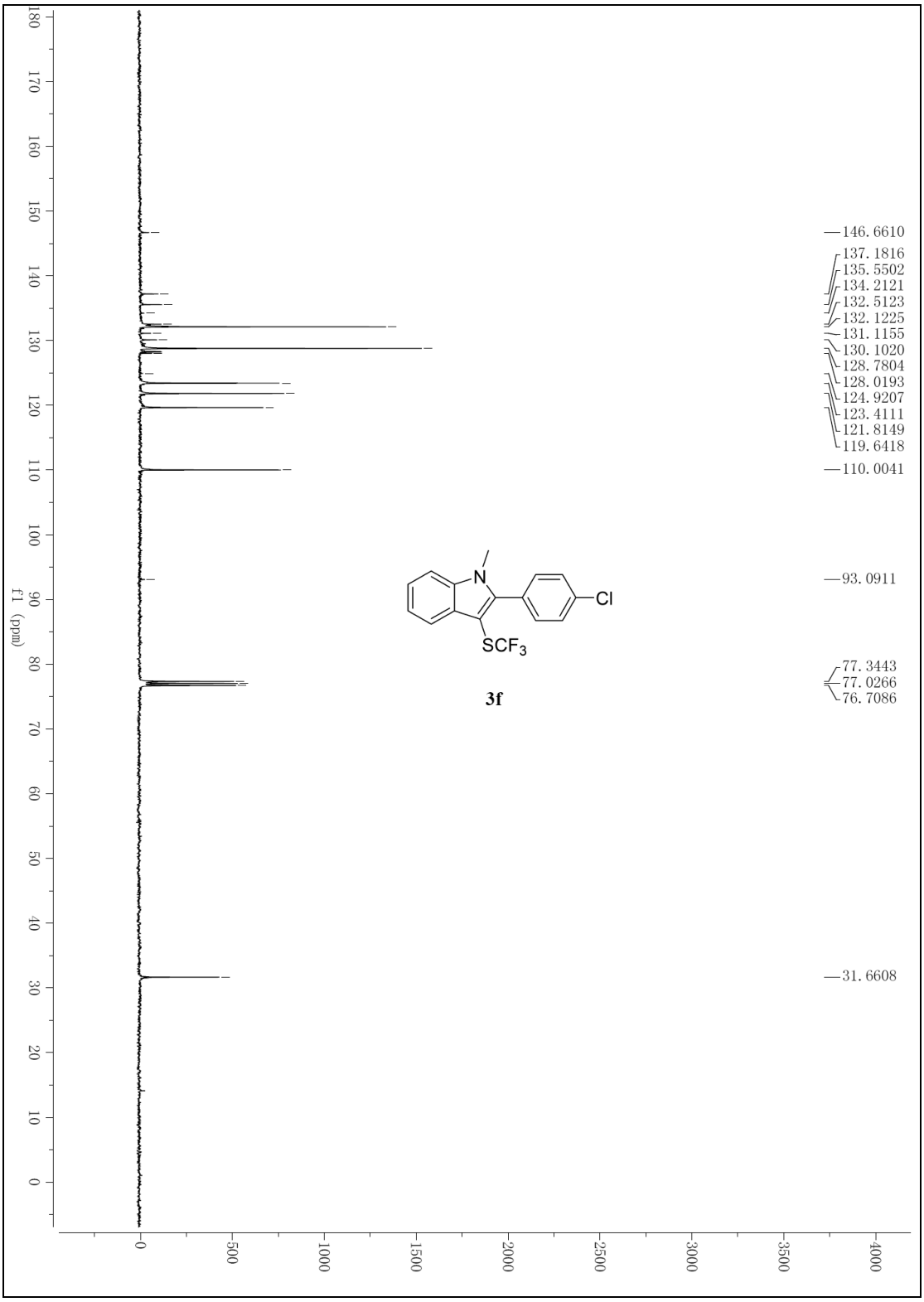
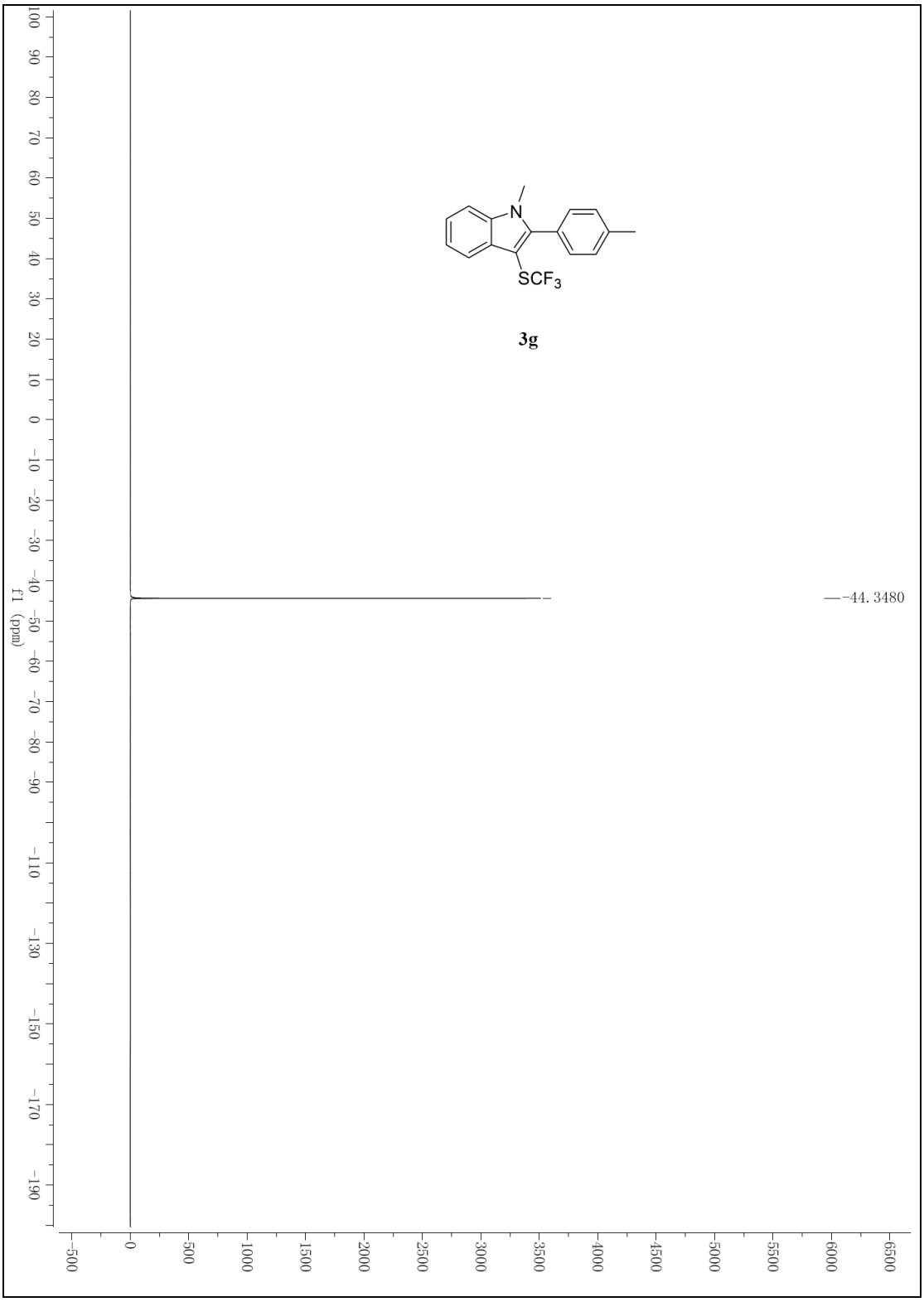
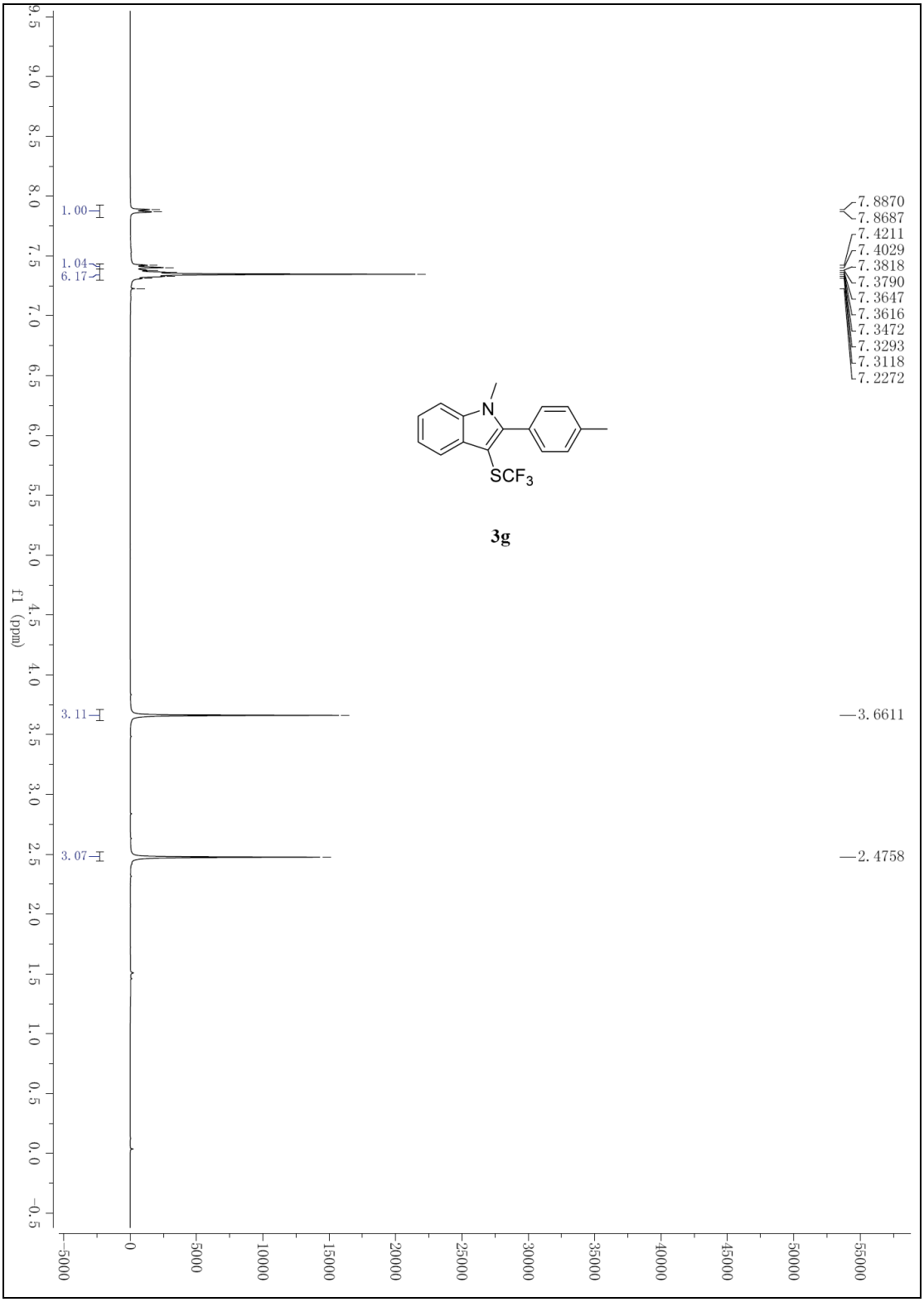
7.3095
7.3063
7.2619
3.6747
N
Cl
SCF3
f1 (ppm)

3f

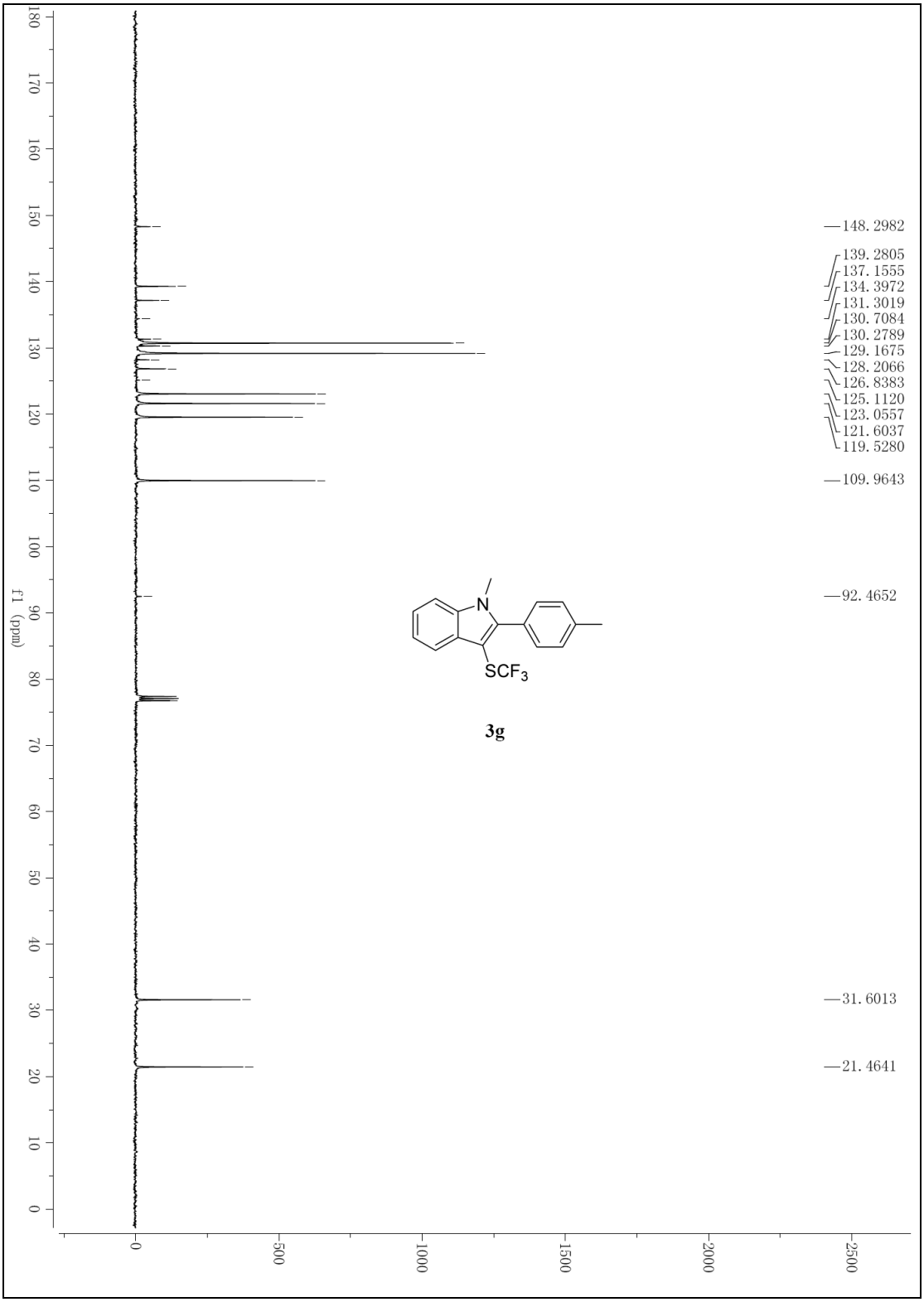

146.6610
137.1816
135.5502
134.2121
132.5123
132.1225
131.1155
130.1020
128.7804
128.0193
124.9207
123.4111
121.8149
119.6418
110.0041
93.0911
77.3443
77.0266
76.7086
31.6608
f1 (ppm)
N
Cl
SCF3

