Electronic Supplementary Information

Trialkylphosphonium Oxoborates as C(sp^3)-H Oxyanion Hole and Their Application in Catalytic Chemoselective Acetalization

Vincent Ming-Yau Leung, Hong-Chai Fabio Wong, Chun-Man Pook, Ying-Lung Steve Tse,* Ying-Yeung Yeung*

Department of Chemistry and State Key Laboratory of Synthetic Chemistry, The Chinese University of Hong Kong, Shatin, NT, Hong Kong

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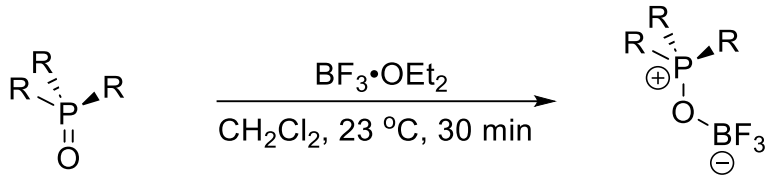
1. General information

Commercially available reagents were used as received. The solvents were dried over a solvent purification system from Innovative Technology. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AMX500 (500 MHz) spectrometer or a Bruker AMX400 (400 MHz) spectrometer, in $CDCl_3$ solutions, unless stated otherwise. All chemical shifts were recorded in ppm downfield from tetramethylsilane (stated otherwise. All chemical shifts were recor3 at $\delta = 7.26$) or carbon signals in NMR solvent ($CDCl_3$ at $\delta = 77.16$). Spin-spin coupling constants (J value) recorded in Hz were measured directly from the spectra. High resolution mass spectra were obtained on a Thermo Q Exactive Focus Orbitrap with ionization mode Electrospray Ionization (Positive) or Atmospheric-pressure Chemical Ionization at the Department of Chemistry, The Chinese University of Hong Kong, Hong Kong Special Administrative Region. Analytical thin layer chromatography (TLC) was performed with Merck pre-coated TLC plates, silica gel 60F-254, layer thickness 0.25 mm. Flash chromatography separations were performed on Merck 60 (0.040-0.063 mm) mesh silica gel.

2. Experimental procedures

(i) Preparation of catalyst

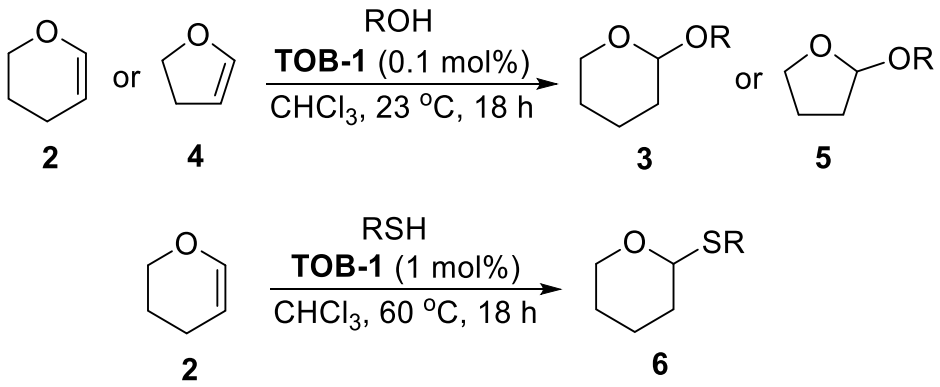


1a, R = Me
1b, R = cyclohexyl
1c, R = Ph

TOB-1, R = Me (84%)
TOB-2, R = cyclohexyl (91%)
TOB-3, R = Ph (95%)

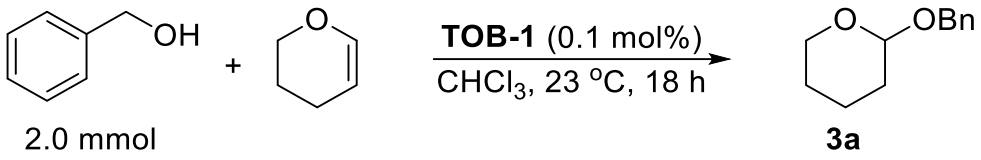
General procedure: To a round bottom flask equipped with a magnetic stirrer bar was added trialkylphosphine oxide **1** (2 mmol) and anhydrous CH_2Cl_2 (1 mL) at 23 °C under inert atmosphere. Boron trifluoride diethyl etherate (0.54 mL, 4 mmol, 2 equiv) was added dropwise using syringe and the resultant mixture was stirred for 30 minutes. Next, diethyl ether was added, and white precipitate was formed. The solution was filtered, and the residue was washed with diethyl ether (5 mL). The residue was dried under high vacuum to give the **TOB** catalyst.

(ii) TOB-catalyzed acetalization reaction



General procedure: To a solution of alcohol or thiol (0.2 mmol, 1 equiv) and **TOB-1** (0.2 μmol, 0.1 mol%) in $CHCl_3$ (0.4 mL) was added 3,4-dihydro-2H-pyran (**2**) (21.9 μL, 0.24 mmol, 1.2 equiv) or 2,3-dihydrofuran (**4**) (18.1 μL, 0.24 mmol, 2 equiv) into a vial (or a resealable tube for reactions at 60 °C). The reaction was stirred at 23 °C (or 60 °C) for 18 hours (or otherwise specified). The solution was concentrated under reduced pressure and the residue was purified by flash column chromatography eluted with hexanes/Et_2O (90:10) to give the desired acetal product.

