

Supporting Information

SO₂ClF-promoted chlorination-oxidation of 2-methylindoles: one-step synthetic method to access 2,3-difunctionalized indoles

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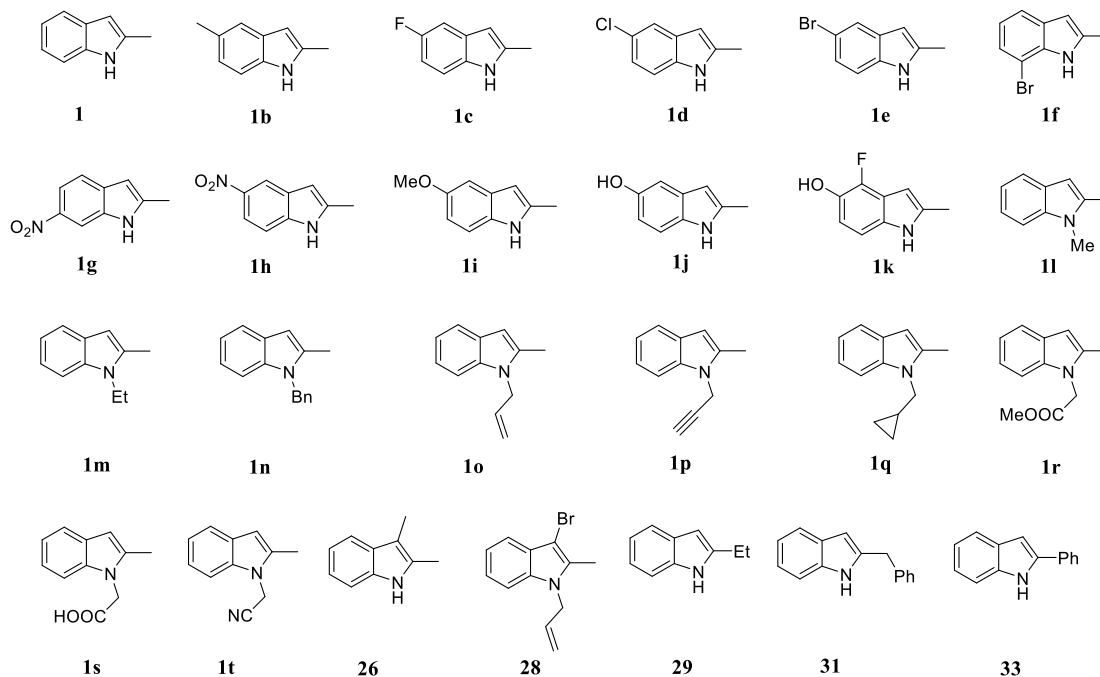
I. General Information

Unless otherwise stated, all glassware was oven-dried. All solvents were distilled from appropriate drying agents prior to use. All reagents were used as received from commercial suppliers unless otherwise indicated. Reactions were monitored using UV light as the visualizing agent. Flash column chromatography was performed using silica gel 60 (200-300 mesh). HRMS data were recorded on ThermoFisher LTQ Orbitrap XL or Agilent 6500QTOFMS-ESI. All ^1H NMR, ^{13}C NMR, and ^{19}F NMR spectra were recorded on Bruker DRX600 instruments. Chemical shifts were given in parts per million (ppm, δ), referenced to the solvent peak of CDCl_3 , defined at $\delta = 7.26$ (^1H NMR), defined at $\delta = 77.16$ (^{13}C NMR); or DMSO-d_6 , defined at 2.50 (^1H NMR), defined at $\delta = 39.52$ (^{13}C NMR). Coupling constants were quoted in Hz (J). ^1H NMR spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), and quartet (q). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br). In addition, SO_2ClF is a low-boiling, volatile chemical that needs to be used in fume hoods.

SO_2ClF was prepared according to the literature procedure.^{S1}

II. Preparation of the Starting Materials

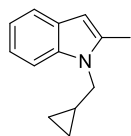
1-1e, **1g**, **1i-1m**, **26**, **29**, and **33** are received from commercial suppliers. **1f**,^{S2} **1h**,^{S3} **1n**,^{S4} **1o**,^{S5} **1p**,^{S6} **1r**,^{S7} **1s**,^{S8} **1t**,^{S9} **28**,^{S5} and **31**^{S10} are known compounds and were synthesized according to the literature. **1q** is an unknown compound and was synthesized similarly to the reported procedure.^{S11}



Synthesis and Characterization of **1q**

According to the literature,^{S11} a 50 mL round-bottom flask was charged with 2-methyl-1H-indole (5 mmol), KOH (10 mmol), 20 mL of DMSO, and (bromomethyl)cyclopropane (10 mmol). The reaction mixture was stirred at room temperature and monitored by TLC. Upon completion, the reaction mixture was quenched with water (20 mL). The mixture was extracted with ethyl acetate (3×30 mL). The combined organic phases were dried over anhydrous Na₂SO₄. The product **1q** was purified by silica gel chromatography with petroleum ether/EtOAc.

1-(Cyclopropylmethyl)-2-methyl-1H-indole (**1q**)

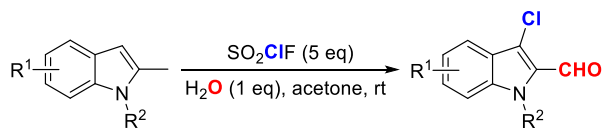


¹H NMR (600 MHz, CDCl₃) δ 7.56 – 7.51 (m, 1H), 7.32 (dd, *J* = 8.2, 0.7 Hz, 1H), 7.15 (td, *J* = 7.0, 1.0 Hz, 1H), 7.08 (ddd, *J* = 8.6, 2.5, 1.3 Hz, 1H), 4.01 (dd, *J* = 6.3, 1.1 Hz, 2H), 2.46 (d, *J* = 1.8 Hz, 3H), 1.21 (ddd, *J* = 8.1, 5.7, 3.4 Hz, 1H), 0.56 (d, *J* = 7.6 Hz, 2H), 0.36 (d, *J* = 4.2 Hz, 2H).

¹³C NMR (150 MHz, CDCl₃) δ 137.1, 136.4, 128.2, 120.5, 119.8, 119.3, 109.3, 100.1, 47.2, 13.2, 11.7, 4.0.

HRMS-ESI *m/z*: [M+H]⁺ Calcd for C₁₃H₁₅N 186.1277; Found 186.1286.

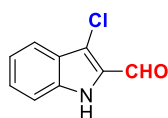
III. General Procedure for Chlorination-Oxidation



To the solution of 2-methylindole (0.2 mmol, 1.0 eq) in acetone (5 mL, 0.04 M) and H₂O (3.6 μL, 1 eq) was added SO₂ClF (1 mmol, 5 eq, 1 M in anhydrous PhCF₃) dropwise, and then stirred at room temperature. After the completion of the reaction, as indicated by TLC, the reaction was quenched with water. The resulting mixture was extracted with ethyl acetate and the combined organic layers were dried over Na₂SO₄ and evaporated under reduced pressure. The residue was purified by column chromatography (petroleum ether/ethyl acetate = 20:1 to 4:1) on silica gel to afford the corresponding products.

IV. Products Characterization

3-Chloro-1*H*-indole-2-carbaldehyde (2)



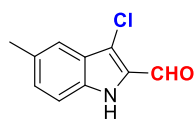
Yellow solid; 3 h; 34.8 mg, 97% yield; R_f = 0.5, petroleum ether/ethyl acetate = 10/1.

¹H NMR (600 MHz, CDCl₃) δ 10.06 (s, 1H), 9.65 (s, 1H), 7.75 (dd, *J* = 8.2, 0.6 Hz, 1H), 7.47 – 7.42 (m, 2H), 7.24 (ddd, *J* = 8.0, 6.7, 3.4 Hz, 1H).

¹³C NMR (150 MHz, CDCl₃) δ 180.2, 136.5, 130.3, 128.5, 125.5, 121.8, 120.6, 117.9, 112.8.

All analytic data match the reported data.^{S12}

3-Chloro-5-methyl-1*H*-indole-2-carbaldehyde (3)



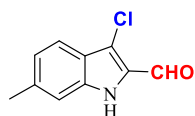
White solid; 6 h; 25.4 mg, 66% yield; R_f = 0.6, petroleum ether/ethyl acetate = 10/1.

¹H NMR (600 MHz, CDCl₃) δ 10.03 (s, 1H), 9.25 (s, 1H), 7.51 (s, 1H), 7.33 (d, *J* = 8.5 Hz, 1H), 7.28 – 7.25 (m, 1H), 2.47 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 180.2, 135.1, 131.6, 130.8, 130.5, 125.9, 119.7, 117.4, 112.6, 21.5.

All analytic data match the reported data.^{S13}

3-Chloro-6-methyl-1*H*-indole-2-carbaldehyde (4)



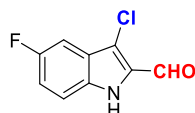
White solid; 14 h; 19 mg, 49% yield; $R_f = 0.6$, petroleum ether/ethyl acetate = 4/1.

$^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.01 (s, 1H), 9.12 (s, 1H), 7.62 (d, $J = 8.3$ Hz, 1H), 7.21 (s, 1H), 7.07 (dd, $J = 8.3, 0.6$ Hz, 1H), 2.49 (s, 3H).

$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 180.1, 139.5, 137.3, 130.1, 124.2, 123.7, 120.3, 118.3, 112.4, 22.3.

HRMS-ESI m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{10}\text{H}_9\text{ClNO}$ 194.0367; Found 194.0364.

3-Chloro-5-fluoro-1H-indole-2-carbaldehyde (5)



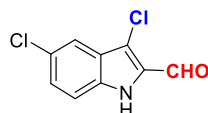
Yellow solid; 10 h; 33.6 mg, 85% yield; $R_f = 0.5$, petroleum ether/ethyl acetate = 4/1.

$^1\text{H NMR}$ (600 MHz, $\text{DMSO}-d_6$) δ 12.38 (s, 1H), 9.98 (s, 1H), 7.49 (dd, $J = 9.1, 4.4$ Hz, 1H), 7.41 (dd, $J = 8.9, 2.4$ Hz, 1H), 7.29 (td, $J = 9.2, 2.5$ Hz, 1H).

$^{13}\text{C NMR}$ (150 MHz, $\text{DMSO}-d_6$) δ 180.8, 158.9, 157.3, 133.6, 132.0, 124.8 (d, $J = 10.6$ Hz), 117.4, 117.2, 115.7 (d, $J = 9.6$ Hz), 114.4 (d, $J = 6.0$ Hz), 104.0, 103.9.

All analytic data match the reported data.^{S12}

3,5-Dichloro-1H-indole-2-carbaldehyde (6)



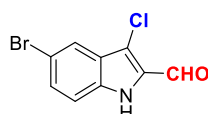
White solid; 6 h; 25.5 mg, 60% yield; $R_f = 0.6$, petroleum ether/ethyl acetate = 10/1.

$^1\text{H NMR}$ (600 MHz, $\text{DMSO}-d_6$) δ 12.46 (s, 1H), 9.99 (s, 1H), 7.70 (d, $J = 1.9$ Hz, 1H), 7.49 (d, $J = 8.8$ Hz, 1H), 7.41 (dd, $J = 8.9, 2.0$ Hz, 1H).

$^{13}\text{C NMR}$ (150 MHz, $\text{DMSO}-d_6$) δ 180.5, 134.8, 131.5, 127.8, 126.1, 125.3, 118.5, 115.4, 113.2.

All analytic data match the reported data.^{S12}

5-Bromo-3-chloro-1H-indole-2-carbaldehyde (7)



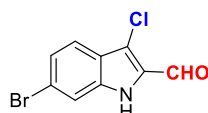
White solid; 8 h; 40 mg, 77% yield; $R_f = 0.7$, petroleum ether/ethyl acetate = 10/1.

$^1\text{H NMR}$ (600 MHz, $\text{DMSO}-d_6$) δ 12.47 (s, 1H), 9.99 (s, 1H), 7.84 (s, 1H), 7.52 (dd, $J = 8.8, 1.6$ Hz, 1H), 7.44 (d, $J = 8.8$ Hz, 1H).

$^{13}\text{C NMR}$ (150 MHz, $\text{DMSO}-d_6$) δ 180.5, 135.0, 131.3, 130.3, 125.9, 121.6, 115.7, 113.9, 113.1.

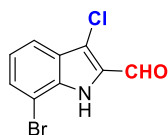
All analytic data match the reported data.^{S12}

6-Bromo-3-chloro-1H-indole-2-carbaldehyde (8)



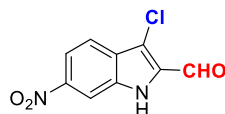
Yellow solid; 7 h; 44.5 mg, 86% yield; $R_f = 0.6$, petroleum ether/ethyl acetate = 4/1.
 $^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 12.39 (s, 1H), 9.99 (s, 1H), 7.63 (d, $J = 9.0$ Hz, 2H), 7.33 (dd, $J = 8.6, 1.7$ Hz, 1H).
 $^{13}\text{C NMR}$ (150 MHz, $\text{DMSO-}d_6$) δ 180.4, 137.0, 131.0, 124.7, 123.4, 121.5, 120.5, 115.9, 114.4.
HRMS-ESI m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_9\text{H}_6\text{BrClNO}$ 257.9316; Found 257.9319.

7-Bromo-3-chloro-1*H*-indole-2-carbaldehyde (9)



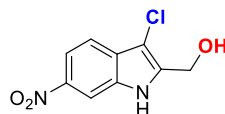
Yellow solid; 6 h; 22.3 mg, 43% yield. $R_f = 0.6$, petroleum ether/ethyl acetate = 10/1.
 $^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.05 (s, 1H), 9.04 (s, 1H), 7.67 (d, $J = 8.1$ Hz, 1H), 7.57 (d, $J = 7.5$ Hz, 1H), 7.10 (t, $J = 7.8$ Hz, 1H).
 $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 179.9, 135.0, 130.8, 130.6, 126.6, 122.9, 119.9, 118.0, 106.1.
All analytic data match the reported data.^{S12}

3-Chloro-6-nitro-1*H*-indole-2-carbaldehyde (10)



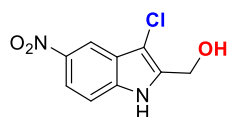
White solid; 31 h; 11.1 mg, 25% yield; $R_f = 0.7$, petroleum ether/ethyl acetate = 4/1.
 $^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 12.94 (s, 1H), 10.07 (s, 1H), 8.30 (s, 1H), 8.00 (d, $J = 8.9$ Hz, 1H), 7.89 (d, $J = 8.9$ Hz, 1H).
 $^{13}\text{C NMR}$ (150 MHz, $\text{DMSO-}d_6$) δ 181.1, 146.1, 134.5, 134.3, 128.2, 120.8, 115.7, 113.4, 110.1.
HRMS-ESI m/z : $[\text{M}-\text{H}]^-$ Calcd for $\text{C}_9\text{H}_4\text{ClN}_2\text{O}_3$ 222.9910; Found 222.9919.

(3-Chloro-6-nitro-1*H*-indol-2-yl)methanol (11)



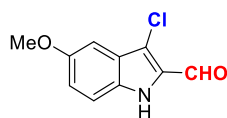
Yellow solid, 31 h, 24.2 mg, 53% yield; $R_f = 0.6$, petroleum ether/ethyl acetate = 4/1.
 $^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 12.52 (s, 1H), 8.34 (d, $J = 1.9$ Hz, 1H), 7.98 (dd, $J = 8.8, 2.1$ Hz, 1H), 7.66 (d, $J = 8.8$ Hz, 1H), 4.98 (s, 2H).
 $^{13}\text{C NMR}$ (150 MHz, $\text{DMSO-}d_6$) δ 143.5, 136.6, 133.0, 128.8, 118.2, 115.3, 109.0, 104.2, 35.4.
HRMS-ESI m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_9\text{H}_8\text{ClN}_2\text{O}_3$ 227.0218; Found 227.0226.

(3-Chloro-5-nitro-1*H*-indol-2-yl)methanol (12)



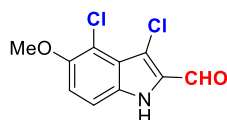
Yellow solid; 29 h; 30.6 mg, 68% yield; $R_f = 0.4$, petroleum ether/ethyl acetate = 4/1.
 $^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 12.51 (s, 1H), 8.36 (d, $J = 2.1$ Hz, 1H), 8.09 (dd, $J = 9.0, 2.3$ Hz, 1H), 7.61 (d, $J = 9.0$ Hz, 1H), 4.95 (s, 2H).
 $^{13}\text{C NMR}$ (150 MHz, $\text{DMSO-}d_6$) δ 141.5, 137.7, 134.1, 123.8, 118.5, 114.5, 113.0, 105.6, 35.4.
HRMS-ESI m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_9\text{H}_8\text{ClN}_2\text{O}_3$ 227.0218; Found 227.0217.

3-Chloro-5-methoxy-1H-indole-2-carbaldehyde (13)



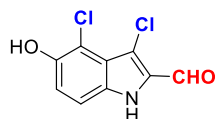
White solid; 7 min; 20.0 mg, 48% yield; $R_f = 0.6$, petroleum ether/ethyl acetate = 4/1.
 $^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 12.17 (s, 1H), 9.95 (s, 1H), 7.38 (d, $J = 9.0$ Hz, 1H), 7.07 (dd, $J = 9.0, 2.4$ Hz, 1H), 7.02 (d, $J = 2.3$ Hz, 1H), 3.82 (s, 3H).
 $^{13}\text{C NMR}$ (150 MHz, $\text{DMSO-}d_6$) δ 180.0, 154.9, 132.0, 130.6, 124.7, 120.0, 114.8, 113.5, 98.5, 55.4.
HRMS-ESI m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{10}\text{H}_9\text{ClNO}_2$ 210.0318; Found 210.0320.

3,4-Dichloro-5-methoxy-1H-indole-2-carbaldehyde (14)



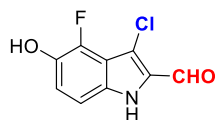
Yellow solid; 7 min; 19.8 mg, 41% yield; $R_f = 0.5$, petroleum ether/ethyl acetate = 4/1.
 $^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 12.39 (s, 1H), 9.98 (s, 1H), 7.40 (d, $J = 9.1$ Hz, 1H), 7.35 (d, $J = 9.1$ Hz, 1H), 3.87 (s, 3H).
 $^{13}\text{C NMR}$ (150 MHz, $\text{DMSO-}d_6$) δ 180.6, 150.0, 133.0, 132.0, 121.0, 116.1, 113.0, 112.6, 111.9, 57.4.
HRMS-ESI m/z : $[\text{M}-\text{H}]^-$ Calcd for $\text{C}_{10}\text{H}_6\text{Cl}_2\text{NO}_2$ 241.9976; Found 241.9773

3,4-Dichloro-5-hydroxy-1H-indole-2-carbaldehyde (15)



Yellow solid; 7 min; 33.2 mg, 72% yield; $R_f = 0.4$, petroleum ether/ethyl acetate = 4/1.
 $^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 12.30 (s, 1H), 9.95 (s, 1H), 9.87 (s, 1H), 7.28 (d, $J = 8.9$ Hz, 1H), 7.13 (d, $J = 8.9$ Hz, 1H).
 $^{13}\text{C NMR}$ (150 MHz, $\text{DMSO-}d_6$) δ 180.4, 148.3, 132.3, 131.4, 121.1, 119.6, 113.0, 112.5, 108.7.
HRMS-ESI m/z : $[\text{M}-\text{H}]^-$ Calcd for $\text{C}_9\text{H}_4\text{Cl}_2\text{NO}_2$ 227.9619; Found 227.9616.

3-Chloro-4-fluoro-5-hydroxy-1H-indole-2-carbaldehyde (16)



Yellow solid; 4 h; 18.5 mg, 43% yield; $R_f = 0.4$, petroleum ether/ethyl acetate = 4/1.

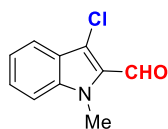
$^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 12.24 (s, 1H), 9.92 (s, 1H), 9.52 (s, 1H), 7.11 (s, 1H).

$^{13}\text{C NMR}$ (150 MHz, $\text{DMSO-}d_6$) δ 180.1, 143.5, 141.8, 137.7 (d, $J = 10.0$ Hz), 132.3 (d, $J = 6.2$ Hz), 130.9, 121.2, 115.0 (d, $J = 15.1$ Hz), 110.5, 109.5 (d, $J = 4.8$ Hz).

$^{19}\text{F NMR}$ (565 MHz, $\text{DMSO-}d_6$) δ -151.1.

HRMS-ESI m/z : $[\text{M-H}]^-$ Calcd for $\text{C}_9\text{H}_4\text{ClFNO}_2$ 211.9915; Found 211.9915.

3-Chloro-1-methyl-1H-indole-2-carbaldehyde (17)



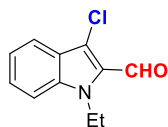
Yellow solid; 11 h; 33.9 mg, 88% yield; $R_f = 0.7$, petroleum ether/ethyl acetate = 10/1.

$^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.15 (s, 1H), 7.72 (d, $J = 8.2$ Hz, 1H), 7.45 (ddd, $J = 8.2, 6.9, 1.1$ Hz, 1H), 7.35 (d, $J = 8.6$ Hz, 1H), 7.25 – 7.19 (m, 1H), 4.04 (s, 3H).

$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 181.4, 138.8, 129.2, 128.2, 124.3, 121.6, 120.6, 119.3, 110.6, 31.9.

All analytic data match the reported data.^{S12}

3-Chloro-1-ethyl-1H-indole-2-carbaldehyde (18)



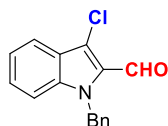
Yellow solid; 11 h; 41.1 mg, 99% yield; $R_f = 0.7$, petroleum ether/ethyl acetate = 10/1.

$^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.17 (s, 1H), 7.74 (d, $J = 8.2$ Hz, 1H), 7.45 (dd, $J = 11.5, 3.9$ Hz, 1H), 7.39 (d, $J = 8.5$ Hz, 1H), 7.22 (t, $J = 7.5$ Hz, 1H), 4.58 (q, $J = 7.2$ Hz, 2H), 1.36 (t, $J = 7.2$ Hz, 3H).

$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 180.9, 137.7, 128.4, 128.1, 124.4, 121.4, 120.6, 119.5, 110.5, 39.9, 15.5.

All analytic data match the reported data.^{S12}

1-Benzyl-3-chloro-1H-indole-2-carbaldehyde (19)



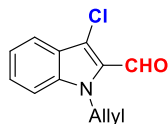
White solid; 12 h; 50.0 mg, 93% yield; $R_f = 0.8$, petroleum ether/ethyl acetate = 10/1.

$^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.21 (s, 1H), 7.78 (d, $J = 8.2$ Hz, 1H), 7.45 – 7.41 (m, 1H), 7.38 (d, $J = 8.5$ Hz, 1H), 7.26 (dt, $J = 16.3, 7.2$ Hz, 4H), 7.11 (d, $J = 7.2$ Hz, 2H), 5.81 (s, 2H).

^{13}C NMR (150 MHz, CDCl_3) δ 181.1, 138.6, 137.4, 128.83, 128.79, 128.5, 127.7, 126.7, 124.7, 121.9, 120.8, 120.4, 111.3, 48.2.

All analytic data match the reported data.^{S12}

1-Allyl-3-chloro-1H-indole-2-carbaldehyde (20)



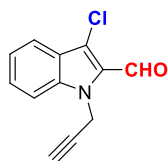
White solid; 10 h; 28.1 mg, 64% yield; R_f = 0.6, petroleum ether/ethyl acetate = 10/1.

^1H NMR (600 MHz, CDCl_3) δ 10.17 (s, 1H), 7.75 (d, J = 8.2 Hz, 1H), 7.44 (ddd, J = 8.2, 6.9, 1.1 Hz, 1H), 7.35 (d, J = 8.6 Hz, 1H), 7.25 – 7.21 (m, 1H), 5.95 (ddt, J = 17.1, 10.3, 5.2 Hz, 1H), 5.18 (dt, J = 5.1, 1.6 Hz, 2H), 5.15 – 5.10 (m, 1H), 4.95 (ddd, J = 17.1, 2.7, 1.6 Hz, 1H).

^{13}C NMR (150 MHz, CDCl_3) δ 181.0, 138.3, 133.2, 128.6, 128.3, 124.6, 121.7, 120.7, 120.0, 116.8, 111.0, 47.0.

All analytic data match the reported data.^{S12}

3-Chloro-1-(prop-2-yn-1-yl)-1H-indole-2-carbaldehyde (21)



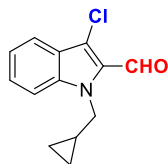
Yellow solid; 10 h; 19.5 mg, 45% yield. R_f = 0.6, petroleum ether/ethyl acetate = 10/1.

^1H NMR (600 MHz, CDCl_3) δ 10.17 (s, 1H), 7.76 (d, J = 8.1 Hz, 1H), 7.51 (d, J = 3.7 Hz, 2H), 7.28 (dt, J = 8.0, 3.9 Hz, 1H), 5.43 (d, J = 2.5 Hz, 2H), 2.28 (s, 1H).

^{13}C NMR (150 MHz, CDCl_3) δ 181.0, 138.0, 128.6, 128.0, 124.8, 122.1, 120.9, 120.8, 110.9, 77.9, 72.8, 34.0.

All analytic data match the reported data.^{S12}

3-Chloro-1-(cyclopropylmethyl)-1H-indole-2-carbaldehyde (22)



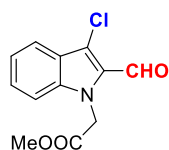
Yellow solid; 14 h; 37.4 mg, 80% yield; R_f = 0.5, petroleum ether/ethyl acetate = 10/1.

^1H NMR (600 MHz, CDCl_3) δ 10.18 (s, 1H), 7.74 (d, J = 8.2 Hz, 1H), 7.46 – 7.43 (m, 1H), 7.40 (d, J = 8.5 Hz, 1H), 7.24 – 7.21 (m, 1H), 4.47 (d, J = 7.0 Hz, 2H), 1.31 – 1.26 (m, 1H), 0.50 – 0.46 (m, 2H), 0.43 – 0.39 (m, 2H).

^{13}C NMR (150 MHz, CDCl_3) δ 181.2, 138.4, 128.7, 128.2, 124.6, 122.1, 121.5, 120.7, 120.0, 111.1, 48.8, 12.0, 3.7.

HRMS-ESI m/z : $[\text{M}+\text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{13}\text{ClNO}$ 234.0680; Found 234.0680.

Methyl 2-(3-chloro-2-formyl-1*H*-indol-1-yl)acetate (23)



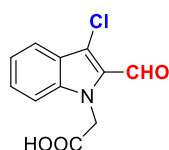
Yellow solid; 10 h; 32.2 mg, 64% yield. $R_f = 0.6$, petroleum ether/ethyl acetate = 10/1.

$^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.13 (s, 1H), 7.77 (d, $J = 8.1$ Hz, 1H), 7.47 (dd, $J = 8.4, 7.0$ Hz, 1H), 7.27 (d, $J = 8.0$ Hz, 2H), 5.30 (s, 2H), 3.75 (s, 3H).

$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 181.2, 168.7, 138.5, 128.9, 128.7, 124.6, 122.1, 120.9, 120.7, 109.9, 52.6, 46.0.

All analytic data match the reported data.^{S14}

2-(3-Chloro-2-formyl-1*H*-indol-1-yl)acetic acid (24)



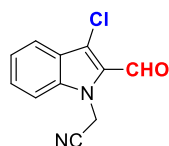
White solid; 7 h; 24.1 mg, 51% yield. $R_f = 0.7$, petroleum ether/ethyl acetate = 6/4.

$^1\text{H NMR}$ (600 MHz, $\text{DMSO-}d_6$) δ 13.07 (s, 1H), 10.06 (s, 1H), 7.74 (t, $J = 7.8$ Hz, 2H), 7.54 – 7.48 (m, 1H), 7.33 – 7.27 (m, 1H), 5.30 (s, 2H).

