Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Synthesis of trifluoromethylated 3,4-dihydroquinolin-2(1*H*)-ones via a photo-induced radical cyclization of benzene-tethered 1,7-enynes with Togni reagent

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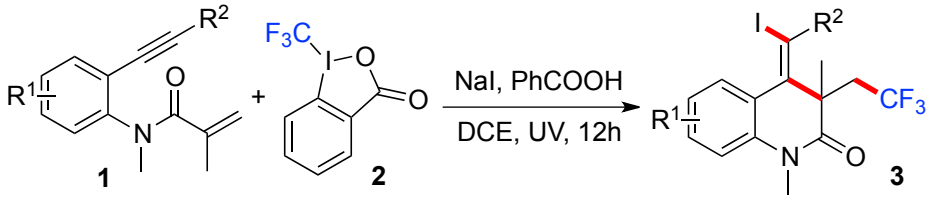
Supporting Information

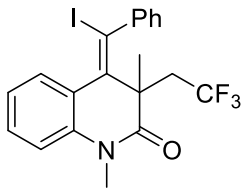
General experimental methods:

Unless otherwise stated, all commercial reagents were used as received. 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 experimental procedure for the photo-induced radical cyclization of benzene-tethered 1,7-enynes **1** *with Togni reagent* **2***:*

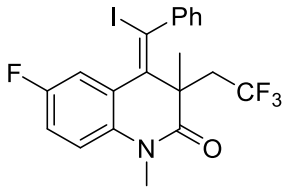


Benzene-tethered 1,7-enynes **1** (0.2 mmol) was added to a mixture of Togni reagent **2** (0.3 mmol), NaI (0.2 mmol) and PhCOOH (0.2 mmol) in DCE (4.0 mL). The mixture, placed around the mercury lamp (purchased from Yuming, Shanghai) with a distance of 10 centimeters, was stirred under UV irradiation (0.67W cm^{-1}) for 12 hours at room temperature. After completion of reaction as indicated by TLC, the solvent was evaporated, and the residue was purified directly by flash column chromatograph (EtOAc/*n*-hexane, 1:8) to give the desired product **3**.



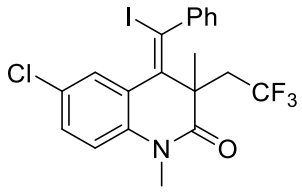
(*E*)-4-(iodo(phenyl)methylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihydroquinolin-2(1*H*)-one (**3a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.07 (s, 3H), 1.95-2.03 (m, 1H), 2.14-2.23 (m, 1H), 3.40 (s, 3H), 7.03 (d, *J* = 8.0 Hz, 1H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.26-7.34 (m, 5H), 7.39-7.43 (m, 1H), 7.87 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 30.9, 41.0 (q, *J* = 27.3 Hz), 48.2, 101.2, 114.2, 123.0, 124.4, 127.2, 127.6, 127.7, 128.1, 128.2, 128.3, 130.0, 132.3, 138.0, 139.1, 146.4, 169.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.1 Hz); HRMS (ESI) calcd for $C_{20}H_{17}F_3INO$: 494.0199 ($M + Na^+$), found: 494.0156.



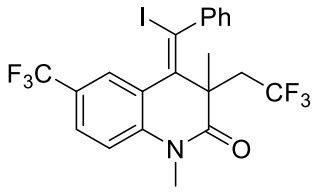
(*E*)-6-fluoro-4-(iodo(phenyl)methylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihydroquinolin-2(1*H*)-one (**3b**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.06 (s, 3H), 1.95-2.02 (m, 1H), 2.16-2.22 (m, 1H), 3.39 (s, 3H), 6.99 (dd, J_1 = 8.9 Hz, J_2 = 4.6 Hz, 1H), 7.10-7.15 (m, 1H), 7.26-7.34 (m, 5H), 7.61 (dd, J_1 = 8.9 Hz, J_2 = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 31.2, 41.0 (q, *J* = 27.3 Hz), 48.1, 102.3, 115.6 (d, $^{3}J_{CF}$ = 8.0 Hz), 116.5 (d, $^{2}J_{CF}$ = 22.8 Hz), 119.3 (d, $^{2}J_{CF}$ = 24.4 Hz), 124.3, 127.1, 127.4, 127.7, 128.1, 128.3, 131.7, 134.3, 138.2, 146.1, 158.3 (d, $^{1}J_{CF}$ = 243.5 Hz), 169.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.4 Hz), -118.7 (td, J_1 = 8.3 Hz, J_2 = 4.9 Hz); HRMS (ESI) calcd for $C_{20}H_{16}F_4INO$: 490.0285 ($M + H^+$), found: 490.0281.



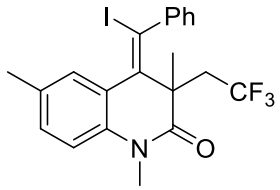
(*E*)-6-chloro-4-(iodo(phenyl)methylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihydroquinolin-2(1*H*)-one (**3c**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.06 (s, 3H), 1.97-2.03 (m, 1H), 2.17-2.23 (m, 1H), 3.38 (s, 3H), 6.97 (d, *J* = 8.7 Hz, 1H), 7.26-7.34 (m, 5H), 7.38 (dd, J_1 = 8.7 Hz, J_2 = 2.2 Hz, 1H), 7.86 (d, *J* = 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 31.0, 41.0 (q, *J* = 27.1 Hz), 48.1, 102.7, 115.5, 124.2, 127.0, 127.4, 127.8, 128.1, 128.1, 128.3, 128.3, 129.7, 131.5, 132.1, 136.6, 146.1, 169.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.3 Hz); HRMS (ESI) calcd for $C_{20}H_{16}ClF_3INO$: 505.9990 ($M + H^+$), found: 505.9980.



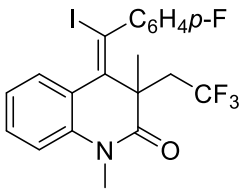
(*E*)-4-(iodo(phenyl)methylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-6-(trifluorometh yl)-3,4-dihydroquinolin-2(1*H*)-one (**3d**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.09 (s, 3H), 1.96-2.07 (m, 1H), 2.11-2.23 (m, 1H), 3.44 (s, 3H), 7.13 (d, *J* = 8.5 Hz, 1H), 7.26-7.35 (m, 5H), 7.67 (d, *J* = 8.4 Hz, 1H), 8.16 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 31.1, 41.1 (q, *J* = 27.6 Hz), 48.1, 103.3, 114.3, 124.1, 124.9, 125.2, 126.8, 127.4, 127.8, 128.0, 128.1, 128.4, 129.8, 130.2, 137.6, 140.8, 146.0, 169.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.9 (t, *J* = 10.4 Hz), -62.2; HRMS (ESI) calcd for $C_{21}H_{16}F_6INO$: 540.0254 ($M + H^+$), found: 540.0254.



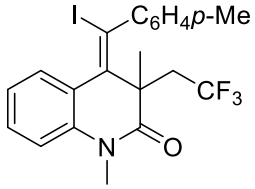
(*E*)-4-(iodo(phenyl)methylene)-1,3,6-trimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihydroqui nolin-2(1*H*)-one (**3e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.05 (s, 3H), 1.91-2.03 (m, 1H), 2.16-2.27 (m, 1H), 2.41 (s, 3H), 3.38 (s, 3H), 6.92 (d, *J* = 8.2 Hz, 1H), 7.20 (d, *J* = 8.2 Hz, 1H), 7.24-7.34 (m, 5H), 7.68 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.7, 21.3, 30.9, 41.0 (q, *J* = 27.1 Hz), 48.1, 100.9, 114.1, 124.4, 127.6, 127.7, 128.0, 128.1, 128.3, 130.0, 130.4, 132.6, 132.7, 135.6, 139.3, 146.5, 169.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.5 Hz); HRMS (ESI) calcd for $C_{21}H_{19}F_3INO$: 486.0536 ($M + H^+$), found: 486.0534.



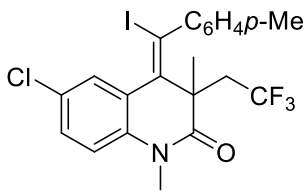
(*E*)-4-((4-fluorophenyl)iodomethylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihydroquinolin-2(1*H*)-one (**3f**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.07 (s, 3H), 1.92-2.04 (m, 1H), 2.14-2.23 (m, 1H), 3.40 (s, 3H), 6.99-7.06 (m, 3H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.26 (t, *J* = 6.8 Hz, 1H), 7.32-7.36 (m, 1H), 7.42 (t, *J* = 7.3 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 31.0, 41.0 (q, *J* = 27.4 Hz), 48.2, 99.7, 114.2, 114.6 (d, $^{2}J_{CF}$ = 21.7 Hz), 115.4 (d, $^{2}J_{CF}$ = 22.1 Hz), 123.1, 124.4, 127.2, 129.4 (d, $^{3}J_{CF}$ = 8.1 Hz), 130.1, 130.3 (d, $^{3}J_{CF}$ = 8.3 Hz), 132.3, 137.9, 139.9, 142.5, 162.2 (d, $^{1}J_{CF}$ = 248.9 Hz), 169.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.5 Hz), -112.5 (ddd, J_1 = 13.7 Hz, J_2 = 8.6 Hz, J_3 = 5.3 Hz); HRMS (ESI) calcd for $C_{20}H_{16}F_4INO$: 490.0285 (M + H^+), found: 490.0288.



(*E*)-4-(iodo(*p*-tolyl)methylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihydroquinolin-2(1*H*)-one (**3g**)

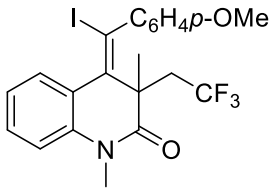
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.08 (s, 3H), 1.92-2.03 (m, 1H), 2.13-2.25 (m, 1H), 2.36 (s, 3H), 3.40 (s, 3H), 7.03 (d, *J* = 8.1 Hz, 1H), 7.10-7.19 (m, 4H), 7.25 (d, *J* = 9.2 Hz, 1H), 7.41 (t, *J* = 7.3 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 21.3, 30.9, 41.0 (q, *J* = 27.4 Hz), 48.1, 101.7, 114.2, 123.0, 124.4, 127.2, 127.5, 128.2, 128.3, 128.8, 129.9, 130.4, 132.4, 138.2, 138.9, 143.7, 169.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.4 Hz); HRMS (ESI) calcd for $C_{21}H_{19}F_3INO$: 486.0536 (M + H^+), found: 486.0519.



(*E*)-6-chloro-4-(iodo(*p*-tolyl)methylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihy

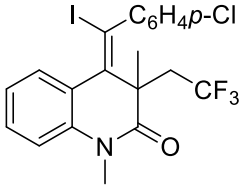
droquinolin-2(1*H*)-one (**3h**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.08 (s, 3H), 1.94-2.05 (m, 1H), 2.13-2.22 (m, 1H), 2.36 (s, 3H), 3.38 (s, 3H), 6.96 (d, *J* = 8.7 Hz, 1H), 7.10-7.15 (m, 3H), 7.22 (d, *J* = 8.1 Hz, 1H), 7.37 (dd, J_1 = 8.7 Hz, J_2 = 2.3 Hz, 1H), 7.85 (d, *J* = 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 21.4, 31.0, 41.0 (q, *J* = 27.3 Hz), 48.0, 103.2, 115.4, 124.3, 127.0, 127.4, 128.0, 128.2, 128.4, 128.9, 129.6, 131.6, 132.1, 136.6, 137.7, 138.4, 143.3, 169.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.4 Hz); HRMS (ESI) calcd for $C_{21}H_{18}ClF_3INO$: 520.0146 (M + H^+), found: 520.0152.



(*E*)-4-(iodo(4-methoxyphenyl)methylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-3,4-di hydroquinolin-2(1*H*)-one (**3i**)

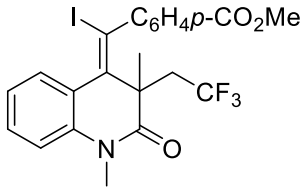
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.10 (s, 3H), 1.92-2.04 (m, 1H), 2.13-2.25 (m, 1H), 3.40 (s, 3H), 3.83 (s, 3H), 6.81 (dd, J_1 = 8.4 Hz, J_2 = 2.6 Hz, 1H), 6.87 (dd, J_1 = 8.6 Hz, J_2 = 2.6 Hz, 1H), 7.03 (d, *J* = 8.1 Hz, 1H), 7.15-7.22 (m, 2H), 7.29 (dd, J_1 = 8.6 Hz, J_2 = 2.2 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 30.9, 41.0 (q, *J* = 26.9 Hz), 48.1, 55.3, 101.8, 112.6, 113.9, 114.1, 123.0, 127.2, 129.0, 129.8, 129.9, 130.5, 132.5, 137.9, 138.9, 139.0, 159.3, 169.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.6 Hz); HRMS (ESI) calcd for $C_{21}H_{19}F_3INO_2$: 502.0485 (M + H^+), found: 502.0496.



(*E*)-4-((4-chlorophenyl)iodomethylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihy droquinolin-2(1*H*)-one (**3j**)

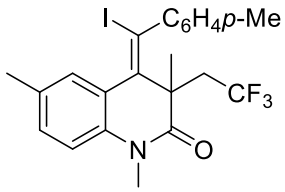
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.09 (s, 3H), 1.92-2.04 (m, 1H), 2.14-2.26 (m, 1H), 3.40 (s, 3H), 7.04 (d, *J* = 8.1 Hz, 1H), 7.19 (dd, J_1 = 16.3 Hz, J_2 = 8.1 Hz, 2H), 7.29-7.33 (m, 3H), 7.41 (dd, J_1 = 11.3 Hz, J_2 = 4.3 Hz, 1H), 7.84 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 21.6, 31.0, 41.0 (q, *J* = 27.5 Hz), 48.3, 99.2, 114.3, 123.1, 124.4, 127.1, 127.9, 128.4, 128.9, 129.7, 130.2, 132.2, 134.0, 138.0, 140.0, 144.9, 169.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.5 Hz); HRMS (ESI) calcd for $C_{20}H_{16}ClF_3INO$: 505.9990 (M + H^+), found: 505.9990.



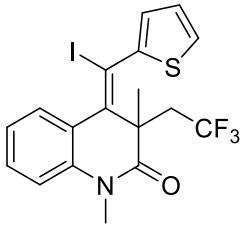
Methyl (*E*)-4-((1,3-dimethyl-2-oxo-3-(2,2,2-trifluoroethyl)-2,3-dihydroquinolin-4(1*H*)-ylidene)iodomethyl)benzoate (**3k**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.05 (s, 3H), 1.93-2.04 (m, 1H), 2.15-2.24 (m, 1H), 3.41 (s, 3H), 3.93 (s, 3H), 7.05 (d, *J* = 8.1 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.35-7.37 (m, 1H), 7.42-7.45 (m, 2H), 7.86 (d, *J* = 7.6 Hz, 1H), 8.01 (dd, J_1 = 5.6 Hz, J_2 = 2.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 31.0, 41.0 (q, *J* = 27.6 Hz), 48.3, 52.2, 99.0, 123.1, 124.3, 127.1, 127.6, 128.4, 129.1, 129.3, 129.6, 129.8, 130.2, 132.2, 138.0, 140.0, 150.8, 166.3, 169.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.2 Hz); HRMS (ESI) calcd for $C_{22}H_{19}F_3INO_3$: 530.0434 (M + H^+), found: 530.0423.



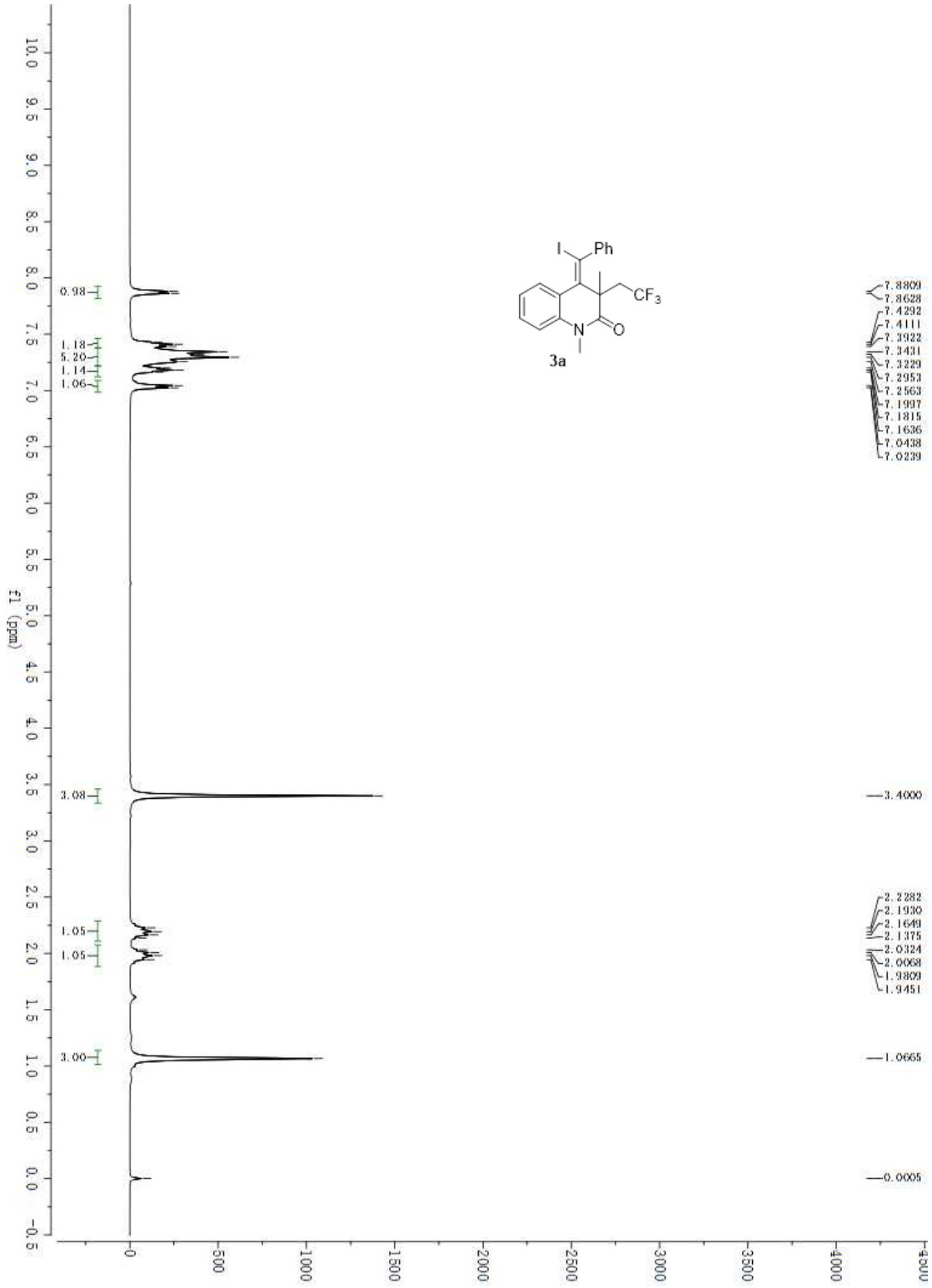
(*E*)-4-(iodo(*p*-tolyl)methylene)-1,3,6-trimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihydroquinolin-2(1*H*)-one (**3l**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.07 (s, 3H), 1.91-2.03 (m, 1H), 2.15-2.24 (m, 1H), 2.36 (s, 3H), 2.40 (s, 3H), 3.37 (s, 3H), 6.91 (d, *J* = 8.2 Hz, 1H), 7.12 (t, *J* = 8.9 Hz, 2H), 7.16-7.20 (m, 2H), 7.24 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.67 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.7, 21.3, 21.4, 30.9, 41.0 (q, *J* = 27.2 Hz), 48.1, 101.4, 114.0, 124.4, 127.2, 127.5, 128.2, 128.3, 128.8, 130.3, 132.5, 132.8, 135.5, 138.1, 139.1, 143.8, 169.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.7 (t, *J* = 10.5 Hz); HRMS (ESI) calcd for $C_{22}H_{21}F_3INO$: 500.0693 (M + H^+), found: 500.0685.