3f

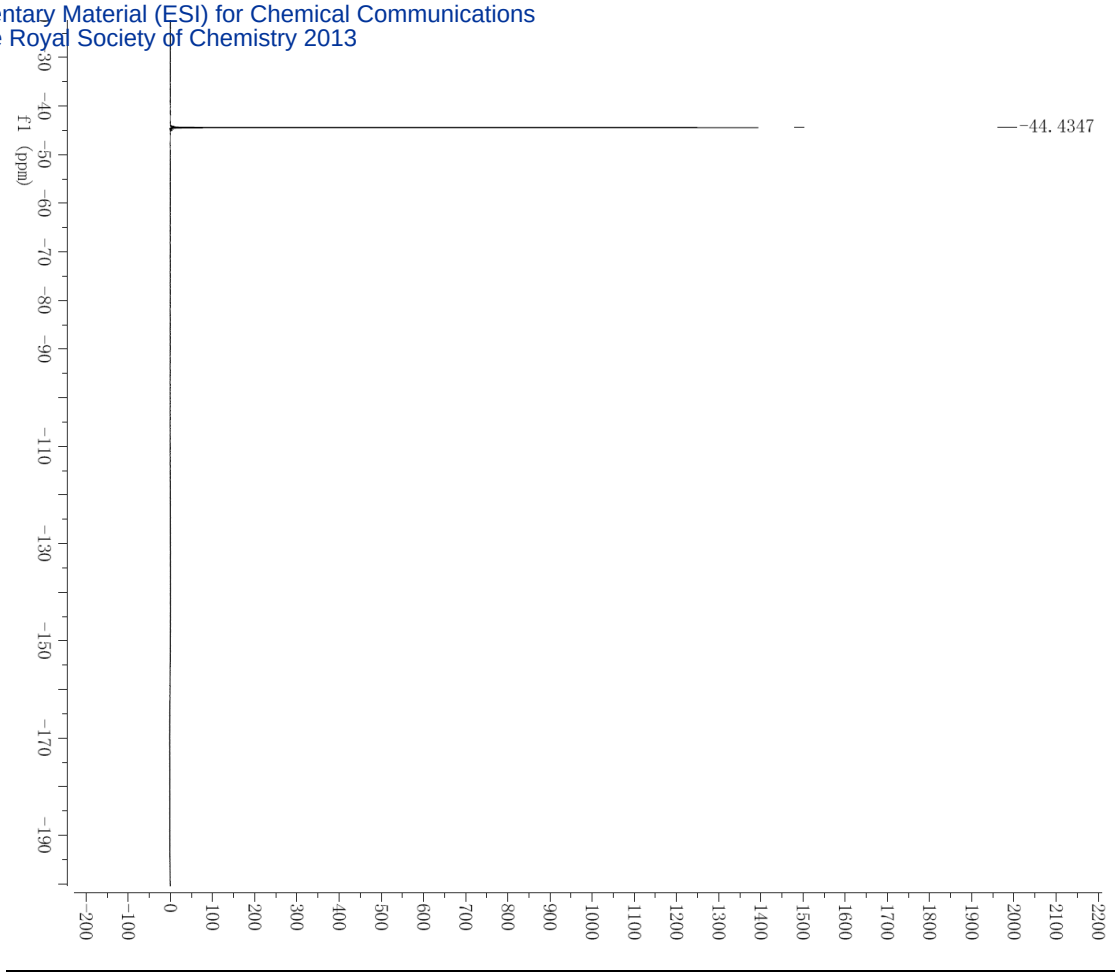

N
SCF3
3g
−44.3480
f1 (ppm)

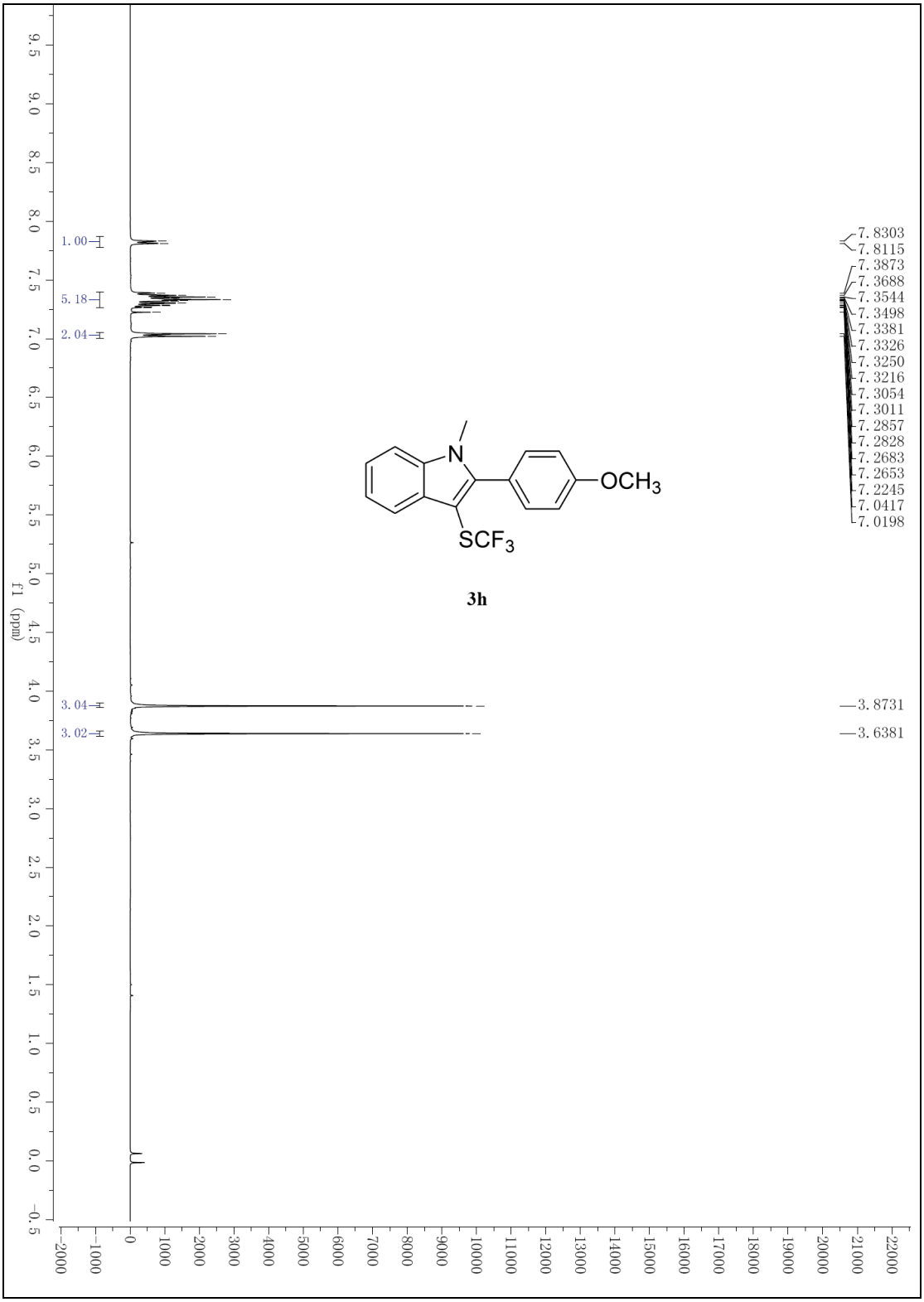

7.8870
7.8687
7.4211
7.4029
7.3818
7.3790
7.3647
7.3616
7.3472
7.3293
7.3118
7.2272
1.00
1.04
6.17
3.11
3.07
3.6611
2.4758
N
SCF3
f1 (ppm)

3g

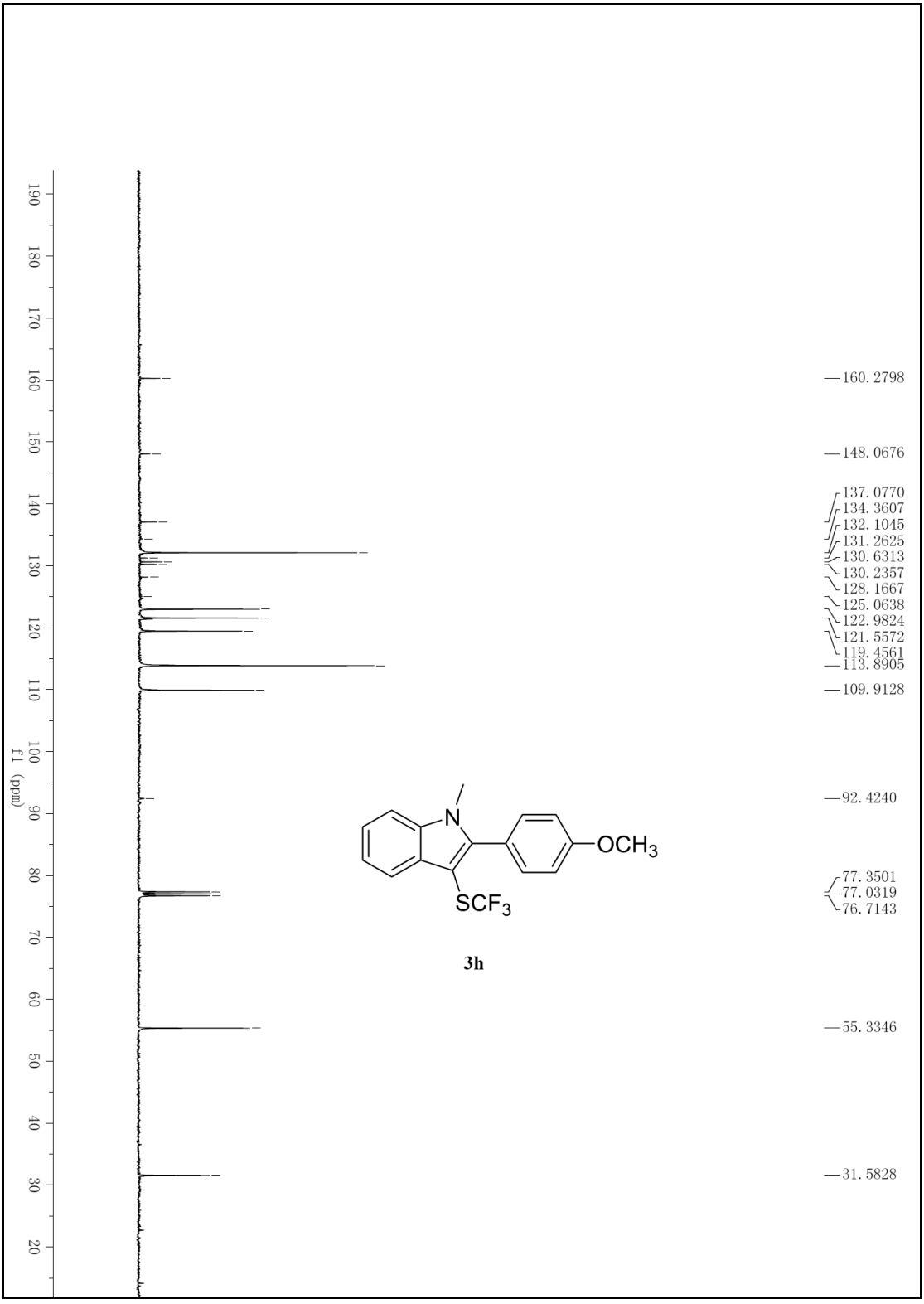

148.2982
139.2805
137.1555
134.3972
131.3019
130.7084
130.2789
129.1675
128.2066
126.8383
125.1120
123.0557
121.6037
119.5280
109.9643
92.4652
31.6013
21.4641
f1 (ppm)
SCF3

3g

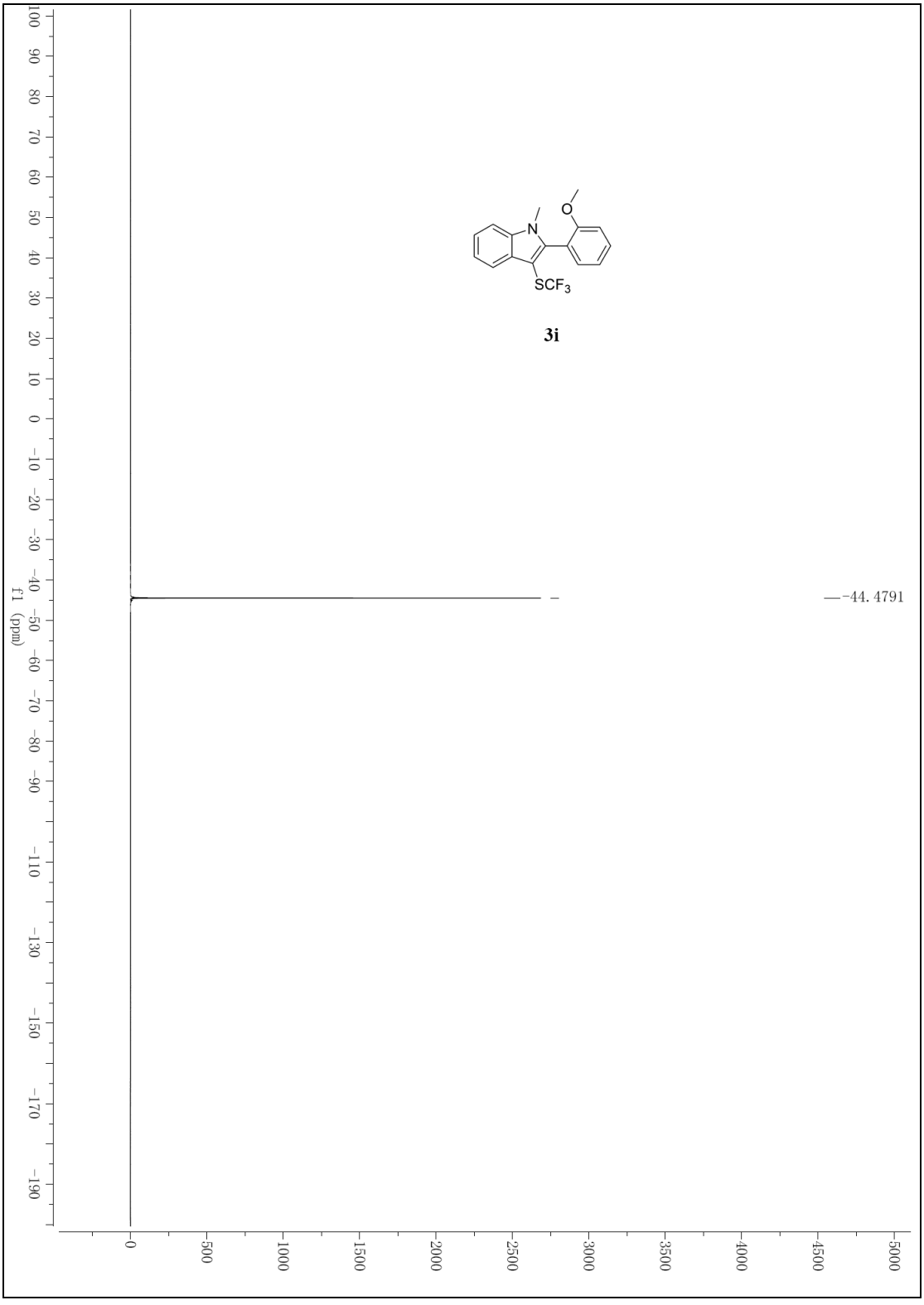

-44.4347
f1 (ppm)
30
40
50
60
70
80
90
110
130
150
170
190
-200
-100
0
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
2000
2100
2200