$^{13}\text{C NMR}$ (150 MHz, $\text{DMSO-}d_6$) δ 181.1, 169.8, 138.2, 128.8, 128.3, 123.4, 122.1, 119.7, 117.6, 111.6, 46.2.

HRMS-ESI m/z : $[\text{M-H}]^-$ Calcd for $\text{C}_{11}\text{H}_7\text{ClNO}_3$ 236.0114; Found 236.0116.

2-(3-Chloro-2-formyl-1*H*-indol-1-yl)acetonitrile (25)



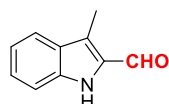
White solid; 4 h; 19.5 mg, 45% yield; $R_f = 0.6$, petroleum ether/ethyl acetate = 4/1.

$^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.16 (s, 1H), 7.80 (d, $J = 8.1$ Hz, 1H), 7.59 (ddd, $J = 8.3, 7.1, 1.1$ Hz, 1H), 7.45 (d, $J = 8.5$ Hz, 1H), 7.38 – 7.34 (m, 1H), 5.60 (s, 2H).

$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 181.3, 137.9, 129.8, 127.9, 125.1, 123.1, 122.6, 121.4, 114.3, 110.1, 32.5.

HRMS-ESI m/z : $[\text{M+H}]^+$ Calcd for $\text{C}_{11}\text{H}_8\text{ClNO}$ 219.0320; Found 219.0325.

3-Chloro-1-(prop-2-yn-1-yl)indolin-2-one (27)



White solid; 1.5 h; 26.1 mg, 82% yield; $R_f = 0.6$, petroleum ether/ethyl acetate = 4/1.

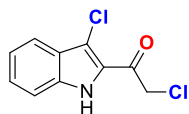
$^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.05 (s, 1H), 9.14 (s, 1H), 7.71 (d, $J = 8.1$ Hz, 1H), 7.43 – 7.37 (m, 2H), 7.16 (ddd, $J = 8.0, 6.2, 1.7$ Hz, 1H), 2.65 (s, 3H).

$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 180.7, 137.7, 132.3, 128.3, 127.8, 125.2, 121.5, 120.6,

112.4, 8.5.

HRMS-ESI m/z : $[M+H]^+$ Calcd for $C_{10}H_{10}NO$ 160.0757; Found 160.0759.

2-Chloro-1-(3-chloro-1*H*-indol-2-yl)ethan-1-one (30)



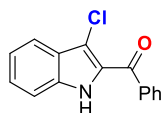
White solid; 7 min; 27.7 mg, 61% yield; R_f = 0.6, petroleum ether/ethyl acetate = 10/1.

1H NMR (600 MHz, $DMSO-d_6$) δ 12.18 (s, 1H), 7.65 (d, J = 8.2 Hz, 1H), 7.50 (d, J = 8.4 Hz, 1H), 7.40 (ddd, J = 8.2, 6.9, 1.0 Hz, 1H), 7.23 – 7.20 (m, 1H), 5.11 (s, 2H).

^{13}C NMR (150 MHz, $DMSO-d_6$) δ 182.9, 135.8, 128.6, 127.1, 125.0, 121.4, 119.7, 113.3, 110.0, 48.3.

HRMS-ESI m/z : $[M+K]^+$ Calcd for $C_{10}H_7Cl_2NOK$ 265.9535; Found 265.9536.

(3-Chloro-1*H*-indol-2-yl)(phenyl)methanone (32)



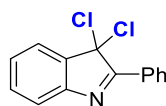
White solid; 7 min; 42.9 mg, 84% yield; R_f = 0.5, petroleum ether/ethyl acetate = 10/1.

1H NMR (600 MHz, $CDCl_3$) δ 9.71 (s, 1H), 7.93 – 7.89 (m, 2H), 7.74 (d, J = 8.1 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H), 7.53 (t, J = 7.7 Hz, 2H), 7.46 (d, J = 8.3 Hz, 1H), 7.44 – 7.40 (m, 1H), 7.26 – 7.21 (m, 1H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 188.1, 137.7, 135.8, 132.8, 130.0, 129.7, 128.4, 127.5, 126.6, 121.6, 120.7, 112.7, 112.6.

HRMS-ESI m/z : $[M+H]^+$ Calcd for $C_{15}H_{11}ClNO$ 256.0524; Found 256.0531.

3,3-Dichloro-2-phenyl-3*H*-indole (34)



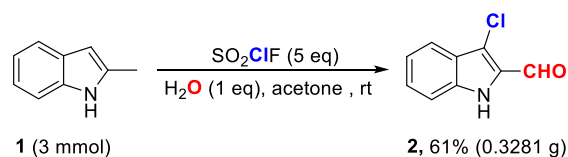
Yellow solid; 40 min; 41.7 mg, 80% yield; R_f = 0.8, petroleum ether/ethyl acetate = 10/1.

1H NMR (600 MHz, $CDCl_3$) δ 8.49 – 8.43 (m, 2H), 7.74 (d, J = 7.4 Hz, 1H), 7.63 (d, J = 7.7 Hz, 1H), 7.59 – 7.51 (m, 3H), 7.47 (td, J = 7.6, 0.4 Hz, 1H), 7.38 (t, J = 7.5 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 172.0, 149.4, 140.0, 132.2, 131.6, 129.5, 128.8, 128.7, 128.0, 122.8, 121.7, 80.3.

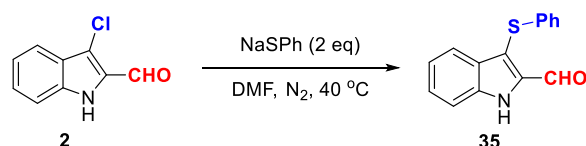
All analytic data match the reported data.^{S15}

V. Scale-Up Experiments



To the solution of **1** (3 mmol, 1.0 eq) in acetone (20 mL) and H₂O (54 μL, 1 eq) was added SO₂ClF (15 mmol, 5 eq, 1 M in anhydrous PhCF₃), and then stirred at room temperature. After the completion of the reaction, as indicated by TLC, the reaction was quenched with water. The resulting mixture was extracted with ethyl acetate and the combined organic layers were dried over Na₂SO₄ and evaporated under reduced pressure. The residue was purified by column chromatography (petroleum ether/ethyl acetate = 50:1 to 10:1) on silica gel to afford **2**.

VI. Synthetic Applications of 3-Chloro-2-Formylindoles

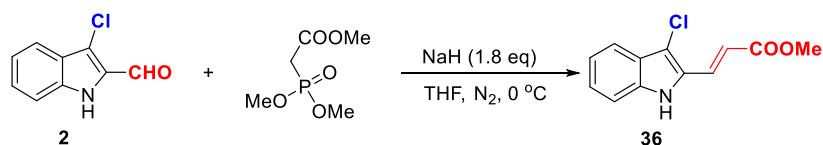


According to the literature,^{S16} to a solution of **2** (35.9 mg, 0.2 mmol, 1.0 eq) in anhydrous DMF (1.0 mL) was added sodium thiophenolate (58.7 mg, 0.4 mmol, 2.0 eq) in one portion at room temperature. The mixture was stirred under an N₂ atmosphere for 43 h and then a saturated aqueous solution of NH₄Cl (5.0 mL) was added. The mixture was extracted with EtOAc (10.0 mL) three times. The combined organic layers were dried over Na₂SO₄, filtered, and evaporated to dryness in vacuo. The residue was purified by column chromatography (petroleum ether/ethyl acetate = 50:1 to 10:1) on silica gel to afford **35** as a white solid (27.9 mg, 55% yield).

¹H NMR (600 MHz, CDCl₃) δ 10.22 (s, 1H), 9.73 (s, 1H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.53 (d, *J* = 8.3 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.20 (dd, *J* = 11.1, 7.0 Hz, 5H), 7.14 (s, 1H).

¹³C NMR (150 MHz, CDCl₃) δ 182.3, 137.6, 137.2, 136.8, 129.6, 129.2, 128.2, 127.4, 126.1, 122.2, 122.1, 116.0, 113.0.

HRMS-ESI *m/z*: [M+H]⁺ Calcd for C₁₅H₁₂NOS 254.0634; Found 254.0640.



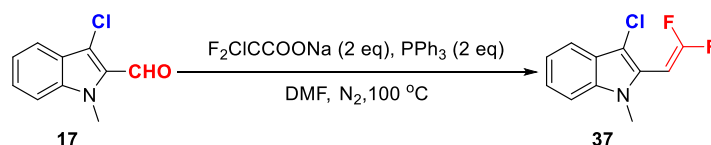
According to the literature,^{S17} to a solution of 60 % sodium hydride (144 mg, 0.36 mmol, 1.8 eq) in 2 mL anhydrous THF, a solution of methyl 2-(dimethoxyphosphoryl)acetate (39.6 μL, 0.24 mmol, 1.2 eq) in THF was added at 0 °C under nitrogen atmosphere. After 20 minutes, **2** (35.9 mg, 0.2 mmol, 1 eq) was added to the flask. After 14 h, the

reaction was hydrolyzed by adding water. The mixture was extracted with ethyl acetate. The organic phase was washed with water and brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by column chromatography (petroleum ether/ethyl acetate = 50:1 to 10:1) on silica gel to afford **36** as a white solid (30.9 mg, 66% yield).

¹H NMR (600 MHz, DMSO-*d*₆) δ 11.94 (s, 1H), 7.64 (d, *J* = 16.0 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.43 (d, *J* = 8.3 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.66 (d, *J* = 16.0 Hz, 1H), 3.75 (s, 3H).

¹³C NMR (150 MHz, DMSO-*d*₆) δ 166.4, 136.2, 129.9, 129.0, 125.5, 125.0, 120.7, 118.2, 116.8, 112.1, 109.1, 51.7.

HRMS-ESI *m/z*: [M+H]⁺ Calcd for C₁₂H₁₁ClNO₂ 236.0473; Found 236.0465.



According to the literature,^{S18} a solution of **17** (38.7 mg, 0.2 mmol, 1.0 eq) and PPh₃ (107.1 mg, 0.4 mmol, 2.0 eq) in DMF (1 mL) was heated to 100 °C. To the reaction mixture at 100 °C was added F₂ClCCOONa (63.5 mg, 0.4 mmol, 2.0 eq) slowly. After the reaction finished according to the TLC (about 3 min), the reaction mixture was cooled to room temperature, quenched with water and extracted with ethyl acetate. The combined organic layers were washed with H₂O₂ (30 wt% in water, 5 mL), brine and dried over Na₂SO₄. After the solvent was removed under reduced pressure, the residue was purified by column chromatography (petroleum ether/ethyl acetate = 80:1 to 20:1) on silica gel to afford **37** as a white oil (34.3 mg, 75% yield).

¹H NMR (600 MHz, CDCl₃) δ 7.63 (d, *J* = 7.9 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.20 (ddd, *J* = 8.0, 5.7, 2.3 Hz, 1H), 5.35 (dd, *J* = 25.1, 1.3 Hz, 1H), 3.67 (d, *J* = 1.1 Hz, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 158.6, 156.7 (d, *J* = 7.1 Hz), 154.7, 136.4, 125.4, 123.2, 120.5, 118.3, 109.6, 71.0 (dd, *J* = 35.1, 18.0 Hz), 31.0 (d, *J* = 2.3 Hz).

¹⁹F NMR (565 MHz, CDCl₃) δ -76.0 (dd, *J* = 25.0, 15.3 Hz), -80.3 (d, *J* = 15.3 Hz).

HRMS-ESI *m/z*: [M+K]⁺ Calcd for C₁₁H₈ClF₂NK 265.9945; Found 265.9950.

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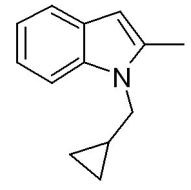
VIII. NMR Spectra

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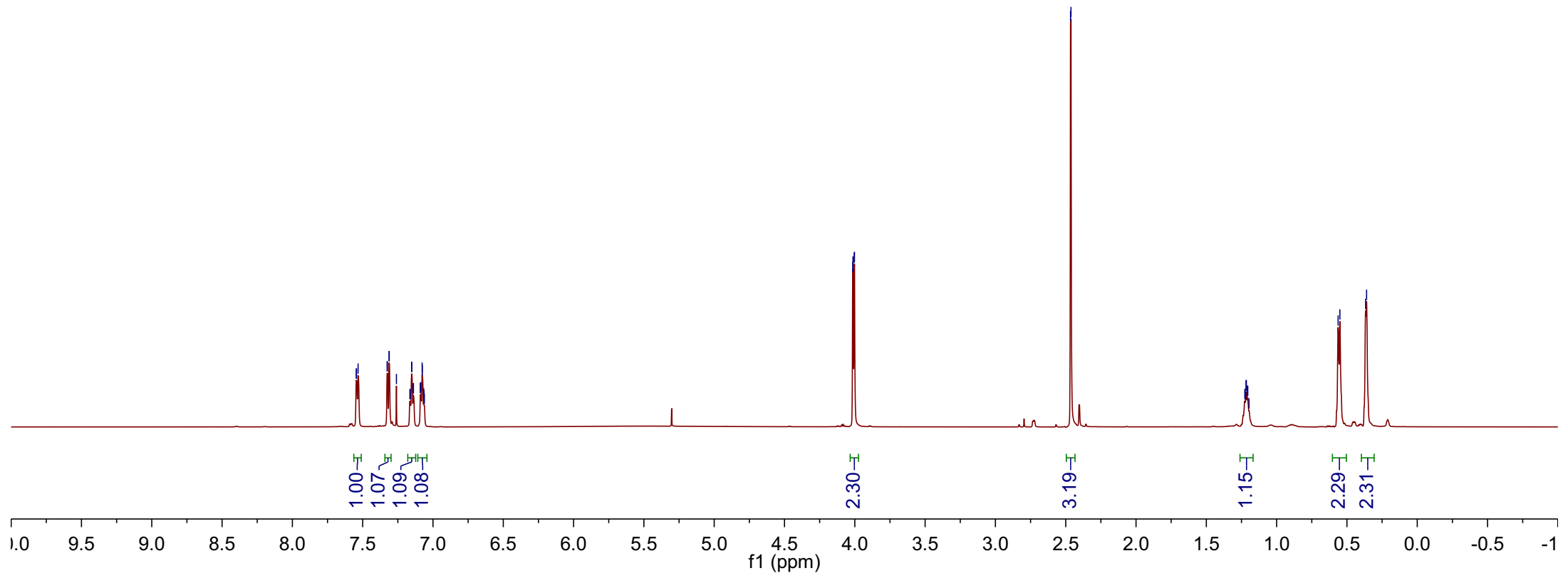
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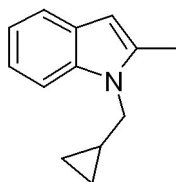
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1q

	Parameter	Value
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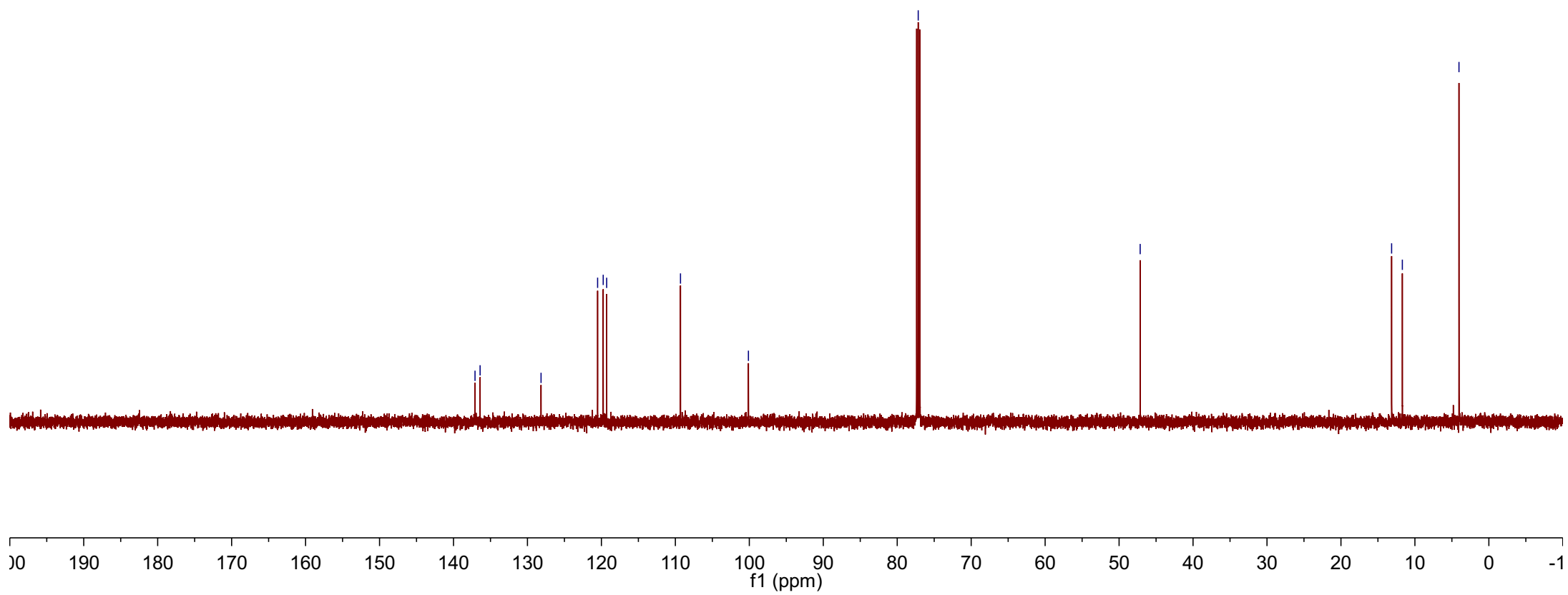


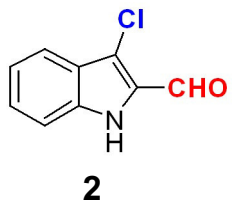


1q

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11.70
4.04

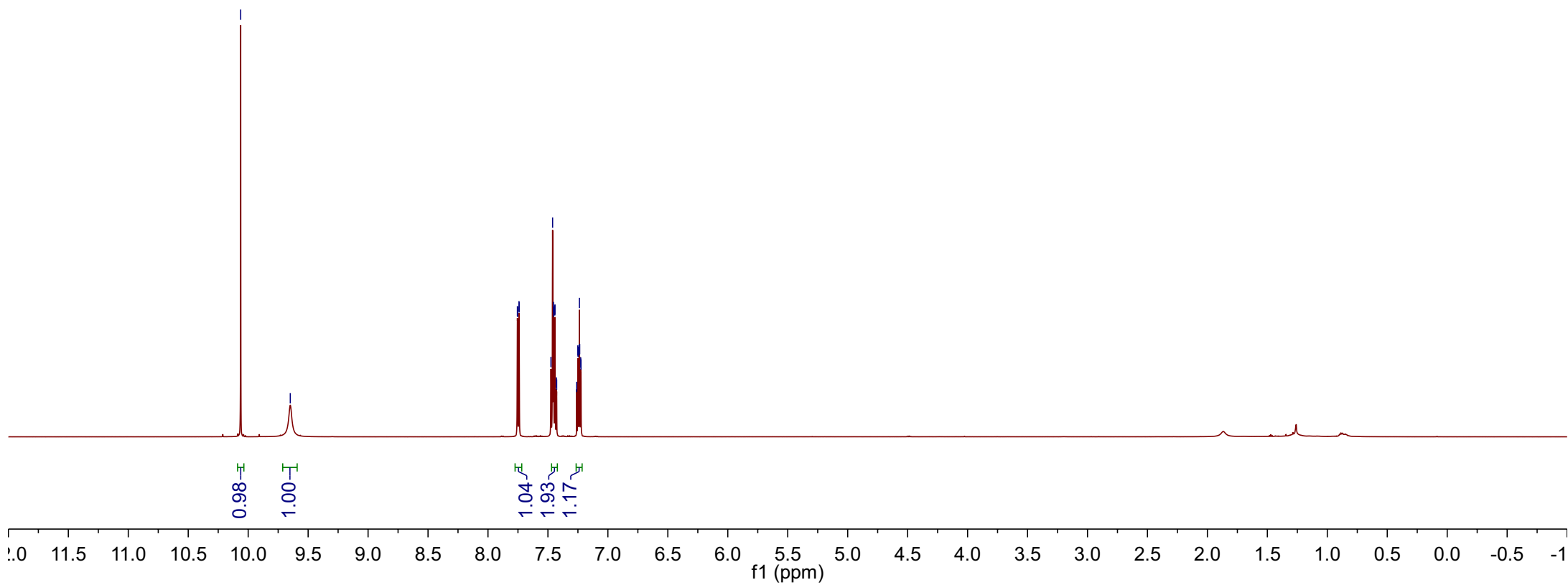
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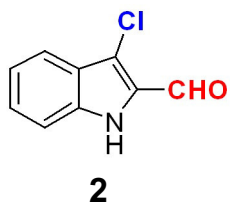




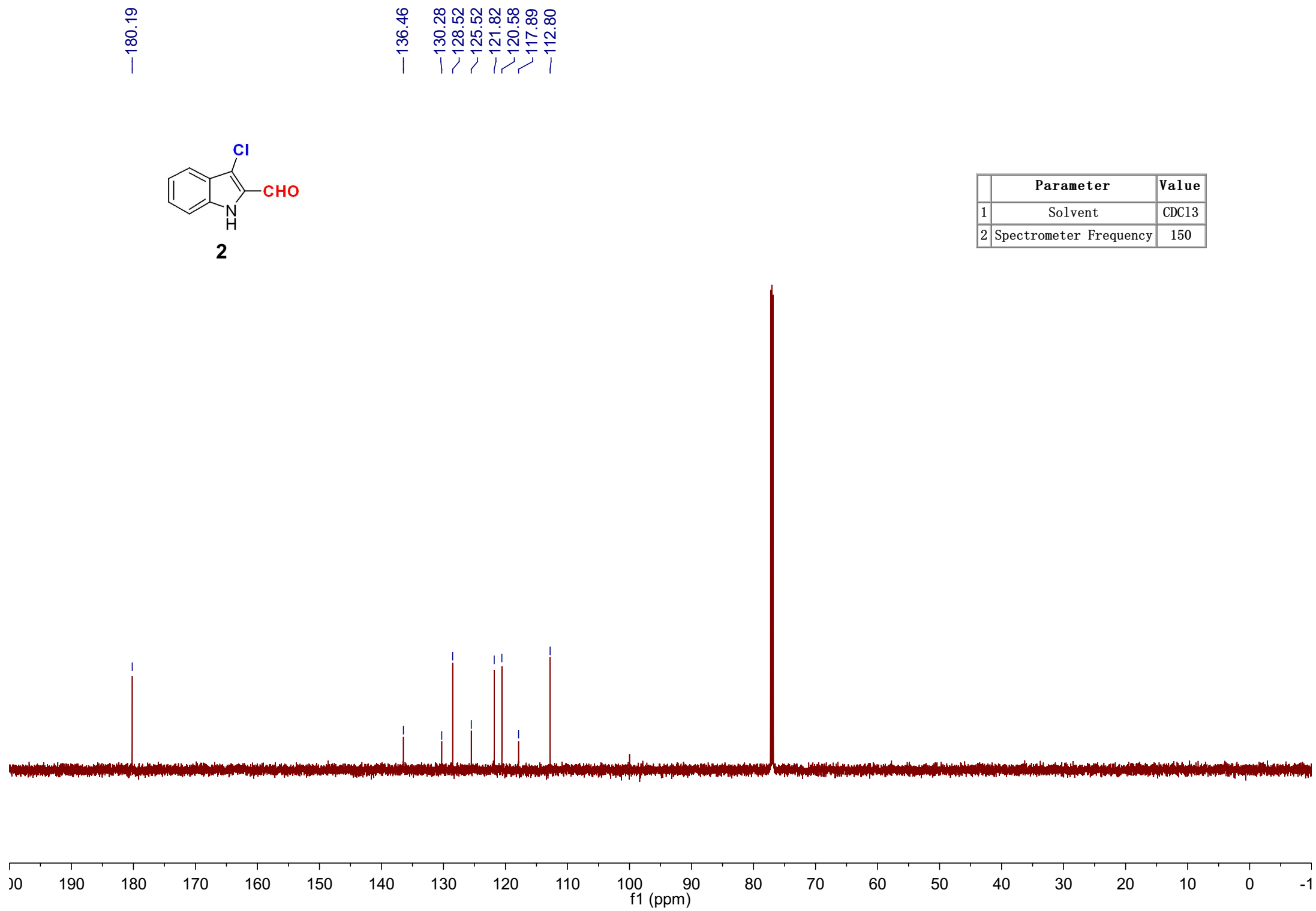
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7.23
7.22

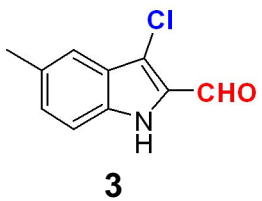
	Parameter	Value
1	Solvent	CDCl ₃
2	Spectrometer Frequency	600