(*E*)-4-(iodo(thiophen-2-yl)methylene)-1,3-dimethyl-3-(2,2,2-trifluoroethyl)-3,4-dihydroquinolin-2(1*H*)-one (**3m**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18 (s, 3H), 1.97-2.08 (m, 1H), 2.15-2.25 (m, 1H), 3.39 (s, 3H), 7.03 (d, *J* = 8.1 Hz, 1H), 7.08 (d, *J* = 4.9 Hz, 1H), 7.16 (d, *J* = 7.5 Hz, 1H), 7.20 (d, *J* = 6.7 Hz, 1H), 7.31 (dd, J_1 = 4.8 Hz, J_2 = 3.0 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.84 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.2, 31.0, 40.8 (q, *J* = 23.7 Hz), 48.3, 114.2, 123.1, 123.4, 124.0, 124.7, 125.4, 128.1, 128.3, 130.0, 130.1, 132.2, 132.7, 137.8, 145.4, 169.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.6 (t, *J* = 10.1 Hz); HRMS (ESI) calcd for $C_{18}H_{15}F_3INOS$: 477.9944 ($M + H^+$), found: 477.9932.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Ph
CF3
N
O
3a
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5.20
1.14
1.06
3.08
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3.00
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7.4292
7.4111
7.3922
7.3431
7.3229
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7.1997
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7.1636
7.0438
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3.4000
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2.1375
2.0324
2.0068
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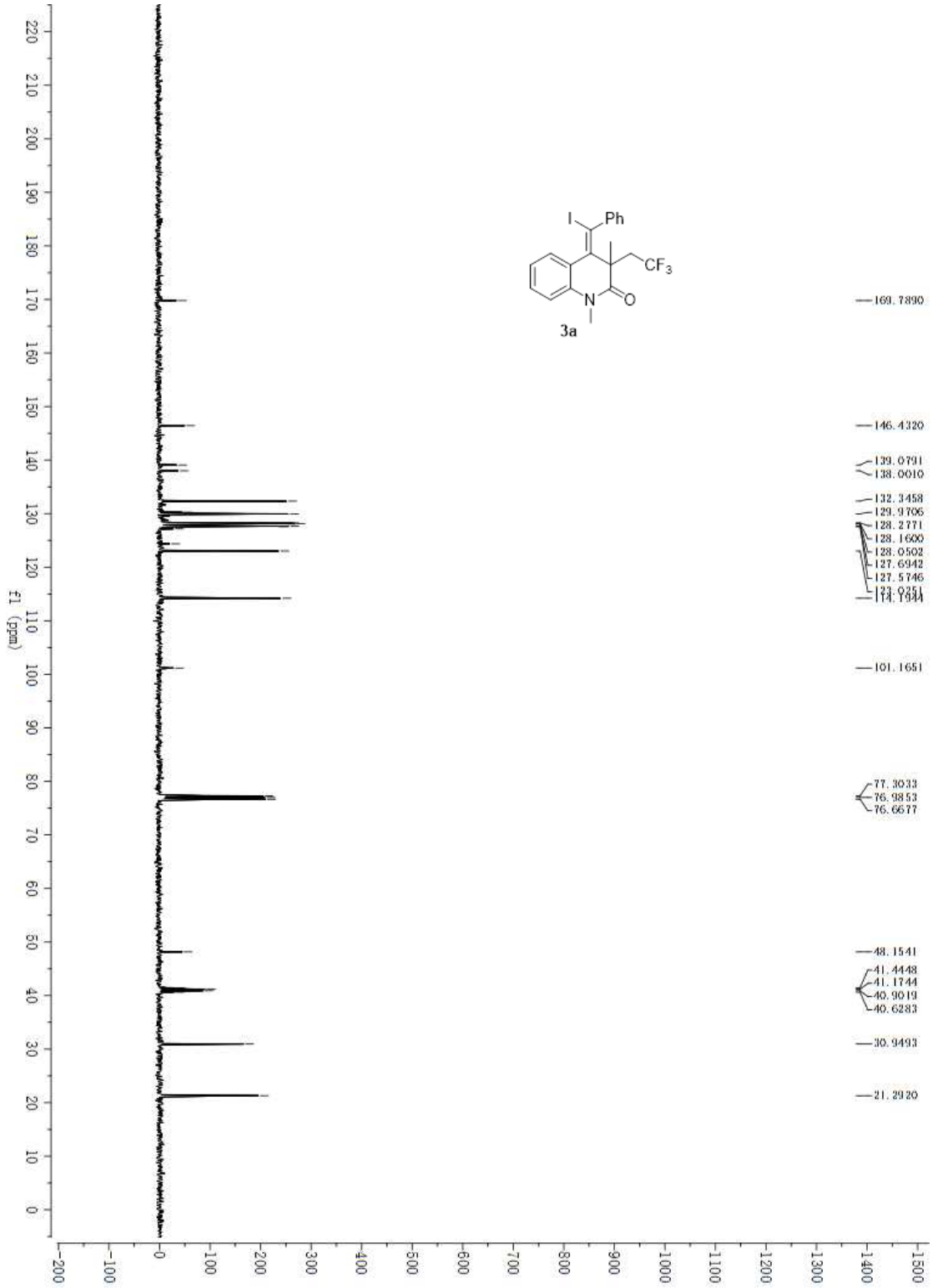
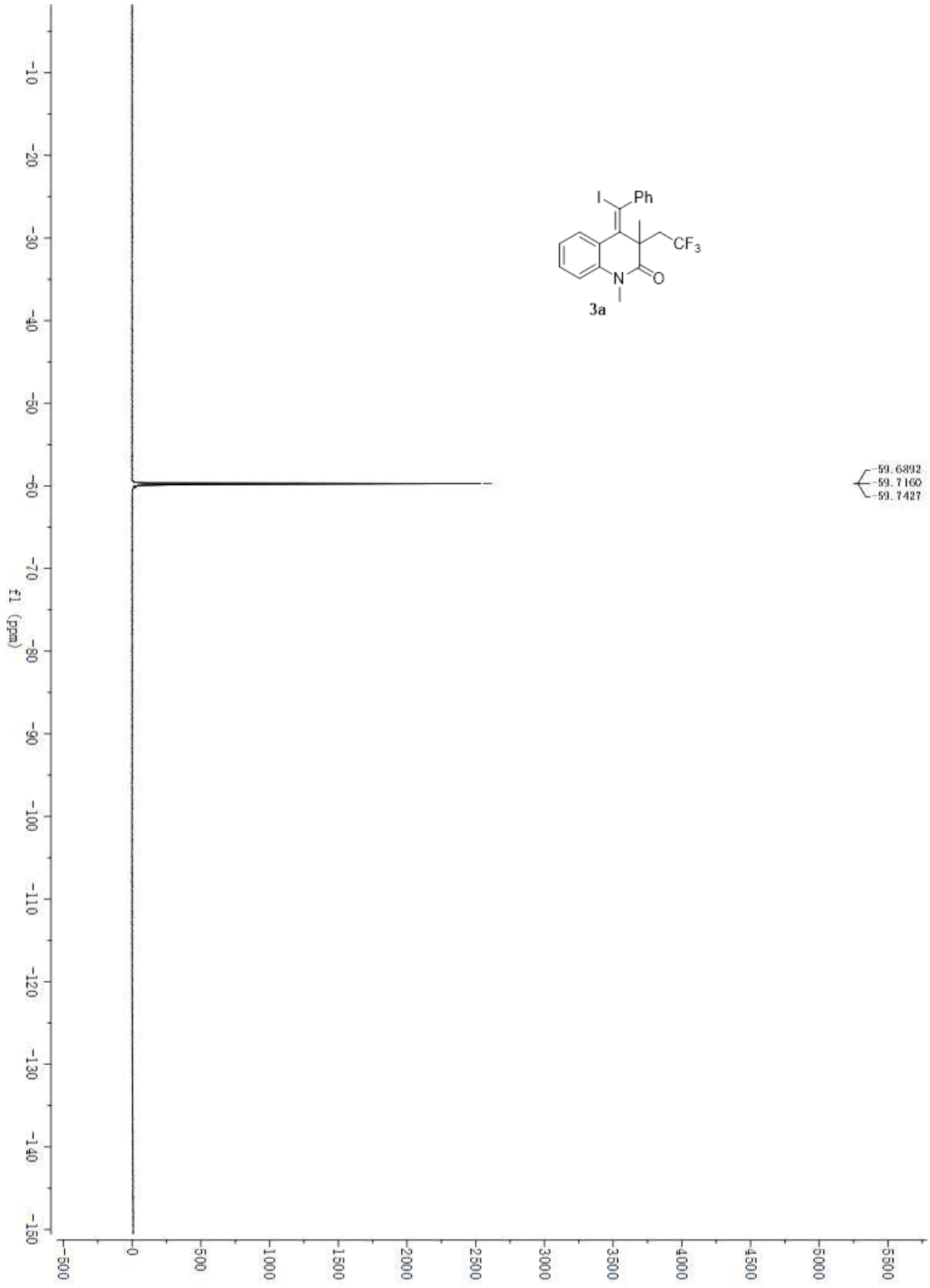
1.9451
1.0665
0.0005


I
Ph
CF3
N
O
3a
169.7890
146.4320
139.0791
138.0010
132.3458
129.9706
128.2771
128.1600
128.0502
127.6942
127.5746
123.0251
114.1944
101.1651
77.3033
76.9853
76.6677
48.1541
41.4448
41.1744
40.9019
40.6283
30.9493
21.2920
f1 (ppm)


I
Ph
CF3
N
O
3a
-59.6892
-59.7160
-59.7427
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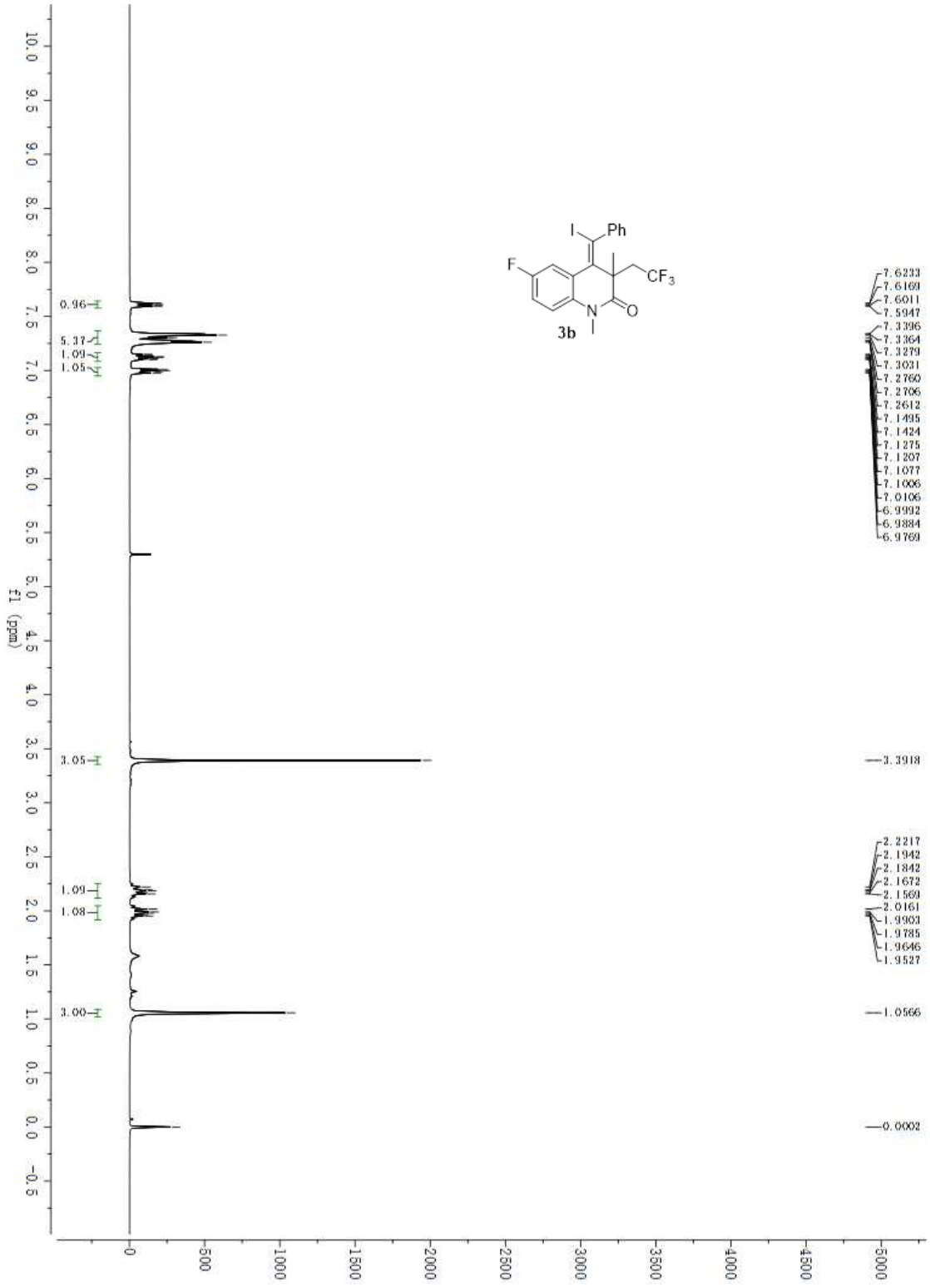
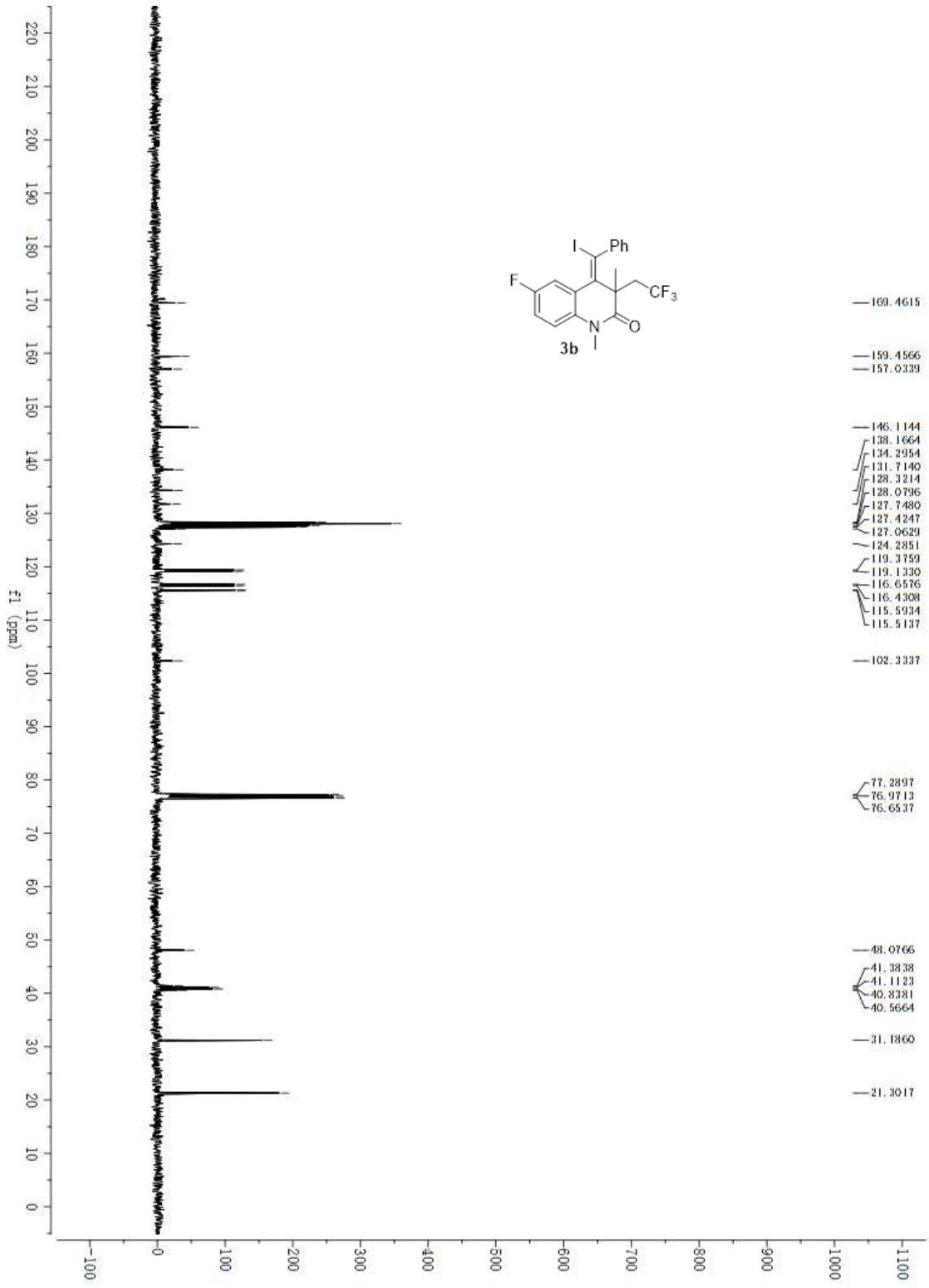
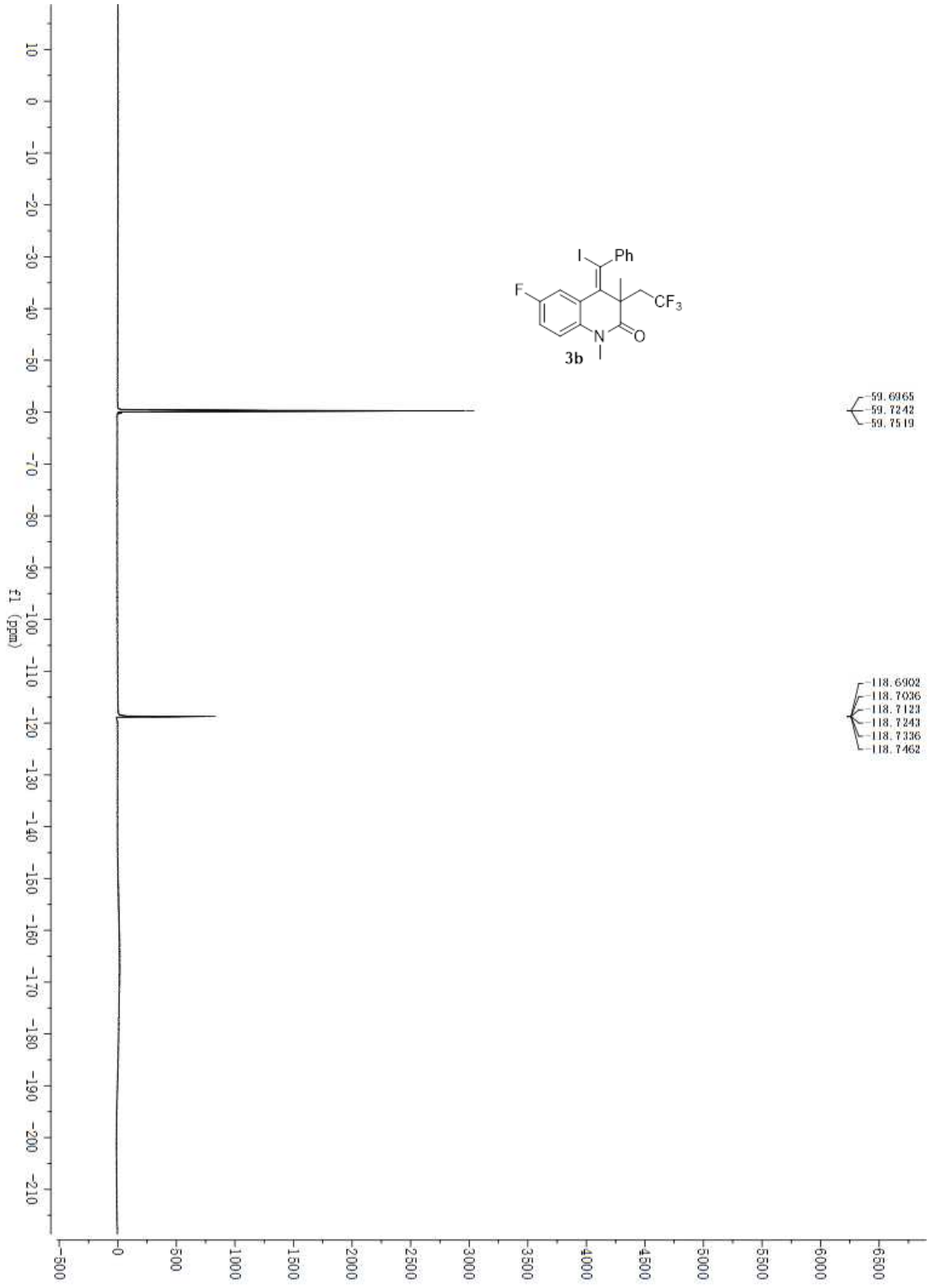
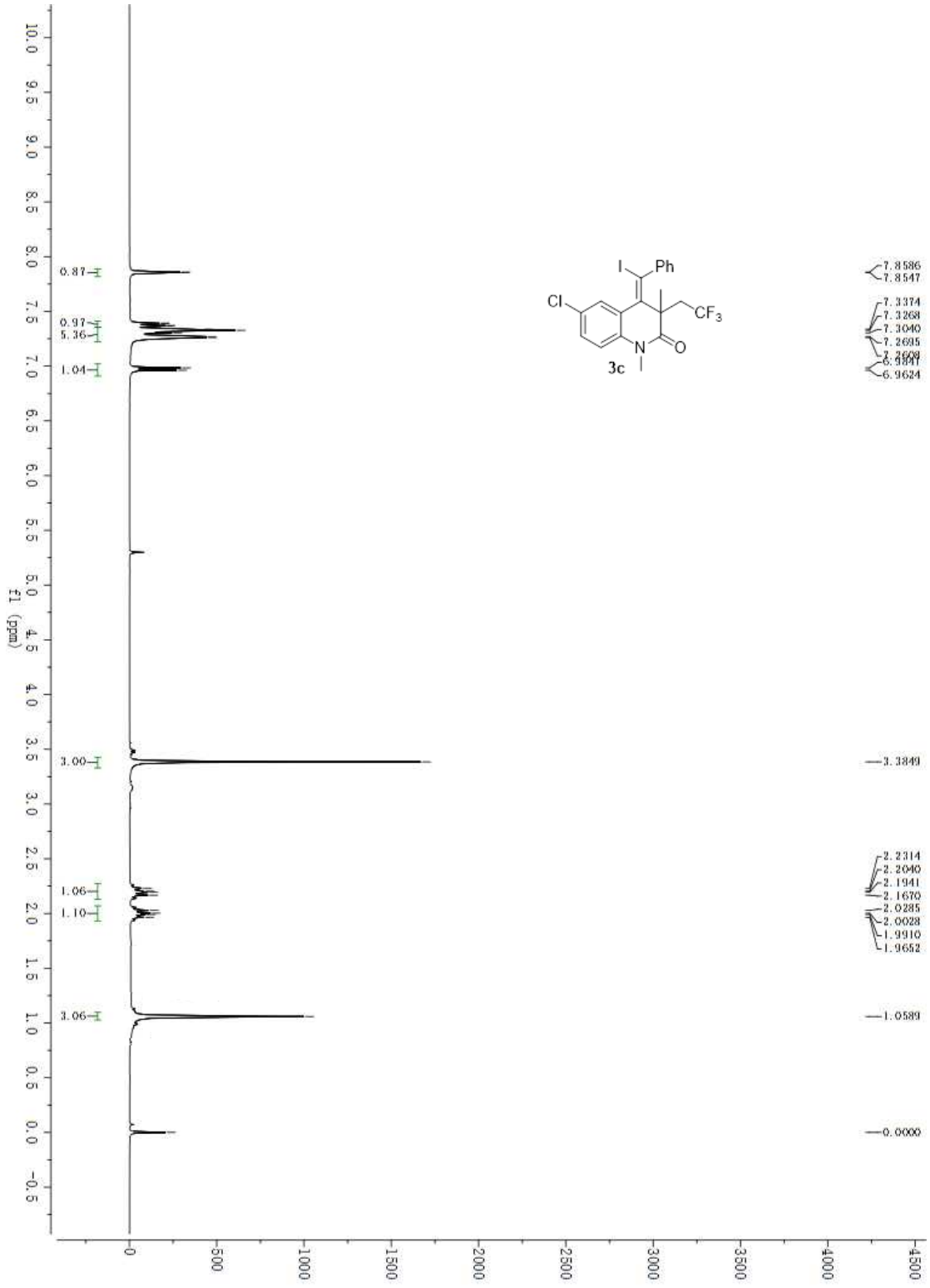
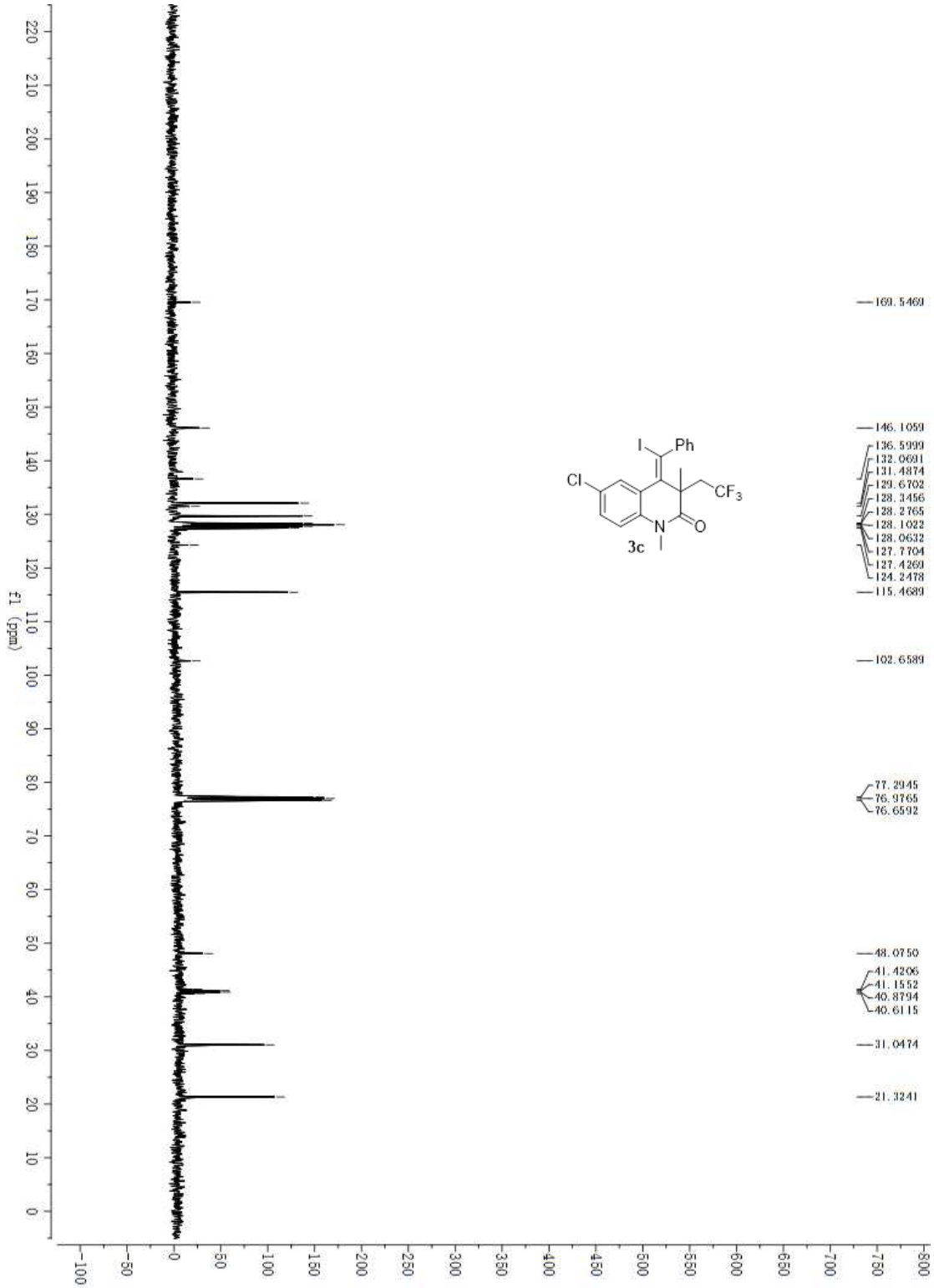
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500


