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Supporting Information

Cobalt(II)-Catalyzed Chelation-Assisted C–H Iodination of Aromatic Amides with I_2

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Contents

I. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer in $CDCl_3$ with tetramethylsilane as the internal standard. Data are reported as follows: chemical shifts in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublet, q = quartet, brs = broad singlet, and m = multiplet), coupling constant (Hz), and integration. Infrared spectra (IR) were obtained using a JASCO FT/IR-4200 spectrometer; absorptions are reported in reciprocal centimeters with the following relative intensities: s (strong), m (medium), or w (weak). Mass spectra and high resolution mass spectra (HRMS) were obtained using a JEOL JMS-700 spectrometer. Melting points were determined using a Stanford Research Systems apparatus. Column chromatography was performed with SiO_2 (Silicycle SiliaFlash F60 (230-400 mesh)). Some compounds were purified by LC-908 HPLC (GPC).

II. Materials

$Co(OAc)_2{\cdot}4H_2O$ (CAS 6147-53-1) was purchased from Wako Pure Chemical Industries, Ltd. Ag_2CO_3 (CAS 534-16-7) was purchased from Nacalai Tesque. Iodine (CAS 7553-56-2) and 8-aminoquinoline (CAS 578-66-5) were purchased from Tokyo Chemical Industry Co., Ltd. KOTf (CAS 2926-27-4) and DCE (CAS 107-06-2) were purchased from Sigma-Aldrich. These reagents were used as received. 5-Chloroquinolin-8-amine (CAS 5432-09-7) and 5-methoxyquinolin-8-amine (CAS 30465-68-0) were prepared by using literature procedures.[1, 2]

III. Synthesis of Starting Amides

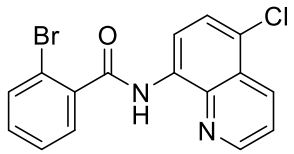
All amides bearing an 5-chloro-8-aminoquinolinyl moiety were prepared by reacting the corresponding acid or acid chloride with 5-chloro-8-aminoquinoline.[3] The amides for **1a**-**1e**, **1g**, and **1i**-**1o** were prepared by using literature procedures.[2]

VI. General Procedure for the Preparation of Starting Amide

To an oven dried two neck round bottom flask, the acid chloride (5.0 mmol) dissolved in CH_2Cl_2 (12 mL) and the resulting reaction mixture was cool to 0 ^{o}C. The solution of 8-amino-5-chloroquinoline (5.5 mmol) and Et_3N (10 mmol) in CH_2Cl_2 (5 mL) was added dropwise to the reaction mixture at 0 ^{o}C. The resulting reaction mixture was allowed to warm to rt and continued for stirring for overnight. The crude reaction mixture was quenched with sat. $NAHCO_3$ and the aqueous layer was extracted with DCM (2 x 15 mL). The combined organic layers were washed with 1 M HCl aq. (30 mL) and brine (30 mL), dried over $MgSO_4$, filtered and evaporated *in vacuo*. The resulting crude amide was purified by column chromatography on silica gel (eluant: hexane/EtOAc = 10/1) to afford the desired amide.

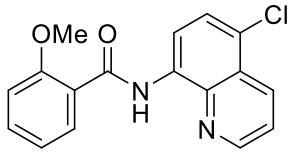
V. Spectroscopic Data for Starting Amides

2-bromo-*N*-(5-chloroquinolin-8-yl)benzamide (1f)



R_f 0.52 (hexane/EtOAc = 4/1). Yellowish green colour solid. MP = 166 °C. ^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.34-7.39 (m, 1H), 7.46 (td, *J* = 7.6, 1.1 Hz, 1H), 7.58 (dd, *J* = 8.5, 4.1 Hz, 1H), 7.67 (d, *J* = 8.5 Hz, 1H), 7.71 (td, *J* = 8.0, 1.2 Hz, 2H), 8.59 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.84 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.90 (d, *J* = 8.5 Hz, 1H), 10.27 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-D) δ: 116.78, 119.65, 122.44, 124.99, 125.99, 127.22, 127.68, 129.61, 131.63, 133.42, 133.56, 133.73, 138.02, 139.14, 148.83, 165.85. IR (neat) 3334 w,2995 w, 1752 s, 1521 w, 1479 w, 1368 s, 1239 s, 1055 w. MS *m/z* (relative intensity, %) 360 (M^+, 36), 281 (10), 253 (5), 185 (97), 183 (100), 157 (20), 155 (21). HRMS calcd for $C_{16}H_{10}BrClN_2O$: 359.9665; found: 359.9669.

N-(5-chloroquinolin-8-yl)-2-methoxybenzamide (1h)



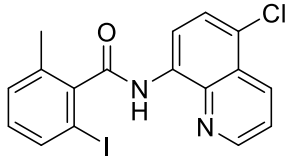
R_f 0.32 (hexane/EtOAc = 4/1). Off white colour solid. MP = 146 °C. ^{1}H-NMR (400 MHz, Chloroform-D) δ: 4.19 (s, 3H), 7.07 (d, *J* = 8.3 Hz, 1H), 7.14 (dt, *J* = 10.2, 3.9 Hz, 1H), 7.49-7.54 (m, 1H), 7.56 (dd, *J* = 8.5, 4.1 Hz, 1H), 7.63 (d, *J* = 8.5 Hz, 1H), 8.34 (dd, *J* = 7.8, 1.8 Hz, 1H), 8.56 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.90 (dd, *J* = 4.1, 1.6 Hz, 1H), 8.98 (d, *J* = 8.5 Hz, 1H), 12.33 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-D) δ: 56.09, 111.56, 117.15, 121.32, 122.01, 122.12, 124.08, 125.97, 127.39, 132.35, 133.20, 133.28, 135.04, 139.75, 148.64, 157.70, 163.59. IR (neat) 3262 w, 1714 s, 1654 m, 1536 s, 1481 m, 1360 m, 1219 m, 1022 w. MS *m/z* (relative intensity, %) 313 (M^+, 35), 178 (25), 136 (9), 135 (100), 92 (7). HRMS calcd for $C_{17}H_{13}ClN_2O_2$: 312.0666; found: 312.0663.

VI. General Procedure for the C-H Iodination

To an oven-dried 5 mL screw-capped vial, *N*-(5-chloroquinolin-8-yl)-2-methylbenzamide **1a** (45 mg, 0.15 mmol), iodine (76 mg, 0.3 mmol), $Co(OAc)_2{\cdot}4H_2O$ (7.6 mg, 0.03 mmol), Ag_2CO_3 (42 mg, 0.15 mmol), KOTf (57 mg, 0.3 mmol) and DCE (0.5 mL) were added. The mixture was stirred for 6 h at 120 °C followed by cooling. The resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc = 10/1) to afford the desired iodinated product **2a** (51 mg, 80%) as a white solid. The compounds **2a**-**2e**, **2g**, **2i**-**2n** were known.[2b]

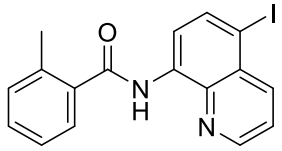
VII. Spectroscopic Data for Iodinated Products

***N*-(5-chloroquinolin-8-yl)-2-iodo-6-methylbenzamide (2a).**



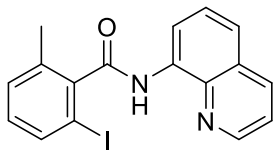
^{1}H-NMR (400 MHz, Chloroform-D) δ: 2.45 (s, 3H), 7.04 (t, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 7.1 Hz, 1H), 7.56 (dd, *J* = 8.2, 4.3 Hz, 1H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 1H), 8.58 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.80 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.90 (d, *J* = 8.2 Hz, 1H), 9.87 (s, 1H).

***N*-(5-iodoquinolin-8-yl)-2-methylbenzamide (1b')**



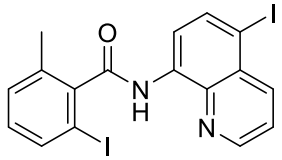
^{1}H-NMR (400 MHz, Chloroform-D) δ: 2.60 (s, 3H), 7.33 (t, *J* = 7.3 Hz, 2H), 7.44-7.40 (m, *J* = 4.0 Hz, 1H), 7.54 (dd, *J* = 8.7, 4.1 Hz, 1H), 7.68 (d, *J* = 7.8 Hz, 1H), 8.14 (d, *J* = 8.7 Hz, 1H), 8.40 (dd, *J* = 8.7, 1.4 Hz, 1H), 8.72 (d, *J* = 8.2 Hz, 1H), 8.75 (dd, *J* = 4.1, 1.8 Hz, 1H), 10.23 (s, 1H).

2-iodo-6-methyl-*N*-(quinolin-8-yl)benzamide (2b)



^{1}H-NMR (400 MHz, Chloroform-D) δ: 2.48 (s, 3H), 7.05 (t, *J* = 7.8 Hz, 1H), 7.26 (t, *J* = 3.7 Hz, 2H), 7.47 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.65-7.58 (m, 2H), 7.73 (d, *J* = 7.8 Hz, 1H), 8.20 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.77 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.97 (dd, *J* = 7.1, 1.6 Hz, 1H), 9.93 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-D) δ: 20.15, 92.94, 117.13, 121.70, 122.25, 127.42, 128.04, 130.06, 130.57, 134.12, 136.44, 136.60, 136.80, 138.48, 143.16, 148.33, 168.18.

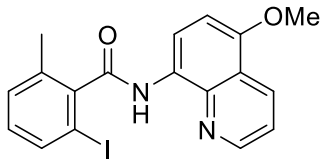
2-iodo-*N*-(5-iodoquinolin-8-yl)-6-methylbenzamide (2b')



R_f 0.52 (hexane/EtOAc = 4/1). Off white colour solid. MP = 173 ^{o}C. ^{1}H-NMR (400 MHz, Chloroform-D) δ: 2.46 (s, 3H), 7.05 (t, *J* = 8.0 Hz, 1H), 7.26 (t, *J* = 3.9 Hz, 1H), 7.54 (dd, *J* = 8.7, 4.1 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 8.16 (d, *J* = 8.3 Hz, 1H), 8.40 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.75-8.73 (m, 2H), 9.93 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-D) δ: 20.13, 76.68, 77.00, 77.32, 90.28, 92.82, 118.33, 123.26, 129.70, 130.10, 130.68, 135.01, 136.61, 136.79, 138.21, 139.07,

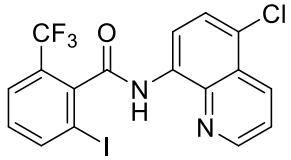
140.74, 142.92, 148.94, 168.17. IR (neat) 3001 w, 1710 s, 1513 w, 1421 w, 1358 s, 1219 s, 1092 w, 906 w. MS *m/z* (relative intensity, %) 514 (M^+, 58), 387 (6), 270 (4), 260 (9), 245 (100), 217 (15), 119 (15). HRMS calcd for $C_{17}H_{12}I_2N_2O$: 513.9039; found: 513.9040.

2-iodo-*N*-(5-methoxyquinolin-8-yl)-6-methylbenzamide (2c).



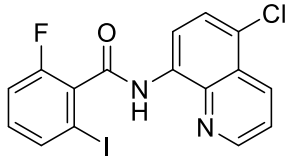
^{1}H-NMR (400 MHz, Chloroform-D) δ: 2.45 (s, 3H), 4.01 (s, 3H), 6.89 (d, *J* = 8.7 Hz, 1H), 7.01 (t, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 1H), 7.42 (dd, *J* = 8.5, 4.4 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 8.58 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.75 (q, *J* = 4.4, 1.6 Hz, 1H), 8.86 (d, *J* = 8.2 Hz, 1H), 9.66 (s, 1H).

***N*-(5-chloroquinolin-8-yl)-2-iodo-6-(trifluoromethyl)benzamide (2d).**



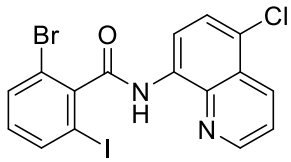
^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.30 (t, *J* = 8.0 Hz, 1H), 7.58 (dd, J = 8.7, 4.1 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H) 7.76 (d, *J* = 8.2 Hz, 1H), 8.13 (d, *J* = 7.8 Hz, 1H), 8.60 (dd, *J* = 8.7, 1.4 Hz, 1H), 8.81 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.87 (d, *J* = 8.7 Hz, 1H), 9.95 (s, 1H).

***N*-(5-chloroquinolin-8-yl)-2-fluoro-6-iodobenzamide (2e).**



^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.14-7.23 (m, 2H), 7.59 (dd, *J* = 8.5, 4.4 Hz, 1H), 7.69 (d, *J* = 8.7 Hz, 1H), 7.73 (dd, *J* = 7.3, 1.4 Hz, 1H), 8.61 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.84 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.90 (d, *J* = 8.2 Hz, 1H), 10.05 (s, 1H).

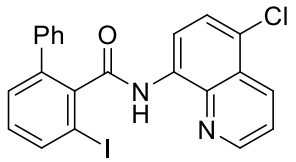
***N*-(5-chloroquinolin-8-yl)-2-bromo-6-iodobenzamide (2f).**



R_f 0.52 (hexane/EtOAc = 4/1). white colour solid. MP = 222 ^{o}C. ^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.02 (t, *J* = 8.0 Hz, 1H), 7.59 (dd, *J* = 8.7, 4.1 Hz, 1H), 7.64 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.69 (d, *J* = 8.7 Hz, 1H), 7.86 (dd, *J* = 7.8, 0.9 Hz, 1H), 8.60 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.84 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.89 (d, *J* = 8.7 Hz, 1H), 9.93 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-D) δ: 93.27,

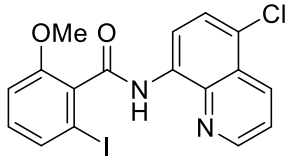
117.17, 119.61, 122.49, 125.39, 126.06, 127.21, 131.84, 132.65, 133.17, 133.47, 138.29, 139.10, 143.60, 148.91, 166.20. IR (neat) 3328 w, 2992 w, 1767 m, 1675 m, 1520 s, 1479 m, 1386 m, 1243 s, 913 s, 745 s. MS *m/z* (relative intensity, %) 486 (M^+, 32), 407 (11), 357 (100), 311 (71), 309 (73), 205 (17), 150 (11). HRMS calcd for $C_{16}H_9BrClIN_2O$: 485.8631; found: 485.8625.

***N*-(5-chloroquinolin-8-yl)-3-iodo-[1,1'-biphenyl]-2-carboxamide (2g).**



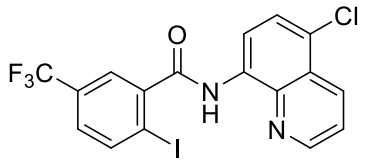
^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.16 (t, *J* = 7.3 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 6H), 7.46 (dd, *J* = 8.7, 4.1 Hz, 1H), 7.48-7.53 (m, 4H), 7.56-7.60 (m, 2H), 7.92 (d, 1H), 8.48 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.55 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.76 (d, *J* = 8.7 Hz, 1H), 9.70 (s, 1H).

***N*-(5-chloroquinolin-8-yl)-2-iodo-6-methoxybenzamide (2h).**



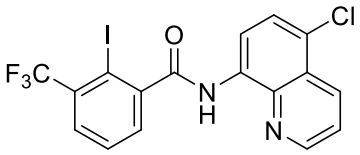
R_f 0.23 (hexane/EtOAc = 4/1). Yellow solid. MP = 224 °C. ^{1}H-NMR (400 MHz, Chloroform-D) δ: 3.83 (s, 3H), 6.98 (d, *J* = 8.2 Hz, 1H), 7.11 (t, *J* = 8.0 Hz, 1H), 7.49 (dd, *J* = 7.8, 0.9 Hz, 1H), 7.57 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.67 (d, *J* = 8.2 Hz, 1H), 8.59 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.82 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.93 (d, *J* = 8.7 Hz, 1H), 9.95 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-D) δ: 56.16, 94.13, 111.10, 117.04, 122.44, 124.91, 126.10, 127.38, 131.39, 131.75, 132.64, 133.47, 133.81, 139.19, 148.81, 157.06, 166.07. IR (neat) 3334 w, 2987 w,1739 s, 1669 m, 1588 w, 1517 s, 1451 w, 1372 m, 1239 s, 1045 m. MS *m/z* (relative intensity, %) 438 (M^+, 25), 262 (9), 261 (100), 203 (6), 166 (45), 135 (14). HRMS calcd for $C_{17}H_{12}ClIN_2O_2$: 437.9632; found: 437.9637.

***N*-(5-chloroquinolin-8-yl)-2-iodo-5-(trifluoromethyl)benzamide (2i).**



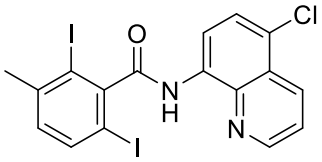
^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.44 (dd, *J* = 8.2, 2.3 Hz, 1H), 7.61 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 1.8 Hz, 1H), 8.12 (d, *J* = 8.2 Hz, 1H), 8.62 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.85-8.87 (m, 2H), 10.14 (s, 1H).

***N*-(5-chloroquinolin-8-yl)-2-iodo-3-(trifluoromethyl)benzamide (2i').**



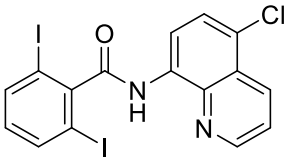
R_f 0.52 (hexane/EtOAc = 4/1). White colour solid. MP = 134 °C. ^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.05 (d, *J* = 8.2 Hz, 1H), 7.45 (dd, *J* = 8.0, 3.9 Hz, 1H), 7.65 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 8.00 (s, 1H), 8.29 (d, *J* = 8.7 Hz, 1H), 8.39 (d, *J* = 8.2 Hz, 1H), 8.53 (d, *J* = 4.1 Hz, 1H), 10.21 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-D) δ: 36.70, 95.57, 116.26, 122.11, 124.24, 124.57, 124.96, 126.33, 127.75, 131.66, 132.84, 132.93, 136.69, 138.02, 148.45, 165.58. IR (neat) 3328 w, 2995 w, 1711 s, 1677 m, 1528 s, 1481 m, 1327 m, 1218 m, 1087 w. MS *m/z* (relative intensity, %) 476 (M^+, 2), 350 (50), 207 (8), 205 (24), 173 (100), 145 (48). HRMS calcd for $C_{17}H_9ClF_3IN_2O$: 475.9400; found: 475.9409.

***N*-(5-chloroquinolin-8-yl)-2, 6-diiodo-3-methylbenzamide (2j)**



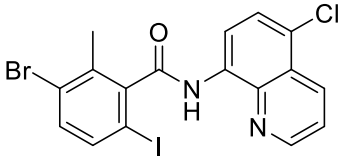
R_f 0.49 (hexane/EtOAc = 4/1). White colour solid. MP = 229 °C. ^{1}H-NMR (400 MHz, Chloroform-D) δ: 2.48 (s, 3H), 7.03 (d, J = 7.8 Hz, 1H), 7.59 (dd, J = 8.3, 4.1 Hz, 1H), 7.70 (d, J = 8.3 Hz, 1H), 7.76 (d, J = 8.3 Hz, 1H), 8.61 (dd, J = 8.5, 1.6 Hz, 1H), 8.84 (dd, J = 4.4, 1.6 Hz, 1H), 8.90 (d, J = 8.7 Hz, 1H), 9.89 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-D) δ: 28.72, 76.68, 77.00, 77.21, 77.32, 88.07, 99.53, 117.16, 122.48, 125.29, 126.06, 127.22, 131.42, 133.24, 133.46, 138.76, 139.10, 142.93, 147.83, 148.89, 168.52. IR (neat) 3335 w, 2922 w, 1677 m, 1517 s, 1477 m, 1386 w, 1320 w, 947 w. MS *m/z* (relative intensity, %) 548 (M^+, 44), 371 (100), 343 (7), 216 (10), 89 (9). HRMS calcd for $C_{17}H_{11}ClI_2N_2O$: 547.8649; found: 547.8647.

***N*-(5-chloroquinolin-8-yl)-2,6-diiodobenzamide (2k)**



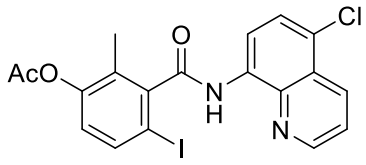
^{1}H-NMR (400 MHz, Chloroform-D) δ: 6.84 (t, *J* = 8.0 Hz, 1H), 7.60 (dd, *J* = 8.5, 4.4 Hz, 1H), 7.70 (d, *J* = 8.3 Hz, 1H), 7.89 (d, *J* = 8.3 Hz, 2H), 8.61 (dd, *J* = 8.7, 1.4 Hz, 1H), 8.85 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.89 (d, *J* = 8.3 Hz, 1H), 9.91 (s, 1H).

3-bromo-*N*-(5-chloroquinolin-8-yl)-6-iodo-2-methylbenzamide (2l).



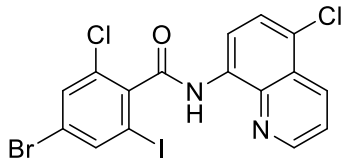
^{1}H-NMR (400 MHz, Chloroform-D) δ: 2.52 (s, 3H), 7.35 (d, *J* = 8.2 Hz, 1H), 7.57-7.61 (m, 2H), 7.69 (d, *J* = 8.2 Hz, 1H), 8.61 (dd, *J* = 8.5, 1.6 Hz 1H), 8.83 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.89 (dd, *J* = 8.2, 6.0 Hz, 1H), 9.88 (s, 1H).

3-((5-chloroquinolin-8-yl)carbamoyl)-4-iodo-2-methylphenyl acetate (2m).



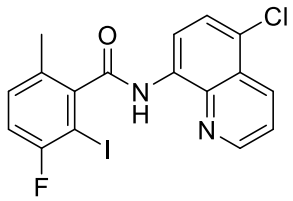
^{1}H-NMR (400 MHz, Chloroform-D) δ: 2.29 (s, 3H), 2.35 (s, 3H), 6.89 (d, *J* = 8.2 Hz, 1H), 7.59 (dd, *J* = 8.7, 4.1 Hz, 1H), 7.68 (d, *J* = 8.2 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 1H), 8.60 (dd, *J* = 8.7, 1.8 Hz, 1H), 8.83 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.89 (d, *J* = 8.7 Hz, 1H), 9.92 (s, 1H).

4-bromo-2-chloro-*N*-(5-chloroquinolin-8-yl)-6-iodobenzamide (2n).



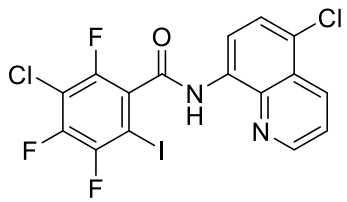
^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.59 (dd, *J* = 8.7, 4.1 Hz, 1H), 7.64 (d, *J* = 1.8 Hz, 1H), 7.68 (d, *J* = 8.2 Hz, 1H), 7.98 (d, *J* = 1.4 Hz, 1H), 8.60 (dd, *J* = 8.5, 1.6 Hz, 1H) , 8.83 (dd, *J* = 4.1, 1.8 Hz, 1H), 8.86 (d, *J* = 8.7 Hz, 1H), 9.94 (s, 1H).

***N*-(5-chloroquinolin-8-yl)-3-fluoro-2-iodo-6-methylbenzamide (2o).**



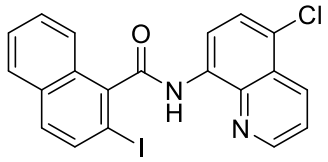
^{1}H-NMR (400 MHz, Chloroform-D) δ: 2.45 (s, 3H), 7.05 (t, *J* = 8.0 Hz, 1H), 7.22 (dd, *J* = 7.8, 5.0 Hz, 1H), 7.58 (dd, *J* = 8.2, 4.1 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 8.60 (dd, *J* = 8.7, 1.4 Hz, 1H), 8.82 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.90 (d, *J* = 8.2 Hz, 1H), 9.89 (s, 1H).

3-chloro-*N*-(5-chloroquinolin-8-yl)-2,4,5-trifluoro-6-iodobenzamide (2p).



^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.59-7.62 (m, 1H), 7.68 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.61 (d, *J* = 8.7 Hz, 1H), 8.82-8.84 (m, 2H), 10.07 (s, 1H).

***N*-(5-chloroquinolin-8-yl)-2-iodo-1-naphthamide (2q)**



R_f 0.48 (hexane/EtOAc = 4/1). Off white colour solid. MP = 256 °C. ^{1}H-NMR (400 MHz, Chloroform-D) δ: 7.50-7.58 (m, 3H), 7.66 (d, *J* = 8.7 Hz, 1H), 7.74 (d, *J* = 8.2 Hz, 1H), 7.89 (m, 2H), 7.97 (d, *J* = 8.7 Hz, 1H), 8.60 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.75 (dd, *J* = 4.1, 1.4 Hz, 1H) , 9.04 (d, J = 8.2 Hz, 1H), 10.08 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-D) δ: 91.35, 117.06, 122.46, 125.09, 125.28, 126.08, 127.02, 127.25, 127.91, 128.21, 130.63, 131.25, 132.54, 133.43, 133.52, 135.28, 139.10, 140.92, 148.86, 167.79. IR (neat) 3334 w, 2987 w, 1746 m, 1588 w, 1517 s, 1466 s, 1374 w, 1242 s, 1047 m. MS *m/z* (relative intensity, %) 458 (M^+, 19), 331 (14), 295 (15), 282 (12), 281 (100), 166 (45), 155 (64), 126 (31). HRMS calcd for $C_{20}H_{12}ClIN_2O$: 457.9683; found: 457.9682.

VIII. Deuterium Labeling Experiments (Scheme 3a)

To an oven-dried 5 mL screw-capped vial, **1a-*d*$_7$** (46 mg, 0.15 mmol), iodine (76 mg, 0.3 mmol), $Co(OAc)_2{\cdot}4H_2O$ (7.6 mg, 0.03 mmol), Ag_2CO_3 (42 mg, 0.15 mmol), KOTf (57 mg, 0.3 mmol) and DCE (0.5 mL) were added. The mixture was stirred at 120 °C followed by cooling. The resulting mixture was filtered through a celite pad and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel (eluent: hexane/EtOAc= 10/1). NMR yields were determined using 1,1,2,2-tetrachloroethane as the reference. The deuterium content was also determined by ^{1}H-NMR.

