Supporting Information

TBAB-Catalyzed Cascade Reactions: Facile Synthesis of 1-Trifluoromethyl-3-alkylidene-1,3-dihydro-furo[3,4-*b*]quinolines *via* 5-*exo*-dig Cyclization of *o*-Arylalkynylquinoline Aldehydes

Kalpana Mishra, Jay bahadur Singh, Tanu Gupta and Radhey M. Singh*

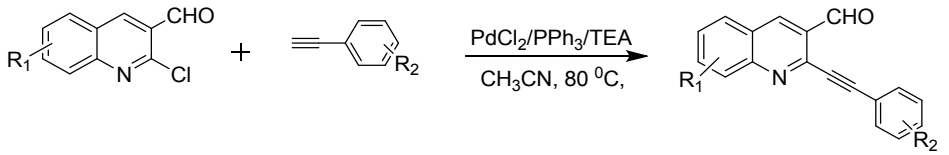
*Department of Chemistry, Center of Advanced study, Institute of Science, Banaras Hindu University, Varanasi, 221005, India. Email: rmohan@bhu.ac.in

Contents	**Page no**
General introduction	2
Experimental procedure for synthesis of starting materials 4 and their corresponding data	2-4
Representative procedure for the synthesis of 1,3-dihydrofuroquinolines 5 and their corresponding data	5-10
X-ray crystallography Data of **5i**	10-13
References	13
^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (500 MHz) spectra of starting materials **4**	14-39
^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (500 MHz) spectra of cyclized product **5**	40-111

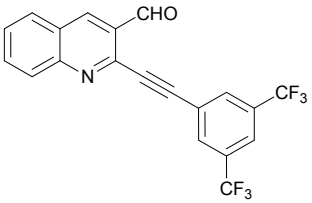
General introduction

^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded at ambient temperature using JEOL at 500 MHz and 125 MHz spectrometer respectively. The data are reported as follows: chemical shift in ppm from internal tetramethylsilane (TMS) on the δ scale, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. Melting points were measured using Buchi melting-point apparatus in an open capillary tube. IR spectra were recorded on VARIAN 3300 FTIR spectrophotometers in cm^{-1} units. High resolution mass spectra (HRMS) were obtained on TOF/6500 SRIES QTOF B.05.00 (B5042.0). $TMSCF_3$, and TBAB are commercially available. Solvents were purified according to standard procedures. The developed chromatogram was analyzed by UV light. Column chromatography was performed using flash silica gel.

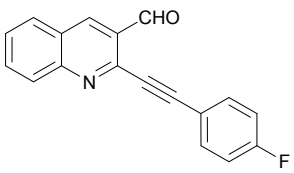
General procedure for synthesis of starting materials 4:



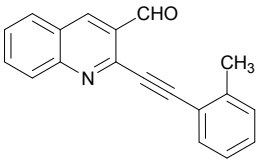
Solution of 2-chloroquinoline-3-carbaldehyde (0.25 mmol), phenyl acetylene (0.26 mmol), $PdCl_2$ (4 mol %), PPh_3(8 mol %), CH_3CN (4 mL) and TEA (0.5 mmol) was stirred under N_2 at 80°C for 1.5-6 h (as monitored by TLC). The reaction mixture was concentrated in vacuo and residue obtained was purified by column chromatography hexane: ethyl acetate to afford 4 (a-z). Data of compounds 4a[1a], 4k-p[1a], 4x[1a], 4e-f,[1b] 4h[1b], 4v[1b], 4z[1b] , 4u[1c] and 4y[1d] is reported in the literature**.**



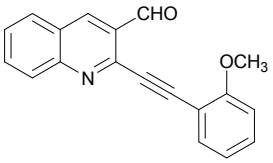
2-((3,5-bis(trifluoromethyl)phenyl)ethynyl)quinoline-3-carbaldehyde (4b): 2-chloroquinoline-3-carbaldehyde (0.09 g, 0.50 mmol), 1-ethynyl-3,5-bis(trifluoromethyl)benzene (0.52 mmol), TEA (1.0 mmol), Reaction time: 2 h, yield: 0.17 g, 88%, yellow solid, mp: 155 °C, IR (KBr): ν 2230, 1697 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.74 (s, 1H), 8.79 (s, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 8.15 (s, 2H), 8.01 (d, *J* = 7.0 Hz, 1H), 7.93 (s, 2H), 7.70 (t, *J* = 7.5 Hz, 1 H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 189.90, 150.18, 142.33, 138.11, 133.47, 132.83, 132.27 (q, *J* = 34.00 Hz), 129.73, 129.56, 129.03, 128.94, 126.79, 123.91, 123.18, 121.75, 91.04, 88.50, ^{19}F NMR (500 MHz, $CDCl_3$): δ -63.02, HRMS (ESI) exact mass calcd. for $C_{20}H_9F_6NOH$: 394.0667 $(M+H)^+$, found: 394.0683 $(M+H)^+$.



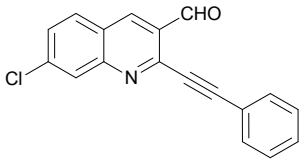
2-((4-fluorophenyl)ethynyl)quinoline-3-carbaldehyde (4c): 2-chloroquinoline-3-carbaldehyde (0.09 g, 0.50 mmol), 1-ethynyl-4-fluorobenzene (0.52 mmol), TEA (1.0 mmol), Reaction time: 2 h, yieid: 0.12 g, 87%, yellow solid, mp: 160°C, IR (KBr): ν 2207, 1693 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.77 (s, 1H), 8.75 (s, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.88 (t, *J* = 8.0 Hz, 1H), 7.70 (t, *J* = 8.0 Hz, 2H), 7.65 (t, *J* = 7.0 Hz, 1H), 7.12 (t, *J* = 8.5 Hz, 2H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 190.72, 161.80 (d, *J* = 250.62 Hz), 150.23, 143.75, 137.44, 134.50 (d, *J* = 8.75 Hz), 133.21, 129.75, 129.39, 128.88, 128.40, 126.52, 117.56 (d, *J* = 13.5 Hz), 116.16 (d, *J* = 21.87 Hz), 94.45, 85.47, ^{19}F NMR (500 MHz, $CDCl_3$): δ -107.79, HRMS (ESI) exact mass calcd. for $C_{18}H_{10}FNOH$: 276.0825 $(M+H)^+$, found: 276.0819 $(M+H)^+$.



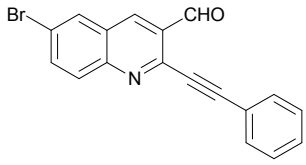
2-(o-tolylethynyl)quinoline-3-carbaldehyde (4d): 2-chloroquinoline-3-carbaldehyde (0.09 g, 0.50 mmol), 1-ethynyl-2-methylbenzene (0.52 mmol), TEA (1.0 mmol), Reaction time: 3 h, yield: 0.12 g, 88 %, yellow solid, mp: 146 °C, IR (KBr): ν 2200, 1691 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.76 (s, 1H), 8.68 (s, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.80 (t, *J* = 8.5 Hz, 1H), 7.66 (d, *J* = 7.5 Hz, 1H)), 7.56 (t, *J* = 8.0 Hz, 1H), 7.28-7.15 (m, 3H), 2.54 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 190.94, 150.35, 144.18, 141.17, 137.20, 133.09, 133.01, 129.92, 129.84, 129.73, 129.43, 128.92, 128.26, 126.48, 125.92, 121.32, 94.62, 89.39, 21.16, HRMS (ESI) exact mass calcd. for $C_{19}H_{13}NOH$: 272.1075 $(M+H)^+$, found 272.1086 $(M+H)^+$.



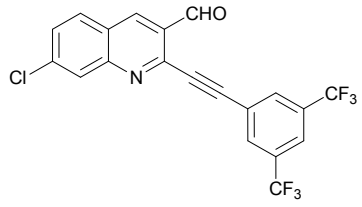
2-(2-methoxyphenyl)ethynyl)quinoline-3-carbaldehyde (4g): 2-chloroquinoline-3-carbaldehyde (0.09 g, 0.50 mmol), 1-ethynyl-2-methoxybenzene (0.52 mmol), TEA (1.0 mmol), Reaction time: 2 h, yield: 0.12 g, 85 %, yellow solid, mp: 158 °C, IR (KBr): ν 2206, 1689 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.93 (s, 1H), 8.73 (s, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 7.5 Hz, 1H), 7.85 (t, *J* = 7.0 Hz, 1H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.61 (d, *J* = 7.0 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.00-6.94 (m, 2H), 3.96 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 192.12, 161.20, 150.19, 144.51, 136.61, 133.88, 132.88, 131.48, 129.71, 129.33, 129.01, 128.03, 126.40, 120.65, 110.67, 110.64, 92.80, 89.86, 55.88, HRMS (ESI) exact mass calcd. for $C_{19}H_{13}NO_2H$: 288.1025 $(M+H)^+$, found 288.1048 $(M+H)^+$.



7-chloro-2-(phenylethynyl)quinoline-3-carbaldehyde (4i): 2,7-dichloroquino line-3-carbaldehyde (0.11 g, 0.50 mmol), ethynylbenzene (0.52 mmol), TEA (1.0 mmol), Reaction time: 3 h, yield: 0.13 g, 86 %, white solid, mp: 150 °C, IR (KBr): ν 2210, 1698 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.78 (s, 1H), 8.72 (s, 1H), 8.16 (s, 1H), 7.90 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 6.0 Hz, 2H), 7.59-7.57 (m, 1H), 7.46-7.41 (m, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 190.48, 150.47, 145.038, 139.461, 136.961, 134.56, 132.45, 130.82, 130.15, 129.44, 128.73, 128.39, 124.87, 121.18, 96.44, 85.34, HRMS (ESI) exact mass calcd. for $C_{18}H_{10}ClNOH$: 292.0529 $(M+H)^+$, found 292.0538 $(M+H)^+$.

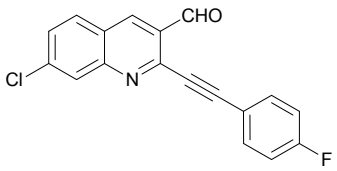


6-bromo-2-(phenylethynyl)quinoline-3-carbaldehyde (4j): 6-bromo-2-(phenylethynyl)quinoline-3-carbaldehyde (0.14 g, 0.50 mmol), ethynylbenzene (0.52 mmol), TEA (1.0 mmol), Reaction time 2 h, yield: 0.14 g, 84%, yellow solid, mp: 160 °C, IR (KBr): ν 2211, 1693 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.80 (s, 1H), 8.69 (s, 1H), 8.13 (d, *J* = 9.0 Hz, 1H), 7.94 (d, *J* = 9.0 Hz, 1H), 7.70 (d, *J* = 7.5 Hz, 1H), 7.60-7.58 (m, 1H), 7.46-7.38(m, 4H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 190.84, 150.24, 143.96, 137.22, 133.10, 132.38 129.93, 129.72, 129.39, 128.91, 128.66, 128.29, 126.50, 121.42, 95.60, 85.61, HRMS (ESI) exact mass calcd. for $C_{18}H_{10}BrNOH$: 336.0024 $(M+H)^+$, found 336.0033 $(M+H)^+$.

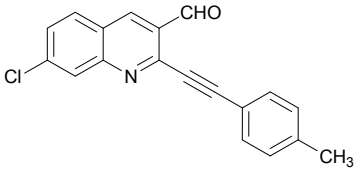


2-((3,5-bis(trifluoromethyl)phenyl)ethynyl)-7-chloroquinoline-3 carbaldehyde (4q): 2,7-dichloroquinoline-3-carbaldehyde (0.11 g, 0.50 mmol), 1-ethynyl-3,5-bis(trifluoromethyl)benzene (0.52 mmol), TEA (1.0 mmol), Reaction time: 2 h, yieid: 0.19 g, 89%, yellow solid, mp: 170°C, IR (KBr): ν 2230, 1697 cm^1, ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.72 (s, 1H), 8.76 (s, 1H), 8.19 (s, 1H), 8.15 (s, 2H), 7.95 (d, *J* = 8.5 Hz, 2H), 7.65-7.63 (m, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 189.51, 150.39, 148.43, 139.87, 137.79, 132.33 (q, *J* = 32.87 Hz), 130.80, 130.08, 129.08, 128.55, 125.15, 123.90, 123.68, 123.38, 121.72, 91.75, 88.12, ^{19}F NMR (500 MHz, $CDCl_3$): δ -63.03, HRMS (ESI) exact mass calcd. for

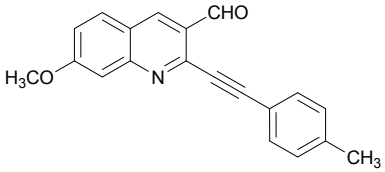
$C_{20}H_8ClF_6NOH$: 428.0277 $(M+H)^+$, found 428.0260 $(M+H)^+$.



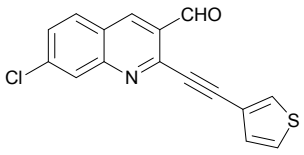
7-chloro-2-((4-fluorophenyl)ethynyl)quinoline-3-carbaldehyde (4r): 2,7-dichloroquinoline-3-carbaldehyde (0.11 g 0.50 mmol), 1-ethynyl-4-fluorobenzene (0.52 mmol), TEA (1.0 mmol), Reaction time: 2 h, Yield: 0.13 g, 87 %, brown solid, mp: 178 °C, IR (KBr): ν 2230, 1697 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 10.75 (s, 1H), 8.72 (s, 1H), 8.16 (s, 1H), 7.92 (d, *J* = 9.0 Hz, 1H), 7.70 (t, *J* = 8.5 Hz, 1H), 7.60-7.58 (m, 1H), 7.13 (t, J = 8.5 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 190.07, 163.52 (d, *J* = 251.12 Hz), 150.49 (d, *J* = 39.75 Hz), 144.24, 139.41, 137.01, 134.49 (d, *J* = 8.5 Hz), 133.43, 132.66, 130.70, 129.39, 128.25 (d, *J* = 7.75 Hz), 128.80 (d, *J* = 12.75 Hz), 117.21, 116.11 (d, *J* = 21.87 Hz), 95.26, 85.10, ^{19}F NMR (500 MHz, $CDCl_3$): δ -107.30, HRMS (ESI) exact mass calcd. for $C_{18}H_9ClFNOH$ 310.0435 $(M+H)^+$, found: 310.0494 $(M+H)^+$.



7-chloro-2-(p-tolylethynyl)quinoline-3-carbaldehyde (4s): 2,7-dichloro quinoline-3-carbaldehyde (0.11 g, 0.50 mmol), 1-ethynyl-4-methylbenzene (0.52 mmol), TEA (1.0 mmol), Reaction time: 3 h, yieid: 0.13 g, 84%, white solid, mp: 150 ^0C, IR (KBr): ν 2209, 1680 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 10.78 (s, 1H), 8.70 (s, 1H), 8.16 (s, 1H), 7.89 (d, *J* = 9.0 Hz, 1H), 7.60-7.56 (m, 3H), 7.23 (d, *J* = 7.5 Hz, 2H), 2.41 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 190.50, 150.44, 145.18, 140.60, 139.30, 136.77, 132.30, 130.70, 129.42, 129.22, 128.86, 128.29, 124.72, 118.02, 96.88, 84.89, 21.69, HRMS (ESI) exact mass calcd. for $C_{19}H_{12}ClNOH$: 306.0686 $(M+H)^+$, found 306.0698 $(M+H)^+$.

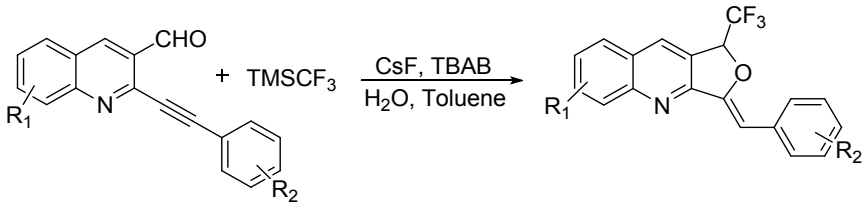


7-methoxy-2-(p-tolylethynyl)quinoline-3-carbaldehyde (4t): 2-chloro-7-methoxyquinoline-3-carbaldehyde (0.11 g, 0.50 mmol), 1-ethynyl-4-methylbenzene(0.52 mmol), TEA (1.0 mmol), Reaction time: 3 h, yield: 0.13 g, 85%, white solid, mp: 178 °C, IR (KBr): ν 2211, 1691 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 10.74 (s, 1H), 8.64 (s, 1H), 7.82 (d, *J* = 9.0, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.46 (s, 1H), 7.26-7.21 (m, 3H), 3.98 (s, 3H), 2.40 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 190.86, 163.74, 152.46, 144.86, 140.33, 136.40, 132.30, 130.81, 130.80, 129.44, 127.36, 121.83, 118.44, 107.15, 95.84, 85.25, 55.90, 21.75, HRMS (ESI) exact mass calcd. for $C_{20}H_{15}NO_2H$: 302.1181 $(M+H)^+$, found 302.1171 $(M+H)^+$.

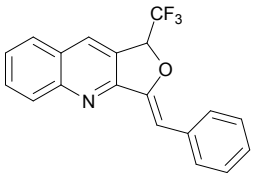


7-chloro-2-(thiophen-3-ylethynyl)quinoline-3-carbaldehyde (4w): 2,7-dichloroquinoline-3-carbaldehyde (0.11 g, 0.50 mmol), 3-ethynylthiophene (0.52 mmol), TEA (1.0 mmol), Reaction time: 3 h, yield: 0.12 g, 83%, white solid, mp: 156 °C, IR (KBr): ν 2218, 1680 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 10.75 (s, 1H), 8.71 (s, 1H), 8.15 (s, 1H), 7.90 (d, *J* = 9.0 Hz, 1H), 7.80 (s, 1H), 7.59-7.56 (m, 1H), 7.39-7.34 (m, 2H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 190.46, 150.49, 145.06, 139.47, 136.96, 132.00, 130.81, 130.04, 129.40, 128.87, 128.36, 126.16, 124.83, 120.34, 91.75, 85.21, HRMS (ESI) exact mass calcd. for $C_{16}H_8ClNOSH$: 298.0093 $(M+H)^+$, found 298.0101 $(M+H)^{\cdot}$

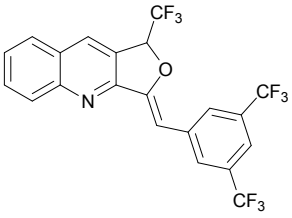
Representative procedure for the synthesis of 1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinolines



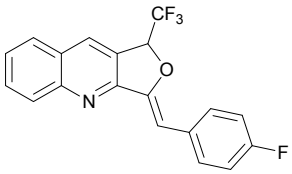
Solution of 2-arylquinoline-3-carbaldehyde (0.25 mmol), $TMSCF_3$ (0.30 mmol), cesium fluoride (0.25 mmol), TBAB (10 mol%) and Toluene (2 mL) was stirred at 0°C for 1-2 h (as monitored by TLC). H_2O (0.50 mmol) was added and mixture was stirred at rt for 1 h. The mixture was then extracted with EtOAc. Organic phase was washed with water, brine and dried over Na_2SO_4. Solvent was then removed under reduced pressure and the residue obtained was purified by column chromatography (hexane: ethyl acetate (18:2) to afford 5(a-x).



3-Benzylidene-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5a): 2-(phenylethynyl)quinoline-3-carbaldehyde (0.06 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol) Reaction time: 2 h, yield: 0.07 g, 88%, yellow solid, mp: 158 °C, IR (KBr): ν 1618, 1275, 1133, 1051, 751 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.18 (s, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.82-7.78 (m, 3H), 7.74 (t, *J* = 7.5 Hz, 1H), 7.53 (t, *J* = 7.0 Hz, 1H), 7.34 (t, *J* = 7.0 Hz, 1H), 7.20 (t, *J* = 7.0 Hz, 2H), 6.74 (s, 1H), 5.94 (q, *J* = 6.0 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.16, 151.03, 150.04, 134.49, 131.29, 131.20, 129.57, 129.43, 128.67, 128.47, 127.46, 127.34, 124.45, 124.07, 121.84, 102.51, 79.31 (q, *J* = 35.12 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.92, HRMS (ESI) exact mass calcd. for $C_{19}H_{12}F_3NOH$: 328.0949 $(M+H)^+$, found: 328.0957 $(M+H)^+$.

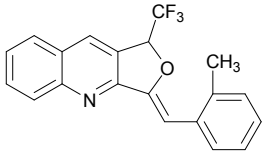


3-(3,5-Bis-trifluoromethyl-benzylidene)-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5b): 2((3,5bis(trifluoromethyl)phenyl)ethynyl)quinoline-3-carbaldehyde (0.09 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2 h, yield: 0.10 g, 90%, yellow solid, mp: 200 °C, IR (KBr): ν 1618, 1287, 1130, 1052, 895 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.31 (s, 1H), 8.26 (s, 2H), 8.19 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 7.5 Hz, 1H), 7.86-7.83 (m, 1H), 7.73 (s, 1H), 7.65 (t, *J* = 8.5 Hz, 1H), 6.85 (s, 1H), 6.08 (q, *J* = 5.5 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.64, 153.02, 150.11, 136.59, 131.92 (q, *J* = 32.87 Hz), 129.80, 128.64, 128.52, 127.96, 127.74, 124.37, 123.83, 122.42, 120.25, 120.22, 120.19, 99.34, 79.91 (q, *J* = 35.62 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -62.99, -77.95, HRMS (ESI) exact mass calcd. for $C_{21}H_{10}F_9NOH$: 464.0697 $(M+H)^+$, found: 464.0710 $(M+H)^+$.

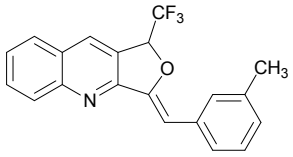


3-(4-Fluoro-benzylidene)-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5c): 2-((4-fluorophenyl)ethynyl)quinoline-3-carbaldehyde (0.06 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2 h, yieid: 0.07 g, 89%, yellow solid, mp: 128°C, IR (KBr): ν 1618, 1275, 1133, 751 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.24 (s, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.88 (d, *J* = 8.0Hz, 1H), 7.84-7.79 (m, 3H), 7.60 (t, *J* = 7.0 Hz, 1H), 7.09 (t, *J* = 8.5 Hz, 2H), 6.78 (s, 1H), 6.00 (q, *J* = 6.0 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.80 (d, *J* = 246.25 Hz), 153.90, 150.50 (d, J = 2.00 Hz), 149.94, 131.17 (d, *J* = 9.50 Hz), 130.95 (d, *J* = 7.87 Hz), 130.61 (d, *J* = 3.00 Hz), 129.44, 128.38, 127.37, 127.26, 124.26, 123.96, 121.72, 115.54 (d, *J* = 21.25 Hz), 101.31, 79.23 (q, *J* = 35.12 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.95, -113.51, HRMS (ESI) exact mass calcd. for $C_{19}H_{11}F_4NOH$: 346.0855 $(M+H)^+$, found:

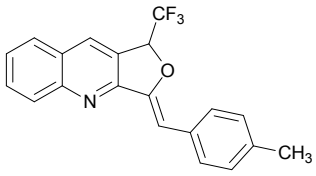
346.0865 $(M+H)^+$.



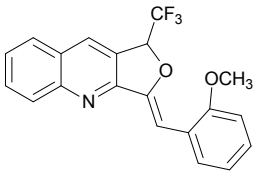
3-(2-methylbenzylidene)-1-(trifluoromethyl)-1,3-dihydrofuro[3,4-b]quinoline (5d): 2-(o-tolylethynyl)quinoline-3-carbaldehyde (0.13 g, 0.50 mmol), $TMSCF_3$ (0.60 mmol), CsF (0.08 g, 0.50 mmol), Reaction time: 3 h, yield: 0.12 g, 75%, light green solid, mp: 98 °C, IR (KBr): ν 1620, 1258, 1138, 1041, 710 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.23 (s, 1H), 8.18 (d, *J* = 8.0 Hz, 2H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.80 (t, *J* = 7.0 Hz, 1H), 7.58 (t, *J* = 8.5 Hz, 2H), 7.29-7.16 (m, 3H), 6.99 (s, 1H), 5.97 (q, *J* = 6.0 Hz, 1H), 2.54 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.21, 151.11, 150.07, 136.72, 132.90, 131.23, 131.08, 130.33, 129.64, 129.39, 128.43, 127.37, 127.27, 126.16, 124.43, 124.11, 121.87, 99.32 , 79.15 (q, *J* = 34.87 Hz), 20.57, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.86, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NOH$: 342.1106 $(M+H)^+$, found 342.1116 $(M+H)^+$.



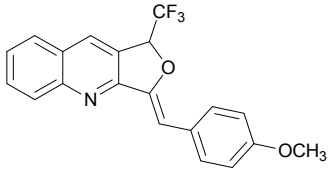
3-(3-Methyl-benzylidene)-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5e): 2-(m-tolylethynyl)quinoline-3-carbaldehyde (0.13 g, 0.50 mmol), $TMSCF_3$ (0.60 mmol), CsF (0.08 g, 0.50 mmol), Reaction time: 3 h, yield: 0.12 g, 74%, yellow solid, mp: 95 °C, IR (KBr): ν 1618, 1272, 1141, 1052, 693 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.24 (s, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.80 (t, *J* = 8.0 Hz, 1H), 7.67 (t, *J* = 8.0 Hz, 2H), 7.59 (t, *J* = 8.0 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 7.5 Hz, 1H), 6.79 (s, 1H), 6.01 (q, *J* = 5.5 Hz, 1H), 2.40 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.23, 150.89, 150.05, 138.13, 134.40, 131.25, 131.15, 130.12, 129.57, 128.56, 128.46, 128.23, 127.28, 126.59, 124.47, 124.09, 121.85, 102.67, 79.26 (q, *J* = 35.00 Hz), 21.65, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.93, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NOH$: 342.1106 $(M+H)^+$, found 342.1114 $(M+H)^+$.



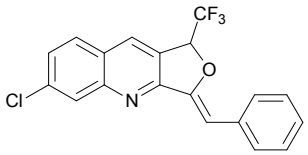
3-(4-Methyl-benzylidene)-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5f): 2-(p-tolylethynyl)quinoline-3-carbaldehyde (0.13 g, 0.50 mmol), $TMSCF_3$ (0.60 mmol), CsF (0.08 g, 0.50mmol), Reaction time: 3 h, yield: 0.11 g, 70 %, yellow solid, mp: 138 °C, IR (KBr): ν 1615, 1175, 1043, 753 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.22 (s, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.80 (t, *J* = 7.5 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.58 (t, *J* = 7.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 6.79 (s, 1H), 5.99 (q, *J* = 5.5 Hz, 1H), 2.38 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.29, 150.41, 150.03, 137.24, 131.66, 131.20, 131.11, 129.51, 129.39, 128.44, 127.39, 127.18, 124.46, 124.10,121.87, 102.61, 79.21 (q, *J* = 35.00 Hz), 21.48, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.94, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NOH$: 342.1106 $(M+H)^+$, found 342.1113 $(M+H)^+$.



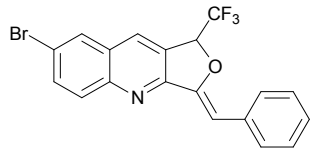
3-(2-methoxybenzylidene)-1-(trifluoromethyl)-1,3-dihydrofuro[3,4-b]quinoline(5g): 2-((2-methoxyphenyl)ethynyl)quinoline-3-carbaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time 2 h, yield: 0.06 g, 73%, yellow solid, mp: 120 °C, IR (KBr): ν 1514, 1233, 1160, 1049, 724 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.26-8.23 (m, 1H), 8.19 (d, *J* = 8.5 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.81-7.78 (m, 1H), 7.58 (t, *J* = 7.0 Hz, 1H), 7.30 (s, 1H), 7.27-7.24 (m, 2H), 7.04 (t, *J* = 7.5 Hz, 1H), 6.92 (d, *J* = 8.5 Hz, 1H), 5.99 (q, *J* = 5.5 Hz, 1H), 3.93 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.04, 154.44, 151.03, 150.12, 131.11, 131.00, 130.14, 129.70, 128.57, 128.39, 127.37, 127.14, 124.44, 124.12, 123.44, 120.73, 110.47, 96.22, 79.16 (q, *J* = 35.12 Hz), 55.63, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.93, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NO_2H$: 358.1055 $(M+H)^+$, found 358.1081 $(M+H)^+$.



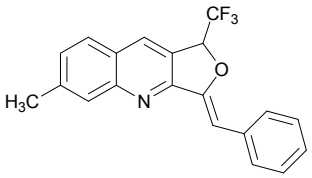
3-(4-Methoxy-benzylidene)-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5h): 2-((4-methoxyphenyl)ethynyl)quinoline-3-carbaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time 2 h, yield: 0.07 g, 76%, light green solid, mp: 154 °C, IR (KBr): ν 1514, 1239, 1177, 1052, 751 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.14 (s, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.74-7.70 (m, 3H), 7.50 (t, *J* = 7.0 Hz, 1 H), 6.88 (d, *J* = 9.0 Hz, 2H), 6.70 (s, 1H), 5.92 (q, *J* = 5.5 Hz, 1H), 3.77 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.96, 154.36, 150.02, 149.53, 131.20, 131.11, 130.85, 129.43, 128.46, 127.32, 127.09, 124.40, 124.11, 121.88, 114.17, 102.36, 79.13 (q, *J* = 35.00 Hz), 55.39, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.01, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NO_2H$: 358.1055 $(M+H)^+$, found 358.1063 $(M+H)^+$.



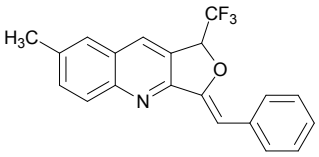
3-Benzylidene-6-chloro-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5i): 7-chloro-2-(phenylethynyl)quinoline-3-carbaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2 h, Yield: 0.08 g, 87 %, yellow solid, mp: 145 °C, IR (KBr): ν 1600, 1218, 1170, 1051, 849 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.17 (s, 1H), 8.14 (s, 1H), 7.83 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.51 (d, *J* = 8.5 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.28-7.24 (m, 1H), 6.78 (s, 1H), 5.95 (q, *J* = 5.0 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.00, 150.55, 150.28, 137.12, 134.16, 130.99, 129.41, 128.58, 128.41, 128.19, 127.45, 125.68, 124.59, 123.86, 121.62, 103.13, 79.18 (q, *J* = 35.12 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.87, HRMS (ESI) exact mass calcd. for $C_{19}H_{11}ClF_3NOH$ 362.0560 $(M+H)^+$, found: 362.0567 $(M+H)^+$.



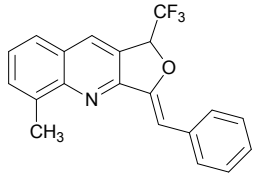
3-Benzylidene-7-bromo-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5j): 6-bromo-2-(phenylethynyl)quinoline-3-carbaldehyde (0.08 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2 h, yield: 0.08 g, 82%, yellow solid, mp: 156 °C, IR (KBr): ν 1619, 1264, 1174, 1050, 846 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.13 (s, 1H), 8.03 (d, *J* = 9.0, 2H), 7.86-7.82 (m, 3H), 7.40 (t, *J* = 7.0 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 1H), 6.79 (s, 1H), 6.00 (q, *J* = 6.0 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.55, 150.67, 148.66, 134.63, 134.29, 131.09, 130.46, 130.21, 129.49, 128.70, 128.46, 127.55, 125.37, 123.96, 121.28, 103.12, 79.11 (q, *J* = 35.00 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.87, HRMS (ESI) exact mass calcd. for $C_{19}H_{11}BrF_3NOH$: 406.0054 $(M+H)^+$, found 406.0062 $(M+H)^+$.



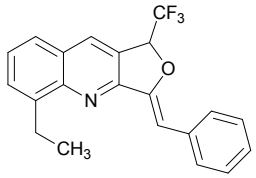
3-Benzylidene-6-methyl-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5k) : 7-methyl-2-(phenylethynyl)quinoline-3-carbaldehyde (0.13 g, 0.50 mmol), $TMSCF_3$ (0.60 mmol), CsF (0.08 g, 0.50 mmol), Reaction time: 3 h, yield: 0.13 g, 75%, yellow solid, mp: 130 °C, IR (KBr): ν 1614, 1261, 1176, 1048, 851 cm^{-1}, ^1H NMR (500 MHz, $CDCl_3$): δ 8.18 (s, 1H), 7.95 (s, 1H), 7.84 (d, *J* = 7.5, 2H), 7.76 (d, *J* = 8.5, 1H), 7.43-7.38 (m, 3H), 7.26 (t, *J* = 7.5 Hz, 1H), 6.78 (s, 1H), 5.97 (q, *J* = 5.5 Hz, 1H), 2.59 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.06, 151.21, 150.30, 141.83, 134.60, 130.90, 129.64, 129.38, 128.64, 128.02, 127.24, 125.60, 124.12, 123.64, 121.89, 102.20, 79.33 (q, *J* = 35.00 Hz), 22.03, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.98, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NOH$: 342.1106 $(M+H)^+$, found 342.1121 $(M+H)^+$.



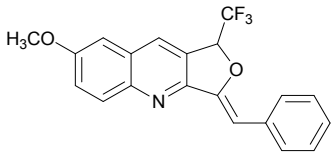
3-Benzylidene-7-methyl-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5l): 6-methyl-2-(phenylethynyl)quinoline-3-carbaldehyde (0.13 g, 0.50 mmol), $TMSCF_3$ (0.60 mmol), CsF (0.08 g, 0.50 mmol), Reaction time: 3 h, Yield: 0.13 g, 77 %, yellow solid, mp: 155 ^{0}C, IR (KBr): ν 1622, 1275, 1127, 1047, 826 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (s, 1H), 8.04 (d, *J* = 8.5, 1H), 7.83 (d, *J* = 7.5 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.25 (t, *J* = 7.0 Hz, 1H), 6.75 (s, 1H), 5.94 (q, *J* = 6.0 Hz, 1H), 2.53 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.26, 151.19, 148.62, 137.52, 134.62, 133.53, 130.50, 129.35, 129.14, 128.66, 127.34, 127.21, 124.43, 124.11, 121.87, 101.96, 79.30 (q, *J* = 34.87 Hz), 21.68, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.94, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NOH$: 342.1106 $(M+H)^+$, found 342.1121 $(M+H)^+$.



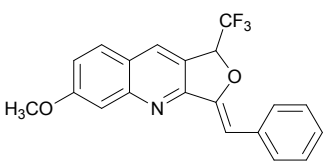
3-Benzylidene-5-methyl-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5m): 8-methyl-2-(phenylethynyl)quinoline-3-carbaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 3 h, yield: 0.06 g, 72%, yellow solid, mp: 110 °C, IR (KBr): ν 1619, 1272, 1130, 1057, 847 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.21 (s, 1H), 7.86 (d, *J* = 7.5, 2H), 7.70 (d, *J* = 8.5 Hz, 1H), 7.64 (d, *J* = 7.0 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 7.0 Hz, 1H), 6.82 (s, 1H), 6.01 (q, *J* = 5.5 Hz, 1H), 2.89 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.95, 151.50, 149.13, 137.81, 134.67, 131.33, 131.12, 129.35, 128.64, 127.42, 127.15, 127.05, 126.35, 123.95, 121.90, 101.84, 79.36 (q, *J* = 34.75 Hz), 18.10, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.93, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NOH$: 342.1106 $(M+H)^+$, found 342.1119 $(M+H)^+$.



3-Benzylidene-5-ethyl-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5n): 8-ethyl-2-(phenylethynyl)quinoline-3-carbaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 4 h, yield: 0.06 g, 70%, yellow solid, mp: 85°C, IR (KBr): ν 1621, 1273, 1135, 1047, 690 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.19 (s, 1H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 7.0 Hz, 1H), 7.50 (t, *J* = 7.5 H, 1H), 7.40 (t, *J* = 7.5 Hz, 2H), 7.26 (t, *J* = 8.0 Hz, 1H), 6.79 (s, 1H), 5.99 (q, *J* = 5.5 Hz, 1H), 3.39 (q, *J* = 7.5 Hz, 2H), 1.43 (t, *J* = 7.5 Hz, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.77, 151.48, 148.45, 143.50, 134.62, 131.25, 129.39, 129.24, 128.52, 127.40, 127.02, 126.20, 124.06, 123.80, 121.83, 101.64, 79.28 (q, *J* = 34.87 Hz), 24.54, 15.09, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.91, HRMS (ESI) exact mass calcd. for $C_{21}H_{16}F_3NOH$: 356.1262 $(M+H)^+$, found 356.1277 $(M+H)^+$.

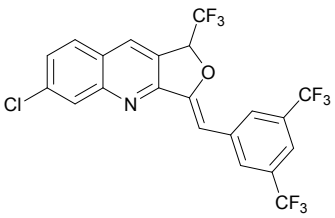


3-Benzylidene-7-methoxy-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5o): 6-methoxy-2-(phenylethynyl)quinoline-3-carbaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2 h, Yield: 0.07 g, 76%, yellow solid, mp: 160 °C, IR (KBr): ν 1625, 1223, 1168, 1036, 836 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.06 (s, 1H), 7.99 (d, *J* = 9.0, 1H), 7.76 (d, *J* = 7.5, 2 H), 7.40-7.37 (m, 1H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.06 (s, 1H), 6.65 (s, 1H), 5.91 (q, *J* = 6.0 Hz, 1H) 3.94 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.50, 151.90, 151.23, 146.20, 134.70, 130.88, 129.66, 129.26, 128.72, 128.62, 127.07, 124.85, 124.11, 121.88, 105.88, 101.42, 79.32 (q, *J* = 35.12 Hz), 55.76, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.88, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NO_2H$: 358.1055 $(M+H)^+$, found 358.1069 $(M+H)^+$.

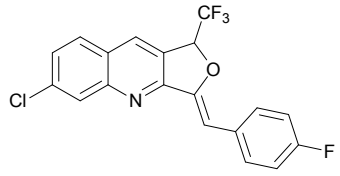


3-Benzylidene-6-methoxy-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5p): 7-methoxy-2-(phenylethynyl)quinoline-3-carbaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2 h, Yield: 0.07 g, 74%, yellow solid, mp: 140 °C, IR (KBr): ν 1615, 1268, 1175, 1043, 849, 753 cm^{-1},

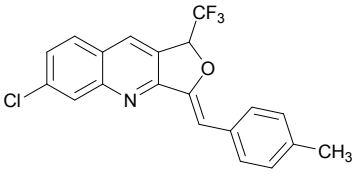
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.16 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 9.5 Hz, 1H), 7.48 (s, 1H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.28-7.24 (m, 2H), 6.76 (s, 1H), 5.98 (q, *J* = 6.0 Hz, 1H), 3.99 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.13, 154.30, 152.03, 151.31, 134.58, 130.90, 129.35, 129.32, 128.65, 127.24, 124.13, 122.86, 122.39, 120.82, 107.28, 102.07, 79.38 (q, *J* = 35.12 Hz), 55.83, ^{19}F NMR (500 MHz, $CDCl_3$): δ -78.06, HRMS (ESI) exact mass calcd. for $C_{20}H_{14}F_3NO_2H$: 358.1055 $(M+H)^+$, found 358.1069 $(M+H)^+$.



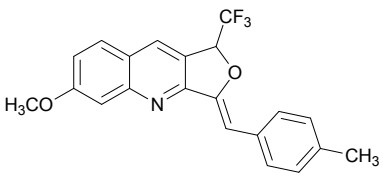
3-(3,5-Bis-trifluoromethyl-benzylidene)-6-chloro-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5q): 2-((3,5-bis(trifluoromethyl)phenyl)ethynyl)-7-chloroquinoline-3-carbaldehyde (0.11 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2 h, yield: 0.01 g, 92%, yellow solid, mp: 160 °C, IR (KBr): ν 1608, 1291, 1175, 1051, 892 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.29 (s, 1H), 8.26(s, 2H), 8.19(s, 1H), 7.86(d, *J* = 9.0 Hz, 1H), 7.74 (s, 1H), 7.61-7.59 (m, 1H), 6.85 (s, 1H), 6.09 (q, *J* = 5.5 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.96, 153.17, 150.37, 137.60, 136.27, 131.89, (q, *J* = 33.00 Hz), 131.32, 129.46, 128.94, 128.66, 125.99, 124.54, 124.47, 123.63, 122.30, 120.37, 99.94, 79.78 (q, *J* = 35.00 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -63.00, -77.92, HRMS (ESI) exact mass calcd. for $C_{21}H_9ClF_9NOH$: 498.0307 $(M+H)^+$, found: 498.0319 $(M+H)^+$.



6-Chloro-3-(4-fluoro-benzylidene)-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5r): 7-chloro-2-((4-fluorophenyl)ethynyl)quinoline-3-carbaldehyde (0.08 g, 0.25 mmol),$TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2 h, yieid: 0.08 g, 90 %, yellow solid, mp: 110 °C, IR (KBr): ν 1600, 1218, 1170, 1051, 849 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.19 (s, 1H), 8.15 (s, 1H), 7.80 (t, *J* = 7.5 Hz, 3H), 7.53 (d, *J* = 10.0 Hz, 1H), 7.08 (t, *J* = 8.5 Hz, 2H), 6.75 (s, 1H), 5.98 (q, *J* = 5.0 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.93 (d, *J* = 246.62 Hz), 154.88, 150.28, 150.14, 137.20, 131.07 (d, *J* = 7.75 Hz), 130.38 (d, *J* = 3.12 Hz), 129.38, 128.33 (d, *J* = 17.5 Hz), 125.69, 124.50, 123.84, 121.80, 115.58 (d, *J* = 21.37 Hz), 102.02, 79.18 (q, *J* = 35.25 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.92, -113.09, HRMS (ESI) exact mass calcd. for$C_{19}H_{10}ClF_4NOH$: 380.0465 $(M+H)^+$, found: 380.0481$(M+H)^+$.

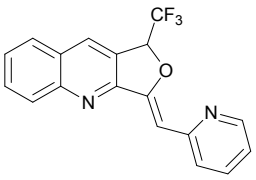


6-Chloro-3-(4-methyl-benzylidene)-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5s): 7-chloro-2-(p-tolylethynyl)quinoline-3-carbaldehyde (0.08 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 3 h, yield: 0.07 g, 80 %, yellow solid, mp: 135 °C IR (KBr): ν 1605, 1273, 1140, 1048, 849 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.18 (s, 1H), 8.15 (s, 1H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.73 (d, *J* = 7.5 Hz, 2H), 7.53-7.51 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.77 (s, 1H), 5.96 (q, *J* = 5.5 Hz, 1H) 2.38 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.28, 150.41, 150.06, 137.62, 137.17, 131.43, 131.04, 129.48, 129.44, 128.49, 128.18, 125.73, 124.71, 123.99, 121.75, 103.35, 79.17 (q, *J* = 34.87 Hz), 21.50, ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.94, HRMS (ESI) exact mass calcd. for $C_{20}H_{13}ClF_3NOH$: 376.0716 $(M+H)^+$, found 376.0724 $(M+H)^+$.

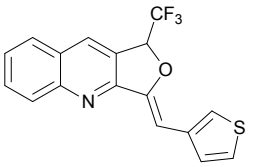


6-Methoxy-3-(4-methyl-benzylidene)-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5t): 7-methoxy-2-(p-tolylethynyl)quinoline-3-carbaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 3 h; yield: 0.07 g, 73%, yellow solid, mp: 140°C, IR (KBr): ν 1611, 1262, 1132, 1022, 853 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.13 (s, 1H), 7.75-7.72 (m, 3H), 7.46 (s, 1H), 7.17-7.12 (m, 3H), 6.73 (s, 1H), 5.95 (q, *J* = 5.5 Hz, 1H), 3.98 (s, 3H), 2.37 (s, 3H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.09,

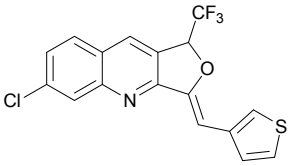
154.44, 152.02, 150.71, 137.22, 131.75, 130.81, 129.38, 129.30, 124.16, 122.78, 122.39, 121.92, 120.63, 107.22, 102.15, 79.29 (q, *J* = 34.87 Hz), 55.79, 21.47, ^{19}F NMR (500 MHz, $CDCl_3$): δ -78.15, HRMS (ESI) exact mass calcd. for $C_{21}H_{16}F_3NO_2H$: 372.1211 $(M+H)^+$, found 372.1226 $(M+H)^+$



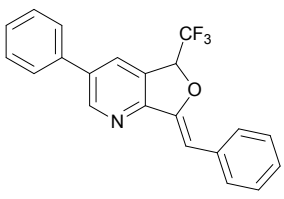
3-(pyridin-2-ylmethylene)-1-(trifluoromethyl)-1,3-dihydrofuro[3,4-b]quinoline (5u): 2-(pyridin-2-ylethynyl)quinoline-3-carbaldehyde (0.13 g, 0.50 mmol), $TMSCF_3$ (0.60 mmol), CsF (0.08 g, 0.50mmol), Reaction time: 3 h, yieid: 0.12 g 79%, brown solid, mp: 150^{0}C, IR (KBr): ν 1668, 1268, 1132, 1050, 756 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.65 (s, 1H), 8.27 (s, 1H), 8.18 (d, *J* = 8.5 Hz, 1H), 8.11 (d, *J* = 7.5 Hz, 1H), 7.90 (d, *J* = 8.5 Hz, 1H), 7.82(t, *J* = 8.5 Hz, 1H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.62 (t, *J* = 7.0 Hz, 1H), 7.13 (t, *J* = 10.0 Hz, 1H), 7.06 (s, 1H), 6.05 (q, *J* = 6.0 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.99, 153.51, 153.42, 150.11, 149.66, 136.17, 131.84, 131.09, 129.98, 128.55, 128.28, 127.59, 127.55, 124.28, 121.29, 115.61, 103.13, 79.63 (q, *J* = 34.75 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.76, HRMS (ESI) exact mass calcd. for $C_{18}H_{11}F_3N_2OH$: 329.0902 $(M+H)^+$, found 329.0915 $(M+H)^+$.



3-(thiophen-3-ylmethylene)-1-(trifluoromethyl)-1,3-dihydrofuro[3,4-b]quinoline (5v): 2-(thiophen-3-ylethynyl)quinoline-3-carbaldehyde (0.06 g 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 3 h, yieid: 0.06 g, 69%, yellow solid, mp: 140°C, IR (KBr): ν 1617, 1278, 1134, 1051, 758 cm^1, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.16 (s, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 8.0 Hz, 1H), 7.63 (s, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.45-7.44 (m, 1H), 7.28-7.26 (m, 1H), 6.82 (s, 1H), 5.92 (q, *J* = 5.5 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.94, 150.23, 150.04, 135.35, 131.22, 131.16, 129.50, 128.81, 128.46, 127.39, 127.23, 125.35, 124.59, 124.07, 121.83, 97.15, 79.18 (q, *J* = 34.87 Hz),^{19}F NMR (500 MHz, $CDCl_3$): δ -77.98, HRMS (ESI) exact mass calcd. for $C_{17}H_{10}F_3NOSH$: 334.0513 $(M+H)^+$, found 334.0523 $(M+H)^+$.



6-Chloro-3-thiophen-2-ylmethylene-1-trifluoromethyl-1,3-dihydro-furo[3,4-b]quinoline (5w): 7-chloro-2-(thiophen-2-ylethynyl)quinoline-3-carbaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2 h, yieid: 0.06 g, 70%, yellow solid, mp: 120 °C, IR (KBr): ν 1618, 1271, 1140, 1048, 842 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.19 (s, 1H), 8.14 (s, 1H), 7.80 (d, *J* = 8.5 Hz, 1H), 7.70 (s, 1H), 7.54-7.50 (m, 2H), 7.35-7.34 (m, 1H), 6.87 (s, 1H), 5.98 (q, *J* = 5.5 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.85, 150.34, 149.80, 137.13, 135.09, 130.96, 129.38, 128.72, 128.41, 128.14, 125.64, 125.37, 124.90, 123.87, 121.64, 97.76, 79.04 (q, *J* = 34.87 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -78.01, HRMS (ESI) exact mass calcd. for $C_{17}H_9ClF_3NOSH$: 368.0124 $(M+H)^+$, found: 368.0131$(M+H)^+$.



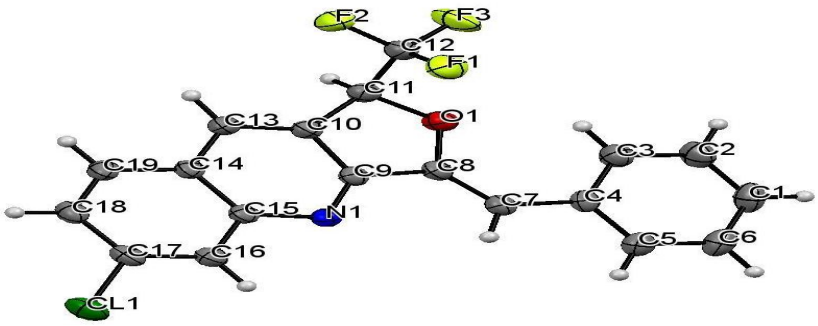
(7-Benzylidene-3-phenyl-5-trifluoromethyl-5,7-dihydro-furo[3,4-b]pyridine (5x): 5-phenyl-2-(phenylethynyl)nicotinaldehyde (0.07 g, 0.25 mmol), $TMSCF_3$ (0.30 mmol), CsF (0.04 g, 0.25 mmol), Reaction time: 2h, yieid: 0.07 g, 84%, white solid, mp: 145 ^{0}C, IR (KBr): ν 1671, 1272, 1132, 1058, 854 cm^{-1}, ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.86 (s, 1H), 7.88 (s, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 7.5 Hz, 2H), 7.45 (t, *J* = 7.0 Hz, 2H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.32 (t *J* = 8.0 Hz, 2H), 7.18 (t, *J* = 7.5 Hz, 2H), 6.51 (s, 1H), 5.87 (q, *J* = 6.0 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.15, 151.50, 151.33, 136.92, 136.86, 134.52, 129.43, 129.16, 128.82, 128,64, 127.37, 127.13, 126.99, 123.96, 121.72, 101.34, 79.83 (q, *J* = 35.37 Hz), ^{19}F NMR (500 MHz, $CDCl_3$): δ -77.70, HRMS (ESI) exact mass calcd. for $C_{21}H_{14}F_3NOH$: 354.1106 $(M+H)^+$, found 354.1123 $(M+H)^+$.

X-Ray Crystallography of compound 5i:

X-ray single crystal structural data of compounds **5i** is collected on Agilent Xcalibur, Eos diffractometer equipped with Enhance (Mo) X-ray source and graphite monochromated Mo-Kα radiation (λ = 0.71073 Å). The program CrysAlis PRO (Agilent, 2012) was used for integration of diffraction profiles and absorption correction was made with SCALE3 ABSPACK scaling algorithm.[2] Structures is solved by SIR 92[3] and refined by full matrix least square method using SHELXL-2014/7[4] and WinGX version 2014.1.[5] All the non-hydrogen atoms were located from the difference Fourier map and refined anisotropically. The crystallographic and structure refinement data of 5i is summarized in Table 1. Selected bond lengths and angles are given in Table 2.

Image of **5i** in mercury

CCDC is **1516018**, Ellipsoid probability = 30%



Oak Ridge Thermal-Ellipsoid Plot (ORTEP) of **5i**
Ellipsoid probability = 30%, Bond line width = 2

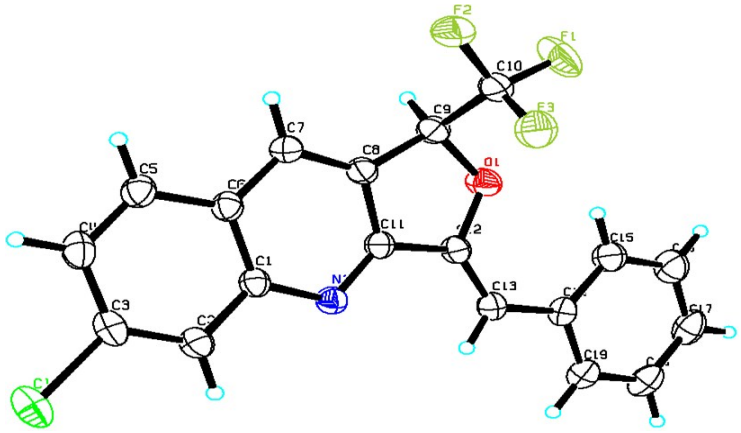


Table 1. Crystal data and structure refinement of **5i**.