	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150





—10.03

—9.25

7.51

7.34

7.32

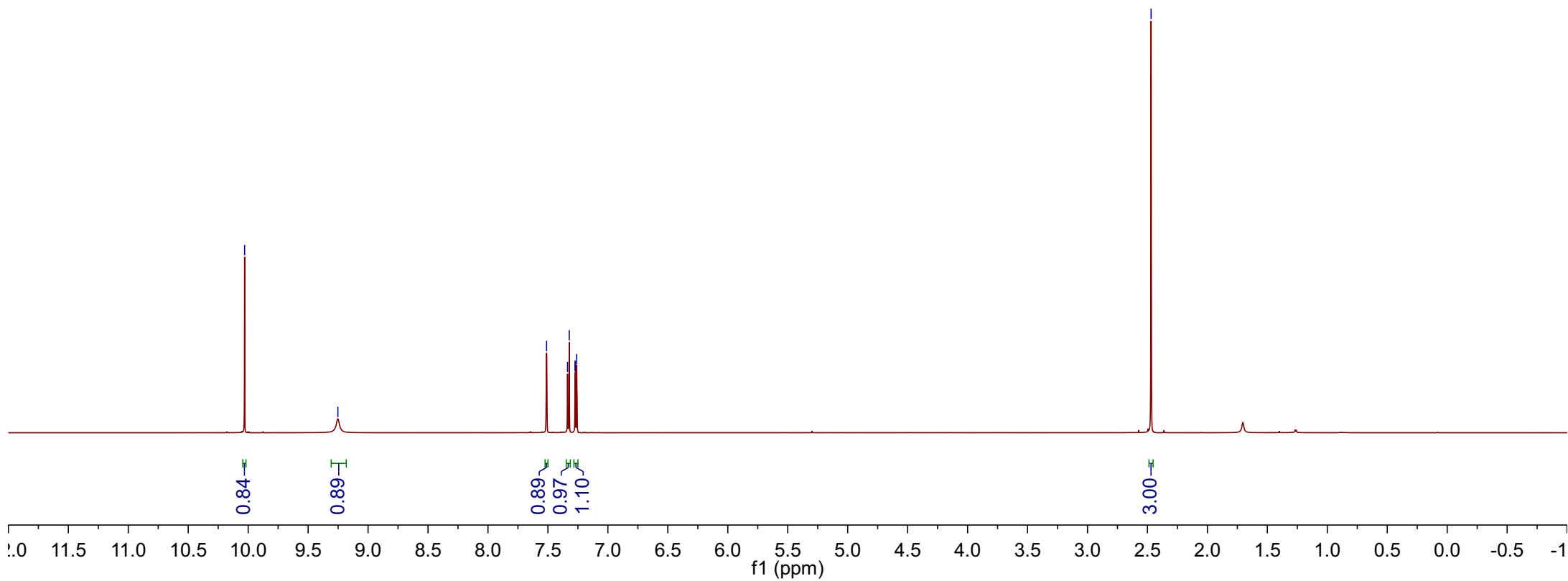
7.27

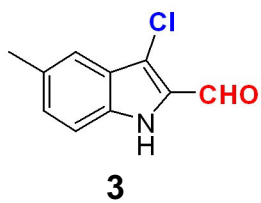
7.27

7.26

—2.47

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600





— 180.18

135.14

131.62

130.81

130.51

125.87

119.68

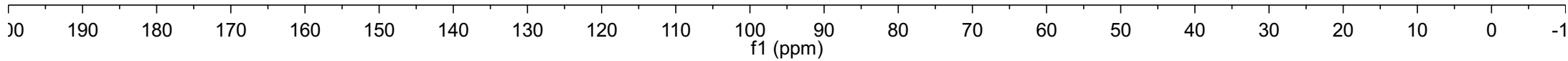
117.36

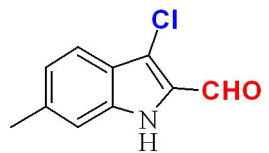
112.62

77.16

— 21.54

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150





4

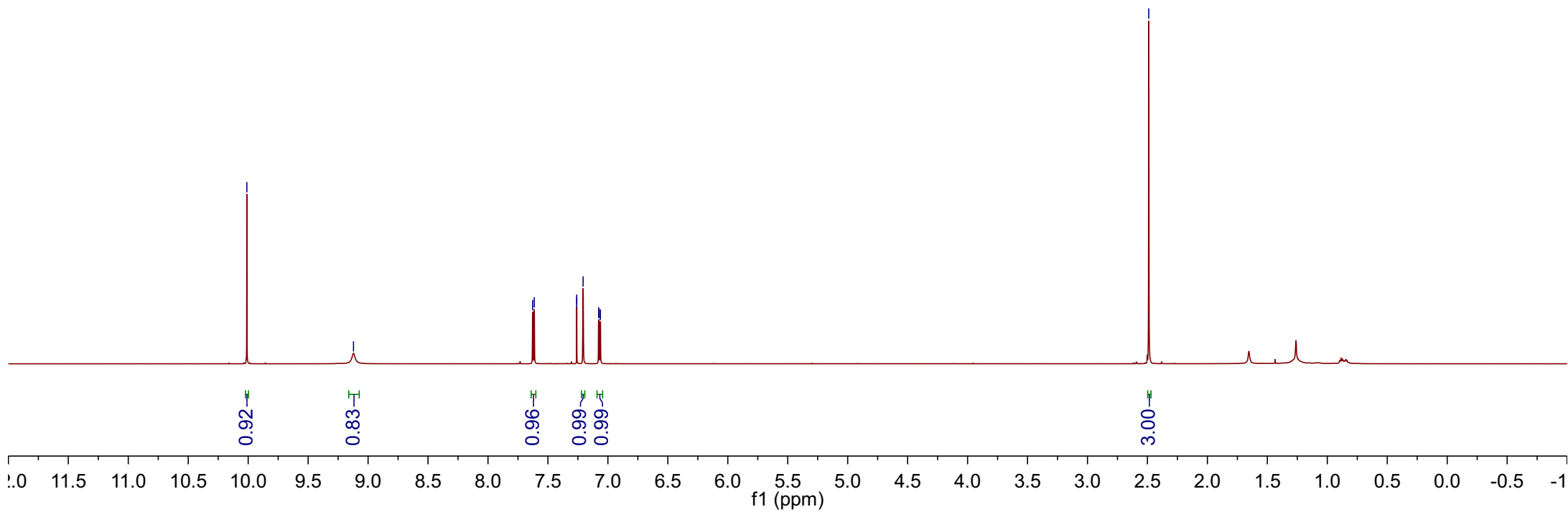
—10.01

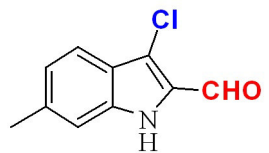
—9.12

7.63
7.61
7.26
7.26
7.21
7.08
7.08
7.06
7.06

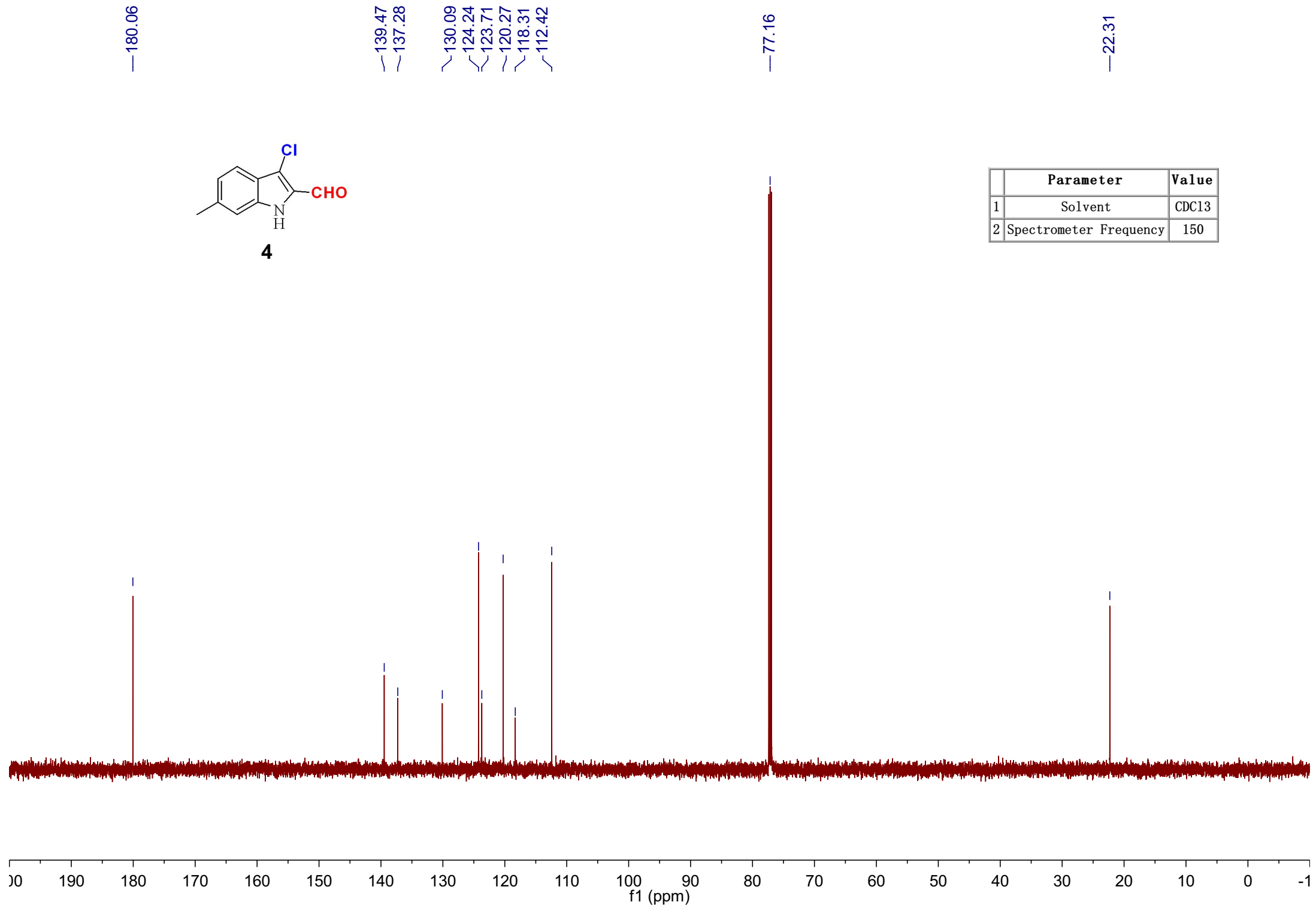
—2.49

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600

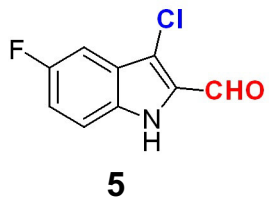




4



	Parameter	Value
1	Solvent	CDCl3
2	Spectrometer Frequency	150



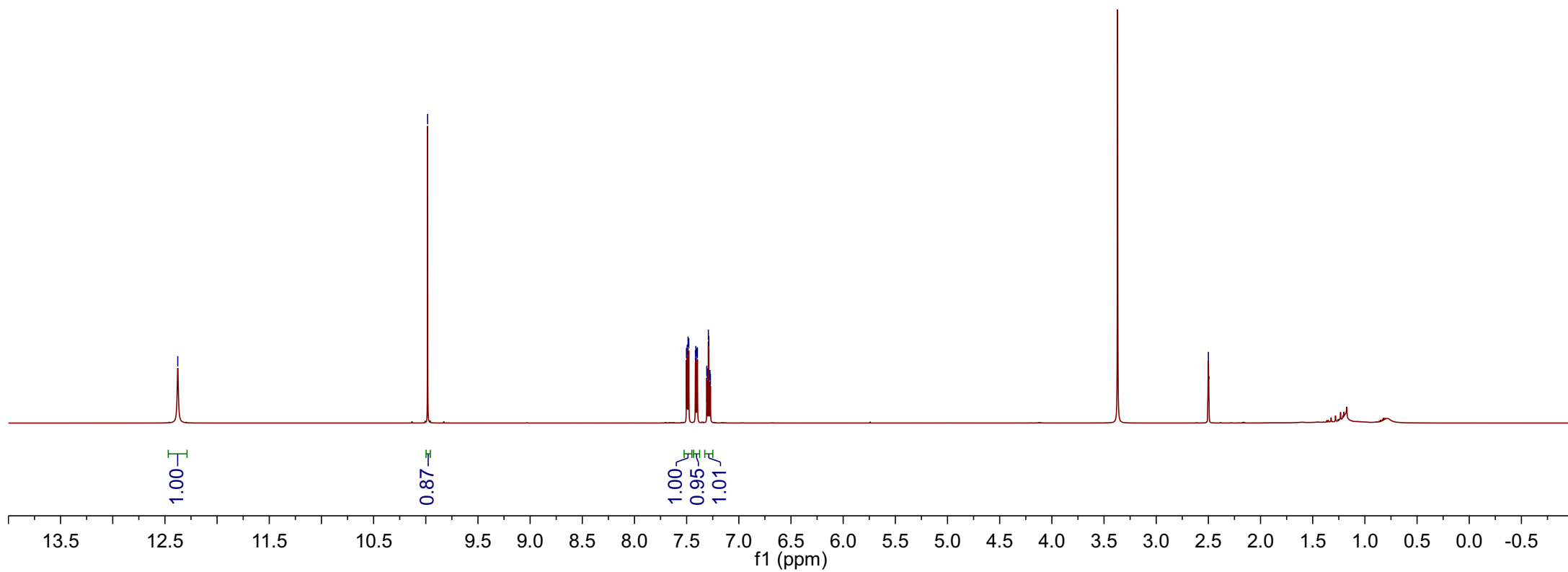
—12.38

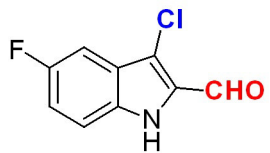
—9.98

7.50
7.49
7.49
7.48
7.42
7.41
7.40
7.40
7.31
7.30
7.29
7.29
7.28
7.27

—2.50

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600





5

—180.79

—158.89

—157.32

—133.56

—132.02

—124.84

—124.77

—117.40

—117.22

—115.73

—115.67

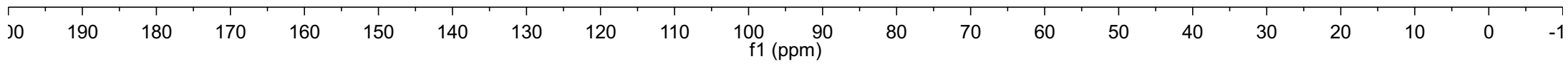
—114.33

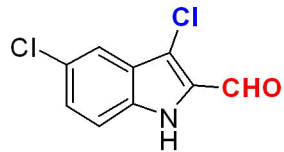
—104.83

—103.87

—39.52

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150





6

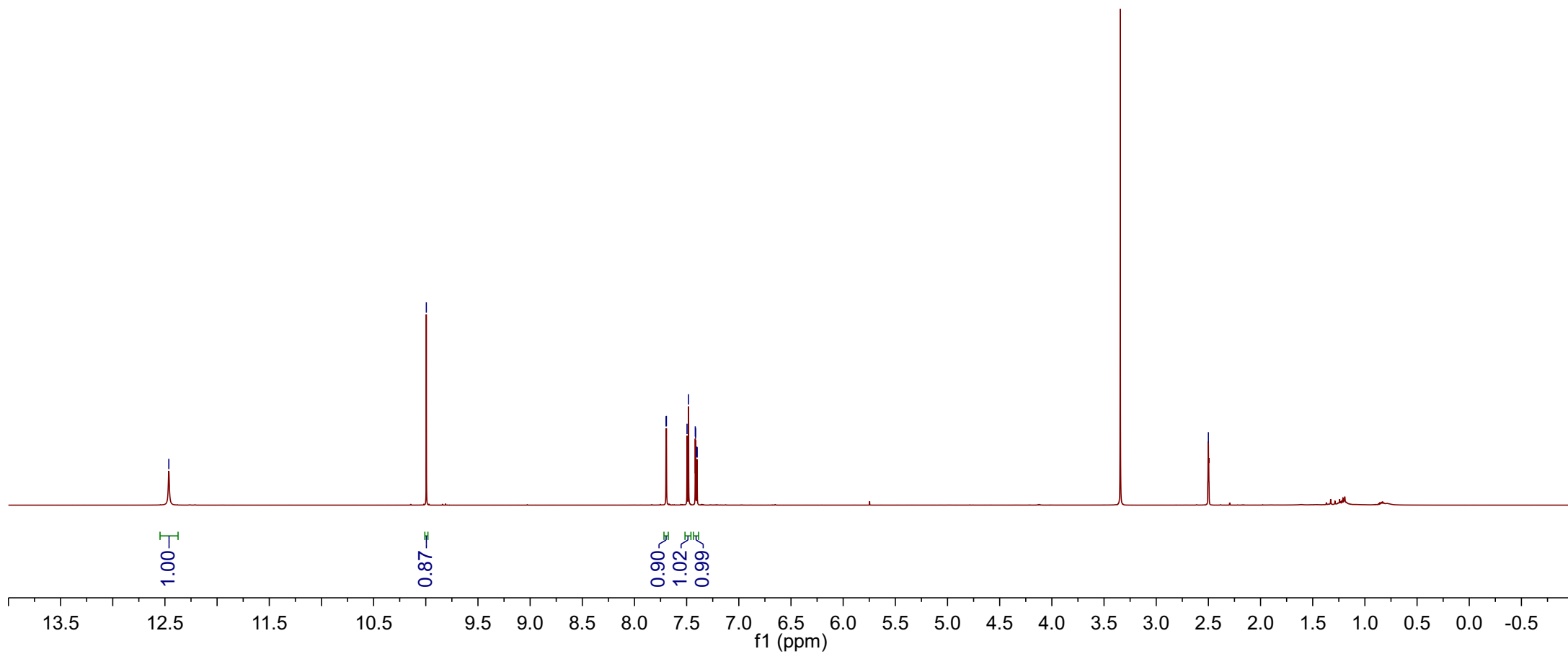
—12.46

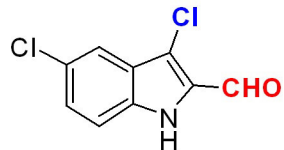
—9.99

7.70
7.69
7.50
7.48
7.42
7.41
7.40
7.40

—2.50

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600





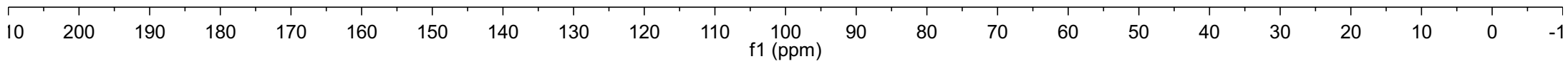
6

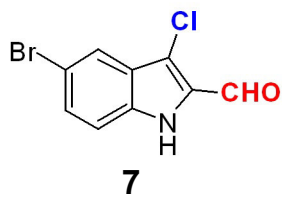
—180.51

134.82
131.47
127.81
126.09
125.25
118.49
115.38
113.24

—39.52

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150





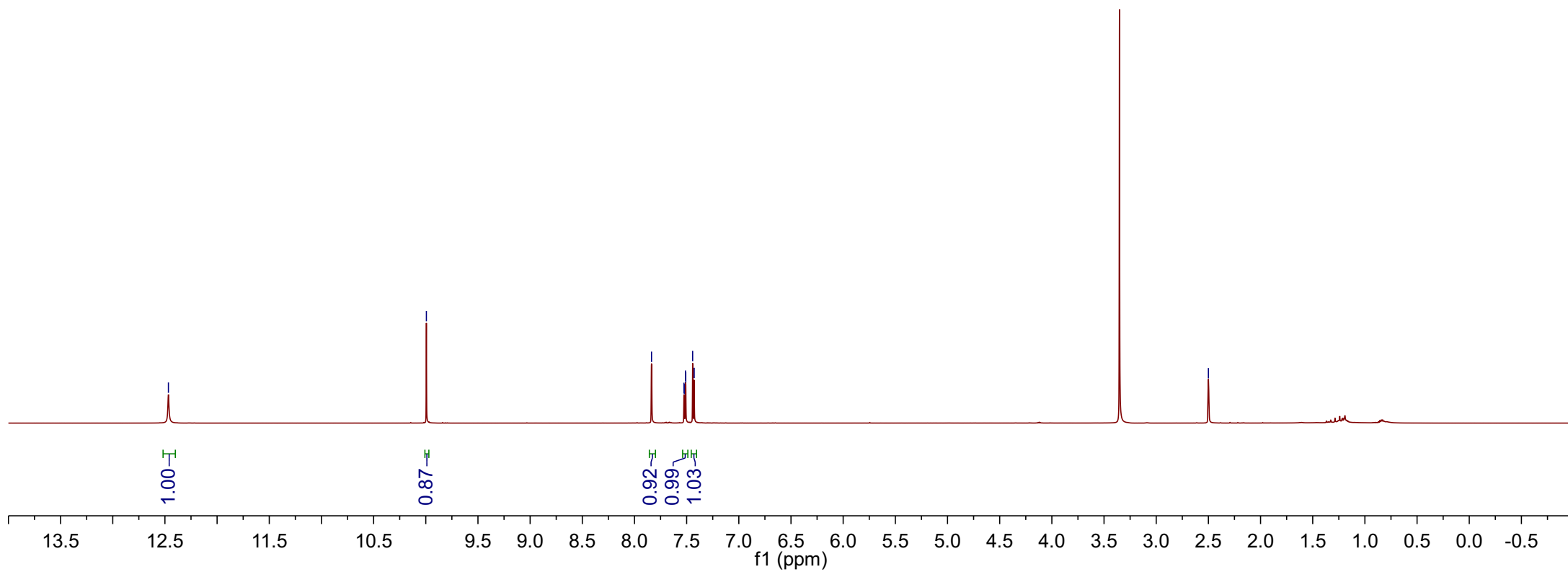
—12.47

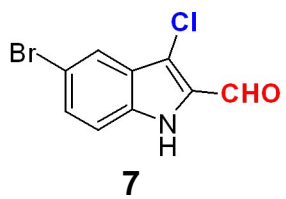
—9.99

7.84
7.53
7.52
7.51
7.51
7.44
7.43

—2.50

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600



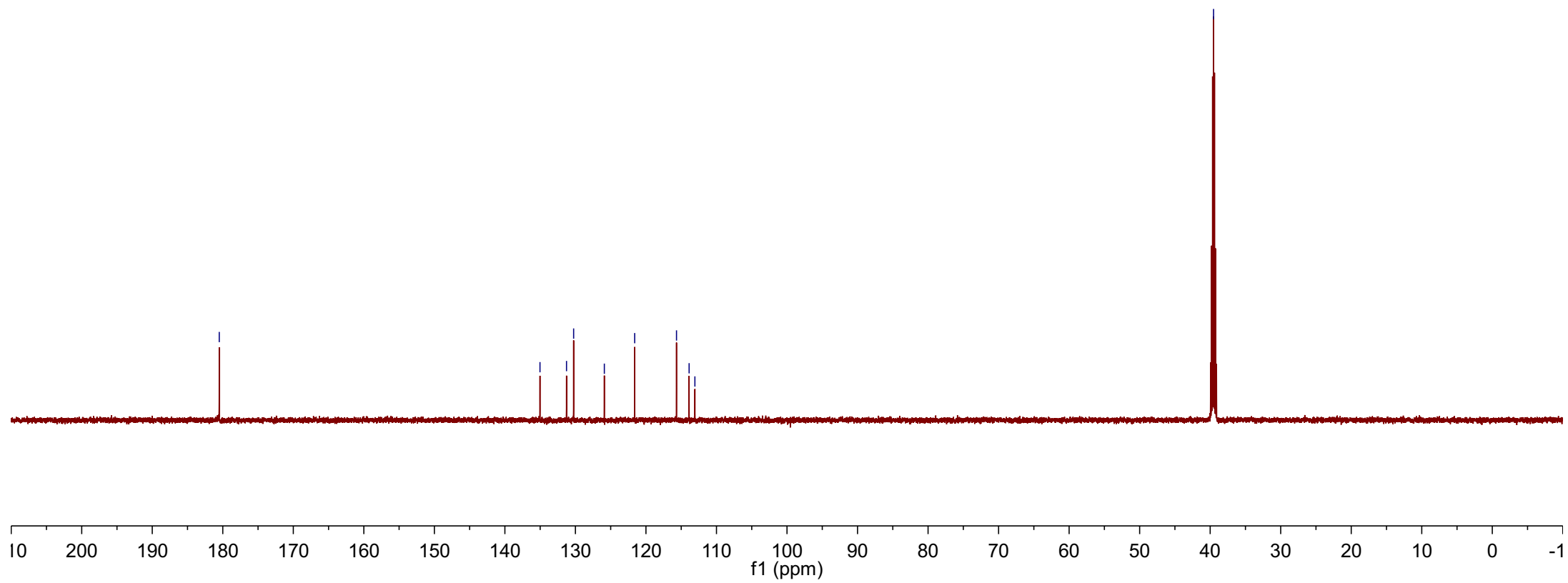


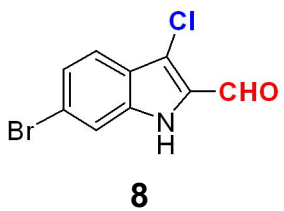
—180.50

—135.02
—131.26
—130.25
—125.90
—121.60
—115.67
—113.88
—113.06

—39.52

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150





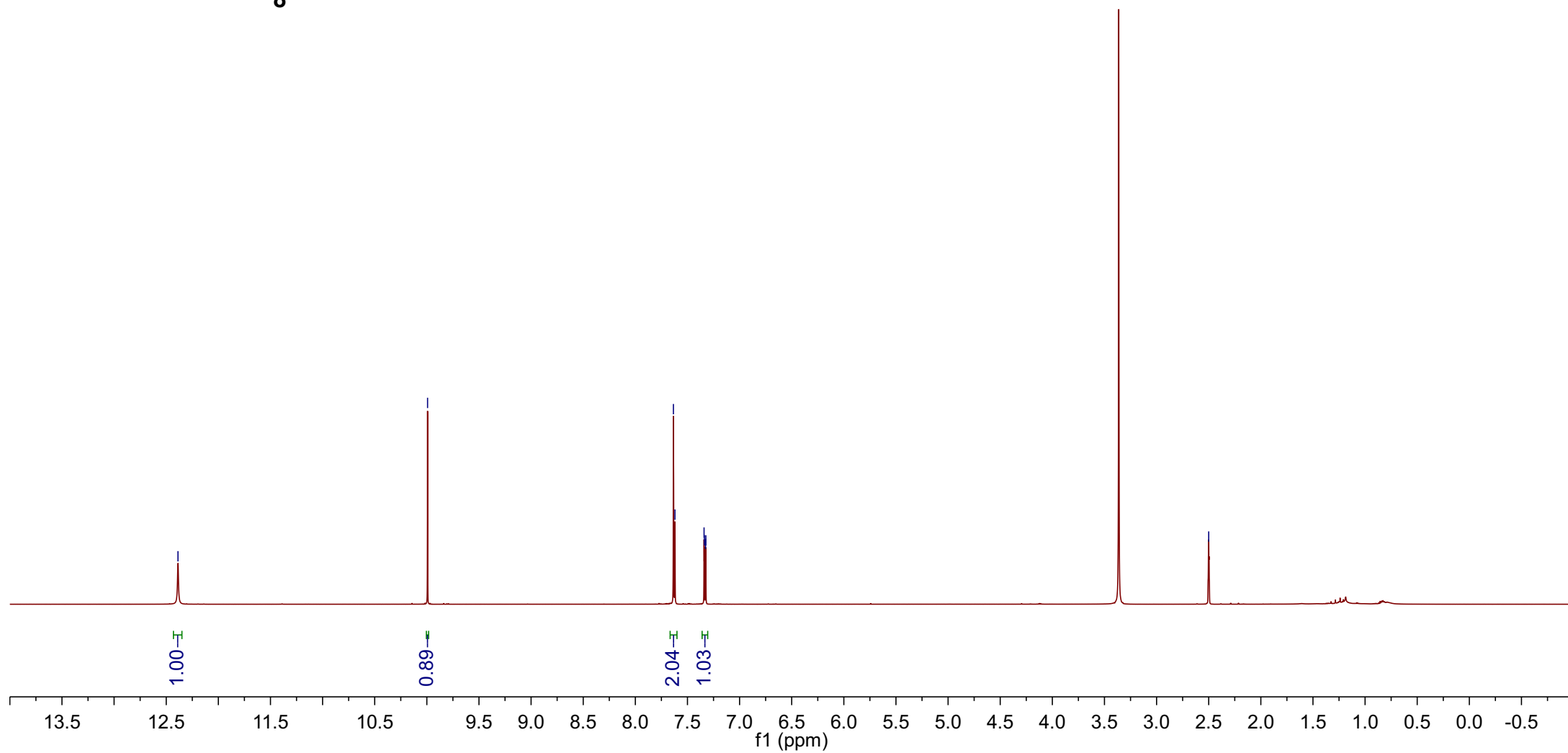
—12.39

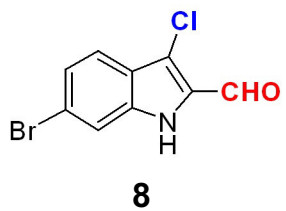
—9.99

7.63
7.62
7.34
7.34
7.33
7.32

—2.50

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600





—180.43

—136.97

—130.94

124.67

123.41

121.51

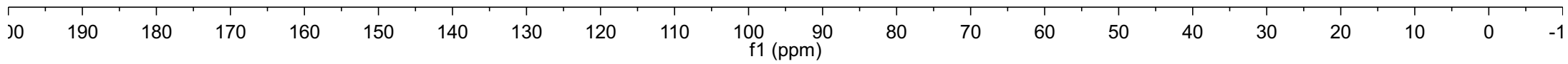
120.45

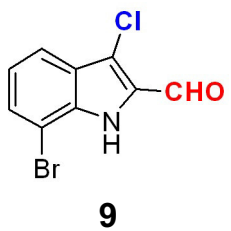
115.85

114.39

—39.52

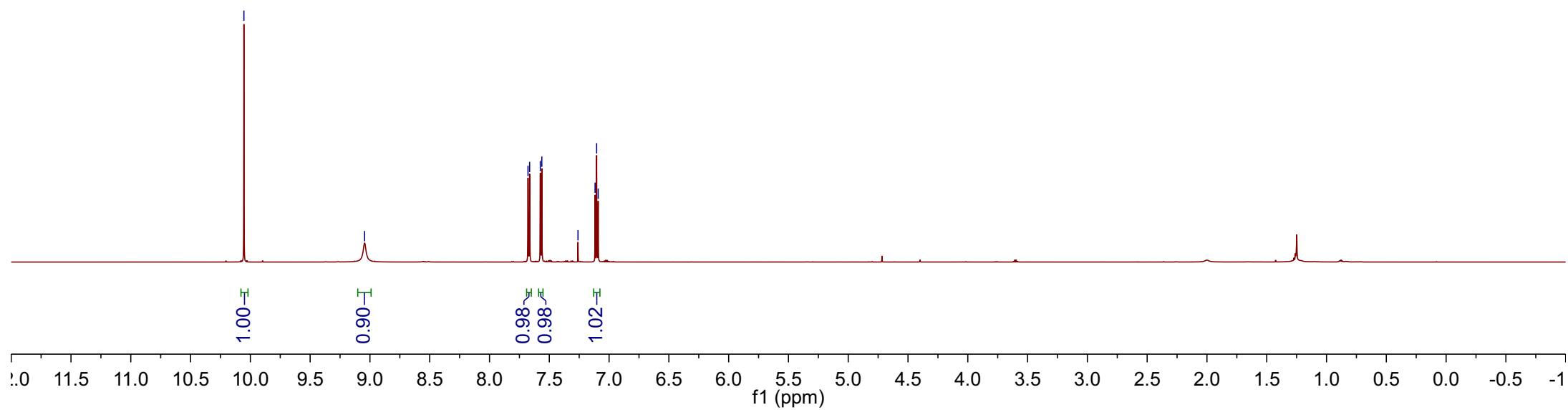
	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150