IX. Reactions with Radical Scavengers (Scheme 3b)

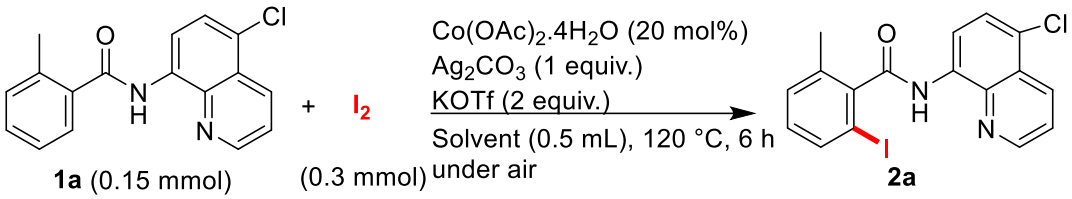
To an oven-dried 5 mL screw-capped vial, **1a** (45 mg, 0.15 mmol), iodine (76 mg, 0.3 mmol), radical scavenger (0.3 mmol), $Co(OAc)_2{\cdot}4H_2O$ (7.6 mg, 0.03 mmol), Ag_2CO_3 (42 mg, 0.15 mmol), KOTf (57 mg, 0.3 mmol), radical scavenger (TEMPO/BHT (0.18 mmol)) and DCE (0.5 mL) were added. The mixture was stirred at 120 °C followed by cooling. The resulting mixture was filtered through a celite pad and concentrated *in vacuo*. The yield of the iodinated product **2a** and the recovery of **1a** were determined by ^{1}H-NMR.

X. Competition Experiment for Kinetic Isotope Effect (Scheme 4)

To an oven-dried 5 mL screw-capped vial, **1a-*d*$_7$** or **1a** (45 mg, 0.15 mmol), iodine (76 mg, 0.3 mmol), $Co(OAc)_2{\cdot}4H_2O$ (7.6 mg, 0.03 mmol), Ag_2CO_3 (42 mg, 0.15 mmol), KOTf (57 mg, 0.3 mmol) and DCE (0.5 mL) were added. The mixture was stirred at 120 °C followed by cooling. The resulting mixture was filtered through a celite pad and concentrated *in vacuo*. The yields of iodinated product and SM was determined by ^{1}H-NMR in $CDCl_3$ as NMR solvent.

XI. Optimization Study

Table S1: Solvent Screening. [a]

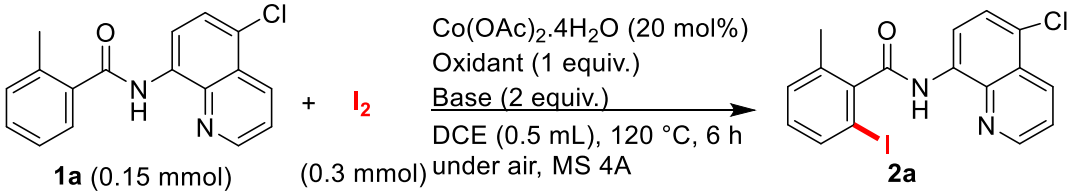


1a (0.15 mmol) (0.3 mmol) **2a**

Entry	Solvent	Yields (**2a**/**1a**)(%)[b, c]	note
1	DCE	85/trace (80)	
2	PhCl	68/14 (62)	
3	CF_3CH_2OH	19/35	
4	DMF	0/100	no reaction
5	DMSO	0/72	no reaction
6	1,4-dioxane	18/45	

[a] All reactions involved treating **1a** (0.15 mmol), **I_2** (0.3 mmol) in a solvent (0.5 mL) in the presence of the $Co(OAc)_2.4H_2O$ (0.03 mmol) and the Ag_2CO_3 (0.15 mmol), KOTf (0.3 mmol) at 120 °C for 6 h under air, unless otherwise stated. [b] Yields were determined by ^1H NMR analysis of the crude reaction mixture using 1,1,2,2-tetrachloroethane as an internal standard. [c] Values given in the parentheses are isolated product yields.

Table S2: Optimization.[a]



1a (0.15 mmol) (0.3 mmol) **2a**

Entry	Base	Oxidant	Yields (**2a**/**1a**)(%)[b, c]
1	CsOAc	Ag_2CO_3	0/83
2[d]	KOTf	$PhI(OAc)_2$	17/69
3[e]	KOTf	Ag_2CO_3	83/trace (79)
4[f]	KOTf	Ag_2CO_3	0/99
5	KOTf	-	0/99

[a] All reactions involved treating **1a** (0.15 mmol), **I_2** (0.3 mmol) in a solvent (0.5 mL) in the presence of the $Co(OAc)_2.4H_2O$ (0.03 mmol) and the Ag_2CO_3 (0.15 mmol), Base (0.3 mmol) at 120 °C for 6 h under air, unless otherwise stated. [b] Yields were determined by ^1H NMR analysis of the crude reaction mixture using 1,1,2,2-tetrachloroethane as an internal standard. [c] Values given in the parentheses are isolated product yields. [d] NaI was used as an iodinating reagent in place of I_2. [e] The reaction was carried out under N_2 atmosphere and $Co(OAc)_2$ (20 mol%) was used. [f] The reaction was carried out in the absence of $Co(OAc)_2.4H_2O$.

Density Functional Theory Calculations

XII. Transition-State Geometry of the CMD Pathway

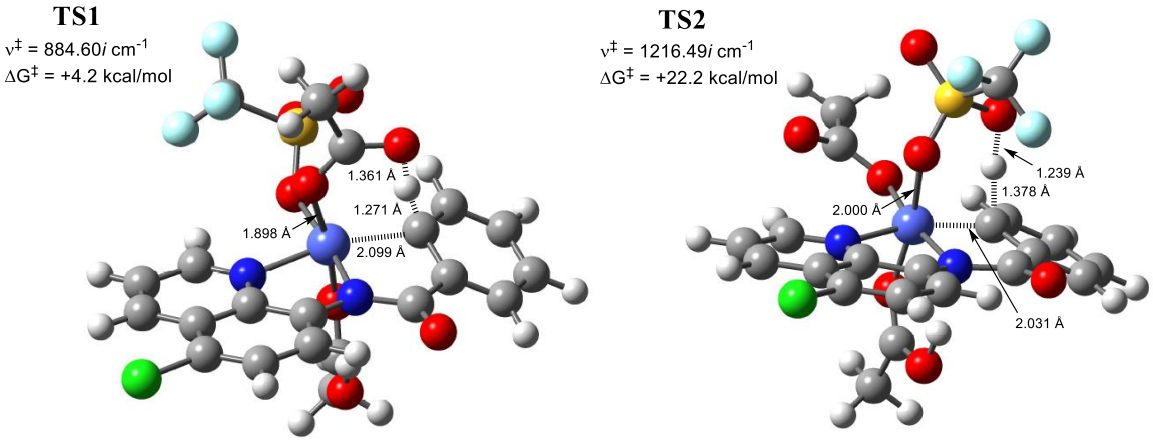


Figure S1. Transition-state geometry of the CMD pathway accelerated by acetate (TS1) and triflate (TS2).

XIII. Energy Surface for CMD Pathway

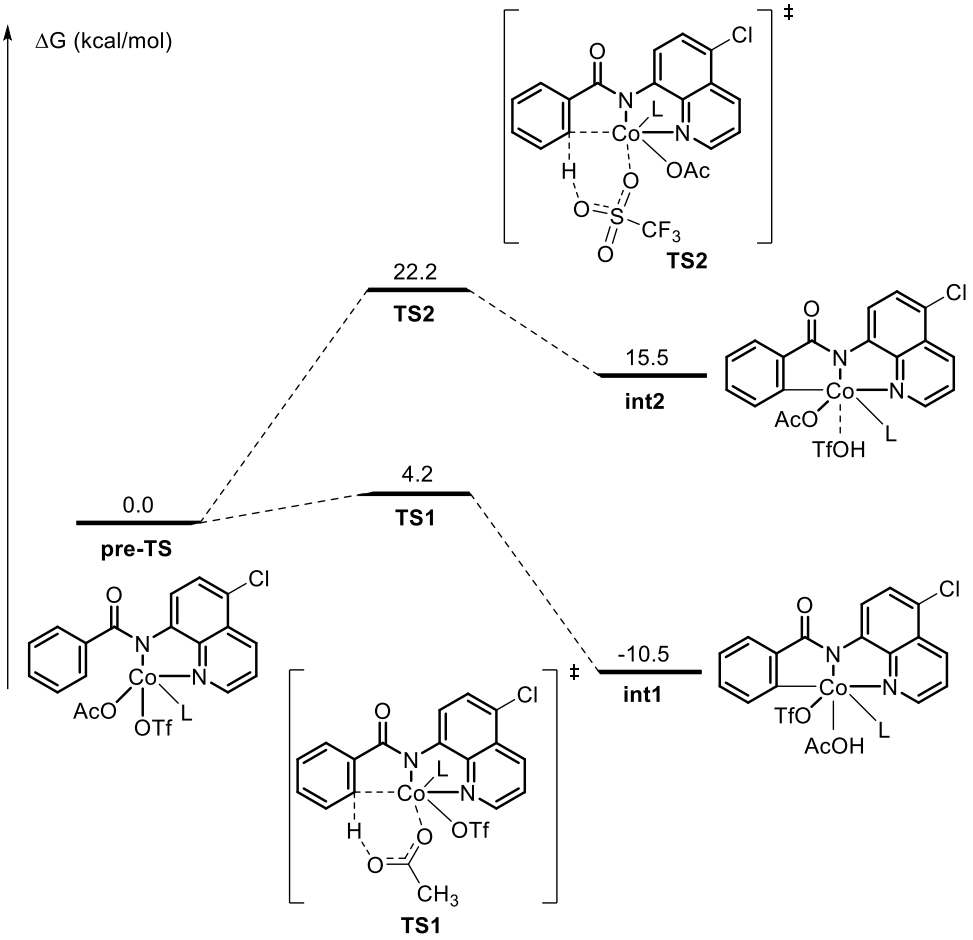


Figure S2. Energy surface for the CMD mechanism accelerated by acetate (TS1) and triflate (TS2). Energies are represented as ΔG (kcal/mol). L = AcOH.

In order to investigate the CMD pathways, we first hypothesized $Co(OAc)_2(OTf)$ generated from the oxidation of $Co(OAc)_2$ by Ag(I) species functions as the actual catalyst. In the CMD pathway, either OAc or OTf can promote the reaction (Figure S2). The energy barrier for the acetate-promoted deprotonation is surprisingly low at 4.2 kcal/mol and is exothermic by 10.5 kcal/mol. On the other hand, the triflate-promoted deprotonation has a high energy barrier of 22.2 kcal/mol. These findings explain the experimental KIE value of 1.08. In addition, we found that the base does not accelerate the CMD process as expected.

XIV. Spin Densities of Proposed Intermediates in SET Pathway

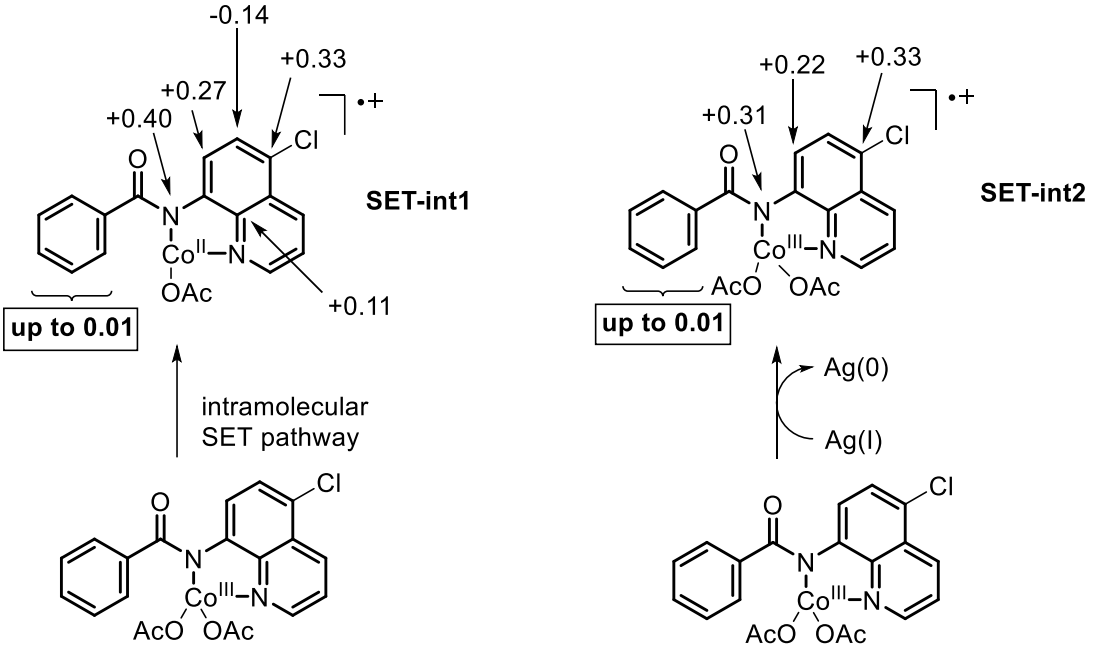


Figure S3. Spin densities of proposed radical cation intermediates in the intra and inter molecular SET pathways. The numbers represent the spin densities.

As demonstrated in Scheme 5, there are two proposed paths for the generation of the key intermediate **E** from **A**. Path a involves a SET process and path b involves a CMD pathway. To gain more insights into the mechanism, the spin densities of the radical cation species were calculated. The calculations show that electron spins exist on the quinoline ring (especially on the C5 and C7 position) rather than on the benzene ring. This result indicates that the SET process is not involved in our catalytic system. This result also supports the experimental results shown in Scheme 2, in which the iodination took place at the C5 position of the quinoline ring in **1b** leading to the production of **1b'** and **2b'** as the major products of the reaction.

XV. Computational Details

Calculations were performed with the Gaussian 09 (G09) program.[4] Geometry optimizations for all reported structures were performed at the B3LYP/{[6-31G(d)](for C, H, N, O, F, S, Cl) + Lanl2dz (for Co) SCRF = (PCM, solvent = dichloroethane)} level of theory with the corresponding effective core potential for Co.[5-7] Single point energy calculations are performed at the B3LYP/{[6-311+G(d,p)] (for C, H, N, O, F, S, Cl) + SDD (for Co) SCRF = (PCM, solvent = dichloroethane)} level of theory with the corresponding effective core potentials for Co.[8-10] PCM[11-13] solvent effects are incorporated for all calculations with dichloroethane as the solvent. TS geometry was characterized by vibrational analysis, which checked whether the obtained geometry has single imaginary frequencies ($v^{‡}$). From TSs, reaction paths were traced by the intrinsic reaction coordinate (IRC) method[14, 15] to obtain the energy-minimum geometries. Energy changes were shown by the use of Gibbs free energies (T = 298.15 K and P = 1 atm).