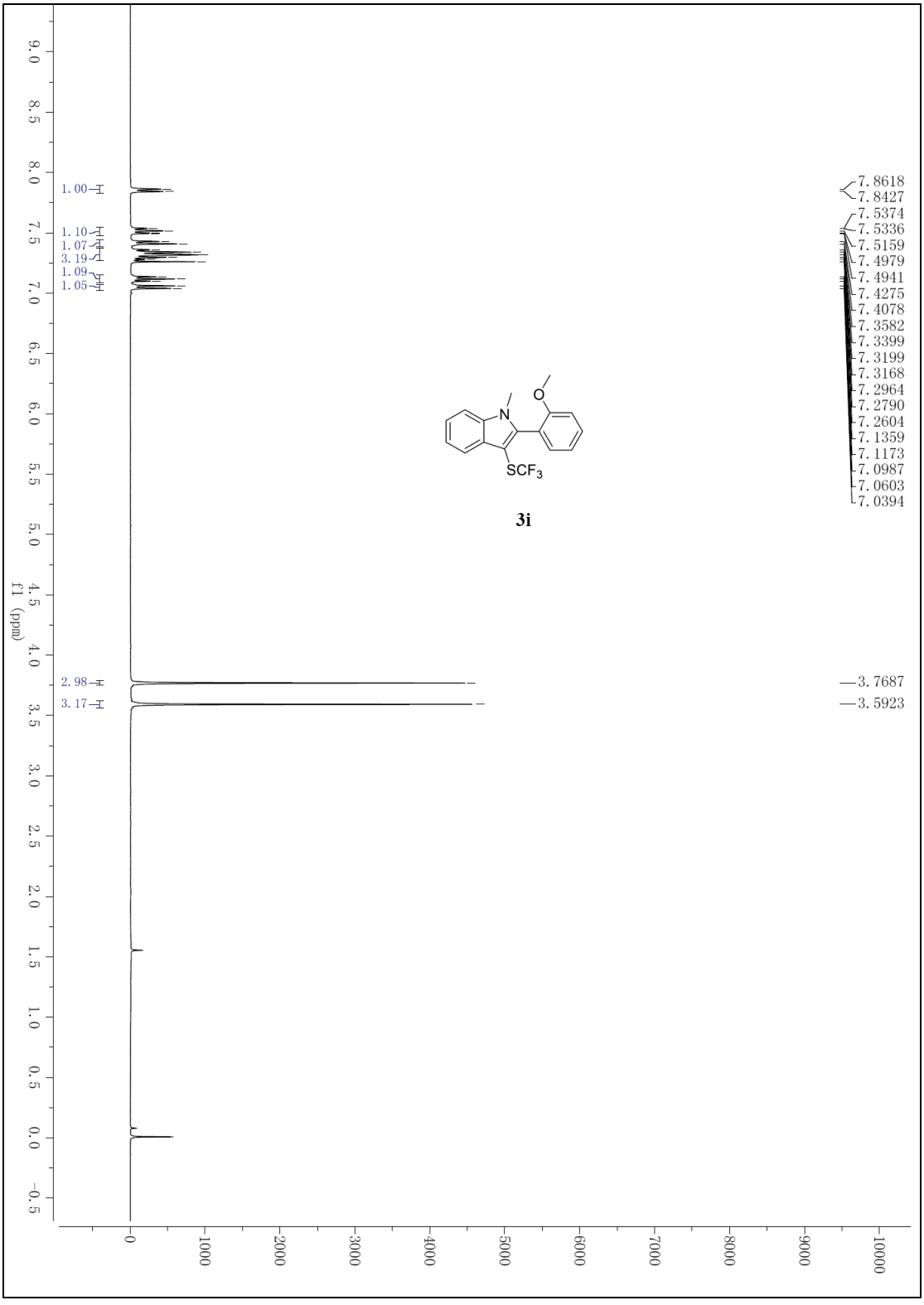

1.00
5.18
2.04
3.04
3.02
7.8303
7.8115
7.3873
7.3688
7.3544
7.3498
7.3381
7.3326
7.3250
7.3216
7.3054
7.3011
7.2857
7.2828
7.2683
7.2653
7.2245
7.0417
7.0198
3.8731
3.6381
N
OCH3
SCF3
f1 (ppm)

3h

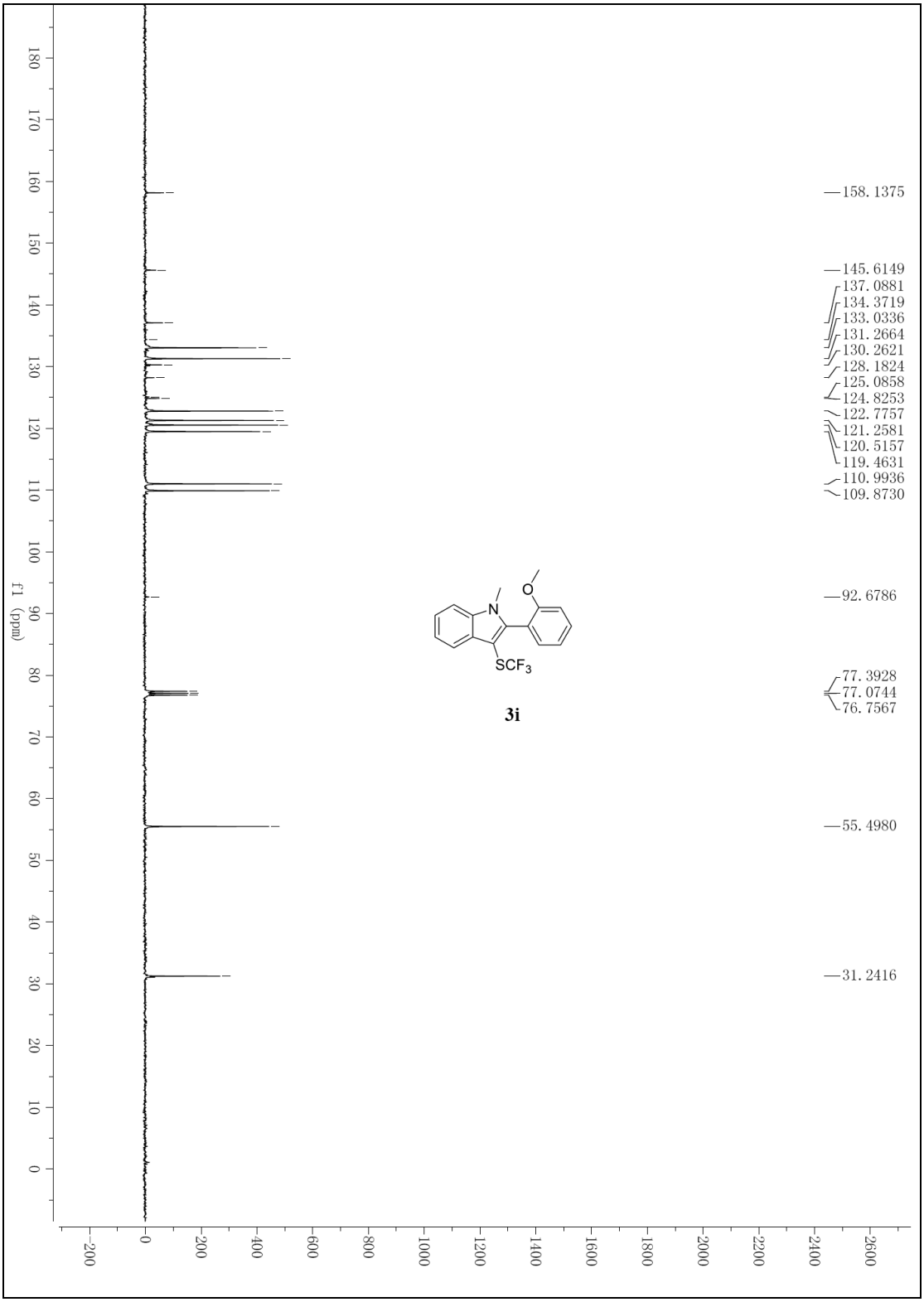

160.2798
148.0676
137.0770
134.3607
132.1045
131.2625
130.6313
130.2357
128.1667
125.0638
122.9824
121.5572
119.4561
113.8905
109.9128
92.4240
77.3501
77.0319
76.7143
55.3346
31.5828
f1 (ppm)
N
OCH3
SCF3

3h

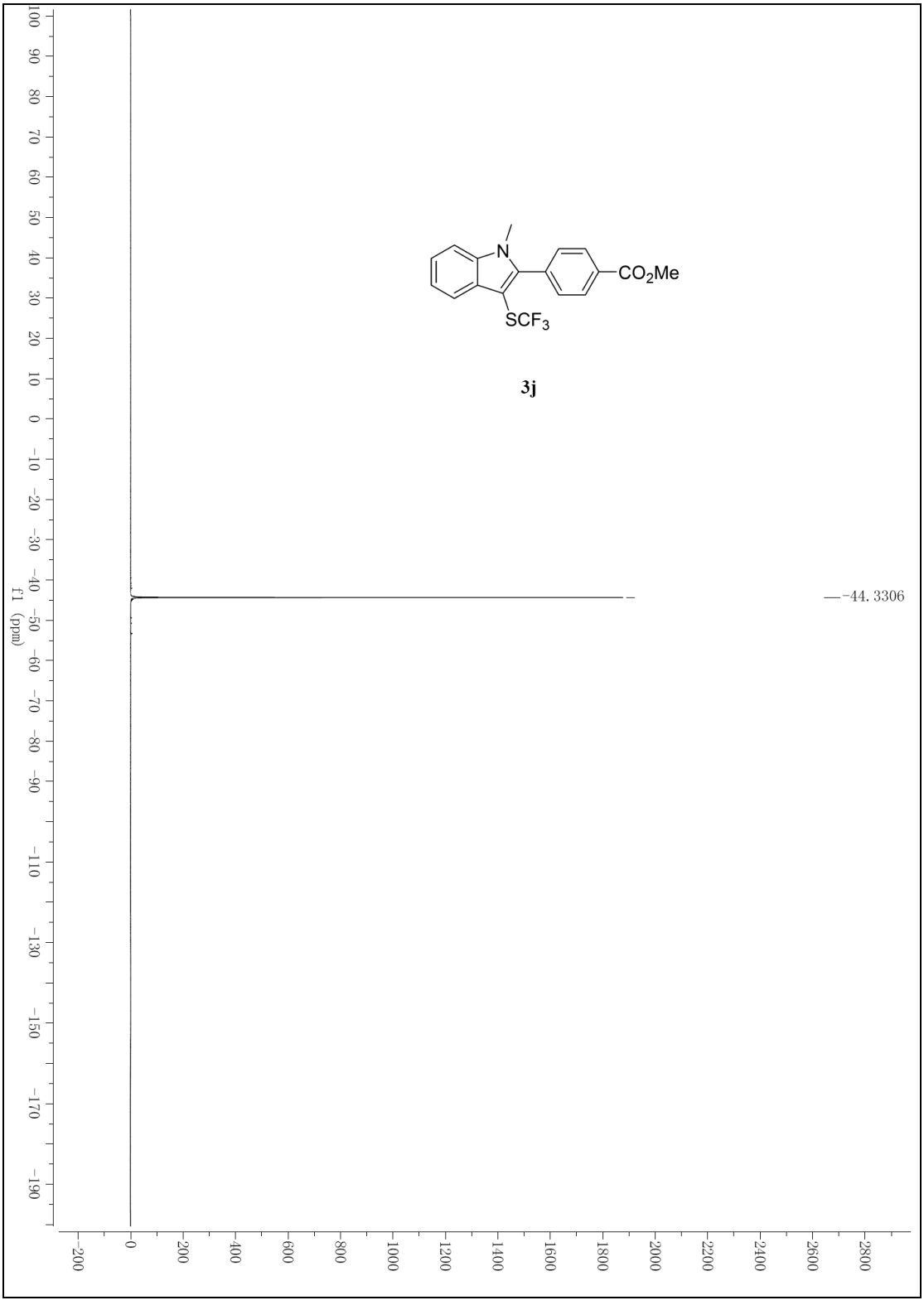

N
O
SCF3
3i
f1 (ppm)
−44.4791

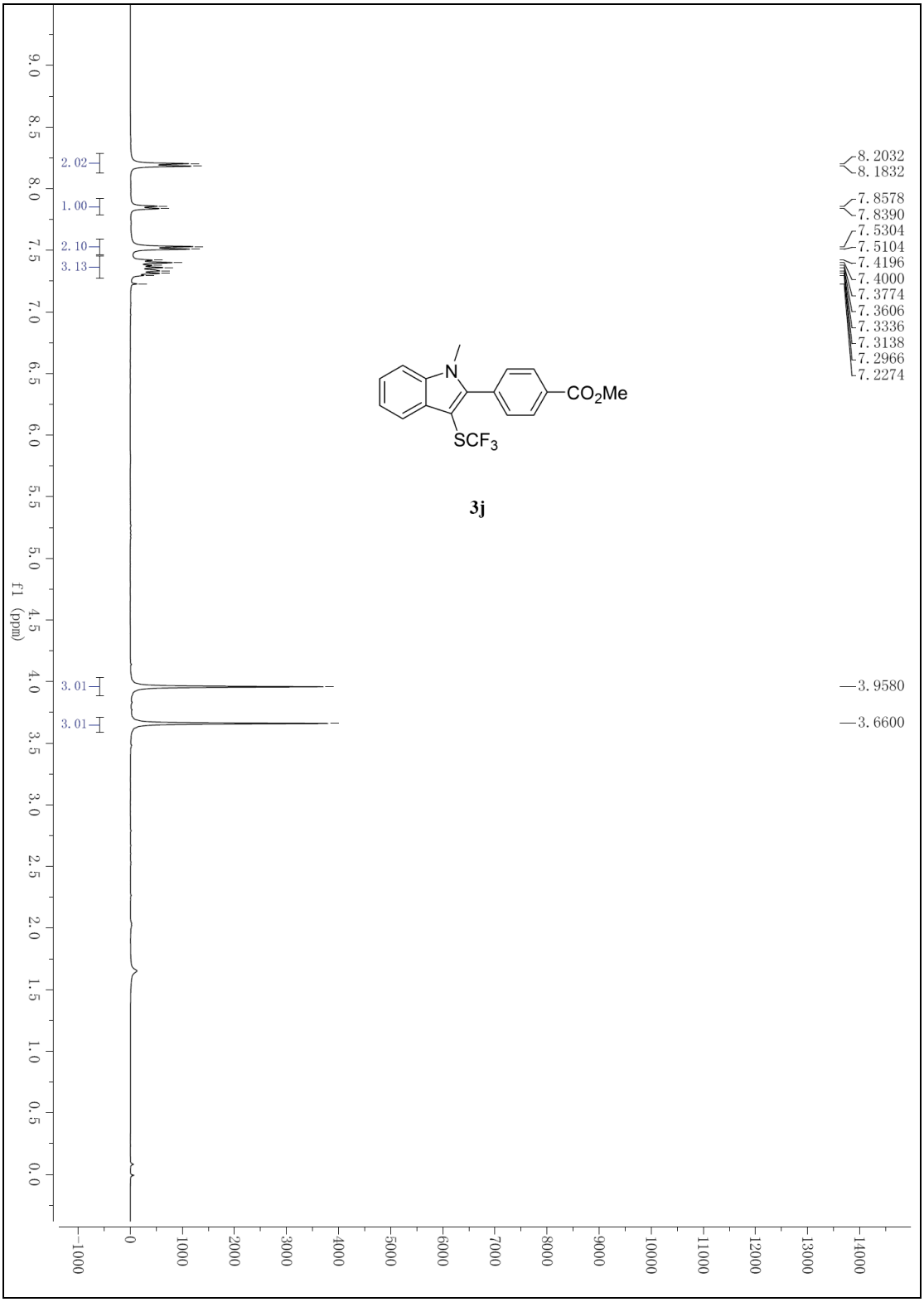

1.00
1.10
1.07
3.19
1.09
1.05
2.98
3.17
7.8618
7.8427
7.5374
7.5336
7.5159
7.4979
7.4941
7.4275
7.4078
7.3582
7.3399
7.3199
7.3168
7.2964
7.2790
7.2604
7.1359
7.1173
7.0987
7.0603
7.0394
3.7687
3.5923
N
O
SCF3
f1 (ppm)