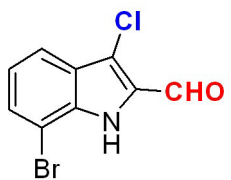




	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600

—10.05
 —9.04
 7.68
 7.66
 7.58
 7.56
 7.26
 7.12
 7.10
 7.09





9

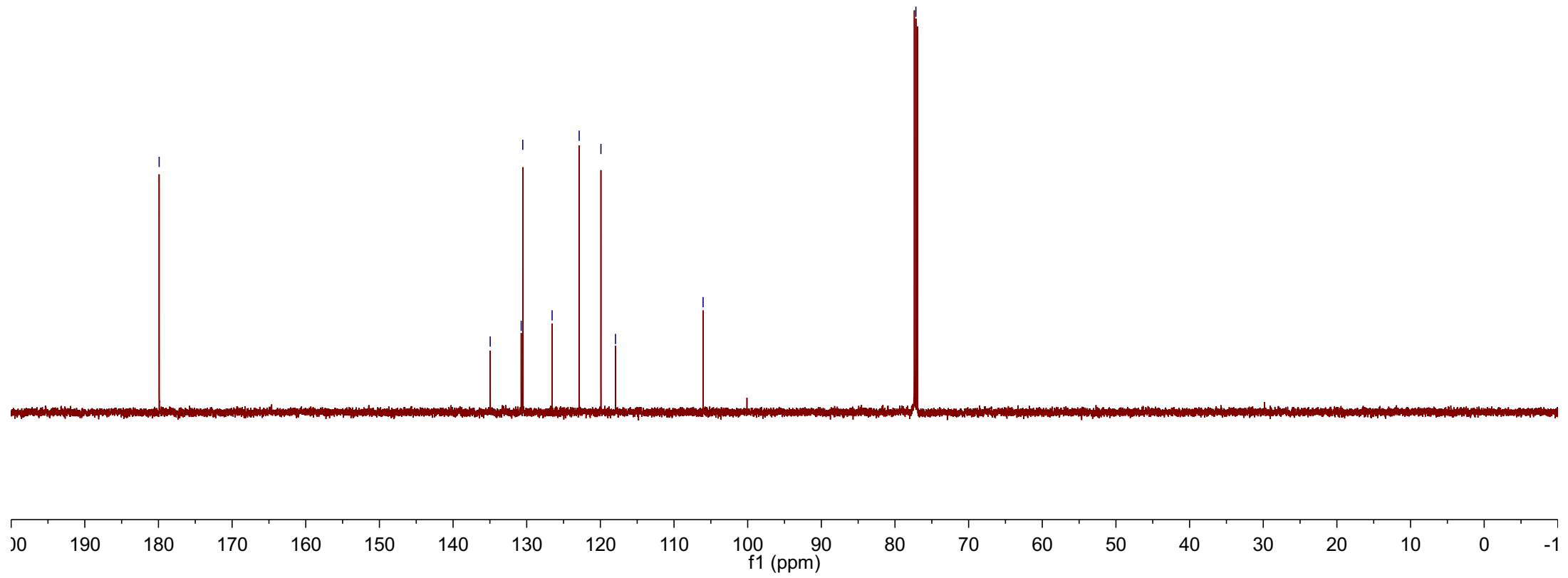
	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150

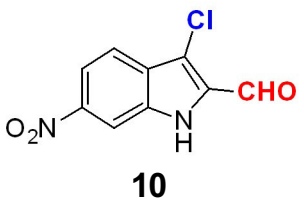
—179.90

—134.96
—130.75
—130.54
—126.55
—122.88
—119.92
—117.95

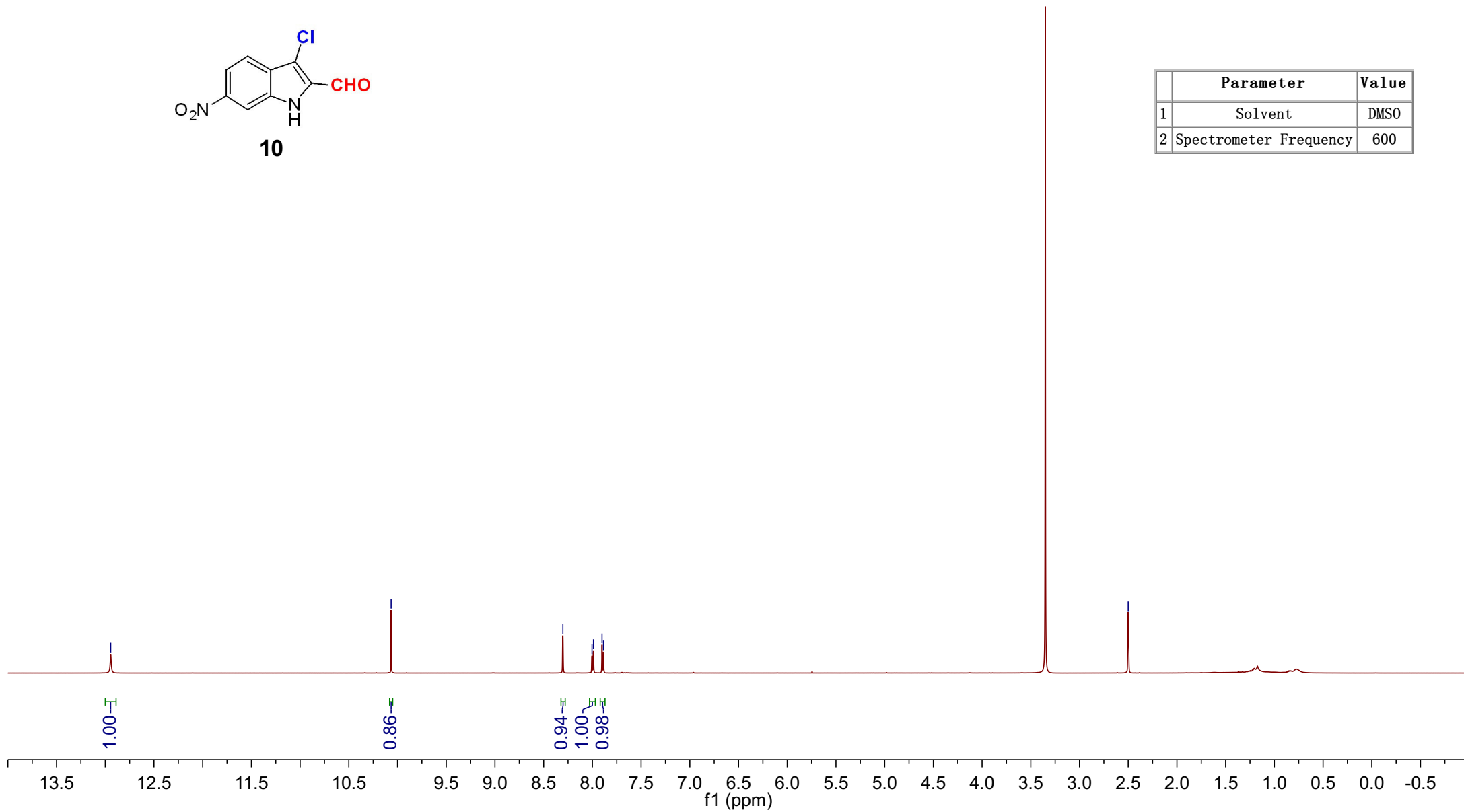
—106.05

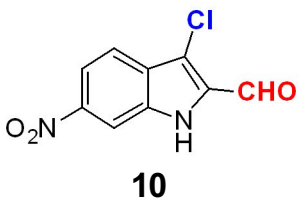
—77.16





	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600





—181.05

—146.11

—134.47

—134.34

—128.24

—120.76

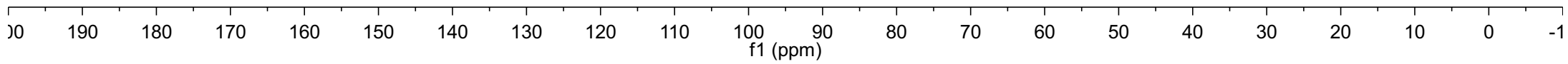
—115.69

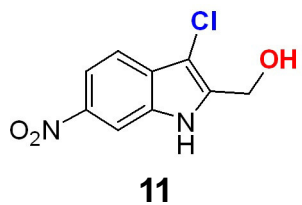
—113.37

—110.08

—39.52

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150





—12.52

8.35
8.34
7.98
7.98
7.97
7.97
7.67
7.65

—4.98

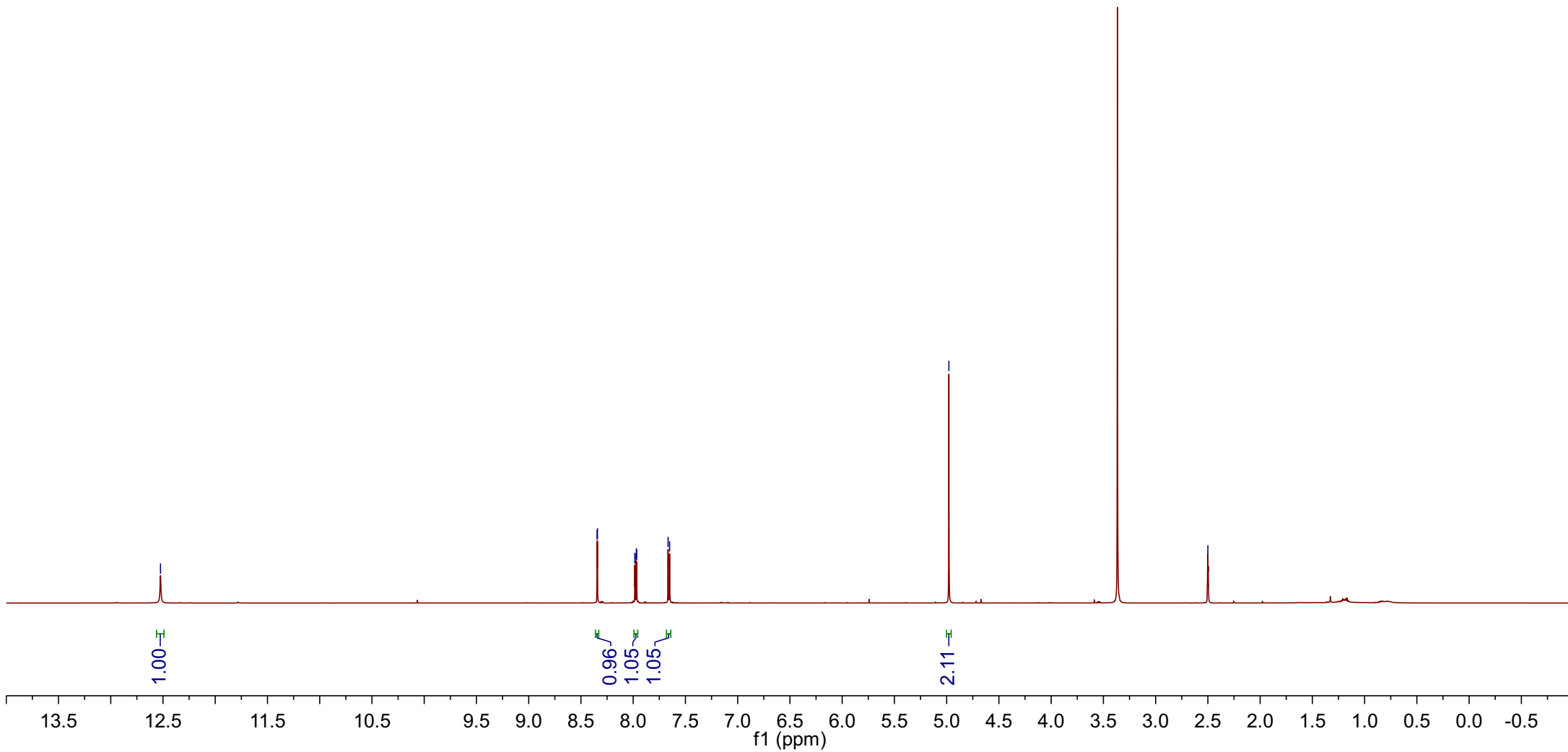
—2.50

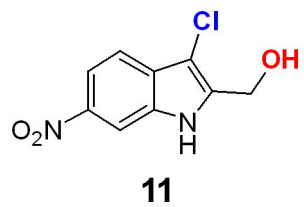
	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600

1.00

0.96
1.05
1.05

2.11





—143.53

—136.60

—132.97

—128.77

—118.19

—115.28

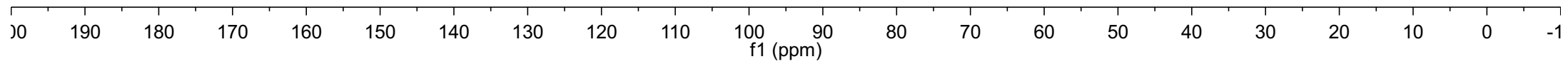
—109.03

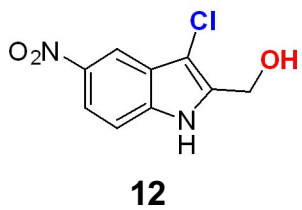
—104.20

—39.52

—35.39

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150





—12.51

8.36
8.36
8.10
8.09
8.08
8.08
7.62
7.60

—4.95

—2.50

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600

1.00

0.93

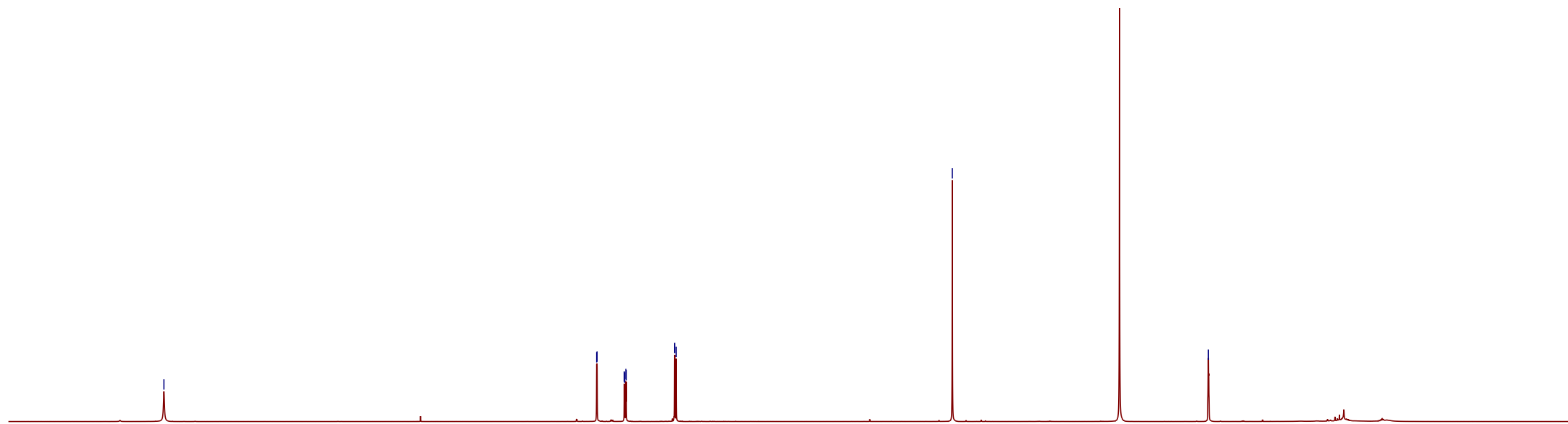
1.01

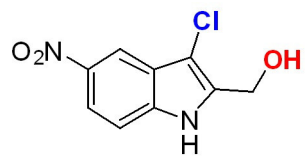
1.03

2.09

13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

f1 (ppm)



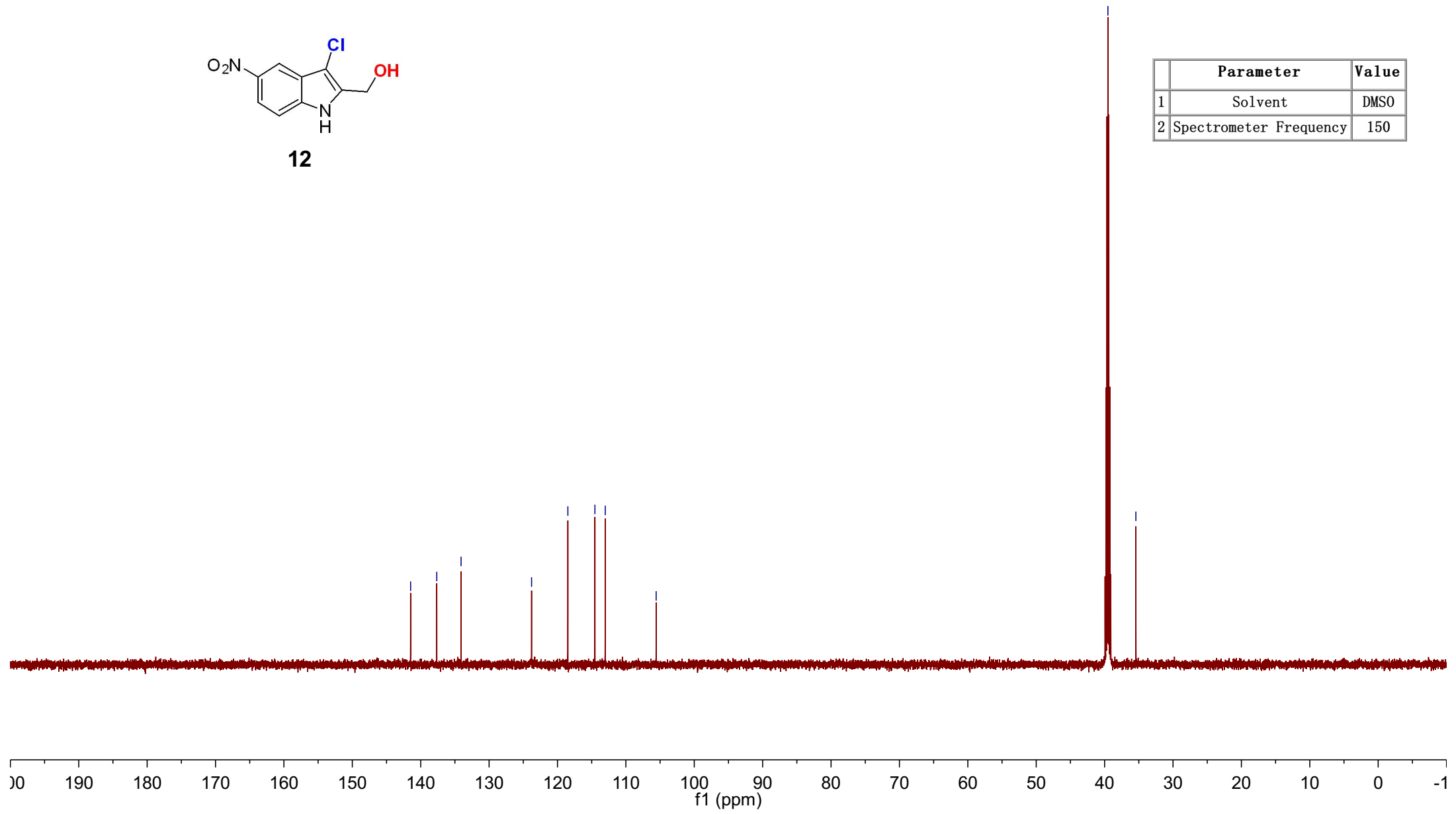


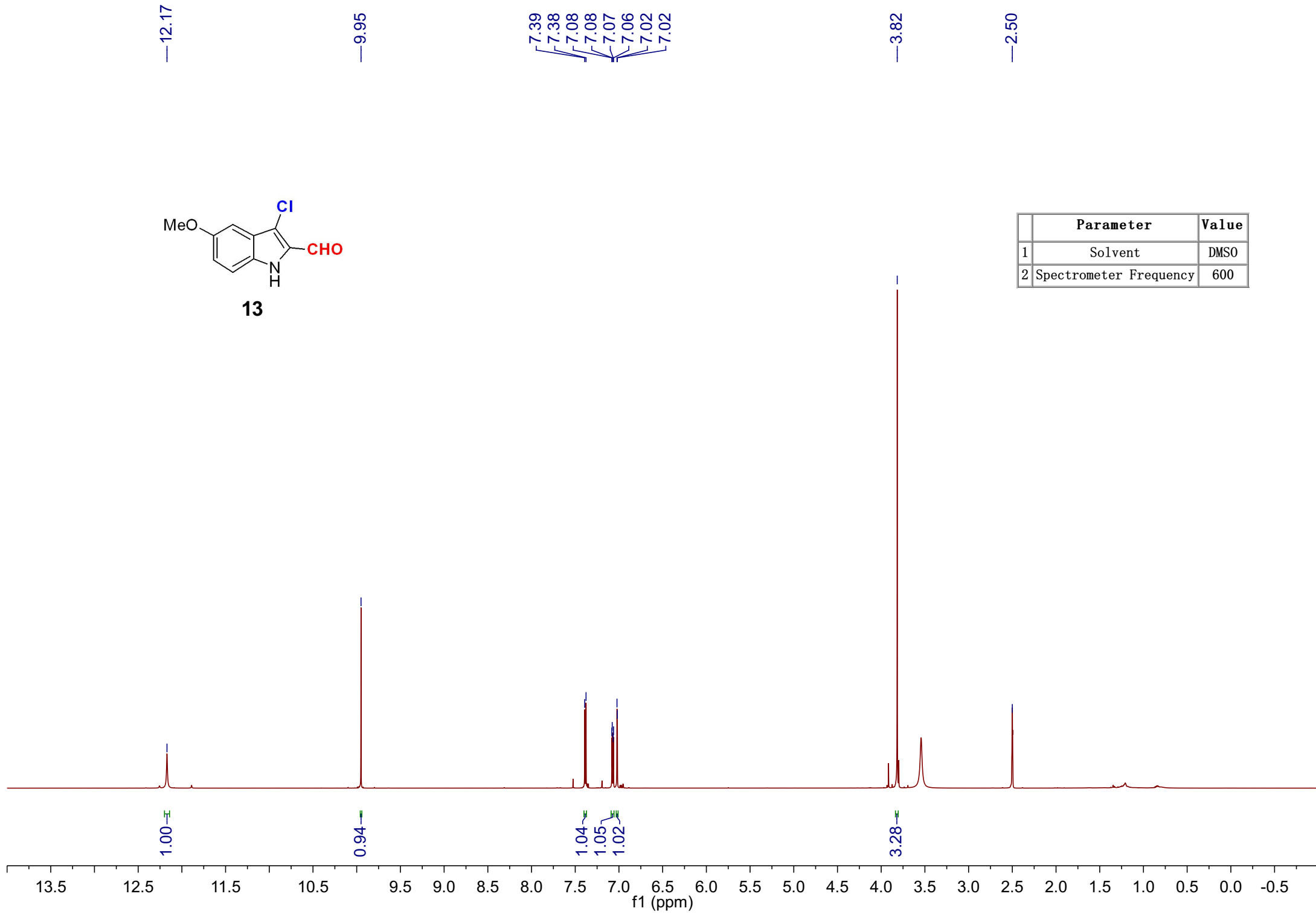
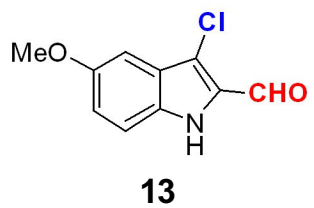
12

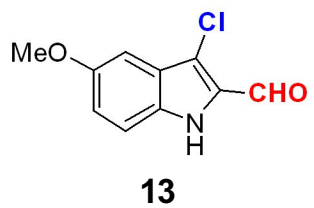
141.47
137.65
134.10
123.79
118.48
114.53
113.02
105.57

39.52
35.43

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150







—179.95

—154.86

—132.00

—130.62

—124.67

—120.00

—114.75

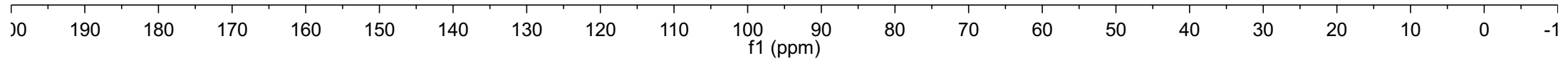
—113.54

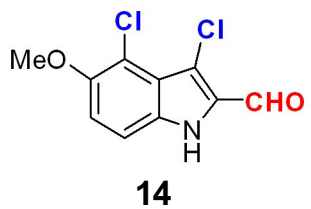
—98.48

—55.41

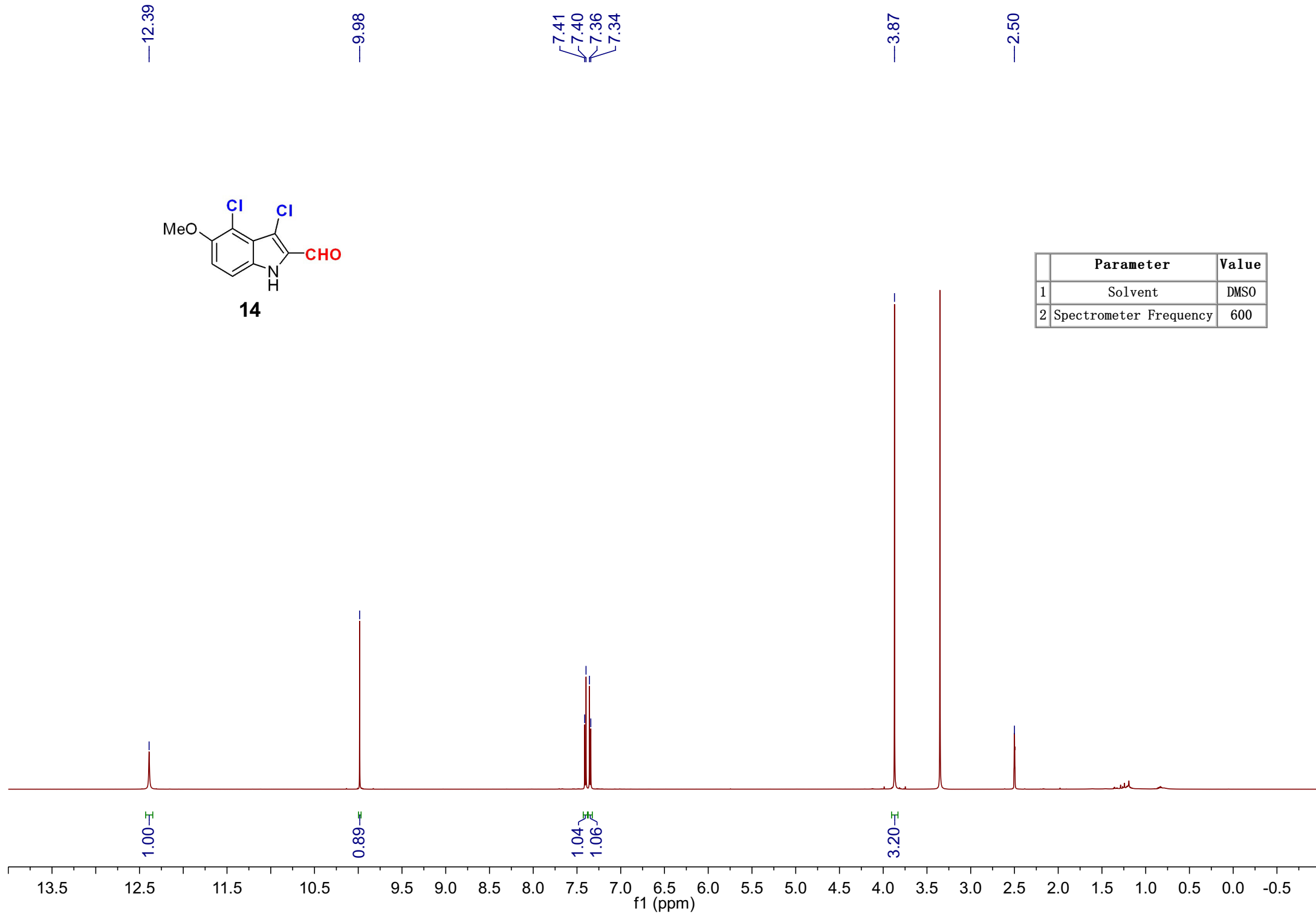
—39.52

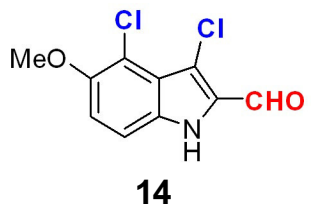
	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150