XVI. References:

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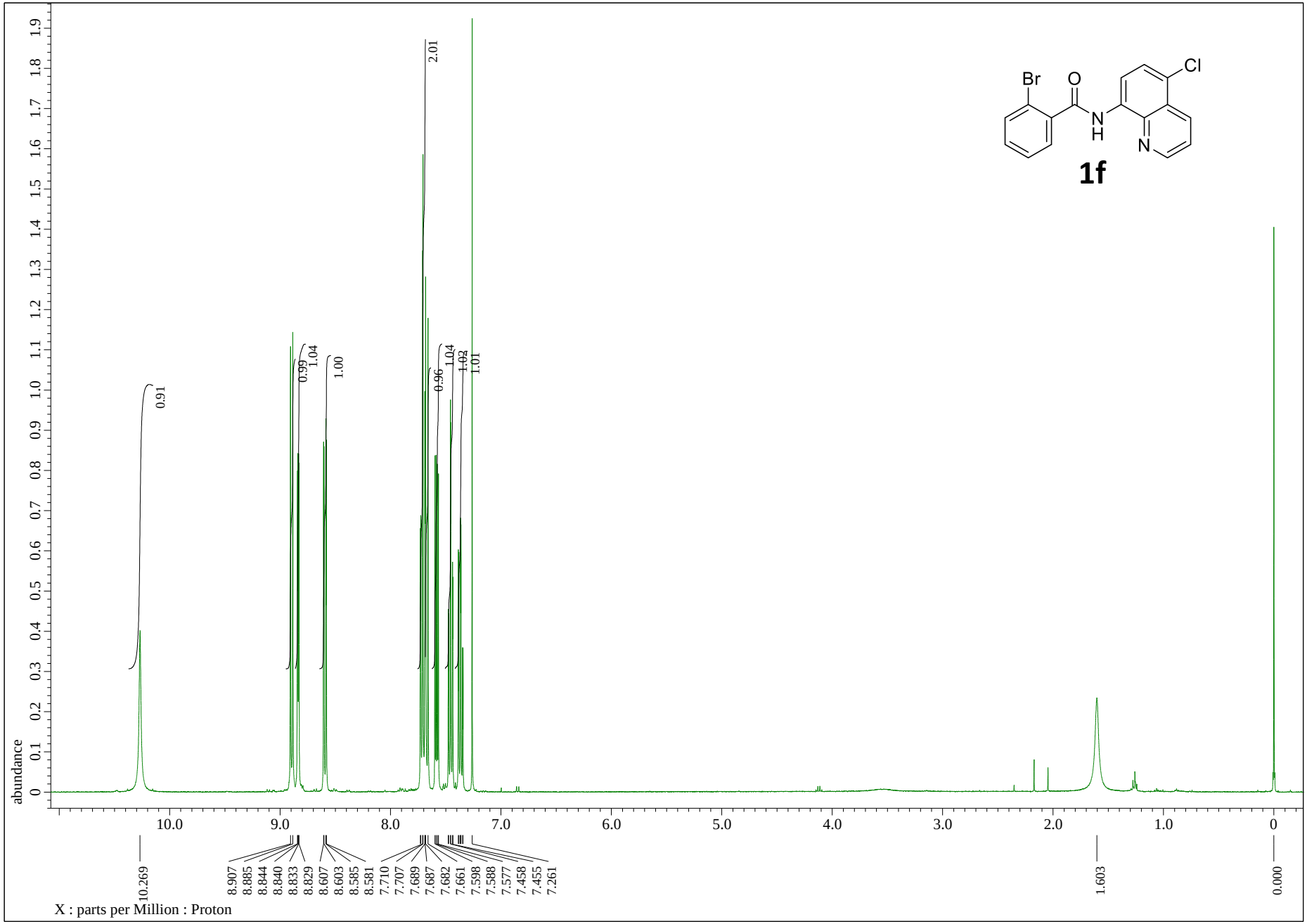
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Cl
N
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abundance
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8.603
8.585
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7.710
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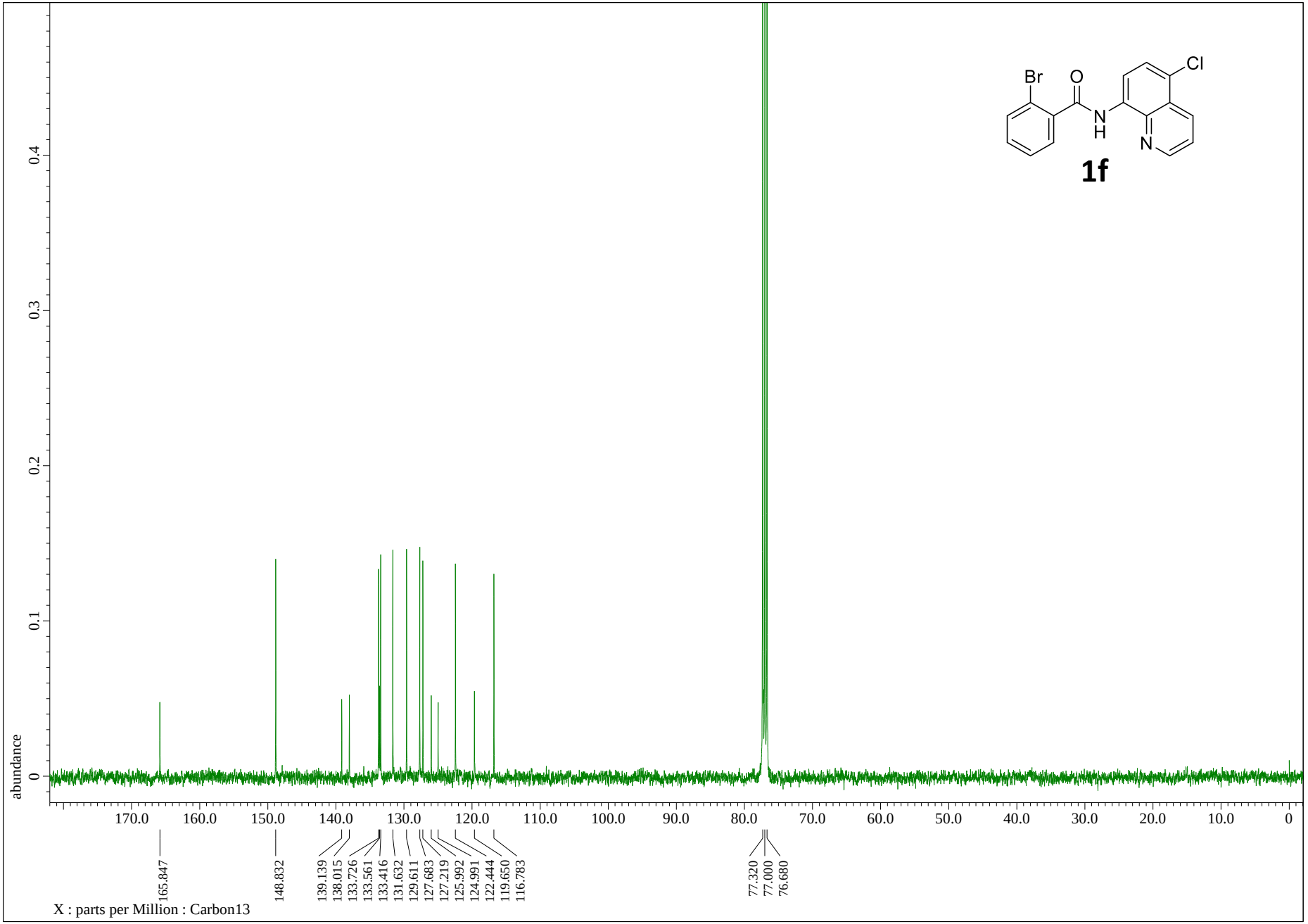
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100.0
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70.0
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30.0
20.0
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0
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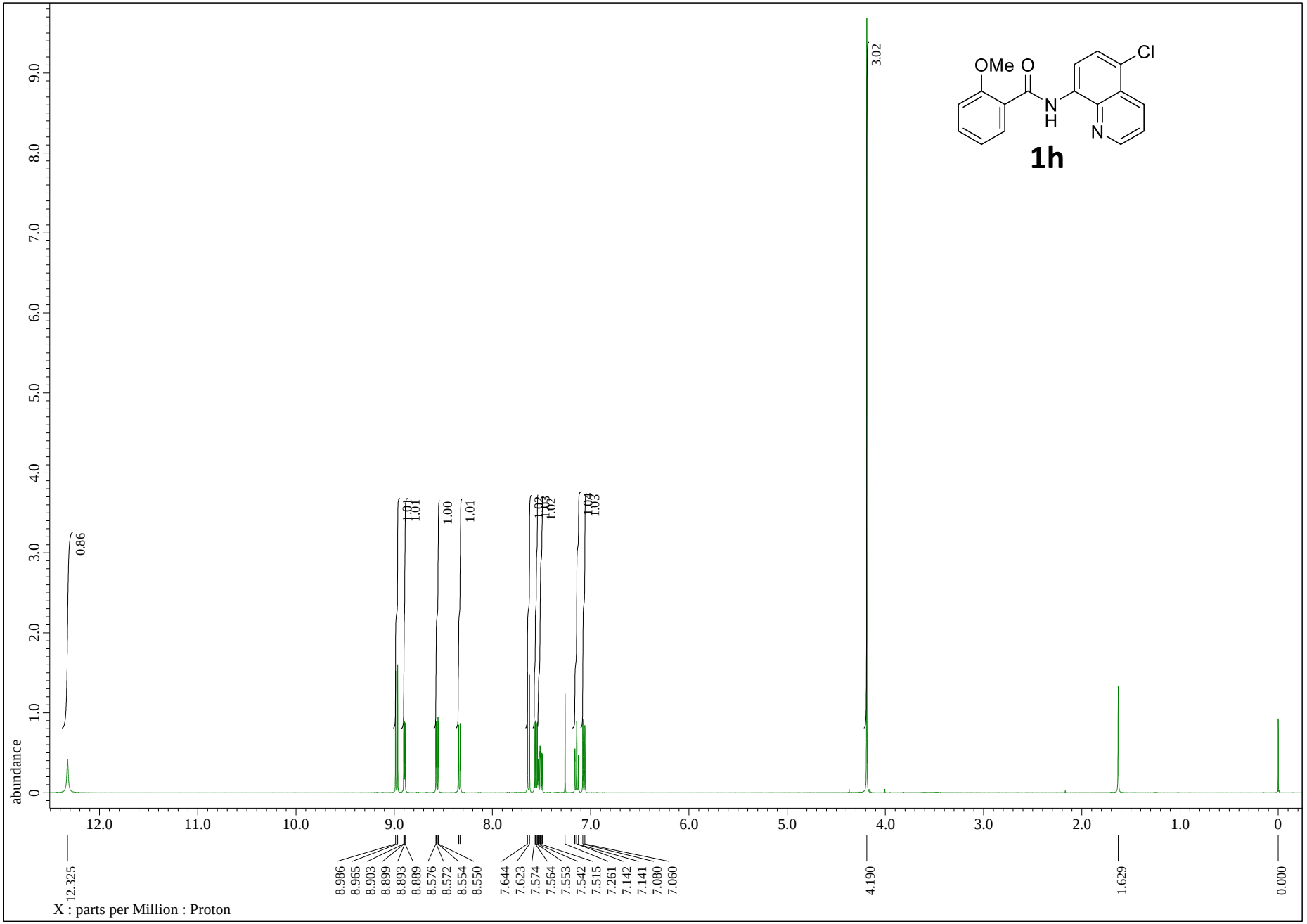
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X : parts per Million : Proton
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8.965
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8.899
8.893
8.889
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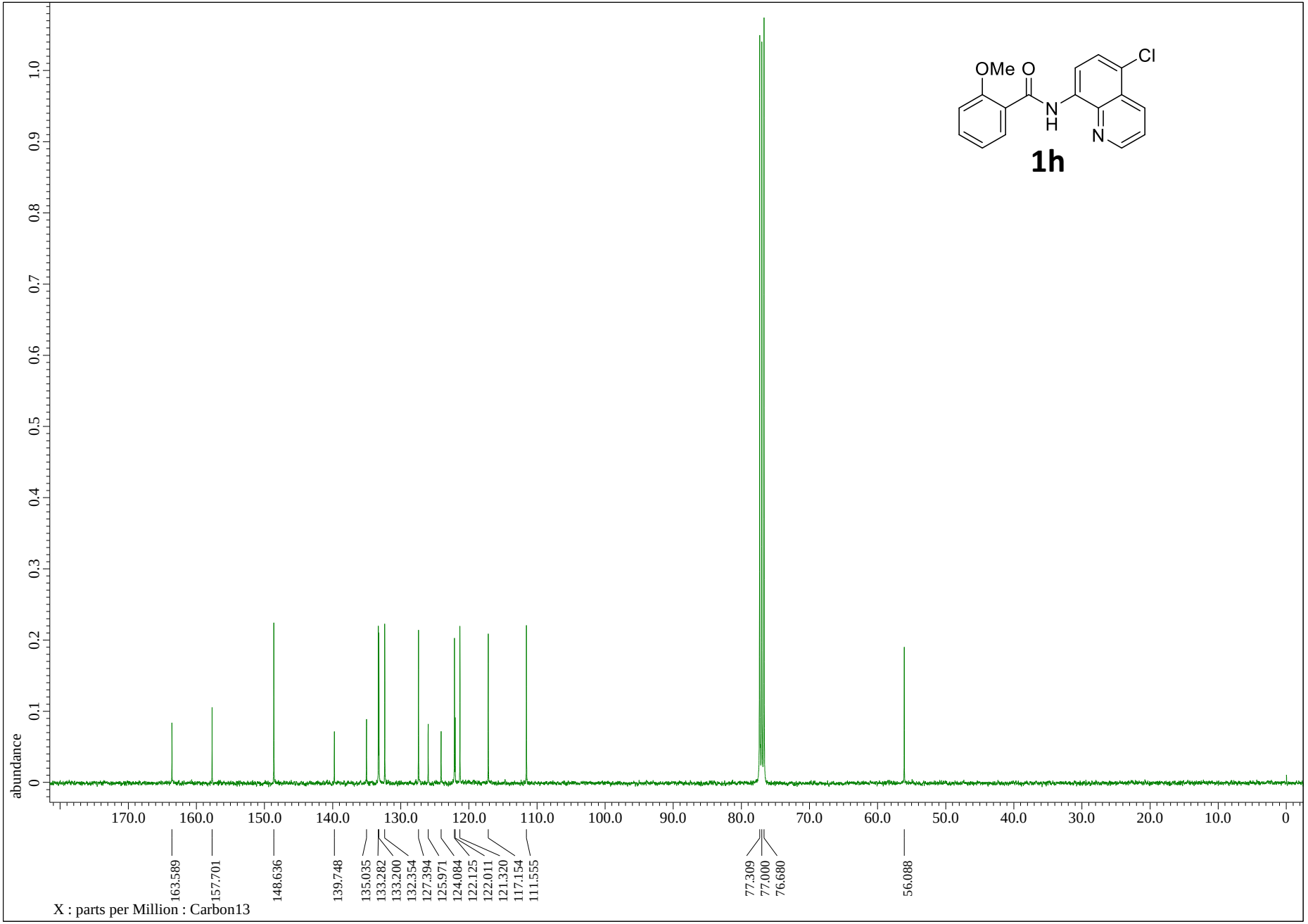
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0.8
0.9
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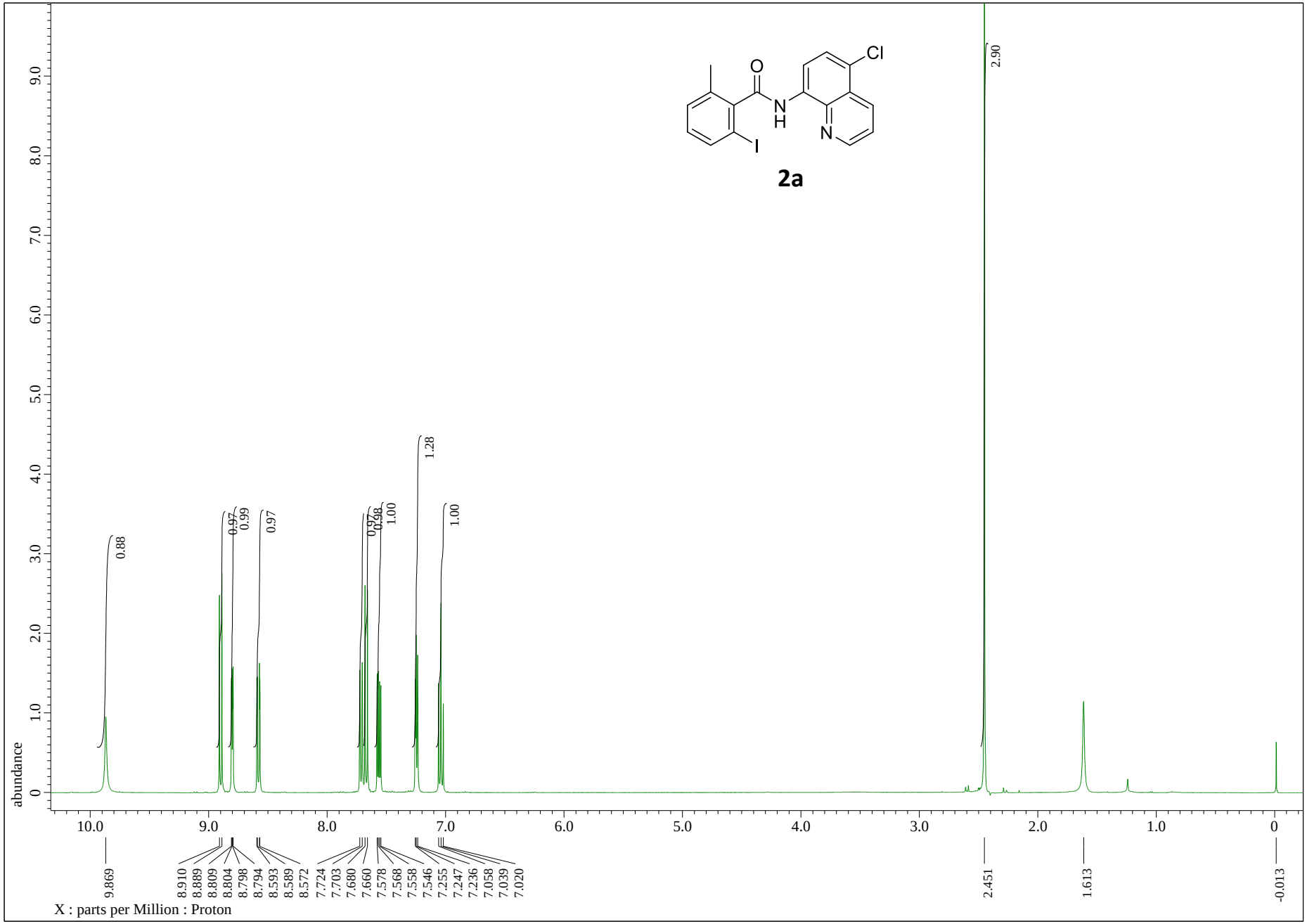
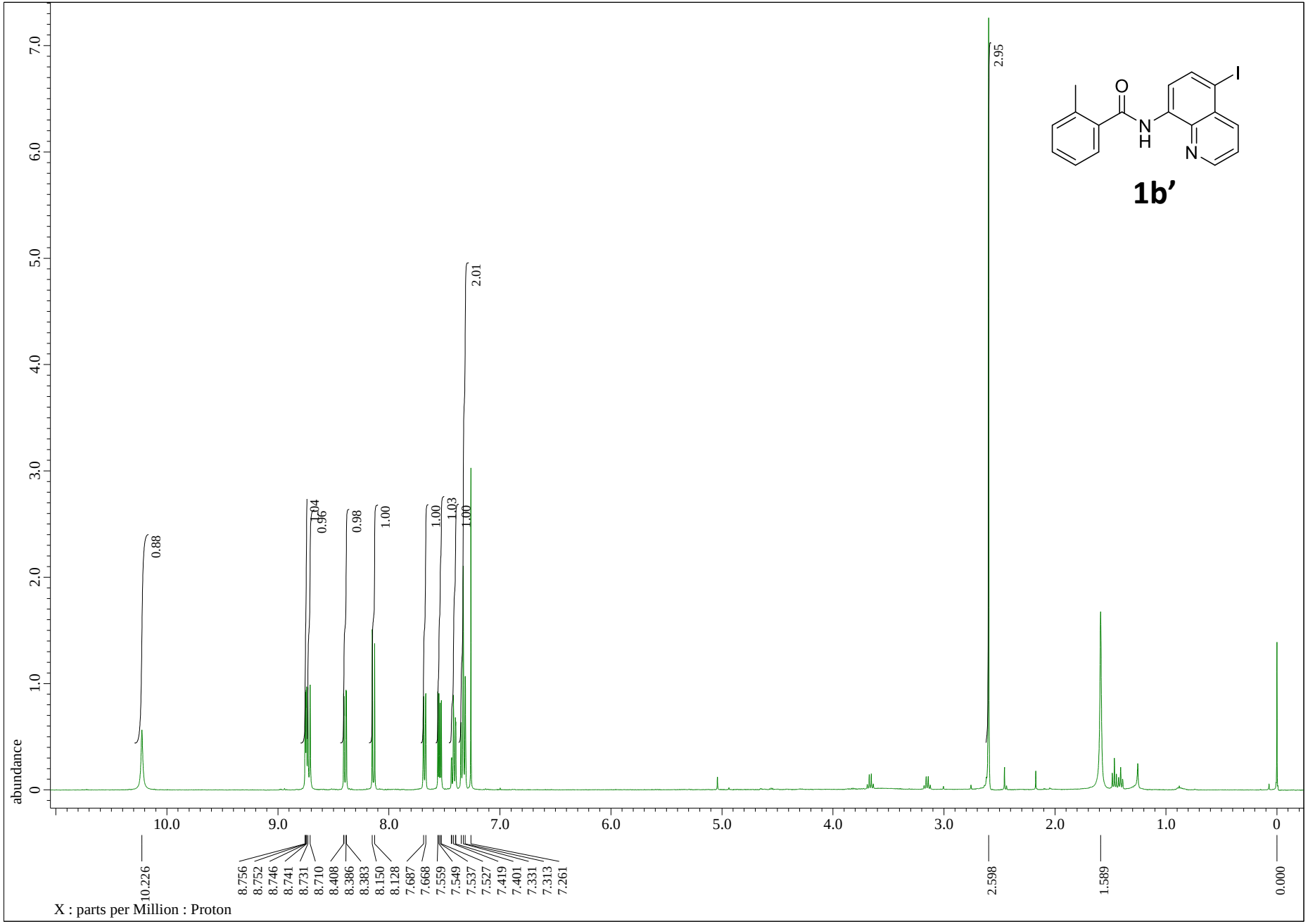
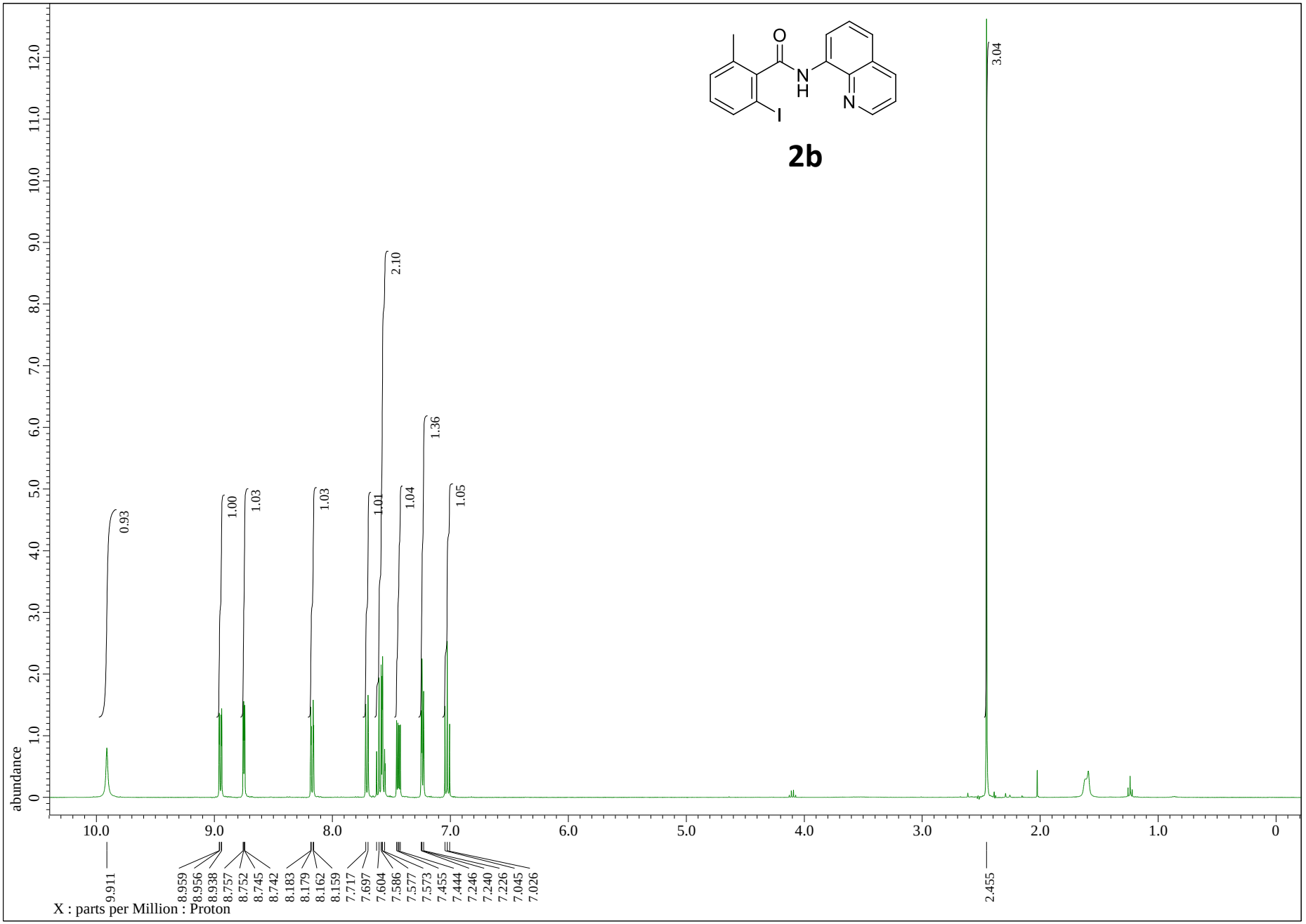
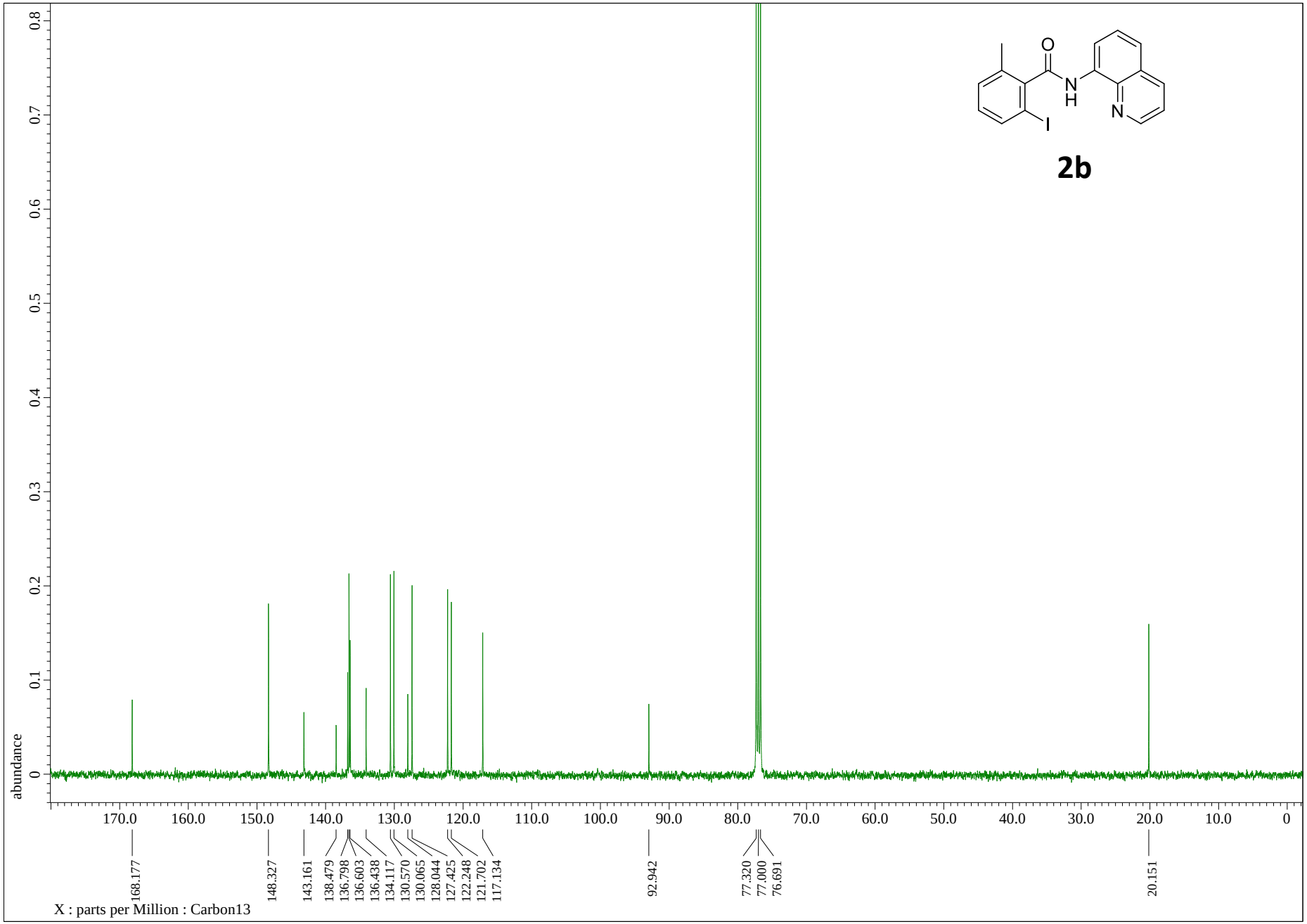
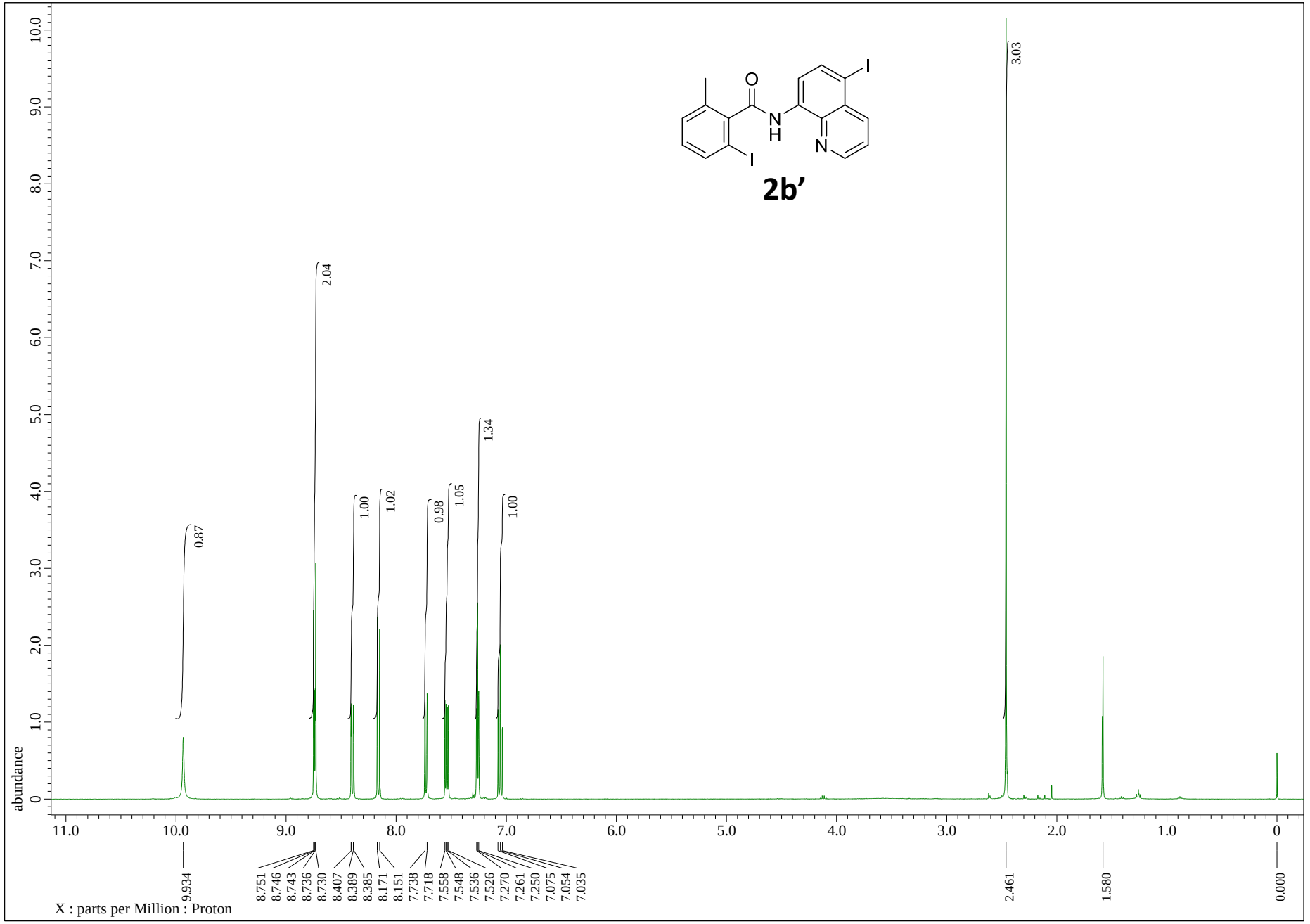
125.971
124.084
122.125
122.011
121.320
117.154
111.555
77.309
77.000
76.680
56.088
X : parts per Million : Carbon13

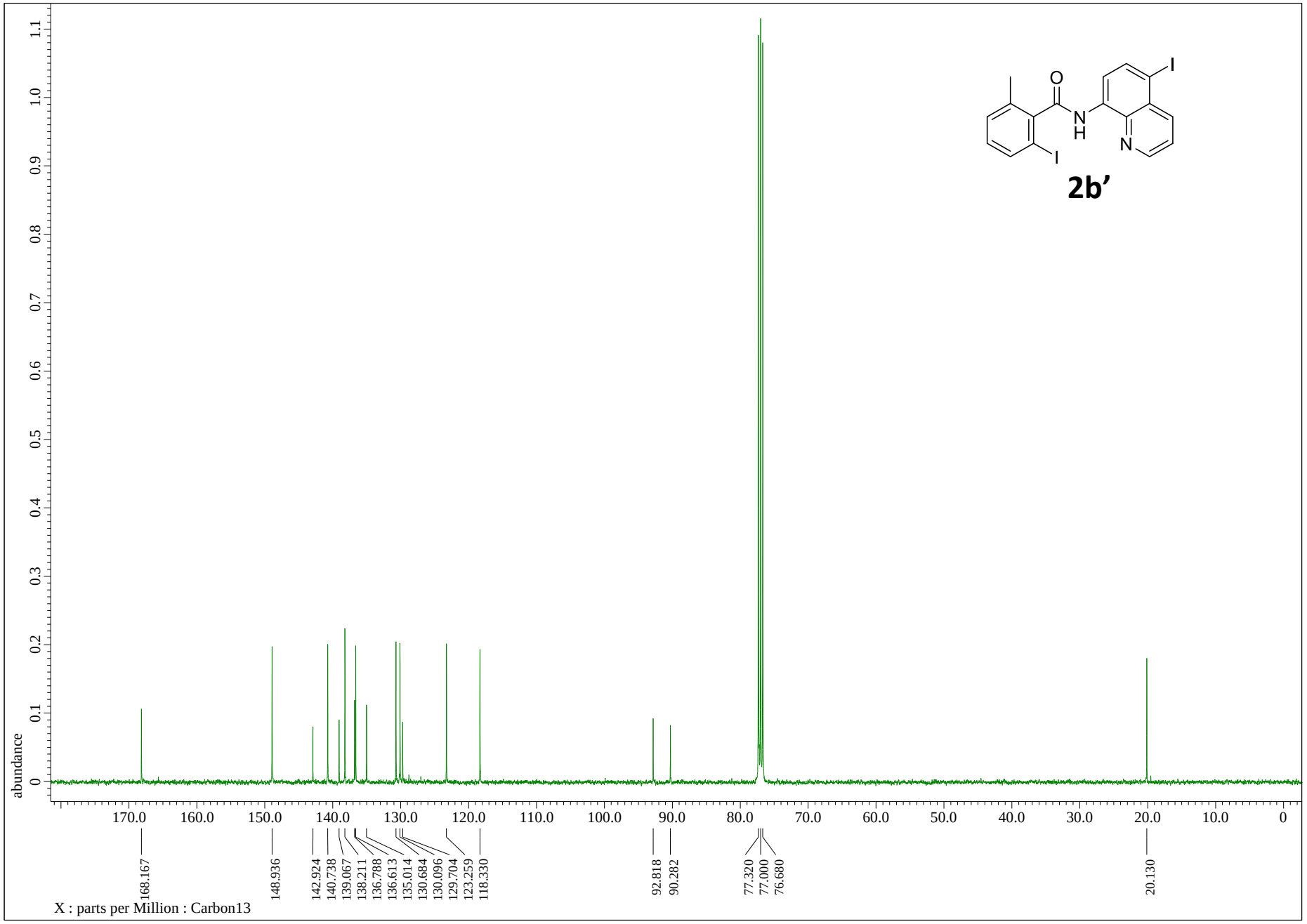

O
N
H
Cl
I
N
2a
2.90
0.88
0.97
0.99
0.97
0.97
0.96
1.00
1.28
1.00
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.869
8.910
8.889
8.809
8.804
8.798
8.794
8.593
8.589
8.572
7.724
7.703
7.680
7.660
7.578
7.568
7.558
7.546
7.255
7.247
7.236
7.058
7.039
7.020
2.451
1.613
-0.013
X : parts per Million : Proton