3i

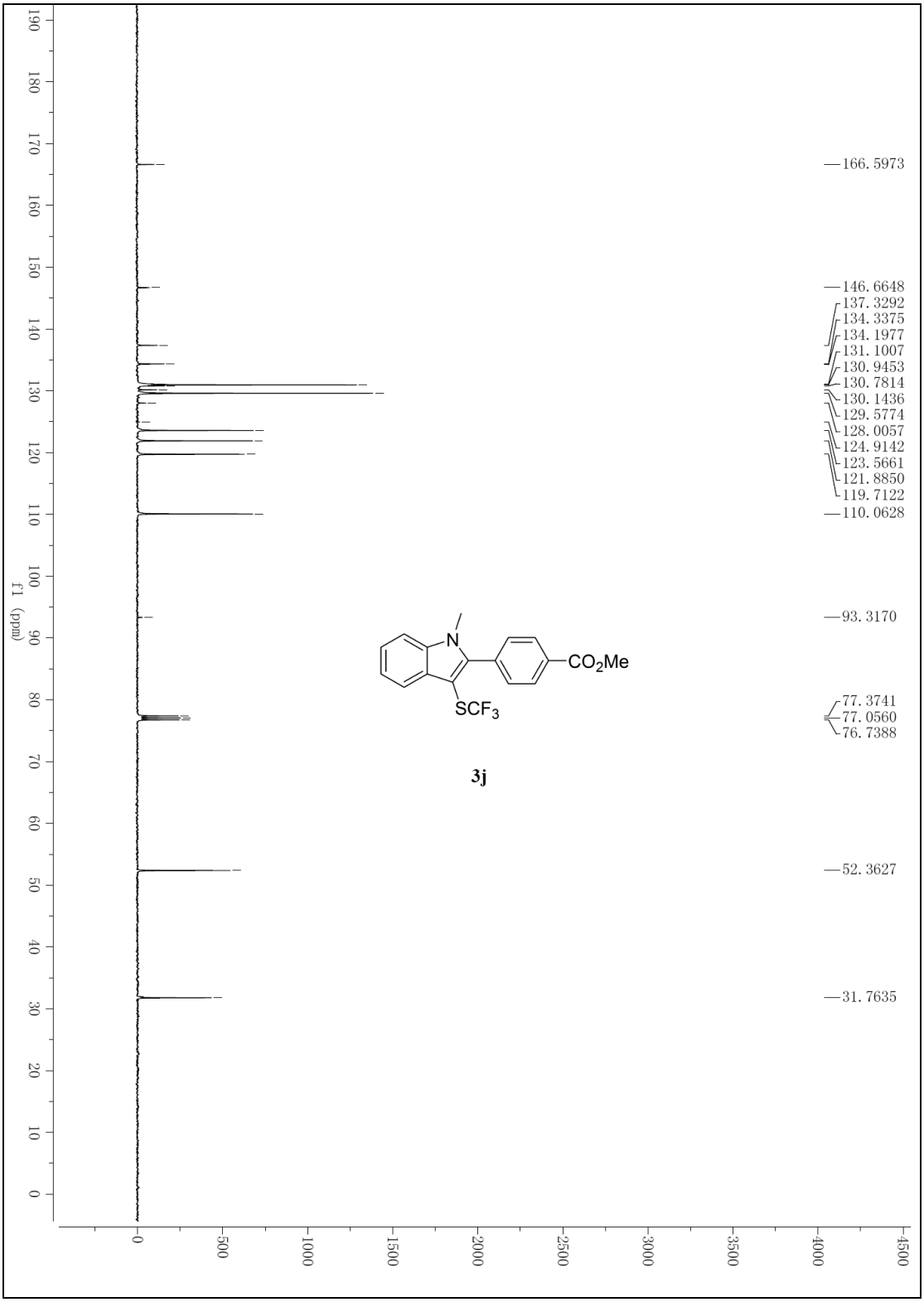

158.1375
145.6149
137.0881
134.3719
133.0336
131.2664
130.2621
128.1824
125.0858
124.8253
122.7757
121.2581
120.5157
119.4631
110.9936
109.8730
92.6786
77.3928
77.0744
76.7567
55.4980
31.2416
f1 (ppm)
N
O
SCF3

3i

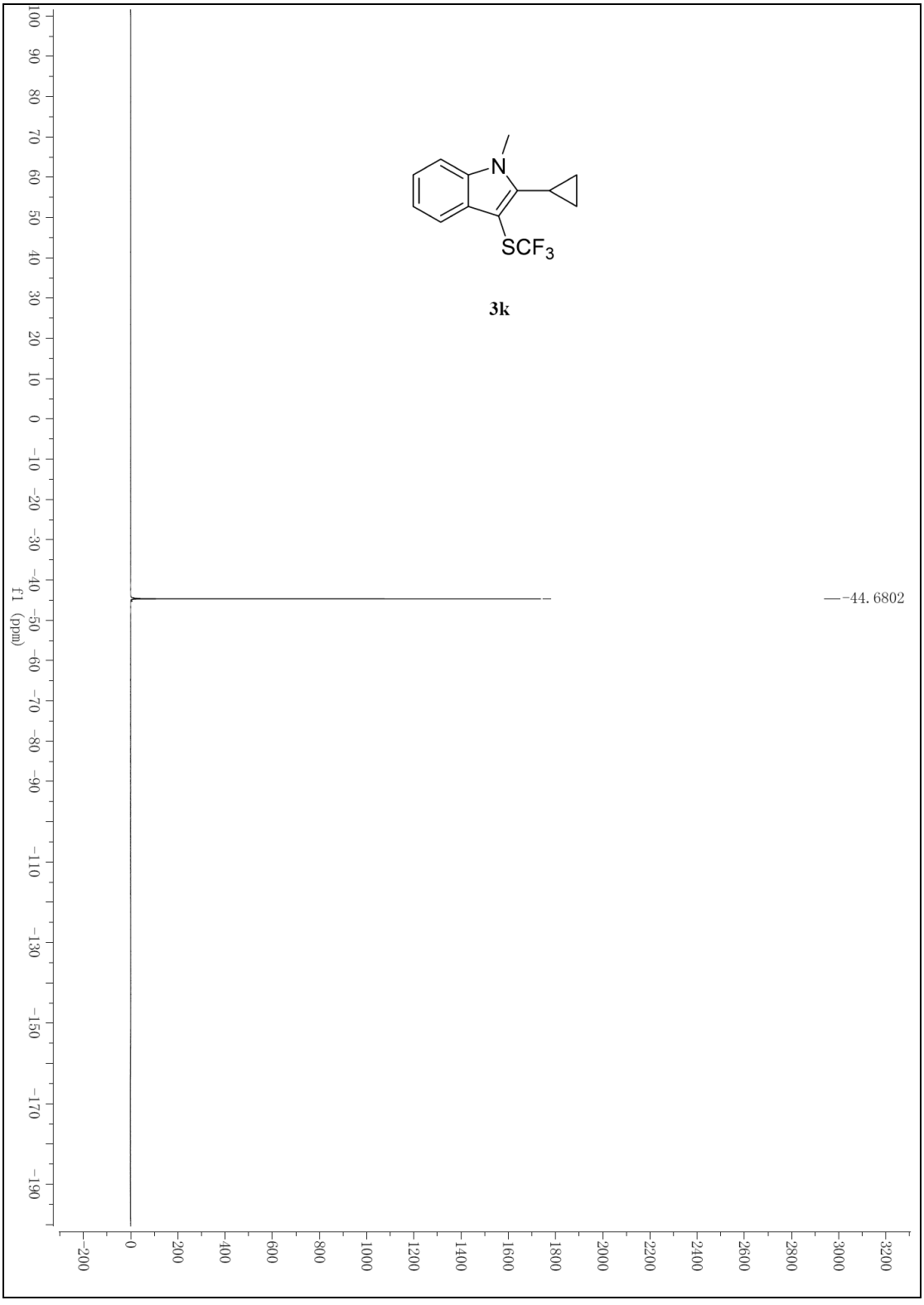

N
CO2Me
SCF3
3j
f1 (ppm)
-44.3306

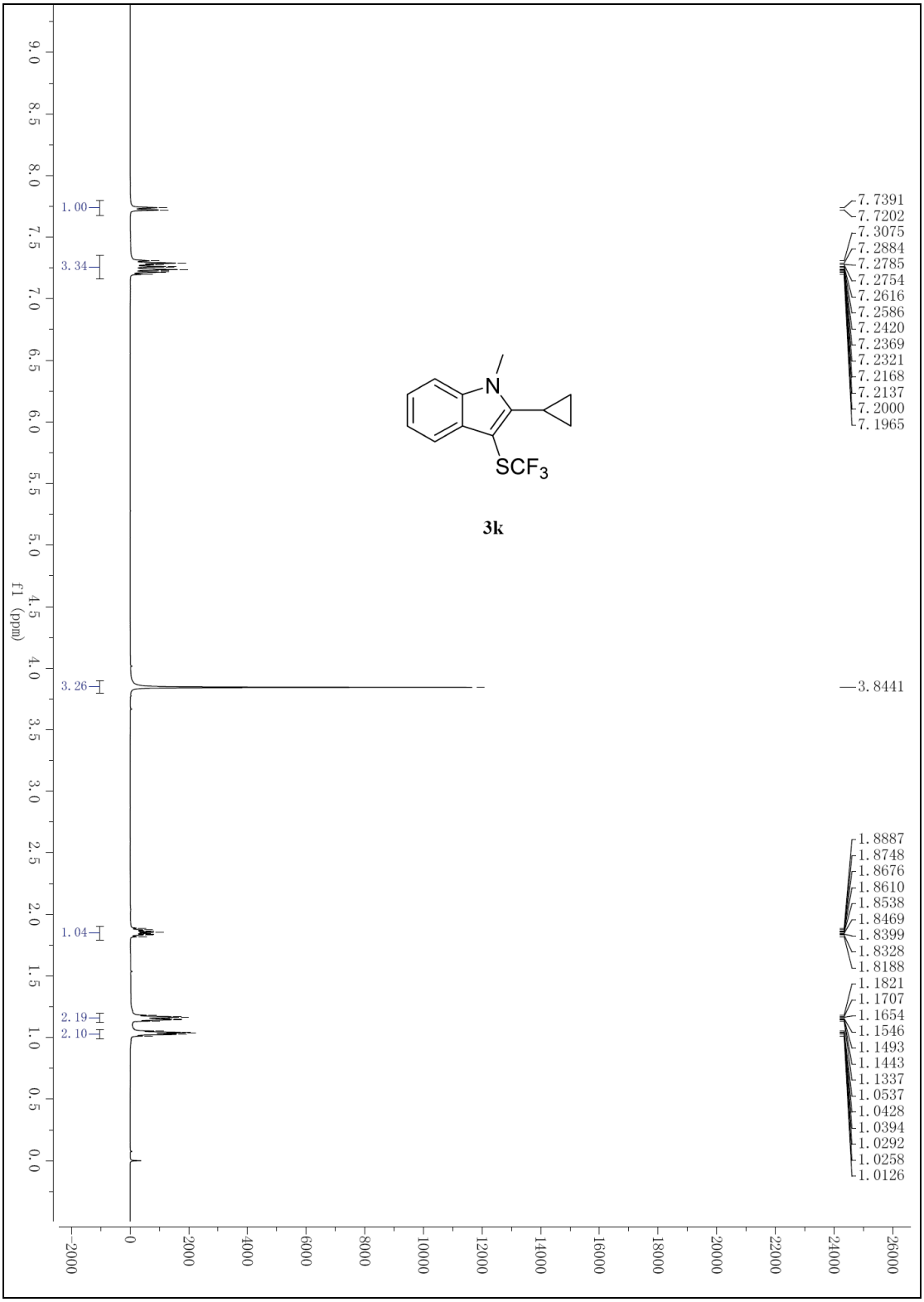

8.2032
8.1832
7.8578
7.8390
7.5304
7.5104
7.4196
7.4000
7.3774
7.3606
7.3336
7.3138
7.2966
7.2274
3.9580
3.6600
2.02
1.00
2.10
3.13
3.01
3.01
N
CO2Me
SCF3
f1 (ppm)

3j

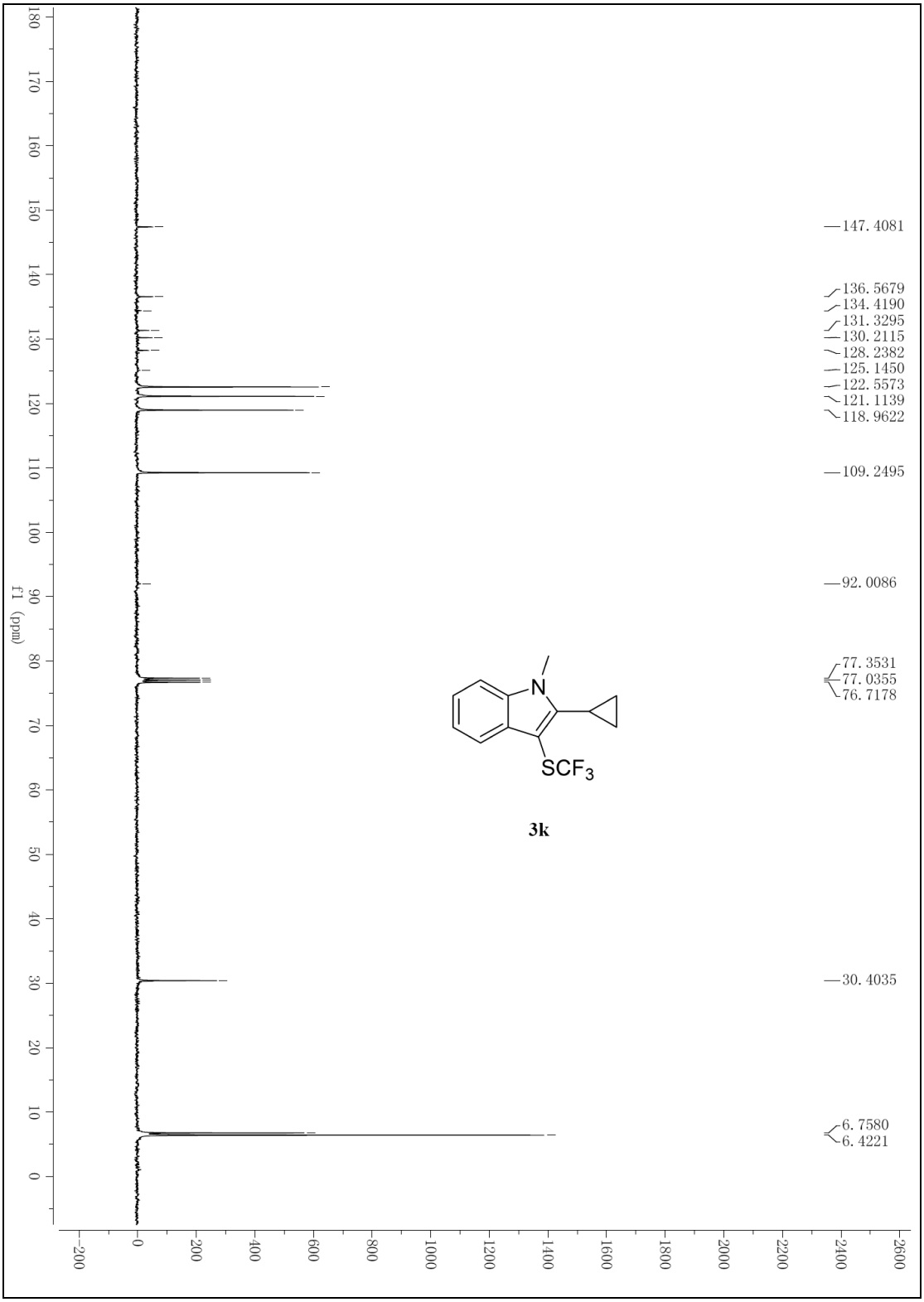

166.5973
146.6648
137.3292
134.3375
134.1977
131.1007
130.9453
130.7814
130.1436
129.5774
128.0057
124.9142
123.5661
121.8850
119.7122
110.0628
93.3170
77.3741
77.0560
76.7388
52.3627
31.7635
f1 (ppm)
N
CO2Me
SCF3

