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Materials and methods

All reagents and solvents were commercial grade and purified prior to use when necessary. All 2-alkynyl alkyl sulfides (except for **5h** and **5q**) were prepared from the corresponding 2-iodoaryl alkyl sulfide and the corresponding alkyne according to the literature procedure.¹ Compounds **5h** and **5q** were prepared from 2-ethynylthioanisole and the corresponding aryl iodide according to the literature procedures.^{1b, 1c} 3-Amino-4-(methylthio)benzotrifluoride (**S4**) was obtained from Acros Organics and was used without further purification. 2-(Ethylthio)aniline (**S6**) was synthesized from 2-aminothiophenol according to literature procedure.² Gold(I) complexes, Au(IPr)Cl and Au(IPr)OH, were prepared as described by Nolan and co-workers.³

Thin layer chromatography (TLC) was performed using glass-backed silica gel (250 μm) plates and flash chromatography utilized 230–400 mesh silica gel from SiliCycle. UV light, and/or the use of potassium permanganate or phosphomolybdic acid solutions were used to visualize products. Anhydrous magnesium or sodium sulfate was used as a drying agent in extractions

Instrumentation

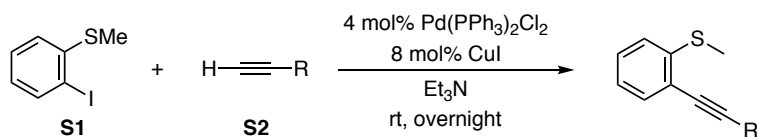
Nuclear magnetic resonance spectra (NMR) were acquired on Bruker FOURIER300 spectrometer. Chemical shifts are measured relative to residual solvent peaks as an internal standard set to δ 7.26 and δ 77.0 (CDCl_3) or δ 2.50 and 39.52 ($\text{DMSO}-d_6$) for ^1H and ^{13}C , respectively. Multiplicities are reported as singlet (s), doublet (d), triplet (t), quartet (q) or combinations thereof while higher coupling patterns are not abbreviated. Quantitative ^1H NMR measurements were performed according to literature procedure as described by Pauli⁴ and used methyl-2,5-dinitrobenzoate (Sigma–Aldrich, TraceCERT) as the internal standard.

Accurate mass measurements were conducted at MS Facility at UC Irvine. Component spectra for $[\text{M}+\text{H}]^+$ or $[\text{M}+\text{Na}]^+$ were lock mass calibrated to the nearest Na.PEG or Na.MePEH standards.

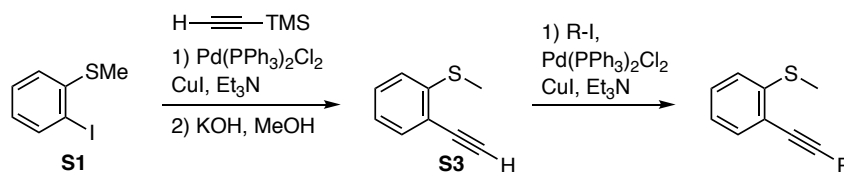
Infrared (IR) spectra were recorded on a Thermo Smart Orbit spectrophotometer and are reported in wavenumbers (cm^{-1}).

Experimental procedures

Synthesis of 2-alkynyl thioanisoles

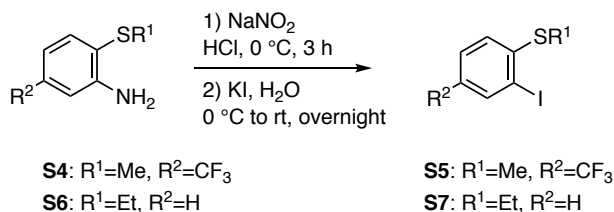


2-Iodothioanisole (**S1**, 1.00 equiv.), Pd(PPh₃)₂Cl₂ (0.04 equiv.) and CuI (0.02 equiv.) were added to a flame-dried, argon flushed flask and dissolved in triethylamine (0.3 M). The flask was flushed with argon and a solution of alkyne (**S2**, 1.10 equiv.) in triethylamine (1 mL) was added dropwise via syringe. The reaction was stirred under argon at rt overnight. The reaction mixture was filtered through Celite®, washed with ethyl acetate, and concentrated. The resulting residue was purified via flash chromatography (SiO₂, ethyl acetate in hexanes).

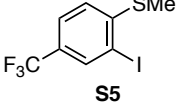
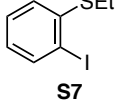
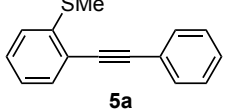
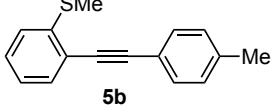
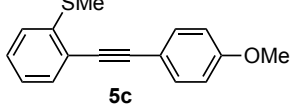
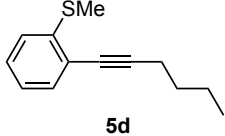


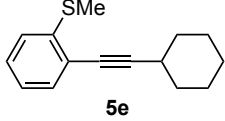

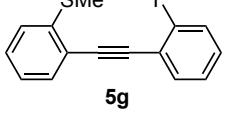
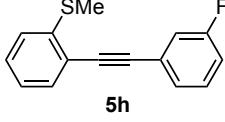
Compounds **5h** and **5q** were prepared by coupling of 2-alkynyl thioanisole (**S3**),^{1b,1c} with aryl iodide according to protocol described above. Compound **5s** and **5t** were prepared by coupling of phenylacetylene with (2-iodo-4-(trifluoromethyl)phenyl)(methyl)sulfane (**S5**) and ethyl(2-iodophenyl)sulfane (**S7**), respectively.

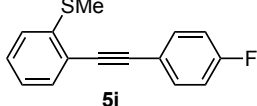
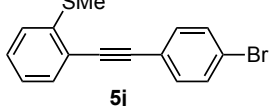
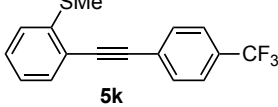
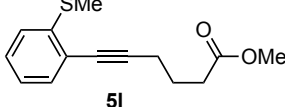
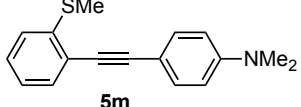
Synthesis of (2-iodo-4-(trifluoromethyl)phenyl)(methyl)sulfane (**S5**) and ethyl(2-iodophenyl)sulfane (**S7**)

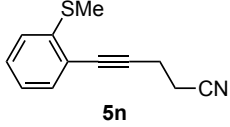
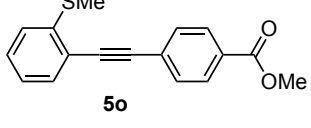
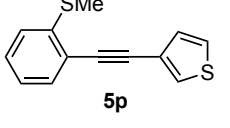
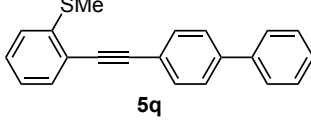
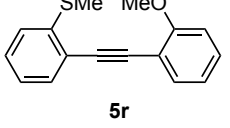


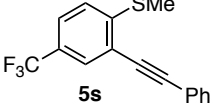
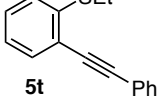
Aryl amines were converted to aryl iodides according to procedure by Shimizu and co-workers.² Substituted aniline (1.00 equiv.) was dissolved in conc. HCl (0.5 mL/mmol) and crushed ice (1 g/mL) was added. While stirring, a solution of sodium nitrite (0.90 equiv.) in water (4.5 mL) was slowly added to the mixture at 0 °C and stirred at room temperature for 2.5 h. To the diazonium salt was added a solution of potassium iodide (4.00 equiv.) in water (12 mL) and stirred overnight at room temperature. The reaction mixture was extracted with diethyl ether, washed with sodium thiosulfate, washed with water, dried with anhydrous sodium sulfate, and concentrated. The resulting oil was purified by flash column chromatography (SiO₂, ethyl acetate in hexanes).

 <p style="text-align: center;">S5</p>	<p>(2-Iodo-4-(trifluoromethyl)phenyl)(methyl)sulfane (S5): Yield 2.83 g (88%); brown oil. $R_f = 0.53$ (5% EtOAc/hexanes); IR (ATR) 2921, 1595, 1434 cm^{-1}; ^1H NMR (300 MHz, CDCl_3) δ 8.01 (dt, $J = 2.0, 0.8$ Hz, 1H), 7.59 (ddt, $J = 8.4, 2.1, 0.8$ Hz, 1H), 7.13 (d, $J = 8.3$ Hz, 1H), 2.51 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 148.73, 135.87 (q, $J = 4.1$ Hz), 127.59 (q, $J = 33.1$ Hz), 125.44, 124.20z, 123.23 (q, $J = 272.2$ Hz), 95.88, 16.90; HRMS (CI): Exact mass calcd for $\text{C}_8\text{H}_6\text{F}_3\text{IS}$ $[\text{M}]^+$ 317.9187, found 317.9172.</p>
 <p style="text-align: center;">S7</p>	<p>Ethyl(2-iodophenyl)sulfane (S7): Yield 1.87 g (63%); brown oil. $R_f = 0.61$ (5% EtOAc/hexanes); ^1H NMR (300 MHz, CDCl_3) δ 7.65–7.53 (m, 2H), 7.49 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.42–7.27 (m, 4H), 7.19 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.12 (td, $J = 7.5, 1.3$ Hz, 1H), 2.52 (s, 3H). This spectrum is in agreement with previously reported spectral data.²</p>
 <p style="text-align: center;">5a</p>	<p>2-(Phenylethynyl)thioanisole (5a): Yield 1.87 g (63%); brown oil. $R_f = 0.61$ (5% EtOAc/hexanes); ^1H NMR (300 MHz, CDCl_3) δ 7.65–7.53 (m, 2H), 7.49 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.42–7.27 (m, 4H), 7.19 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.12 (td, $J = 7.5, 1.3$ Hz, 1H), 2.52 (s, 3H). This spectrum is in agreement with previously reported spectral data.^{1b}</p>
 <p style="text-align: center;">5b</p>	<p>1-((4-Methylphenyl)ethynyl)-2-(methylsulfanyl)benzene (5b): Yield 1.42 g (99%); orange solid. $R_f = 0.41$ (1% EtOAc/hexanes); ^1H NMR (300 MHz, CDCl_3) δ 7.52–7.42 (m, 3H), 7.35–7.22 (m, 1H), 7.22–7.11 (m, 3H), 7.11 (td, $J = 7.5, 1.3$ Hz, 1H), 2.51 (s, 3H), 2.37 (s, 3H). This spectrum is in agreement with previously reported spectral data.^{1c}</p>
 <p style="text-align: center;">5c</p>	<p>1-((4-Methoxyphenyl)ethynyl)-2-(methylsulfanyl)benzene (5c): Yield 0.62 g (61%); brown solid. $R_f = 0.37$ (10% EtOAc/hexanes); ^1H NMR (300 MHz, CDCl_3) δ 7.57–7.46 (m, 2H), 7.46 (ddd, $J = 7.6, 1.5, 0.5$ Hz, 1H), 7.36–7.23 (m, 1H), 7.17 (dd, $J = 8.0, 1.3$ Hz, 1H), 7.10 (td, $J = 7.5, 1.3$ Hz, 1H), 6.94–6.83 (m, 2H), 3.83 (s, 3H), 2.51 (s, 3H). This spectrum is in agreement with previously reported spectral data.^{1c}</p>
 <p style="text-align: center;">5d</p>	<p>1-(Hex-1-yn-1-yl)-2-(methylsulfanyl)benzene (5d): Yield 0.58 g (39%); yellow oil. $R_f = 0.68$ (2% EtOAc/hexanes); ^1H NMR (300 MHz, CDCl_3) δ 7.35 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.24 (ddd, $J = 8.0, 7.3, 1.5$ Hz, 1H), 7.12 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.05 (td, $J = 7.5, 1.3$ Hz, 1H), 2.50 (t, $J = 6.8$ Hz, 2H), 2.47 (s, 3H), 1.72–1.58 (m, 2H), 1.58–1.43 (m, 2H), 0.96 (t, $J = 7.2$ Hz, 3H). This spectrum is in agreement with previously reported spectral data.^{1b}</p>

 <p style="text-align: center;">5e</p>	<p>1-(Cyclohexylethynyl)-2-(methylsulfanyl)benzene (5e): Yield 1.13 g (92%); yellow orange oil. $R_f = 0.63$ (10% EtOAc/hexanes);</p> <p>IR (ATR) 2924, 2850, 2360, 1462, 1434 cm^{-1};</p> <p>^1H NMR (300 MHz, CDCl_3) δ 7.37 (dd, $J=7.6, 1.5$ Hz, 1H), 7.24 (ddd, $J=8.3, 7.3, 1.5$ Hz, 1H), 7.11 (dd, $J=8.1, 1.3$ Hz, 1H), 7.05 (td, $J=7.5, 1.3$ Hz, 1H), 2.72 (tt, $J=8.8, 3.7$ Hz, 1H), 2.46 (s, 3H), 1.99 – 1.74 (m, 4H), 1.71 – 1.48 (m, 3H), 1.49 – 1.23 (m, 3H);</p> <p>^{13}C NMR (75 MHz, CDCl_3) δ 141.32, 132.12, 127.97, 124.02, 123.69, 122.07, 101.36, 78.20, 32.62, 29.88, 26.03, 24.77, 14.94;</p> <p>HRMS (CI): Exact mass calcd for $\text{C}_{15}\text{H}_{18}\text{S}$ $[\text{M}+\text{H}]^+$ 231.1207, found 231.1206.</p>
 <p style="text-align: center;">5f</p>	<p>tert-Butyl(dimethyl)((5-(2-(methylsulfanyl)phenyl)pent-4-yn-1-yl)oxy)silane (5f): Yield 0.571 g (44%); off-white oil. $R_f = 0.42$ (2% EtOAc/hexanes);</p> <p>IR (ATR) 2951, 2925, 2855, 1493, 1463, 1435 cm^{-1};</p> <p>^1H NMR (300 MHz, CDCl_3) δ 7.39–7.19 (m, 2H), 7.16–6.99 (m, 2H), 3.80 (t, $J = 6.1$ Hz, 2H), 2.57 (t, $J = 7.0$ Hz, 2H), 2.47 (s, 3H), 1.92–1.78 (m, 2H), 0.91 (s, 9H), 0.08 (s, 6H);</p> <p>^{13}C NMR (75 MHz, CDCl_3) δ; 146.35, 140.38, 139.50, 124.17, 123.51, 122.81, 122.24, 120.81, 62.09, 34.22, 27.23, 26.11, 18.47, -5.12, -5.15;</p> <p>HRMS (CI): Exact mass calcd for $\text{C}_{18}\text{H}_{28}\text{OSSiNa}$ $[\text{M}+\text{Na}]^+$ 343.1528, found 343.1423.</p>
 <p style="text-align: center;">5g</p>	<p>1-Fluoro-2-((2-(methylsulfanyl)phenyl)ethynyl)benzene (5g): Yield 1.13 g (77%); orange solid. Mp: 47-50; $R_f = 0.38$ (2% EtOAc/hexanes);</p> <p>IR (ATR) 3063, 2925, 2360, 2342, 1569, 1491, 1436, 1427 cm^{-1};</p> <p>^1H NMR (300 MHz, CDCl_3) δ; 7.65 – 7.47 (m, 2H), 7.39 – 7.28 (m, 2H), 7.21 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.19 – 7.04 (m, 3H), 2.53 (s, 3H);</p> <p>^{13}C NMR (75 MHz, CDCl_3) δ; 164.36, 161.02, 141.94, 133.65, 133.63, 132.63, 130.30, 130.19, 129.21, 124.50, 124.46, 124.11, 124.06, 121.27, 115.82, 115.55, 112.12, 111.91, 91.99, 91.95, 89.21, 15.33;</p> <p>HRMS (CI): Exact mass calcd for $\text{C}_{15}\text{H}_{11}\text{FS}$ $[\text{M}]^+$ 242.0565, found 242.0554.</p>
 <p style="text-align: center;">5h</p>	<p>1-((3-Fluorophenyl)ethynyl)-2-(methylsulfanyl)benzene (5h): Yield 0.48 mg (37%); yellow solid. $R_f = 0.31$ (2% EtOAc/hexanes); ^1H NMR (300 MHz, CDCl_3) δ 7.49 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.40–7.24 (m, 4H), 7.19 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.12 (td, $J = 7.5, 1.2$ Hz, 1H), 7.09–6.98 (m, 1H), 2.52 (s, 3H). This spectrum is in agreement with previously reported spectral data.⁵</p>

 <p style="text-align: center;">5i</p>	<p>1-((4-Fluorophenyl)ethynyl)-2-(methylsulfanyl)benzene (5i): Yield 0.64 g (66%); brown crystal solid. $R_f = 0.29$ (1% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.66–7.52 (m, 2H), 7.48 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.31 (td, $J = 7.7, 1.5$ Hz, 1H), 7.18 (dd, $J = 8.0, 1.3$ Hz, 1H), 7.12 (dd, $J = 8.2, 6.9$ Hz, 1H), 7.06 (td, $J = 8.5, 1.5$ Hz, 2H), 2.52 (s, 3H). This spectrum is in agreement with previously reported spectral data.^{1c}</p>
 <p style="text-align: center;">5j</p>	<p>1-((4-bromophenyl)ethynyl)-2-(methylsulfanyl)benzene (5j): Yield 1.52 g (74%); yellow crystal solid. $R_f = 0.31$ (5% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.53–7.39 (m, 5H), 7.32 (ddd, $J = 8.1, 7.4, 1.5$ Hz, 1H), 7.18 (d, $J = 7.9$ Hz, 1H), 7.12 (td, $J = 7.5, 1.3$ Hz, 1H), 2.52 (s, 3H). This spectrum is in agreement with previously reported spectral data.^{1c}</p>
 <p style="text-align: center;">5k</p>	<p>1-(Methylsulfanyl)-2-((4-(trifluoromethyl)phenyl)ethynyl)benzene (5k): Yield 1.20 g (86%); yellow solid. $R_f = 0.55$ (10% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.68 (dt, $J = 7.9, 0.8$ Hz, 2H), 7.66–7.56 (m, 2H), 7.50 (ddd, $J = 7.6, 1.6, 0.5$ Hz, 1H), 7.34 (ddd, $J = 8.1, 7.4, 1.5$ Hz, 1H), 7.20 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.13 (td, $J = 7.5, 1.2$ Hz, 1H), 2.53 (s, 3H). This spectrum is in agreement with previously reported spectral data.^{1c}</p>
 <p style="text-align: center;">5l</p>	<p>Methyl 6-(2-(methylsulfanyl)phenyl)hex-5-ynoate (5l): Yield 1.67 g (68%); yellow oil. $R_f = 0.18$ (5% EtOAc/hexanes);</p> <p>IR (ATR) 2949, 2921, 1732, 1464, 1434 cm^{-1};</p> <p>$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.49 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.39 (td, $J = 7.6, 1.4$ Hz, 1H), 7.29–7.22 (m, 1H), 7.18 (td, $J = 7.5, 1.3$ Hz, 1H), 3.82 (d, $J = 1.5$ Hz, 3H), 2.71 (td, $J = 7.2, 2.9$ Hz, 4H), 2.60 (s, 3H), 2.11 (td, $J = 14.6, 7.5$ Hz, 2H);</p> <p>$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ; 173.69, 145.15, 140.21, 139.47, 124.23, 123.66, 122.89, 122.24, 121.21, 121.18, 51.70, 51.64, 33.15, 30.05, 29.81, 26.21;</p> <p>HRMS (ESI): Exact mass calcd for $\text{C}_{14}\text{H}_{16}\text{O}_2\text{SNa}$ $[\text{M}+\text{Na}]^+$ 271.0769, found 271.0769.</p>
 <p style="text-align: center;">5m</p>	<p>N,N-Dimethyl-4-((2-(methylsulfanyl)phenyl)ethynyl)aniline (5m): Yield 0.74 g (76%); yellow solid. $R_f = 0.31$ (10% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.50 (d, $J=8.9$ Hz, 3H), 7.33 – 7.23 (m, 1H), 7.18 (dd, $J=8.1, 1.3$ Hz, 1H), 7.12 (td, $J=7.4, 1.3$ Hz, 1H), 6.68 (d, $J=8.9$ Hz, 2H), 2.99 (s, 6H), 2.52 (s, 3H) This spectrum is in agreement with previously reported spectral data.^{1b}</p>

 <p style="text-align: center;">5n</p>	<p>5-(2-(Methylsulfonyl)phenyl)pent-4-ynenitrile (5n): Yield 0.95 g (78%); green solid. $R_f = 0.40$ (20% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.38 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.29 (ddd, $J = 8.1, 7.4, 1.5$ Hz, 1H), 7.14 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.07 (td, $J = 7.5, 1.2$ Hz, 1H), 2.88 (ddd, $J = 7.8, 6.9, 1.0$ Hz, 2H), 2.70 (ddd, $J = 7.7, 6.8, 1.0$ Hz, 2H), 2.48 (s, 3H). This spectrum is in agreement with previously reported spectral data.^{1b}</p>
 <p style="text-align: center;">5o</p>	<p>Methyl 4-((2-(methylsulfonyl)phenyl)ethynyl)benzoate (5o): Yield 0.99 g (87%); Brown/yellow solid. $R_f = 0.34$ (10% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.07 – 7.97 (m, 2H), 7.67 – 7.57 (m, 2H), 7.48 (dd, $J = 7.7, 1.5$ Hz, 1H), 7.30 (ddd, $J = 8.0, 7.4, 1.5$ Hz, 1H), 7.16 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.10 (td, $J = 7.5, 1.2$ Hz, 1H), 3.90 (s, 3H), 2.49 (s, 3H). This spectrum is in agreement with previously reported spectral data.^{1c}</p>
 <p style="text-align: center;">5p</p>	<p>3-((2-(Methylsulfonyl)phenyl)ethynyl)thiophene (5p): Yield 0.68 g (64%); light green oil. $R_f = 0.26$ (1% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.47 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.37–7.25 (m, 3H), 7.18 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.11 (td, $J = 7.5, 1.2$ Hz, 1H), 7.02 (dd, $J = 5.1, 3.6$ Hz, 1H), 2.51 (s, 3H). This spectrum is in agreement with previously reported spectral data.^{1b}</p>
 <p style="text-align: center;">5q</p>	<p>4-((2-(Methylsulfonyl)phenyl)ethynyl)-1,1'-biphenyl (5q): Yield 0.69 g (64%); orange solid powder. Mp: 90-94; $R_f = 0.5$ (10% EtOAc/hexanes); IR (ATR) 3055, 1580, 1521, 1427 cm^{-1};</p> <p>$^1\text{H NMR}$ (300 MHz, CDCl_3) δ: 7.71–7.57 (m, 6H), 7.56–7.42 (m, 3H), 7.42–7.26 (m, 2H), 7.20 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.13 (td, $J = 7.5, 1.3$ Hz, 1H), 2.54 (s, 3H);</p> <p>$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ: 141.85, 141.27, 140.54, 132.38, 132.17, 129.00, 128.92, 127.78, 127.18, 127.16, 124.44, 124.33, 122.24, 121.56, 95.95, 87.74, 15.29;</p> <p>HRMS (CI): Exact mass calcd for $\text{C}_{14}\text{H}_{16}\text{NO}_2\text{S}$ [$\text{M}-\text{C}_6\text{H}_5-\text{CH}_3+\text{O}_2+3\text{H}+\text{NH}_4$]$^+$ 262.0896, found 262.0922.</p>
 <p style="text-align: center;">5r</p>	<p>1-methoxy-2-((2-(methylsulfonyl)phenyl)ethynyl)benzene (5r): Yield 1.14 g (74%); yellow crystal solid. $R_f = 0.37$ (2% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ (ppm) 7.54 (dddd, $J = 9.3, 7.6, 1.7, 0.5$ Hz, 1H), 7.37–7.23 (m, 1H), 7.19 (dd, $J = 8.0, 1.3$ Hz, 1H), 7.11 (td, $J = 7.4, 1.3$ Hz, 0H), 3.93 (s, 1H), 2.52 (s, 1H). This spectrum is in agreement with previously reported spectral data.⁶</p>

 <p style="text-align: center;">5s</p>	<p>Methyl(2-(phenylethynyl)-4-(trifluoromethyl)phenyl)sulfane (5s): Yield 1.04 g (71%); clear yellow solid. Mp: 41–42; $R_f = 0.57$ (5% EtOAc/hexanes);</p> <p>IR (ATR) 2356, 1774, 1576, 1490 cm^{-1};</p> <p>^1H NMR (300 MHz, CDCl_3) δ: 7.75 (dt, $J = 2.1, 0.6$ Hz, 1H), 7.68 – 7.58 (m, 2H), 7.53 (ddt, $J = 8.4, 1.5, 0.8$ Hz, 1H), 7.45 – 7.30 (m, 3H), 7.23 (d, $J = 8.4$ Hz, 1H), 2.54 (s, 3H);</p> <p>^{13}C NMR (75 MHz, CDCl_3) δ 147.0, 131.9, 129.1, 128.8, 128.6, 126.5 (q, $J = 31.3$ Hz), 125.2 (q, $J = 3.9$ Hz), 124.1 (q, $J = 271$ Hz), 123.48, 122.73, 121.43, 97.61, 85.65, 14.88;</p> <p>HRMS (CI): Exact mass calcd for $\text{C}_{16}\text{H}_{11}\text{F}_3\text{S}$ $[\text{M}]^+$ 292.0533, found 292.0548.</p>
 <p style="text-align: center;">5t</p>	<p>Ethyl(2-(phenylethynyl)phenyl)sulfane (5t): Yield 577 mg (49%); orange oil. $R_f = 0.29$ (2% EtOAc/hexanes);</p> <p>IR (ATR) cm^{-1}; 3080, 3055, 2966, 2925, 2869, 2853, 1597, 1580, 1570, 1557, 1490, 1459, 1441, 1434</p> <p>^1H NMR (300 MHz, CDCl_3) δ 7.67 – 7.56 (m, 2H), 7.53 (dt, $J = 7.6, 1.1$ Hz, 1H), 7.43 – 7.32 (m, 3H), 7.32 – 7.23 (m, 2H), 7.20 – 7.06 (m, 1H), 3.04 (q, $J = 7.4$ Hz, 2H), 1.40 (t, $J = 7.4$ Hz, 3H).</p> <p>^{13}C NMR (75 MHz, CDCl_3) δ 140.19, 132.62, 131.68, 128.68, 128.45, 128.39, 126.35, 124.86, 123.31, 122.56, 95.56, 87.30, 26.34, 14.01.</p> <p>HRMS (CI): Exact mass calcd for $\text{C}_{16}\text{H}_{14}\text{S}$ $[\text{M}]^+$ 238.0816, found 238.0807.</p>

Optimization of reaction conditions

Entry	Catalyst (mol%)	Additive	Solvent	T (°C)	Time (h)	Conv. (%) ^a	Yield (%) ^b
1	AuCl (5)	none	toluene	80	20	<5	—
2	Au(PPh ₃)Cl (5)	none	toluene	80	20	<5	—
3	Au(PPh ₃)BF ₄ (5)	none	toluene	80	20	<5	—
4	Au(IPr)OH (5)	none	toluene	80	20	<5	—
5	Au(IPr)OH (20)	none	toluene	80	20	15	—
6	Au(IPr)OH (5)	H ₂ O	toluene	80	20	<5	—
7	Au(IPr)OH (5)	MeOH	toluene	80	20	<5	—
8	none	AcOH	toluene	80	20	0	—
9	Au(IPr)OH (5)	AcOH	toluene	80	20	n.d.	>95
10	Au(IPr)OH (2)	AcOH	toluene	80	20	n.d.	>95
11	Au(IPr)OH (1)	AcOH	toluene	80	20	n.d.	>95
12	Au(IPr)OH (0.5)	AcOH	toluene	80	20	99	97
13	Au(IPr)OH (1)	AcOH	toluene	100	6	92	—
14	Au(IPr)OH (0.5)	AcOH	toluene	100	20	99	97
15	Au(IPr)Cl (0.5)	AcOH	toluene	100	20	99	90
16	Au(IPr)Cl (0.5)	AcOH	toluene	100	20	99	94
17	Au(IPr)OH (1)	AcOH	toluene	rt	20	<5	—
18	Au(IPr)Cl (1)	AcOH	toluene	70	6	38 ^a	—
19	Au(IPr)Cl (1)	AcOH	toluene	80	6	75 ^a	—
20	Au(IPr)Cl (1)	AcOH	none	80	6	91 ^a	—
21	Au(IPr)Cl (1)	AcOH	EtOH	80	6	29 ^a	—
22	Au(IPr)Cl (1)	AcOH	CH ₃ CN	80	6	22 ^a	—
23	Au(IPr)Cl (1)	—	AcOH	80	6	71 ^a	—
24	Au(IPr)Cl (1)	AcOH	EtOAc	80	6	18 ^a	—
25	Au(IPr)OH (5)	Et ₃ N	toluene	100	20	n.d.	—

n.d. = not determined

^a Determined by quantitative ¹H NMR spectroscopy as described by Pauli and co-workers⁴ using methyl-2,5-dinitrobenzoate as internal standard

Comparison of catalytic activity of Au(IPr)Cl and Au(IPr)OH by qHNMR

Gold(I) complex (67.0 μmol), 2-(phenylethynyl)thioanisole (0.670 mmol), glacial acetic acid (39.0 μL), and toluene- d_8 (630 μL) were added to a vial and the mixture was heated at 100 $^\circ\text{C}$. At time intervals listed below, an aliquot (10 μL) of the reaction mixture was removed and transferred to an NMR tube. To the tube was added qNMR standard (methyl-2,5-dinitrobenzoate, 500 μL , 9.9 mM in CDCl_3) and an ^1H NMR spectrum was acquired.

Concentration was calculated by first normalizing the integral value of the resonance for qNMR standard ($n\text{Int}_{\text{std}}$, singlet at 4.10 ppm) to 1.000 and then comparing this signal to the thioanisole SMe resonance (singlet at 2.55 ppm). Concentration of the substrate was calculated according to the following formula: $[\text{thioanisole}] = \text{Int}_{\text{SMe}} * [\text{std}]$, where $[\text{thioanisole}]$ is the molar concentration of the substrate analyte, Int_{SMe} is the integral value of thioanisoles SMe after the standard's signal is normalized, and $[\text{std}]$ is the molar concentration of qNMR standard in the sample (9.7 mM for all samples).

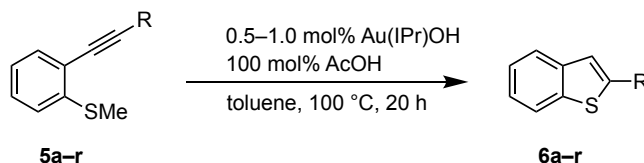
Table 1. Conversion of alkyne **5a** in reaction catalyzed by Au(IPr)Cl

Time (min)	nInt(std)	nInt(SMe)	Conc (mM)
0	1.000	1.473	14.3
60	1.000	1.437	14.0
120	1.000	1.085	10.6
180	1.000	0.948	9.23
240	1.000	0.689	6.71
360	1.000	0.365	3.55

Table 2. Conversion of alkyne **5a** in reaction catalyzed by Au(IPr)OH

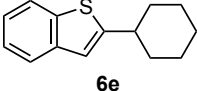
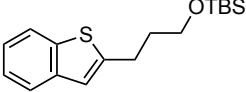
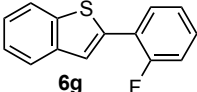
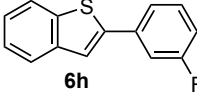
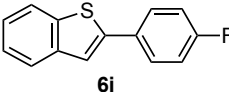
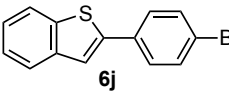
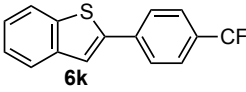
Time (min)	nInt(std)	nInt(SMe)	Conc (mM)
0	1.000	1.451	14.1
60	1.000	0.607	5.91
120	1.000	0.314	3.06
180	1.000	0.243	2.37
240	1.000	0.192	1.87
360	1.000	0.156	1.52

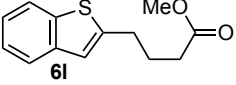
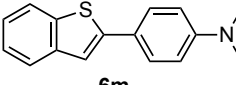
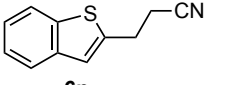
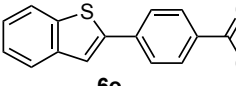
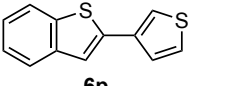
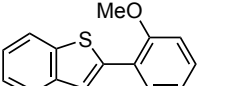
Gold(I)-catalyzed synthesis of benzo[b]thiophenes

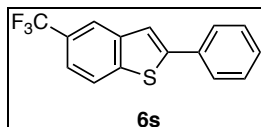


In a 2-dram vial was added the catalyst (2.50 μmol), alkyne (0.250 mmol) acetic acid (15.0 μL , 0.250 mmol) and toluene (240 μL). The vial was capped, and the mixture heated at 100 $^\circ\text{C}$ for 20 h. The mixture was then cooled to rt and the product was purified by flash column chromatography (SiO_2 , ethyl acetate in hexanes).

<p>6a</p>	<p>2-Phenyl-1-benzothiophene (6a): Yield 51.0 mg (97%); white solid. $R_f = 0.51$ (2% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.87 (ddd, $J = 7.2, 1.9, 0.8$ Hz, 1H), 7.85 – 7.79 (m, 1H), 7.79 – 7.72 (m, 2H), 7.59 (d, $J = 0.8$ Hz, 1H), 7.51 – 7.43 (m, 2H), 7.43 – 7.32 (m, 3H). This spectrum is in agreement with previously reported spectral data.⁷</p>
<p>6b</p>	<p>2-(4-Methylphenyl)-1-benzothiophene (6b): Yield 50.9 mg (89%); white solid. $R_f = 0.58$ (20% DCM/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.83 (ddd, $J = 7.4, 1.8, 0.8$ Hz, 1H), 7.80–7.72 (m, 1H), 7.70–7.57 (m, 2H), 7.52 (d, $J = 0.8$ Hz, 1H), 7.43–7.28 (m, 2H), 7.27–7.19 (m, 2H), 2.41 (s, 3H). This spectrum is in agreement with previously reported spectral data.⁸</p>
<p>6c</p>	<p>2-(4-Methoxyphenyl)-1-benzothiophene (6c): Yield 57.9 mg (94%); white solid. $R_f = 0.49$ (10% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.81 (ddd, $J = 7.5, 1.6, 0.7$ Hz, 1H), 7.74 (ddd, $J = 7.9, 1.7, 0.7$ Hz, 1H), 7.67 (dd, $J = 3.0, 2.2$ Hz, 1H), 7.63 (dd, $J = 2.8, 2.2$ Hz, 1H), 7.43 (d, $J = 0.8$ Hz, 1H), 7.37–7.25 (m, 2H), 6.97 (dd, $J = 3.1, 2.3$ Hz, 1H), 6.95 (dd, $J = 3.0, 2.2$ Hz, 1H), 3.86 (s, 3H). This spectrum is in agreement with previously reported spectral data.⁹</p>
<p>6d</p>	<p>2-Butyl-1-benzothiophene (6d): Yield 87.5 mg (92%); colorless oil. $R_f = 0.63$ (2% EtOAc/hexanes);</p> <p>IR (ATR) 3057, 2955, 2927, 2856 cm^{-1};</p> <p>$^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.85 (ddd, $J = 7.8, 1.4, 0.7$ Hz, 1H), 7.74 (dd, $J = 7.6, 1.6$ Hz, 1H), 7.46–7.27 (m, 2H), 7.07 (t, $J = 1.0$ Hz, 1H), 3.04–2.91 (m, 2H), 1.90–1.73 (m, 2H), 1.51 (dt, $J = 14.5, 7.3$ Hz, 2H), 1.05 (t, $J = 7.3$ Hz, 3H);</p> <p>$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 146.90, 140.36, 139.43, 124.11, 123.42, 122.75, 122.20, 120.50, 33.34, 30.59, 22.33, 13.94;</p> <p>HRMS (CI): Exact mass calcd for $\text{C}_{12}\text{H}_{14}\text{S}$ $[\text{M}+]$⁺ 190.0816, found 190.0816.</p>

 <p style="text-align: center;">6e</p>	<p>2-Cyclohexyl-1-benzothiophene (6e): Yield 98.3 mg (91%); white solid. $R_f = 0.56$ (2% EtOAc/hexanes); $^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.81 (dd, $J = 8.0, 1.0$ Hz, 1H), 7.75–7.67 (m, 1H), 7.39–7.28 (m, 1H), 7.27 (td, $J = 7.5, 1.5$ Hz, 1H), 7.04 (s, 1H), 3.02–2.82 (m, 1H), 2.24–2.09 (m, 2H), 1.90 (dt, $J = 11.8, 3.0$ Hz, 2H), 1.79 (dddd, $J = 12.4, 5.0, 3.2, 1.5$ Hz, 1H), 1.67–1.23 (m, 5H). This spectrum is in agreement with previously reported spectral data.¹⁰</p>
 <p style="text-align: center;">6f</p>	<p>(3-(1-benzothiophen-2-yl)propoxy)(tert-butyl)dimethylsilane (6f): Yield (200 mg scale) 109.6 mg (57%); colorless oil. $R_f = 0.42$ (2% EtOAc/hexanes); IR (ATR) 2950, 2927, 2854, 1435 cm^{-1};</p> <p>$^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.80 (ddt, $J = 7.7, 1.6, 0.8$ Hz, 1H), 7.74 – 7.65 (m, 1H), 7.41 – 7.21 (m, 2H), 7.05 (q, $J = 1.0$ Hz, 1H), 3.74 (t, $J = 6.1$ Hz, 2H), 3.03 (ddd, $J = 7.7, 7.0, 1.1$ Hz, 2H), 2.11 – 1.92 (m, 2H), 0.97 (s, 9H), 0.12 (s, 6H);</p> <p>$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 173.69, 145.15, 140.21, 139.47, 124.23, 123.66, 122.89, 122.24, 121.21, 121.18, 51.70, 51.64, 33.15, 30.05, 29.81, 26.21;</p> <p>HRMS (ESI): Exact mass calcd for $\text{C}_{17}\text{H}_{26}\text{OSSi}$ [$\text{M}+\text{Na}$]$^+$ 343.1528, found 343.1523.</p>
 <p style="text-align: center;">6g</p>	<p>2-(2-Fluorophenyl)-1-benzothiophene (6g): Yield 49.7 mg (87%); white solid. $R_f = 0.54$ (2% EtOAc/hexanes); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.91–7.78 (m, 2H), 7.77–7.67 (m, 2H), 7.44–7.27 (m, 3H), 7.25–7.14 (m, 2H). This spectrum is in agreement with previously reported spectral data.¹⁰</p>
 <p style="text-align: center;">6h</p>	<p>2-(3-fluorophenyl)-1-benzothiophene (6h): Yield 48.2 mg (84%); white solid. $R_f = 0.54$ (2% EtOAc/hexanes); $^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.92–7.68 (m, 2H), 7.56 (d, $J = 0.8$ Hz, 1H), 7.50 (ddd, $J = 7.8, 1.7, 1.0$ Hz, 1H), 7.46–7.29 (m, 4H), 7.04 (tdd, $J = 8.3, 2.6, 1.0$ Hz, 1H). This spectrum is in agreement with previously reported spectral data.¹¹</p>
 <p style="text-align: center;">6i</p>	<p>2-(4-Fluorophenyl)-1-benzothiophene (6i): Yield 44.2 mg (74%); white solid. $R_f = 0.50$ (2% EtOAc/hexanes); $^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.82 (ddd, $J = 7.2, 1.9, 0.8$ Hz, 1H), 7.79 – 7.71 (m, 1H), 7.71 – 7.61 (m, 2H), 7.46 (d, $J = 0.7$ Hz, 1H), 7.40 – 7.27 (m, 2H), 7.17 – 7.05 (m, 2H). This spectrum is in agreement with previously reported spectral data.⁷</p>
 <p style="text-align: center;">6j</p>	<p>2-(4-Bromophenyl)-1-benzothiophene (6j): Yield 70.0 mg (97%); off-white solid. $R_f = 0.51$ (2% EtOAc/hexanes); $^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.87–7.81 (m, 1H), 7.80–7.74 (m, 1H), 7.62–7.49 (m, 5H), 7.42–7.29 (m, 2H). This spectrum is in agreement with previously reported spectral data.¹¹</p>
 <p style="text-align: center;">6k</p>	<p>2-(4-(Trifluoromethyl)phenyl)-1-benzothiophene (6k): Yield 347.0 mg (87%); white solid. $R_f = 0.44$ (2% EtOAc/hexanes); $^1\text{H NMR}$($\text{DMSO}-d_6$, 300 MHz): δ (ppm) 8.07 (d, $J = 0.7$ Hz, 1H), 8.06–7.97 (m, 3H), 7.90 (ddt, $J = 7.3, 3.4, 1.7$ Hz, 1H), 7.84 (d, $J = 8.4$ Hz, 1H), 7.52–7.31 (m, 2H). This spectrum is in agreement with previously reported spectral data.¹²</p>

 <p>6l</p>	<p>Methyl 4-(1-benzothiophen-2-yl)butanoate (6l): Yield 54.6 mg (93%); colorless oil. $R_f = 0.47$ (50% DCM/hexanes);</p> <p>IR (ATR) 3057, 2949, 2923, 2850, 2360, 2342, 1733, 1435 cm^{-1};</p> <p>$^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.77 (dd, $J = 7.8, 1.3$ Hz, 1H), 7.68 (dd, $J = 7.4, 1.3$ Hz, 1H), 7.37–7.20 (m, 2H), 7.03 (d, $J = 1.0$ Hz, 1H), 3.69 (s, 3H), 2.97 (td, $J = 7.4, 1.0$ Hz, 2H), 2.42 (t, $J = 7.4$ Hz, 2H), 2.09 (p, $J = 7.4$ Hz, 2H);</p> <p>$^{13}\text{C NMR}$ (75 MHz, CDCl_3) δ 173.69, 145.15, 140.21, 139.47, 124.23, 123.66, 122.89, 122.24, 121.21, 121.18, 51.70, 51.64, 33.15, 30.05, 29.81, 26.21;</p> <p>HRMS (CI): Exact mass calcd for $\text{C}_{14}\text{H}_{13}\text{O}_2\text{S}$ [M^+]$^+$ 234.0715, found 234.0712.</p>
 <p>6m</p>	<p>4-(1-Benzothiophen-2-yl)-N,N-dimethylaniline (6m): Reaction was carried out using 2 mol% of catalyst. Yield 82 mg (88%); white solid. $R_f = 0.68$ (20% EtOAc/hexanes); $^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.80 (ddt, $J = 7.7, 1.4, 0.7$ Hz, 1H), 7.73 (ddd, $J = 7.8, 1.5, 0.7$ Hz, 1H), 7.67 – 7.55 (m, 2H), 7.39 (s, 1H), 7.37 – 7.20 (m, 2H), 6.87 – 6.65 (m, 2H), 3.02 (s, 6H). This spectrum is in agreement with previously reported spectral data.⁸</p>
 <p>6n</p>	<p>3-(1-Benzothiophen-2-yl)propanenitrile (6n): Reaction was carried out using 2 mol% of catalyst. Yield 35.0 mg (75%); pale yellow oil. $R_f = 0.40$ (50% DCM/hexanes);</p> <p>IR (ATR) 3057, 2925, 2360, 2342, 2247, 1435 cm^{-1};</p> <p>$^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.83–7.75 (m, 1H), 7.75–7.67 (m, 1H), 7.41–7.23 (m, 3H), 7.16 (q, $J = 1.0$ Hz, 1H), 3.27 (td, $J = 7.3, 1.0$ Hz, 2H), 2.76 (t, $J = 7.3$ Hz, 2H);</p> <p>$^{13}\text{C NMR}$(CDCl_3, 75 MHz): δ (ppm) 140.90, 139.87, 139.54, 124.63, 124.42, 123.44, 122.48, 122.35, 118.66, 26.94, 19.37;</p> <p>HRMS (CI): Exact mass calcd for $\text{C}_{11}\text{H}_9\text{NS}$ [M^+]$^+$ 187.0456, found 187.0454.</p>
 <p>6o</p>	<p>Methyl 4-(1-benzothiophen-2-yl)benzoate (6o): Yield 50.1 mg (75%); white solid. $R_f = 0.49$ (10% EtOAc/hexanes); $^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 8.16 – 8.03 (m, 2H), 7.92 – 7.71 (m, 4H), 7.66 (d, $J = 0.8$ Hz, 1H), 7.47 – 7.29 (m, 2H), 3.95 (s, 3H). This spectrum is in agreement with previously reported spectral data.¹³</p>
 <p>6p</p>	<p>2-(Thiophen-3-yl)-1-benzothiophene (6p): Yield 46.5 mg (86%); off-white solid. $R_f = 0.71$ (2% EtOAc/hexanes); $^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.79 (ddd, $J = 7.1, 2.0, 0.8$ Hz, 1H), 7.76–7.69 (m, 1H), 7.41 (d, $J = 0.8$ Hz, 1H), 7.38–7.23 (m, 4H), 7.07 (dd, $J = 5.0, 3.7$ Hz, 1H). This spectrum is in agreement with previously reported spectral data.⁷</p>
 <p>6r</p>	<p>2-(2-Methoxyphenyl)-1-benzothiophene (6r): Yield 58.0 mg (97%); colorless oil. $R_f = 0.37$ (2% EtOAc/hexanes); $^1\text{H NMR}$(CDCl_3, 300 MHz): δ (ppm) 7.97–7.80 (m, 3H), 7.77 (dd, $J = 7.7, 1.7$ Hz, 1H), 7.45–7.29 (m, 3H), 7.10 (dd, $J = 7.5, 1.2$ Hz, 1H), 7.04 (dd, $J = 8.2, 1.1$ Hz, 1H), 3.99 (s, 3H). This spectrum is in agreement with previously reported spectral data.⁹</p>



2-Phenyl-5-(trifluoromethyl)benzo[*b*]thiophene (6s): Purified by filtration. Yield 273 mg (82%); white solid. Mp 178–180 °C; $R_f = 0.61$ (2% EtOAc/hexanes); IR (ATR) 2924, 2360, 2214, 1899, 1595 cm^{-1} ;
 ^1H NMR (300 MHz, CDCl_3) δ 8.05 (s, 1H), 7.93 (d, $J = 8.4$ Hz, 1H), 7.77 – 7.66 (m, 2H), 7.61 (d, $J = 2.1$ Hz, 1H), 7.58 – 7.32 (m, 4H);
 ^{13}C NMR(CDCl_3 , 75 MHz): δ (ppm) 146.71, 142.60, 140.38, 133.76, 129.25, 129.01, 127.30 (q, $J = 32.3$ Hz), 126.77, 124.74 (q, $J = 271.9$ Hz), 122.91, 120.71 (q, $J = 8.2$ Hz), 119.51, 119.46;
HRMS (CI): Exact mass calcd for $\text{C}_{15}\text{H}_9\text{F}_3\text{S}$ $[\text{M}]^+$ 278.0377, found 278.0381.

Mechanistic studies

Migration of the alkyl group

The reaction was carried out according to general protocol. The reaction mixture was not concentrated but immediately analyzed by ^1H NMR. Figure 1 shows ^1H NMR spectrum of the reaction of **5a** in toluene. Figure 2 and Figure 3 show ^1H NMR spectrum of the reaction of **5t** (SEt) carried out in toluene- d_8 as solvent.

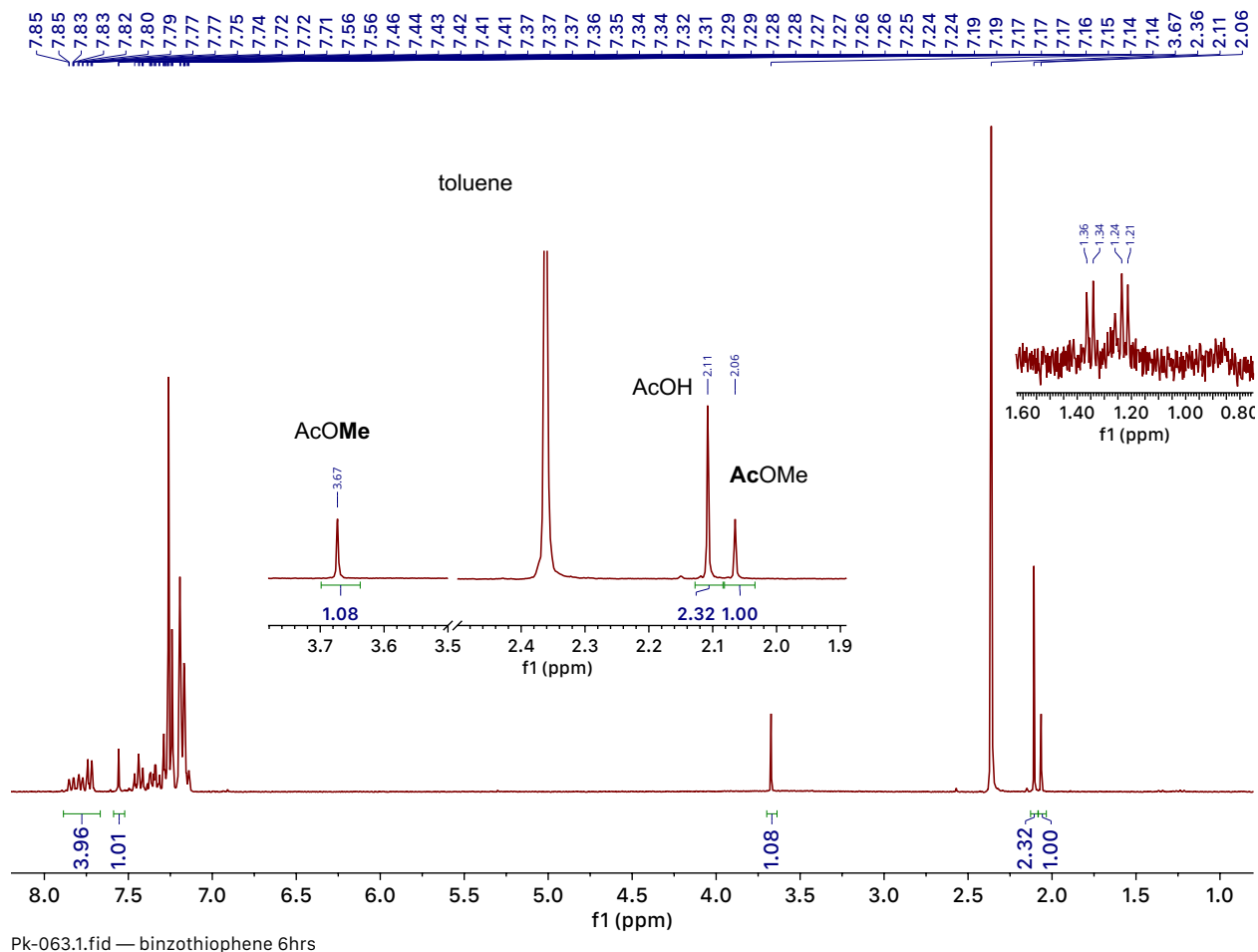


Figure 1. ^1H NMR of a post-reaction mixture containing benzo[b]thiophene **6a** as the main product (7.84 ppm) as well as methyl acetate (3.67 and 2.06 ppm) and remaining acetic acid (2.11 ppm). Resonances at 1.35 and 1.23 ppm correspond to the catalyst.

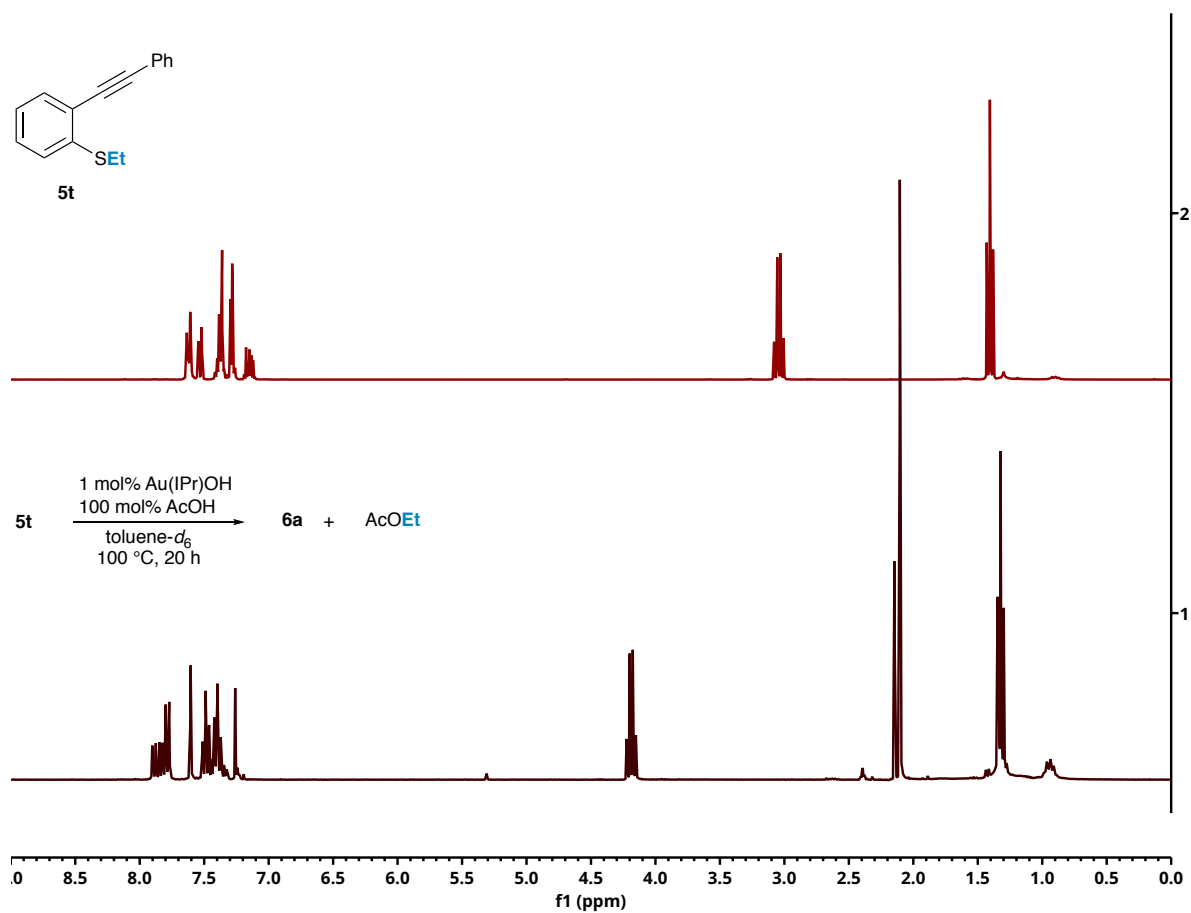


Figure 2. ¹H NMR spectra (CDCl₃) of alkyne **6t** (top) and unpurified post-reaction mixture (bottom spectrum) with benzo[b]thiophene **6a** (7.84 ppm), ethyl acetate (4.3, 2.1, and 1.3 ppm), and remaining acetic acid (2.11 ppm).

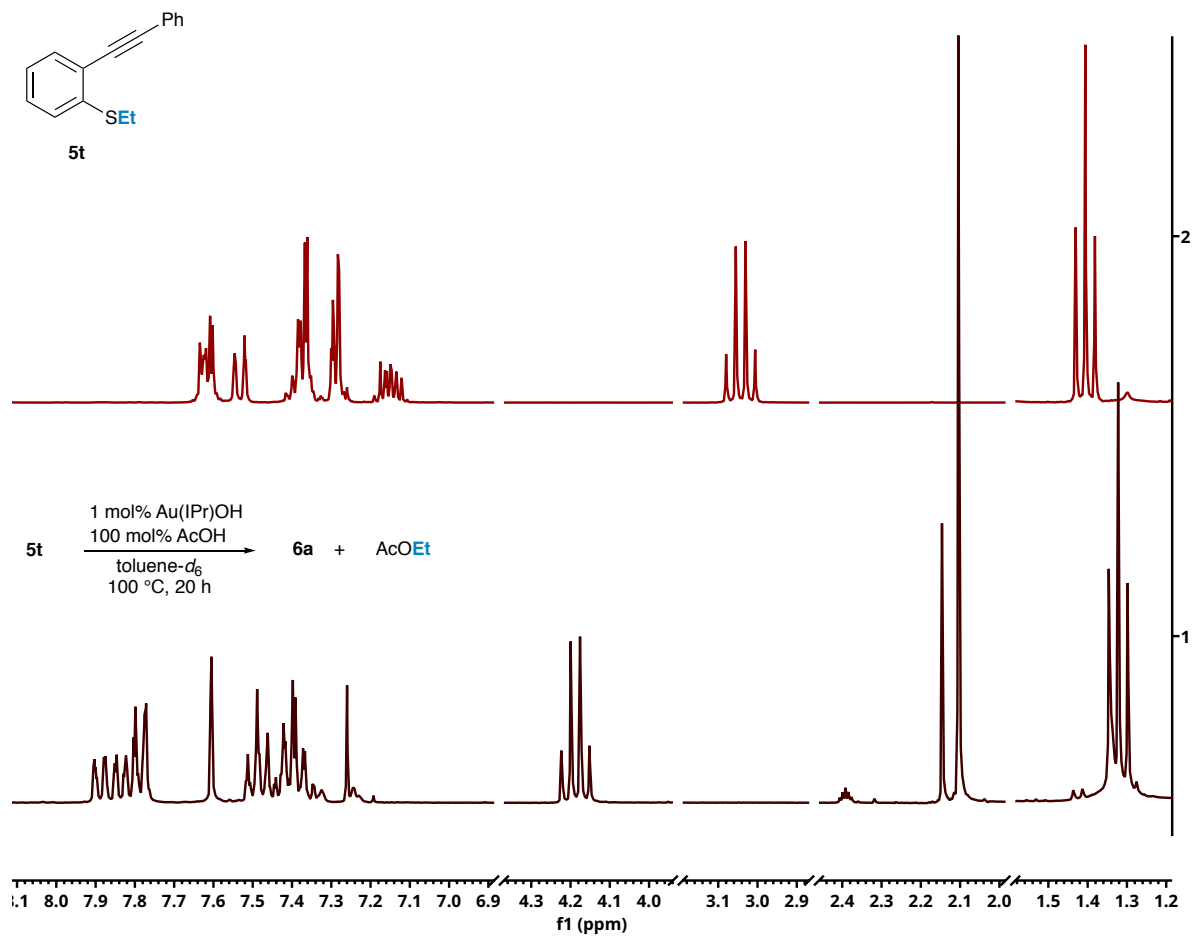


Figure 3. Expanded regions in spectra from Figure 2. Resonance at 2.4 is from toluene- d_8 .

Reaction in presence of acetic acid-*d*

In a 2-dram vial was added the catalyst (2.2 μmmol), alkyne (0.45 mmol) acetic acid-*d* (26 μL , 0.45 mmol) and toluene (480 μL). The vial was capped, and the mixture heated at 100 $^{\circ}\text{C}$ for 20 h. The mixture was then cooled to rt and the product was purified by trituration with cold diethyl ether.

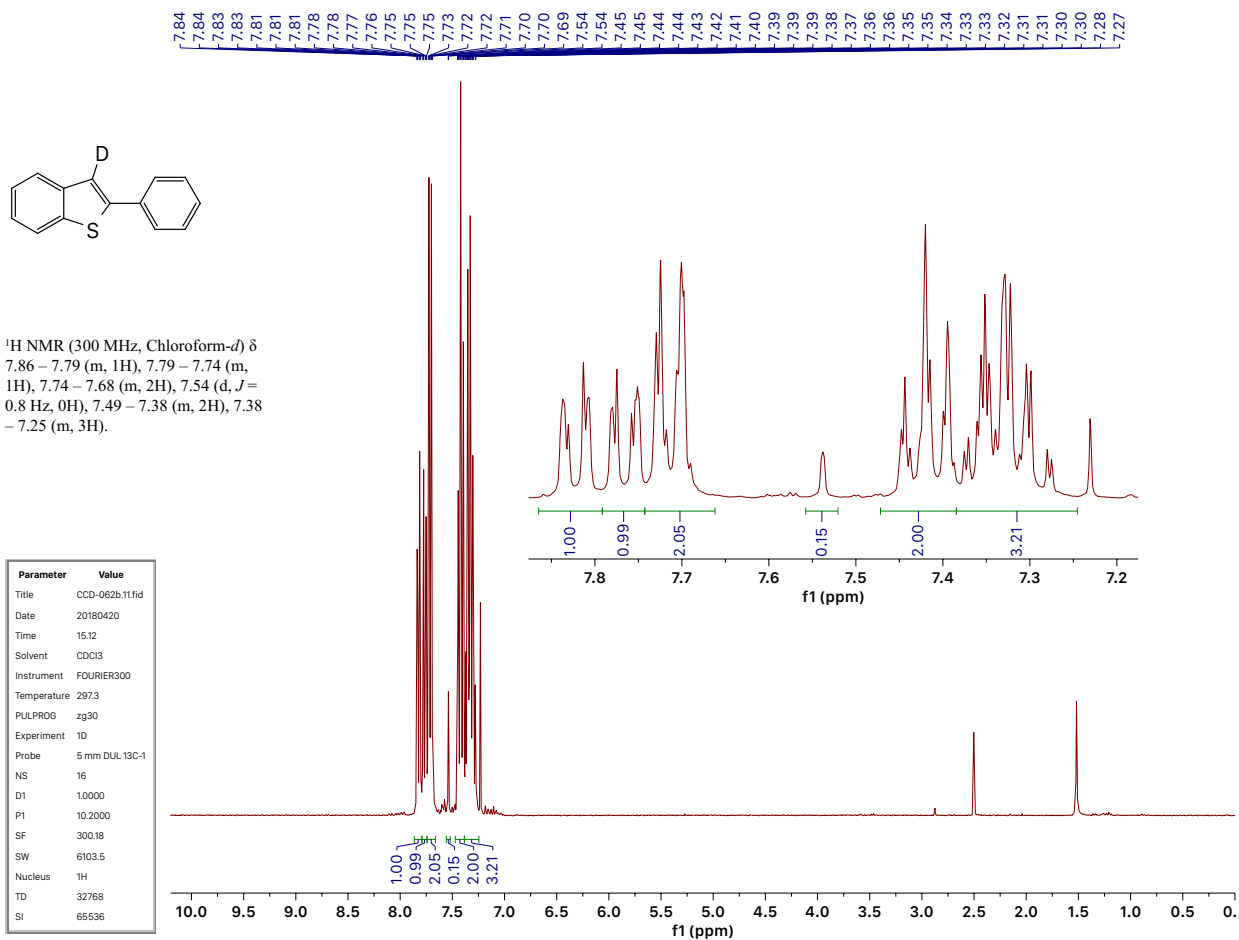
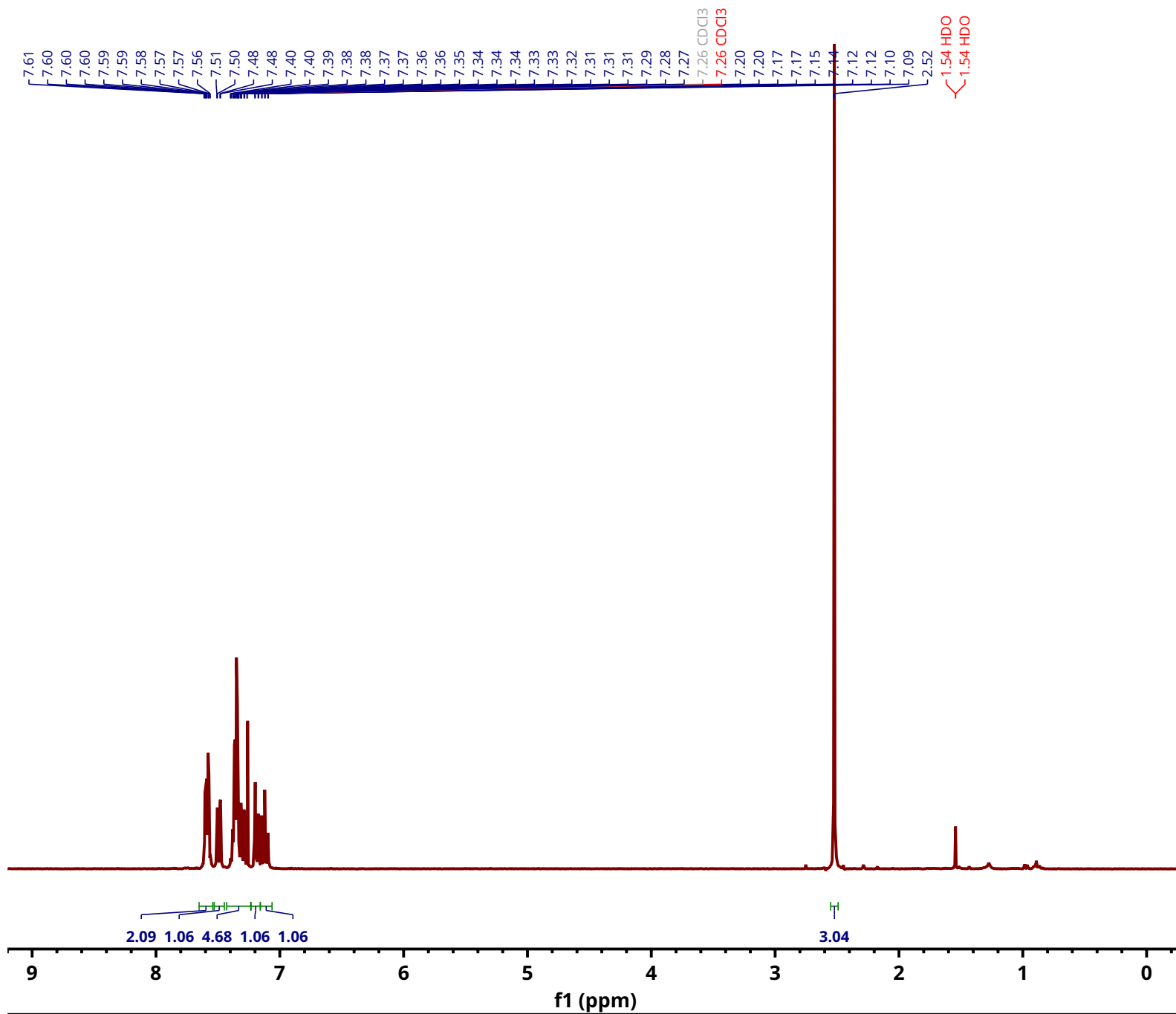


Figure 4. ¹H NMR spectrum (CDCl₃) of 2-phenylbenzo[b]thiophene-*d*. Isotopic enrichment is estimated at 85% (resonance at 7.54 ppm).