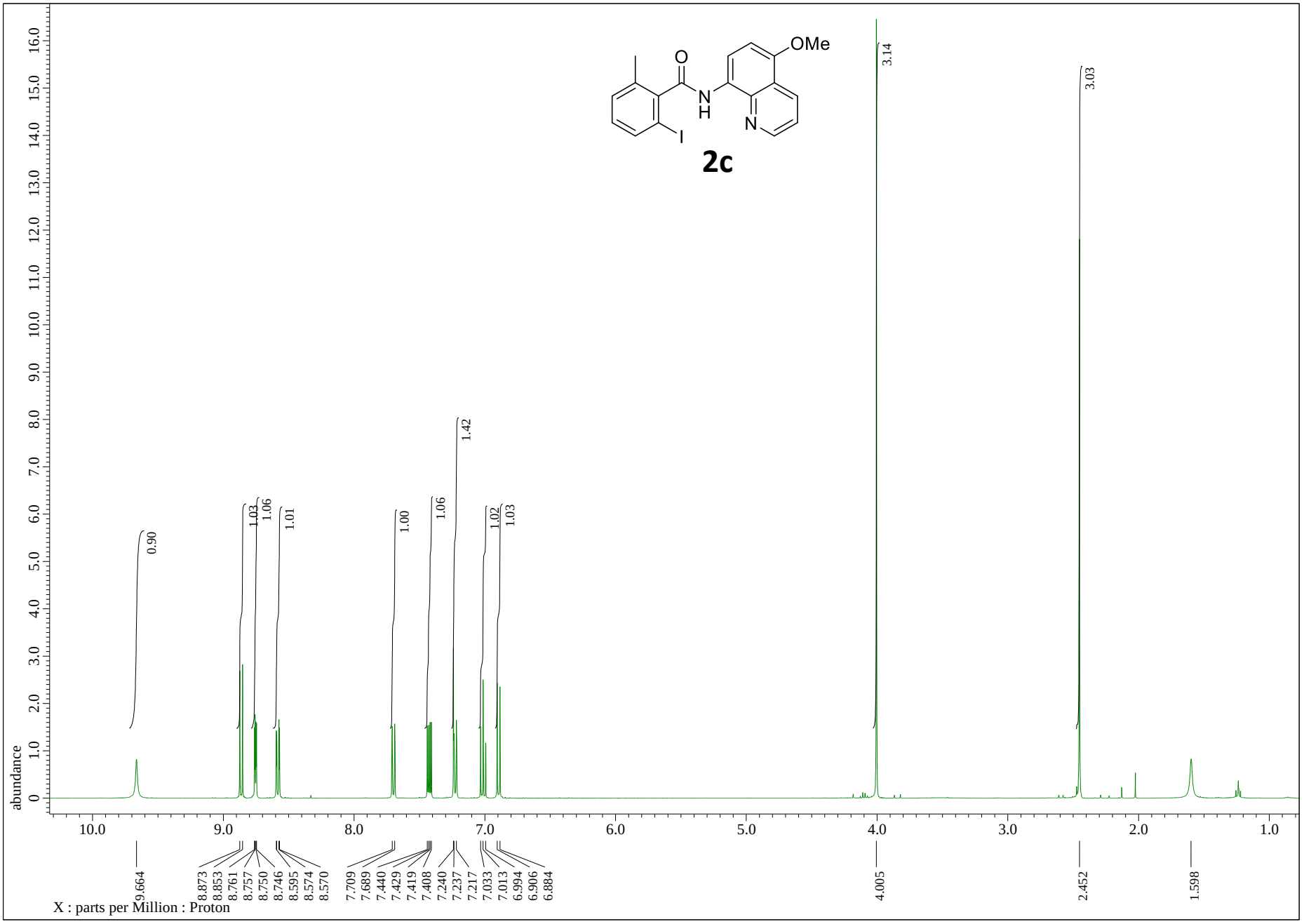

1b’
abundance
X : parts per Million : Proton
10.226
8.756
8.752
8.746
8.741
8.731
8.710
8.408
8.386
8.383
8.150
8.128
7.687
7.668
7.559
7.549
7.537
7.527
7.419
7.401
7.331
7.313
7.261
2.598
1.589
0.000
0.88
1.04
0.96
0.98
1.00
1.00
1.03
1.00
2.01
2.95

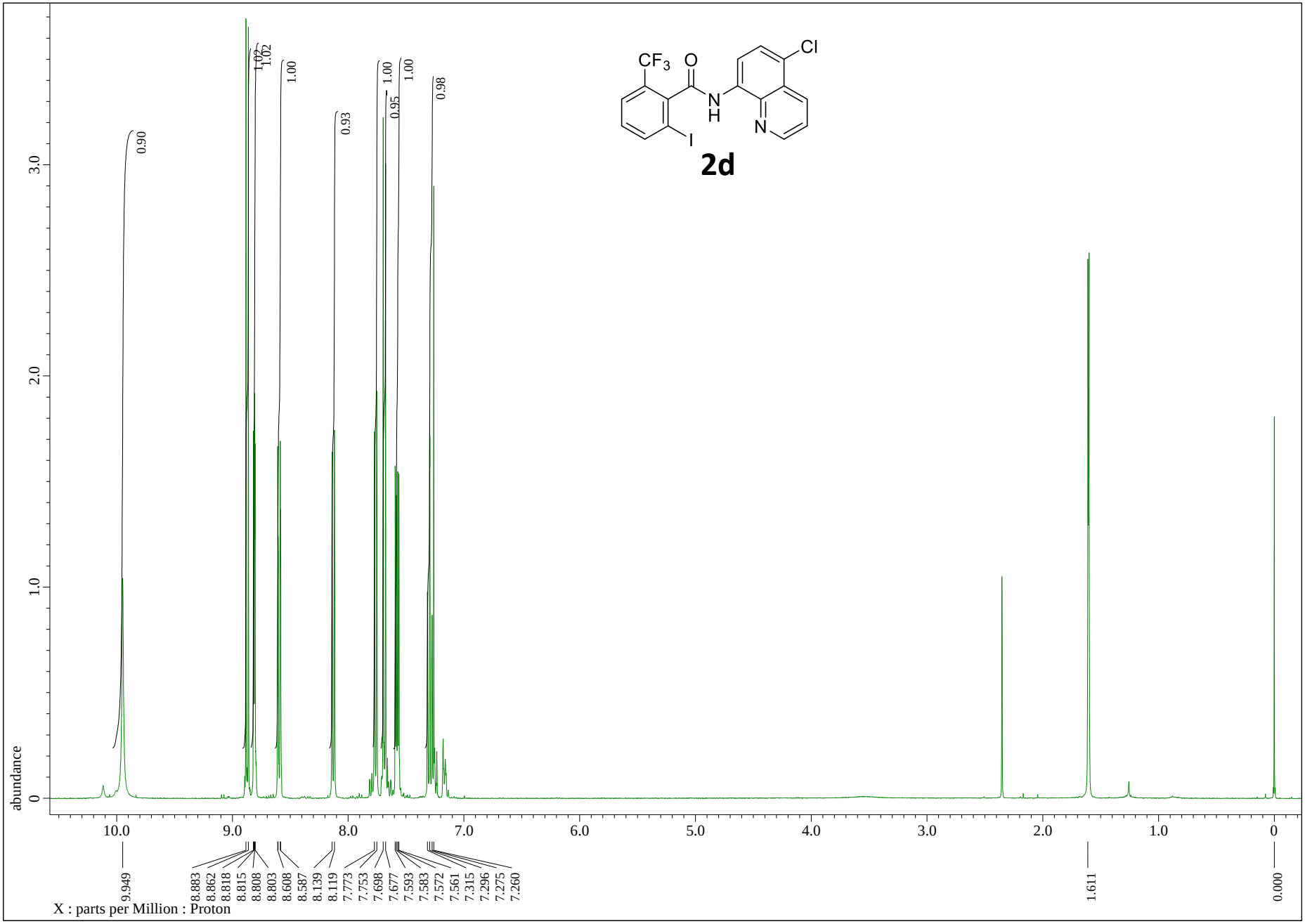

2b
abundance
X : parts per Million : Proton
0.93
1.00
1.03
1.03
1.01
2.10
1.04
1.36
1.05
3.04
9.911
8.959
8.956
8.938
8.757
8.752
8.745
8.742
8.183
8.179
8.162
8.159
7.717
7.697
7.604
7.586
7.577
7.573
7.455
7.444
7.246
7.240
7.226
7.045
7.026
2.455

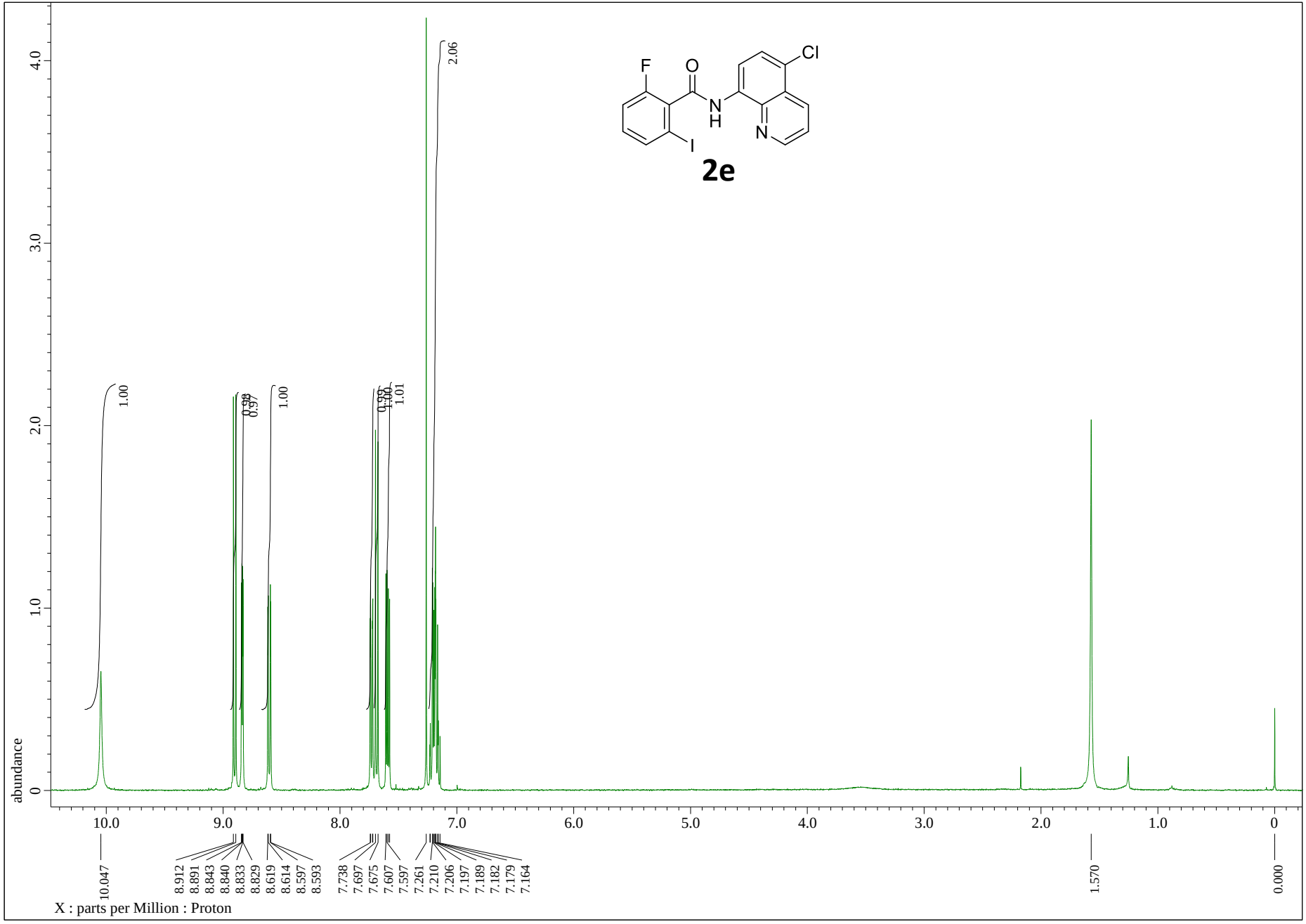

O
N
H
N
I
2b
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
168.177
148.327
143.161
138.479
136.798
136.603
136.438
134.117
130.570
130.065
128.044
127.425
122.248
121.702
117.134
92.942
77.320
77.000
76.691
20.151
X : parts per Million : Carbon13

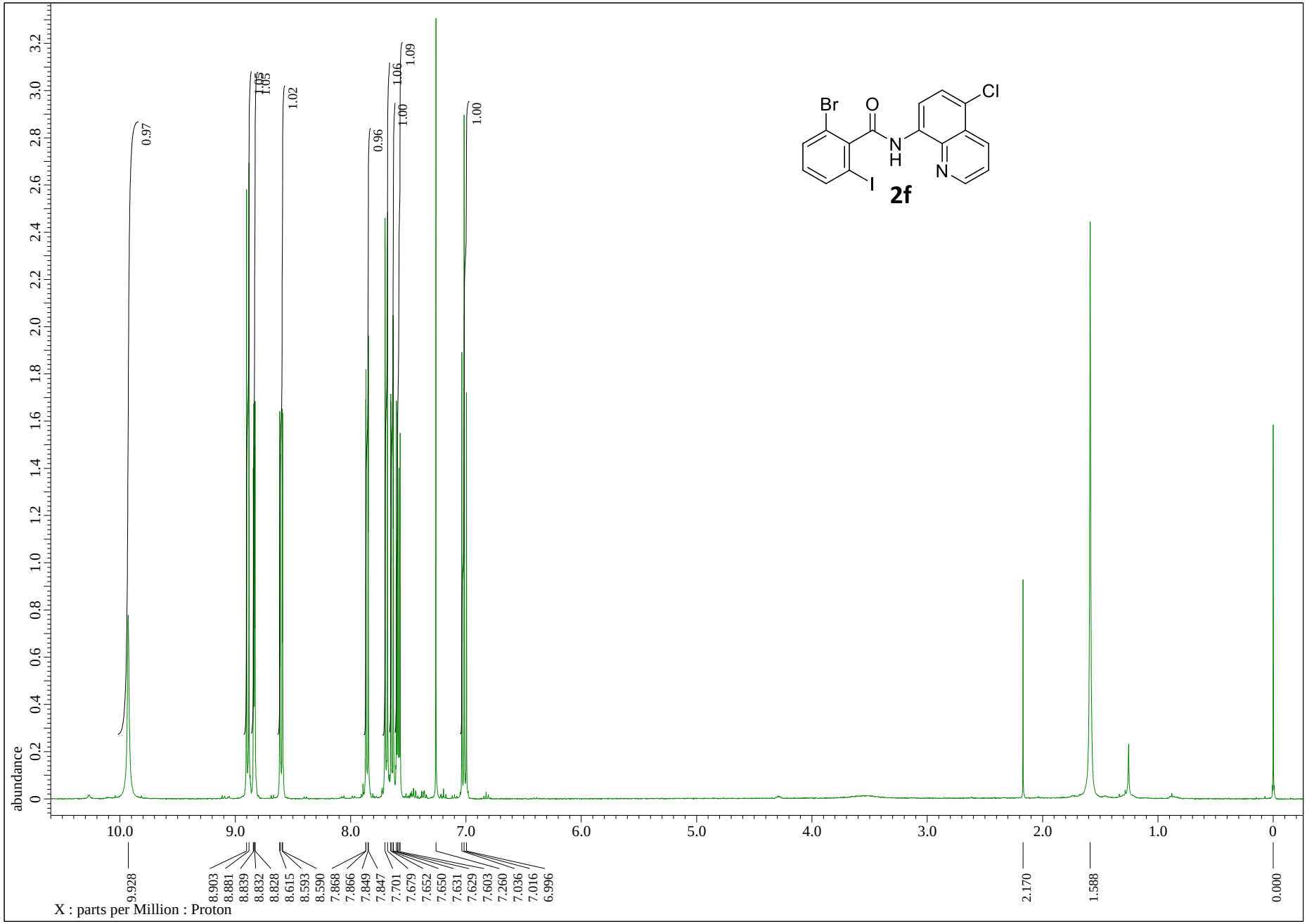

O
N
H
I
I
N
2b’
abundance
X : parts per Million : Proton
0.87
2.04
1.00
1.02
0.98
1.05
1.34
1.00
3.03
9.934
8.751
8.746
8.743
8.736
8.730
8.407
8.389
8.385
8.171
8.151
7.738
7.718
7.558
7.548
7.536
7.526
7.270
7.261
7.250
7.075
7.054
7.035
2.461
1.580
0.000

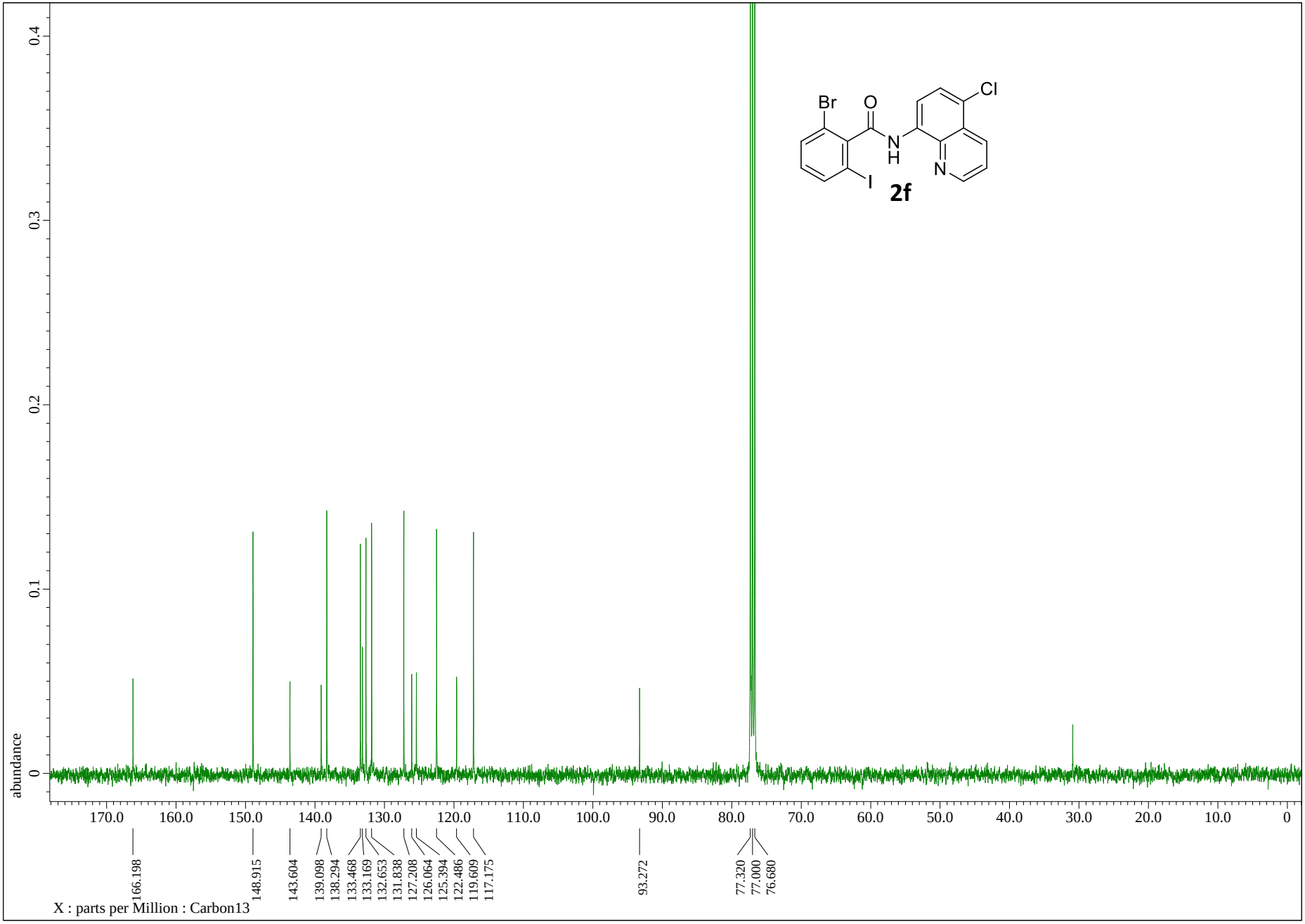

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
168.167
148.936
142.924
140.738
139.067
138.211
136.788
136.613
135.014
130.684
130.096
129.704
123.259
118.330
92.818
90.282
77.320
77.000
76.680
20.130
X : parts per Million : Carbon13
O
N
H
N
I
I
2b’

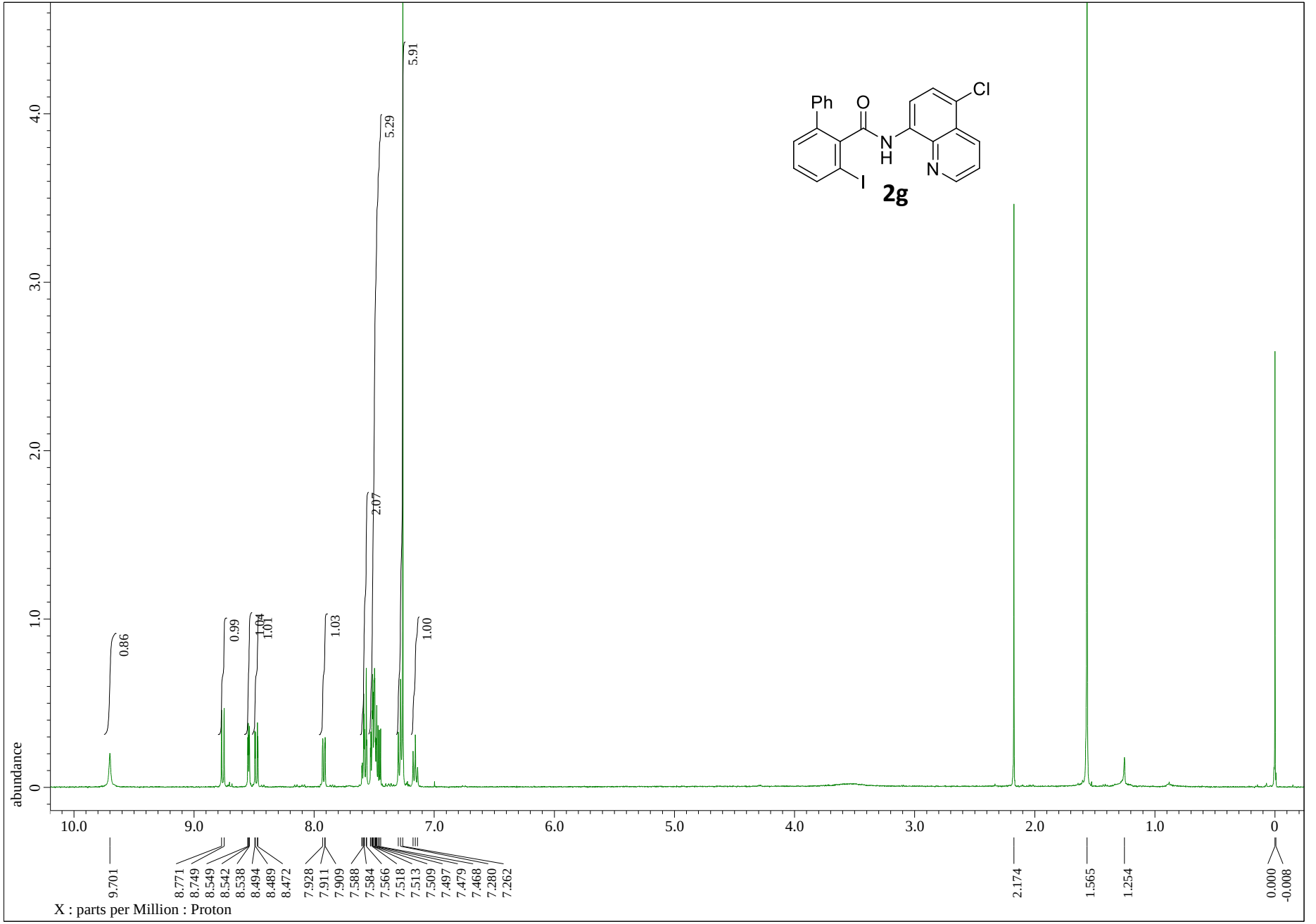

OMe
O
N
H
N
I
2c
3.14
3.03
1.42
0.90
1.03
1.06
1.01
1.00
1.06
1.02
1.03
abundance
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
9.664
8.873
8.853
8.761
8.757
8.750
8.746
8.595
8.574
8.570
7.709
7.689
7.440
7.429
7.419
7.408
7.240
7.237
7.217
7.033
7.013
6.994
6.906
6.884
4.005
2.452
1.598
X : parts per Million : Proton