	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600





—180.62

—149.97

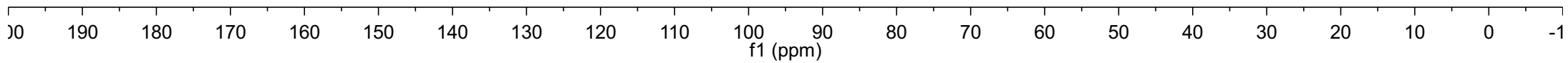
132.99
132.00

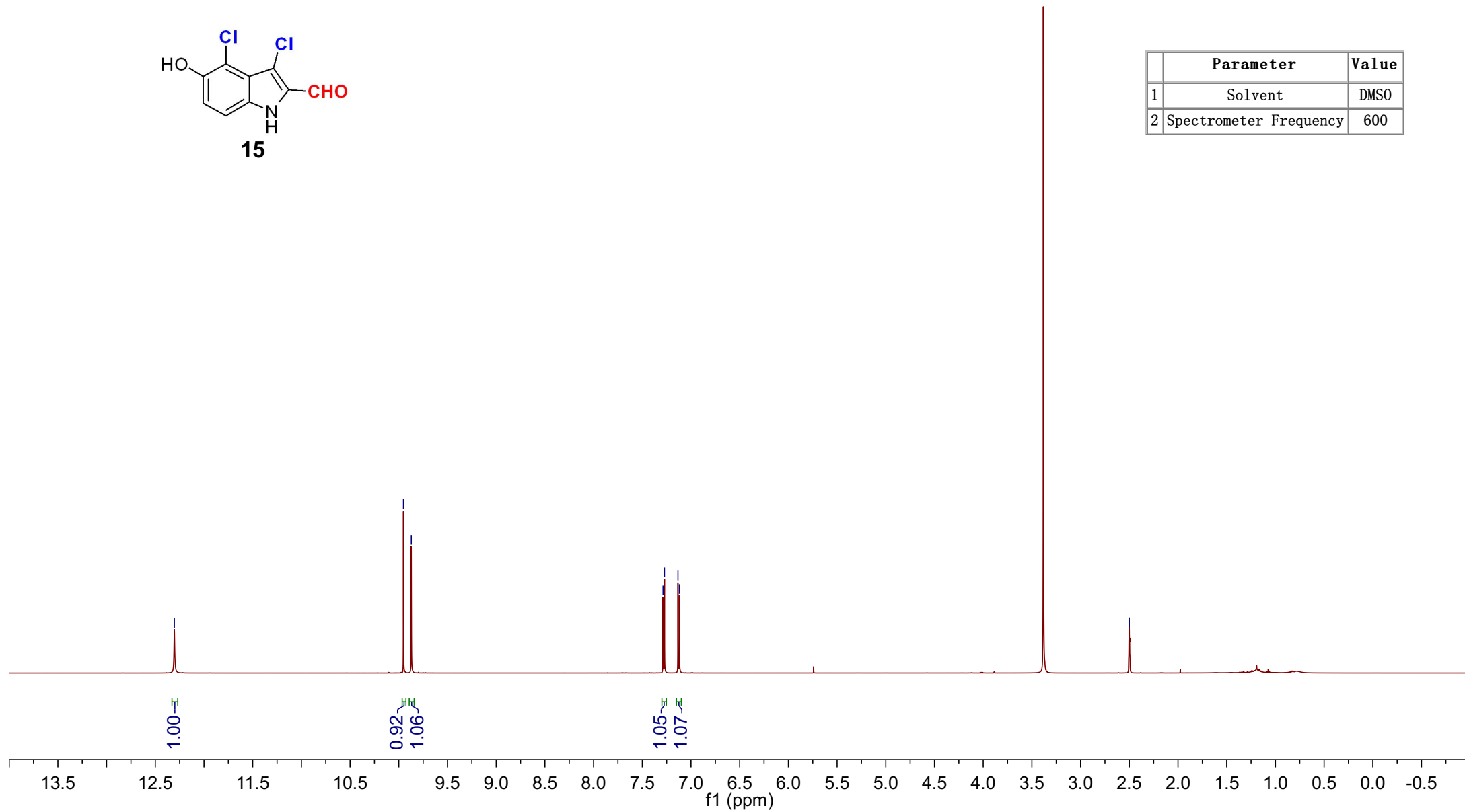
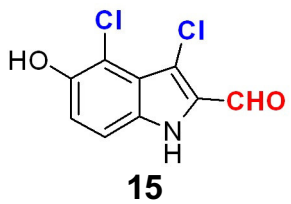
121.02
116.05
113.04
112.56
111.88

—57.37

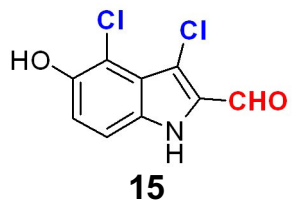
—39.52

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150





	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600



—180.38

—148.27

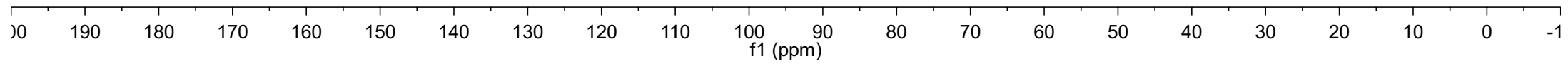
—132.26
—131.37

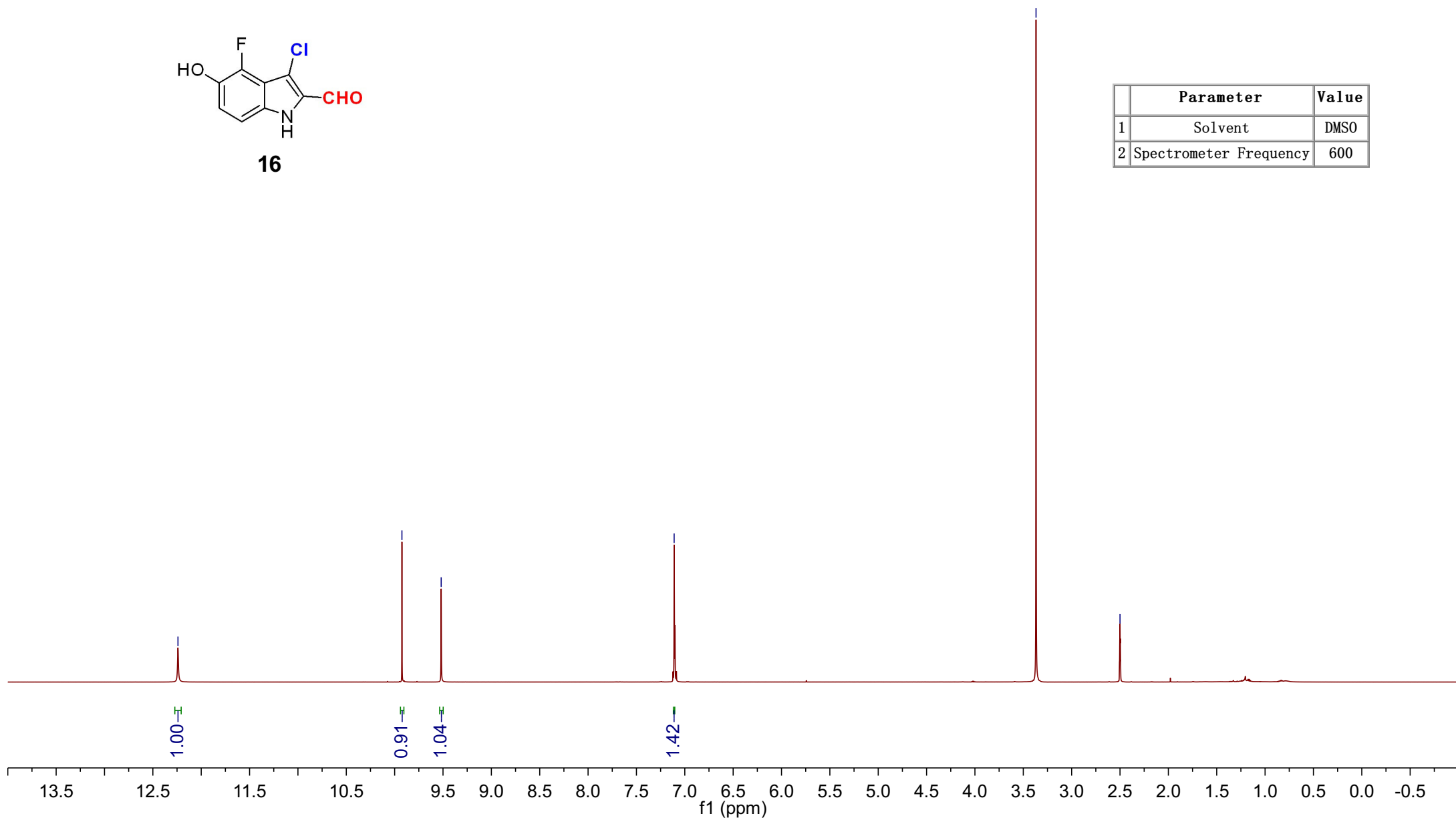
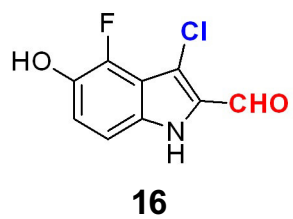
—121.07
—119.56

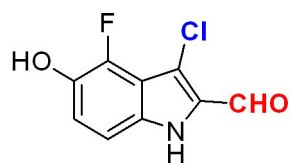
—113.02
—112.47
—108.71

—39.52

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150







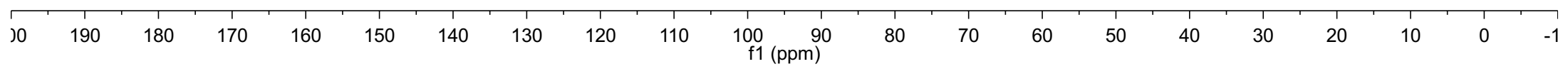
16

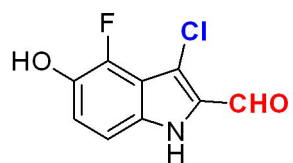
—180.13

143.45
141.83
137.73
137.66
132.31
132.27
130.93
121.19
115.07
114.97
110.51
109.48
109.45

39.52

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150

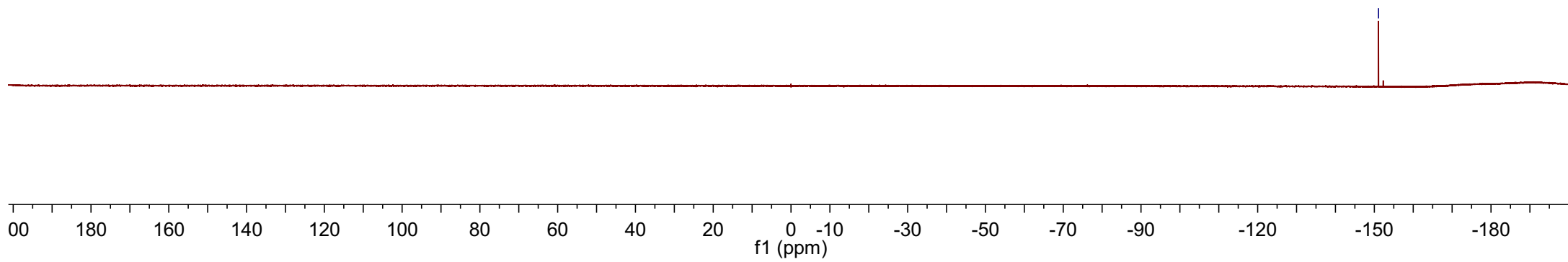


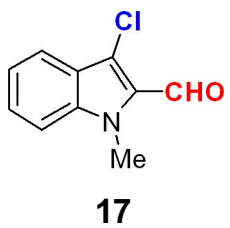


16

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	565

---151.07





—10.15

7.73
7.71
7.47
7.47
7.46
7.45
7.45
7.44
7.44
7.36
7.34
7.26
7.24
7.24
7.23
7.22
7.21
7.21

—4.04

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600

0.95

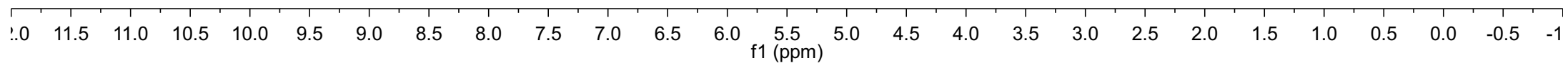
1.00

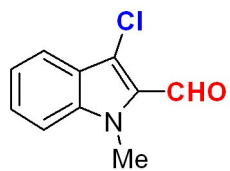
1.02

1.05

1.03

3.11





17

—181.36

—138.75

—129.16

—128.19

—124.33

—121.57

—120.61

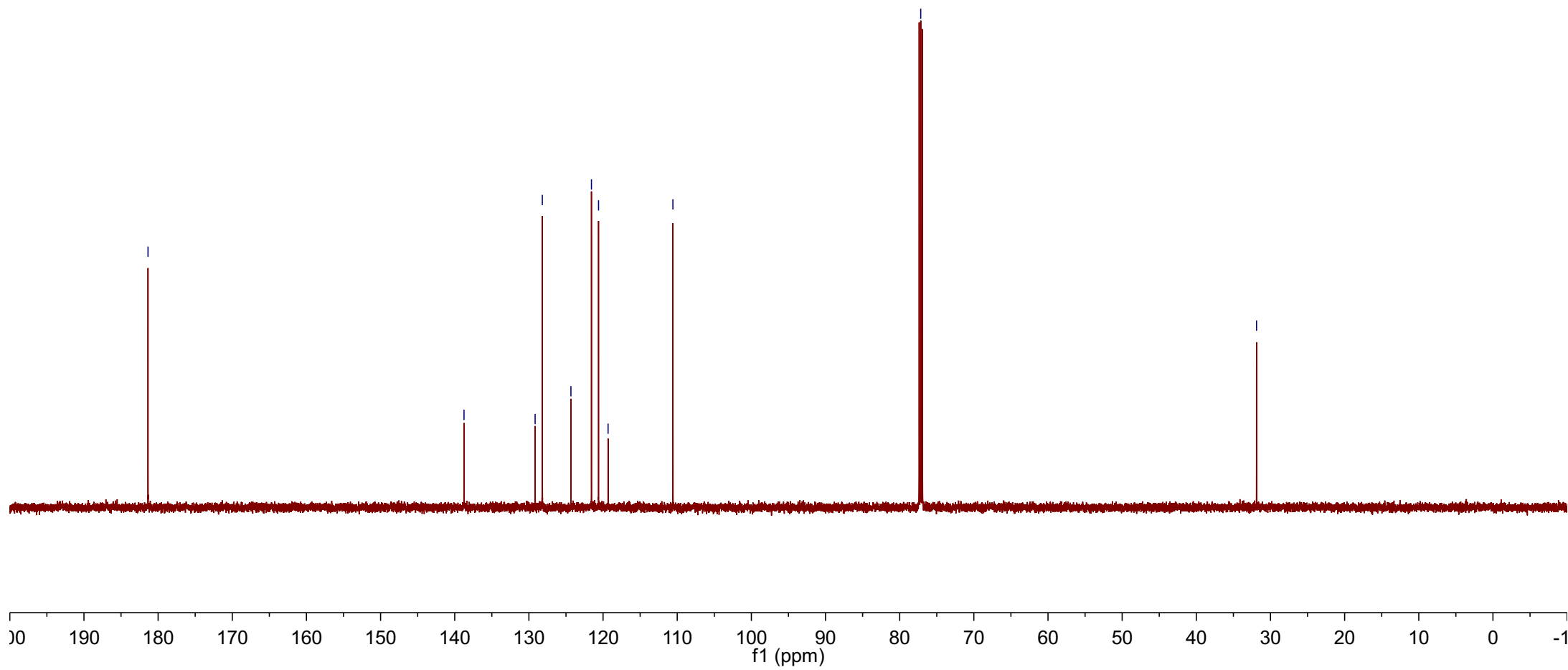
—119.32

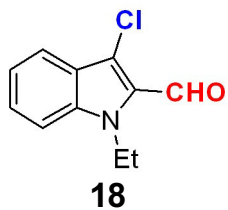
—110.58

—77.16

—31.88

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150





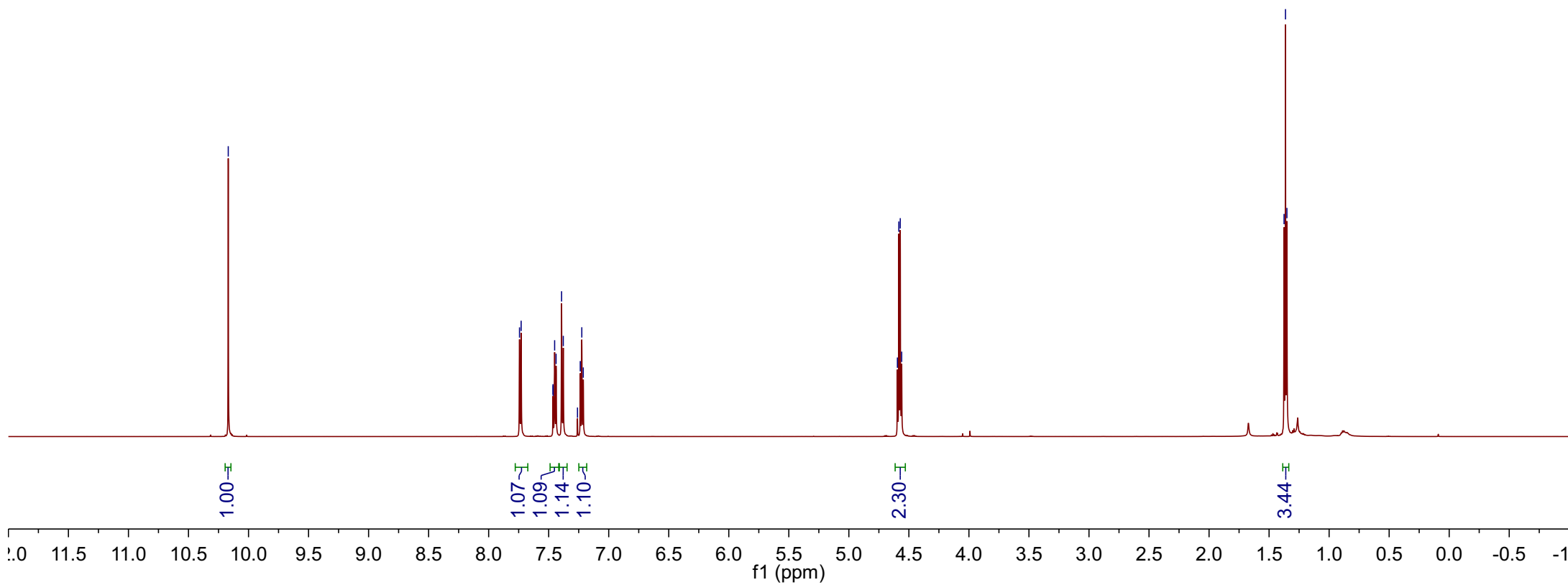
10.17

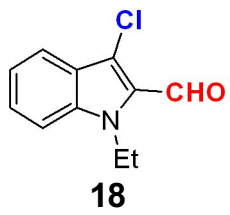
7.74
7.73
7.46
7.46
7.45
7.44
7.39
7.38
7.26
7.24
7.22
7.21

4.60
4.58
4.57
4.56

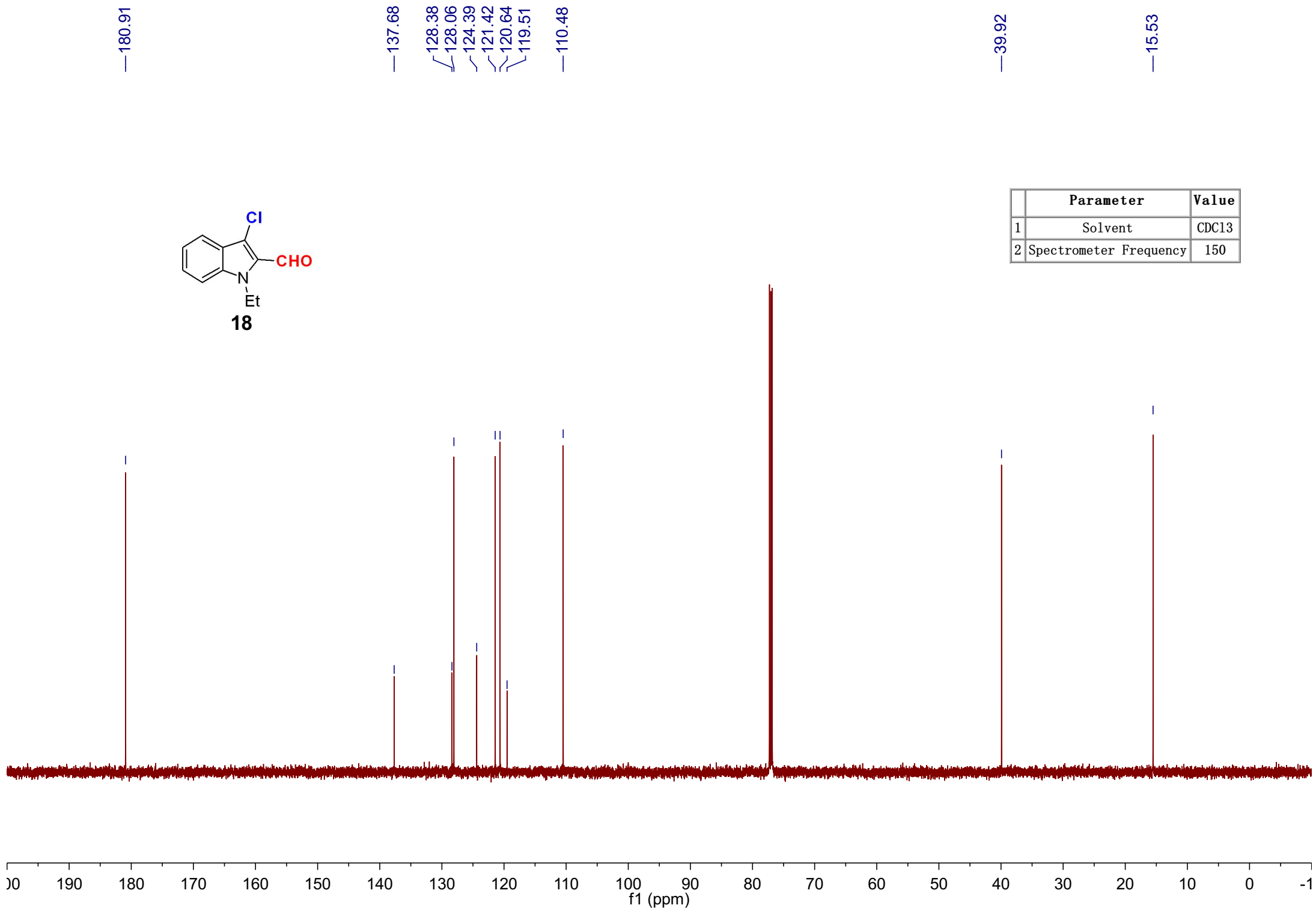
1.38
1.36
1.35

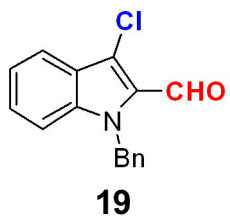
	Parameter	Value
1	Solvent	CDCl3
2	Spectrometer Frequency	600



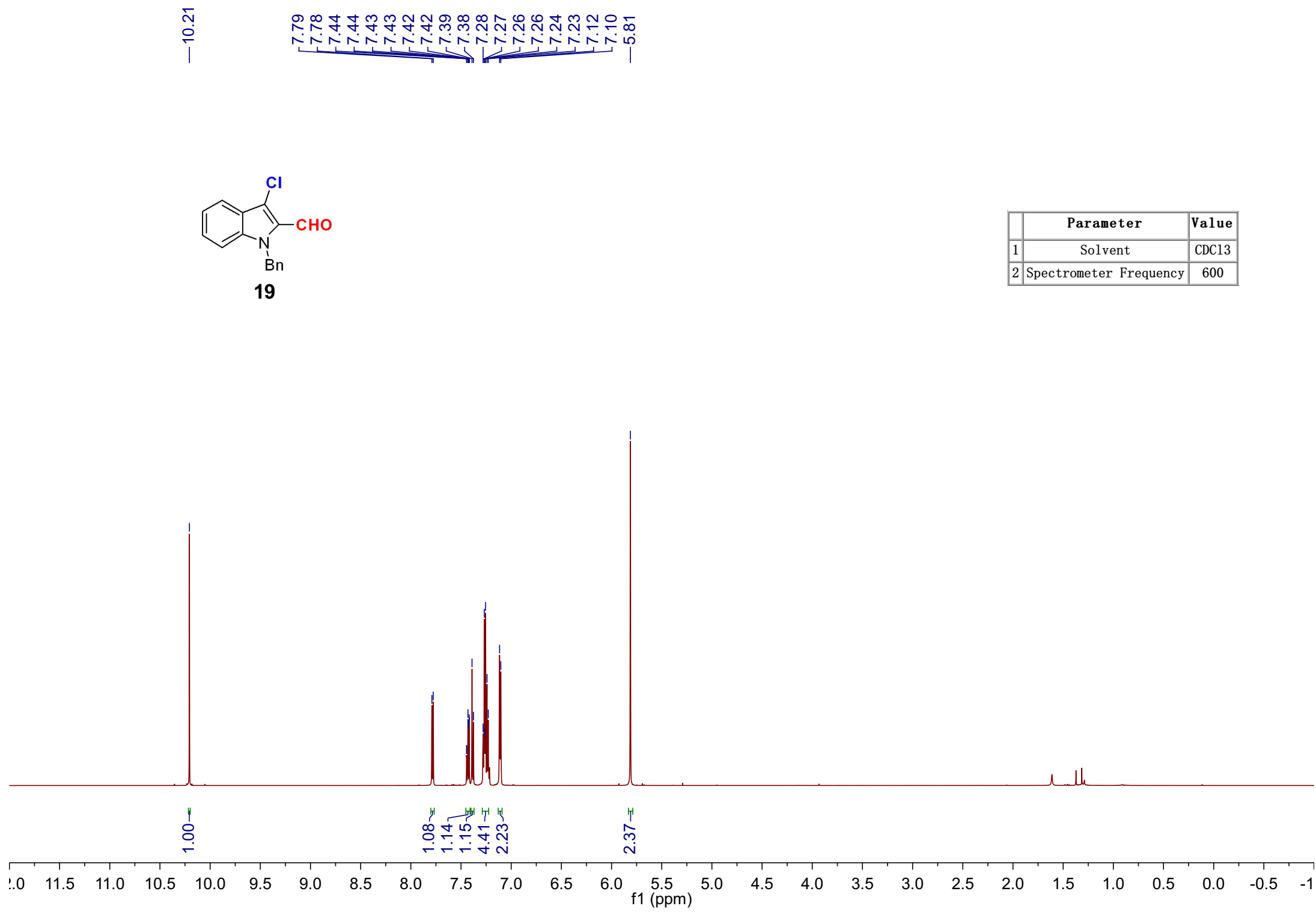


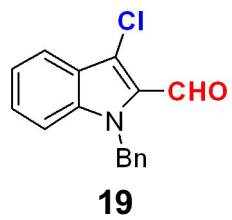
	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150