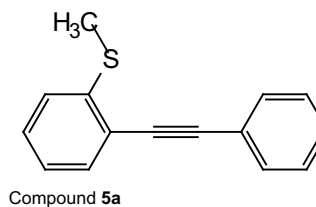
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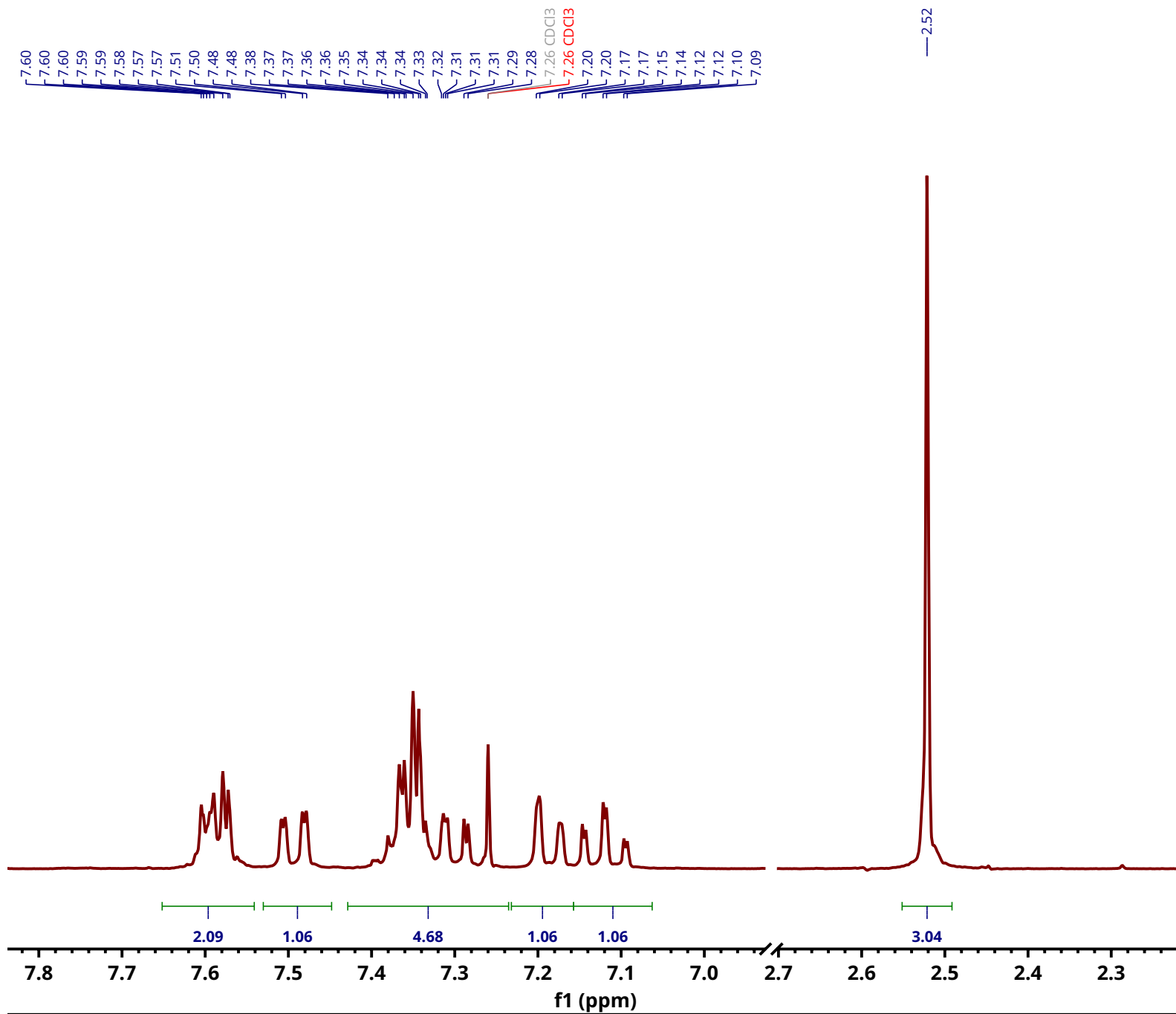
Digital images of NMR spectra



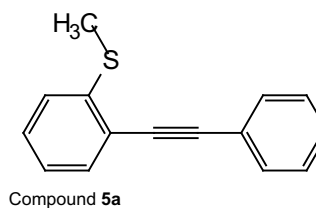
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6 Experiment	1D
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9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-03-02T14:38:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



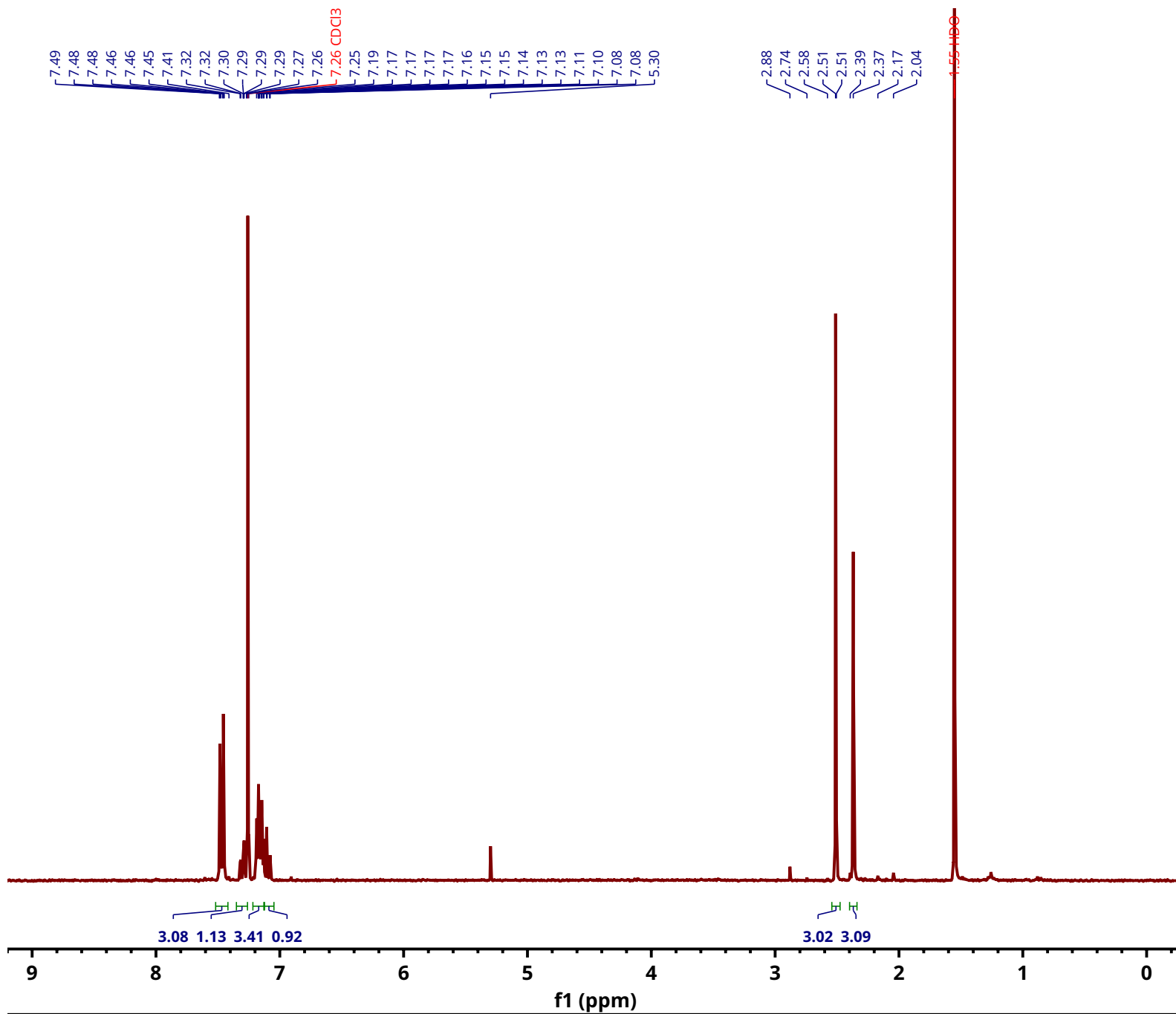
¹H NMR (300 MHz, Chloroform-*d*) δ 7.65 – 7.53 (m, 2H), 7.49 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.42 – 7.27 (m, 4H), 7.19 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.12 (td, *J* = 7.5, 1.3 Hz, 1H), 2.52 (s, 3H).



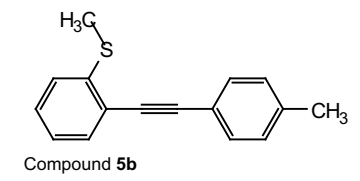
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5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	56.1
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
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14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
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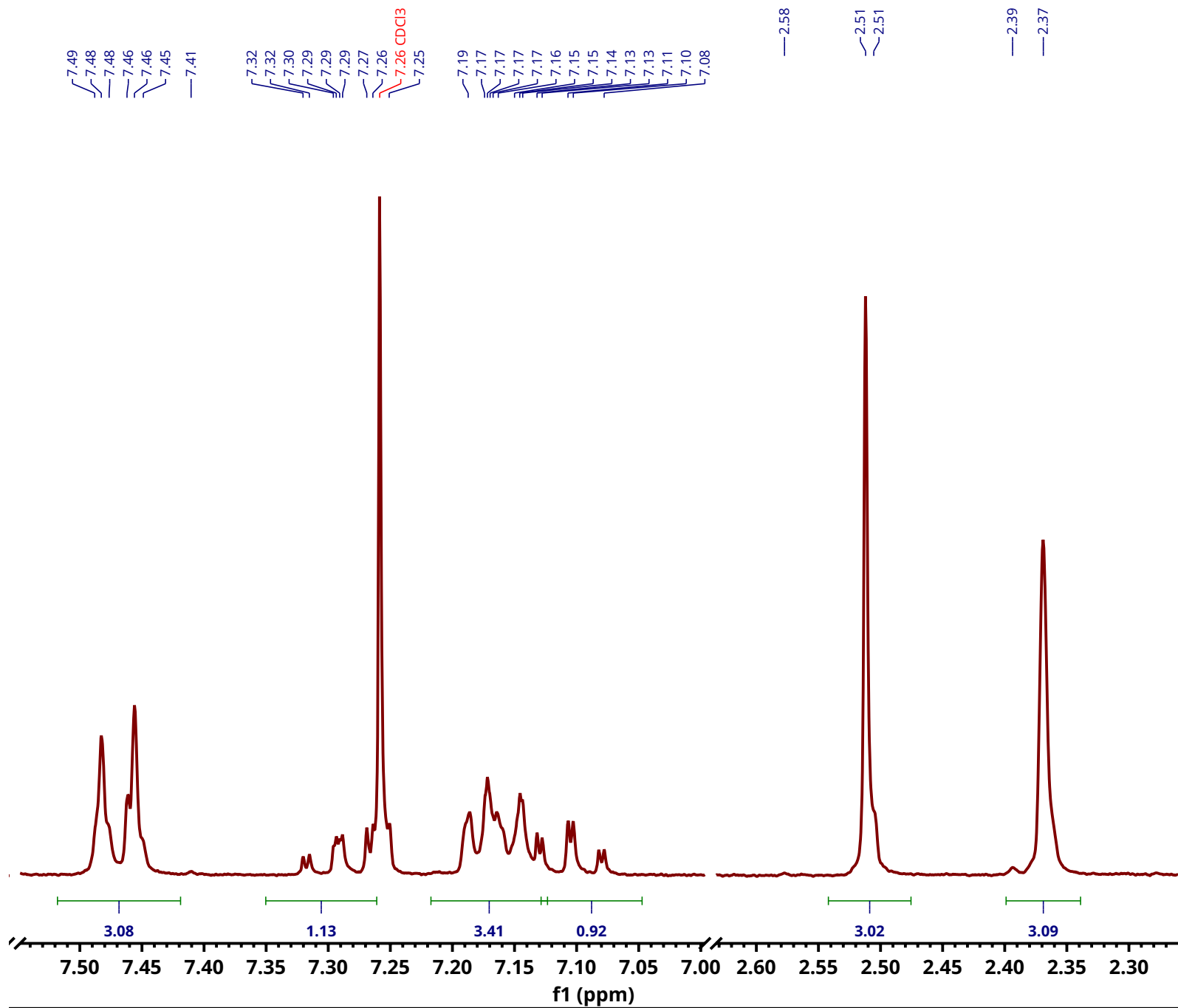
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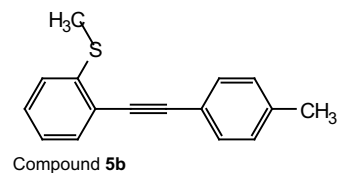
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15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



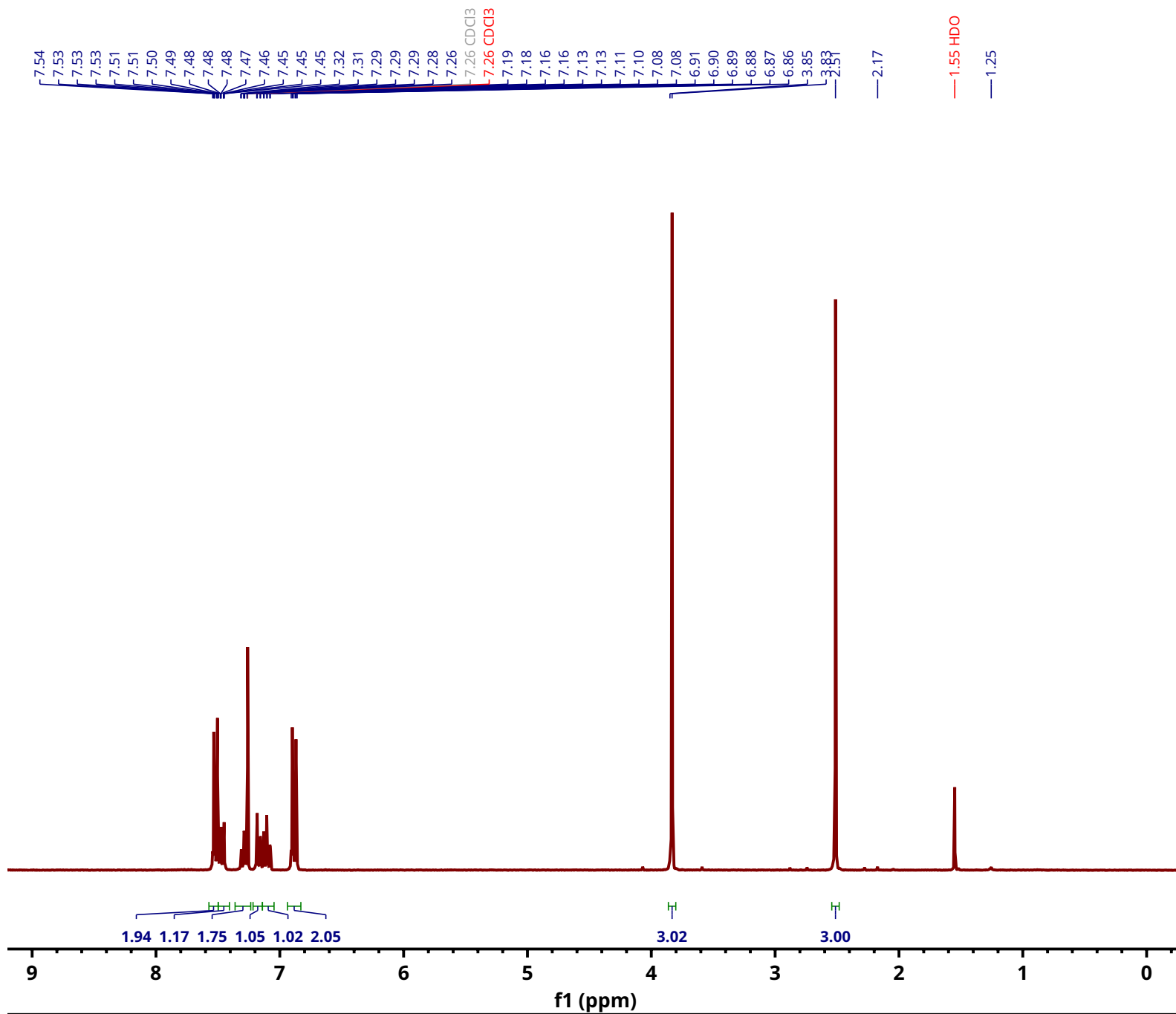
¹H NMR (300 MHz, Chloroform-*d*) δ 7.52 – 7.42 (m, 3H), 7.35 – 7.22 (m, 1H), 7.22 – 7.11 (m, 3H), 7.11 (td, *J* = 7.5, 1.3 Hz, 1H), 2.51 (s, 3H), 2.37 (s, 3H).



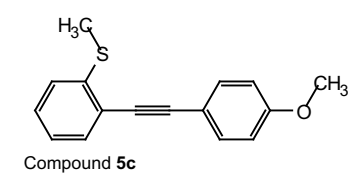
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6 Experiment	1D
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9 Relaxation Decay	1.0000
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16 Acquired Size	32768
17 Spectral Size	65536



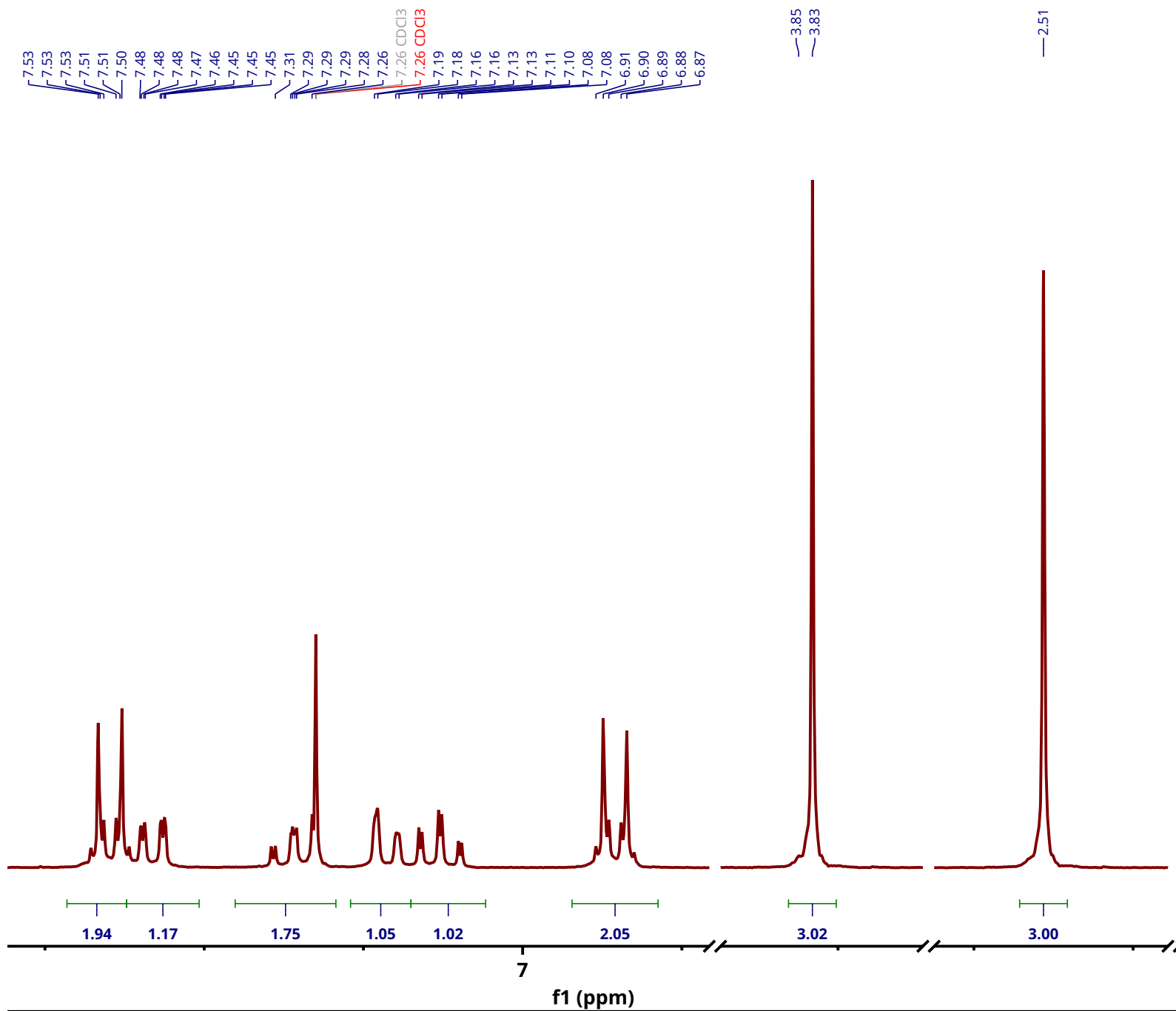
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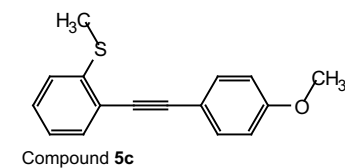
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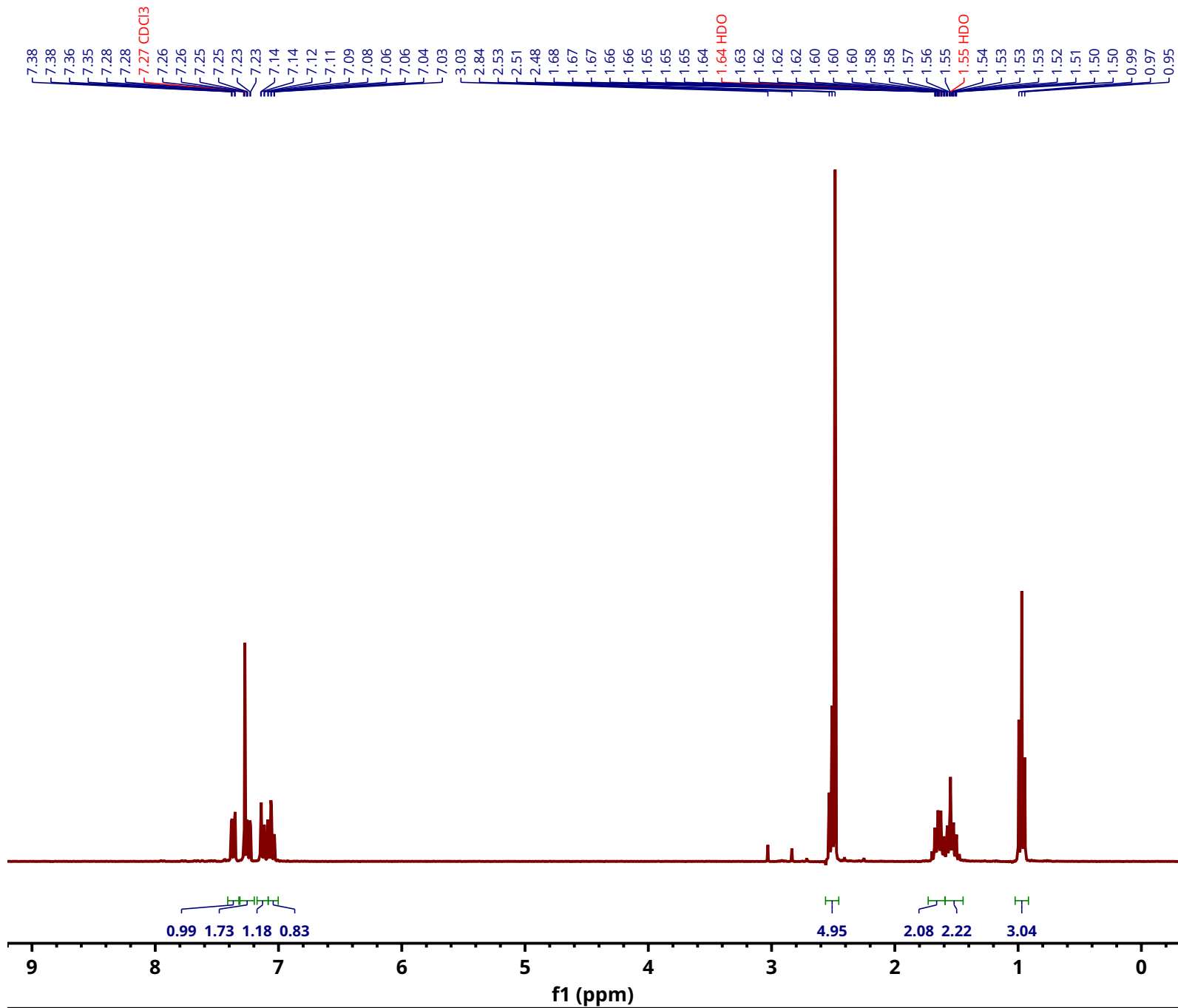
¹H NMR (300 MHz, Chloroform-*d*) δ 7.57 – 7.46 (m, 2H), 7.46 (ddd, *J* = 7.6, 1.5, 0.5 Hz, 1H), 7.36 – 7.23 (m, 1H), 7.17 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.10 (td, *J* = 7.5, 1.3 Hz, 1H), 6.94 – 6.83 (m, 2H), 3.83 (s, 3H), 2.51 (s, 3H).



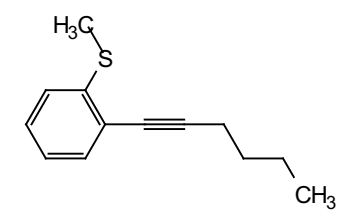
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3 Solvent	CDCl3
4 Temperature	294.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
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9 Relaxation Decay	1.0000
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14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



¹H NMR (300 MHz, Chloroform-*d*) δ 7.57 – 7.46 (m, 2H), 7.46 (ddd, *J* = 7.6, 1.5, 0.5 Hz, 1H), 7.36 – 7.23 (m, 1H), 7.17 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.10 (td, *J* = 7.5, 1.3 Hz, 1H), 6.94 – 6.83 (m, 2H), 3.83 (s, 3H), 2.51 (s, 3H).

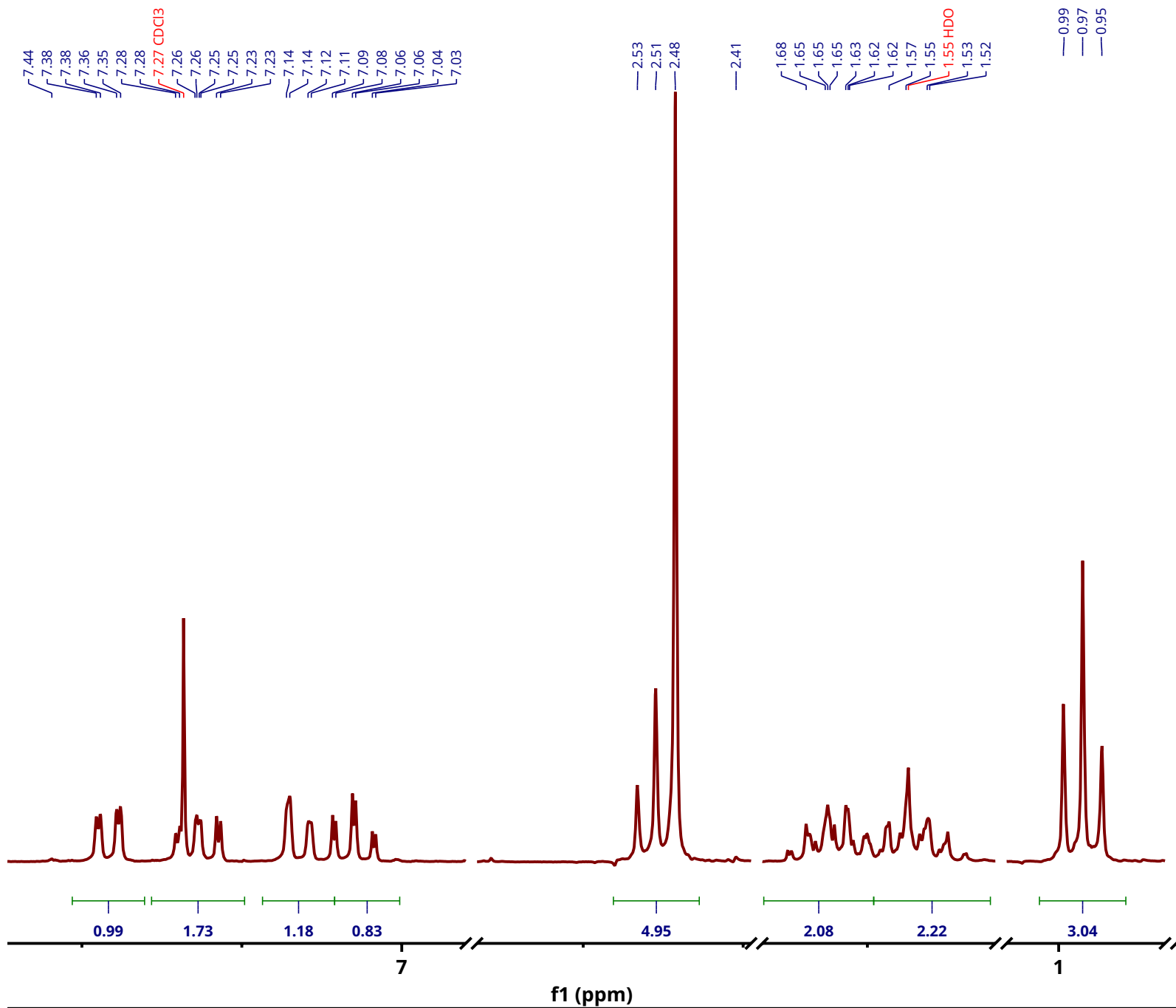


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17 Spectral Size	65536

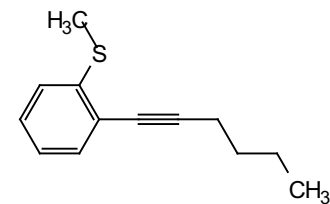


Compound 5d

¹H NMR (300 MHz, Chloroform-*d*) δ 7.35 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.24 (ddd, *J* = 8.0, 7.3, 1.5 Hz, 1H), 7.12 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.05 (td, *J* = 7.5, 1.3 Hz, 1H), 2.50 (t, *J* = 6.8 Hz, 2H), 2.47 (s, 3H), 1.72 – 1.58 (m, 2H), 1.58 – 1.43 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H).

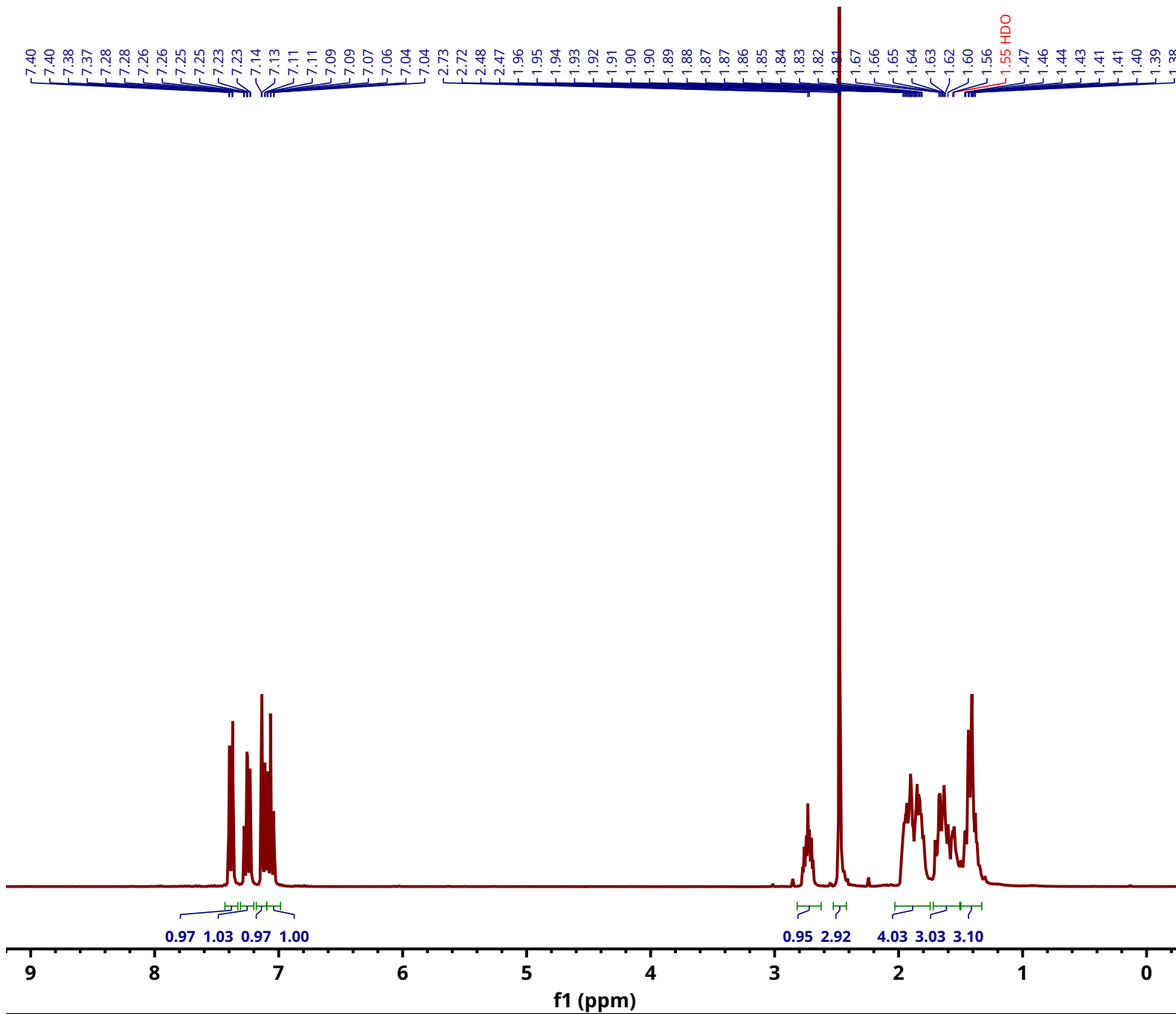


Parameter	Value
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6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	58.6
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
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15 Nucleus	¹ H
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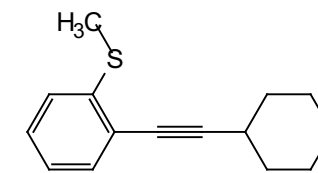


Compound 5d

¹H NMR (300 MHz, Chloroform-*d*) δ 7.35 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.24 (ddd, *J* = 8.0, 7.3, 1.5 Hz, 1H), 7.12 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.05 (td, *J* = 7.5, 1.3 Hz, 1H), 2.50 (t, *J* = 6.8 Hz, 2H), 2.47 (s, 3H), 1.72 – 1.58 (m, 2H), 1.58 – 1.43 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H).

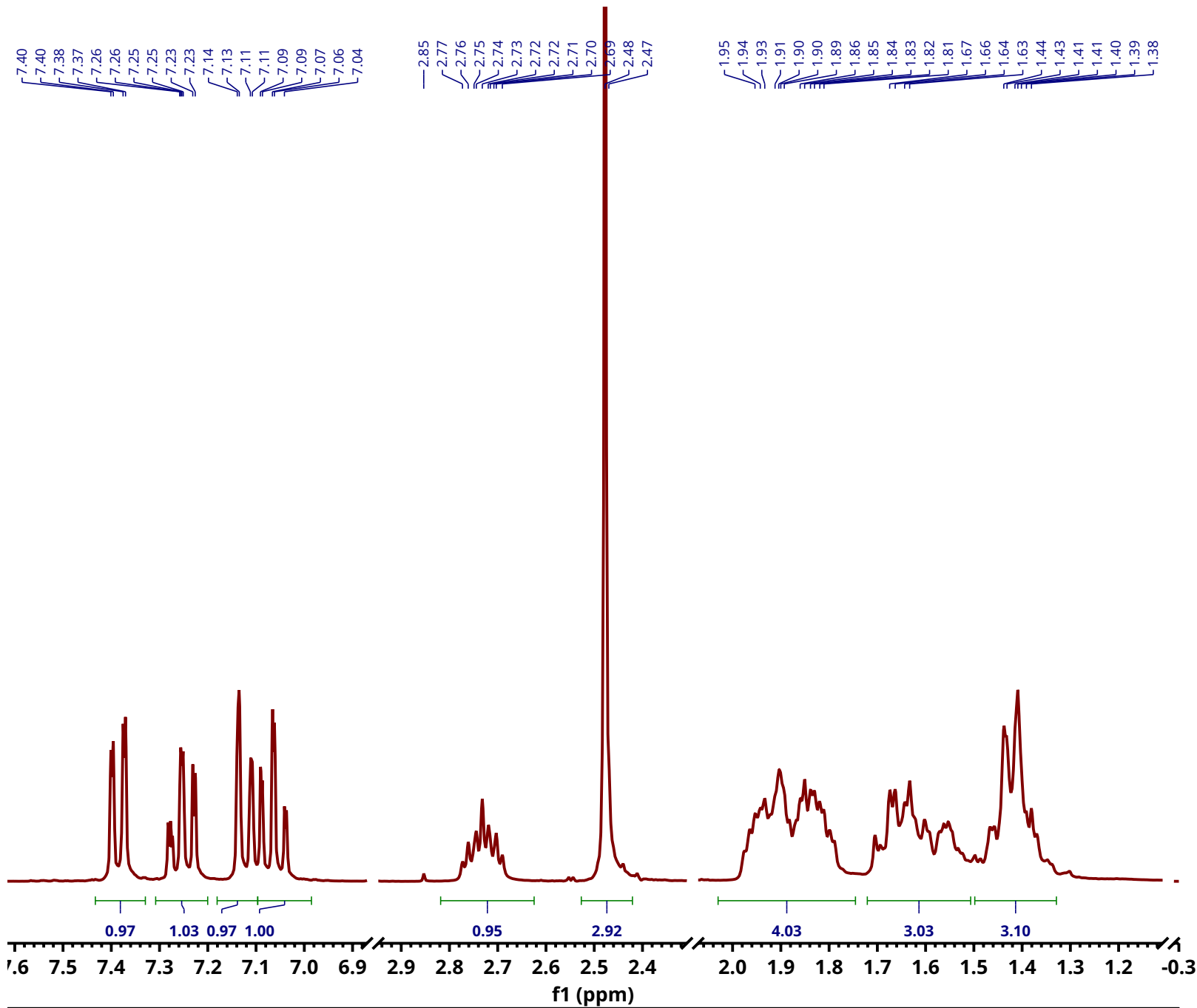


Parameter	Value
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16 Acquired Size	32768
17 Spectral Size	65536

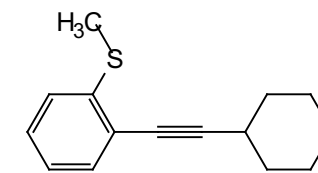


Compound 5e

¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.37 (dd, *J*=7.6, 1.5 Hz, 1H), 7.24 (ddd, *J*=8.3, 7.3, 1.5 Hz, 1H), 7.11 (dd, *J*=8.1, 1.3 Hz, 1H), 7.05 (td, *J*=7.5, 1.3 Hz, 1H), 2.72 (tt, *J*=8.8, 3.7 Hz, 1H), 2.46 (s, 3H), 1.99 – 1.74 (m, 4H), 1.71 – 1.48 (m, 3H), 1.49 – 1.23 (m, 3H)



Parameter	Value
1 Title	MS-078.101.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	1021.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	4.2
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-25T19:03:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

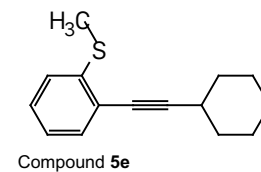
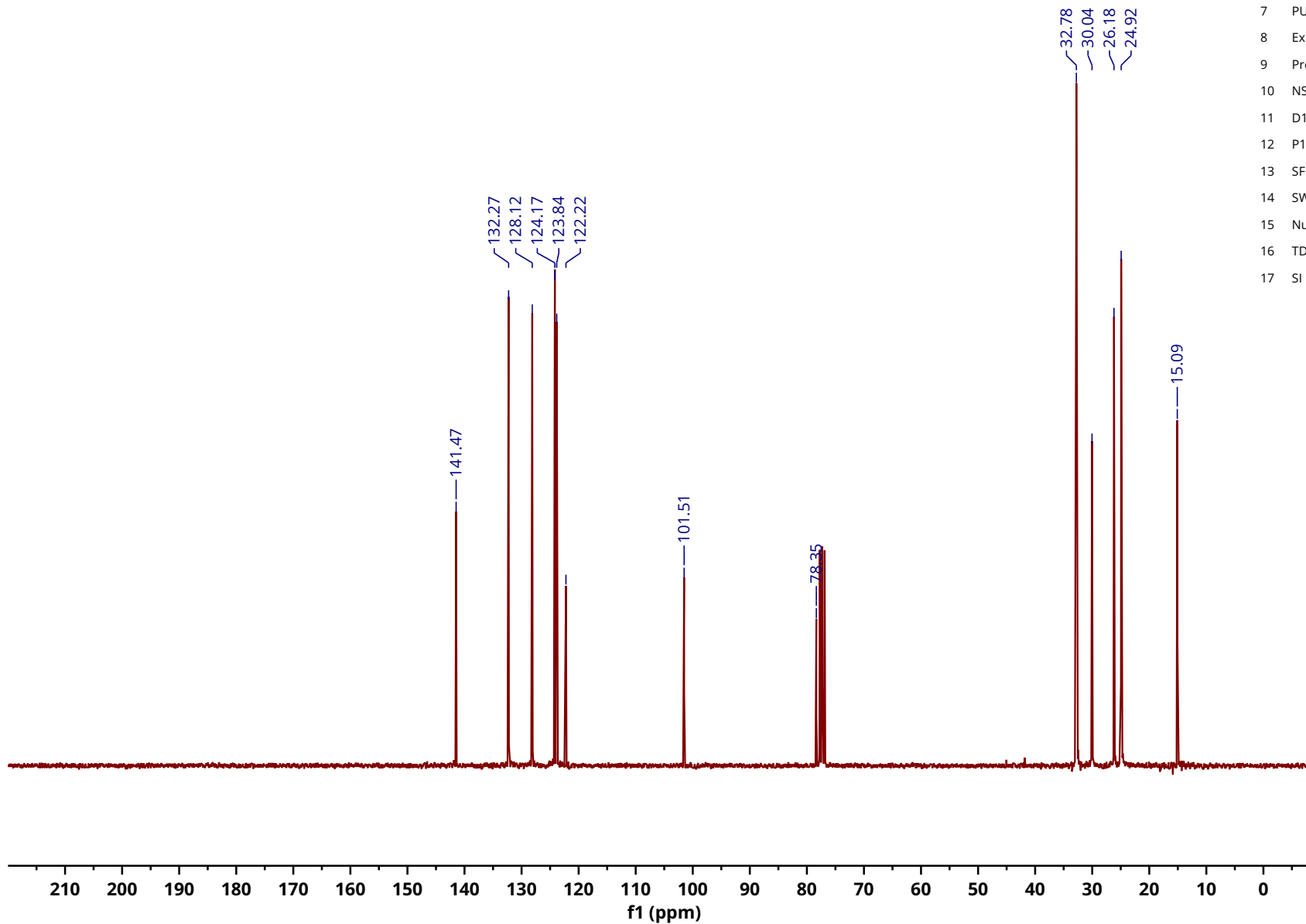


Compound 5e

¹H NMR (Chloroform-*d*, 300 MHz): δ (ppm) 7.37 (dd, *J*=7.6, 1.5 Hz, 1H), 7.24 (ddd, *J*=8.3, 7.3, 1.5 Hz, 1H), 7.11 (dd, *J*=8.1, 1.3 Hz, 1H), 7.05 (td, *J*=7.5, 1.3 Hz, 1H), 2.72 (tt, *J*=8.8, 3.7 Hz, 1H), 2.46 (s, 3H), 1.99 – 1.74 (m, 4H), 1.71 – 1.48 (m, 3H), 1.49 – 1.23 (m, 3H)

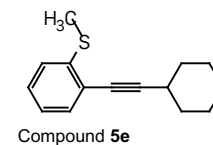
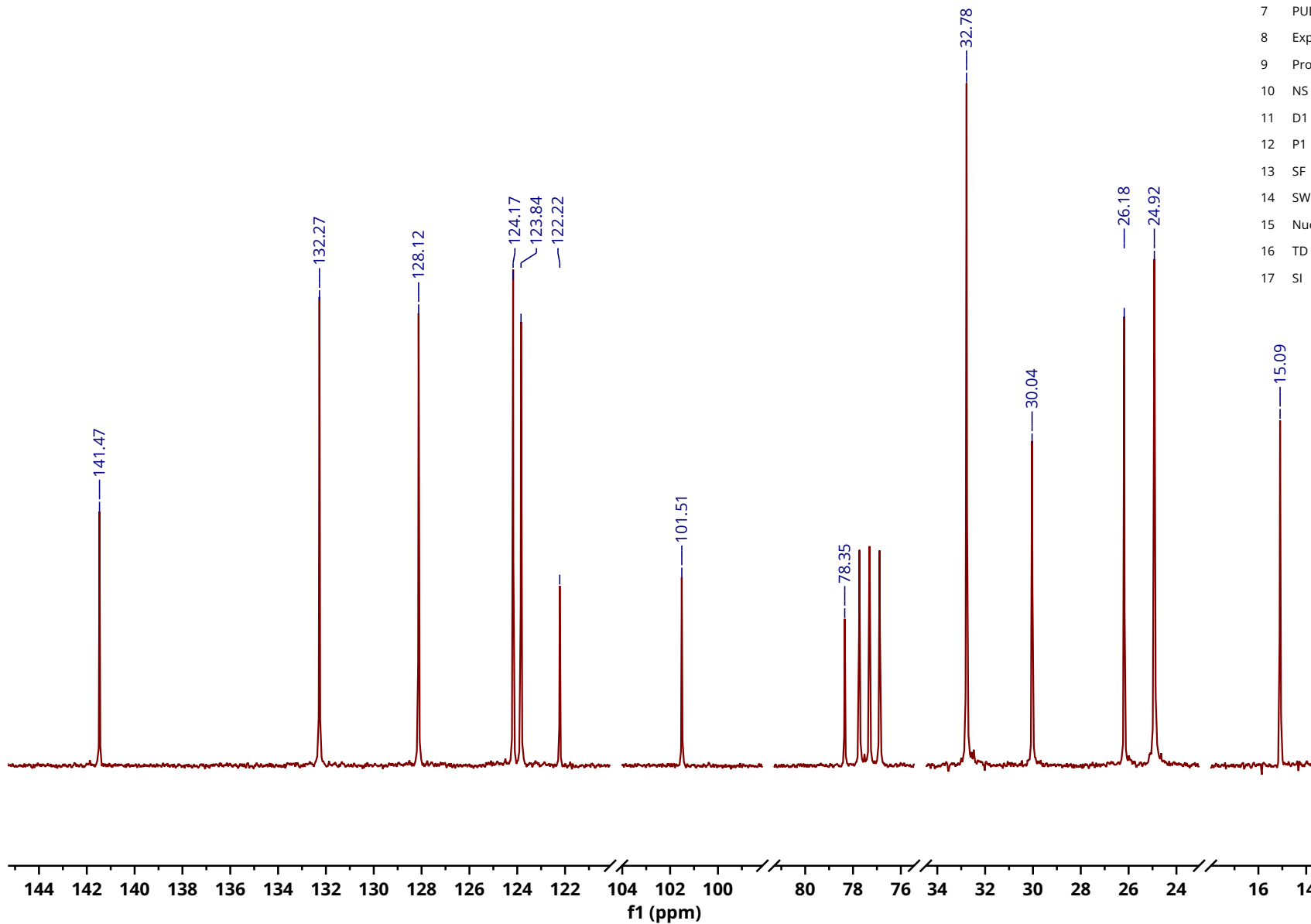
^{13}C NMR (75 MHz, CDCl_3) δ 141.32, 132.12, 127.97, 124.02, 123.69, 122.07, 101.36, 78.20, 32.62, 29.88, 26.03, 24.77, 14.94.

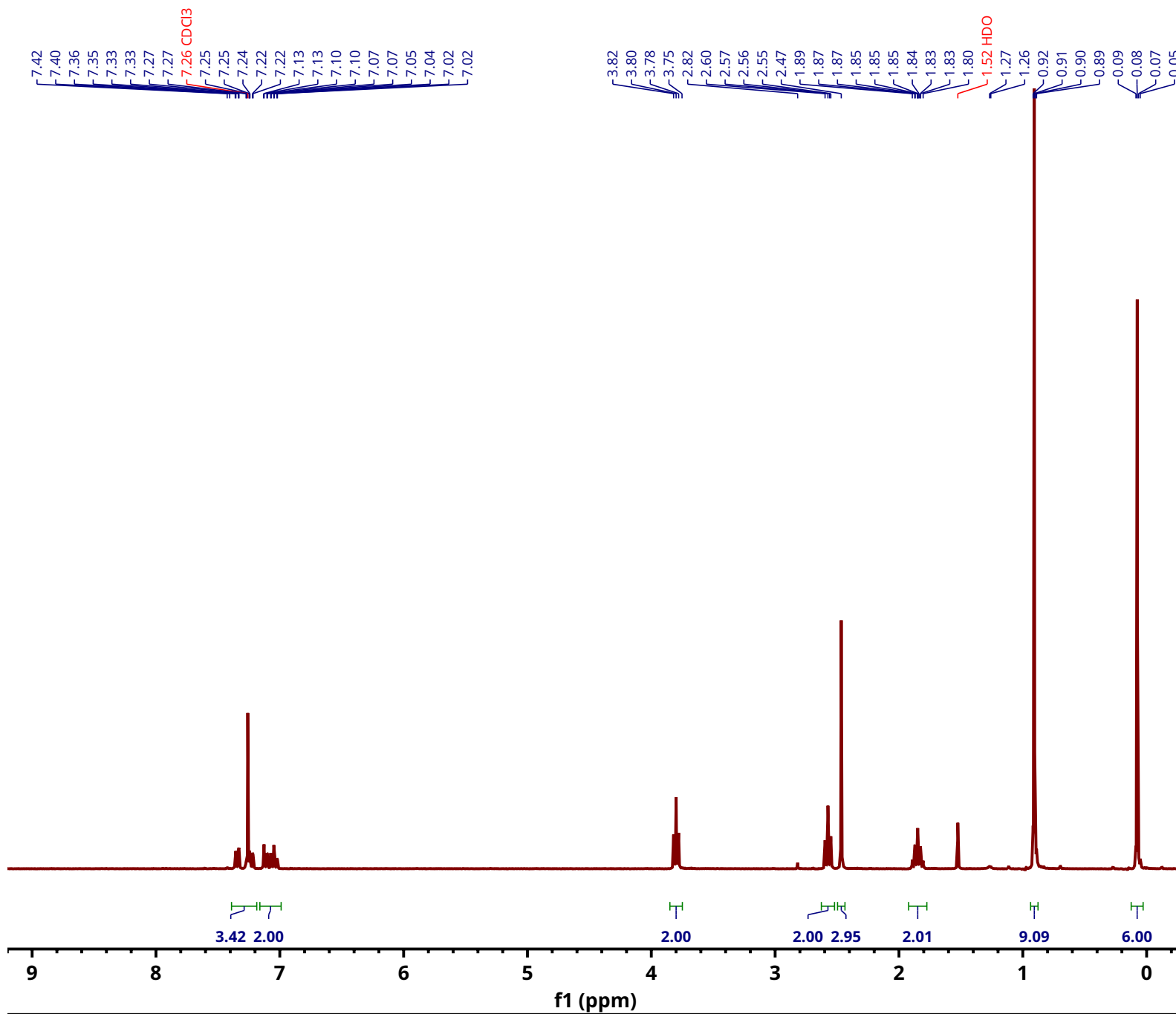
Parameter	Value
1 Title	MS-078.102.fid
2 Date	20180725
3 Time	19.11
4 Solvent	CDCl_3
5 Instrument	FOURIER300
6 Temperature	1021.9
7 PULPROG	zgpg30
8 Experiment	1D
9 Probe	5 mm DUL 13C-1
10 NS	1024
11 D1	2.0000
12 P1	11.0000
13 SF	75.49
14 SW	24414.1
15 Nucleus	^{13}C
16 TD	32768
17 SI	65536



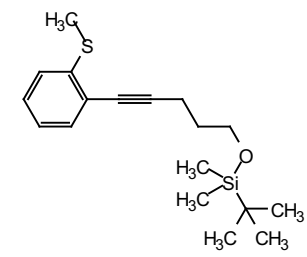
^{13}C NMR (75 MHz, CDCl_3) δ 141.32, 132.12, 127.97, 124.02, 123.69, 122.07, 101.36, 78.20, 32.62, 29.88, 26.03, 24.77, 14.94.

Parameter	Value
1 Title	MS-078.102.fid
2 Date	20180725
3 Time	19.11
4 Solvent	CDCl_3
5 Instrument	FOURIER300
6 Temperature	1021.9
7 PULPROG	zgpg30
8 Experiment	1D
9 Probe	5 mm DUL 13C-1
10 NS	1024
11 D1	2.0000
12 P1	11.0000
13 SF	75.49
14 SW	24414.1
15 Nucleus	^{13}C
16 TD	32768
17 SI	65536



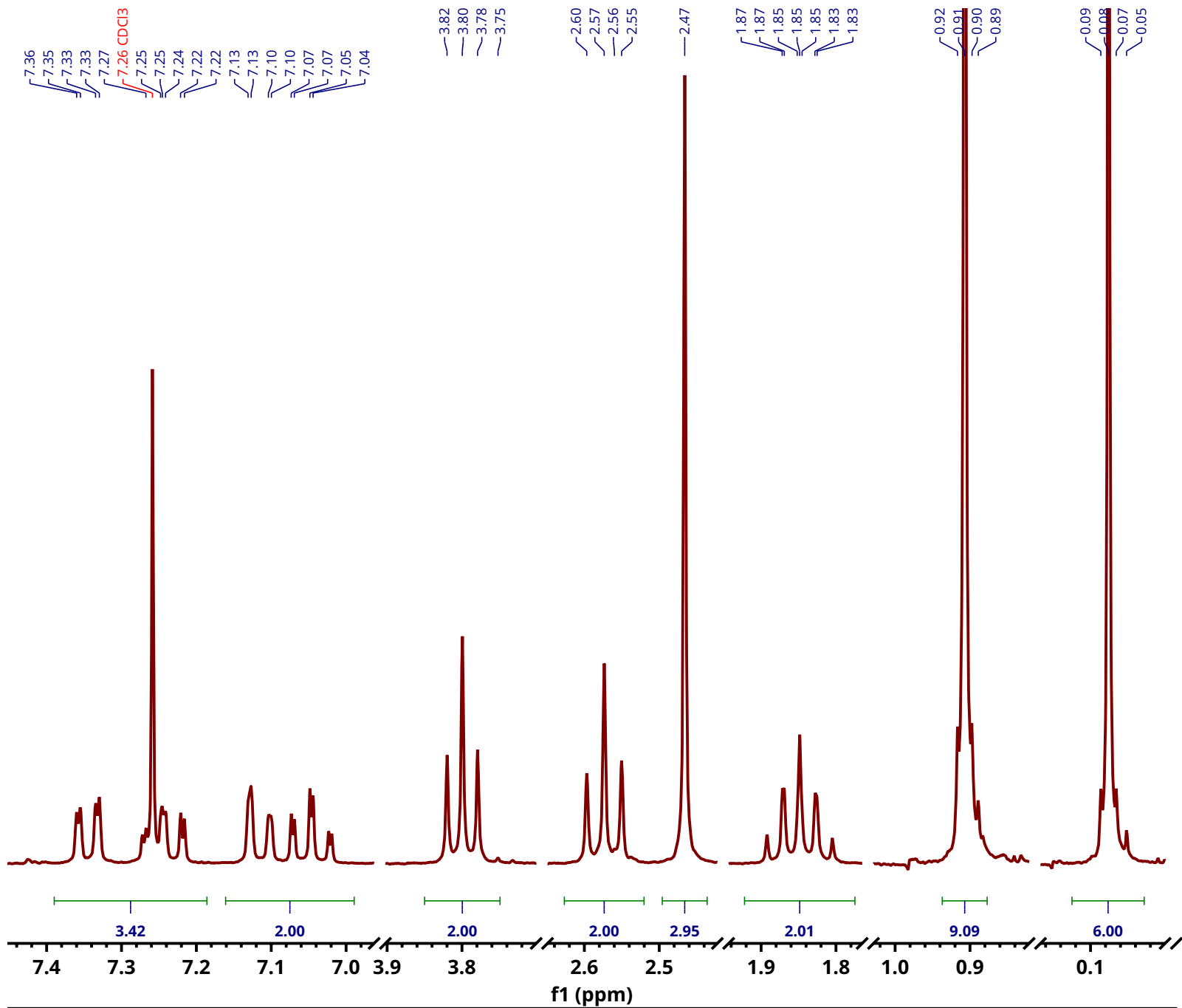


Parameter	Value
1 Title	DAL-086.2.fid
2 Instrument	FOURIER300
3 Solvent	CDCl ₃
4 Temperature	298.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	89.6
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-13T15:42:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	¹ H
16 Acquired Size	32768
17 Spectral Size	65536

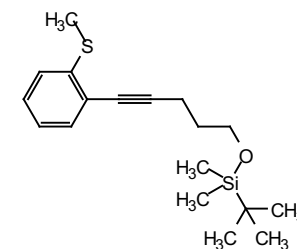


Compound 5f

¹H NMR (300 MHz, Chloroform-*d*) δ 7.39 – 7.19 (m, 2H), 7.16 – 6.99 (m, 2H), 3.80 (t, *J* = 6.1 Hz, 2H), 2.57 (t, *J* = 7.0 Hz, 2H), 2.47 (s, 3H), 1.92 – 1.78 (m, 2H), 0.91 (s, 9H), 0.08 (s, 6H).



Parameter	Value
1 Title	DAL-086.2.fid
2 Instrument	FOURIER300
3 Solvent	CDCl ₃
4 Temperature	298.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	89.6
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-13T15:42:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	¹ H
16 Acquired Size	32768
17 Spectral Size	65536

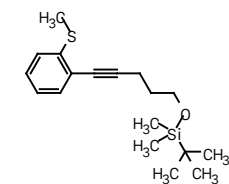
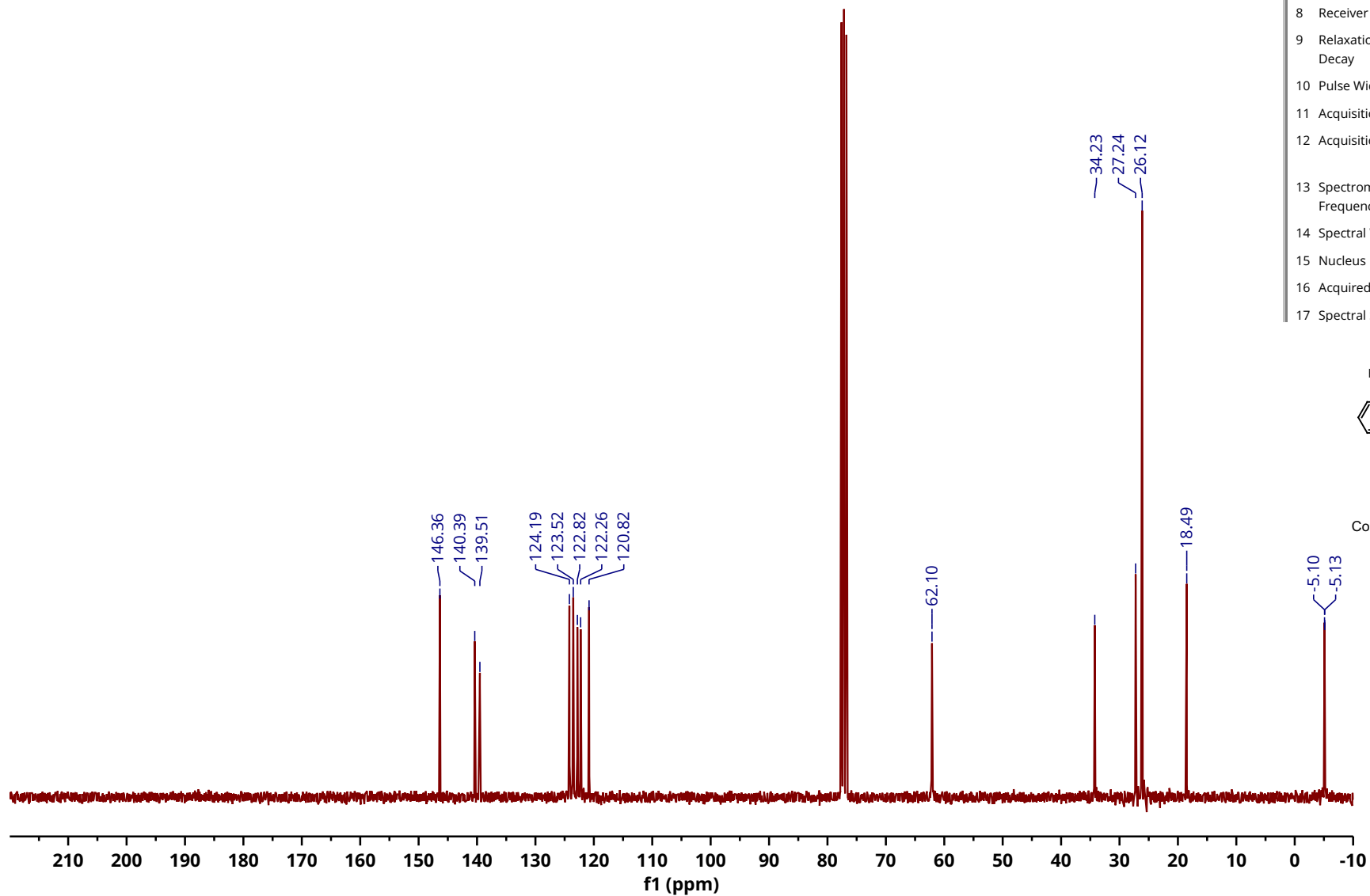


Compound **5f**

¹H NMR (300 MHz, Chloroform-*d*) δ 7.39 – 7.19 (m, 2H), 7.16 – 6.99 (m, 2H), 3.80 (t, *J* = 6.1 Hz, 2H), 2.57 (t, *J* = 7.0 Hz, 2H), 2.47 (s, 3H), 1.92 – 1.78 (m, 2H), 0.91 (s, 9H), 0.08 (s, 6H).