3j

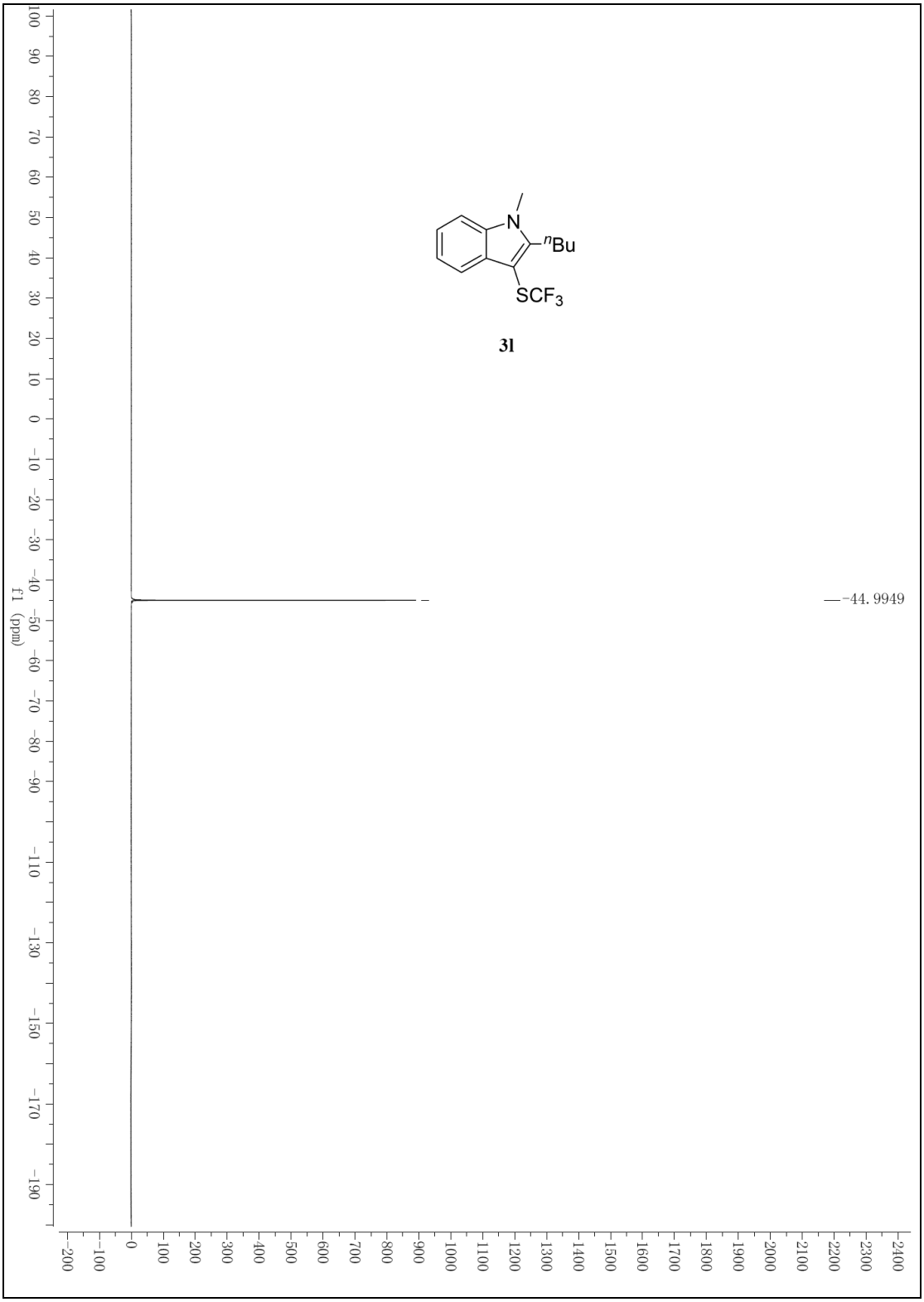

N
SCF3
3k
f1 (ppm)
-44.6802

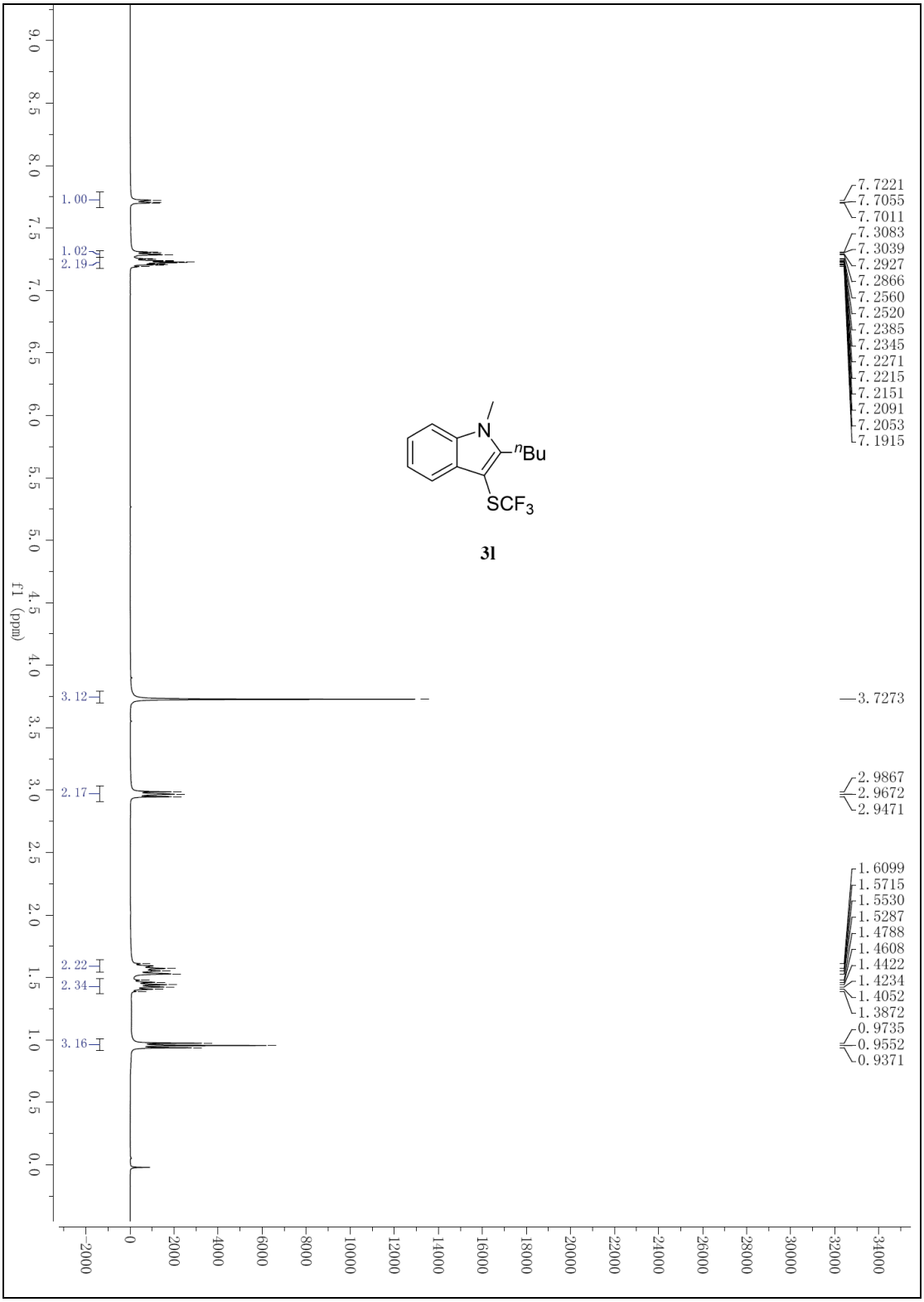

f1 (ppm)
1.00
3.34
3.26
1.04
2.19
2.10
7.7391
7.7202
7.3075
7.2884
7.2785
7.2754
7.2616
7.2586
7.2420
7.2369
7.2321
7.2168
7.2137
7.2000
7.1965
3.8441
1.8887
1.8748
1.8676
1.8610
1.8538
1.8469
1.8399
1.8328
1.8188
1.1821
1.1707
1.1654
1.1546
1.1493
1.1443
1.1337
1.0537
1.0428
1.0394
1.0292
1.0258
1.0126
N
SCF3

3k

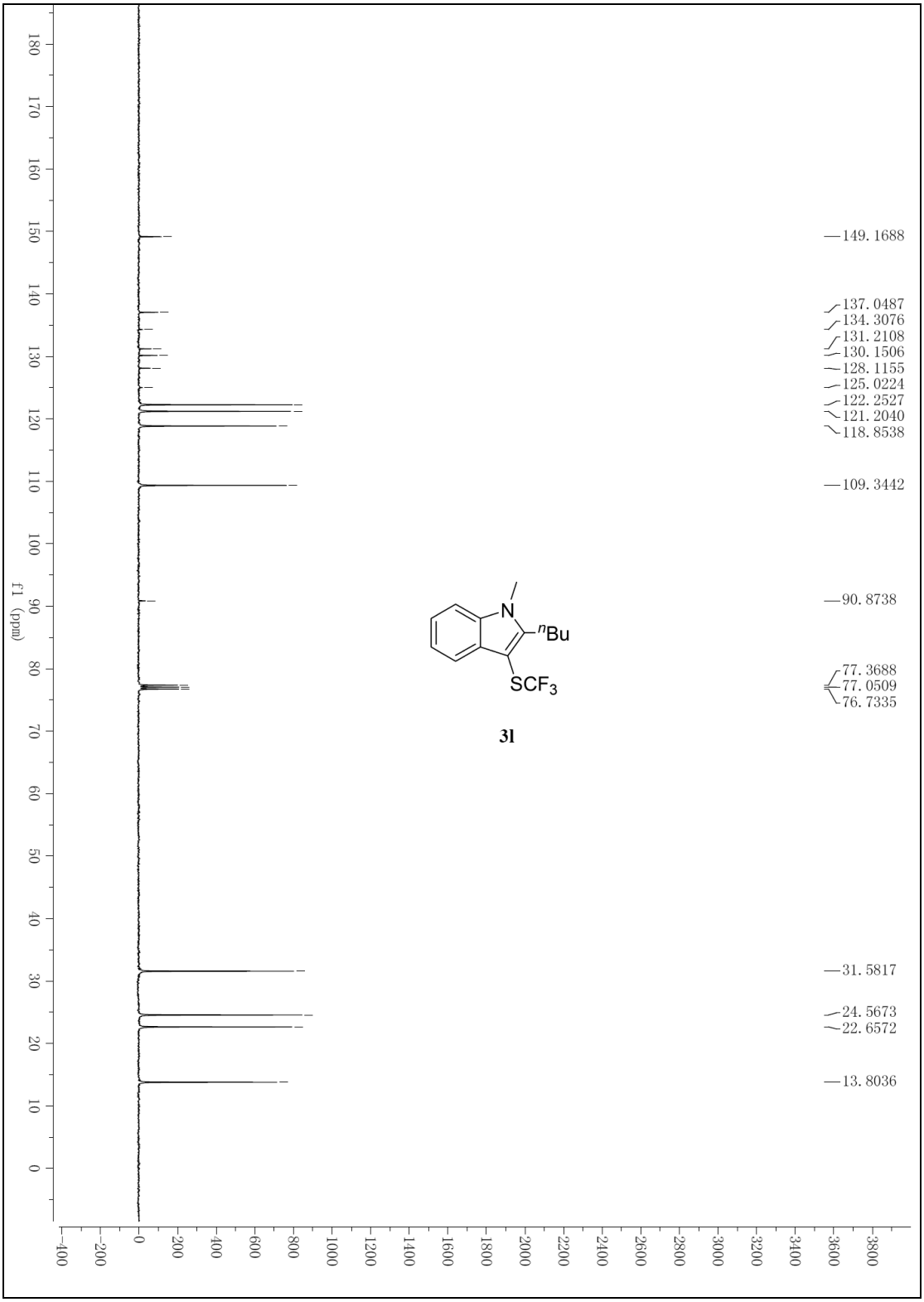

147.4081
136.5679
134.4190
131.3295
130.2115
128.2382
125.1450
122.5573
121.1139
118.9622
109.2495
92.0086
77.3531
77.0355
76.7178
30.4035
6.7580
6.4221
f1 (ppm)
N
SCF3

3k

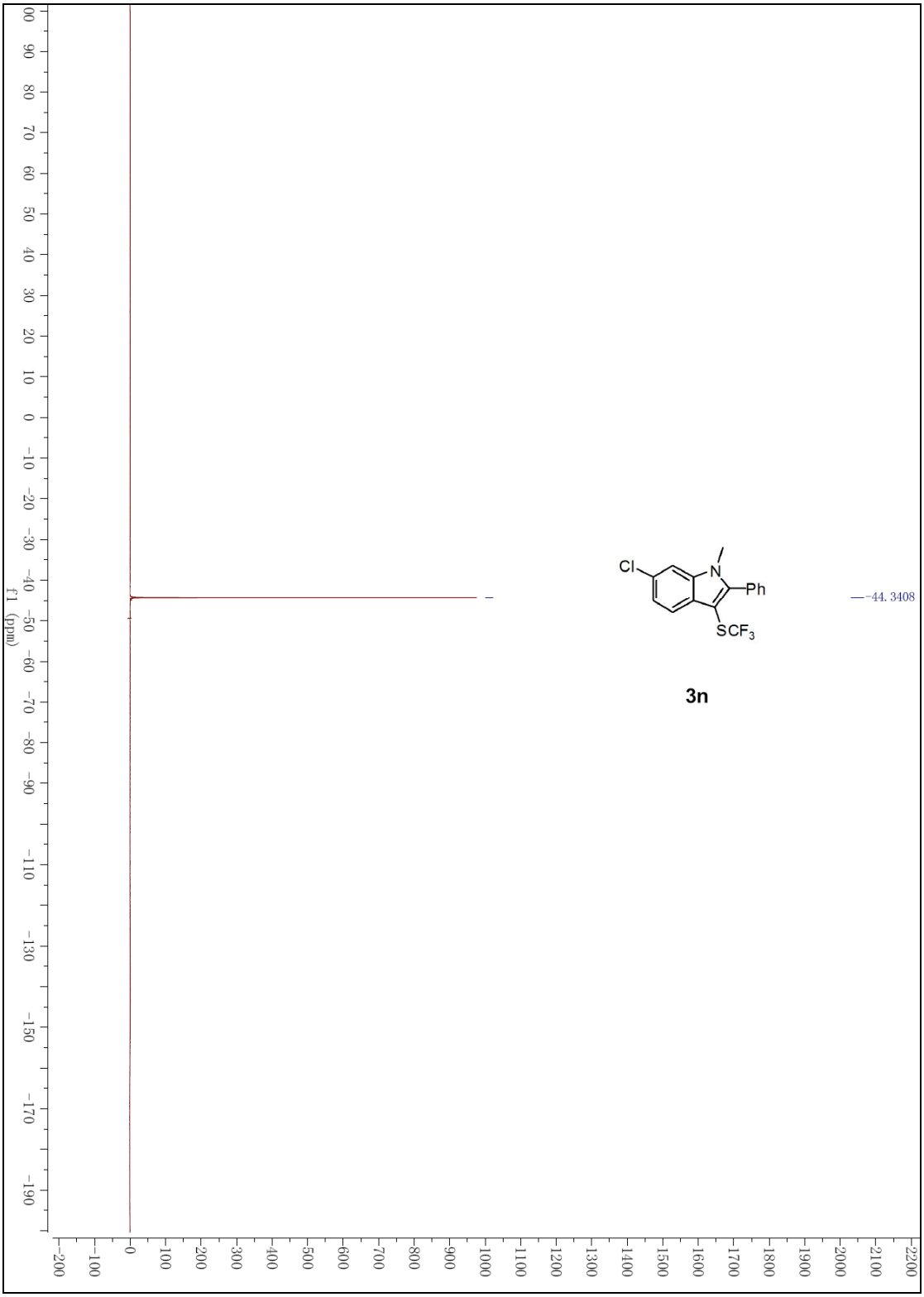

N
nBu
SCF3
31
f1 (ppm)
-44.9949


f1 (ppm)
1.00
1.02
2.19
3.12
2.17
2.22
2.34
3.16
7.7221
7.7055
7.7011
7.3083
7.3039
7.2927
7.2866
7.2560
7.2520
7.2385
7.2345
7.2271
7.2215
7.2151
7.2091
7.2053
7.1915
3.7273
2.9867
2.9672
2.9471
1.6099
1.5715
1.5530
1.5287
1.4788
1.4608
1.4422
1.4234
1.4052
1.3872
0.9735
0.9552
0.9371
N
nBu
SCF3