Parameters	Molecule 5i
CCDC No.	1516018
Empirical formula	$C_{19}H_{11}F_3NO$
Formula Weight	361.74
Crystal system	monoclinic

Space group	C2/c
a (Å) b (Å) c (Å)	17.5265(8) 18.9585(9) 11.1154(5)
α (°) β (°) γ (°)	90 120.995(2) 90
V (A^3)	3166.0(3)
Z	8
D_c (g cm^{-3})	1.518
μ (mm^{-1})	0.280
F (000)	1472
T (K)	298
λ (Mo K_α)(Å)	0.71073
Crystal size (mm)	0.13 x 0.22 x 0.32
Θ_{min}(°) Θ_{max}(°)	2.7 28.3
Total data Unique data	51891 3960
R_{int}	0.037
Data [I>2σ(I)]	3027
R^a	0.0439
$R_w{}^b$	0.1244
S	1.03

bTable 2. Selected bond distance (Å) and angles (º) in **5i.**

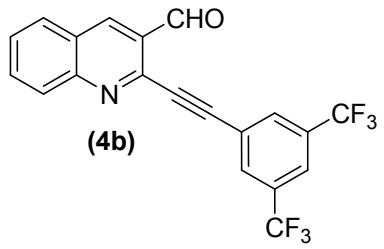
Cl1-C3	1.7365(18)	C12-C13	1.329(3)
F1-C10	1.324(2)	C13-C14	1.457(3)
F2-C10	1.329(2)	C14 -C15	1.399(3)
F3-C10	1.323(3)	C14 -C19	1.390(3)
O1-C9	1.435(2)	C15-C16	1.378(3)
O1-C19	1.308(5)	C13-C141.497(3)	
O -C12	1.390(2)	C16-C17	1.377(4)
N1 -C1	1.367(2)	C17-C18	1.377(3)
N1-C11	1.316(2)	C18-C19	1.380(3)
C1-C2	1.412(2)	C2 -H2	0.9300
C1-C6	1.425(2)	C4-H4	0.9300
C2-C3	1.360(3)	C5-H5	0.9300
C3-C4	1.407(3)	C7 -H7	0.9300
C4-C5	1.357(3)	C9-H9	0.9800
C5-C6	1.413(3)	C13-H13	0.92(2)
C6 -C7	1.412(2)	C15-H15	0.9300
C7-C8	1.356(2)	C16-H16	0.9300
C8-C9	1.495(2)	C17-H17	0.9300
C8-C11	1.407(2)	C18-H18	0.9300

C9 -C10	1.508(3)	C19 -H19	0.9300
C11 -C12	1.459(2)		
C9 -O1-C12	110.44(12)	N1 -C11-C12	125.97(14)
C1-N1-C11	115.27(14)	C8 -C11 -C12	108.47(13)
N1-C1-C2	118.11(15)	O1-C12 -C11	107.89(13)
N1-C1 -C6	123.12(14)	O1-C12-C13	123.63(15)
C2 -C1-C6	118.77(15)	C11-C12-C13	128.48(15)
C1-C2-C3	119.95(16)	C12 -C13 -C14	130.17(17)
Cl1-C3-C2	119.62(15)	C13-C14-C15	123.52(17)
Cl1 -C3-C4	118.28(14)	C13 -C14-C19	118.80(16)
C2 -C3-C4	122.10(17)	C15-C14-C19	117.66(17)
C3-C4-C5	118.71(17)	C14-C15-C16	120.37(19)
C4-C5-C6	121.77(17)	C15-C16-C17	121.1(2)
C1-C6-C5	118.65(15)	C16-C17-C18	119.2(2)
C1-C6-C7	118.67(15)	C17-C18-C19	120.1(2)
C5-C6-C7	122.68(16)	C14-C19-C18	121.52(18)
C6 -C7-C8	117.37(16)	C1-C2-H2	120.00
C7-C8 -C9	132.56(16)	C3-C2-H2	120.00
C7-C8-C11	119.90(15)	C3-C4-H4	121.00
C9-C8-C11	107.52(14)	C5 -C4-H4	121.00
O1-C9-C8	105.47(13)	C4-C5-H5	119.00
O1-C9-C10	107.27(15)	C6-C5-H5	119.00
C8-C9-C10	113.68(18)	C6-C7-H7	121.00
F1-C10-F2	106.83(16)	C8-C7-H7	121.00
F1-C10-F3	107.56(18)	O1-C9-H9	110.00
F1-C10-C9	111.8(2)	C8-C9-H9	110.00
F2-C10-F3	106.6(2)	C10-C9-H9	110.00
F2-C10-C9	111.41(17)	C12-C13-H13	113.4(12)
F3-C10-C9	112.37(15)	C14-C13-H13	116.4(12)
N1-C11-C8	125.55(14)	C14-C14-H15	120.00

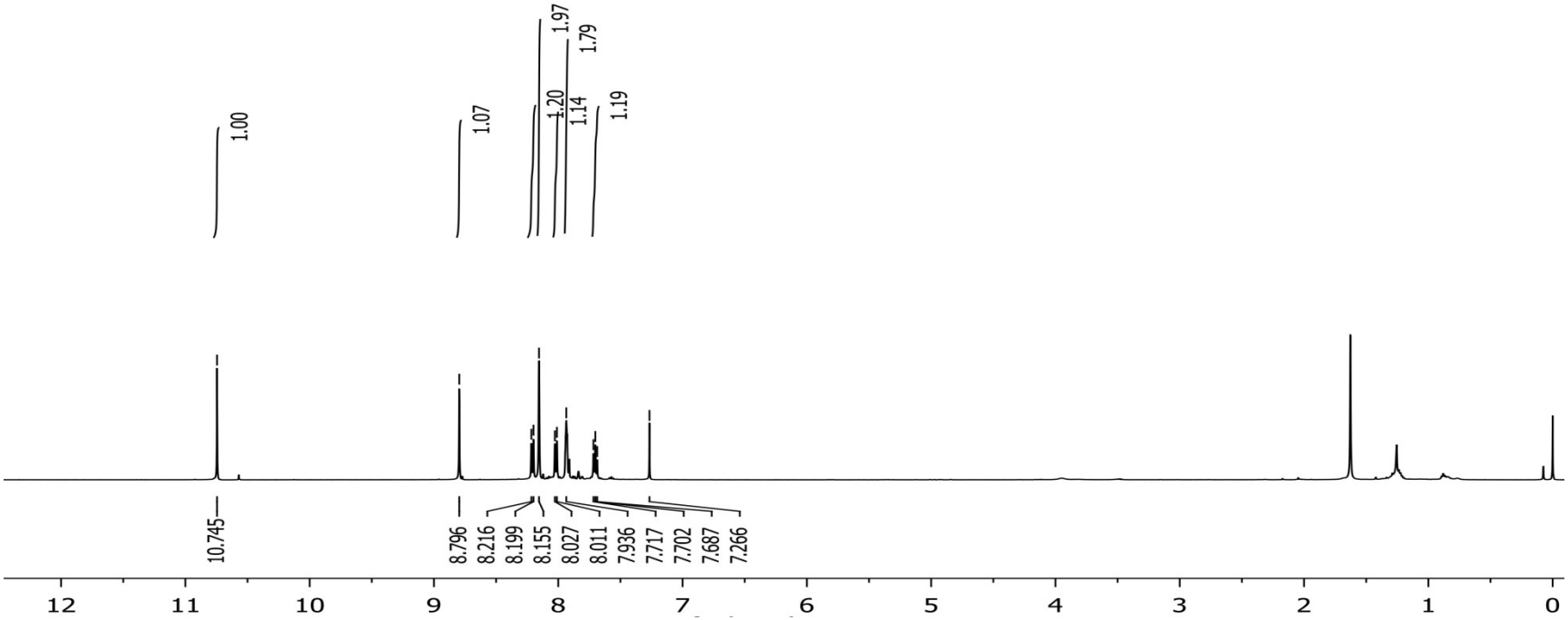
References

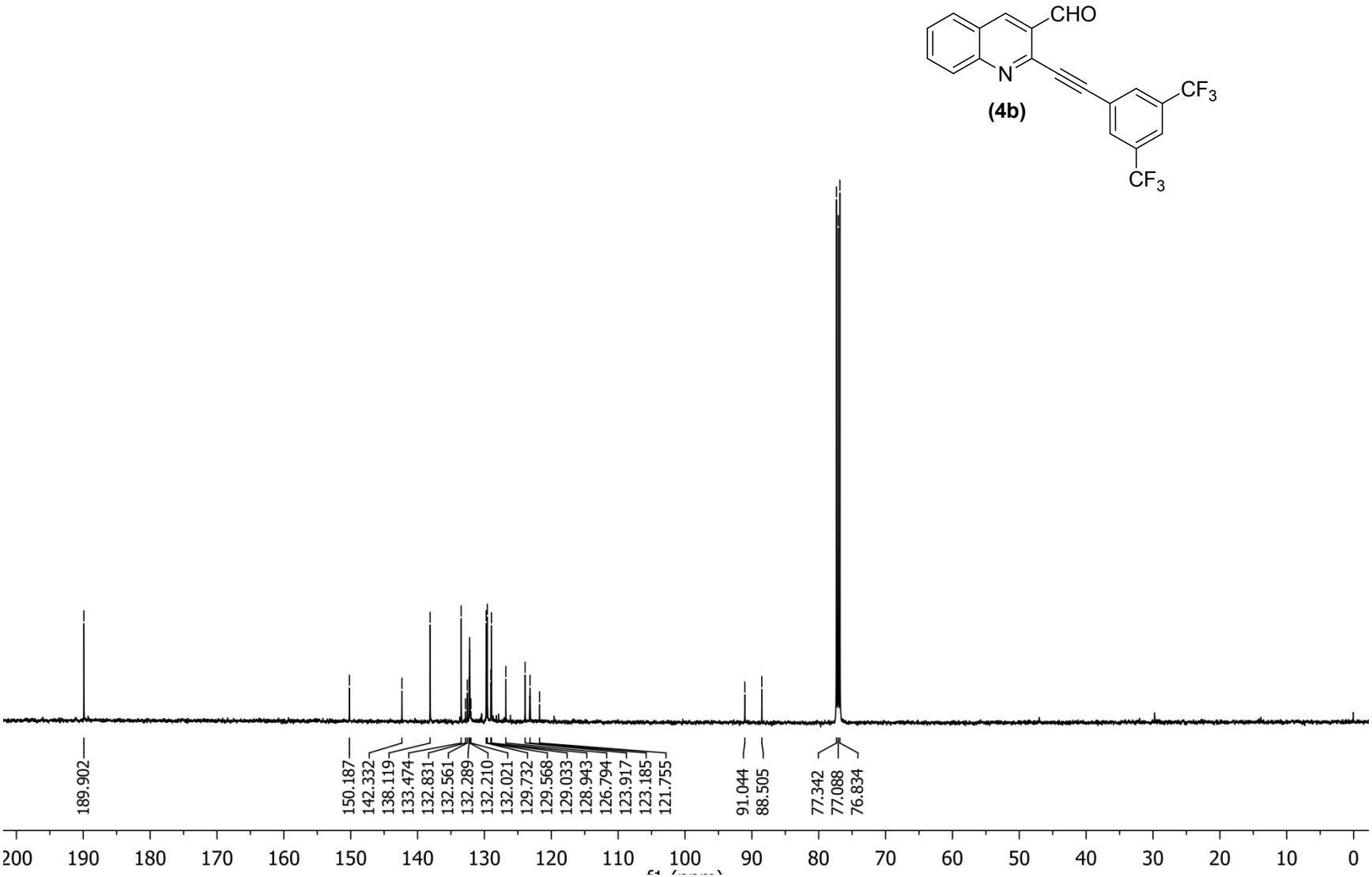
1. a) R. M Singh, A. Chandra,B.Singh, S. Upadhyay, *Tetrahedron* 2008, **64**, 11680; b) A. K. Verma, T. Aggarwal, V. Rustagia and R. C. Larock, *Chem. Commun*., 2010, **46**, 4064; c) P. Belmont and T. Belhadj, *Org. Lett*., 2005, **7**, 1793; d) A. B. G. Mariaulea, S. D.-Fincka, P. Helisseya, S. G.-Renaulta, V. Michelet, P. Belmont *Synthesis,* , **47***,* 2015, A.
2. Agilent, (2012) *CrysAlis PRO* Agilent Technologies, Yarnton, England.
3. a) A. Altomare, G. Cascarano, C. Giacovazzo, and A. Gualaradi, *J. Appl. Cryst*. 1993, **26**, 343; b) A. Altomare, M. C. Burla, G. Camalli, G. Cascarano, C. Giacovazzo, A. Gualiardi and G. Polidori, J. Appl. Cryst. 1994, **27**, 435.
4. G. M. Sheldrick, *ActaCryst.,* 2008, **A64**, 112-122.
5. L. J. Farrugia, WinGX-A Windows Program for Crystal Structure Analysis, *J. Appl. Cryst.,* 2012, **45**, 849-854.

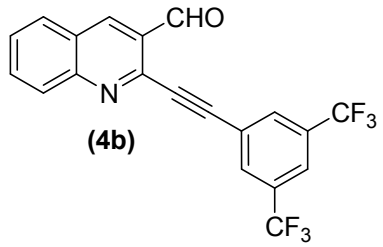
^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (500 MHz) spectra of starting materials



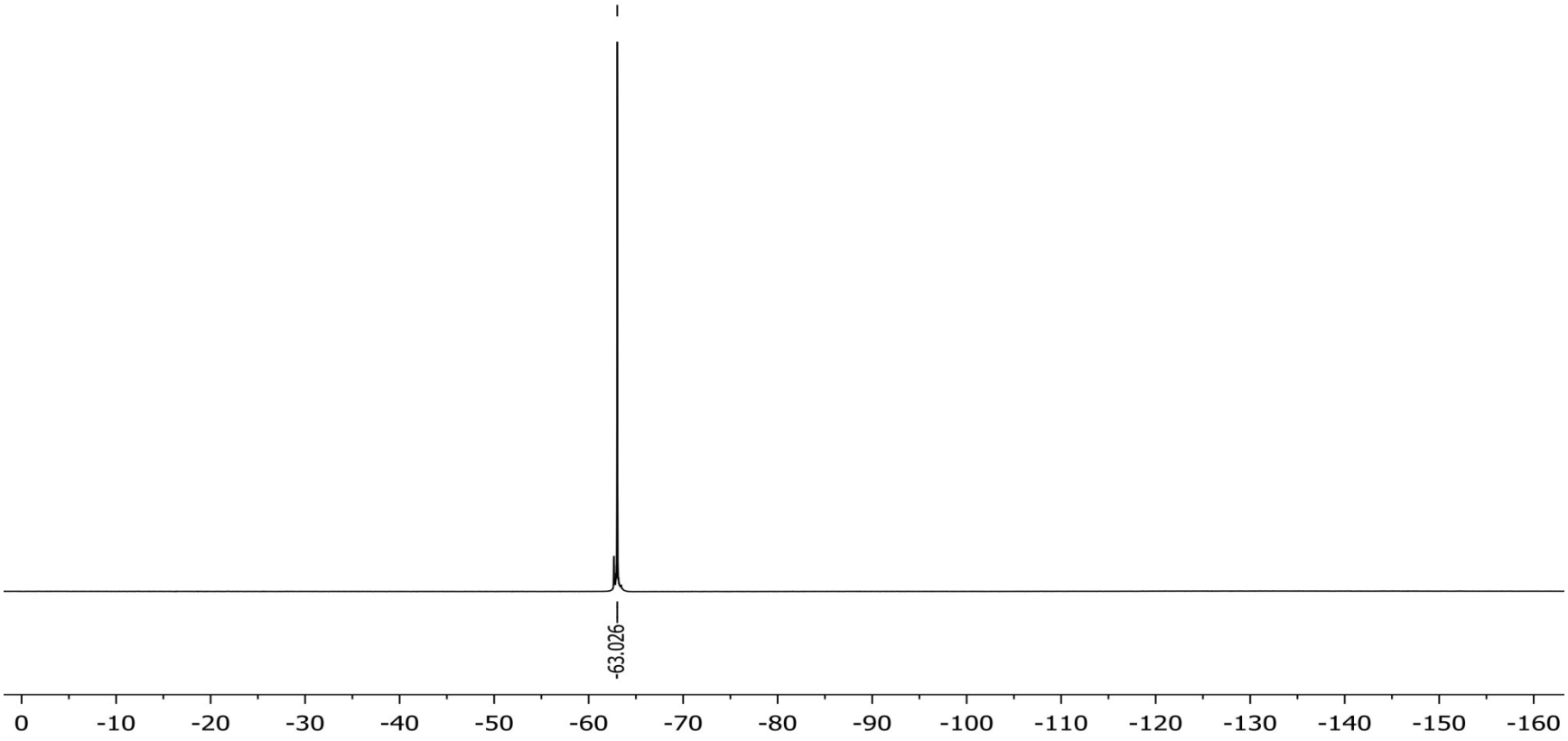
(4b)

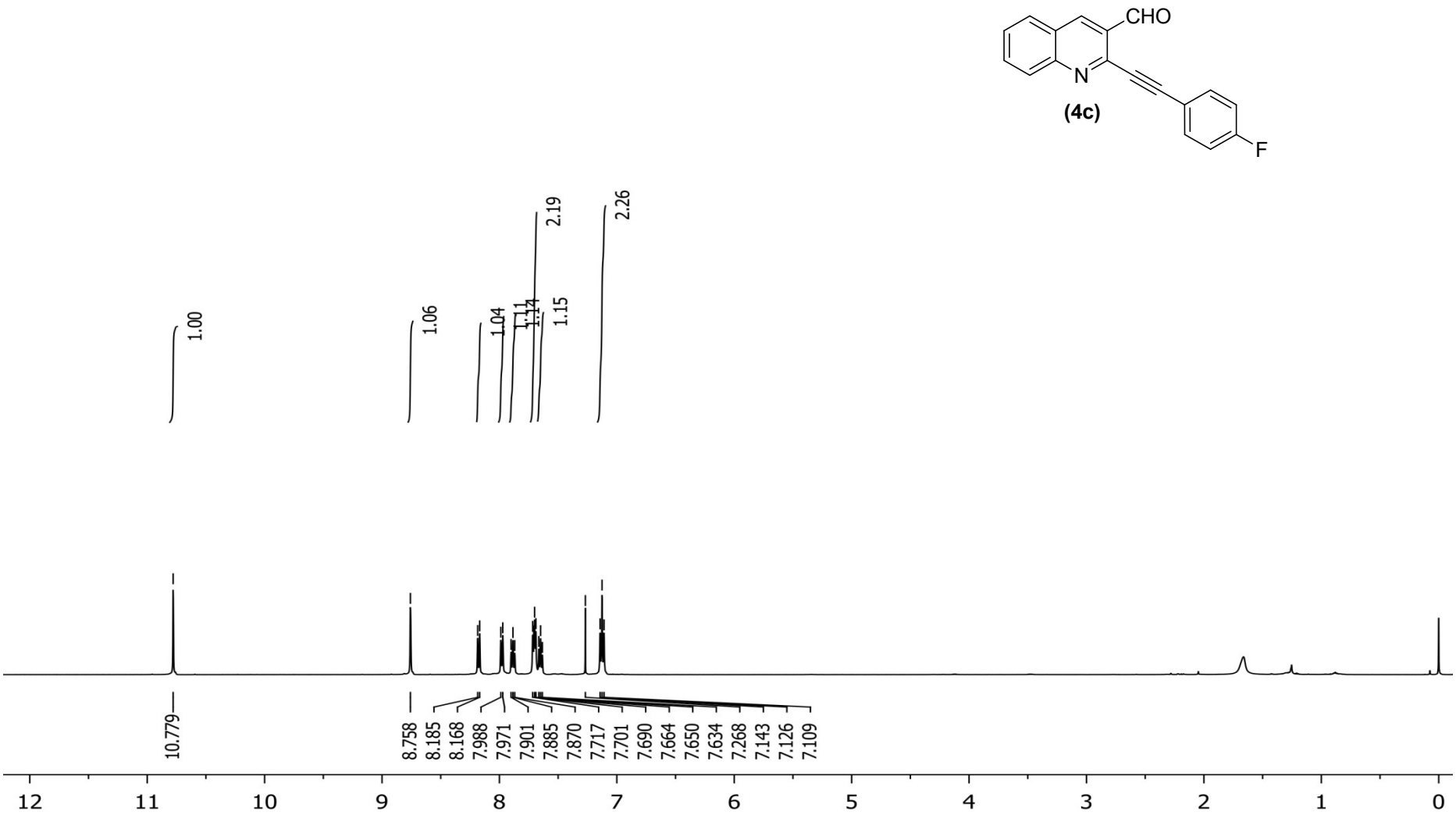


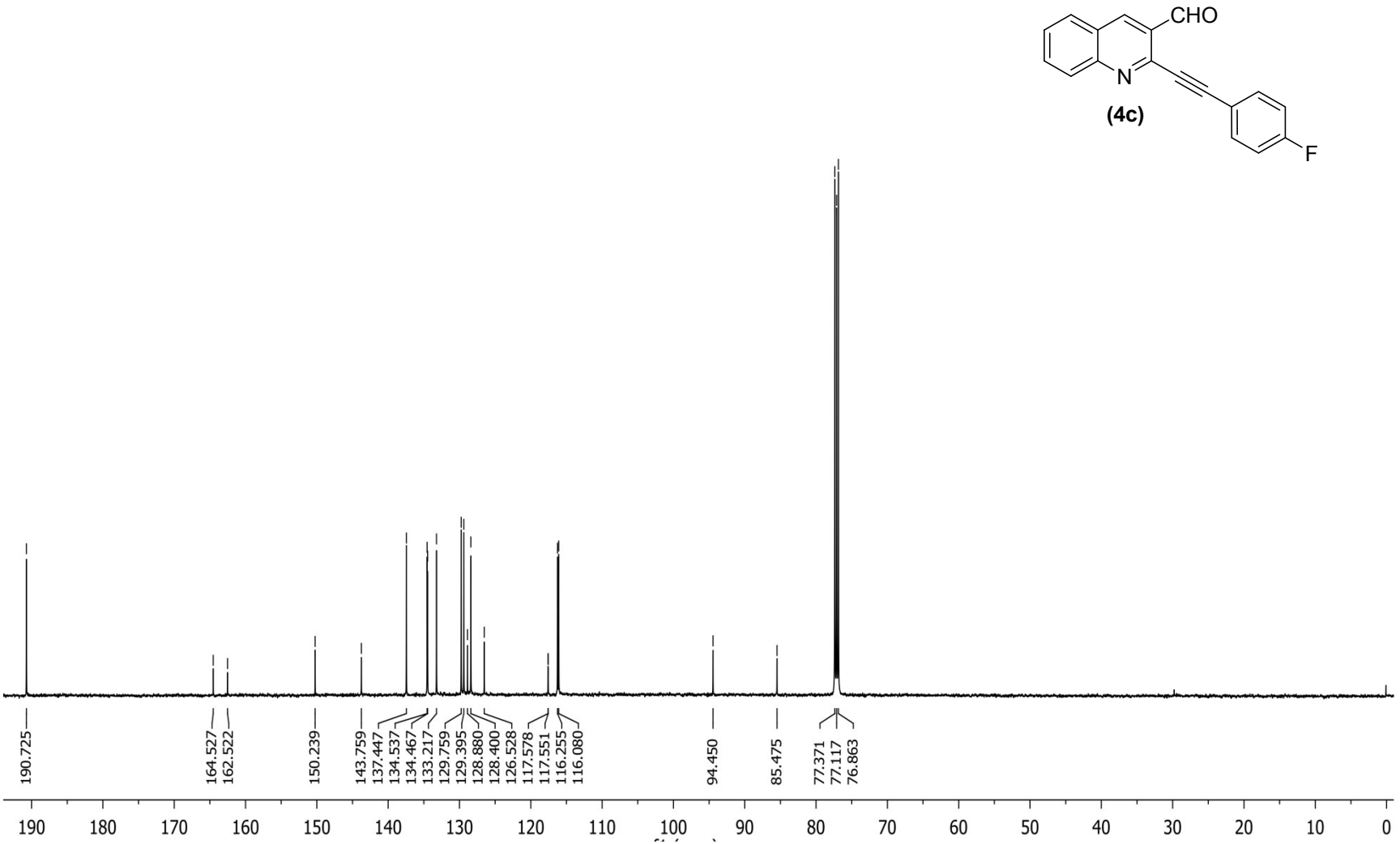

CHO
N
CF3
CF3
(4b)
189.902
150.187
142.332
138.119
133.474
132.831
132.561
132.289
132.210
132.021
129.732
129.568
129.033
128.943
126.794
123.917
123.185
121.755
91.044
88.505
77.342
77.088
76.834
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

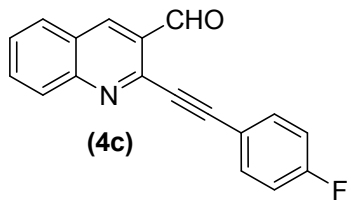

CHO
N
CF3
CF3

(4b)

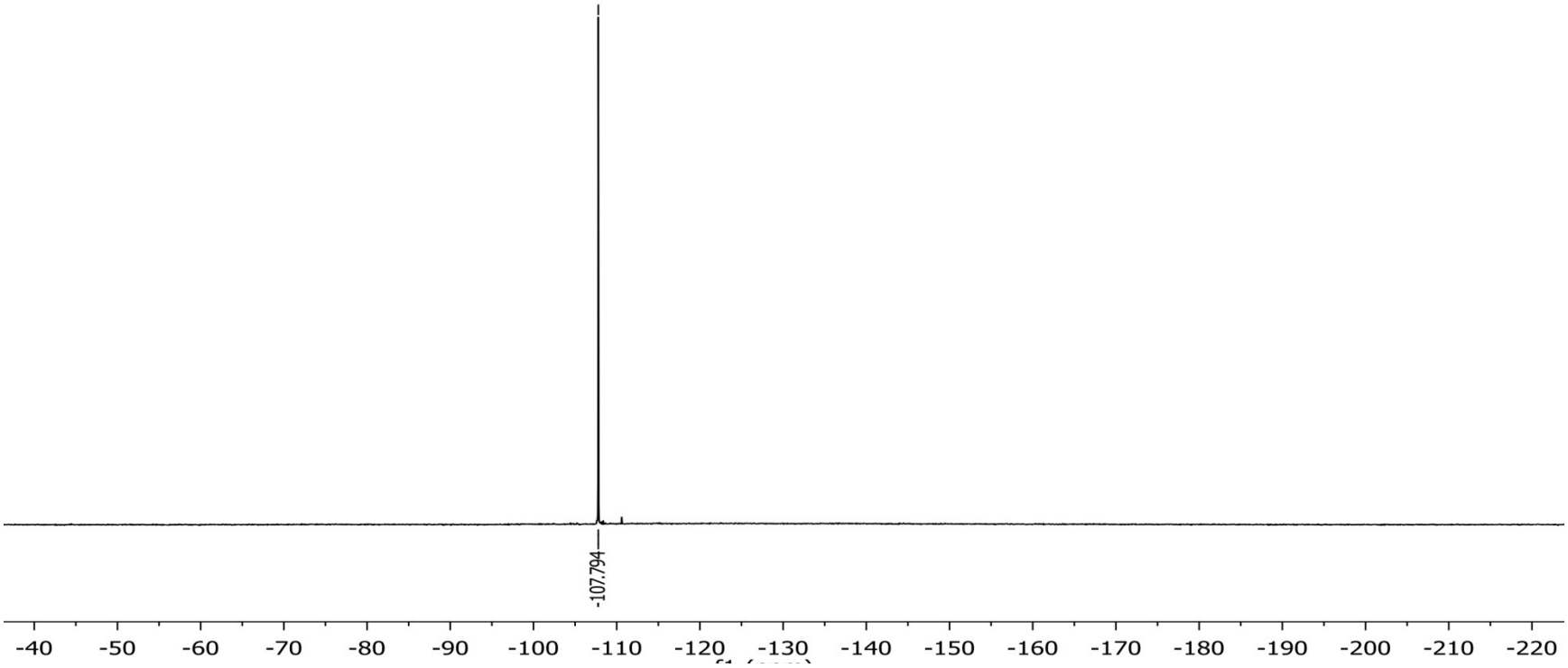

-63.026
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160

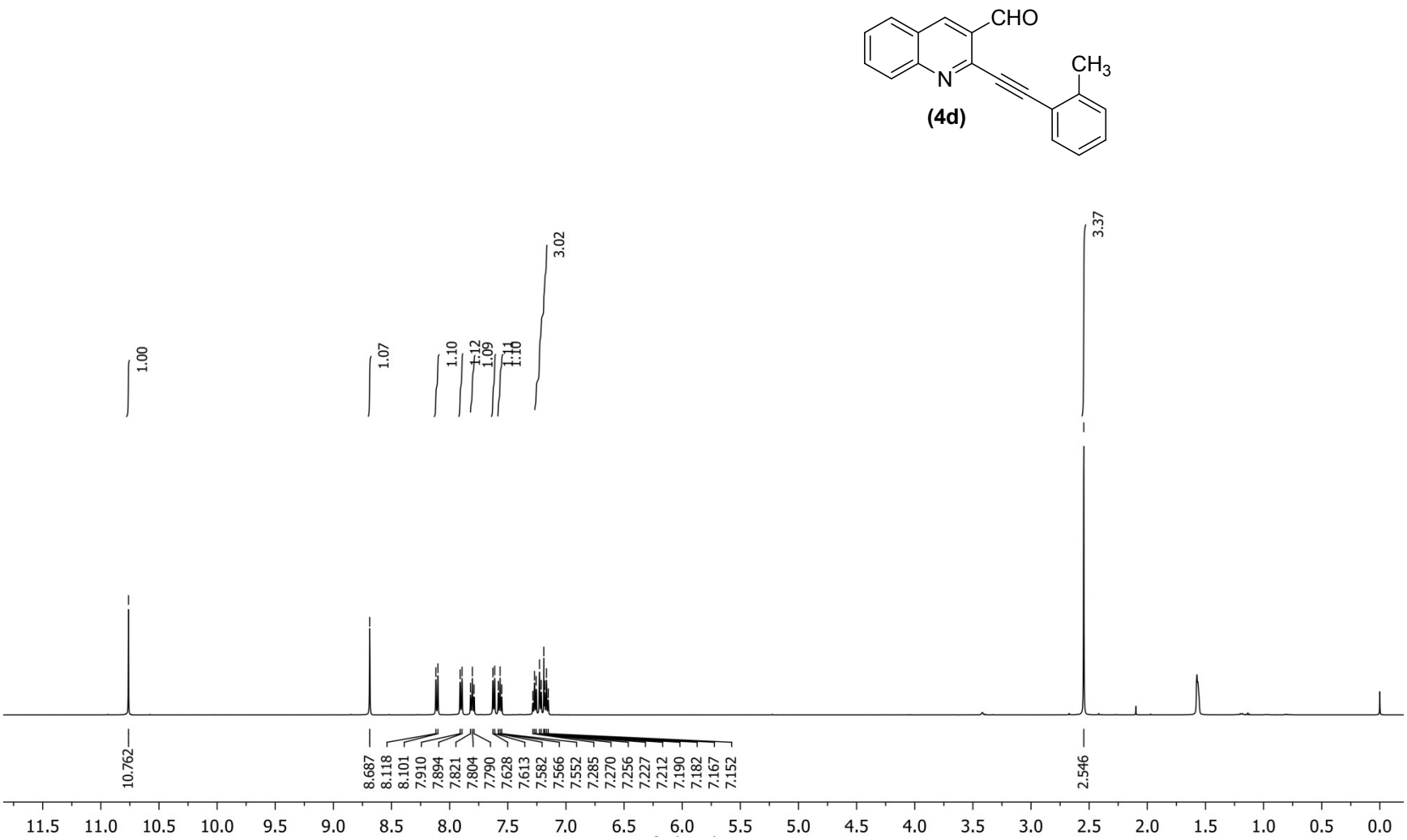

CHO
N
F
(4c)
1.00
1.06
1.04
1.11
1.14
1.15
2.19
2.26
10.779
8.758
8.185
8.168
7.988
7.971
7.901
7.885
7.870
7.717
7.701
7.690
7.664
7.650
7.634
7.268
7.143
7.126
7.109
12
11
10
9
8
7
6
5
4
3
2
1
0

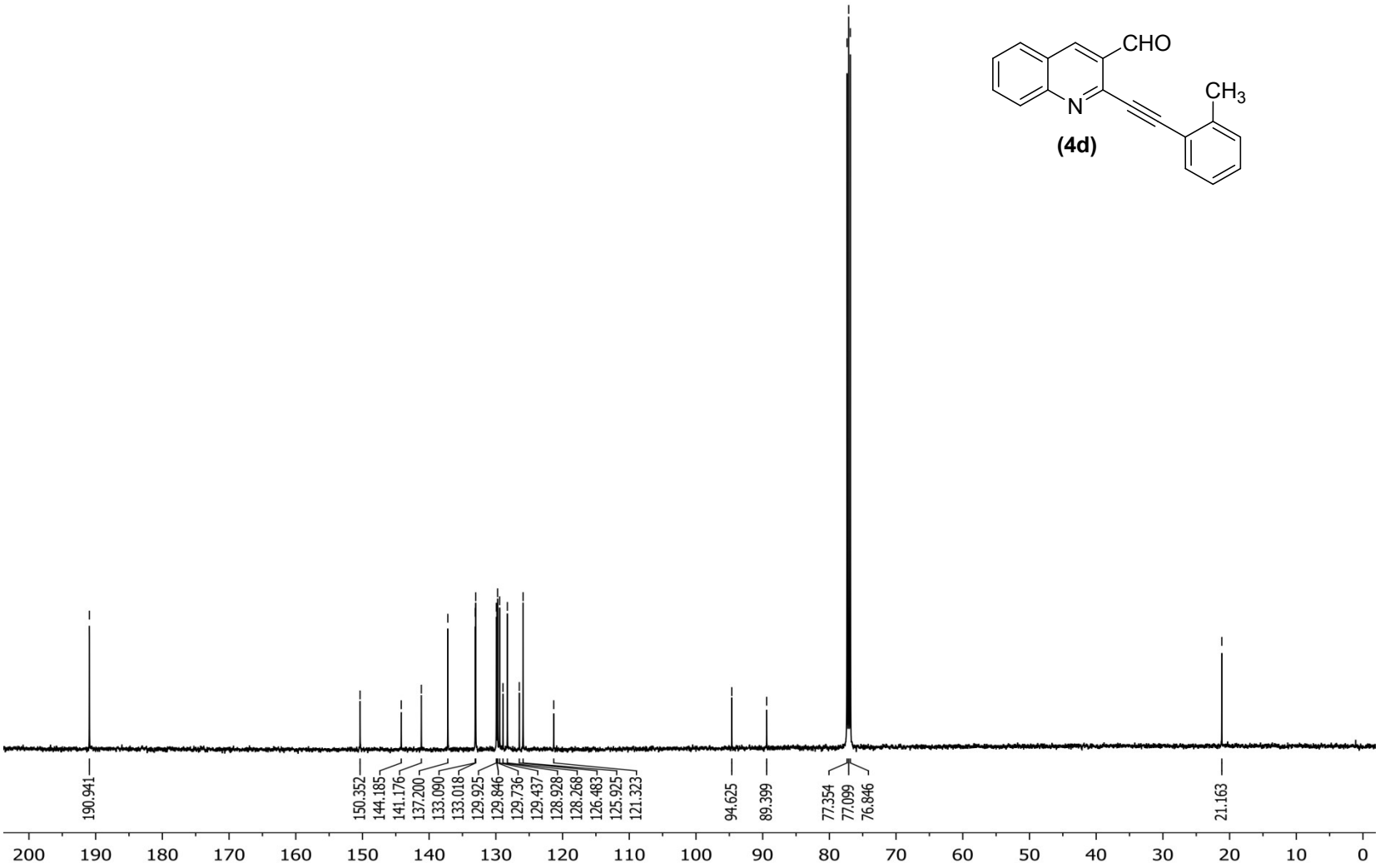

CHO
N
F
(4c)
190.725
164.527
162.522
150.239
143.759
137.447
134.537
134.467
133.217
129.759
129.395
128.880
128.400
126.528
117.578
117.551
116.255
116.080
94.450
85.475
77.371
77.117
76.863
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

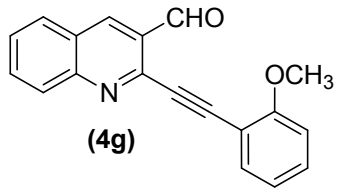

CHO
N
F

(4c)

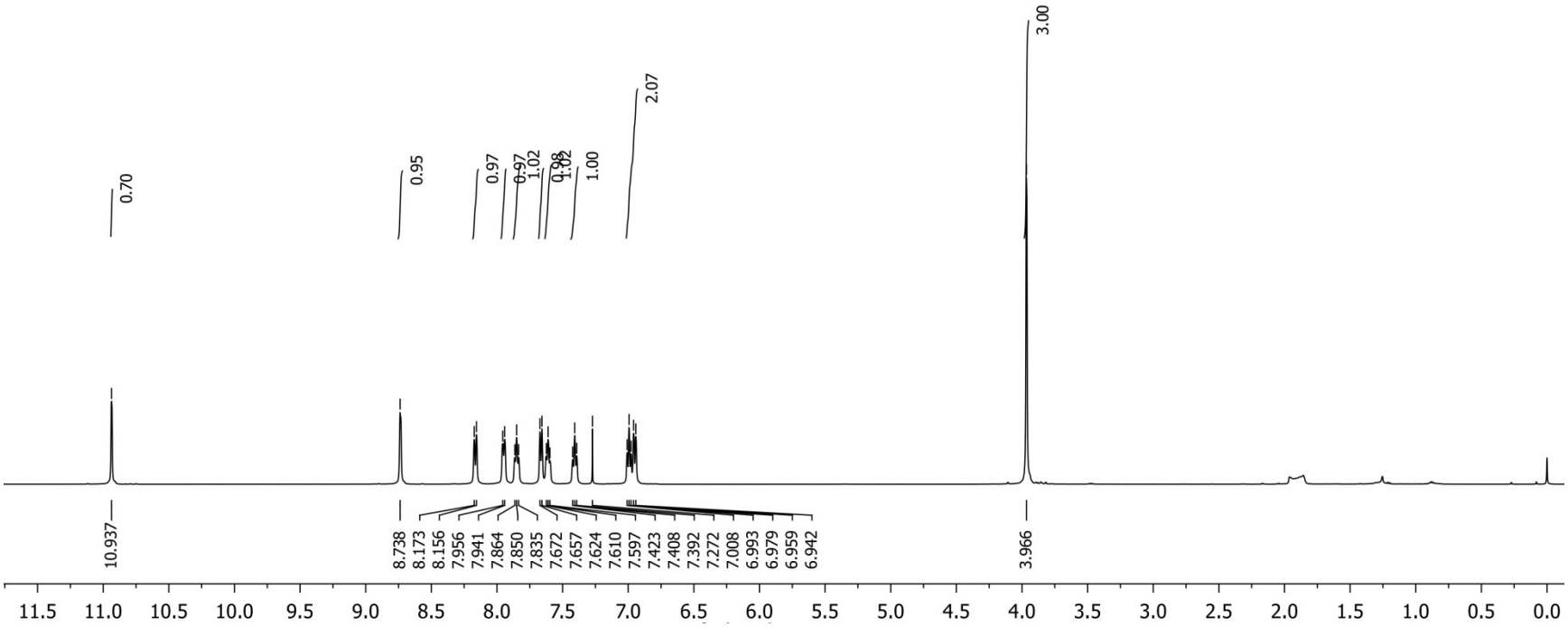

-107.794
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220

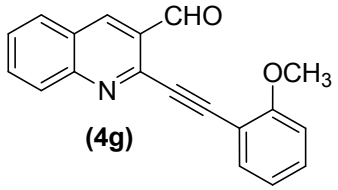

CHO
N
CH3
(4d)
1.00
1.07
1.10
1.12
1.09
1.11
1.10
3.02
3.37
10.762
8.687
8.118
8.101
7.910
7.894
7.821
7.804
7.790
7.628
7.613
7.582
7.566
7.552
7.285
7.270
7.256
7.227
7.212
7.190
7.182
7.167
7.152
2.546
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


CHO
N
CH3
(4d)
190.941
150.352
144.185
141.176
137.200
133.090
133.018
129.925
129.846
129.736
129.437
128.928
128.268
126.483
125.925
121.323
94.625
89.399
77.354
77.099
76.846
21.163
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

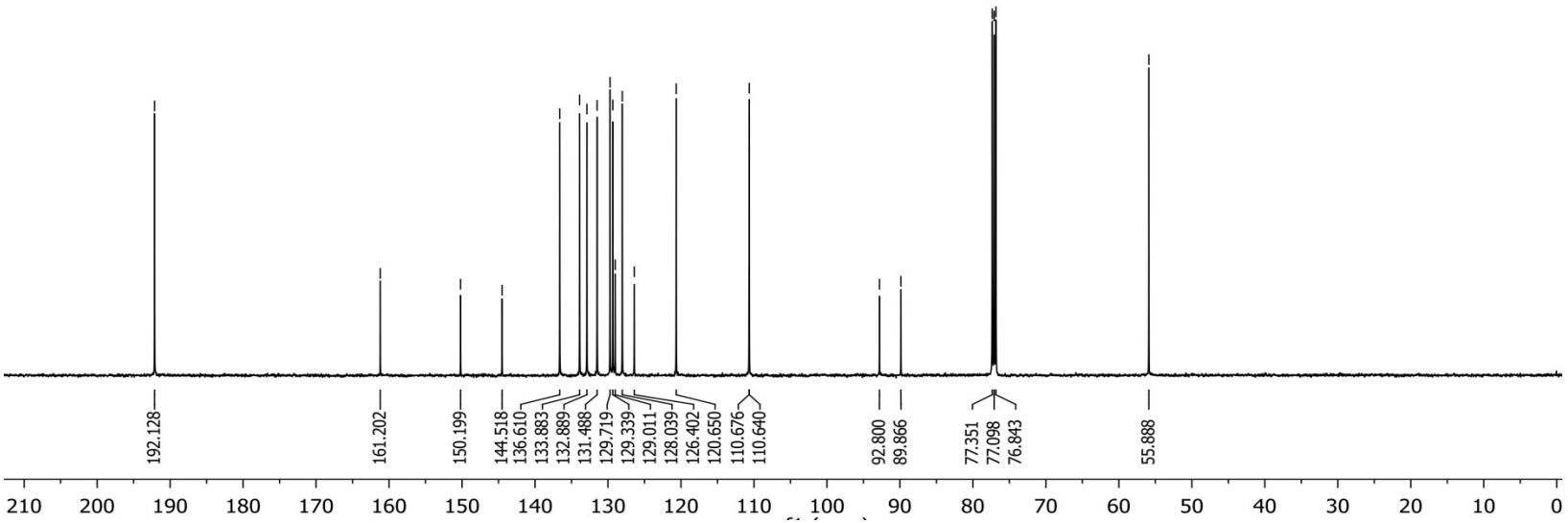

CHO
N
OCH3

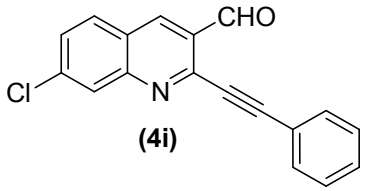
(4g)


0.70
0.95
0.97
0.97
1.02
0.98
1.02
1.00
2.07
3.00
10.937
8.738
8.173
8.156
7.956
7.941
7.864
7.850
7.835
7.672
7.657
7.624
7.610
7.597
7.423
7.408
7.392
7.272
7.008
6.993
6.979
6.959
6.942
3.966
11.5
11.0
10.5
10.0
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

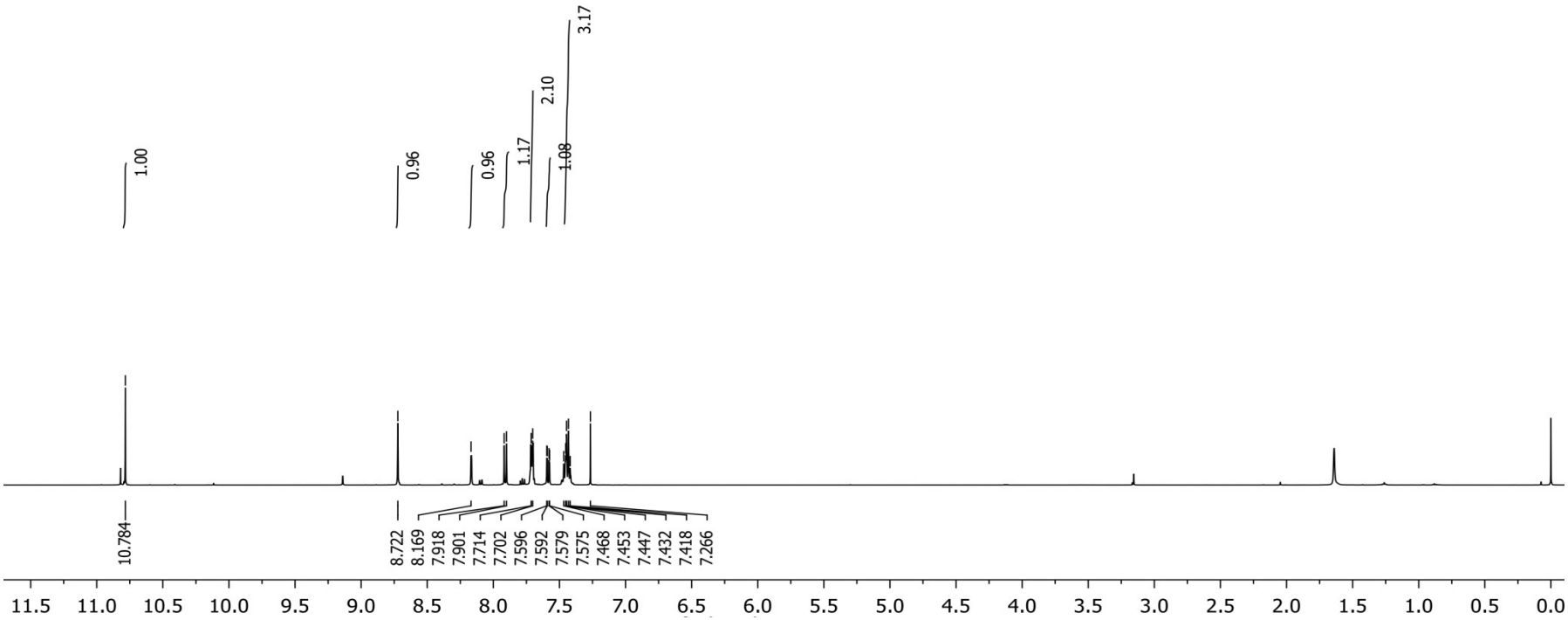

CHO
N
OCH3

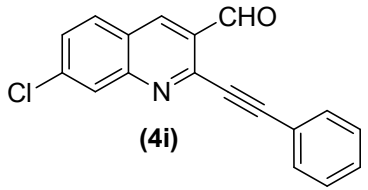
(4g)


192.128
161.202
150.199
144.518
136.610
133.883
132.889
131.488
129.719
129.339
129.011
128.039
126.402
120.650
110.676
110.640
92.800
89.866
77.351
77.098
76.843
55.888
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

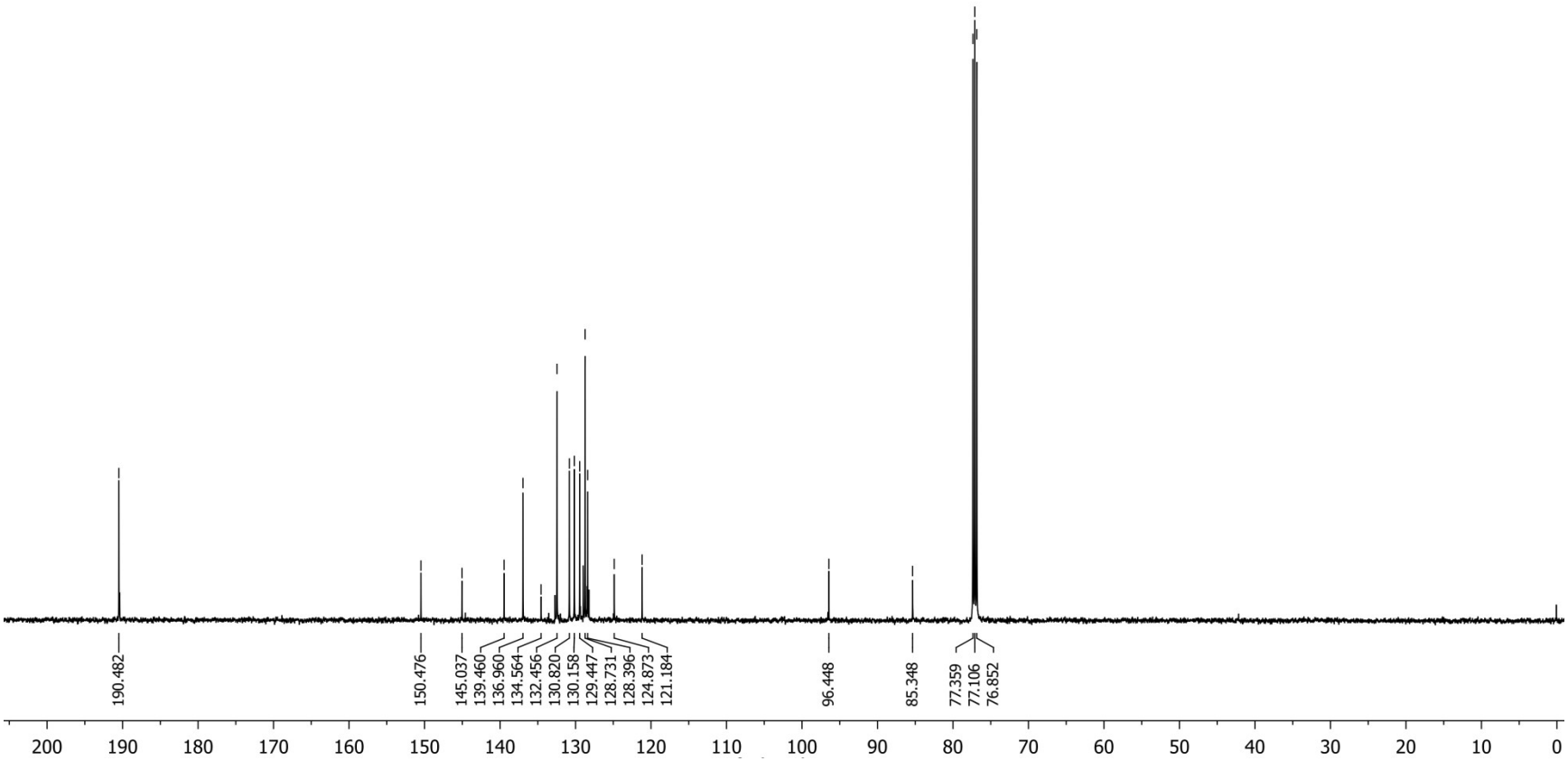

CHO
Cl
N

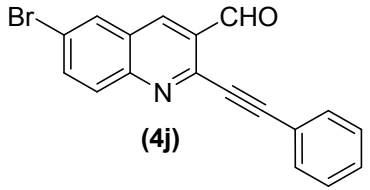
(4i)


1.00
0.96
0.96
1.17
2.10
1.08
3.17
10.784
8.722
8.169
7.918
7.901
7.714
7.702
7.596
7.592
7.579
7.575
7.468
7.453
7.447
7.432
7.418
7.266
11.5
11.0
10.5
10.0
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

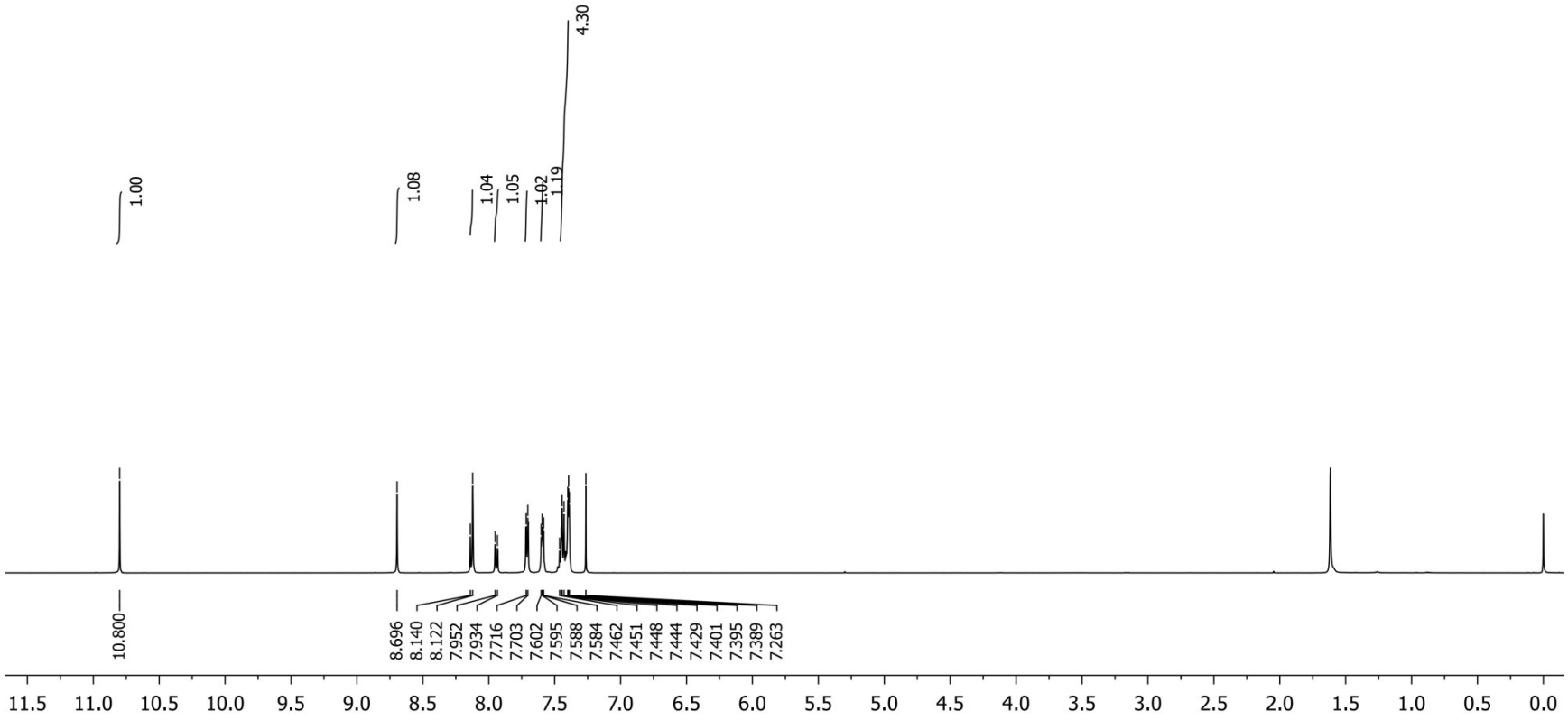

CHO
Cl
N

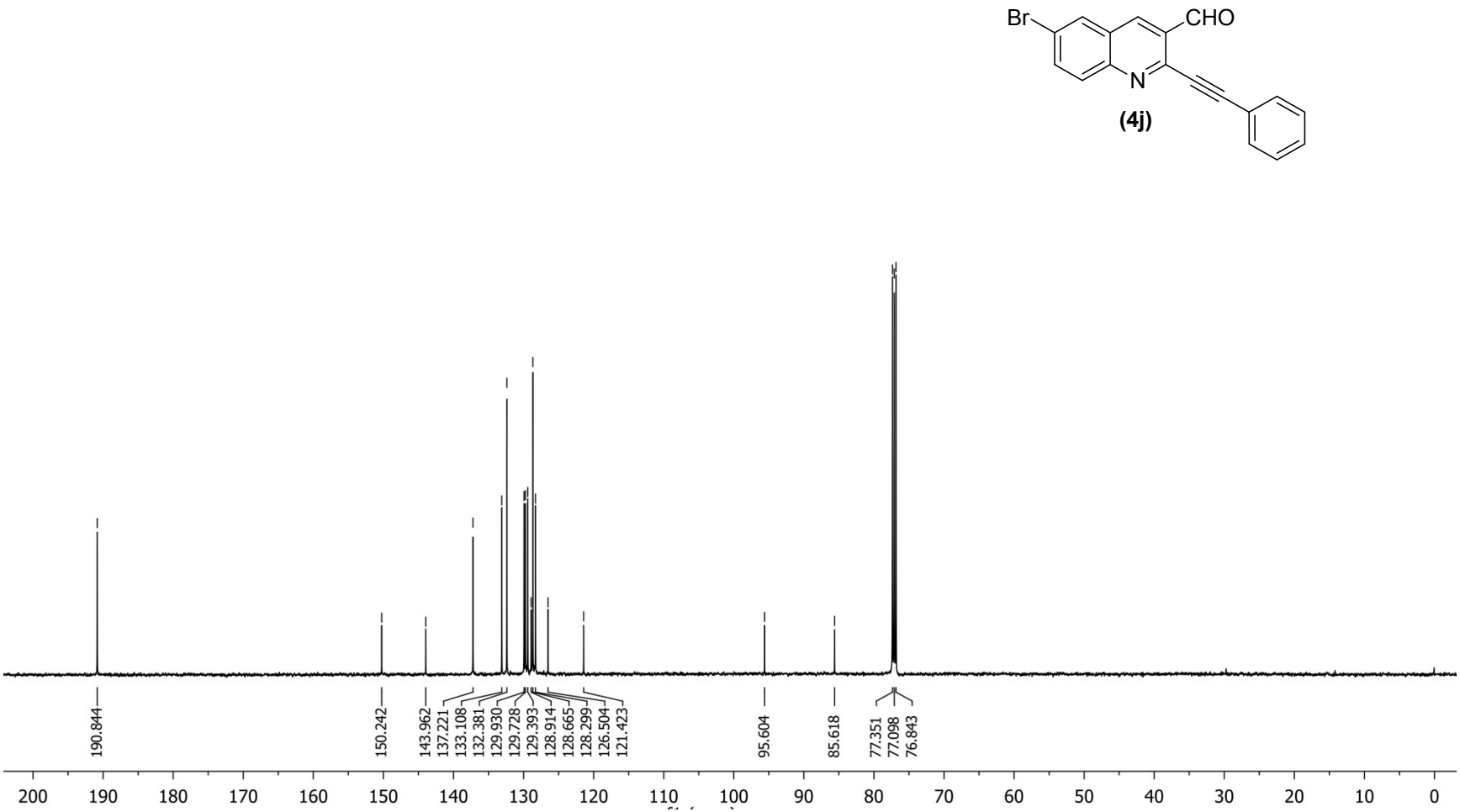
(4i)