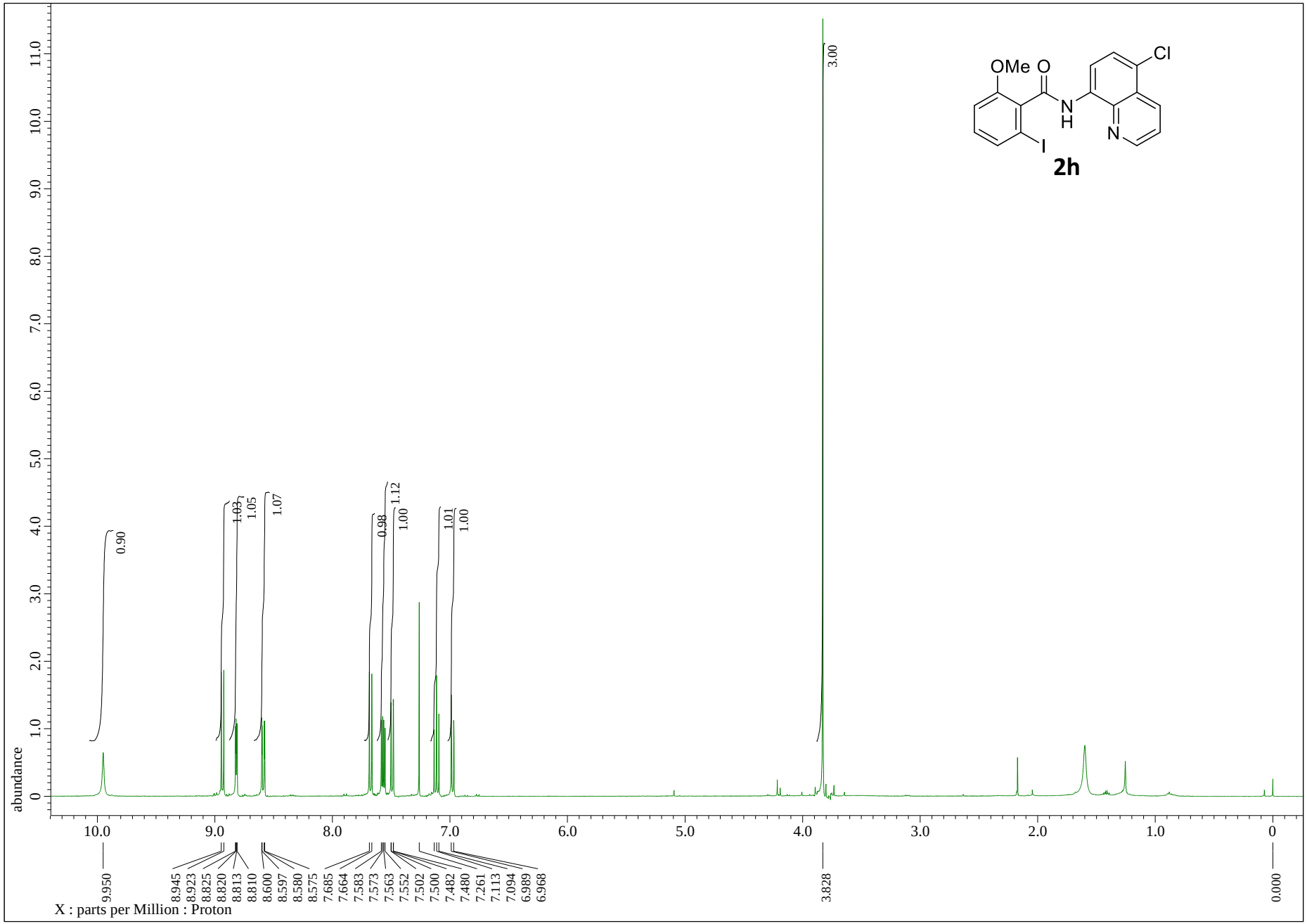

CF3
O
N
H
Cl
N
I
2d
0.90
1.02
1.02
1.00
0.93
1.00
0.95
1.00
0.98
abundance
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.949
8.883
8.862
8.818
8.815
8.808
8.803
8.608
8.587
8.139
8.119
7.773
7.753
7.698
7.677
7.593
7.583
7.572
7.561
7.315
7.296
7.275
7.260
1.611
0.000
X : parts per Million : Proton

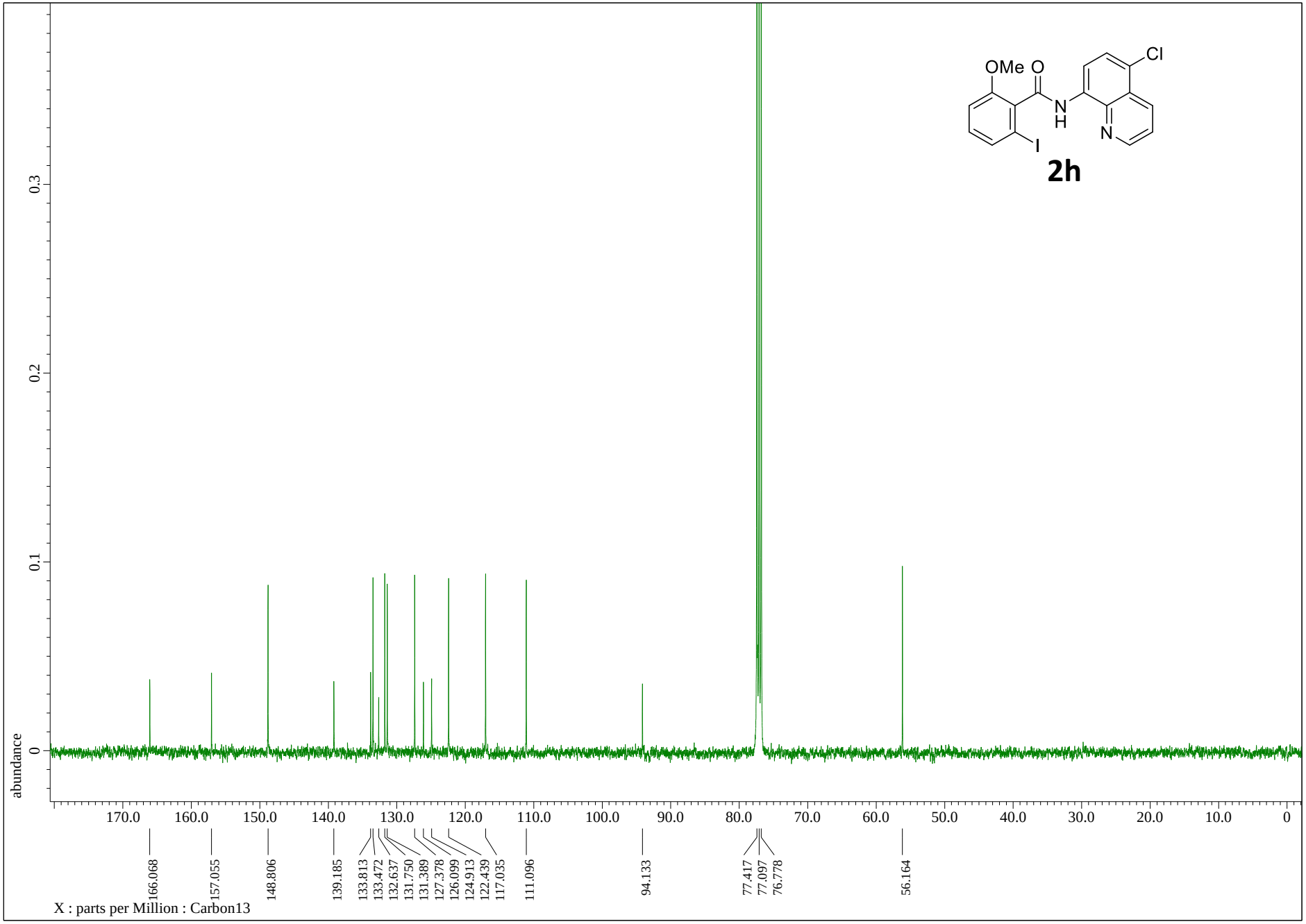

F
O
N
H
Cl
N
I
2e
abundance
X : parts per Million : Proton
10.047
8.912
8.891
8.843
8.840
8.833
8.829
8.619
8.614
8.597
8.593
7.738
7.697
7.675
7.607
7.597
7.261
7.210
7.206
7.197
7.189
7.182
7.179
7.164
1.570
0.000

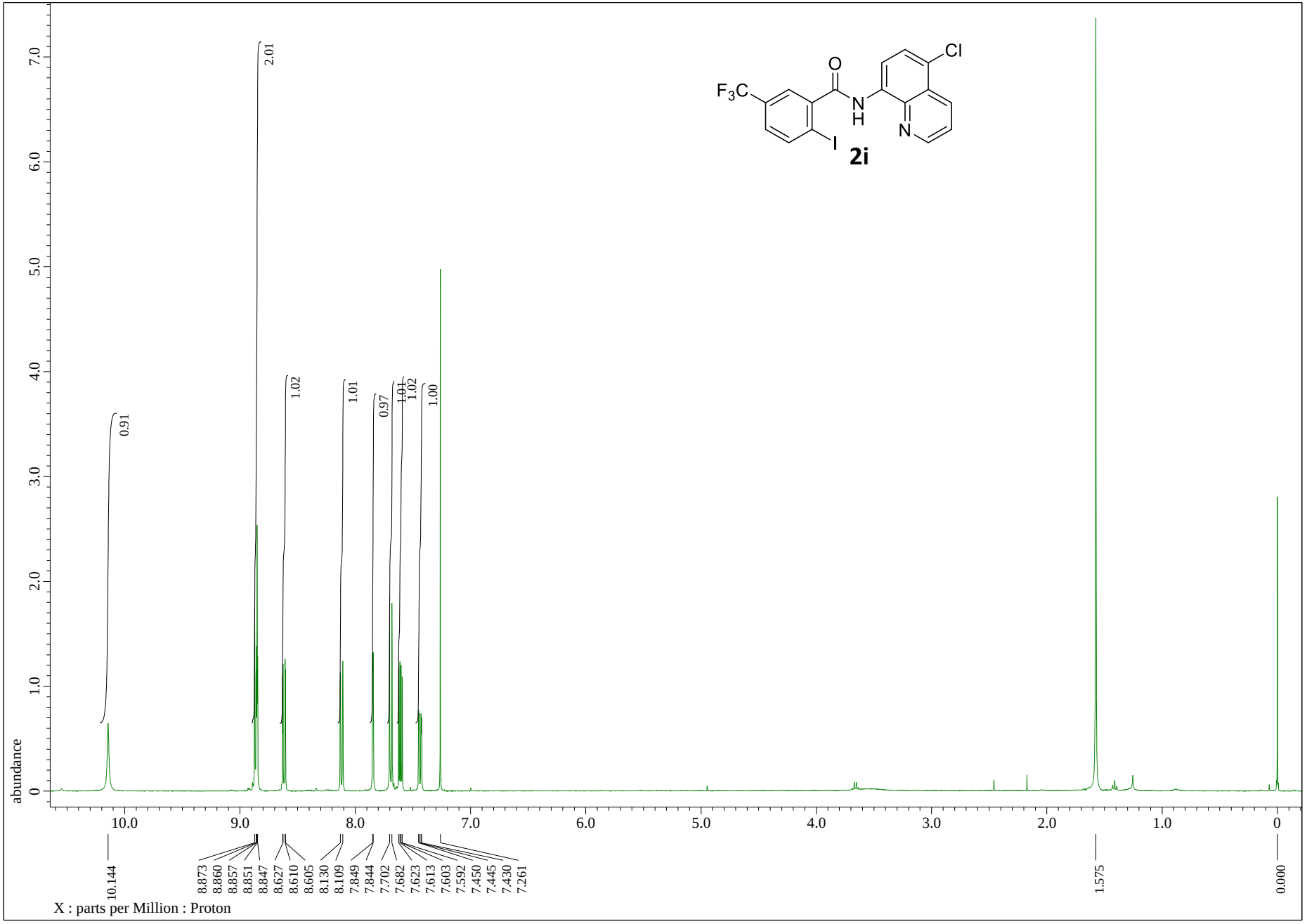

Br
O
N
H
Cl
N
I
2f
abundance
X : parts per Million : Proton
0.97
1.05
1.05
1.02
0.96
1.06
1.09
1.00
1.00
9.928
8.903
8.881
8.839
8.832
8.828
8.615
8.593
8.590
7.868
7.866
7.849
7.847
7.701
7.679
7.652
7.650
7.631
7.629
7.603
7.260
7.036
7.016
6.996
2.170
1.588
0.000

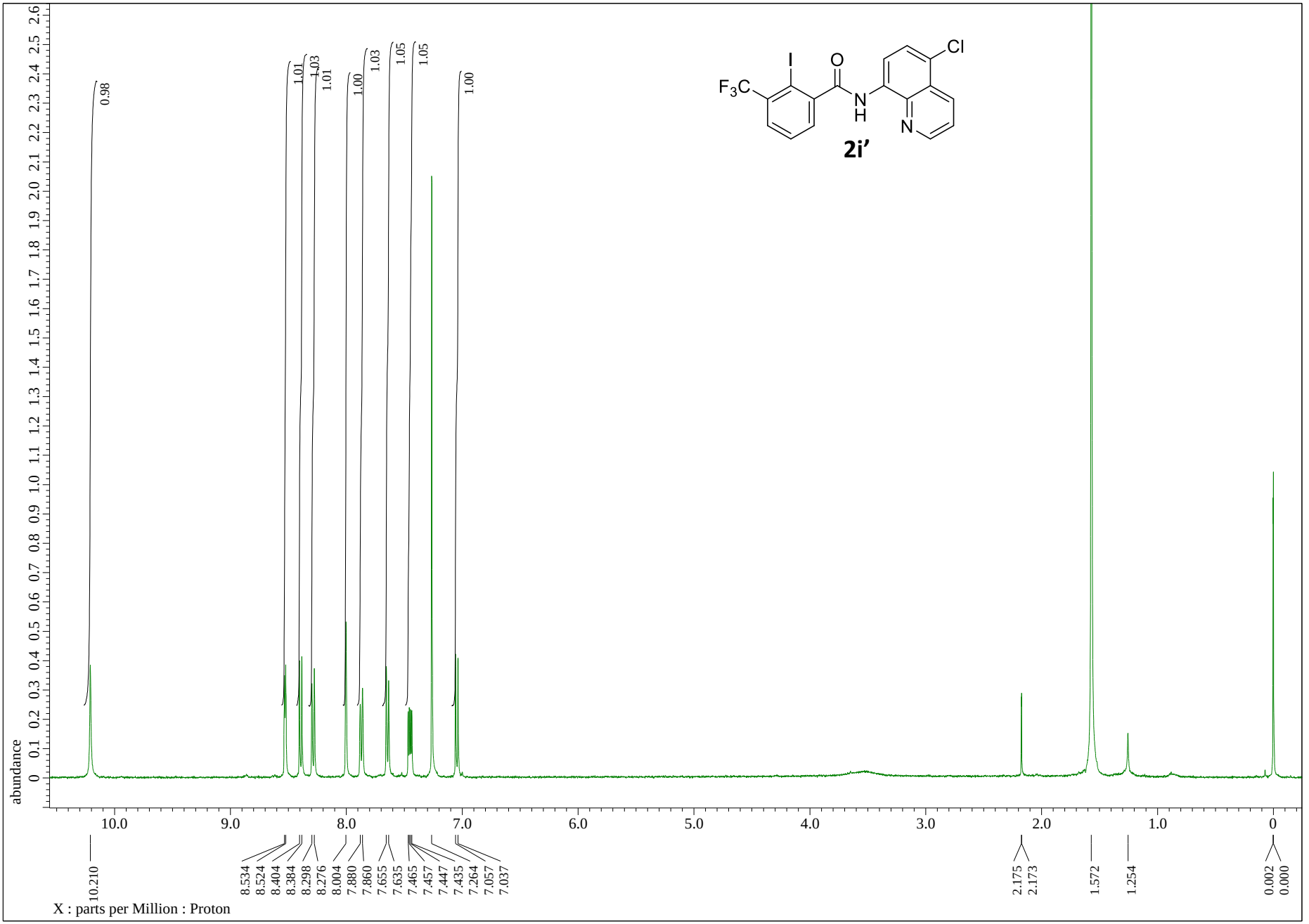

Br
O
N
H
Cl
N
I
2f
abundance
0.4
0.3
0.2
0.1
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.198
148.915
143.604
139.098
138.294
133.468
133.169
132.653
131.838
127.208
126.064
125.394
122.486
119.609
117.175
93.272
77.320
77.000
76.680
X : parts per Million : Carbon13

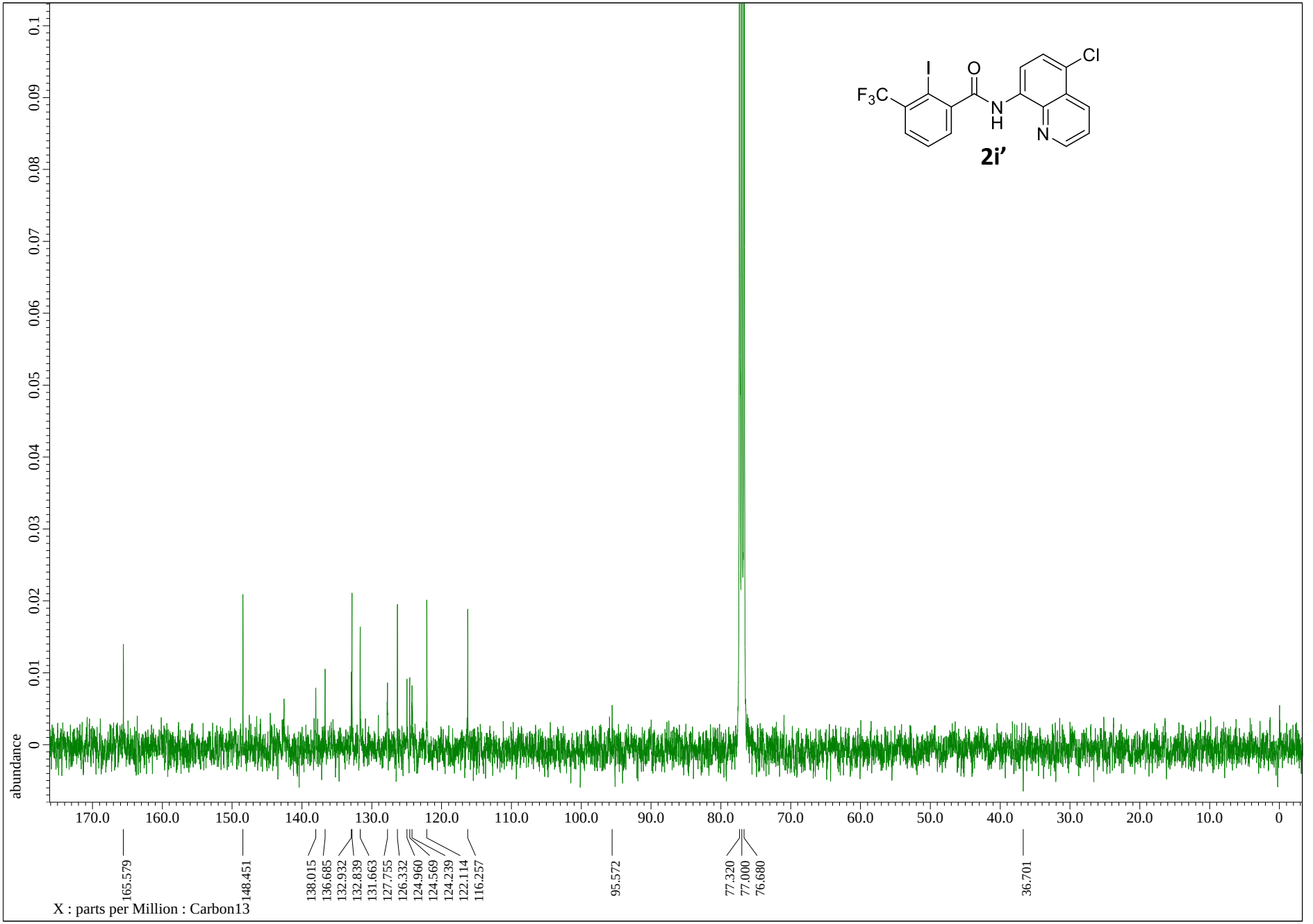

Ph
O
N
H
Cl
N
I
2g
abundance
X : parts per Million : Proton
9.701
8.771
8.749
8.549
8.542
8.538
8.494
8.489
8.472
7.928
7.911
7.909
7.588
7.584
7.566
7.518
7.513
7.509
7.497
7.479
7.468
7.280
7.262
2.174
1.565
1.254
0.000
-0.008
0.86
0.99
1.04
1.01
1.03
2.07
5.29
5.91
1.00

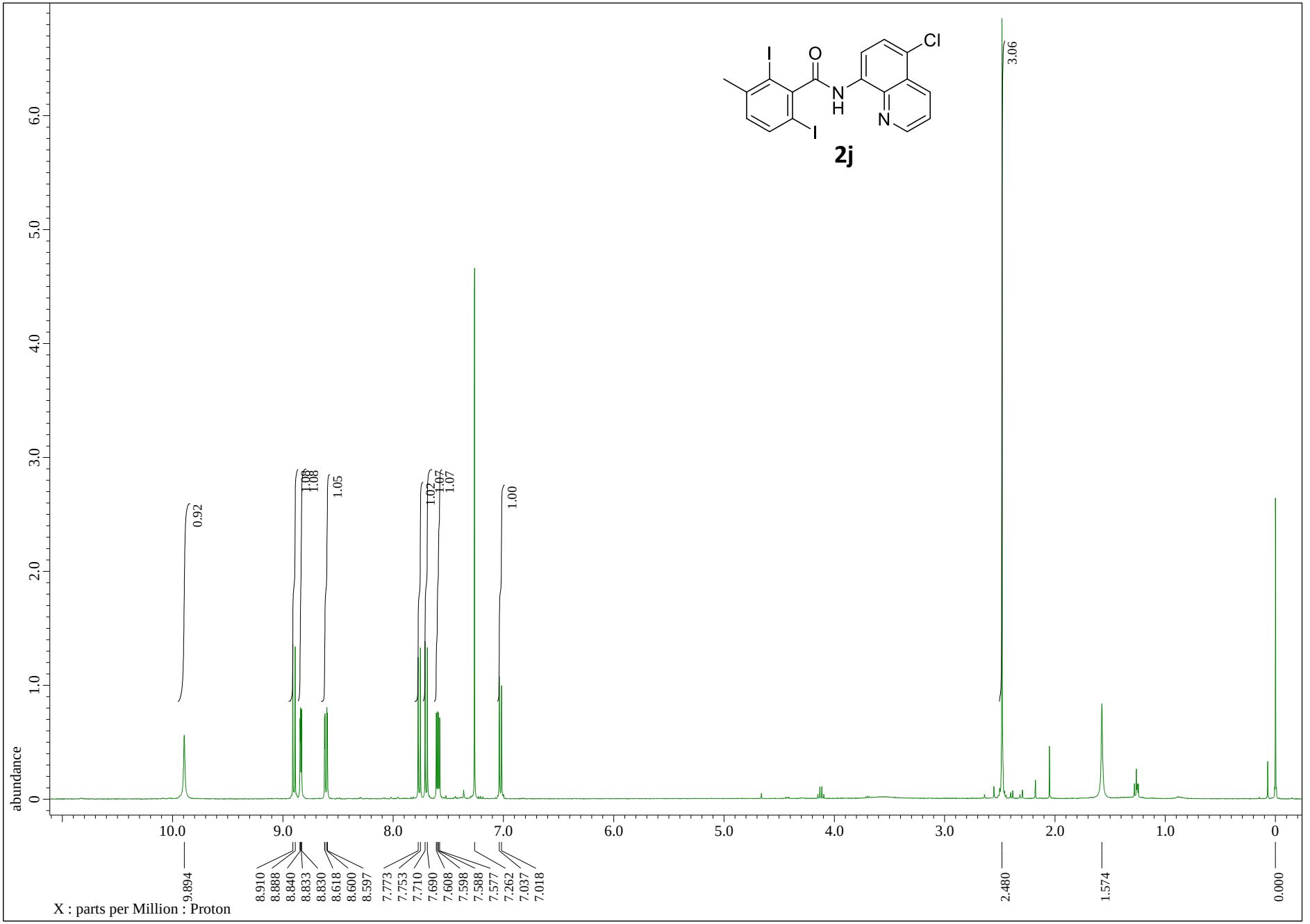

OMe
O
N
H
Cl
N
I
2h
abundance
X : parts per Million : Proton
0.90
1.03
1.05
1.07
0.98
1.12
1.00
1.01
1.00
3.00
9.950
8.945
8.923
8.825
8.820
8.813
8.810
8.600
8.597
8.580
8.575
7.685
7.664
7.583
7.573
7.563
7.552
7.502
7.500
7.482
7.480
7.261
7.113
7.094
6.989
6.968
3.828
0.000