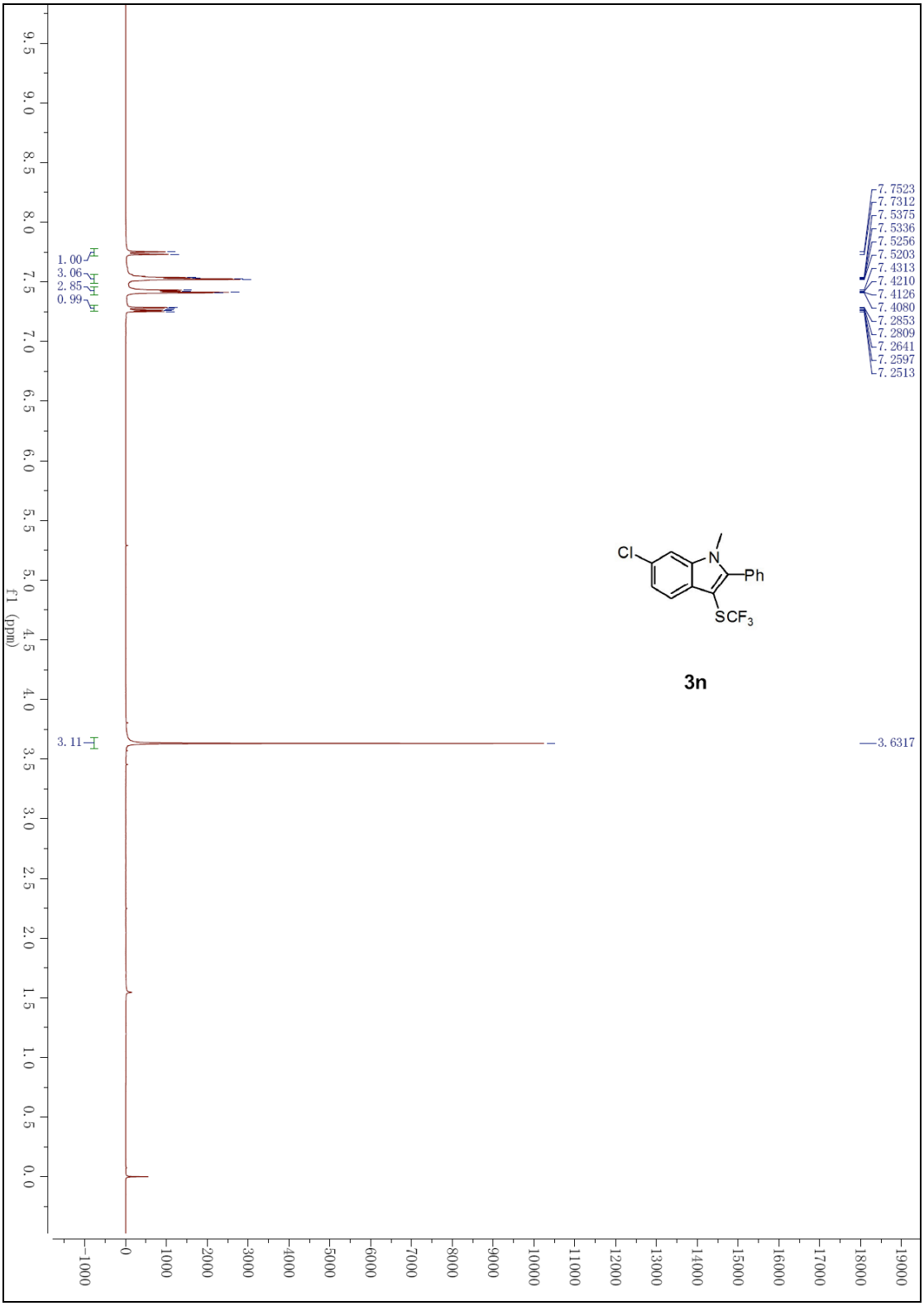
3l

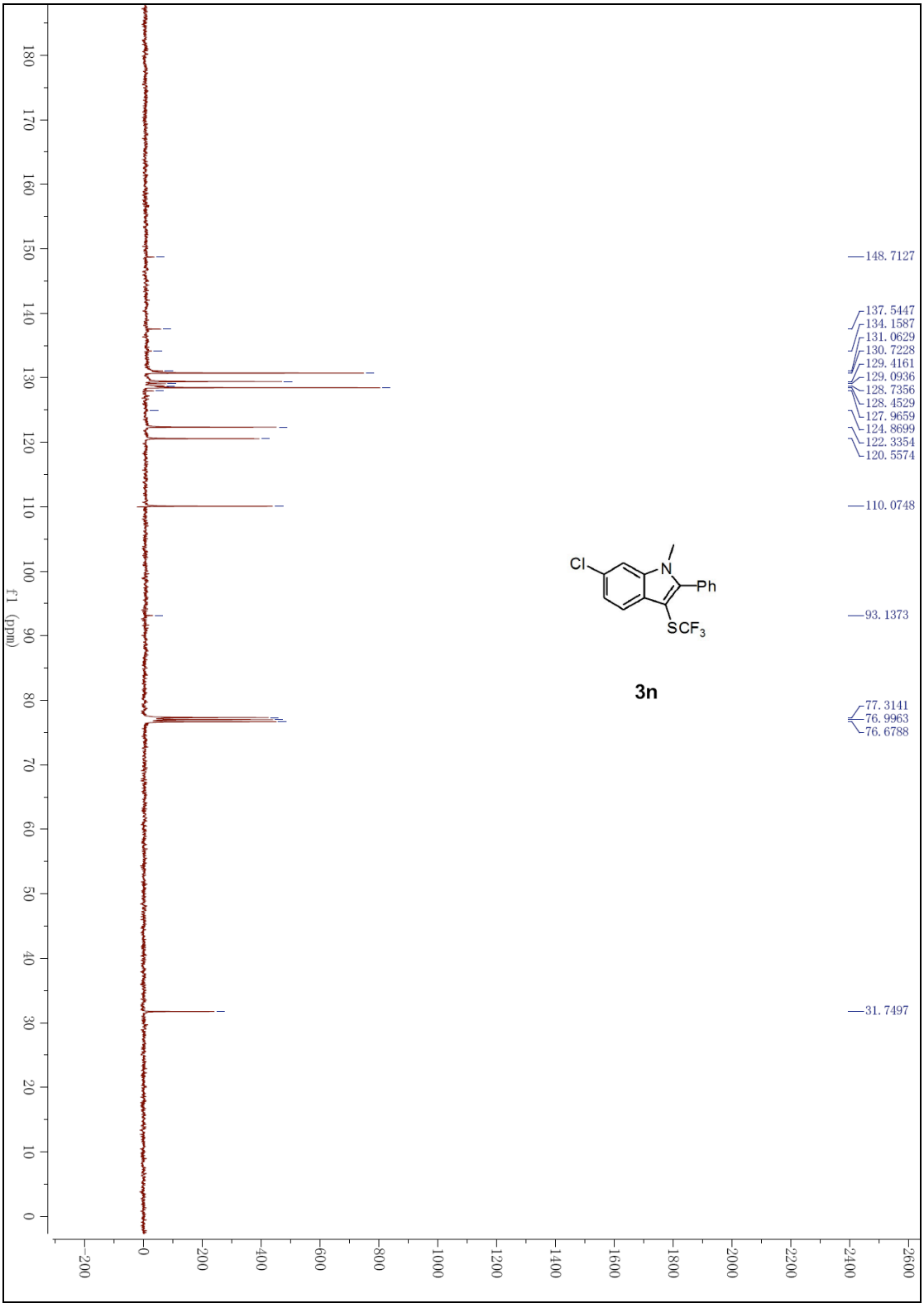

149.1688
137.0487
134.3076
131.2108
130.1506
128.1155
125.0224
122.2527
121.2040
118.8538
109.3442
90.8738
77.3688
77.0509
76.7335
31.5817
24.5673
22.6572
13.8036
f1 (ppm)
N
nBu
SCF3

3l



3n


1.00
3.06
2.85
0.99
3.11
7.7523
7.7312
7.5375
7.5336
7.5256
7.5203
7.4313
7.4210
7.4126
7.4080
7.2853
7.2809
7.2641
7.2597
7.2513
3.6317
Cl
N
Ph
SCF3
3n
f1 (ppm)