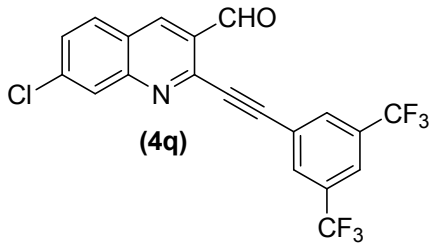

190.482
150.476
145.037
139.460
136.960
134.564
132.456
130.820
130.158
129.447
128.731
128.396
124.873
121.184
96.448
85.348
77.359
77.106
76.852
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


Br
CHO
N

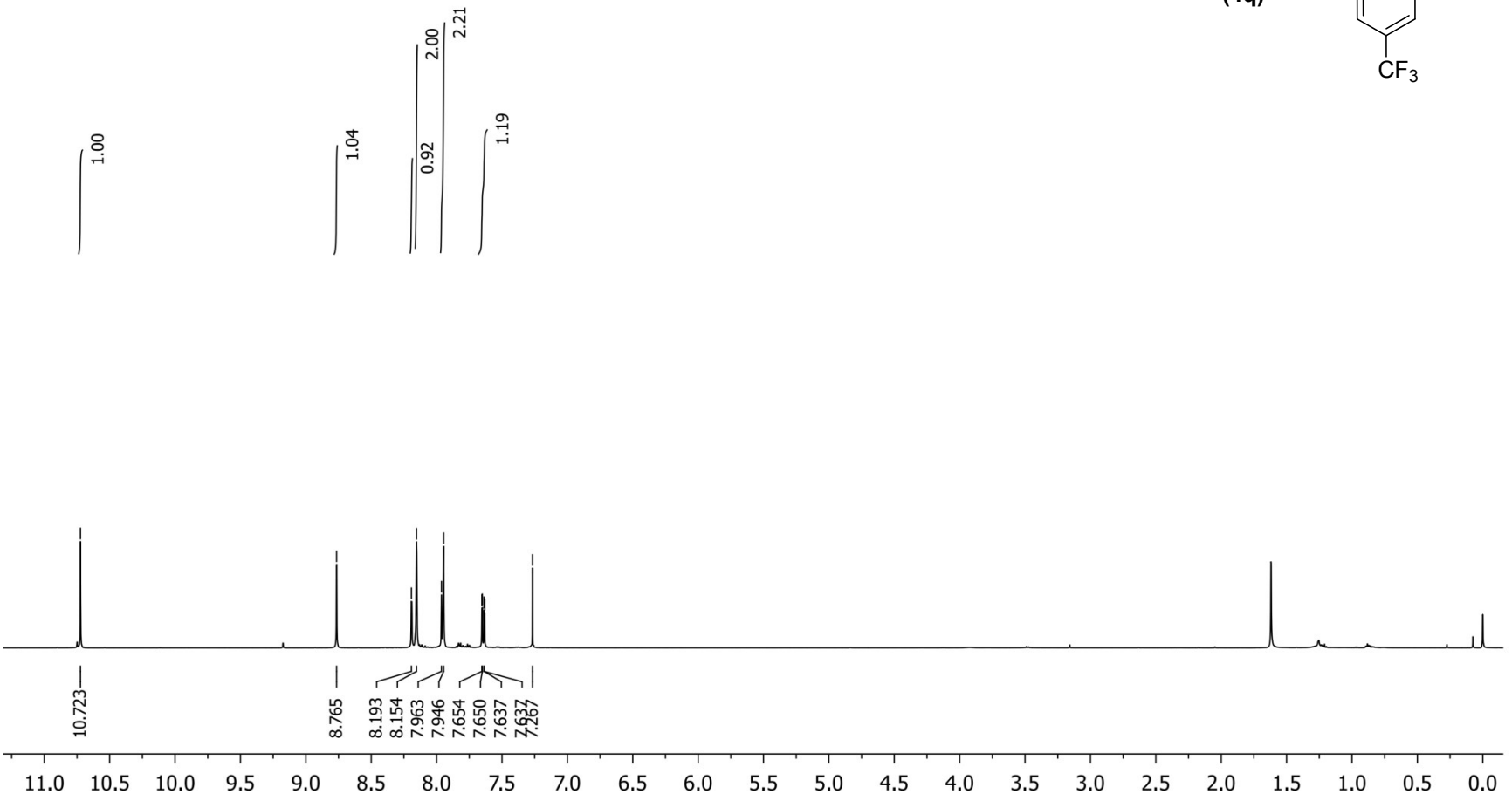
(4j)

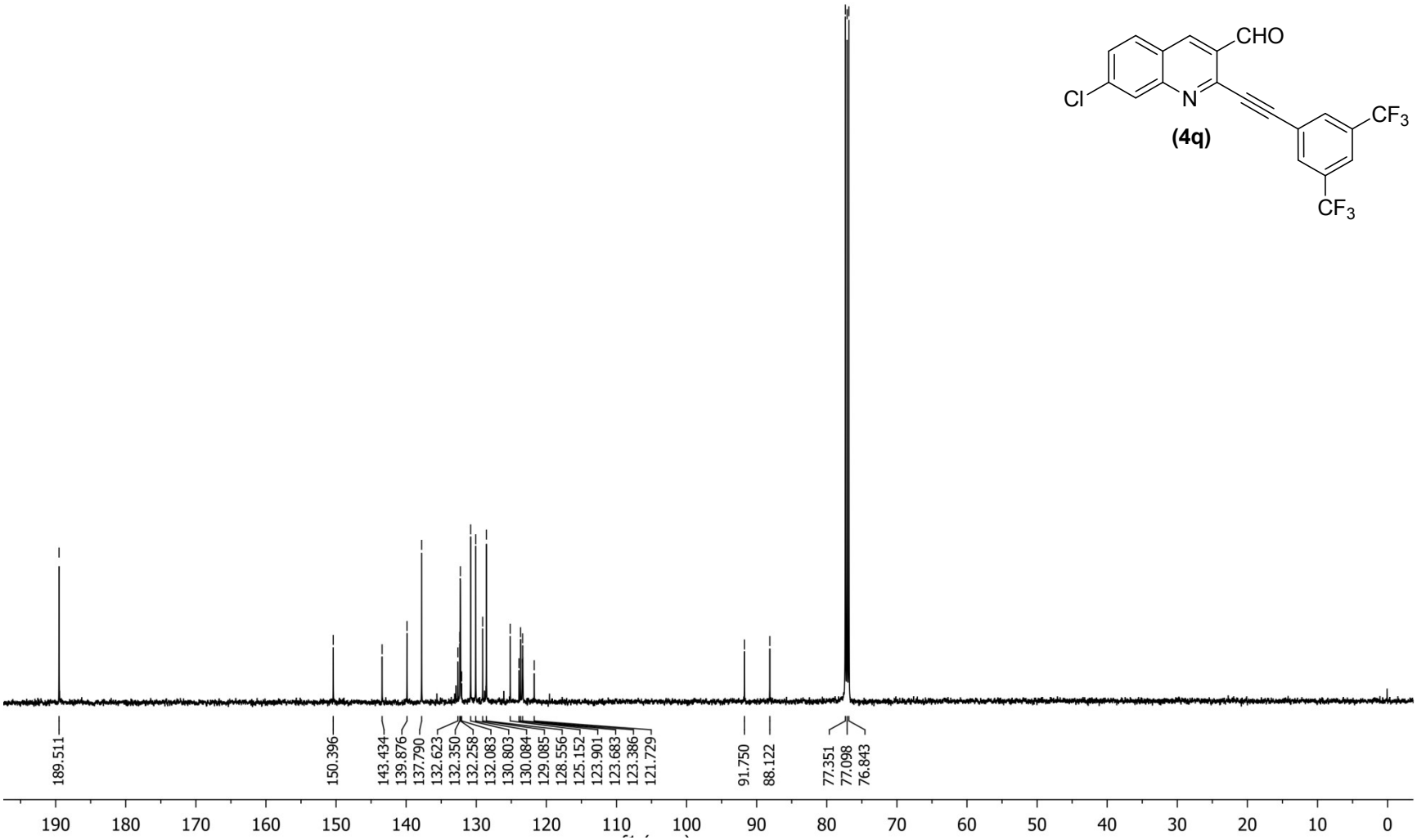

1.00
1.08
1.04
1.05
1.02
1.19
4.30
10.800
8.696
8.140
8.122
7.952
7.934
7.716
7.703
7.602
7.595
7.588
7.584
7.462
7.451
7.448
7.444
7.429
7.401
7.395
7.389
7.263
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

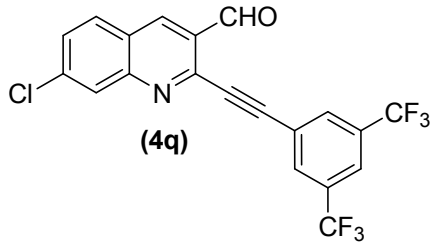

Br
CHO
N
(4j)
190.844
150.242
143.962
137.221
133.108
132.381
129.930
129.728
129.393
128.914
128.665
128.299
126.504
121.423
95.604
85.618
77.351
77.098
76.843
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


CHO
Cl
N
CF3
CF3

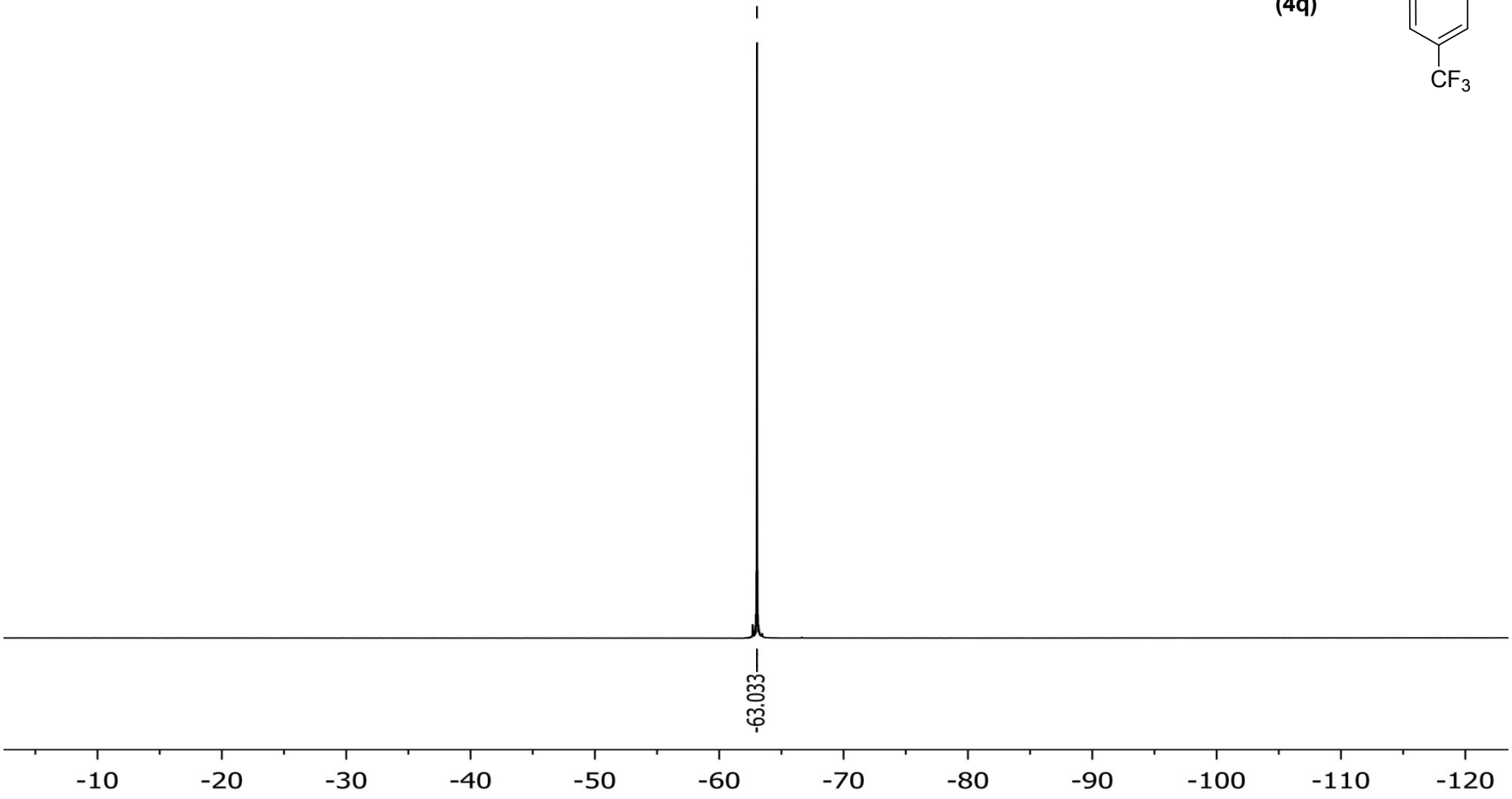
(4q)

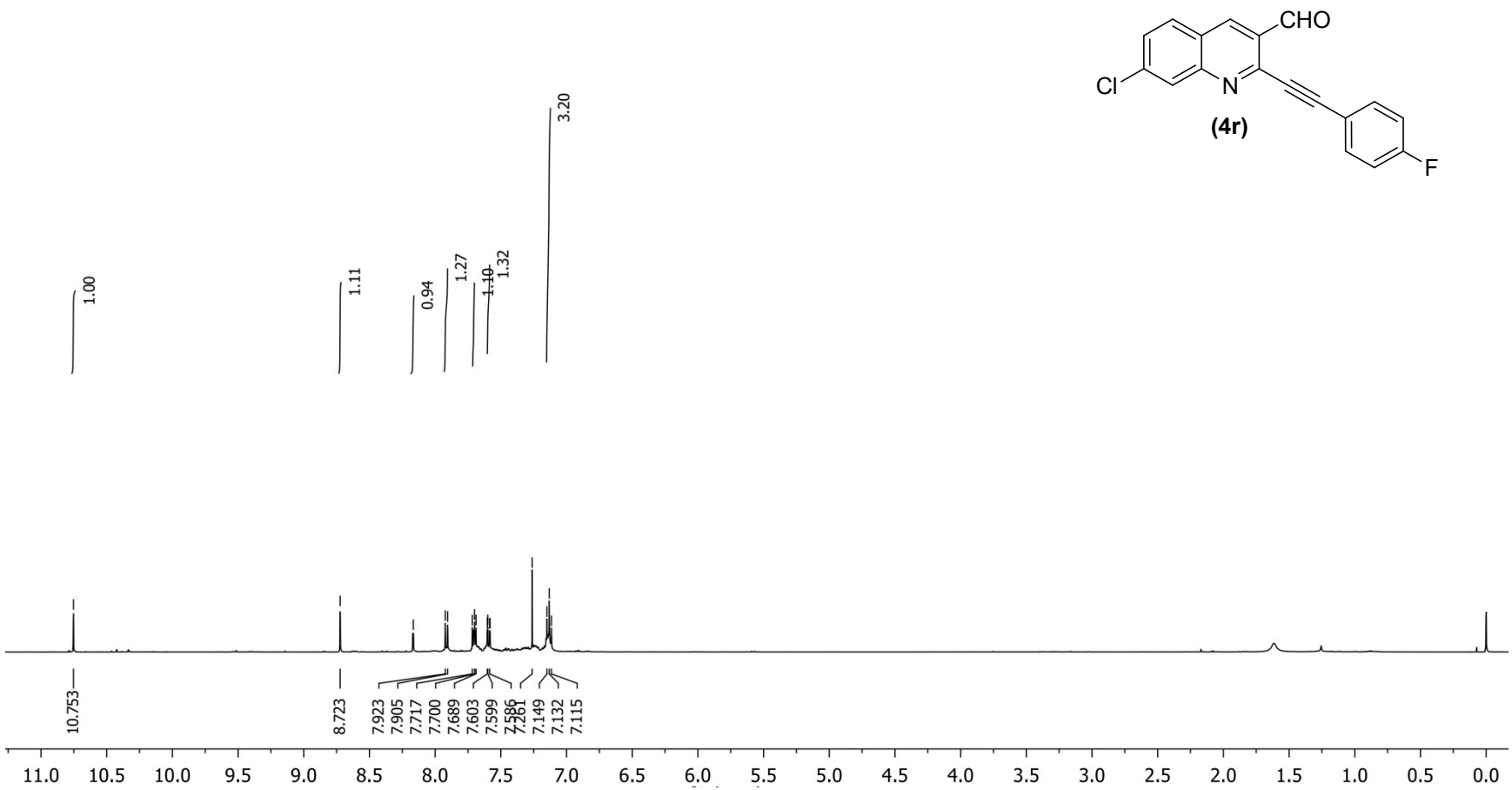

1.00
1.04
0.92
2.00
2.21
1.19
10.723
8.765
8.193
8.154
7.963
7.946
7.654
7.650
7.637
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

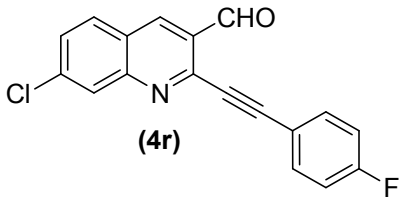

CHO
Cl
N
CF3
CF3
(4q)
189.511
150.396
143.434
139.876
137.790
132.623
132.350
132.258
132.083
130.803
130.084
129.085
128.556
125.152
123.901
123.683
123.386
121.729
91.750
88.122
77.351
77.098
76.843
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



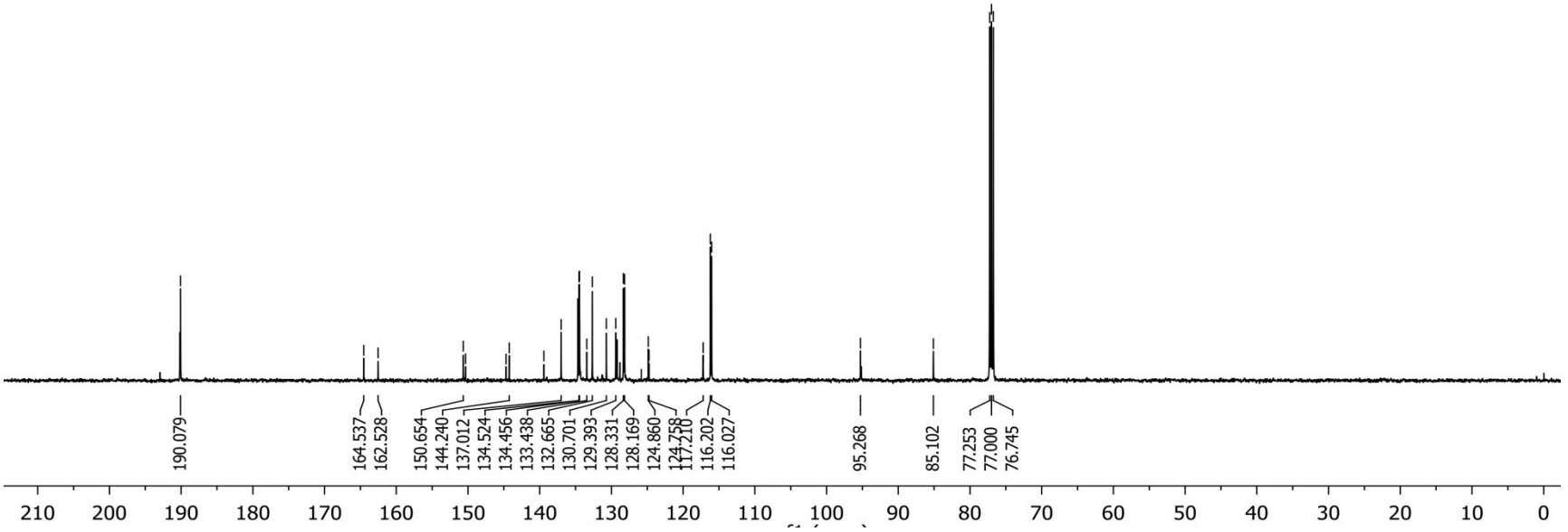
(4q)

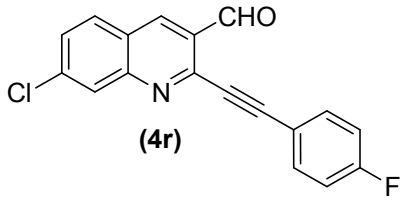



CHO
Cl
N
F
(4r)
1.00
1.11
0.94
1.27
1.10
1.32
3.20
10.753
8.723
7.923
7.905
7.717
7.700
7.689
7.603
7.599
7.586
7.281
7.149
7.132
7.115
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

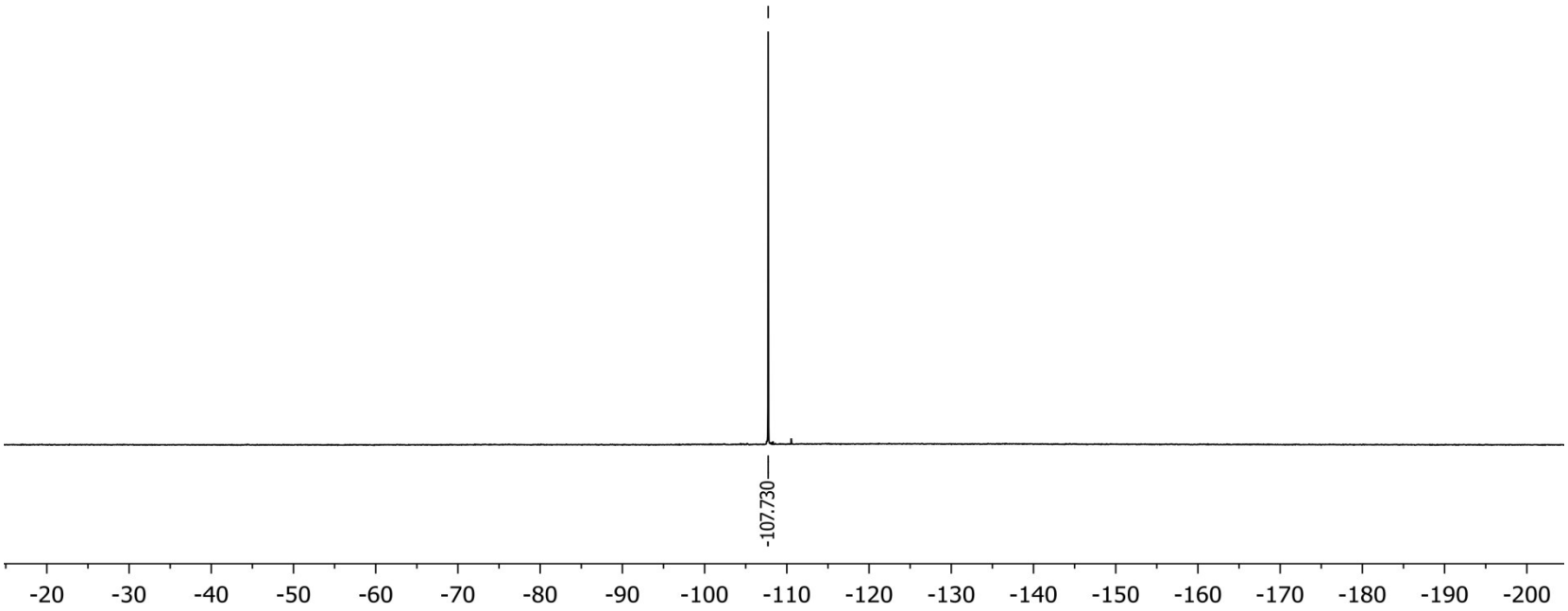

CHO
Cl
N
F

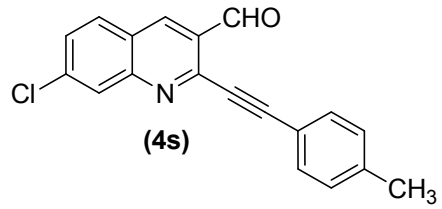
(4r)


190.079
164.537
162.528
150.654
144.240
137.012
134.524
134.456
133.438
132.665
130.701
129.393
128.331
128.169
124.860
124.758
117.210
116.202
116.027
95.268
85.102
77.253
77.000
76.745
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

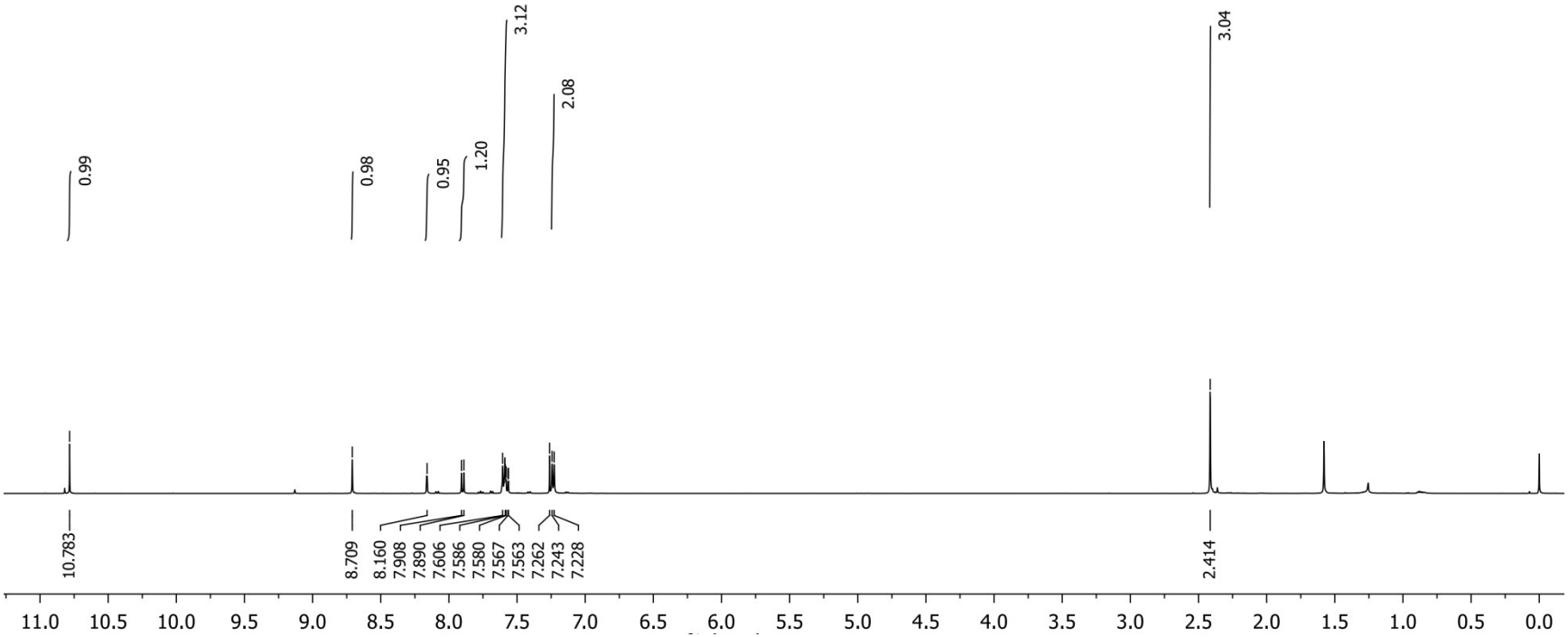

CHO
Cl
N
F

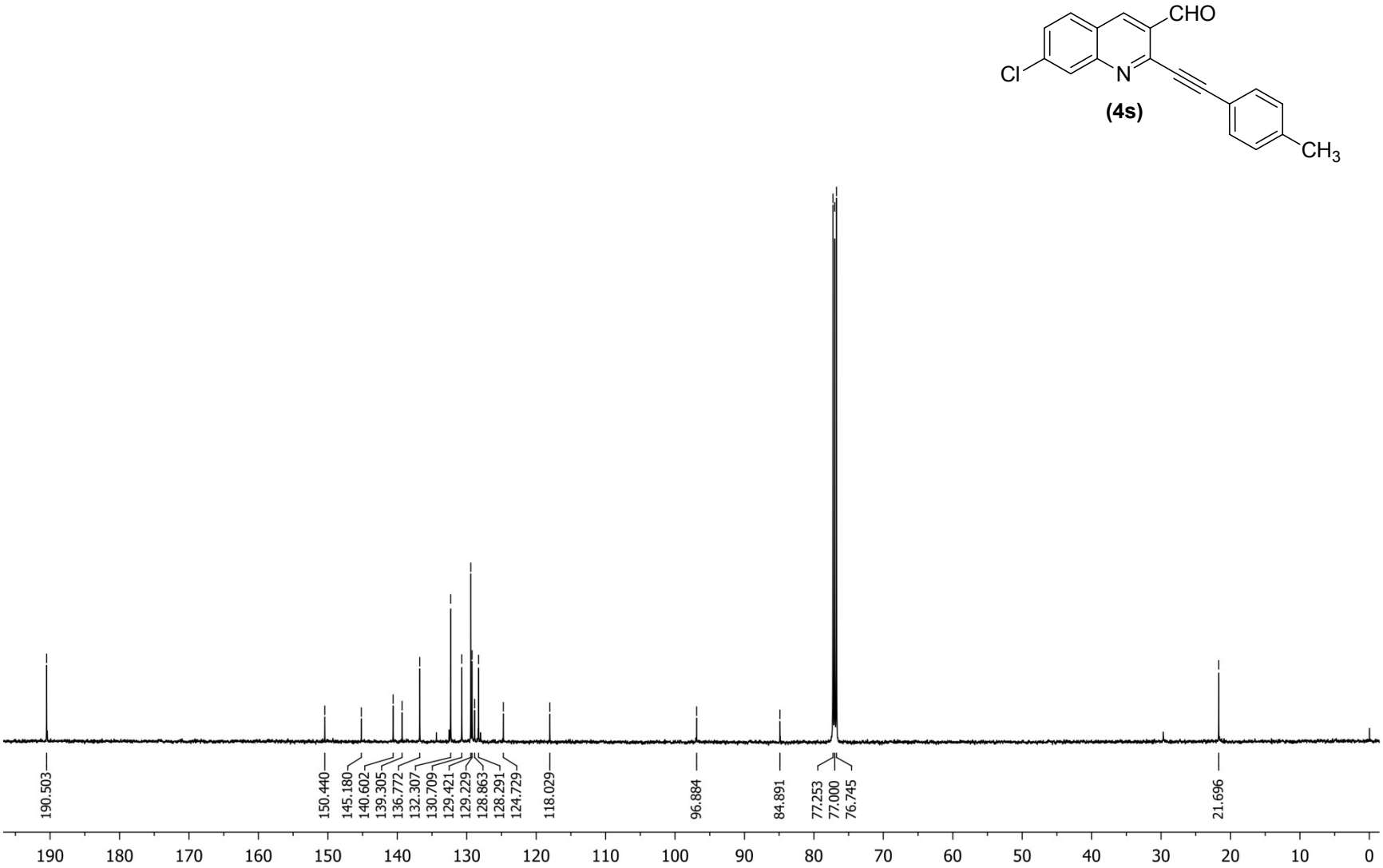
(4r)

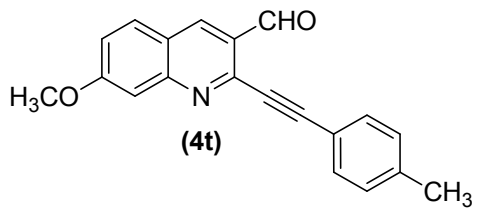

-107.730
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200


CHO
Cl
N
CH3

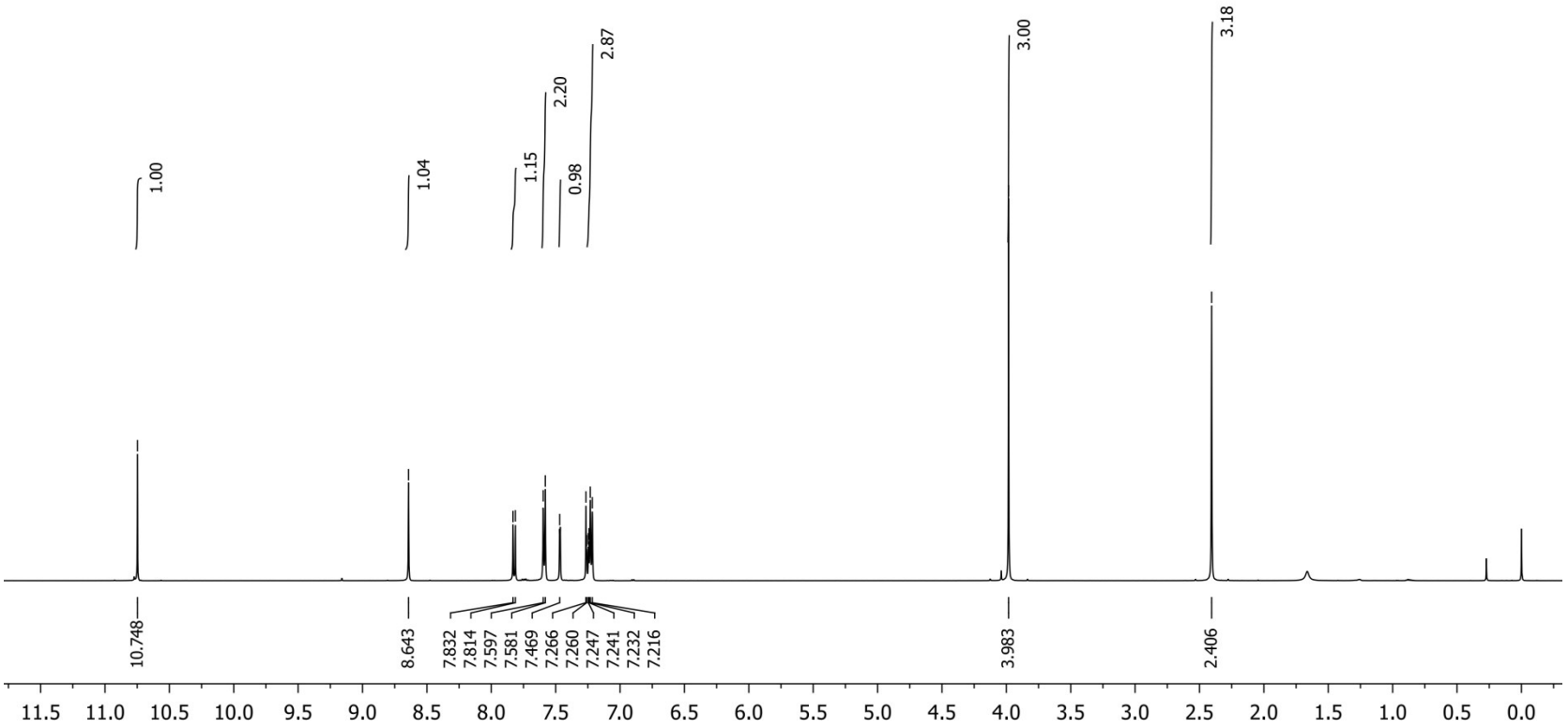
(4s)

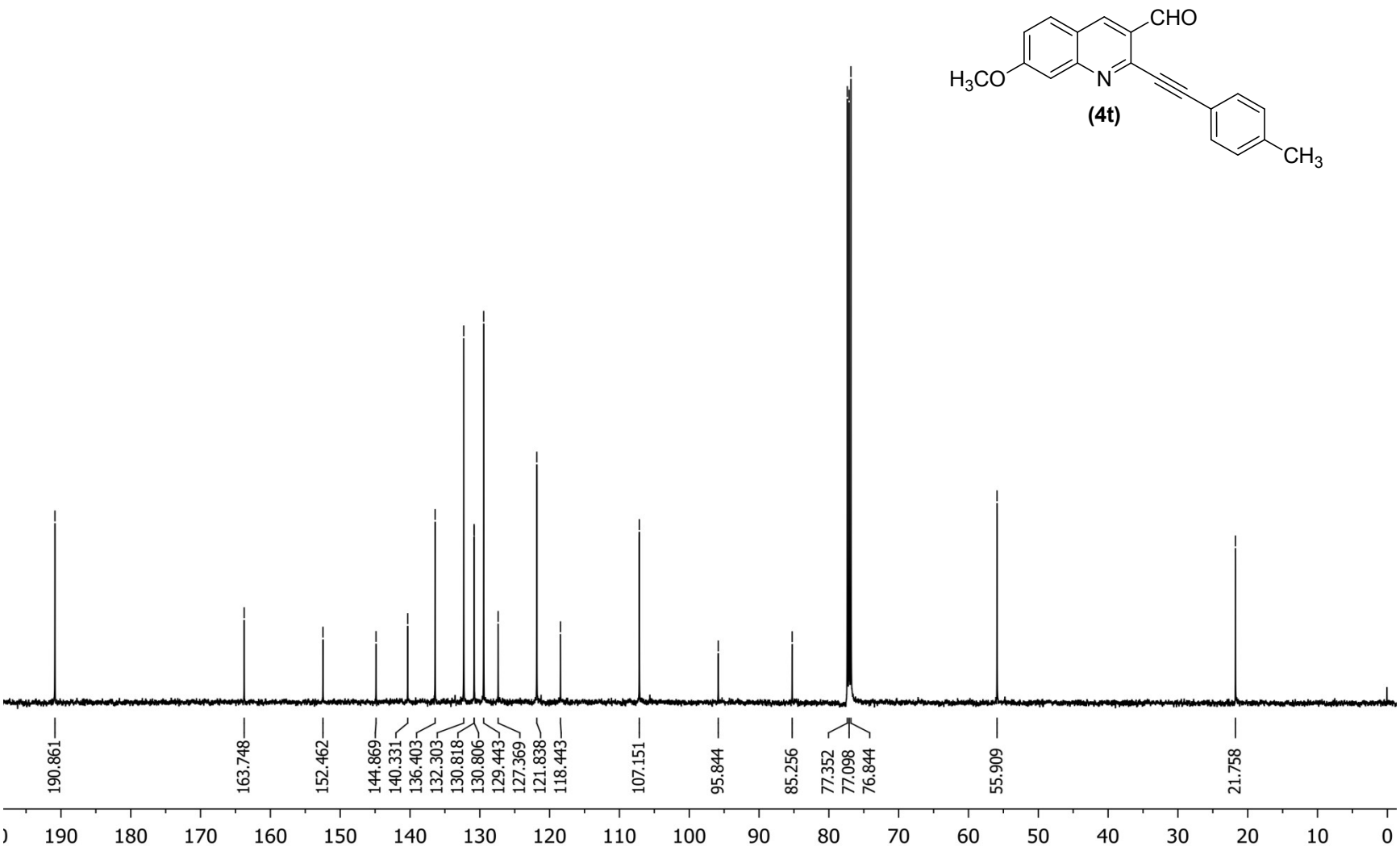

0.99
0.98
0.95
1.20
3.12
2.08
3.04
10.783
8.709
8.160
7.908
7.890
7.606
7.586
7.580
7.567
7.563
7.262
7.243
7.228
2.414
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

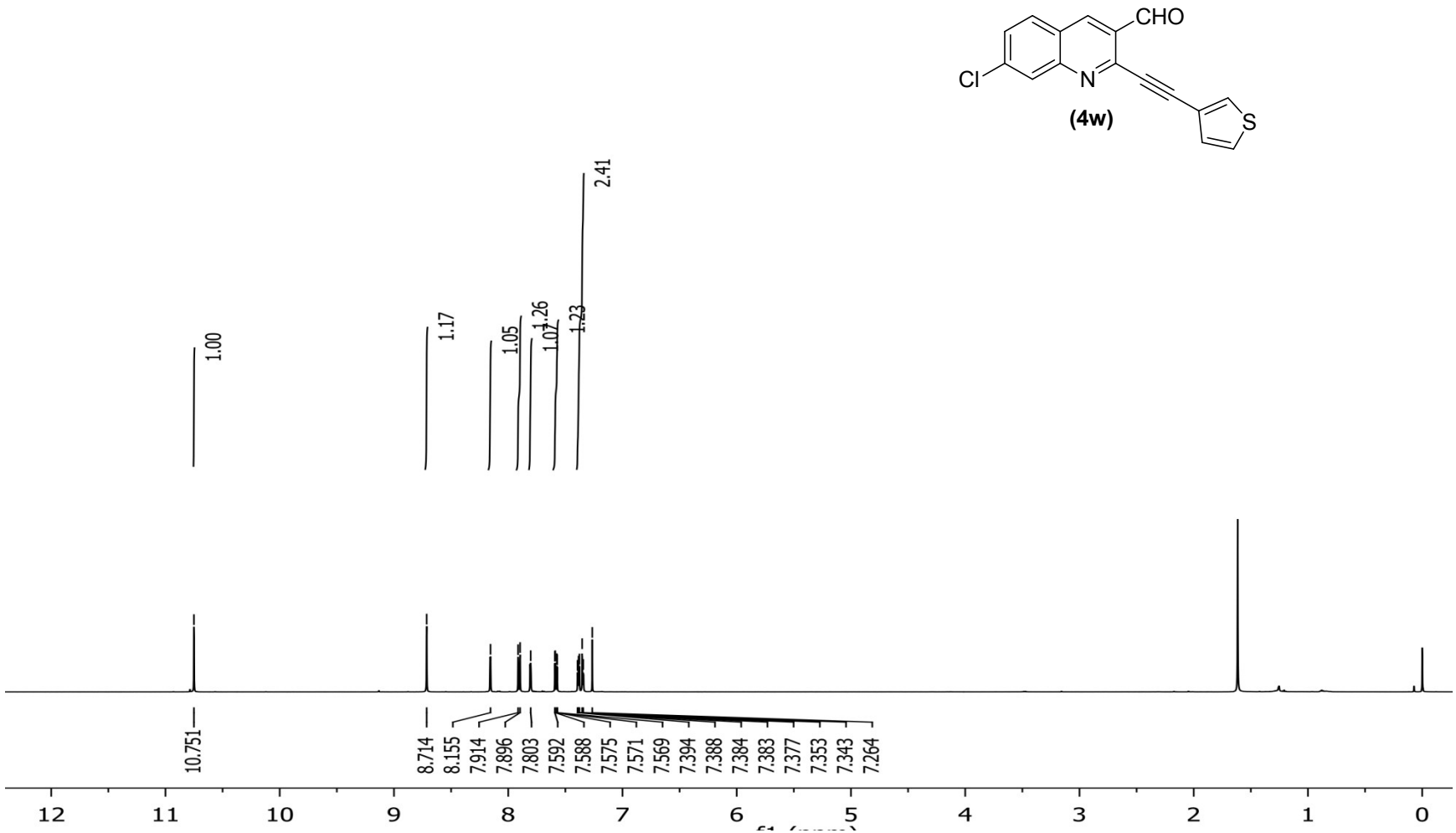

CHO
Cl
N
(4s)
CH3
190.503
150.440
145.180
140.602
139.305
136.772
132.307
130.709
129.421
129.229
128.863
128.291
124.729
118.029
96.884
84.891
77.253
77.000
76.745
21.696
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

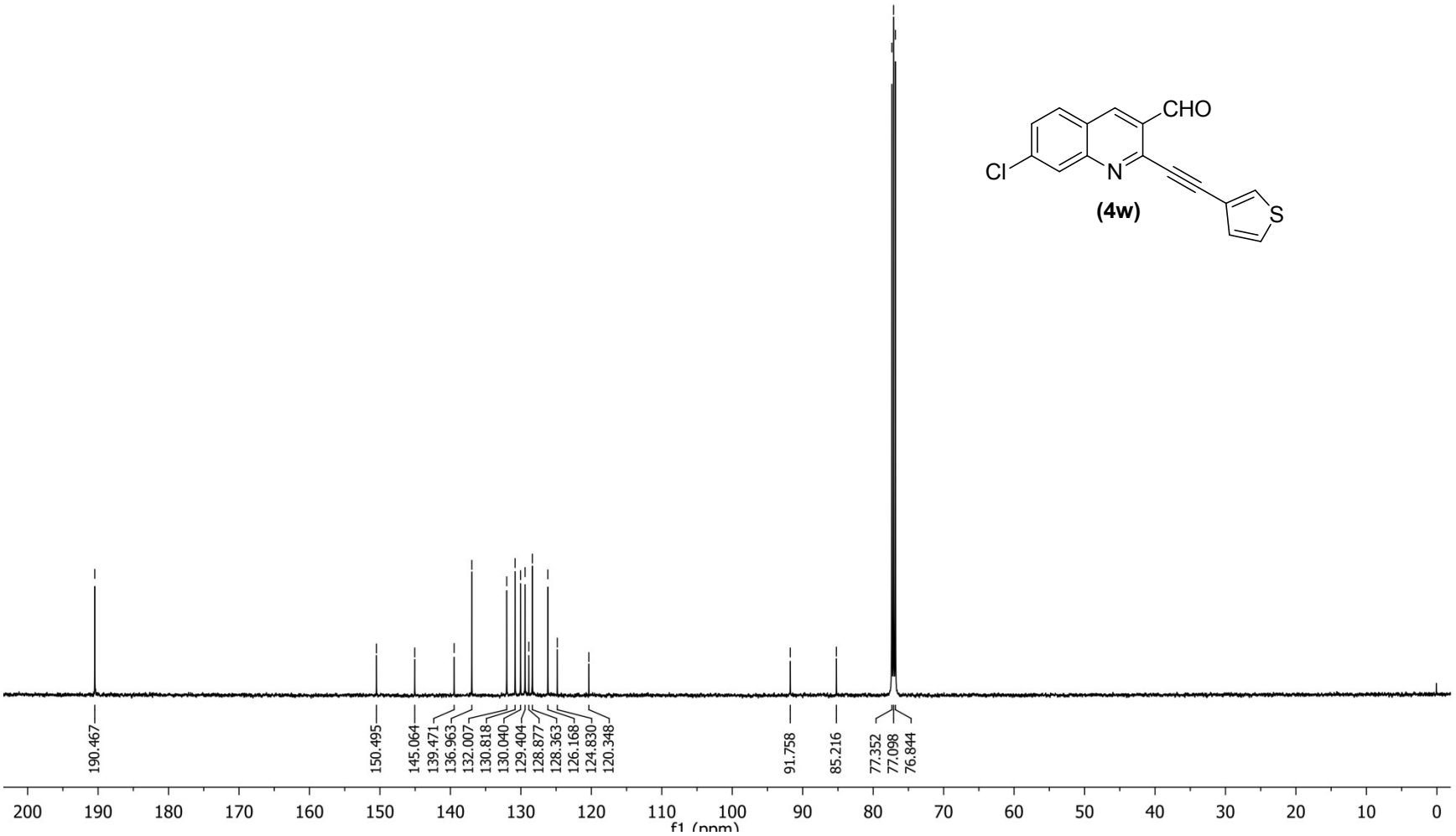

CHO
H_3CO
N
CH_3

(4t)

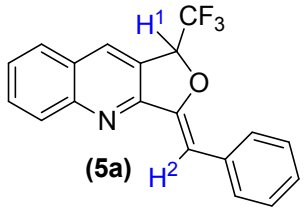

1.00
1.04
1.15
2.20
0.98
2.87
3.00
3.18
10.748
8.643
7.832
7.814
7.597
7.581
7.469
7.266
7.260
7.247
7.241
7.232
7.216
3.983
2.406
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


CHO
H3CO
N
(4t)
CH3
190.861
163.748
152.462
144.869
140.331
136.403
132.303
130.818
130.806
129.443
127.369
121.838
118.443
107.151
95.844
85.256
77.352
77.098
76.844
55.909
21.758
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

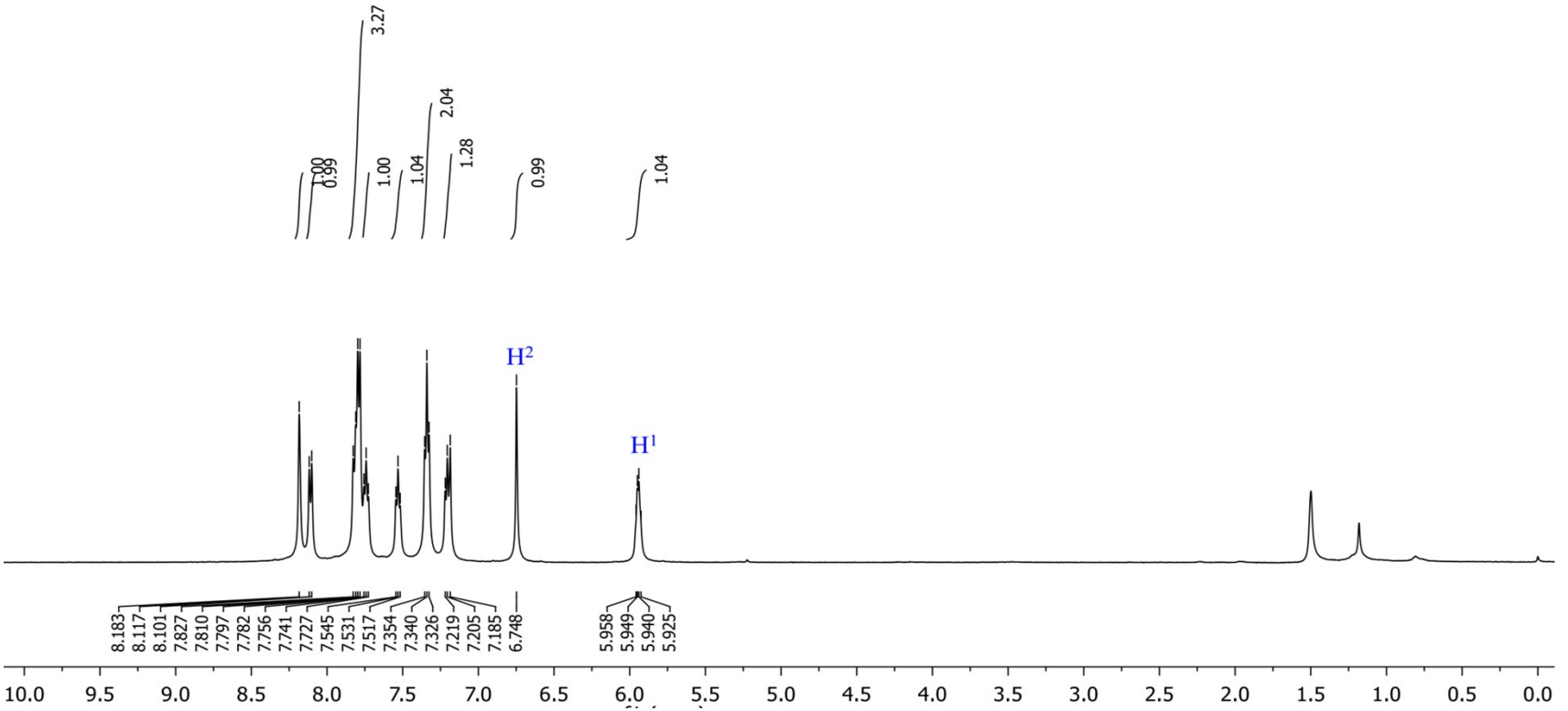

CHO
Cl
N
S
(4w)
1.00
1.17
1.05
1.07
1.26
1.23
2.41
10.751
8.714
8.155
7.914
7.896
7.803
7.592
7.588
7.575
7.571
7.569
7.394
7.388
7.384
7.383
7.377
7.353
7.343
7.264
12
11
10
9
8
7
6
5
4
3
2
1
0