	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600





—181.08

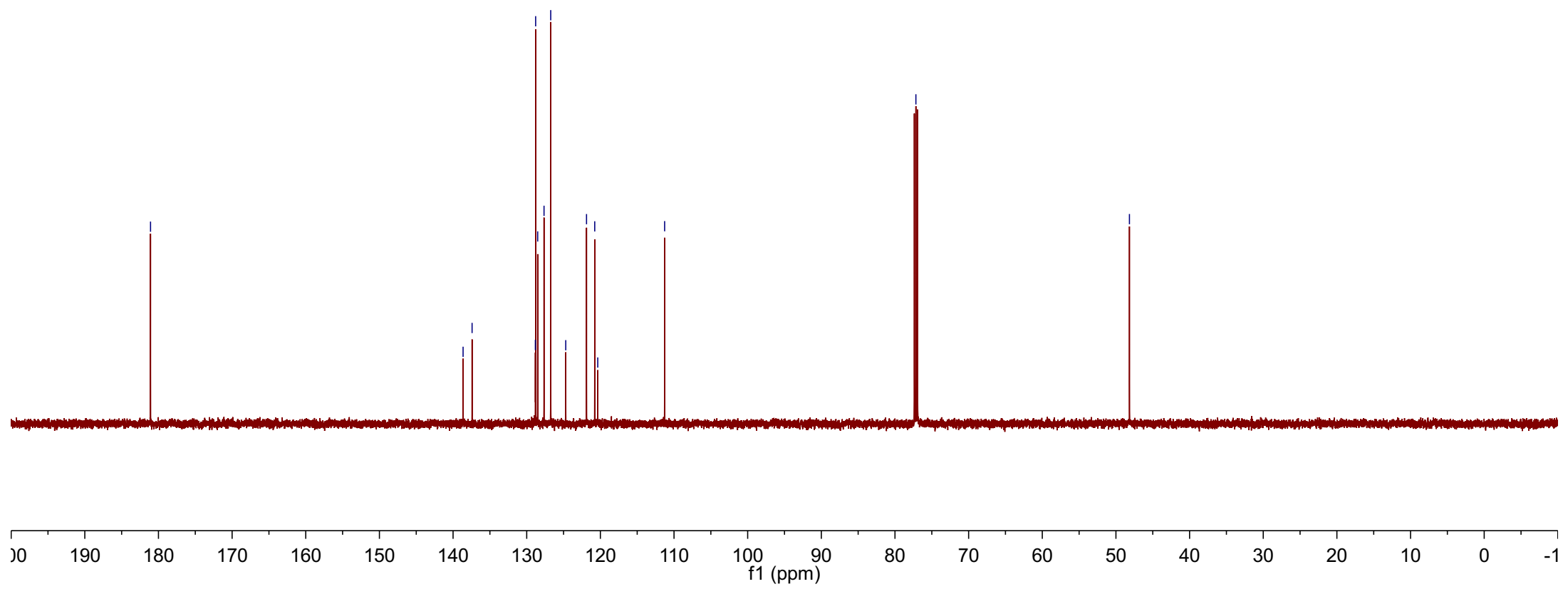
138.64
137.42

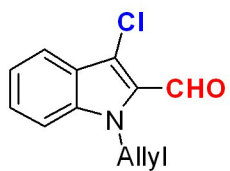
128.83
128.79
128.51
127.65
126.74
121.88
111.28

—77.16

—48.17

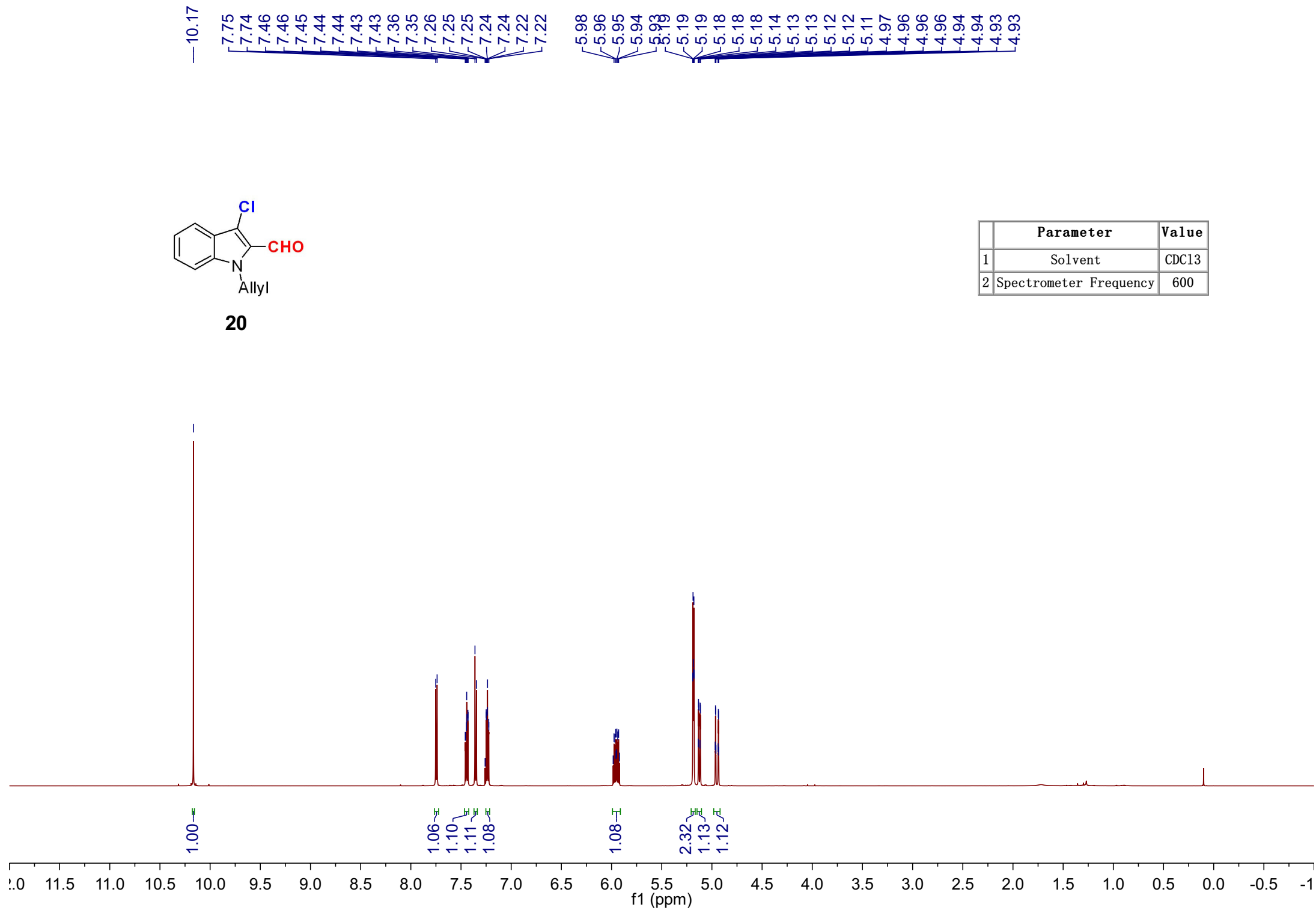
	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150

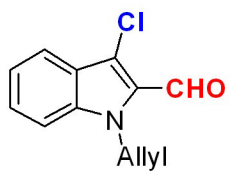




20

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600





20

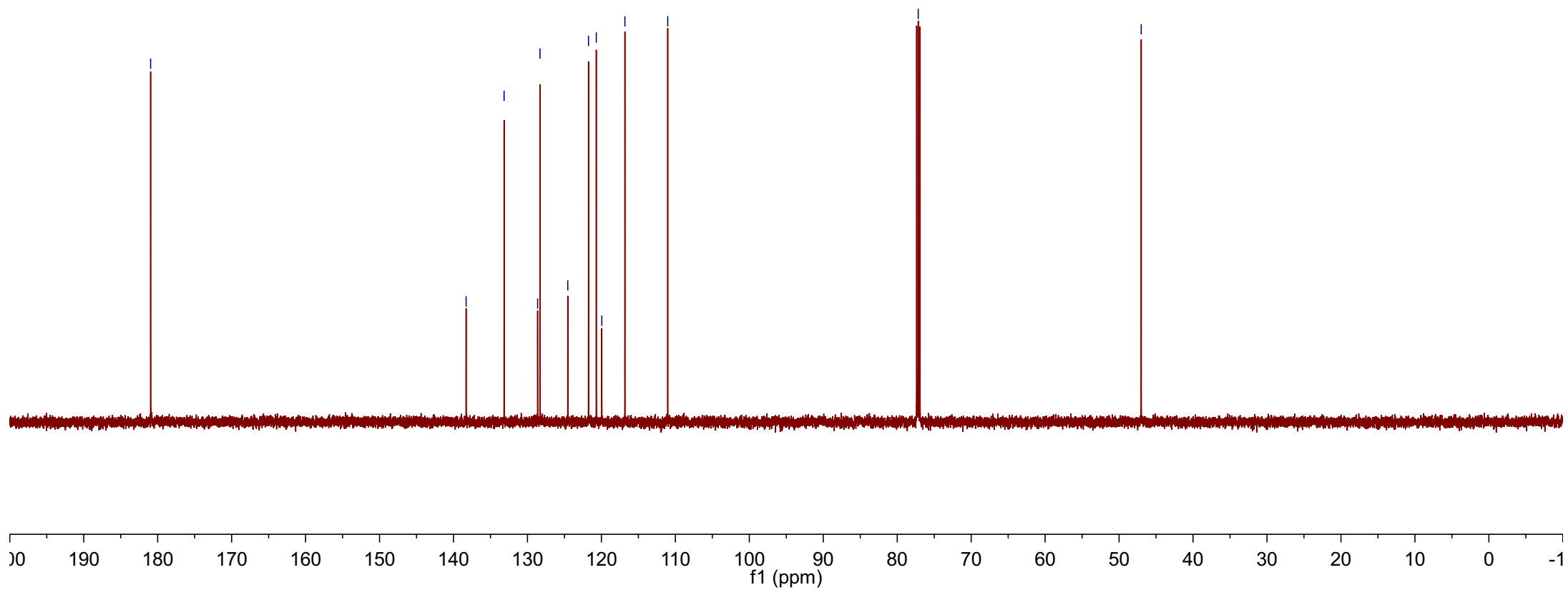
—180.95

—138.29
—133.16
—128.63
—128.30
—124.55
—121.74
—120.69
—119.95
—116.82
—111.03

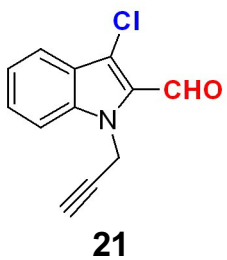
—77.16

—47.01

	Parameter	Value
1	Solvent	CDCl ₃
2	Spectrometer Frequency	150



—10.17

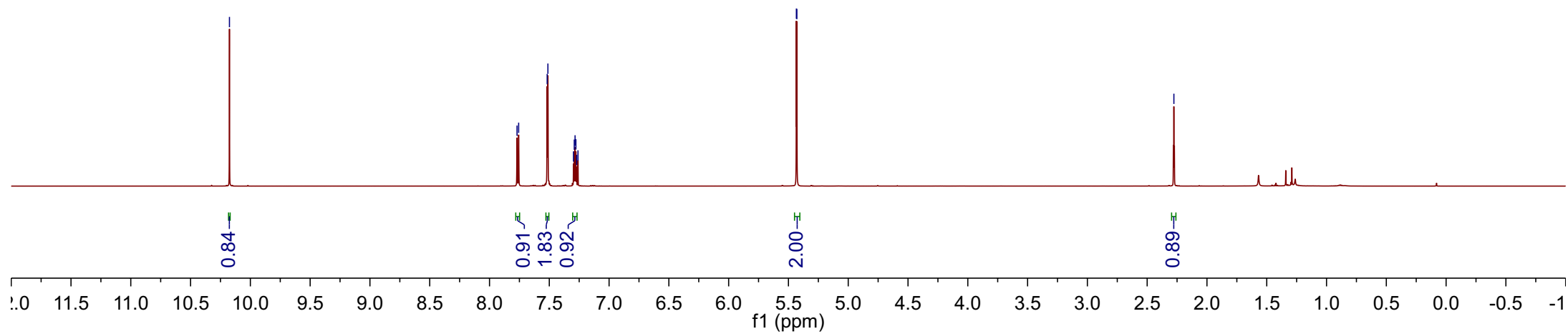


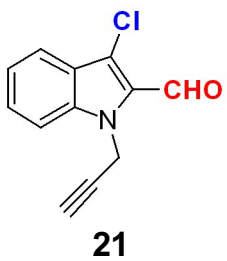
7.77
7.76
7.52
7.51
7.30
7.29
7.28
7.28
7.27
7.26

5.43
5.43

—2.28

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600





—181.03

—138.01

128.61

128.02

124.78

122.10

120.89

120.78

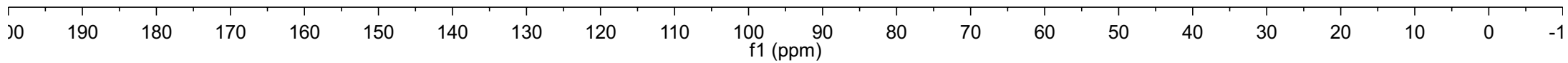
—110.93

—77.85

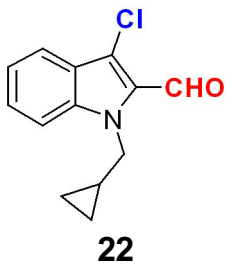
—72.80

—34.03

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150



—10.18

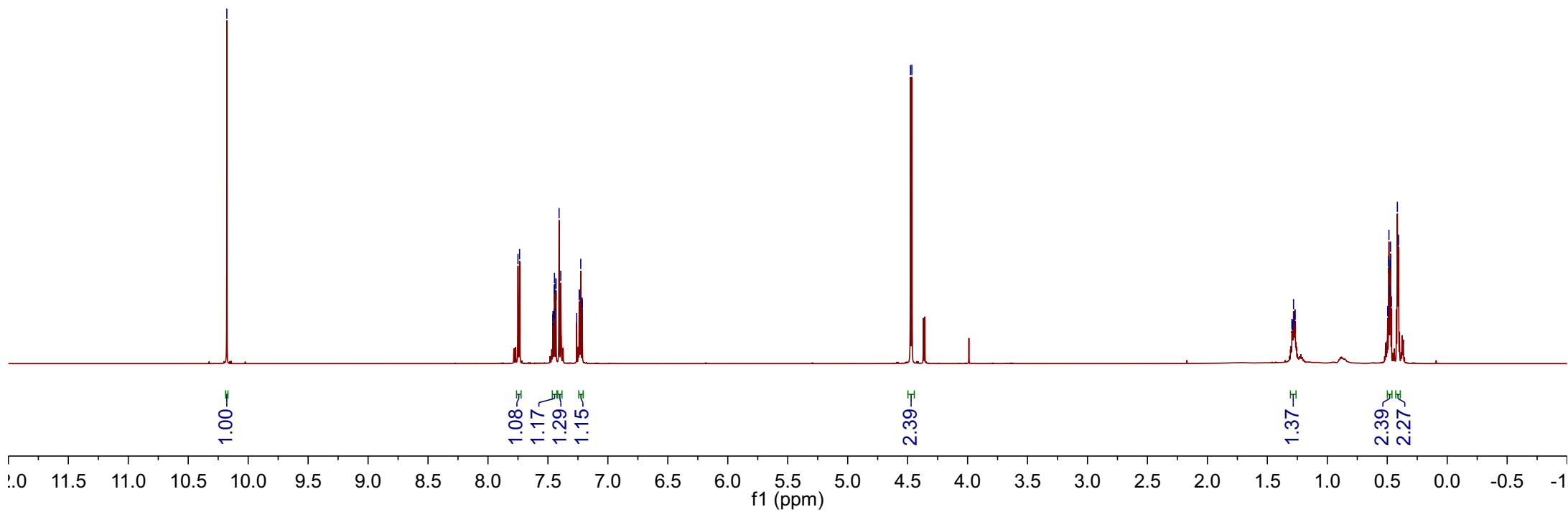


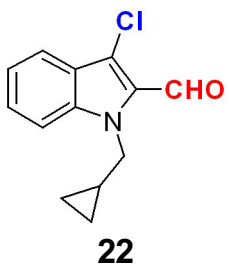
7.75
7.74
7.46
7.46
7.45
7.45
7.44
7.43
7.43
7.41
7.39
7.26
7.24
7.24
7.23
7.21
7.21

4.48
4.46

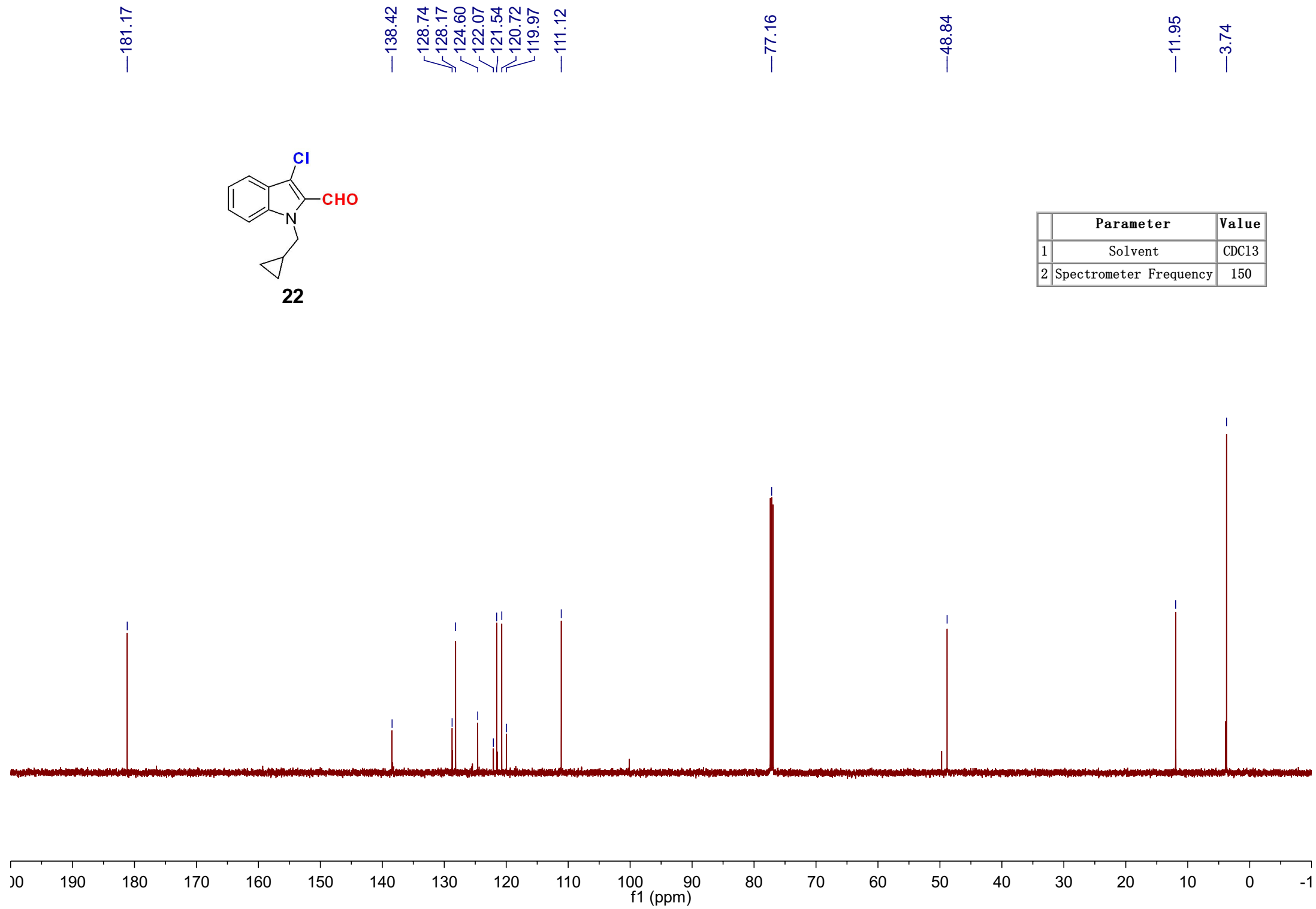
1.30
1.29
1.29
1.28
1.27
1.27
1.27
0.50
0.49
0.49
0.48
0.48
0.47
0.47
0.42
0.41
0.41

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600





	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150

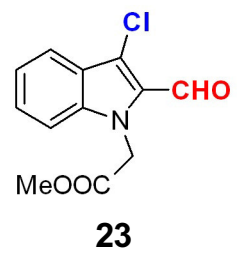


—10.13

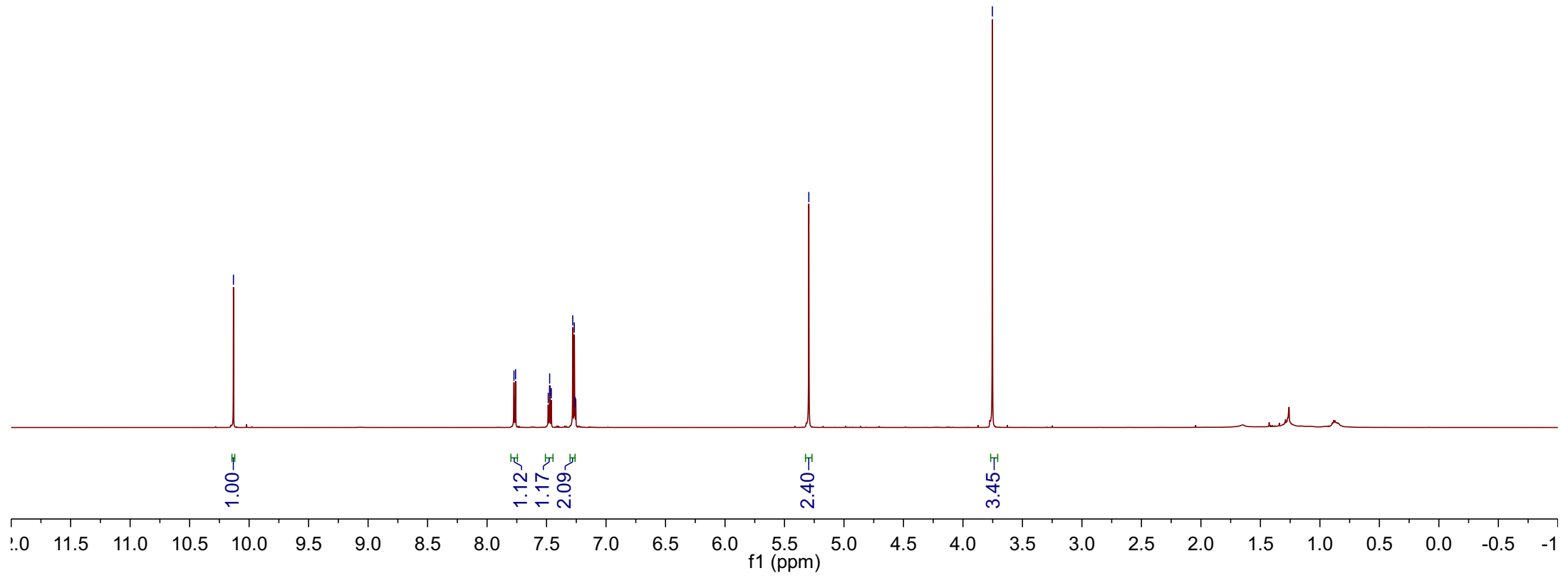
7.77
7.76
7.49
7.47
7.47
7.46
7.28
7.27
7.26

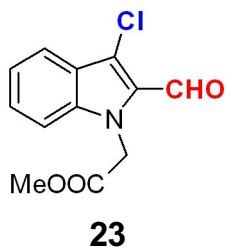
—5.30

—3.75

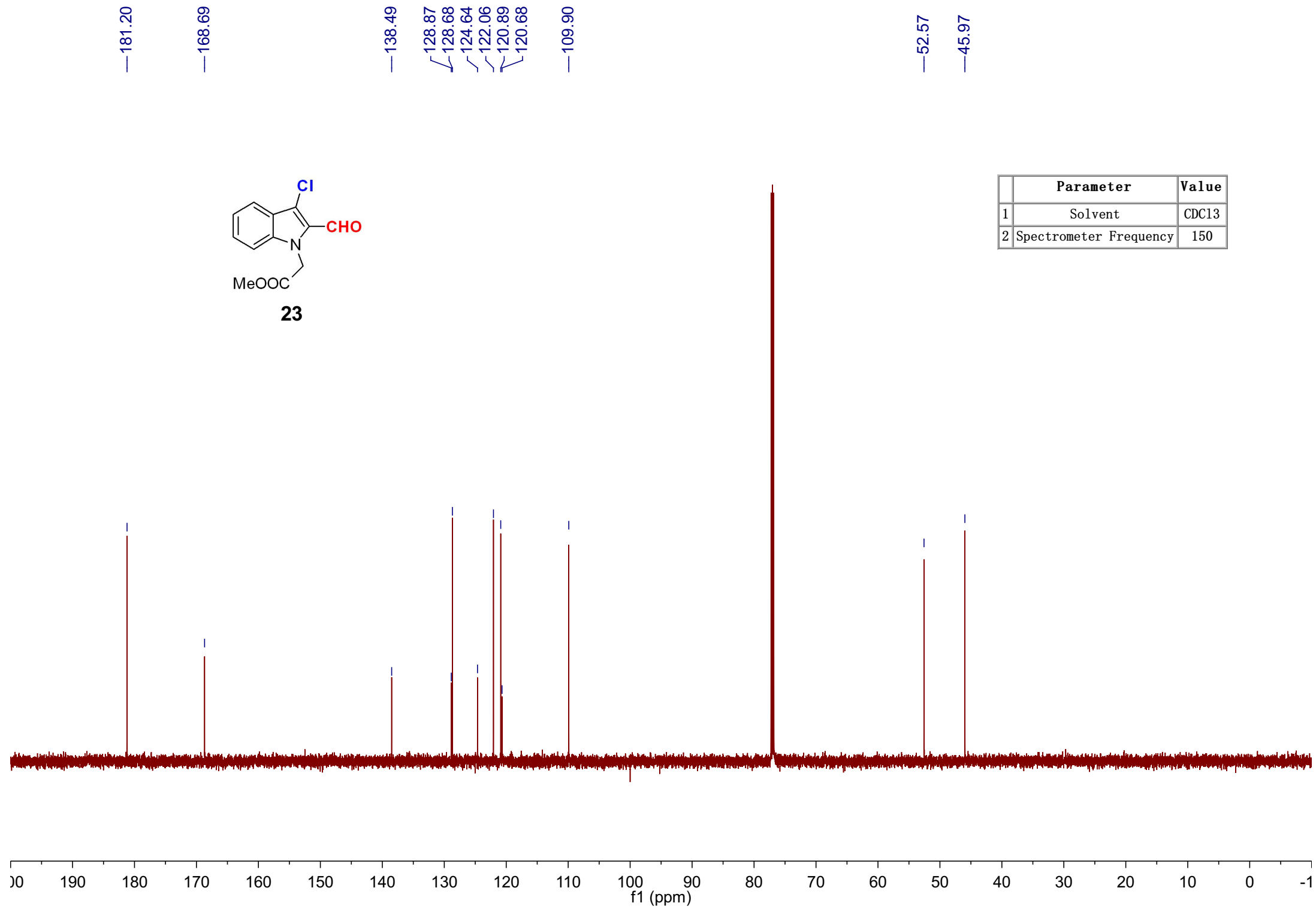


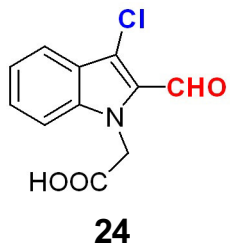
	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600