I
Ph
F
CF3
N
O
3b
f1 (ppm)
0.96
5.37
1.09
1.05
3.05
1.09
1.08
3.00
7.6233
7.6169
7.6011
7.5947
7.3396
7.3364
7.3279
7.3031
7.2760
7.2706
7.2612
7.1495
7.1424
7.1275
7.1207
7.1077
7.1006
7.0106
6.9992
6.9884
6.9769
3.3918
2.2217
2.1942
2.1842
2.1672
2.1569
2.0161
1.9903
1.9785
1.9646
1.9527
1.0566
0.0002


I
Ph
F
CF3
N
O
3b
f1 (ppm)
169.4615
159.4566
157.0339
146.1144
138.1664
134.2954
131.7140
128.3214
128.0796
127.7480
127.4247
127.0629
124.2851
119.3759
119.1330
116.6576
116.4308
115.5934
115.5137
102.3337
77.2897
76.9713
76.6537
48.0766
41.3838
41.1123
40.8381
40.5664
31.1860
21.3017


I
Ph
F
CF3
N
O
3b
59.6965
59.7242
59.7519
118.6902
118.7036
118.7123
118.7243
118.7336
118.7462
f1 (ppm)


I
Ph
Cl
CF3
N
O
3c
7.8586
7.8547
7.3374
7.3268
7.3040
7.2695
6.9641
6.9624
3.3849
2.2314
2.2040
2.1941
2.1670
2.0285
2.0028
1.9910
1.9652
1.0589
0.0000
0.87
0.97
5.36
1.04
3.00
1.06
1.10
3.06
f1 (ppm)


f1 (ppm)
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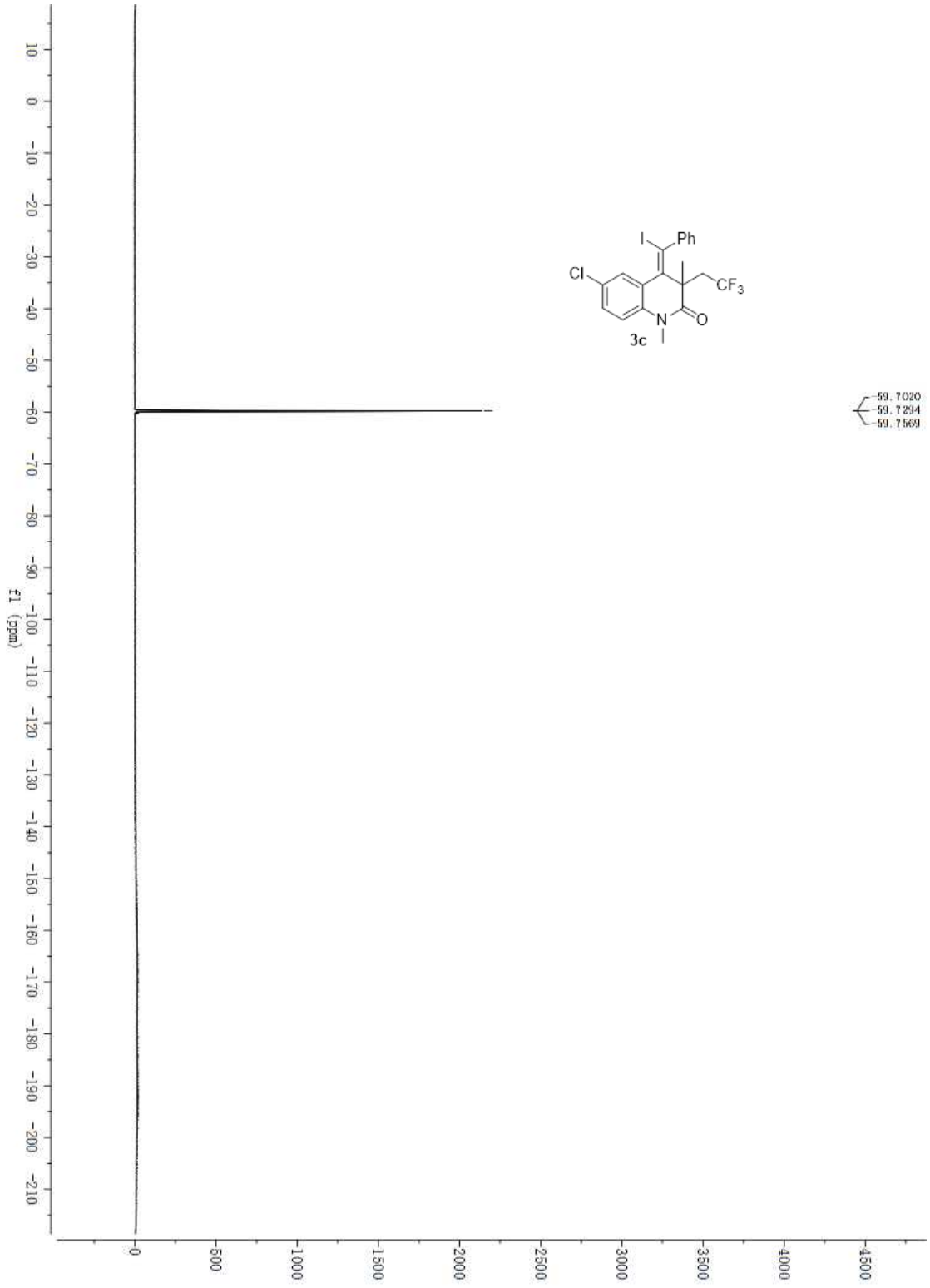
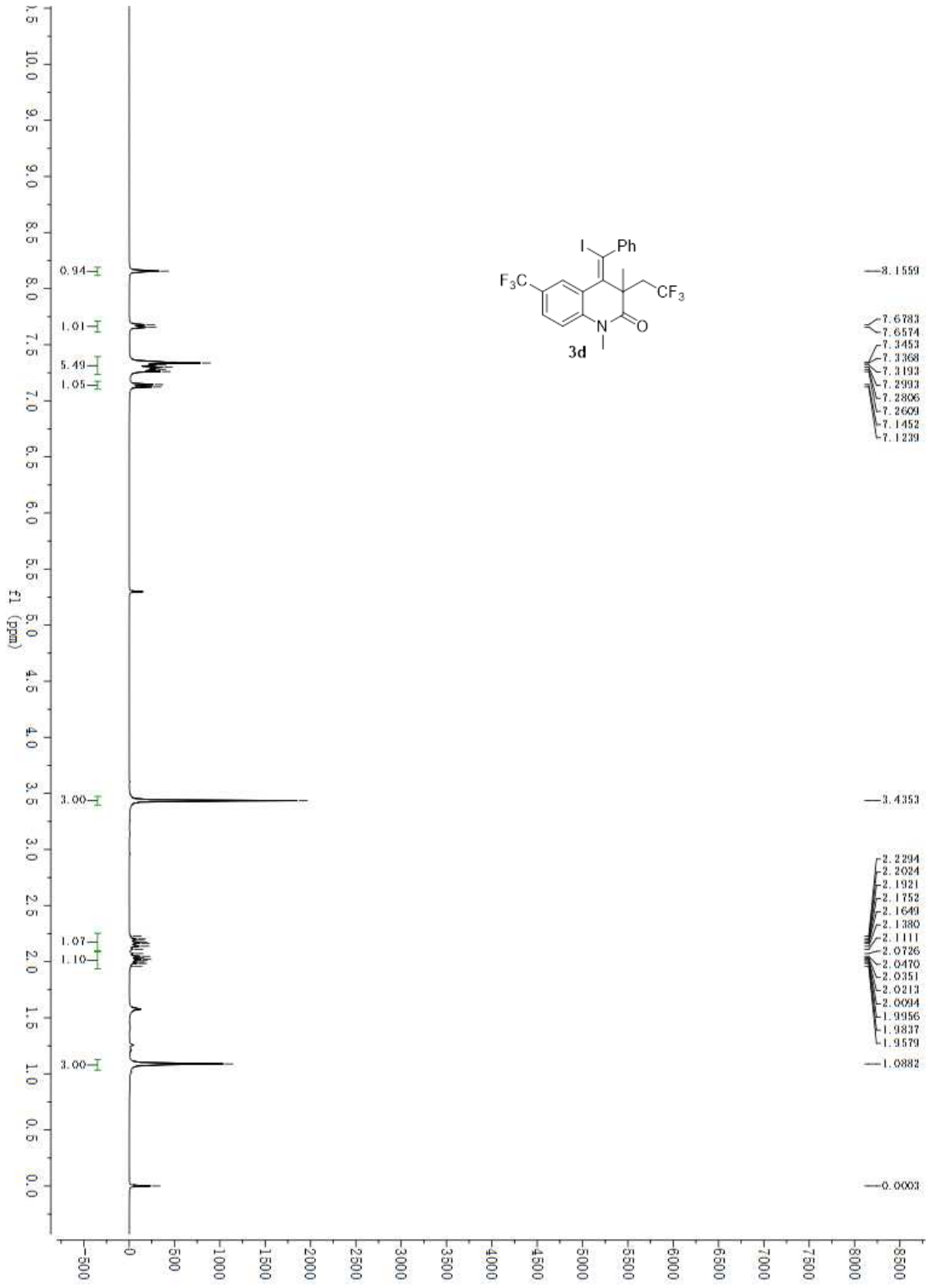
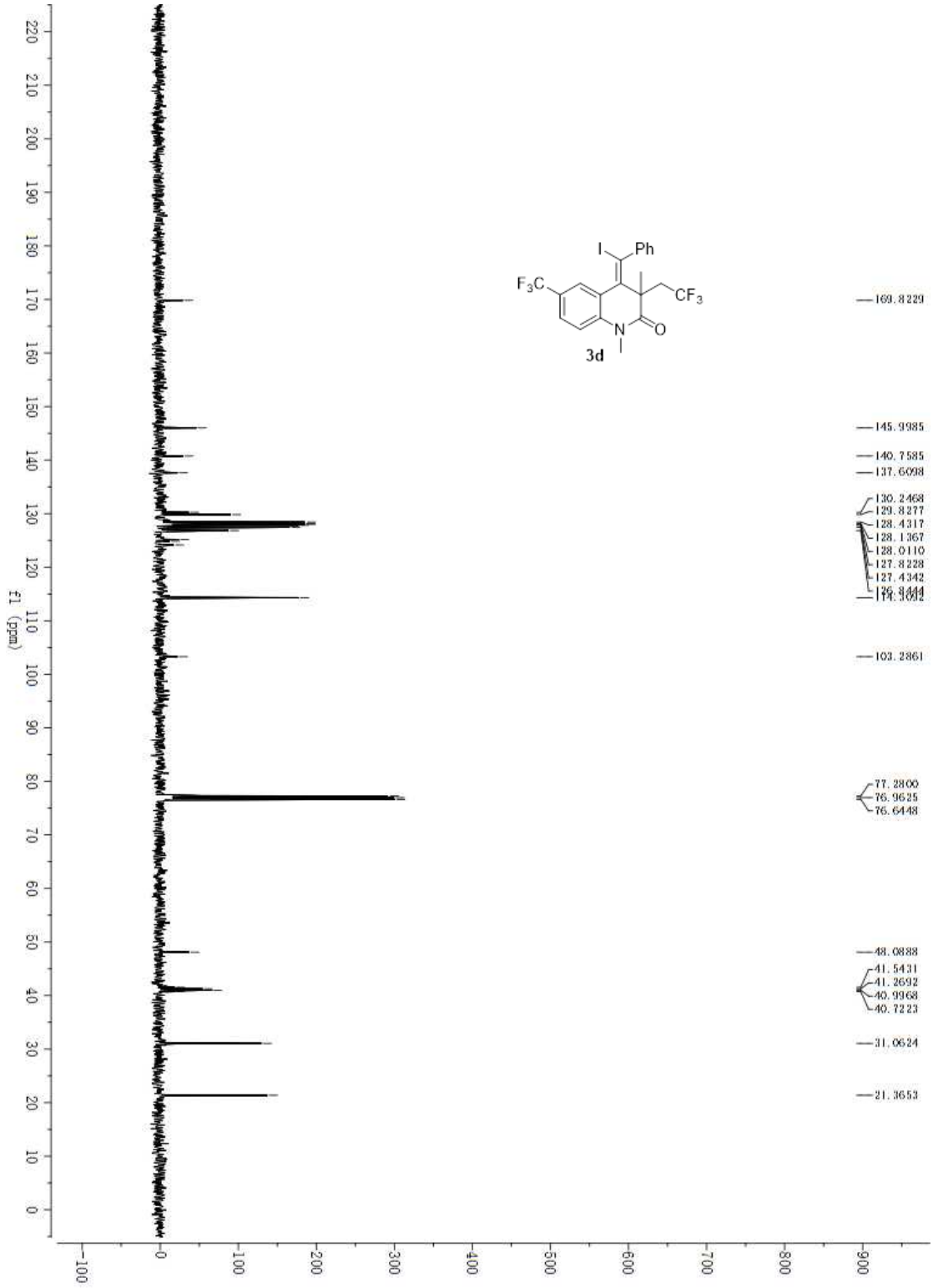
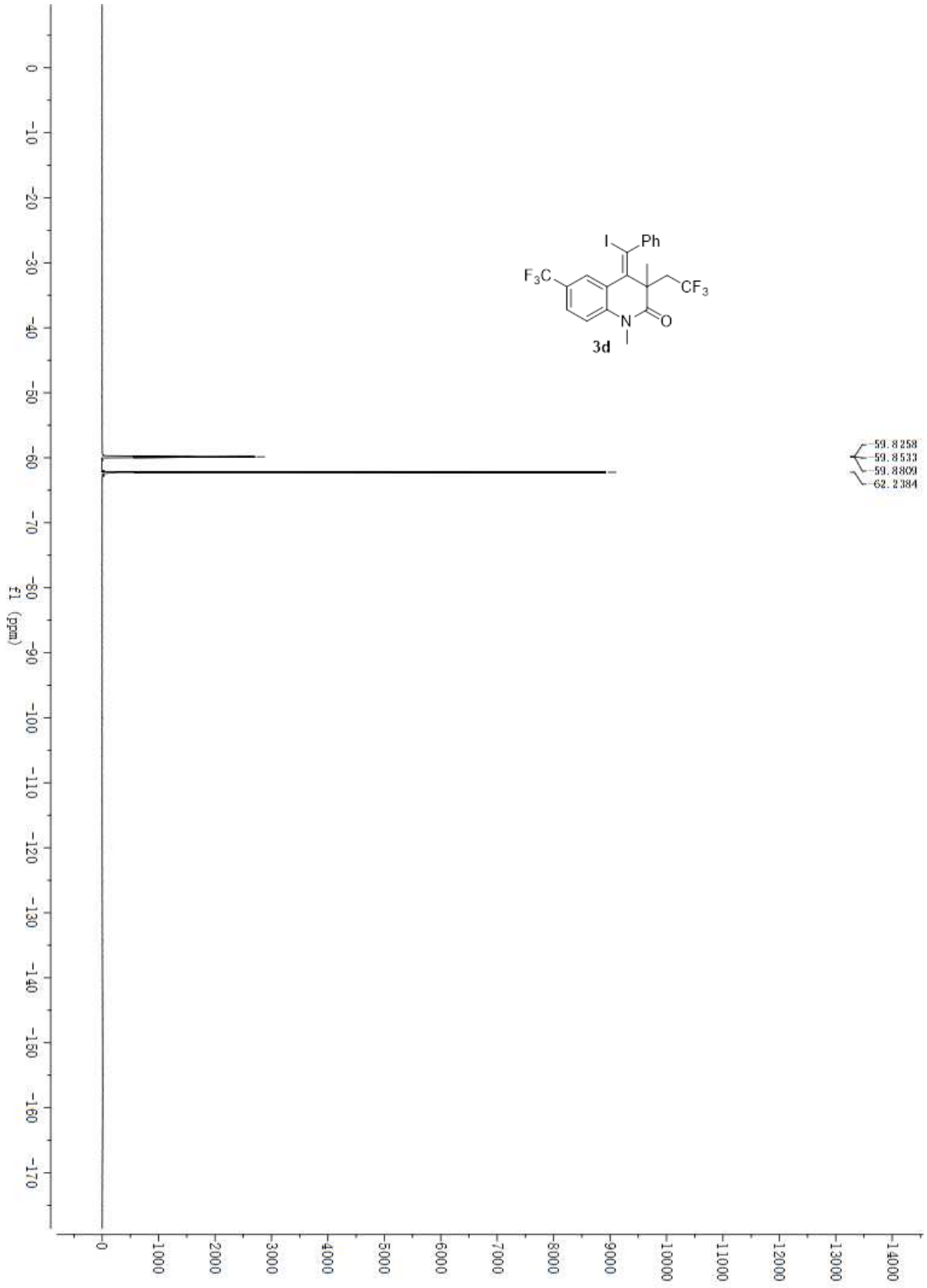
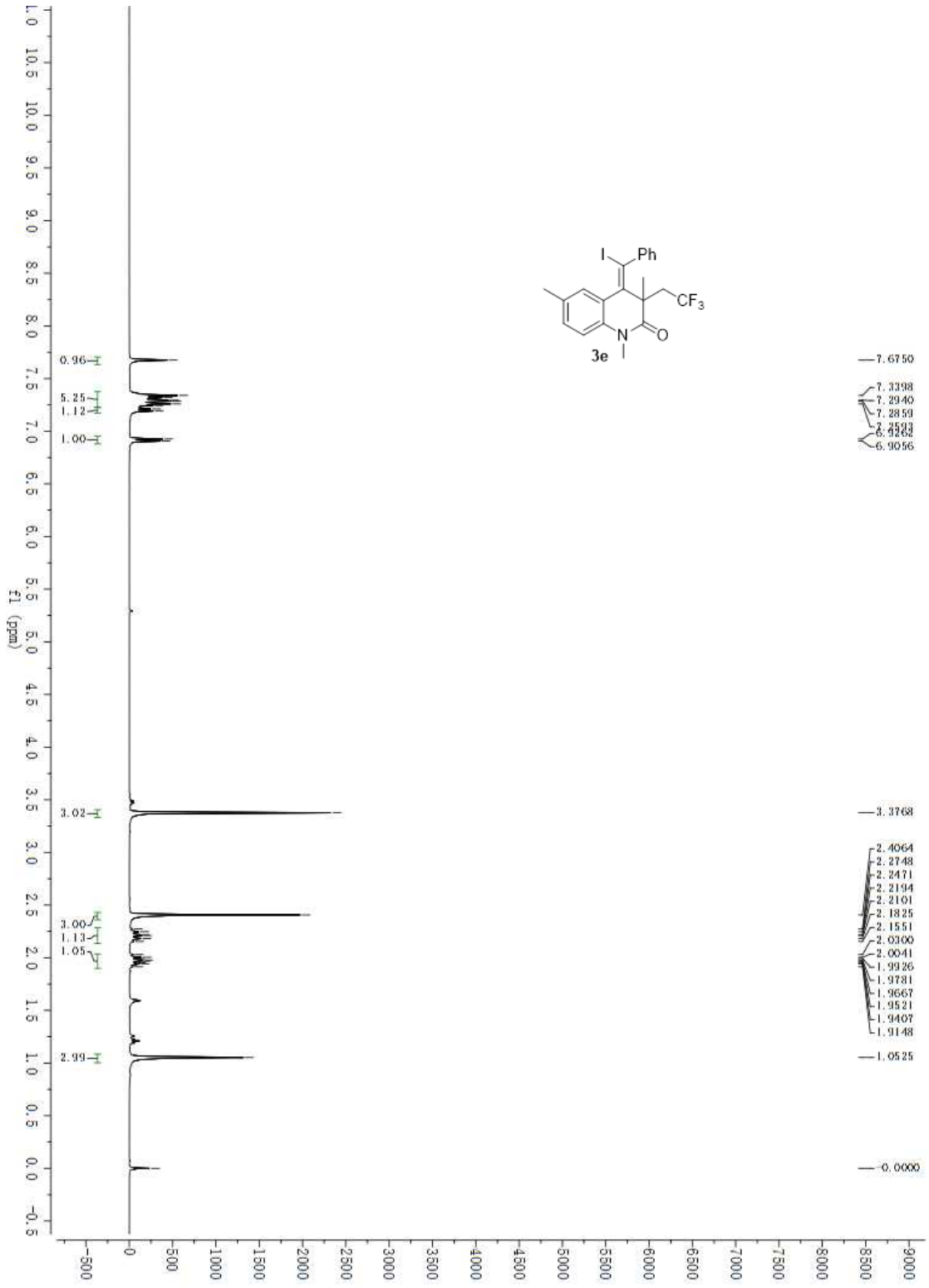
136.5999
132.0691
131.4874
129.6702
128.3456
128.2765
128.1022
128.0632
127.7704
127.4269
124.2478
115.4689
102.6589
77.2945
76.9765
76.6592
48.0750
41.4206
41.1552
40.8794
40.6115
31.0474
21.3241
I
Ph
Cl
CF3
N
O
3c