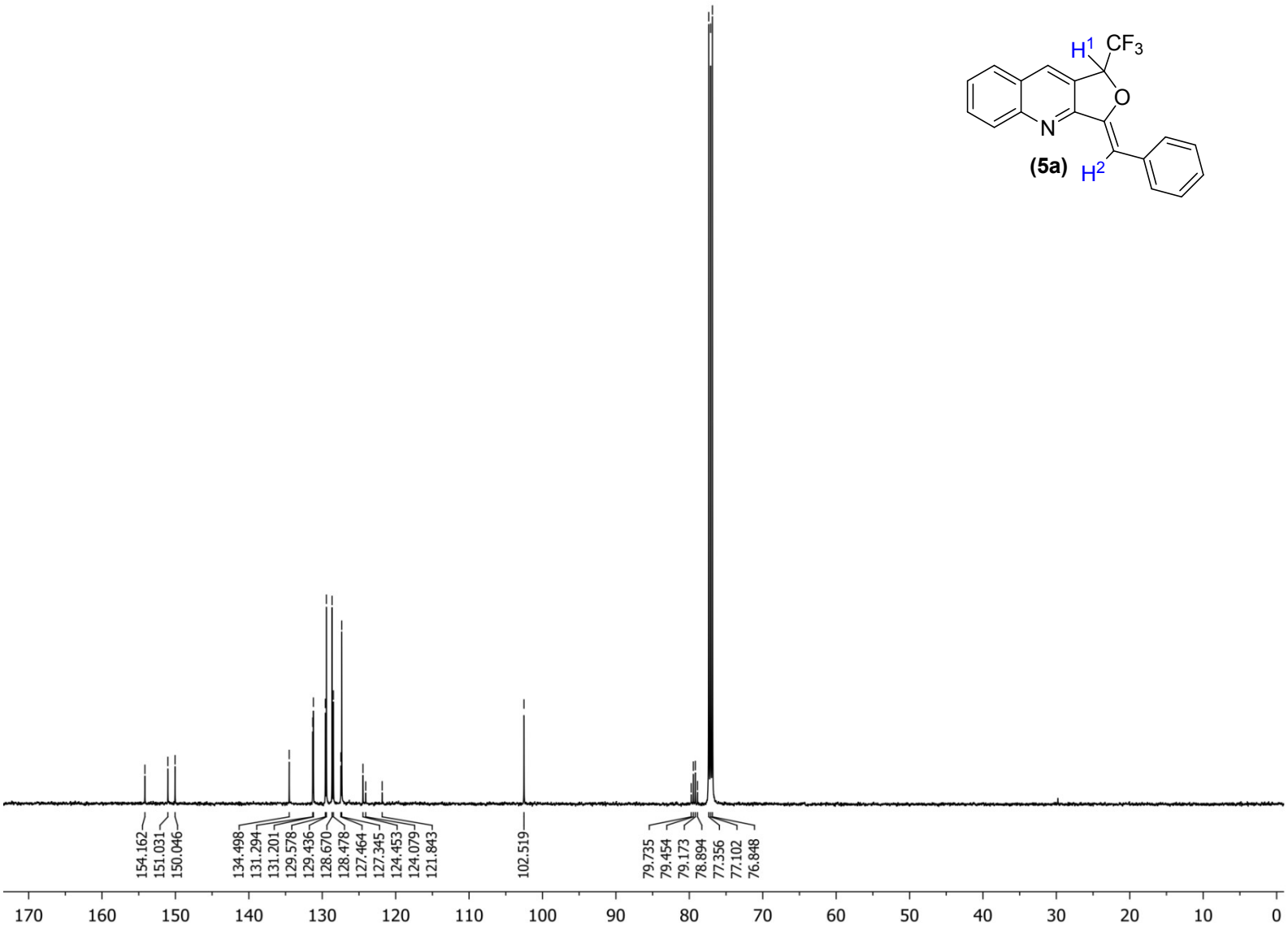

CHO
Cl
N
S
(4w)
190.467
150.495
145.064
139.471
136.963
132.007
130.818
130.040
129.404
128.877
128.363
126.168
124.830
120.348
91.758
85.216
77.352
77.098
76.844
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

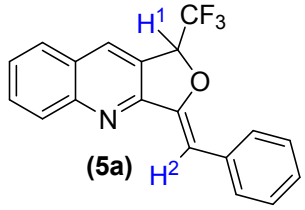
^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (500 MHz) spectra of annulated product



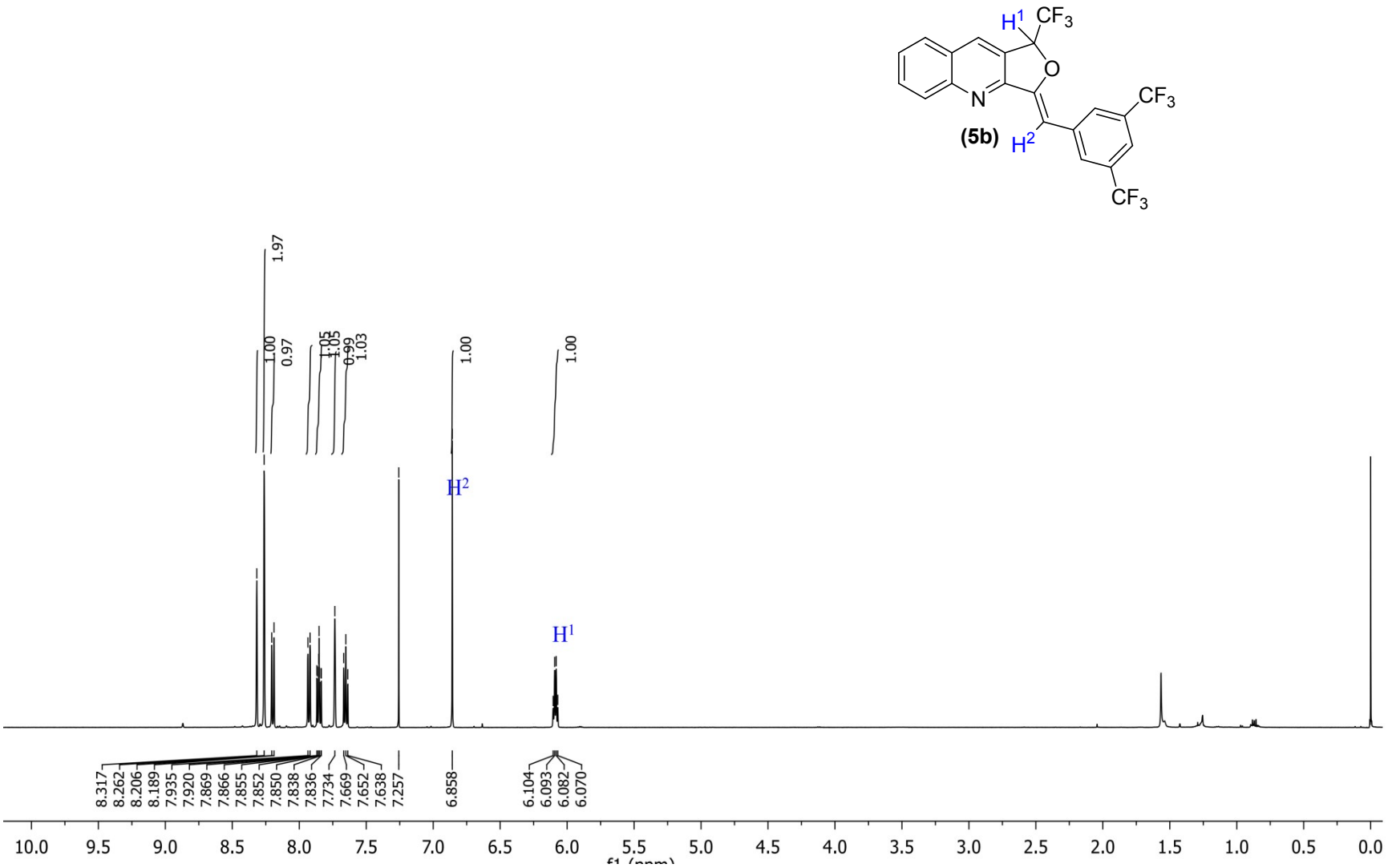
(5a)

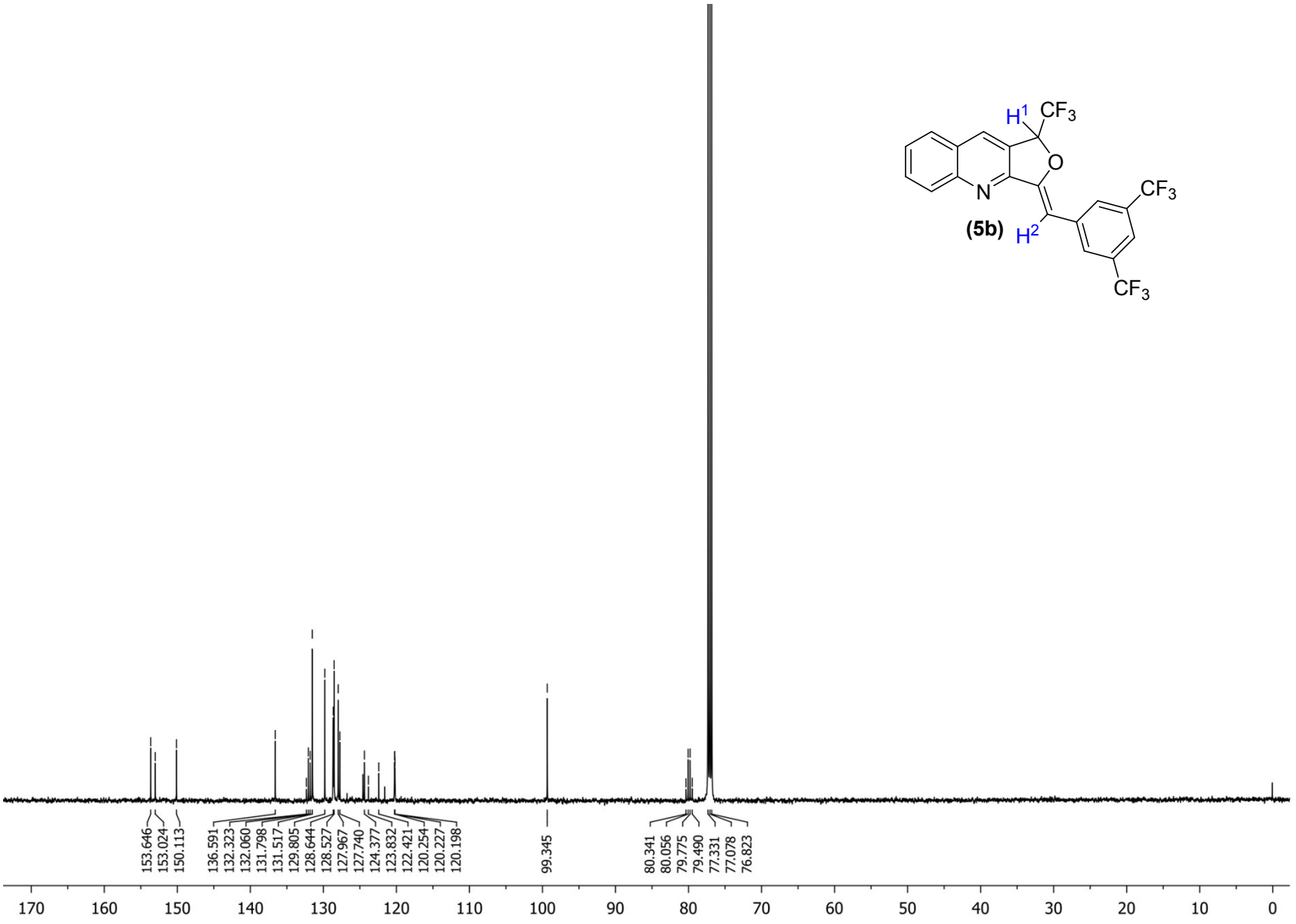


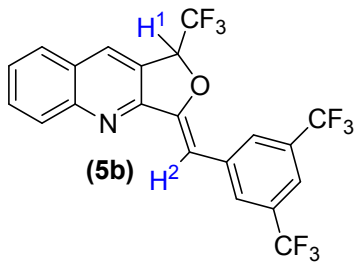

H1
CF3
O
N
(5a)
H2
154.162
151.031
150.046
134.498
131.294
131.201
129.578
129.436
128.670
128.478
127.464
127.345
124.453
124.079
121.843
102.519
79.735
79.454
79.173
78.894
77.356
77.102
76.848
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

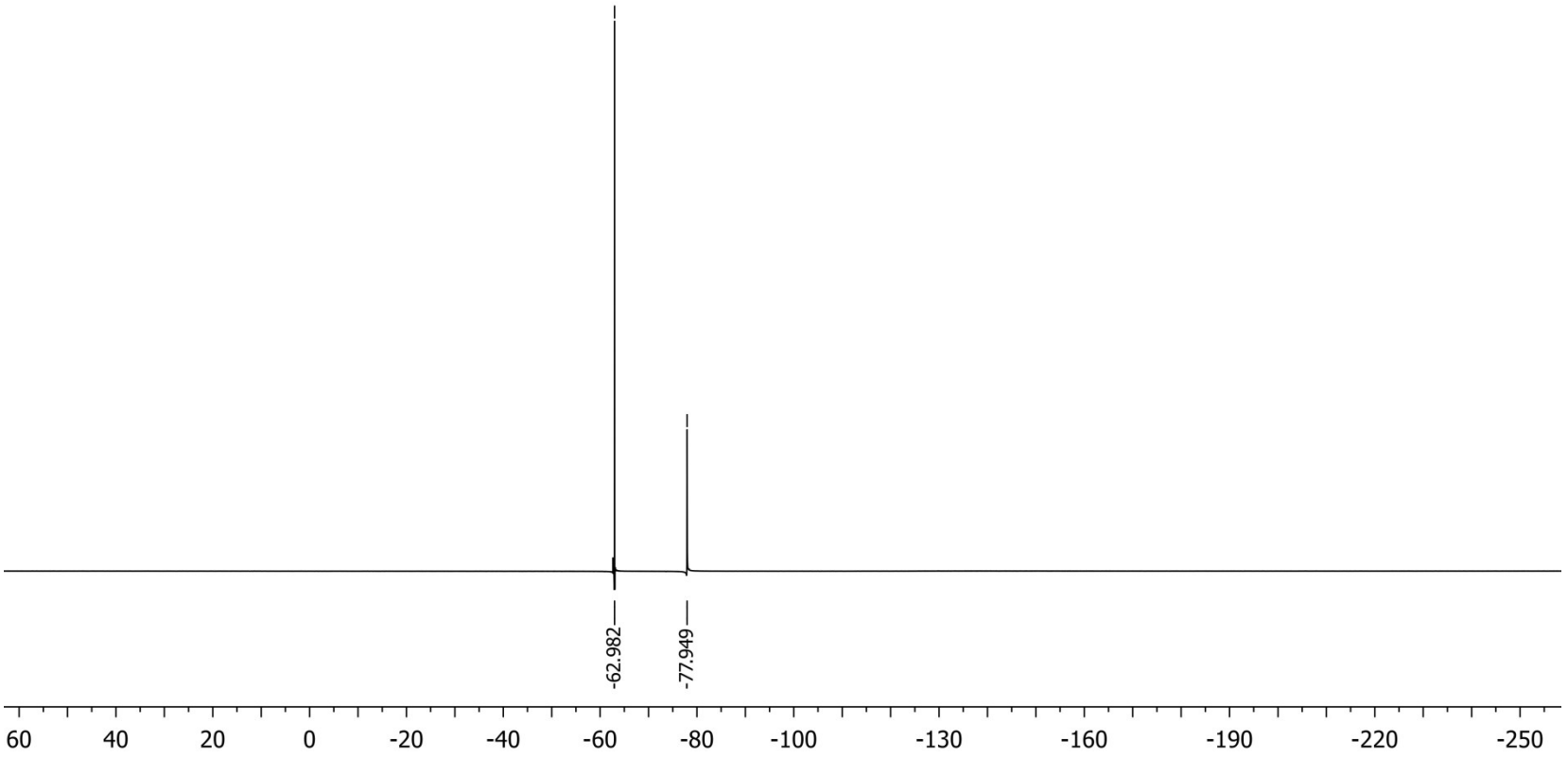

H1
CF3
O
N
(5a)
H2

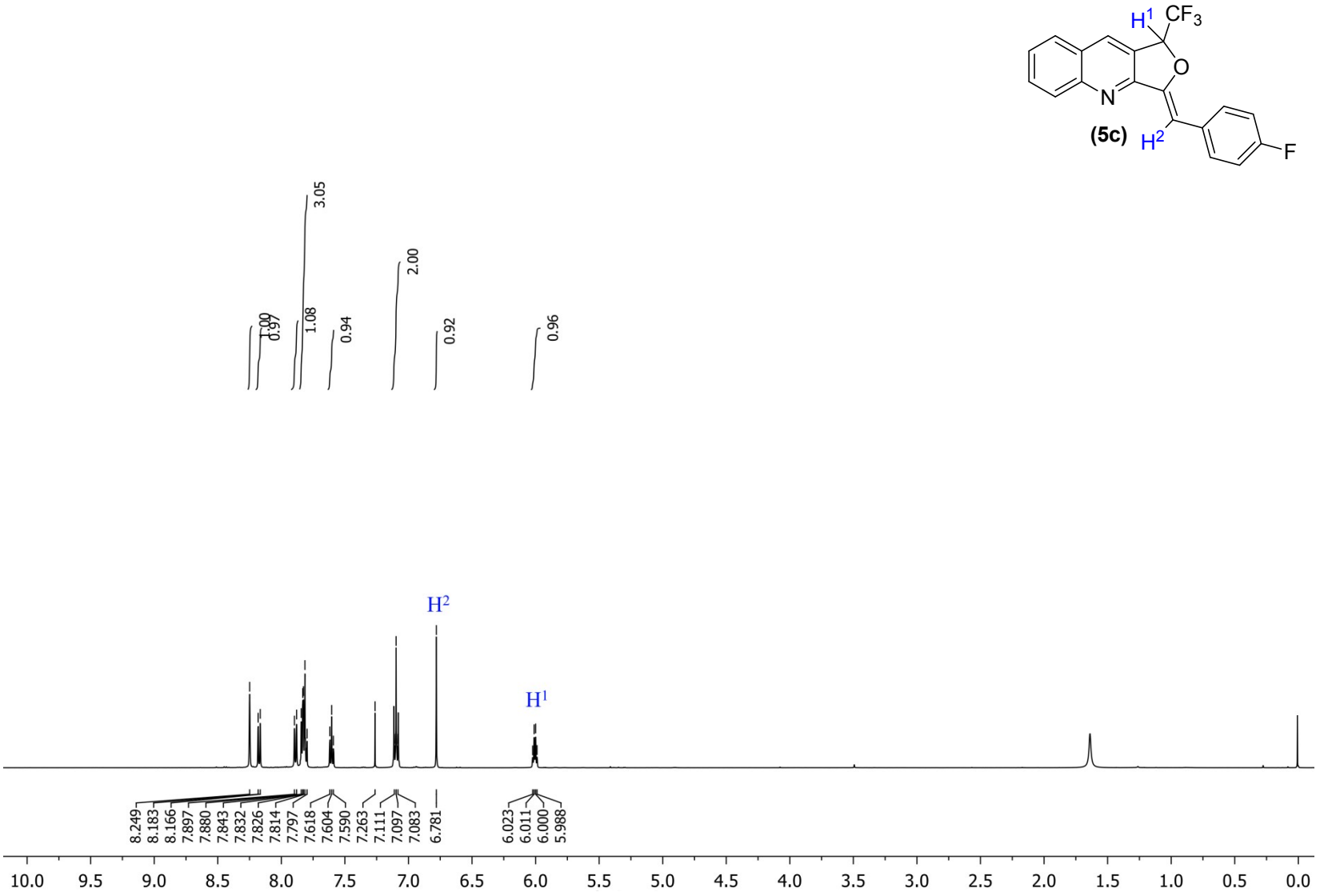
-77.928
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250

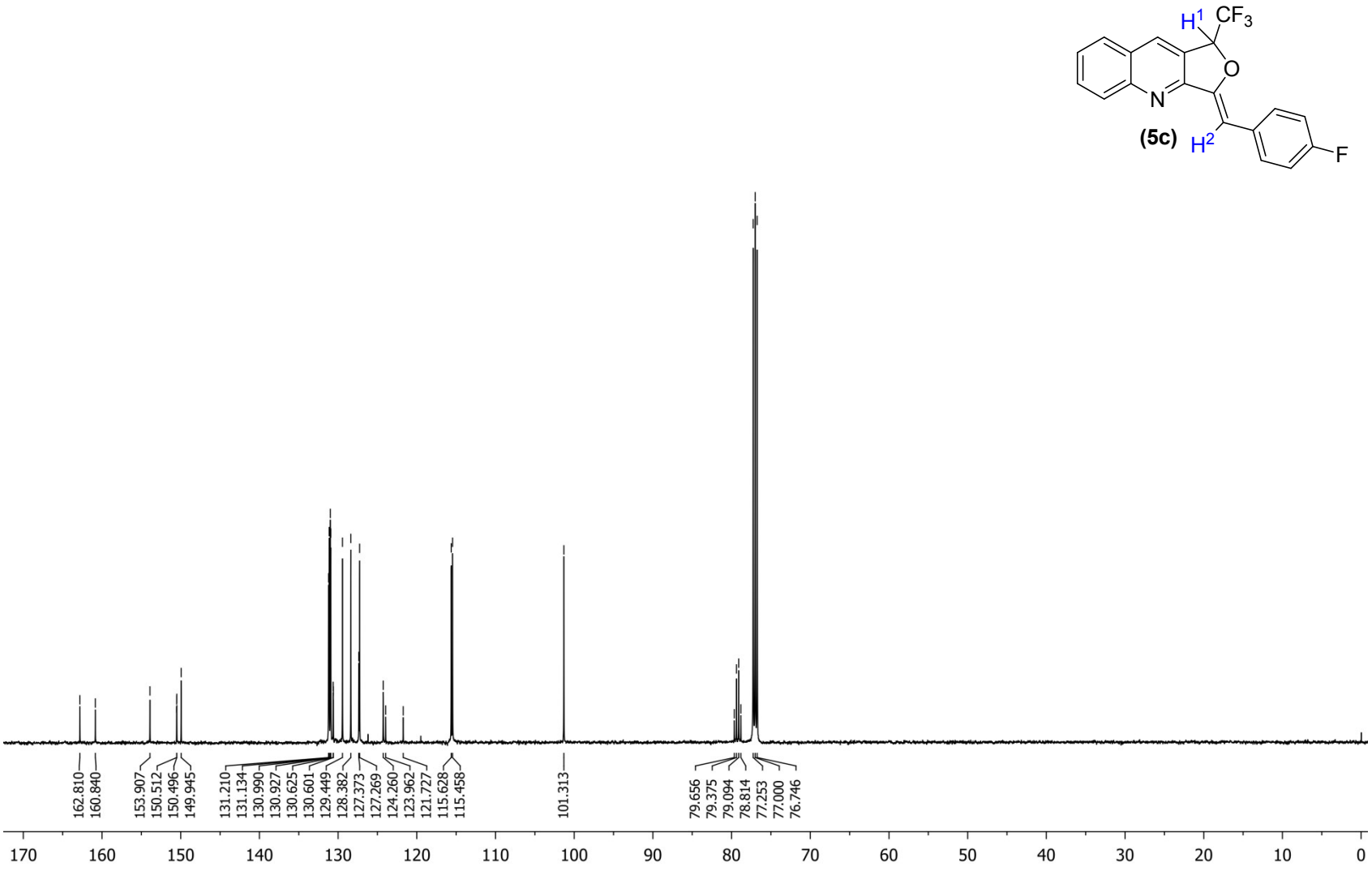

H1
CF3
O
N
CF3
(5b)
H2
CF3
1.97
1.00
0.97
1.05
1.05
0.99
1.03
1.00
1.00
H2
H1
8.317
8.262
8.206
8.189
7.935
7.920
7.869
7.866
7.855
7.852
7.850
7.838
7.836
7.734
7.669
7.652
7.638
7.257
6.858
6.104
6.093
6.082
6.070
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

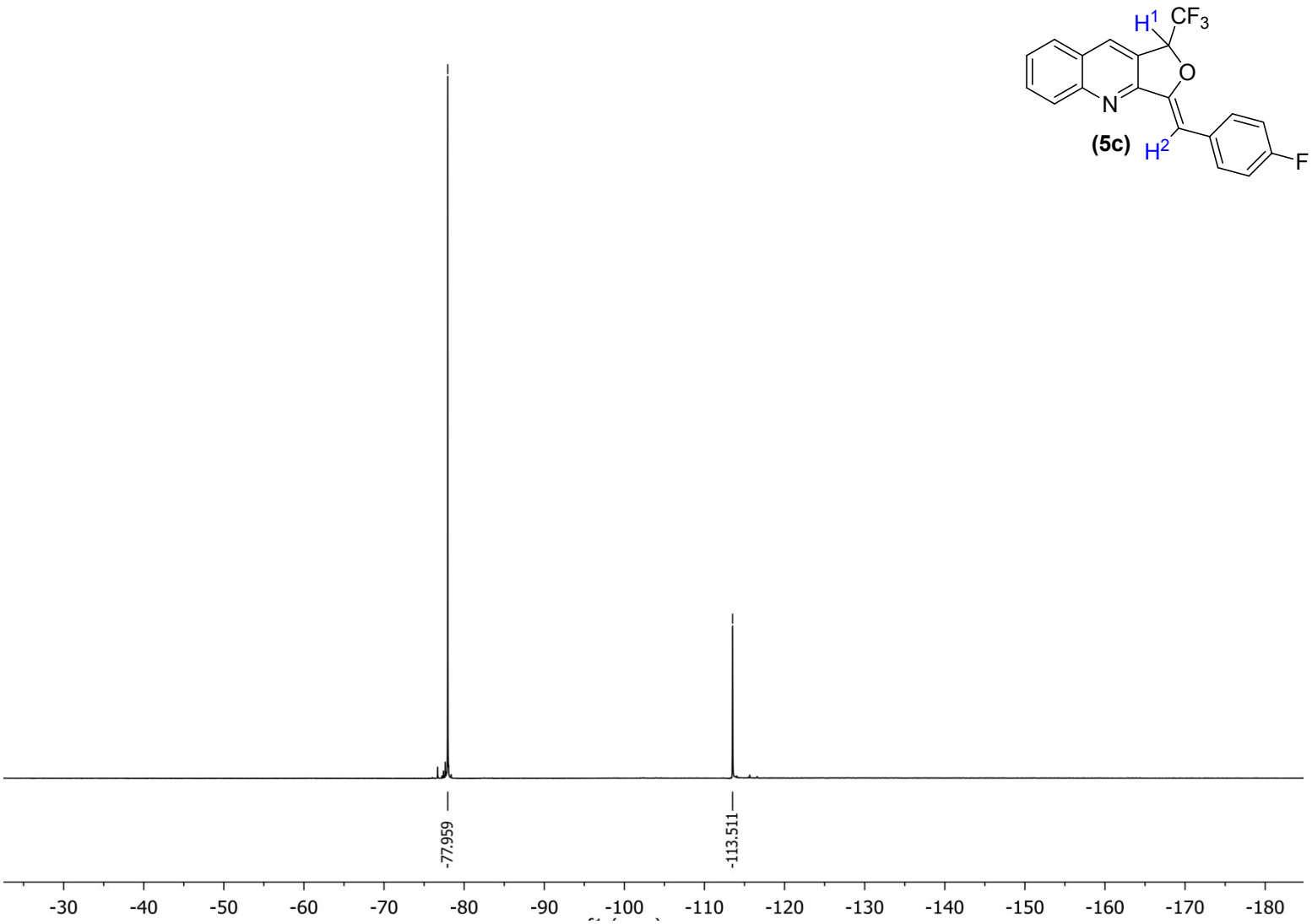

H1
CF3
O
N
CF3
(5b)
H2
CF3
153.646
153.024
150.113
136.591
132.323
132.060
131.798
131.517
129.805
128.644
128.527
127.967
127.740
124.377
123.832
122.421
120.254
120.227
120.198
99.345
80.341
80.056
79.775
79.490
77.331
77.078
76.823
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

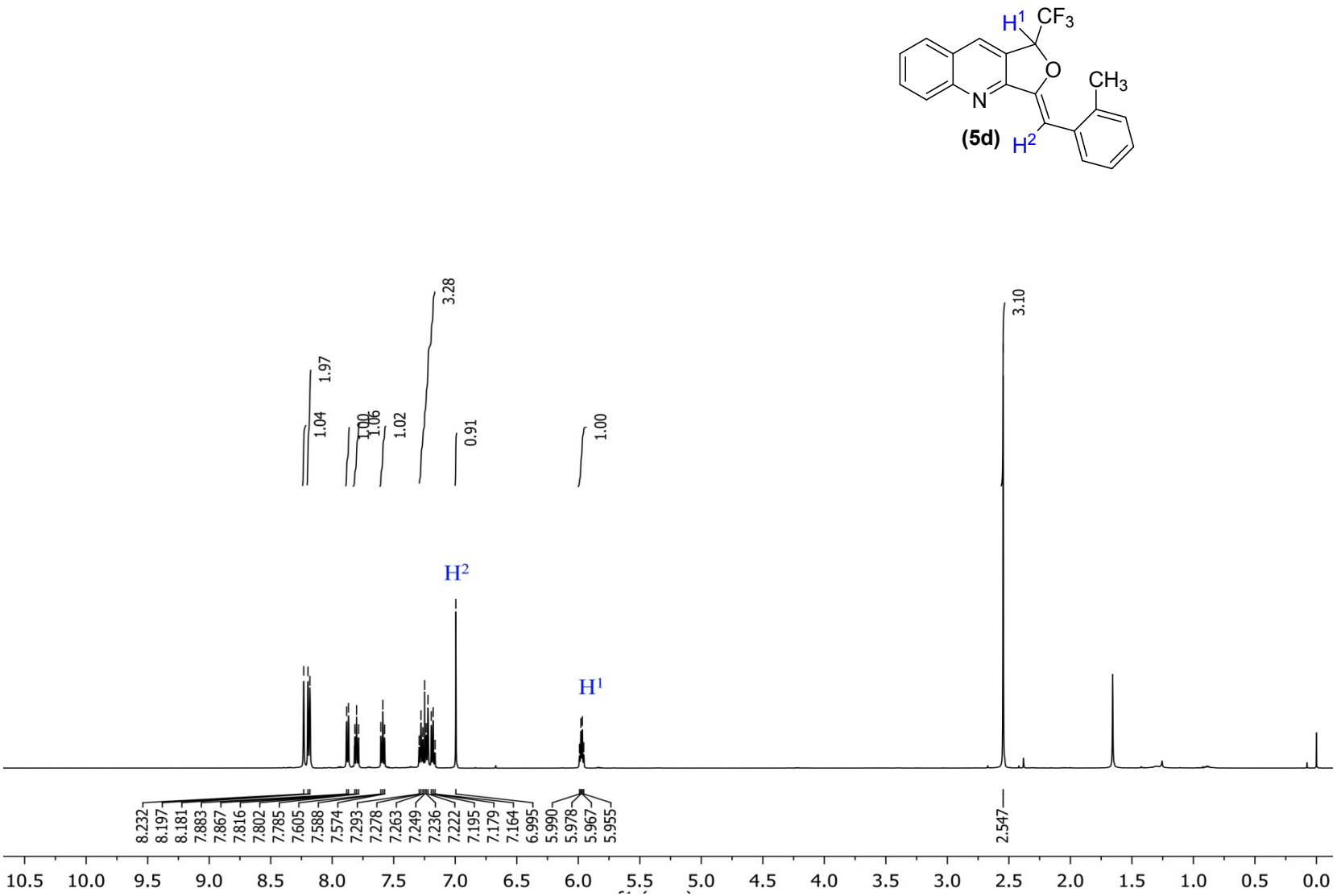

H1
CF3
O
N
CF3
(5b)
H2
CF3

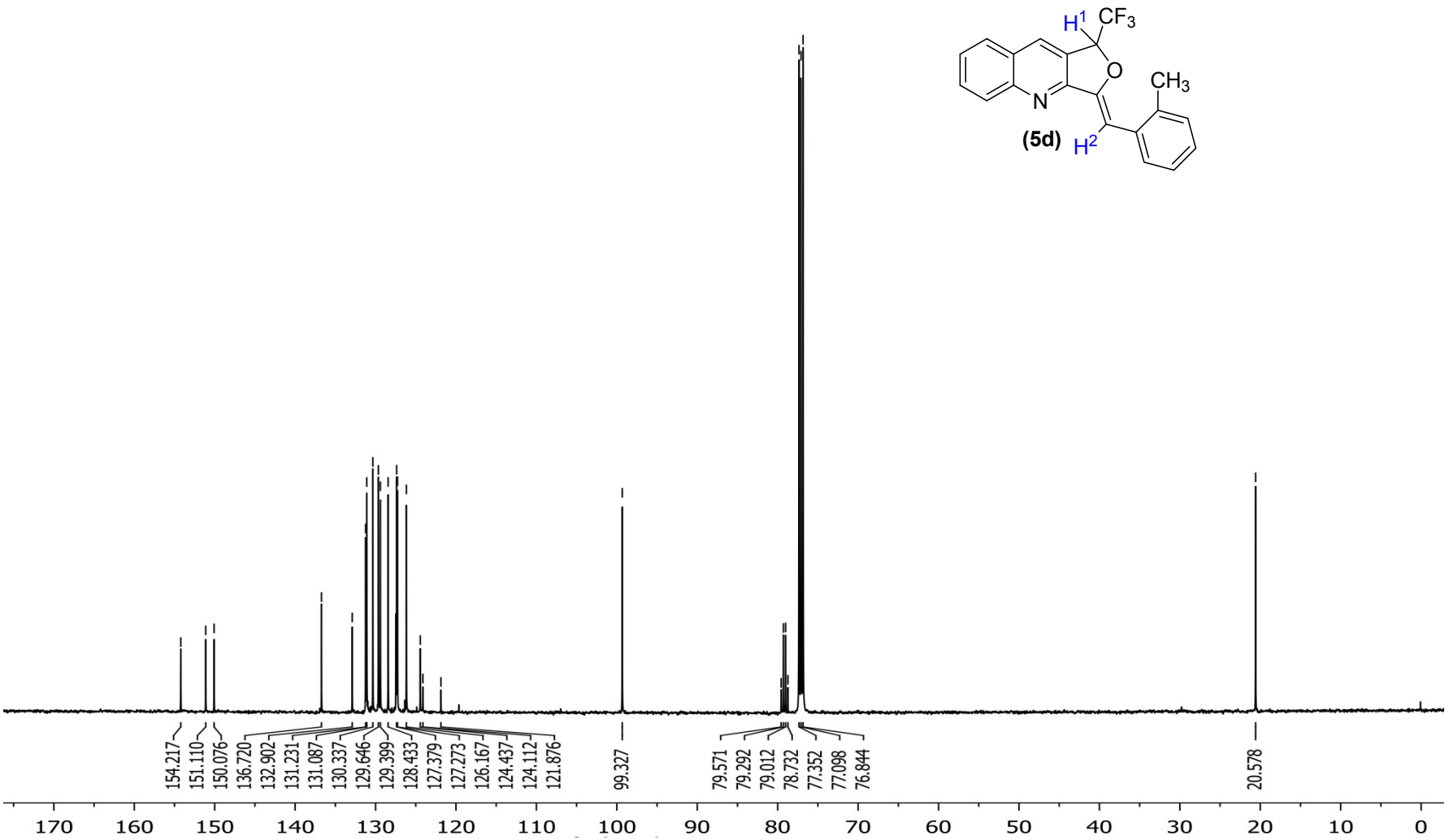

-62.982
-77.949
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250

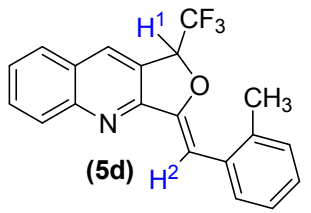

H1
CF3
O
N
(5c)
H2
F
3.05
2.00
1.08
1.00
0.97
0.94
0.92
0.96
H2
H1
8.249
8.183
8.166
7.897
7.880
7.843
7.832
7.826
7.814
7.797
7.618
7.604
7.590
7.263
7.111
7.097
7.083
6.781
6.023
6.011
6.000
5.988
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

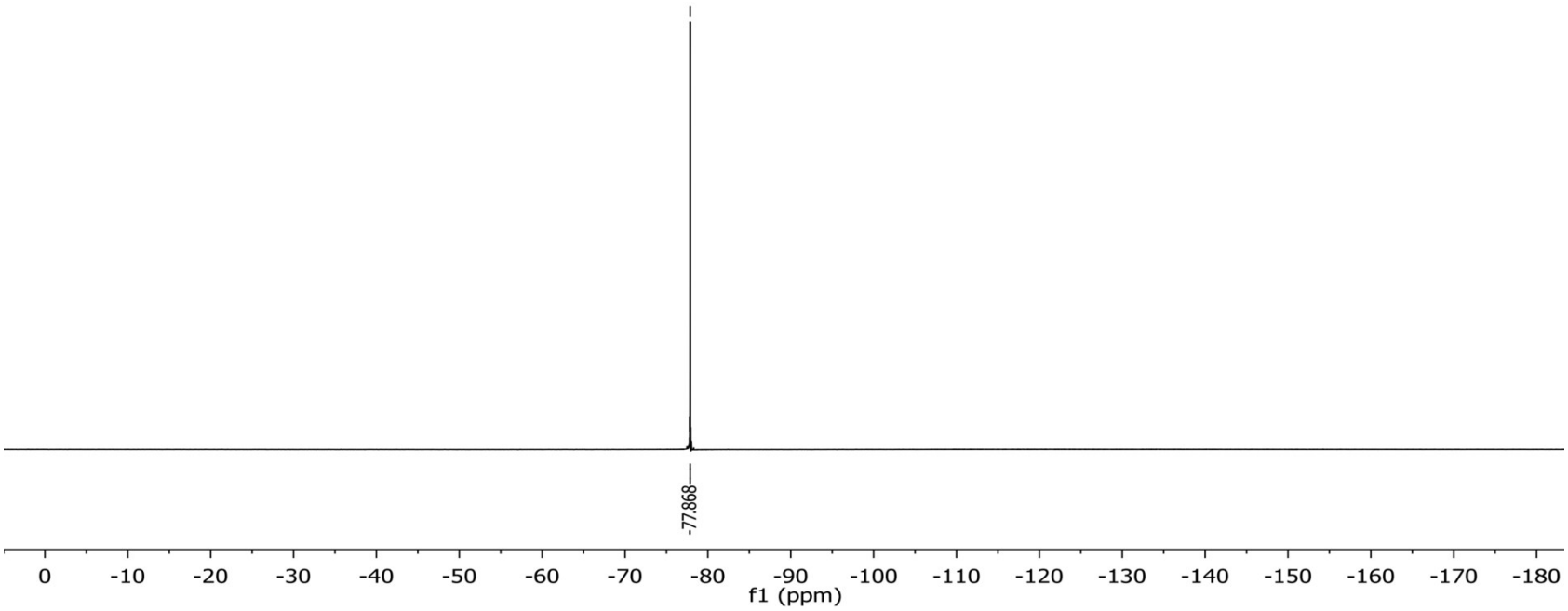

H1
CF3
O
N
(5c)
H2
F
162.810
160.840
153.907
150.512
150.496
149.945
131.210
131.134
130.990
130.927
130.625
130.601
129.449
128.382
127.373
127.269
124.260
123.962
121.727
115.628
115.458
101.313
79.656
79.375
79.094
78.814
77.253
77.000
76.746
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

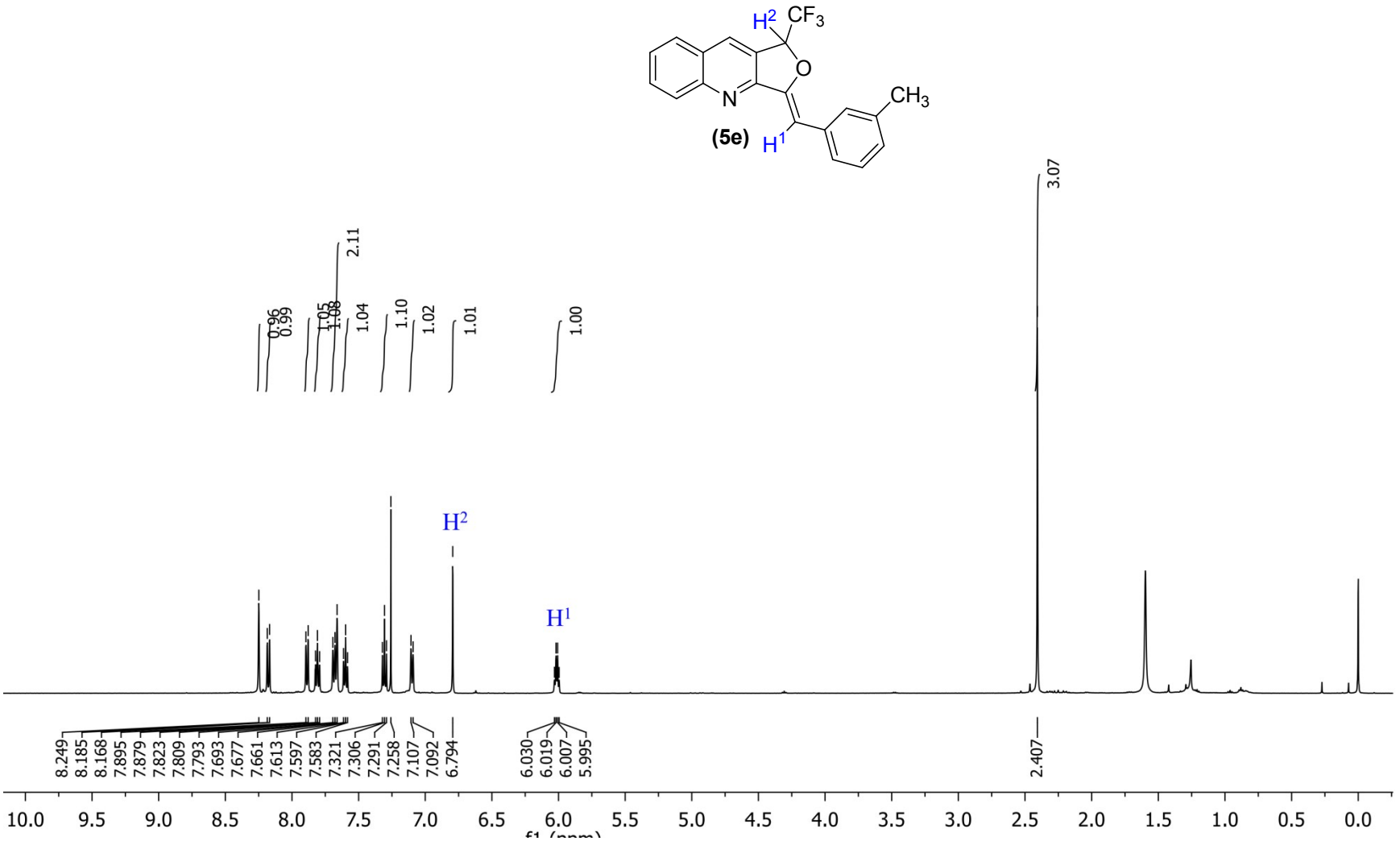

H1
CF3
O
N
(5c)
H2
F
-77.959
-113.511
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180

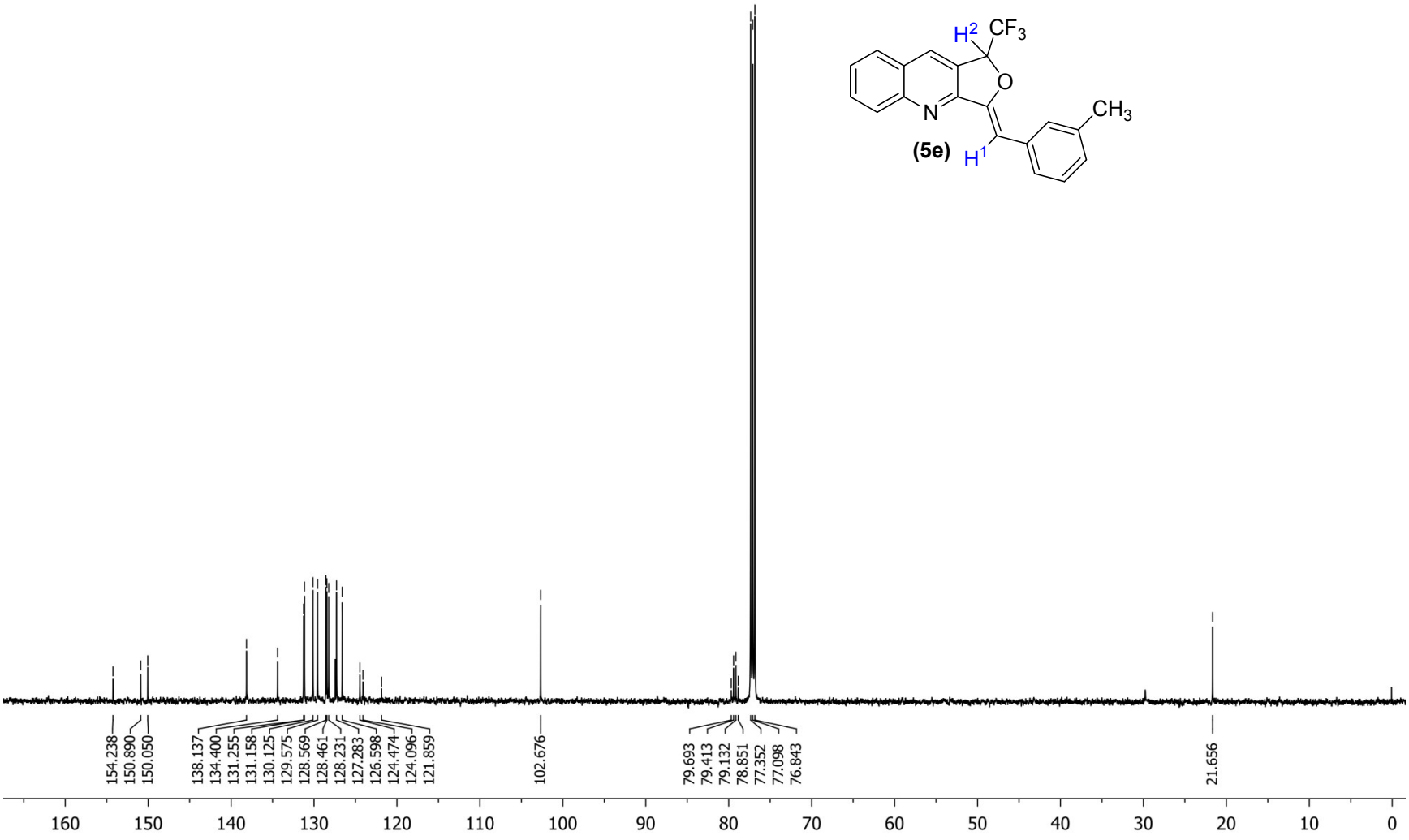

H1
CF3
O
N
CH3
(5d)
H2
3.28
1.97
1.04
1.00
1.06
1.02
0.91
1.00
3.10
H2
H1
8.232
8.197
8.181
7.883
7.867
7.816
7.802
7.785
7.605
7.588
7.574
7.293
7.278
7.263
7.249
7.236
7.222
7.195
7.179
7.164
6.995
5.990
5.978
5.967
5.955
2.547
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

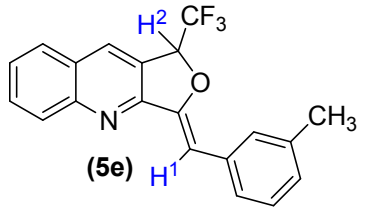

H1
CF3
O
CH3
N
(5d)
H2
154.217
151.110
150.076
136.720
132.902
131.231
131.087
130.337
129.646
129.399
128.433
127.379
127.273
126.167
124.437
124.112
121.876
99.327
79.571
79.292
79.012
78.732
77.352
77.098
76.844
20.578
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


H1
CF3
O
CH3
N
(5d)
H2

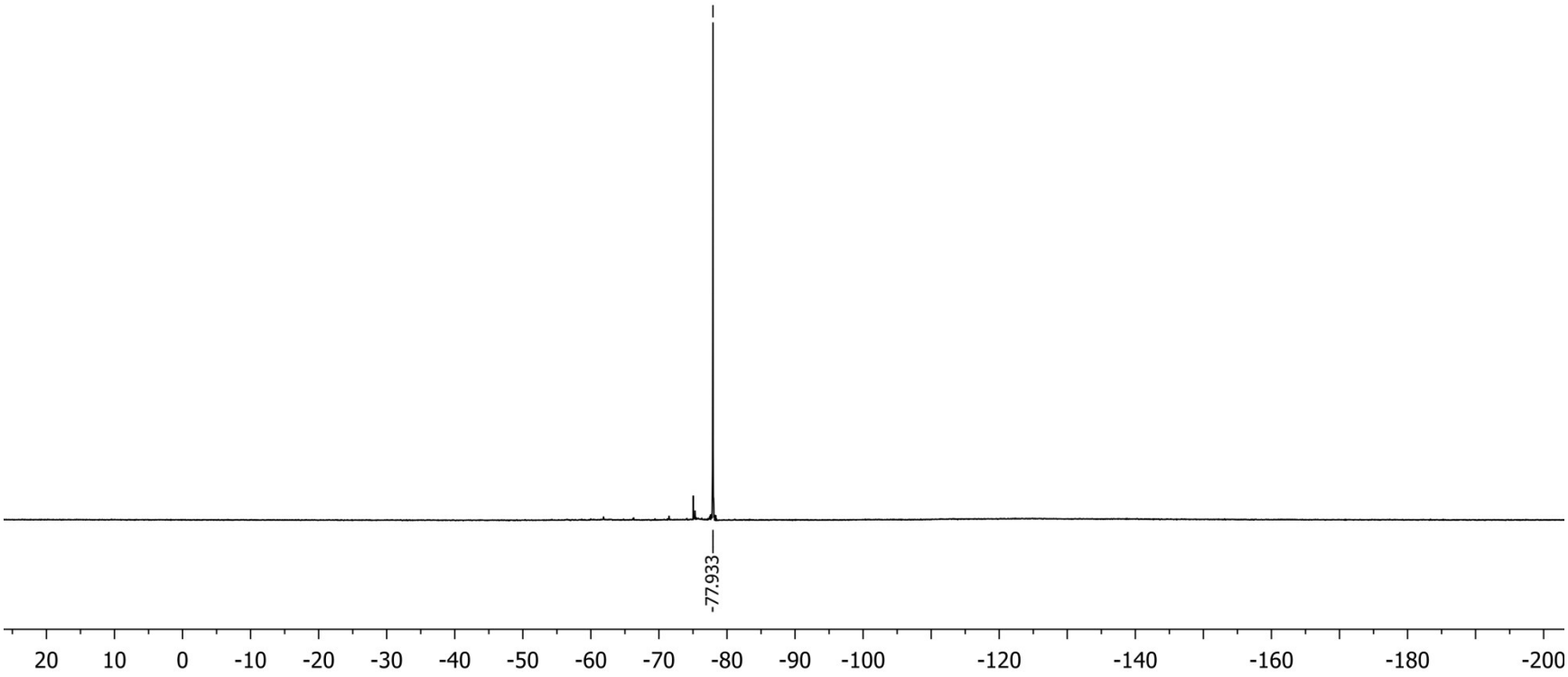

-77.868
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)

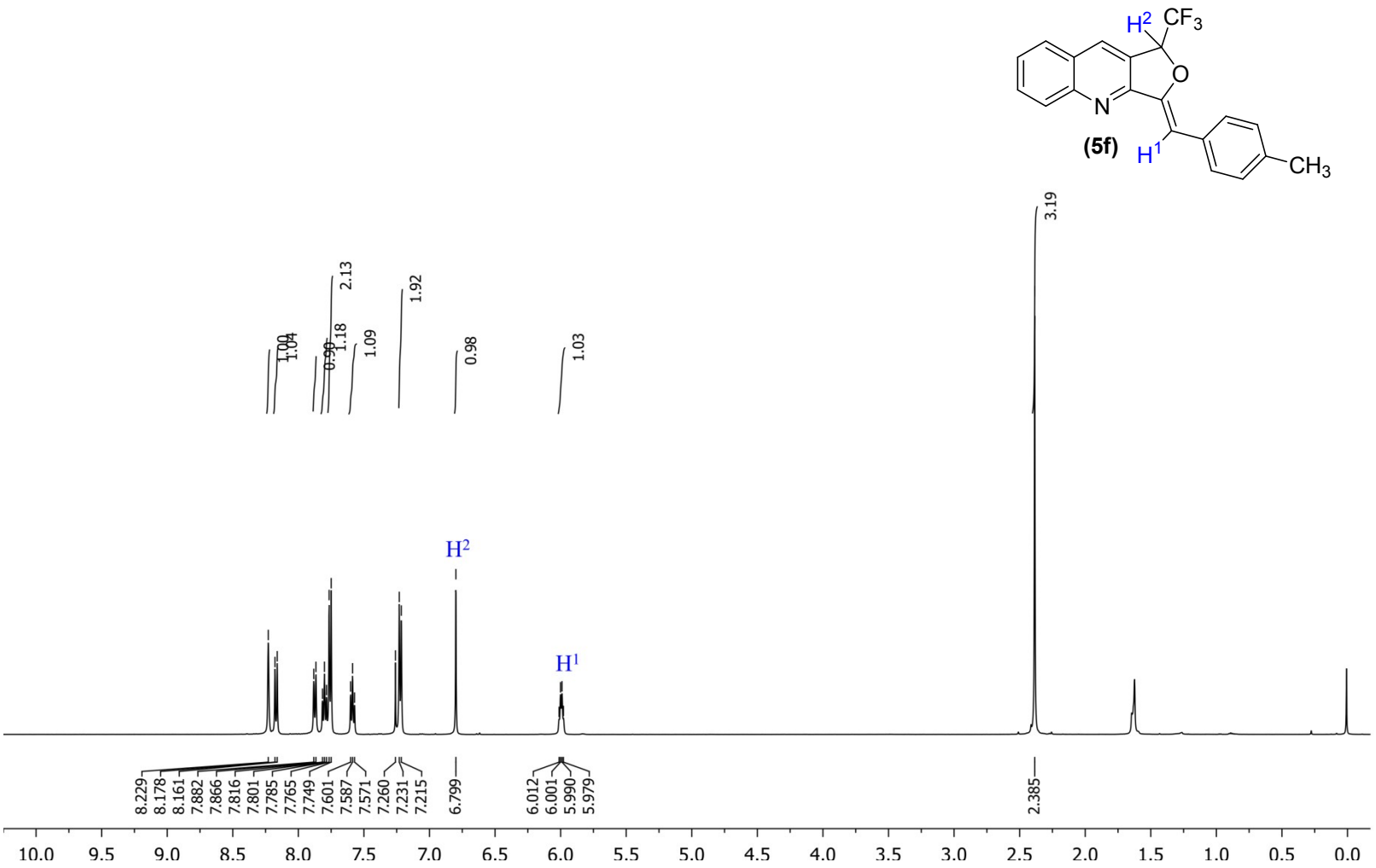

H2
CF3
O
N
CH3
(5e)
H1
3.07
2.11
0.96
0.99
1.05
1.08
1.04
1.10
1.02
1.01
1.00
H2
H1
8.249
8.185
8.168
7.895
7.879
7.823
7.809
7.793
7.693
7.677
7.661
7.613
7.597
7.583
7.321
7.306
7.291
7.258
7.107
7.092
6.794
6.030
6.019
6.007
5.995
2.407
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