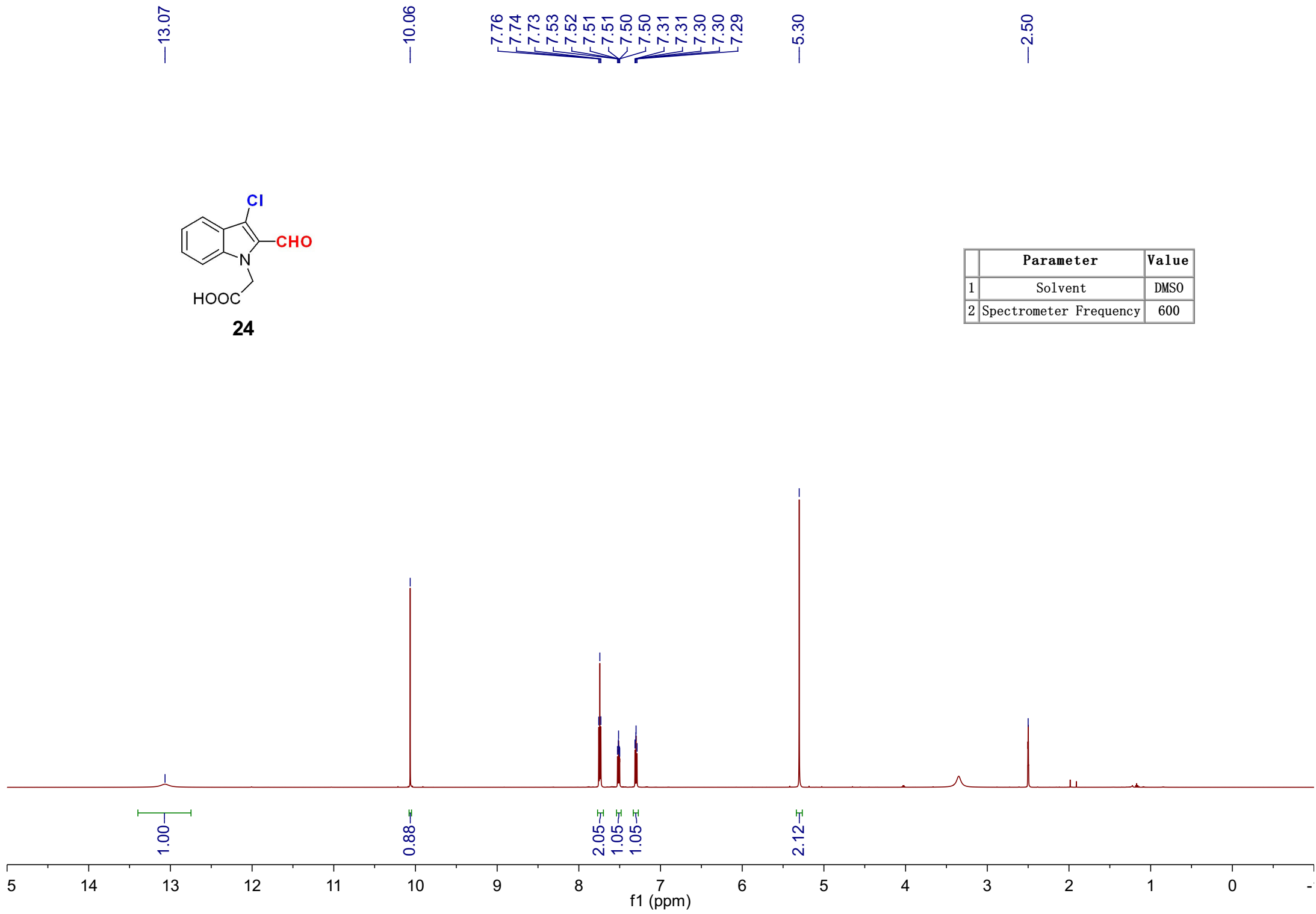


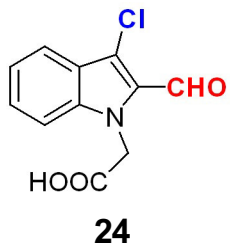
	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150





	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600

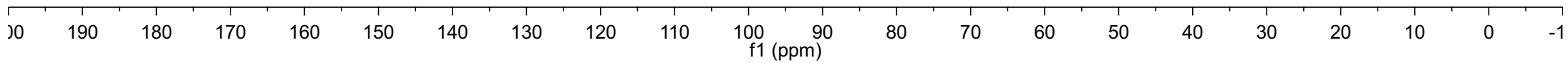


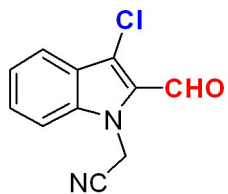


—181.07
—169.82
—138.24
128.76
128.32
123.40
122.08
119.73
117.62
—111.56

—46.18
—39.52

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150





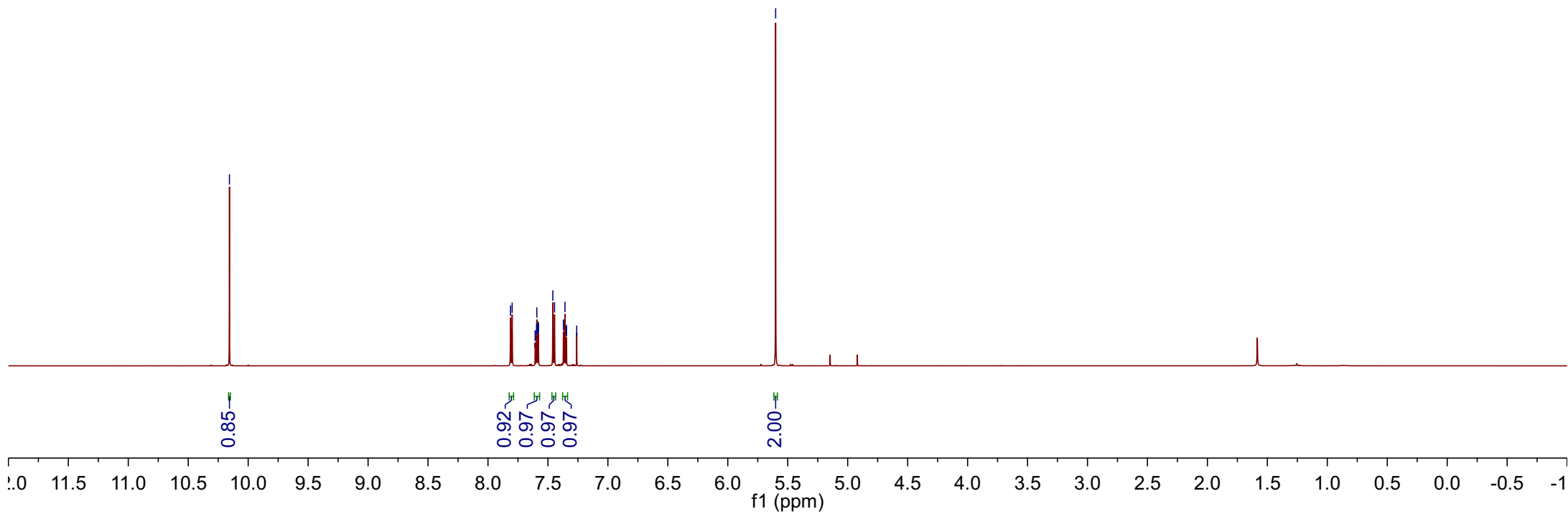
25

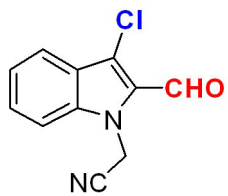
—10.16

7.81
7.80
7.61
7.60
7.59
7.59
7.59
7.58
7.58
7.46
7.44
7.37
7.37
7.36
7.35
7.34
7.26

—5.60

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600





25

—181.26

—137.94

—129.79

—127.88

—125.14

—123.14

—122.58

—121.44

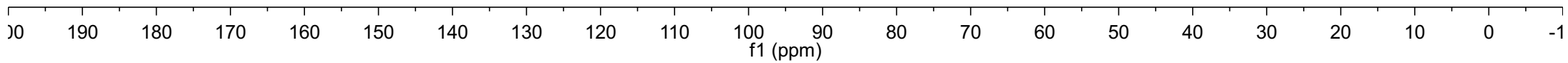
—114.34

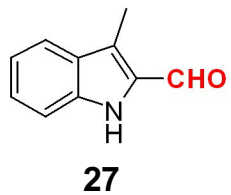
—110.07

—77.16

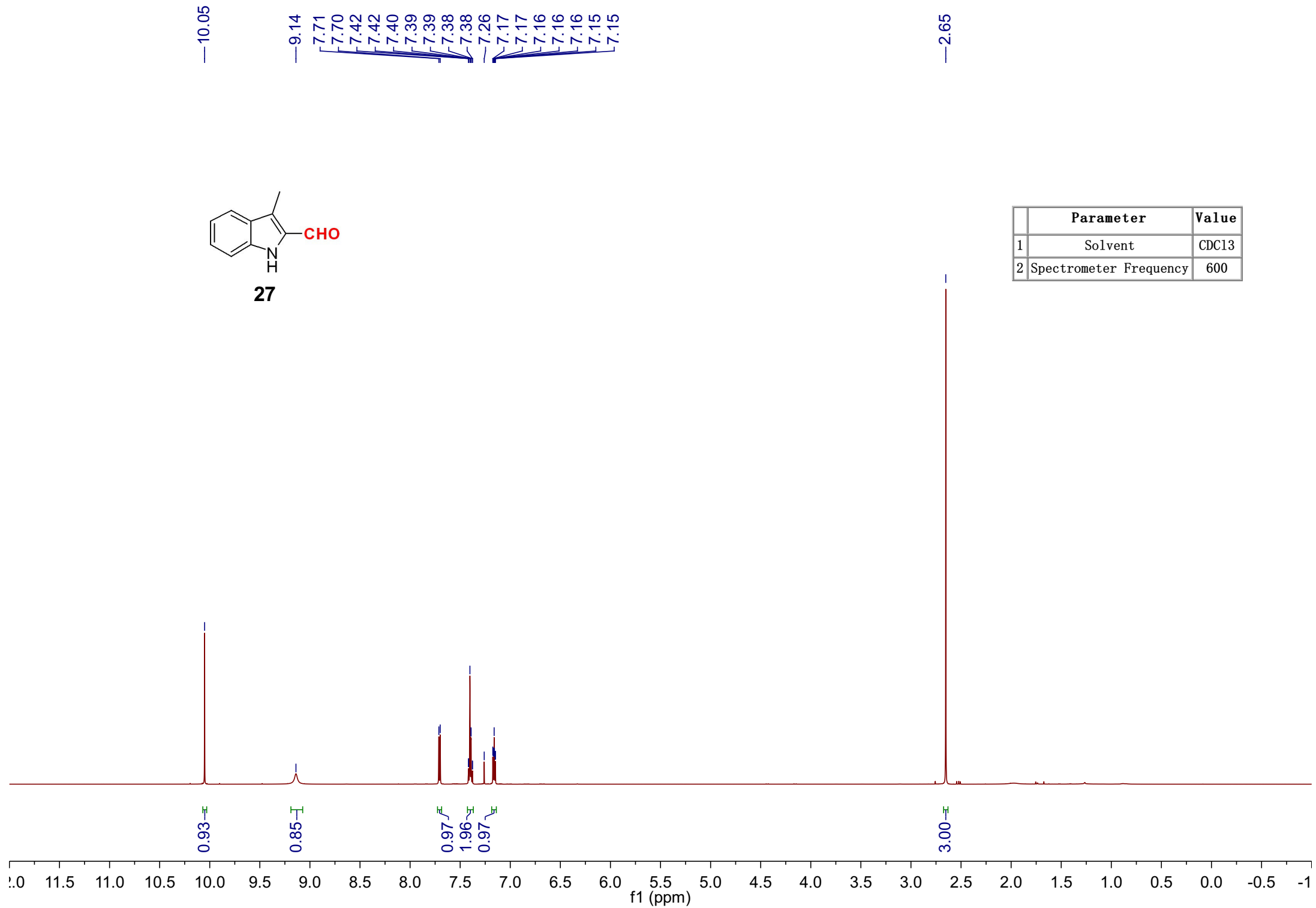
—32.52

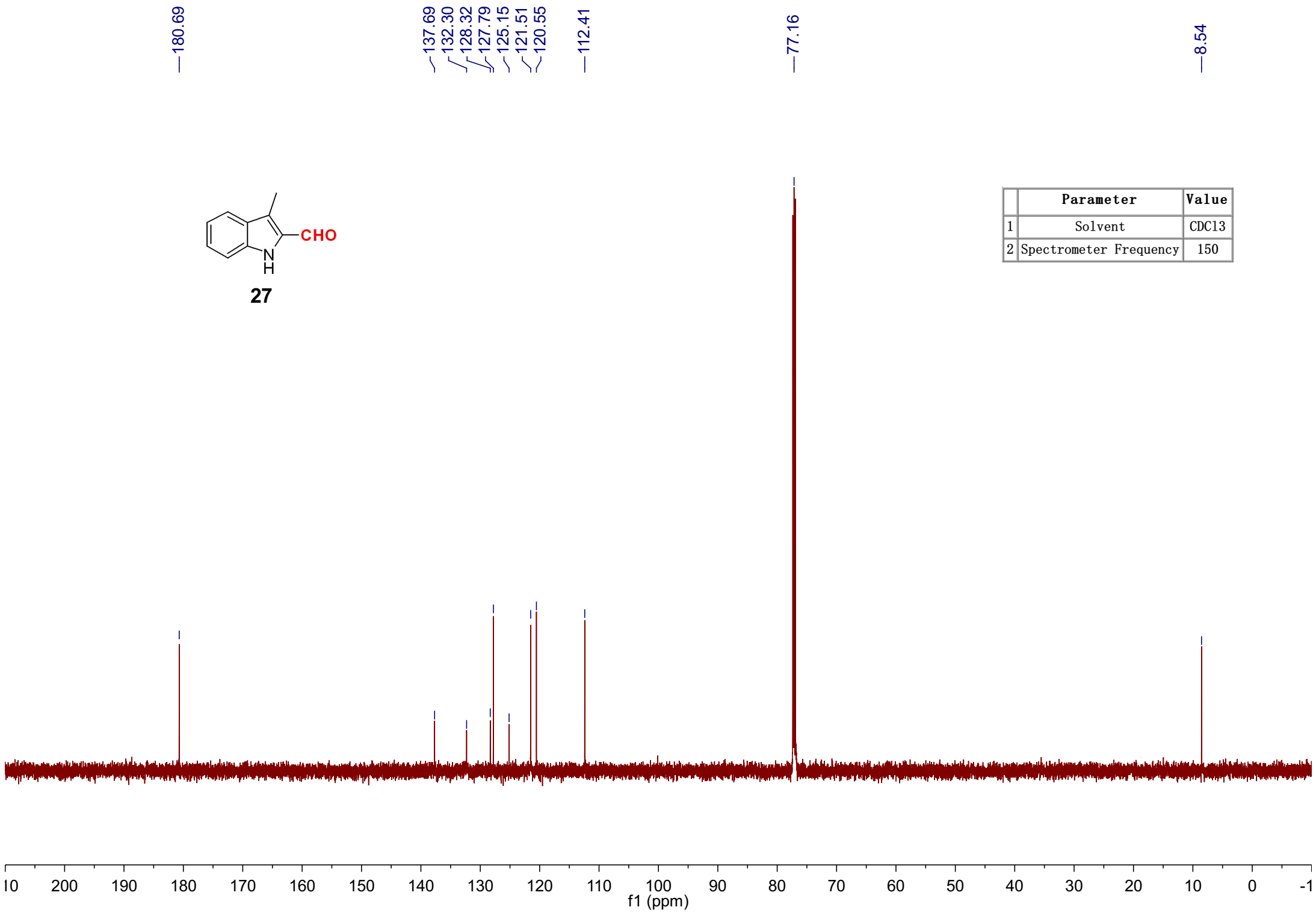
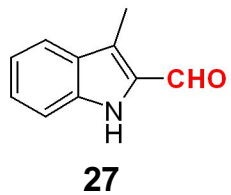
	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150



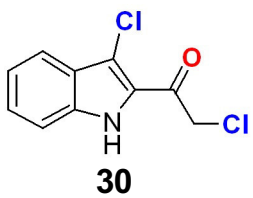


	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600





	Parameter	Value
1	Solvent	CDCl3
2	Spectrometer Frequency	150



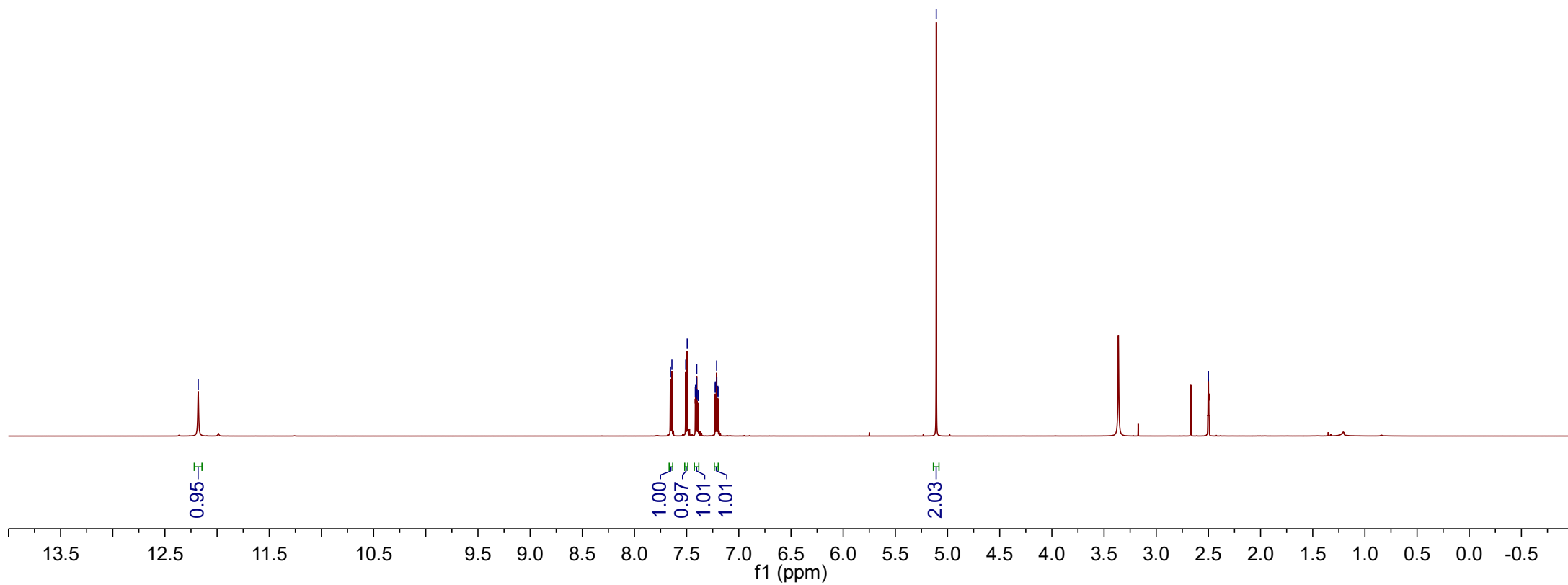
—12.18

7.65
7.64
7.51
7.49
7.42
7.42
7.41
7.40
7.40
7.39
7.39
7.23
7.22
7.21
7.21
7.20
7.20

—5.11

—2.50

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	600



—182.86

—135.78

—128.59

—127.08

—124.95

—121.43

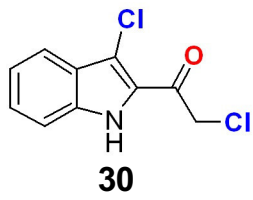
—119.65

—113.28

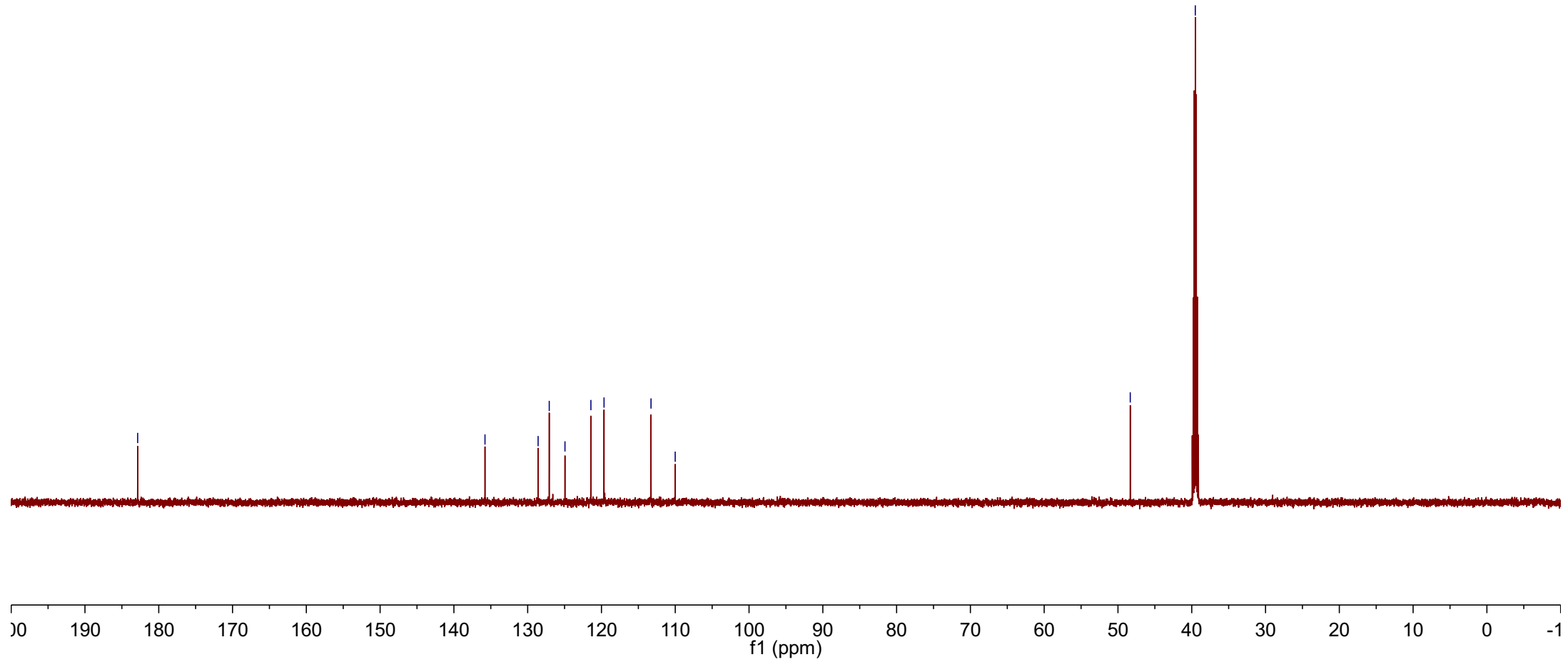
—110.01

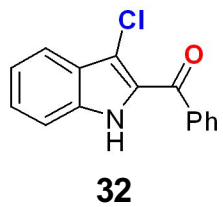
—48.34

—39.52



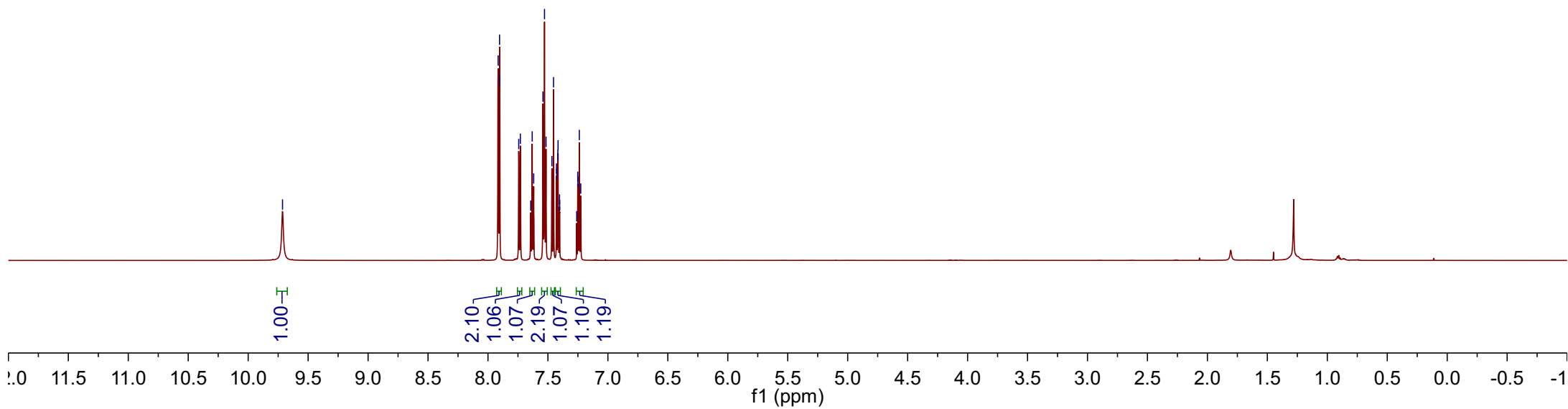
	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150





	Parameter	Value
1	Solvent	CDCl ₃
2	Spectrometer Frequency	600

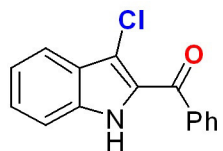
9.71
7.92
7.90
7.90
7.74
7.73
7.64
7.63
7.62
7.54
7.53
7.52
7.47
7.45
7.43
7.43
7.42
7.42
7.40
7.40
7.26
7.25
7.25
7.24
7.23