148.7127
137.5447
134.1587
131.0629
130.7228
129.4161
129.0936
128.7356
128.4529
127.9659
124.8699
122.3354
120.5574
110.0748
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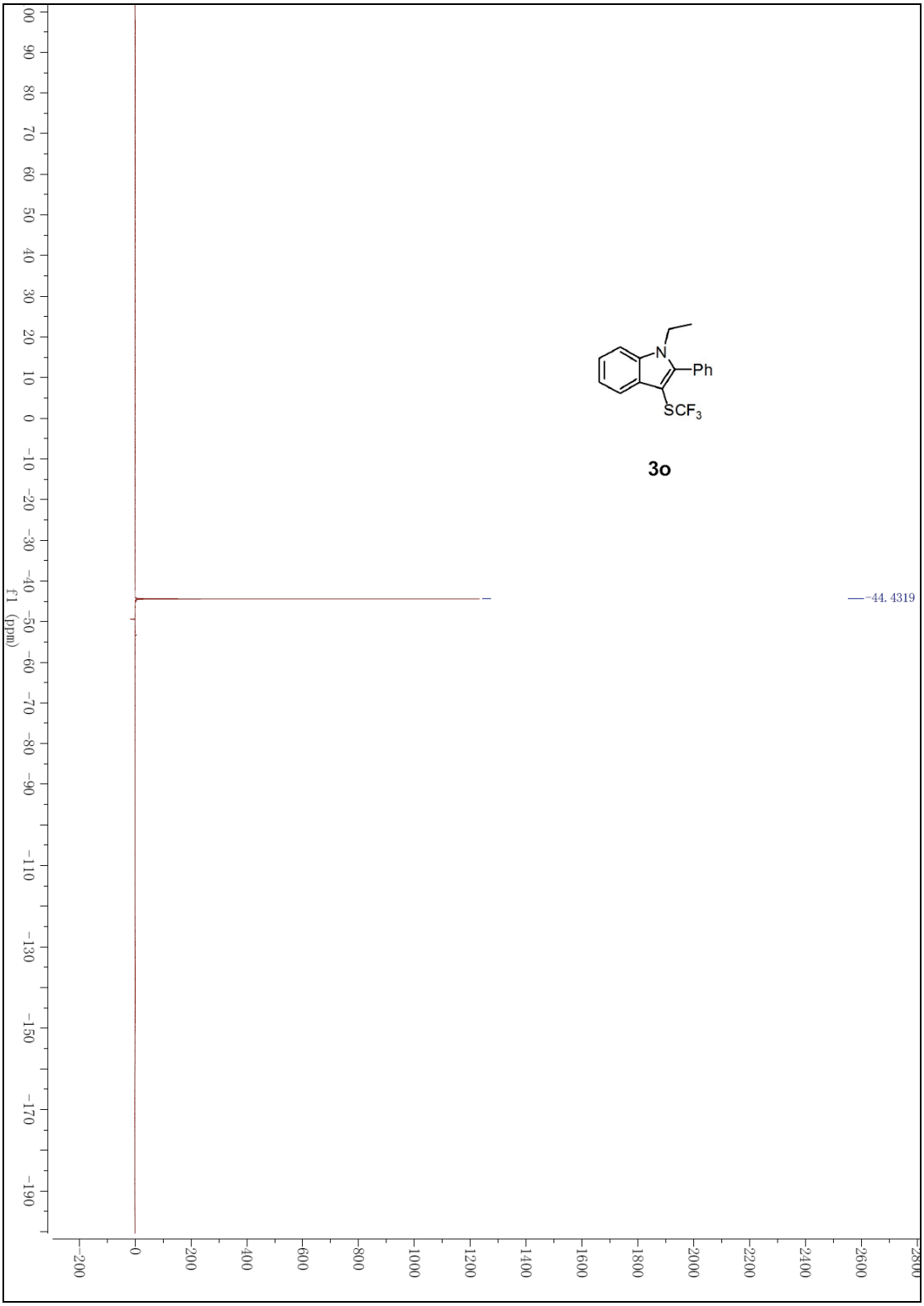
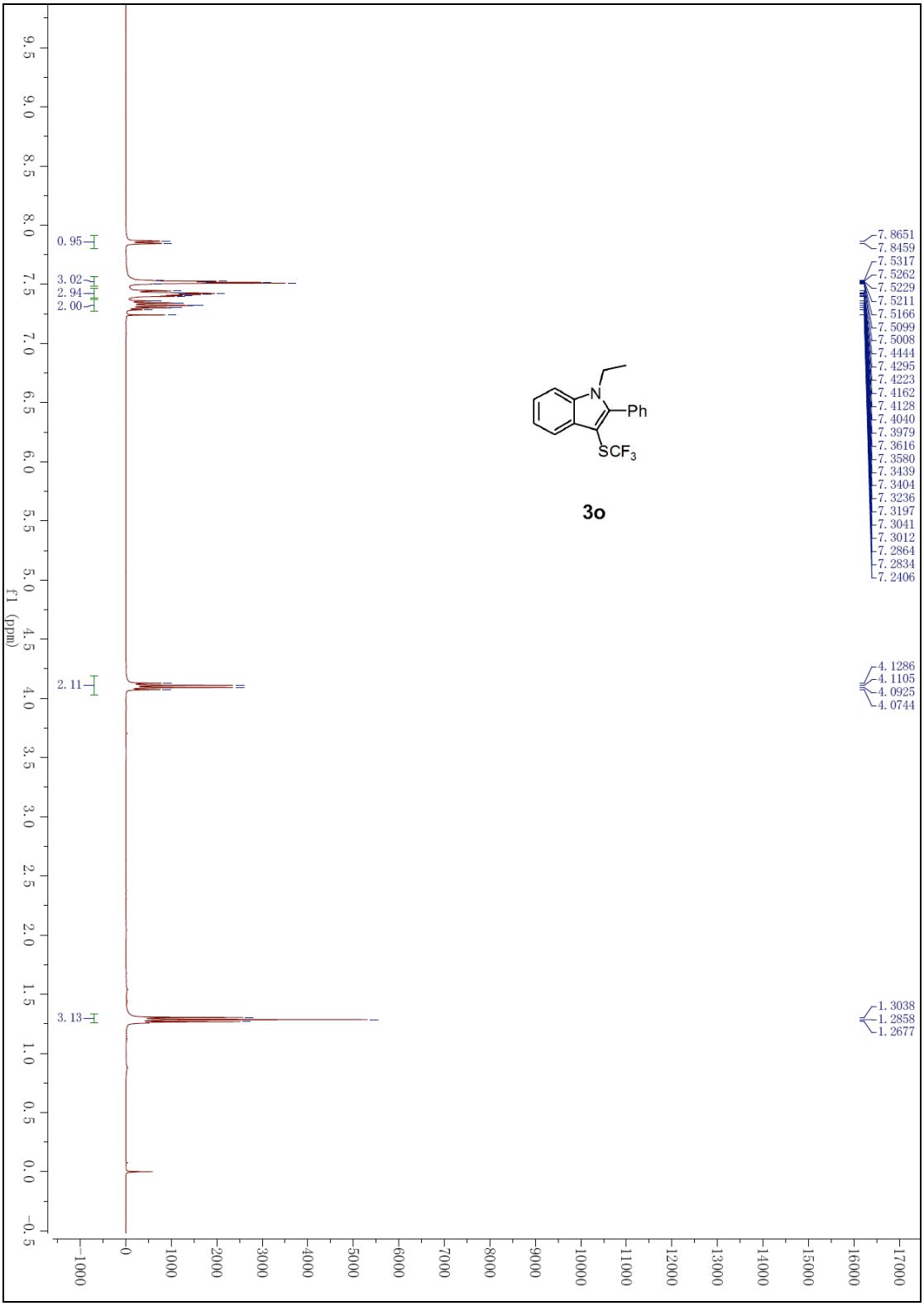
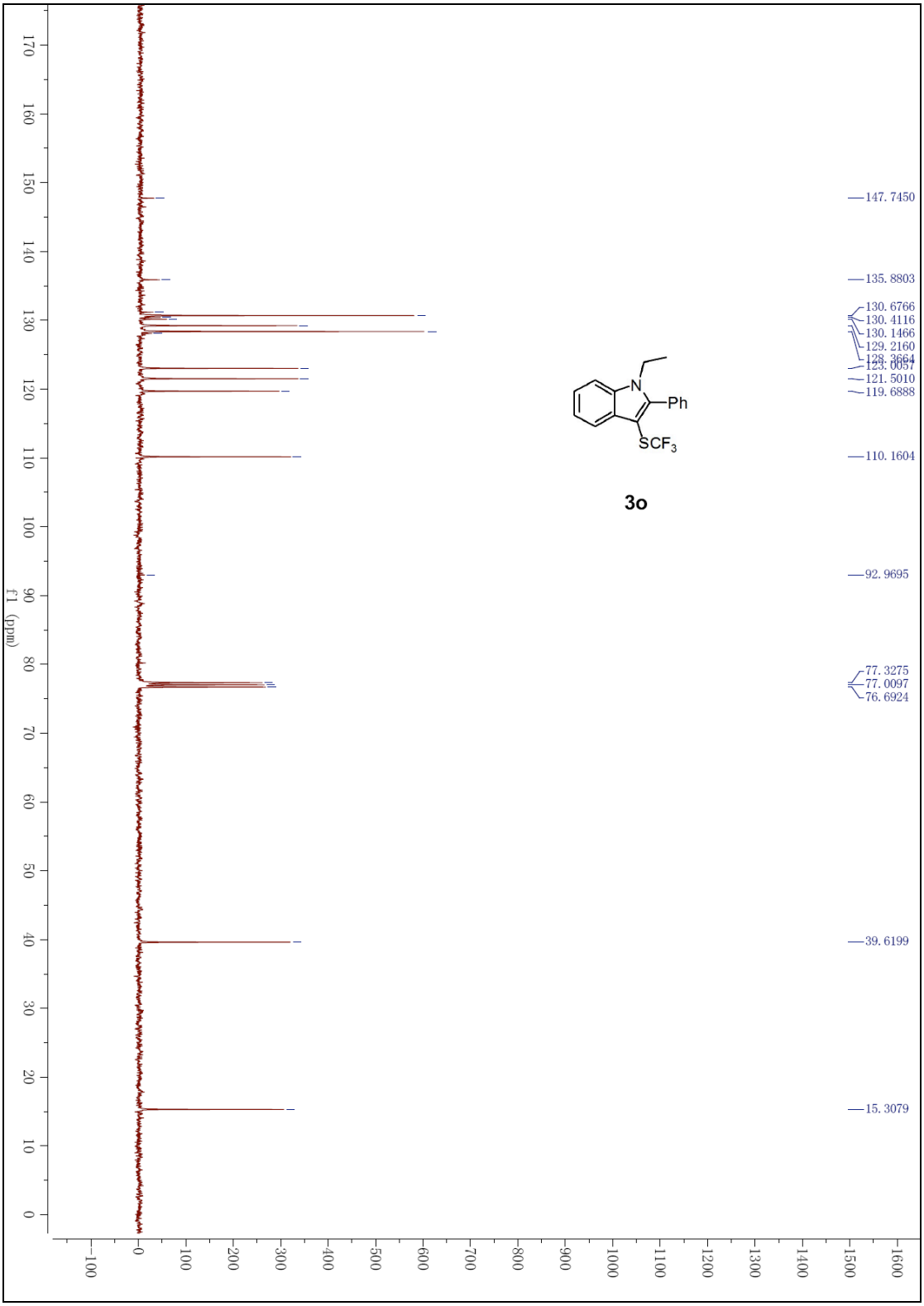
77.3141
76.9963
76.6788
31.7497
Cl
N
Ph
SCF3
3n
f1 (ppm)



3o


0.95
3.02
2.94
2.00
2.11
3.13
7.8651
7.8459
7.5317
7.5262
7.5229
7.5211
7.5166
7.5099
7.5008
7.4444
7.4295
7.4223
7.4162
7.4128
7.4040
7.3979
7.3616
7.3580
7.3439
7.3404
7.3236
7.3197
7.3041
7.3012
7.2864
7.2834
7.2406
4.1286
4.1105
4.0925
4.0744
1.3038
1.2858
1.2677
N
Ph
SCF3
3o
f1 (ppm)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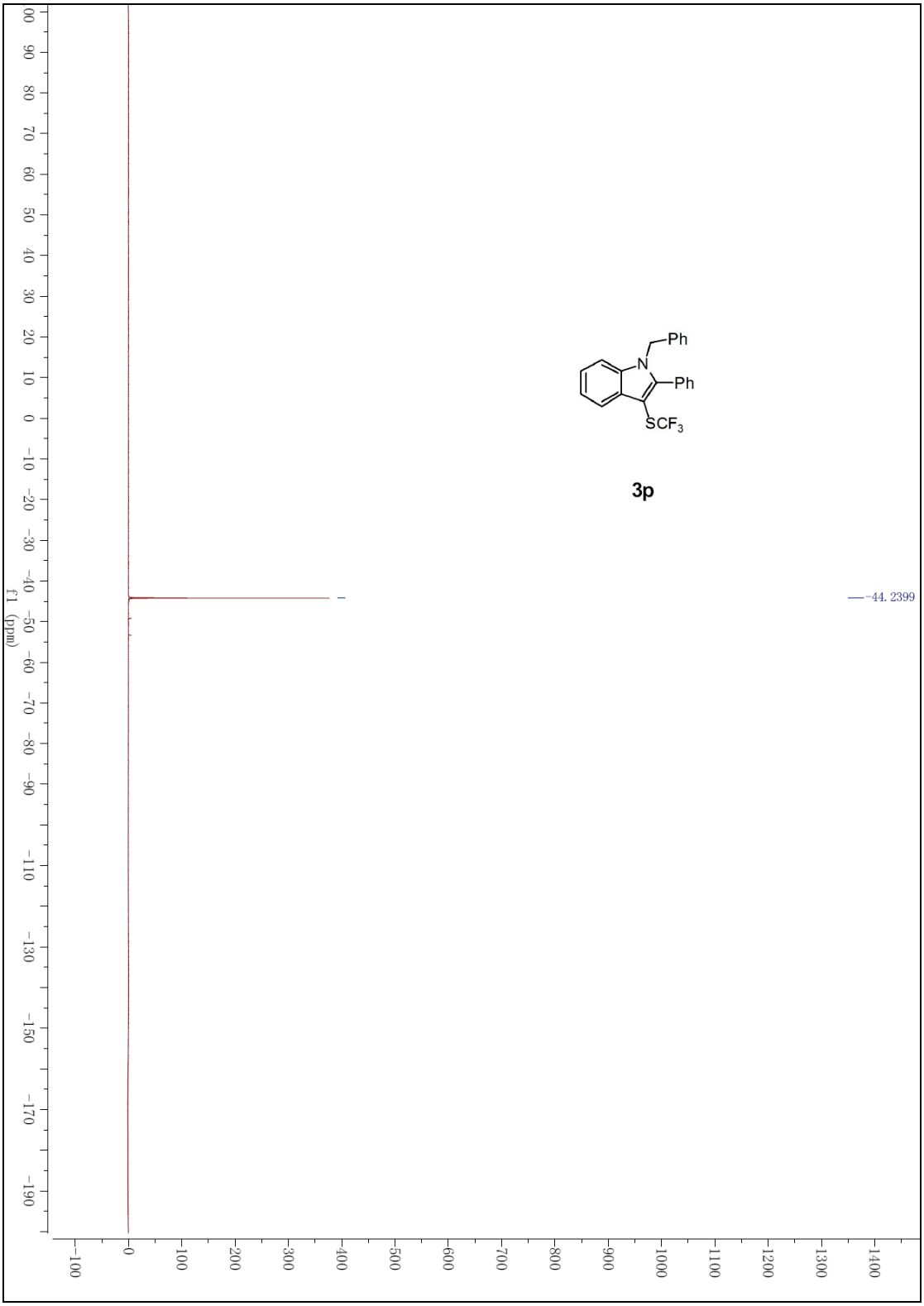
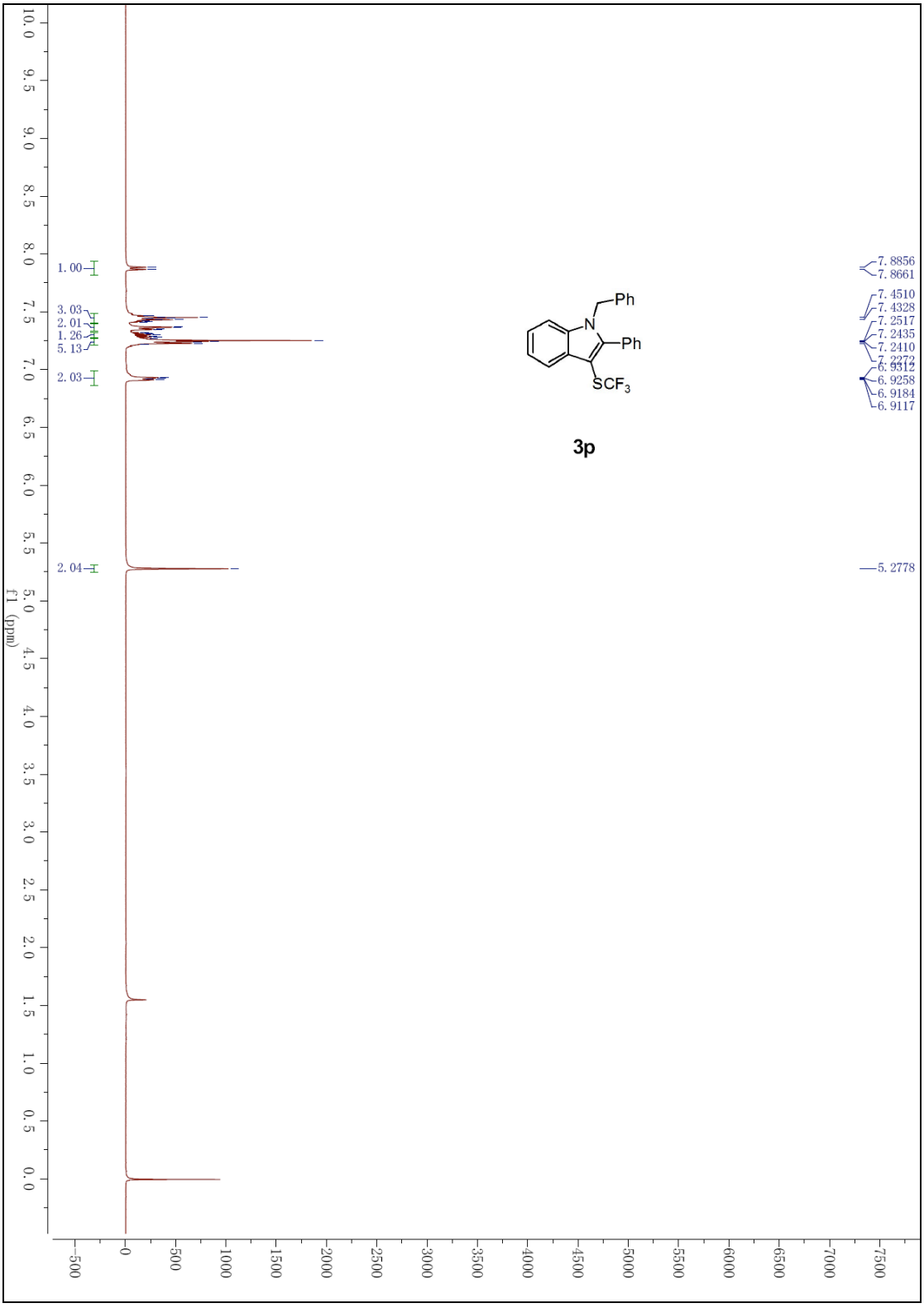
135.8803
130.6766
130.4116
130.1466
129.2160
128.3664
123.0057
121.5010
119.6888
110.1604
92.9695
77.3275
77.0097
76.6924
39.6199
15.3079
f1 (ppm)
Ph
SCF3
3o