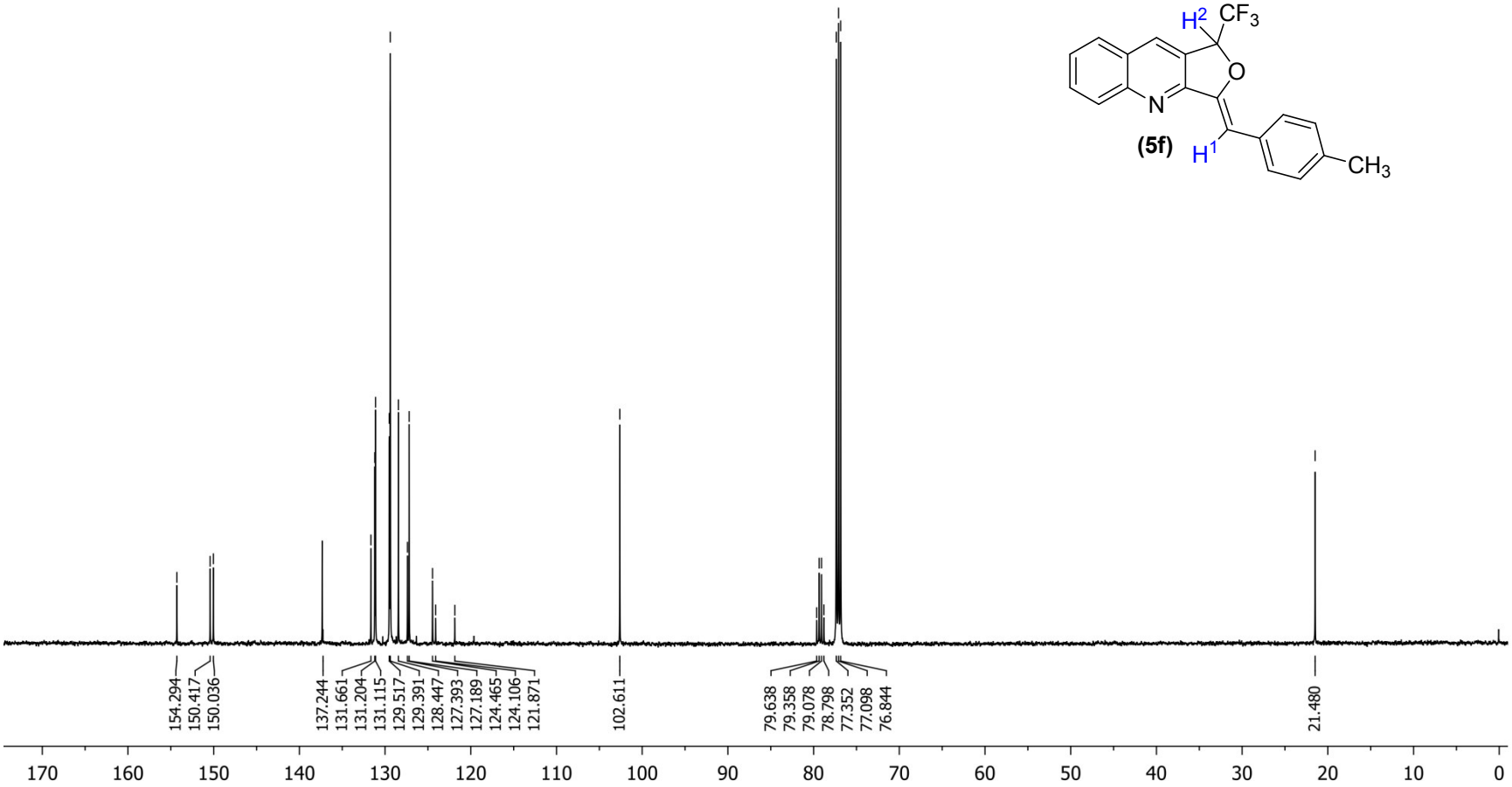

H2
CF3
O
N
CH3
(5e)
H1
154.238
150.890
150.050
138.137
134.400
131.255
131.158
130.125
129.575
128.569
128.461
128.231
127.283
126.598
124.474
124.096
121.859
102.676
79.693
79.413
79.132
78.851
77.352
77.098
76.843
21.656
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

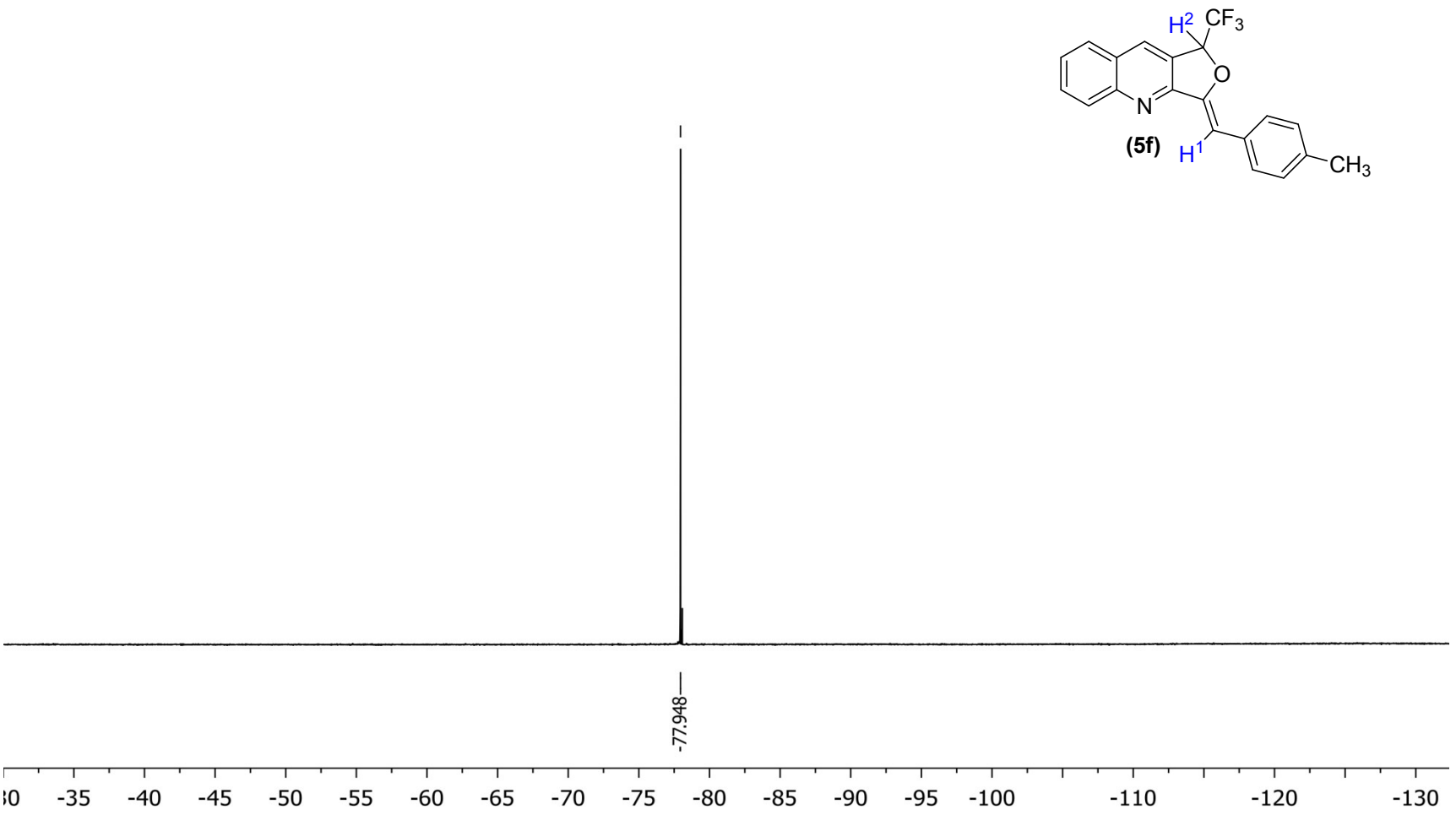

H2
CF3
O
N
CH3
H1

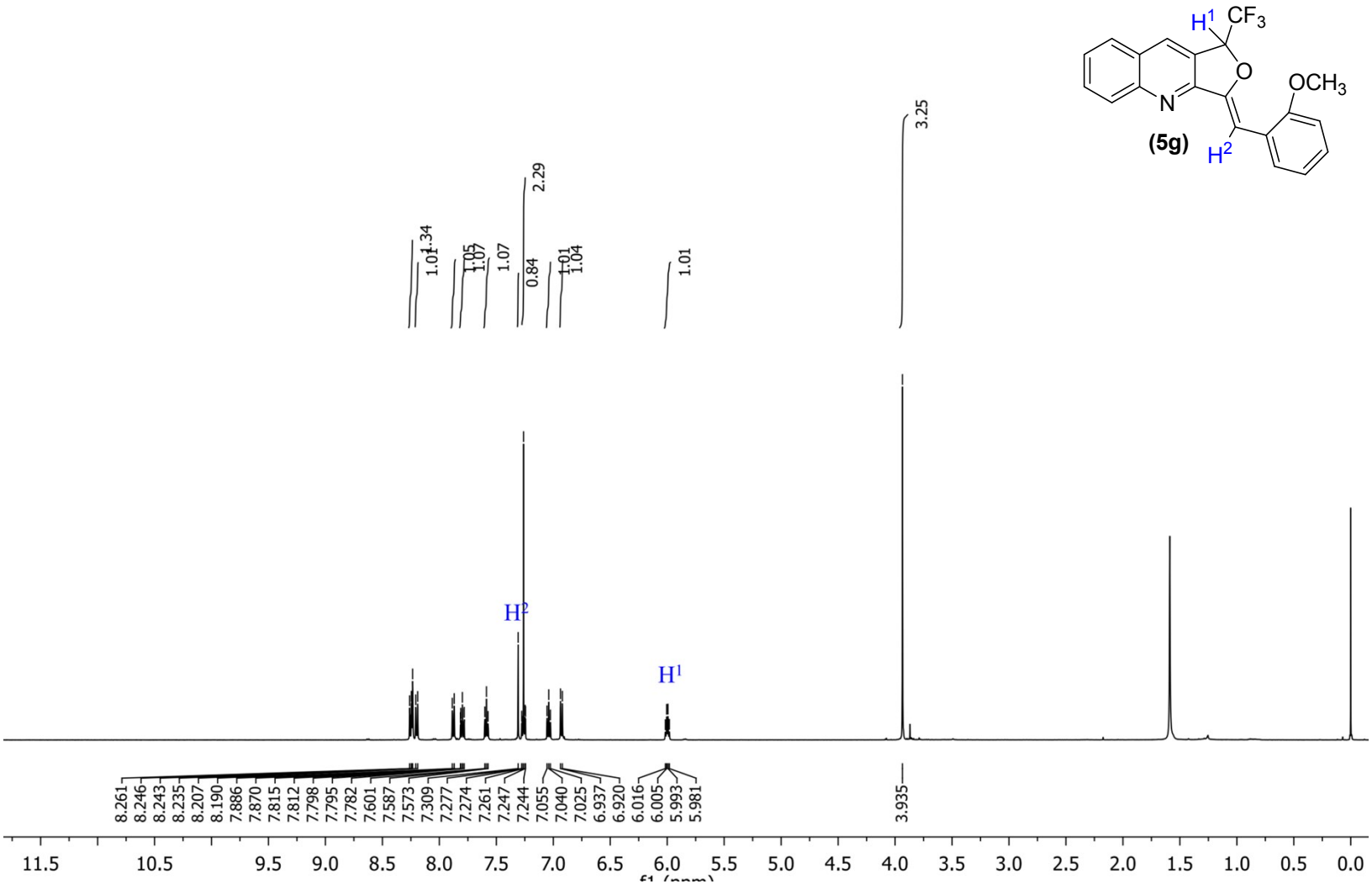
(5e)

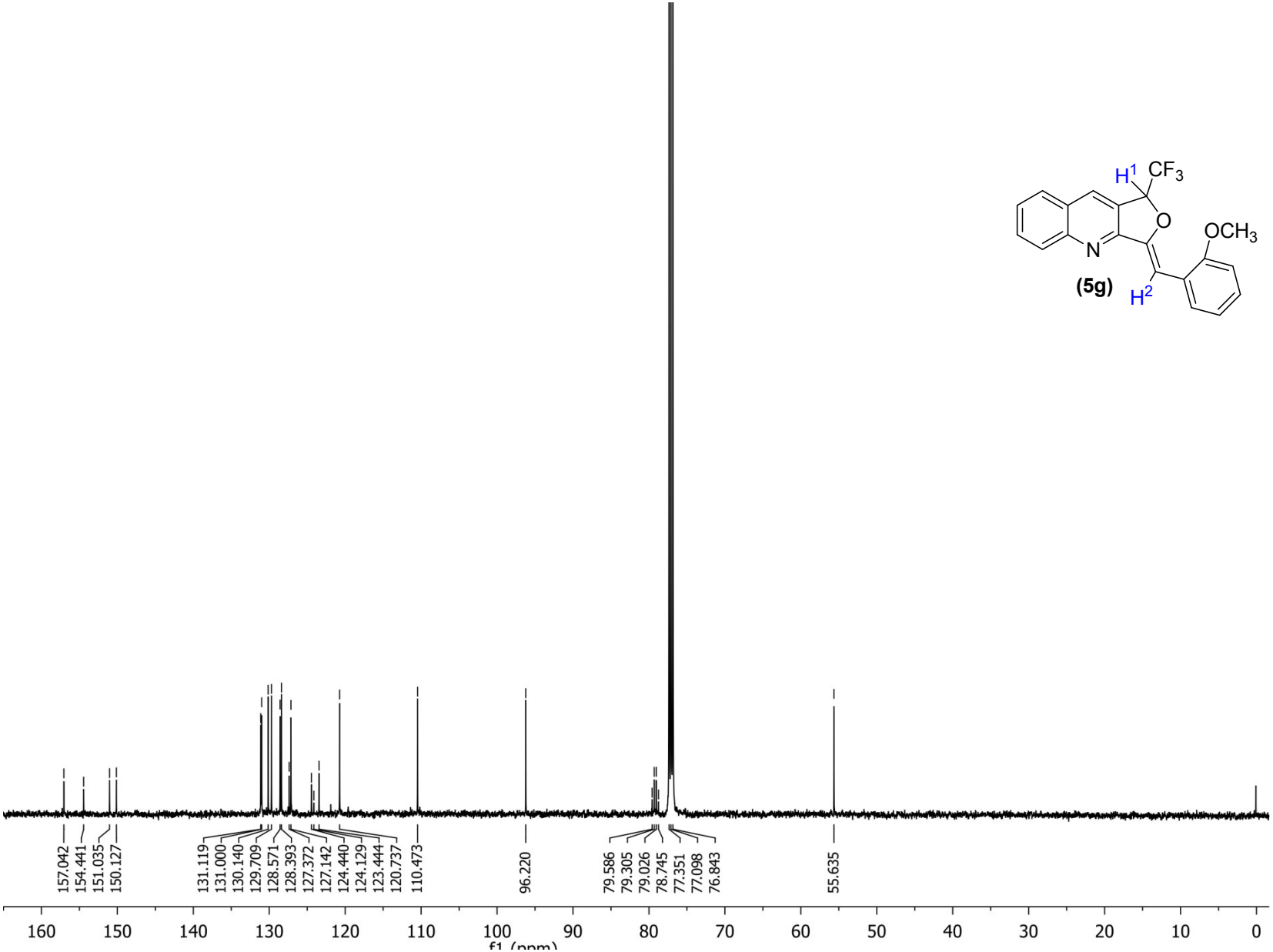

-77.933
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200

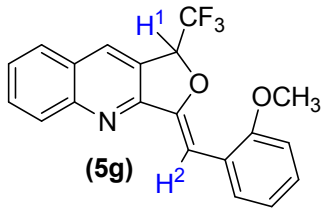

H2
CF3
O
N
(5f)
H1
CH3
3.19
2.13
1.92
1.18
1.09
1.04
1.00
0.98
1.03
H2
H1
8.229
8.178
8.161
7.882
7.866
7.816
7.801
7.785
7.765
7.749
7.601
7.587
7.571
7.260
7.231
7.215
6.799
6.012
6.001
5.990
5.979
2.385
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


H2
CF3
O
N
(5f)
H1
CH3
154.294
150.417
150.036
137.244
131.661
131.204
131.115
129.517
129.391
128.447
127.393
127.189
124.465
124.106
121.871
102.611
79.638
79.358
79.078
78.798
77.352
77.098
76.844
21.480
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

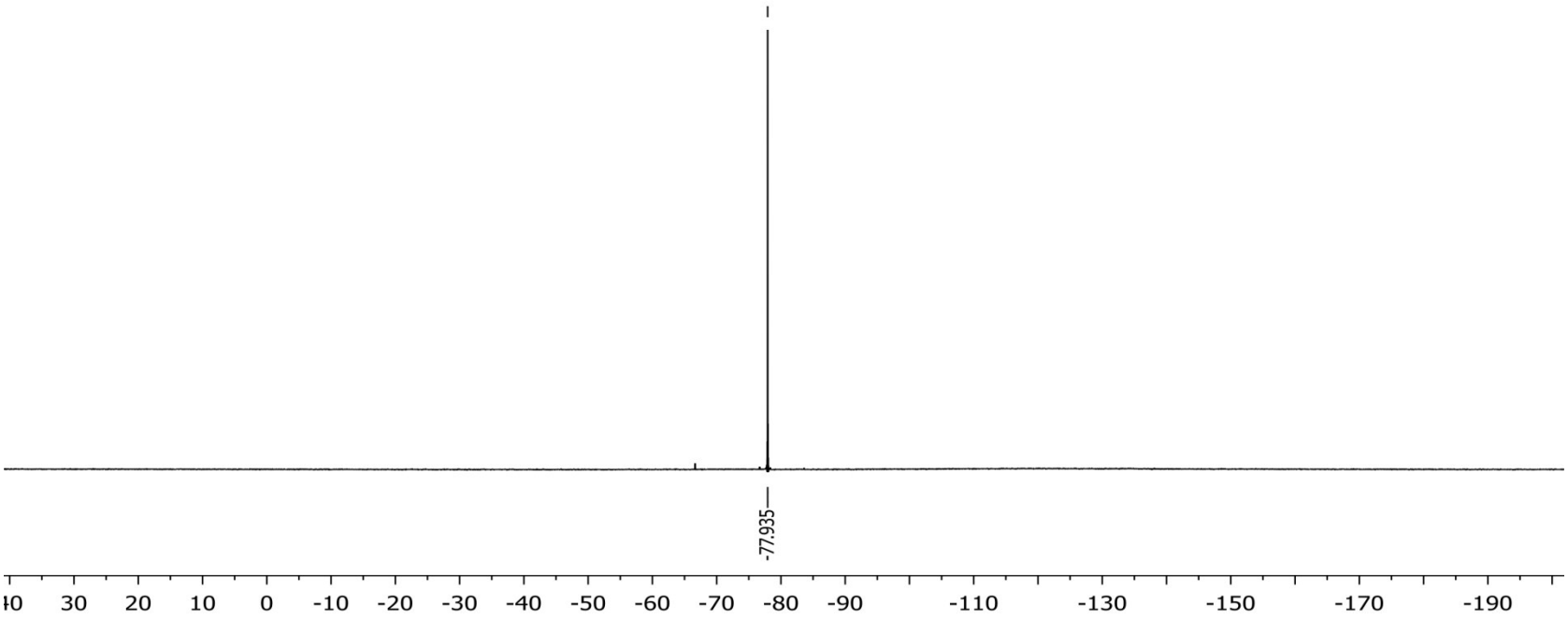

H2
CF3
O
N
(5f)
H1
CH3
-77.948
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-110
-120
-130

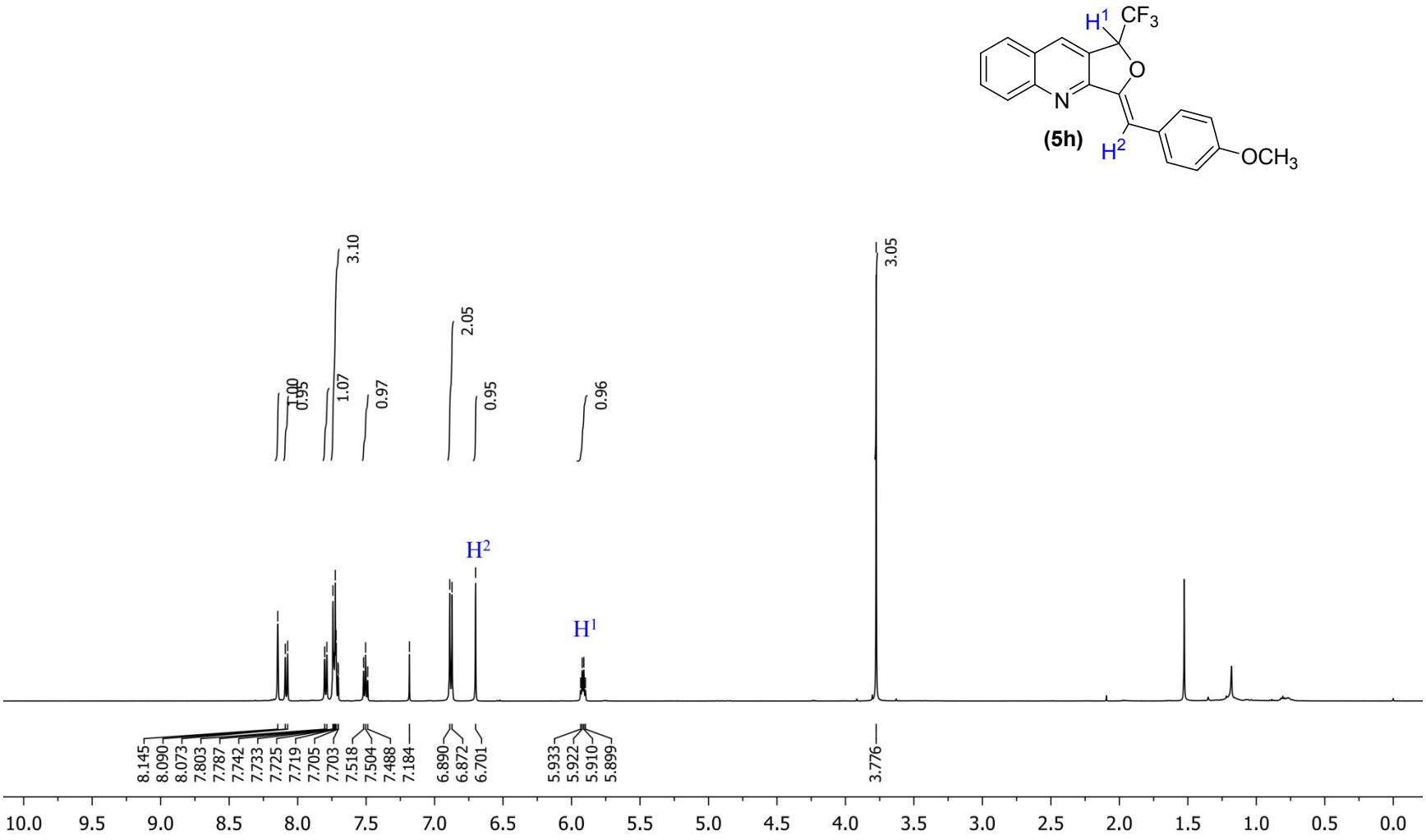

H1
CF3
O
N
OCH3
(5g)
H2
3.25
2.29
1.34
1.01
1.05
1.07
1.07
0.84
1.01
1.04
1.01
H2
H1
8.261
8.246
8.243
8.235
8.207
8.190
7.886
7.870
7.815
7.812
7.798
7.795
7.782
7.601
7.587
7.573
7.309
7.277
7.274
7.261
7.247
7.244
7.055
7.040
7.025
6.937
6.920
6.016
6.005
5.993
5.981
3.935
11.5
10.5
9.5
9.0
8.5
8.0
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

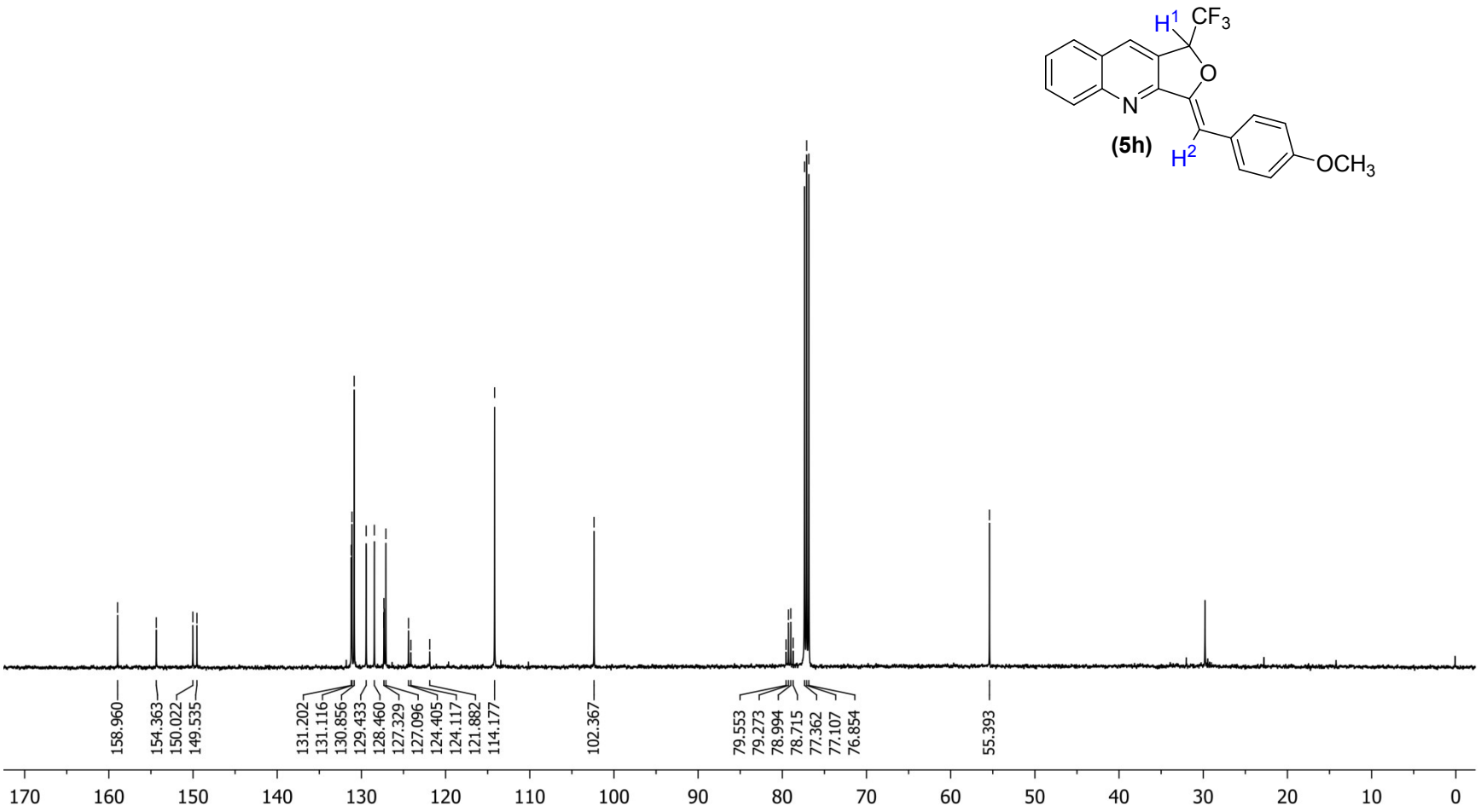

H1
CF3
O
OCH3
N
H2
(5g)
157.042
154.441
151.035
150.127
131.119
131.000
130.140
129.709
128.571
128.393
127.372
127.142
124.440
124.129
123.444
120.737
110.473
96.220
79.586
79.305
79.026
78.745
77.351
77.098
76.843
55.635
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

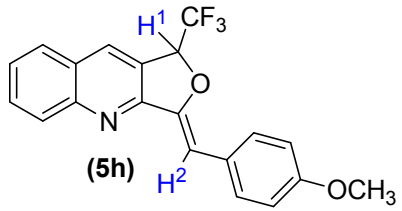

H1
CF3
O
OCH3
N
H2

(5g)

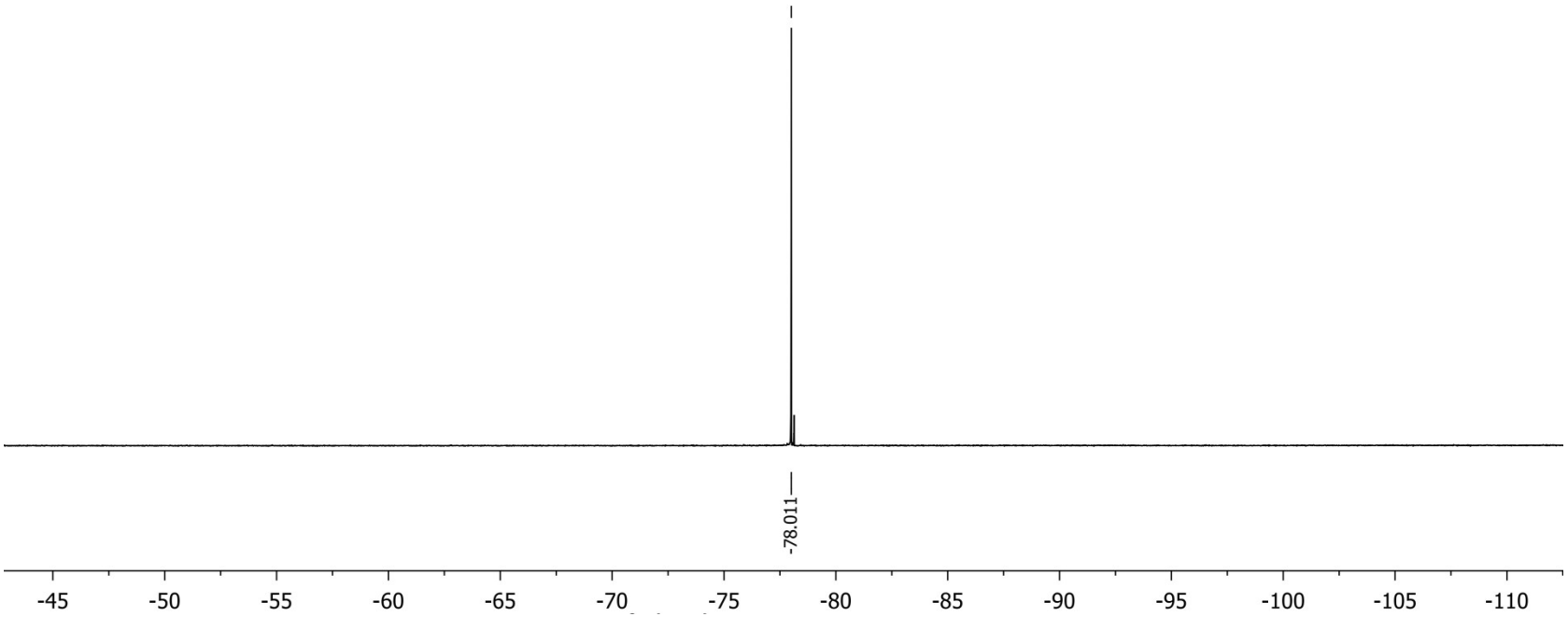

-77.935
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190

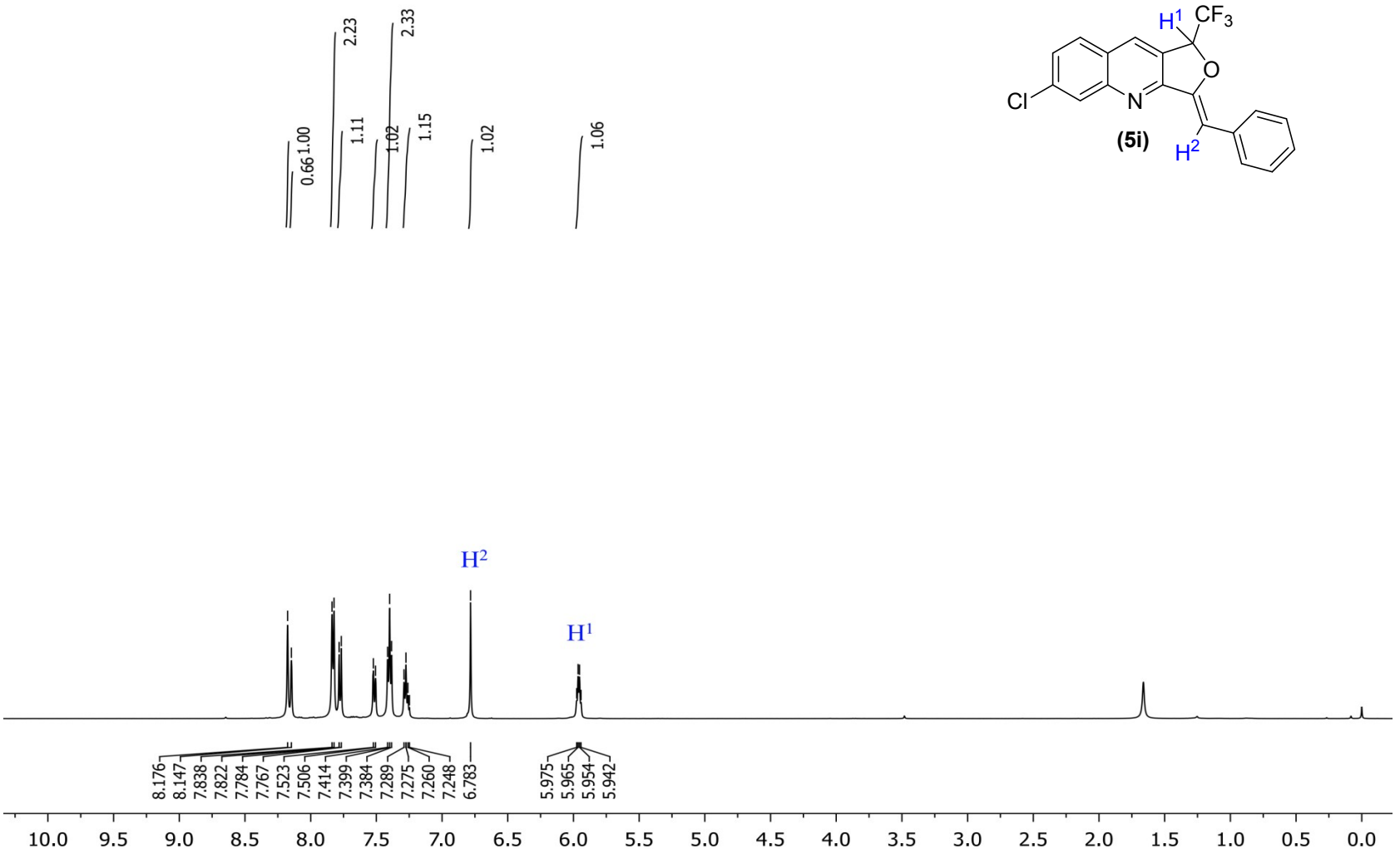

H1
CF3
O
N
(5h)
H2
OCH3
3.10
2.05
3.05
1.00
0.95
1.07
0.97
0.95
0.96
H2
H1
8.145
8.090
8.073
7.803
7.787
7.742
7.733
7.725
7.719
7.705
7.703
7.518
7.504
7.488
7.184
6.890
6.872
6.701
5.933
5.922
5.910
5.899
3.776
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

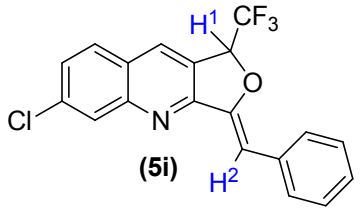

H1
CF3
O
N
(5h)
H2
OCH3
158.960
154.363
150.022
149.535
131.202
131.116
130.856
129.433
128.460
127.329
127.096
124.405
124.117
121.882
114.177
102.367
79.553
79.273
78.994
78.715
77.362
77.107
76.854
55.393
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



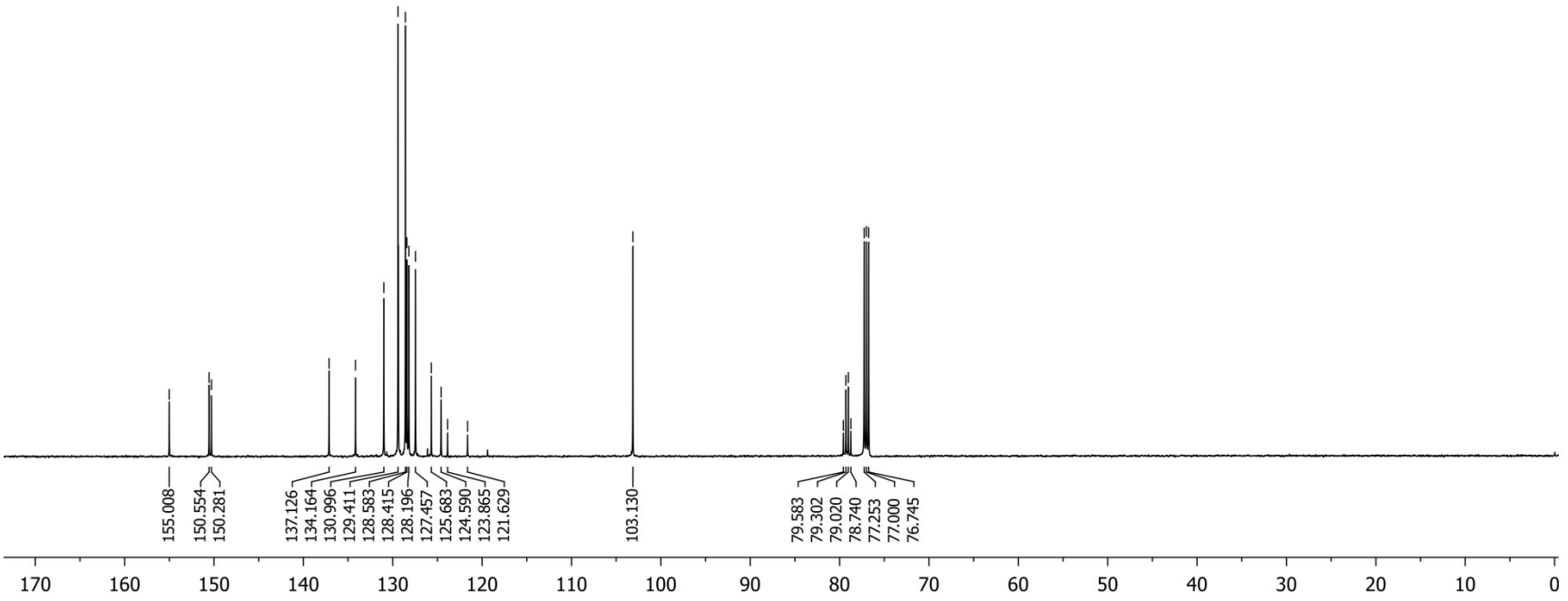
(5h)

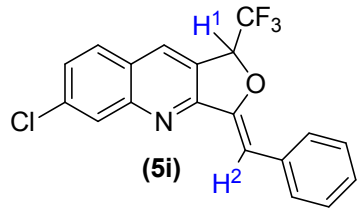



0.66
1.00
2.23
1.11
2.33
1.02
1.15
1.02
1.06
H1
CF3
O
Cl
N
(5i)
H2
H2
H1
8.176
8.147
7.838
7.822
7.784
7.767
7.523
7.506
7.414
7.399
7.384
7.289
7.275
7.260
7.248
6.783
5.975
5.965
5.954
5.942
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

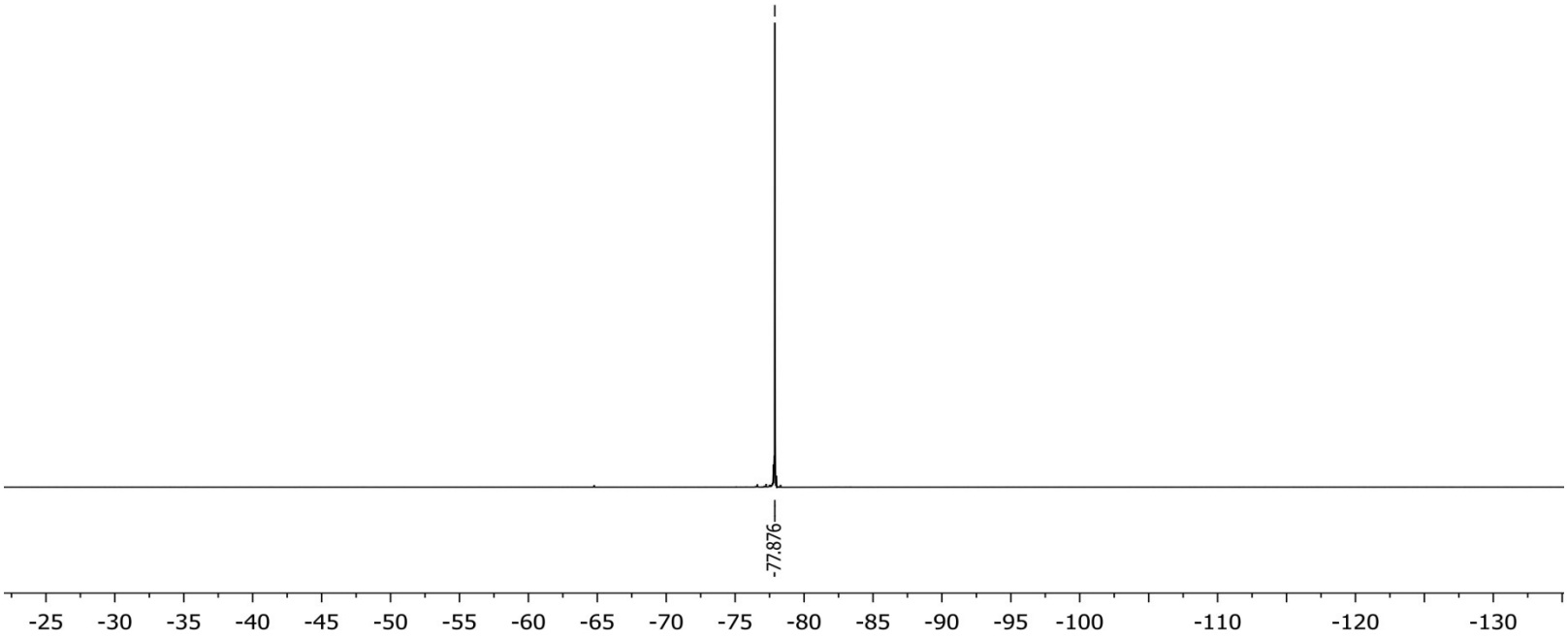

H1
CF3
O
Cl
N
H2

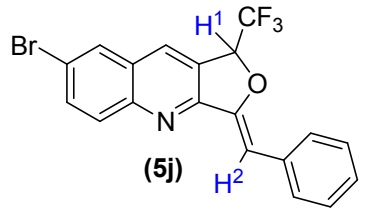
(5i)


155.008
150.554
150.281
137.126
134.164
130.996
129.411
128.583
128.415
128.196
127.457
125.683
124.590
123.865
121.629
103.130
79.583
79.302
79.020
78.740
77.253
77.000
76.745
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

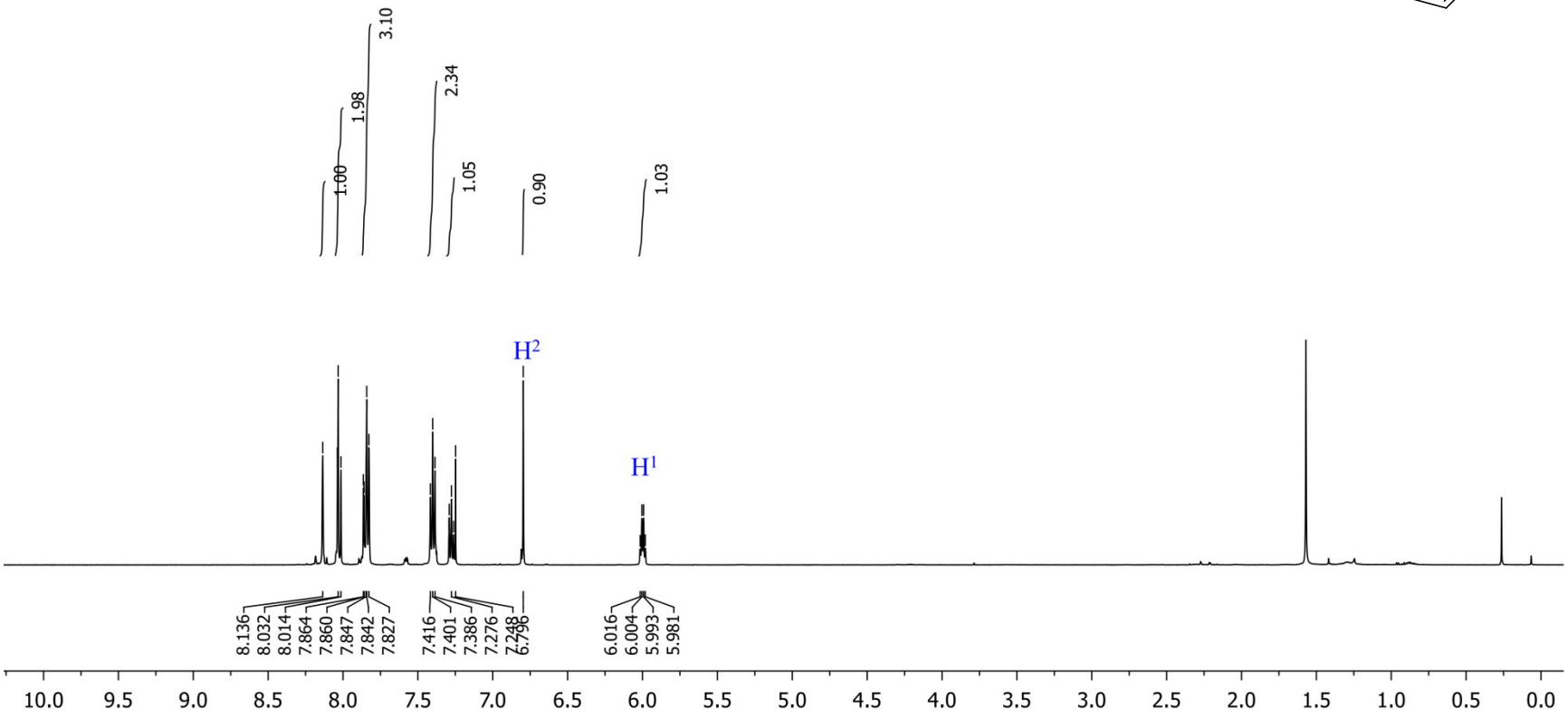

H1
CF3
O
Cl
N
H2

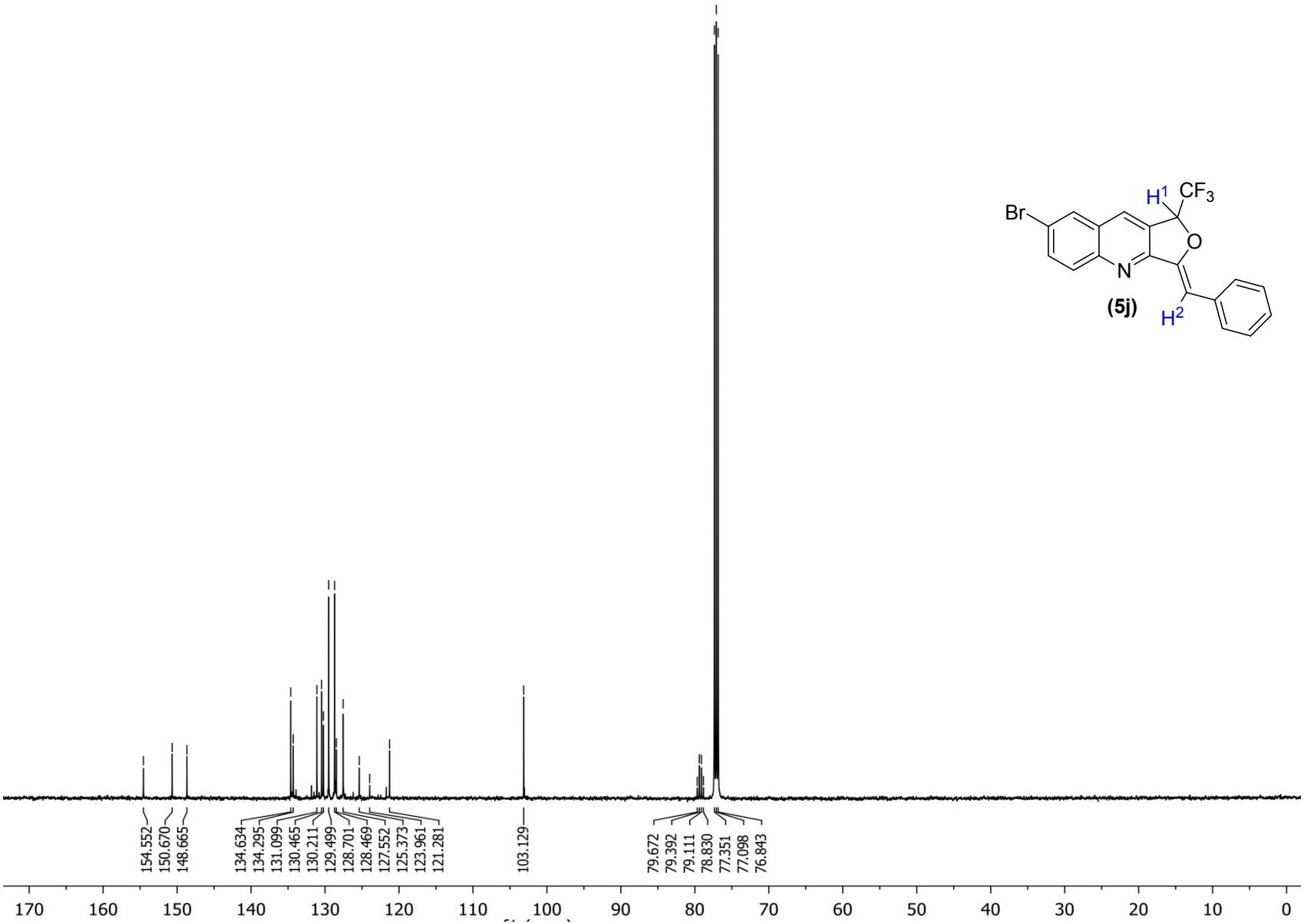
(5i)

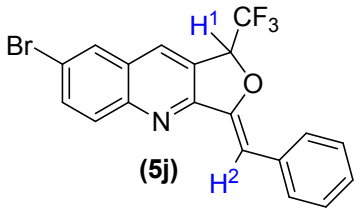

-77.876
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-110
-120
-130


H1
CF3
Br
O
N
H2

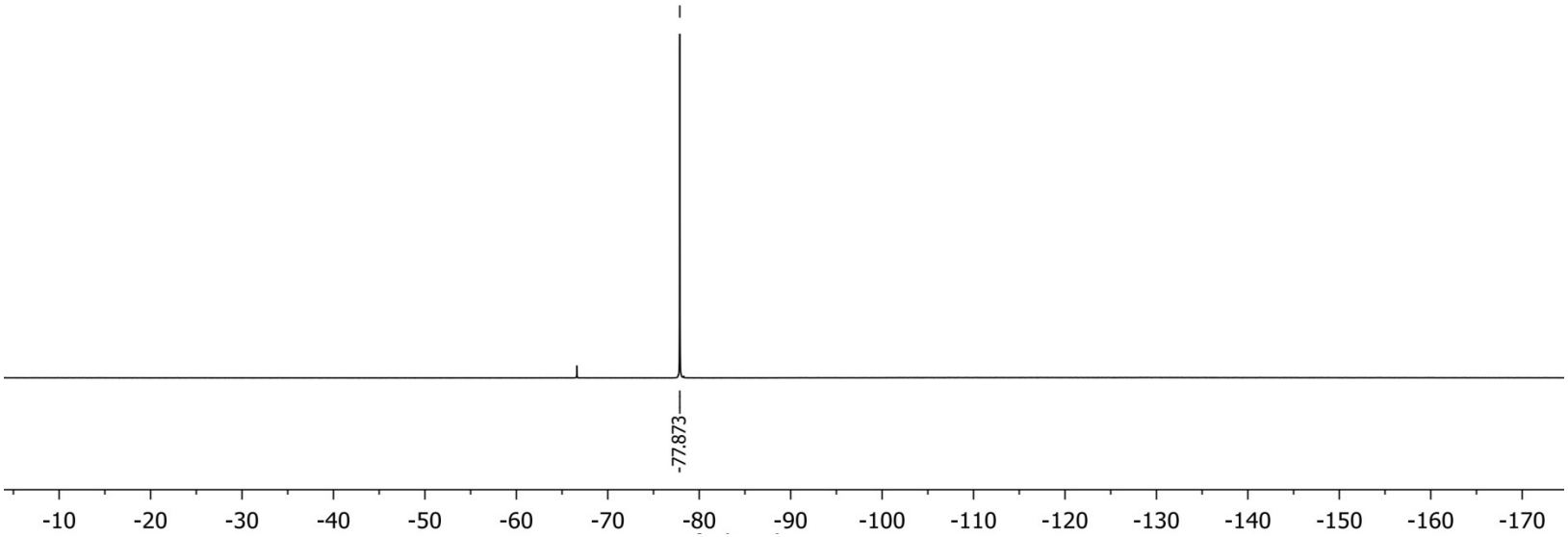
(5j)