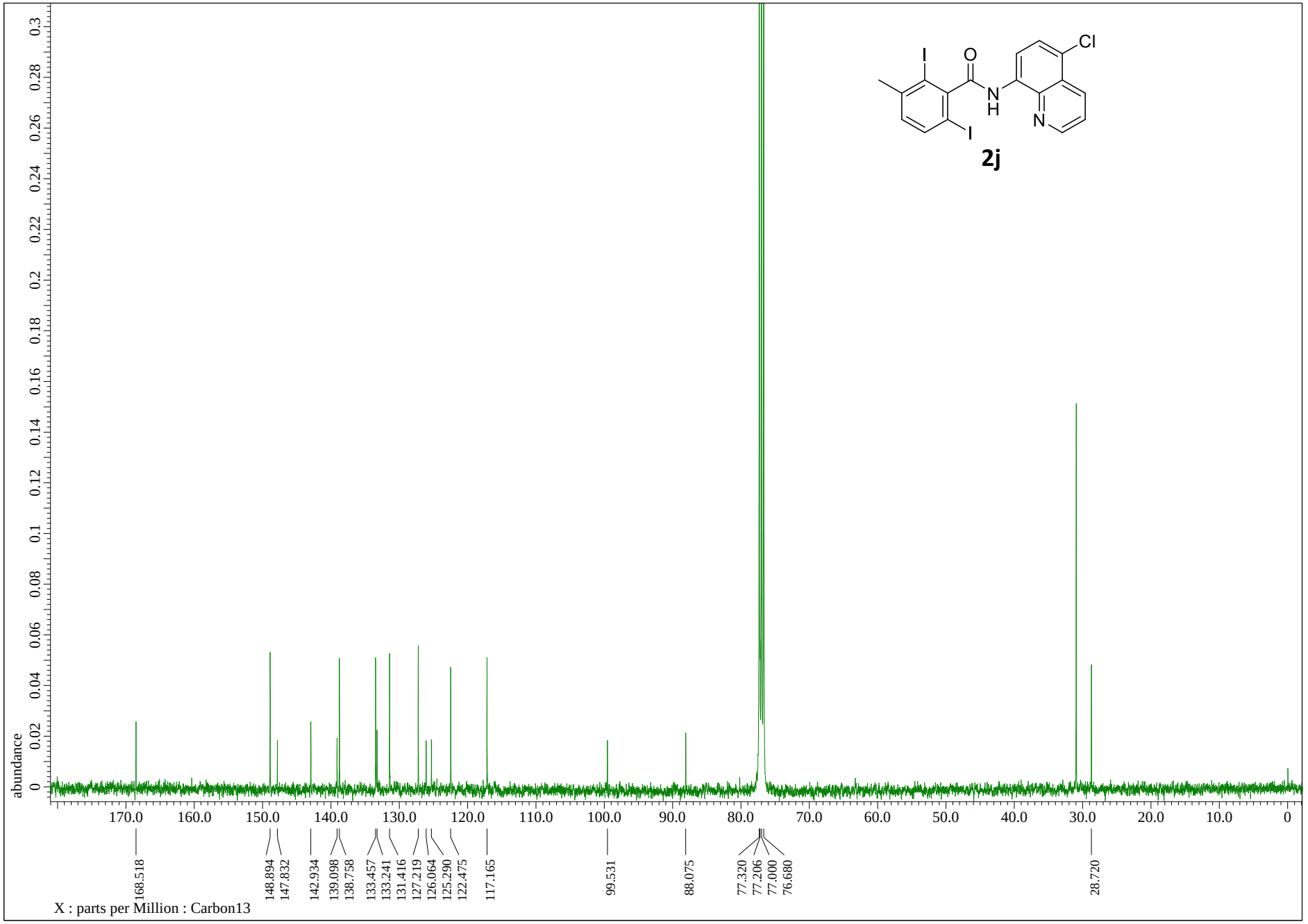

OMe
O
N
H
Cl
N
I
2h
abundance
0
0.1
0.2
0.3
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
166.068
157.055
148.806
139.185
133.813
133.472
132.637
131.750
131.389
127.378
126.099
124.913
122.439
117.035
111.096
94.133
77.417
77.097
76.778
56.164
X : parts per Million : Carbon13

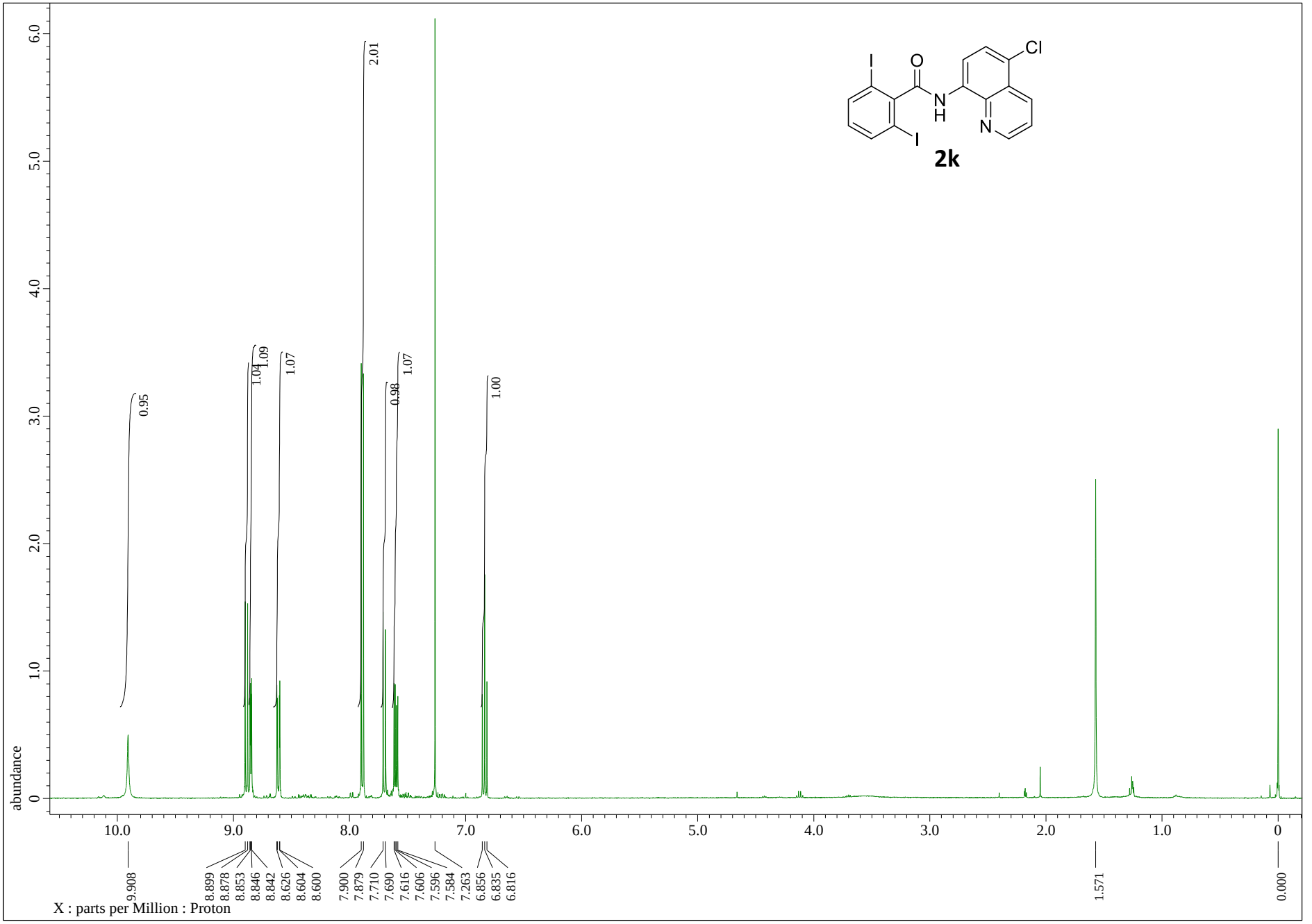

2i
abundance
X : parts per Million : Proton
2.01
1.02
1.01
0.97
1.01
1.02
1.00
0.91
10.144
8.873
8.860
8.857
8.851
8.847
8.627
8.610
8.605
8.130
8.109
7.849
7.844
7.702
7.682
7.623
7.613
7.603
7.592
7.450
7.445
7.430
7.261
1.575
0.000

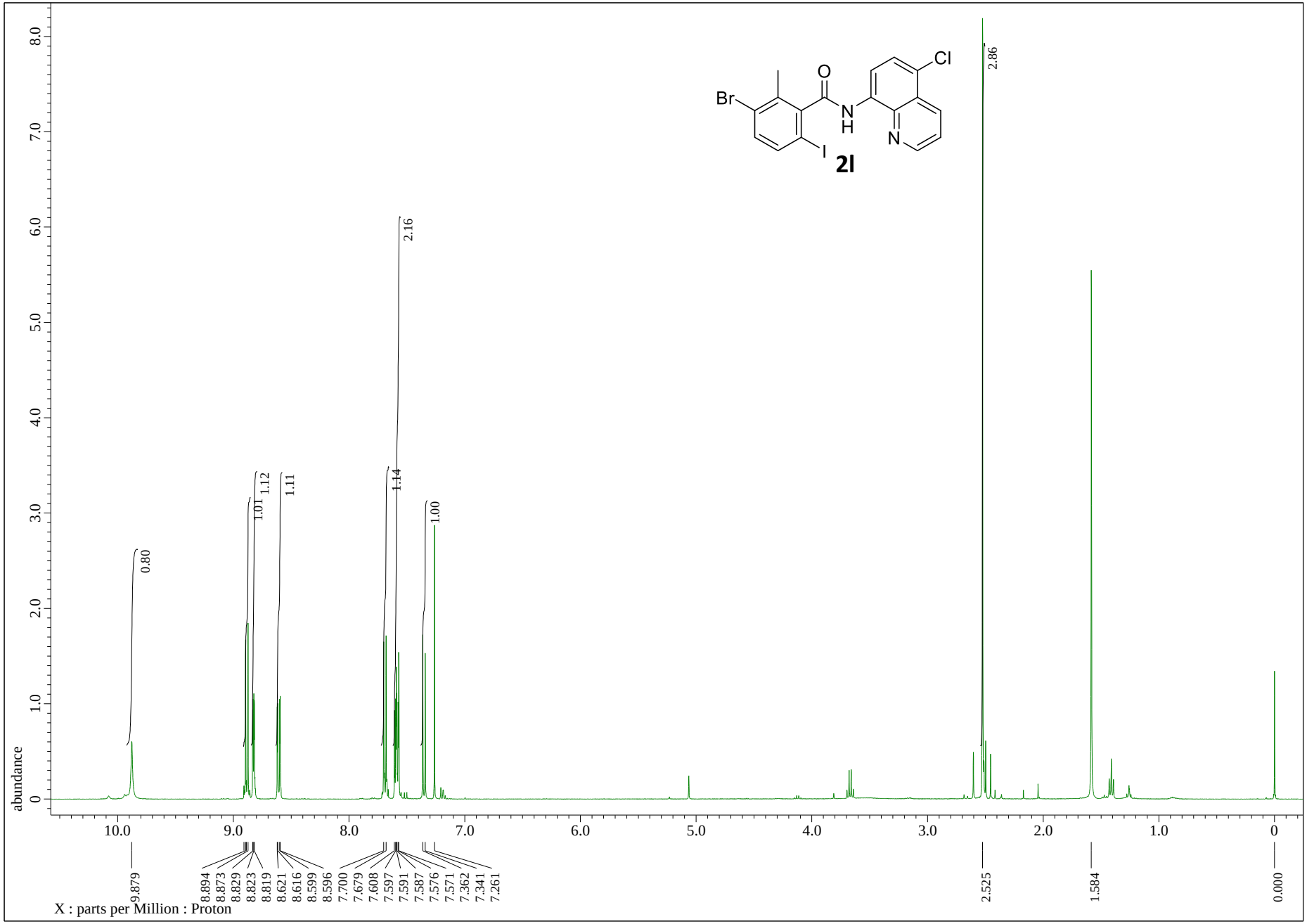

I
O
Cl
F3C
N
H
N
2i'
0.98
1.01
1.03
1.01
1.00
1.03
1.05
1.05
1.00
abundance
X : parts per Million : Proton
10.210
8.534
8.524
8.404
8.384
8.298
8.276
8.004
7.880
7.860
7.655
7.635
7.465
7.457
7.447
7.435
7.264
7.057
7.037
2.175
2.173
1.572
1.254
0.002
0.000

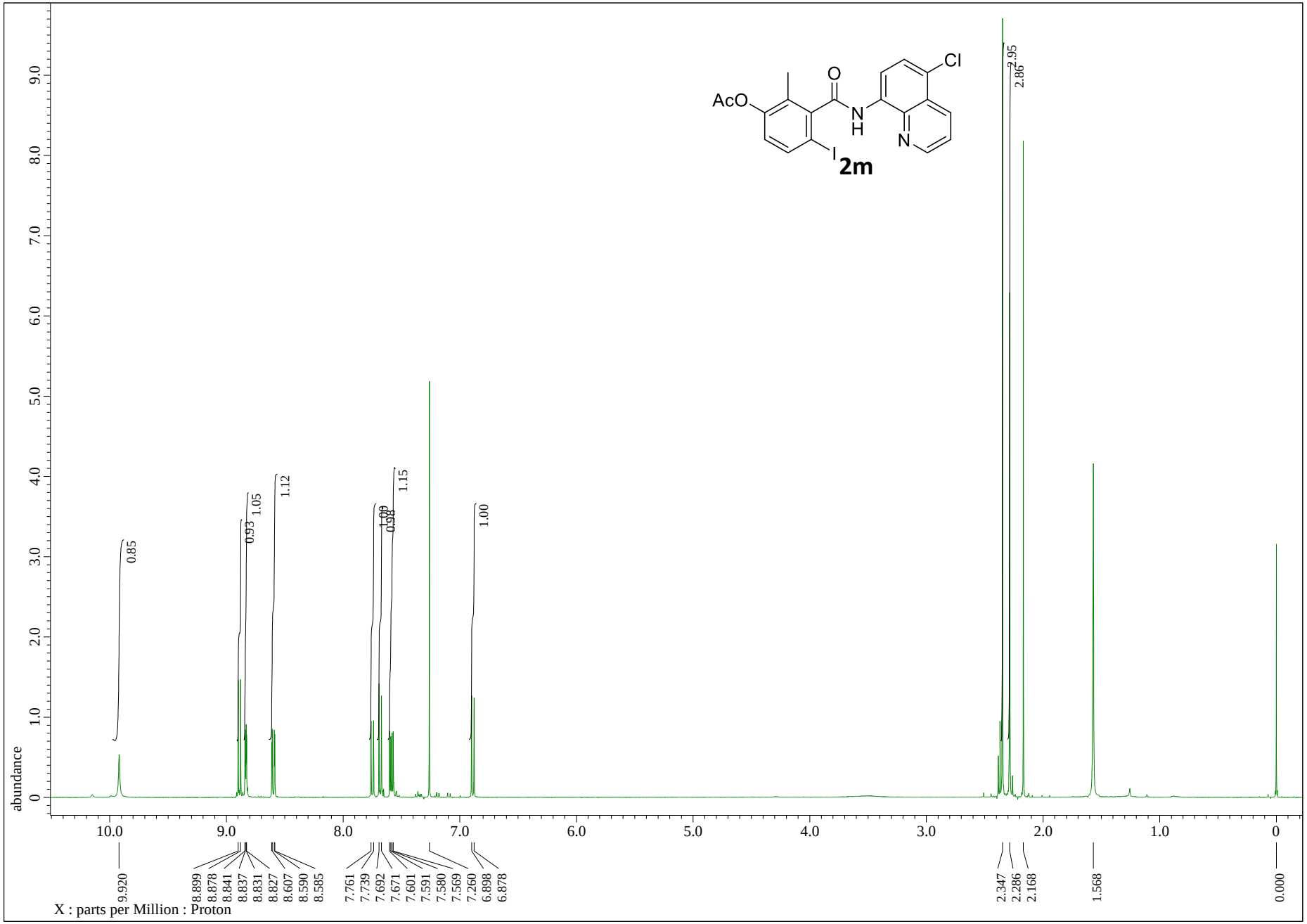

I
O
Cl
F3C
N
H
N
2i'
abundance
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
165.579
148.451
138.015
136.685
132.932
132.839
131.663
127.755
126.332
124.960
124.569
124.239
122.114
116.257
95.572
77.320
77.000
76.680
36.701
X : parts per Million : Carbon13

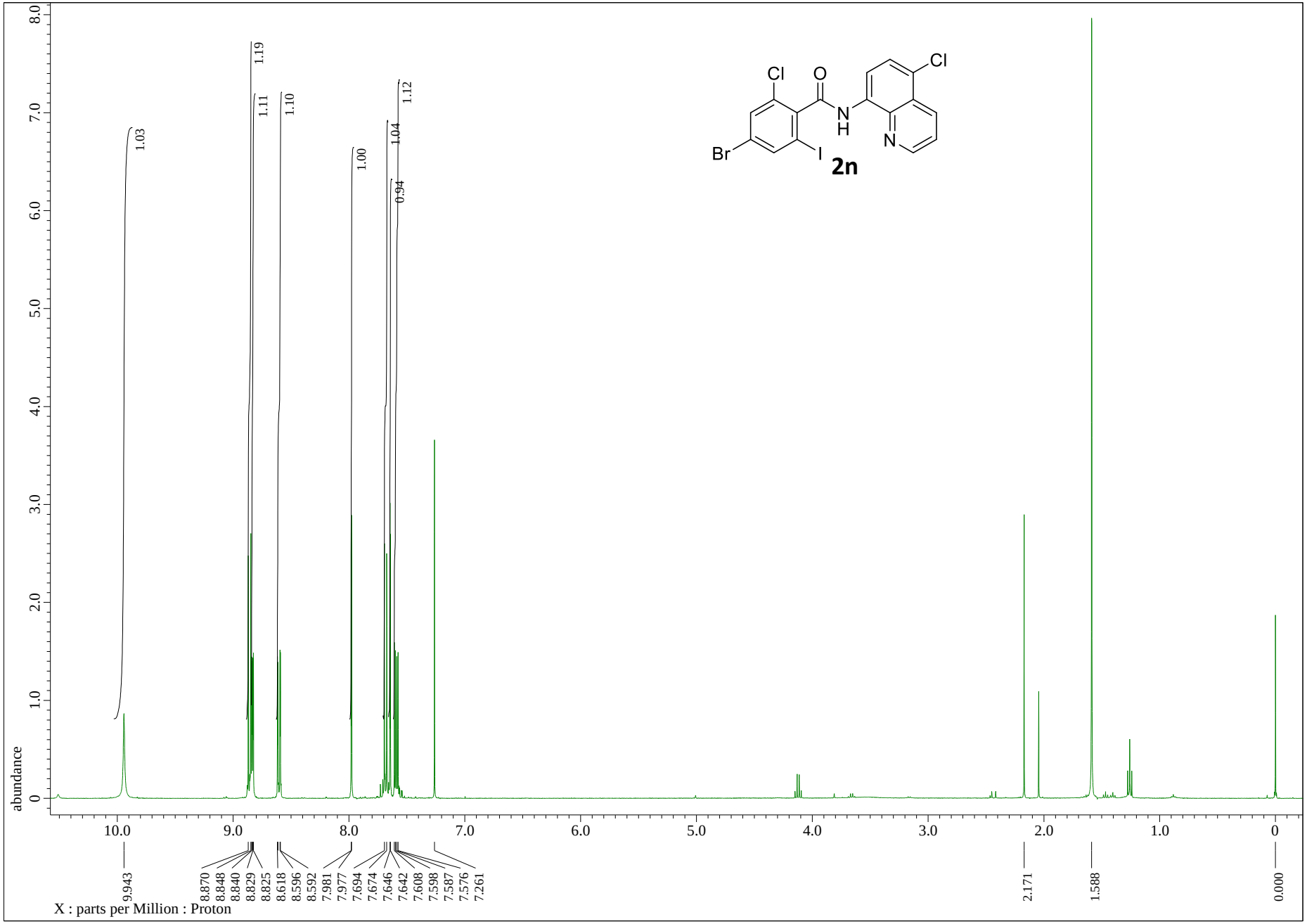

I
O
Cl
N
H
N
I
2j
3.06
0.92
1.08
1.08
1.05
1.02
1.07
1.07
1.00
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.894
8.910
8.888
8.840
8.833
8.830
8.618
8.600
8.597
7.773
7.753
7.710
7.690
7.608
7.598
7.588
7.577
7.262
7.037
7.018
2.480
1.574
0.000
X : parts per Million : Proton

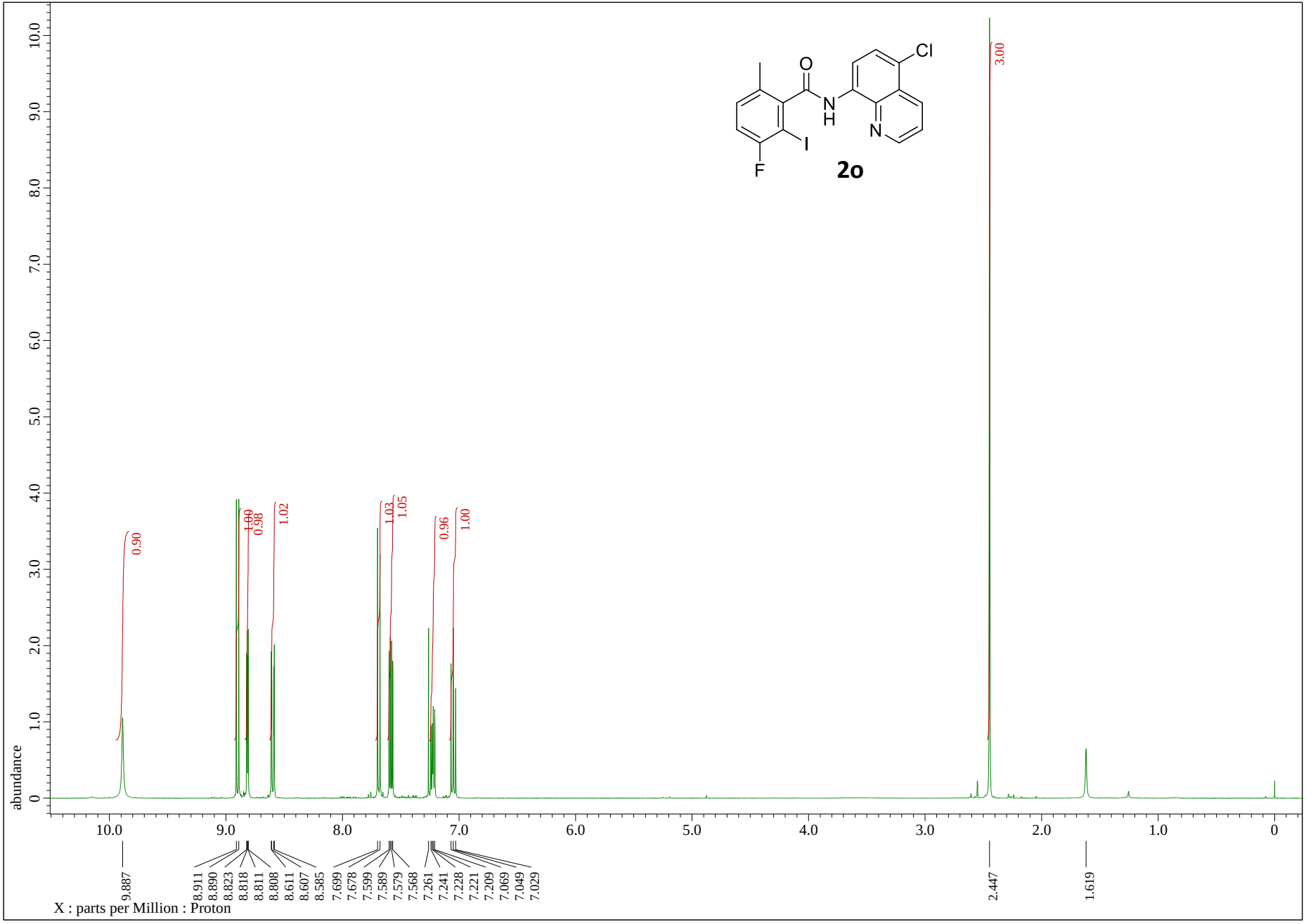

I
O
Cl
N
H
N
I
2j
abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
0.28
0.3
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
168.518
148.894
147.832
142.934
139.098
138.758
133.457
133.241
131.416
127.219
126.064
125.290
122.475
117.165
99.531
88.075
77.320
77.206
77.000
76.680
28.720
X : parts per Million : Carbon13