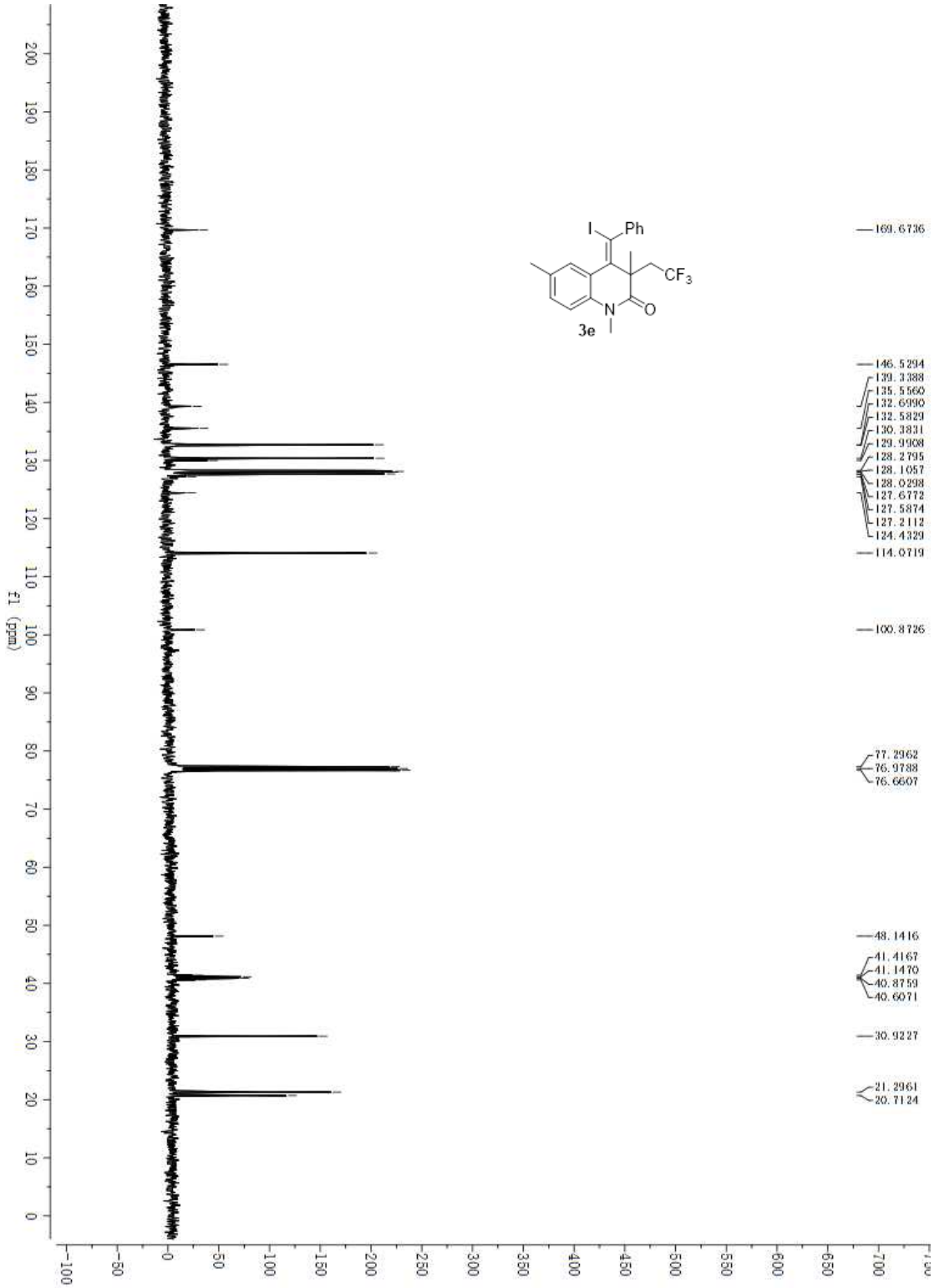

I
Ph
Cl
CF3
N
O
3c
-59.7020
-59.7294
-59.7569
f1 (ppm)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
0
500
1000
1500
2000
2500
3000
3500
4000
4500

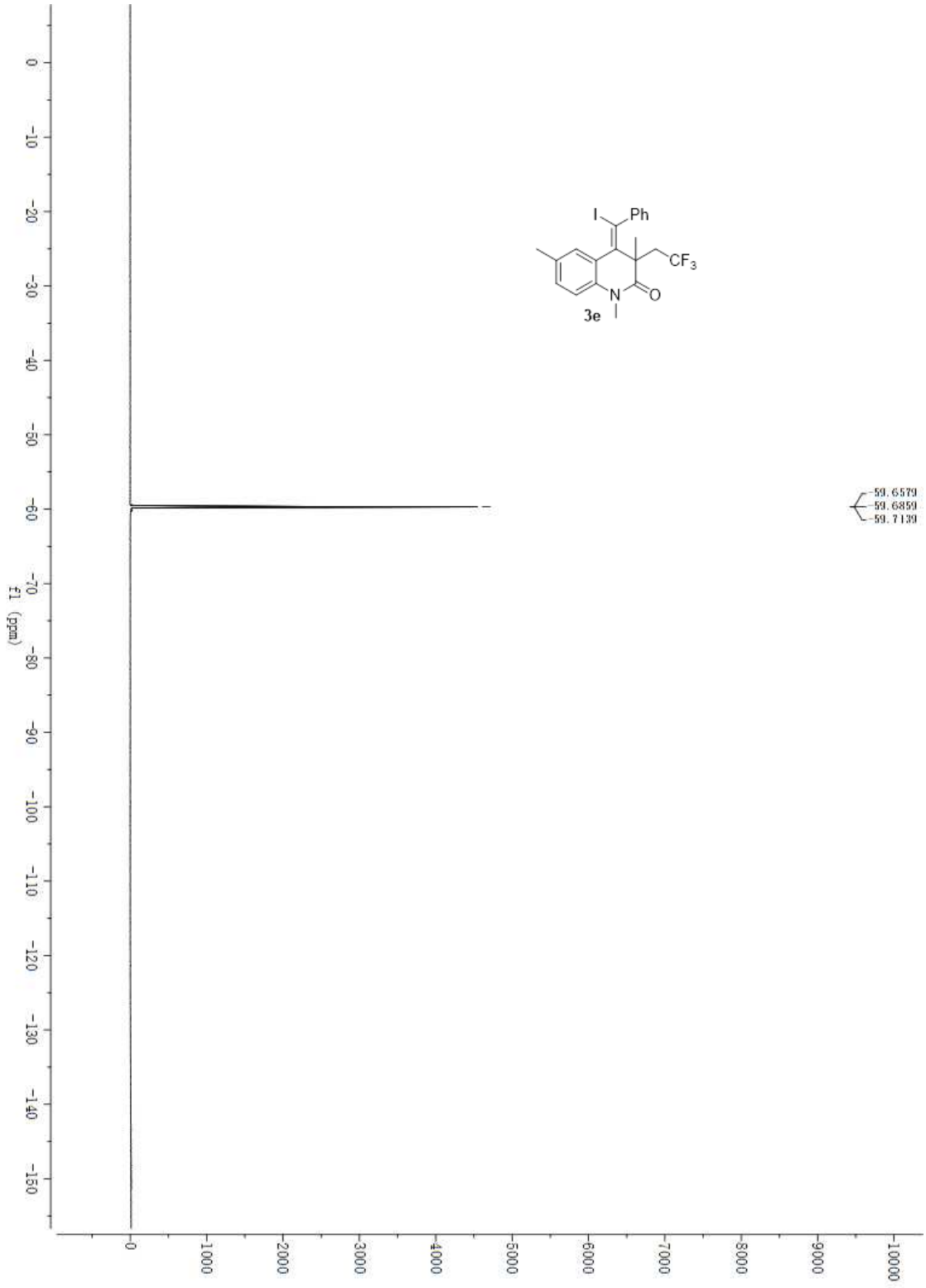

I
Ph
F3C
CF3
N
O
3d
f1 (ppm)
0.94
1.01
5.49
1.05
3.00
1.07
1.10
3.00
8.1559
7.6783
7.6574
7.3453
7.3368
7.3193
7.2993
7.2806
7.2609
7.1452
7.1239
3.4353
2.2294
2.2024
2.1921
2.1752
2.1649
2.1380
2.1111
2.0726
2.0470
2.0351
2.0213
2.0094
1.9956
1.9837
1.9579
1.0882
0.0003

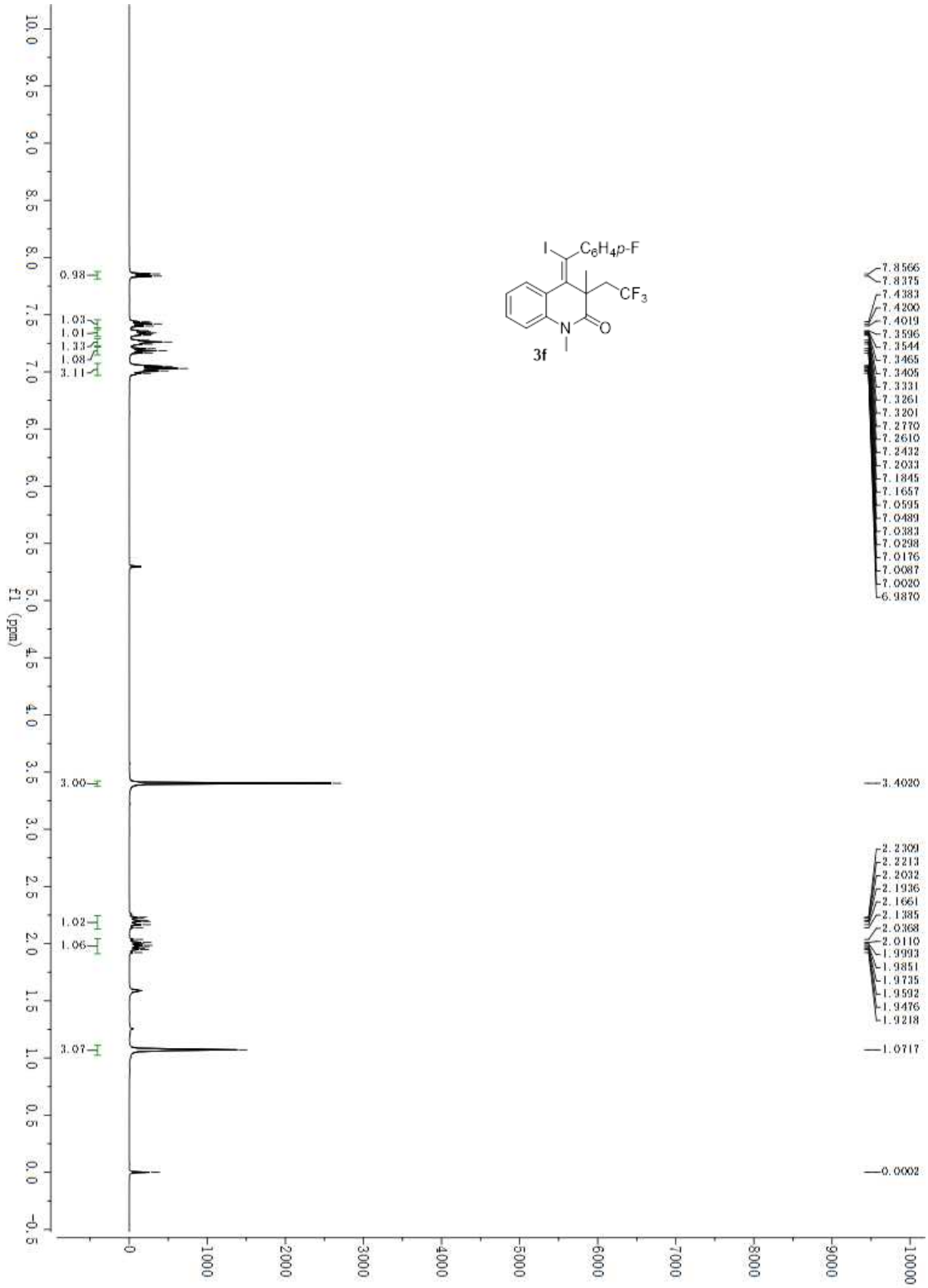

I
Ph
F3C
CF3
N
O
3d
169.8229
145.9985
140.7585
137.6098
130.2468
129.8277
128.4317
128.1367
128.0110
127.8228
127.4342
126.8444
114.3092
103.2861
77.2800
76.9625
76.6448
48.0888
41.5431
41.2692
40.9968
40.7223
31.0624
21.3653
f1 (ppm)

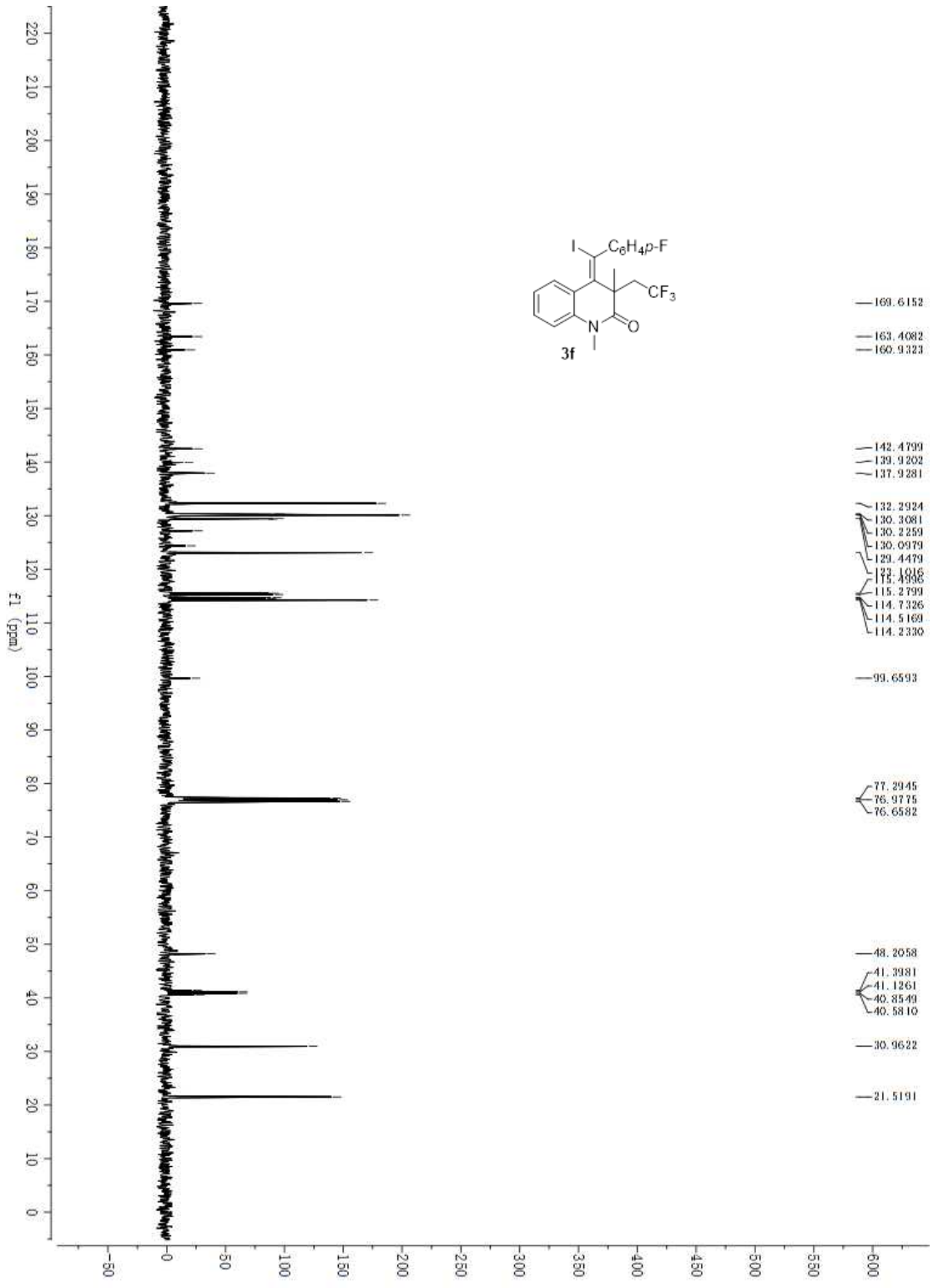

I
Ph
F3C
CF3
N
O
3d
59.8258
59.8533
59.8809
62.2384
f1 (ppm)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000
11000
12000
13000
14000


I
Ph
CF3
N
O
3e
f1 (ppm)
0.96
5.25
1.12
1.00
3.02
3.00
1.13
1.05
2.99
7.6750
7.3398
7.2940
7.2859
6.9056
3.3768
2.4064
2.2748
2.2471
2.2194
2.2101
2.1825
2.1551
2.0300
2.0041
1.9926
1.9781
1.9667
1.9521
1.9407
1.9148
1.0525
0.0000