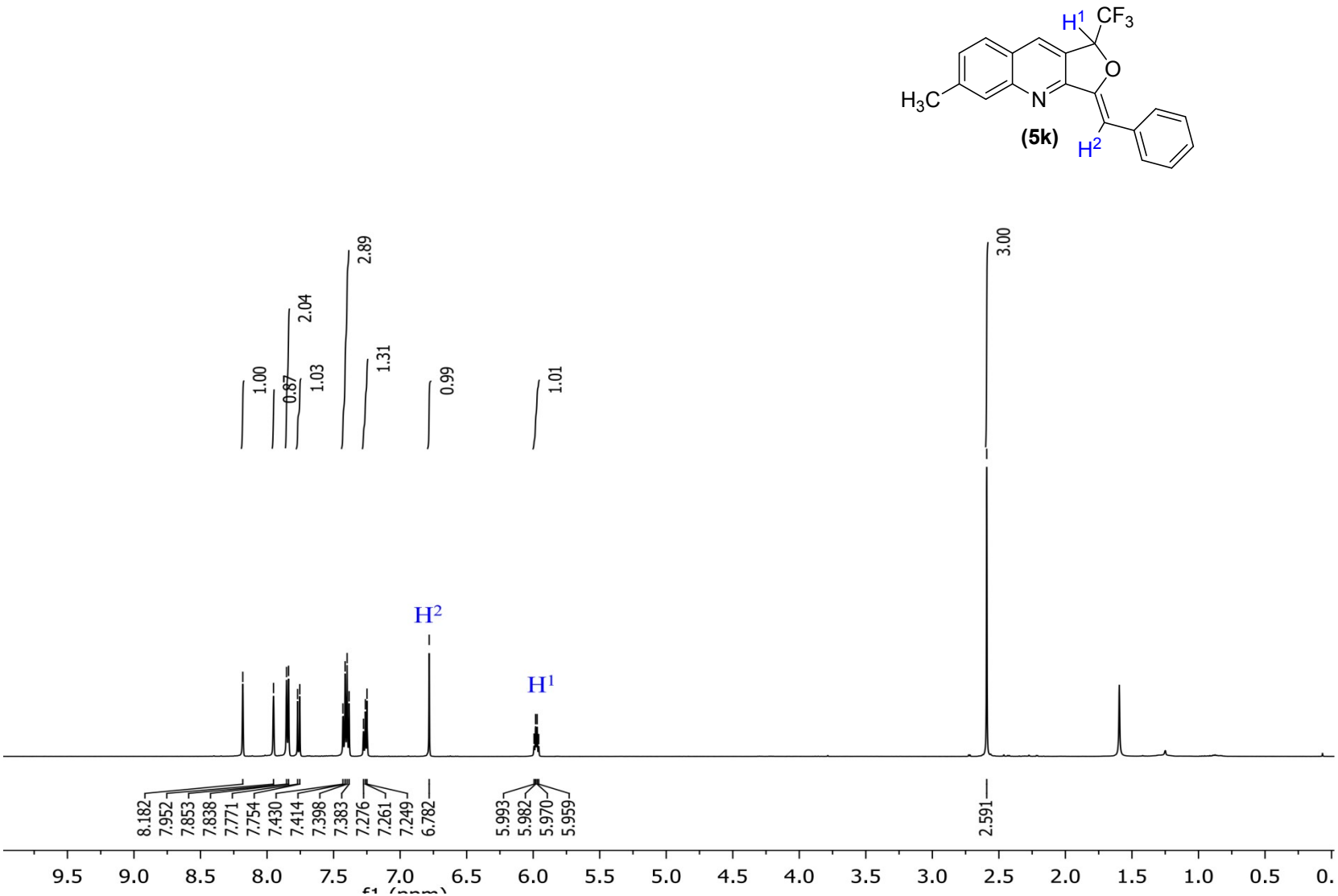

3.10
2.34
1.98
1.00
1.05
0.90
1.03
H2
H1
8.136
8.032
8.014
7.864
7.860
7.847
7.842
7.827
7.416
7.401
7.386
7.276
6.016
6.004
5.993
5.981
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

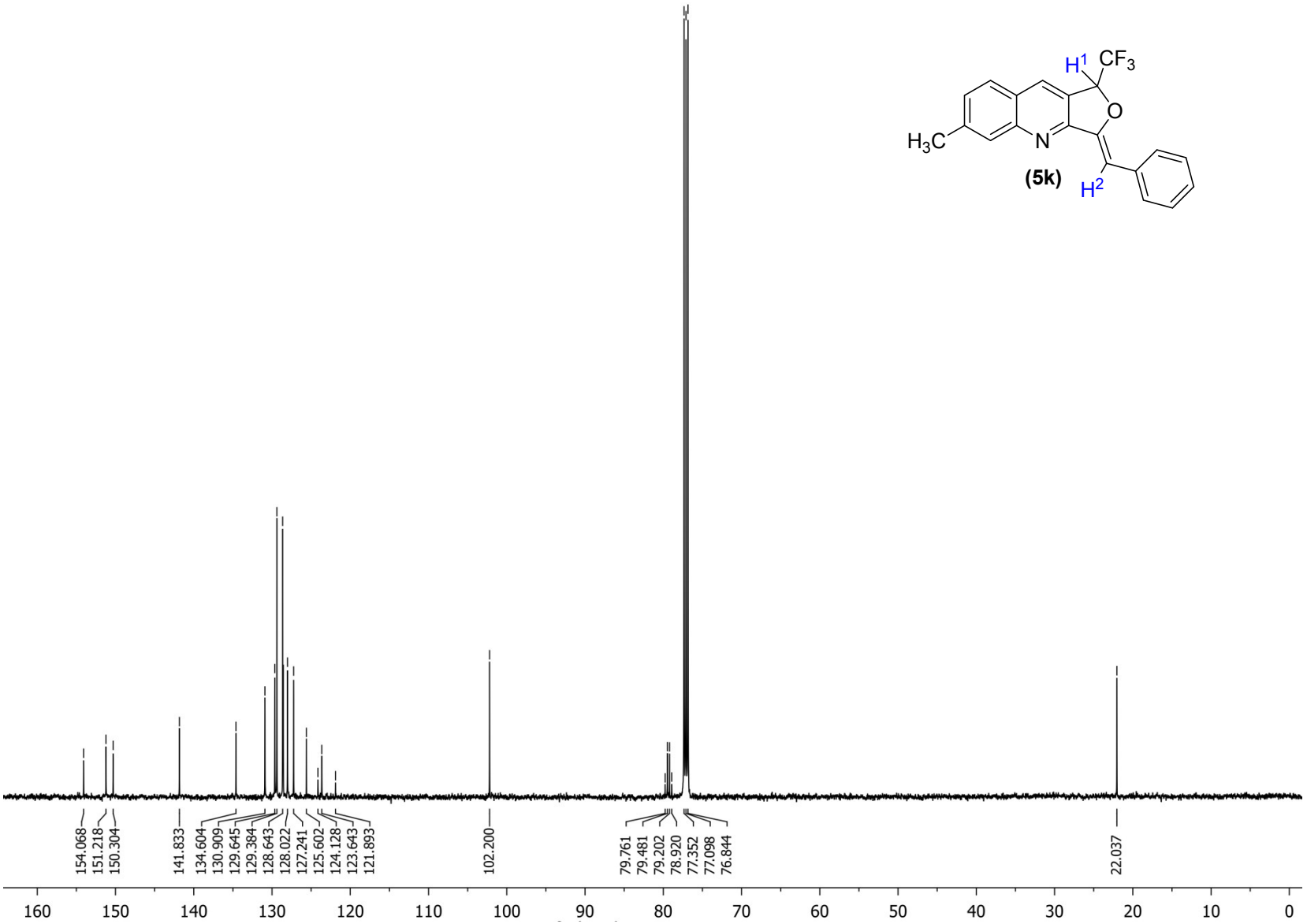

Br
H1
CF3
O
N
H2
(5j)
154.552
150.670
148.665
134.634
134.295
131.099
130.465
130.211
129.499
128.701
128.469
127.552
125.373
123.961
121.281
103.129
79.672
79.392
79.111
78.830
77.351
77.098
76.843
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

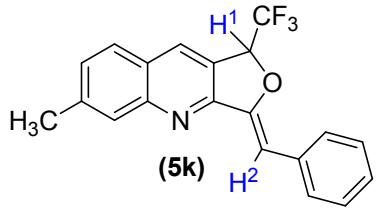

Br
H1
CF3
O
N
H2

(5j)

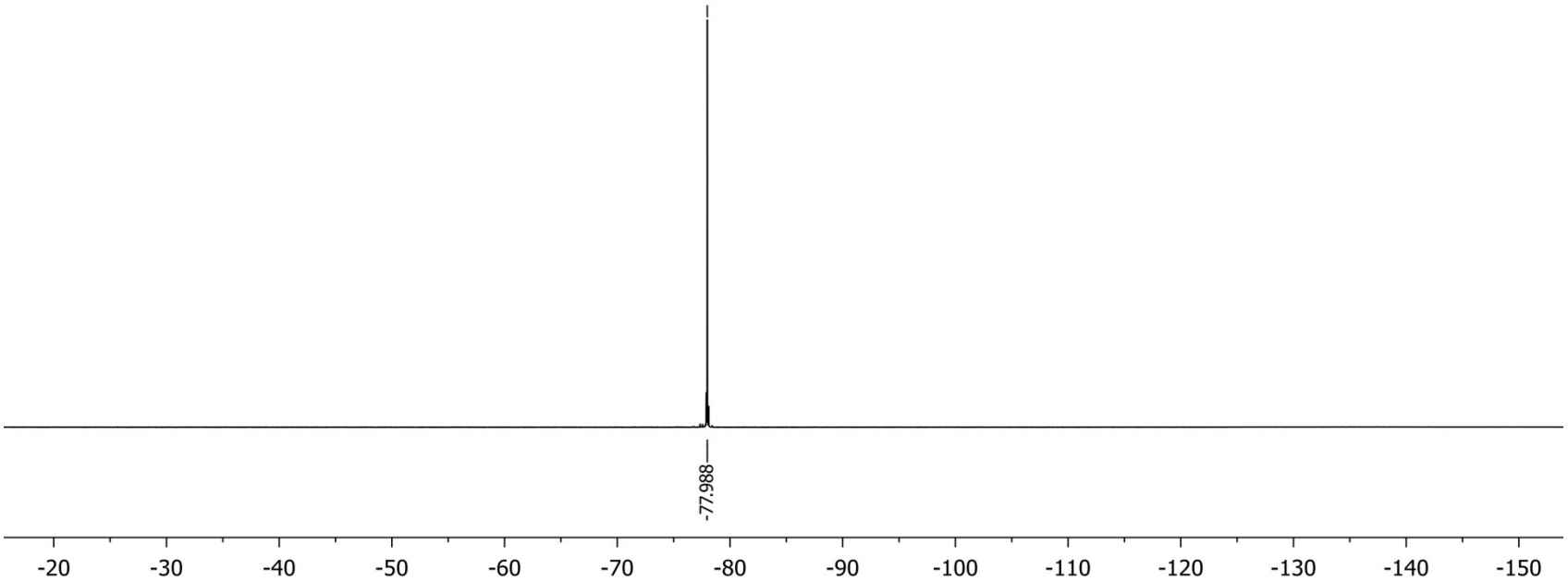

-77.873
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170

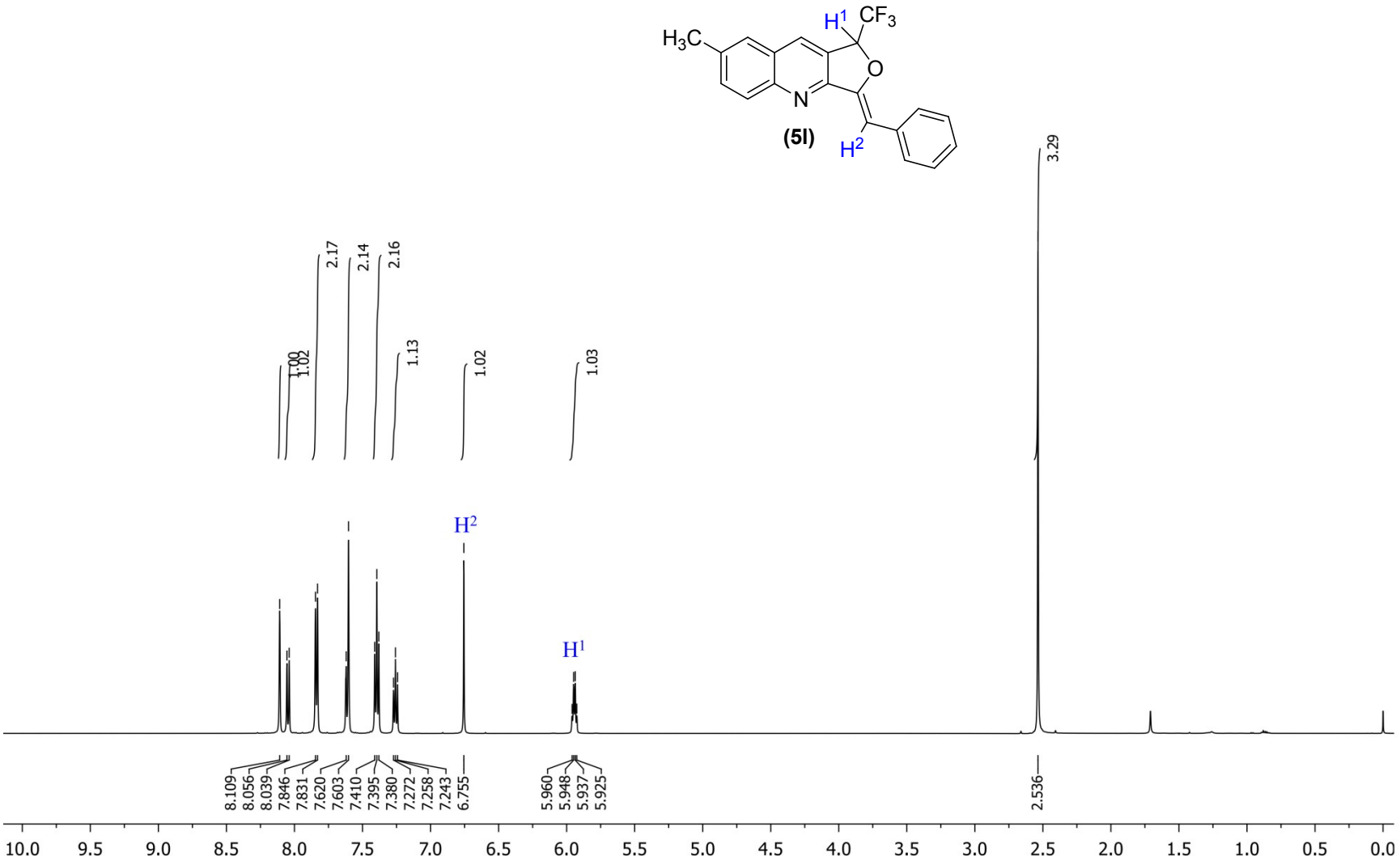

H1
CF3
O
H3C
N
(5k)
H2
1.00
0.87
2.04
1.03
2.89
1.31
0.99
1.01
3.00
H2
H1
8.182
7.952
7.853
7.838
7.771
7.754
7.430
7.414
7.398
7.383
7.276
7.261
7.249
6.782
5.993
5.982
5.970
5.959
2.591
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.

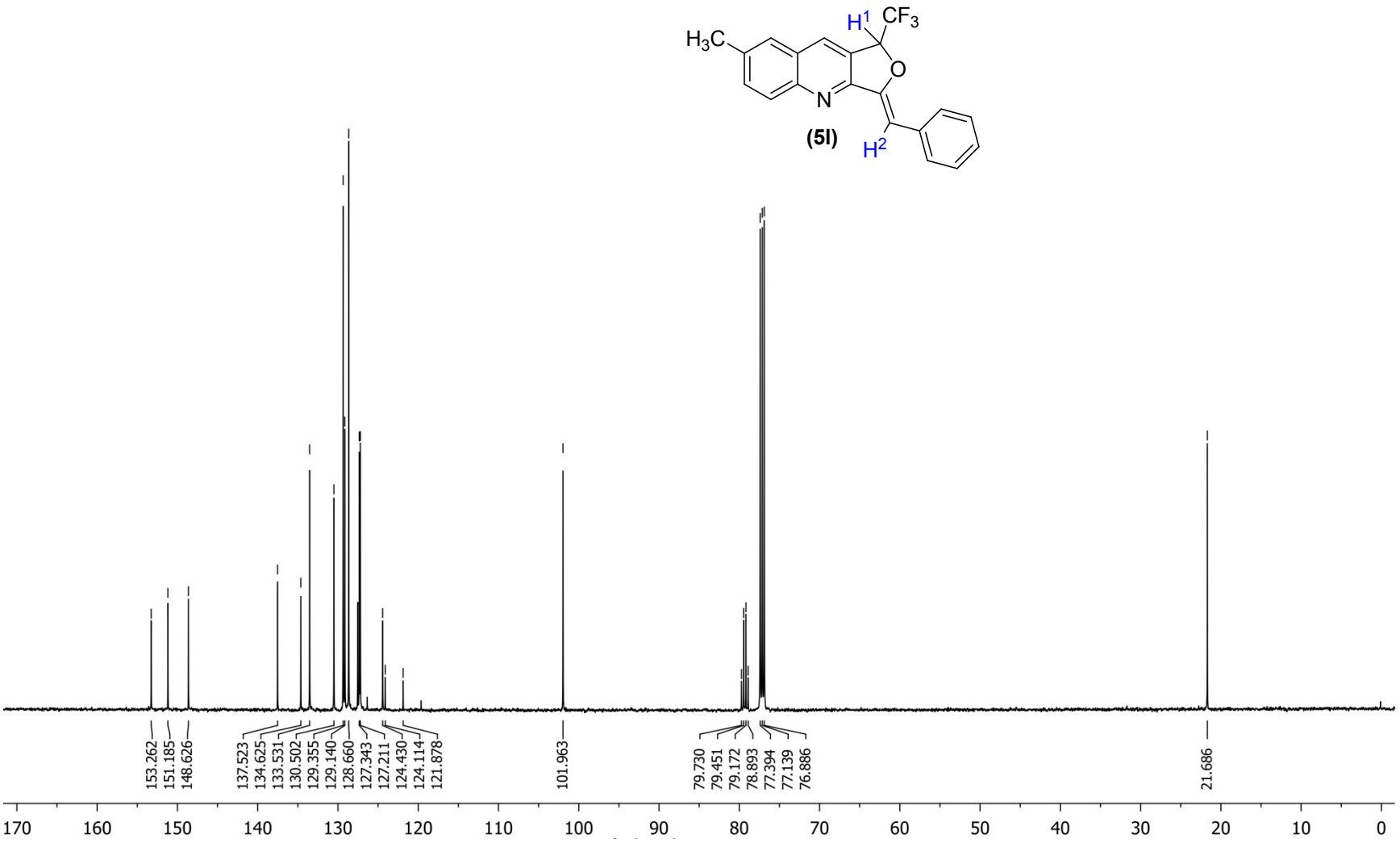

H1
CF3
O
H3C
N
(5k)
H2
154.068
151.218
150.304
141.833
134.604
130.909
129.645
129.384
128.643
128.022
127.241
125.602
124.128
123.643
121.893
102.200
79.761
79.481
79.202
78.920
77.352
77.098
76.844
22.037
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

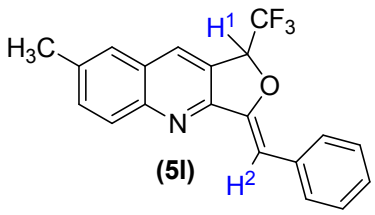

H1
CF3
O
H3C
N
H2

(5k)


-77.988
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150

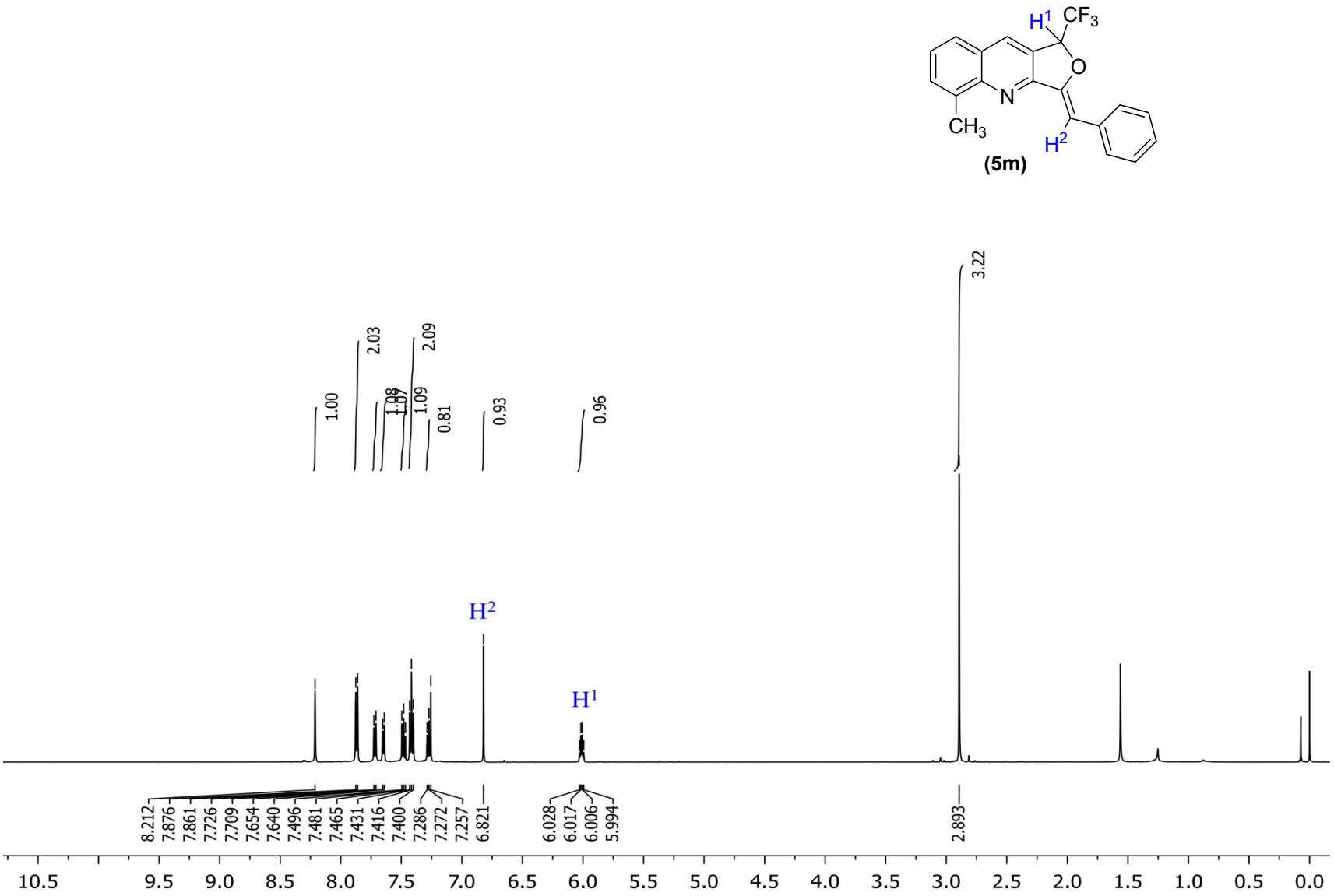

H1
CF3
H3C
O
N
(5l)
H2
3.29
2.17
2.14
2.16
1.13
1.02
1.03
1.00
1.02
H2
H1
8.109
8.056
8.039
7.846
7.831
7.620
7.603
7.410
7.395
7.380
7.272
7.258
7.243
6.755
5.960
5.948
5.937
5.925
2.536
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

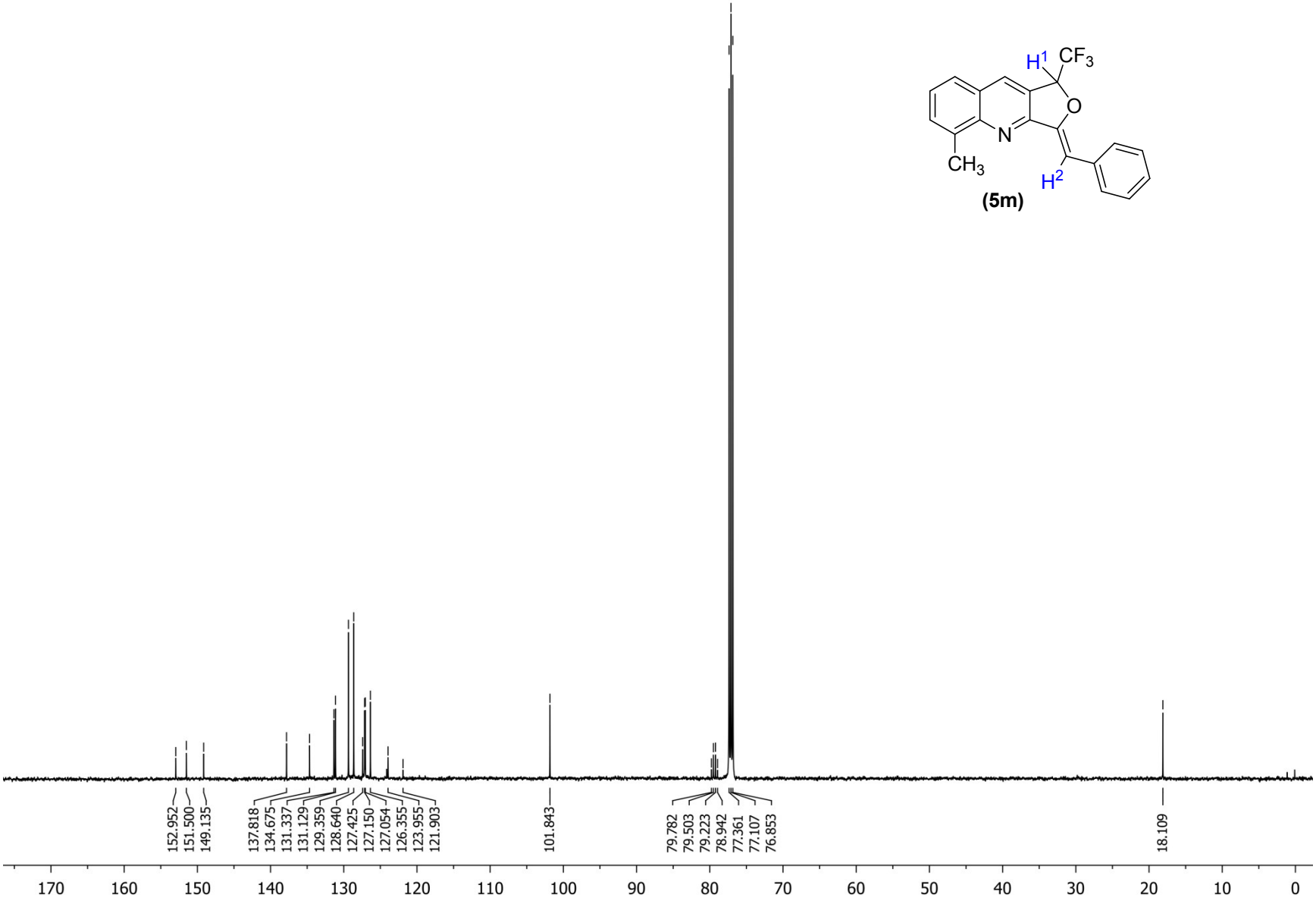

H1
CF3
H3C
O
N
(5l)
H2
153.262
151.185
148.626
137.523
134.625
133.531
130.502
129.355
129.140
128.660
127.343
127.211
124.430
124.114
121.878
101.963
79.730
79.451
79.172
78.893
77.394
77.139
76.886
21.686
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

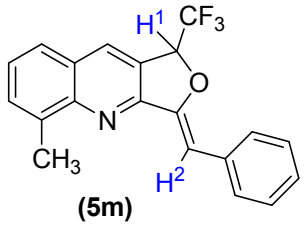

H1
CF3
H3C
O
N
H2

(5l)

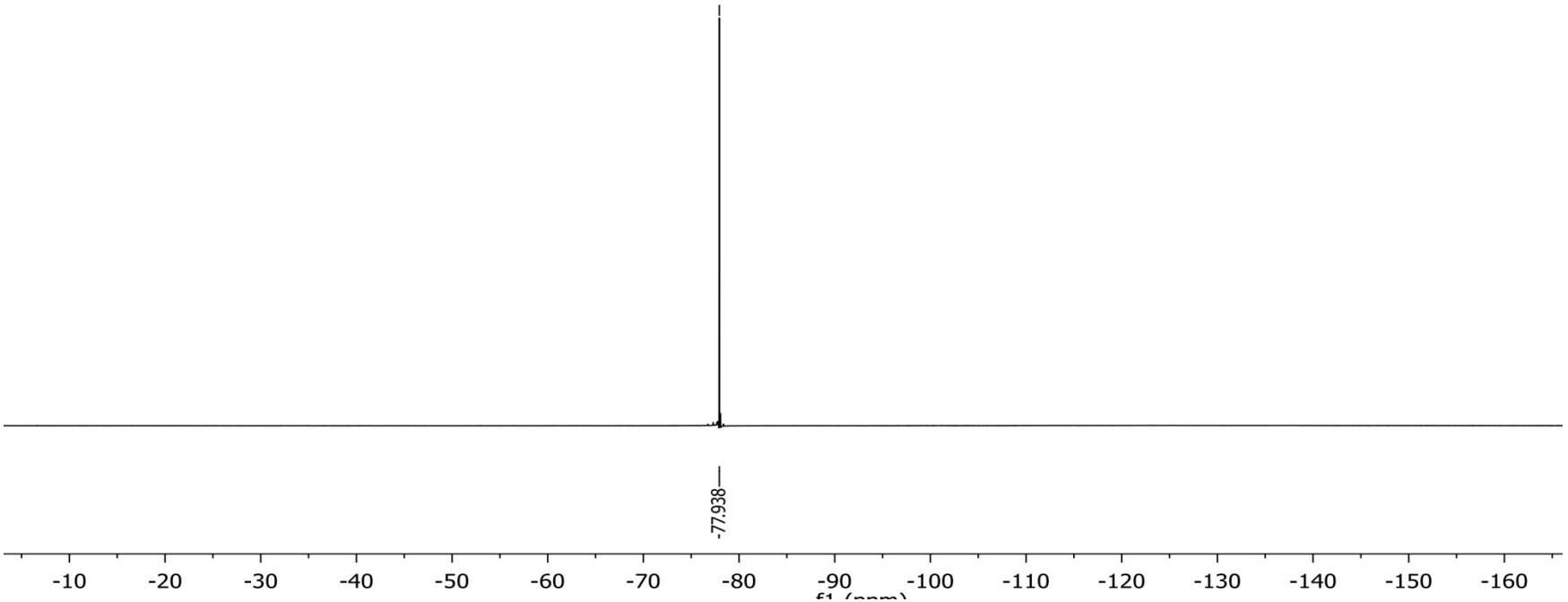
-77.948
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200

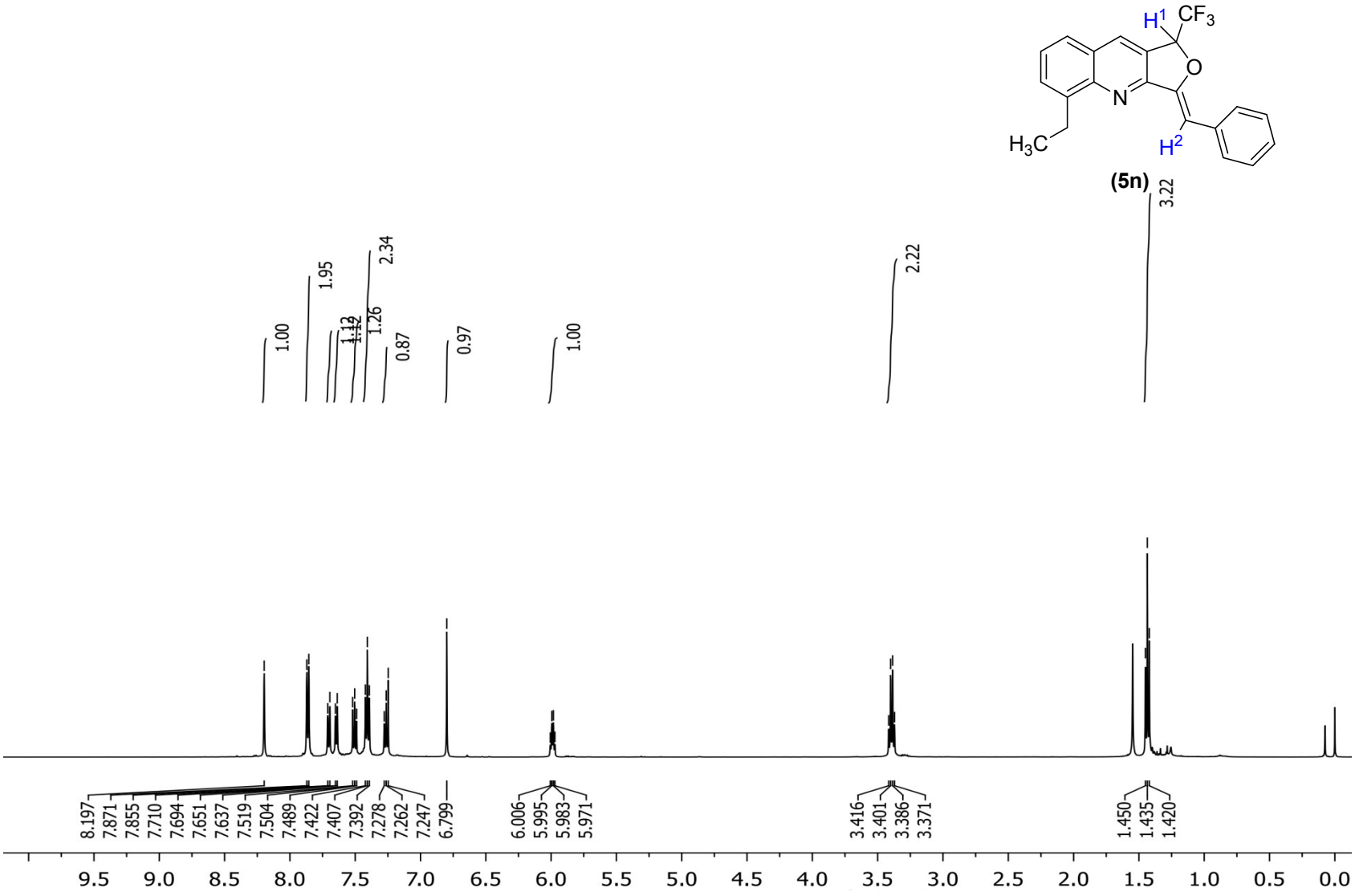

H1
CF3
O
N
CH3
H2
(5m)
3.22
2.03
2.09
1.00
1.09
0.81
0.93
0.96
H2
H1
8.212
7.876
7.861
7.726
7.709
7.654
7.640
7.496
7.481
7.465
7.431
7.416
7.400
7.286
7.272
7.257
6.821
6.028
6.017
6.006
5.994
2.893
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

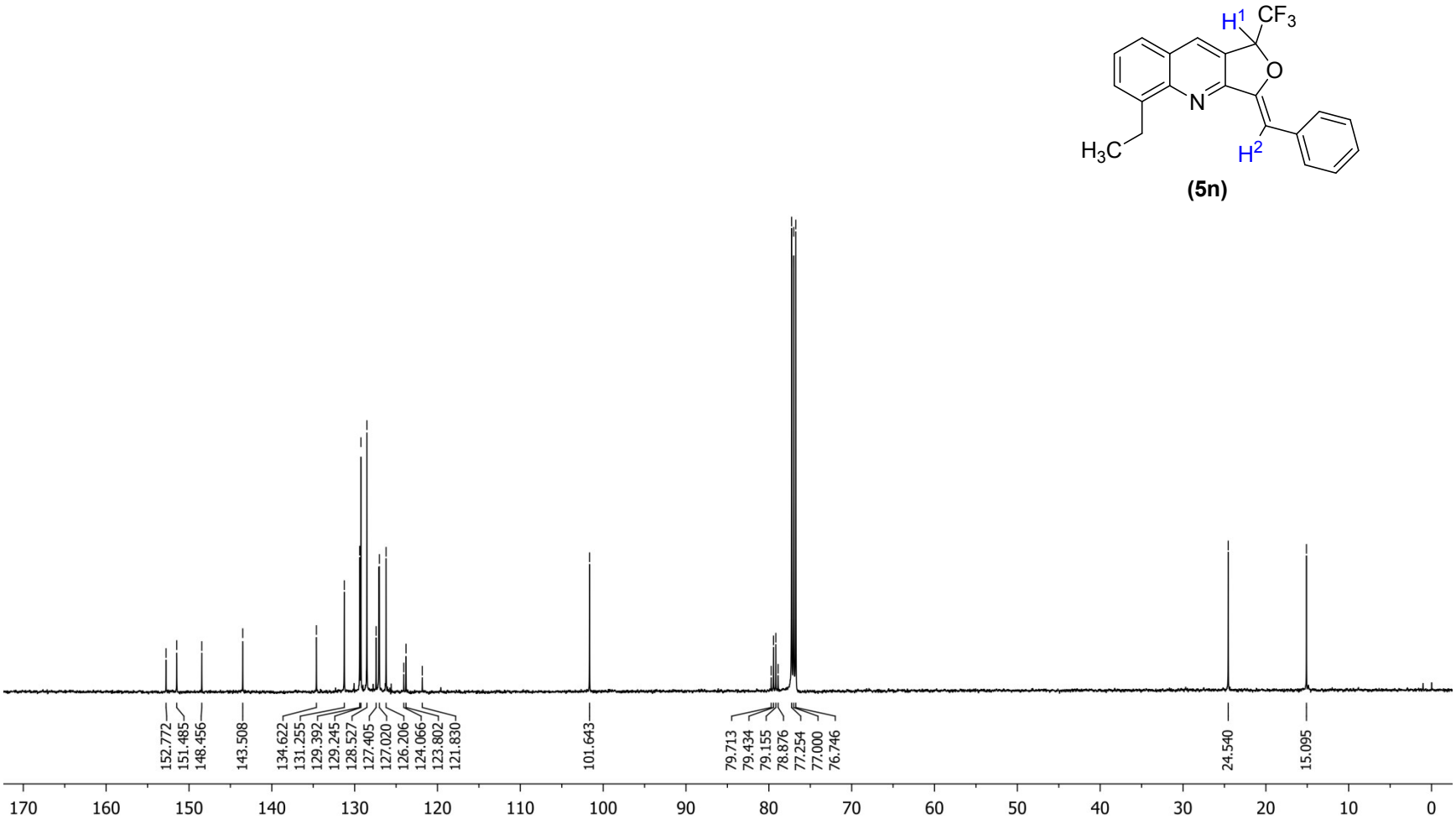

H1
CF3
O
N
CH3
H2
(5m)
152.952
151.500
149.135
137.818
134.675
131.337
131.129
129.359
128.640
127.425
127.150
127.054
126.355
123.955
121.903
101.843
79.782
79.503
79.223
78.942
77.361
77.107
76.853
18.109
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

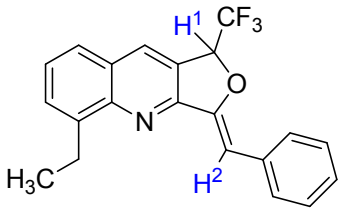

H1
CF3
O
N
CH3
H2

(5m)

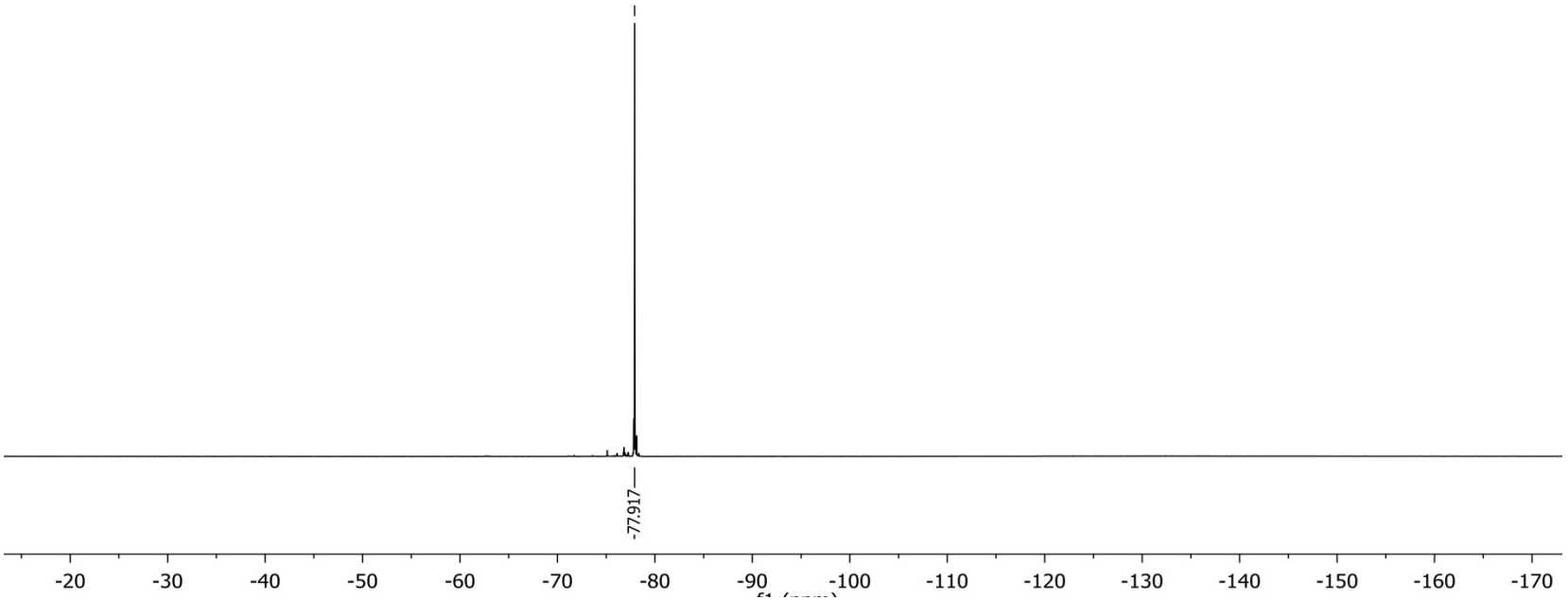

-77.938
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160

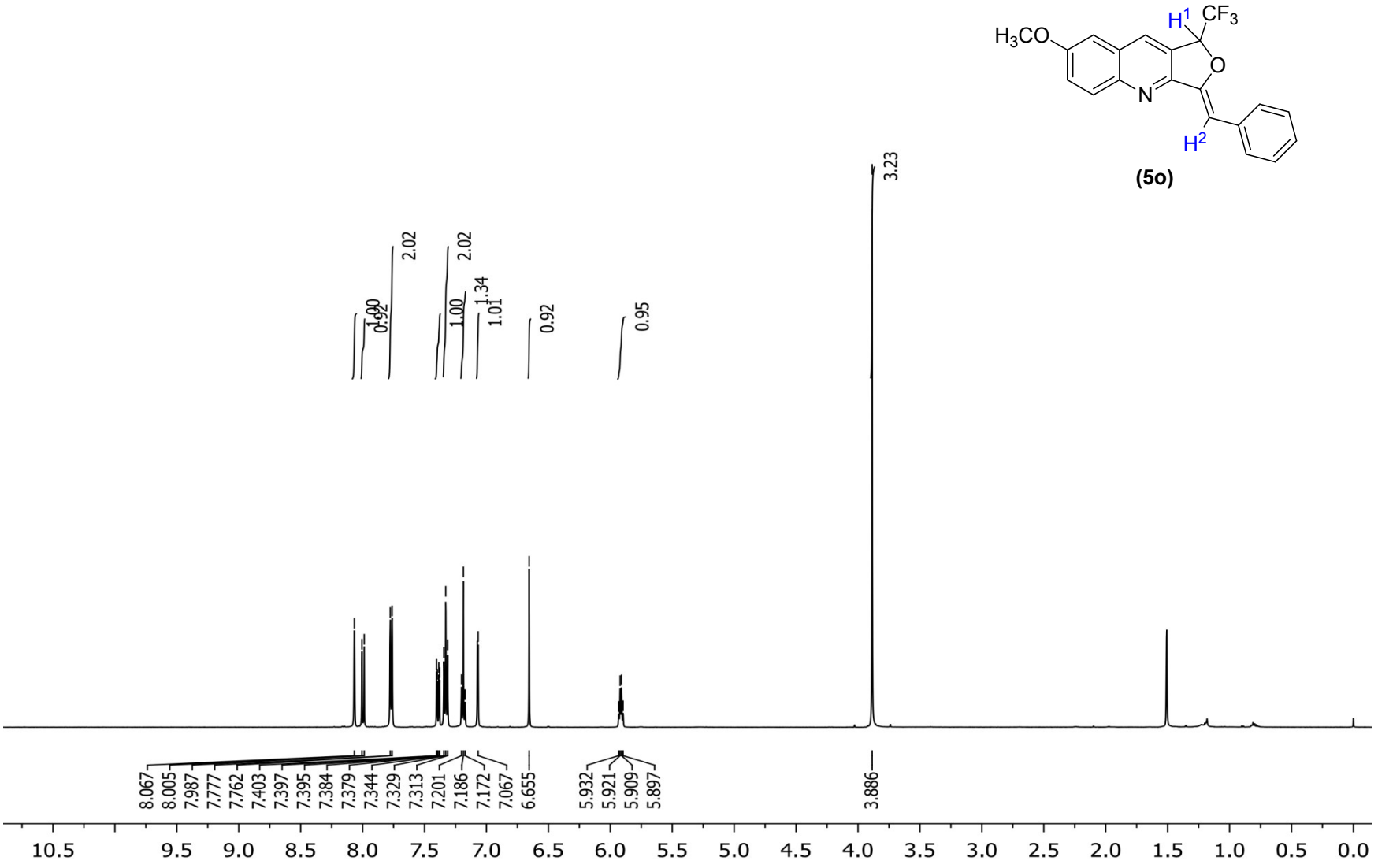

H1
CF3
O
N
H3C
H2
(5n)
1.00
1.95
2.34
1.26
0.87
0.97
1.00
2.22
3.22
8.197
7.871
7.855
7.710
7.694
7.651
7.637
7.519
7.504
7.489
7.422
7.407
7.392
7.278
7.262
7.247
6.799
6.006
5.995
5.983
5.971
3.416
3.401
3.386
3.371
1.450
1.435
1.420
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

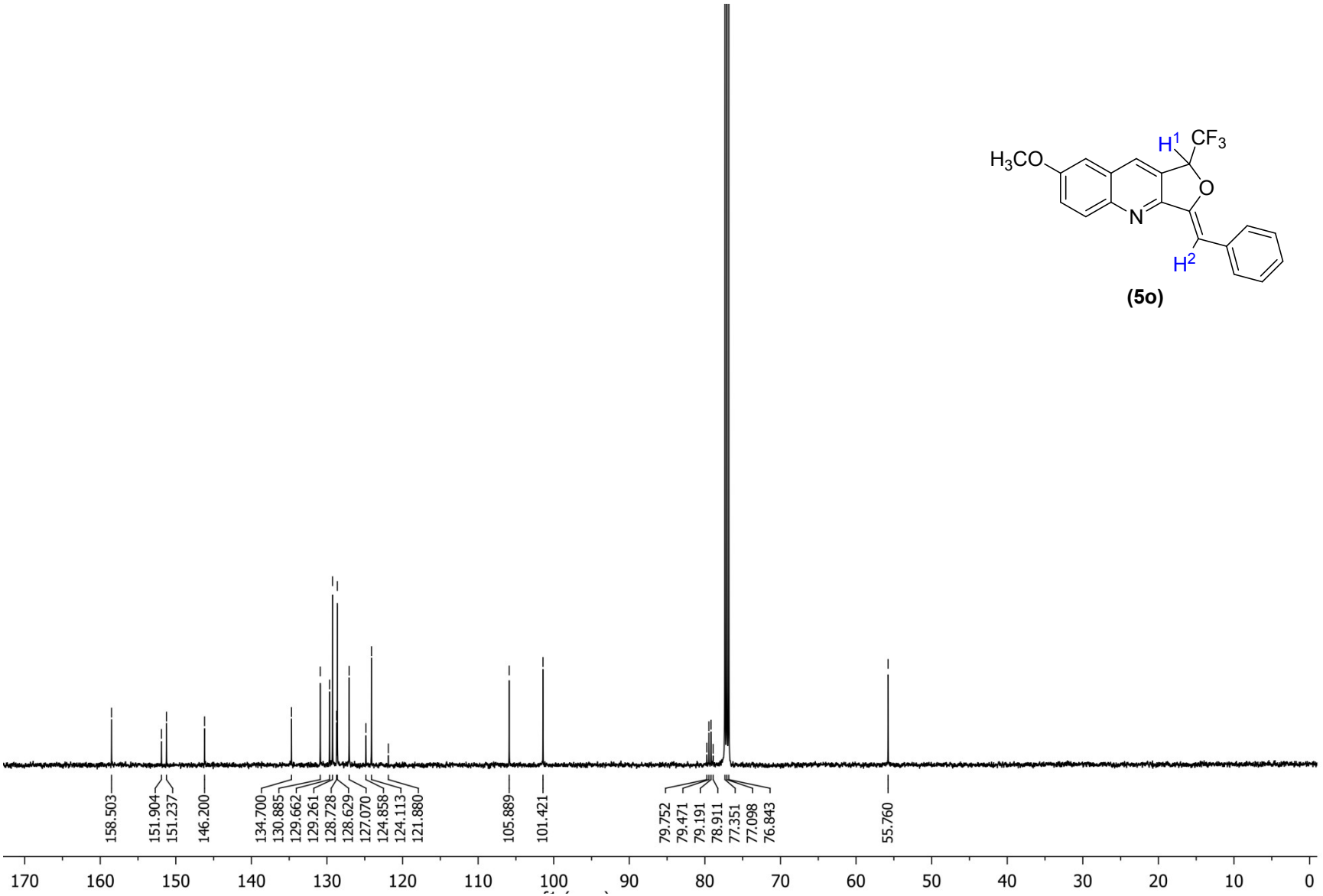

H1
CF3
O
N
H3C
H2
(5n)
152.772
151.485
148.456
143.508
134.622
131.255
129.392
129.245
128.527
127.405
127.020
126.206
124.066
123.802
121.830
101.643
79.713
79.434
79.155
78.876
77.254
77.000
76.746
24.540
15.095
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

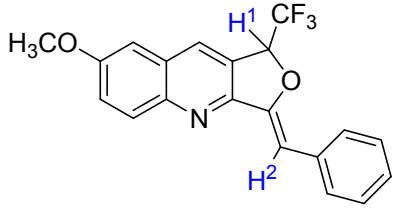

H1
CF3
O
N
H3C
H2

(5n)

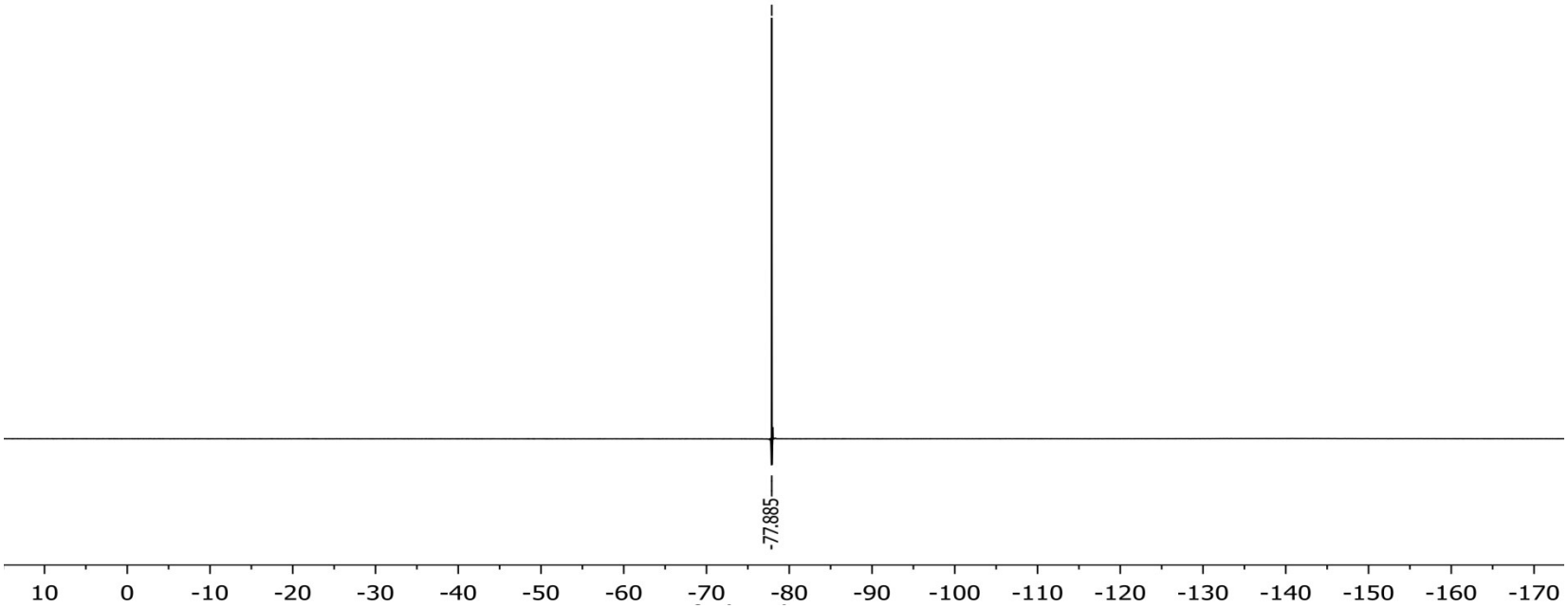

-77.917
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170

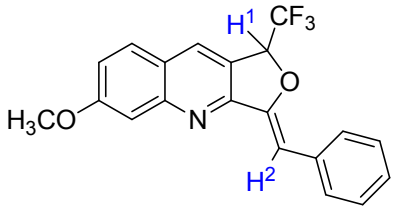

H1
CF3
H3CO
O
N
H2
(5o)
3.23
2.02
2.02
1.34
1.01
1.00
1.00
0.92
0.92
0.95
8.067
8.005
7.987
7.777
7.762
7.403
7.397
7.395
7.384
7.379
7.344
7.329
7.313
7.201
7.186
7.172
7.067
6.655
5.932
5.921
5.909
5.897
3.886
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