^{13}C NMR(Chloroform-*d*, 75 MHz): δ (ppm) 146.35, 140.38, 139.50, 124.17, 123.51, 122.81, 122.24, 120.81, 62.09, 34.22, 27.23, 26.11, 18.47, -5.12, -5.15

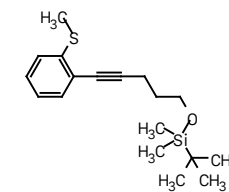
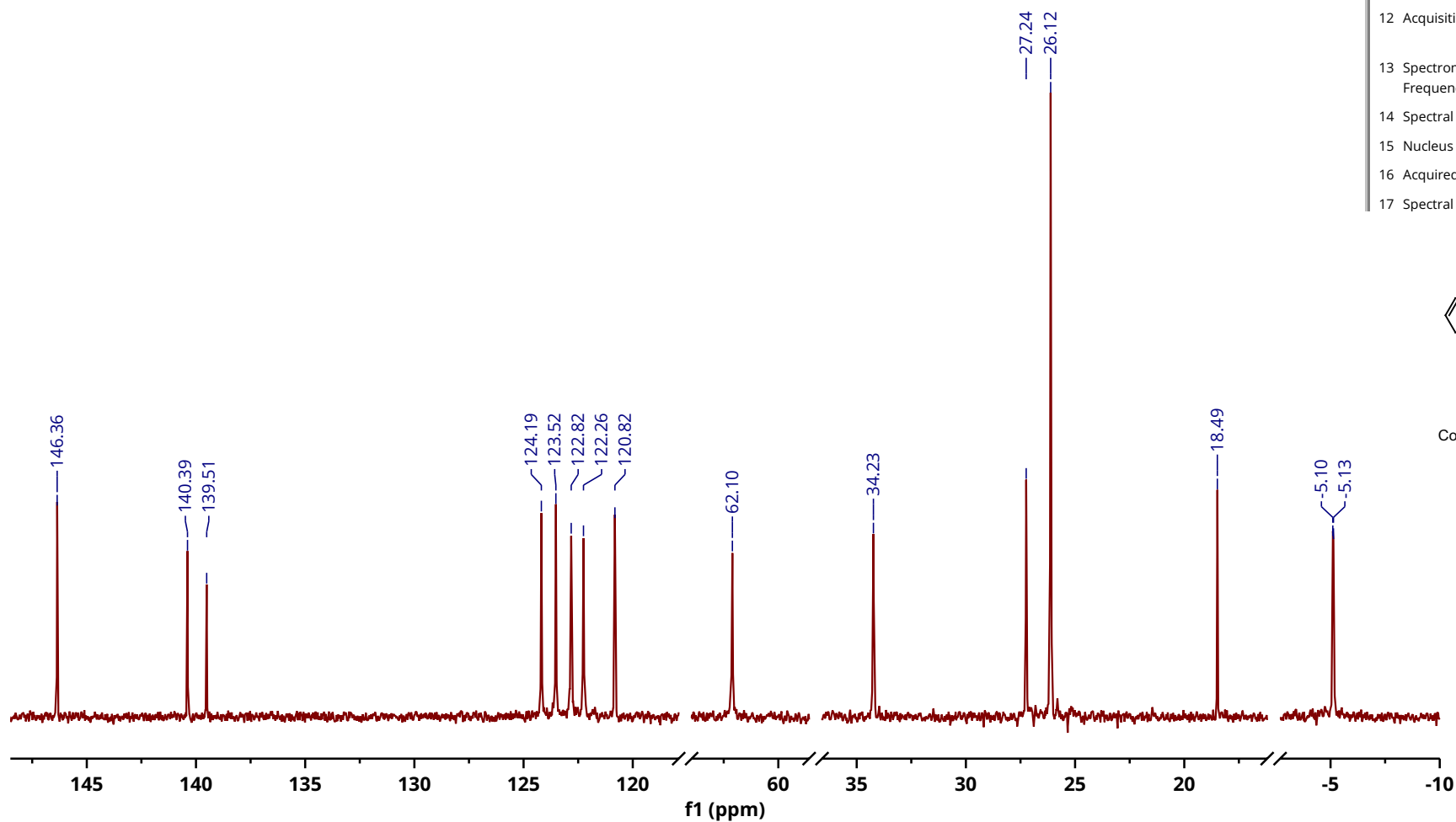
Parameter	Value
1 Title	CCD-097.12.fid
2 Instrument	FOURIER300
3 Solvent	CDCl ₃
4 Temperature	300.7
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	2048
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-19T19:04:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	^{13}C
16 Acquired Size	32768
17 Spectral Size	65536



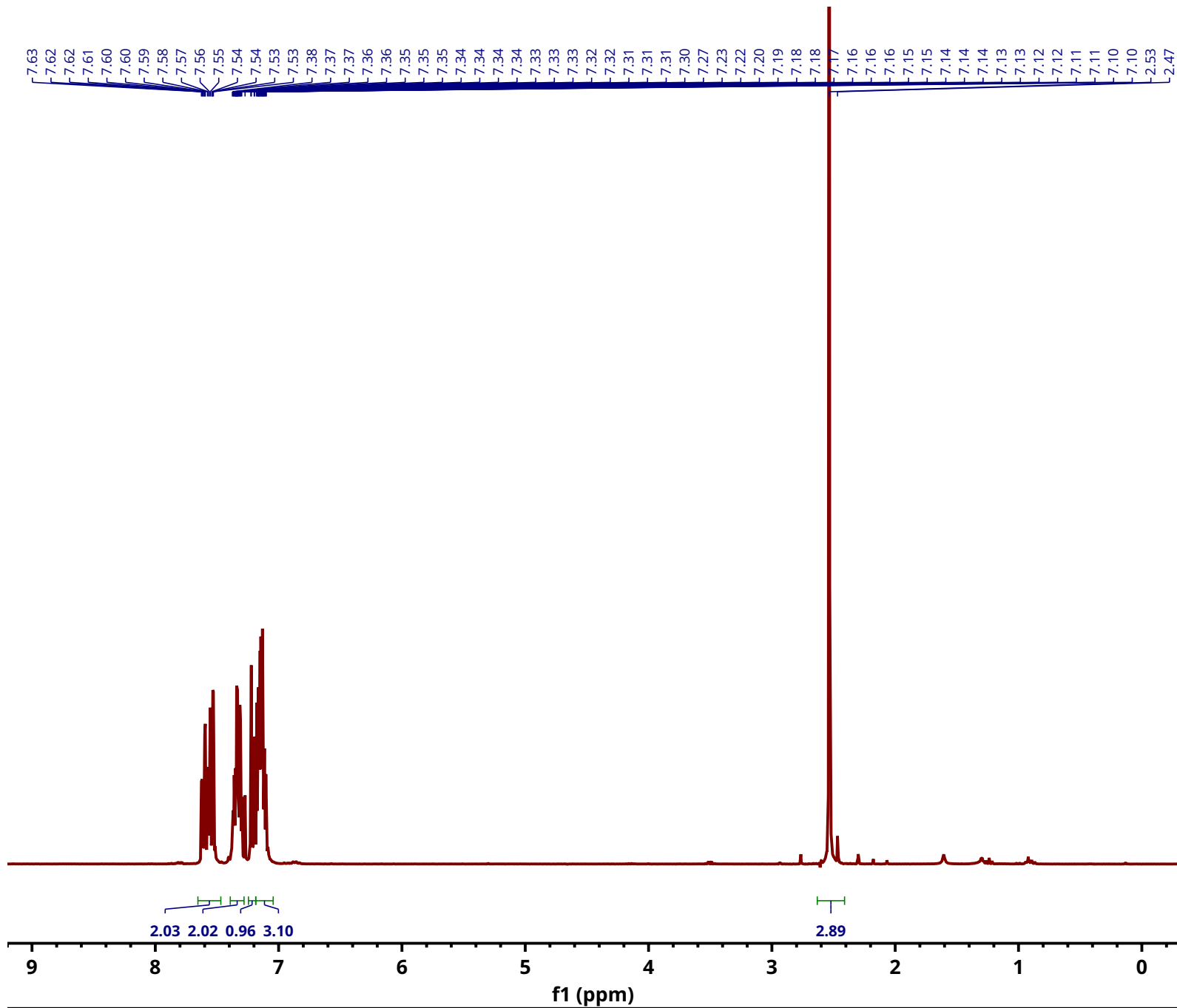
Compound 5f

^{13}C NMR(Chloroform-*d*, 75 MHz): δ (ppm) 146.35, 140.38, 139.50, 124.17, 123.51, 122.81, 122.24, 120.81, 62.09, 34.22, 27.23, 26.11, 18.47, -5.12, -5.15

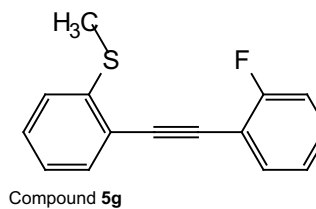
Parameter	Value
1 Title	CCD-097.12.fid
2 Instrument	FOURIER300
3 Solvent	CDCl ₃
4 Temperature	300.7
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	2048
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-19T19:04:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	¹³ C
16 Acquired Size	32768
17 Spectral Size	65536



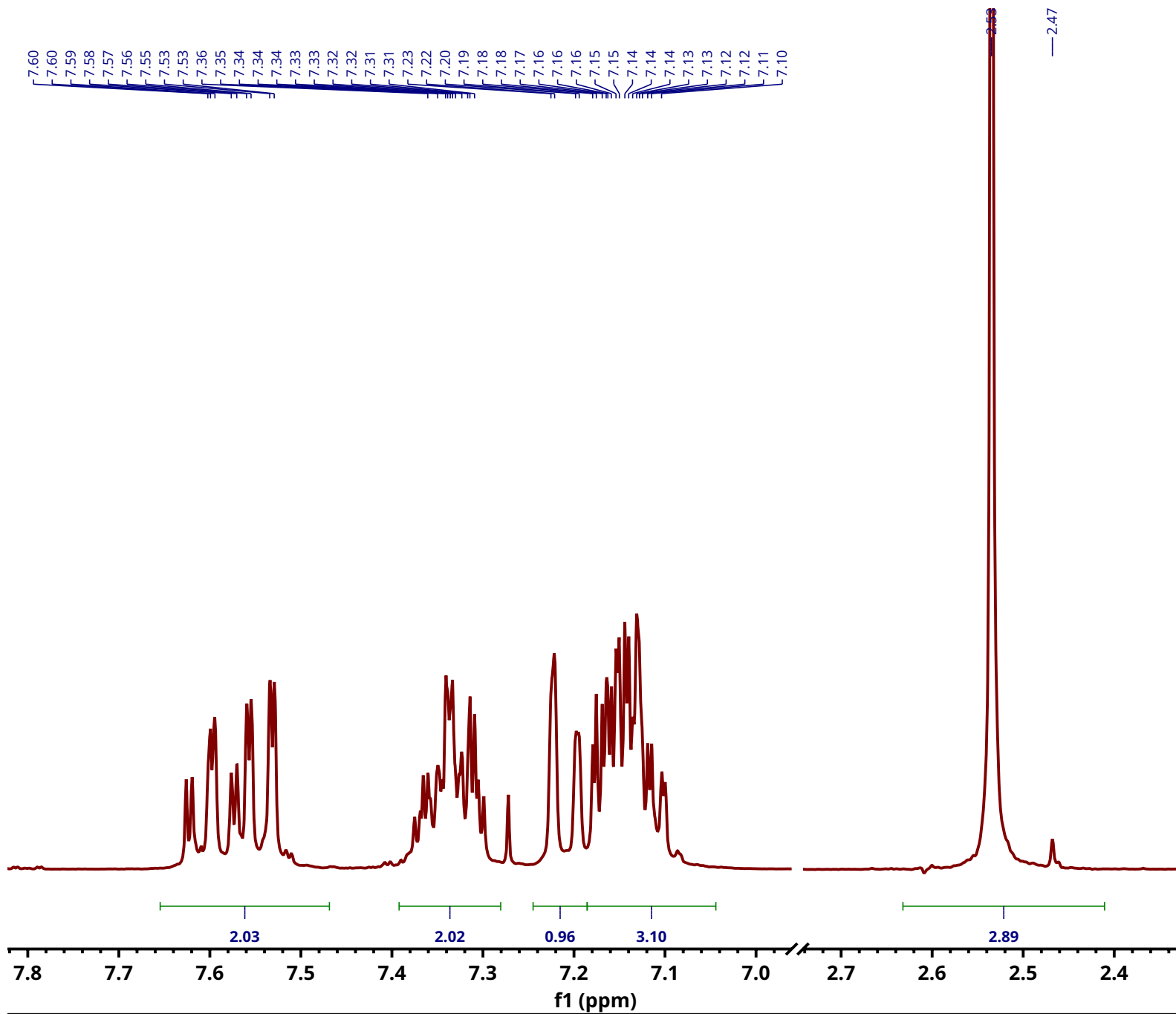
Compound 5f



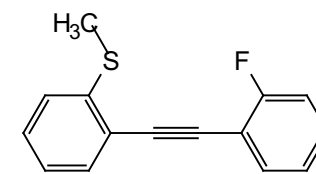
Parameter	Value
Title	PK-904.101.fid
Date	20181018
Time	12.55
Solvent	CDCl3
Instrument	FOURIER300
Temperature	296.9
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	16
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536



¹H NMR (300 MHz, Chloroform-*d*) δ 7.65 – 7.47 (m, 2H), 7.39 – 7.28 (m, 2H), 7.21 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.19 – 7.04 (m, 3H), 2.53 (s, 3H).



Parameter	Value
Title	PK-904.101.fid
Date	20181018
Time	12.55
Solvent	CDCl3
Instrument	FOURIER300
Temperature	296.9
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	16
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

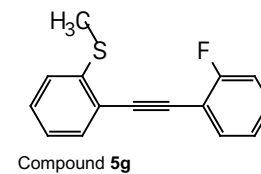
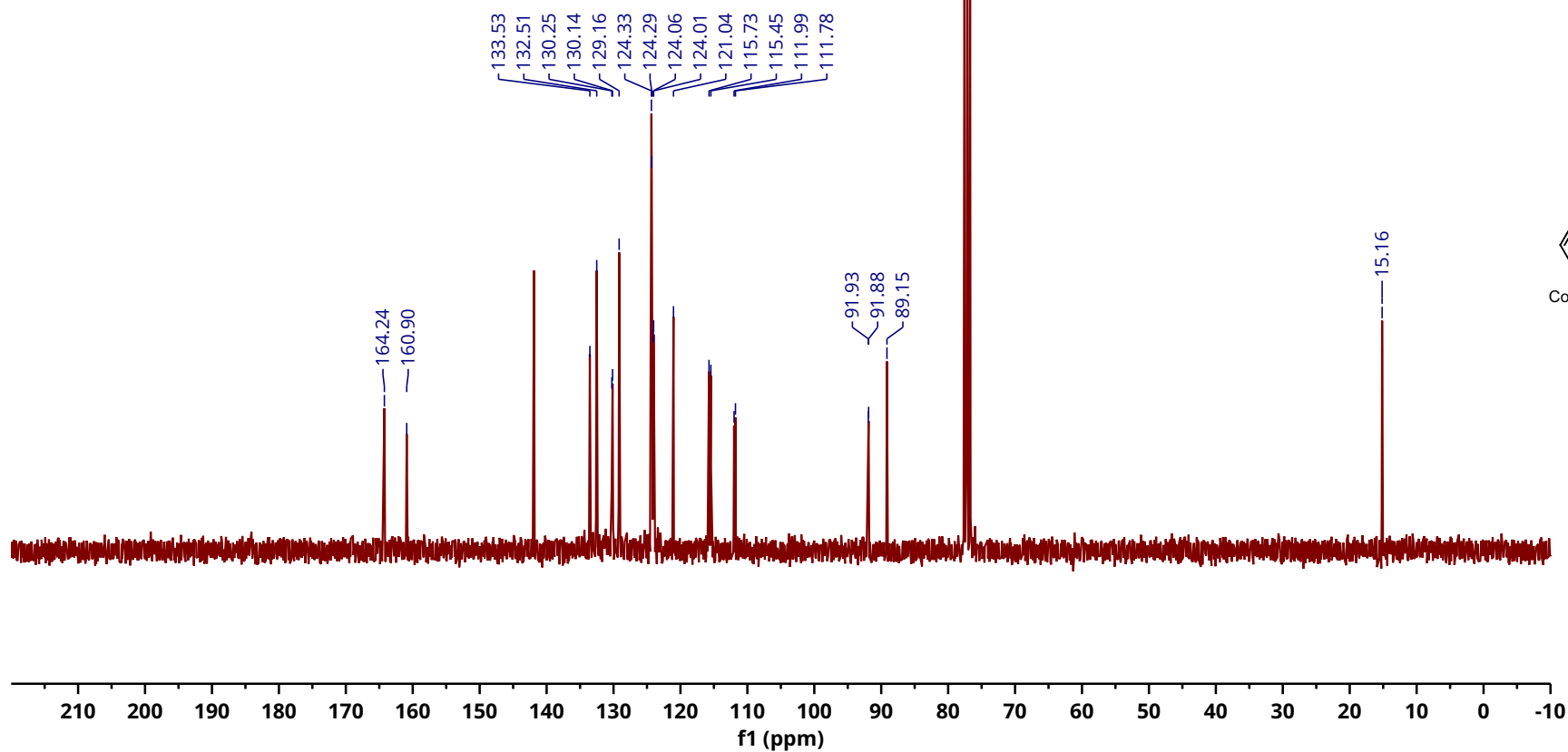


Compound 5g

$^1\text{H NMR}$ (300 MHz, Chloroform-*d*) δ 7.65 – 7.47 (m, 2H), 7.39 – 7.28 (m, 2H), 7.21 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.19 – 7.04 (m, 3H), 2.53 (s, 3H).

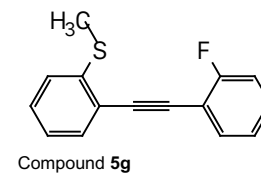
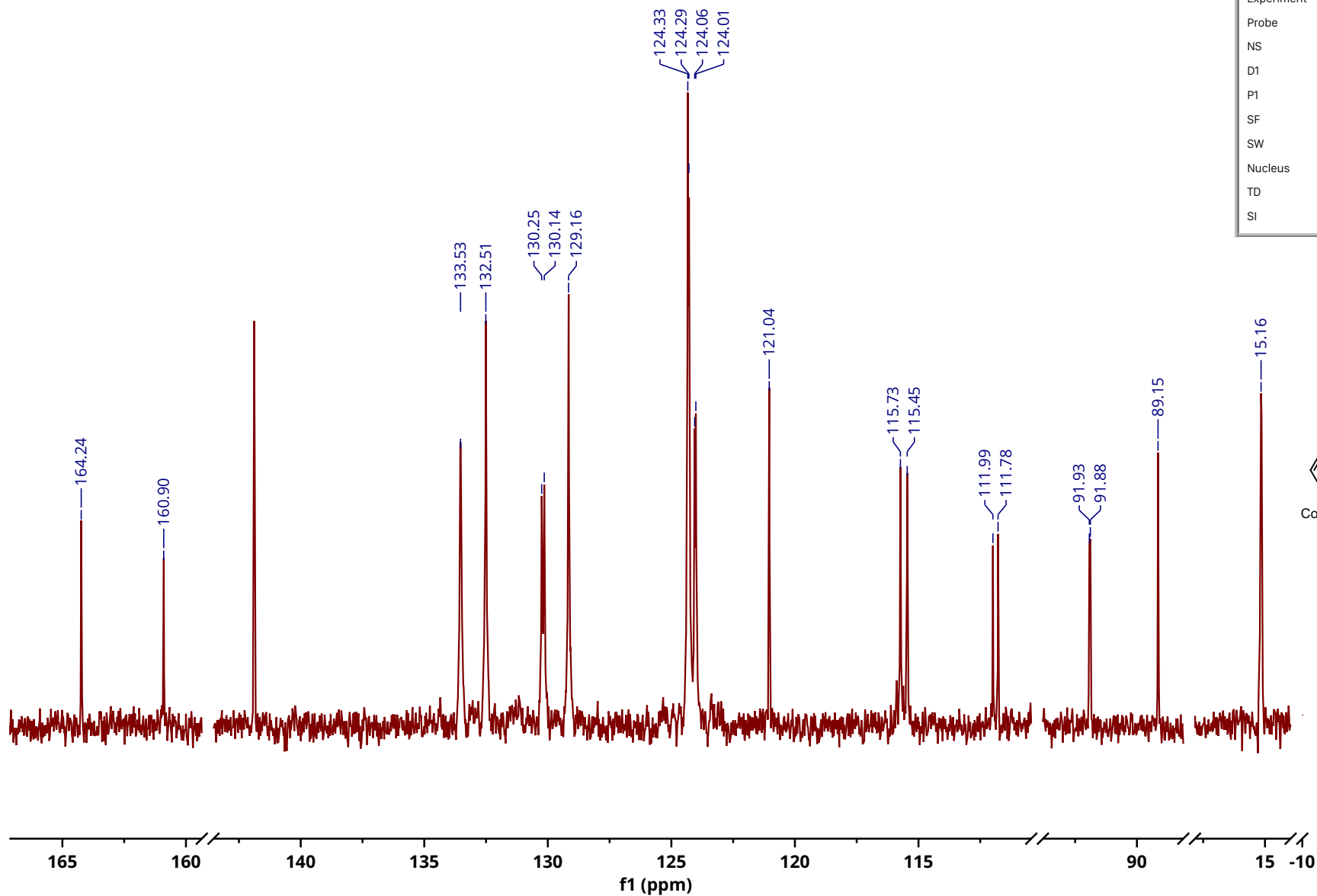
^{13}C NMR (75 MHz, CDCl_3) δ 164.24, 160.90, 133.53, 132.51, 130.25, 130.14, 129.16, 124.33, 124.29, 124.06, 124.01, 121.04, 115.73, 115.45, 111.99, 111.78, 91.93, 91.88, 89.15, 15.16.

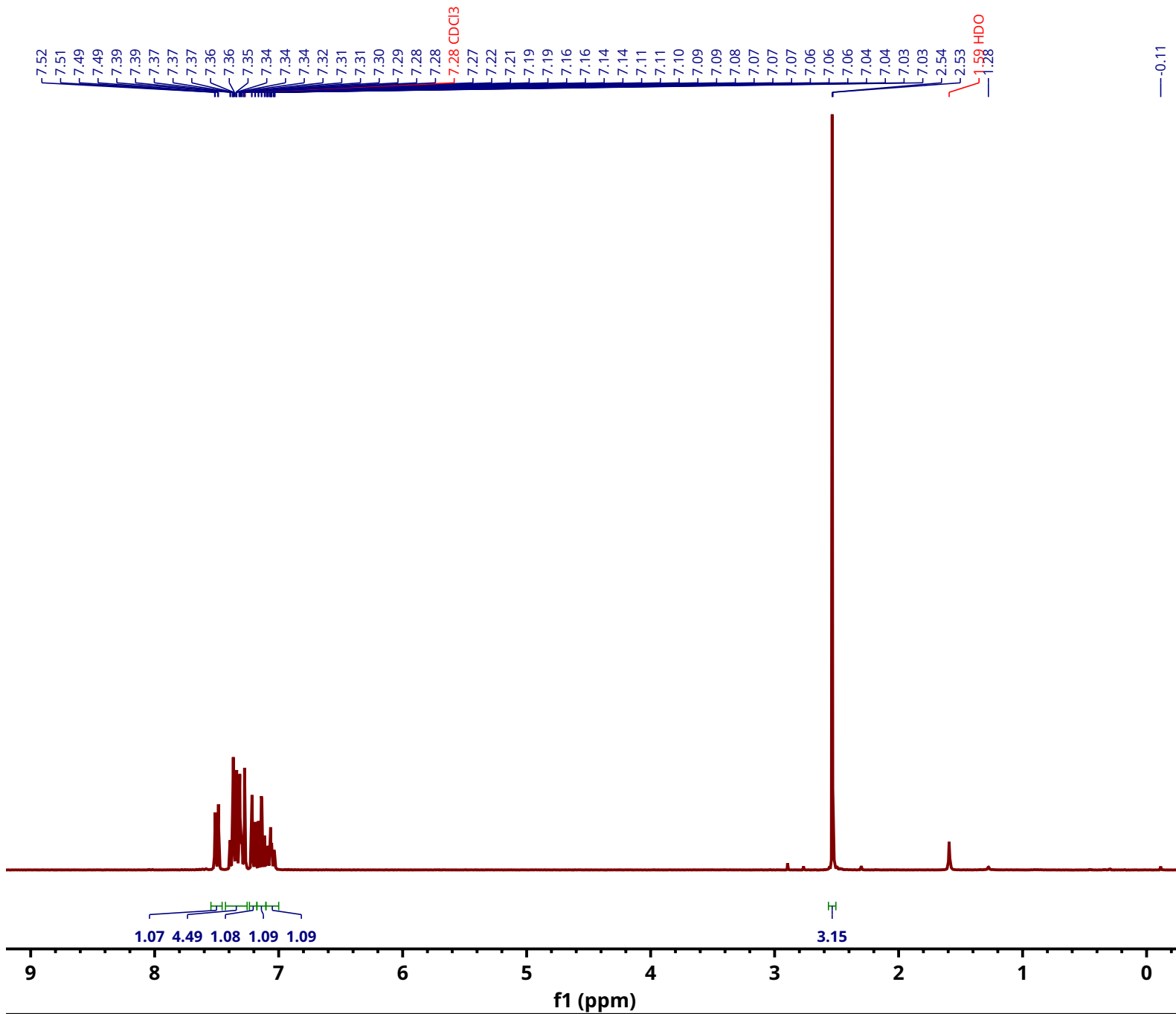
Parameter	Value
Title	PK-904.100.fid
Date	20181018
Time	12.58
Solvent	CDCl_3
Instrument	FOURIER300
Temperature	297.0
PULPROG	zgpg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	256
D1	2.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536



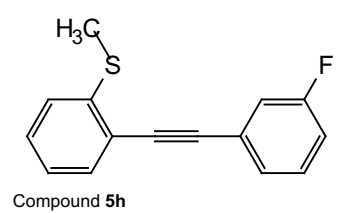
^{13}C NMR (75 MHz, CDCl_3) δ 164.24, 160.90, 133.53, 132.51, 130.25, 130.14, 129.16, 124.33, 124.29, 124.06, 124.01, 121.04, 115.73, 115.45, 111.99, 111.78, 91.93, 91.88, 89.15, 15.16.

Parameter	Value
Title	PK-904.100.fid
Date	20181018
Time	12.58
Solvent	CDCl_3
Instrument	FOURIER300
Temperature	297.0
PULPROG	zgpg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	256
D1	2.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536

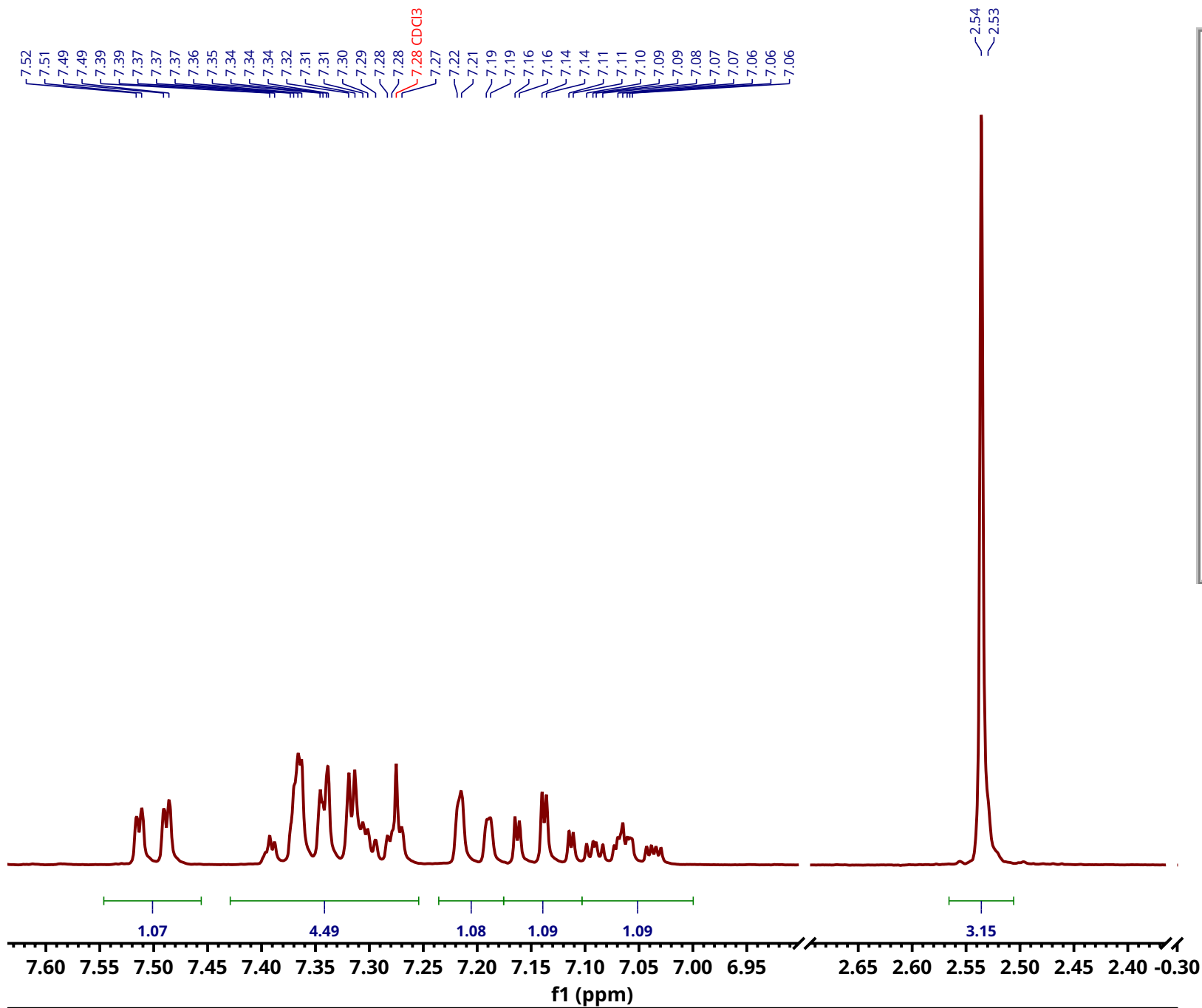




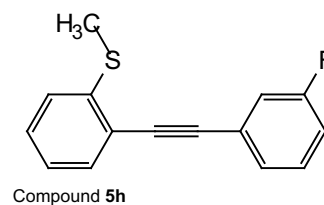
Parameter	Value
1 Title	AP-055.2.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	295.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	48.8
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-03-16T11:27:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



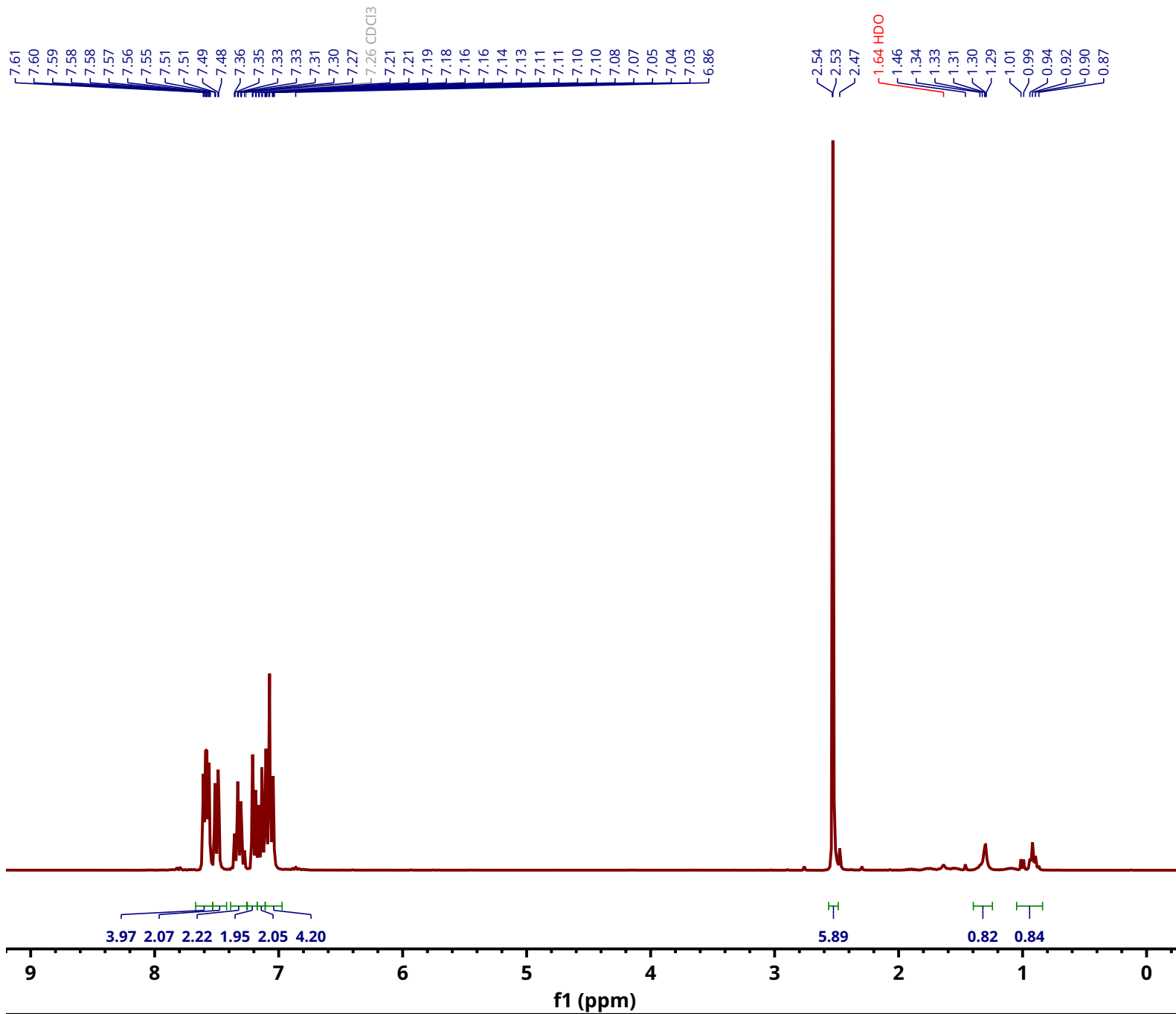
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.49 (dd, *J*=7.6, 1.5 Hz, 1H), 7.40 – 7.24 (m, 4H), 7.19 (dd, *J*=8.1, 1.2 Hz, 1H), 7.12 (td, *J*=7.5, 1.2 Hz, 1H), 7.09 – 6.98 (m, 1H), 2.52 (s, 3H)



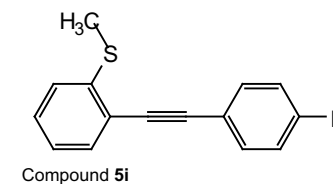
Parameter	Value
1 Title	AP-055.2.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	295.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	48.8
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-03-16T11:27:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



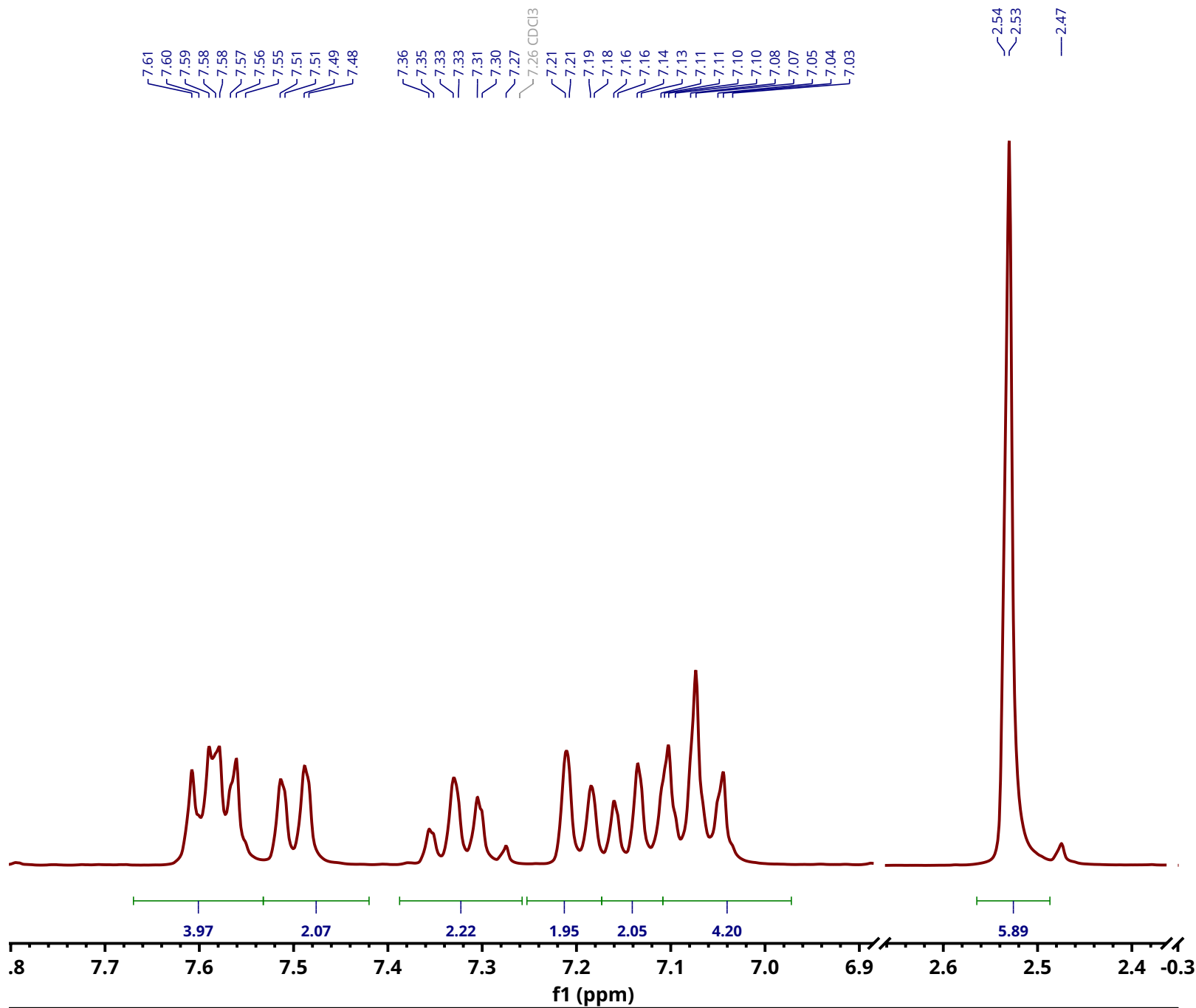
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.49 (dd, *J*=7.6, 1.5 Hz, 1H), 7.40 – 7.24 (m, 4H), 7.19 (dd, *J*=8.1, 1.2 Hz, 1H), 7.12 (td, *J*=7.5, 1.2 Hz, 1H), 7.09 – 6.98 (m, 1H), 2.52 (s, 3H)



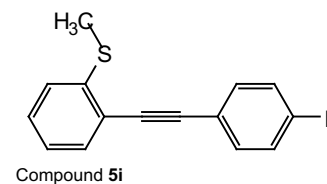
Parameter	Value
1 Title	MS-071.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	296.6
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	128
8 Receiver Gain	15.5
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2017-12-21T11:40:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



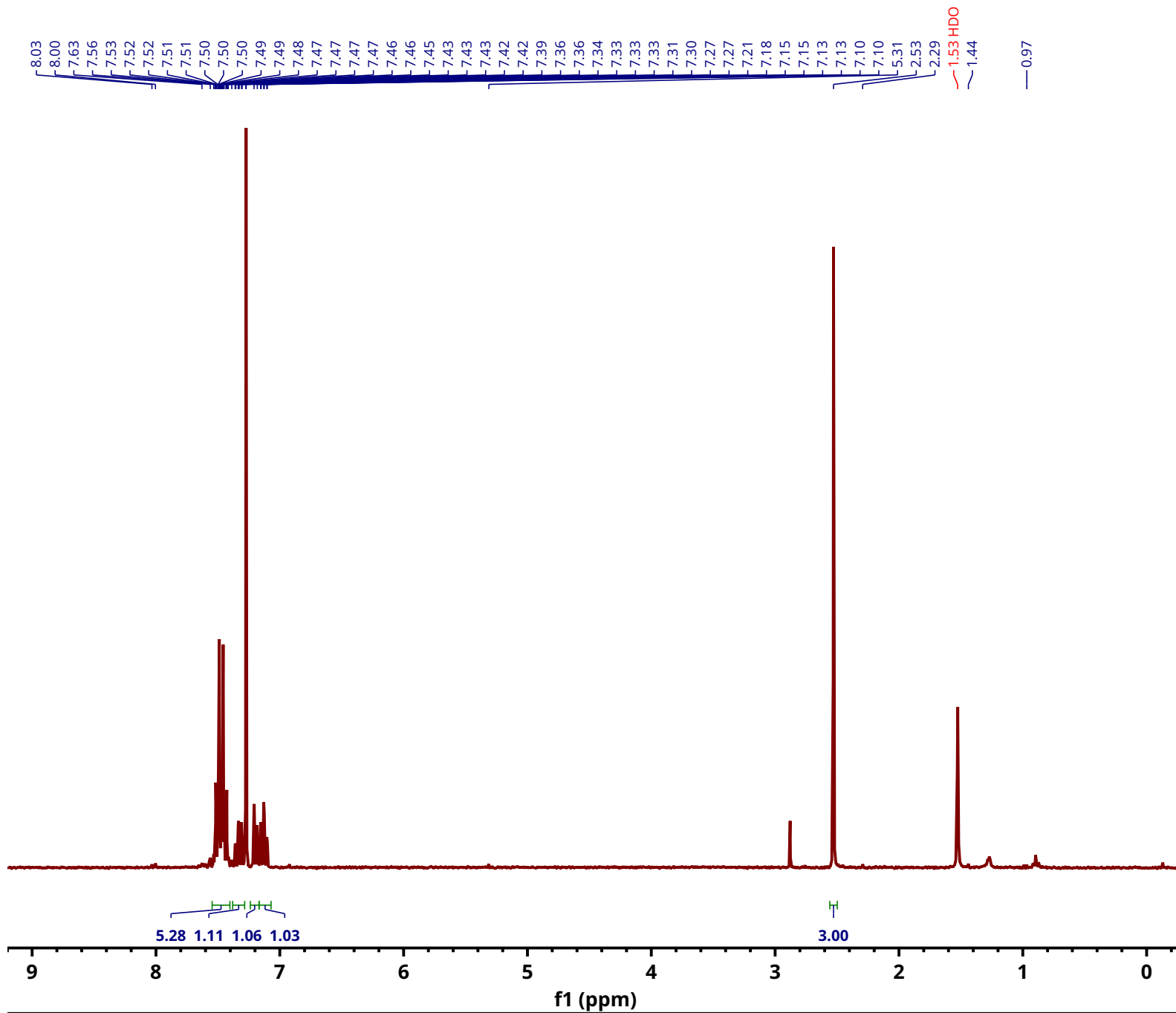
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.66 – 7.52 (m, 2H), 7.48 (dd, *J*=7.6, 1.5 Hz, 1H), 7.31 (td, *J*=7.7, 1.5 Hz, 1H), 7.18 (dd, *J*=8.0, 1.3 Hz, 1H), 7.12 (dd, *J*=8.2, 6.9 Hz, 1H), 7.06 (td, *J*=8.5, 1.5 Hz, 2H), 2.52 (s, 3H)



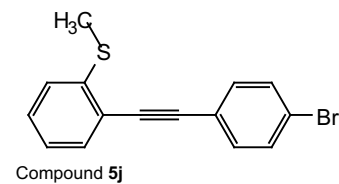
Parameter	Value
1 Title	MS-071.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	296.6
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	128
8 Receiver Gain	15.5
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2017-12-21T11:40:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



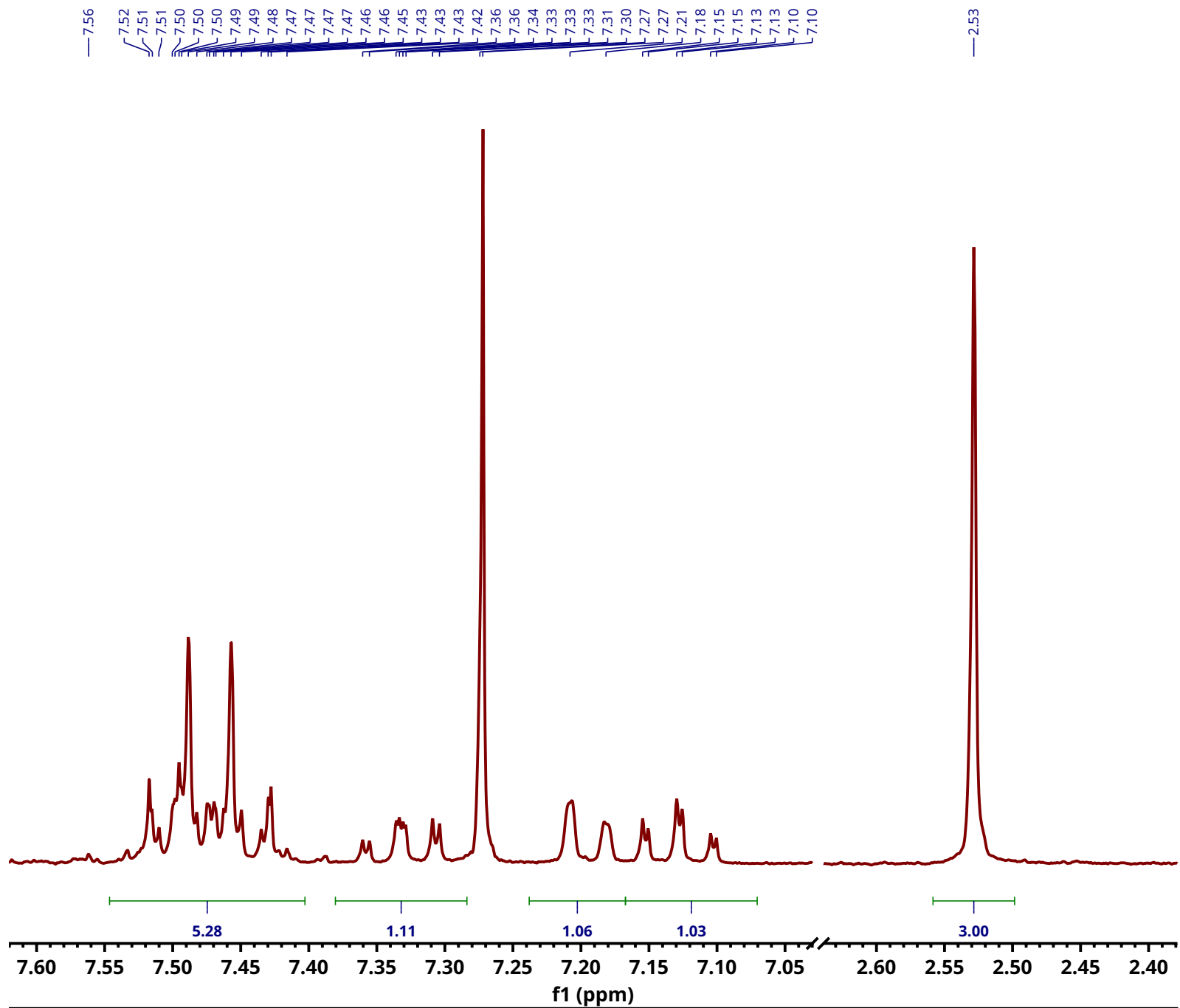
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.66 – 7.52 (m, 2H), 7.48 (dd, *J*=7.6, 1.5 Hz, 1H), 7.31 (td, *J*=7.7, 1.5 Hz, 1H), 7.18 (dd, *J*=8.0, 1.3 Hz, 1H), 7.12 (dd, *J*=8.2, 6.9 Hz, 1H), 7.06 (td, *J*=8.5, 1.5 Hz, 2H), 2.52 (s, 3H)



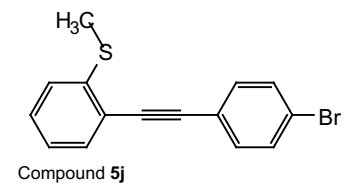
Parameter	Value
1 Title	JWP-047.1.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	258.3
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-14T10:48:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



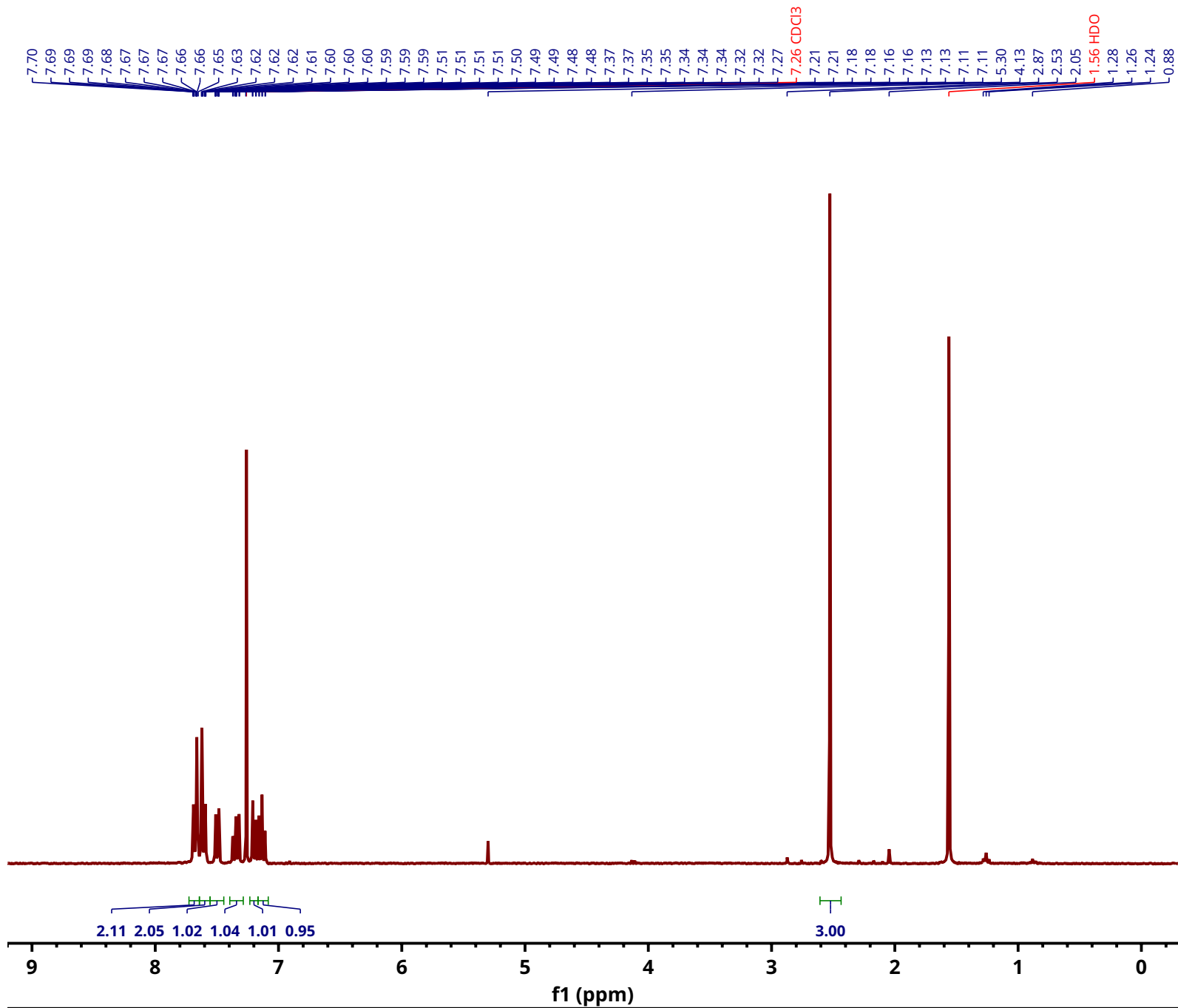
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.53 – 7.39 (m, 5H), 7.32 (ddd, *J*=8.1, 7.4, 1.5 Hz, 1H), 7.18 (d, *J*=7.9 Hz, 1H), 7.12 (td, *J*=7.5, 1.3 Hz, 1H), 2.52 (s, 3H)



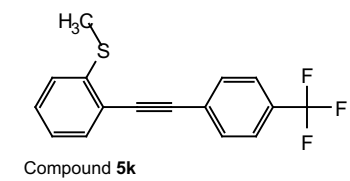
Parameter	Value
1 Title	JWP-047.1.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	258.3
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-14T10:48:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



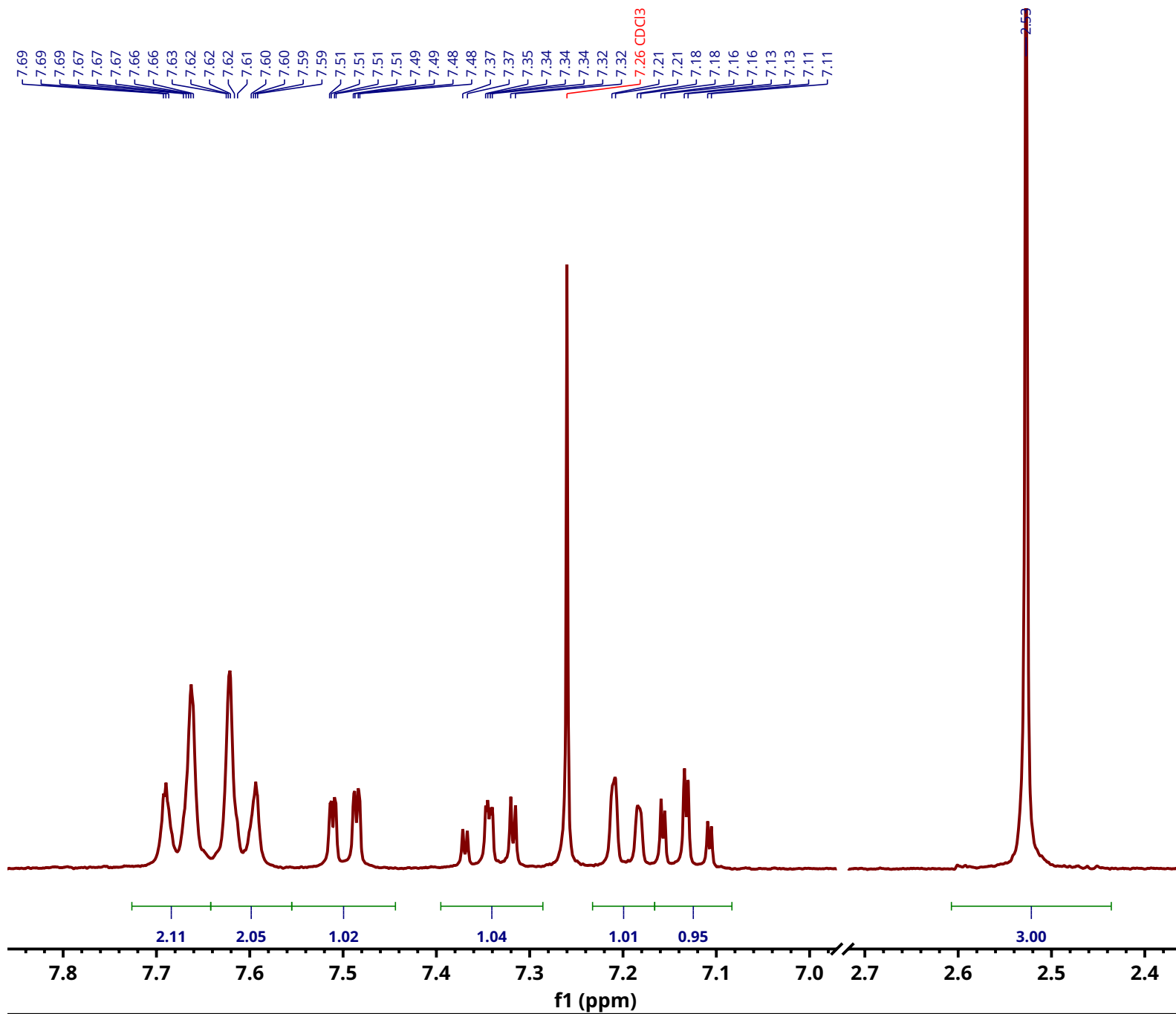
$^1\text{H NMR}$ (Chloroform-*d*, 300 MHz): δ (ppm) 7.53 – 7.39 (m, 5H), 7.32 (ddd, $J=8.1, 7.4, 1.5$ Hz, 1H), 7.18 (d, $J=7.9$ Hz, 1H), 7.12 (td, $J=7.5, 1.3$ Hz, 1H), 2.52 (s, 3H)



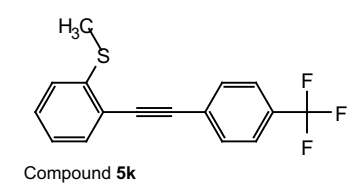
Parameter	Value
1 Title	DAL-071.3.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	296.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	120.0
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-05-31T10:49:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



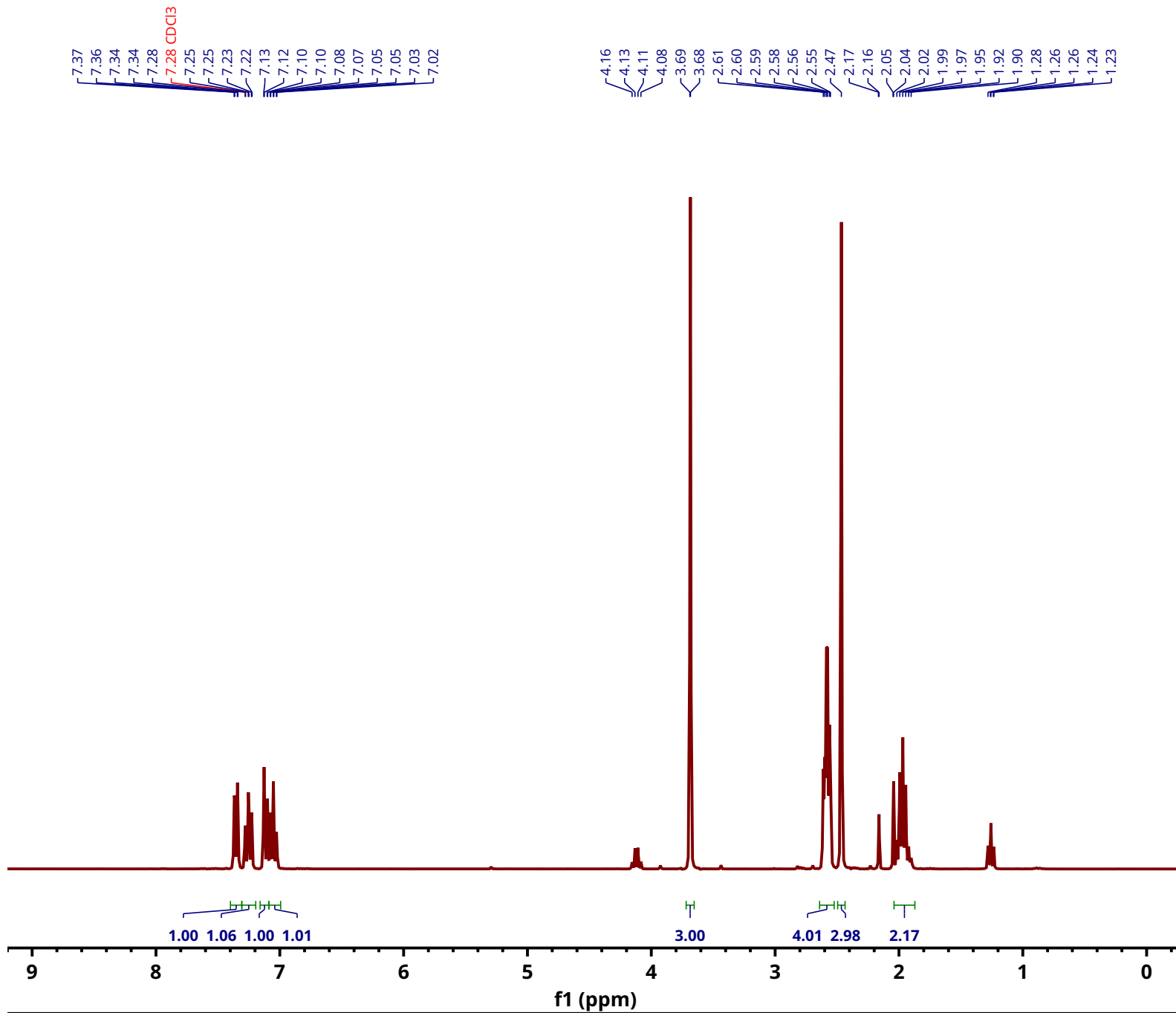
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.68 (dt, *J*=7.9, 0.8 Hz, 2H), 7.66 – 7.56 (m, 2H), 7.50 (ddd, *J*=7.6, 1.6, 0.5 Hz, 1H), 7.34 (ddd, *J*=8.1, 7.4, 1.5 Hz, 1H), 7.20 (dd, *J*=8.1, 1.2 Hz, 1H), 7.13 (td, *J*=7.5, 1.2 Hz, 1H), 2.53 (s, 3H)



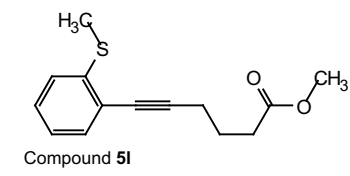
Parameter	Value
1 Title	DAL-071.3.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	296.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	120.0
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-05-31T10:49:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



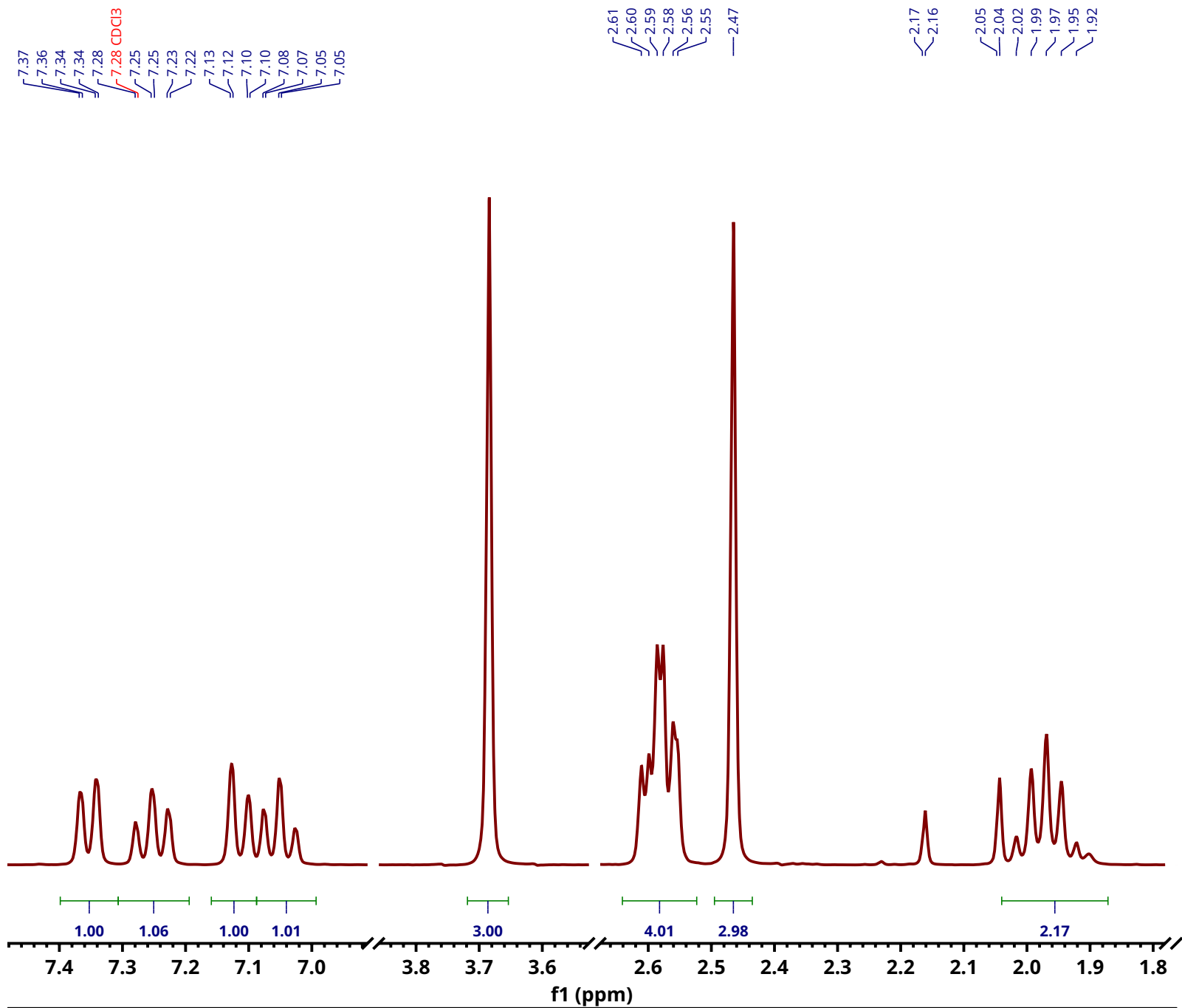
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.68 (dt, *J*=7.9, 0.8 Hz, 2H), 7.66 – 7.56 (m, 2H), 7.50 (ddd, *J*=7.6, 1.6, 0.5 Hz, 1H), 7.34 (ddd, *J*=8.1, 7.4, 1.5 Hz, 1H), 7.20 (dd, *J*=8.1, 1.2 Hz, 1H), 7.13 (td, *J*=7.5, 1.2 Hz, 1H), 2.53 (s, 3H)



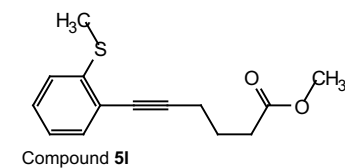
Parameter	Value
1 Title	MS-076.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	295.6
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	128
8 Receiver Gain	8.9
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-03-15T11:31:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



¹H NMR (300 MHz, Chloroform-*d*) δ 7.49 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.39 (td, *J* = 7.6, 1.4 Hz, 1H), 7.29 – 7.22 (m, 1H), 7.18 (td, *J* = 7.5, 1.3 Hz, 1H), 3.82 (d, *J* = 1.5 Hz, 3H), 2.71 (td, *J* = 7.2, 2.9 Hz, 4H), 2.60 (s, 3H), 2.11 (td, *J* = 14.6, 7.5 Hz, 2H).



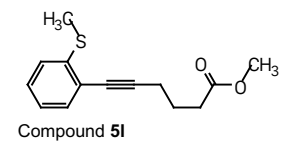
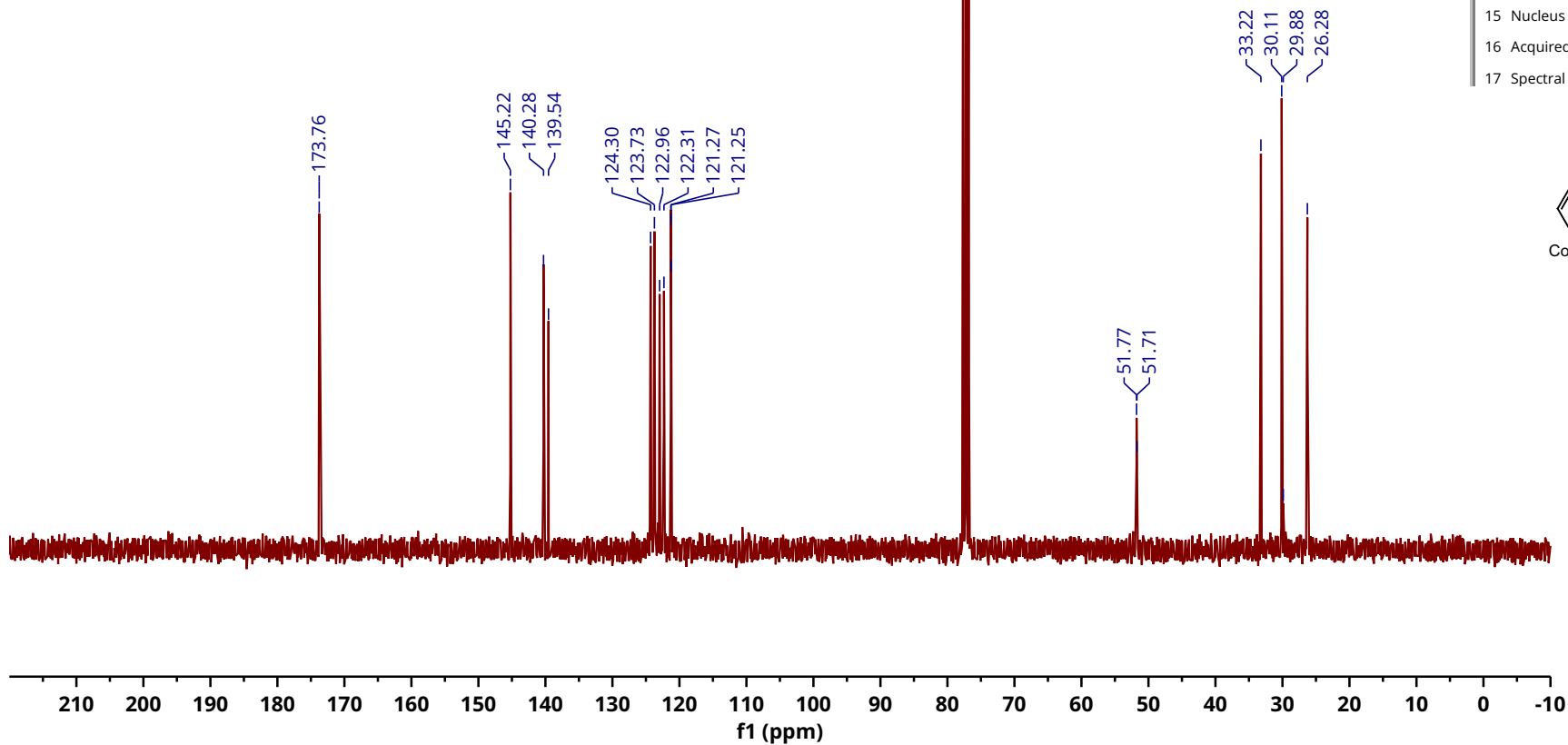
Parameter	Value
1 Title	MS-076.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	295.6
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	128
8 Receiver Gain	8.9
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-03-15T11:31:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



^1H NMR (300 MHz, Chloroform-*d*) δ 7.49 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.39 (td, $J = 7.6, 1.4$ Hz, 1H), 7.29 – 7.22 (m, 1H), 7.18 (td, $J = 7.5, 1.3$ Hz, 1H), 3.82 (d, $J = 1.5$ Hz, 3H), 2.71 (td, $J = 7.2, 2.9$ Hz, 4H), 2.60 (s, 3H), 2.11 (td, $J = 14.6, 7.5$ Hz, 2H).