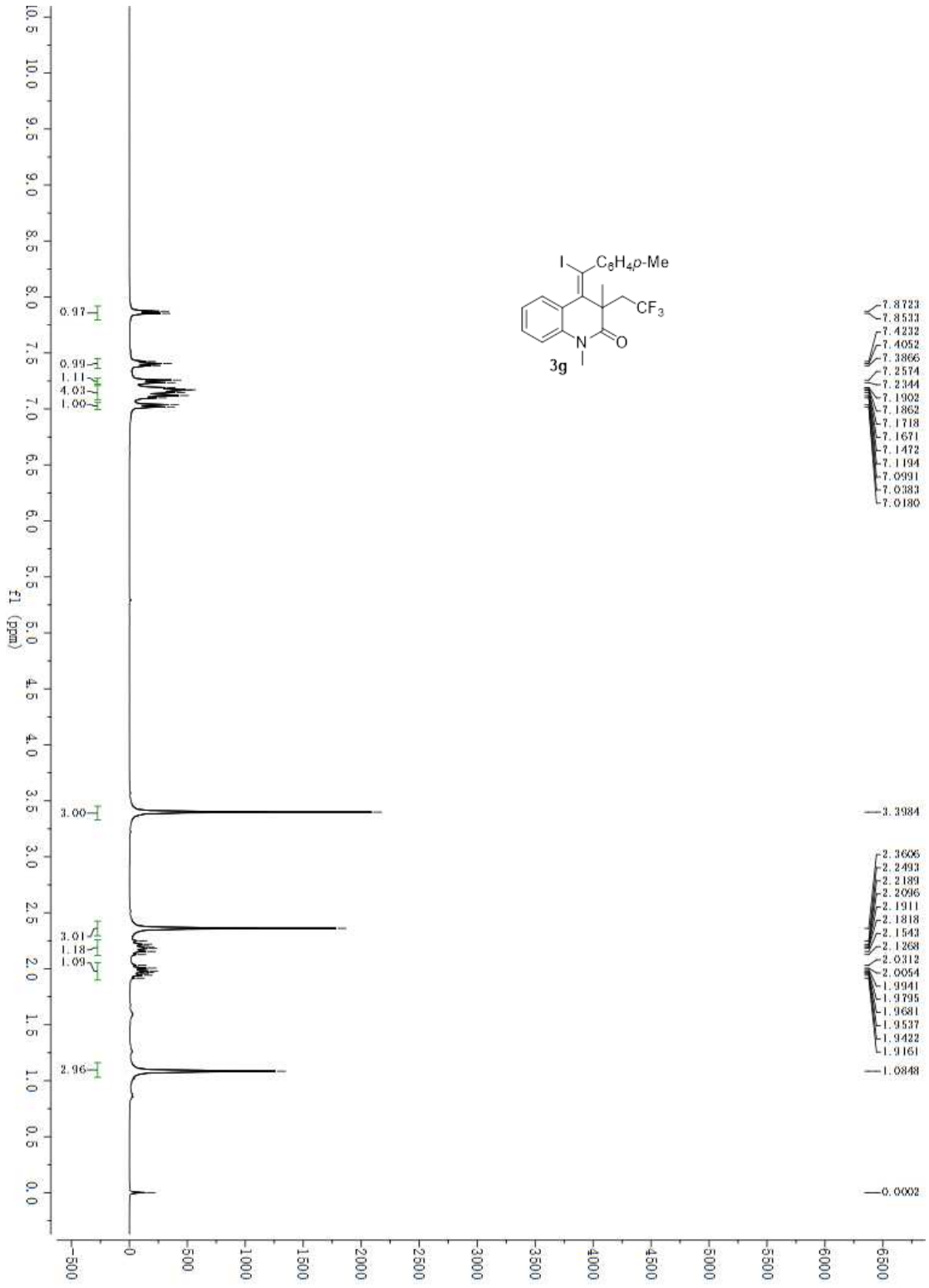

I
Ph
CF3
N
O
3e
169.6736
146.5294
139.3388
135.5560
132.6990
132.5829
130.3831
129.9908
128.2795
128.1057
128.0298
127.6772
127.5874
127.2112
124.4329
114.0719
100.8726
77.2962
76.9788
76.6607
48.1416
41.4167
41.1470
40.8759
40.6071
30.9227
21.2961
20.7124
f1 (ppm)

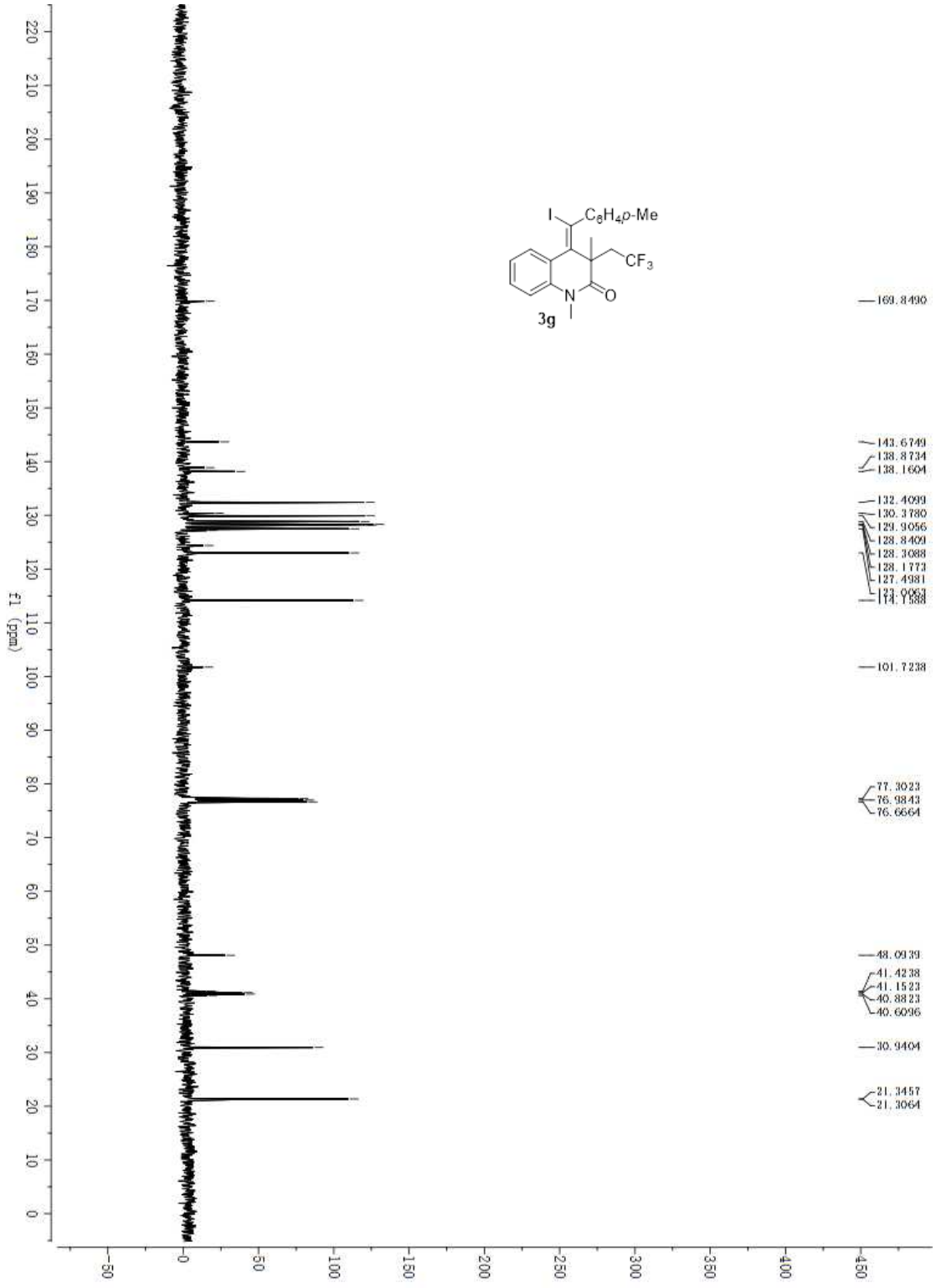

I
Ph
CF3
N
O
3e
-59.6579
-59.6859
-59.7139
f1 (ppm)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000

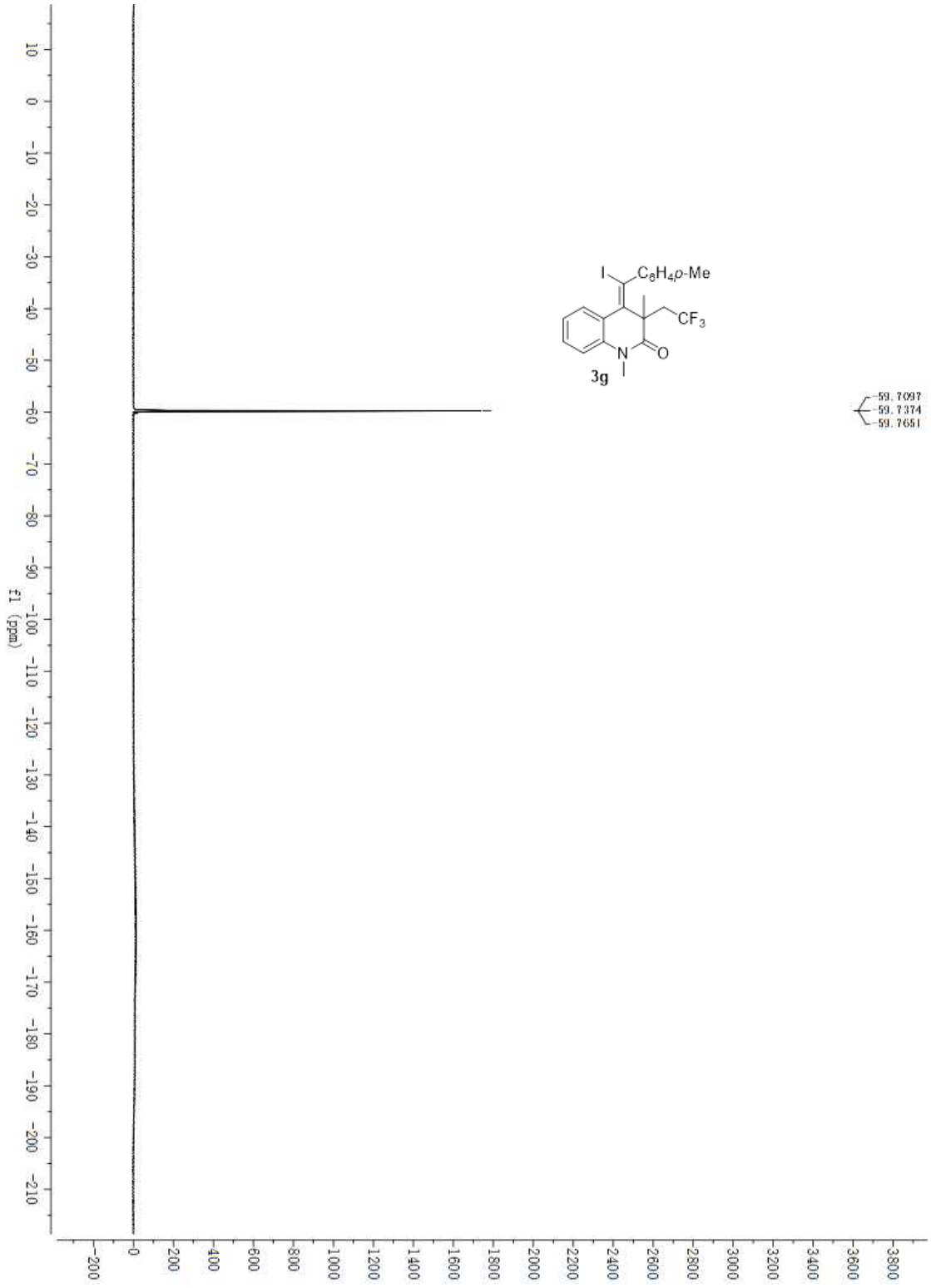

I
C6H4p-F
CF3
N
O
3f
f1 (ppm)
0.98
1.03
1.01
1.33
1.08
3.11
3.00
1.02
1.06
3.07
7.8566
7.8375
7.4383
7.4200
7.4019
7.3596
7.3544
7.3465
7.3405
7.3331
7.3261
7.3201
7.2770
7.2610
7.2432
7.2033
7.1845
7.1657
7.0595
7.0489
7.0383
7.0298
7.0176
7.0087
7.0020
6.9870
3.4020
2.2309
2.2213
2.2032
2.1936
2.1661
2.1385
2.0368
2.0110
1.9993
1.9851
1.9735
1.9592
1.9476
1.9218
1.0717
0.0002

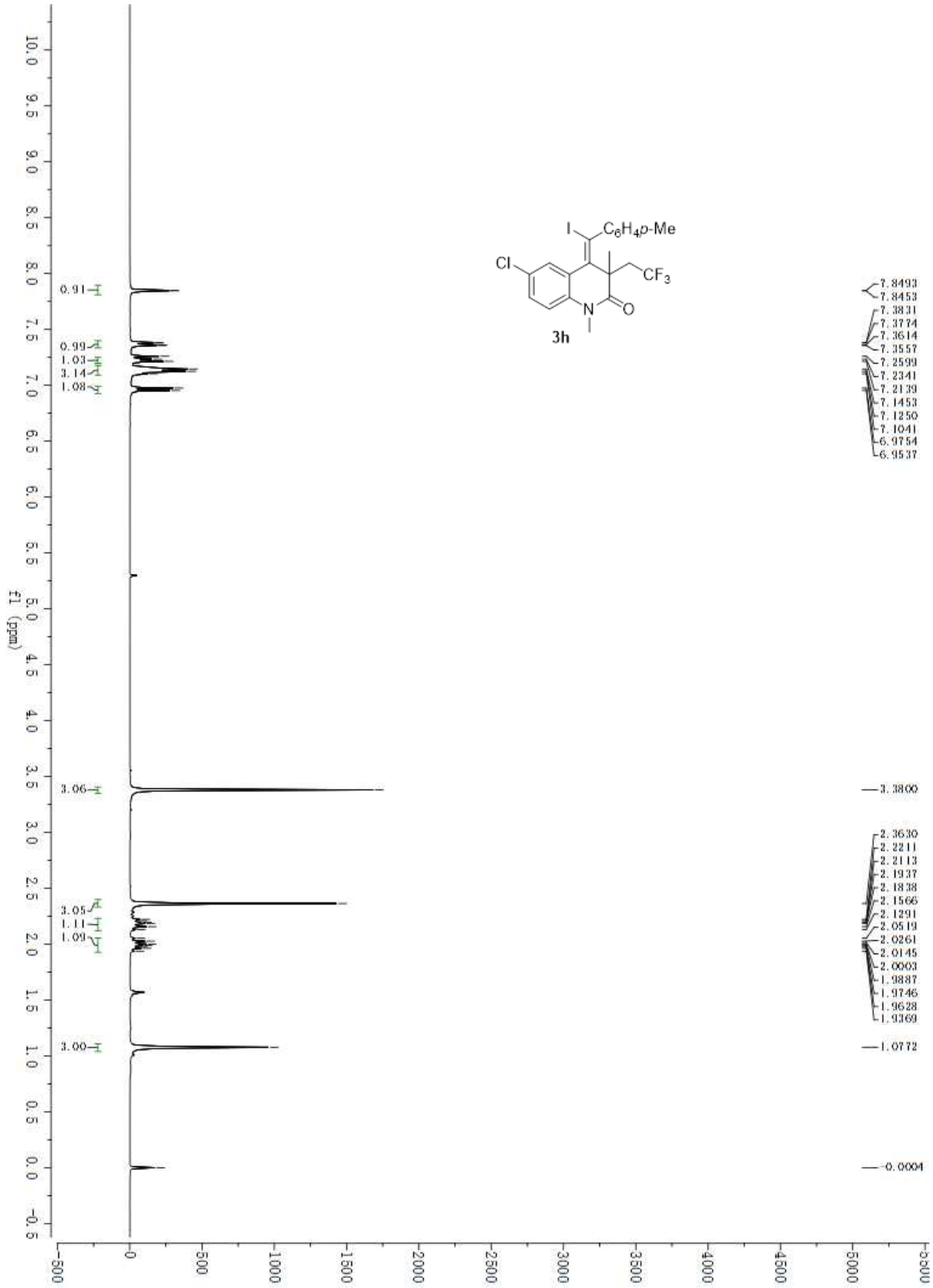

I
C6H4p-F
CF3
N
O
3f
169.6152
163.4082
160.9323
142.4799
139.9202
137.9281
132.2924
130.3081
130.2259
130.0979
129.4479
123.1016
115.4996
115.2799
114.7326
114.5169
114.2330
99.6593
77.2945
76.9775
76.6582
48.2058
41.3981
41.1261
40.8549
40.5840
30.9622
21.5191
f1 (ppm)

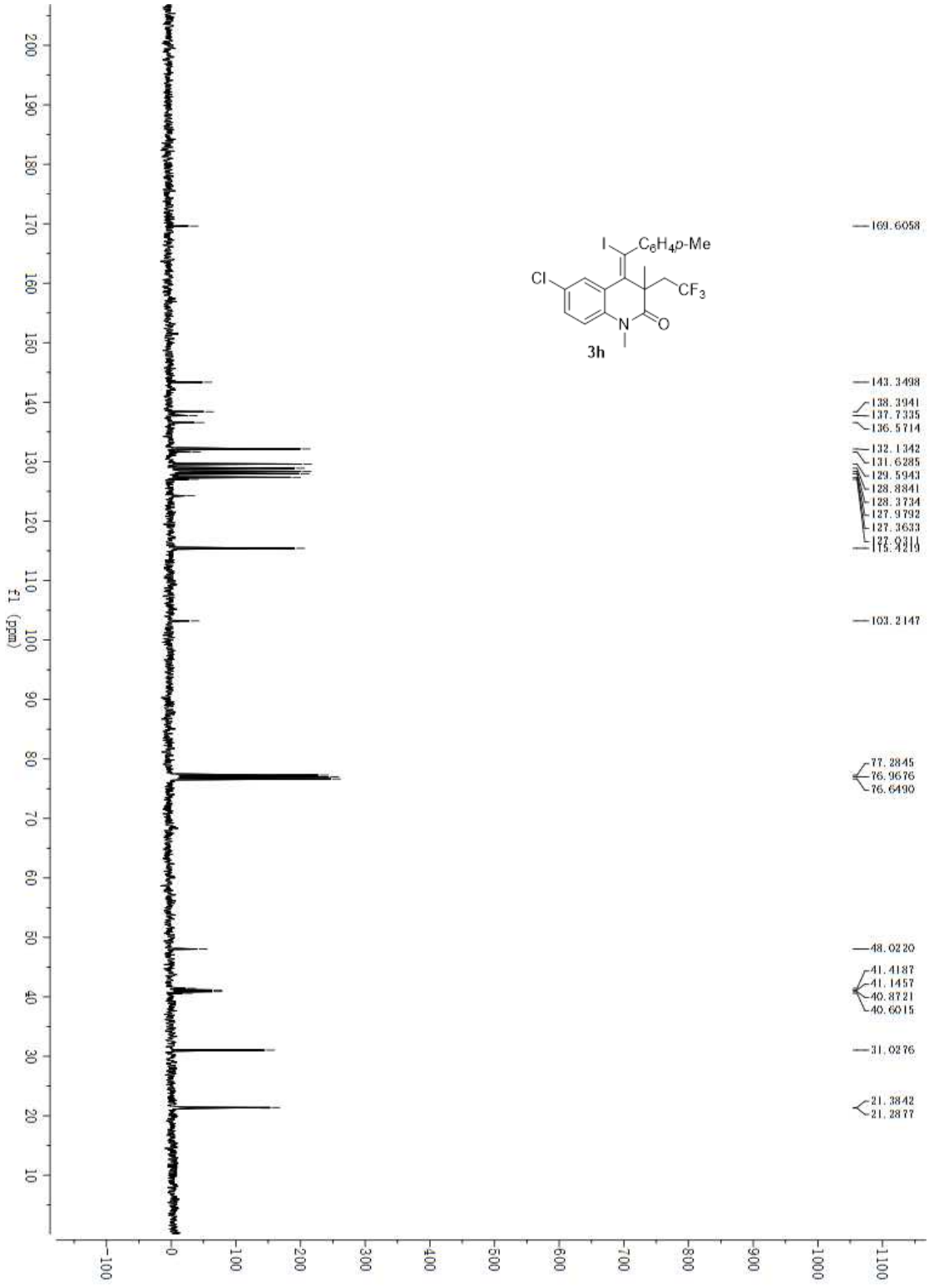

I
C6H4p-F
CF3
N
O
3f
-59.6840
-59.7118
-59.7397
-112.4317
-112.4459
-112.4546
-112.4681
-112.4820
-112.4908
-112.5046
f1 (ppm)

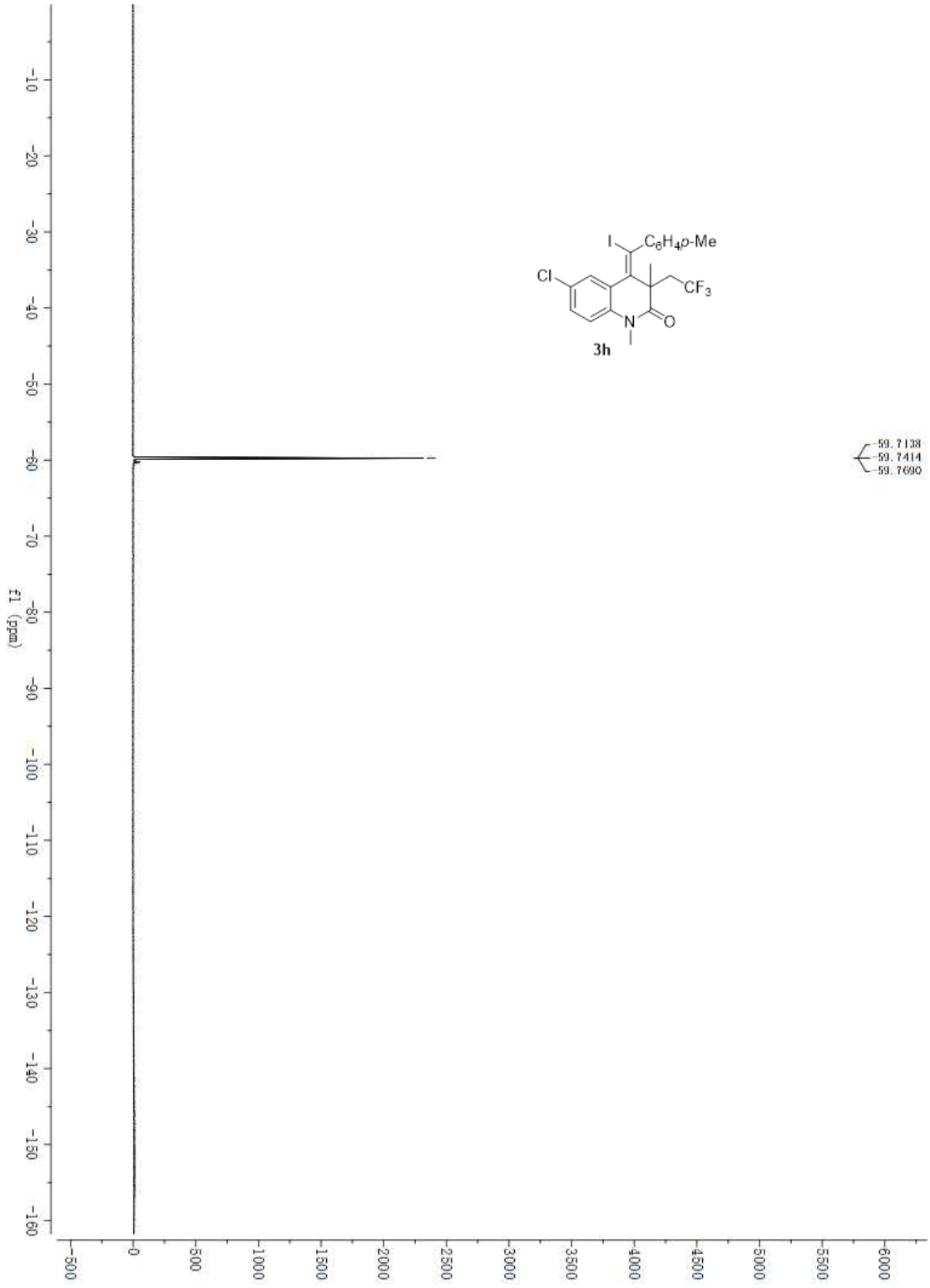

I
C6H4p-Me
CF3
N
O
3g
f1 (ppm)
0.97
0.99
1.11
4.03
1.00
3.00
3.01
1.18
1.09
2.96
7.8723
7.8533
7.4232
7.4052
7.3866
7.2574
7.2344
7.1902
7.1862
7.1718
7.1671
7.1472
7.1194
7.0991
7.0383
7.0180
3.3984
2.3606
2.2493
2.2189
2.2096
2.1911
2.1818
2.1543
2.1268
2.0312
2.0054
1.9941
1.9795
1.9681
1.9537
1.9422
1.9161
1.0848
0.0002