H1
CF3
H3CO
O
N
H2
(5o)
158.503
151.904
151.237
146.200
134.700
130.885
129.662
129.261
128.728
128.629
127.070
124.858
124.113
121.880
105.889
101.421
79.752
79.471
79.191
78.911
77.351
77.098
76.843
55.760
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

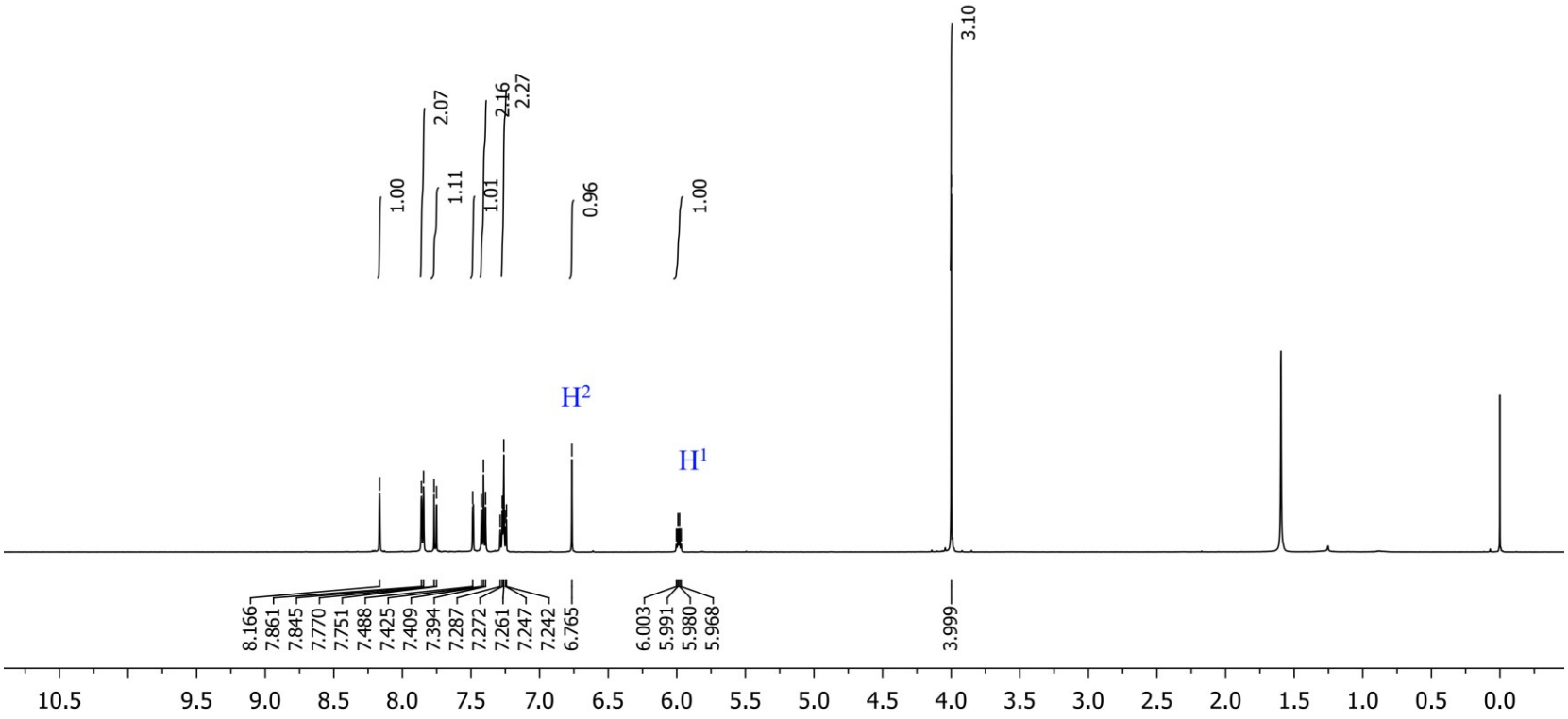

H1
CF3
H3CO
O
N
H2

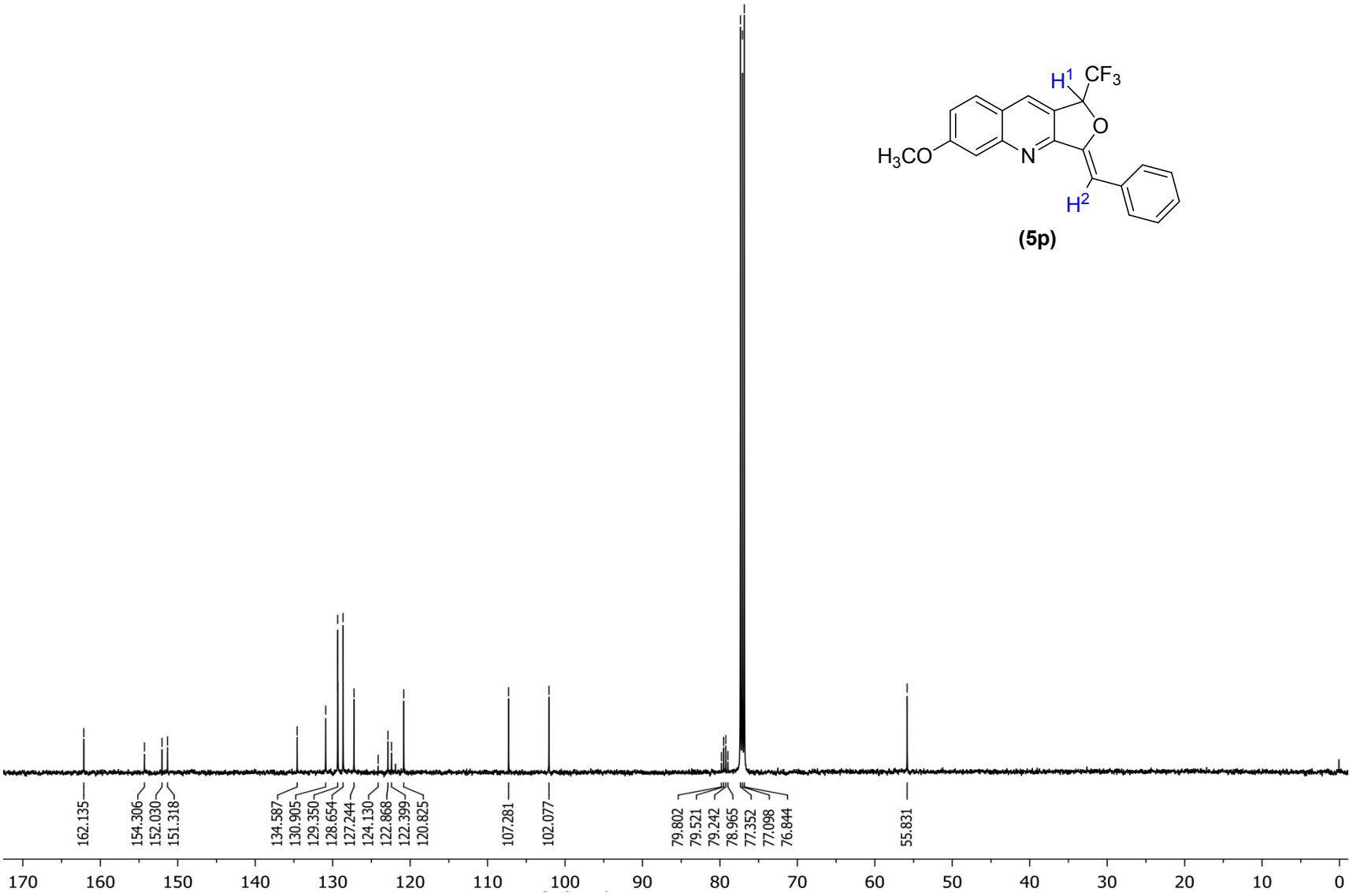
(5o)

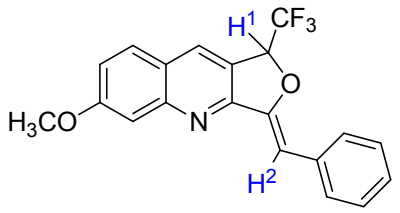

-77.885
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170


H1
CF3
O
H3CO
N
H2

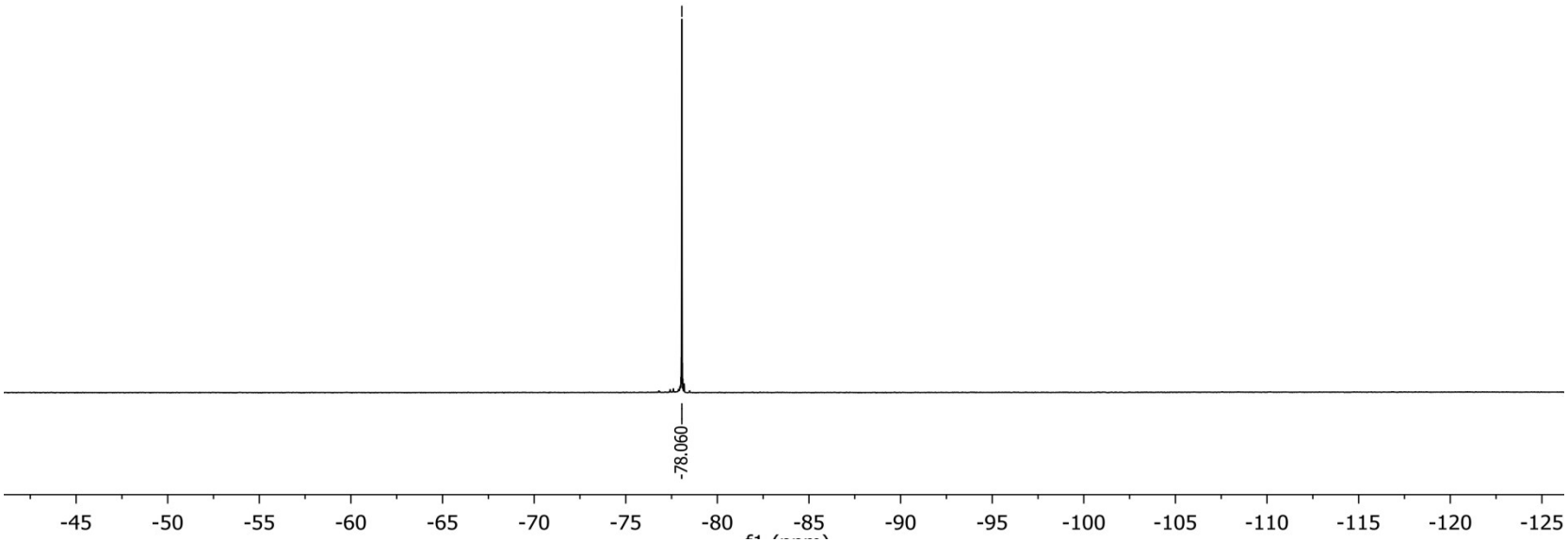
(5p)

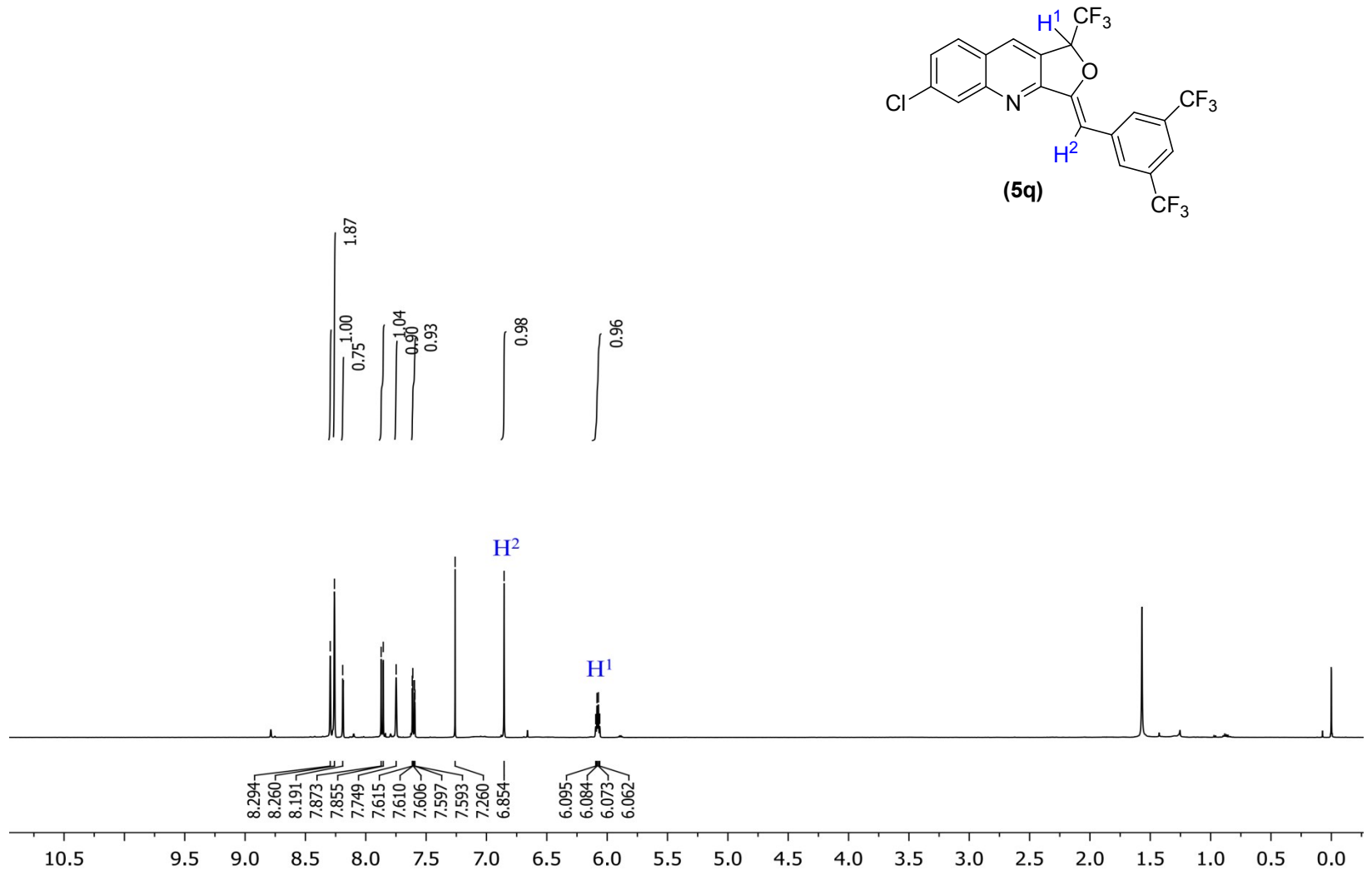

3.10
2.07
2.16
2.27
1.00
1.11
1.01
0.96
1.00
H2
H1
8.166
7.861
7.845
7.770
7.751
7.488
7.425
7.409
7.394
7.287
7.272
7.261
7.247
7.242
6.765
6.003
5.991
5.980
5.968
3.999
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

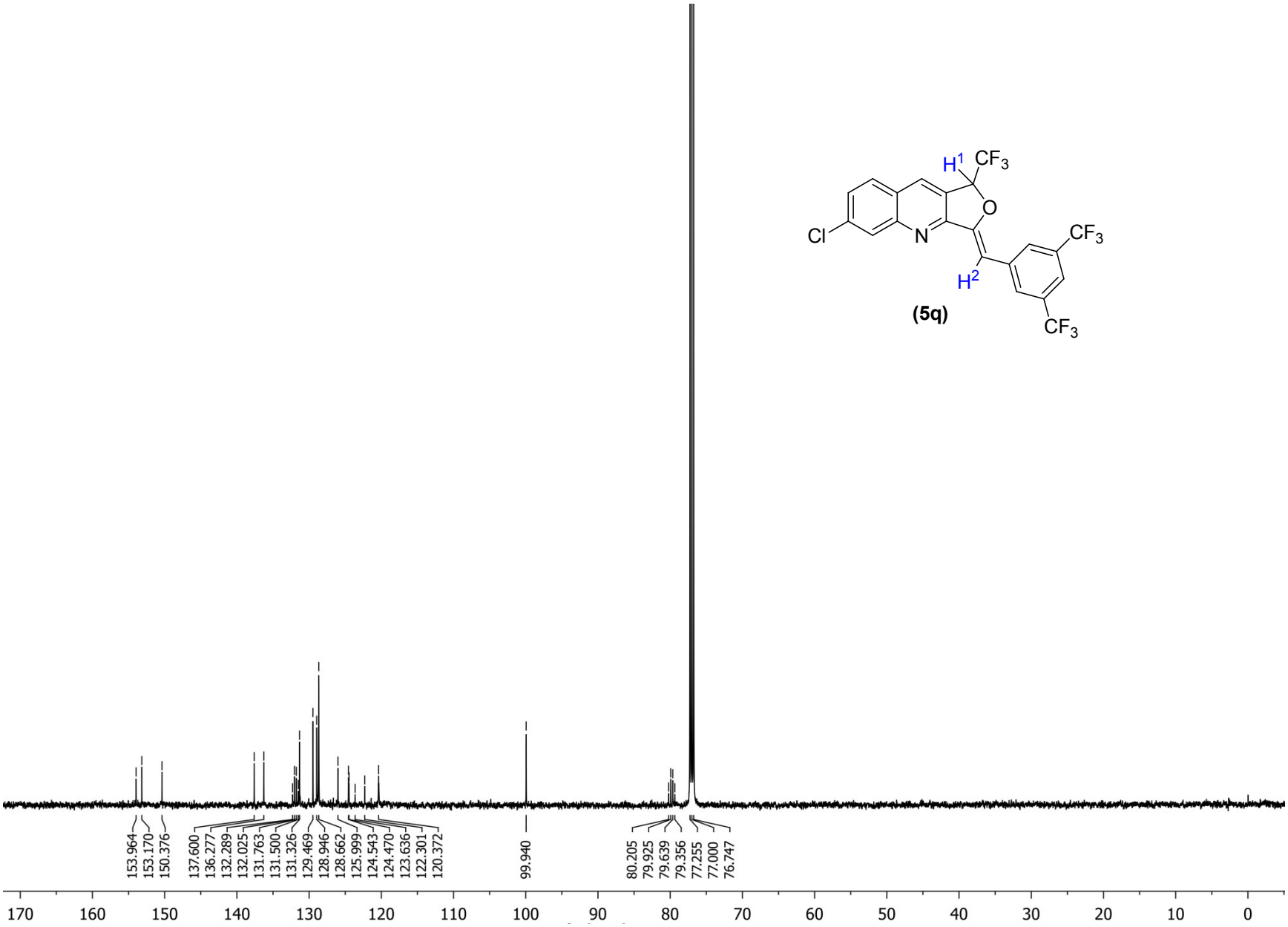

H1
CF3
O
H3CO
N
H2
(5p)
162.135
154.306
152.030
151.318
134.587
130.905
129.350
128.654
127.244
124.130
122.868
122.399
120.825
107.281
102.077
79.802
79.521
79.242
78.965
77.352
77.098
76.844
55.831
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

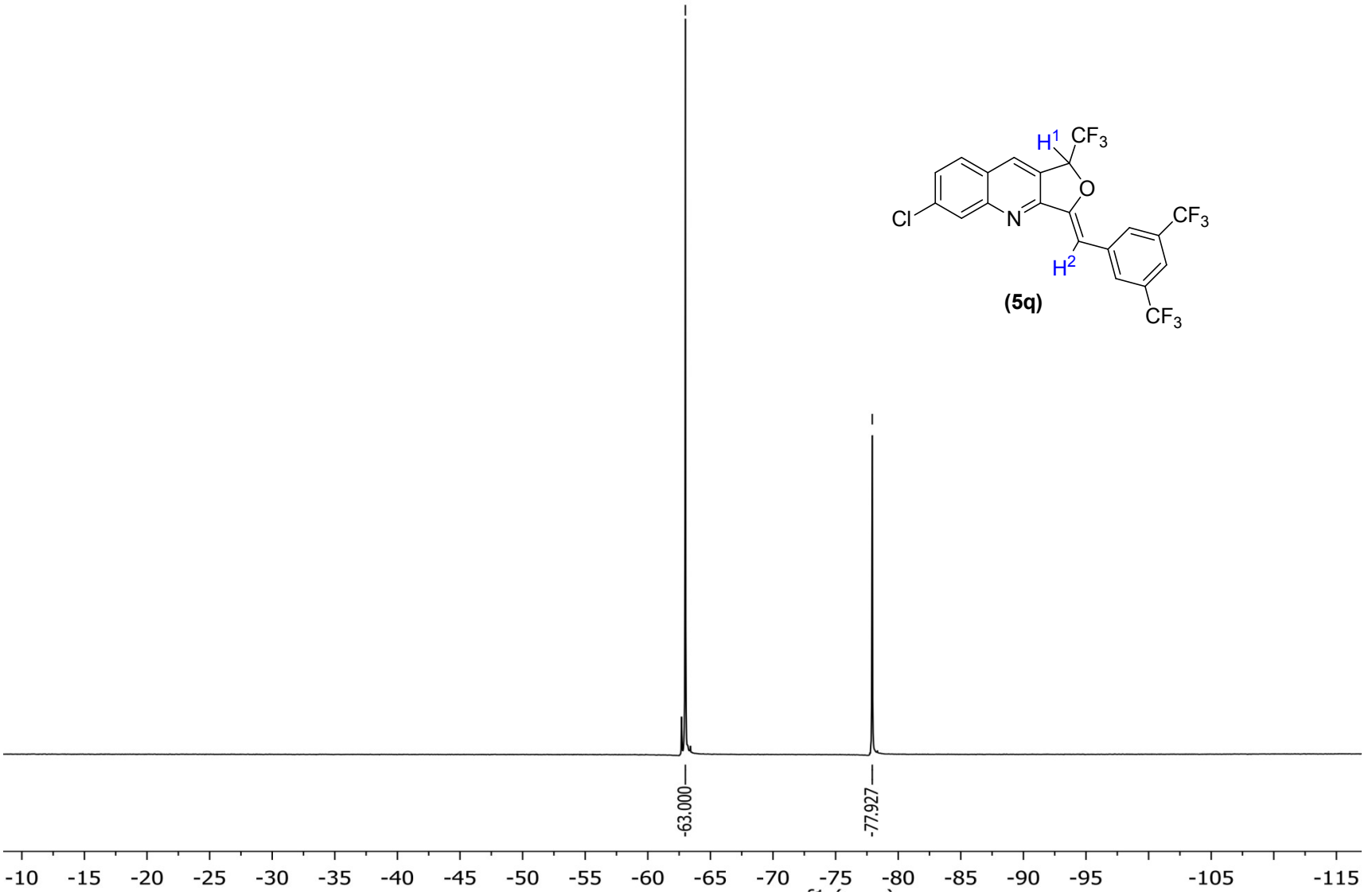

H1
CF3
O
H3CO
N
H2

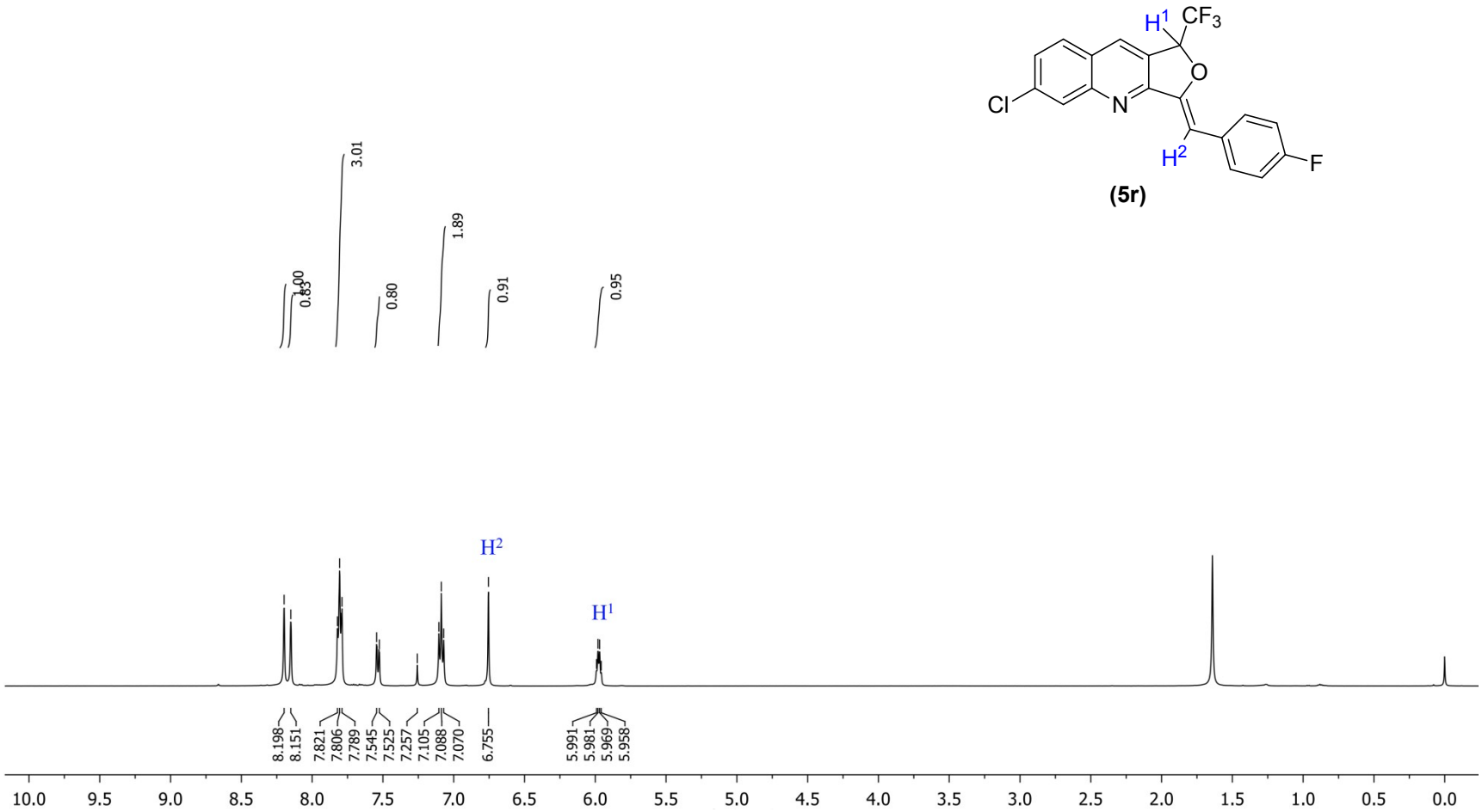
(5p)

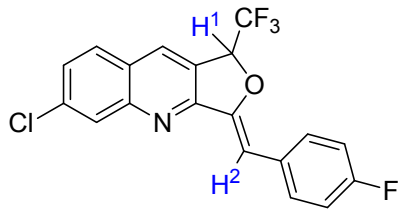

-78.060
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125


H1
CF3
O
Cl
N
CF3
H2
CF3
(5q)
1.87
1.00
0.75
1.04
0.90
0.93
0.98
0.96
H2
H1
8.294
8.260
8.191
7.873
7.855
7.749
7.615
7.610
7.606
7.597
7.593
7.260
6.854
6.095
6.084
6.073
6.062
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

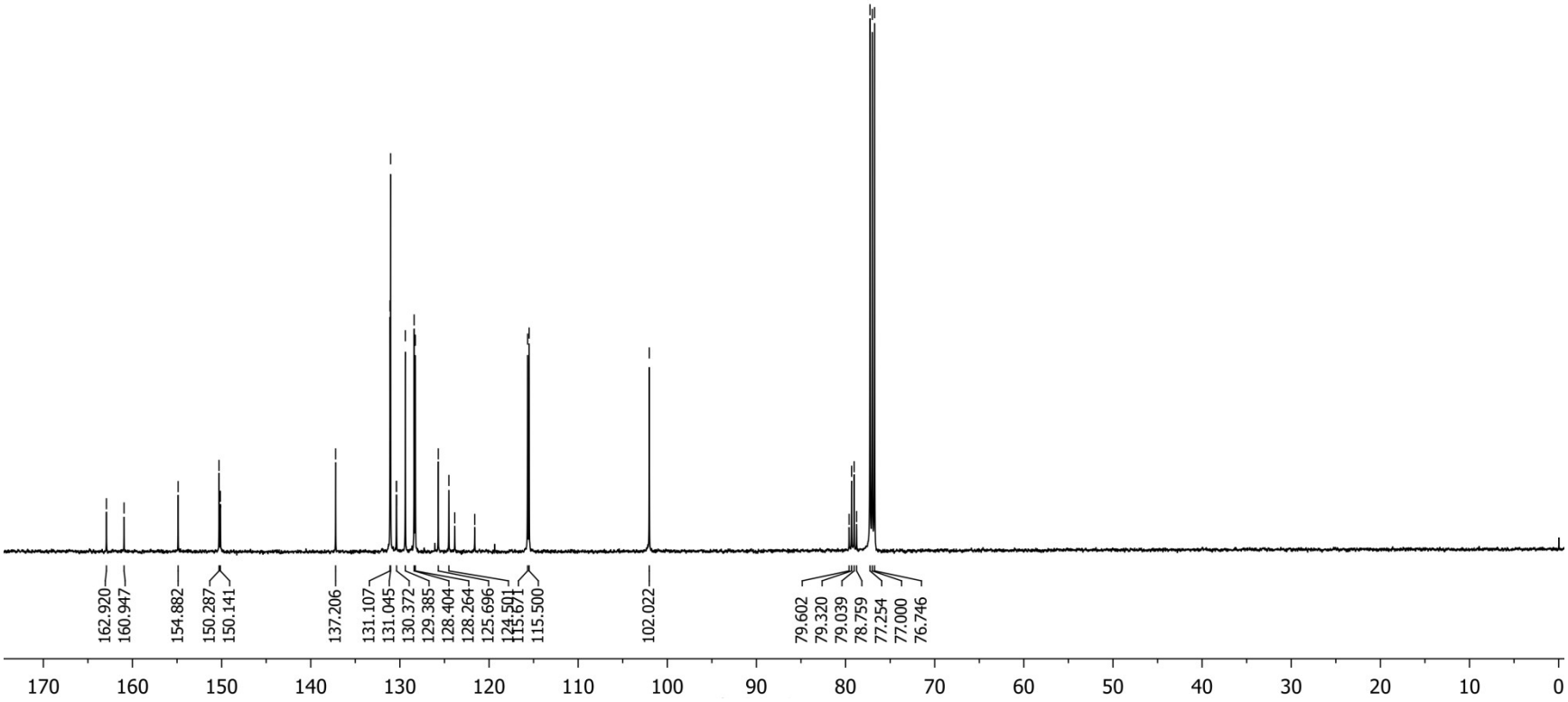

H1
CF3
O
Cl
N
CF3
H2
CF3
(5q)
153.964
153.170
150.376
137.600
136.277
132.289
132.025
131.763
131.500
131.326
129.469
128.946
128.662
125.999
124.543
124.470
123.636
122.301
120.372
99.940
80.205
79.925
79.639
79.356
77.255
77.000
76.747
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

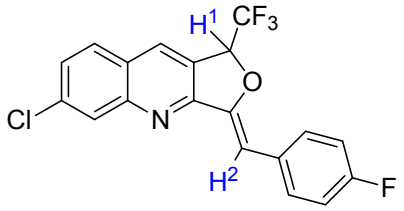

H1
CF3
O
Cl
N
CF3
H2
CF3
(5q)
-63.000
-77.927
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-105
-115


H1
CF3
O
Cl
N
H2
F
(5r)
3.01
1.89
0.80
0.91
0.95
0.83
1.00
H2
H1
8.198
8.151
7.821
7.806
7.789
7.545
7.525
7.257
7.105
7.088
7.070
6.755
5.991
5.981
5.969
5.958
10.0
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

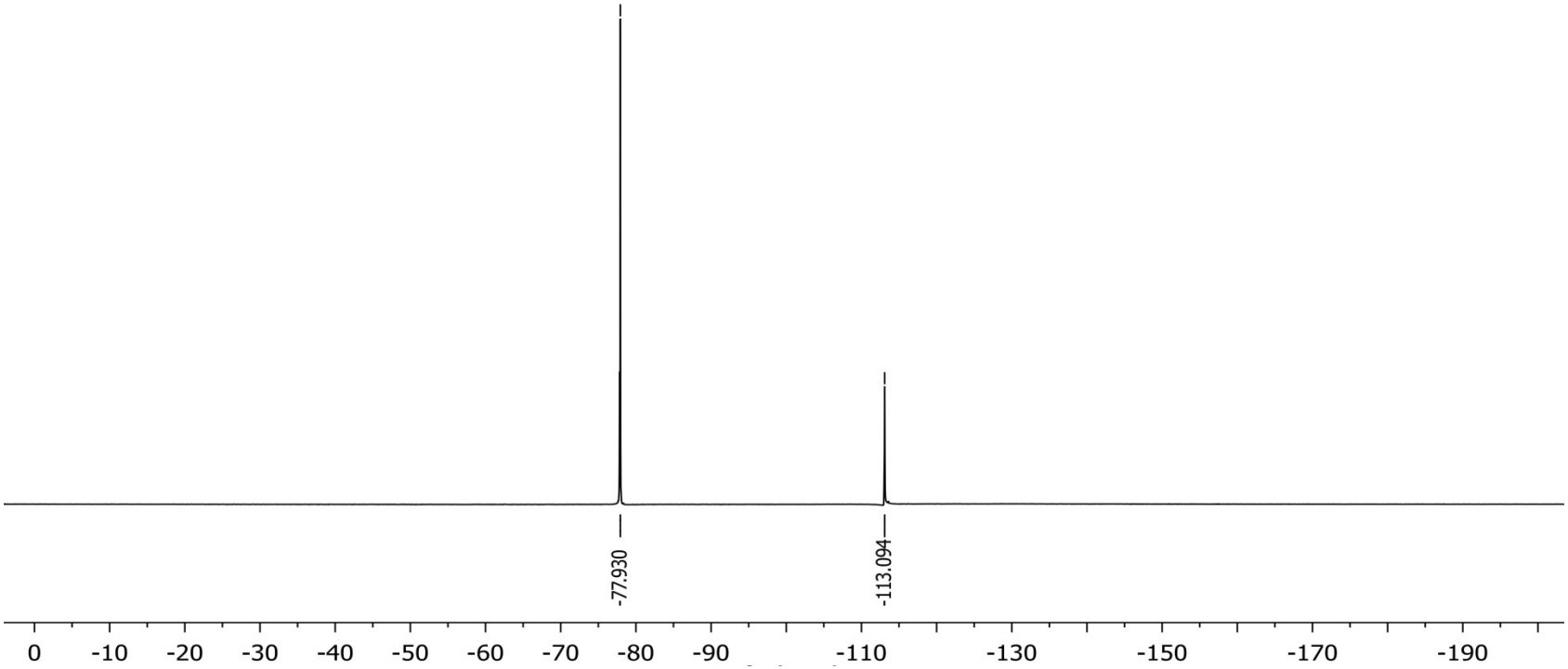

H1
CF3
O
Cl
N
H2
F

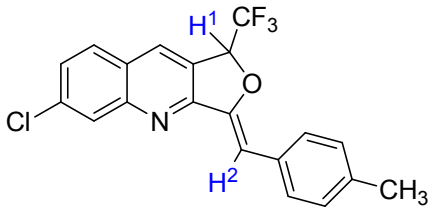
(5r)


162.920
160.947
154.882
150.287
150.141
137.206
131.107
131.045
130.372
129.385
128.404
128.264
125.696
124.501
115.671
115.500
102.022
79.602
79.320
79.039
78.759
77.254
77.000
76.746
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

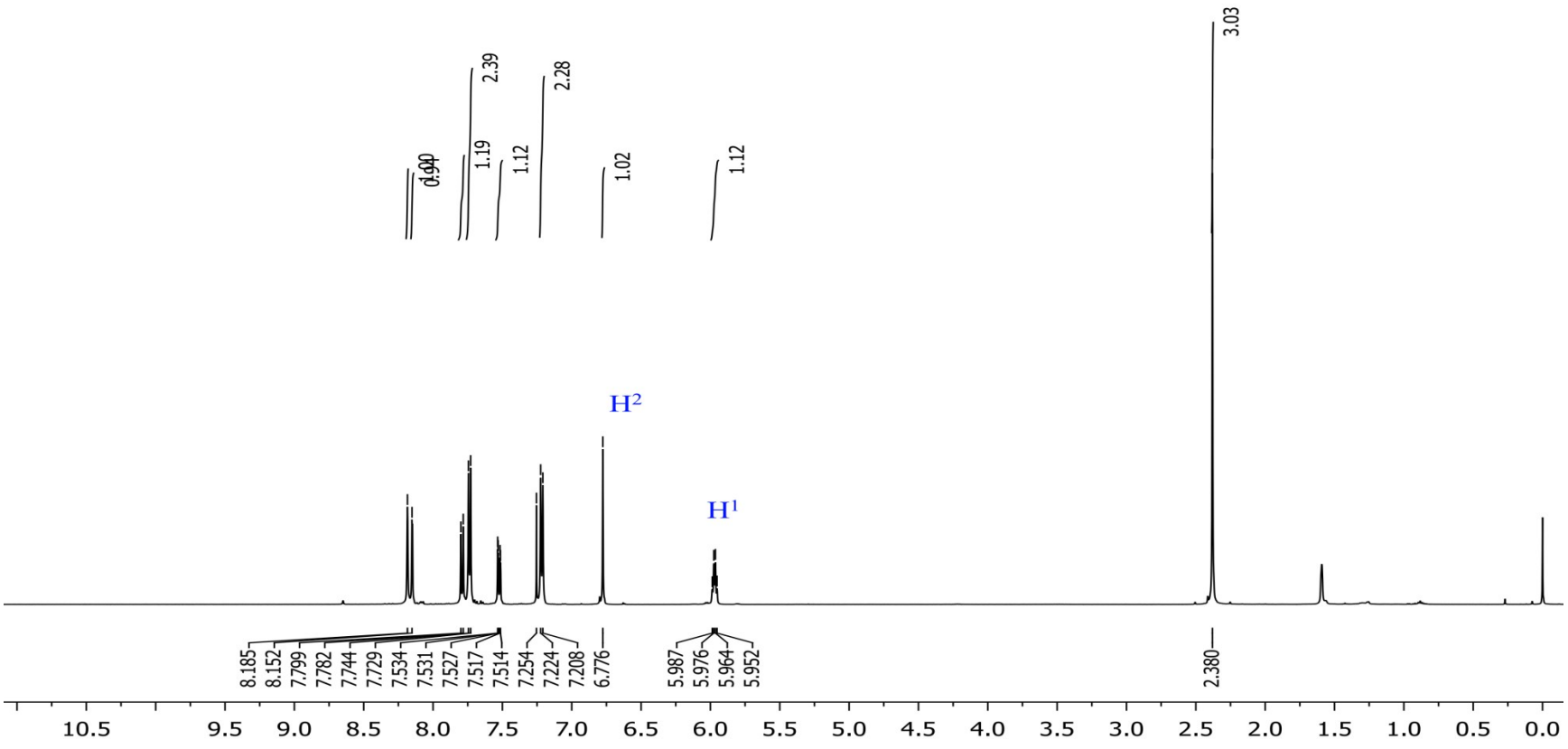

H1
CF3
O
Cl
N
H2
F

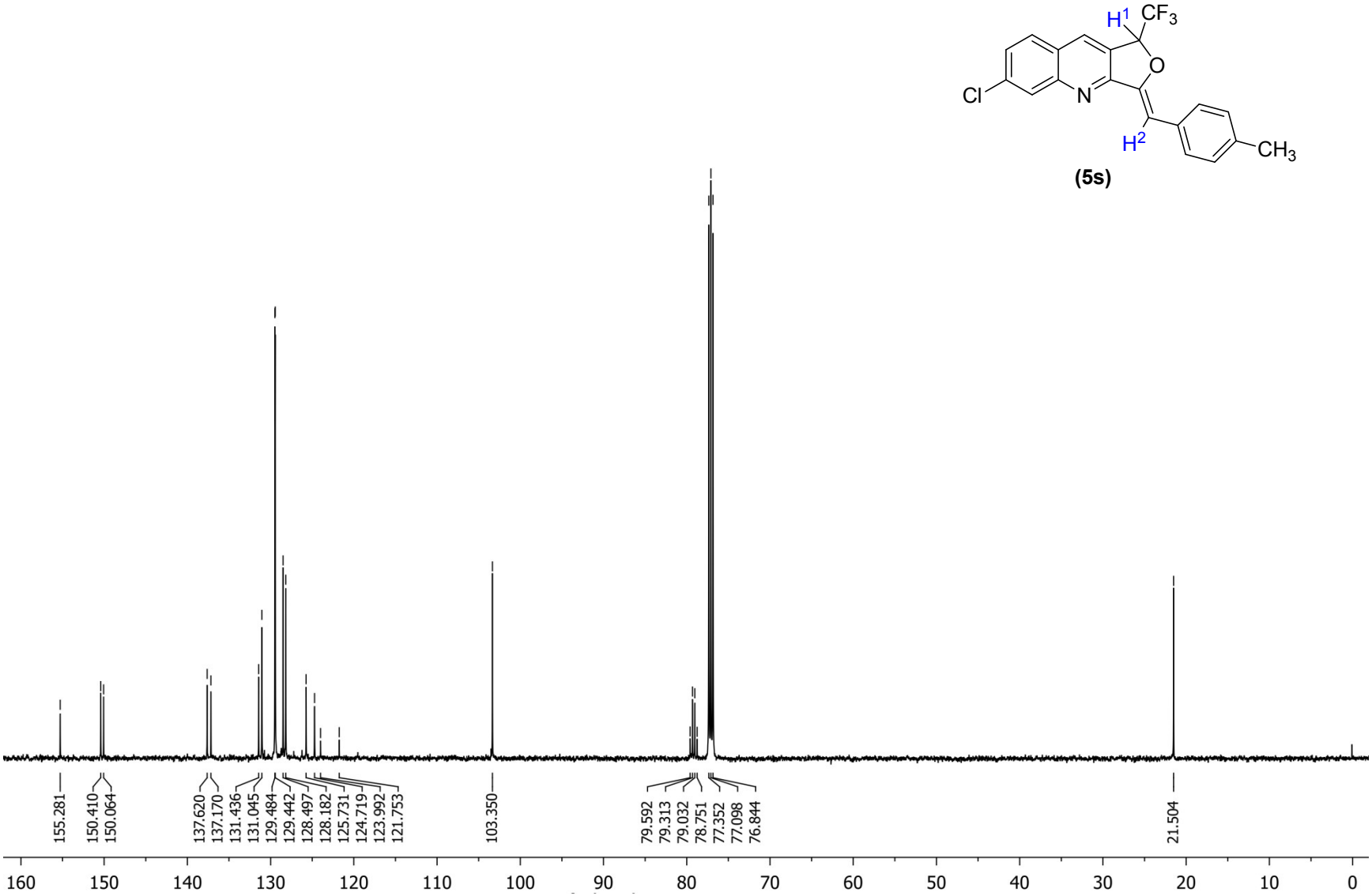
(5r)


-77.930
-113.094
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190

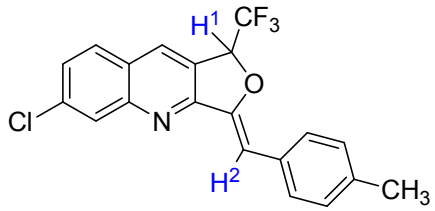

H1
CF3
O
Cl
N
H2
CH3

(5s)

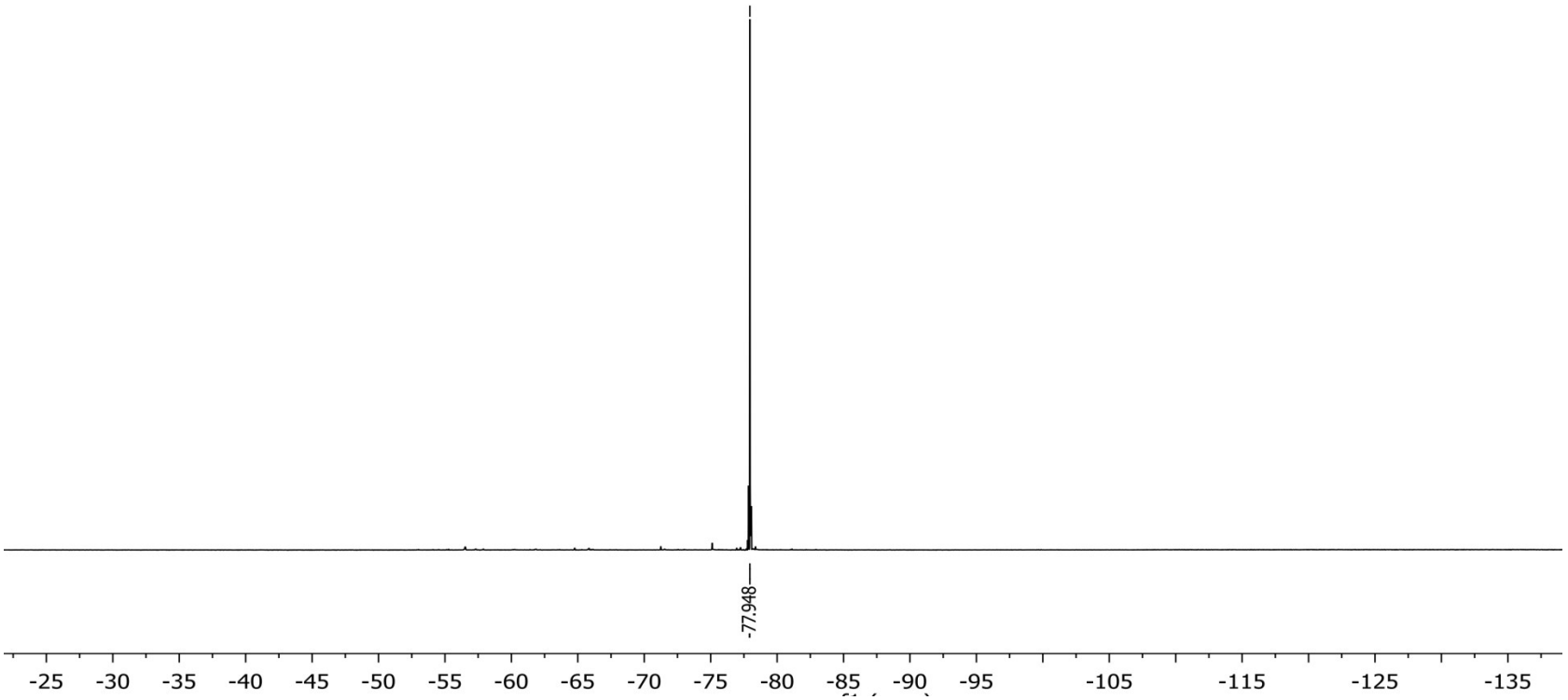

3.03
2.39
2.28
1.19
1.12
1.02
1.12
H2
H1
8.185
8.152
7.799
7.782
7.744
7.729
7.534
7.531
7.527
7.517
7.514
7.254
7.224
7.208
6.776
5.987
5.976
5.964
5.952
2.380
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

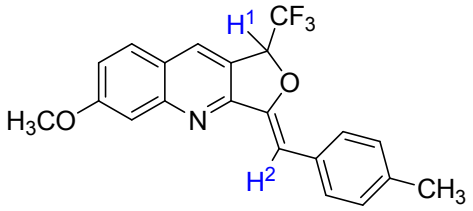

H1
CF3
O
Cl
N
H2
CH3
155.281
150.410
150.064
137.620
137.170
131.436
131.045
129.484
129.442
128.497
128.182
125.731
124.719
123.992
121.753
103.350
79.592
79.313
79.032
78.751
77.352
77.098
76.844
21.504
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

(5s)

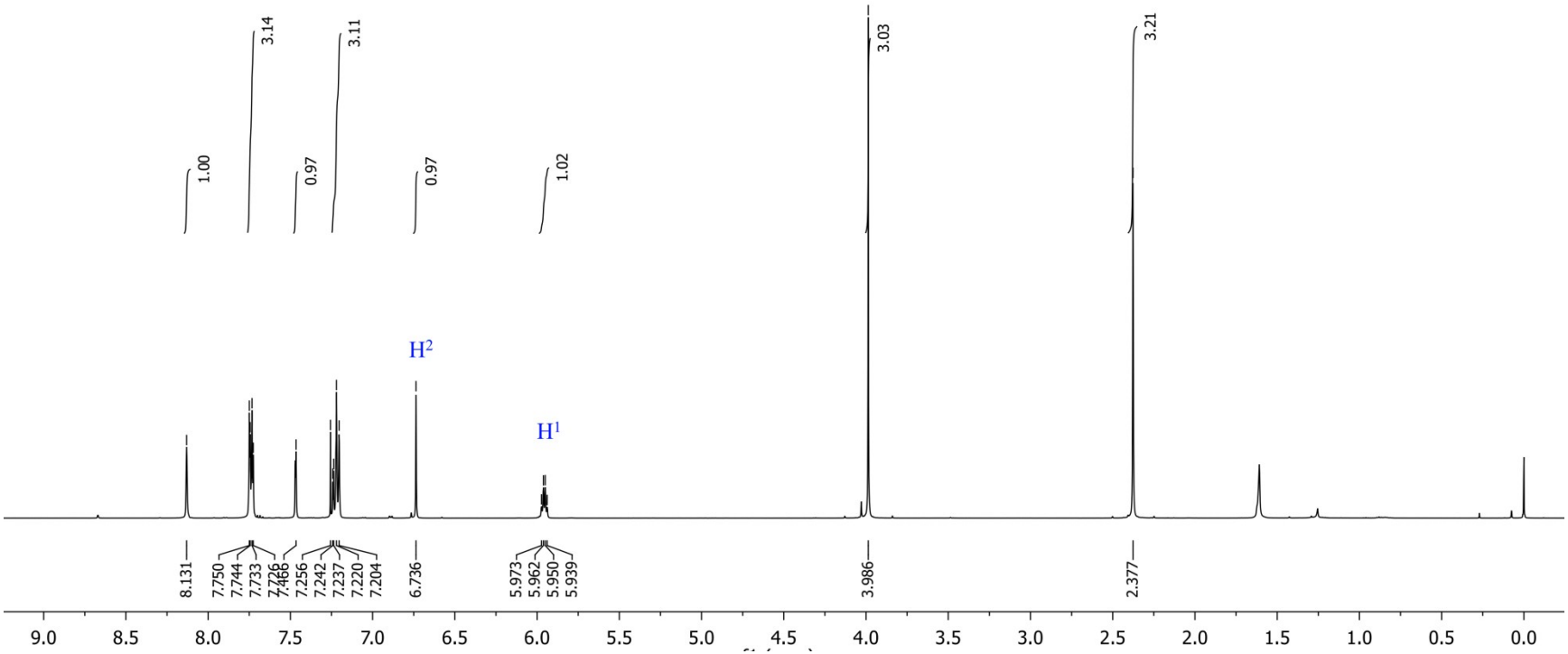

H1
CF3
O
Cl
N
H2
CH3

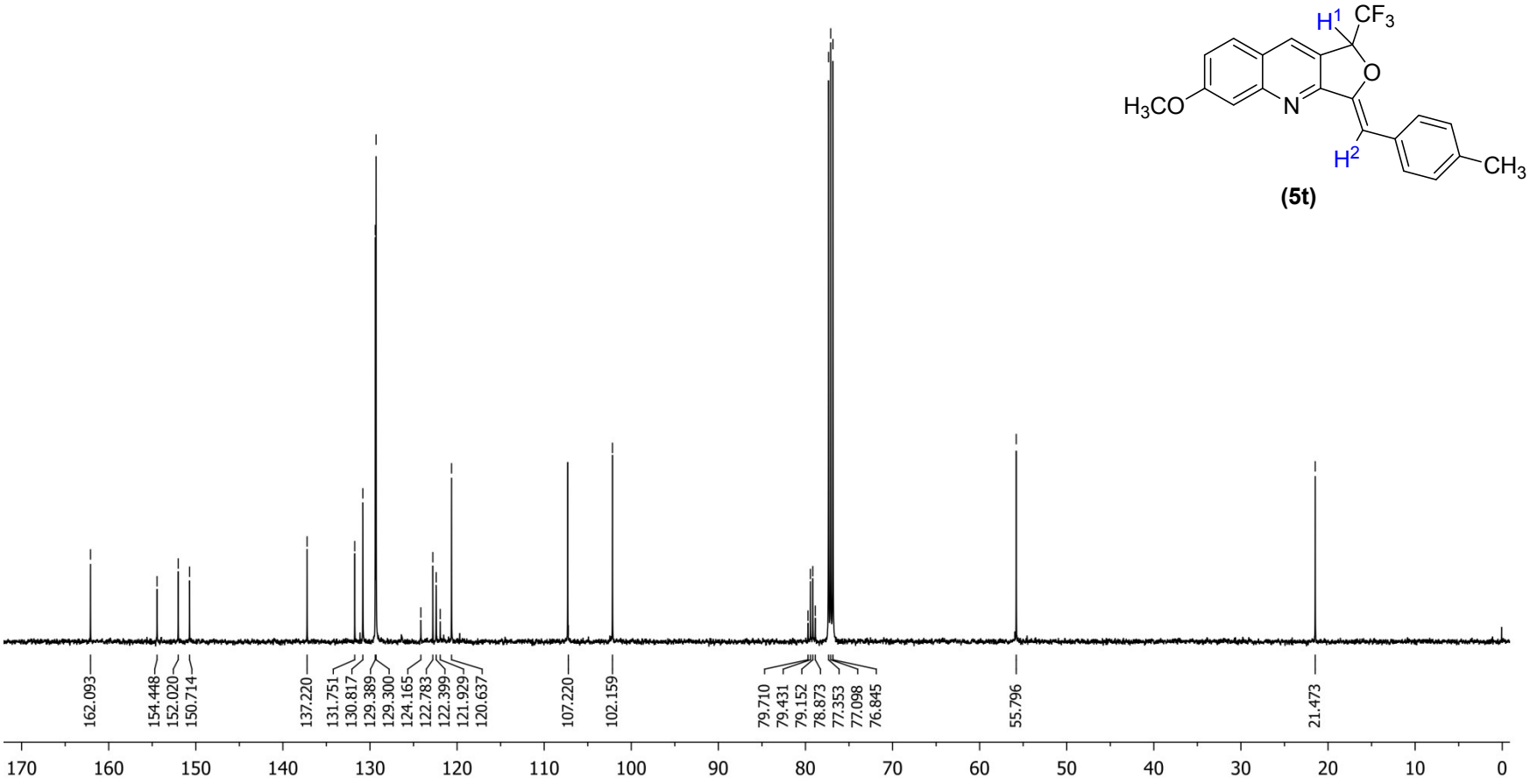
(5s)