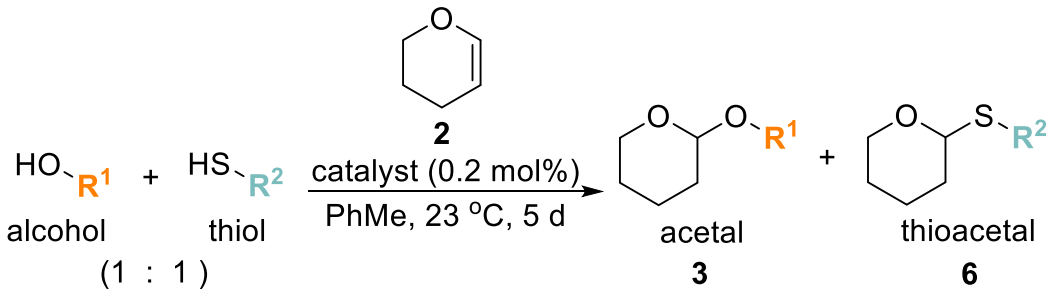
(iii) Scale-up reaction



2.0 mmol **3a**

To a solution of benzyl alcohol (207 µL, 2.0 mmol, 1 equiv) and **TOB-1** (2.0 µmol, 0.1 mol%) in $CHCl_3$ (4.0 mL) was added 3,4-dihydropyran **2** (219 µL, 2.4 mmol, 1.2 equiv). The reaction was stirred at 23 °C for 18 hours. The solution was concentrated under reduced pressure and the residue was purified by flash column chromatography eluted with hexanes/Et_2O = 90:10 to give the desired acetal product **3a** (0.31 g, 1.63 mmol, 81% yield).

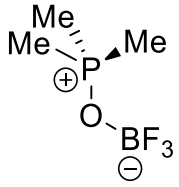
(iv) O/S Chemoselective acetalization



alcohol (1 : 1) thiol acetal **3** thioacetal **6**

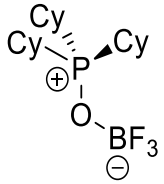
To a solution of alcohol (0.2 mmol, 1 equiv), thiol (0.2 mmol, 1 equiv) and **TOB-1** (0.4 µmol, 0.2 mol%) in toluene (0.4 mL) was added 3,4-dihydro-2H-pyran (**2**) (18.1 µL, 0.2 mmol, 1 equiv) into a vial. The reaction was stirred at 23 °C for 5 days. The reaction mixture was then filtered through a thin plug of silica gel column and the filtrate was concentrated under reduced pressure. The reaction yield and ratio were determined using NMR with dibromomethane (14.0 µL, 0.2 mmol, 1 equiv) as the internal standard.

3. Physical data



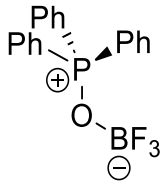
TOB-1

84% yield. White solid. mp 154.7-156.1 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.89 (d, J = 13.5 Hz, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 14.8 (d, J = 71.3 Hz). ^{11}B NMR (160 MHz, $CDCl_3$): δ -0.93. ^{19}F NMR (470 MHz, $CDCl_3$): δ -146.0 (s, 3F). ^{31}P NMR (200 MHz, $CDCl_3$): δ 67.9 (m). FTICR MS (APCI) calcd for $[C_3H_9BF_3OP + Cl]^-$: 195.01308, found: 195.01285.



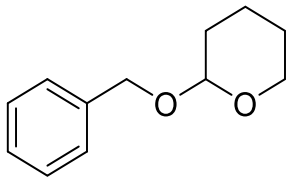
TOB-2

91% yield. White solid. mp 204.2-206.9 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.23 (qt, J = 12.5 Hz, 2.7 Hz, 3H), 2.00-1.97 (m, 6H), 1.93-1.88 (m, 6H), 1.78 (m, 3H), 1.60-1.51 (m, 6H), 1.36-1.23 (m, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 34.1, 33.6, 26.7 (d, J = 12.5 Hz), 25.8 (d, J = 11.3 Hz). ^{11}B NMR (160 MHz, $CDCl_3$): δ -1.03. ^{19}F NMR (470 MHz, $CDCl_3$): δ -145.9 (s, 3F). ^{31}P NMR (200 MHz, $CDCl_3$): δ 70.1 (m). FTICR MS (APCI) calcd for $[C_{18}H_{33}BF_3OP + Cl]^-$: 399.20115, found: 399.20146.



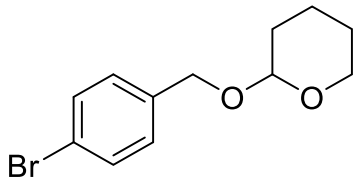
TOB-3[1]

95% yield. White solid. mp 243.5-244.3 ºC. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.77-7.70 (m, 9H), 7.60-7.56 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 134.4 (d, J = 2.7 Hz), 133.2 (d, J = 11.7 Hz), 129.4 (d, J = 13.3 Hz), 124.9 (d, J = 111.6 Hz). ^{11}B NMR (160 MHz, $CDCl_3$): δ -0.46. ^{19}F NMR (470 MHz, $CDCl_3$): δ -144.1 (s, 3F). ^{31}P NMR (200 MHz, $CDCl_3$): δ 44.5 (s).



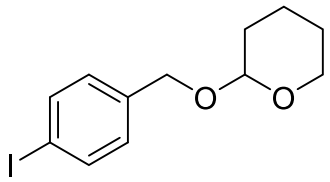
3a

Colorless liquid. 93% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.40-7.26 (m, 5H), 4.81 (d, J = 15 Hz, 1H), 4.73 (t, J = 4.4 Hz, 1H), 4.52 (d, J = 15 Hz, 1H), 3.97-3.91 (m, 1H), 3.59-3.54 (m, 1H), 1.93-1.84 (m, 1H), 1.79-1.52 (m, 5H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 138.4, 128.5, 127.9, 127.6, 97.8, 68.9, 62.2, 30.7, 25.6, 19.5. QEFMS calcd for $[C_{12}H_{16}O_2Na]^+$: 215.10425, found: 215.10390.



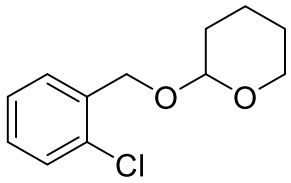
3b

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.46 (d, J = 8.6 Hz, 2H), 7.24 (d, J = 8.4 Hz, 2H), 4.73 (d, J = 12.3 Hz, 1H), 4.69 (t, J = 3.5 Hz, 1H), 4.45 (d, J = 12.3Hz, 1H), 3.91-3.87 (m, 1H), 3.56-3.52 (m, 1H) 1.89-1.50 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 137.4, 131.1, 129.5, 121.4, 97.9, 68.1, 62.2, 30.6, 25.5, 19.4. QEFMS calcd for $[C_{12}H_{15}BrO_2Na]^+$: 293.01476, found: 293.01405.