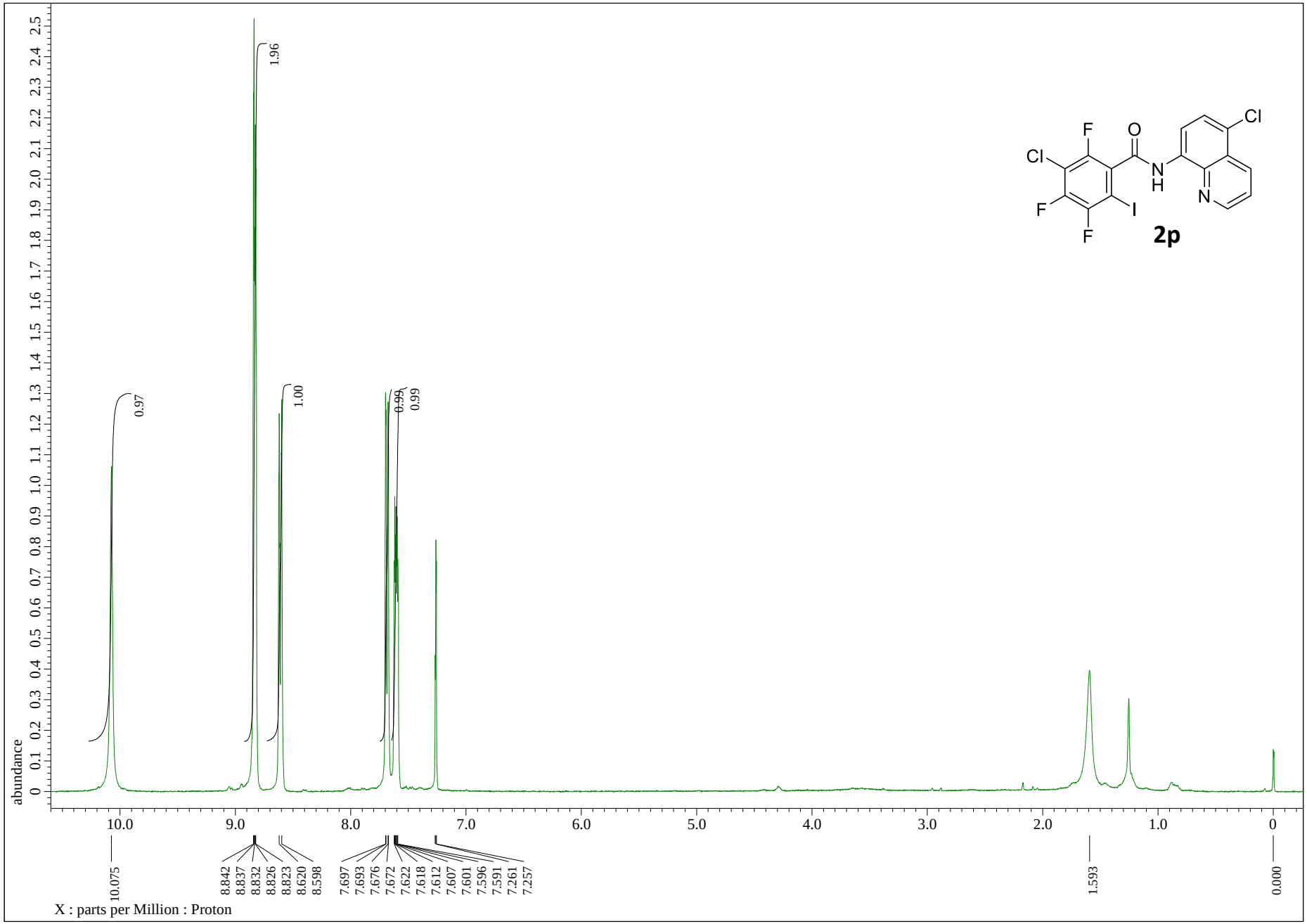

I
O
Cl
N
H
N
I
2k
abundance
X : parts per Million : Proton
0.95
1.04
1.09
1.07
2.01
0.98
1.07
1.00
9.908
8.899
8.878
8.853
8.846
8.842
8.626
8.604
8.600
7.900
7.879
7.710
7.690
7.616
7.606
7.596
7.584
7.263
6.856
6.835
6.816
1.571
0.000

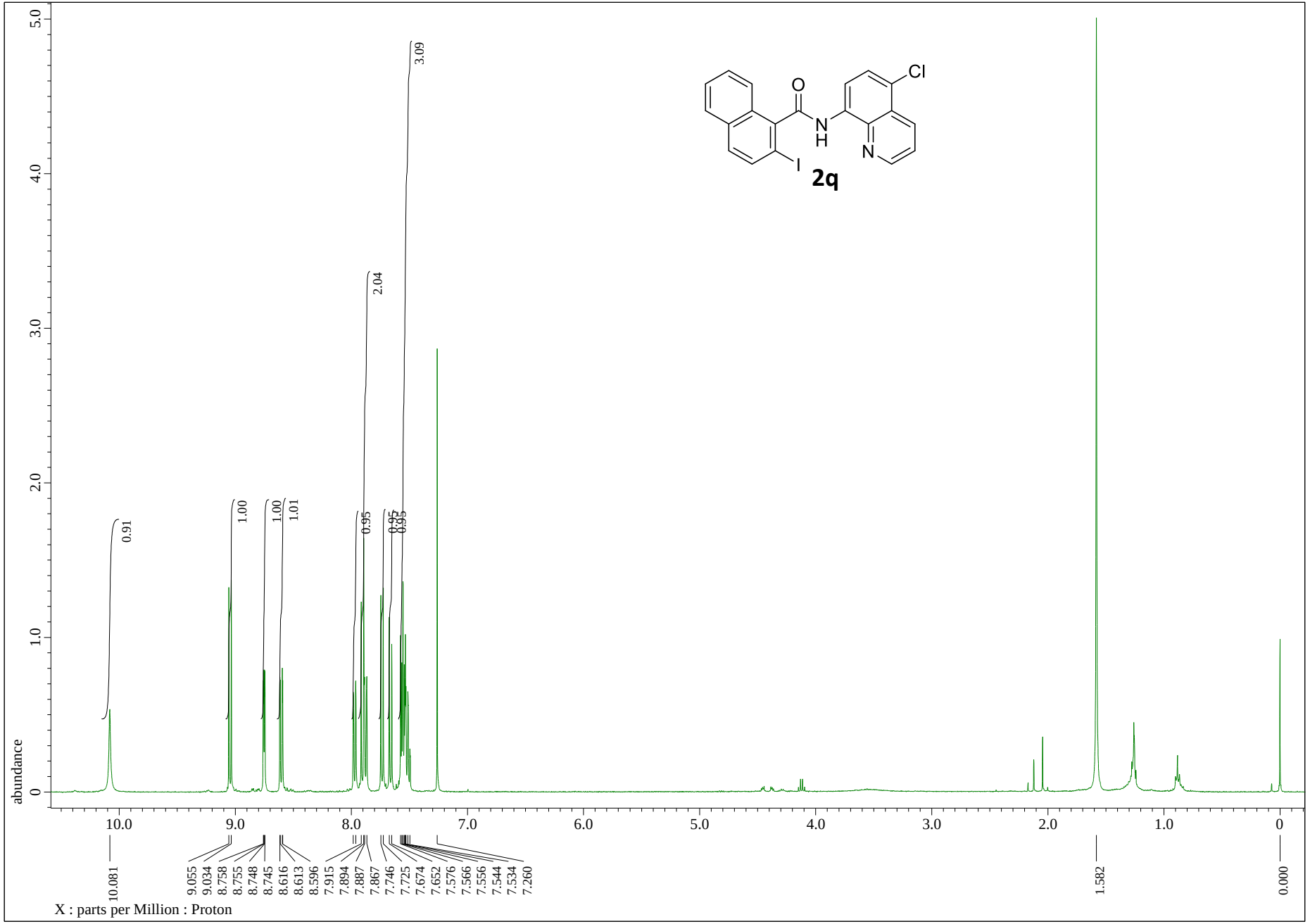

Br
O
N
H
Cl
N
I
2l
abundance
X : parts per Million : Proton
0.80
1.01
1.12
1.11
2.16
1.14
1.00
2.86
9.879
8.894
8.873
8.829
8.823
8.819
8.621
8.616
8.599
8.596
7.700
7.679
7.608
7.597
7.591
7.587
7.576
7.571
7.362
7.341
7.261
2.525
1.584
0.000

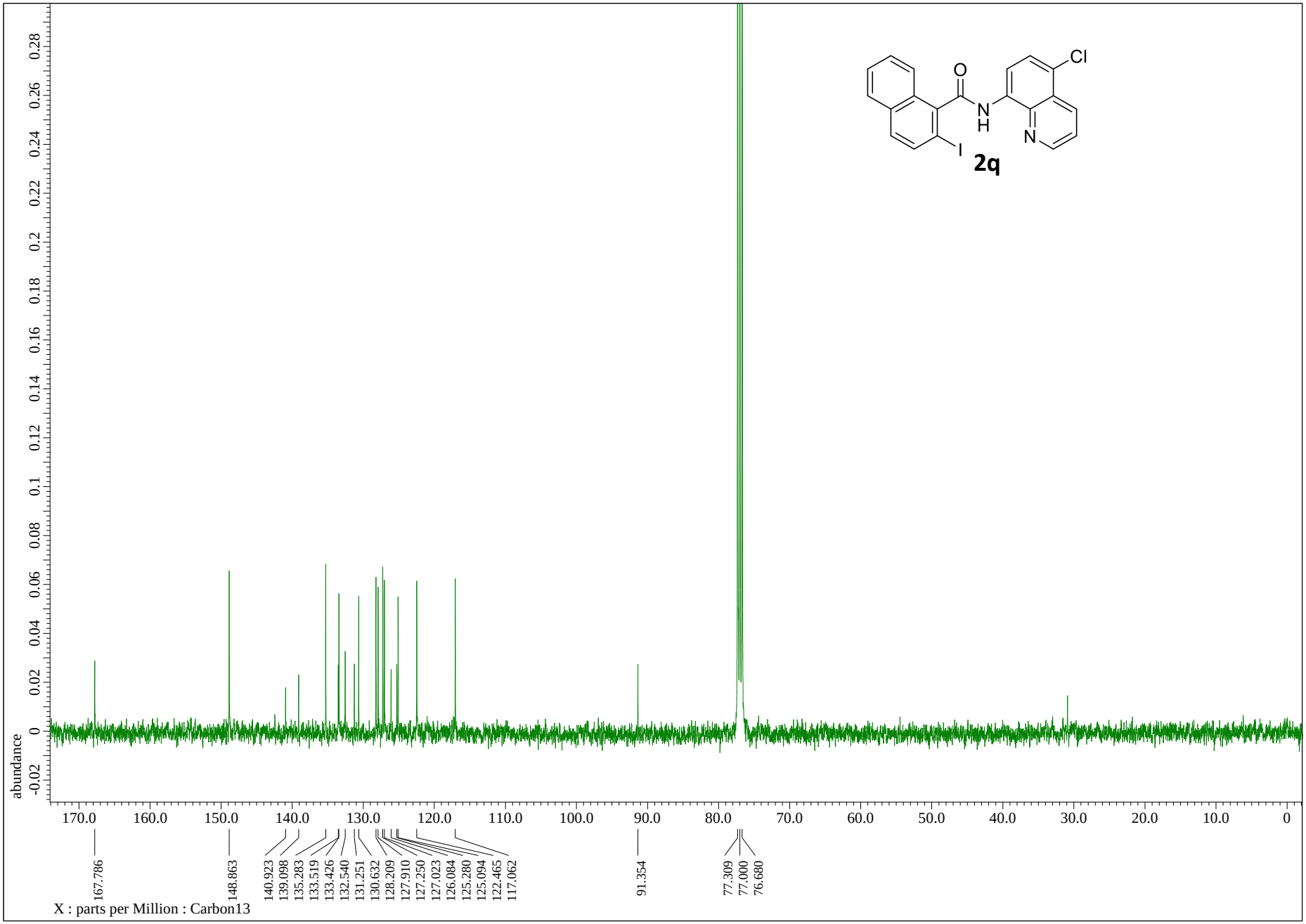

AcO
O
N
H
Cl
N
I
2m
abundance
X : parts per Million : Proton
0.85
0.93
1.05
1.12
1.15
1.00
2.95
2.86
9.920
8.899
8.878
8.841
8.837
8.831
8.827
8.607
8.590
8.585
7.761
7.739
7.692
7.671
7.601
7.591
7.580
7.569
7.260
6.898
6.878
2.347
2.286
2.168
1.568
0.000

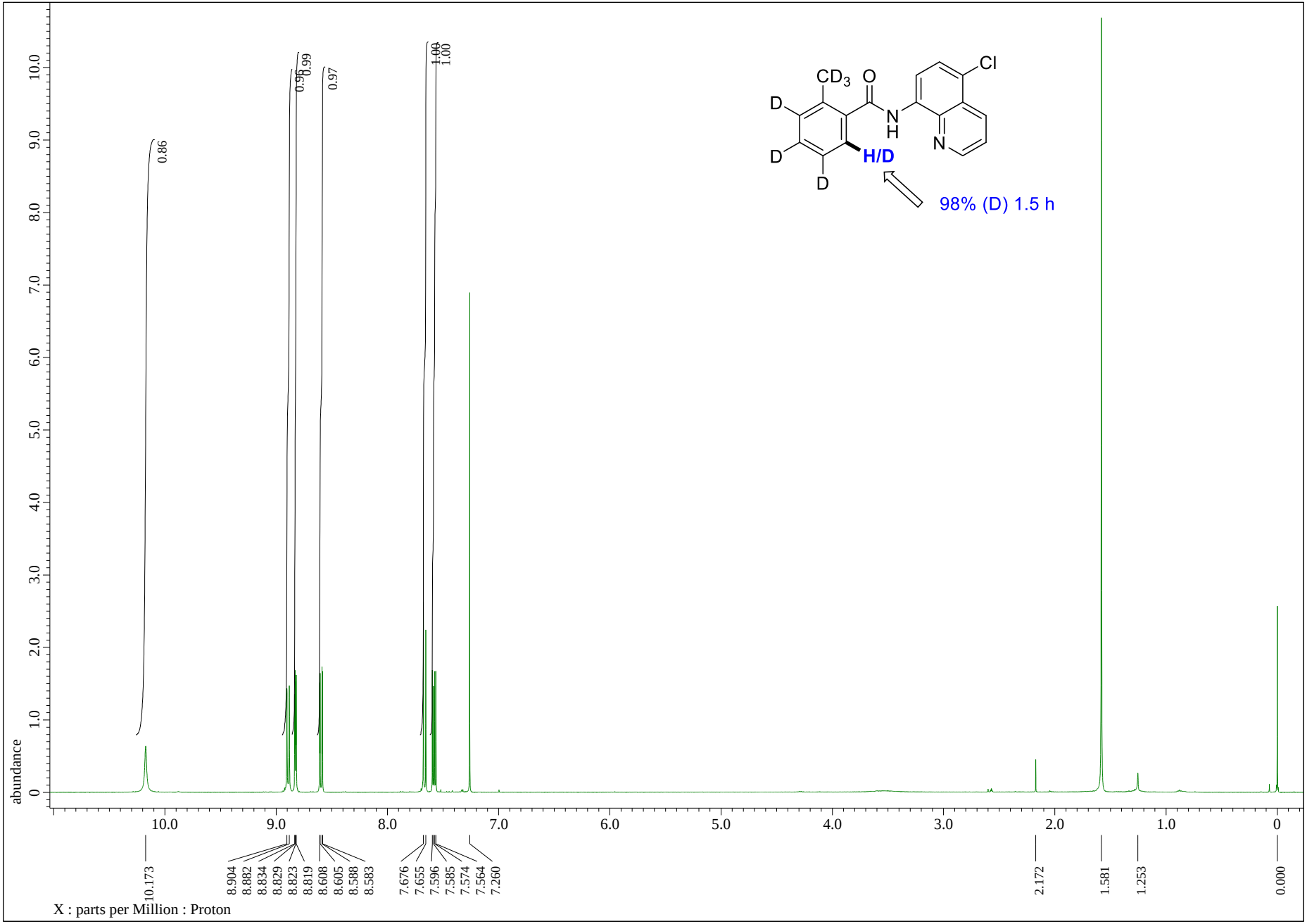

Cl
O
N
H
Cl
Br
I
N
2n
1.03
1.19
1.11
1.10
1.00
1.04
0.94
1.12
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.943
8.870
8.848
8.840
8.829
8.825
8.618
8.596
8.592
7.981
7.977
7.694
7.674
7.646
7.642
7.608
7.598
7.587
7.576
7.261
2.171
1.588
0.000
X : parts per Million : Proton

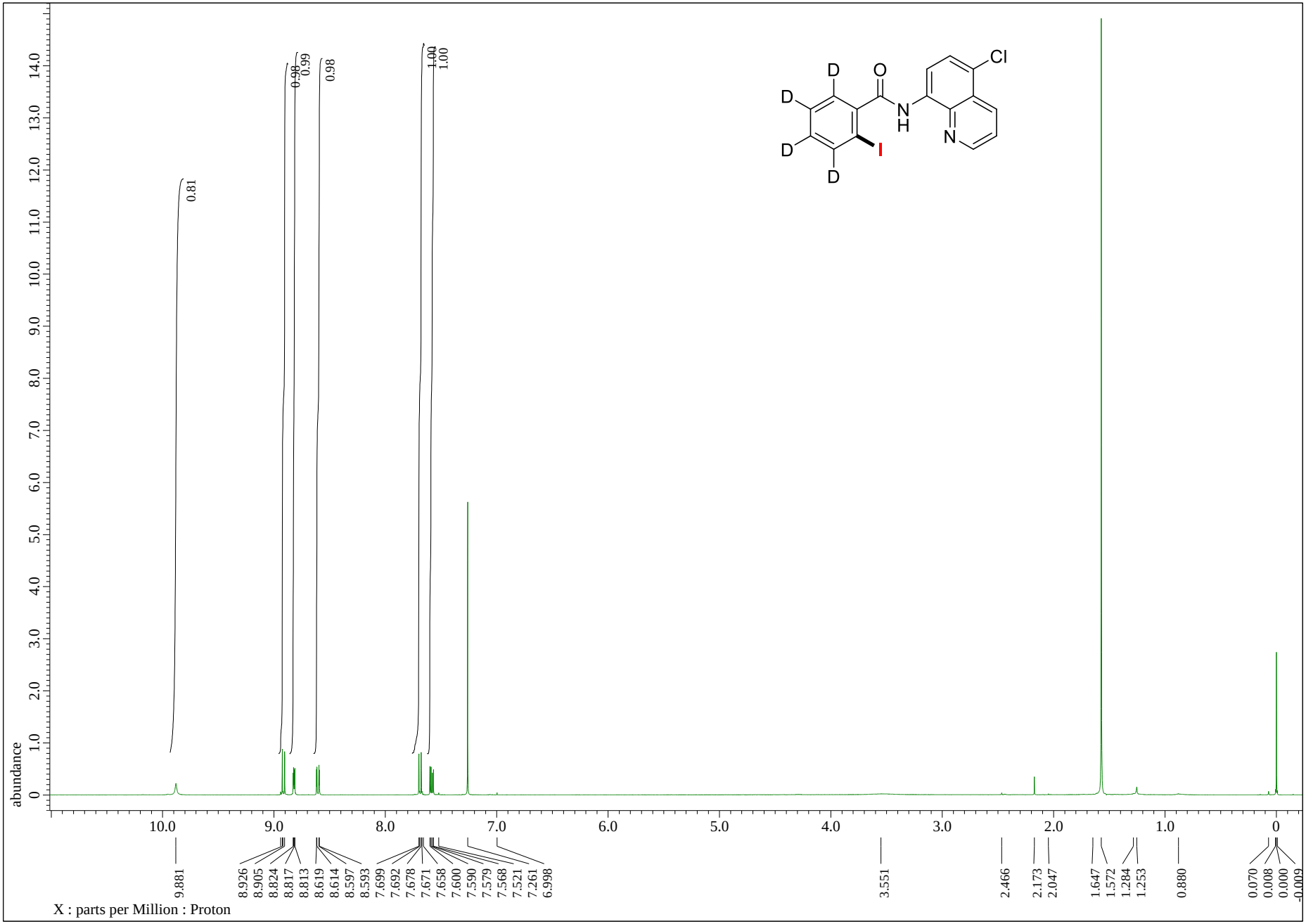

Cl
O
N
H
N
I
F
2o
3.00
0.90
1.00
0.98
1.02
1.03
1.05
0.96
1.00
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.887
8.911
8.890
8.823
8.818
8.811
8.808
8.611
8.607
8.585
7.699
7.678
7.599
7.589
7.579
7.568
7.261
7.241
7.228
7.221
7.209
7.069
7.049
7.029
2.447
1.619
X : parts per Million : Proton

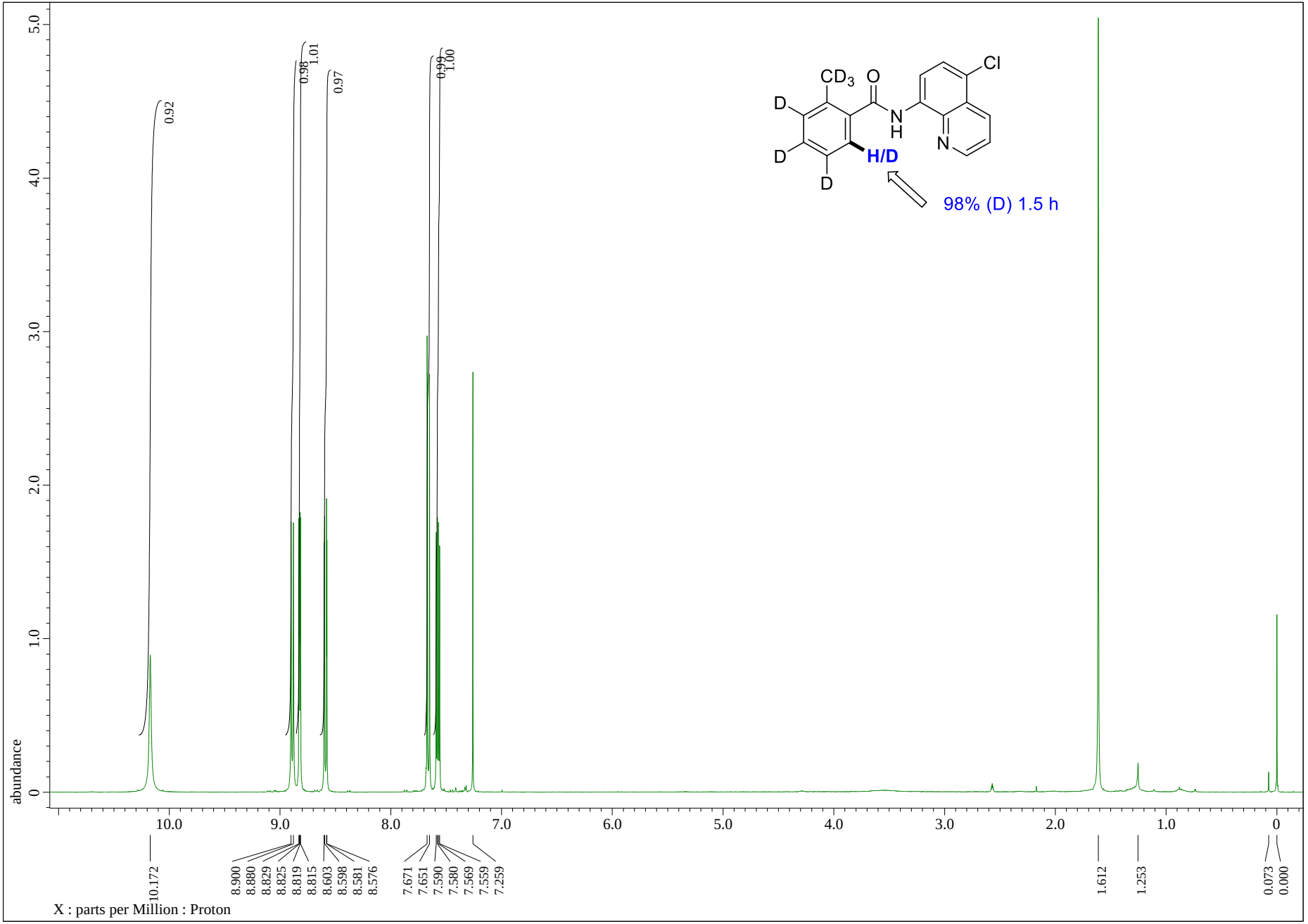

abundance
0.97
1.96
1.00
0.99
0.99
10.075
8.842
8.837
8.832
8.826
8.823
8.620
8.598
7.697
7.693
7.676
7.672
7.622
7.618
7.612
7.607
7.601
7.596
7.591
7.261
7.257
1.593
0.000
X : parts per Million : Proton
Cl
F
O
N
H
Cl
F
I
F
N
2p


2q
abundance
X : parts per Million : Proton
0.91
1.00
1.00
1.01
0.95
2.04
3.09
10.081
9.055
9.034
8.758
8.755
8.748
8.745
8.616
8.613
8.596
7.915
7.894
7.887
7.867
7.746
7.725
7.674
7.652
7.576
7.566
7.556
7.544
7.534
7.260
1.582
0.000


O
N
H
Cl
N
I
2q
abundance
0.28
0.26
0.24
0.22
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
-0.02
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
167.786
148.863
140.923
139.098
135.283
133.519
133.426
132.540
131.251
130.632
128.209
127.910
127.250
127.023
126.084
125.280
125.094
122.465
117.062
91.354
77.309
77.000
76.680
X : parts per Million : Carbon13


abundance
X : parts per Million : Proton
0.86
0.96
0.99
0.97
1.00
1.00
CD3
O
Cl
D
N
H
D
N
D
H/D
98% (D) 1.5 h
10.173
8.904
8.882
8.834
8.829
8.823
8.819
8.608
8.605
8.588
8.583
7.676
7.655
7.596
7.585
7.574
7.564
7.260
2.172
1.581
1.253
0.000


abundance
X : parts per Million : Proton
0.81
0.98
0.99
0.98
1.00
1.00
D
O
Cl
D
N
H
D
N
D
I
D
9.881
8.926
8.905
8.824
8.817
8.813
8.619
8.614
8.597
8.593
7.699
7.692
7.678
7.671
7.658
7.600
7.590
7.579
7.568
7.521
7.261
6.998
3.551
2.466
2.173
2.047
1.647
1.572
1.284
1.253
0.880
0.070
0.008
0.000
-0.009