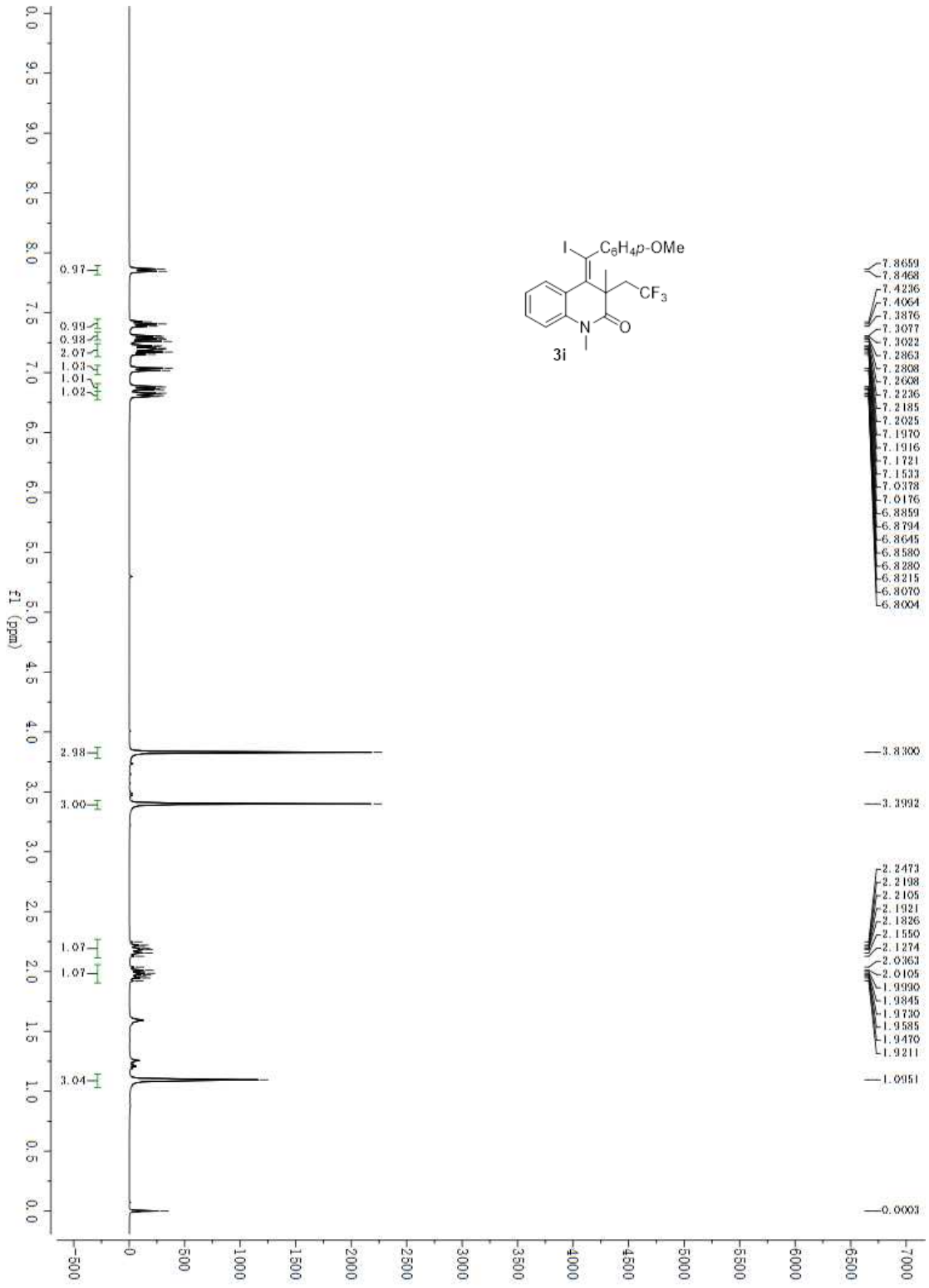

I
C6H4p-Me
CF3
N
O
3g
169.8490
143.6749
138.8734
138.1604
132.4099
130.3780
129.9056
128.8409
128.3088
128.1773
127.4981
123.0063
114.7588
101.7238
77.3023
76.9843
76.6664
48.0939
41.4238
41.1523
40.8823
40.6096
30.9404
21.3457
21.3064
f1 (ppm)

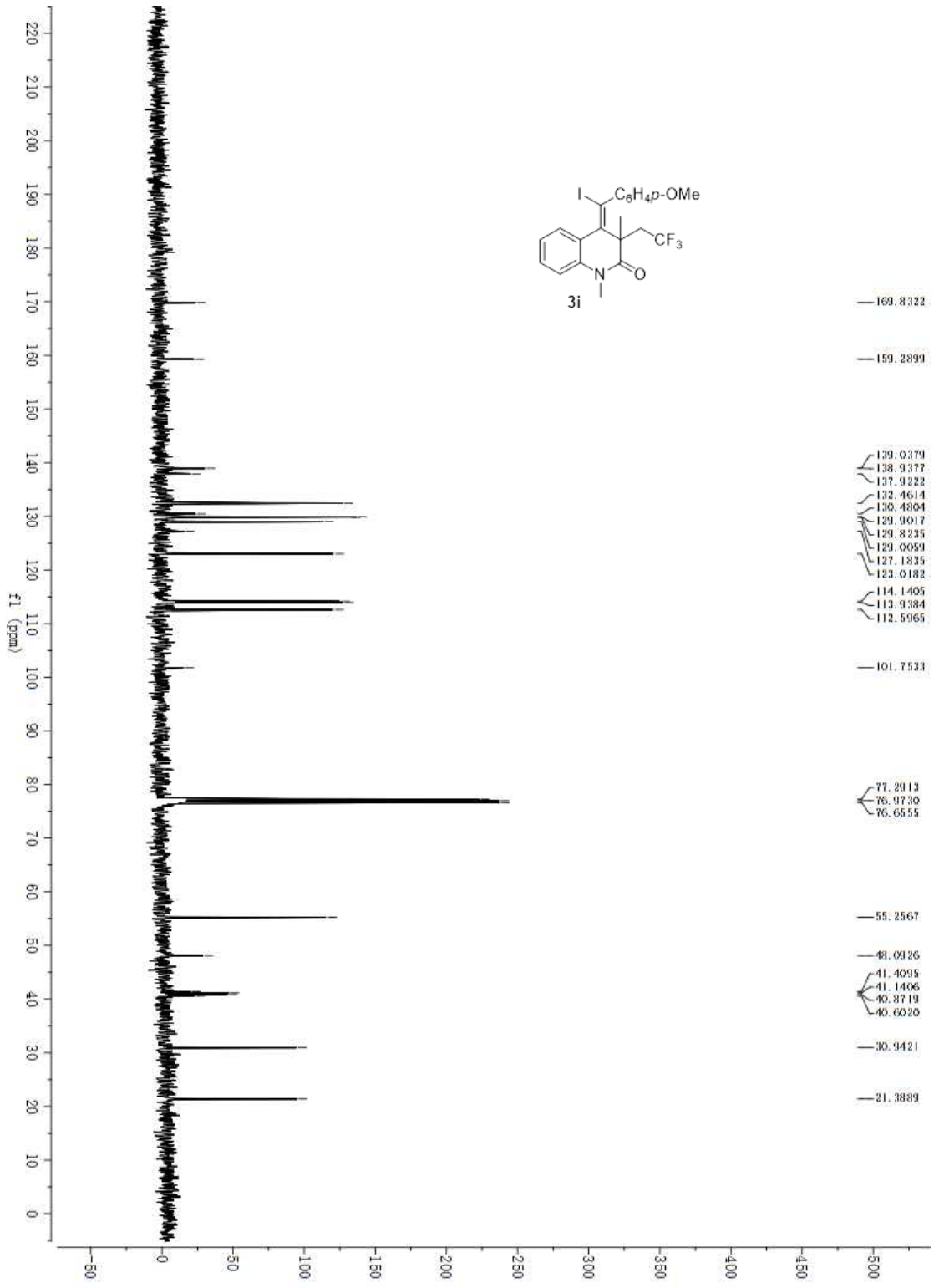

I
C6H4p-Me
CF3
N
O
3g
-59.7097
-59.7374
-59.7651
f1 (ppm)

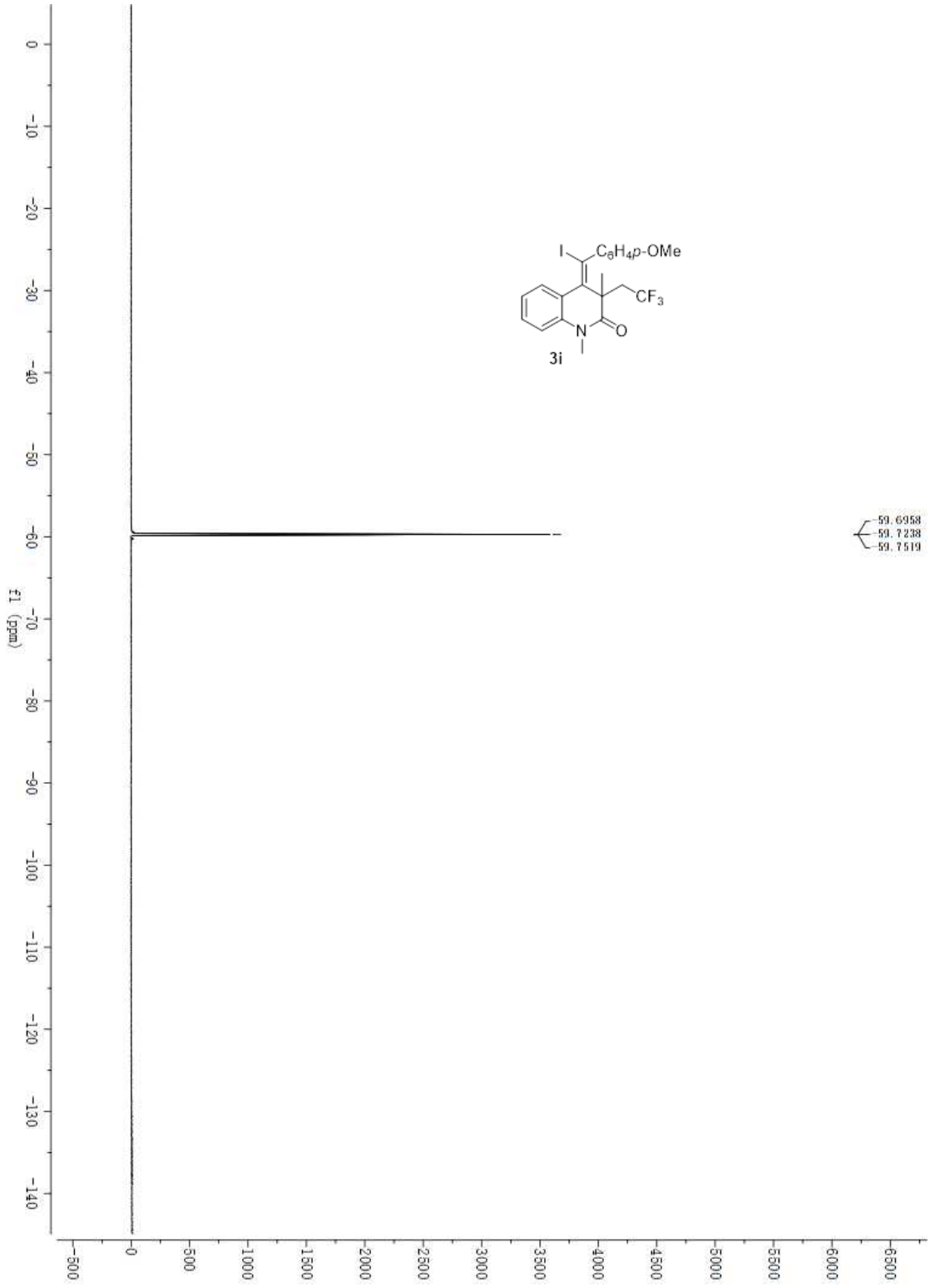

I
C6H4p-Me
Cl
CF3
N
O
3h
f1 (ppm)
0.91
0.99
1.03
3.14
1.08
3.06
3.05
1.11
1.09
3.00
7.8493
7.8453
7.3831
7.3774
7.3614
7.3557
7.2599
7.2341
7.2139
7.1453
7.1250
7.1041
6.9754
6.9537
3.3800
2.3630
2.2211
2.2113
2.1937
2.1838
2.1566
2.1291
2.0519
2.0261
2.0145
2.0003
1.9887
1.9746
1.9628
1.9369
1.0772
0.0004

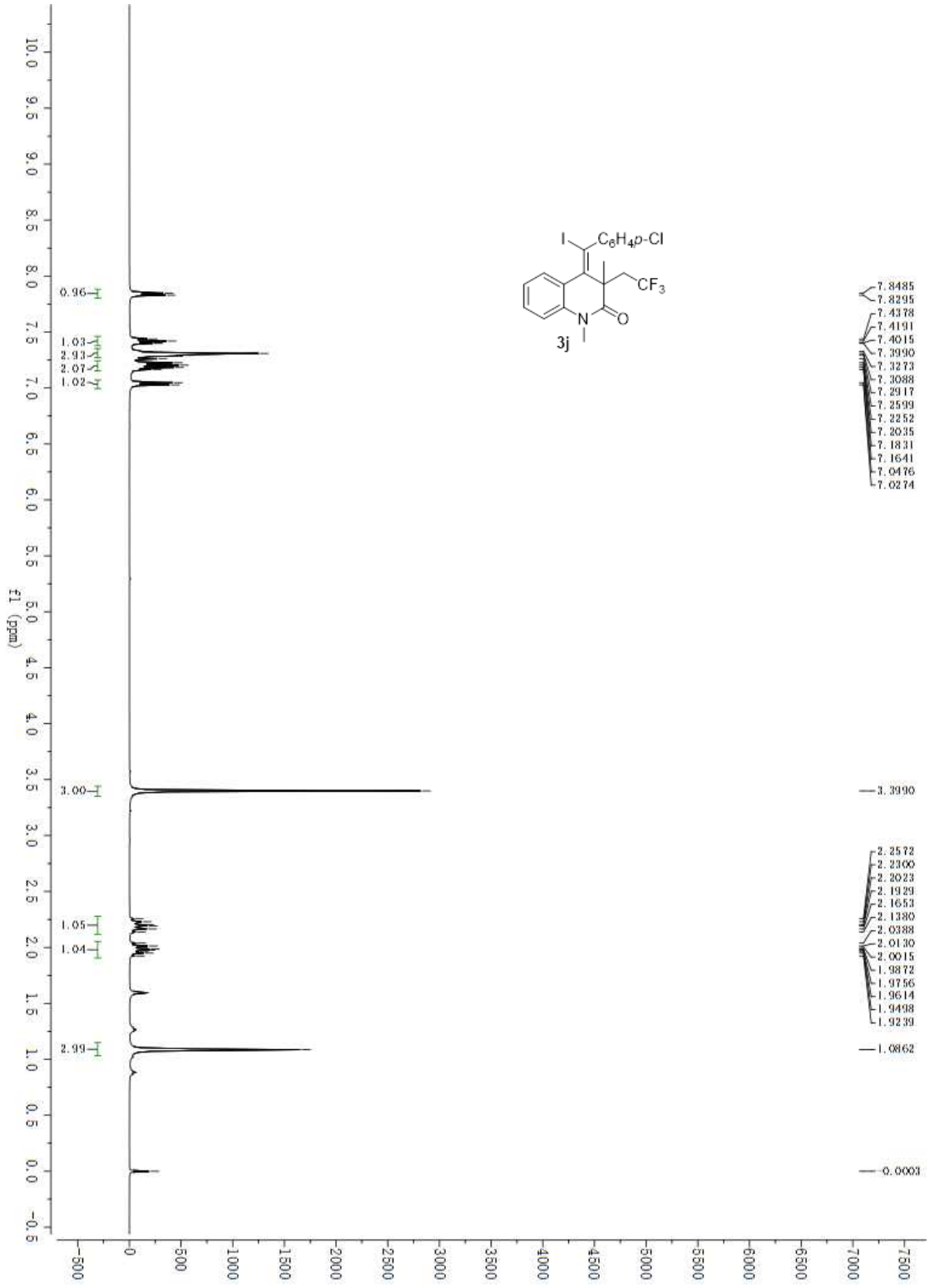

I
C6H4p-Me
Cl
CF3
N
O
3h
169.6058
143.3498
138.3941
137.7335
136.5714
132.1342
131.6285
129.5943
128.8841
128.3734
127.9792
127.3633
103.2147
77.2845
76.9676
76.6490
48.0220
41.4187
41.1457
40.8721
40.6015
31.0276
21.3842
21.2877
f1 (ppm)

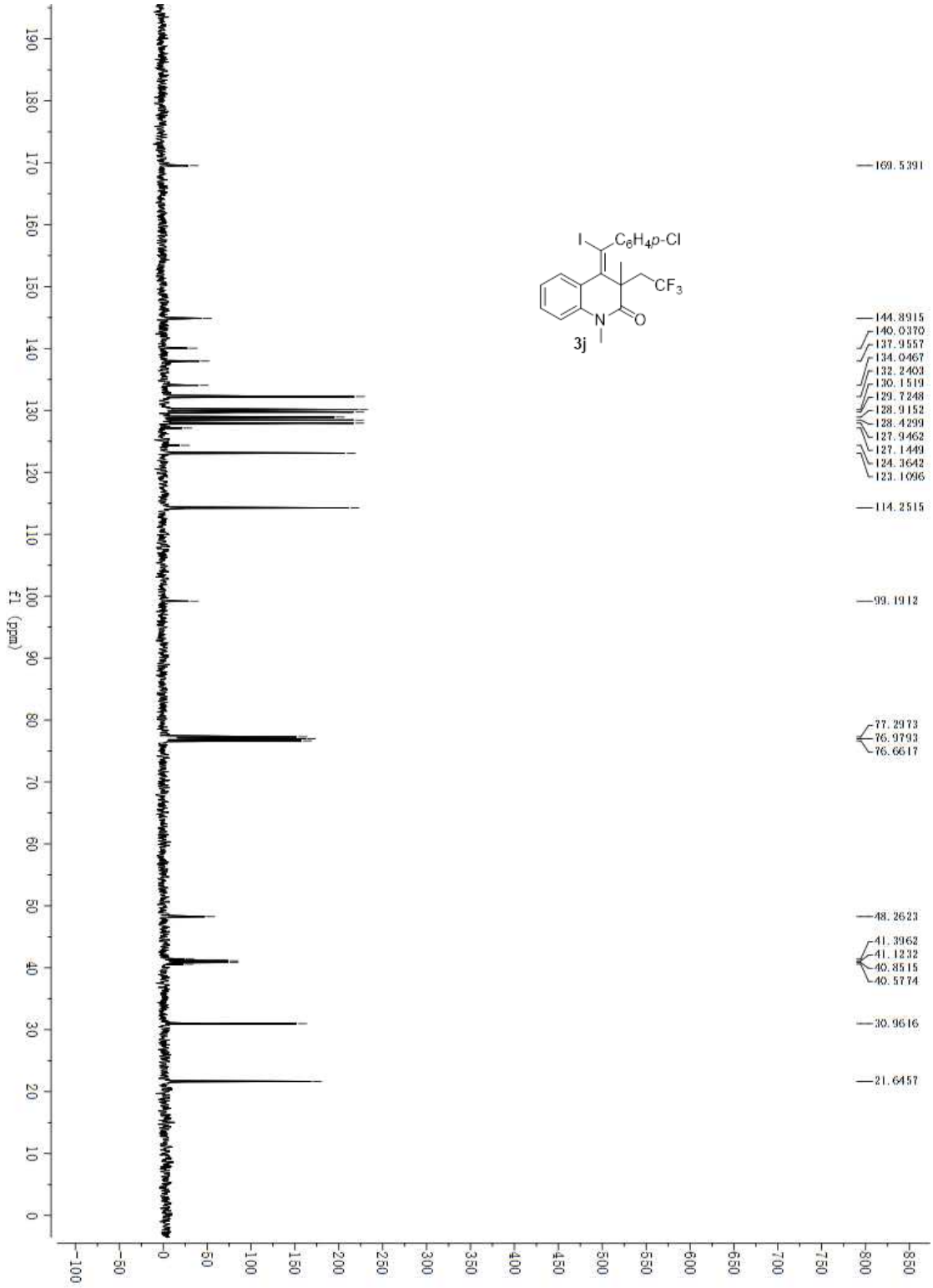

I
C6H4p-Me
Cl
CF3
N
O
3h
-59.7138
-59.7414
-59.7690
f1 (ppm)
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000