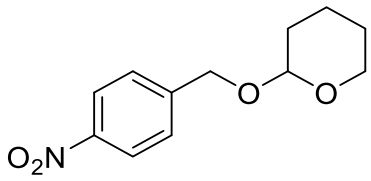
3c

Colorless liquid. 91% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.68-7.65 (m, 2H), 7.11-7.09 (m, 2H), 4.71 (d, J = 12.3 Hz, 1H), 4.68 (t, J = 3.6 Hz, 1H), 4.45 (d, J = 12.4 Hz, 1H), 3.90-3.86 (m, 1H), 3.56-3.52 (m, 1H) 1.87-1.51 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 138.1, 137.5, 129.7, 128.7, 97.9, 68.2, 62.3, 30.6, 25.5, 19.4. QEFMS calcd for $[C_{12}H_{15}IO_2Na]^+$: 341.00089, found: 341.00039.



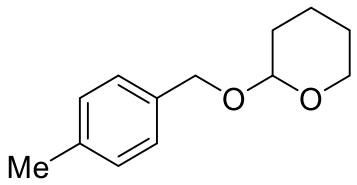
3d

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.52 (d, J = 7.5 Hz, 1H), 7.34 (d, J = 7.8 Hz, 1H), 7.24 (dt, J = 25.7 Hz, 7.8 Hz, 2H) , 4.86 (d, J = 13.2 Hz, 1H), 4.77 (s, 1H), 4.60 (d, J = 13.2 Hz, 1H), 3.92 (t, J = 10.6 Hz, 1H), 3.57-3.55 (m, 1H), 1.90-1.55 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 136.3, 133.0, 129.3, 129.0, 128.6, 126.8, 98.4, 66.4, 62.2, 30.6, 25.5, 19.4. QEFMS calcd for $[C_{12}H_{15}ClO_2Na]^+$: 249.06528, found: 249.06500.



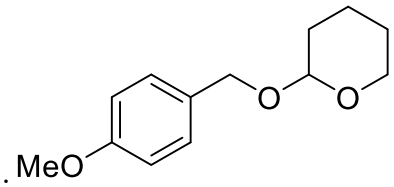
3e

Colorless liquid. 88% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.19 (d, J = 8.8 Hz, 2H), 7.52 (d, J = 8.8 Hz, 2H), 4.87 (d, J = 13.5 Hz, 1H), 4.72 (t, J = 3.5 Hz, 1H), 4.59 (d, J = 13.5 Hz, 1H), 3.89-3.85 (m, 1H), 3.57-3.53 (m, 1H), 1.89-1.53 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 146.2, 127.9, 127.1, 123.7, 98.4, 67.7, 62.4, 30.5, 25.4, 19.4. QEFMS calcd for $[C_{12}H_{15}NO_4Na]^+$: 260.08933, found: 260.08915.



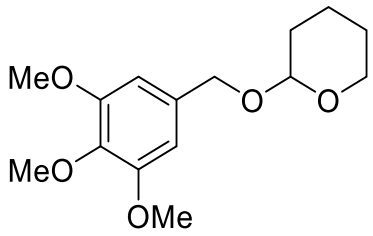
3f

Colorless liquid. 93% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.27(d, J = 8 Hz, 2H), 7.17 (d, J = 7.8 Hz, 2H), 4.76 (d, J = 11.8 Hz, 1H), 4.71 (t, J = 3.6 Hz, 1H), 4.48 (d, J = 11.8 Hz, 1H), 3.96-3.92 (m, 1H), 3.58-3.54 (m, 1H), 2.36 (s, 3H) 1.92-1.50 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 137.3, 135.3, 129.1, 128.1, 97.6, 68.8, 62.2, 30.7, 25.6, 21.3, 19.5. QEFMS calcd for $[C_{13}H_{18}O_2Na]^+$: 229.11990, found: 229.11954



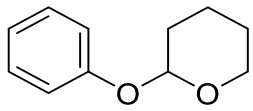
3g

Colorless liquid. 92% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.30 (d, J = 8.7 Hz, 2H), 6.88 (d, J = 8.7 Hz, 2H), 4.72 (d, J = 11.6 Hz, 1H), 4.69 (t, J = 3.6 Hz, 1H), 4.44 (d, J = 11.6 Hz, 1H), 3.95-3.90 (m, 1H), 3.8 (s, 3H), 3.55 (m, 1H), 1.88-1.50 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.2, 130.4, 129.6, 113.9, 97.6, 68.6, 62.3, 55.4, 30.7, 25.6, 19.5. QEFMS calcd for $[C_{13}H_{18}O_3Na]^+$: 245.11482, found: 229.11456.



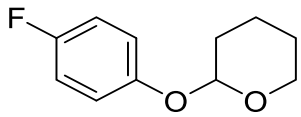
3h

Colorless liquid. 93% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.60 (d, J = 3.7 Hz, 2H), 4.72 (d, J = 11.9 Hz, 1H), 4.70 (t, J = 3.7 Hz, 1H), 4.43 (d, J = 10.7 Hz, 1H), 3.96-3.91 (m, 1H), 3.86 (s, 6H), 3.83 (s, 3H), 3.58-3.54 (m, 1H), 1.90-1.52 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.4, 137.4, 134.0, 105.0, 97.9, 69.2, 62.5, 61.0, 56.2, 30.8, 25.6, 19.7. QEFMS calcd for $[C_{15}H_{22}O_5Na]^+$: 305.13594, found: 305.13538.



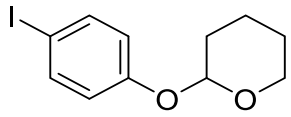
3i

Colorless liquid. 98% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.29 (t, J = 7.3 Hz, 2H), 7.07 (d, J = 7.9 Hz, 2H), 7.00 (t, J = 7.3 Hz, 1H), 5.43 (s, 1H), 3.93 (t, J = 11.3 Hz, 1H), 3.63-3.60 (m, 1H), 2.06-1.56 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.2, 129.5, 121.7, 116.6, 96.4, 62.1, 30.5, 25.3, 18.9. QEFMS calcd for $[C_{11}H_{14}O_2Na]^+$: 201.08819, found: 201.08858.