—188.06

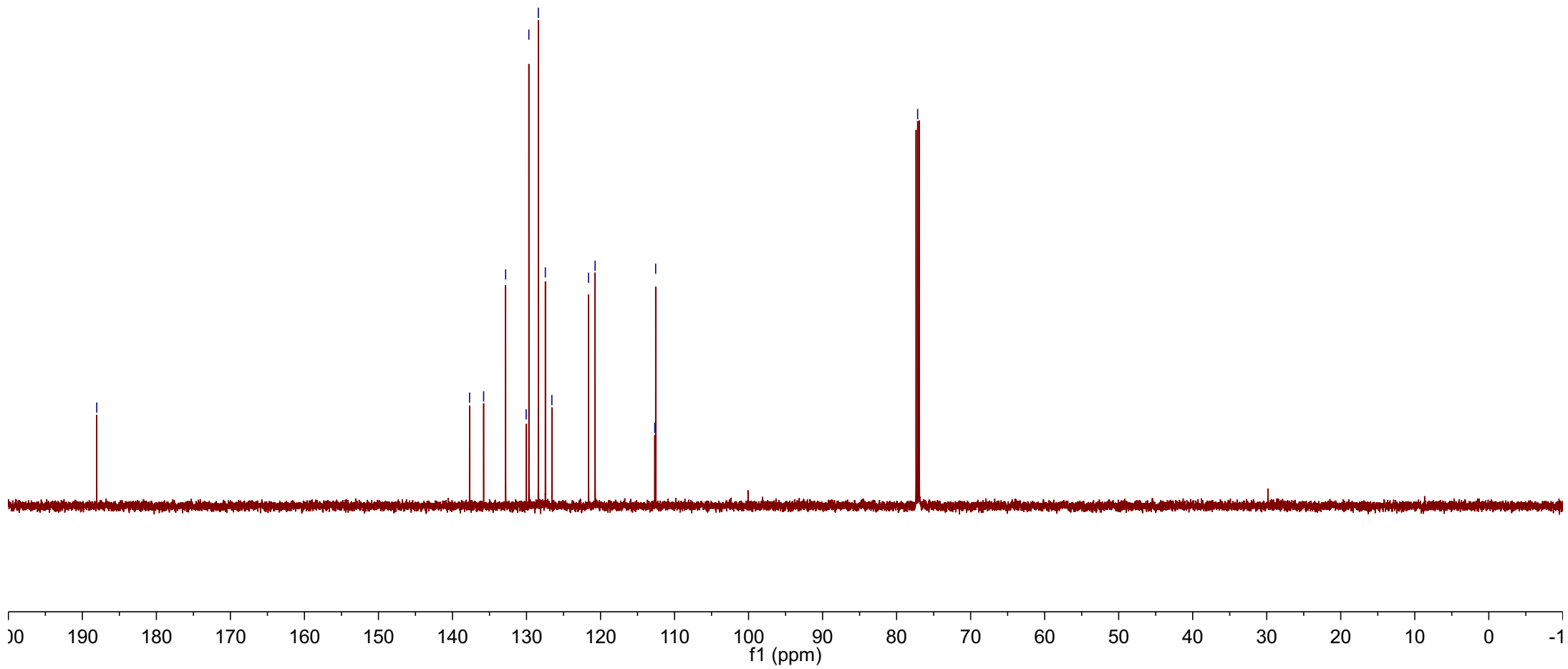
137.69
135.79
132.82
130.04
129.68
128.40
127.46
126.57
121.62
120.73
112.67
112.55

—77.16

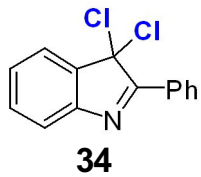


32

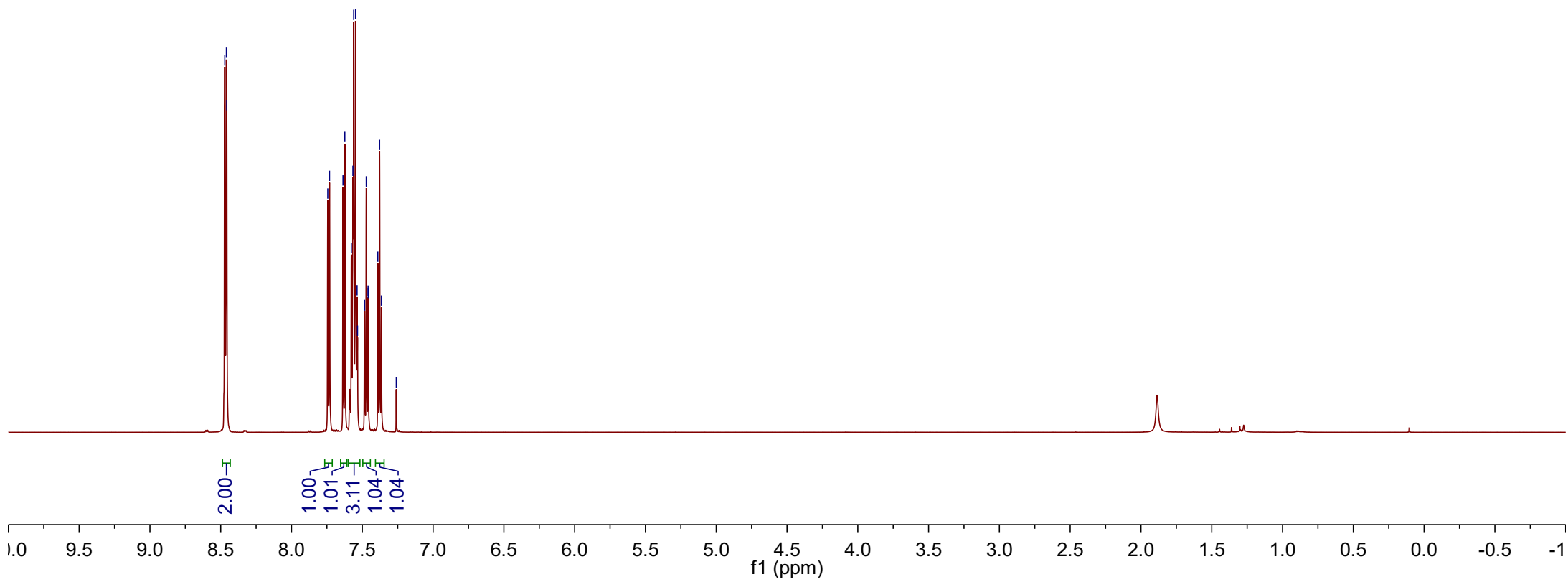
	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150



8.47
8.46
8.46
7.74
7.73
7.64
7.62
7.58
7.57
7.56
7.55
7.54
7.53
7.48
7.48
7.47
7.47
7.46
7.46
7.39
7.38
7.37
7.26



	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600



—172.00

—149.43

—139.95

132.20

131.64

129.53

128.79

128.71

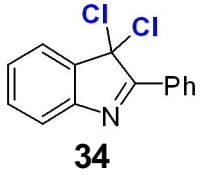
128.00

122.82

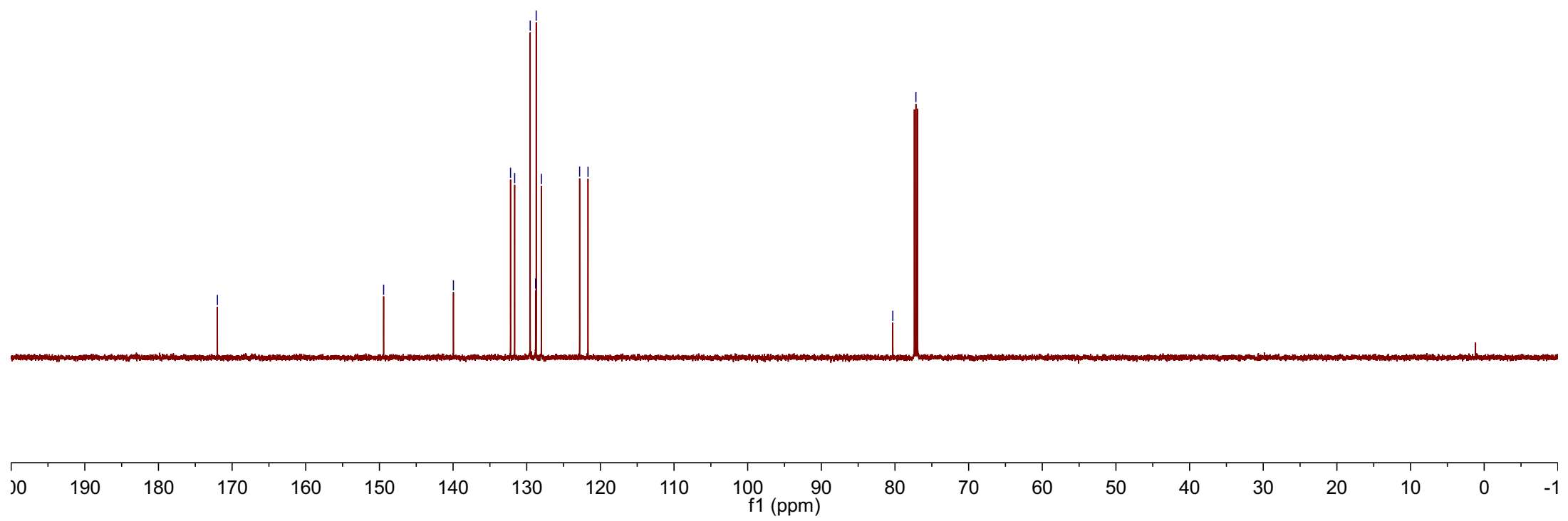
121.68

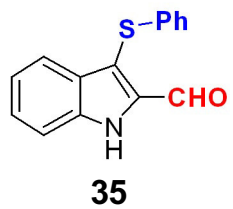
—80.30

—77.16



	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150



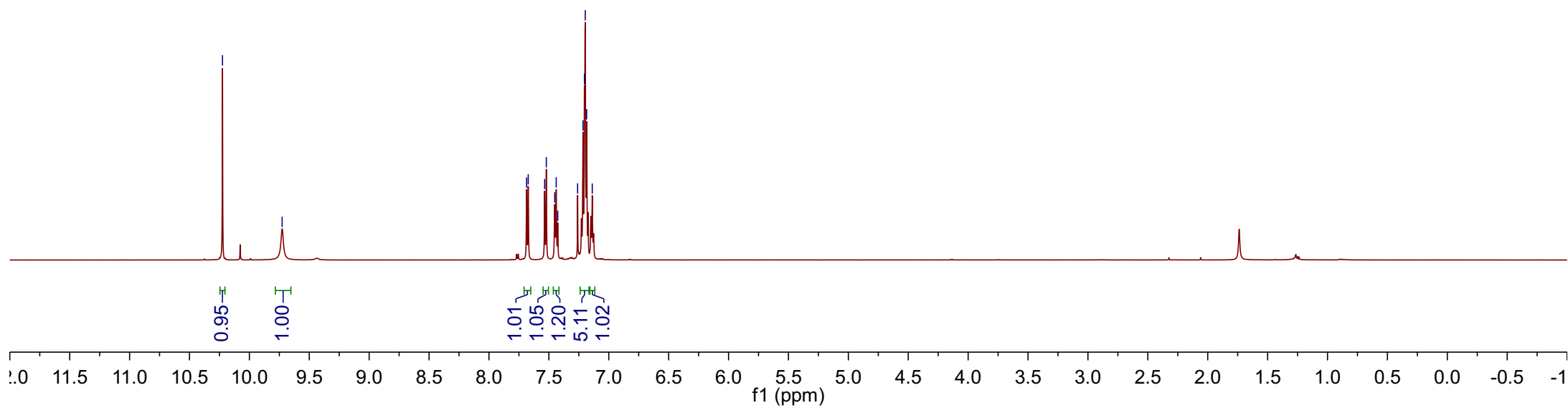


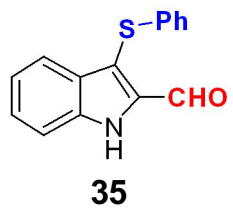
—10.22

—9.73

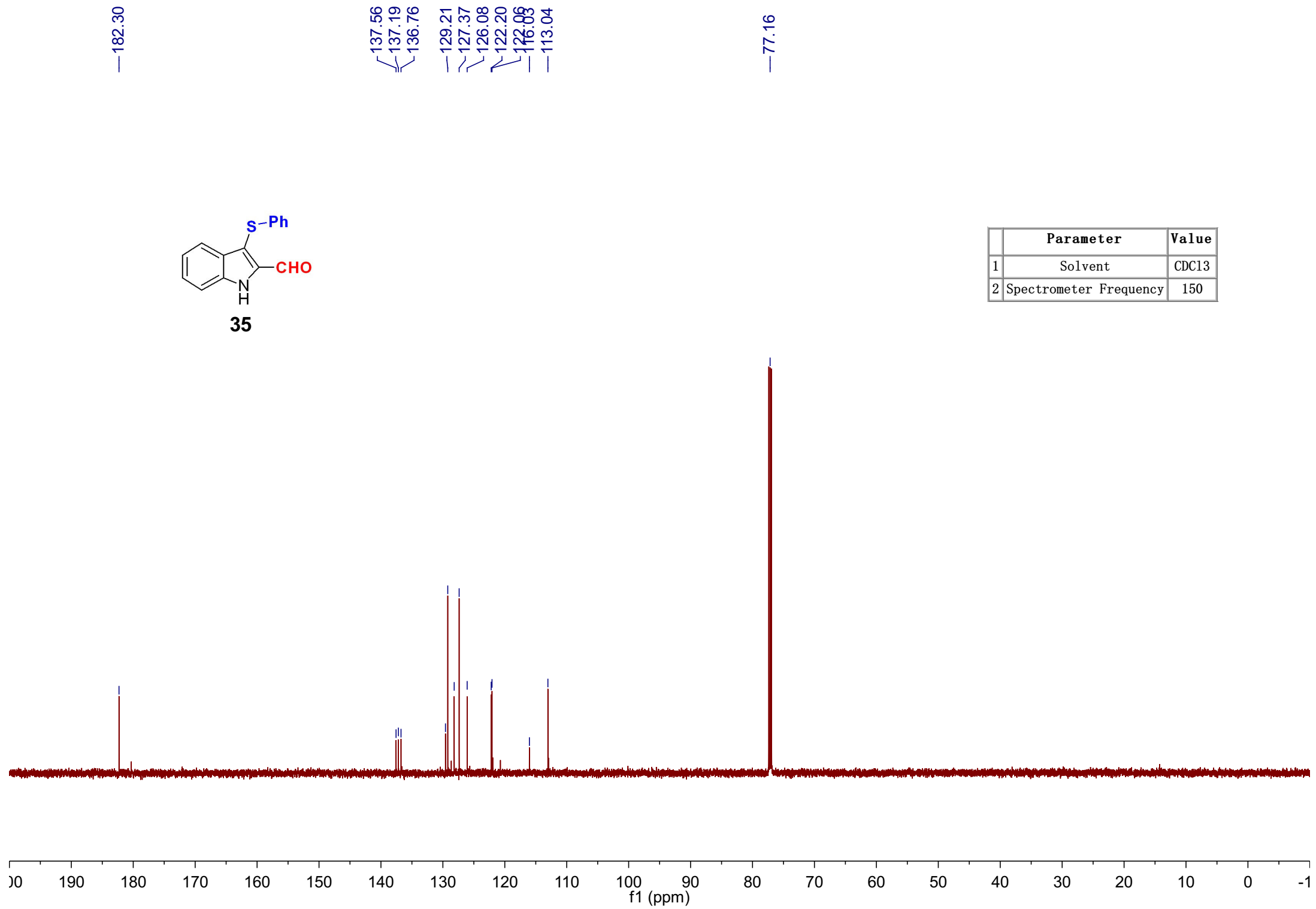
7.69
7.67
7.54
7.52
7.45
7.44
7.43
7.26
7.21
7.20
7.20
7.18
7.14

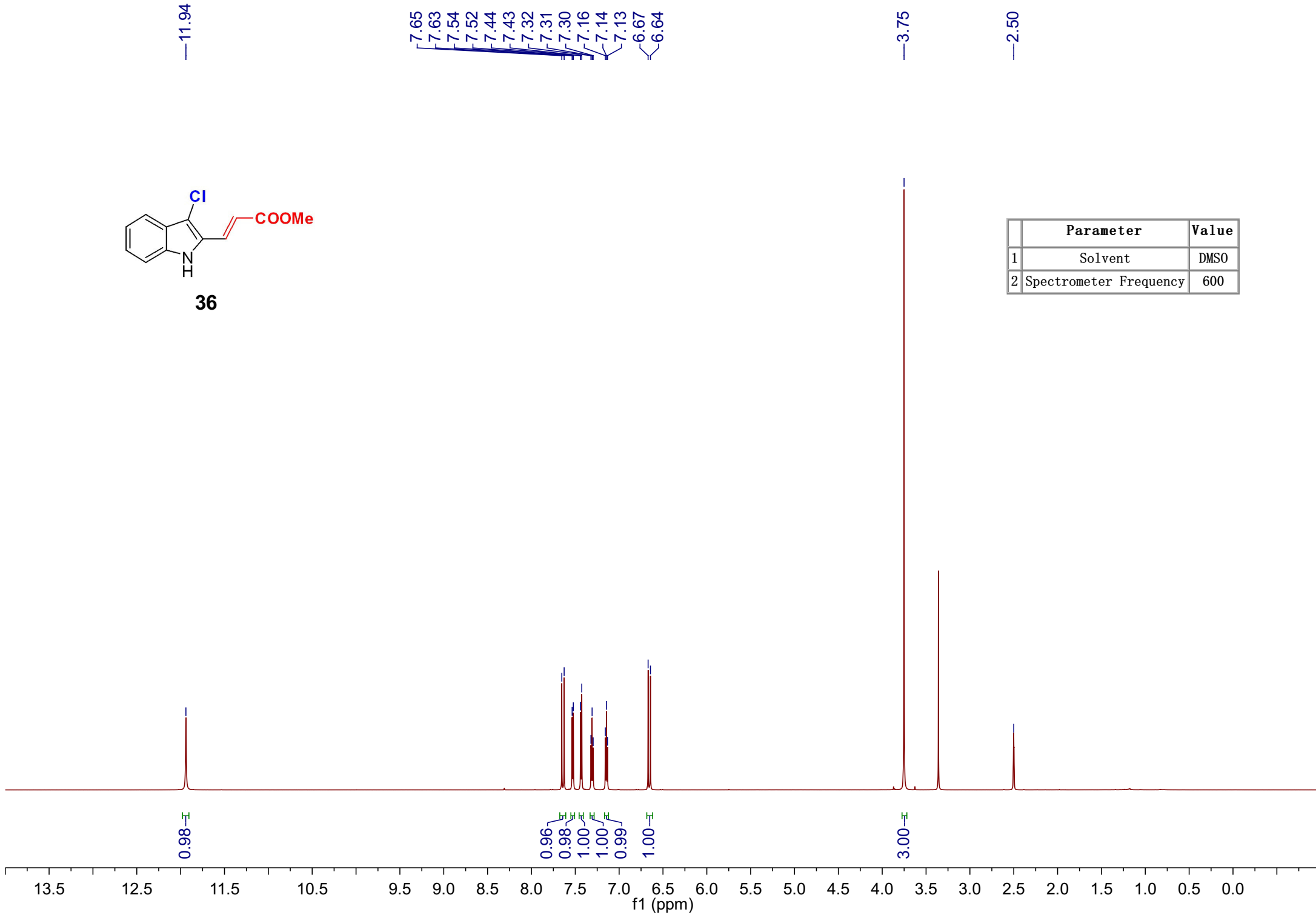
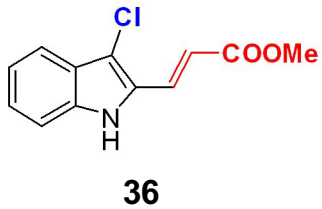
	Parameter	Value
1	Solvent	CDCl3
2	Spectrometer Frequency	600





	Parameter	Value
1	Solvent	CDCl ₃
2	Spectrometer Frequency	150





11.94

7.65
7.63
7.54
7.52
7.44
7.43
7.32
7.31
7.30
7.16
7.14
7.13
6.67
6.64

3.75

2.50

0.98

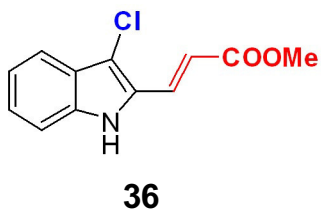
0.96
0.98
1.00
1.00
0.99

1.00

3.00

13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

f1 (ppm)



—166.44

—136.24

—129.86

—128.99

—125.47

—124.98

—120.74

—118.18

—116.84

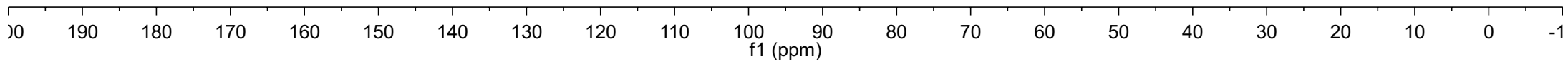
—112.14

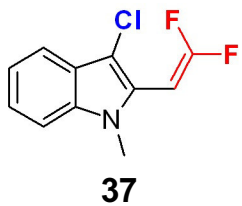
—109.14

—51.68

—39.52

	Parameter	Value
1	Solvent	DMSO
2	Spectrometer Frequency	150



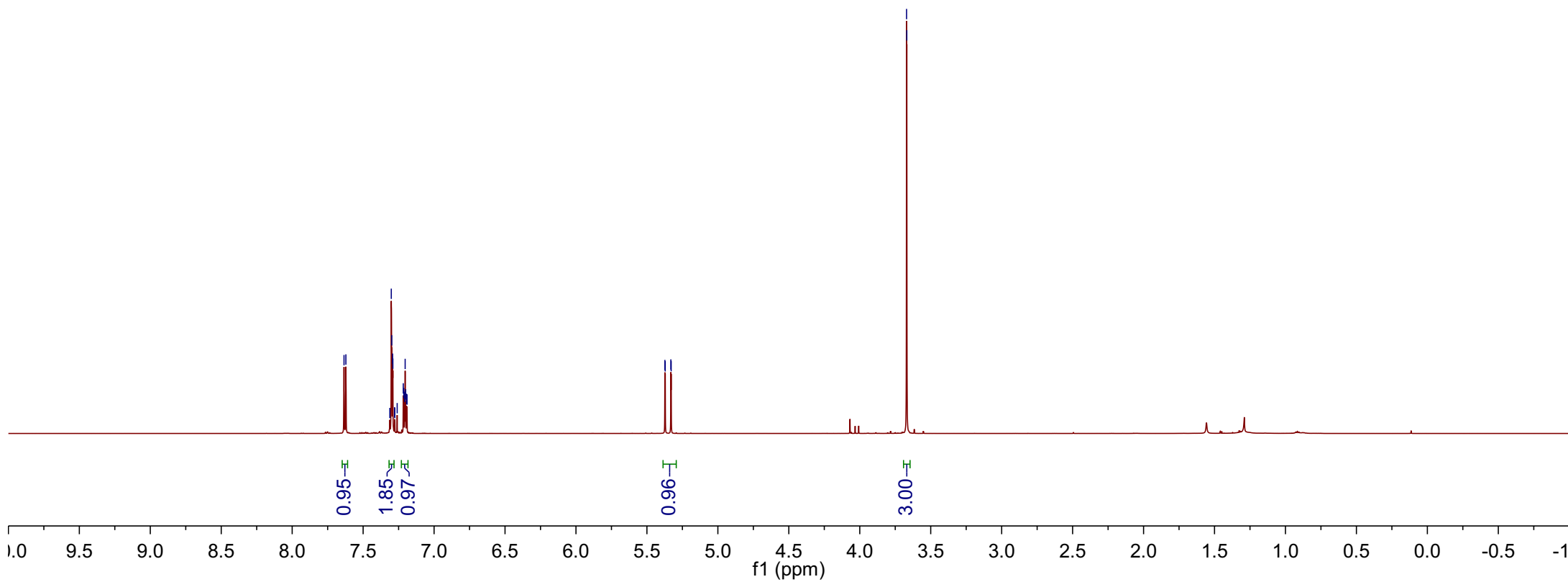


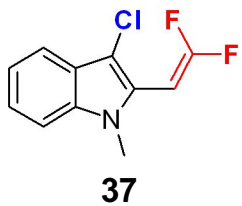
7.63
7.62
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.26
7.22
7.21
7.21
7.20
7.20
7.19
7.19

5.37
5.37
5.33
5.33

3.67
3.67

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	600





158.63
156.70
156.65
154.71

136.39

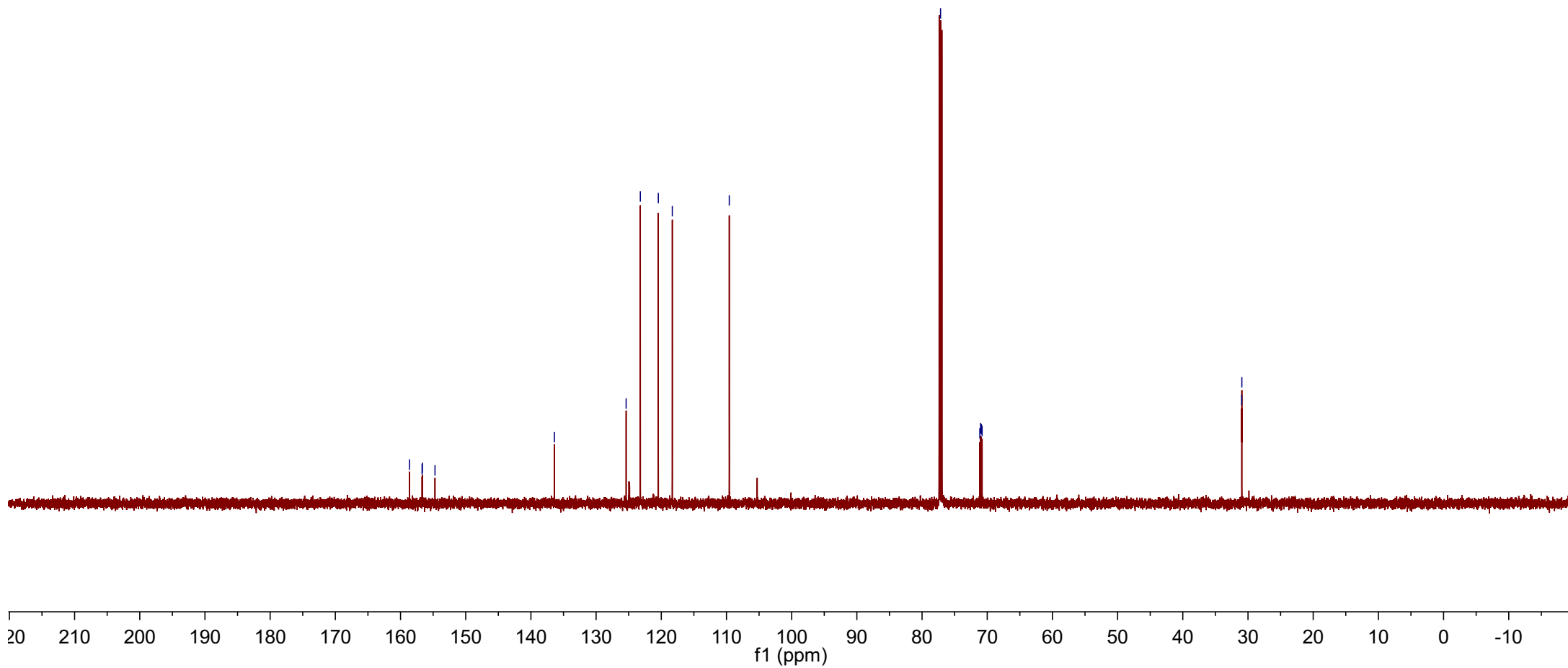
125.39
123.21
120.46
118.31

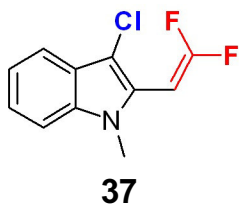
109.57

77.16
71.14
71.02
70.90
70.79

30.96
30.94

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	150





75.98
76.00
76.02
76.05
80.26
80.28

	Parameter	Value
1	Solvent	CDC13
2	Spectrometer Frequency	565