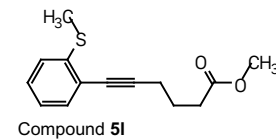
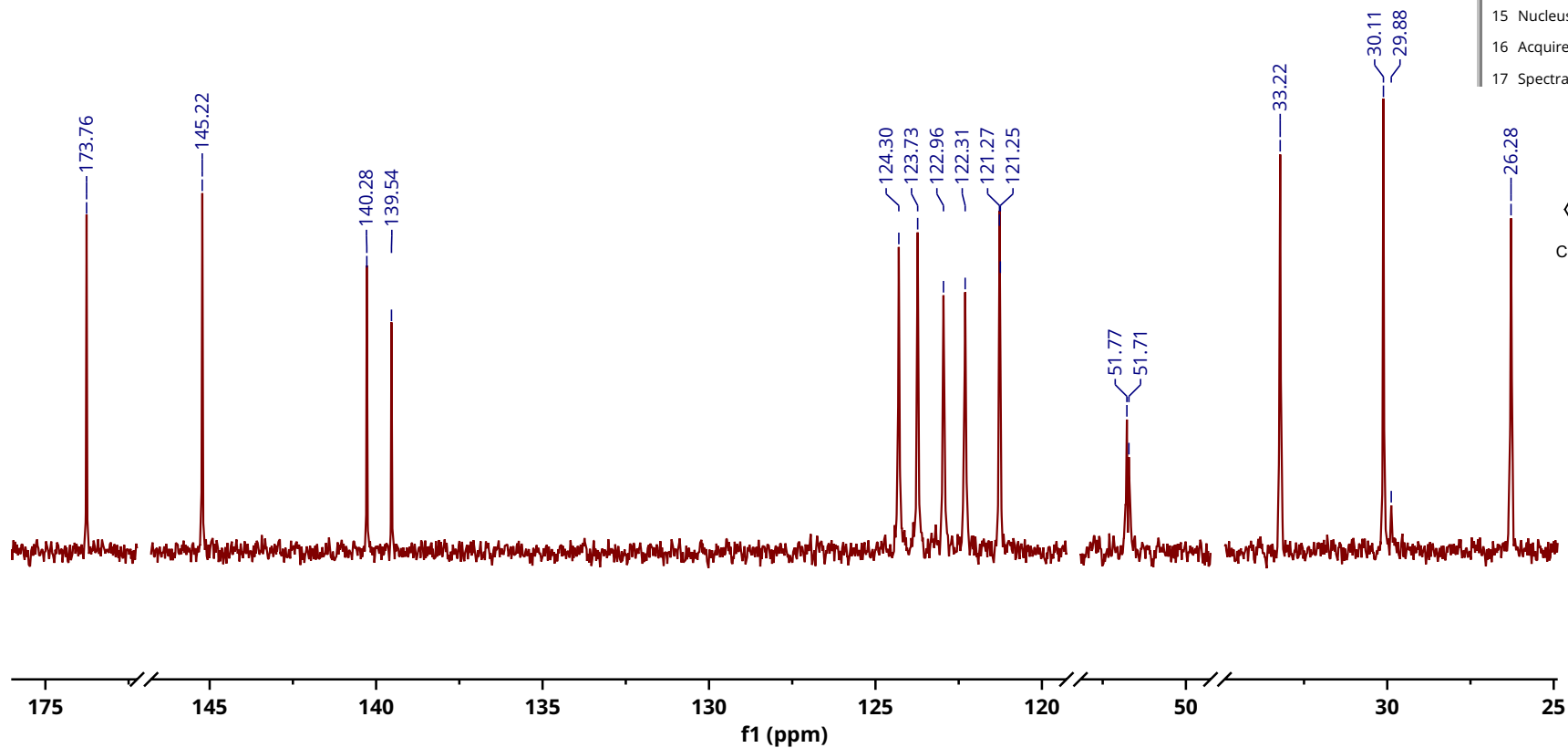
^{13}C NMR (75 MHz, CDCl_3) δ 173.69, 145.15, 140.21, 139.47, 124.23, 123.66, 122.89, 122.24, 121.21, 121.18, 51.70, 51.64, 33.15, 30.05, 29.81, 26.21.

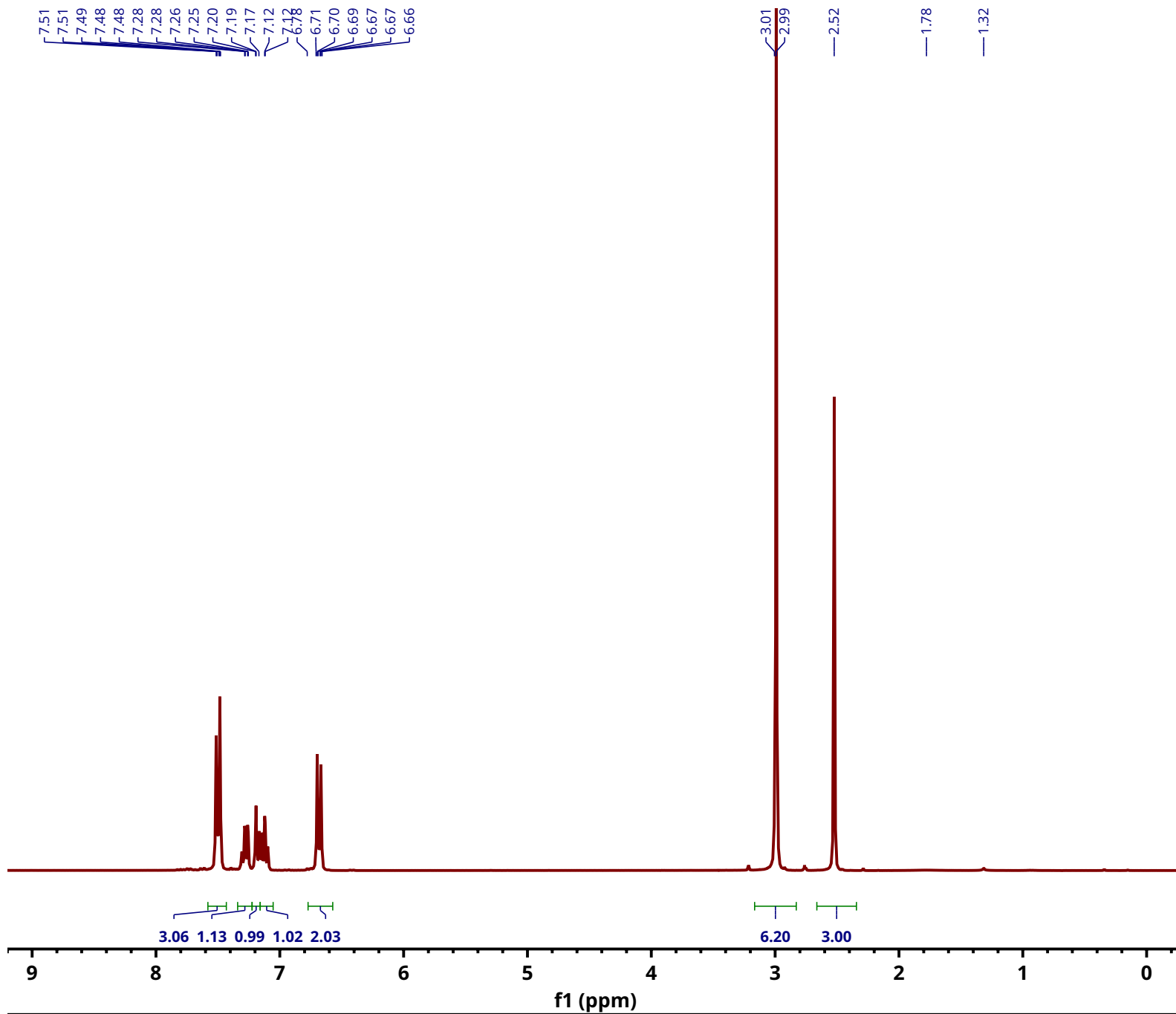
Parameter	Value
1 Title	CCD-093.111.fid
2 Instrument	FOURIER300
3 Solvent	CDCl_3
4 Temperature	299.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	403
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-13T11:24:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	^{13}C
16 Acquired Size	32768
17 Spectral Size	65536



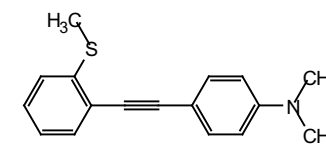
^{13}C NMR (75 MHz, CDCl_3) δ 173.69, 145.15, 140.21, 139.47, 124.23, 123.66, 122.89, 122.24, 121.21, 121.18, 51.70, 51.64, 33.15, 30.05, 29.81, 26.21.

Parameter	Value
1 Title	CCD-093.111.fid
2 Instrument	FOURIER300
3 Solvent	CDCl_3
4 Temperature	299.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	403
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-13T11:24:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	^{13}C
16 Acquired Size	32768
17 Spectral Size	65536



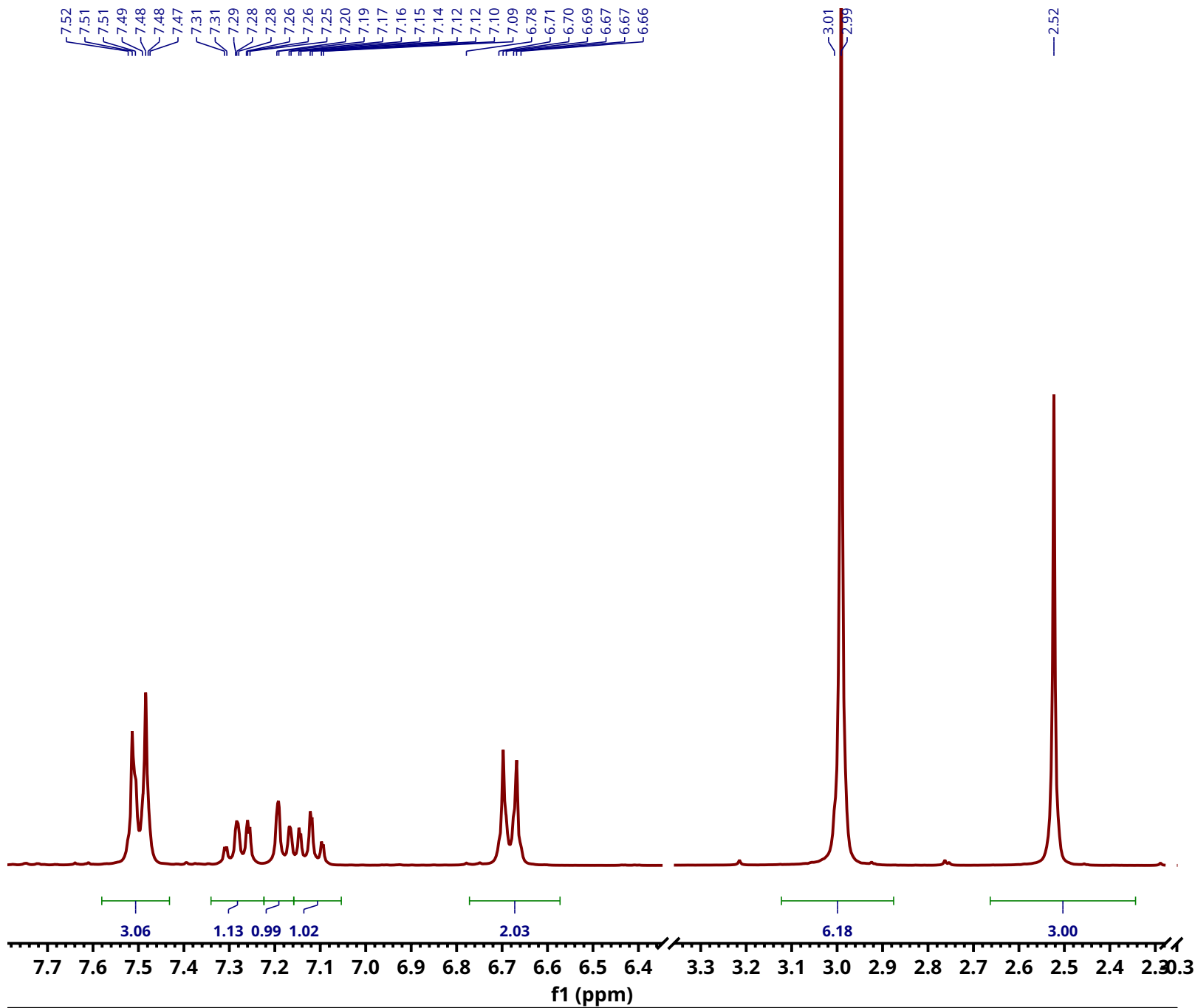


Parameter	Value
1 Title	BK-061.21.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	1032.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	6.8
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-08-17T14:37:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

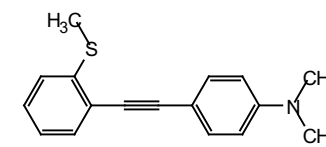


Compound 5m

¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.50 (d, *J*=8.9 Hz, 3H), 7.33 – 7.23 (m, 1H), 7.18 (dd, *J*=8.1, 1.3 Hz, 1H), 7.12 (td, *J*=7.4, 1.3 Hz, 1H), 6.68 (d, *J*=8.9 Hz, 2H), 2.99 (s, 6H), 2.52 (s, 3H)

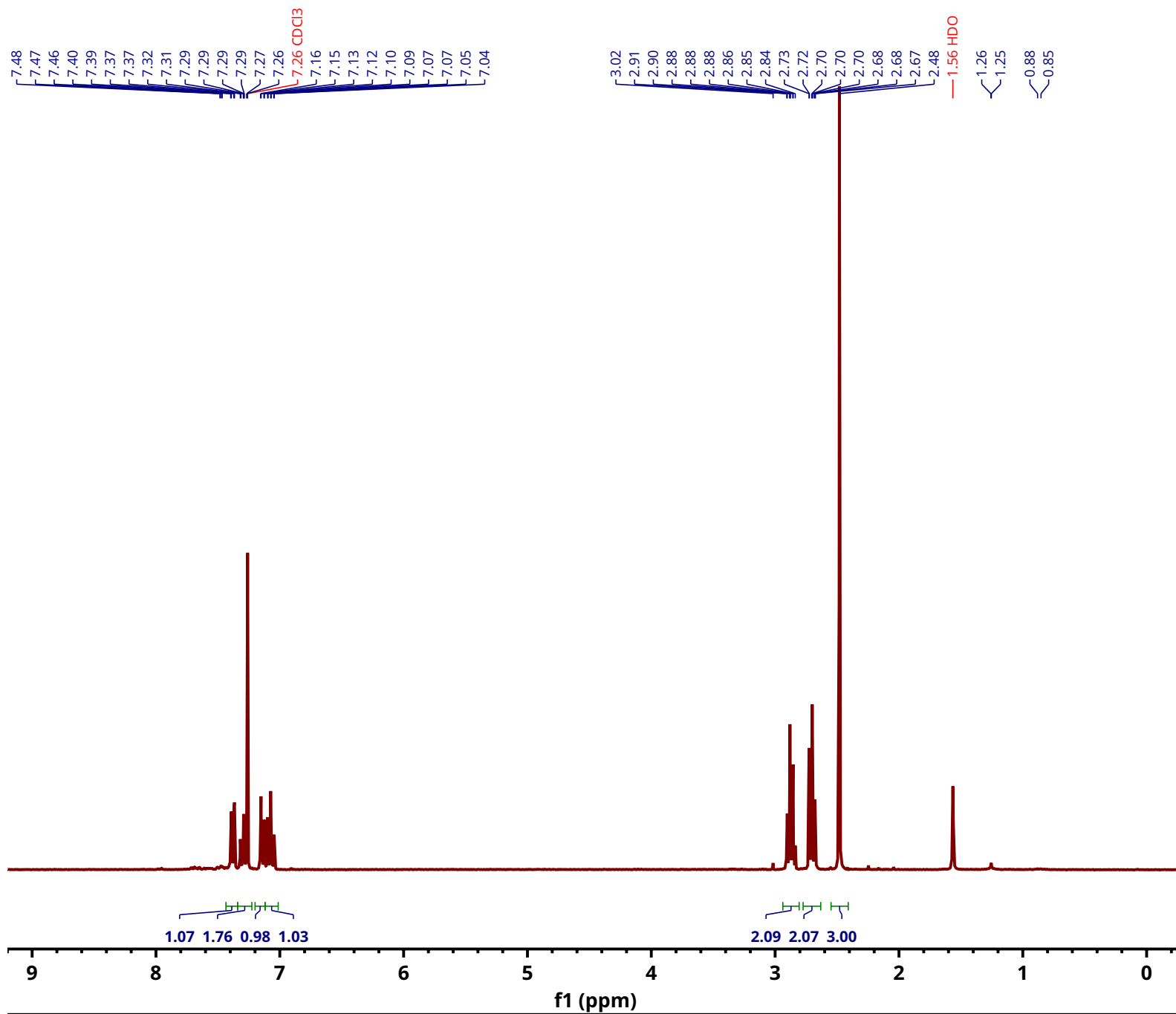


Parameter	Value
1 Title	BK-061.21.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	1032.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	6.8
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-08-17T14:37:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

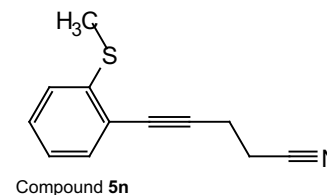


Compound 5m

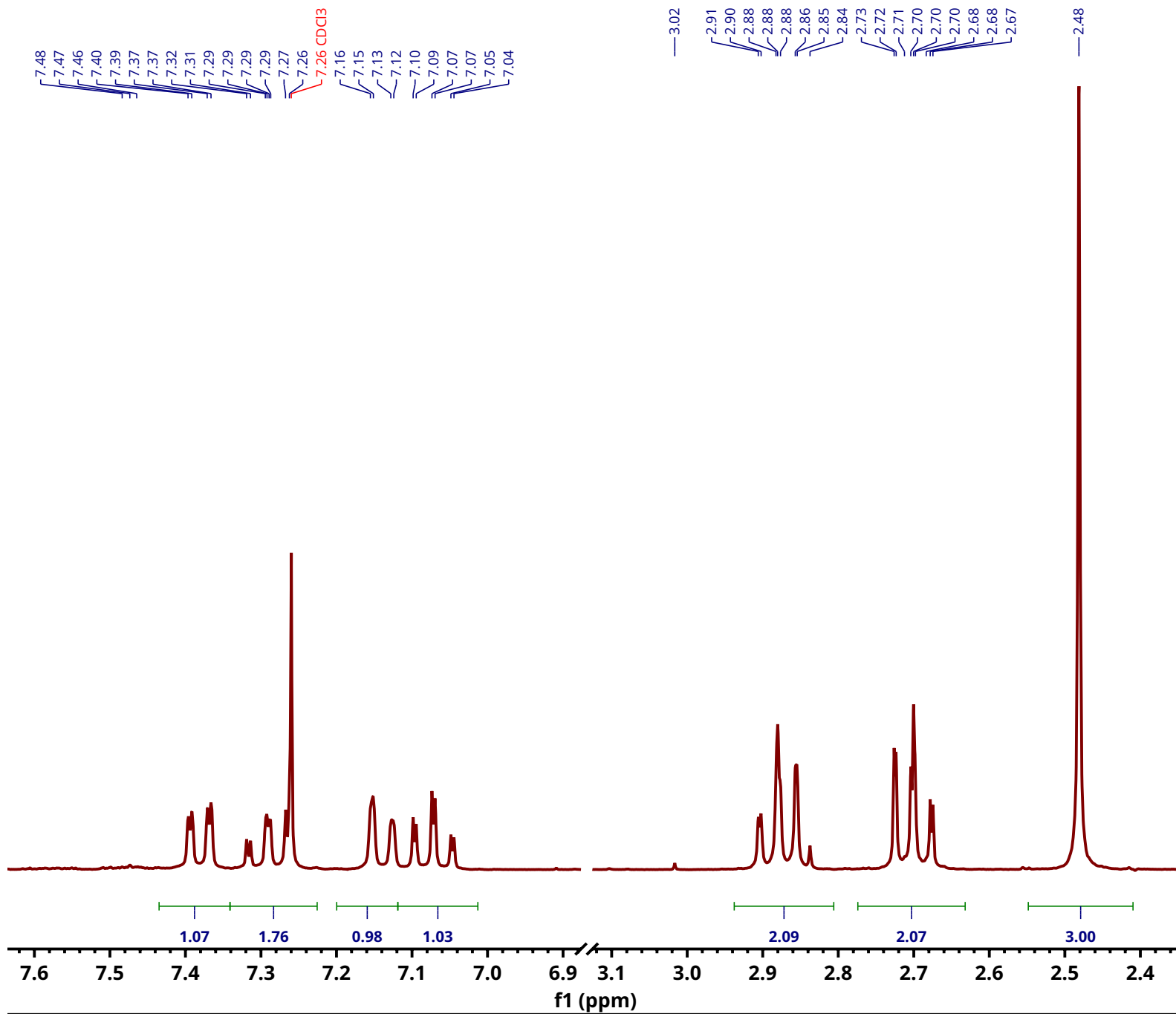
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.50 (d, *J*=8.9 Hz, 3H), 7.33 – 7.23 (m, 1H), 7.18 (dd, *J*=8.1, 1.3 Hz, 1H), 7.12 (td, *J*=7.4, 1.3 Hz, 1H), 6.68 (d, *J*=8.9 Hz, 2H), 2.99 (s, 6H), 2.52 (s, 3H)



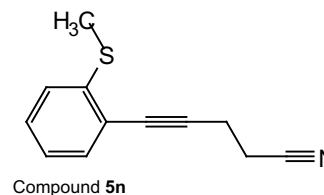
Parameter	Value
1 Title	BK-083.13.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	124.5
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-17T11:46:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



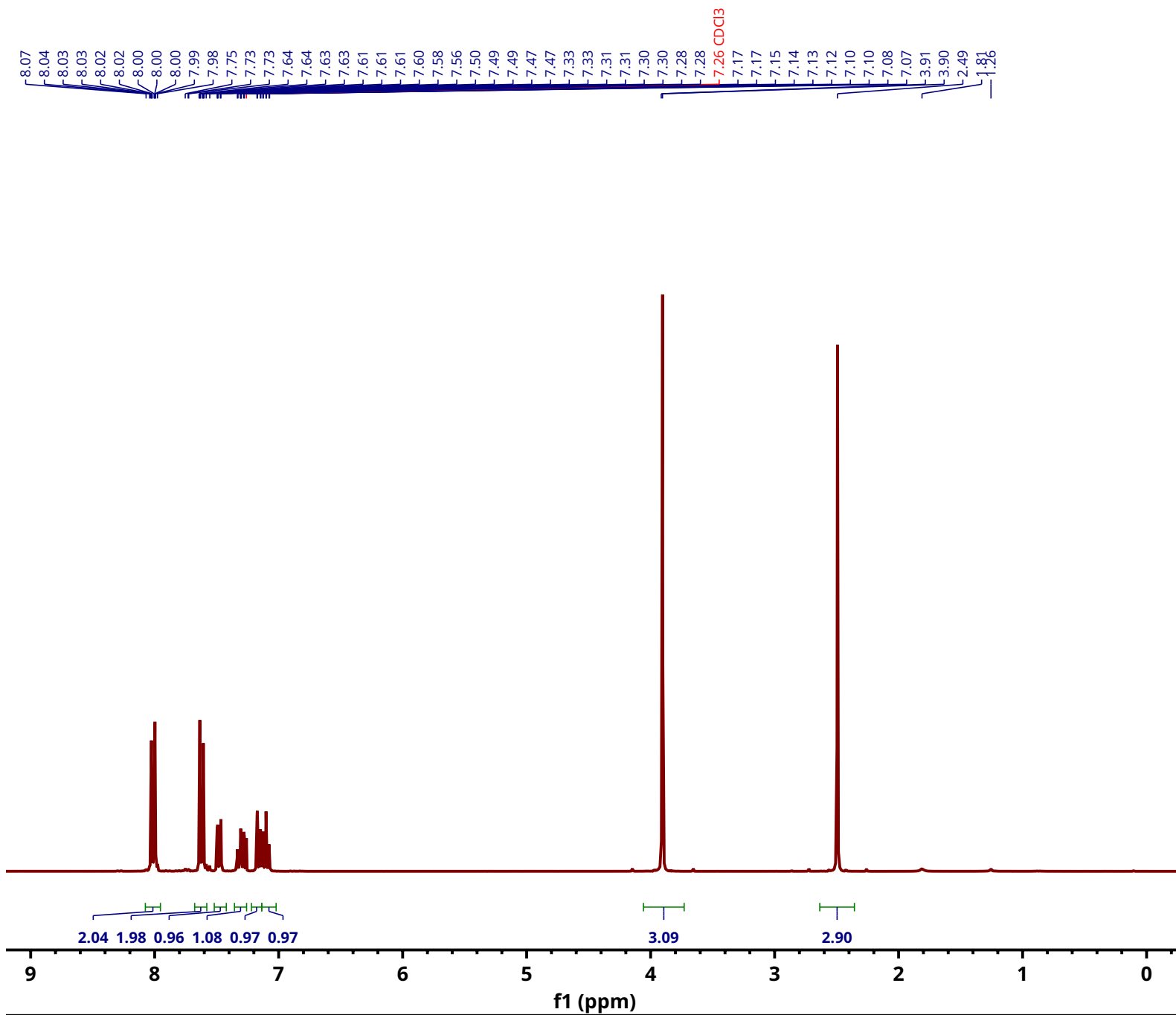
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.38 (dd, *J*=7.6, 1.5 Hz, 1H), 7.29 (ddd, *J*=8.1, 7.4, 1.5 Hz, 1H), 7.14 (dd, *J*=8.1, 1.2 Hz, 1H), 7.07 (td, *J*=7.5, 1.2 Hz, 1H), 2.88 (ddd, *J*=7.8, 6.9, 1.0 Hz, 2H), 2.70 (ddd, *J*=7.7, 6.8, 1.0 Hz, 2H), 2.48 (s, 3H)



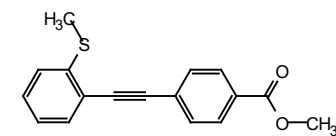
Parameter	Value
1 Title	BK-083.13.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	124.5
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-17T11:46:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



¹H NMR (Chloroform-*d*, 300 MHz): δ (ppm) 7.38 (dd, *J*=7.6, 1.5 Hz, 1H), 7.29 (ddd, *J*=8.1, 7.4, 1.5 Hz, 1H), 7.14 (dd, *J*=8.1, 1.2 Hz, 1H), 7.07 (td, *J*=7.5, 1.2 Hz, 1H), 2.88 (ddd, *J*=7.8, 6.9, 1.0 Hz, 2H), 2.70 (ddd, *J*=7.7, 6.8, 1.0 Hz, 2H), 2.48 (s, 3H)

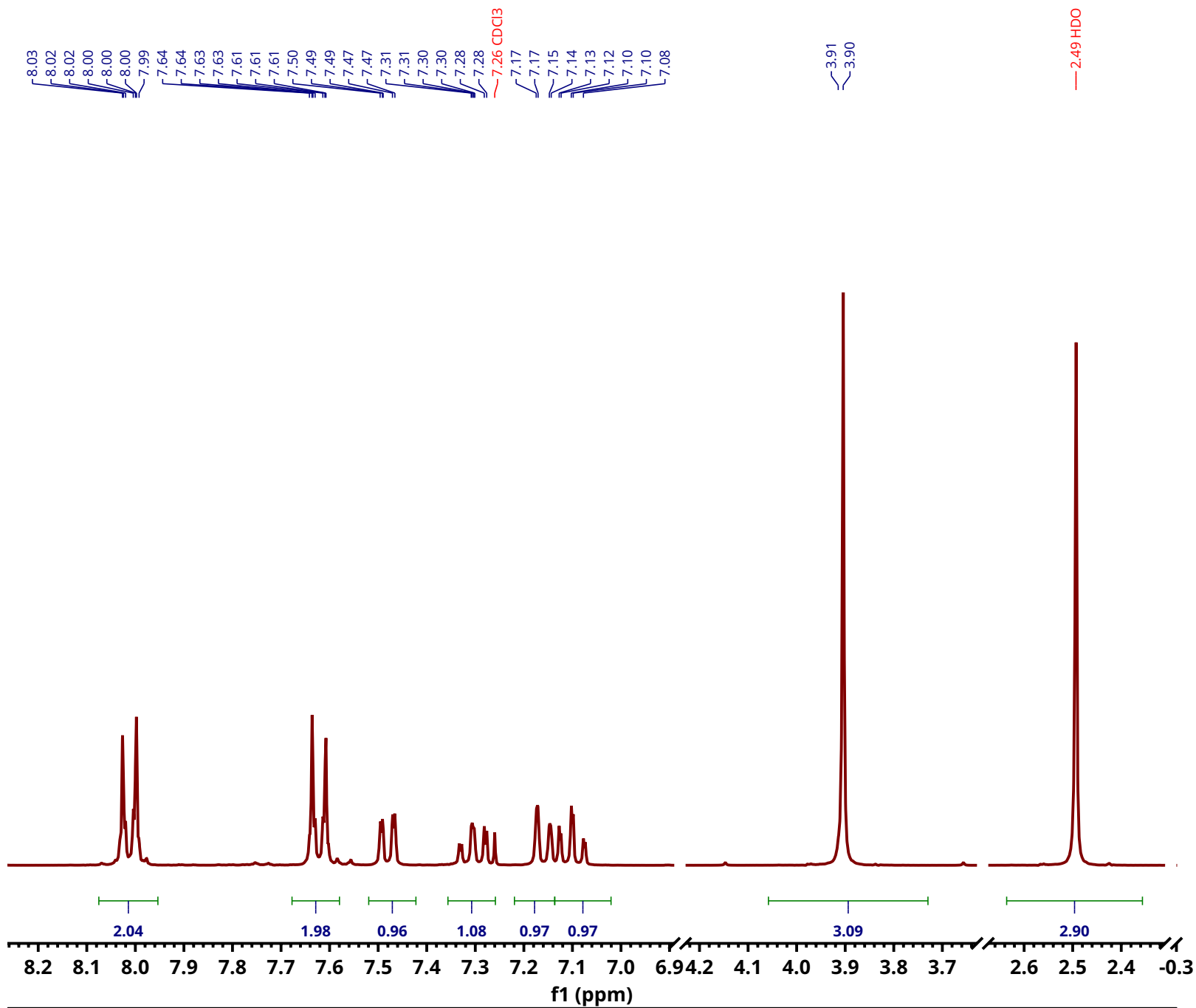


Parameter	Value
1 Title	DAL-051.7.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	1032.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	9.6
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-08-17T14:48:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

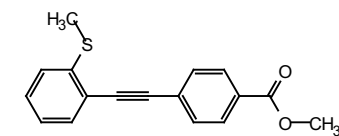


Compound 5o

¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 8.07 – 7.97 (m, 2H), 7.67 – 7.57 (m, 2H), 7.48 (dd, *J*=7.7, 1.5 Hz, 1H), 7.30 (ddd, *J*=8.0, 7.4, 1.5 Hz, 1H), 7.16 (dd, *J*=8.1, 1.2 Hz, 1H), 7.10 (td, *J*=7.5, 1.2 Hz, 1H), 3.90 (s, 3H), 2.49 (s, 3H)

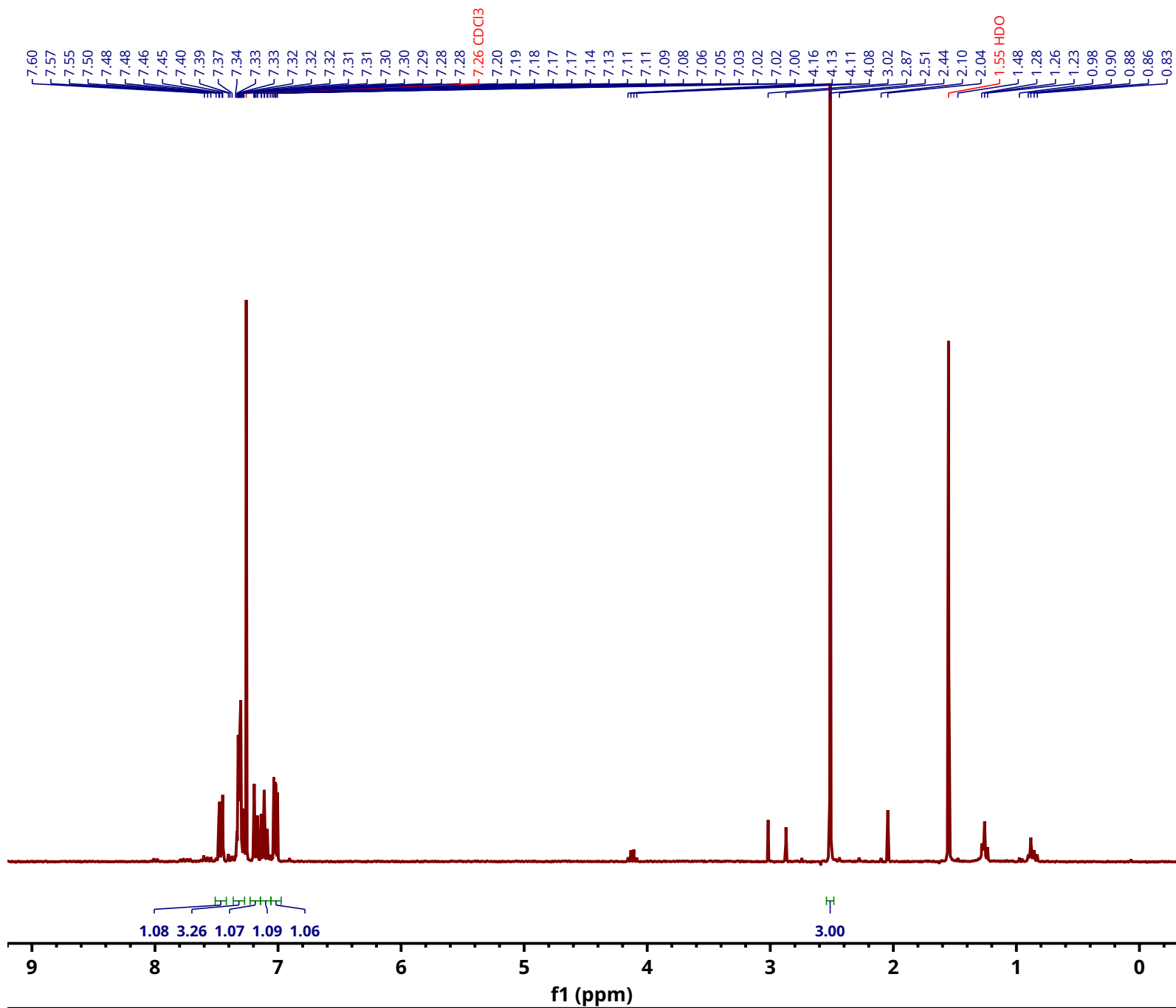


Parameter	Value
1 Title	DAL-051.7.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	1032.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	9.6
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-08-17T14:48:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

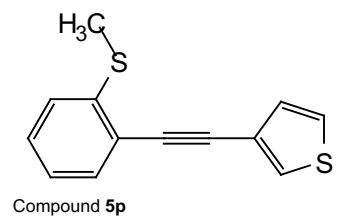


Compound 5o

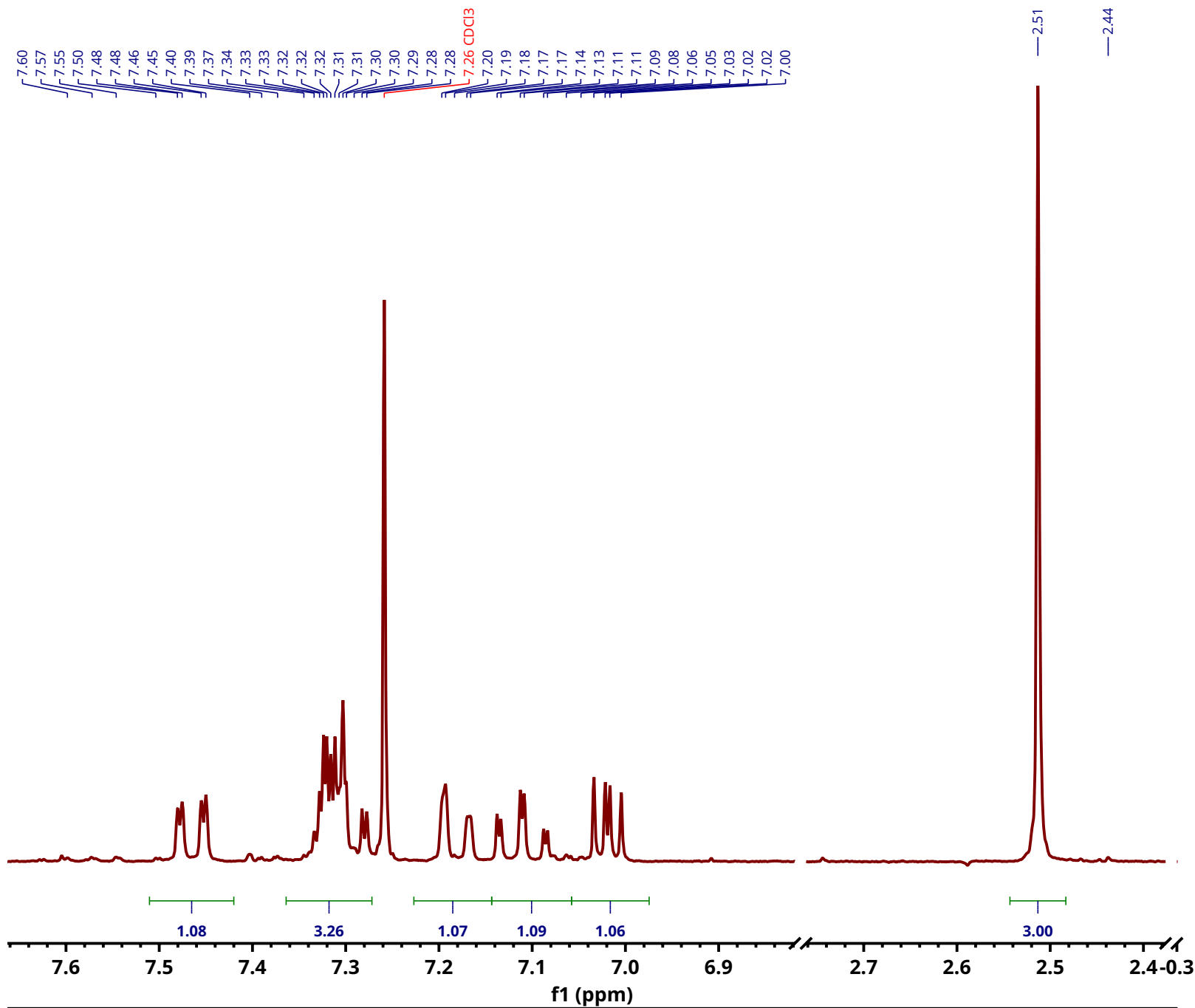
$^1\text{H NMR}$ (Chloroform-*d*, 300 MHz): δ (ppm) 8.07 – 7.97 (m, 2H), 7.67 – 7.57 (m, 2H), 7.48 (dd, $J=7.7, 1.5$ Hz, 1H), 7.30 (ddd, $J=8.0, 7.4, 1.5$ Hz, 1H), 7.16 (dd, $J=8.1, 1.2$ Hz, 1H), 7.10 (td, $J=7.5, 1.2$ Hz, 1H), 3.90 (s, 3H), 2.49 (s, 3H)



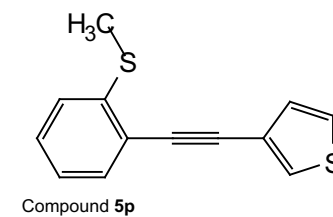
Parameter	Value
1 Title	DAL-079.5.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	297.2
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	126.9
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-08T12:50:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



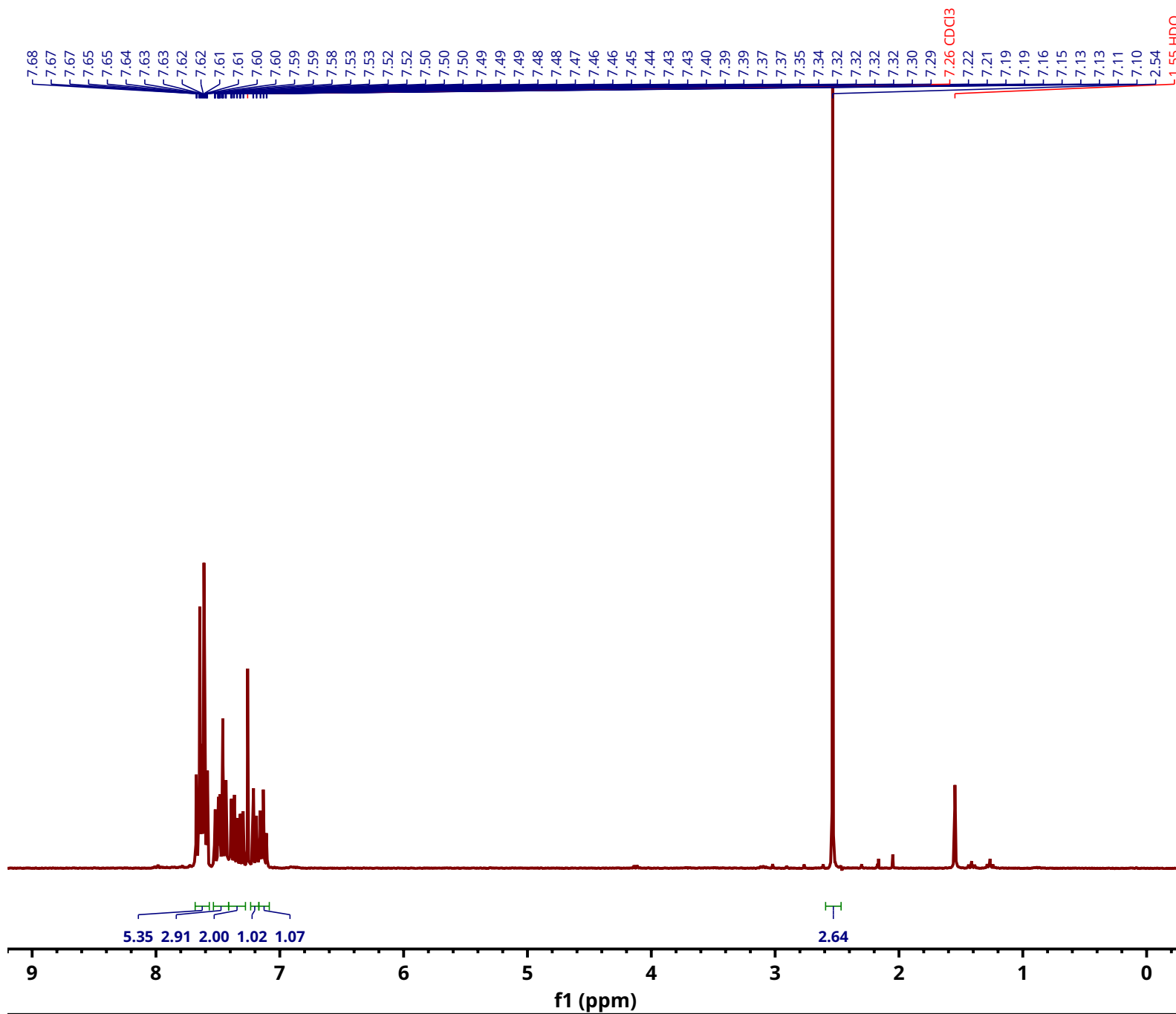
¹H NMR (300 MHz, Chloroform-*d*) δ 7.47 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.37 – 7.25 (m, 3H), 7.18 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.11 (td, *J* = 7.5, 1.2 Hz, 1H), 7.02 (dd, *J* = 5.1, 3.6 Hz, 1H), 2.51 (s, 3H).



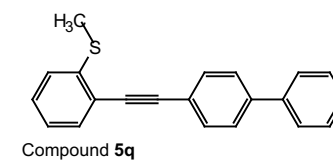
Parameter	Value
1 Title	DAL-079.5.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	297.2
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	126.9
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-08T12:50:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



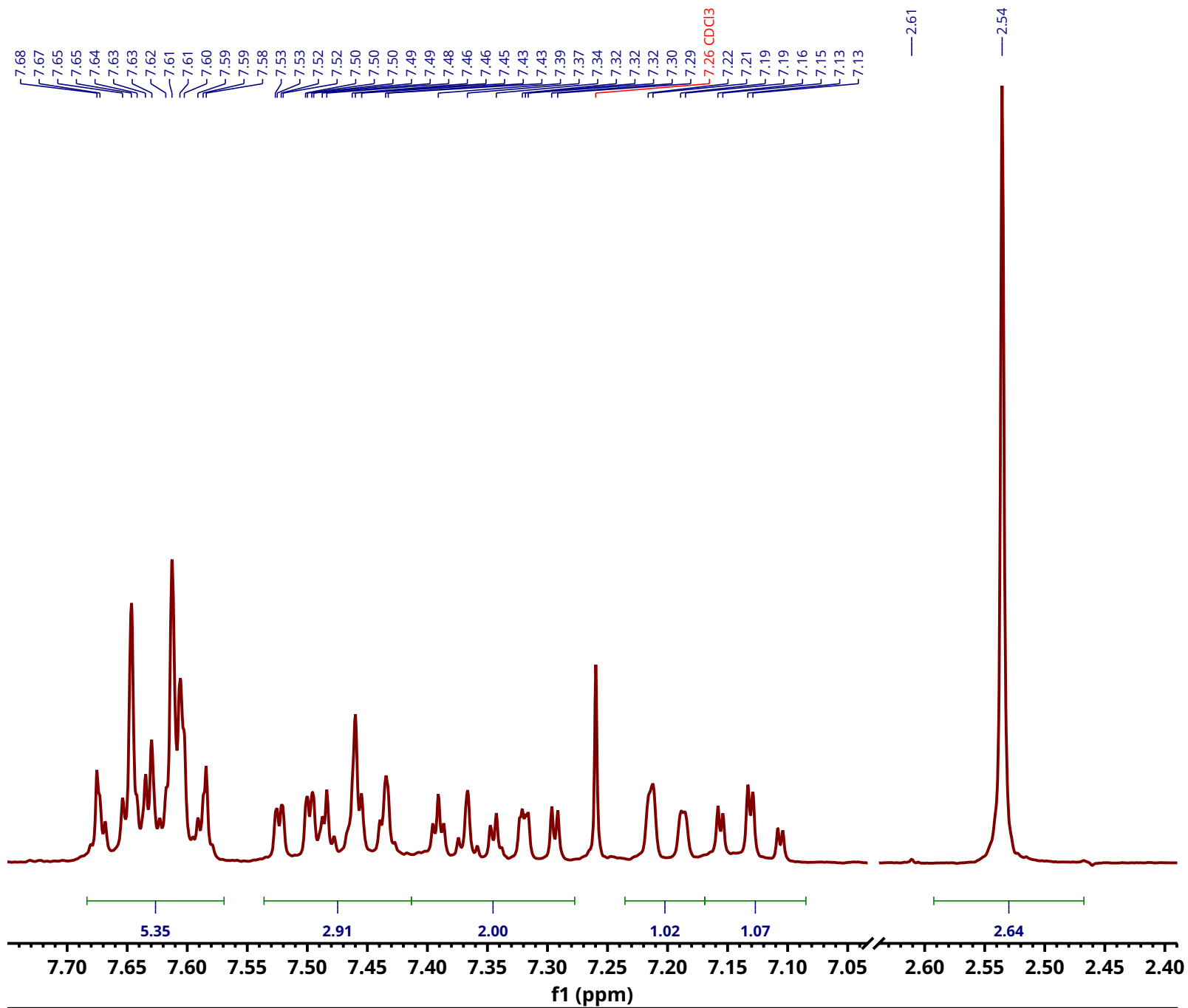
¹H NMR (300 MHz, Chloroform-*d*) δ 7.47 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.37 – 7.25 (m, 3H), 7.18 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.11 (td, *J* = 7.5, 1.2 Hz, 1H), 7.02 (dd, *J* = 5.1, 3.6 Hz, 1H), 2.51 (s, 3H).



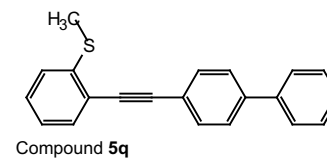
Parameter	Value
1 Title	AP-058.101.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.7
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	74.9
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-20T12:59:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



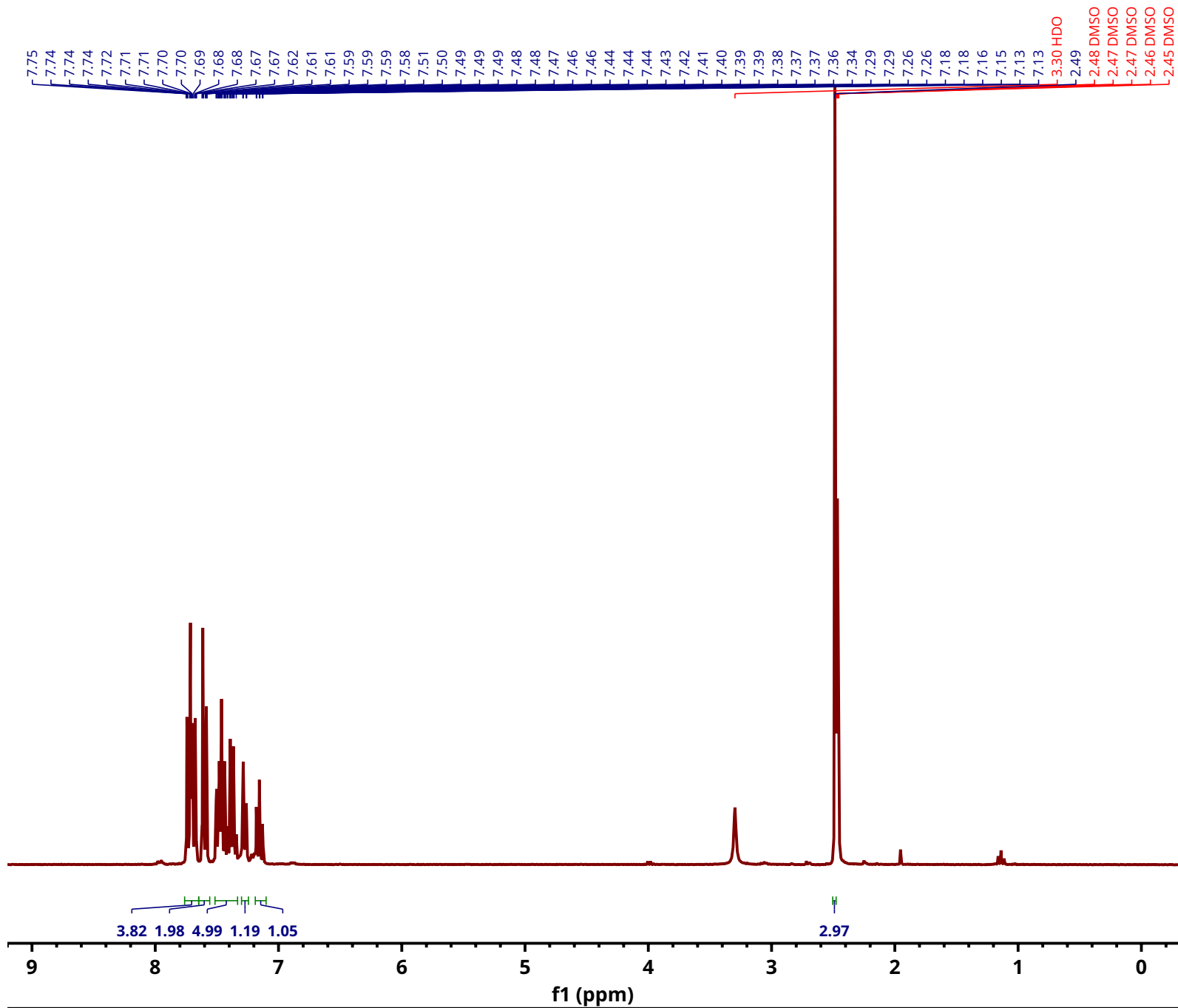
^1H NMR (300 MHz, Chloroform-*d*) δ 7.71 – 7.57 (m, 6H), 7.56 – 7.42 (m, 3H), 7.42 – 7.26 (m, 2H), 7.20 (dd, J = 8.1, 1.2 Hz, 1H), 7.13 (td, J = 7.5, 1.3 Hz, 1H), 2.54 (s, 3H).



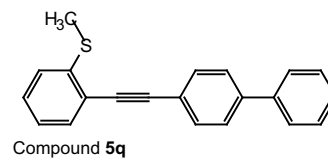
Parameter	Value
1 Title	AP-058.101.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.7
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	74.9
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-20T12:59:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



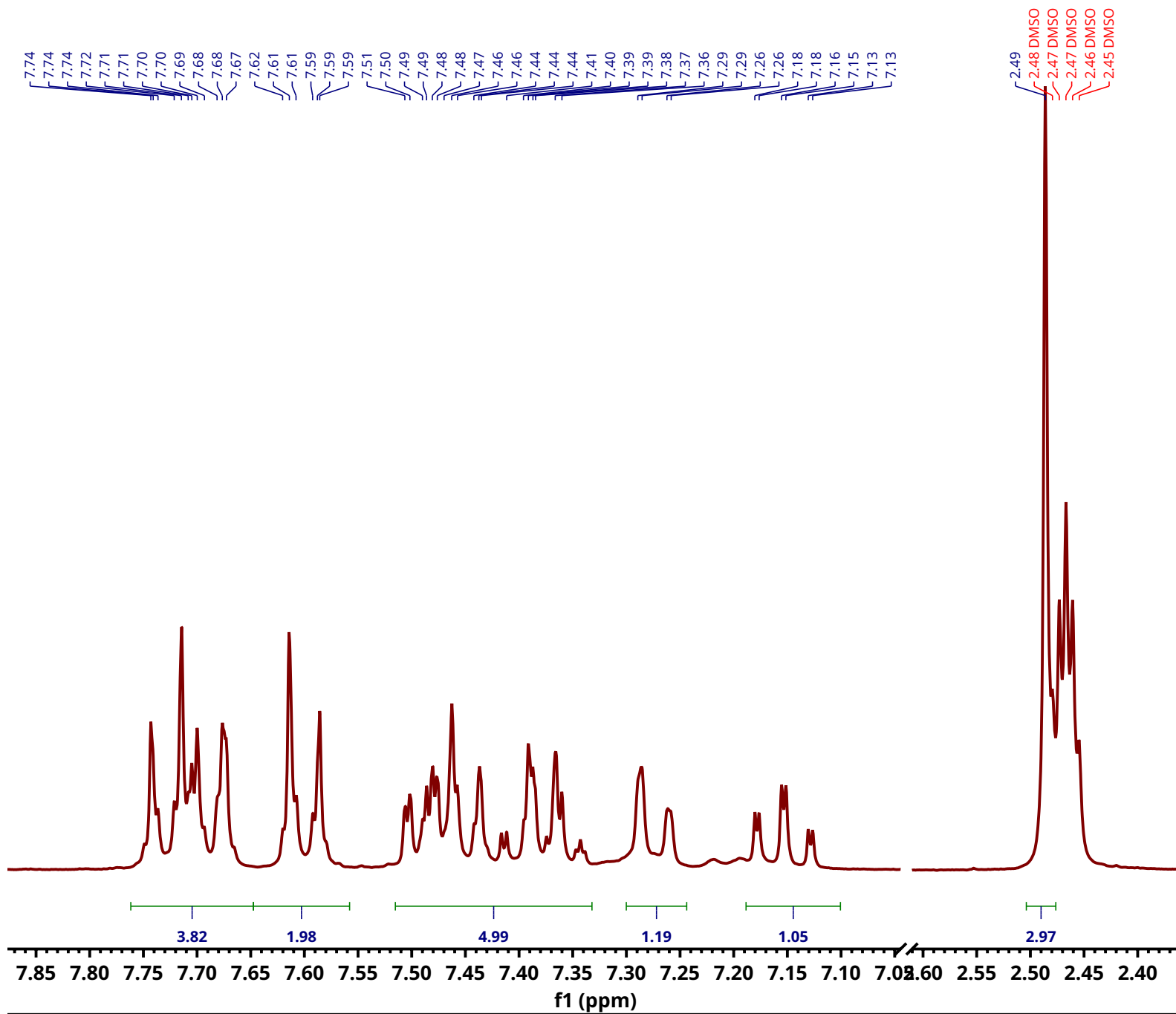
¹H NMR (300 MHz, Chloroform-*d*) δ 7.71 – 7.57 (m, 6H), 7.56 – 7.42 (m, 3H), 7.42 – 7.26 (m, 2H), 7.20 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.13 (td, *J* = 7.5, 1.3 Hz, 1H), 2.54 (s, 3H).



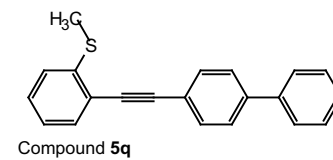
Parameter	Value
Title	PK-901.401.fid
Date	20181002
Time	18.05
Solvent	DMSO
Instrument	FOURIER300
Temperature	297.2
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	64
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	¹ H
TD	32768
SI	65536



¹H NMR (300 MHz, DMSO-*d*₆) δ 7.76 – 7.65 (m, 4H), 7.65 – 7.56 (m, 2H), 7.52 – 7.33 (m, 5H), 7.27 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.15 (td, *J* = 7.5, 1.2 Hz, 1H), 2.49 (s, 3H).



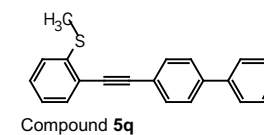
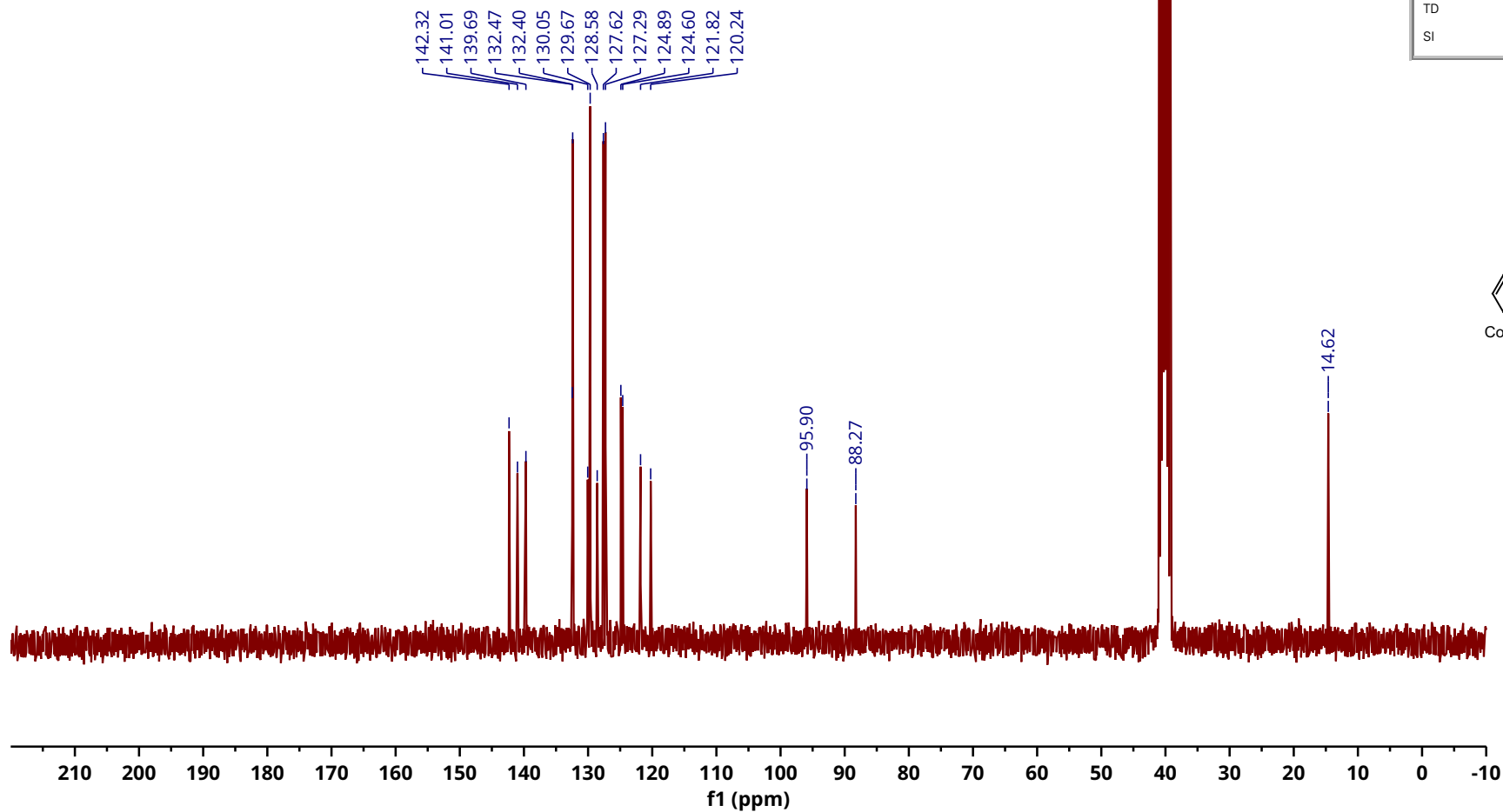
Parameter	Value
Title	PK-901.401.fid
Date	20181002
Time	18.05
Solvent	DMSO
Instrument	FOURIER300
Temperature	297.2
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	64
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	¹ H
TD	32768
SI	65536



¹H NMR (300 MHz, DMSO-*d*₆) δ 7.76 – 7.65 (m, 4H), 7.65 – 7.56 (m, 2H), 7.52 – 7.33 (m, 5H), 7.27 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.15 (td, *J* = 7.5, 1.2 Hz, 1H), 2.49 (s, 3H).

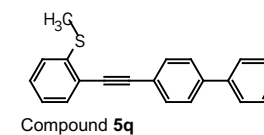
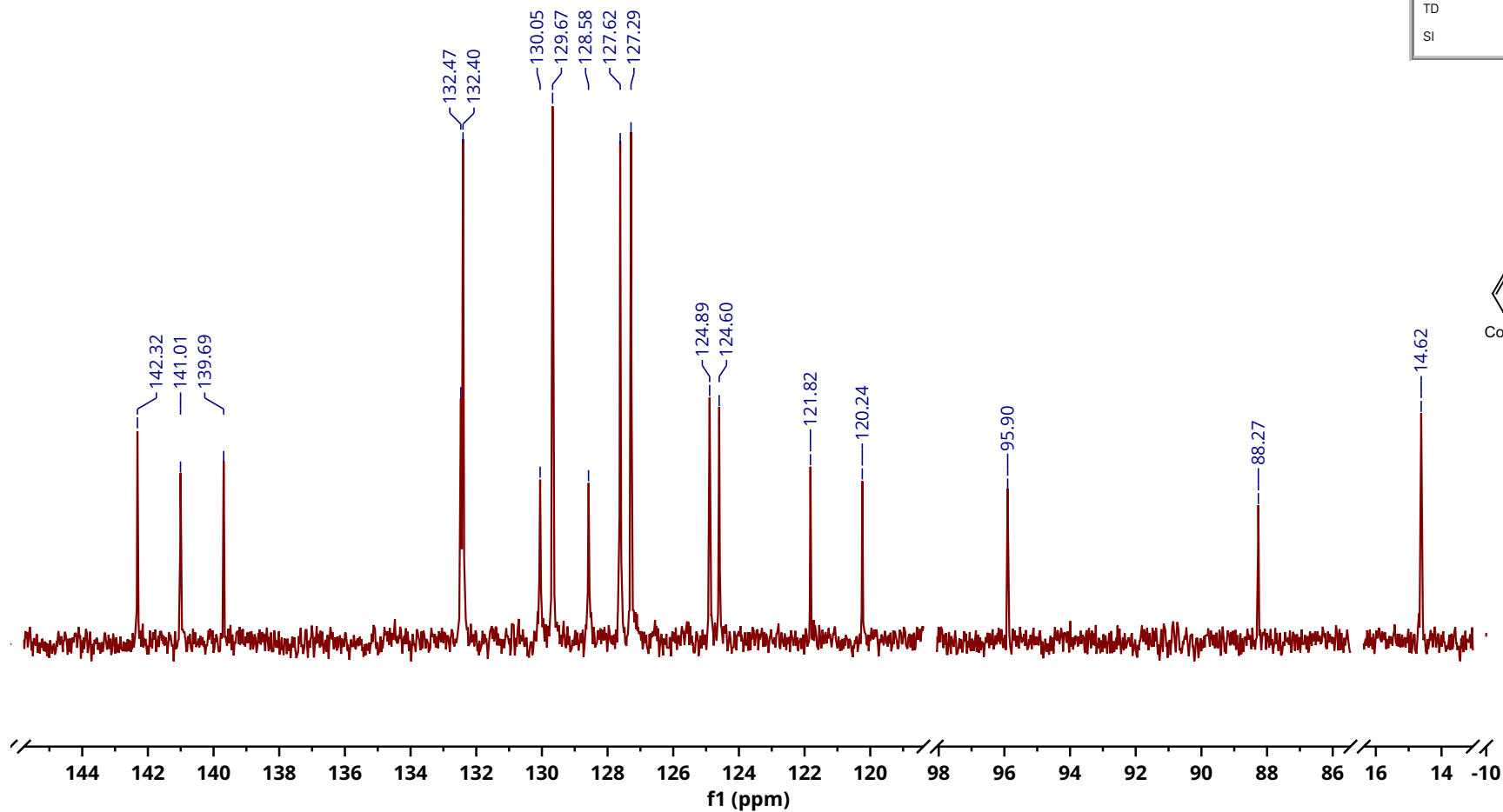
^{13}C NMR (75 MHz, DMSO) δ 142.32, 141.01, 139.69, 132.47, 132.40, 130.05, 129.67, 128.58, 127.62, 127.29, 124.89, 124.60, 121.82, 120.24, 95.90, 88.27, 14.62.