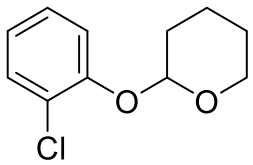
3j

Colorless liquid. 95% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.01-6.94 (m, 4H), 5.32 (t, J=3.29 1H), 3.93-3.88 (m, 1H), 3.62-3.58 (m, 1H), 2.07-1.93 (m, 1H), 1.89-1.80 (m, 2H), 1.72-1.58 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.9 (d, J_{CF} = 237.5 Hz), 153.3 (d, J_{CF} = 3.75 Hz), 117.9 (d, J_{CF} = 7.5 Hz), 115.9 (d, J_{CF} = 22.5 Hz), 97.2, 62.2, 30.5, 25.3, 18.9. ^{19}F NMR (470 MHz, $CDCl_3$): δ -122.9 (sept, J_{CF} = 4.7 Hz). QEFMS calcd for $[C_{11}H_{13}FO_2Na]^+$: 219.07918, found: 219.07886.



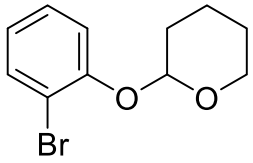
3k

Colorless liquid. 95% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.55 (d, J = 7.8 Hz, 2H), 6.83 (d, J =7.8 Hz, 2H), 5.38 (s, 1H), 3.86 (t, J = 11.2 Hz, 1H), 3.60-3.58 (m, 1H), 2.00-1.58 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.0, 138.4, 118.9, 96.4, 84.0, 62.1, 30.3, 25.2, 18.7. QEFMS calcd for $[C_{11}H_{13}IO_2Na]^+$: 326.98524, found: 326.98498.



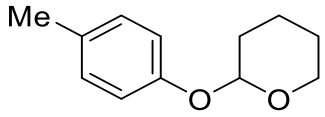
3l

Colorless liquid. 83% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37-7.35 (m, 1H), 7.19-7.18 (m, 2H), 6.95-6.89 (m, 1H), 5.50 (t, J = 2.9 Hz, 1H), 3.96-3.90 (m, 1H), 3.64-3.59 (m, 1H), 2.15-2.04 (m, 1H), 2.00-1.95 (m, 1H), 1.92-1.84 (m, 1H), 1.77-1.61 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.7, 130.3, 127.7, 124.0, 122.5, 117.1, 96.9, 62.0, 30.3, 25.3, 18.9. QEFMS calcd for $[C_{11}H_{13}ClO_2Na]^+$: 235.04963, found: 235.04948.



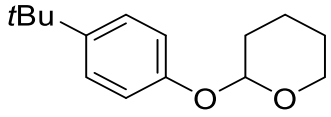
3m

Colorless liquid. 74% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.24 (d, J = 12.4 Hz, 1H), 7.13-7.12 (m, 2H), 6.98 (d, J =7.6 Hz, 1H), 5.40 (t, J = 2.8 Hz, 1H), 3.87 (td, J = 10.6 Hz, 2.8Hz, 1H), 3.63-3.59 (m, 1H), 1.99-1.57 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.0, 130.6, 124.8, 122.7, 120.0, 115.3, 96.9, 62.1, 30.3, 25.2, 18.7. QEFMS calcd for $[C_{11}H_{13}BrO_2Na]^+$: 278.99911, found: 278.99906.



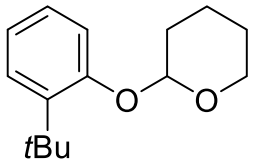
3n

Colorless liquid. 82% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.08 (d, J = 8.3 Hz, 2H), 6.95 (d, J = 8.6 Hz, 2H), 5.37 (t, J = 3.3 Hz, 1H), 3.94-3.89 (m, 1H), 3.61-3.57 (m, 1H), 2.28 (s, 3H), 2.05-1.96 (m, 1H), 1.87-1.83 (m, 2H), 1.71-1.57 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.0, 131.0, 130.0, 116.5, 96.7, 62.2, 30.6, 25.4, 20.7, 19.0. QEFMS calcd for $[C_{12}H_{16}O_2Na]^+$: 215.10425, found: 215.10387.



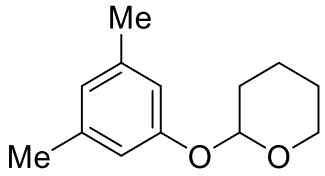
3o

Colorless liquid. 89% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.31 (d, J = 8.7 Hz, 2H), 7.0 (d, J = 8.7 Hz, 2H), 5.41 (s, 1H), 3.95 (t, J = 9.9 Hz, 1H), 3.62-3.60 (m, 1H), 2.03-1.60 (m, 6H), 1.31 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.9, 144.3, 126.3, 116.0, 96.5, 62.1, 34.2, 31.6, 30.6, 25.3, 19.0. QEFMS calcd for $[C_{15}H_{22}O_2Na]^+$: 257.15120, found: 257.15080.



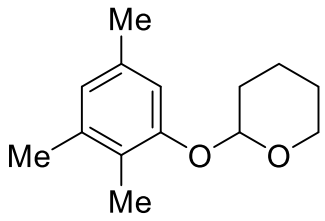
3p

Colorless liquid. 92% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31-7.29 (m, 1H), 7.21-7.14 (m, 2H), 6.94-6.90 (m, 1H), 5.49 (t, J = 2.9 Hz, 1H), 3.95-3.89 (m, 1H), 3.69-3.64 (m, 1H), 2.10-2.01 (m, 1H), 1.95-1.90 (m, 2H), 1.89-1.69 (m, 2H), 1.67-1.61 (m, 1H), 1.43 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.2, 138.0, 127.3, 126.7, 121.0, 114.4, 96.2, 61.9, 35.0, 30.7, 30.1, 25.5, 19.1. QEFMS calcd for $[C_{15}H_{22}O_2Na]^+$: 257.15120, found: 257.15090.