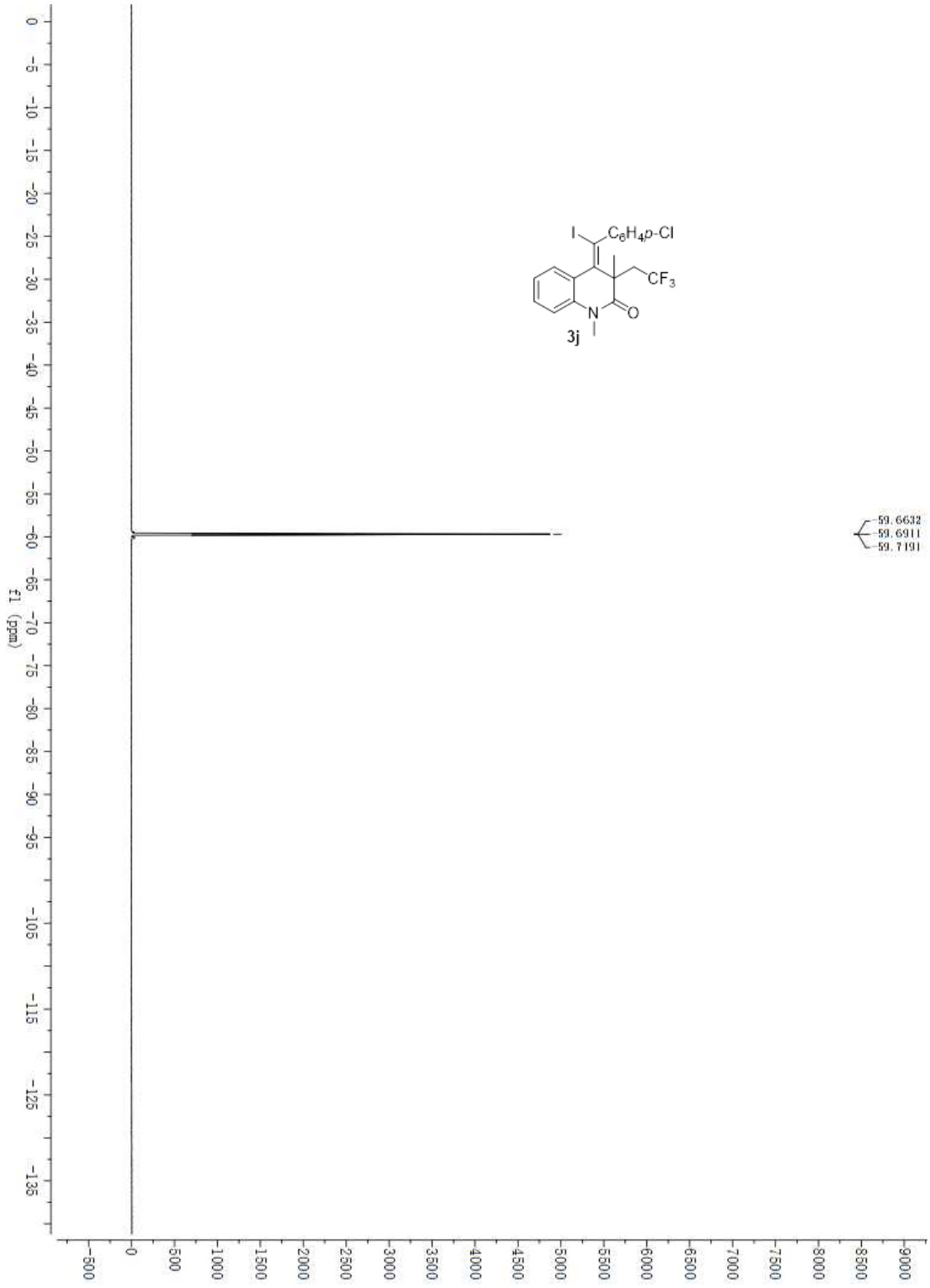

I
C6H4p-OMe
CF3
N
O
3i
f1 (ppm)
0.97
0.99
0.98
2.07
1.03
1.01
1.02
2.98
3.00
1.07
1.07
3.04
7.8659
7.8468
7.4236
7.4064
7.3876
7.3077
7.3022
7.2863
7.2808
7.2608
7.2236
7.2185
7.2025
7.1970
7.1916
7.1721
7.1533
7.0378
7.0176
6.8859
6.8794
6.8645
6.8580
6.8280
6.8215
6.8070
6.8004
3.8300
3.3992
2.2473
2.2198
2.2105
2.1921
2.1826
2.1550
2.1274
2.0363
2.0105
1.9990
1.9845
1.9730
1.9585
1.9470
1.9211
1.0951
0.0000

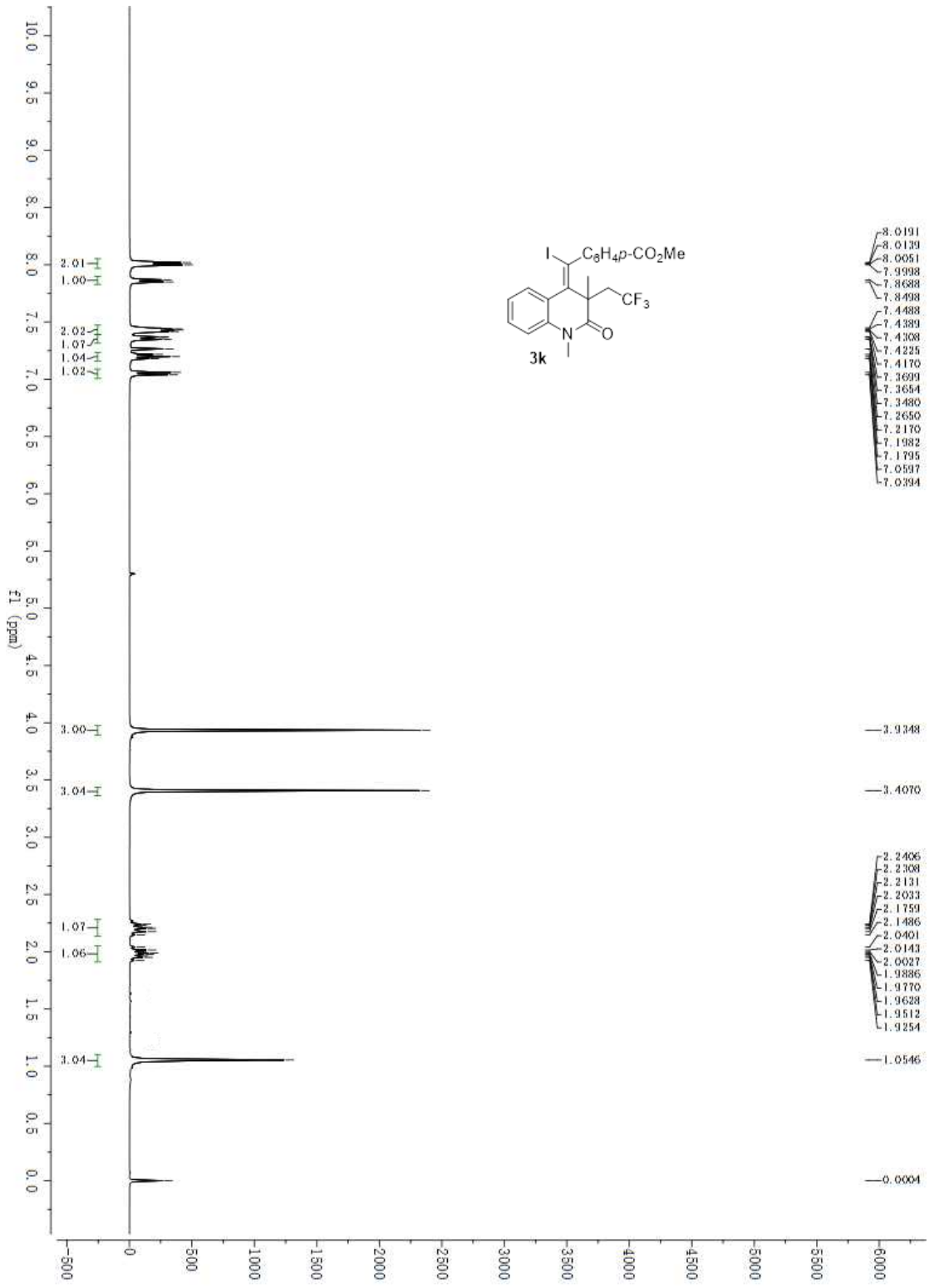

I
C6H4p-OMe
CF3
N
O
3i
169.8322
159.2899
139.0379
138.9377
137.9222
132.4614
130.4804
129.9017
129.8235
129.0059
127.1835
123.0182
114.1405
113.9384
112.5965
101.7533
77.2913
76.9730
76.6555
55.2567
48.0926
41.4095
41.1406
40.8719
40.6020
30.9421
21.3889
f1 (ppm)

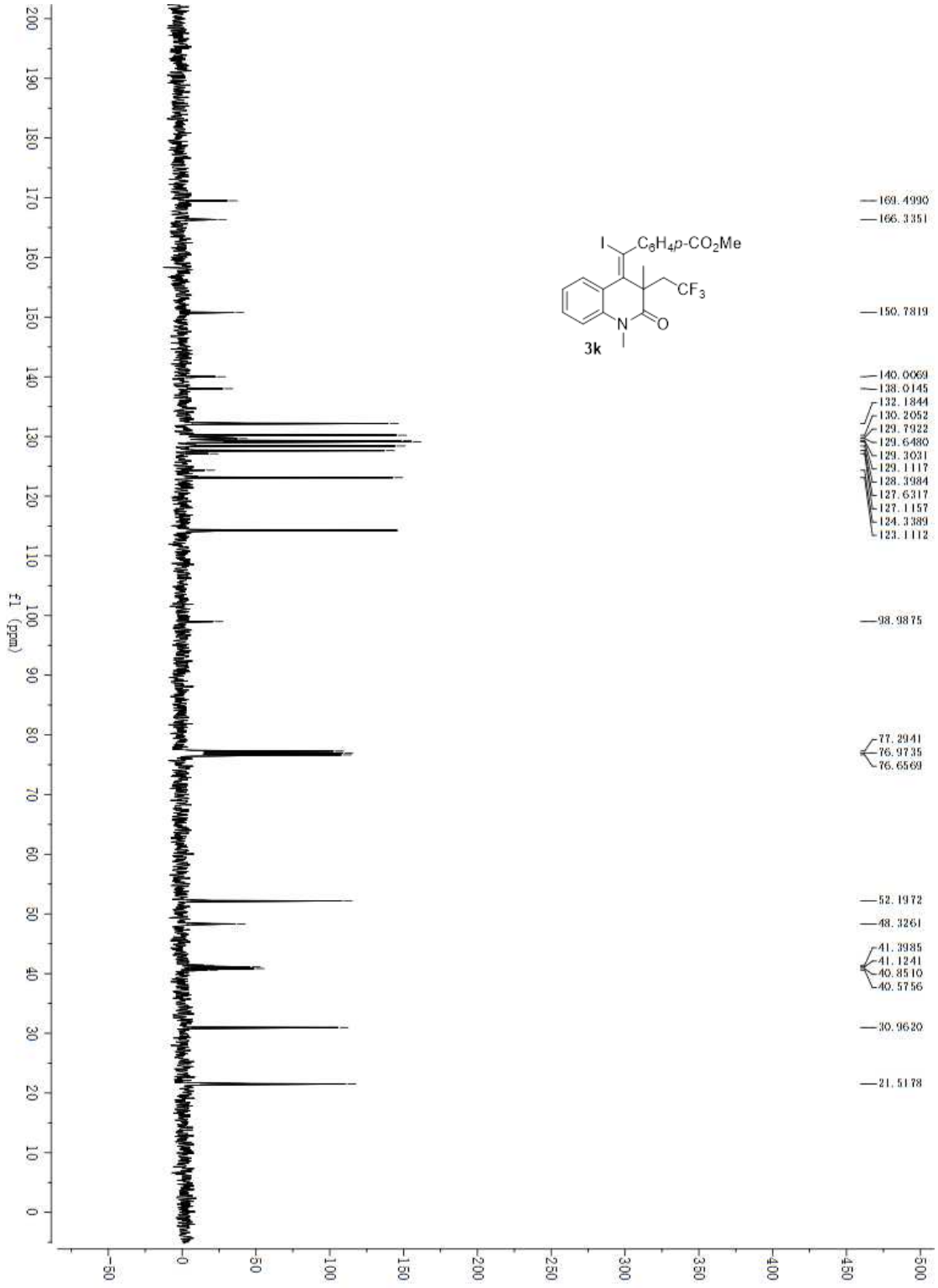

I
C6H4p-OMe
CF3
N
O
3i
59.6958
59.7238
59.7519
f1 (ppm)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000
6500


I
C6H4p-Cl
CF3
O
N
3j
f1 (ppm)
0.96
1.03
2.93
2.07
1.02
3.00
1.05
1.04
2.99
7.8485
7.8295
7.4378
7.4191
7.4015
7.3990
7.3273
7.3088
7.2917
7.2599
7.2252
7.2035
7.1831
7.1641
7.0476
7.0274
3.3990
2.2572
2.2360
2.2023
2.1929
2.1653
2.1380
2.0388
2.0130
2.0015
1.9872
1.9756
1.9614
1.9498
1.9239
1.0862
0.0003


I
C6H4p-Cl
CF3
N
O
3j
f1 (ppm)
169.5391
144.8915
140.0370
137.9557
134.0467
132.2403
130.1519
129.7248
128.9152
128.4299
127.9462
127.1449
124.3642
123.1096
114.2515
99.1912
77.2973
76.9793
76.6617
48.2623
41.3962
41.1232
40.8515
40.5774
30.9616
21.6457


I
C6H4p-Cl
CF3
N
O
3j
-59.6632
-59.6911
-59.7191
f1 (ppm)
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-105
-115
-125
-135
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000
6500
7000
7500
8000
8500
9000


I
C6H4p-CO2Me
CF3
N
O
3k
8.0191
8.0139
8.0051
7.9998
7.8688
7.8498
7.4488
7.4389
7.4308
7.4225
7.4170
7.3699
7.3654
7.3480
7.2650
7.2170
7.1982
7.1795
7.0597
7.0394
3.9348
3.4070
2.2406
2.2308
2.2131
2.2033
2.1759
2.1486
2.0401
2.0143
2.0027
1.9886
1.9770
1.9628
1.9512
1.9254
1.0546
0.0004
2.01
1.00
2.02
1.07
1.04
1.02
3.00
3.04
1.07
1.06
3.04
f1 (ppm)