Ph
N
Ph
SCF3
3p
−44.2399
f1 (ppm)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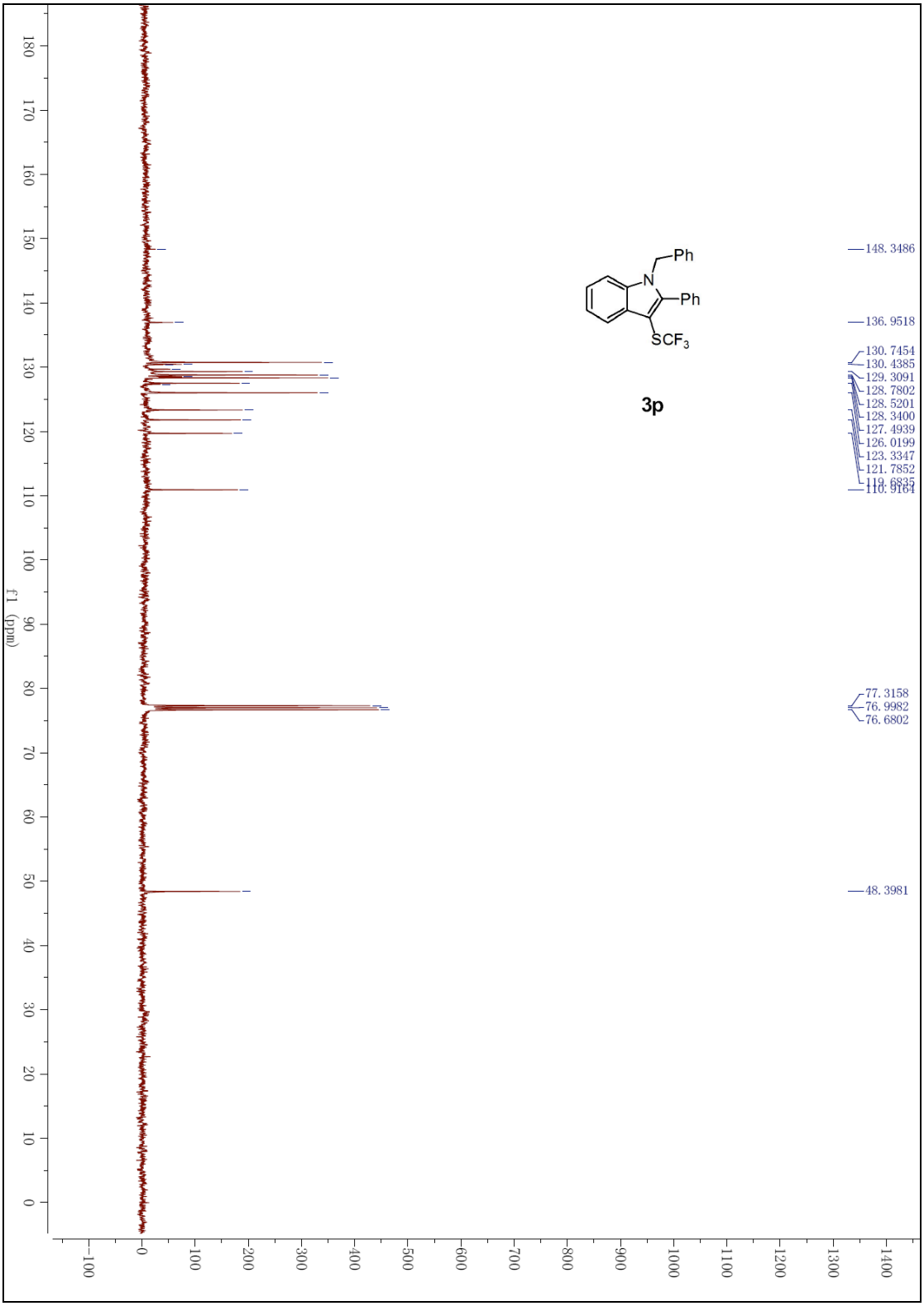
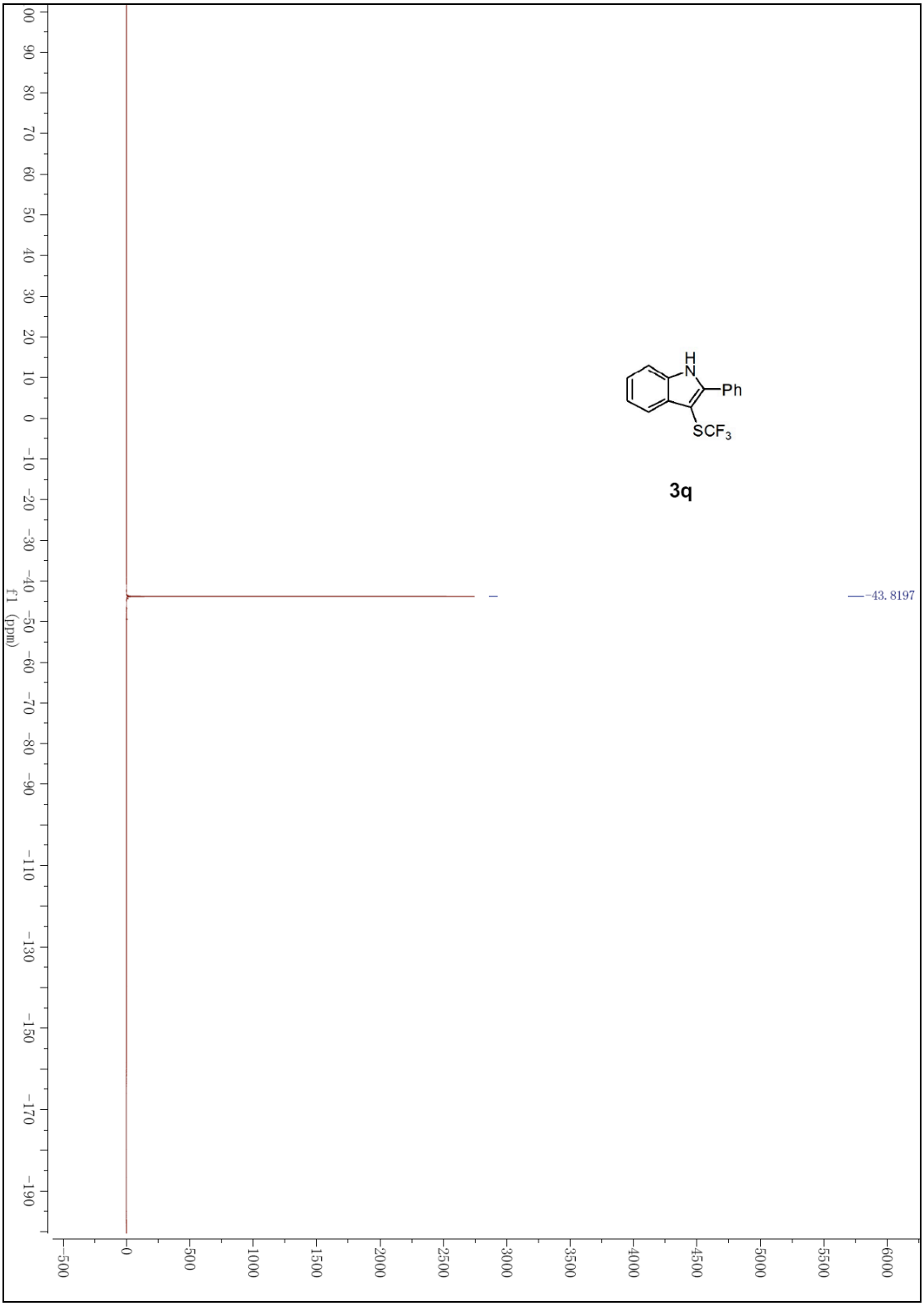
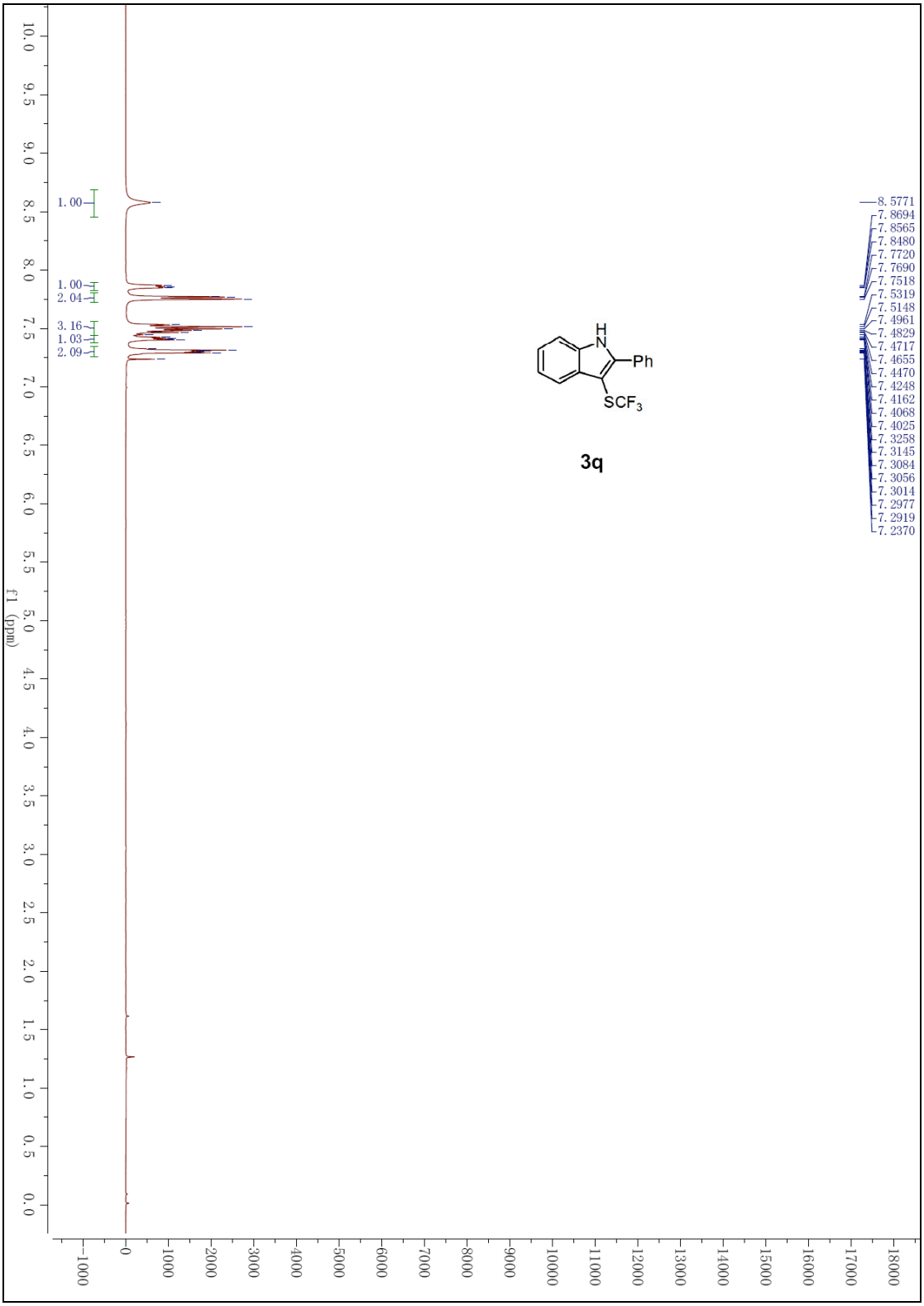
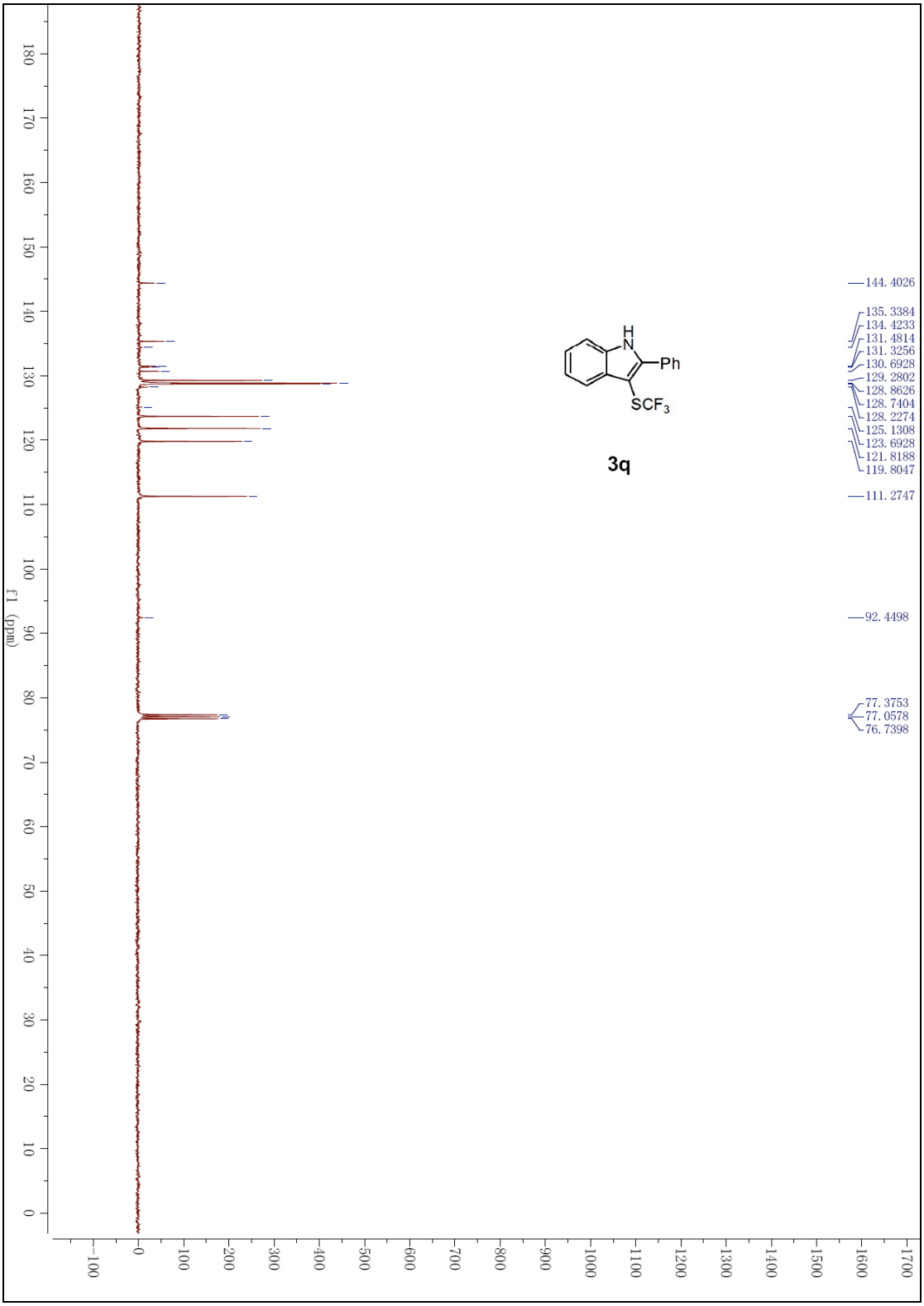
3.03
2.01
1.26
5.13
2.03
2.04
7.8856
7.8661
7.4510
7.4328
7.2517
7.2435
7.2410
7.2272
6.9312
6.9258
6.9184
6.9117
5.2778
Ph
N
Ph
SCF3
3p
f1 (ppm)


Ph
N
Ph
SCF3
3p
148.3486
136.9518
130.7454
130.4385
129.3091
128.7802
128.5201
128.3400
127.4939
126.0199
123.3347
121.7852
110.9164
77.3158
76.9982
76.6802
48.3981
f1 (ppm)


H
N
Ph
SCF3
3q
−43.8197
f1 (ppm)


1.00
1.00
2.04
3.16
1.03
2.09
8.5771
7.8694
7.8565
7.8480
7.7720
7.7690
7.7518
7.5319
7.5148
7.4961
7.4829
7.4717
7.4655
7.4470
7.4248
7.4162
7.4068
7.4025
7.3258
7.3145
7.3084
7.3056
7.3014
7.2977
7.2919
7.2370
H
N
Ph
SCF3
f1 (ppm)

3q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135.3384
134.4233
131.4814
131.3256
130.6928
129.2802
128.8626
128.7404
128.2274
125.1308
123.6928
121.8188
119.8047
111.2747
92.4498
77.3753
77.0578
76.7398
f1 (ppm)
H
N
Ph
SCF3
3q