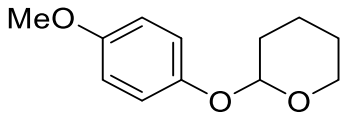
3q

Colorless liquid. 93% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.70 (s, 2H), 6.65 (s, 1H), 5.42 (t, J = 3.2 Hz, 1H), 3.94 (td, J = 9.8 Hz, 3.1 Hz, 1H), 3.63-3.60 (m, 1H), 2.30 (s, 6H) 2.04-1.56 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.2, 139.2, 123.5, 114.3, 96.3, 62.1, 30.6, 25.4, 21.5, 18.9. QEFMS calcd for $[C_{13}H_{18}O_2Na]^+$: 229.11990, found: 229.11988.



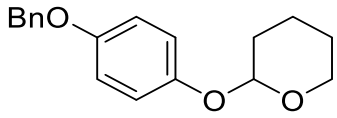
3r

Colorless liquid. 71% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.80 (s, 1H), 6.66 (s, 1H), 5.40 (s, 1H), 3.92 (td, J = 9.9 Hz, 2.6 Hz, 1H), 3.64-3.60 (m, 1H), 2.28 (s, 3H), 2.25 (s, 3H), 2.16 (s, 3H), 2.06-2.01 (m, 1H), 1.90-1.88 (m, 2H), 1.74-1.61 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.9, 137.6, 135.6, 124.0, 122.7, 112.9, 96.4, 62.1, 30.8, 25.5, 21.4, 20.2, 19.1, 11.6. QEFMS calcd for $[C_{14}H_{20}O_2Na]^+$: 243.13555, found: 243.13525.



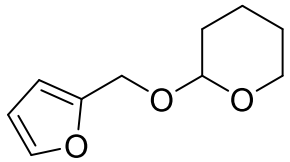
3s

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.00 (d, J = 7.9 Hz, 2H), 6.82 (d, J = 7.9 Hz, 2H), 5.30 (s, 1H), 3.94 (t, J = 11.1 Hz, 1H), 3.76 (s, 3H), 3.60-3.58 (m, 1H), 2.00-1.55 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.6, 151.2, 117.9, 114.6, 97.4, 62.2, 55.7, 30.6, 25.3, 19.0. QEFMS calcd for $[C_{12}H_{16}O_3Na]^+$: 231.09917, found: 231.09923.



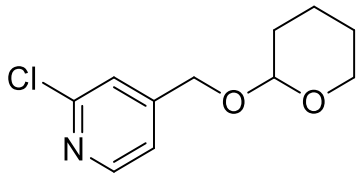
3t

Colorless liquid. 86% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.45 (d, J = 7.5 Hz, 2H), 7.40 (t, J = 7.3 Hz, 2H), 7.33 (t, J = 7.2 Hz, 1H), 7.02 (d, J = 9.0 Hz, 2H), 6.92 (d, J = 9.0 Hz, 2H), 5.32 (t, J = 3.1 Hz, 1H), 5.03 (s, 2H) 3.96 (td, J = 12.0 Hz, 2.9 Hz, 1H), 3.63-3.59 (m, 1H), 2.07-1.60 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.8, 151.4, 137.4, 128.6, 128.0, 127.6, 117.8, 115.7, 97.4, 70.6, 62.2, 30.6, 25.4, 19.0. QEFMS calcd for $[C_{18}H_{20}O_3Na]^+$: 307.13047, found: 307.13000.



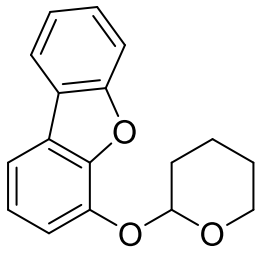
3u

Colorless liquid. 70% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.41 (m, 1H), 6.33 (d, J = 2.5 Hz, 2H), 4.71 (m, 1H), 4.67 (d, J = 12.8 Hz, 1H), 4.49 (d, J = 12.8 Hz, 1H) 3.90 (t, J = 10.2 Hz, 1H), 3.55 (m, 1H), 1.87-1.80 (m, 1H), 1.74-1.69 (m, 1H), 1.63-1.59 (m, 2H), 1.54-1.52 (m, 2H) . ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.9, 142.9, 110.4, 109.4, 97.4, 62.1, 60.7, 30.5, 25.5., 19.3. QEFMS calcd for $[C_{10}H_{14}O_3Na]^+$: 205.08352, found: 205.08313.



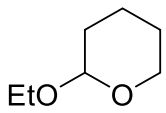
3v

Colorless liquid. 65% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 2.1 Hz, 1H), 7.66 (dd, J = 8.2, 2.4 Hz, 1H), 7.30 (d, J = 8.1 Hz, 1H), 4.76 (d, J = 12.4 Hz, 1H), 4.67 (t, J = 3.4 Hz, 1H), 4.48 (d, J = 12.4 Hz, 1H), 3.88-3.82 (m, 1H), 3.56-3.51 (m, 1H), 1.87-1.70 (m, 2H), 1.66-1.52 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.7, 149.1, 138.5, 132.9, 124.1, 98.3, 65.7, 62.4, 30.5, 25.4, 19.3. QEFMS calcd for $[C_{11}H_{14}NO_2Cl+H]^+$: 228.07858, found: 228.07822.



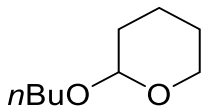
3w

Colorless liquid. 69% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (dd, J = 7.6, 0.5 Hz, 1H), 7.62 (d, J = 8.2 Hz, 1H), 7.59 (d, J = 4.4 Hz, 1H), 7.45 (td, J = 7.4, 1.3 Hz, 1H), 7.33 (td, J = 7.7, 0.8 Hz, 1H), 7.25 (d, J = 4.1 Hz, 2H), 5.74 (t, J = 3.1 Hz, 1H), 4.03 (td, J = 11.4, 3.0 Hz, 1H), 3.64 (dtd, J = 11.2, 3.8, 1.1 Hz, 1H), 2.22-2.05 (m, 2H), 2.01-1.93 (m, 1H), 1.79-1.63 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 146.2, 142.7, 127.2, 126.2, 124.6, 123.5, 122.8, 120.8, 114.7, 114.0, 112.1, 97.5, 62.2, 30.4, 25.3, 18.7. QEFMS calcd for $[C_{17}H_{16}O_3Na]^+$: 291.09917, found: 291.09847.