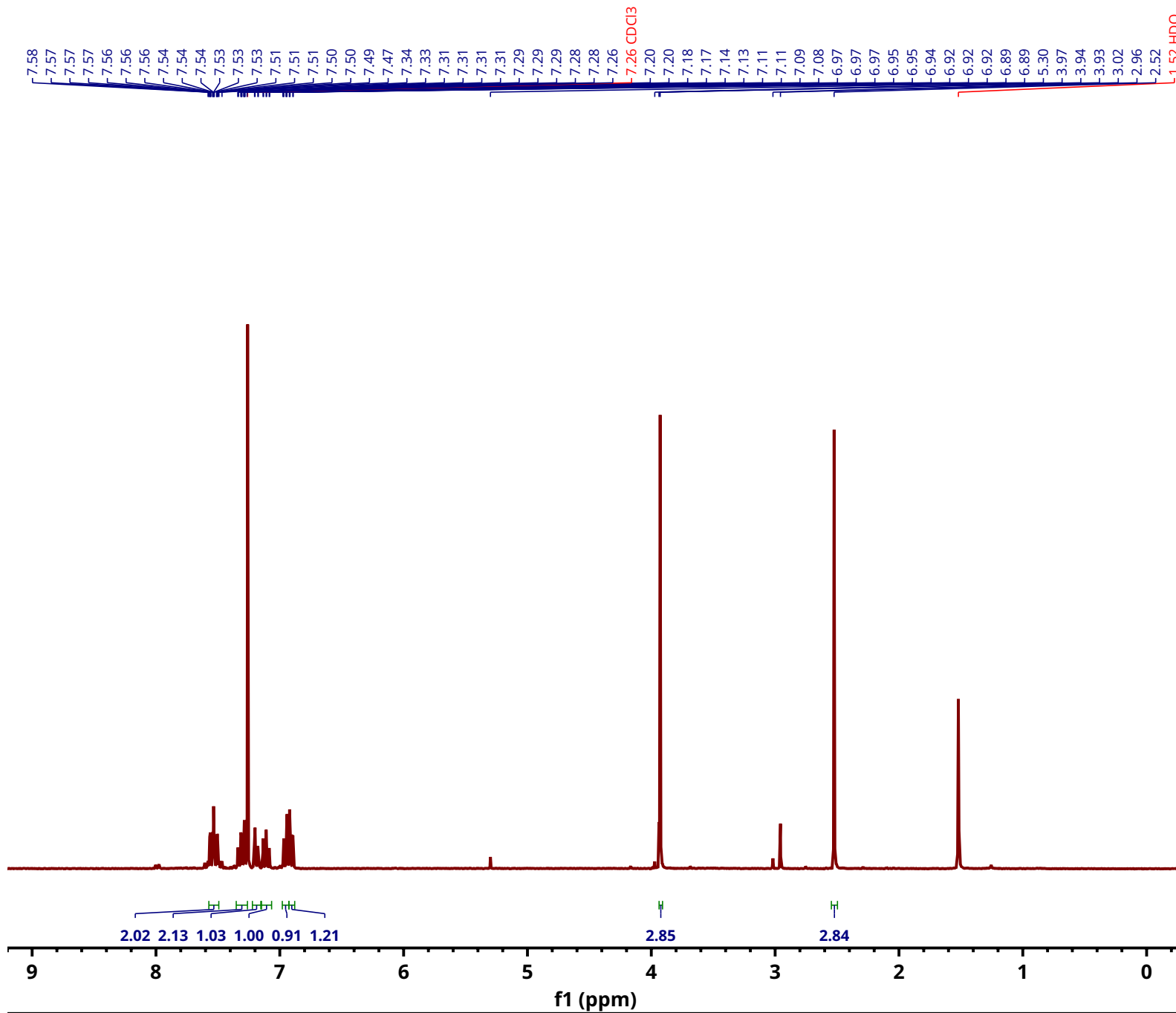
Parameter	Value
Title	PK-901.402.fid
Date	20181002
Time	18.13
Solvent	DMSO
Instrument	FOURIER300
Temperature	297.2
PULPROG	zgpg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	6144
D1	2.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536



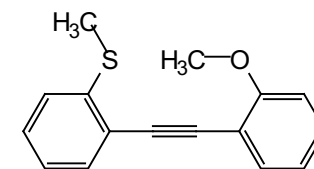
^{13}C NMR (75 MHz, DMSO) δ 142.32, 141.01, 139.69, 132.47, 132.40, 130.05, 129.67, 128.58, 127.62, 127.29, 124.89, 124.60, 121.82, 120.24, 95.90, 88.27, 14.62.

Parameter	Value
Title	PK-901.402.fid
Date	20181002
Time	18.13
Solvent	DMSO
Instrument	FOURIER300
Temperature	297.2
PULPROG	zgpg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	6144
D1	2.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536



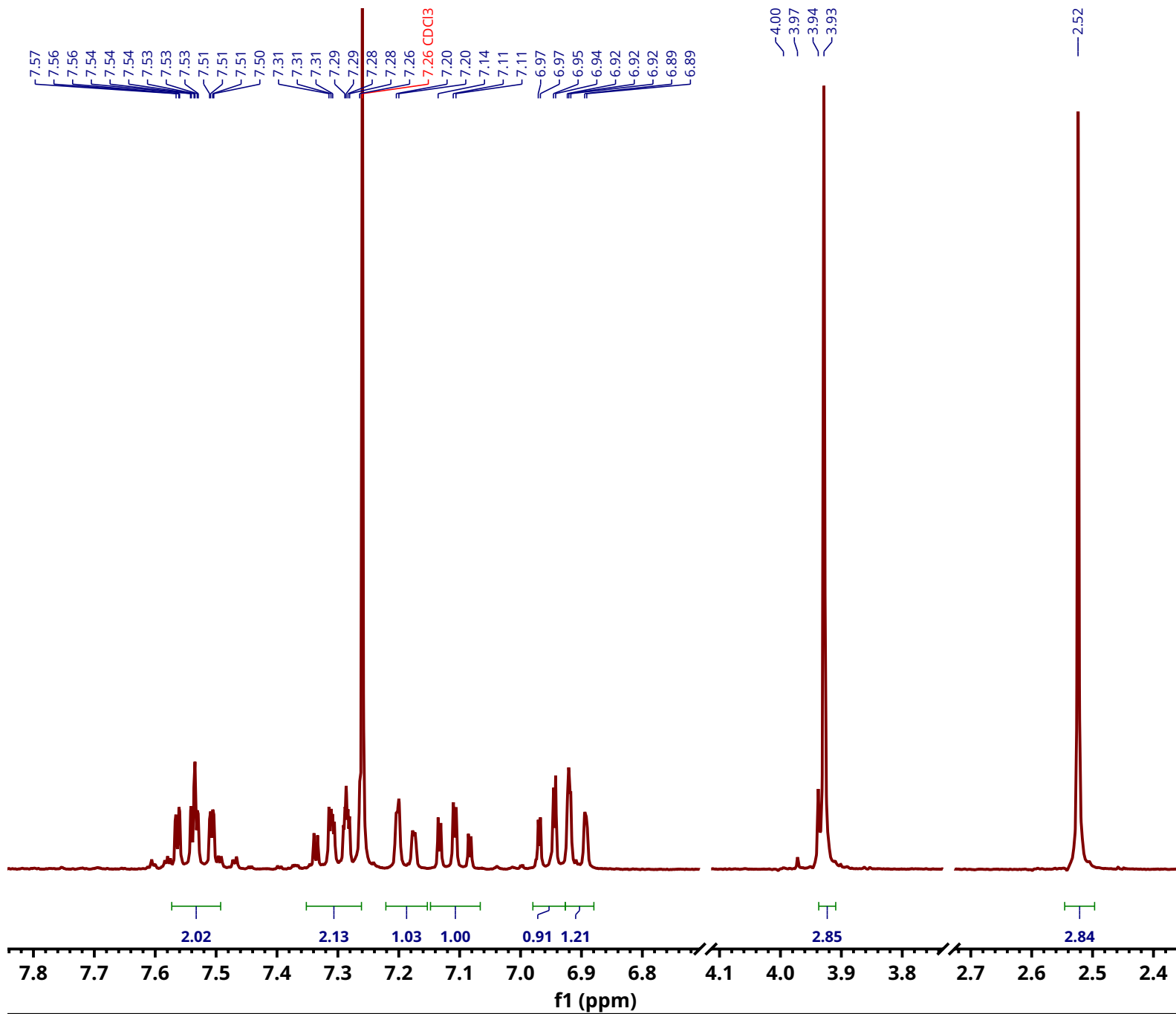


Parameter	Value
1 Title	BK-113.11.fid
2 Date	20180717
3 Time	11.11
4 Solvent	CDCl3
5 Instrument	FOURIER300
6 Temperature	299.3
7 PULPROG	zg30
8 Experiment	1D
9 Probe	5 mm DUL 13C-1
10 NS	64
11 D1	1.0000
12 P1	10.2000
13 SF	300.18
14 SW	6103.5
15 Nucleus	1H
16 TD	32768
17 SI	65536

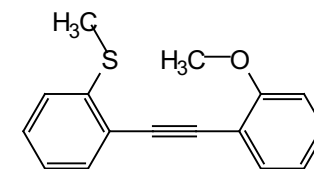


Compound 5r

^1H NMR (300 MHz, Chloroform-*d*) δ 7.54 (dddd, J = 9.3, 7.6, 1.7, 0.5 Hz, 2H), 7.37 – 7.23 (m, 2H), 7.19 (dd, J = 8.0, 1.3 Hz, 1H), 7.11 (td, J = 7.4, 1.3 Hz, 1H), 6.96 (dd, J = 7.5, 1.1 Hz, 1H), 6.93 – 6.88 (m, 1H), 3.93 (s, 3H), 2.52 (s, 3H).

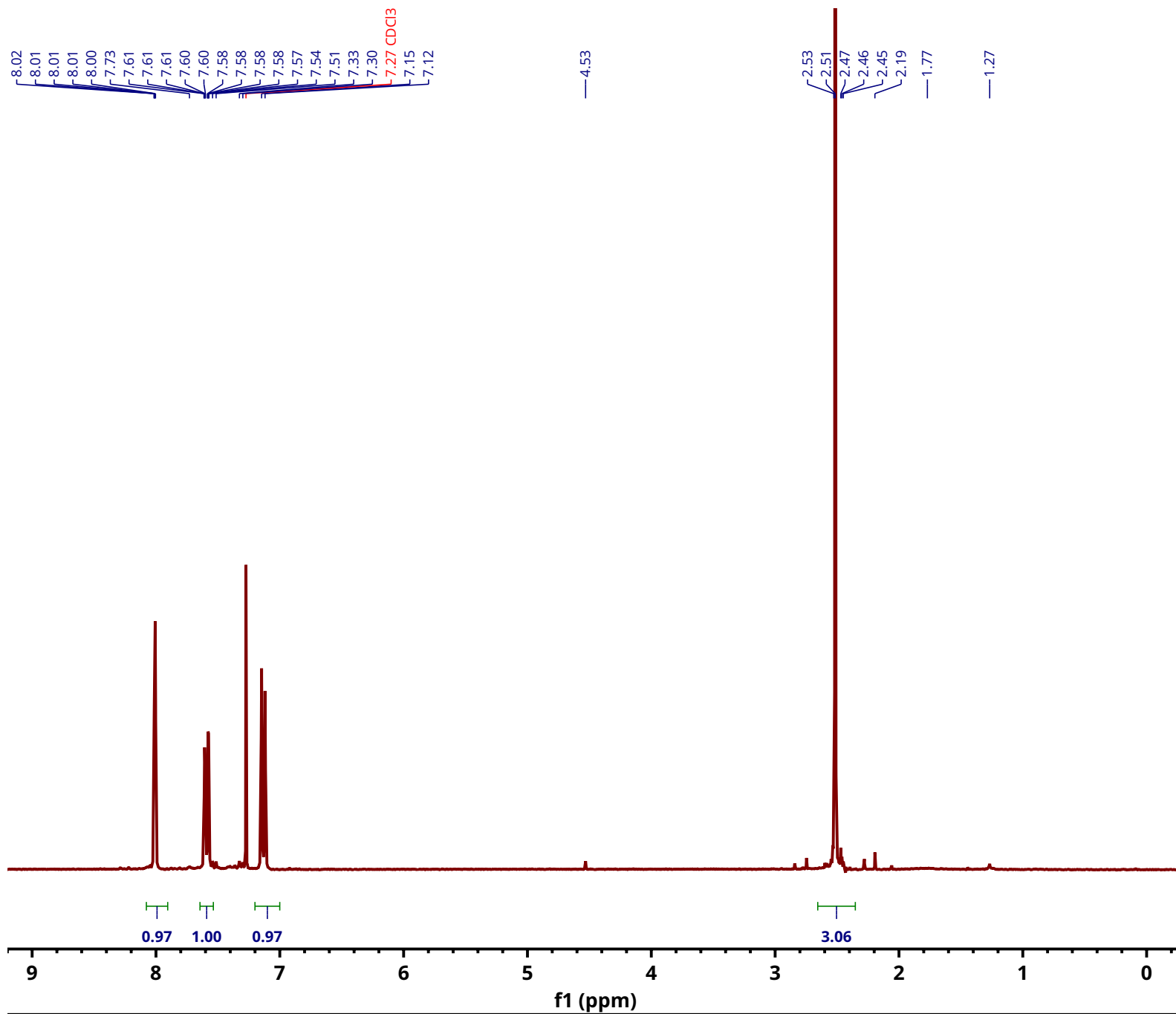


Parameter	Value
1 Title	BK-113.11.fid
2 Date	20180717
3 Time	11.11
4 Solvent	CDCl ₃
5 Instrument	FOURIER300
6 Temperature	299.3
7 PULPROG	zg30
8 Experiment	1D
9 Probe	5 mm DUL 13C-1
10 NS	64
11 D1	1.0000
12 P1	10.2000
13 SF	300.18
14 SW	6103.5
15 Nucleus	1H
16 TD	32768
17 SI	65536

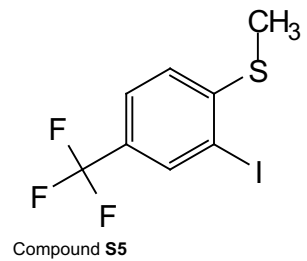


Compound 5r

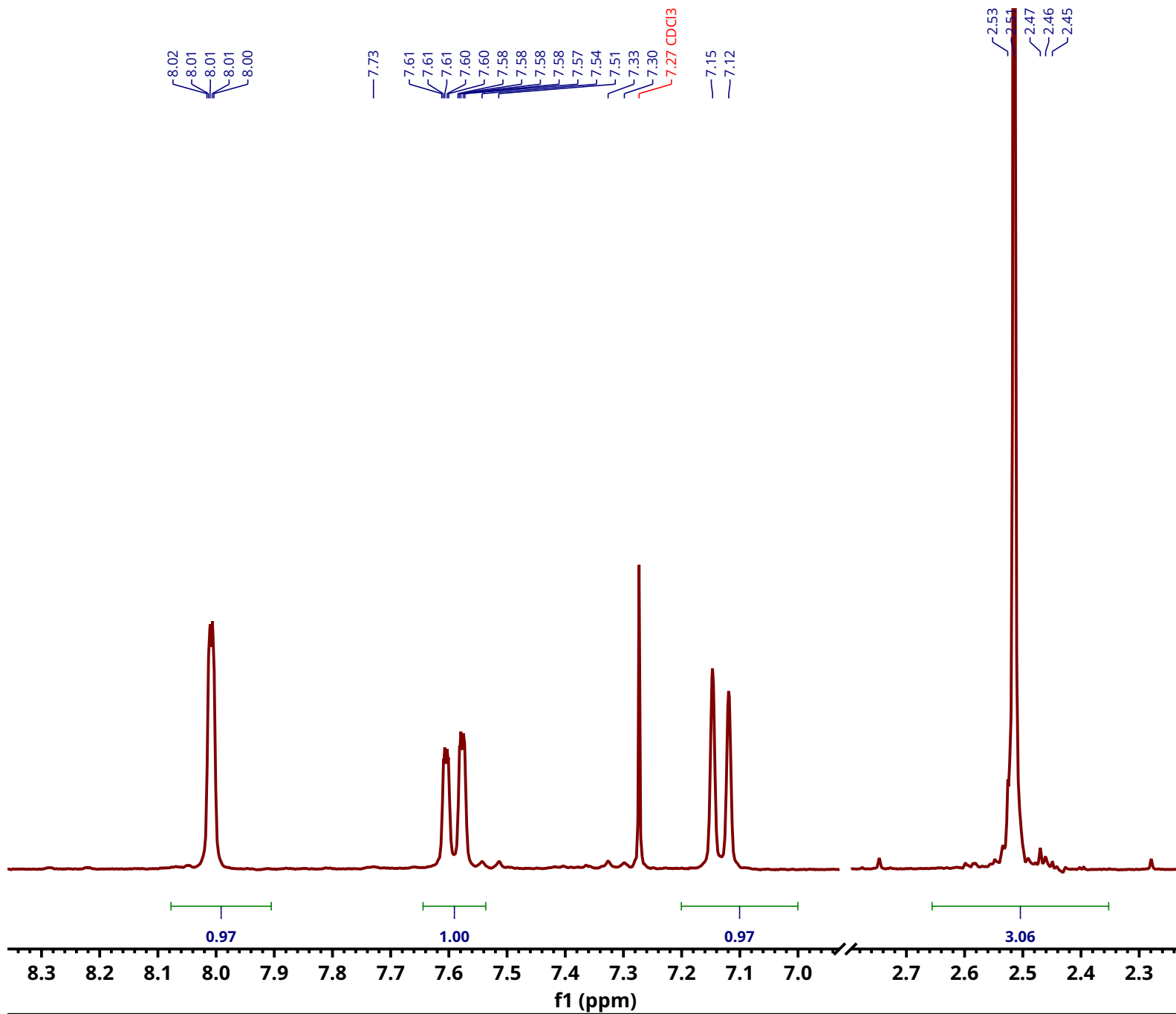
¹H NMR (300 MHz, Chloroform-*d*) δ 7.54 (dddd, *J* = 9.3, 7.6, 1.7, 0.5 Hz, 2H), 7.37 – 7.23 (m, 2H), 7.19 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.11 (td, *J* = 7.4, 1.3 Hz, 1H), 6.96 (dd, *J* = 7.5, 1.1 Hz, 1H), 6.93 – 6.88 (m, 1H), 3.93 (s, 3H), 2.52 (s, 3H).



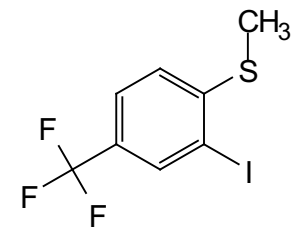
Parameter	Value
Title	MS-096.101.fid
Date	20181019
Time	15.51
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.8
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	16
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536



$^1\text{H NMR}$ (300 MHz, Chloroform-*d*) δ 8.01 (dt, $J = 2.0, 0.8$ Hz, 1H), 7.59 (ddt, $J = 8.4, 2.1, 0.8$ Hz, 1H), 7.13 (d, $J = 8.3$ Hz, 1H), 2.51 (s, 3H).



Parameter	Value
Title	MS-096.101.fid
Date	20181019
Time	15.51
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.8
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	16
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

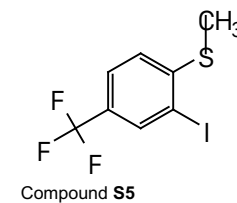
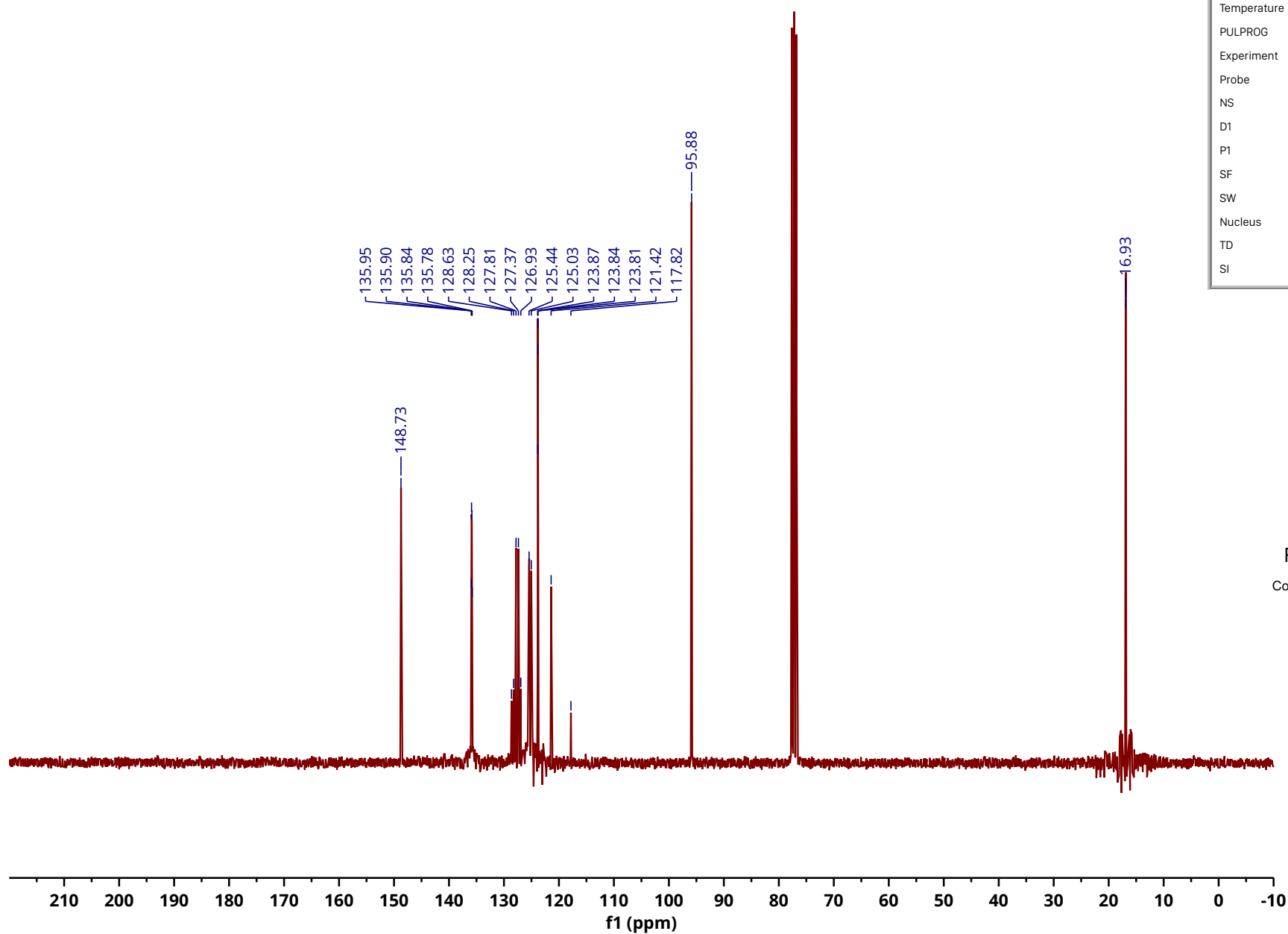


Compound S5

^1H NMR (300 MHz, Chloroform-*d*) δ 8.01 (dt, $J = 2.0, 0.8$ Hz, 1H), 7.59 (ddt, $J = 8.4, 2.1, 0.8$ Hz, 1H), 7.13 (d, $J = 8.3$ Hz, 1H), 2.51 (s, 3H).

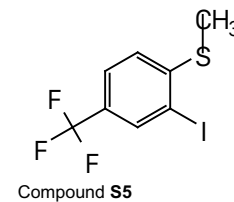
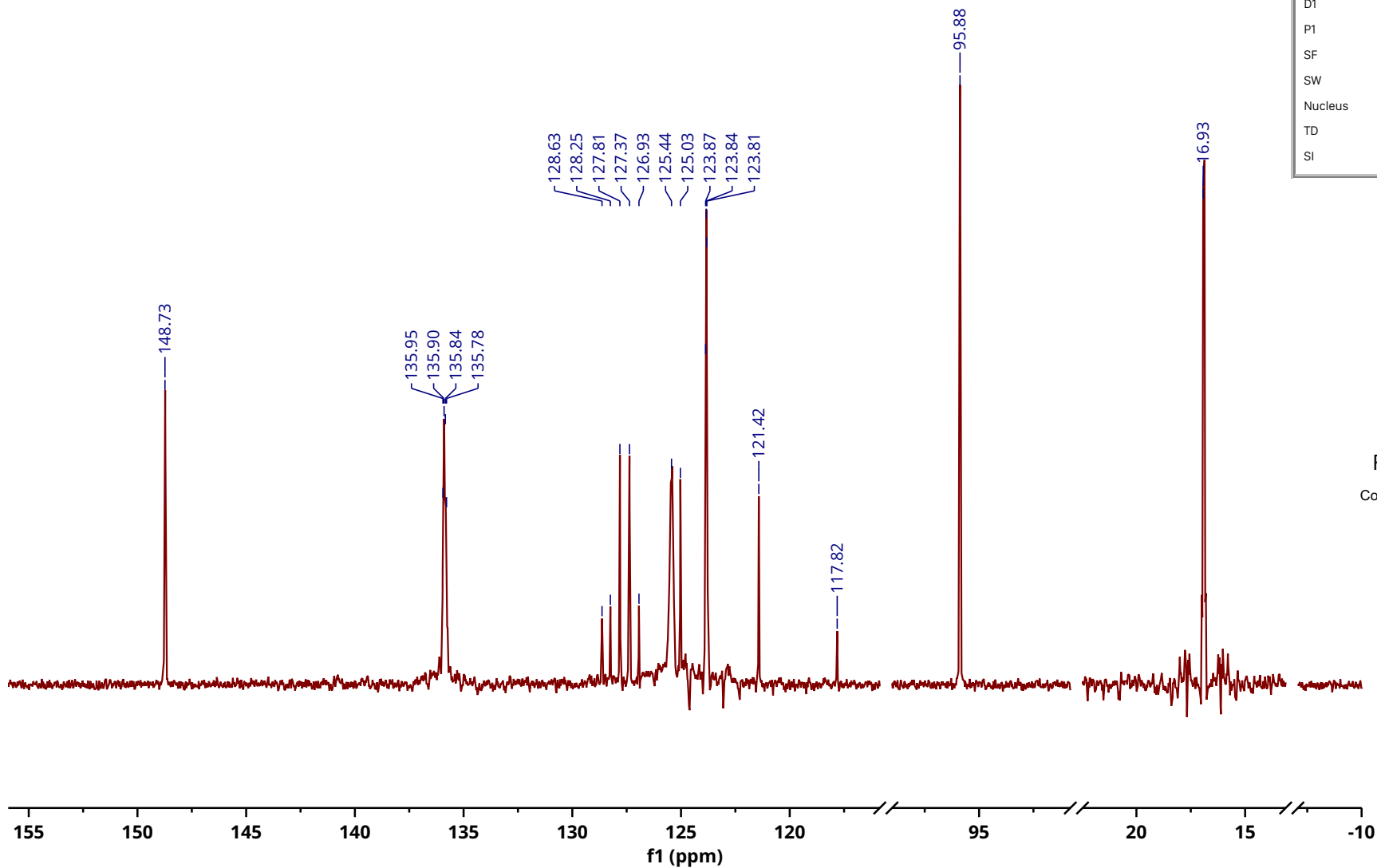
^{13}C NMR (75 MHz, CDCl_3) δ 148.73, 135.87 (q, $J = 4.1$ Hz), 127.59 (q, $J = 33.1$ Hz), 125.44, 124.20z, 123.23 (q, $J = 272.2$ Hz), 95.88, 16.90

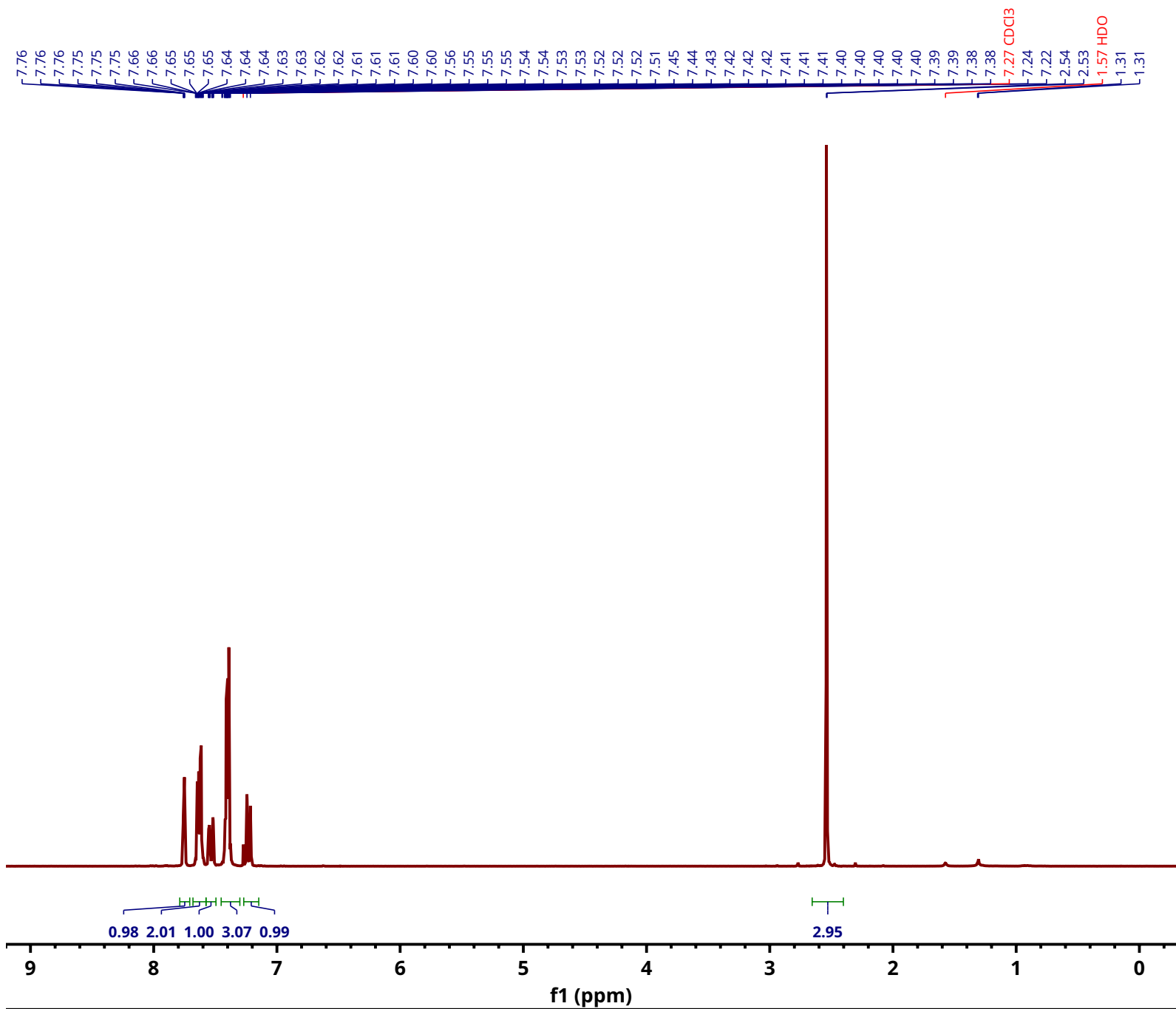
Parameter	Value
Title	MS-096.112.fid
Date	20181025
Time	18.05
Solvent	CDCl_3
Instrument	FOURIER300
Temperature	296.7
PULPROG	zgpg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	2048
D1	2.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536



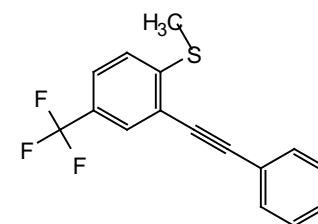
^{13}C NMR (75 MHz, CDCl_3) δ 148.73, 135.87 (q, $J = 4.1$ Hz), 127.59 (q, $J = 33.1$ Hz), 125.44, 124.20z, 123.23 (q, $J = 272.2$ Hz), 95.88, 16.90

Parameter	Value
Title	MS-096.112.fid
Date	20181025
Time	18.05
Solvent	CDCl_3
Instrument	FOURIER300
Temperature	296.7
PULPROG	zgpg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	2048
D1	2.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536



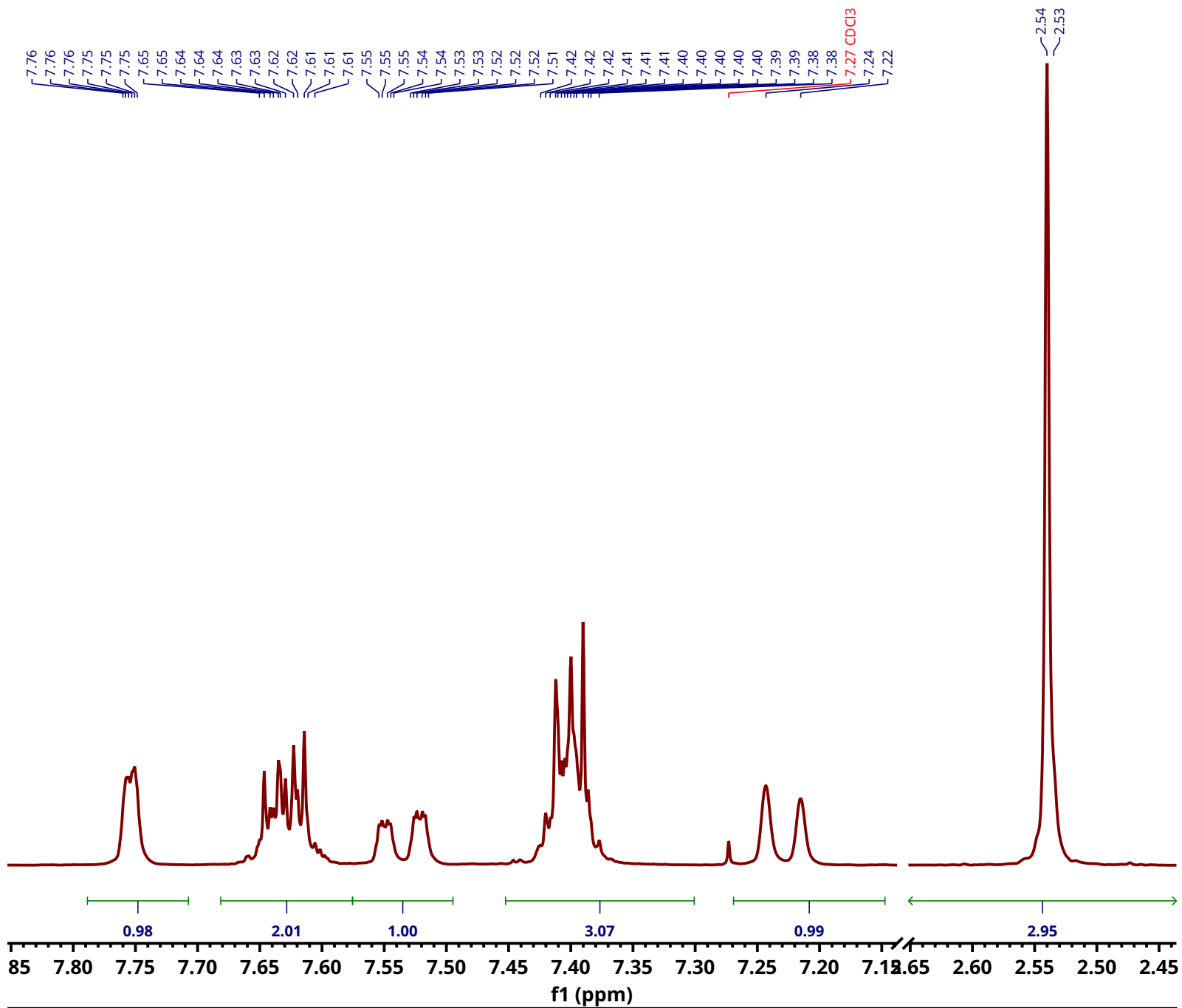


Parameter	Value
Title	MS-097.2010.fid
Date	
Time	
Solvent	CDCl3
Instrument	FOURIER300
Temperature	296.5
PULPROG	zg30
Experiment	1D
Probe	
NS	16
D1	2.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

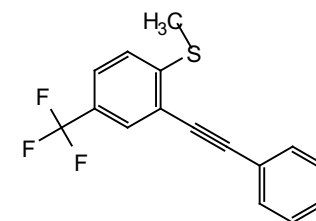


Compound 5s

^1H NMR (300 MHz, Chloroform-*d*) δ 7.75 (dt, $J = 2.1, 0.6$ Hz, 1H), 7.68 – 7.58 (m, 2H), 7.53 (ddt, $J = 8.4, 1.5, 0.8$ Hz, 1H), 7.45 – 7.30 (m, 3H), 7.23 (d, $J = 8.4$ Hz, 1H), 2.54 (s, 3H).



Parameter	Value
Title	MS-097.2010.fid
Date	
Time	
Solvent	CDCl3
Instrument	FOURIER300
Temperature	296.5
PULPROG	zg30
Experiment	1D
Probe	
NS	16
D1	2.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

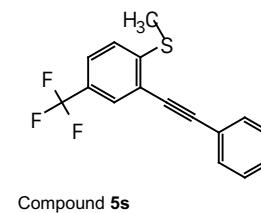
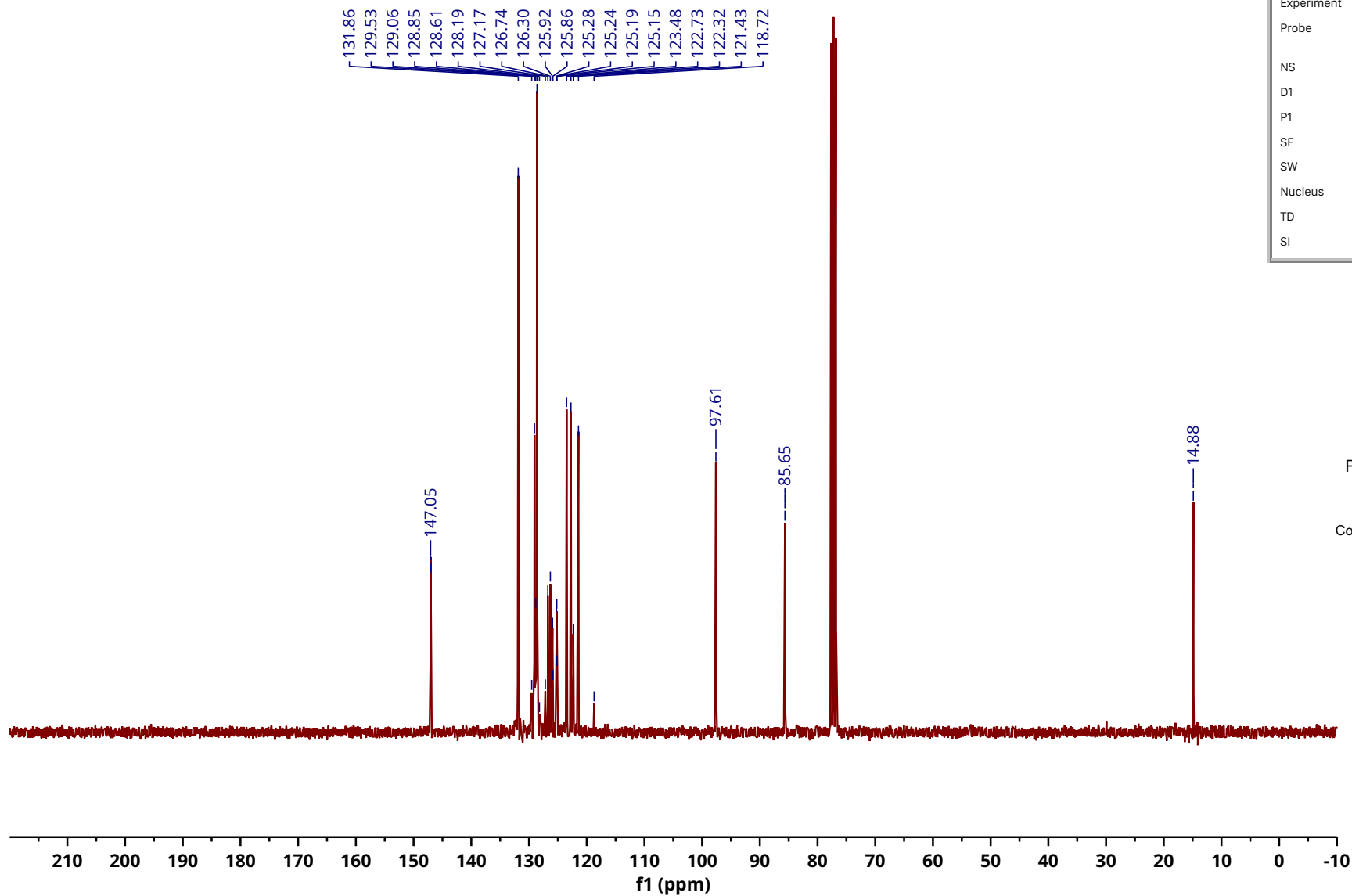


Compound 5s

^1H NMR (300 MHz, Chloroform-*d*) δ 7.75 (dt, $J = 2.1, 0.6$ Hz, 1H), 7.68 – 7.58 (m, 2H), 7.53 (ddt, $J = 8.4, 1.5, 0.8$ Hz, 1H), 7.45 – 7.30 (m, 3H), 7.23 (d, $J = 8.4$ Hz, 1H), 2.54 (s, 3H).

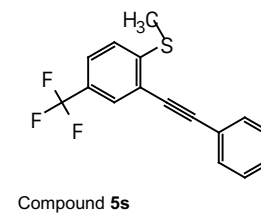
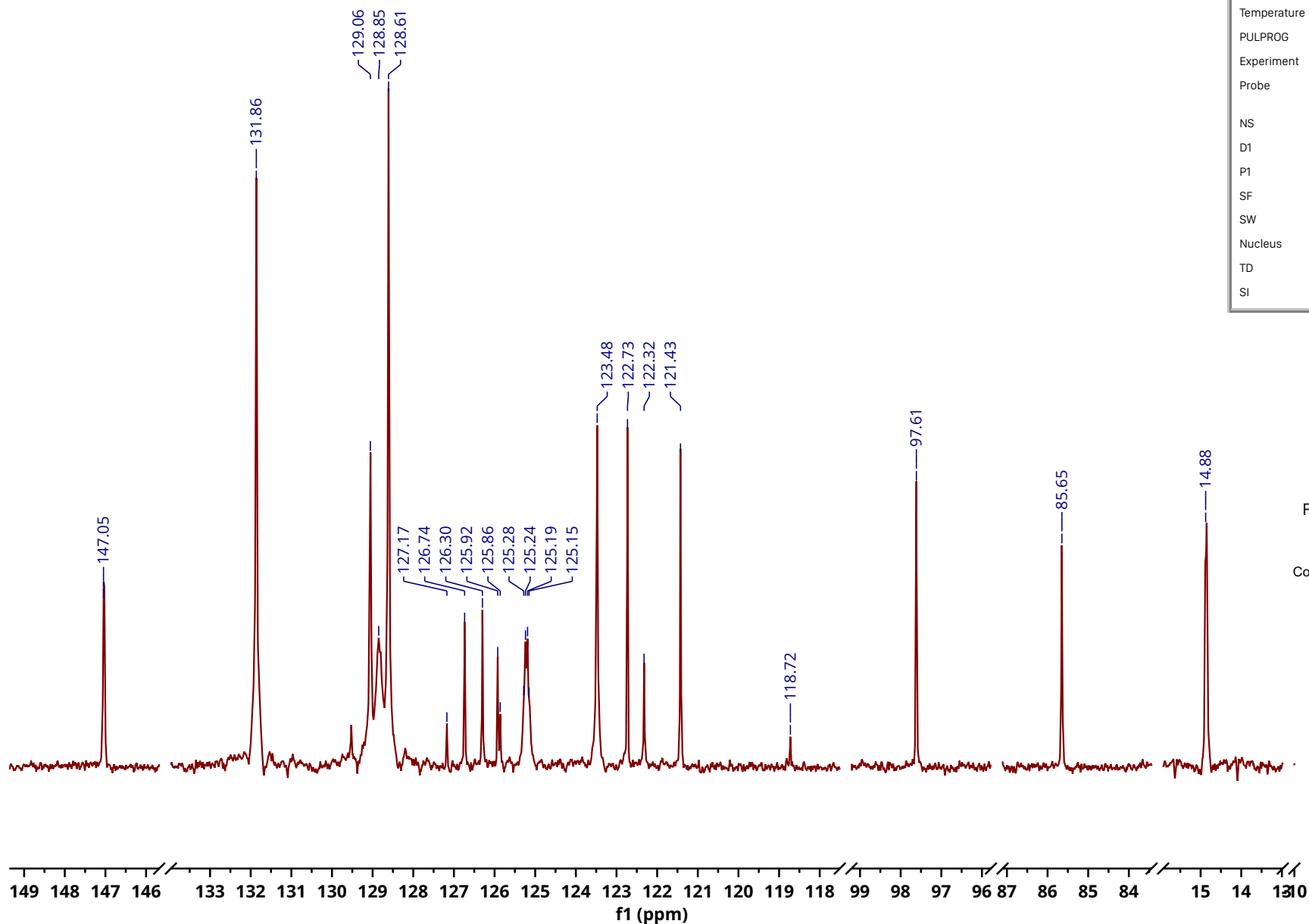
^{13}C NMR (75 MHz, CDCl_3) δ 147.0, 131.9, 129.1, 128.8, 128.6, 126.5 (q, $J = 31.3$ Hz), 125.2 (q, $J = 3.9$ Hz), 124.1 (q, $J = 271$ Hz), 123.48, 122.73, 121.43, 97.61, 85.65, 14.88.

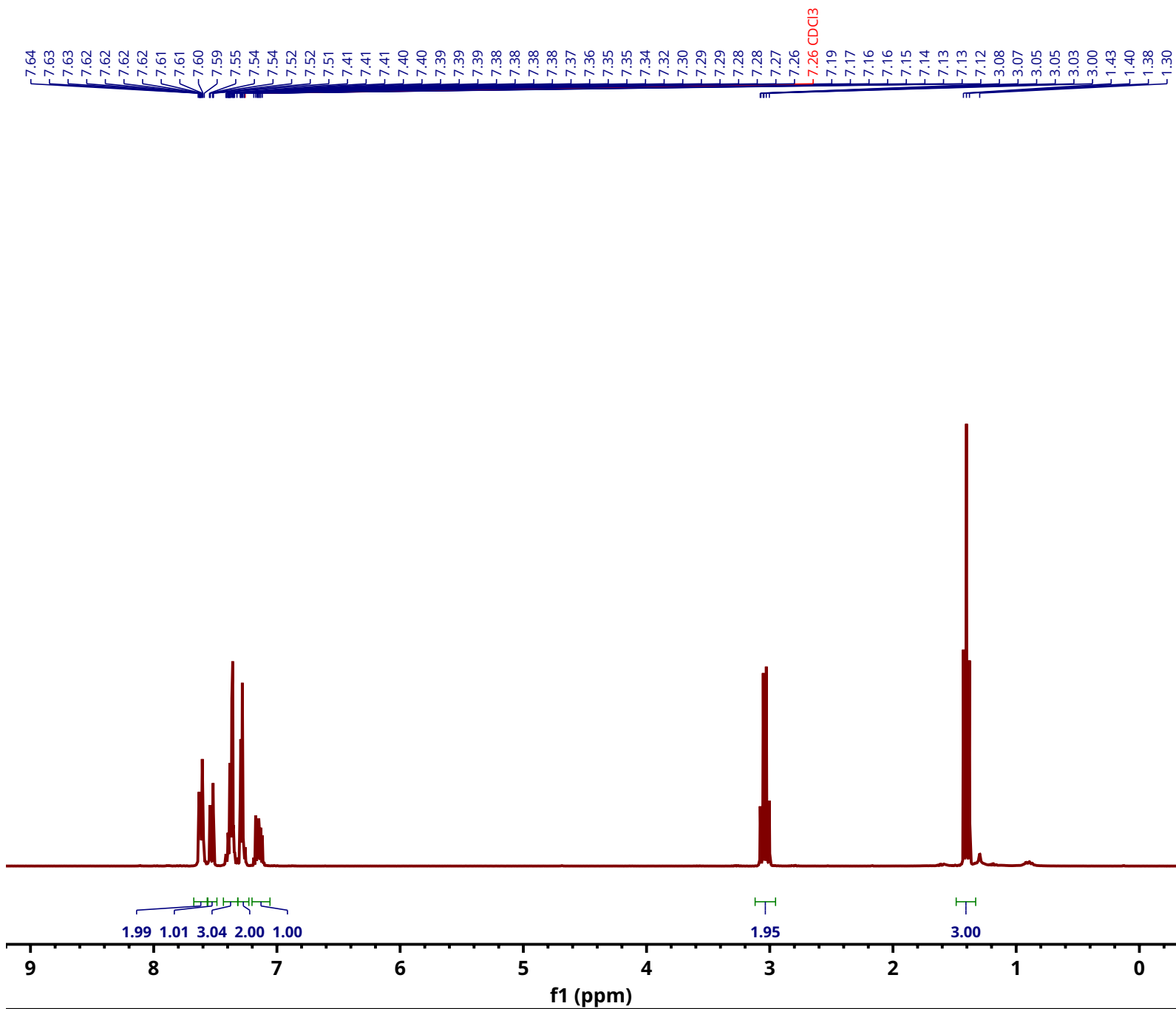
Parameter	Value
Title	MS-097.2020.fid
Date	
Time	
Solvent	CDCl_3
Instrument	FOURIER300
Temperature	297.1
PULPROG	zgpg30
Experiment	1D
Probe	
NS	841
D1	4.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536



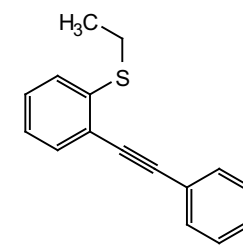
^{13}C NMR (75 MHz, CDCl_3) δ 147.0, 131.9, 129.1, 128.8, 128.6, 126.5 (q, $J = 31.3$ Hz), 125.2 (q, $J = 3.9$ Hz), 124.1 (q, $J = 271$ Hz), 123.48, 122.73, 121.43, 97.61, 85.65, 14.88.

Parameter	Value
Title	MS-097.2020.fid
Date	
Time	
Solvent	CDCl_3
Instrument	FOURIER300
Temperature	2971
PULPROG	zgpg30
Experiment	1D
Probe	
NS	841
D1	4.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536



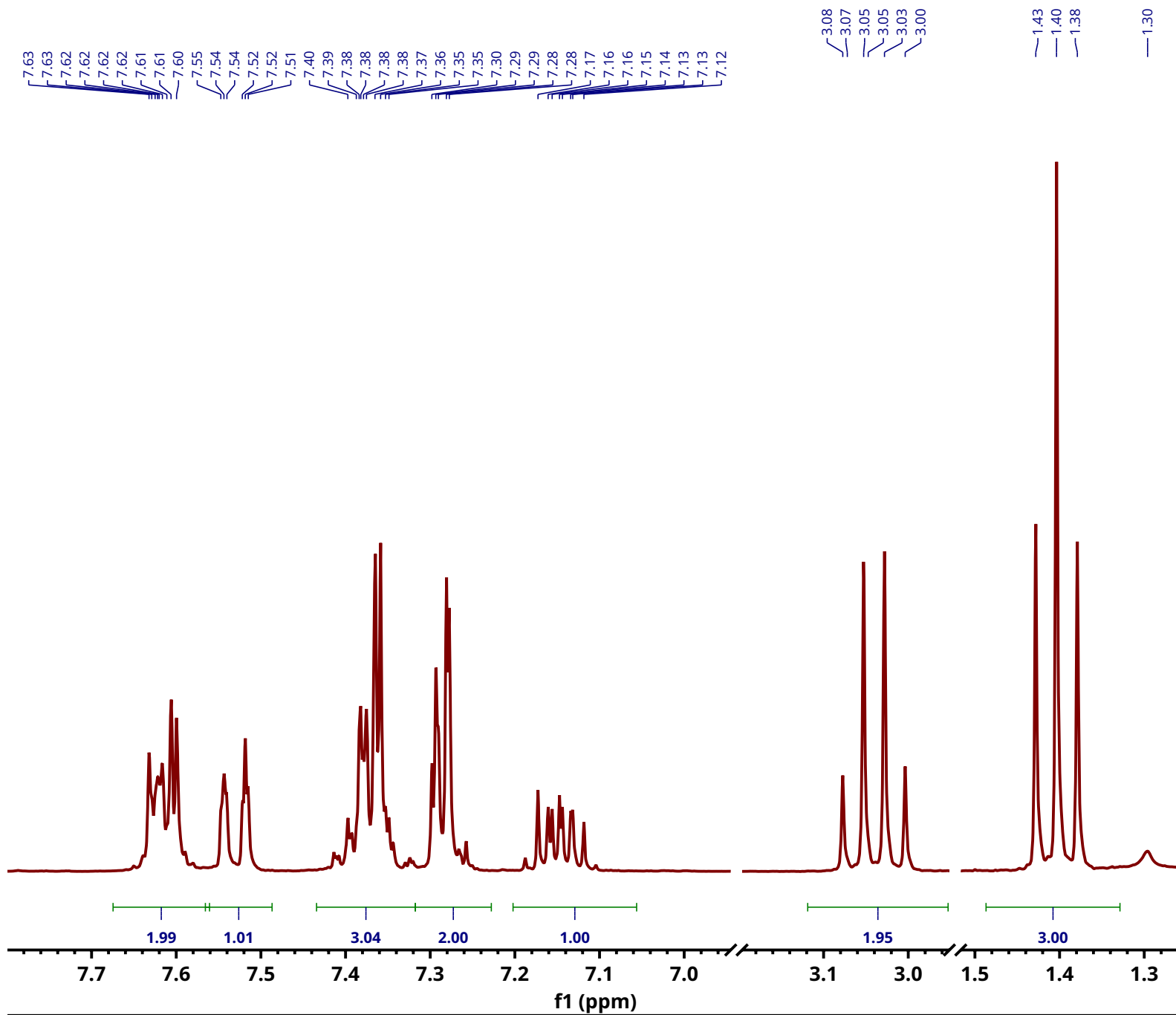


Parameter	Value
Title	CCD-116.2001.fid
Date	
Time	
Solvent	CDCl3
Instrument	FOURIER300
Temperature	295.9
PULPROG	zg30
Experiment	1D
Probe	
NS	16
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

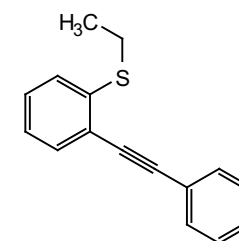


Compound 5t

^1H NMR (300 MHz, Chloroform-*d*) δ 7.67 – 7.56 (m, 2H), 7.53 (dt, $J = 7.6, 1.1$ Hz, 1H), 7.43 – 7.32 (m, 3H), 7.32 – 7.23 (m, 2H), 7.20 – 7.06 (m, 1H), 3.04 (q, $J = 7.4$ Hz, 2H), 1.40 (t, $J = 7.4$ Hz, 3H).



Parameter	Value
Title	CCD-116.2001.fid
Date	
Time	
Solvent	CDCl3
Instrument	FOURIER300
Temperature	295.9
PULPROG	zg30
Experiment	1D
Probe	
NS	16
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

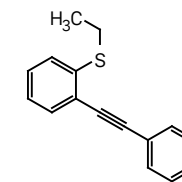
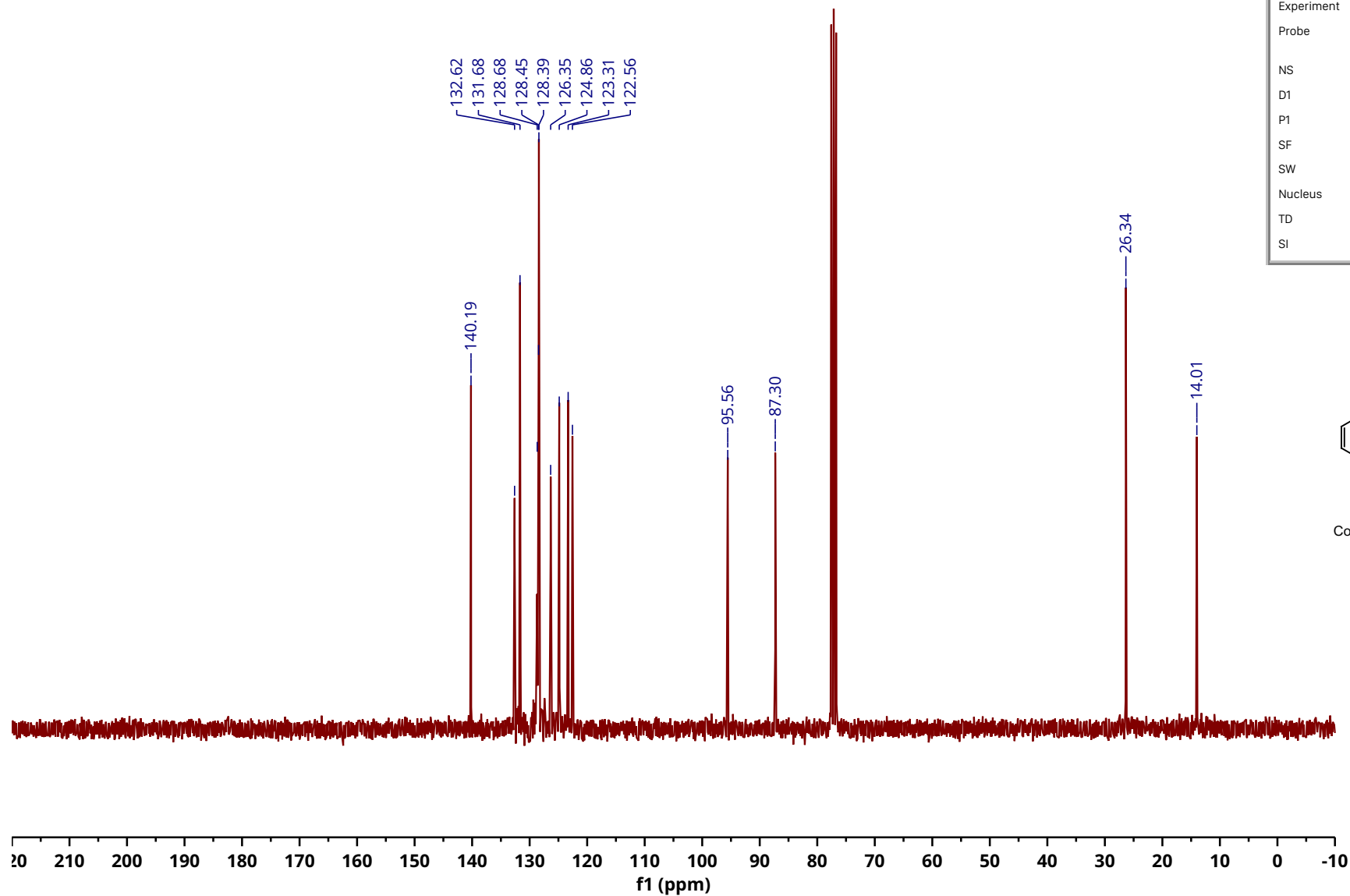


Compound 5t

^1H NMR (300 MHz, Chloroform-*d*) δ 7.67 – 7.56 (m, 2H), 7.53 (dt, $J = 7.6, 1.1$ Hz, 1H), 7.43 – 7.32 (m, 3H), 7.32 – 7.23 (m, 2H), 7.20 – 7.06 (m, 1H), 3.04 (q, $J = 7.4$ Hz, 2H), 1.40 (t, $J = 7.4$ Hz, 3H).

^{13}C NMR (75 MHz, CDCl_3) δ 140.19, 132.62, 131.68, 128.68, 128.45, 128.39, 126.35, 124.86, 123.31, 122.56, 95.56, 87.30, 26.34, 14.01.

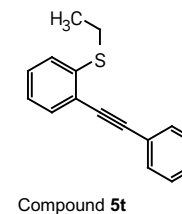
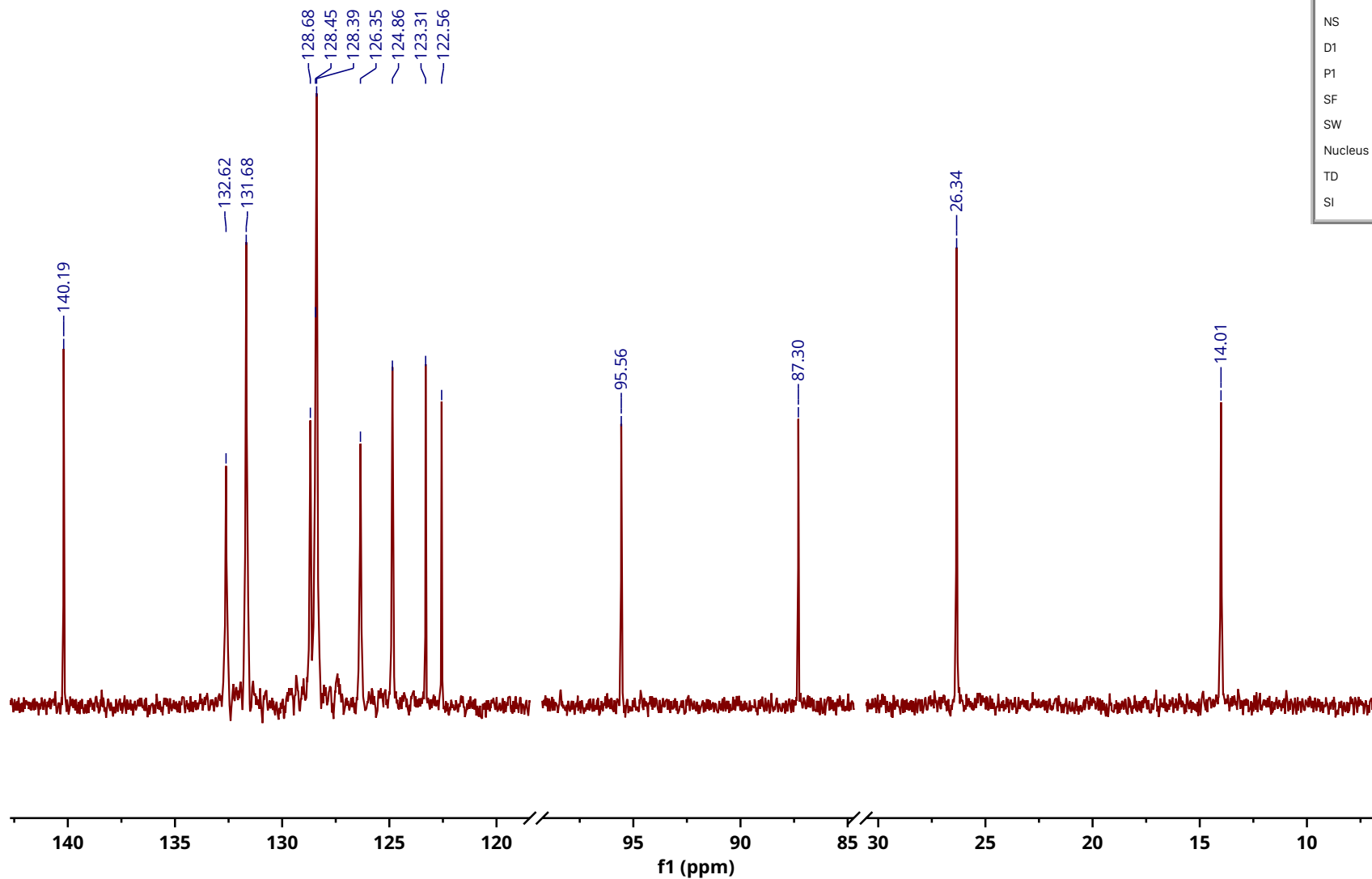
Parameter	Value
Title	CCD-116.2002.fid
Date	
Time	
Solvent	CDCl_3
Instrument	FOURIER300
Temperature	296.0
PULPROG	zgpg30
Experiment	1D
Probe	
NS	513
D1	2.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536

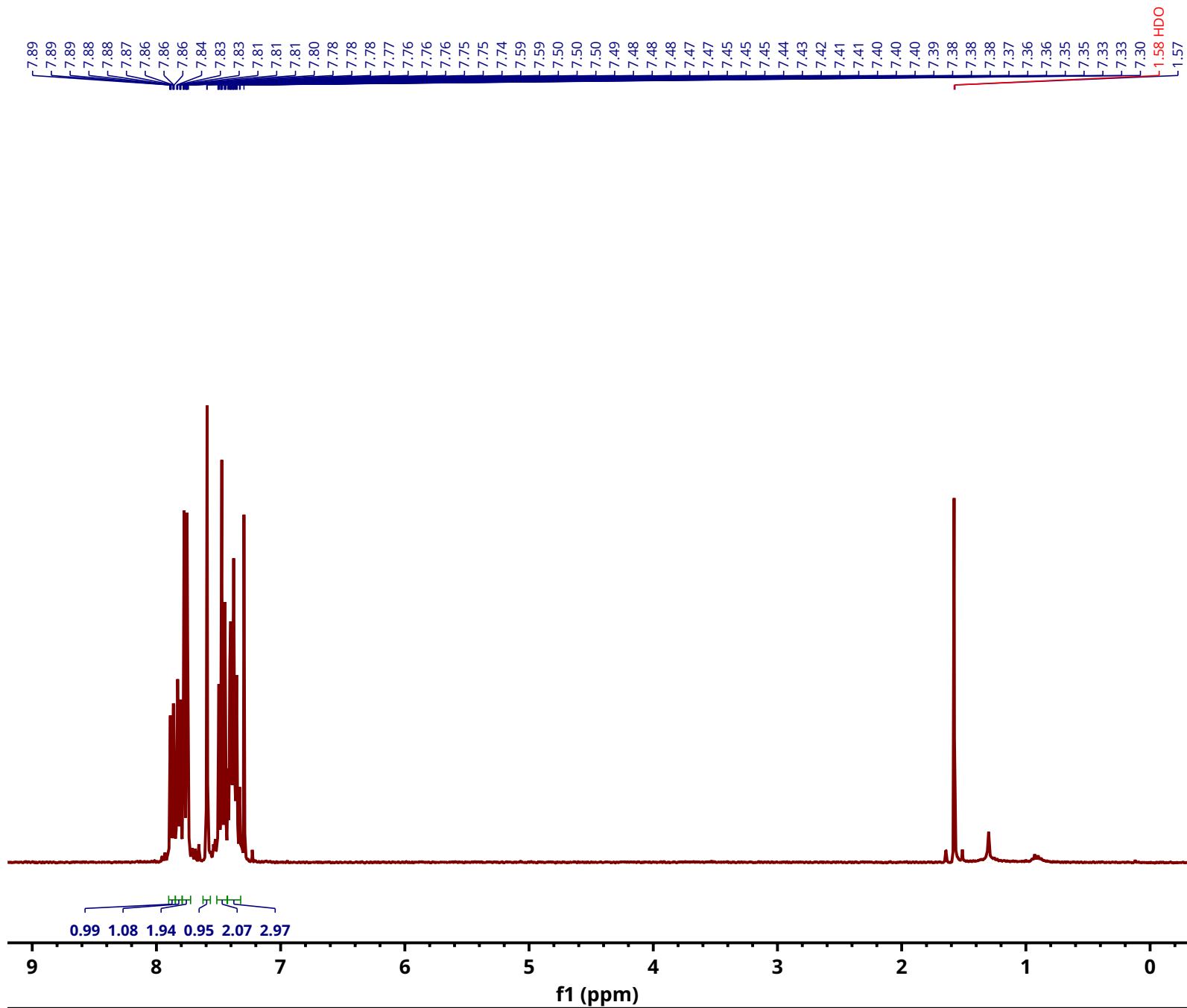


Compound 5t

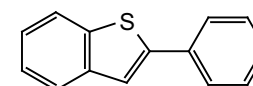
^{13}C NMR (75 MHz, CDCl_3) δ 140.19, 132.62, 131.68, 128.68, 128.45, 128.39, 126.35, 124.86, 123.31, 122.56, 95.56, 87.30, 26.34, 14.01.