I
C6H4p-CO2Me
CF3
N
O
3k
169.4990
166.3351
150.7819
140.0069
138.0145
132.1844
130.2052
129.7922
129.6480
129.3031
129.1117
128.3984
127.6317
127.1157
124.3389
123.1112
98.9875
77.2941
76.9735
76.6569
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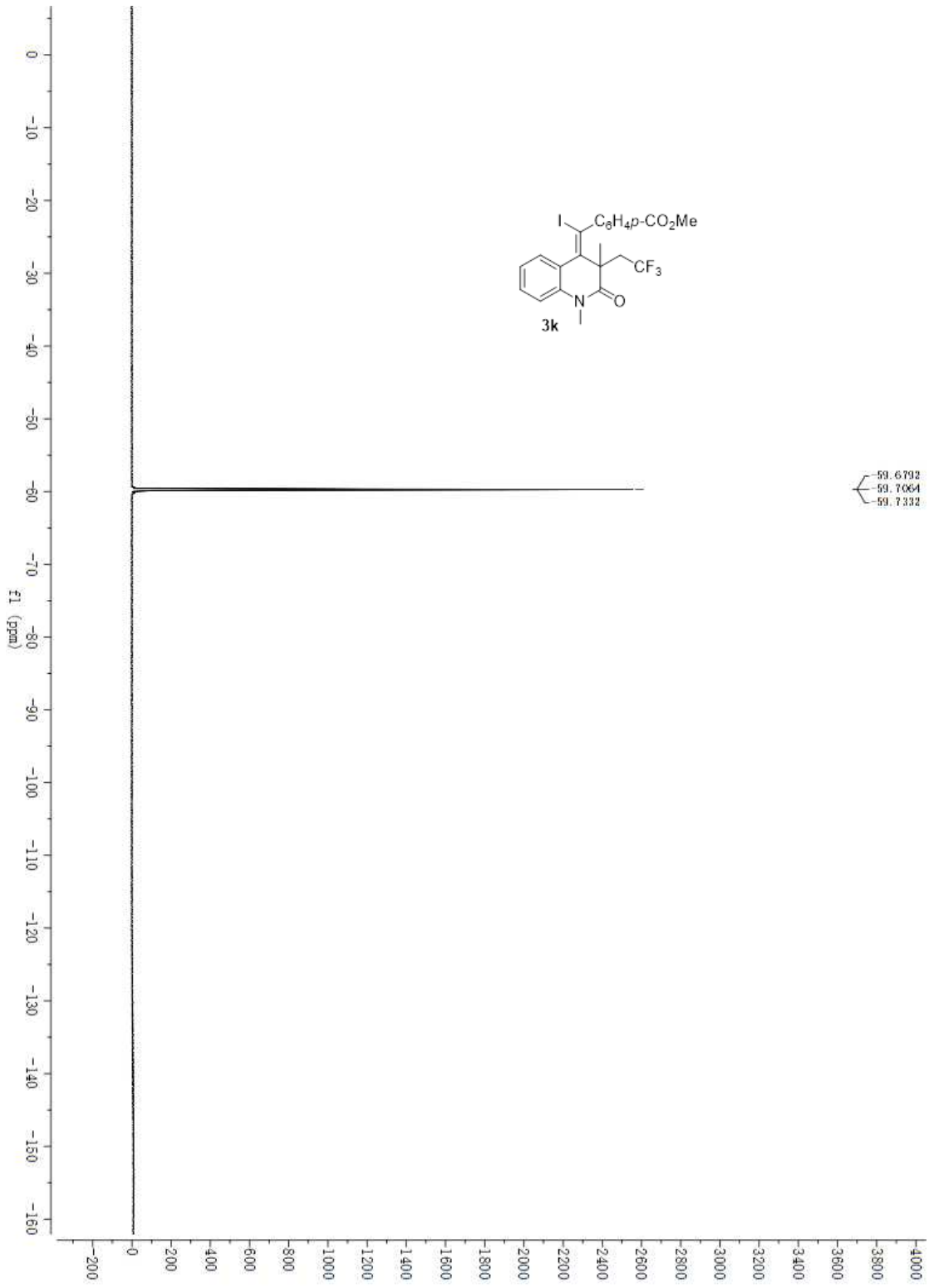
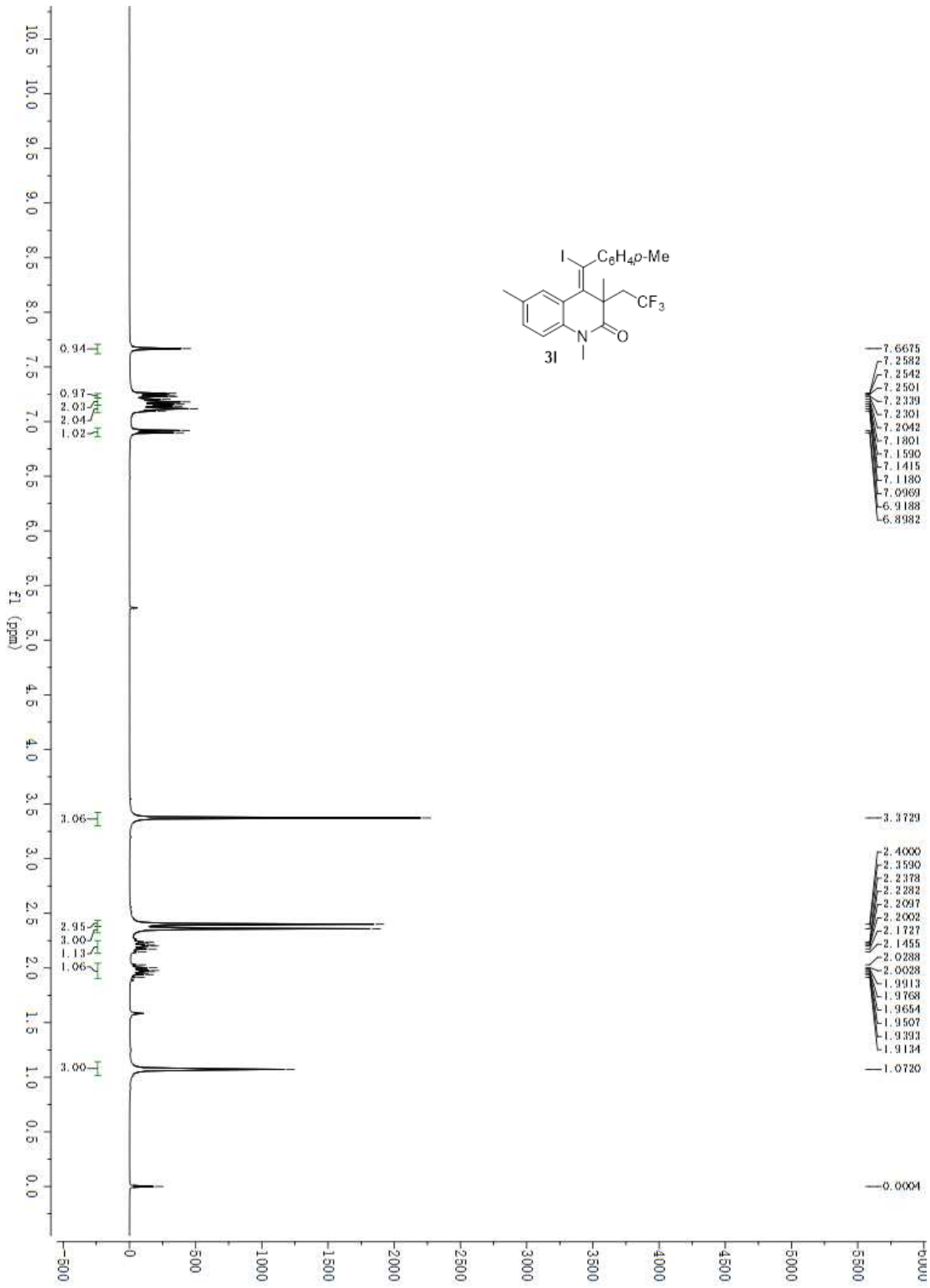
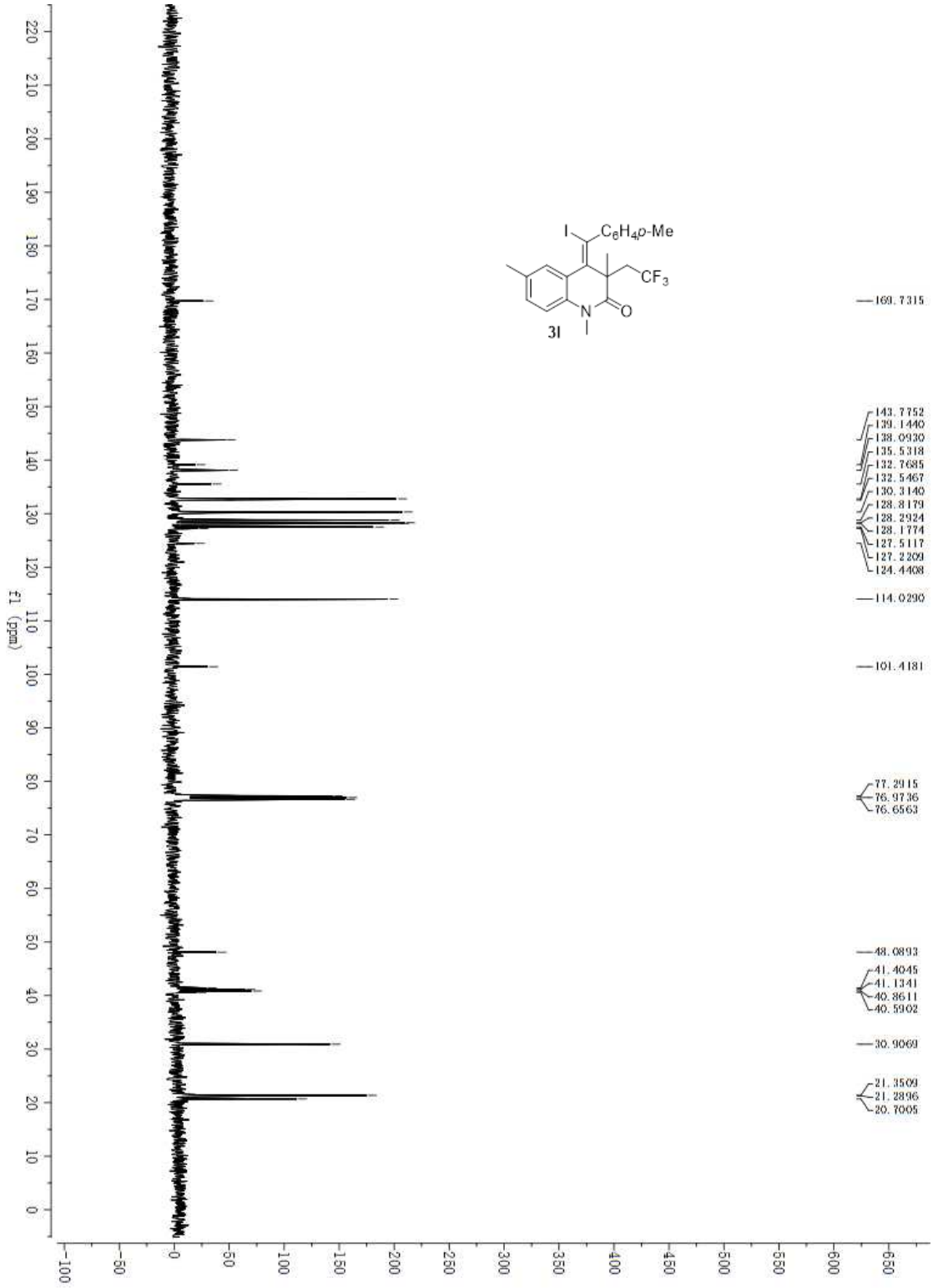
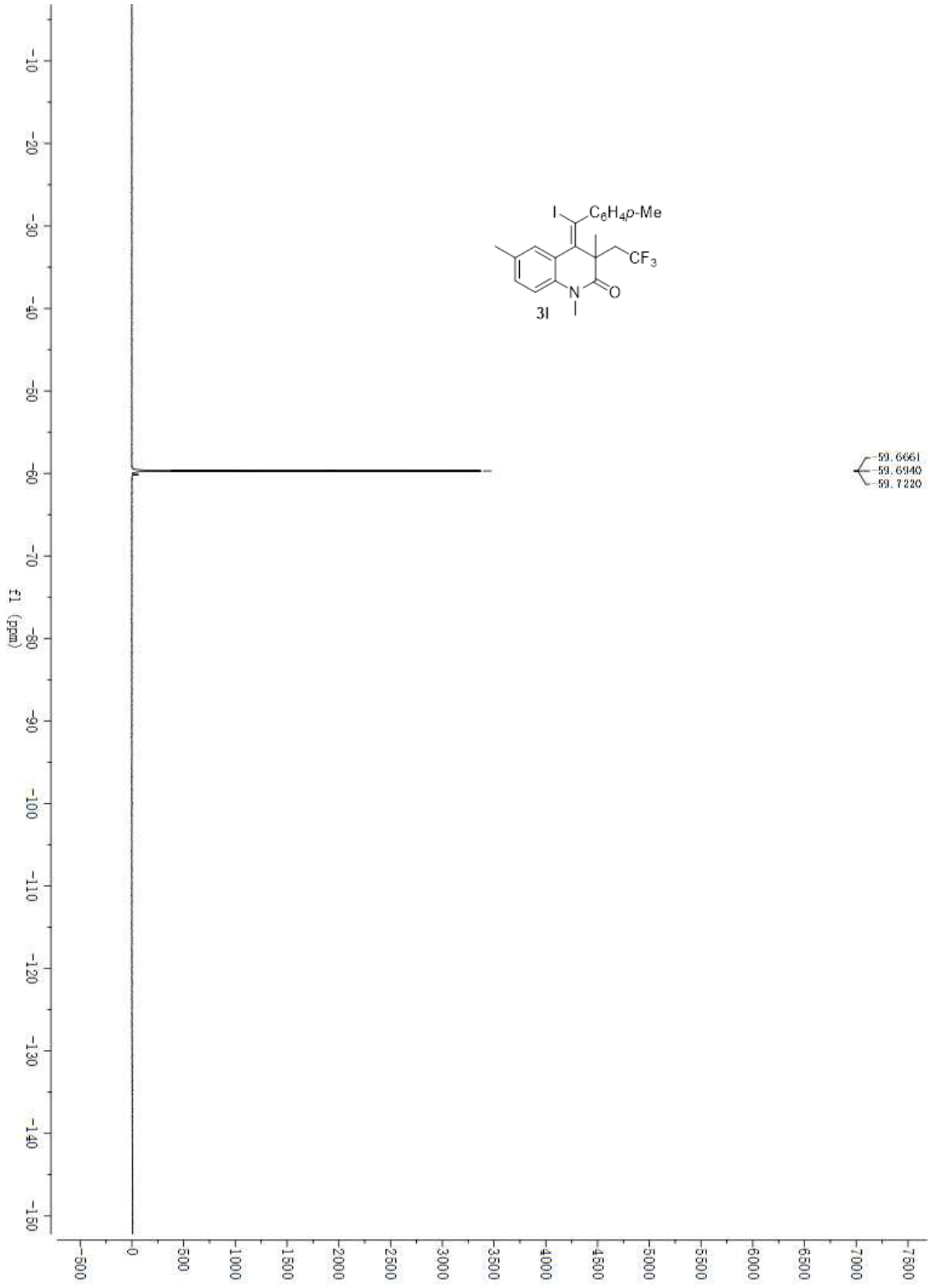
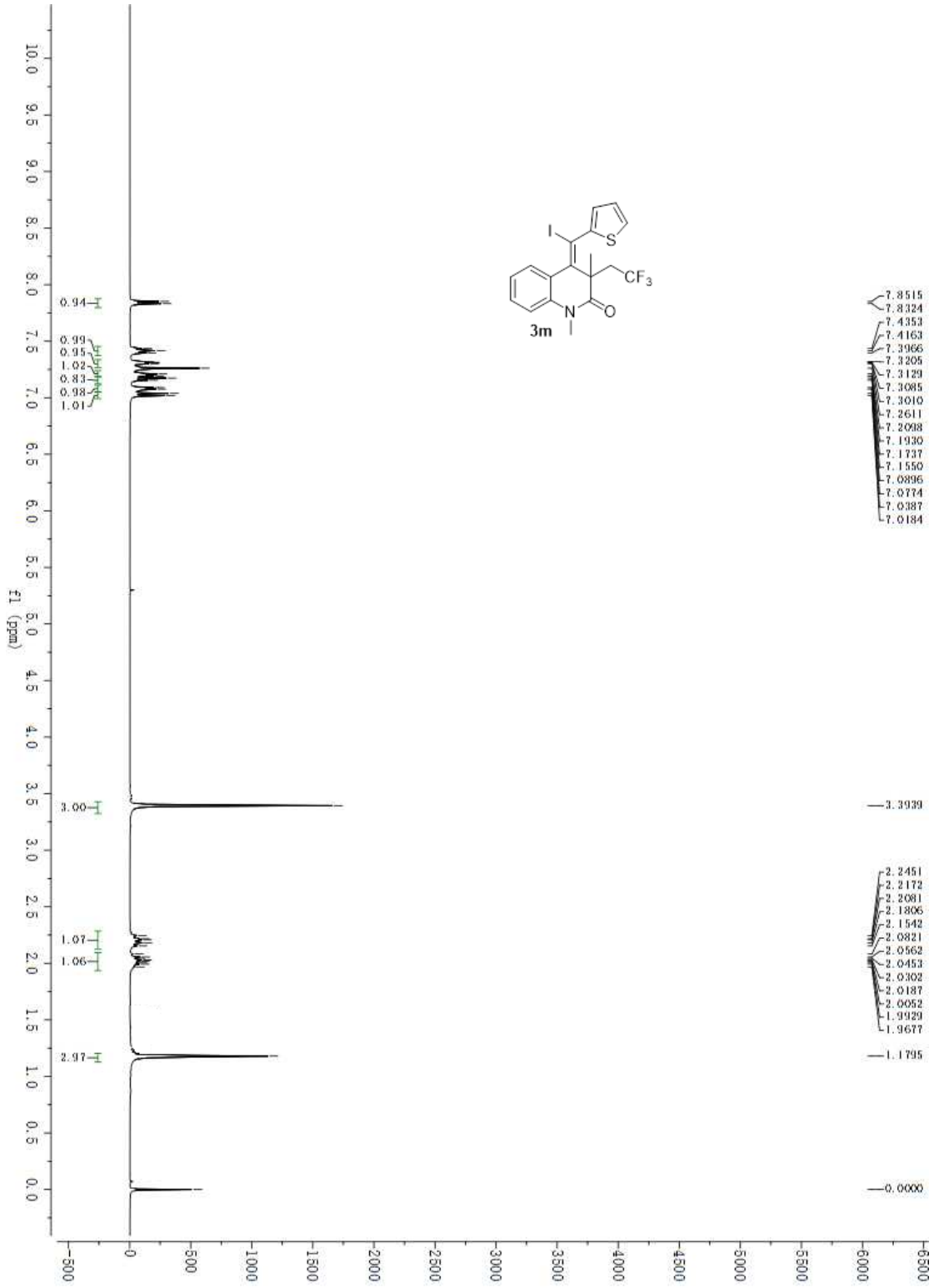
48.3261
41.3985
41.1241
40.8510
40.5756
30.9620
21.5178
f1 (ppm)

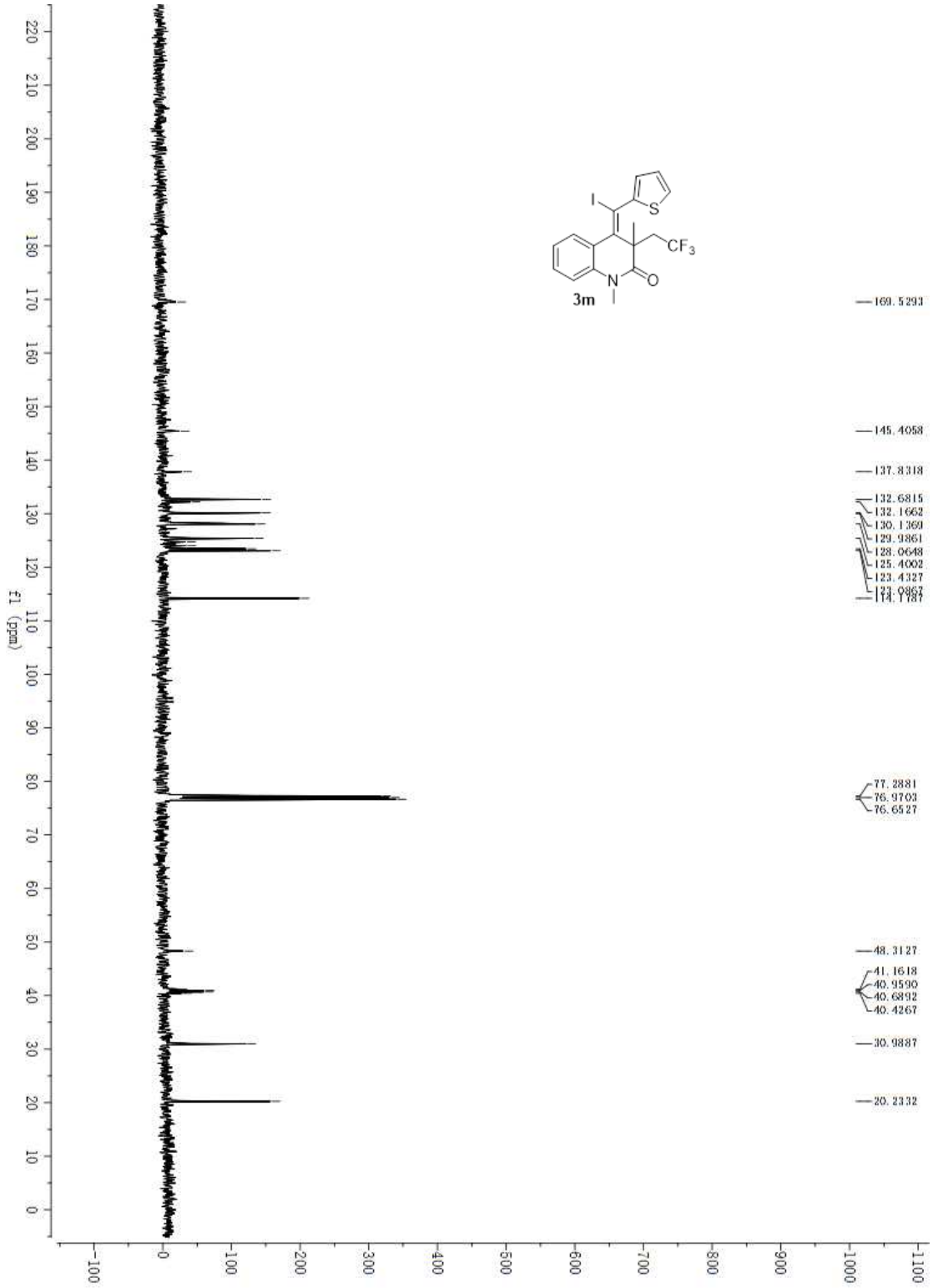

I
C6H4p-CO2Me
CF3
N
O
3k
-59.6792
-59.7064
-59.7332
f1 (ppm)

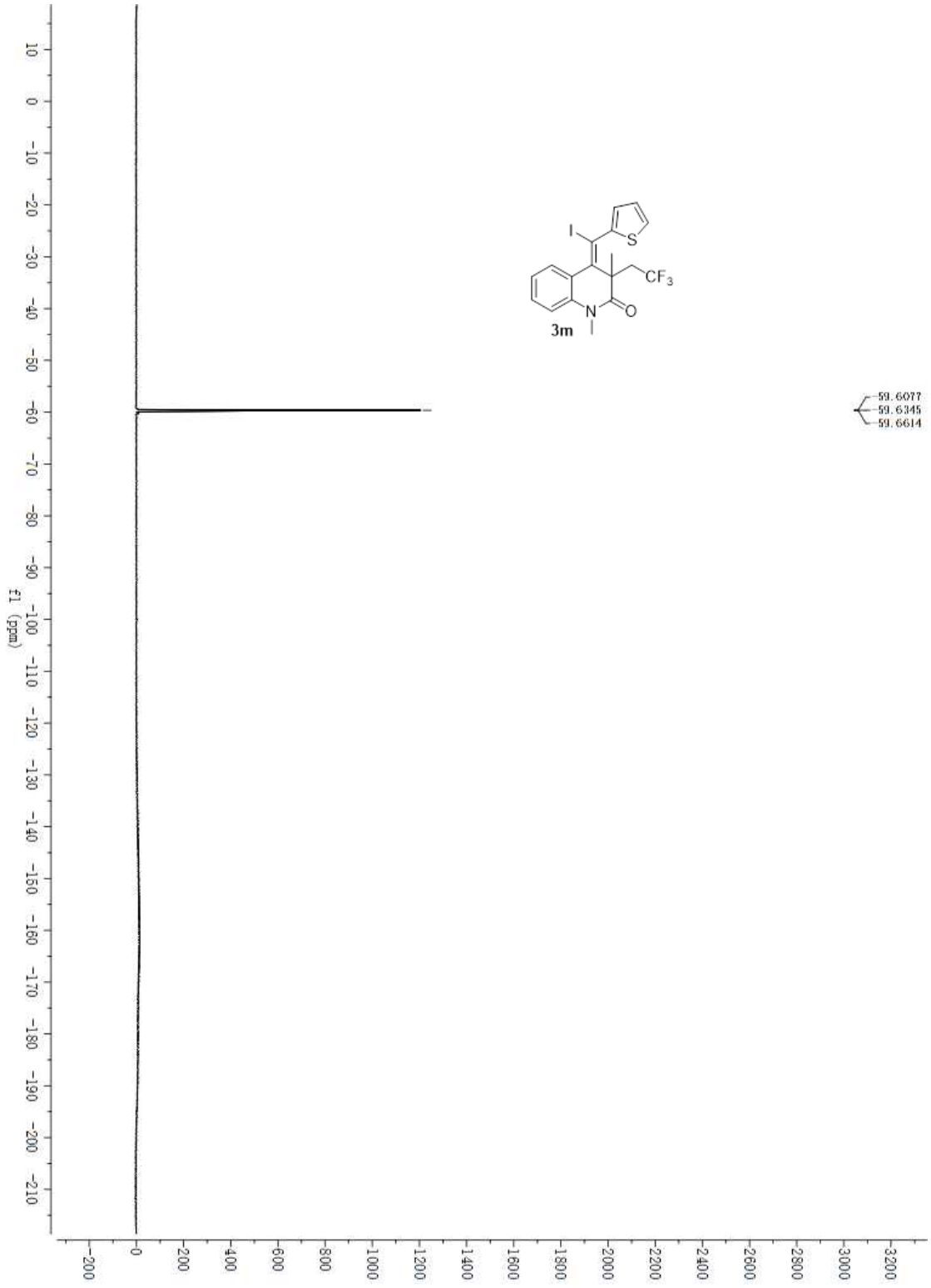

I
C6H4p-Me
CF3
N
O
3l
f1 (ppm)
0.94
0.97
2.03
2.04
1.02
3.06
2.95
3.00
1.13
1.06
3.00
7.6675
7.2582
7.2542
7.2501
7.2339
7.2301
7.2042
7.1801
7.1590
7.1415
7.1180
7.0969
6.9188
6.8982
3.3729
2.4000
2.3590
2.2378
2.2282
2.2097
2.2002
2.1727
2.1455
2.0288
2.0028
1.9913
1.9768
1.9654
1.9507
1.9393
1.9134
1.0720
0.0000


I
C6H4p-Me
CF3
N
O
3l
f1 (ppm)
169.7315
143.7752
139.1440
138.0930
135.5318
132.7685
132.5467
130.3140
128.8179
128.2924
128.1774
127.5117
127.2309
124.4408
114.0290
101.4181
77.2915
76.9736
76.6563
48.0893
41.4045
41.1341
40.8611
40.5902
30.9069
21.3509
21.2896
20.7005


I
C6H4p-Me
CF3
N
O
3l
-59.6661
-59.6940
-59.7220
f1 (ppm)
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-500
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
5500
6000
6500
7000
7500


I
S
CF3
N
O
3m
f1 (ppm)
0.94
0.99
0.95
1.02
0.83
0.98
1.01
3.00
1.07
1.06
2.97
7.8515
7.8324
7.4353
7.4163
7.3966
7.3205
7.3129
7.3085
7.3010
7.2611
7.2098
7.1930
7.1737
7.1550
7.0896
7.0774
7.0387
7.0184
3.3939
2.2451
2.2172
2.2081
2.1806
2.1542
2.0821
2.0562
2.0453
2.0302
2.0187
2.0052
1.9929
1.9677
1.1795
0.0000


3m
169.5293
145.4058
137.8318
132.6815
132.1662
130.1369
129.9861
128.0648
125.4002
123.4327
123.0867
114.7187
77.2881
76.9703
76.6527
48.3127
41.1618
40.9590
40.6892
40.4267
30.9887
20.2332
f1 (ppm)


I
S
CF3
N
O
3m
-59.6077
-59.6345
-59.6614
f1 (ppm)