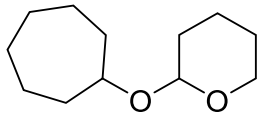
3x

Colorless liquid. 99% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.57 (dd, J = 2.7, 4.5 Hz, 1H), 3.89-3.83 (m, 1H), 3.81-3.77 (m, 1H), 3.51-3.40 (m, 2H), 1.88-1.76 (m, 1H), 1.74-1.66 (m, 1H), 1.60-1.48 (m, 4H), 1.21 (t, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 98.8, 63.0, 62.6, 30.9, 25.6, 19.9, 15.3. QEFMS calcd for $[C_7H_{14}O_2Na]^+$: 153.08860, found: 183.08840.



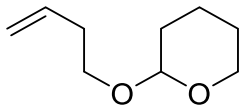
3y

Colorless liquid. 99% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.56 (t, J = 2.6 Hz, 1H), 3.88-3.83 (m, 1H), 3.72 (dt, J = 9.6 Hz, 6.8 Hz, 1H), 3.51-3.46 (m, 1H), 3.37 (dt, J = 9.6 Hz, 6.8 Hz, 1H), 1.85-1.77 (m, 1H), 1.73-1.67 (m, 1H), 1.60-1.47 (m, 6H), 1.42-1.33 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 98.9, 67.5, 62.4, 32.0, 30.9, 25.6, 19.8, 19.6, 14.0. QEFMS calcd for $[C_9H_{18}O_2Na]^+$: 181.1199, found: 181.1197.



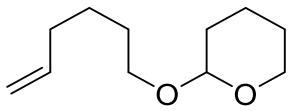
3z

Colorless liquid. 90% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.64 (t, J = 3.7 1H), 3.90 (sept, J = 3.6 Hz, 1H), 3.78 (sept, J = 4.2 Hz, 1H), 1.98-1.93 (m, 1H), 1.86-1.81 (m, 2H), 1.72-1.61 (m, 5H), 1.59-1.49 (m, 9H), 1.42-1.34 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 96.9, 76.8, 62.9, 35.8, 33.4, 31.5, 28.4, 28.2, 25.7, 23.3, 23.0, 20.2. QEFMS calcd for $[C_{12}H_{22}O_2Na]^+$: 221.15120, found: 221.15098.



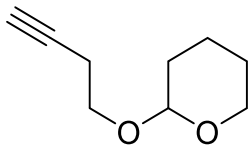
3aa

Colorless liquid. 70% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.88-5.80 (m, 1H), 5.10 (d, J = 17.2 Hz, 1H), 5.03 (d, J = 10.3 Hz, 1H), 4.59 (t, J = 3.5 Hz, 1H), 3.86 (t, J = 9.3 Hz, 1H), 3.78 (q, J = 7.1 Hz, 1H), 3.52-3.43 (m, 2H), 5.10 (q, J = 17 Hz, 2H), 1.85-1.79 (m, 1H), 1.74-1.68 (m, 1H), 1.61-1.50 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.4, 116.4, 98.9, 66.9, 62.4, 34.3, 30.8, 25.6, 19.7. QEFMS calcd for $[C_9H_{16}O_2Na]^+$: 179.10425, found: 179.10409.



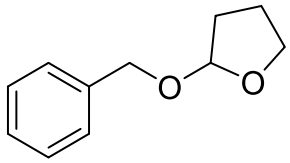
3ab

Colorless liquid. 92% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.80 (sext, J = 8.1 Hz, 1H), 4.99 (d, J = 17.2 Hz, 1H), 4.93 (d, J = 10.2 Hz, 1H), 4.56 (s, 1H), 3.85 (t, J = 9.5 Hz, 1H), 3.73 (q, J = 7.7 Hz, 1H), 3.48 (t, J = 5.5 Hz, 1H), 3.37 (q, J = 7.5 Hz, 1H), 2.07 (q, J = 7.1 Hz, 2H), 1.81 (q, J = 8.8 Hz, 1H), 1.69 (t, J = 11.1 Hz, 1H), 1.63-1.45 (m, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 138.9, 114.6, 98.9, 67.5, 62.4, 33.7, 30.9, 29.3, 25.7, 25.6, 19.8. QEFMS calcd for $[C_{11}H_{20}O_2Na]^+$: 207.13555, found: 207.13535.



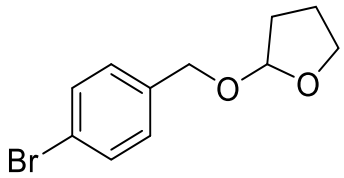
3ac

Colorless liquid. 94% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.64 (t, J = 3.4 Hz, 1H), 3.89-3.80 (m, 2H), 3.58-3.48 (m, 2H), 2.48 (td, J = 7 Hz, 2.5 Hz, 2H), 1.97 (t, J = 2.4 Hz, 1H), 1.85-1.50 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 98.9, 81.6, 69.3, 65.6, 62.3, 30.6, 25.5, 20.1, 19.5. QEFMS calcd for $[C_9H_{14}O_2Na]^+$: 177.08860, found: 177.08848.



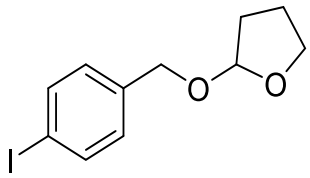
5a

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.38 (m, 4H), 7.26 (m, 1H), 5.23 (d, J = 4.4 Hz, 1H), 4.73 (d, J = 11.9 Hz, 1H), 4.49 (d, J = 11.9 Hz, 1H), 3.99-3.89 (m, 2H), 2.09-1.82 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 138.4, 128.5, 128.0, 127.6, 103.2, 68.9, 67.1, 32.4, 23.6. QEFMS calcd for $[C_{11}H_{14}O_2Na]^+$: 201.08860, found: 201.08832.



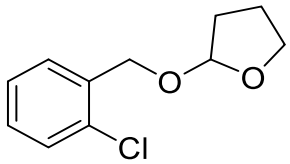
5b

Colorless liquid. 94% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.45 (d, J = 7.6 Hz, 2H), 7.21 (d, J = 7.7 Hz, 2H), 5.19 (s, 1H), 4.65 (d, J = 12.2 Hz, 1H), 4.45 (d, J = 12.1 Hz, 1H), 3.91 (sext, J = 7.2 Hz, 2H), 2.05-1.81 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 137.5, 131.5, 129.5, 121.4, 103.3, 68.1, 67.2, 32.5, 23.5. QEFMS calcd for $[C_{11}H_{13}BrO_2Na]^+$: 278.99911, found: 278.99890.