Parameter	Value
Title	CCD-116.2002.fid
Date	
Time	
Solvent	CDCl_3
Instrument	FOURIER300
Temperature	296.0
PULPROG	zgpg30
Experiment	1D
Probe	
NS	513
D1	2.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	^{13}C
TD	32768
SI	65536



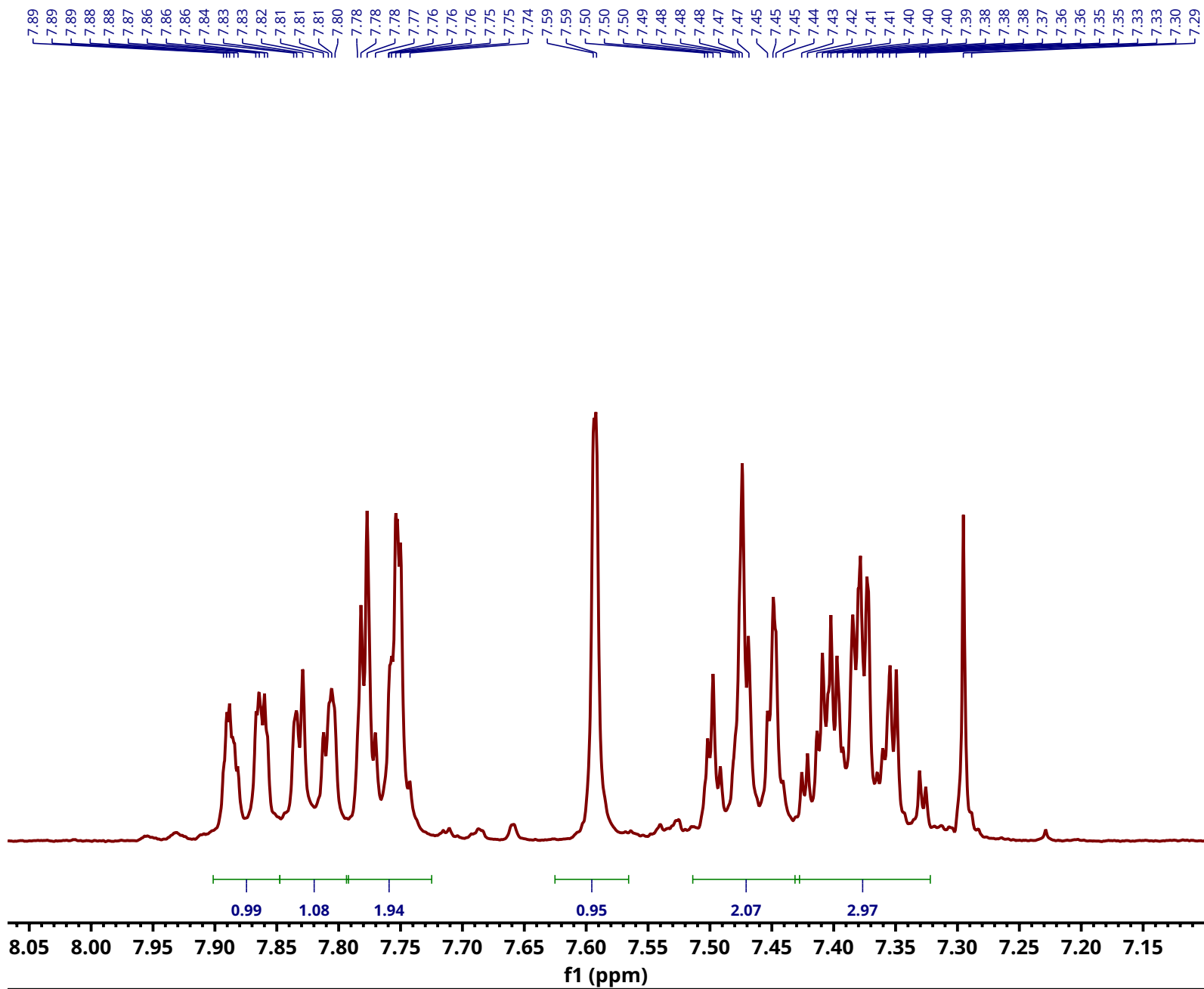


Parameter	Value
Title	JEM-030.21.fid
Date	
Time	
Solvent	CDCl3
Instrument	FOURIER300
Temperature	296.8
PULPROG	zg30
Experiment	1D
Probe	
NS	16
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

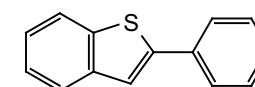


Compound 6a

^1H NMR (300 MHz, Chloroform-*d*) δ 7.87 (ddd, $J = 7.2, 1.9, 0.8$ Hz, 1H), 7.85 – 7.79 (m, 1H), 7.79 – 7.72 (m, 2H), 7.59 (d, $J = 0.8$ Hz, 1H), 7.51 – 7.43 (m, 2H), 7.43 – 7.32 (m, 3H).

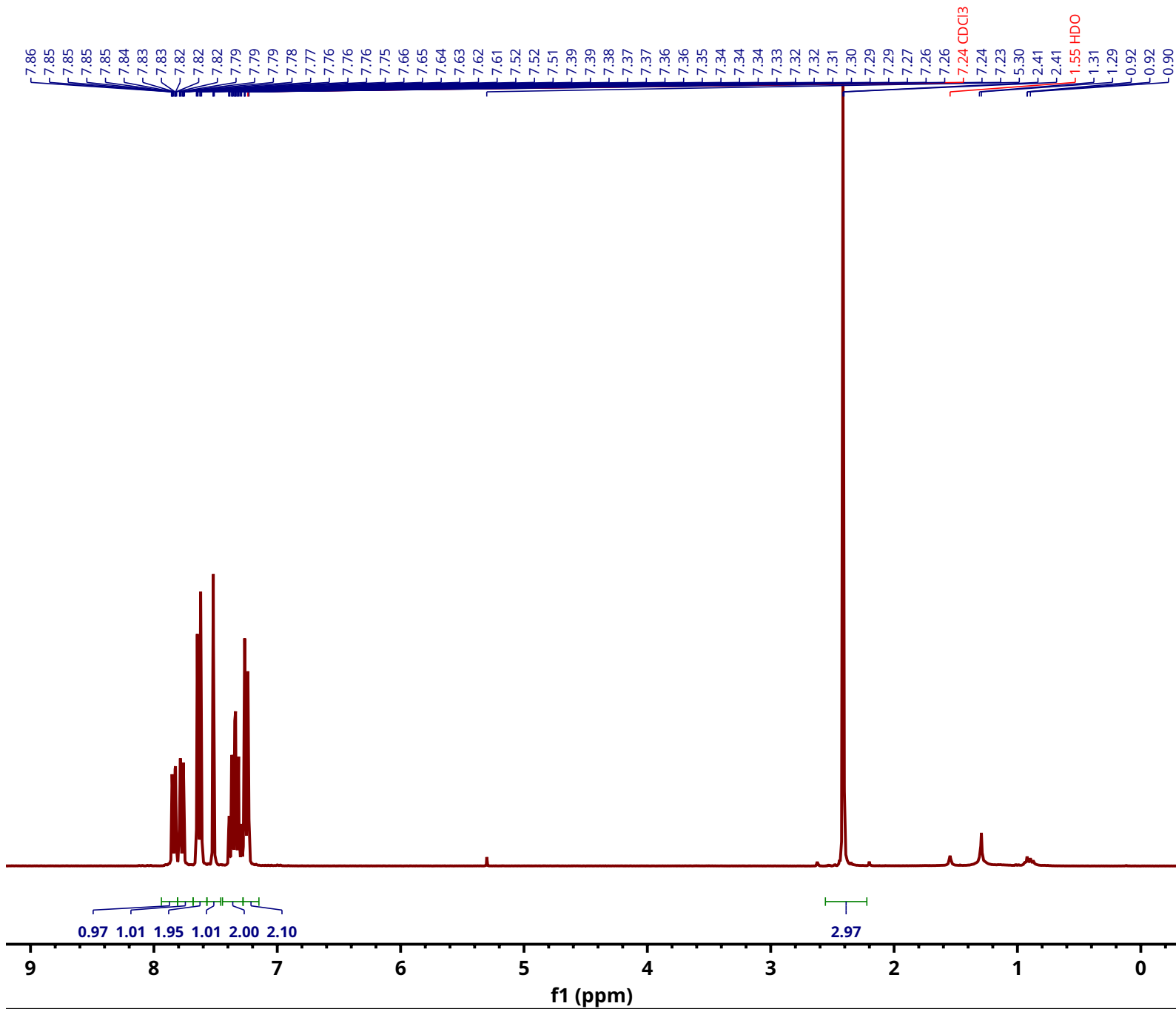


Parameter	Value
Title	JEM-030.21.fid
Date	
Time	
Solvent	CDCl3
Instrument	FOURIER300
Temperature	296.8
PULPROG	zg30
Experiment	1D
Probe	
NS	16
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

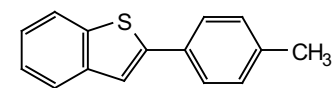


Compound 6a

¹H NMR (300 MHz, Chloroform-*d*) δ 7.87 (ddd, *J* = 7.2, 1.9, 0.8 Hz, 1H), 7.85 – 7.79 (m, 1H), 7.79 – 7.72 (m, 2H), 7.59 (d, *J* = 0.8 Hz, 1H), 7.51 – 7.43 (m, 2H), 7.43 – 7.32 (m, 3H).

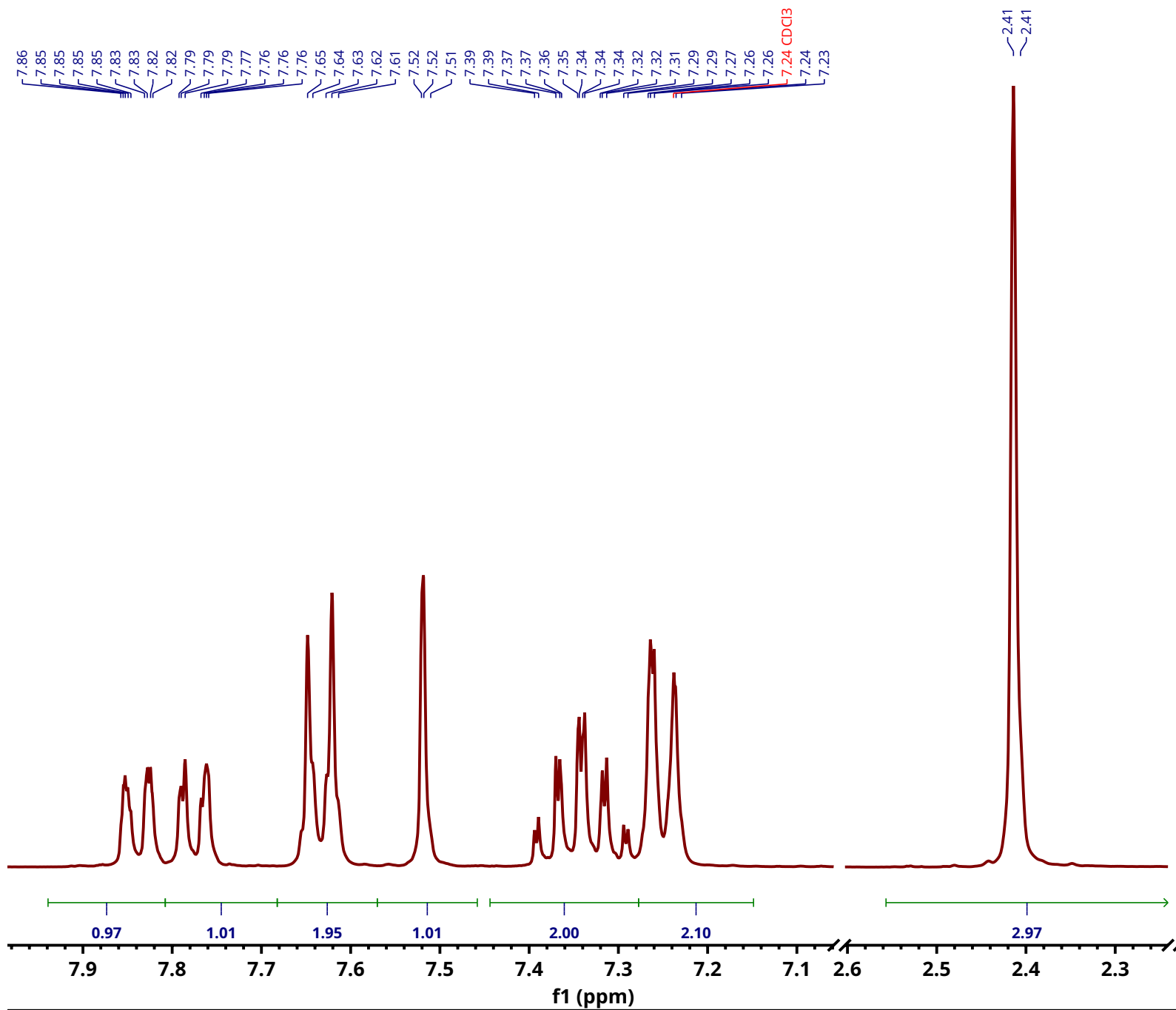


Parameter	Value
1 Title	CCD-089.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	31.6
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-09T17:28:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

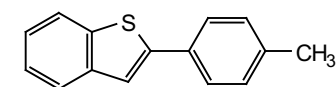


Compound 6b

^1H NMR (300 MHz, Chloroform-*d*) δ 7.83 (ddd, $J = 7.4, 1.8, 0.8$ Hz, 1H), 7.80 – 7.72 (m, 1H), 7.70 – 7.57 (m, 2H), 7.52 (d, $J = 0.8$ Hz, 1H), 7.43 – 7.28 (m, 2H), 7.27 – 7.19 (m, 2H), 2.41 (s, 3H).

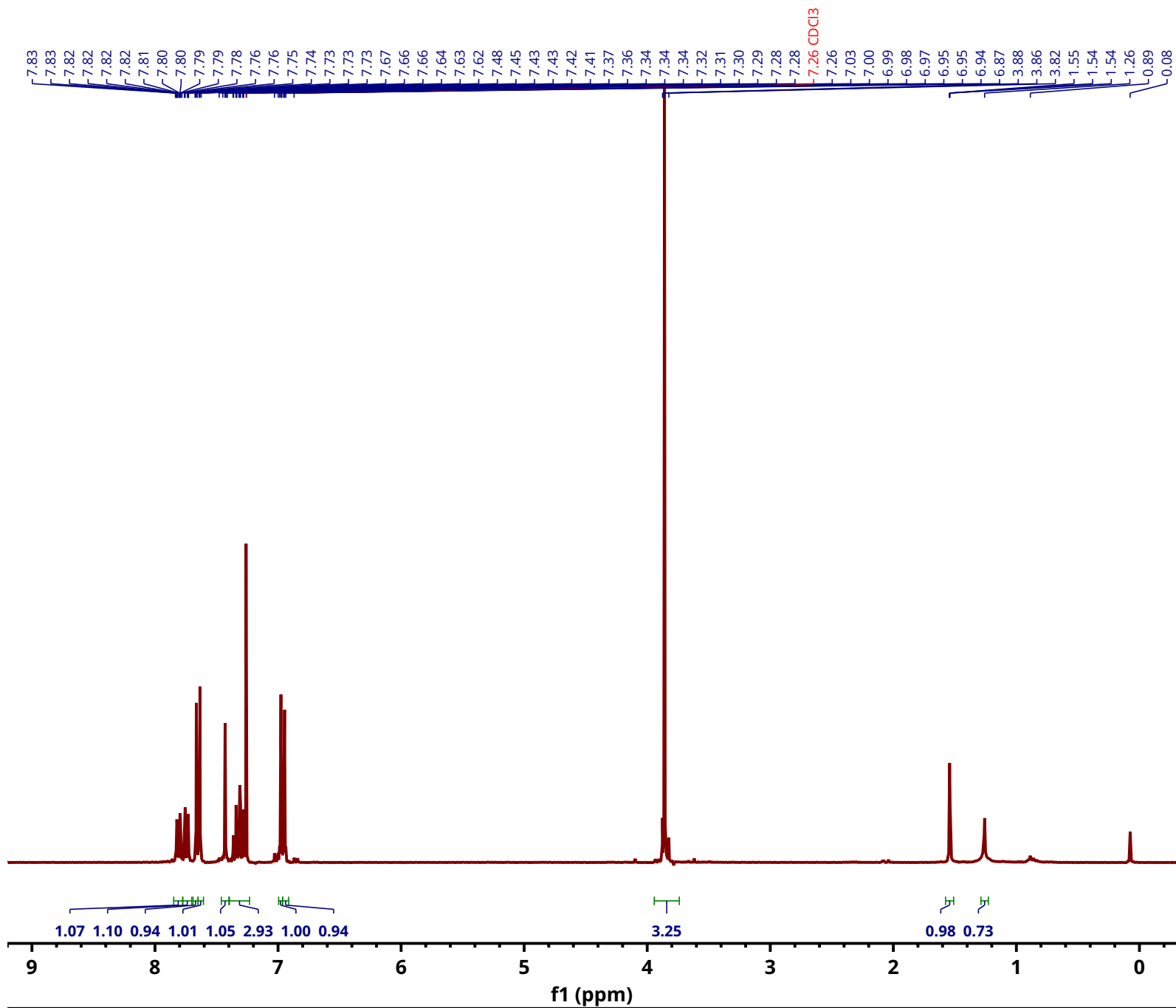


Parameter	Value
1 Title	CCD-089.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	31.6
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-09T17:28:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

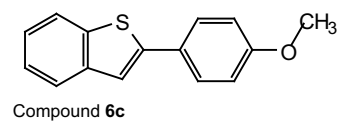


Compound **6b**

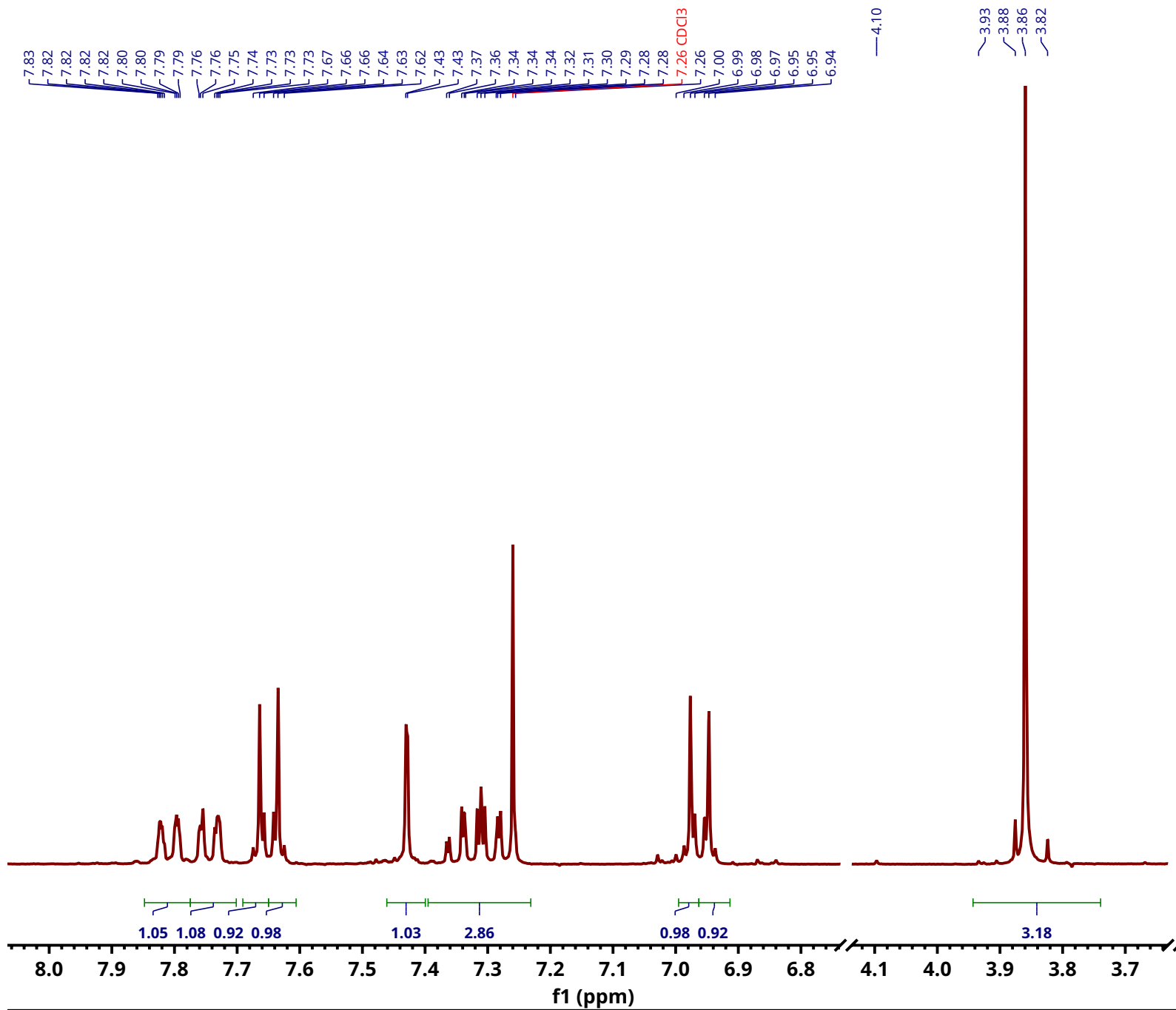
^1H NMR (300 MHz, Chloroform-*d*) δ 7.83 (ddd, $J = 7.4, 1.8, 0.8$ Hz, 1H), 7.80 – 7.72 (m, 1H), 7.70 – 7.57 (m, 2H), 7.52 (d, $J = 0.8$ Hz, 1H), 7.43 – 7.28 (m, 2H), 7.27 – 7.19 (m, 2H), 2.41 (s, 3H).



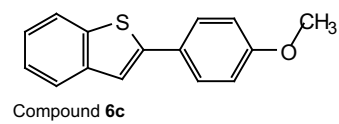
Parameter	Value
1 Title	CCD-072.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.1
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	122.2
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-25T10:56:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



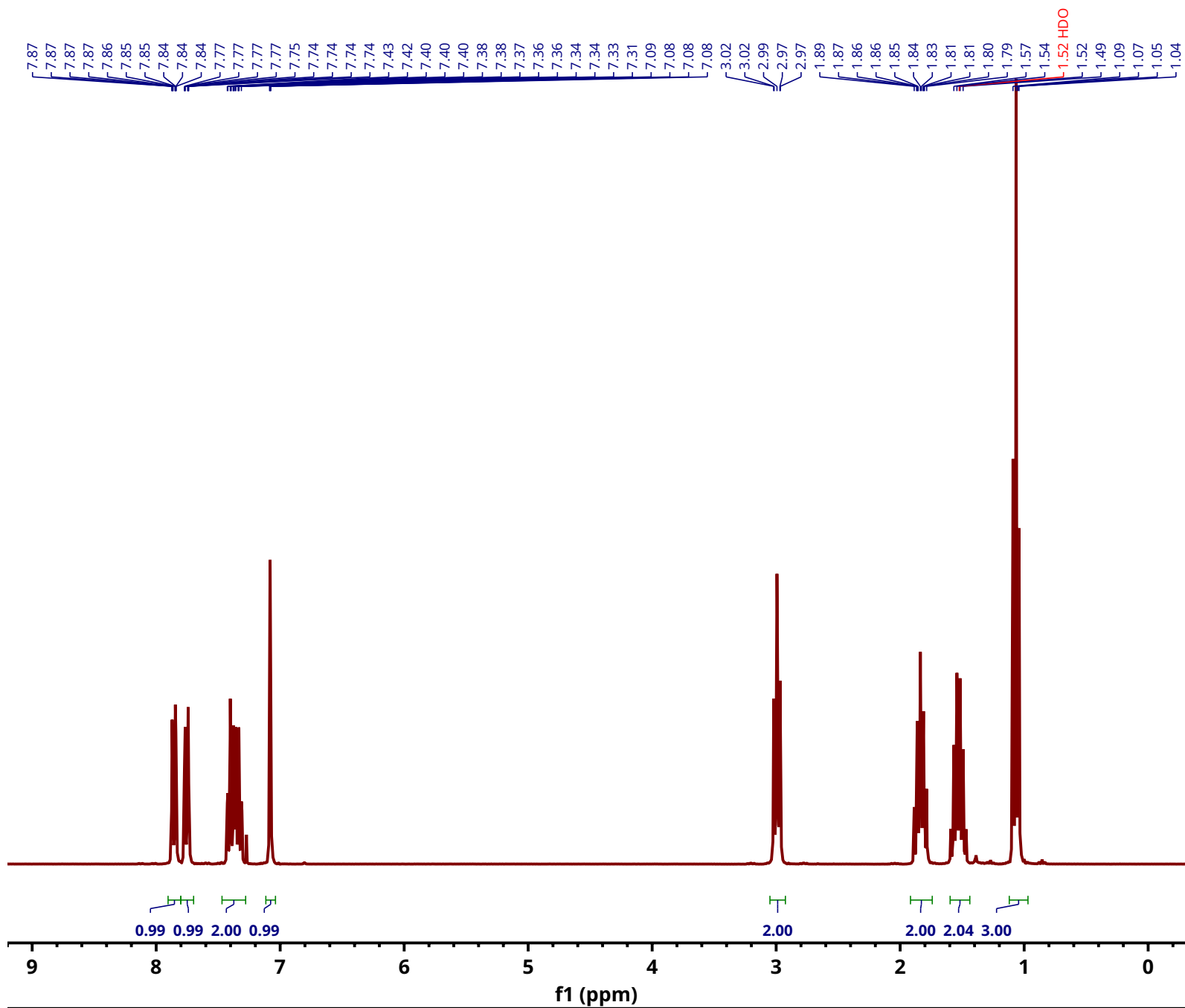
¹H NMR (300 MHz, Chloroform-*d*) δ 7.81 (ddd, *J* = 7.5, 1.6, 0.7 Hz, 1H), 7.74 (ddd, *J* = 7.9, 1.7, 0.7 Hz, 1H), 7.67 (dd, *J* = 3.0, 2.2 Hz, 1H), 7.63 (dd, *J* = 2.8, 2.2 Hz, 1H), 7.43 (d, *J* = 0.8 Hz, 1H), 7.37 – 7.25 (m, 2H), 6.97 (dd, *J* = 3.1, 2.3 Hz, 1H), 6.95 (dd, *J* = 3.0, 2.2 Hz, 1H), 3.86 (s, 3H)



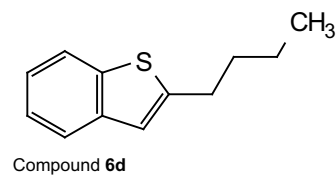
Parameter	Value
1 Title	CCD-072.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.1
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	122.2
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-25T10:56:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



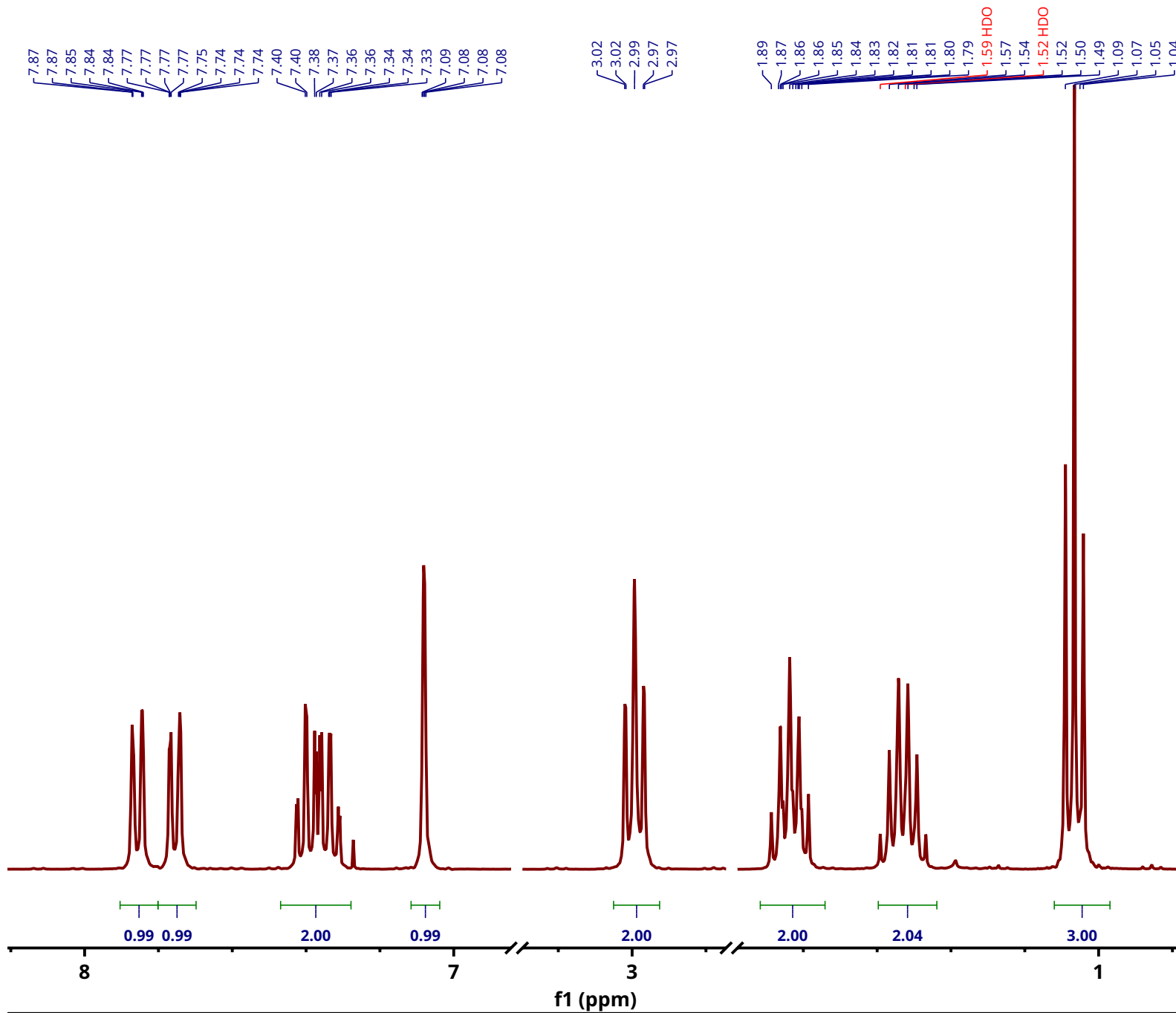
¹H NMR (300 MHz, Chloroform-*d*) δ 7.81 (ddd, *J* = 7.5, 1.6, 0.7 Hz, 1H), 7.74 (ddd, *J* = 7.9, 1.7, 0.7 Hz, 1H), 7.67 (dd, *J* = 3.0, 2.2 Hz, 1H), 7.63 (dd, *J* = 2.8, 2.2 Hz, 1H), 7.43 (d, *J* = 0.8 Hz, 1H), 7.37 – 7.25 (m, 2H), 6.97 (dd, *J* = 3.1, 2.3 Hz, 1H), 6.95 (dd, *J* = 3.0, 2.2 Hz, 1H), 3.86 (s, 3H)



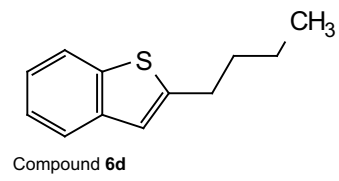
Parameter	Value
1 Title	CCD-084.13.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	6.4
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-06T11:47:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



¹H NMR (Chloroform-*d*, 300 MHz): δ (ppm) 7.85 (ddd, *J*=7.8, 1.4, 0.7 Hz, 1H), 7.74 (dd, *J*=7.6, 1.6 Hz, 1H), 7.46 – 7.27 (m, 2H), 7.07 (t, *J*=1.0 Hz, 1H), 3.04 – 2.91 (m, 2H), 1.90 – 1.73 (m, 2H), 1.51 (dt, *J*=14.5, 7.3 Hz, 2H), 1.05 (t, *J*=7.3 Hz, 3H)



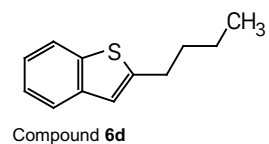
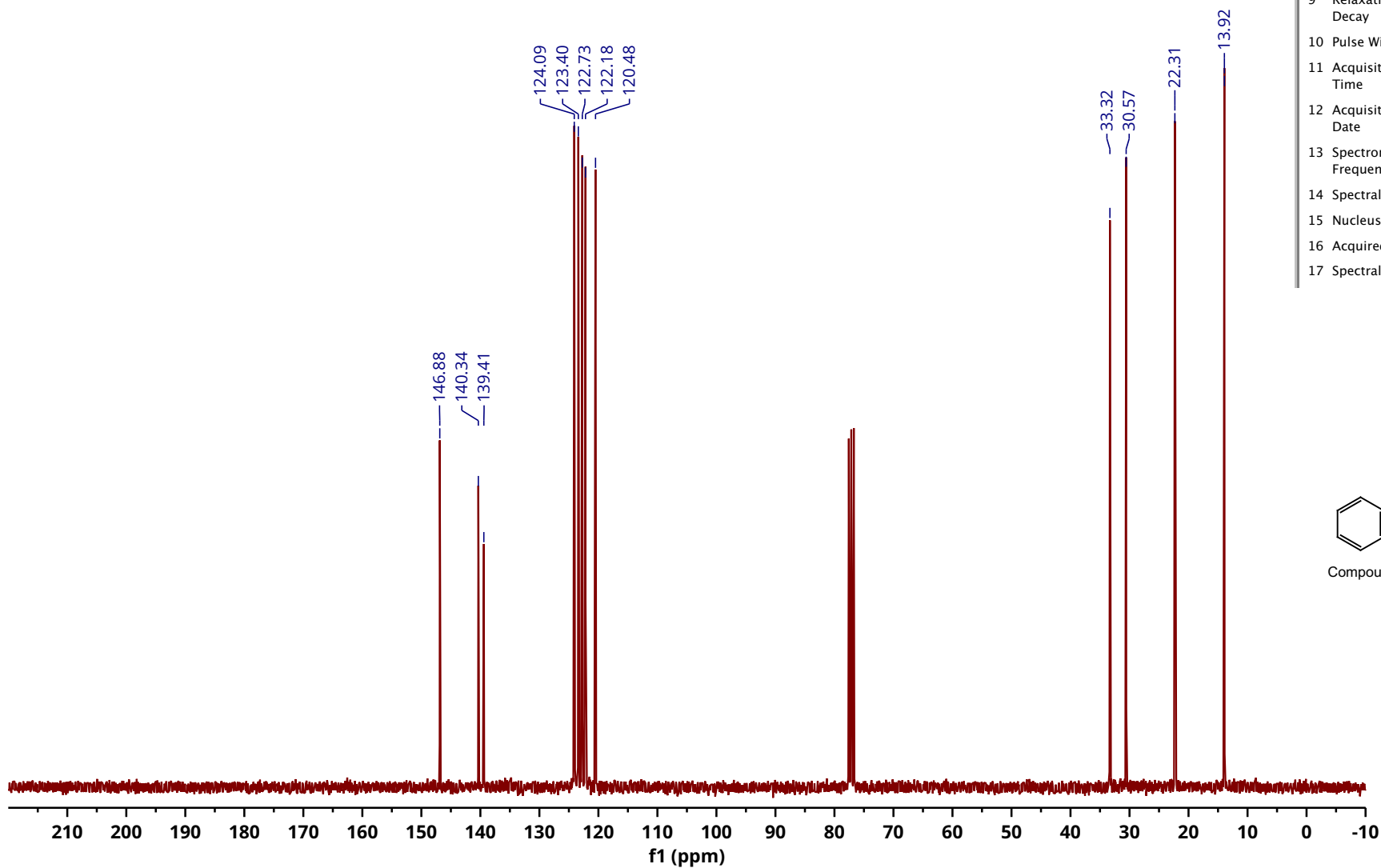
Parameter	Value
1 Title	CCD-084.13.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.3
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	6.4
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-06T11:47:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



¹H NMR (Chloroform-*d*, 300 MHz): δ (ppm) 7.85 (ddd, *J*=7.8, 1.4, 0.7 Hz, 1H), 7.74 (dd, *J*=7.6, 1.6 Hz, 1H), 7.46 – 7.27 (m, 2H), 7.07 (t, *J*=1.0 Hz, 1H), 3.04 – 2.91 (m, 2H), 1.90 – 1.73 (m, 2H), 1.51 (dt, *J*=14.5, 7.3 Hz, 2H), 1.05 (t, *J*=7.3 Hz, 3H)

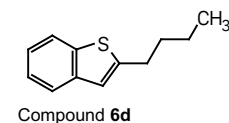
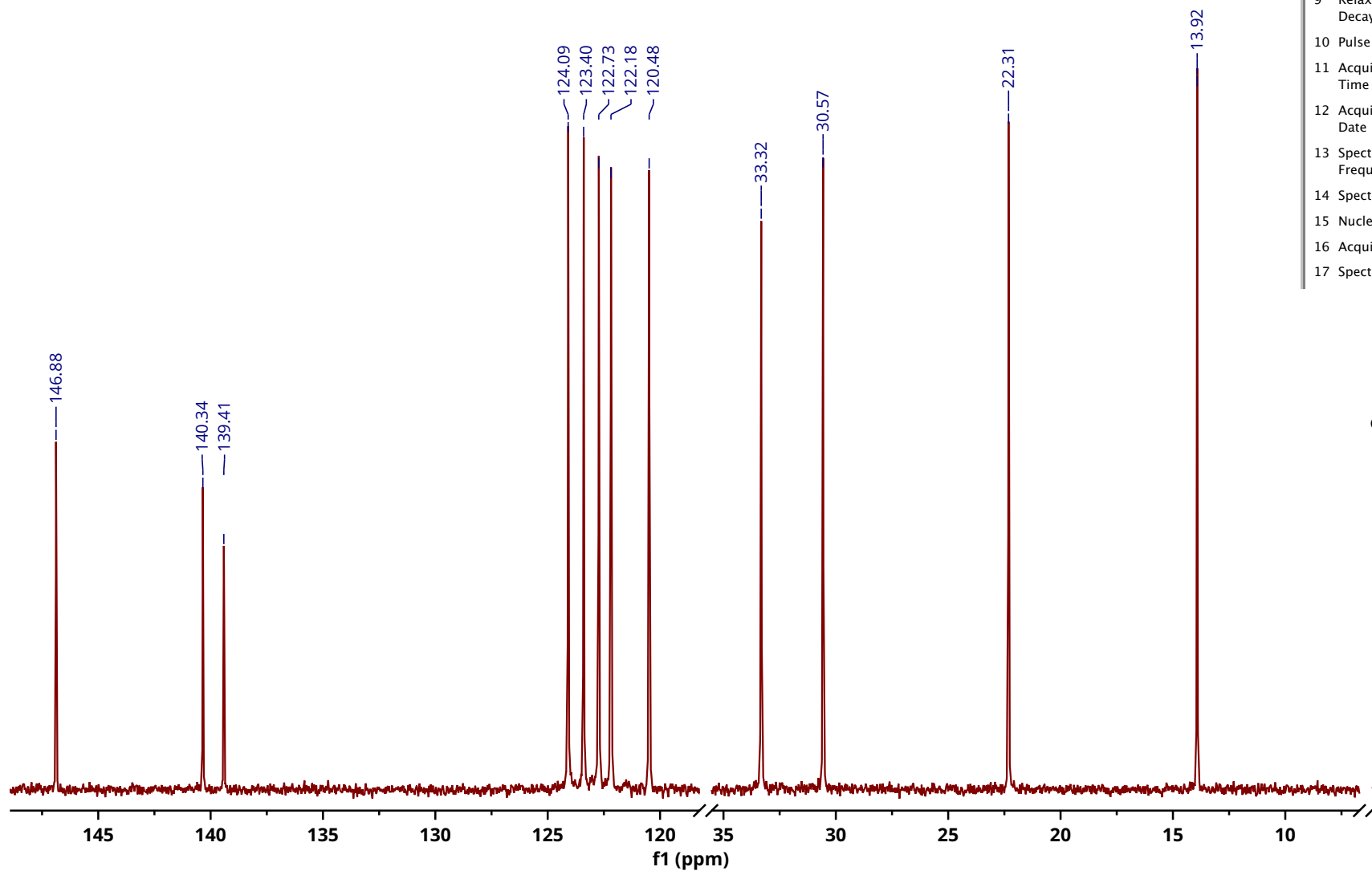
^{13}C NMR (75 MHz, CDCl_3) δ 146.90, 140.36, 139.43, 124.11, 123.42, 122.75, 122.20, 120.50, 33.34, 30.59, 22.33, 13.94.

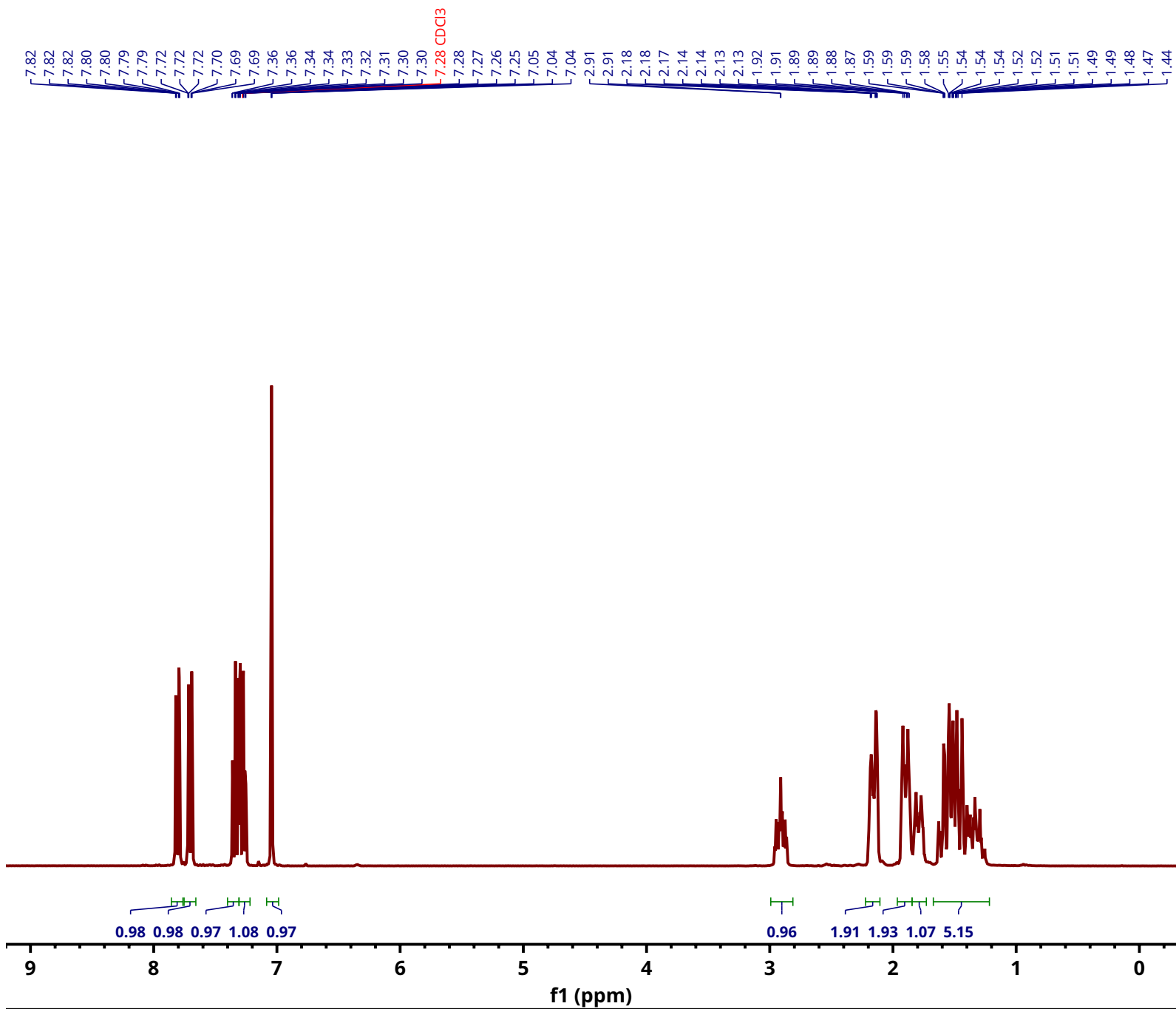
Parameter	Value
1 Title	CCD-084.111.fid
2 Instrument	FOURIER300
3 Solvent	CDCl_3
4 Temperature	298.8
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	400
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-06T14:57:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	^{13}C
16 Acquired Size	32768
17 Spectral Size	65536



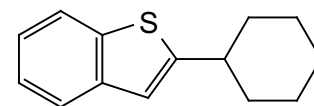
^{13}C NMR (75 MHz, CDCl_3) δ 146.90, 140.36, 139.43, 124.11, 123.42, 122.75, 122.20, 120.50, 33.34, 30.59, 22.33, 13.94.

Parameter	Value
1 Title	CCD-084.111.fid
2 Instrument	FOURIER300
3 Solvent	CDCl_3
4 Temperature	298.8
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	400
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-06T14:57:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	^{13}C
16 Acquired Size	32768
17 Spectral Size	65536



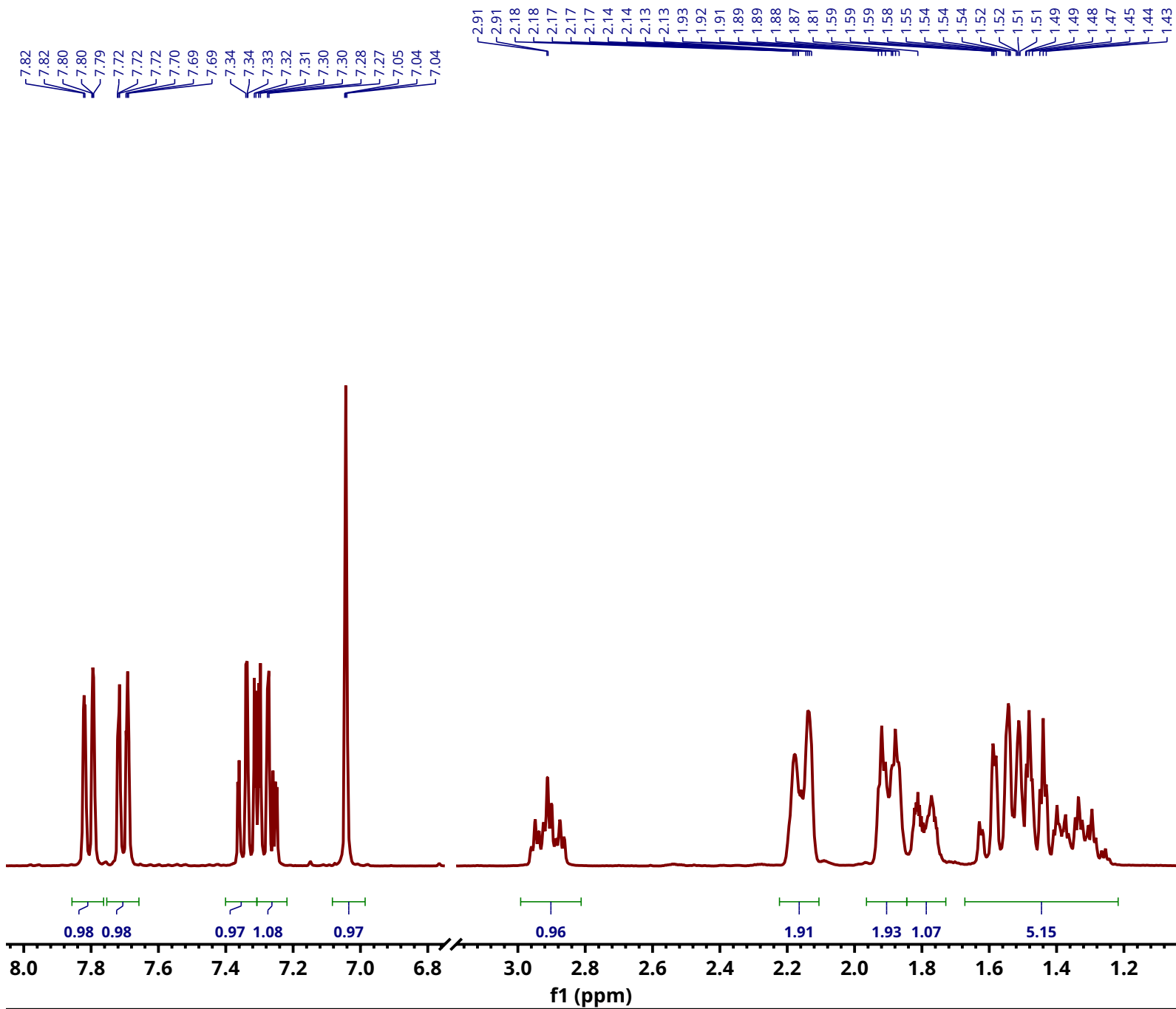


Parameter	Value
1 Title	BK-112.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.0
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	11.1
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-10T12:20:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

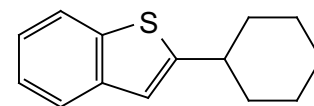


Compound 6e

¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.81 (dd, *J*=8.0, 1.0 Hz, 1H), 7.75 – 7.67 (m, 1H), 7.39 – 7.28 (m, 1H), 7.27 (td, *J*=7.5, 1.5 Hz, 1H), 7.04 (s, 1H), 3.02 – 2.82 (m, 1H), 2.24 – 2.09 (m, 2H), 1.90 (dt, *J*=11.8, 3.0 Hz, 2H), 1.79 (dddd, *J*=12.4, 5.0, 3.2, 1.5 Hz, 1H), 1.67 – 1.53 (m, 5H)

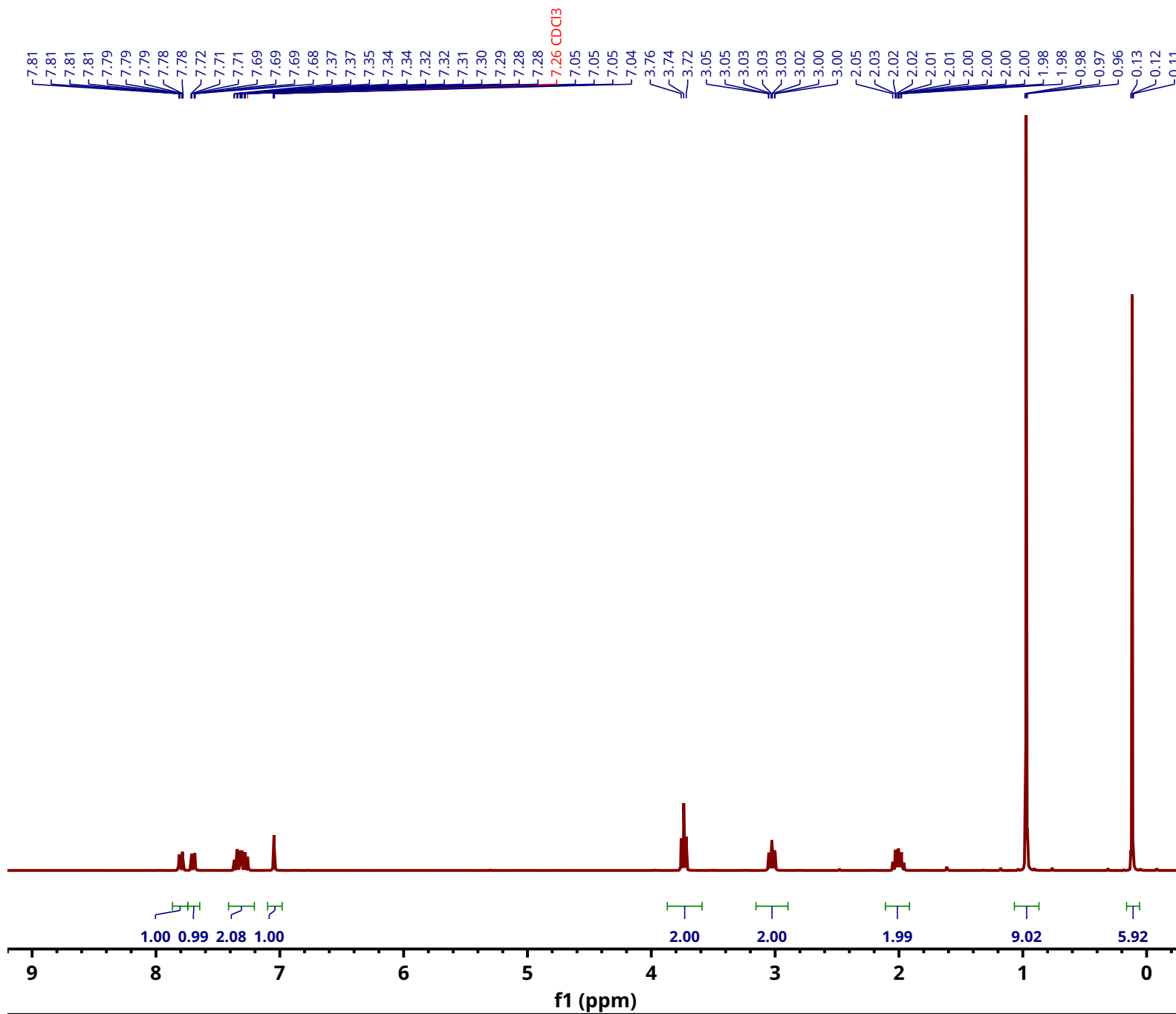


Parameter	Value
1 Title	BK-112.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.0
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	11.1
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-10T12:20:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

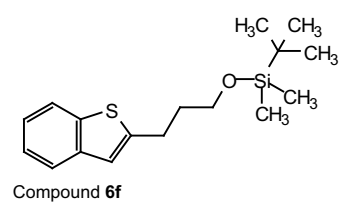


Compound 6e

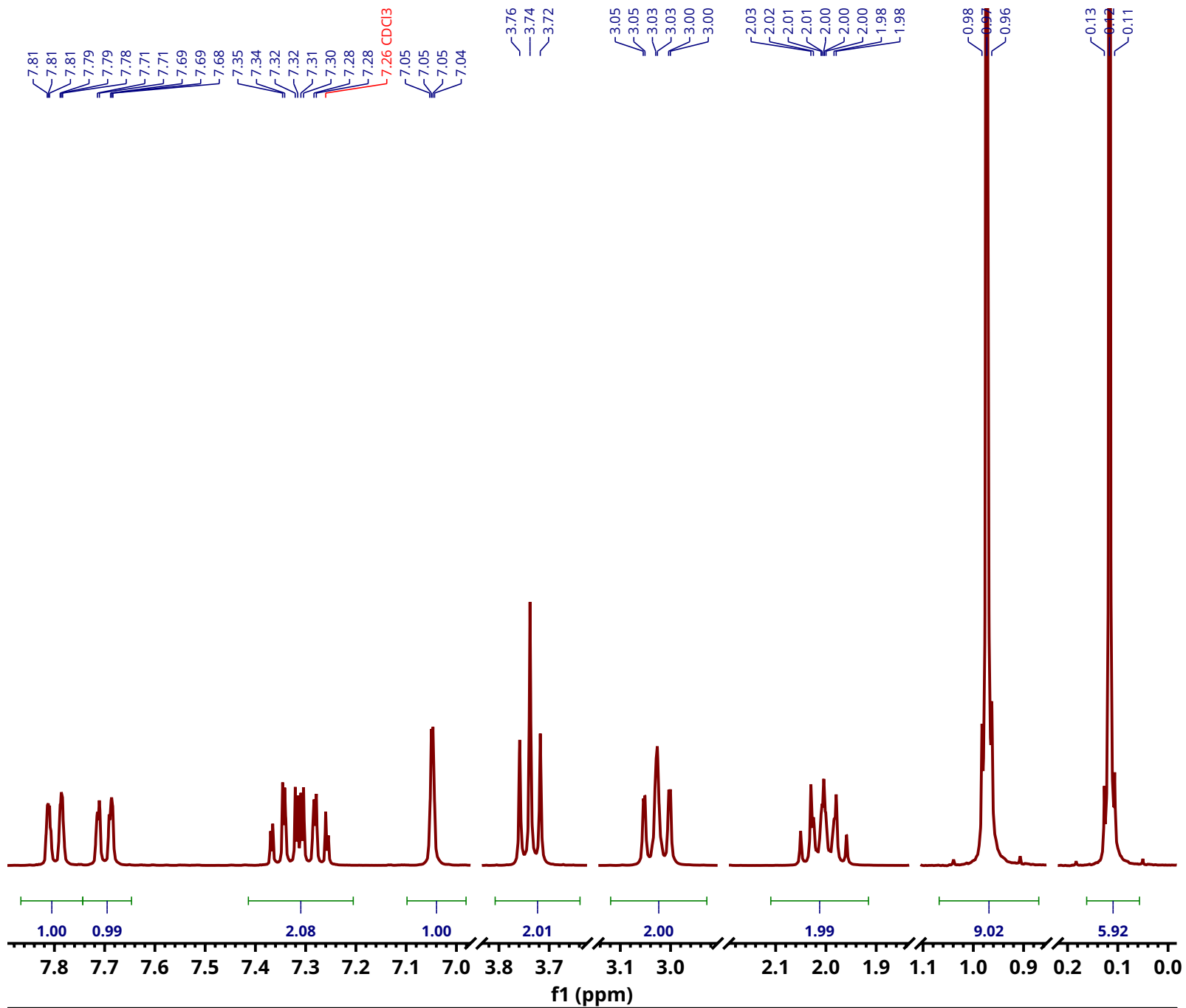
¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.81 (dd, *J*=8.0, 1.0 Hz, 1H), 7.75 – 7.67 (m, 1H), 7.39 – 7.28 (m, 1H), 7.27 (td, *J*=7.5, 1.5 Hz, 1H), 7.04 (s, 1H), 3.02 – 2.82 (m, 1H), 2.24 – 2.09 (m, 2H), 1.90 (dt, *J*=11.8, 3.0 Hz, 2H), 1.79 (dddd, *J*=12.4, 5.0, 3.2, 1.5 Hz, 1H), 1.67 – 1.53 (m, 5H)



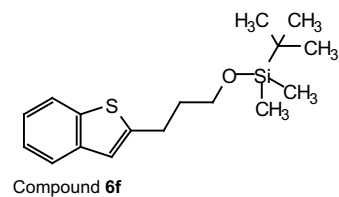
Parameter	Value
Title	BK-114.11.fid
Date	20181015
Time	17.37
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.2
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	64
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536



¹H NMR (300 MHz, Chloroform-*d*) δ 7.80 (ddt, *J* = 7.7, 1.6, 0.8 Hz, 1H), 7.74 – 7.65 (m, 1H), 7.41 – 7.21 (m, 2H), 7.05 (q, *J* = 1.0 Hz, 1H), 3.74 (t, *J* = 6.1 Hz, 2H), 3.03 (ddd, *J* = 7.7, 7.0, 1.1 Hz, 2H), 2.11 – 1.92 (m, 2H), 0.97 (s, 9H), 0.12 (s, 6H).



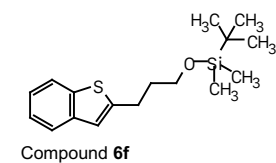
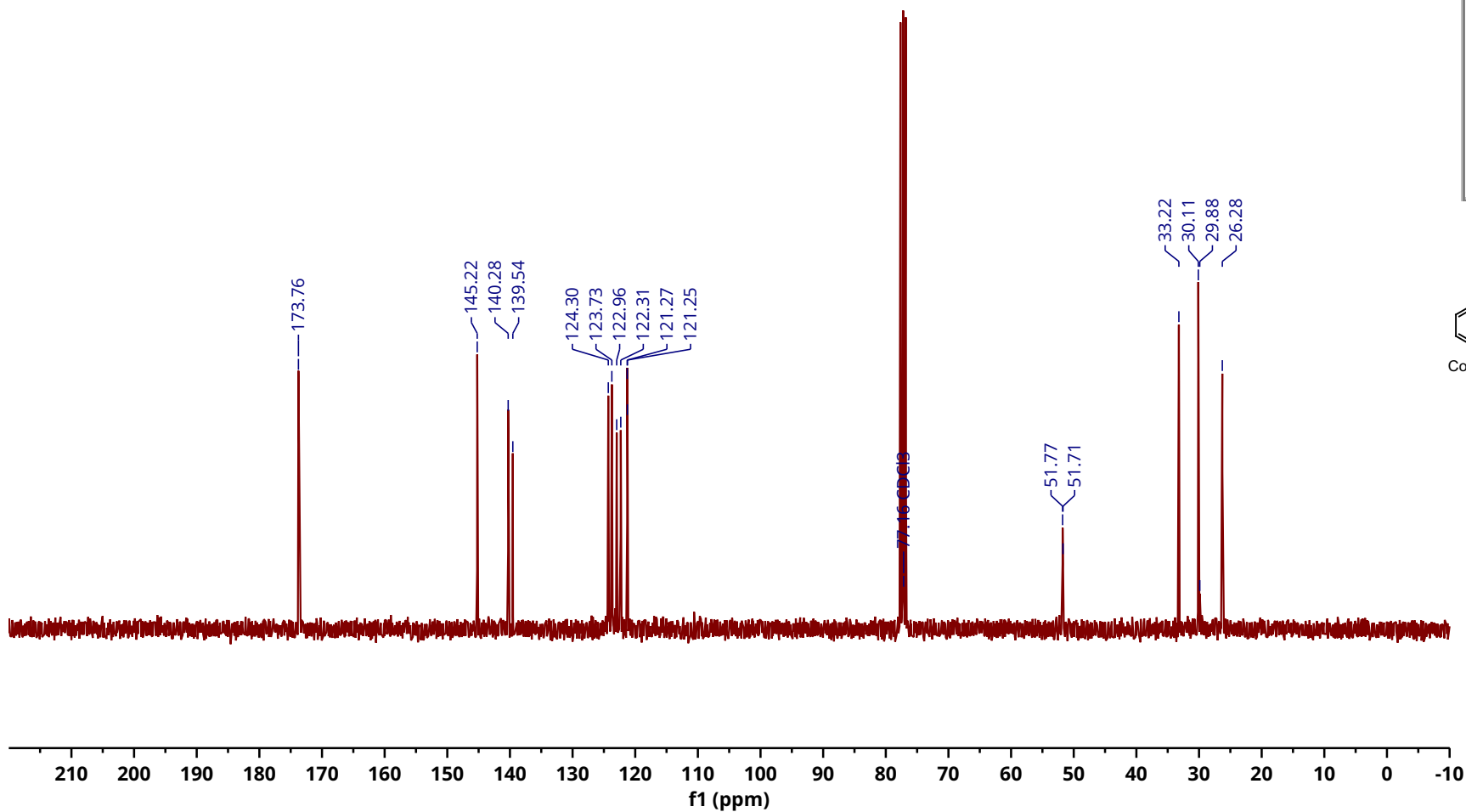
Parameter	Value
Title	BK-114.11.fid
Date	20181015
Time	17.37
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.2
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	64
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536



¹H NMR (300 MHz, Chloroform-*d*) δ 7.80 (ddt, *J* = 7.7, 1.6, 0.8 Hz, 1H), 7.74 – 7.65 (m, 1H), 7.41 – 7.21 (m, 2H), 7.05 (q, *J* = 1.0 Hz, 1H), 3.74 (t, *J* = 6.1 Hz, 2H), 3.03 (ddd, *J* = 7.7, 7.0, 1.1 Hz, 2H), 2.11 – 1.92 (m, 2H), 0.97 (s, 9H), 0.12 (s, 6H).