CD3
O
N
H
Cl
N
D
D
D
H/D
98% (D) 1.5 h
abundance
X : parts per Million : Proton

Calculated data of Cartesian coordinates and energies

Figure S1

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.001517	2.145892	-0.188157
2	6	0	1.660445	1.924450	-0.557956
3	6	0	0.816037	3.052285	-0.727682
4	6	0	1.296723	4.349834	-0.583937
5	6	0	2.634424	4.540869	-0.221835
6	6	0	3.482139	3.445314	-0.020113
7	6	0	-0.627322	2.775985	-0.998842
8	8	0	-1.401597	3.561338	-1.543731
9	7	0	-0.969866	1.549789	-0.458915
10	6	0	-2.227871	0.936674	-0.529547
11	6	0	-2.288183	-0.293650	0.190103
12	6	0	-3.382084	1.402770	-1.141506
13	6	0	-3.493752	-1.035700	0.322753
14	6	0	-4.583672	0.665713	-1.038371
15	6	0	-1.088215	-1.838685	1.467978
16	6	0	-3.436729	-2.225125	1.092272
17	6	0	-4.647028	-0.511078	-0.325481
18	6	0	-2.247501	-2.616088	1.667839
19	7	0	-1.119753	-0.724033	0.757192
20	17	0	-6.175276	-1.372301	-0.213059
21	1	0	3.676130	1.301770	-0.089292
22	1	0	1.601782	1.170818	-1.579892
23	1	0	0.629276	5.193453	-0.731864
24	1	0	3.018370	5.549339	-0.096537
25	1	0	4.520172	3.609517	0.254262
26	1	0	-3.364371	2.336077	-1.686231
27	1	0	-5.475272	1.045203	-1.525628
28	1	0	-0.124450	-2.132132	1.866591
29	1	0	-4.333520	-2.820626	1.222299
30	1	0	-2.182700	-3.520596	2.261720
31	27	0	0.416454	0.380180	0.130424
32	6	0	0.795088	-0.435117	-2.568151
33	8	0	0.234073	-0.669394	-1.440277
34	8	0	1.521711	0.565660	-2.796494
35	6	0	0.559553	-1.461196	-3.649129
36	1	0	0.915002	-1.091883	-4.611563
37	1	0	1.106281	-2.370834	-3.380045
38	1	0	-0.502884	-1.711889	-3.704411
39	8	0	1.751818	-0.899211	0.884543
40	16	0	2.958827	-1.635693	0.321393

41	8	0	3.993665	-1.816942	1.348048
42	8	0	3.381364	-1.166782	-1.006153
43	6	0	2.286257	-3.352893	0.044173
44	9	0	1.751129	-3.826837	1.180169
45	9	0	1.339711	-3.355168	-0.903021
46	9	0	3.276651	-4.166272	-0.336992
47	6	0	-0.052893	1.921088	2.653761
48	8	0	0.651306	1.180816	1.951378
49	8	0	-1.169617	2.474919	2.226262
50	1	0	-1.283755	2.227578	1.272861
51	6	0	0.314867	2.258691	4.064480
52	1	0	0.492518	3.336412	4.142379
53	1	0	-0.519692	2.012562	4.728192
54	1	0	1.208677	1.711371	4.361542

SCF Done: E(RB3LYP) = -2826.20867693 A.U. after 23 cycles

Zero-point correction= 0.365512 (Hartree/Particle)
Thermal correction to Energy= 0.400525
Thermal correction to Enthalpy= 0.401470
Thermal correction to Gibbs Free Energy= 0.297462
Sum of electronic and zero-point Energies= -2824.462024
Sum of electronic and thermal Energies= -2824.427010
Sum of electronic and thermal Enthalpies= -2824.426066
Sum of electronic and thermal Free Energies= -2824.530074

TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.460533	-1.350256	-0.396851
2	6	0	-2.225477	-0.760260	-0.733304
3	6	0	-1.860477	-0.704301	-2.102755
4	6	0	-2.732920	-1.117352	-3.104141
5	6	0	-3.975791	-1.651995	-2.744665
6	6	0	-4.335231	-1.778278	-1.398661
7	6	0	-0.459938	-0.274366	-2.404892
8	8	0	-0.090628	0.153991	-3.496796
9	7	0	0.343171	-0.521514	-1.302327
10	6	0	1.694824	-0.155054	-1.206535
11	6	0	2.245114	-0.351138	0.095868
12	6	0	2.529395	0.294598	-2.219693
13	6	0	3.632393	-0.158300	0.356823
14	6	0	3.897624	0.532855	-1.963542
15	6	0	1.841301	-1.033311	2.289332
16	6	0	4.094389	-0.456242	1.663321
17	6	0	4.439824	0.302680	-0.719977

18	6	0	3.208797	-0.909836	2.612941
19	7	0	1.378504	-0.750225	1.081901
20	17	0	6.159736	0.576972	-0.465611
21	8	0	-1.706464	-0.731865	1.969905
22	6	0	-1.512353	-0.383959	3.213249
23	8	0	-0.462979	0.027012	3.710809
24	6	0	-2.777710	-0.540037	4.055669
25	1	0	-3.741386	-1.413513	0.649686
26	1	0	-2.472003	0.502504	-0.238789
27	1	0	-2.430944	-1.048352	-4.144979
28	1	0	-4.661612	-1.984331	-3.518834
29	1	0	-5.296611	-2.208997	-1.133633
30	1	0	2.131230	0.452773	-3.211508
31	1	0	4.530931	0.887275	-2.769624
32	1	0	1.108952	-1.313655	3.032864
33	1	0	5.144689	-0.329152	1.901227
34	1	0	3.537996	-1.153831	3.616738
35	1	0	-3.576860	0.088406	3.648428
36	1	0	-3.128176	-1.577230	4.021777
37	1	0	-2.579940	-0.253676	5.090564
38	8	0	-0.355881	1.295786	0.587637
39	16	0	-1.490286	2.274194	0.726624
40	8	0	-1.675588	2.929378	2.011998
41	8	0	-2.755283	1.650881	0.130835
42	6	0	-1.032908	3.598558	-0.510702
43	9	0	0.116630	4.156563	-0.140854
44	9	0	-0.899394	3.046103	-1.715416
45	9	0	-1.994252	4.517744	-0.541227
46	8	0	-0.642664	-2.629385	0.544623
47	6	0	-0.156200	-3.510593	-0.190174
48	27	0	-0.558163	-0.687205	0.424522
49	8	0	0.486864	-3.251911	-1.300255
50	1	0	0.494866	-2.252979	-1.430680
51	6	0	-0.283778	-4.961060	0.156188
52	1	0	-0.816306	-5.478269	-0.648439
53	1	0	0.714277	-5.404309	0.230650
54	1	0	-0.819287	-5.080477	1.097282

SCF Done: E(RB3LYP) = -2826.17759399 A.U. after 28 cycles

Zero-point correction= 0.363705 (Hartree/Particle)
Thermal correction to Energy= 0.398836
Thermal correction to Enthalpy= 0.399780
Thermal correction to Gibbs Free Energy= 0.295014
Sum of electronic and zero-point Energies= -2824.430573
Sum of electronic and thermal Energies= -2824.395443
Sum of electronic and thermal Enthalpies= -2824.394498
Sum of electronic and thermal Free Energies= -2824.499264

Figure S2

pre-TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.145821	2.321332	-0.347423
2	6	0	1.851665	1.992978	-0.768453
3	6	0	0.859181	2.986979	-0.866843
4	6	0	1.182321	4.313965	-0.575280
5	6	0	2.476114	4.638593	-0.160725
6	6	0	3.454227	3.645475	-0.036787
7	6	0	-0.566482	2.622542	-1.151989
8	8	0	-1.335971	3.340897	-1.781990
9	7	0	-0.937083	1.475157	-0.469028
10	6	0	-2.208378	0.884437	-0.506210
11	6	0	-2.273175	-0.303161	0.272914
12	6	0	-3.369657	1.330492	-1.119184
13	6	0	-3.478699	-1.023516	0.482650
14	6	0	-4.576944	0.614990	-0.945708
15	6	0	-1.041051	-1.801925	1.595832
16	6	0	-3.408915	-2.167484	1.316293
17	6	0	-4.641392	-0.518177	-0.164434
18	6	0	-2.205941	-2.542966	1.876157
19	7	0	-1.095668	-0.726216	0.826381
20	17	0	-6.175793	-1.346365	0.038307
21	1	0	3.905248	1.547903	-0.307074
22	1	0	1.705585	1.025053	-1.263682
23	1	0	0.415625	5.078102	-0.655075
24	1	0	2.721595	5.670916	0.071203
25	1	0	4.458085	3.909292	0.281999
26	1	0	-3.353693	2.229499	-1.718225
27	1	0	-5.474712	0.978949	-1.433361
28	1	0	-0.064693	-2.088969	1.966028
29	1	0	-4.306870	-2.744417	1.507331
30	1	0	-2.132247	-3.413424	2.517488
31	27	0	0.390693	0.257050	0.156142
32	6	0	0.250976	-0.494434	-2.610419
33	8	0	0.226618	-0.842003	-1.340522
34	8	0	0.411698	0.640990	-3.046755
35	6	0	0.067831	-1.701819	-3.519006
36	1	0	0.133878	-1.390127	-4.562723
37	1	0	0.836572	-2.448261	-3.300691
38	1	0	-0.906293	-2.165814	-3.332826
39	8	0	1.723364	-0.997375	0.907702
40	16	0	2.996898	-1.559271	0.275286
41	8	0	4.074735	-1.650911	1.267839
42	8	0	3.314754	-0.974829	-1.035812
43	6	0	2.523461	-3.335060	-0.047603

44	9	0	2.050826	-3.885704	1.079885
45	9	0	1.586171	-3.430746	-0.994420
46	9	0	3.605918	-4.014265	-0.441808
47	6	0	0.085095	2.002577	2.576837
48	8	0	0.715980	1.153728	1.925722
49	8	0	-0.991669	2.605093	2.119728
50	1	0	-1.141373	2.291664	1.187686
51	6	0	0.508942	2.422191	3.948769
52	1	0	0.789464	3.480601	3.929225
53	1	0	-0.332731	2.316303	4.640020
54	1	0	1.352911	1.819995	4.283055

SCF Done: E(RB3LYP) = -2826.21712751 A.U. after 26 cycles

Zero-point correction= 0.369715 (Hartree/Particle)
Thermal correction to Energy= 0.405546
Thermal correction to Enthalpy= 0.406491
Thermal correction to Gibbs Free Energy= 0.299209
Sum of electronic and zero-point Energies= -2824.466401
Sum of electronic and thermal Energies= -2824.430570
Sum of electronic and thermal Enthalpies= -2824.429625
Sum of electronic and thermal Free Energies= -2824.536907

Int1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.983333	2.015579	0.257632
2	6	0	1.619747	1.894119	-0.020724
3	6	0	0.944784	2.979113	-0.609809
4	6	0	1.614214	4.160324	-0.944507
5	6	0	2.977055	4.270470	-0.669272
6	6	0	3.654655	3.204935	-0.067905
7	6	0	-0.511998	2.794902	-0.847754
8	8	0	-1.219326	3.555589	-1.505009
9	7	0	-0.955393	1.654036	-0.175757
10	6	0	-2.218183	1.063765	-0.364078
11	6	0	-2.334039	-0.260976	0.161531
12	6	0	-3.340006	1.644053	-0.939472
13	6	0	-3.567930	-0.974324	0.136526
14	6	0	-4.562724	0.938536	-0.992429
15	6	0	-1.239787	-2.020906	1.225271
16	6	0	-3.577658	-2.269403	0.714200
17	6	0	-4.681902	-0.327315	-0.465618
18	6	0	-2.425001	-2.785041	1.262865
19	7	0	-1.200540	-0.812990	0.690472
20	17	0	-6.236070	-1.150985	-0.540147

```
     21         1          0        3.532982    1.204866    0.724401
     22         1          0        2.201104    1.111688   -1.887095
     23         1          0        1.062056    4.972720   -1.408696
     24         1          0        3.511888    5.182088   -0.919411
     25         1          0        4.715530    3.295077    0.150828
     26         1          0       -3.278565    2.644091   -1.343422
     27         1          0       -5.424273    1.414020   -1.448874
     28         1          0       -0.306612   -2.404228    1.621830
     29         1          0       -4.497115   -2.844223    0.719333
     30         1          0       -2.410282   -3.771531    1.712560
     31        27          0        0.424316    0.424770    0.348160
     32         6          0        0.994589   -0.182874   -2.537496
     33         8          0        0.374374   -0.312548   -1.467966
     34         8          0        1.971664    0.668320   -2.737511
     35         6          0        0.659157   -1.045562   -3.714058
     36         1          0        1.055195   -0.622336   -4.637630
     37         1          0        1.115297   -2.027612   -3.543873
     38         1          0       -0.422131   -1.180665   -3.779396
     39         8          0        1.749523   -0.960903    0.942215
     40        16          0        2.899575   -1.719119    0.303315
     41         8          0        3.952721   -2.021584    1.281102
     42         8          0        3.314823   -1.195980   -1.008200
     43         6          0        2.123722   -3.369801   -0.076676
     44         9          0        1.622886   -3.921658    1.039095
     45         9          0        1.127439   -3.230530   -0.964795
     46         9          0        3.042097   -4.194563   -0.588984
     47         6          0       -0.147216    1.711600    2.923036
     48         8          0        0.487858    0.881625    2.246741
     49         8          0       -1.051530    2.513580    2.417587
     50         1          0       -1.115498    2.321044    1.431704
     51         6          0        0.089225    1.857429    4.393891
     52         1          0        0.478582    2.860927    4.595767
     53         1          0       -0.860174    1.757209    4.928471
     54         1          0        0.800145    1.107635    4.739155
 ---------------------------------------------------------------------
SCF Done:  E(RB3LYP) =  -2826.23563497     A.U. after   28 cycles

Zero-point correction=                           0.370536 (Hartree/Particle)
 Thermal correction to Energy=                    0.406080
 Thermal correction to Enthalpy=                  0.407025
 Thermal correction to Gibbs Free Energy=         0.300963
 Sum of electronic and zero-point Energies=          -2824.482139
 Sum of electronic and thermal Energies=             -2824.446594
 Sum of electronic and thermal Enthalpies=           -2824.445650
 Sum of electronic and thermal Free Energies=        -2824.551711


Int2

                      Standard orientation:
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.141083	1.638452	-0.480152
2	6	0	1.901296	1.086555	-0.812573
3	6	0	1.712265	0.538667	-2.092322
4	6	0	2.750055	0.514499	-3.027993
5	6	0	3.991987	1.054245	-2.687531
6	6	0	4.184646	1.615412	-1.422378
7	6	0	0.358834	-0.012434	-2.382439
8	8	0	0.080081	-0.683287	-3.374767
9	7	0	-0.530765	0.372565	-1.378637
10	6	0	-1.814853	-0.175935	-1.221379
11	6	0	-2.390079	0.029086	0.072361
12	6	0	-2.571914	-0.826344	-2.185922
13	6	0	-3.725468	-0.378574	0.366857
14	6	0	-3.883572	-1.261493	-1.896371
15	6	0	-2.096186	0.892592	2.214313
16	6	0	-4.221223	-0.090638	1.663203
17	6	0	-4.451140	-1.037532	-0.663366
18	6	0	-3.416218	0.551519	2.575407
19	7	0	-1.601138	0.635964	1.014837
20	17	0	-6.101539	-1.576442	-0.363991
21	8	0	1.337296	1.476124	1.832631
22	6	0	1.274979	1.003147	3.046378
23	8	0	0.587037	0.049638	3.420744
24	6	0	2.181307	1.755957	4.017536
25	1	0	3.291510	2.095182	0.494041
26	1	0	3.017209	-0.219272	0.699633
27	1	0	2.574771	0.075576	-4.006451
28	1	0	4.805893	1.042953	-3.406720
29	1	0	5.149320	2.044476	-1.163112
30	1	0	-2.153568	-0.997267	-3.167274
31	1	0	-4.453420	-1.768861	-2.667457
32	1	0	-1.426210	1.355199	2.926751
33	1	0	-5.233556	-0.378716	1.924178
34	1	0	-3.772846	0.785892	3.572222
35	1	0	3.225617	1.665087	3.698933
36	1	0	1.932993	2.822562	4.018423
37	1	0	2.074174	1.352075	5.026197
38	8	0	0.653192	-1.093638	0.563696
39	16	0	1.748733	-1.914272	1.126187
40	8	0	1.569633	-2.704483	2.323257
41	8	0	3.079390	-1.043823	1.255624
42	6	0	2.201257	-3.097609	-0.259661
43	9	0	1.115186	-3.790818	-0.578183
44	9	0	2.624472	-2.399751	-1.308504
45	9	0	3.159744	-3.910425	0.165459
46	8	0	-0.004593	2.834840	0.130206
47	6	0	-0.540232	3.497404	-0.781199
48	27	0	0.325827	0.935552	0.281766

49	8	0	-1.002624	2.971141	-1.883608
50	1	0	-0.857671	1.967460	-1.832591
51	6	0	-0.687318	4.982850	-0.661823
52	1	0	-0.158312	5.464076	-1.490768
53	1	0	-1.745400	5.250498	-0.744630
54	1	0	-0.285030	5.329222	0.289496

SCF Done: E(RB3LYP) = -2826.19175886 A.U. after 27 cycles

Zero-point correction= 0.368382 (Hartree/Particle)
Thermal correction to Energy= 0.404242
Thermal correction to Enthalpy= 0.405186
Thermal correction to Gibbs Free Energy= 0.298530
Sum of electronic and zero-point Energies= -2824.439950
Sum of electronic and thermal Energies= -2824.404090
Sum of electronic and thermal Enthalpies= -2824.403146
Sum of electronic and thermal Free Energies= -2824.509802

Figure S3

SET-int1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.579019	-1.680906	-2.047486
2	6	0	-2.468368	-1.361770	-1.269384
3	6	0	-2.420883	-1.753907	0.078934
4	6	0	-3.492729	-2.473986	0.635036
5	6	0	-4.603136	-2.781358	-0.143516
6	6	0	-4.647026	-2.385305	-1.484915
7	6	0	-1.251405	-1.483027	0.938398
8	8	0	-1.068917	-1.982254	2.035686
9	7	0	-0.286953	-0.533916	0.437171
10	6	0	1.014709	-0.851287	0.350921
11	6	0	1.874025	0.249612	-0.021516
12	6	0	1.608692	-2.123517	0.542174
13	6	0	3.264257	0.094048	-0.205644
14	6	0	2.979851	-2.288330	0.366996
15	6	0	1.958051	2.518983	-0.530217
16	6	0	4.001217	1.243707	-0.575200
17	6	0	3.800371	-1.220117	0.002085
18	6	0	3.345381	2.449246	-0.738142
19	7	0	1.251693	1.444671	-0.181866
20	17	0	5.496568	-1.496763	-0.201888
21	8	0	-1.217647	3.202615	0.022709
22	6	0	-2.412740	2.843401	0.330715
23	8	0	-2.568544	1.592094	0.548076

24	6	0	-3.528941	3.826599	0.455969
25	1	0	-3.611650	-1.382411	-3.090781
26	1	0	-1.637259	-0.821212	-1.712077
27	1	0	-3.439508	-2.777964	1.675009
28	1	0	-5.433821	-3.329518	0.290348
29	1	0	-5.513817	-2.628754	-2.092527
30	1	0	0.999545	-2.970278	0.832354
31	1	0	3.422945	-3.266249	0.515589
32	1	0	1.406592	3.445986	-0.641896
33	1	0	5.072101	1.174507	-0.728003
34	1	0	3.885870	3.344503	-1.021892
35	1	0	-3.510278	4.256023	1.464793
36	1	0	-3.397474	4.639315	-0.262055
37	1	0	-4.490036	3.330923	0.306756
38	27	0	-0.657816	1.356394	0.190605

SCF Done: E(UB3LYP) = -1635.18696290 A.U. after 65 cycles

Zero-point correction= 0.276838 (Hartree/Particle)
Thermal correction to Energy= 0.298619
Thermal correction to Enthalpy= 0.299563
Thermal correction to Gibbs Free Energy= 0.222748
Sum of electronic and zero-point Energies= -1633.870077
Sum of electronic and thermal Energies= -1633.848296
Sum of electronic and thermal Enthalpies= -1633.847351
Sum of electronic and thermal Free Energies= -1633.924166

SET-int2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.086367	0.249501	0.059804
2	6	0	-2.787394	0.620148	0.421475
3	6	0	-2.318632	1.920956	0.143690
4	6	0	-3.168004	2.848006	-0.468424
5	6	0	-4.463488	2.470789	-0.824773
6	6	0	-4.921077	1.172772	-0.571293
7	6	0	-0.904757	2.298966	0.384091
8	8	0	-0.508221	3.437343	0.561179
9	7	0	-0.037047	1.178757	0.272150
10	6	0	1.299623	1.237306	0.187280
11	6	0	1.902407	-0.023160	-0.187946
12	6	0	2.155700	2.352574	0.397117
13	6	0	3.295707	-0.182303	-0.335326
14	6	0	3.529403	2.205592	0.260552
15	6	0	1.497430	-2.252656	-0.755312
16	6	0	3.771951	-1.457476	-0.714194

```
     17         6          0        4.105024    0.979564   -0.093312
     18         6          0        2.871295   -2.485999   -0.920473
     19         7          0        1.045475   -1.049025   -0.412309
     20        17          0        5.816065    0.875251   -0.245625
     21         8          0       -1.540483   -2.206129   -0.711842
     22         6          0       -1.679239   -1.638201   -1.855086
     23         8          0       -1.241381   -0.437350   -1.912384
     24         6          0       -2.284680   -2.335402   -3.025619
     25         1          0       -4.441490   -0.745146    0.308408
     26         1          0       -2.312177   -0.052309    1.158400
     27         1          0       -2.799472    3.845418   -0.683594
     28         1          0       -5.117087    3.190159   -1.308104
     29         1          0       -5.931017    0.889748   -0.850935
     30         1          0        1.728958    3.305723    0.672705
     31         1          0        4.176205    3.057972    0.433887
     32         1          0        0.757438   -3.031657   -0.890999
     33         1          0        4.835513   -1.624874   -0.838493
     34         1          0        3.207727   -3.475831   -1.204820
     35         1          0       -1.551531   -3.037574   -3.439480
     36         1          0       -3.157028   -2.910470   -2.704515
     37         1          0       -2.562374   -1.614221   -3.795831
     38         8          0       -0.305596   -1.055408    1.746091
     39         6          0       -1.179807   -1.644270    2.536327
     40         8          0       -2.386367   -1.719392    2.309678
     41        27          0       -0.754196   -0.569018   -0.017403
     42         6          0       -0.539486   -2.218939    3.787858
     43         1          0       -1.311057   -2.618139    4.448060
     44         1          0        0.158575   -3.016396    3.512402
     45         1          0        0.032728   -1.445441    4.309125
 ---------------------------------------------------------------------
SCF Done:  E(UB3LYP) =  -1863.74504969     A.U. after   42 cycles

Zero-point correction=                          0.328860 (Hartree/Particle)
 Thermal correction to Energy=                   0.355534
 Thermal correction to Enthalpy=                 0.356478
 Thermal correction to Gibbs Free Energy=        0.269376
 Sum of electronic and zero-point Energies=         -1862.266166
 Sum of electronic and thermal Energies=            -1862.239492
 Sum of electronic and thermal Enthalpies=          -1862.238548
 Sum of electronic and thermal Free Energies=       -1862.325650


Calculated data of spin densities

SET-int1

Mulliken charges and spin densities:
              1         2
     1  C   -0.143441   0.001903
     2  C   -0.169837   0.000251
     3  C    0.090015   0.005666
```

```
     4  C   -0.156239  -0.002494
     5  C   -0.141285   0.002143
     6  C   -0.119675  -0.002862
     7  C    0.546792  -0.029498
     8  O   -0.464606   0.047317
     9  N   -0.708402   0.403125
    10  C    0.429157  -0.074084
    11  C    0.318155   0.110322
    12  C   -0.126098   0.273143
    13  C    0.190776  -0.081297
    14  C   -0.127768  -0.136505
    15  C    0.111712   0.038083
    16  C   -0.123813   0.055754
    17  C   -0.134483   0.328056
    18  C   -0.149929  -0.034994
    19  N   -0.664538  -0.033411
    20  Cl   0.086650   0.049567
    21  O   -0.545827  -0.023296
    22  C    0.718584   0.004903
    23  O   -0.530360  -0.023323
    24  C   -0.553281  -0.000543
    25  H    0.165368  -0.000077
    26  H    0.181081  -0.001222
    27  H    0.173757   0.000044
    28  H    0.166199  -0.000001
    29  H    0.167734   0.000171
    30  H    0.215846  -0.011899
    31  H    0.213253   0.004355
    32  H    0.233817  -0.002327
    33  H    0.217288  -0.002341
    34  H    0.208883   0.001246
    35  H    0.220421   0.000226
    36  H    0.206928  -0.000246
    37  H    0.206564  -0.000313
    38  Co   0.790603   1.134458
 Sum of Mulliken charges =   1.00000   2.00000


SET-int2

Mulliken charges and spin densities:
              1         2
     1  C   -0.137223  -0.003557
     2  C   -0.271812   0.006931
     3  C    0.092878   0.001638
     4  C   -0.140557   0.009191
     5  C   -0.125413  -0.005337
     6  C   -0.112432   0.014399
     7  C    0.596068  -0.027673
     8  O   -0.469858   0.079114
     9  N   -0.707588   0.306693
```

```
   10  C    0.444455   0.021990
   11  C    0.346340   0.087825
   12  C   -0.106381   0.223968
   13  C    0.195816  -0.071400
   14  C   -0.119107  -0.106070
   15  C    0.110204   0.026825
   16  C   -0.116526   0.054931
   17  C   -0.124872   0.333149
   18  C   -0.143836  -0.017917
   19  N   -0.622677  -0.005501
   20  Cl   0.123756   0.066315
   21  O   -0.507879  -0.002580
   22  C    0.711419   0.000111
   23  O   -0.491984   0.007912
   24  C   -0.552256   0.000023
   25  H    0.195892   0.000116
   26  H    0.299136   0.000012
   27  H    0.187178  -0.000490
   28  H    0.184143   0.000129
   29  H    0.182289  -0.000603
   30  H    0.238864  -0.010065
   31  H    0.223240   0.003050
   32  H    0.243422  -0.001442
   33  H    0.226782  -0.002322
   34  H    0.219527   0.000634
   35  H    0.222678   0.000100
   36  H    0.218918   0.000041
   37  H    0.211678  -0.000020
   38  O   -0.554996  -0.000589
   39  C    0.663185   0.000224
   40  O   -0.526901  -0.000532
   41  Co   0.657514   0.010489
   42  C   -0.529067   0.000226
   43  H    0.182116   0.000073
   44  H    0.192648  -0.000010
   45  H    0.191217   0.000001
Sum of Mulliken charges =   1.00000   1.00000
```