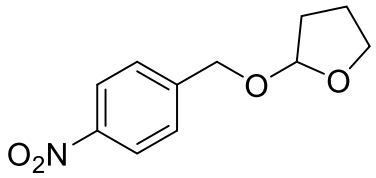
5c

Colorless liquid. 97% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.66 (d, J = 7.5 Hz, 2H), 7.08 (d, J = 7.6 Hz, 2H), 5.19 (s, 1H), 4.64 (d, J = 12.2 Hz, 1H), 4.41 (d, J = 12.2 Hz, 1H), 3.91 (sext, J = 7.3 Hz, 2H), 2.05-1.80 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 138.2, 137.5, 129.8, 103.3, 93.0, 68.1, 67.2, 32.4, 23.5. QEFMS calcd for $[C_{11}H_{13}IO_2Na]^+$: 326.98524, found: 326.98447.



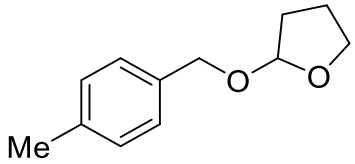
5d

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.46 (d, J = 7.4 Hz, 1H), 7.34 (d, J = 7.5 Hz, 1H), 7.28-7.19 (m, 2H), 5.26 (d, J = 4.1 Hz, 1H) 4.80 (d, J = 13.0 Hz, 1H), 4.57 (d, J = 13.0 Hz, 1H), 3.94 (dq, J = 5.1 Hz, 7 Hz, 2H), 2.08-1.85 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 136.3, 133.2, 129.4, 129.3, 128.7, 126.8, 103.7, 67.3, 66.2, 32.5, 23.5. QEFMS calcd for $[C_{11}H_{13}ClO_2Na]^+$: 235.04963, found: 235.04924.



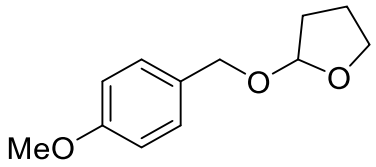
5e

Colorless liquid. 92% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.17(d, J = 7.9 Hz, 2H), 7.48 (d, J = 7.9Hz, 2H), 5.21 (s, 1H), 4.79 (d, J = 13.5 Hz, 1H), 4.56 (d, J = 13.4 Hz, 1H), 3.91 (sext, J = 7.5 Hz, 2H), 2.07-1.87 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 147.3, 146.4, 127.9, 123.6, 103.8, 67.6, 67.4, 32.5, 23.5. QEFMS calcd for $[C_{11}H_{13}NO_4Na]^+$: 246.07368, found: 246.07359.



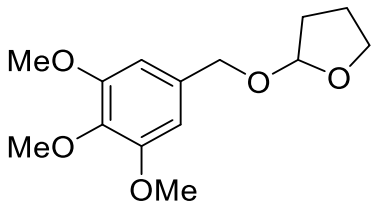
5f

Colorless liquid. 87% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.25 (d, J = 7.6 Hz, 2H), 7.16 (d, J = 7.7 Hz, 2H), 5.22 (s, 1H), 4.69 (d, J = 11.7 Hz, 1H), 4.45 (d, J = 11.6 Hz, 1H), 3.91 (dq, J = 26.1 Hz, 7.2 Hz, 2H), 2.35 (s, 3H), 2.08-1.81 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 137.3, 135.3, 129.1, 128.1, 103.0, 68.7, 67.1, 32.4, 23.6, 21.2. QEFMS calcd for $[C_{12}H_{16}O_2Na]^+$: 215.10425, found: 216.10402.



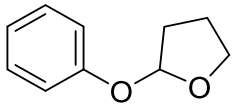
5g

Colorless liquid. 98% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.27 (d, J = 8.2 Hz, 2H), 6.88 (d, J = 7.6 Hz, 2H), 5.20 (s, 1H) 4.65 (d, J = 11.4 Hz, 1H), 4.41 (d, J = 11.4 Hz, 1H), 3.92 (sept, J = 7.3 Hz, 2H), 3.8 (s, 3H), 2.07-1.80 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.2, 130.5, 129.6, 113.8, 102.9, 68.5, 67.1, 55.4, 32.4, 23.6. QEFMS calcd for $[C_{12}H_{16}O_3Na]^+$: 231.09859, found: 231.09917.



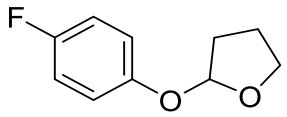
5h

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.5 (s, 2H), 5.22 (t, J = 3.2 Hz, 1H), 4.63 (d, J = 11.7 Hz, 1H), 4.40 (d, J = 11.7 Hz, 1H), 3.98-3.89 (m, 2H), 3.86 (s, 6H), 3.82 (s, 3H), 2.07-1.82 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.4, 137.4, 134.0, 105.0, 103.2, 69.2, 67.2, 60.9, 56.2, 32.5, 23.6. QEFMS calcd for $[C_{14}H_{20}O_5Na]^+$: 291.12029, found: 291.11961.



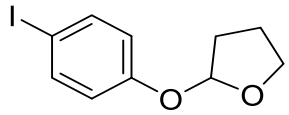
5i

Colorless liquid. 96% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.28 (t, J = 7.6 Hz, 2H), 7.03 (d, J = 7.9 Hz, 2H), 6.98 (t, J = 7.4 Hz, 1H), 5.81 (d, J = 4.7 Hz, 1H), 4.07-4.03 (m, 1H), 3.97-3.93 (m, 1H), 2.21-2.10 (m, 3H), 1.99-1.90 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.3, 129.5, 121.6, 116.6, 102.4, 68.2, 32.8, 23.6. QEFMS calcd for $[C_{10}H_{12}O_2Na]^+$: 187.07295, found: 187.07261.