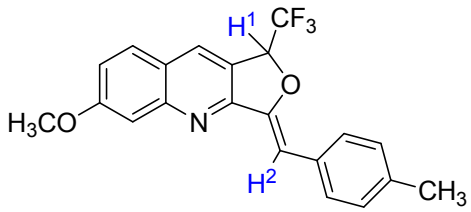

-77.948
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-105
-115
-125
-135


H1
CF3
O
H3CO
N
H2
CH3

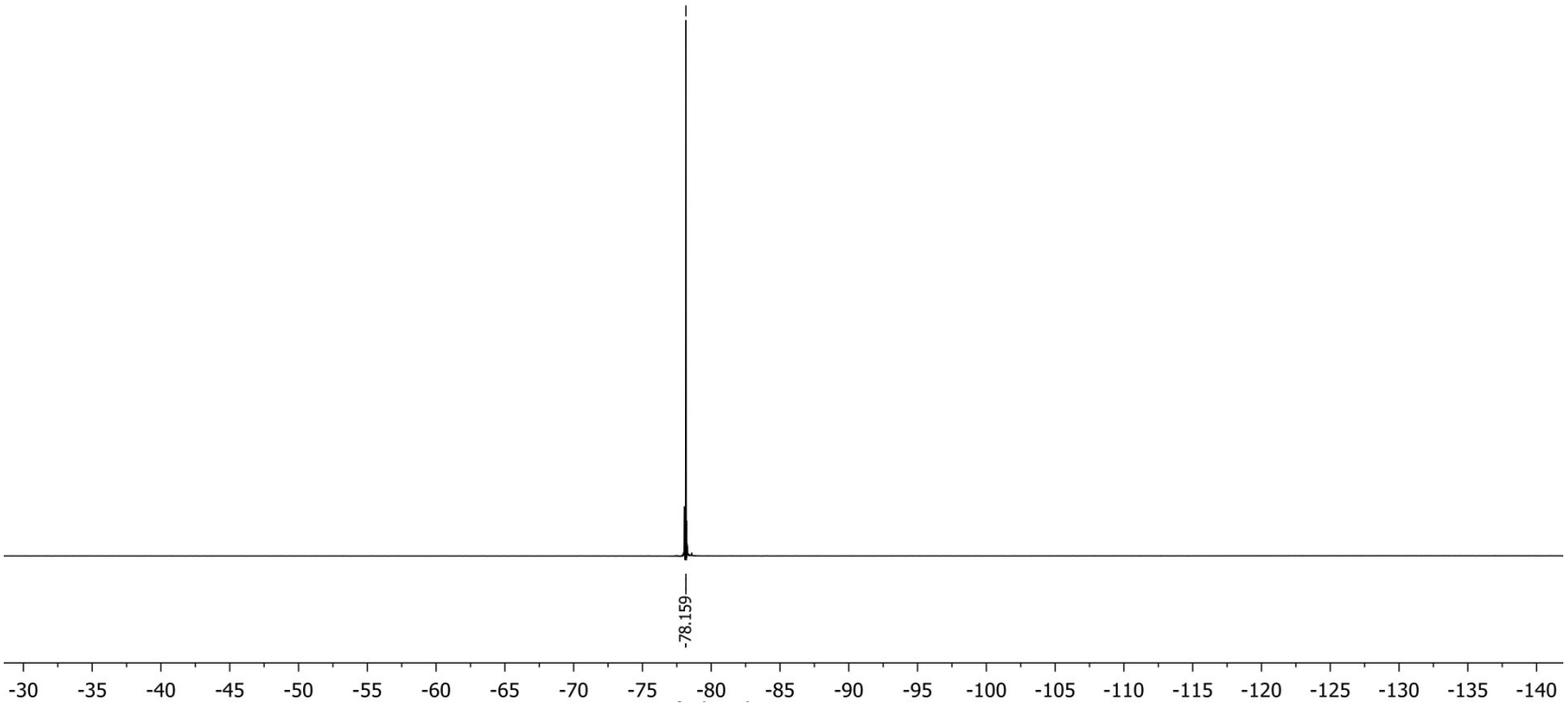
(5t)

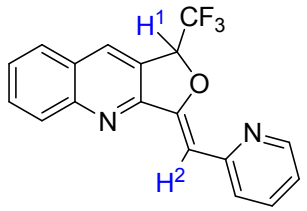

3.14
3.11
3.03
3.21
1.00
0.97
0.97
1.02
H2
H1
8.131
7.750
7.744
7.733
7.256
7.242
7.237
7.220
7.204
6.736
5.973
5.962
5.950
5.939
3.986
2.377
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


H1
CF3
O
H3CO
N
H2
CH3
(5t)
162.093
154.448
152.020
150.714
137.220
131.751
130.817
129.389
129.300
124.165
122.783
122.399
121.929
120.637
107.220
102.159
79.710
79.431
79.152
78.873
77.353
77.098
76.845
55.796
21.473
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

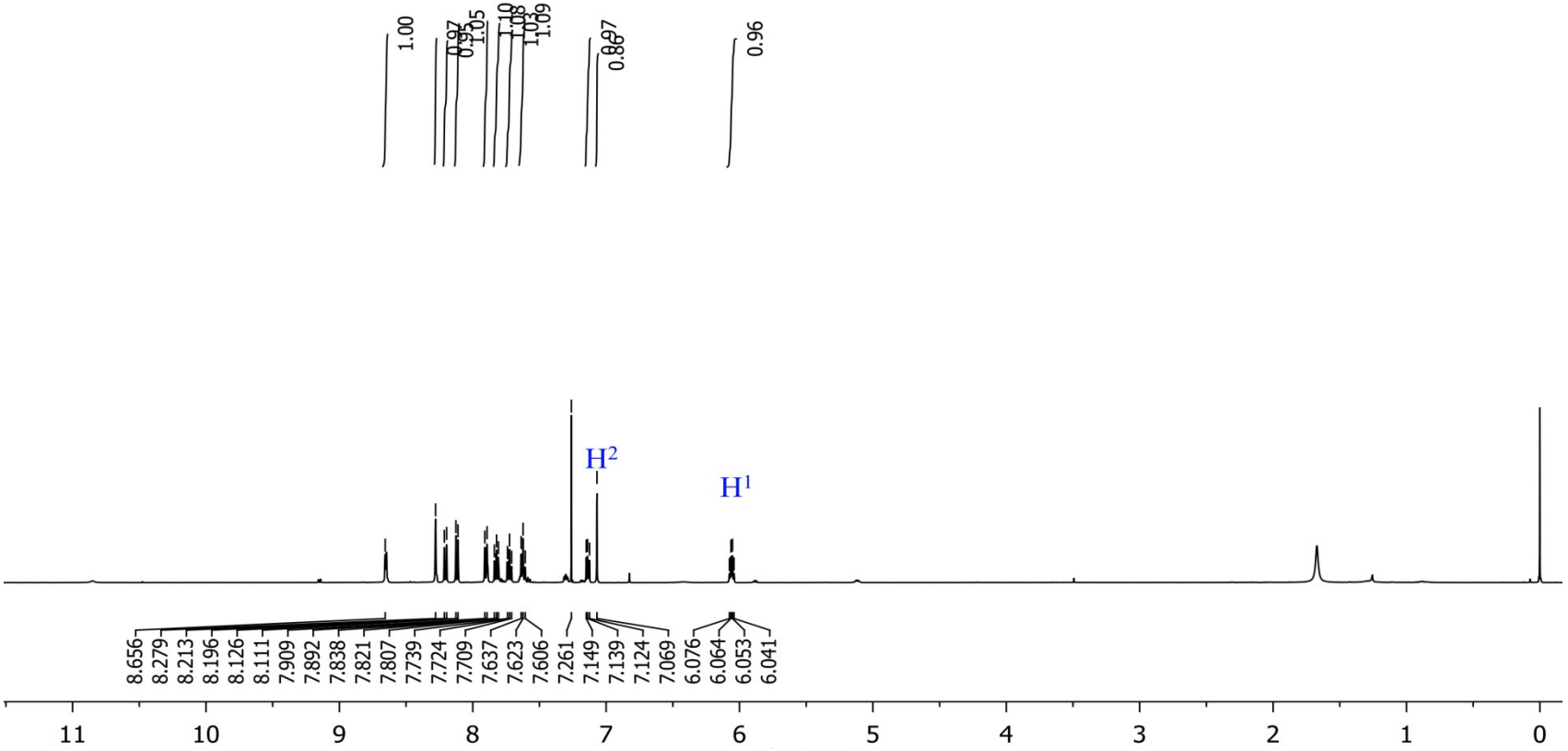

H1
CF3
O
H3CO
N
H2
CH3

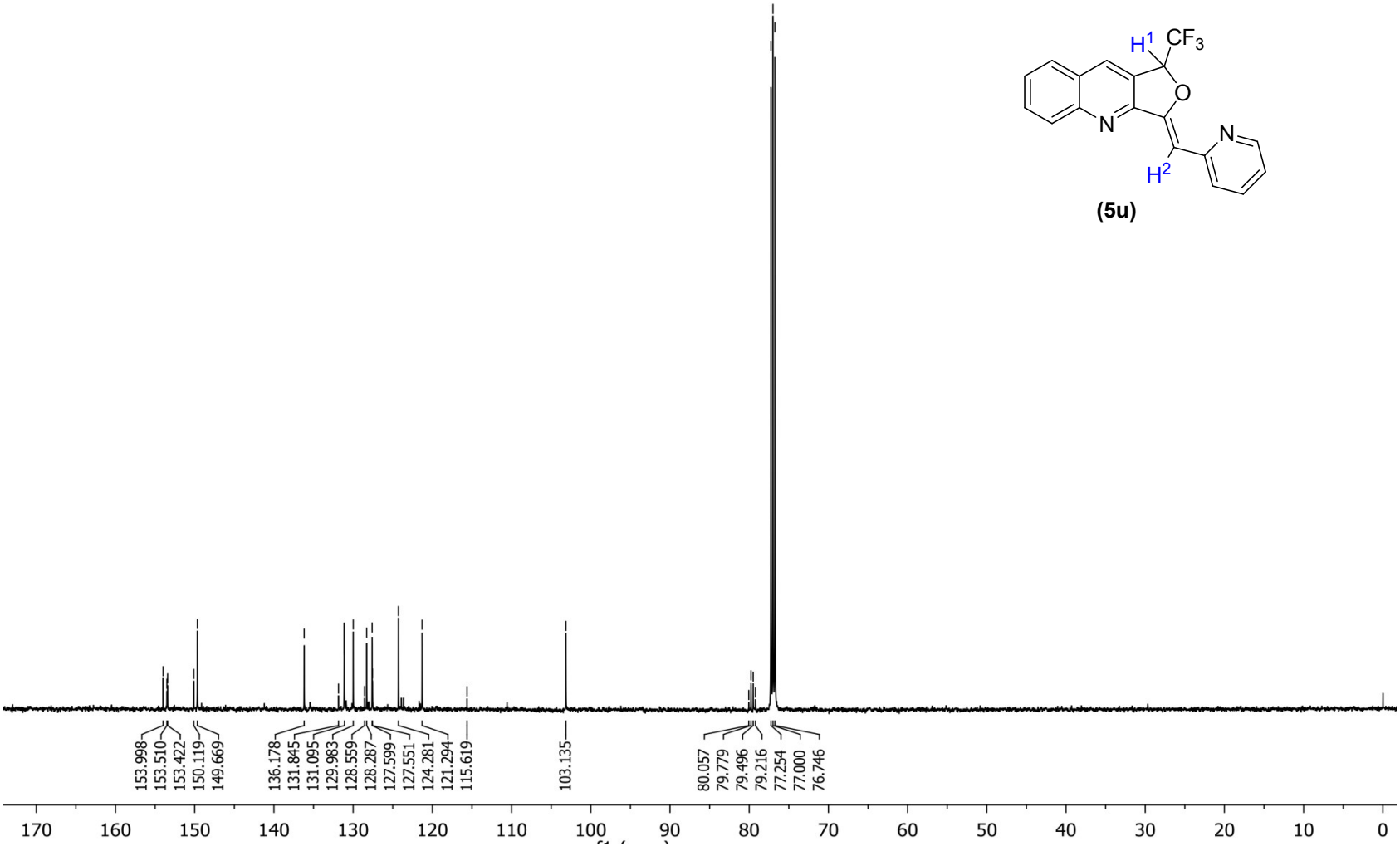
(5t)


-78.159
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140

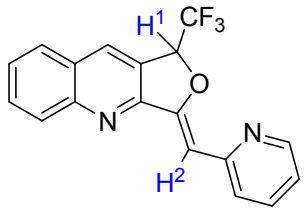

H1
CF3
O
N
N
H2

(5u)

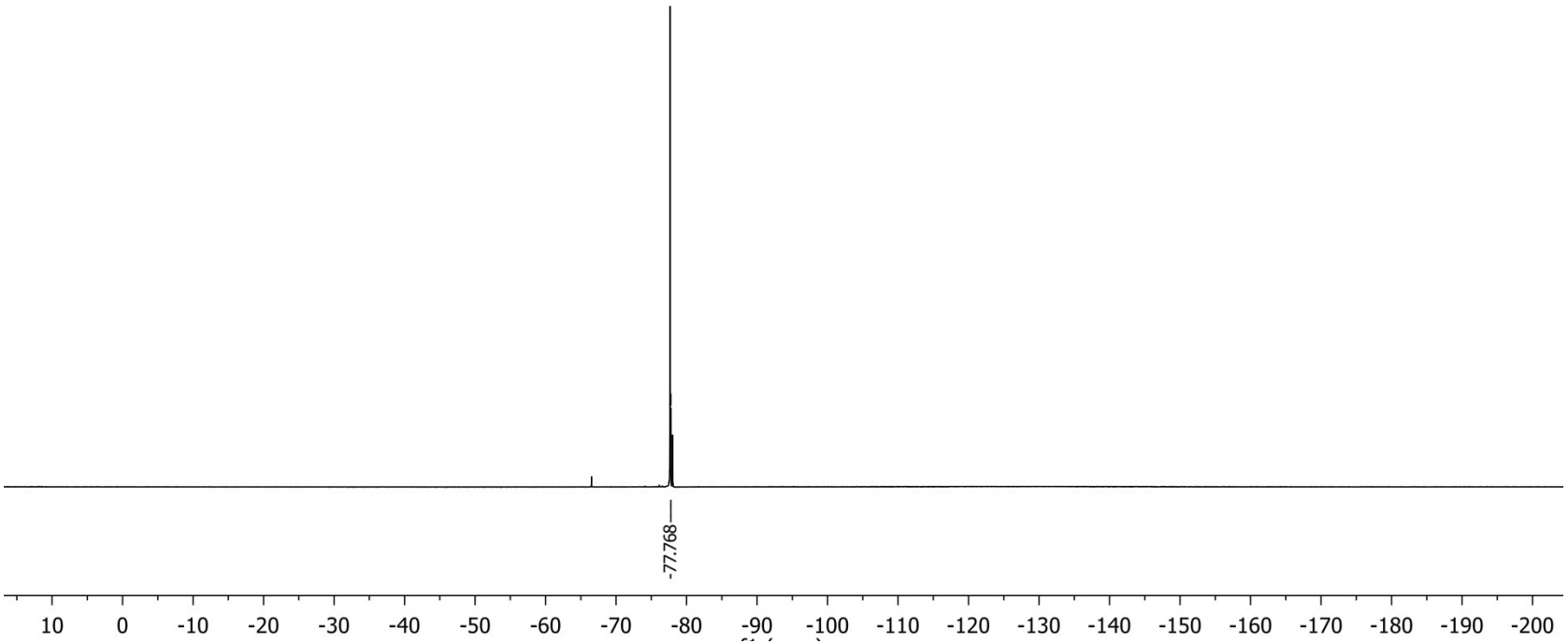

1.00
0.97
0.95
1.05
1.10
1.08
1.03
1.09
0.86
0.97
0.96
H2
H1
8.656
8.279
8.213
8.196
8.126
8.111
7.909
7.892
7.838
7.821
7.807
7.739
7.724
7.709
7.637
7.623
7.606
7.261
7.149
7.139
7.124
7.069
6.076
6.064
6.053
6.041
11
10
9
8
7
6
5
4
3
2
1
0

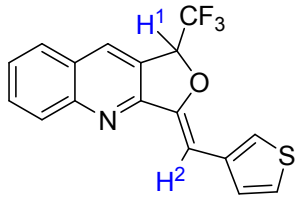

H1
CF3
O
N
N
H2
153.998
153.510
153.422
150.119
149.669
136.178
131.845
131.095
129.983
128.559
128.287
127.599
127.551
124.281
121.294
115.619
103.135
80.057
79.779
79.496
79.216
77.254
77.000
76.746
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

(5u)

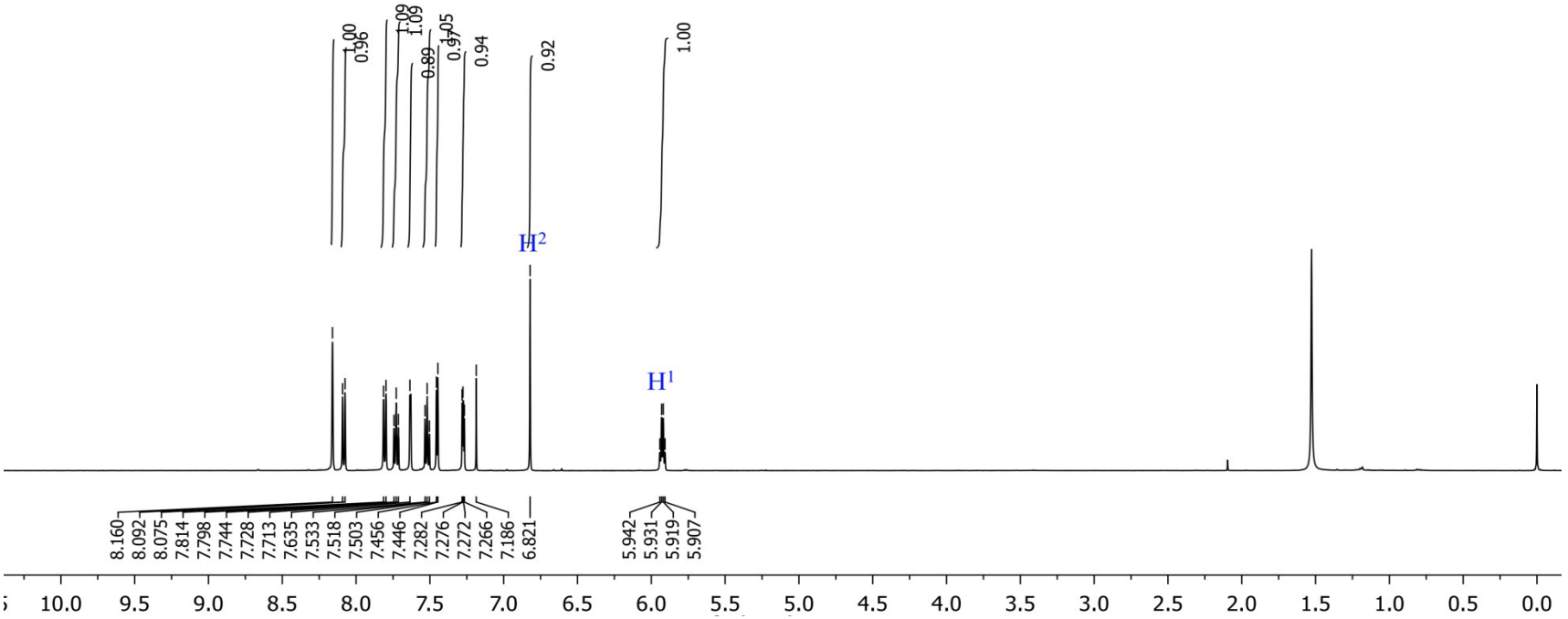

H1
CF3
O
N
N
H2

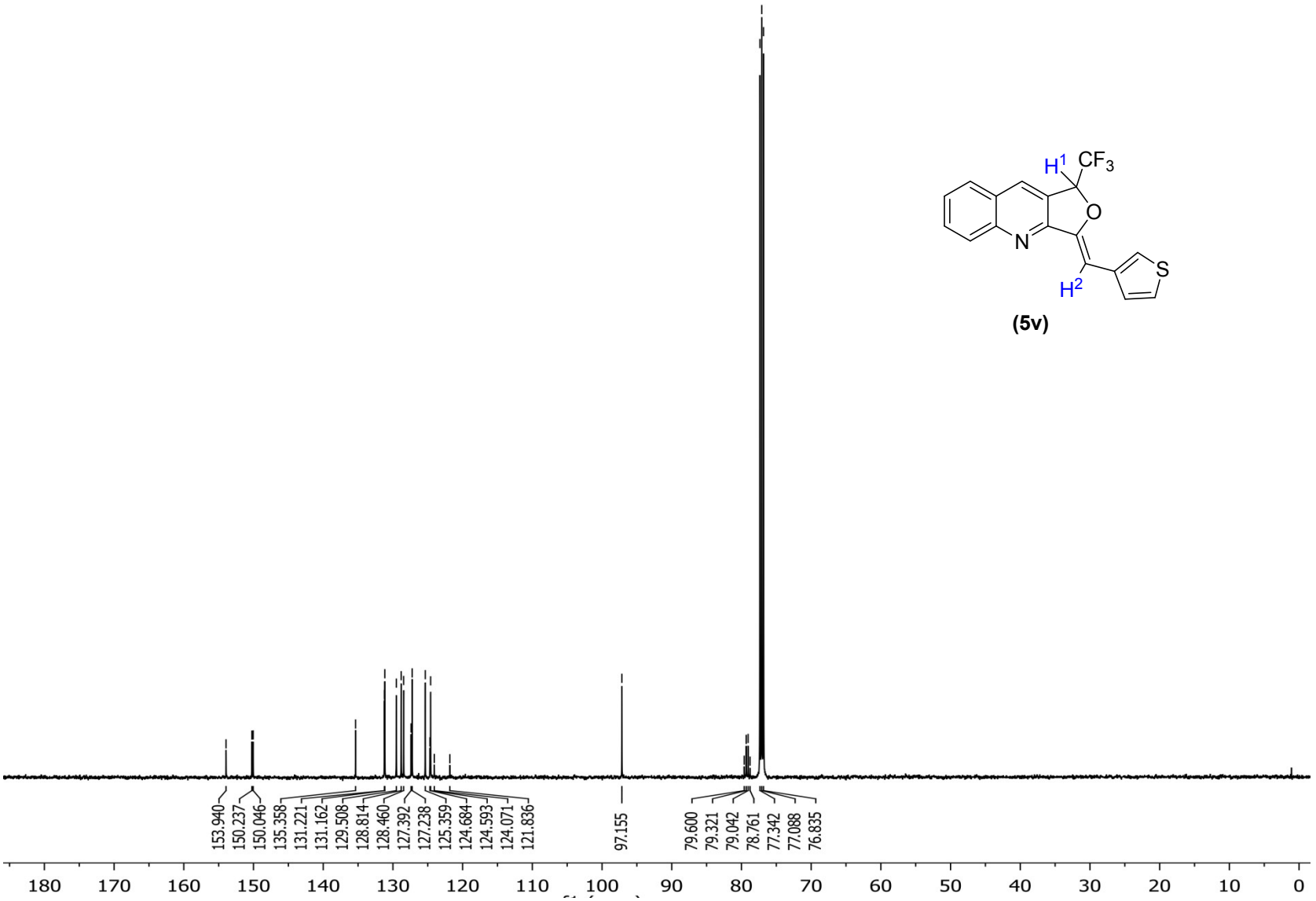
(5u)


-77.768
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200


H1
CF3
O
N
S
H2

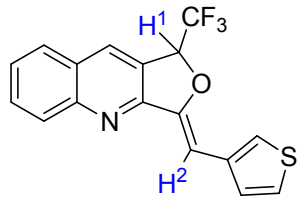
(5v)


1.00
0.96
1.09
1.09
0.89
1.05
0.97
0.94
0.92
1.00
H2
H1
8.160
8.092
8.075
7.814
7.798
7.744
7.728
7.713
7.635
7.533
7.518
7.503
7.456
7.446
7.282
7.276
7.272
7.266
7.186
6.821
5.942
5.931
5.919
5.907
10.0
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

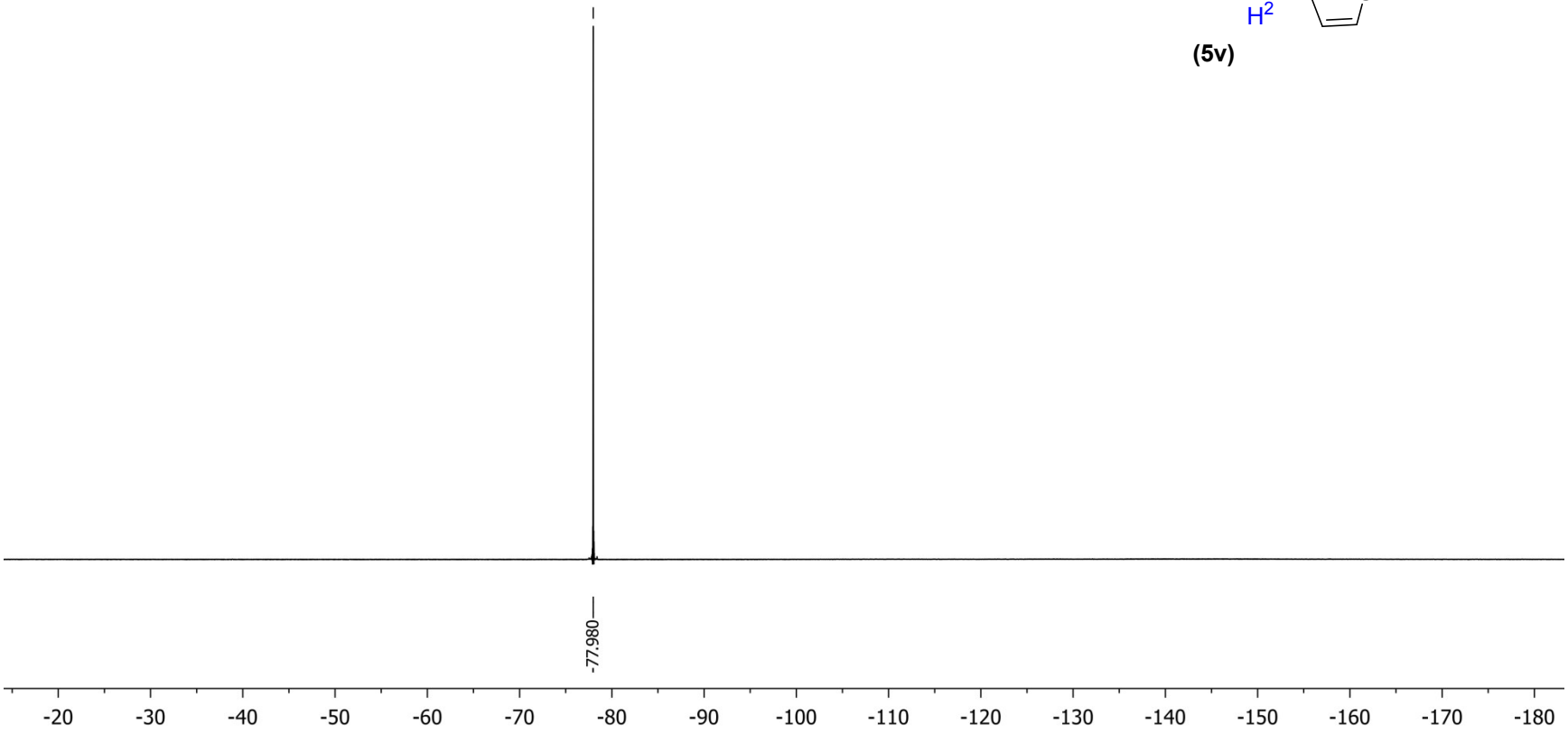

153.940
150.237
150.046
135.358
131.221
131.162
129.508
128.814
128.460
127.392
127.238
125.359
124.684
124.593
124.071
121.836
97.155
79.600
79.321
79.042
78.761
77.342
77.088
76.835
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

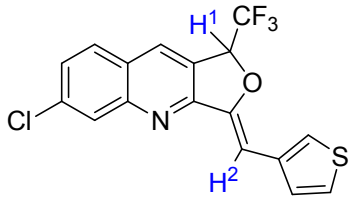
H1
CF3
O
N
S
H2

(5v)

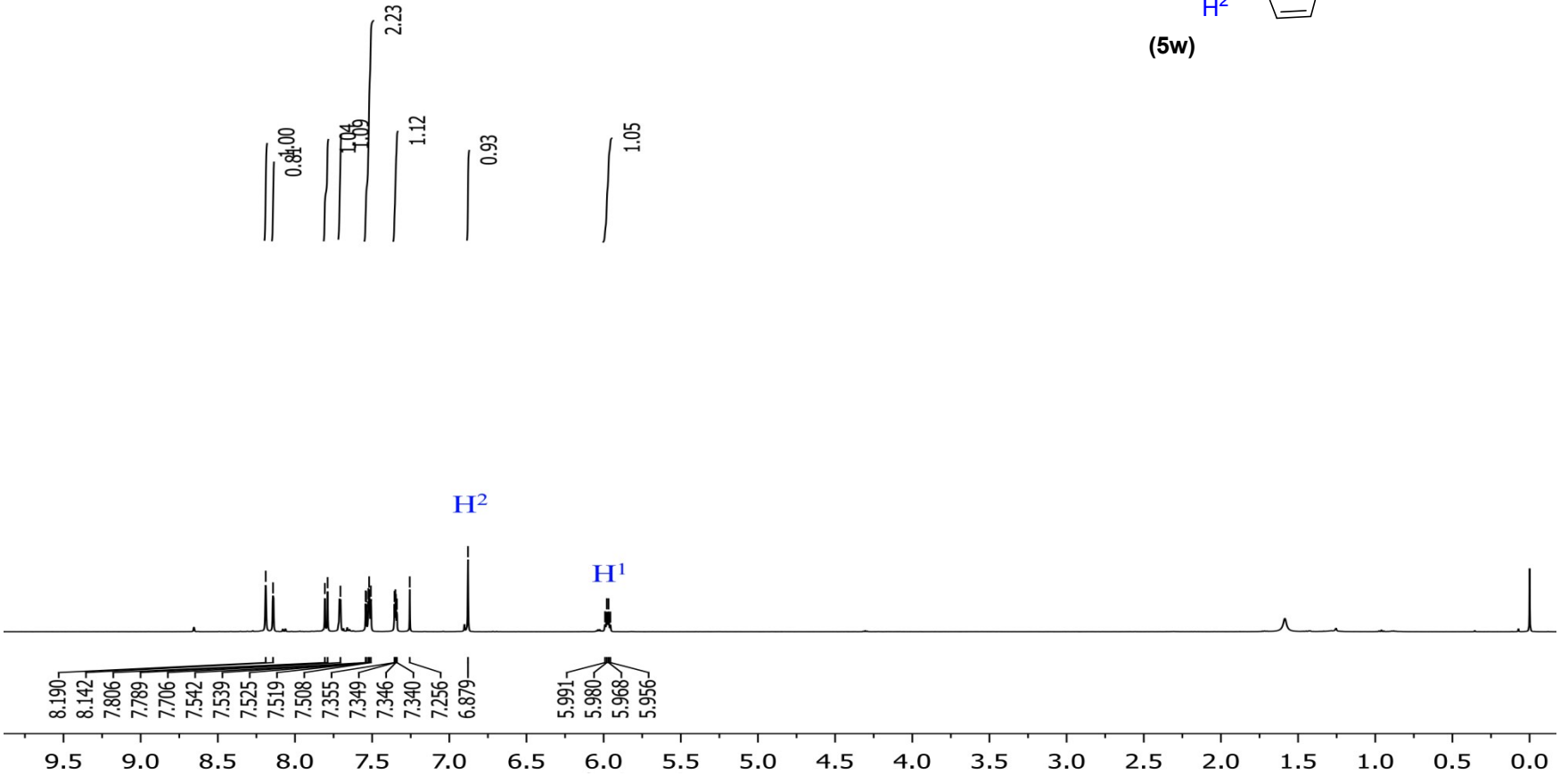

H1
CF3
O
N
S
H2

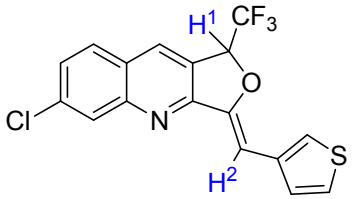
(5v)


-77.980
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180

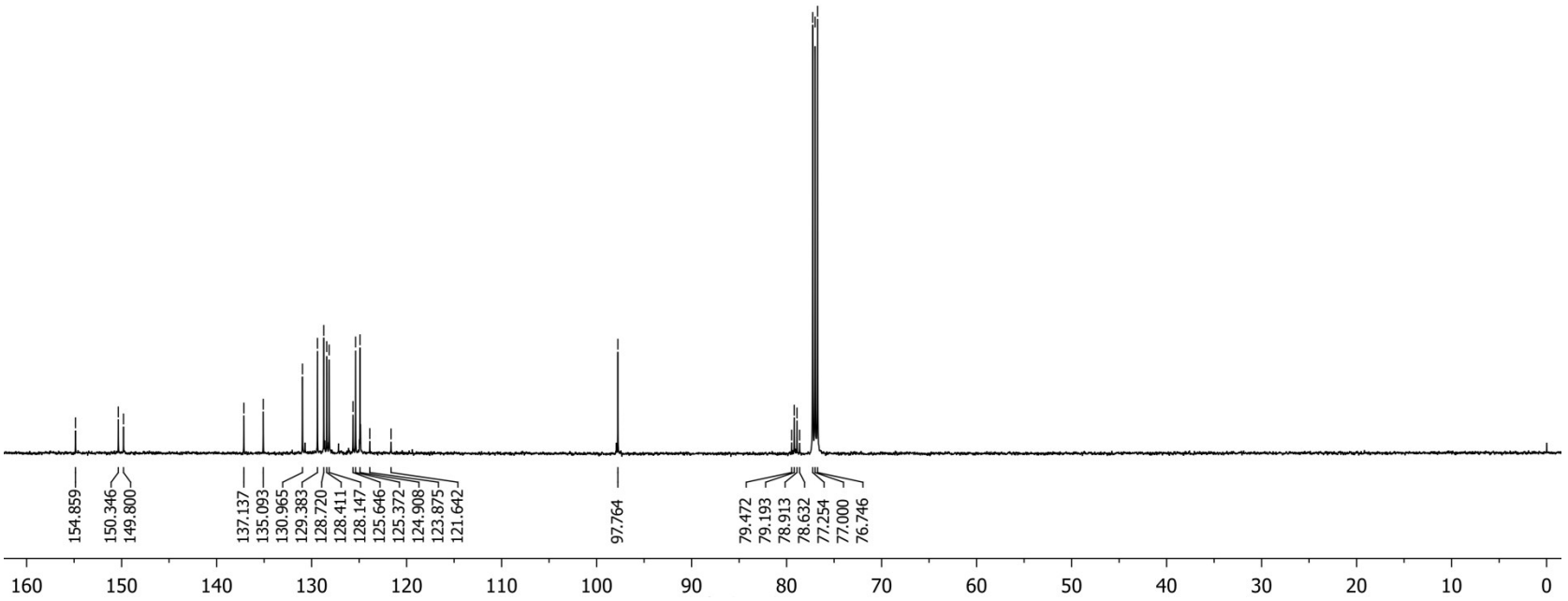

H1
CF3
O
Cl
N
S
H2

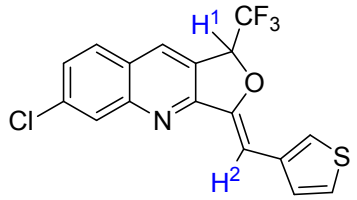
(5w)


2.23
1.12
0.93
1.05
H2
H1
8.190
8.142
7.806
7.789
7.706
7.542
7.539
7.525
7.519
7.508
7.355
7.349
7.346
7.340
7.256
6.879
5.991
5.980
5.968
5.956
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

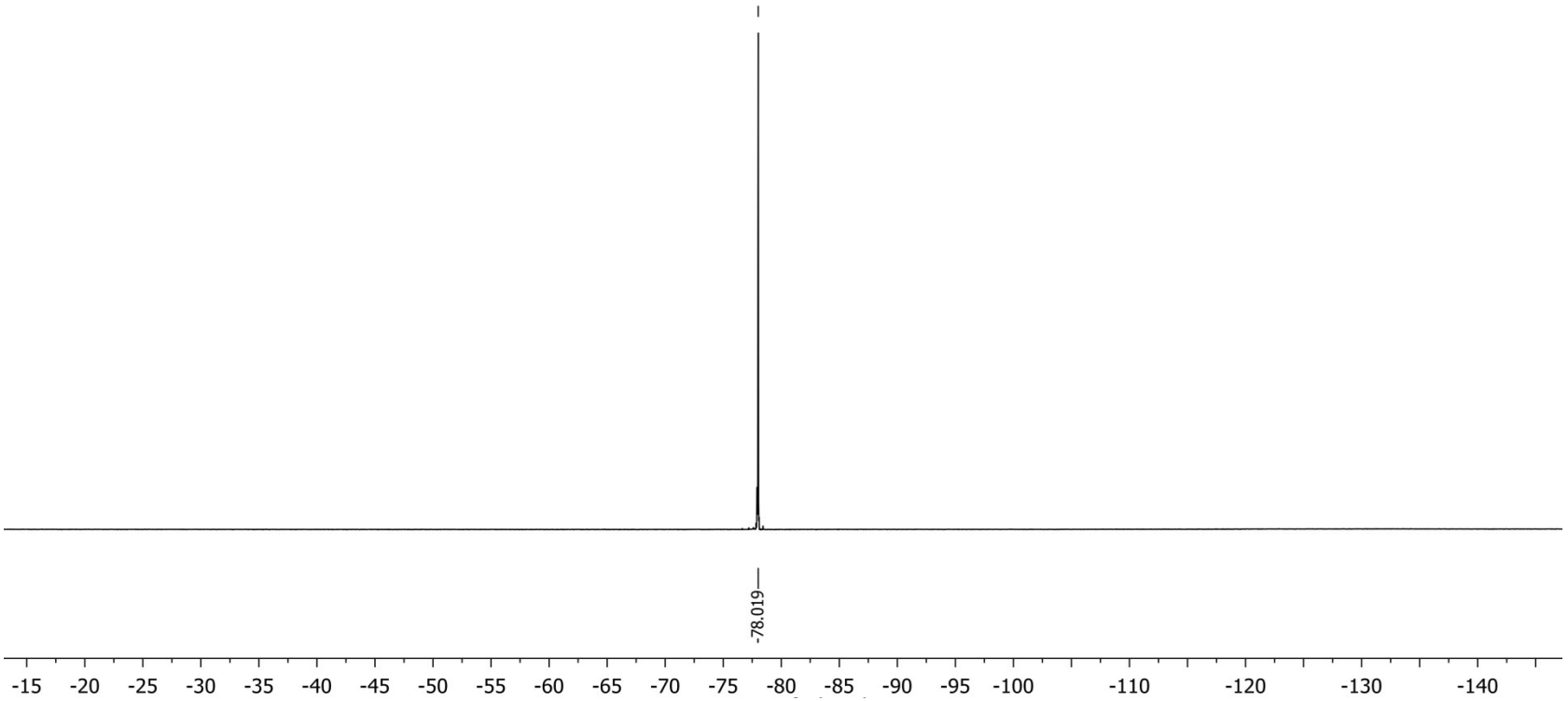

H1
CF3
O
Cl
N
S
H2

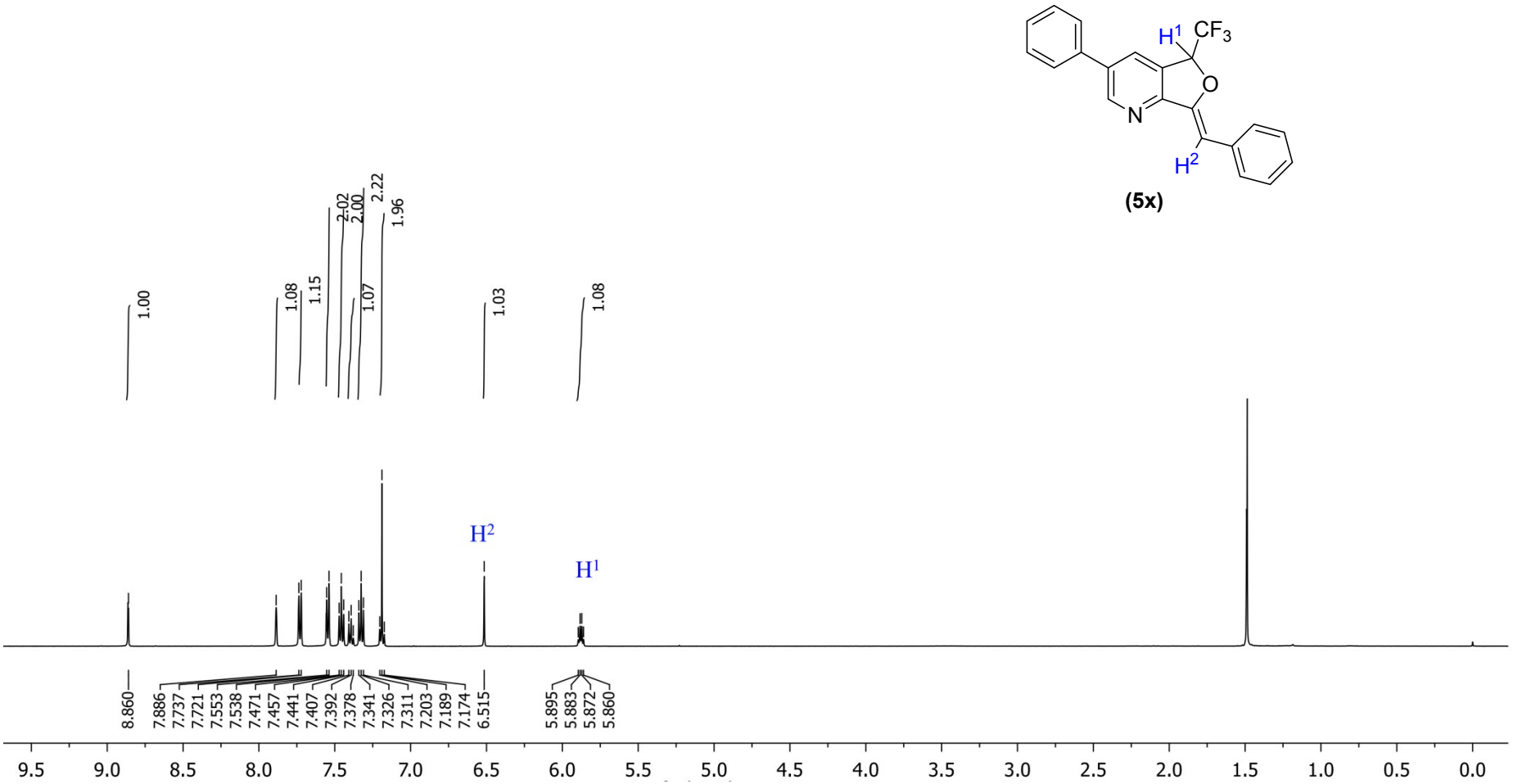
(5w)

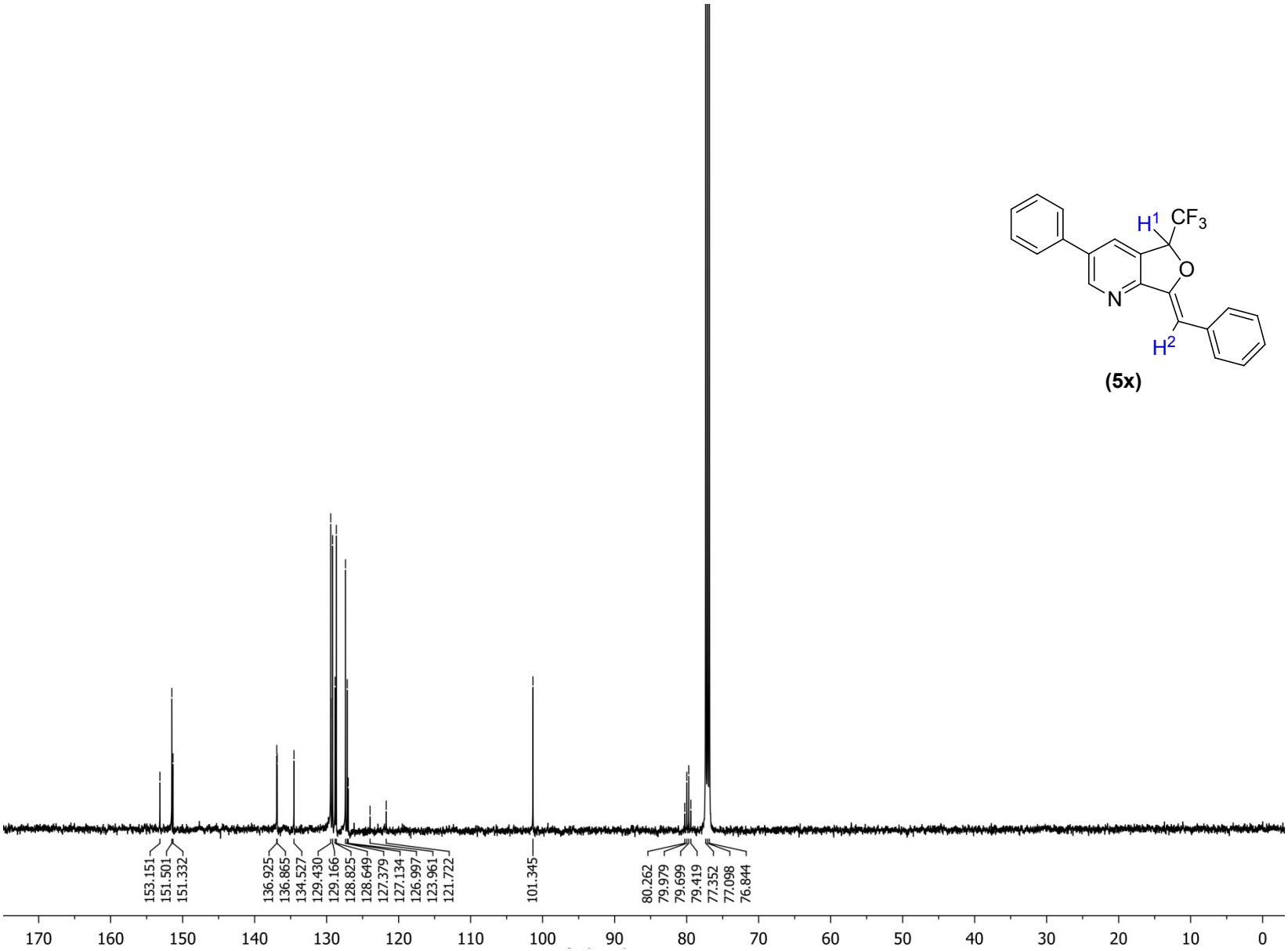

154.859
150.346
149.800
137.137
135.093
130.965
129.383
128.720
128.411
128.147
125.646
125.372
124.908
123.875
121.642
97.764
79.472
79.193
78.913
78.632
77.254
77.000
76.746
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


H1
CF3
O
Cl
N
S
H2

(5w)

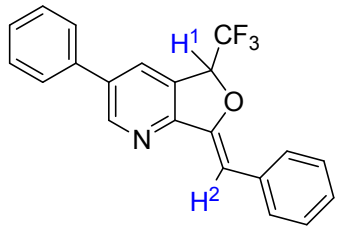

-78.019
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-110
-120
-130
-140


H1
CF3
O
N
H2
(5x)
1.00
1.08
1.15
2.02
2.00
1.07
2.22
1.96
1.03
1.08
H2
H1
8.860
7.886
7.737
7.721
7.553
7.538
7.471
7.457
7.441
7.407
7.392
7.378
7.341
7.326
7.311
7.203
7.189
7.174
6.515
5.895
5.883
5.872
5.860
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

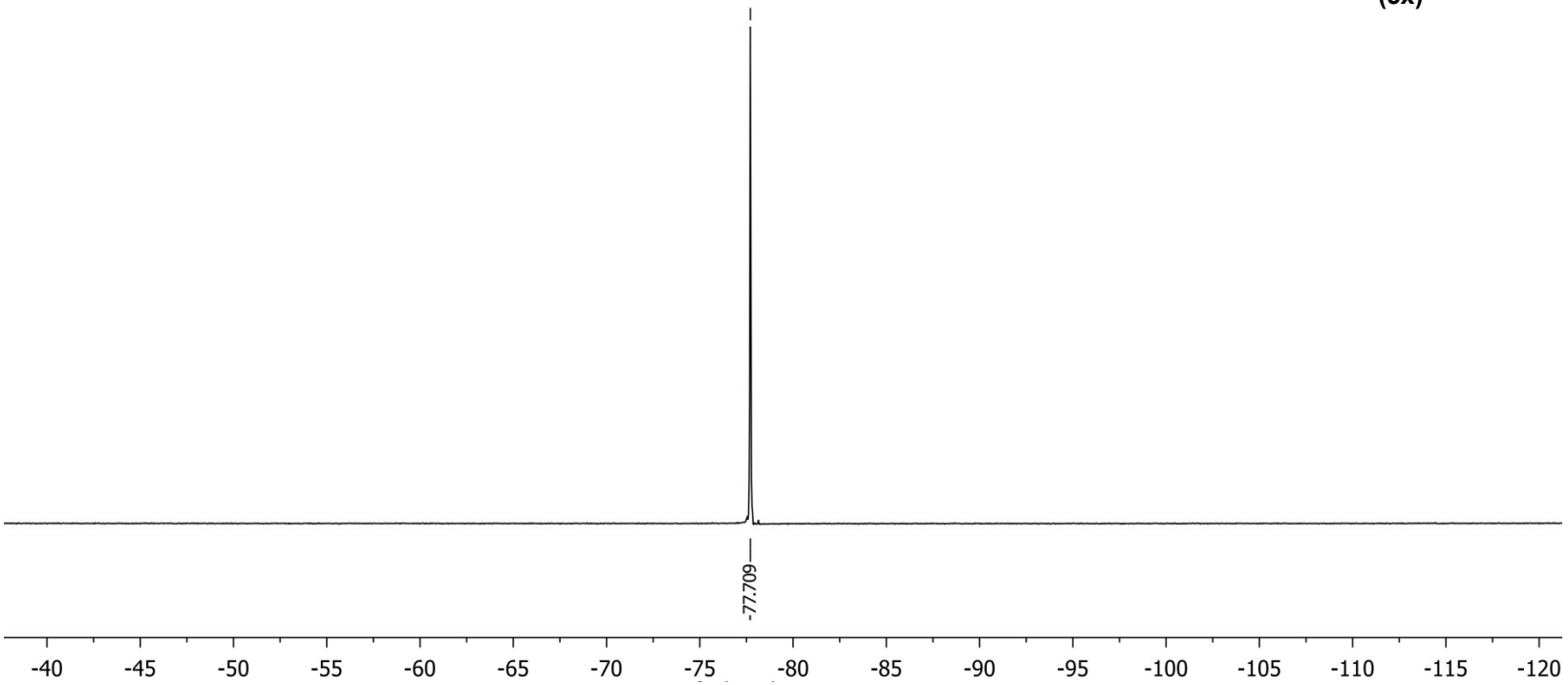

153.151
151.501
151.332
136.925
136.865
134.527
129.430
129.166
128.825
128.649
127.379
127.134
126.997
123.961
121.722
101.345
80.262
79.979
79.699
79.419
77.352
77.098
76.844
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

H1
CF3
O
N
H2

(5x)


H1
CF3
O
N
H2

(5x)


-77.709
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120