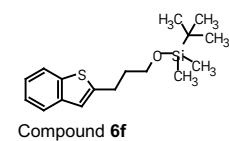
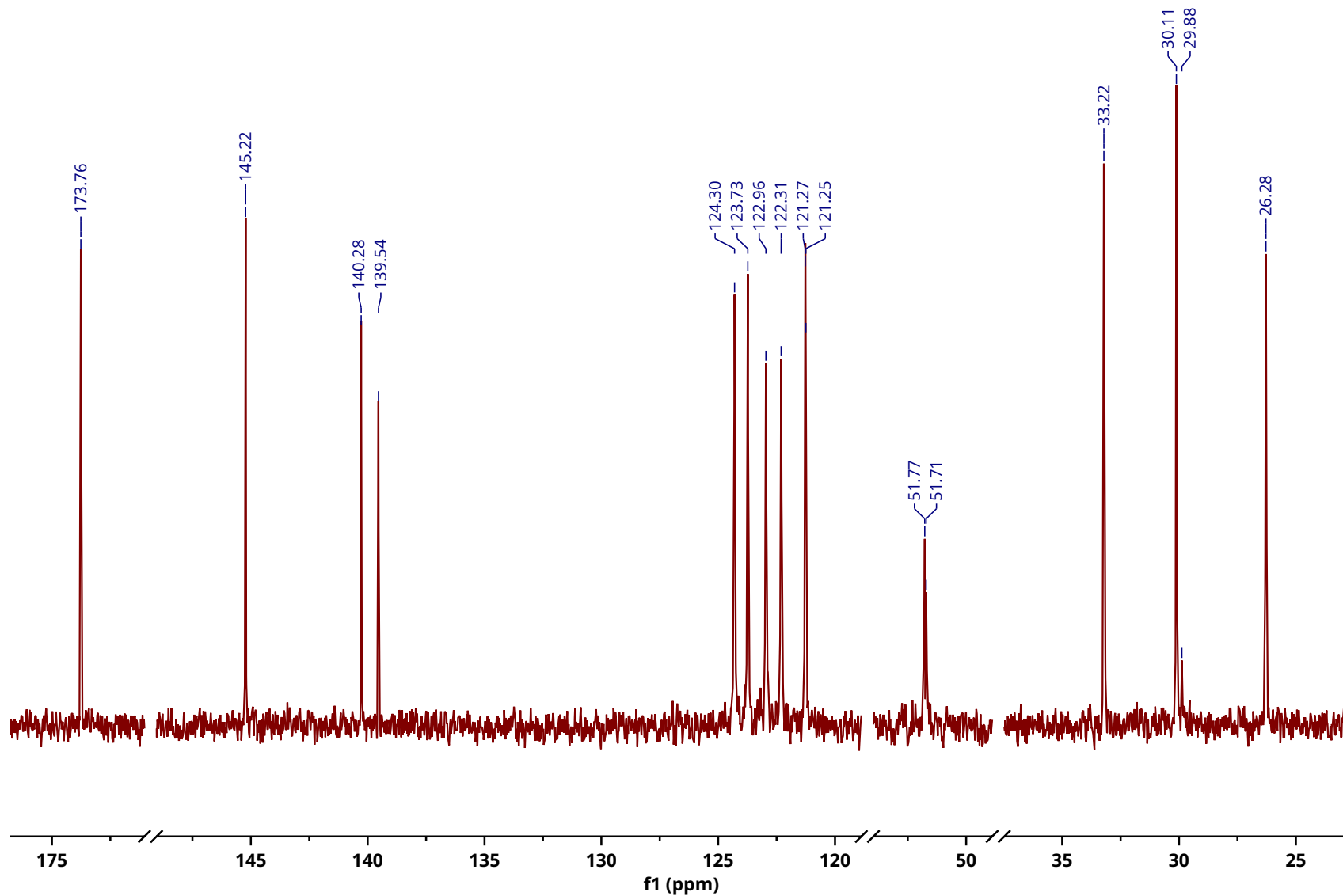
^{13}C NMR (75 MHz, CDCl_3) δ 173.69, 145.15, 140.21, 139.47, 124.23, 123.66, 122.89, 122.24, 121.21, 121.18, 51.70, 51.64, 33.15, 30.05, 29.81, 26.21.

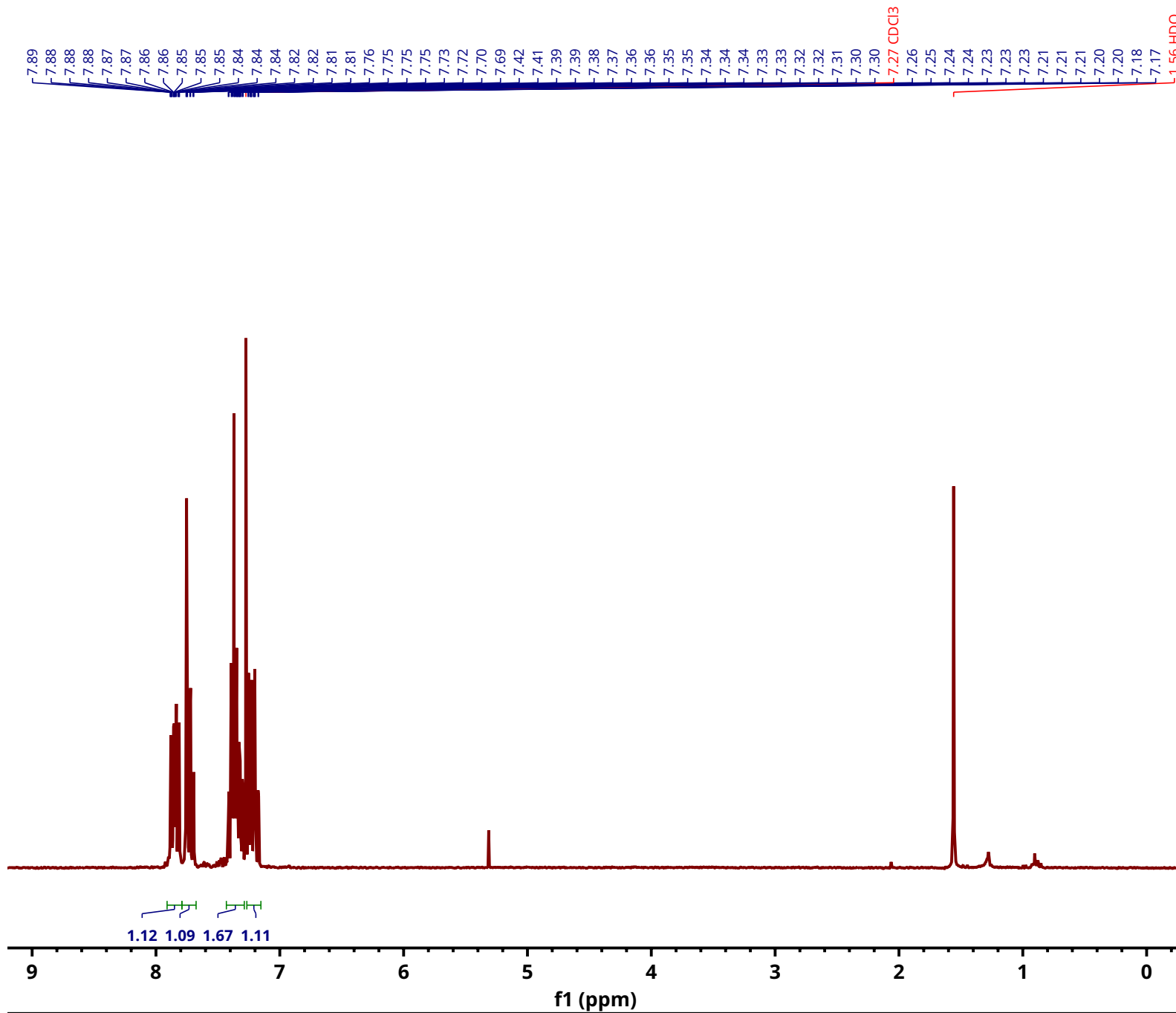
Parameter	Value
1 Title	CCD-093.111.fid
2 Instrument	FOURIER300
3 Solvent	CDCl_3
4 Temperature	299.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	403
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-13T11:24:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	^{13}C
16 Acquired Size	32768
17 Spectral Size	65536



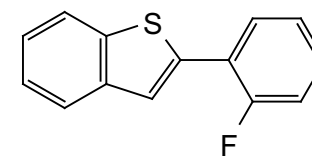
^{13}C NMR (75 MHz, CDCl_3) δ 173.69, 145.15, 140.21, 139.47, 124.23, 123.66, 122.89, 122.24, 121.21, 121.18, 51.70, 51.64, 33.15, 30.05, 29.81, 26.21.

Parameter	Value
1 Title	CCD-093.111.fid
2 Instrument	FOURIER300
3 Solvent	CDCl_3
4 Temperature	299.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	403
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-13T11:24:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	^{13}C
16 Acquired Size	32768
17 Spectral Size	65536



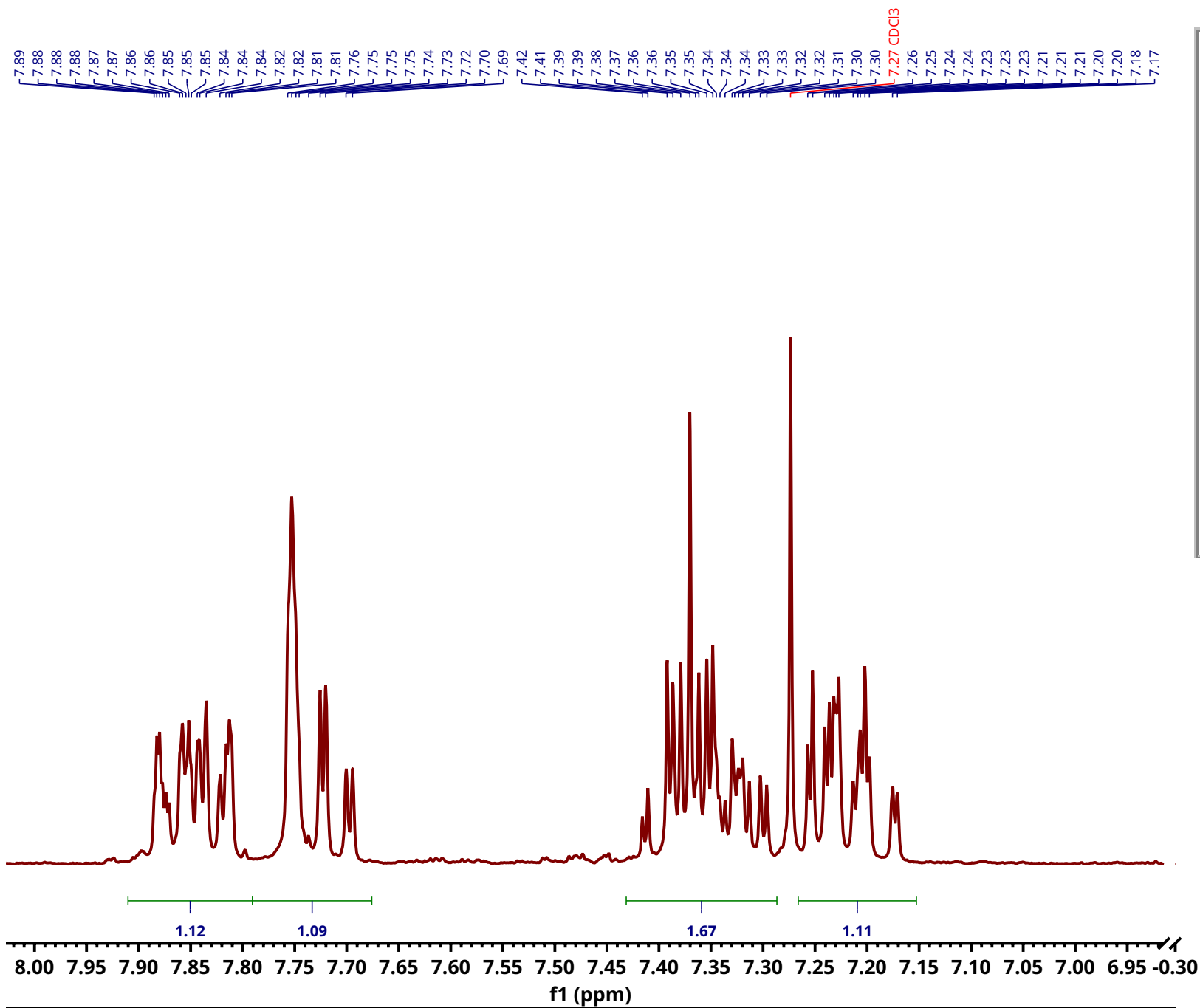


Parameter	Value
1 Title	BK-104.101.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	97.3
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-29T2 2:31:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

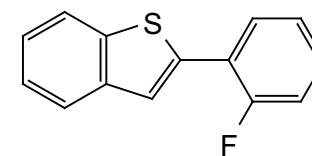


Compound 6g

$^1\text{H NMR}$ (300 MHz, Chloroform-*d*) δ 7.91 – 7.78 (m, 2H), 7.77 – 7.67 (m, 2H), 7.44 – 7.27 (m, 3H), 7.25 – 7.14 (m, 2H).

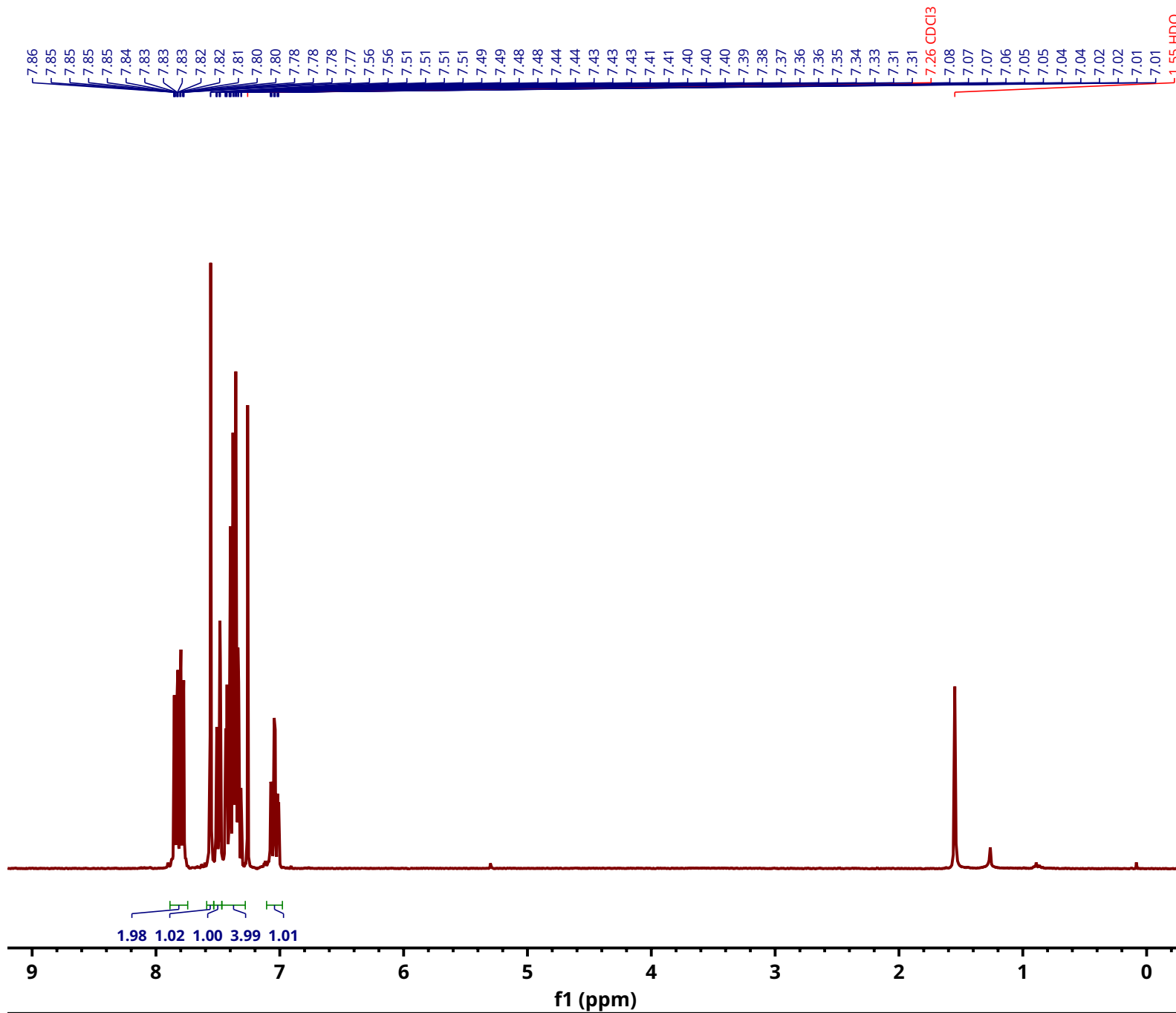


Parameter	Value
1 Title	BK-104.101.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	16
8 Receiver Gain	97.3
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-29T2 2:31:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

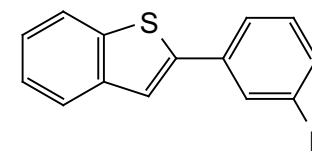


Compound 6g

$^1\text{H NMR}$ (300 MHz, Chloroform-*d*) δ 7.91 – 7.78 (m, 2H), 7.77 – 7.67 (m, 2H), 7.44 – 7.27 (m, 3H), 7.25 – 7.14 (m, 2H).

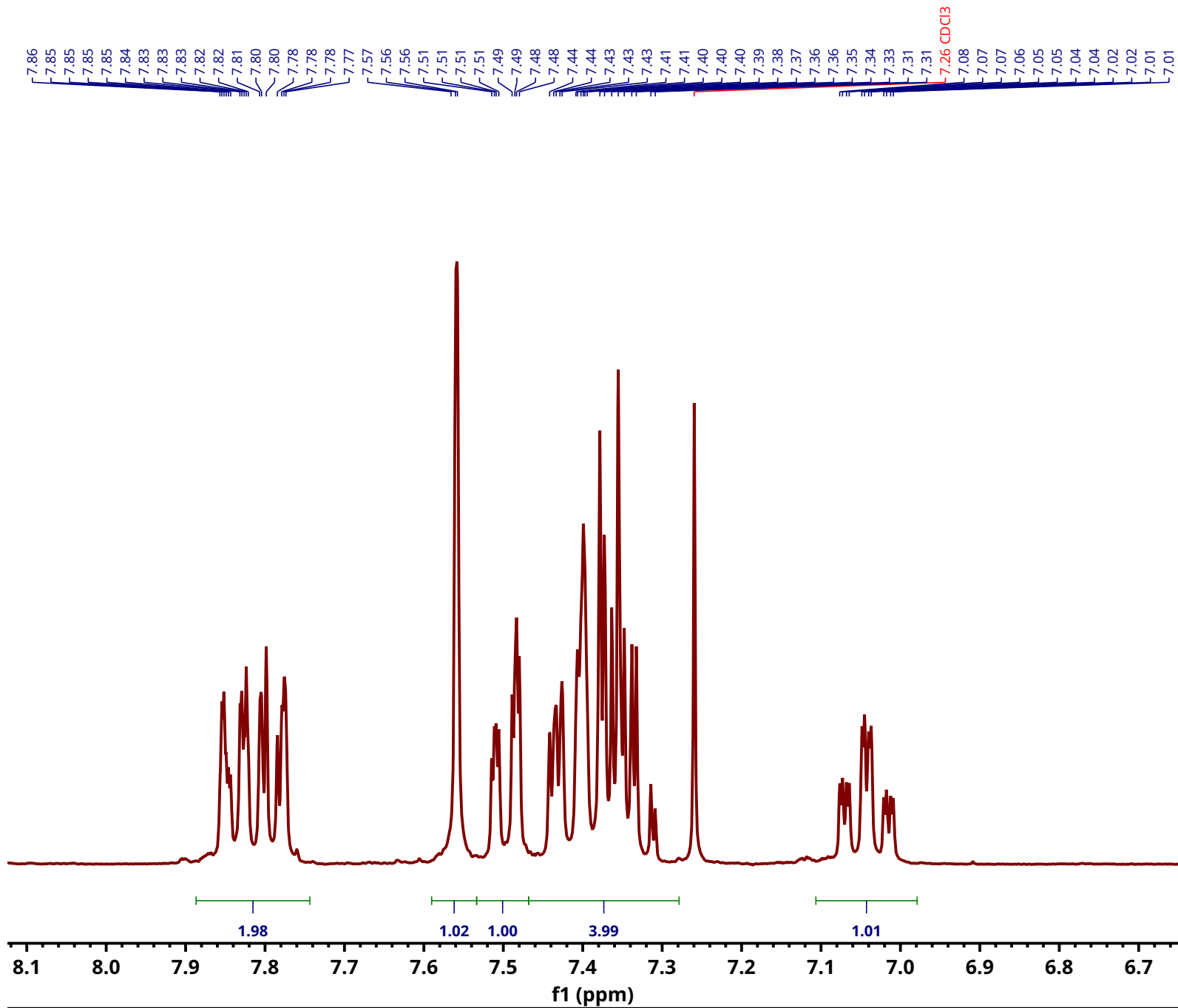


Parameter	Value
1 Title	BK-105.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.6
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	71.8
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-28T15:21:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

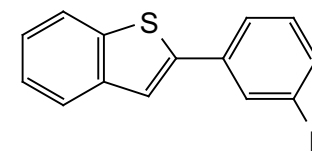


Compound 6h

¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.92 – 7.68 (m, 2H), 7.56 (d, *J*=0.8 Hz, 1H), 7.50 (ddd, *J*=7.8, 1.7, 1.0 Hz, 1H), 7.46 – 7.29 (m, 4H), 7.04 (tdd, *J*=8.3, 2.6, 1.0 Hz, 1H)

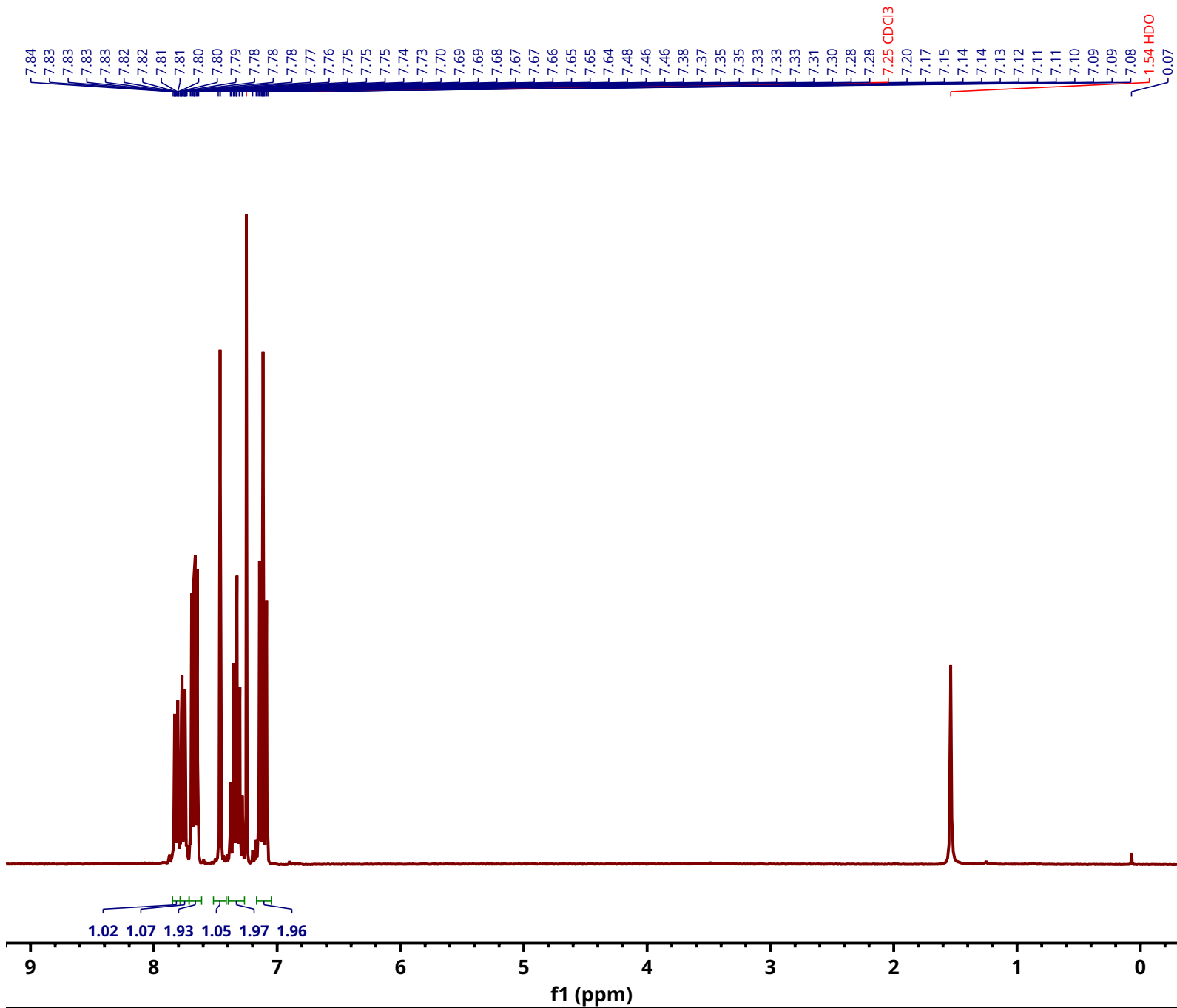


Parameter	Value
1 Title	BK-105.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	298.6
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	71.8
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-06-28T15:21:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

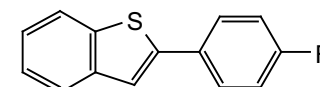


Compound 6h

¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.92 – 7.68 (m, 2H), 7.56 (d, *J*=0.8 Hz, 1H), 7.50 (ddd, *J*=7.8, 1.7, 1.0 Hz, 1H), 7.46 – 7.29 (m, 4H), 7.04 (tdd, *J*=8.3, 2.6, 1.0 Hz, 1H)

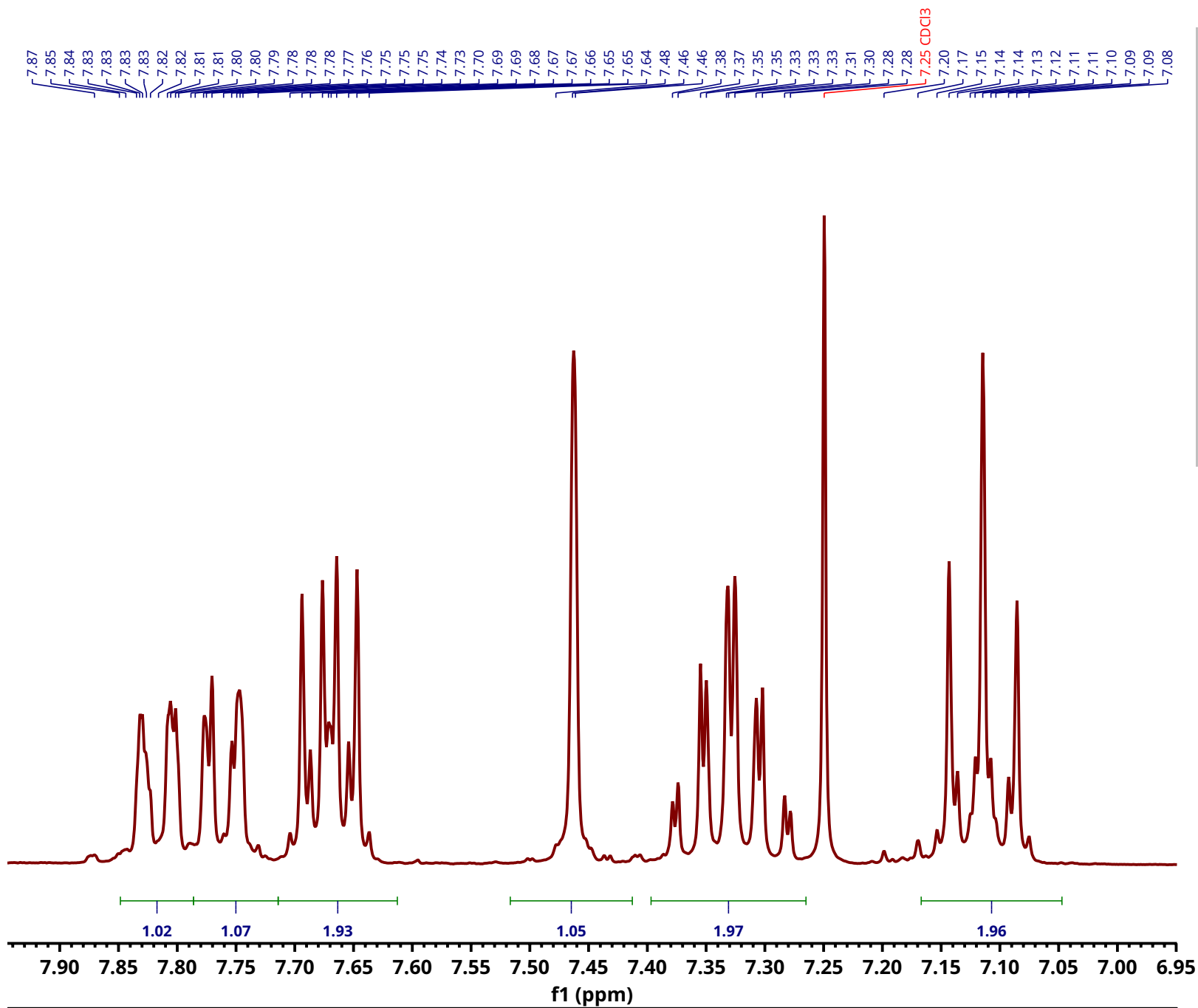


Parameter	Value
Title	PK-901.101.fid
Date	20181002
Time	17.04
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.3
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	256
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

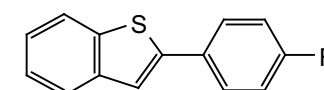


Compound 6i

¹H NMR (300 MHz, Chloroform-*d*) δ 7.82 (ddd, *J* = 7.2, 1.9, 0.8 Hz, 1H), 7.79 – 7.71 (m, 1H), 7.71 – 7.61 (m, 2H), 7.46 (d, *J* = 0.7 Hz, 1H), 7.40 – 7.27 (m, 2H), 7.17 – 7.05 (m, 2H).

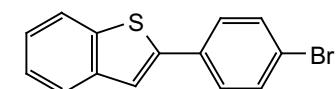
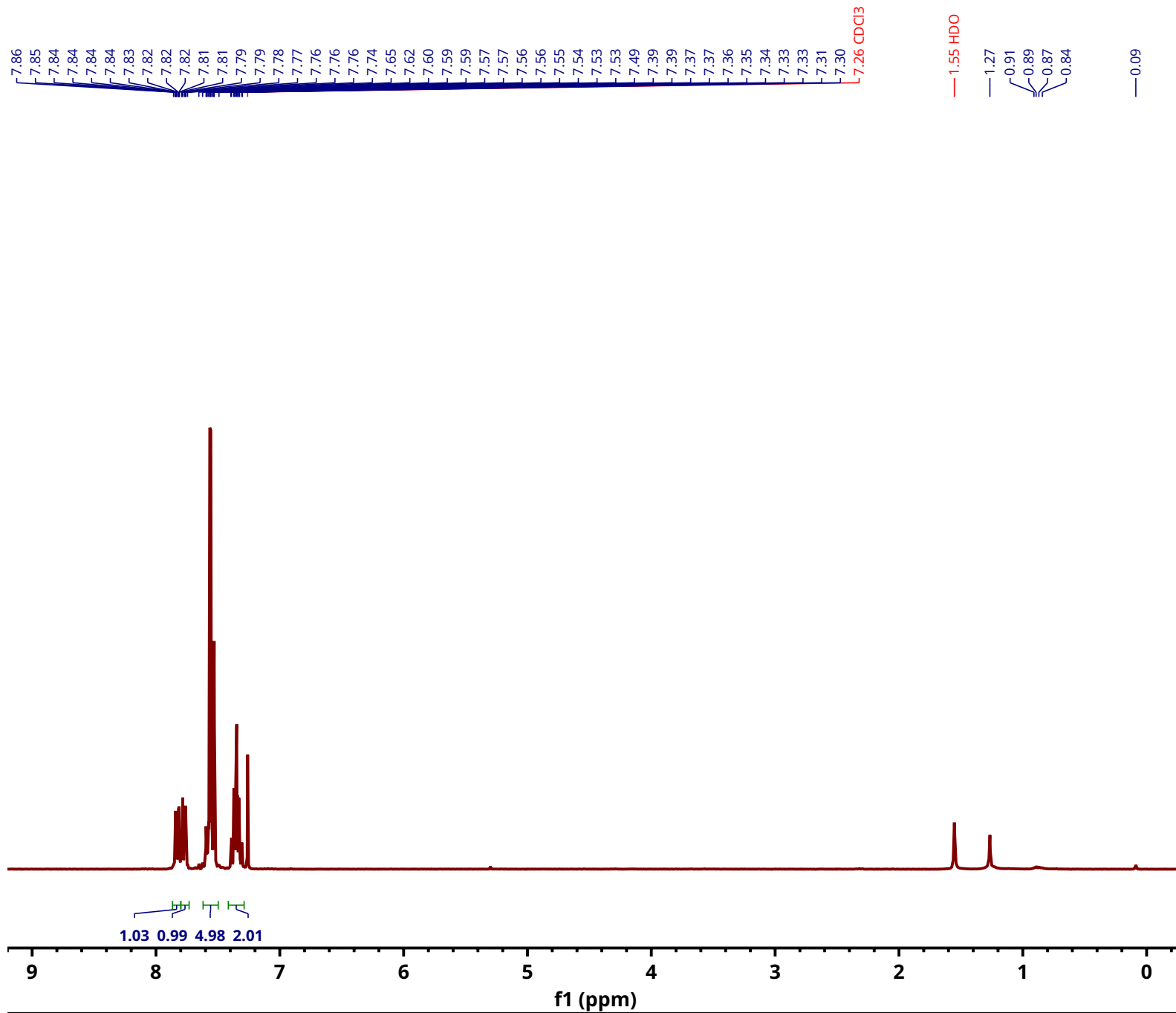


Parameter	Value
Title	PK-901.101.fid
Date	20181002
Time	17.04
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.3
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	256
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536



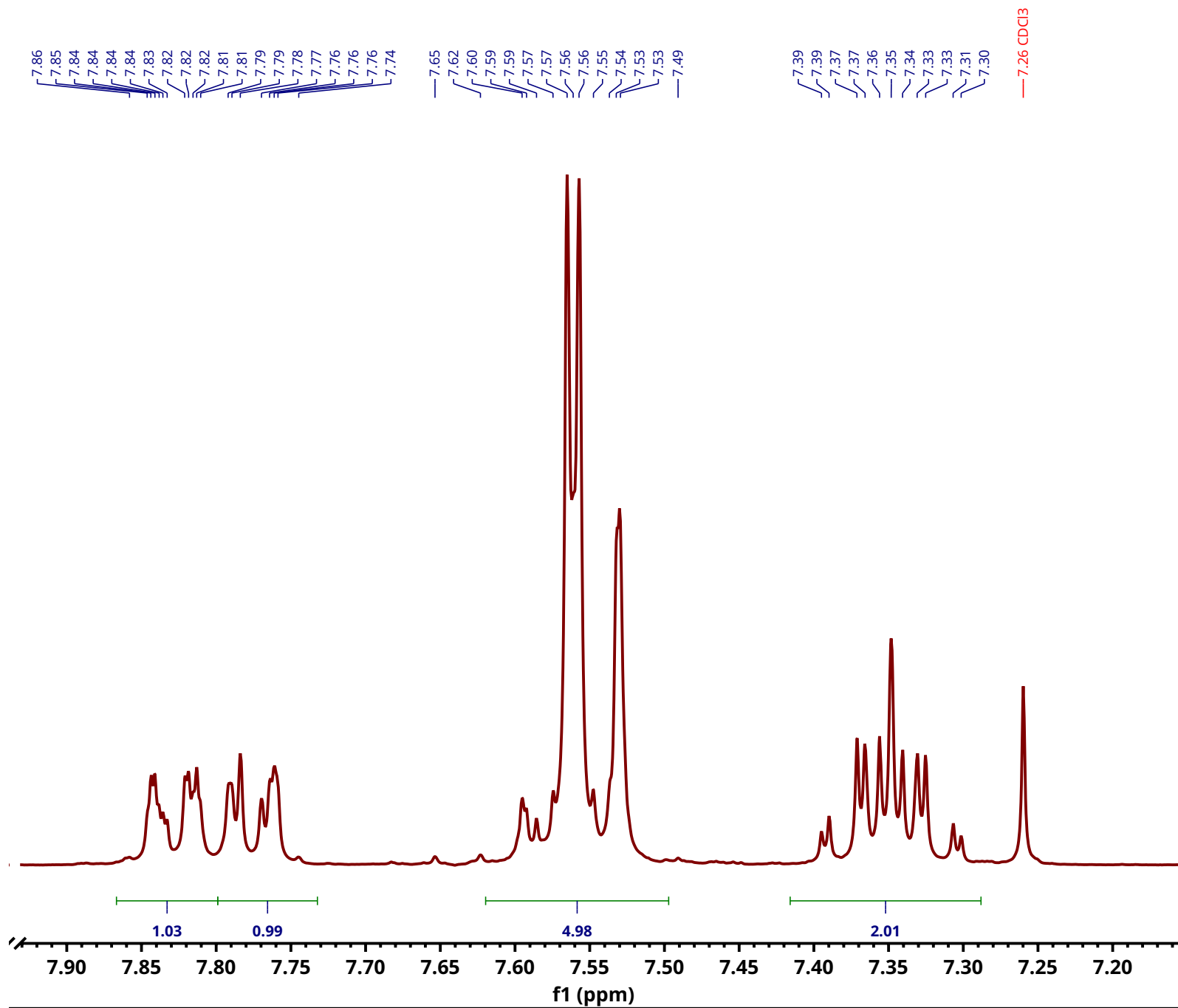
Compound 6i

^1H NMR (300 MHz, Chloroform-*d*) δ 7.82 (ddd, $J = 7.2, 1.9, 0.8$ Hz, 1H), 7.79 – 7.71 (m, 1H), 7.71 – 7.61 (m, 2H), 7.46 (d, $J = 0.7$ Hz, 1H), 7.40 – 7.27 (m, 2H), 7.17 – 7.05 (m, 2H).

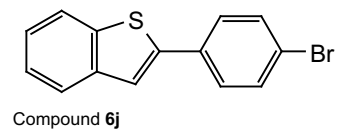


Compound 6j

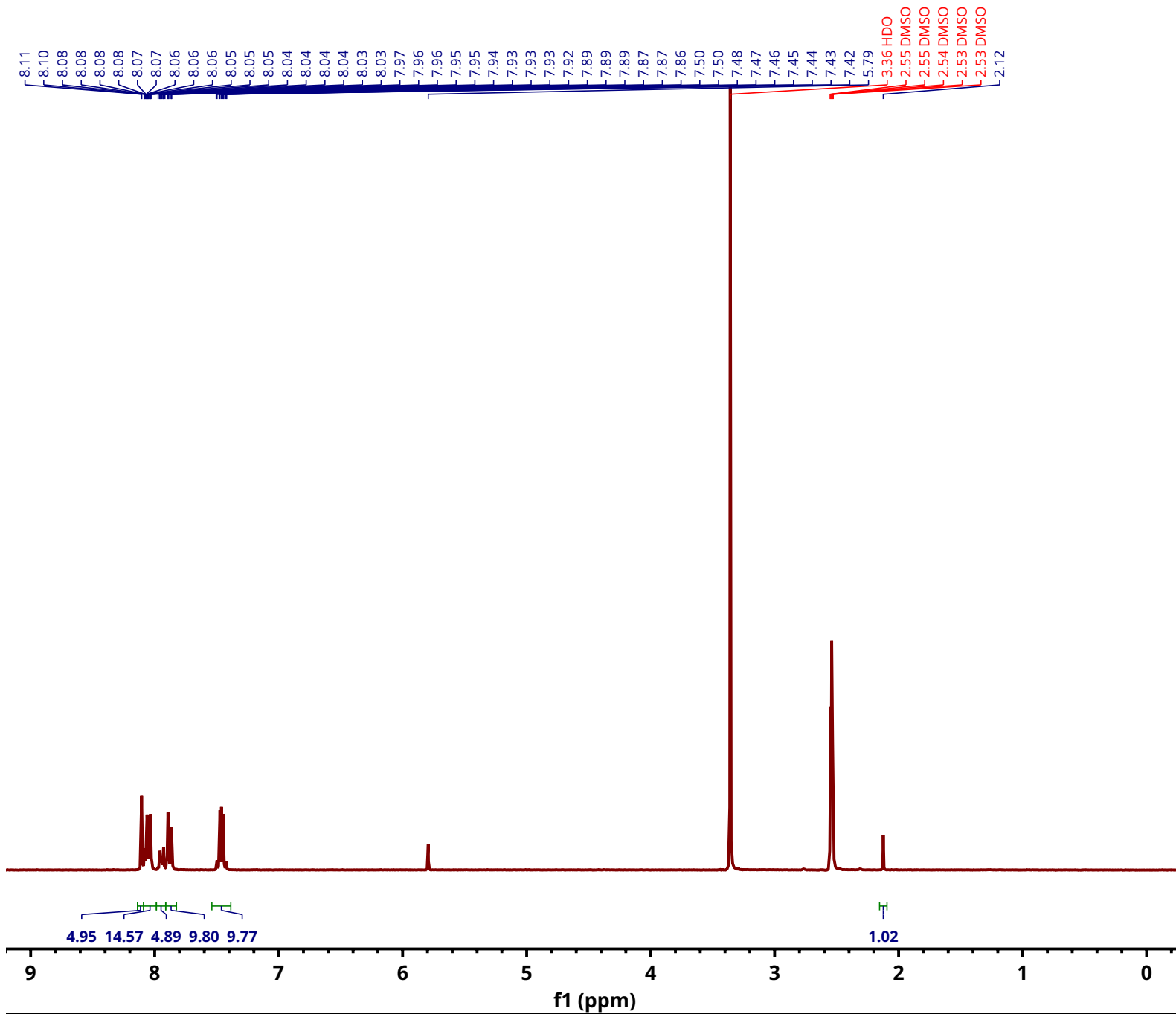
$^1\text{H NMR}$ (Chloroform-*d*, 300 MHz): δ (ppm) 7.87 – 7.81 (m, 1H), 7.80 – 7.74 (m, 1H), 7.62 – 7.49 (m, 5H), 7.42 – 7.29 (m, 2H)



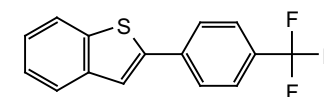
Parameter	Value
1 Title	CCD-076.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.5
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	63.8
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-13T11:06:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536



¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.87 – 7.81 (m, 1H), 7.80 – 7.74 (m, 1H), 7.62 – 7.49 (m, 5H), 7.42 – 7.29 (m, 2H)

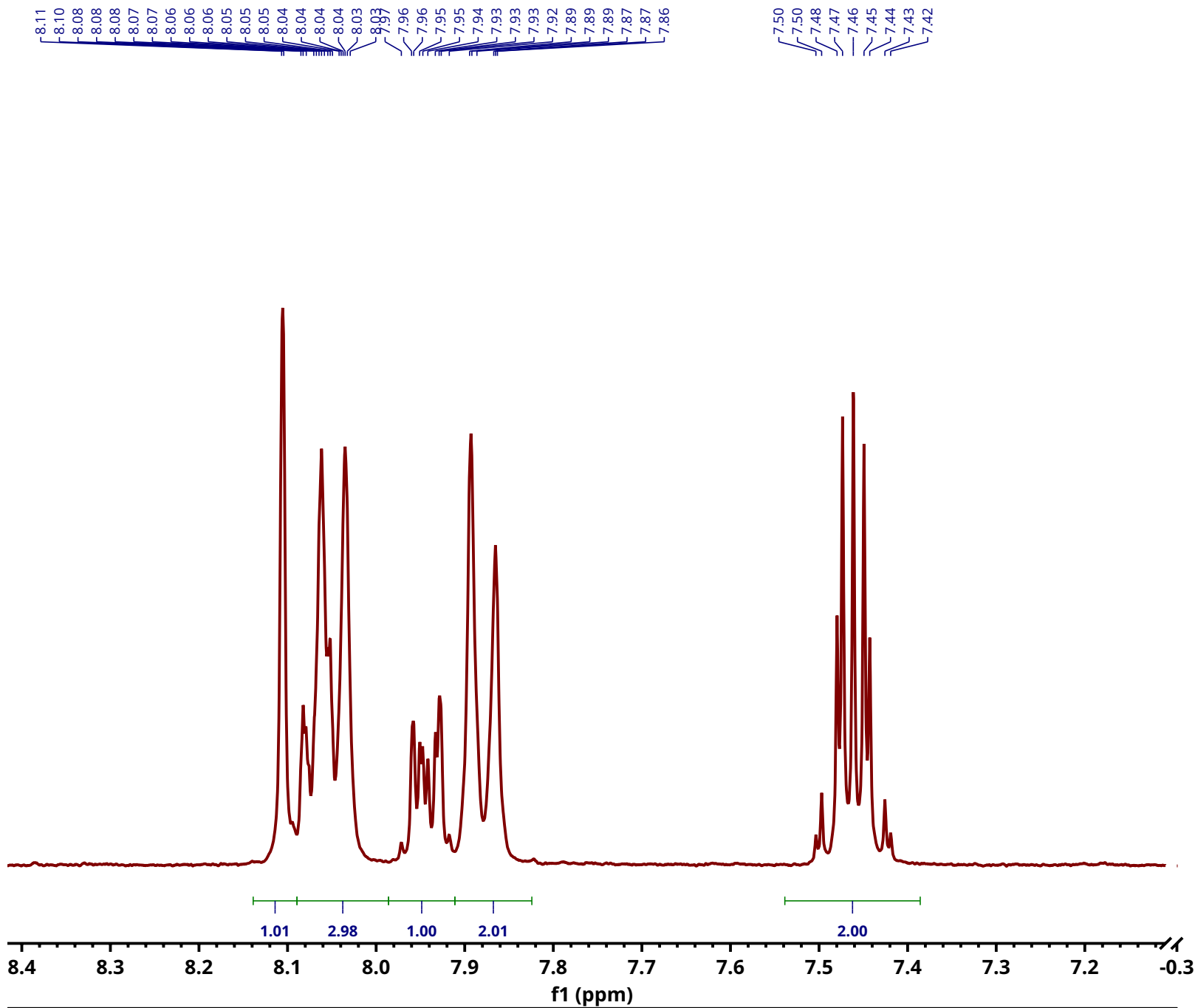


Parameter	Value
1 Title	CCD-083.11.fid
2 Instrument	FOURIER300
3 Solvent	DMSO
4 Temperature	299.6
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	143.0
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-10T16:41:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

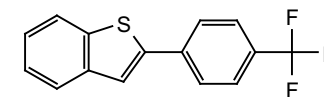


Compound 6k

¹H NMR(DMSO-*d*₆, 300 MHz): δ (ppm) 8.07 (d, *J*=0.7 Hz, 1H), 8.06 – 7.97 (m, 3H), 7.90 (ddt, *J*=7.3, 3.4, 1.7 Hz, 1H), 7.84 (d, *J*=8.4 Hz, 1H), 7.52 – 7.31 (m, 2H)

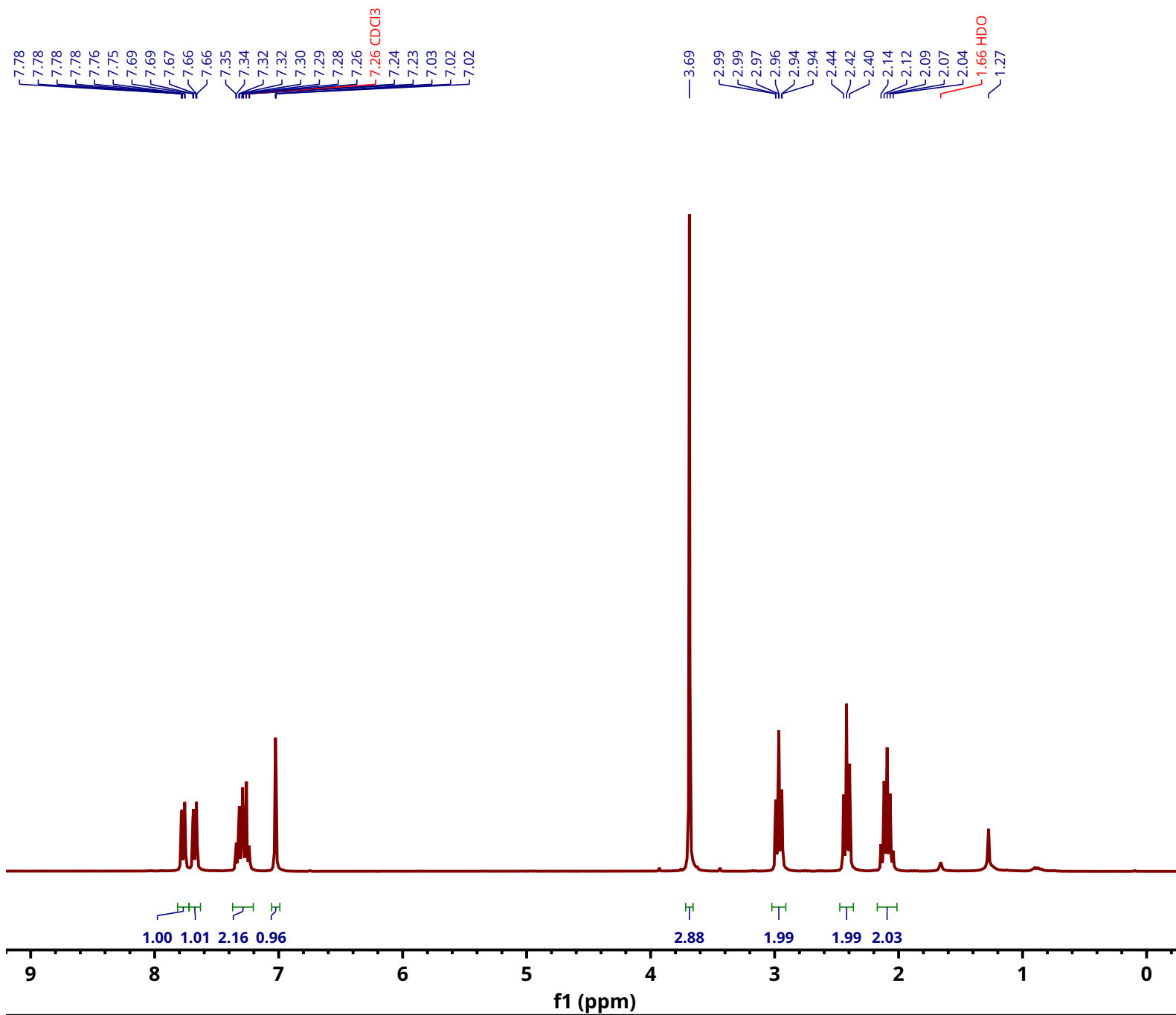


Parameter	Value
1 Title	CCD-083.11.fid
2 Instrument	FOURIER300
3 Solvent	DMSO
4 Temperature	299.6
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	143.0
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-10T16:41:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

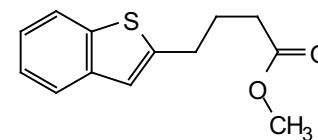


Compound 6k

^1H NMR(DMSO- d_6 , 300 MHz): δ (ppm) 8.07 (d, $J=0.7$ Hz, 1H), 8.06 – 7.97 (m, 3H), 7.90 (ddt, $J=7.3, 3.4, 1.7$ Hz, 1H), 7.84 (d, $J=8.4$ Hz, 1H), 7.52 – 7.31 (m, 2H)

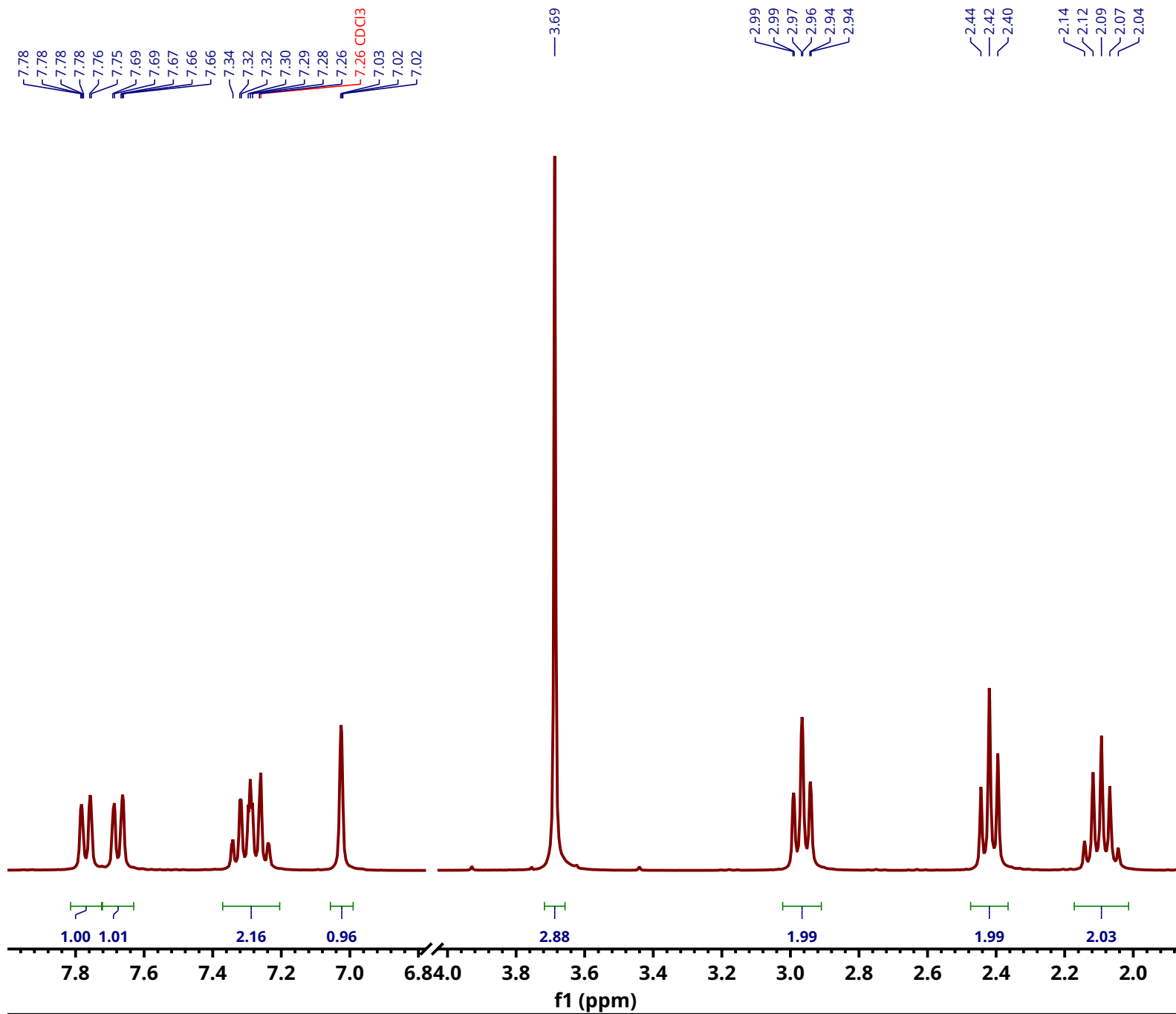


Parameter	Value
1 Title	CCD-085.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl ₃
4 Temperature	299.0
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	20.0
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-10T12:10:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	¹ H
16 Acquired Size	32768
17 Spectral Size	65536

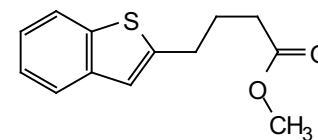


Compound 6l

¹H NMR (Chloroform-*d*, 300 MHz): δ (ppm) 7.77 (dd, *J*=7.8, 1.3 Hz, 1H), 7.68 (dd, *J*=7.4, 1.3 Hz, 1H), 7.37 – 7.20 (m, 2H), 7.03 (d, *J*=1.0 Hz, 1H), 3.69 (s, 3H), 2.97 (td, *J*=7.4, 1.0 Hz, 2H), 2.42 (t, *J*=7.4 Hz, 2H), 2.09 (p, *J*=7.4 Hz, 2H)



Parameter	Value
1 Title	CCD-085.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.0
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	20.0
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-10T12:10:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

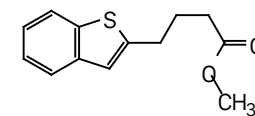
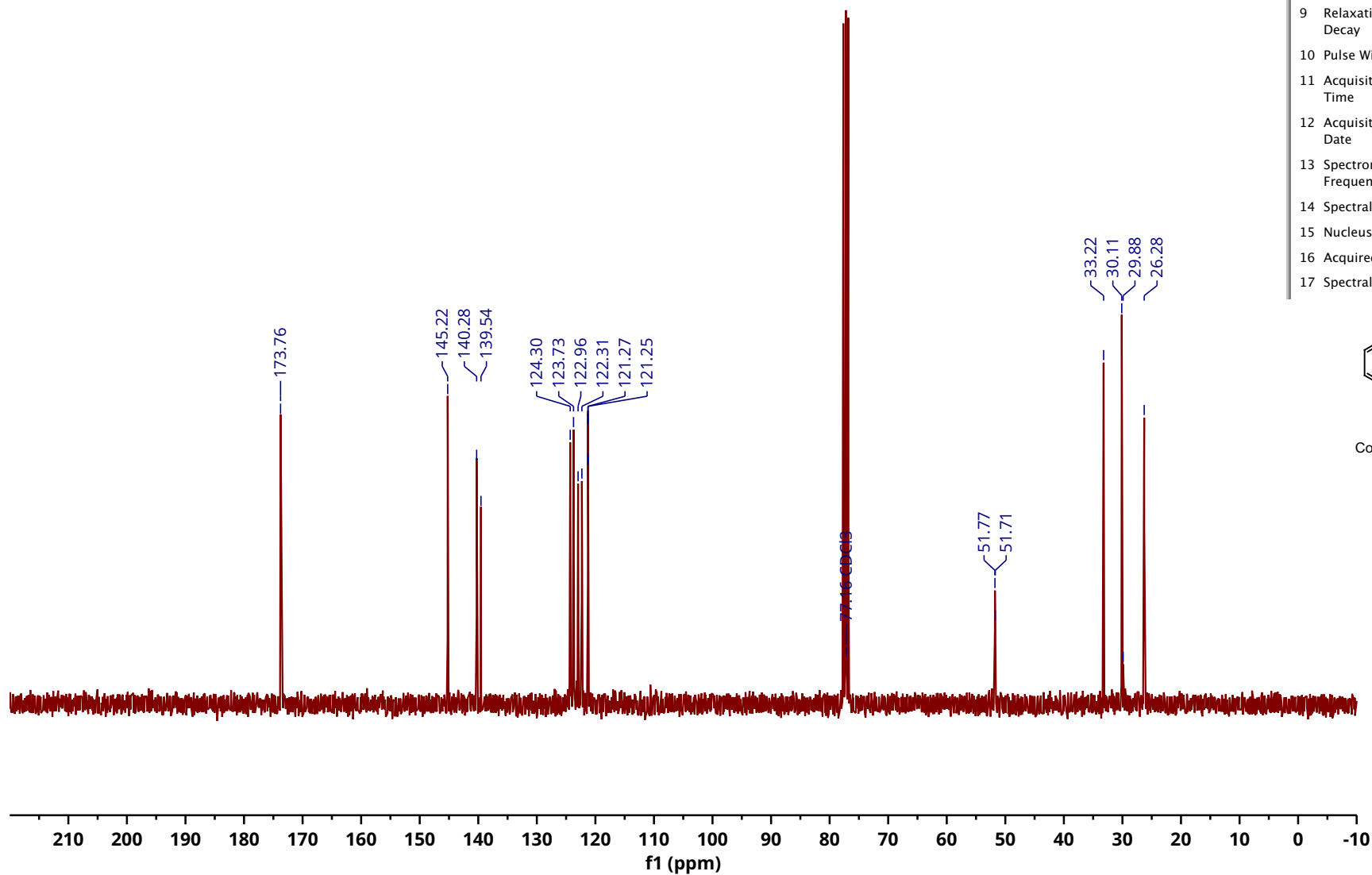


Compound 6I

¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.77 (dd, *J*=7.8, 1.3 Hz, 1H), 7.68 (dd, *J*=7.4, 1.3 Hz, 1H), 7.37 – 7.20 (m, 2H), 7.03 (d, *J*=1.0 Hz, 1H), 3.69 (s, 3H), 2.97 (td, *J*=7.4, 1.0 Hz, 2H), 2.42 (t, *J*=7.4 Hz, 2H), 2.09 (p, *J*=7.4 Hz, 2H)

^{13}C NMR (75 MHz, CDCl_3) δ 173.69, 145.15, 140.21, 139.47, 124.23, 123.66, 122.89, 122.24, 121.21, 121.18, 51.70, 51.64, 33.15, 30.05, 29.81, 26.21.

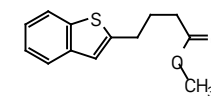
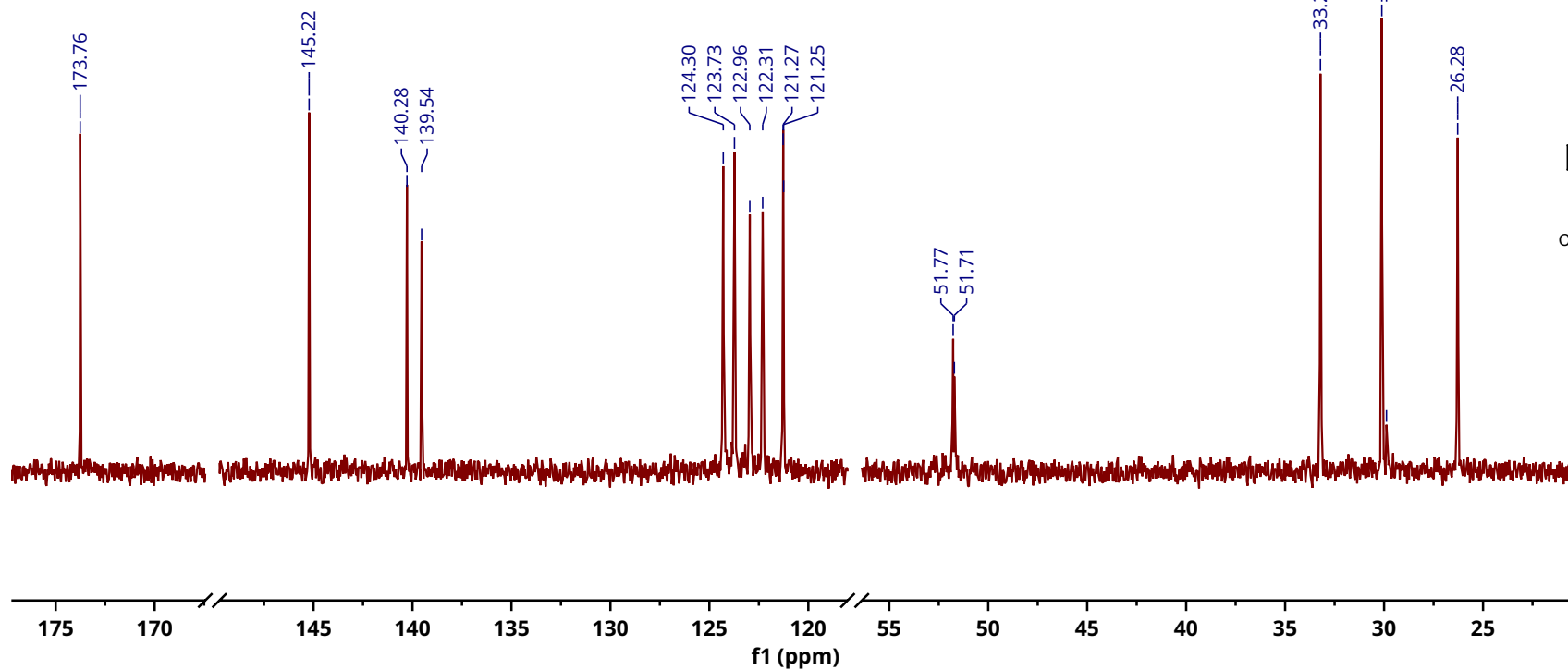
Parameter	Value
1 Title	CCD-093.111.fid
2 Instrument	FOURIER300
3 Solvent	CDCl_3
4 Temperature	299.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	403
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-13T11:24:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	^{13}C
16 Acquired Size	32768
17 Spectral Size	65536



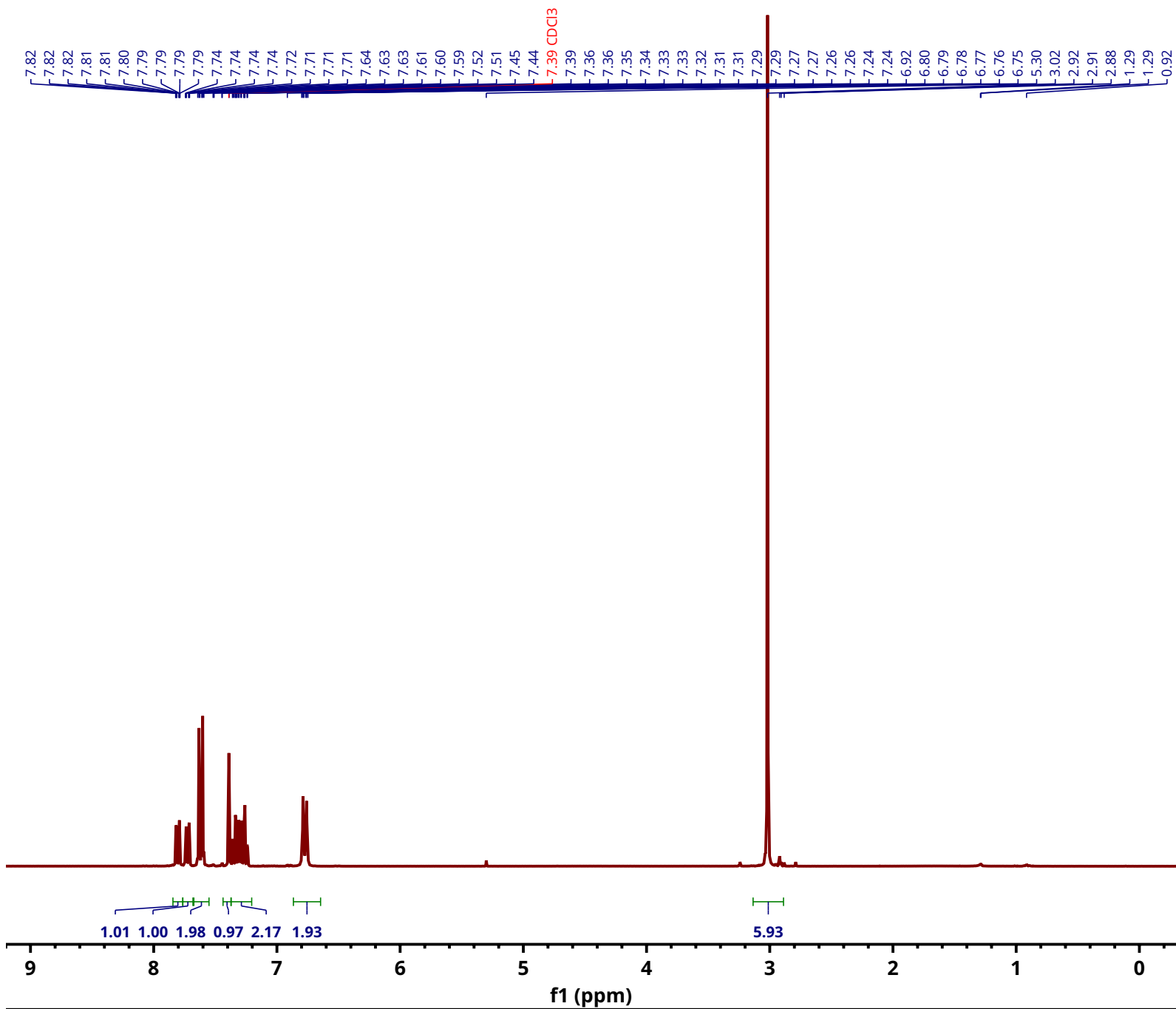
Compound 6I

^{13}C NMR (75 MHz, CDCl_3) δ 173.69, 145.15, 140.21, 139.47, 124.23, 123.66, 122.89, 122.24, 121.21, 121.18, 51.70, 51.64, 33.15, 30.05, 29.81, 26.21.

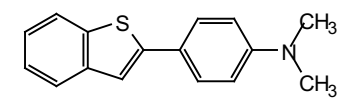
Parameter	Value
1 Title	CCD-093.111.fid
2 Instrument	FOURIER300
3 Solvent	CDCl_3
4 Temperature	299.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Number of Scans	403
8 Receiver Gain	501.2
9 Relaxation Decay	2.0000
10 Pulse Width	11.0000
11 Acquisition Time	1.3422
12 Acquisition Date	2018-07-13T11:24:00
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Nucleus	^{13}C
16 Acquired Size	32768
17 Spectral Size	65536



Compound **6i**

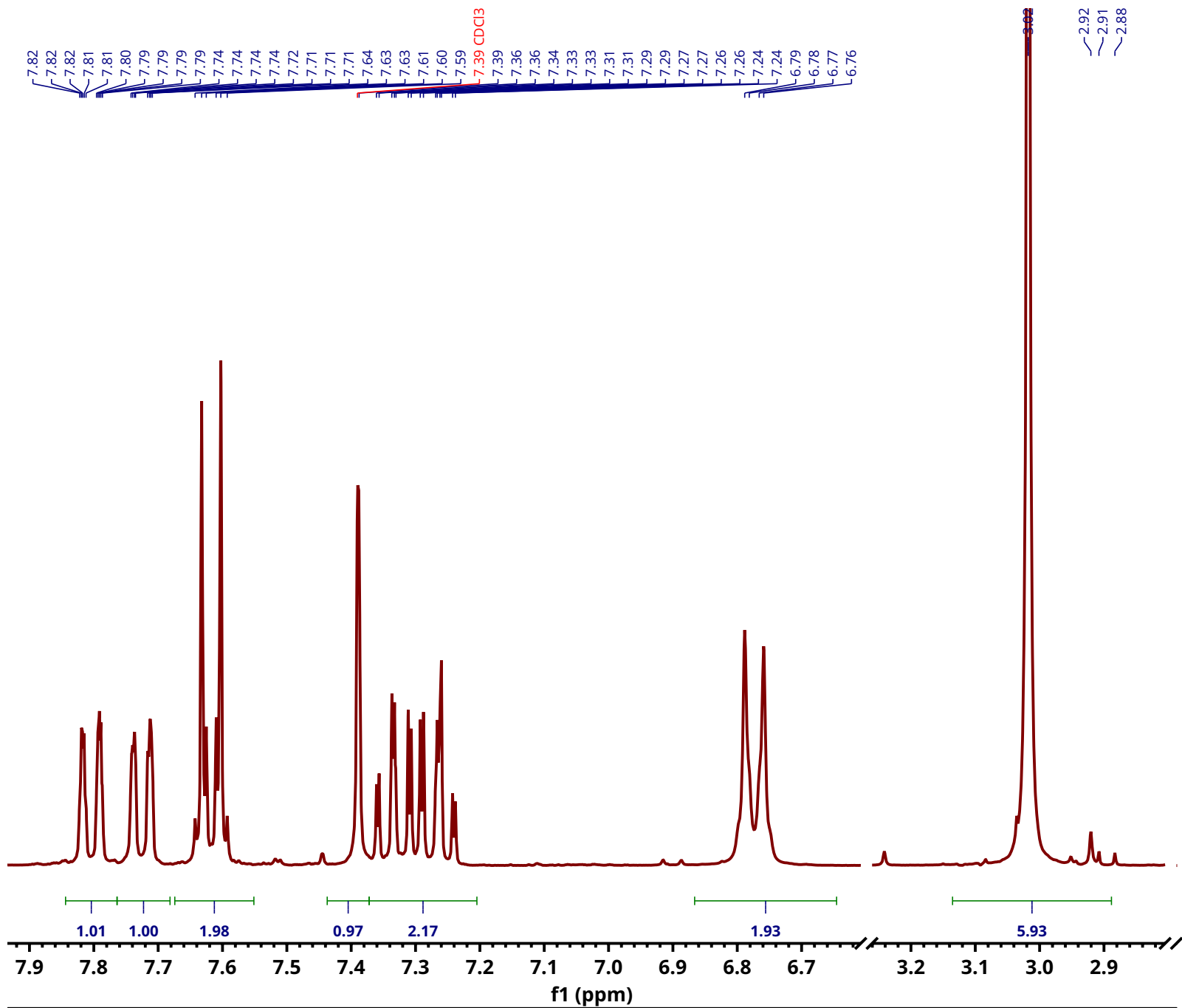


Parameter	Value
Title	BK-115.11.fid
Date	20181012
Time	14.21
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.3
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	64
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

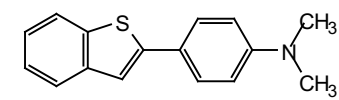


Compound **6m**

¹H NMR (300 MHz, Chloroform-*d*) δ 7.80 (ddt, *J* = 7.7, 1.4, 0.7 Hz, 1H), 7.73 (ddd, *J* = 7.8, 1.5, 0.7 Hz, 1H), 7.67 – 7.55 (m, 2H), 7.39 (s, 1H), 7.37 – 7.20 (m, 2H), 6.87 – 6.65 (m, 2H), 3.02 (s, 6H).

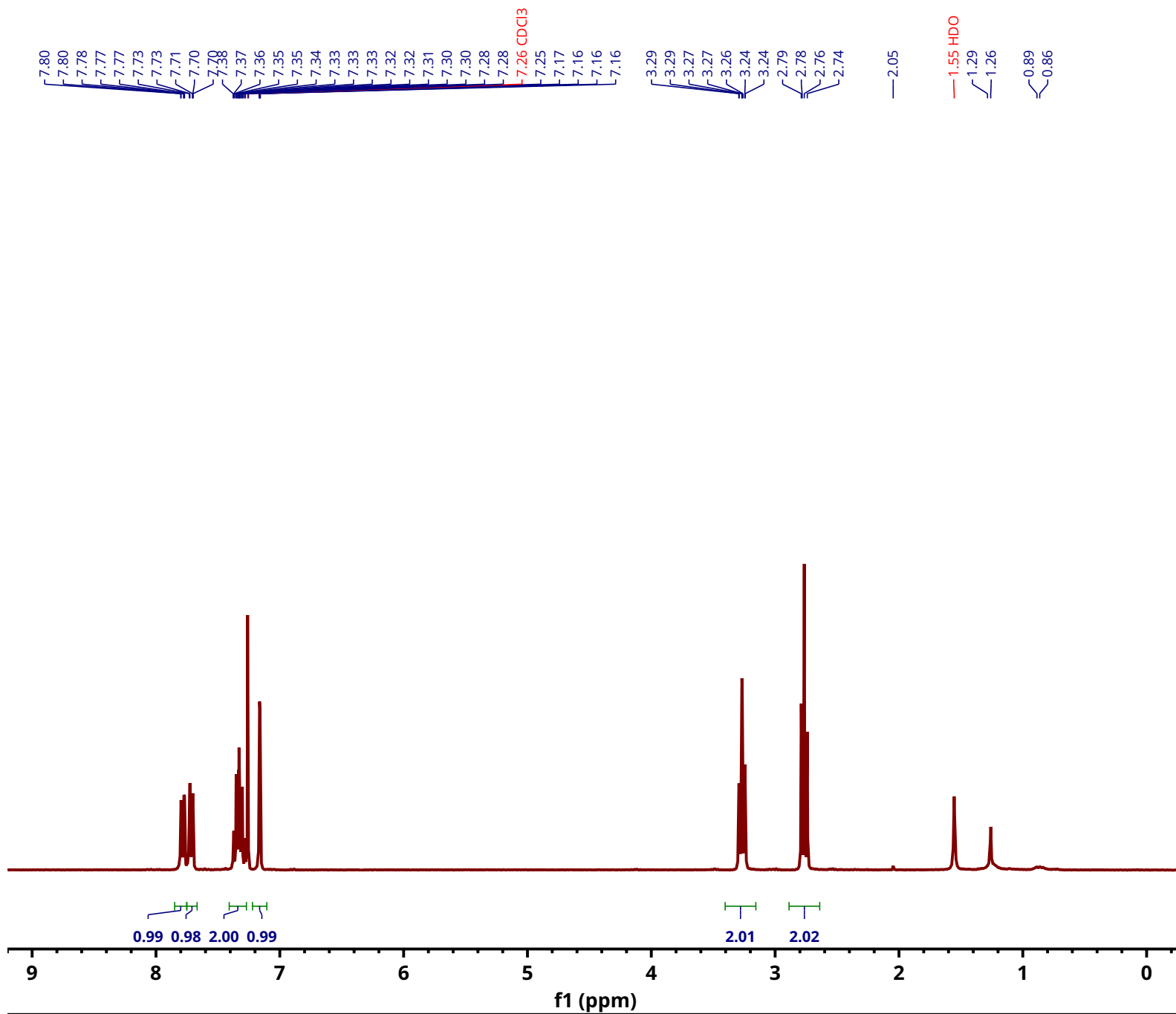


Parameter	Value
Title	BK-115.11.fid
Date	20181012
Time	14.21
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.3
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	64
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536

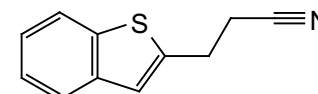


Compound 6m

¹H NMR (300 MHz, Chloroform-*d*) δ 7.80 (ddt, *J* = 7.7, 1.4, 0.7 Hz, 1H), 7.73 (ddd, *J* = 7.8, 1.5, 0.7 Hz, 1H), 7.67 – 7.55 (m, 2H), 7.39 (s, 1H), 7.37 – 7.20 (m, 2H), 6.87 – 6.65 (m, 2H), 3.02 (s, 6H).

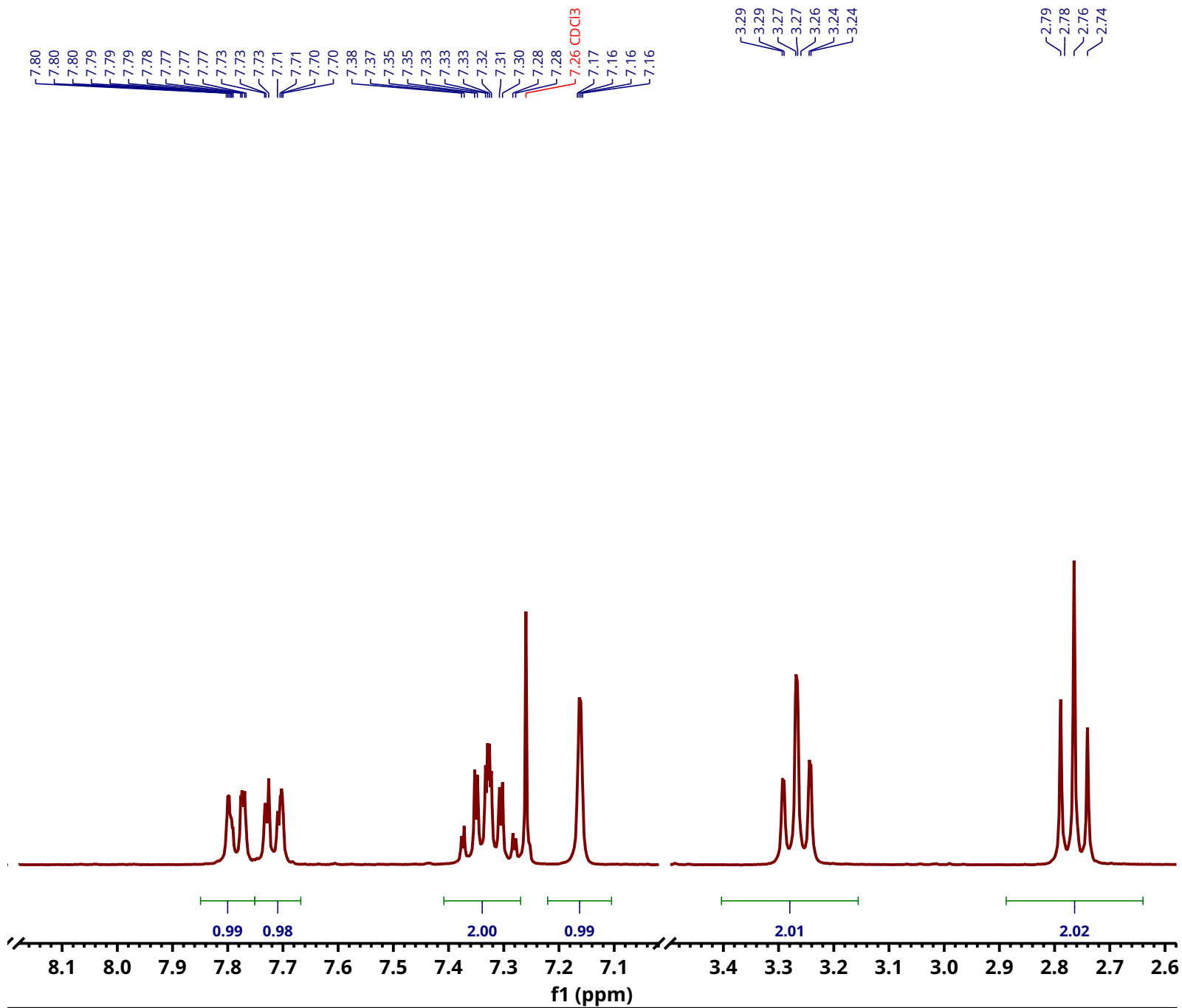


Parameter	Value
1 Title	CCD-091.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	106.8
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-11T15:03:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

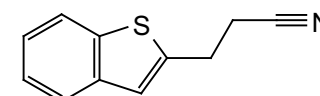


Compound 6n

¹H NMR (Chloroform-*d*, 300 MHz): δ (ppm) 7.83 – 7.75 (m, 1H), 7.75 – 7.67 (m, 1H), 7.41 – 7.23 (m, 3H), 7.16 (q, *J*=1.0 Hz, 1H), 3.27 (td, *J*=7.3, 1.0 Hz, 2H), 2.76 (t, *J*=7.3 Hz, 2H)



Parameter	Value
1 Title	CCD-091.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.9
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	106.8
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-11T15:03:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

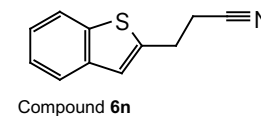
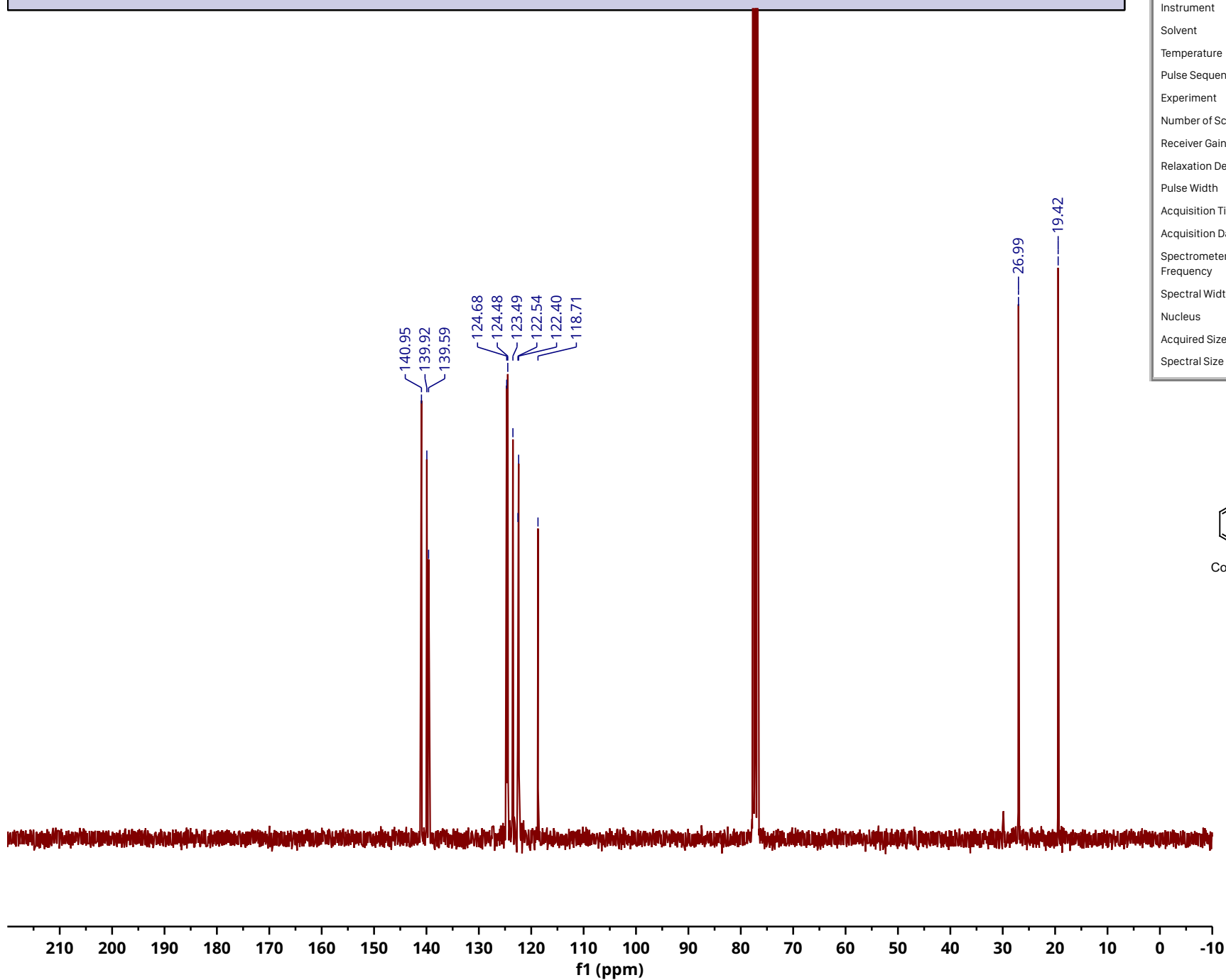


Compound 6n

$^1\text{H NMR}$ (Chloroform-*d*, 300 MHz): δ (ppm) 7.83 – 7.75 (m, 1H), 7.75 – 7.67 (m, 1H), 7.41 – 7.23 (m, 3H), 7.16 (q, $J=1.0$ Hz, 1H), 3.27 (td, $J=7.3, 1.0$ Hz, 2H), 2.76 (t, $J=7.3$ Hz, 2H)

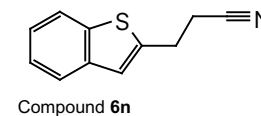
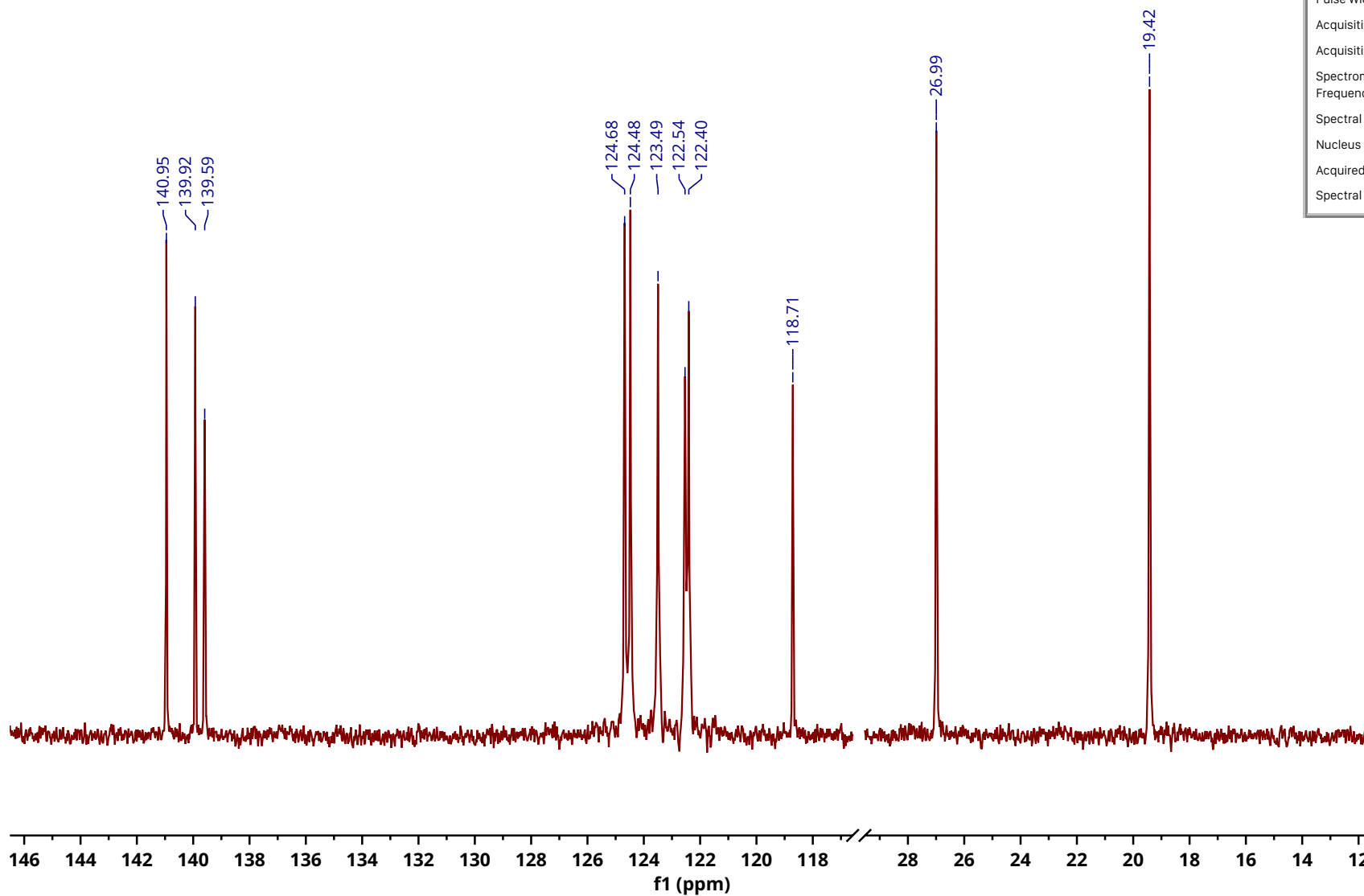
^{13}C NMR(Chloroform-*d*, 75 MHz): δ (ppm) 140.90, 139.87, 139.54, 124.63, 124.42, 123.44, 122.48, 122.35, 118.66, 26.94, 19.37

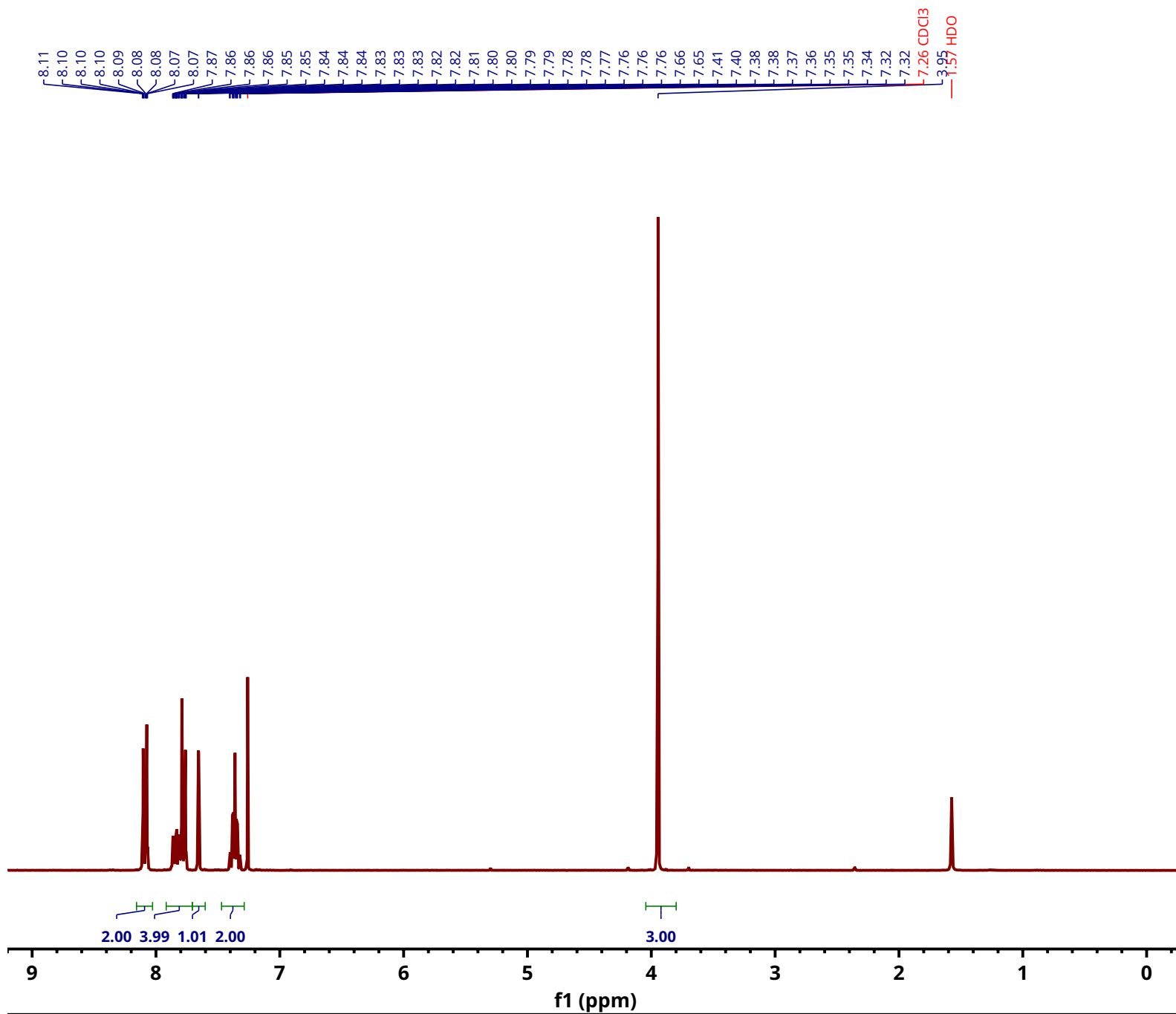
Parameter	Value
Title	CCD-101102.fid
Instrument	FOURIER300
Solvent	CDCl ₃
Temperature	433.8
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	4096
Receiver Gain	501.2
Relaxation Decay	2.0000
Pulse Width	11.0000
Acquisition Time	1.3422
Acquisition Date	2018-07-20T19:06:00
Spectrometer	75.49
Frequency	
Spectral Width	24414.1
Nucleus	^{13}C
Acquired Size	32768
Spectral Size	65536



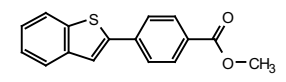
^{13}C NMR(Chloroform-*d*, 75 MHz): δ (ppm) 140.90, 139.87, 139.54, 124.63, 124.42, 123.44, 122.48, 122.35, 118.66, 26.94, 19.37

Parameter	Value
Title	CCD-101102.fid
Instrument	FOURIER300
Solvent	CDCl ₃
Temperature	433.8
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	4096
Receiver Gain	501.2
Relaxation Decay	2.0000
Pulse Width	11.0000
Acquisition Time	1.3422
Acquisition Date	2018-07-20T19:06:00
Spectrometer	75.49
Frequency	
Spectral Width	24414.1
Nucleus	^{13}C
Acquired Size	32768
Spectral Size	65536



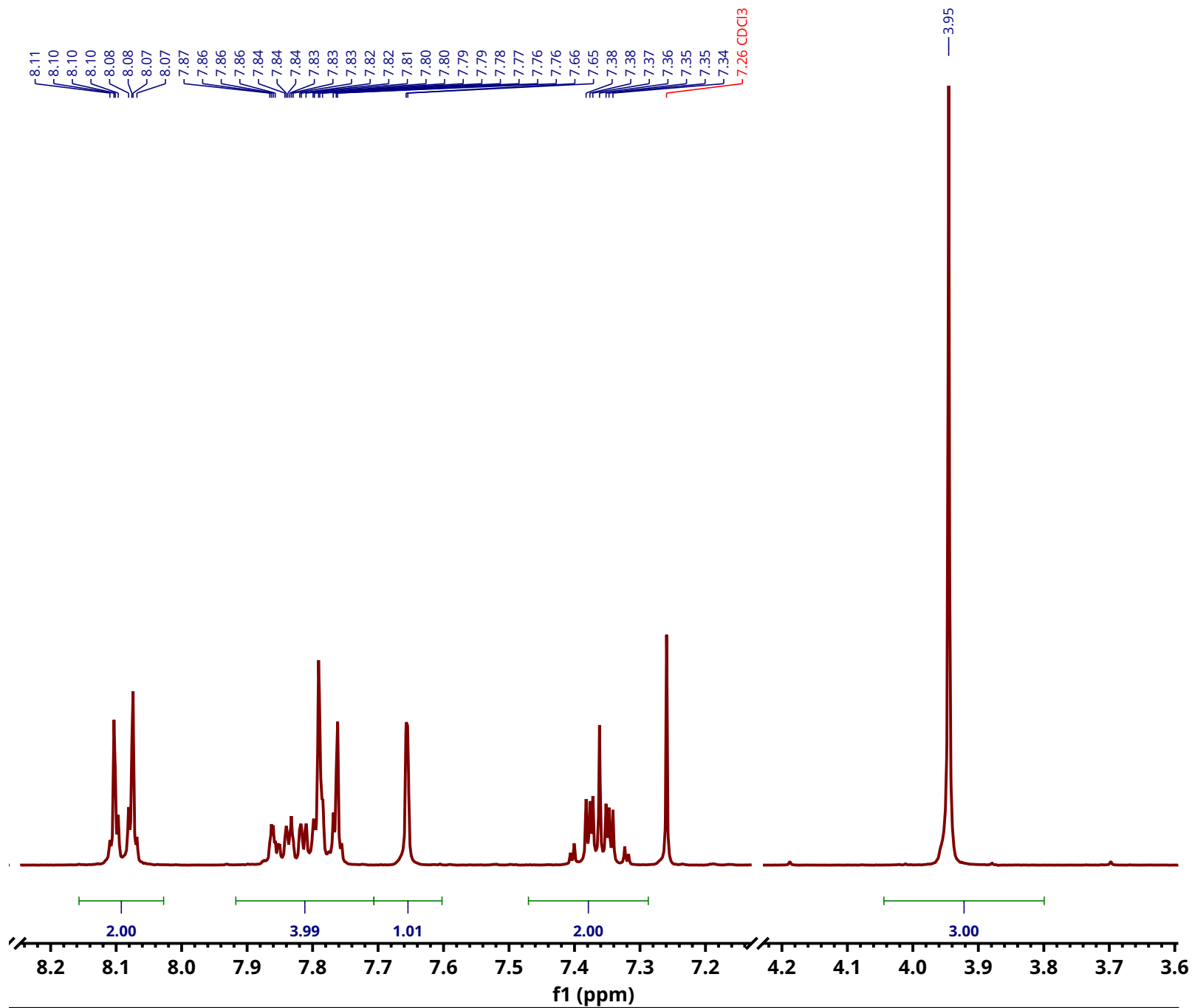


Parameter	Value
Title	BK-118.11.fid
Date	20181022
Time	12.21
Solvent	CDCl ₃
Instrument	FOURIER300
Temperature	297.7
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	64
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	¹ H
TD	32768
SI	65536

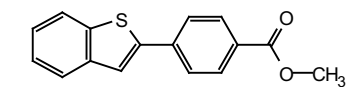


Compound 6o

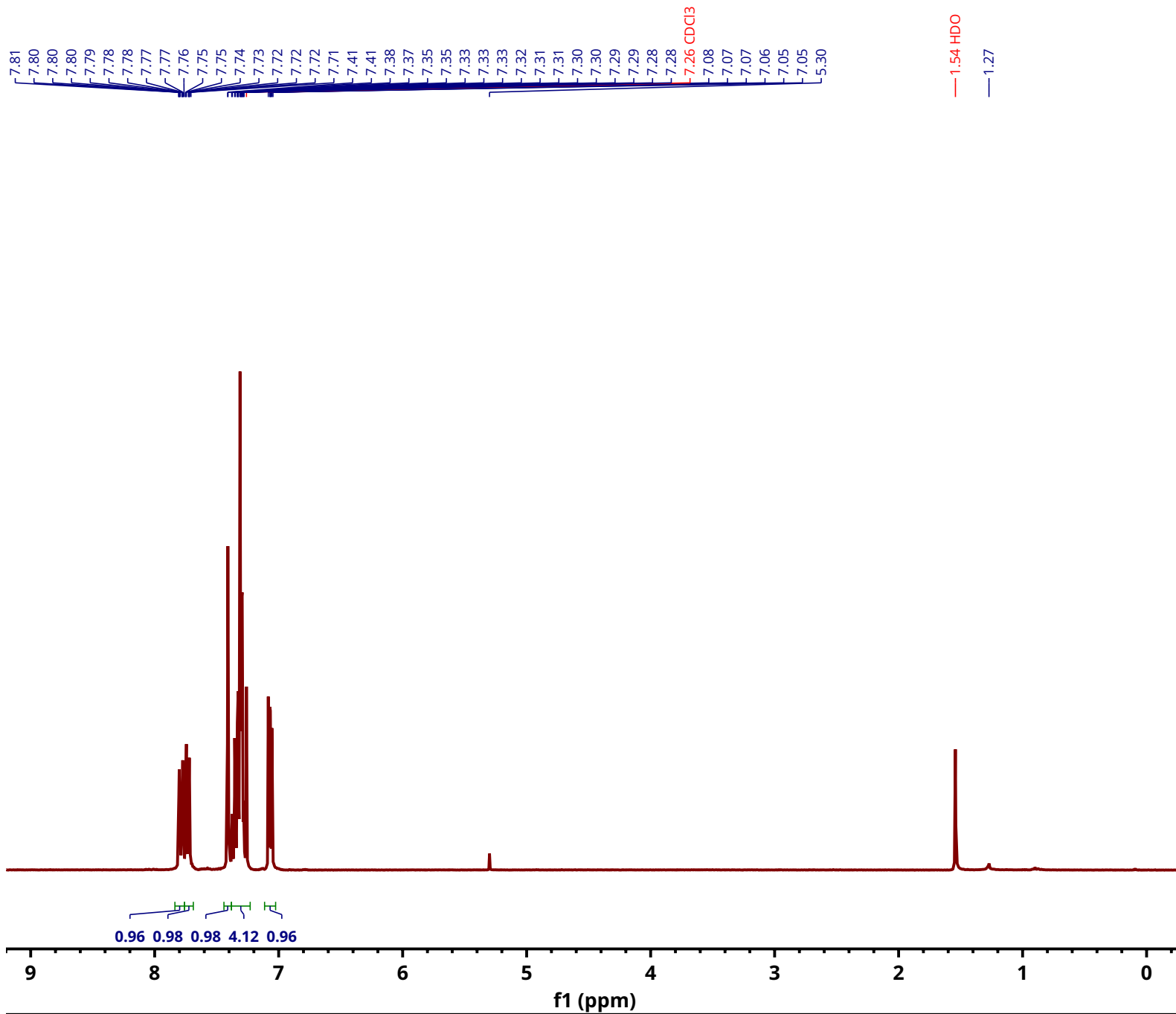
¹H NMR (300 MHz, Chloroform-*d*) δ 8.16 – 8.03 (m, 2H), 7.92 – 7.71 (m, 4H), 7.66 (d, *J* = 0.8 Hz, 1H), 7.47 – 7.29 (m, 2H), 3.95 (s, 3H).



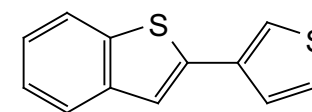
Parameter	Value
Title	BK-118.11.fid
Date	20181022
Time	12.21
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.7
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	64
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536



Compound 6o

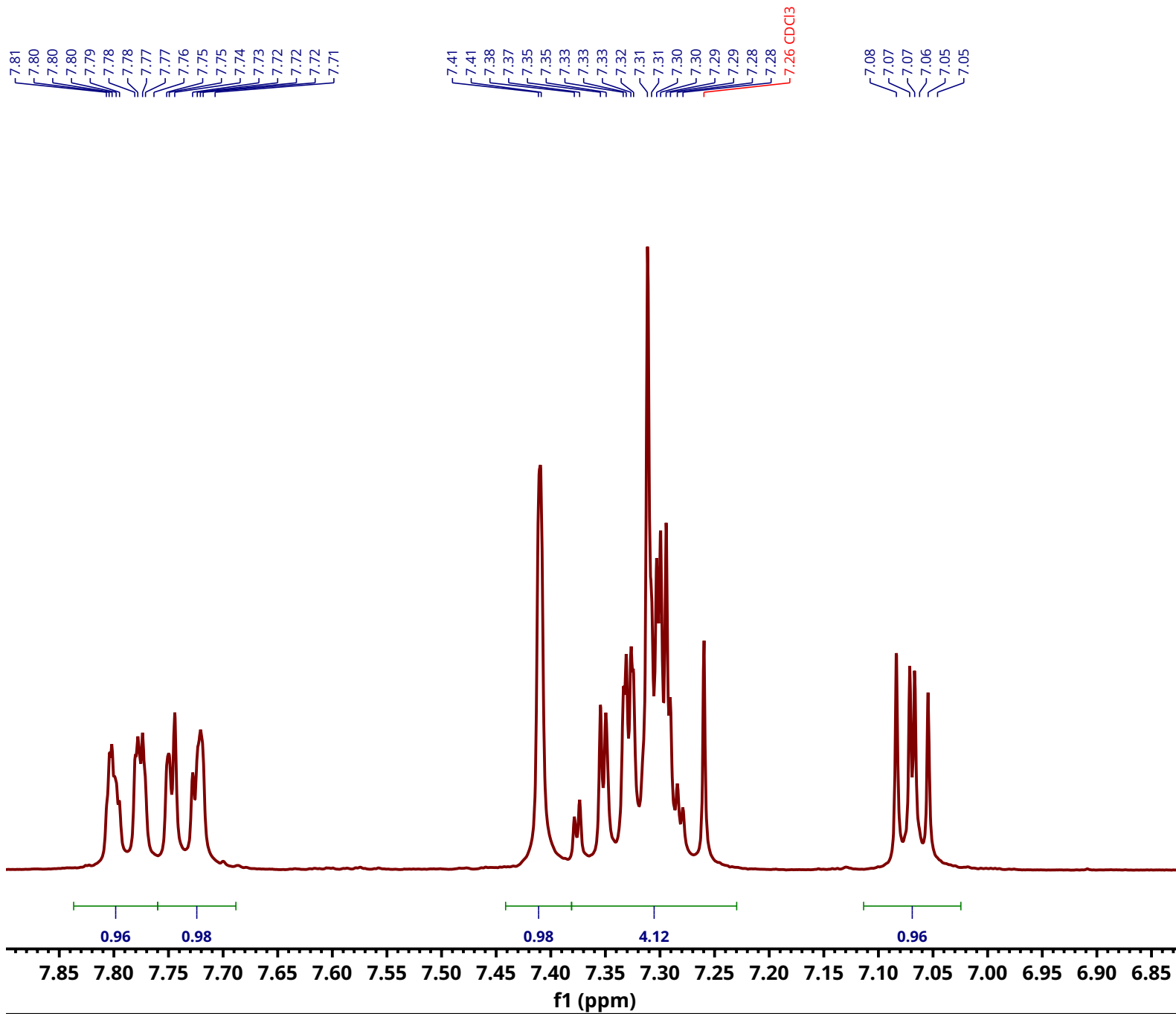


Parameter	Value
1 Title	CCD-090.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.5
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	56.4
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-10T15:21:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

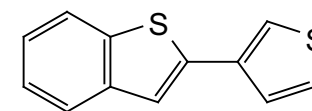


Compound 6p

¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.79 (ddd, *J*=7.1, 2.0, 0.8 Hz, 1H), 7.76 – 7.69 (m, 1H), 7.41 (d, *J*=0.8 Hz, 1H), 7.38 – 7.23 (m, 4H), 7.07 (dd, *J*=5.0, 3.7 Hz, 1H)

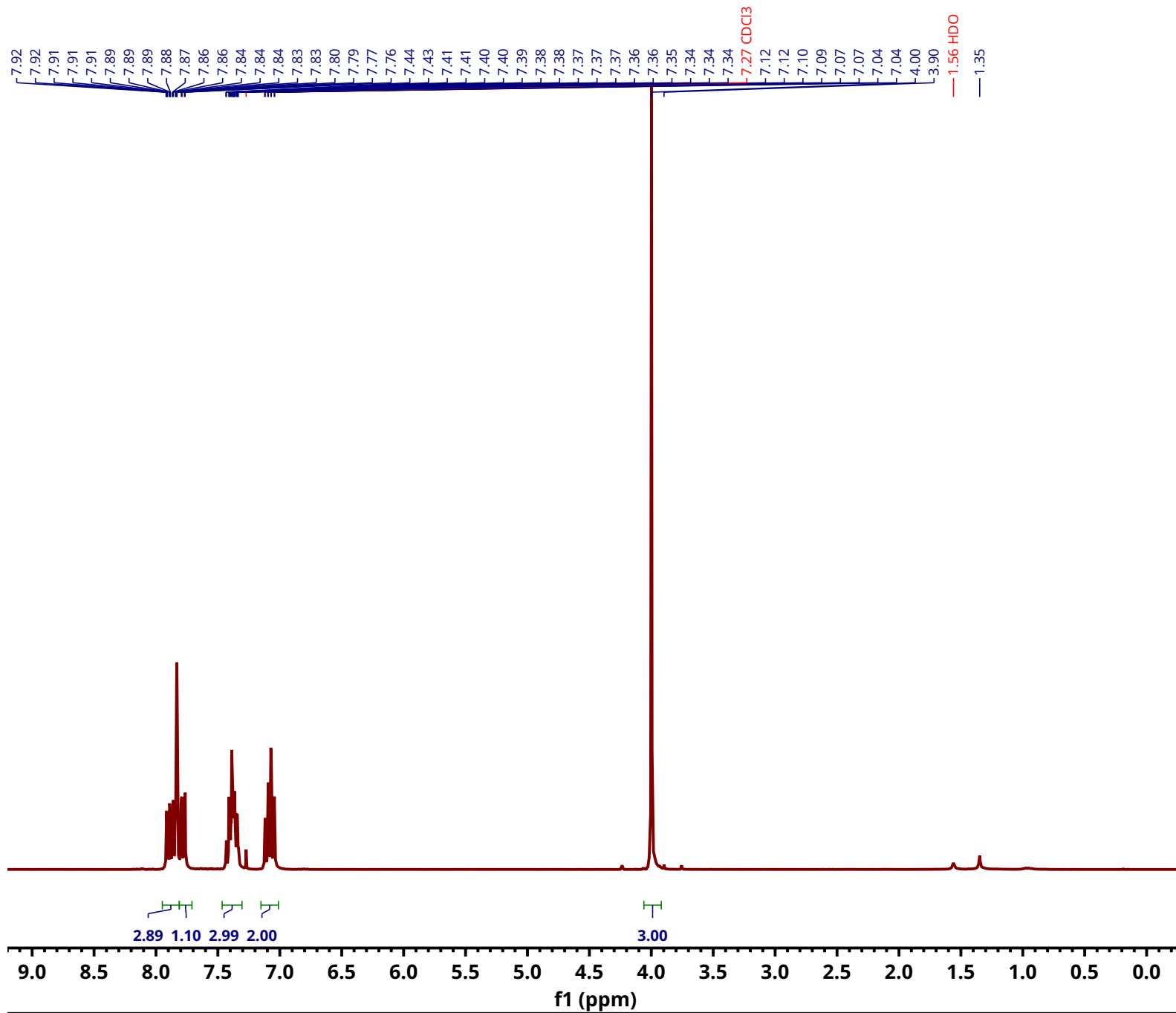


Parameter	Value
1 Title	CCD-090.11.fid
2 Instrument	FOURIER300
3 Solvent	CDCl3
4 Temperature	299.5
5 Pulse Sequence	zg30
6 Experiment	1D
7 Number of Scans	64
8 Receiver Gain	56.4
9 Relaxation Decay	1.0000
10 Pulse Width	10.2000
11 Acquisition Time	5.3687
12 Acquisition Date	2018-07-10T15:21:00
13 Spectrometer Frequency	300.18
14 Spectral Width	6103.5
15 Nucleus	1H
16 Acquired Size	32768
17 Spectral Size	65536

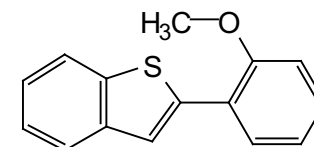


Compound 6p

¹H NMR (Chloroform-*d*, 300 MHz): δ (ppm) 7.79 (ddd, $J=7.1, 2.0, 0.8$ Hz, 1H), 7.76 – 7.69 (m, 1H), 7.41 (d, $J=0.8$ Hz, 1H), 7.38 – 7.23 (m, 4H), 7.07 (dd, $J=5.0, 3.7$ Hz, 1H)

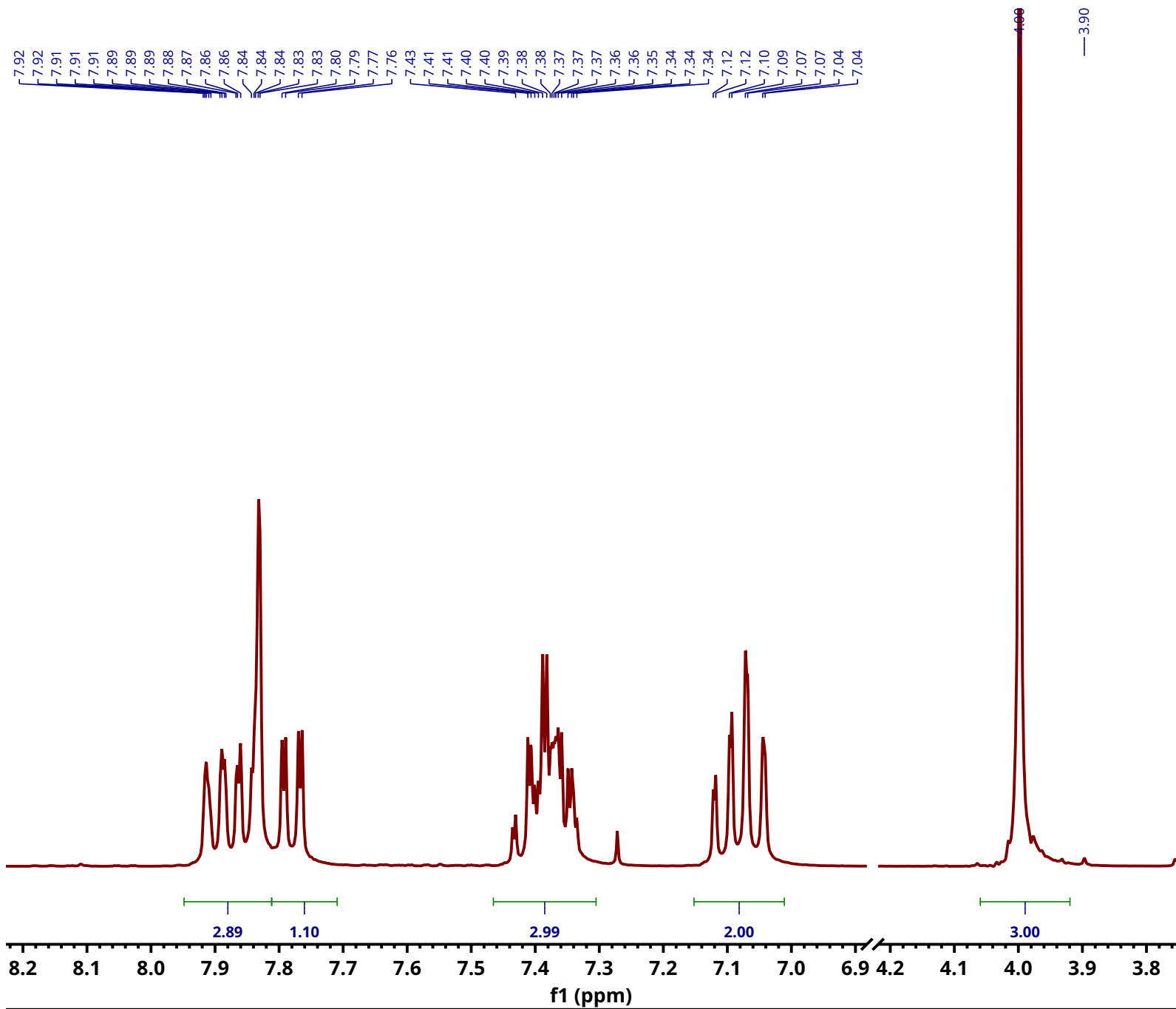


Parameter	Value
1 Title	CCD-102.11.fid
2 Date	20180719
3 Time	14.14
4 Solvent	CDCl3
5 Instrument	FOURIER300
6 Temperature	300.2
7 PULPROG	zg30
8 Experiment	1D
9 Probe	5 mm DUL 13C-1
10 NS	64
11 D1	1.0000
12 P1	10.2000
13 SF	300.18
14 SW	6103.5
15 Nucleus	1H
16 TD	32768
17 SI	65536

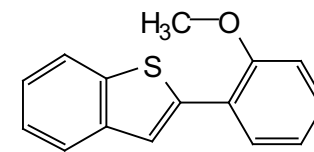


Compound 6r

¹H NMR(Chloroform-*d*, 300 MHz): δ (ppm) 7.97 – 7.80 (m, 3H), 7.77 (dd, *J*=7.7, 1.7 Hz, 1H), 7.45 – 7.29 (m, 3H), 7.10 (dd, *J*=7.5, 1.2 Hz, 1H), 7.04 (dd, *J*=8.2, 1.1 Hz, 1H), 3.99 (s, 3H)



Parameter	Value
1 Title	CCD-102.11.fid
2 Date	20180719
3 Time	14.14
4 Solvent	CDCl3
5 Instrument	FOURIER300
6 Temperature	300.2
7 PULPROG	zg30
8 Experiment	1D
9 Probe	5 mm DUL 13C-1
10 NS	64
11 D1	1.0000
12 P1	10.2000
13 SF	300.18
14 SW	6103.5
15 Nucleus	1H
16 TD	32768
17 SI	65536

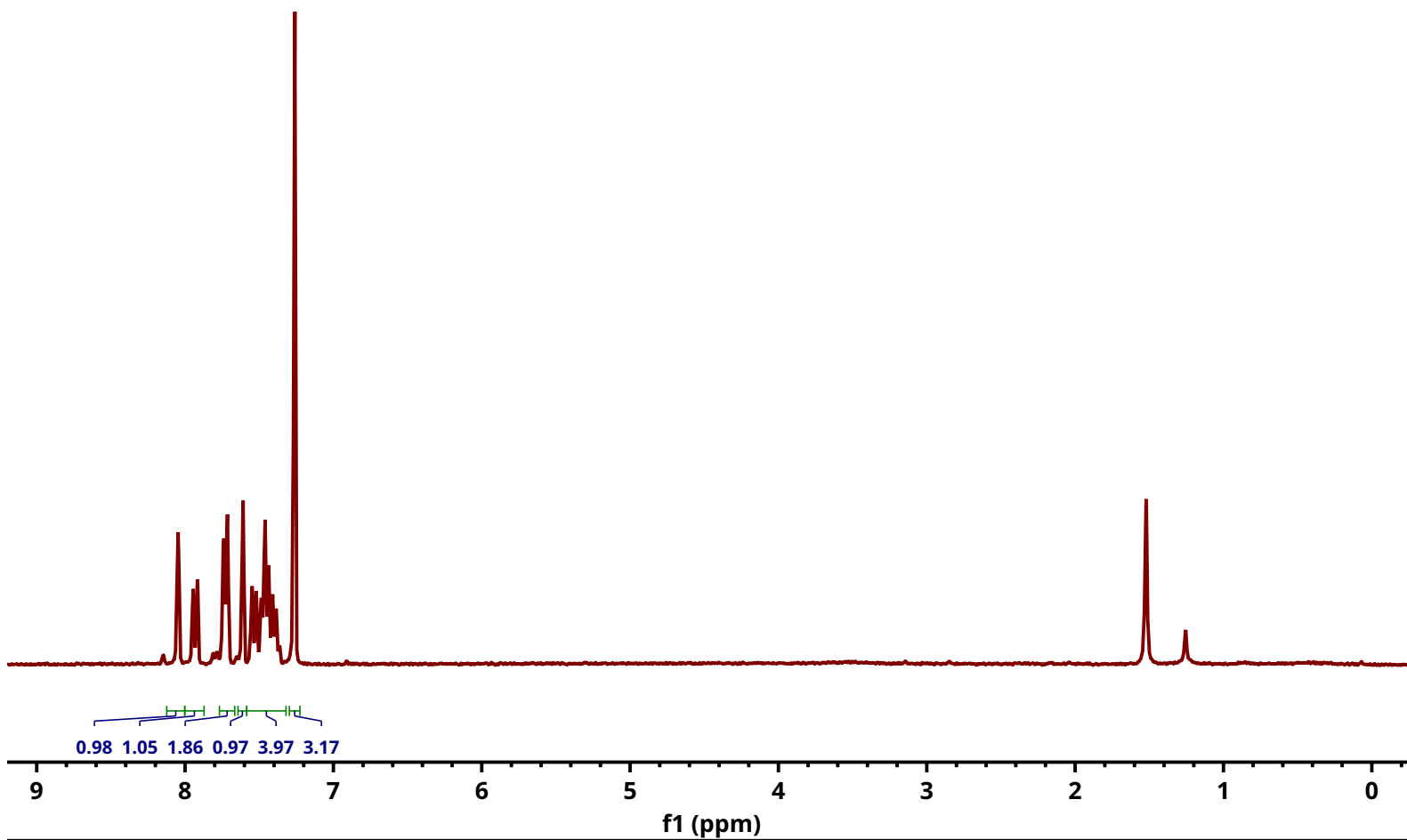


Compound 6r

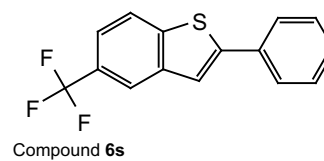
¹H NMR (Chloroform-*d*, 300 MHz): δ (ppm) 7.97 – 7.80 (m, 3H), 7.77 (dd, *J*=7.7, 1.7 Hz, 1H), 7.45 – 7.29 (m, 3H), 7.10 (dd, *J*=7.5, 1.2 Hz, 1H), 7.04 (dd, *J*=8.2, 1.1 Hz, 1H), 3.99 (s, 3H)

8.15
8.05
7.94
7.92
7.81
7.78
7.74
7.74
7.72
7.71
7.71
7.65
7.61
7.61
7.55
7.52
7.49
7.46
7.44
7.41
7.41
7.39
7.37
7.36
7.27
7.26 CDCl₃
7.26

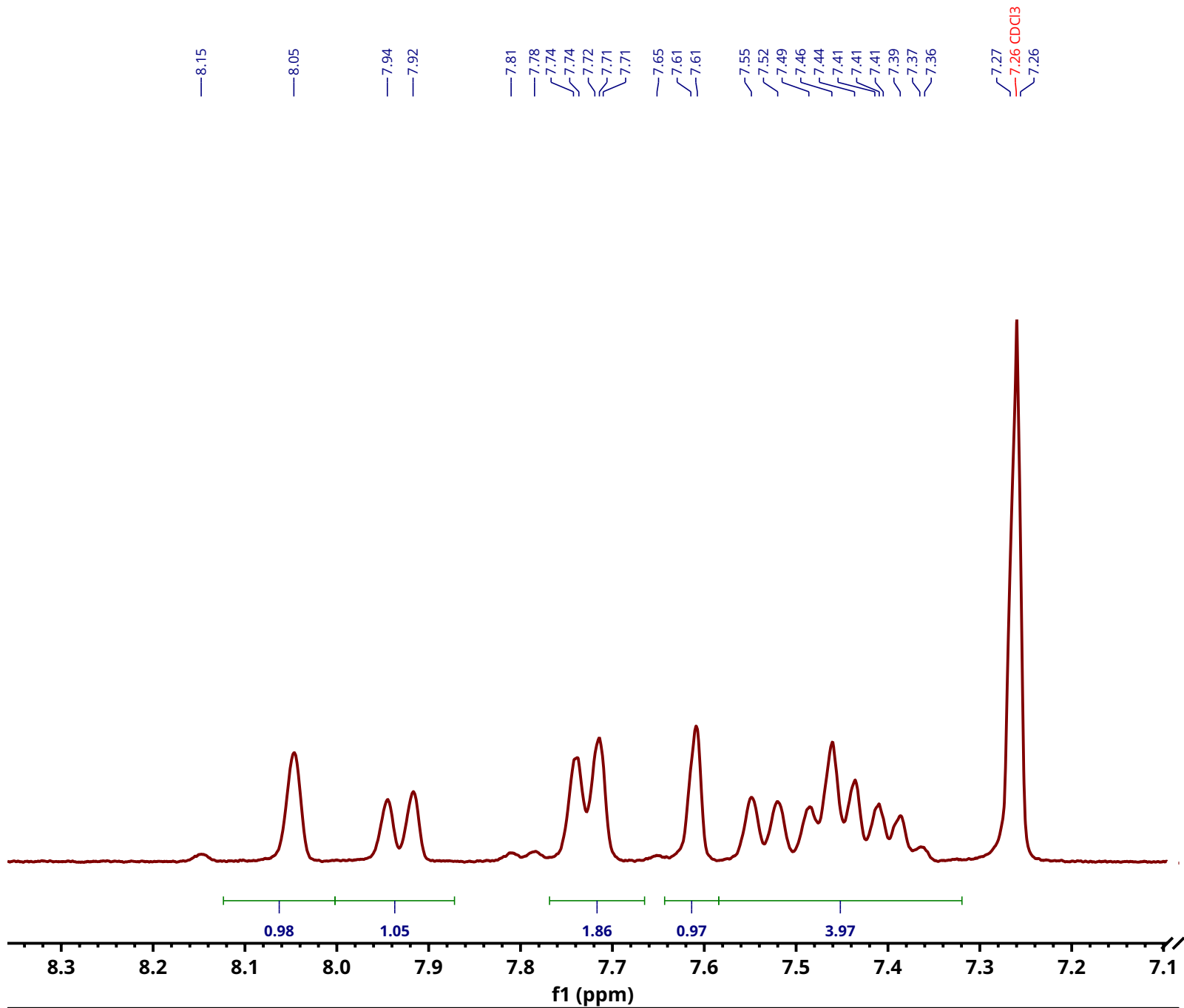
1.52 H₂O
1.25



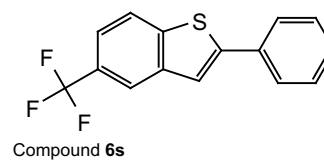
Parameter	Value
Title	MS-099.11.fid
Date	20181019
Time	14.01
Solvent	CDCl ₃
Instrument	FOURIER300
Temperature	297.6
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	128
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	¹ H
TD	32768
SI	65536



¹H NMR (300 MHz, Chloroform-*d*) δ 8.05 (s, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.77 – 7.66 (m, 2H), 7.61 (d, *J* = 2.1 Hz, 1H), 7.58 – 7.32 (m, 4H).



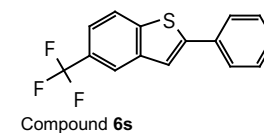
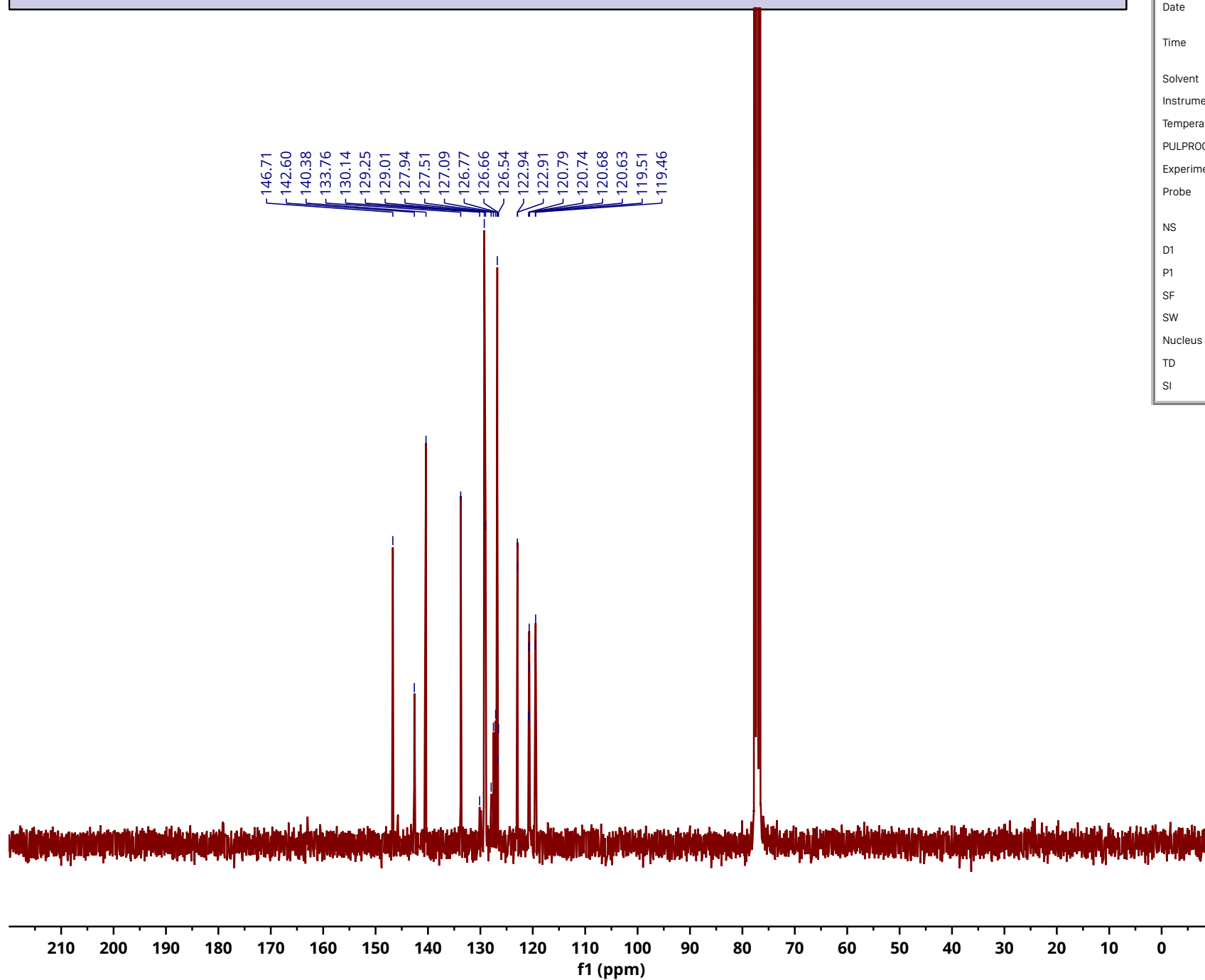
Parameter	Value
Title	MS-099.11.fid
Date	20181019
Time	14.01
Solvent	CDCl3
Instrument	FOURIER300
Temperature	297.6
PULPROG	zg30
Experiment	1D
Probe	5 mm DUL 13C-1
NS	128
D1	1.0000
P1	10.2000
SF	300.18
SW	6103.5
Nucleus	1H
TD	32768
SI	65536



$^1\text{H NMR}$ (300 MHz, Chloroform-*d*) δ 8.05 (s, 1H), 7.93 (d, $J = 8.4$ Hz, 1H), 7.77 – 7.66 (m, 2H), 7.61 (d, $J = 2.1$ Hz, 1H), 7.58 – 7.32 (m, 4H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 146.71, 142.60, 140.38, 133.76, 130.14, 129.25, 129.01, 127.94, 127.51, 127.09, 126.77, 126.66, 126.54, 122.94, 122.91, 120.79, 120.74, 120.68, 120.63, 119.51, 119.46.

Parameter	Value
Title	MS-099-2.502.fid
Date	
Time	
Solvent	CDCl ₃
Instrument	FOURIER300
Temperature	298.2
PULPROG	zgpg30
Experiment	1D
Probe	
NS	10240
D1	4.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	¹³ C
TD	32768
SI	65536



^{13}C NMR (75 MHz, Chloroform-*d*) δ 146.71, 142.60, 140.38, 133.76, 129.25, 129.01, 127.30 (q, $J = 32.3$ Hz), 126.77, 124.74 (q, $J = 271.9$ Hz), 122.91, 120.71 (q, $J = 8.2$ Hz), 119.51, 119.46.

Parameter	Value
Title	MS-099-2.502.fid
Date	
Time	
Solvent	CDCl ₃
Instrument	FOURIER300
Temperature	298.2
PULPROG	zgpg30
Experiment	1D
Probe	
NS	10240
D1	4.0000
P1	11.0000
SF	75.49
SW	24414.1
Nucleus	¹³ C
TD	32768
SI	65536