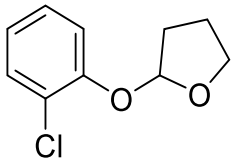
5j

Colorless liquid. 71% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.99-6.94 (m, 4H), 4.76 (d, J = 4.8 Hz, 1H), 4.07-4.02 (m, 1H), 3.97-3.92 (m, 1H), 2.21-2.06 (m, 3H), 1.99-1.89 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.0 (d, J_{CF} = 237.5 Hz), 153.4 (d, J_{CF} = 1.25 Hz), 118.0 (d, J_{CF} = 8.75 Hz), 115.84 (d, J_{CF} = 22.5 Hz), 103.1, 68.1, 32.8, 23.5. ^{19}F NMR (470 MHz, $CDCl_3$): δ -123.0 (sext, J_{CF} = 4.7 Hz). QEFMS calcd for $[C_{10}H_{11}FO_2Na]^+$: 205.06353, found: 205.06357.



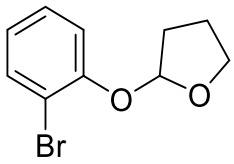
5k

Colorless liquid. 88% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.54 (d, J = 8.8 Hz, 2H), 6.80 (d, J =8.8 Hz, 2H), 5.74 (d, J =4.6 Hz, 1H), 4.02 (q, J = 7.6 Hz, 1H), 3.94 (q, J = 7.9 Hz, 1H), 2.19-1.92 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.2, 138.2, 119.0, 102.4, 84.0, 68.3, 32.8, 23.5. QEFMS calcd for $[C_{10}H_{11}IO_2Na]^+$: 312.96959, found: 312.96946.



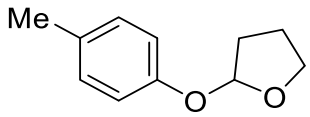
5l

Colorless liquid. 72% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.52 (dd, J = 7.9 Hz, 1.5 Hz, 1H), 7.23-7.18 (m, 2H), 6.87 (td, J = 7.9 Hz, 1.7 Hz, 1H), 5.82 (d, J = 4.5 Hz, 1H), 4.10 (dt, J = 8.1 Hz, 5.6 Hz, 1H), 3.96 (q, J =6.7 Hz, 1H), 2.35-1.93 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.8, 133.3, 128.5, 123.0, 117.4, 113.7, 103.5, 68.5, 32.9, 23.4. QEFMS calcd for $[C_{10}H_{11}ClO_2Na]^+$: 221.0339, found: 221.0336.



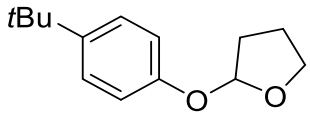
5m

Colorless liquid. 94% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35 (dd, J = 7.9 Hz, 6.5 Hz, 1H), 7.23 (m, 2H), 6.95-6.91 (m, 1H), 5.81 (d, J = 4.5 Hz, 1H), 4.10 (dd, J = 13.8 Hz, 5.8 Hz, 1H), 3.97 (dd, J =14.3 Hz, 7.7 Hz, 1H), 2.34-2.29 (m, 1H), 2.27-2.10 (m, 2H), 2.00-1.93(m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.9, 130.3, 127.7, 124.2, 122.6, 117.6, 103.5, 68.5, 32.9, 23.4. QEFMS calcd for $[C_{10}H_{11}BrO_2Na]^+$: 264.98346, found: 264.98317.



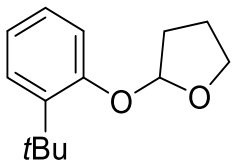
5n

Colorless liquid. 85% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.22 (d, J = 9.0 Hz, 2H), 6.98 (d, J = 9.0 Hz, 2H), 5.37 (t, J = 3.2 Hz, 1H), 3.90-3.85 (m, 1H), 3.62-3.57 (m, 1H), 2.03-1.95 (m, 1H), 1.87-1.84 (m, 2H), 1.73-1.56 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.8, 129.4, 126.6, 117.9, 96.7, 62.1, 30.4, 25.3, 18.8. QEFMS calcd for $[C_{11}H_{14}O_2Na]^+$: 201.08860, found: 201.08839.



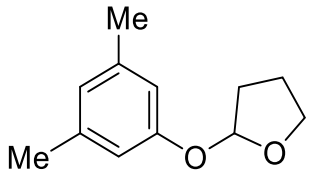
5o

Colorless liquid. 99% Isolated yield, 33% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.29 (dt, J = 8.8 Hz, 2.1 Hz, 2H), 6.96 (dt, J = 8.8 Hz, 2.2 Hz, 2H), 5.80 (d, J = 4.8 Hz, 1H), 4.06-4.02 (m, 1H), 3.96-3.92 (m, 1H), 2.20-1.89 (m, 4H), 1.29 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.9, 144.3, 126.3, 116.0, 102.4, 68.1, 34.2, 32.8, 31.6, 23.6. QEFMS calcd for $[C_{14}H_{20}O_2Na]^+$: 243.13555, found: 243.13538.



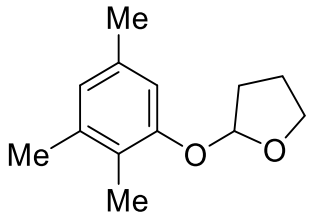
5p

Colorless liquid. 75% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.26 (m, 1H), 7.23-7.15 (m, 2H), 6.94-6.90 (m, 1H), 5.87 (d, J = 4.6 Hz, 1H), 4.09-4.04 (m, 1H), 4.01-3.96 (m, 1H), 2.30 (m, 3H), 2.05-1.97 (m, 1H), 1.38 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.0, 138.2, 127.1, 126.7, 121.0, 114.6, 101.8, 68.0, 34.9, 32.9, 30.0, 23.7. QEFMS calcd for $[C_{14}H_{20}O_2Na]^+$: 243.13555, found: 243.13533.



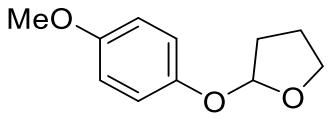
5q

Colorless liquid. 81% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.69 (s, 2H), 6.65 (s, 1H), 5.81 (d, J = 4.8 Hz, 1H), 4.09-4.04 (m, 1H), 3.98-3.93 (m, 1H), 2.30 (s, 6H), 2.20-1.92 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.2, 139.2, 123.4, 114.3, 102.2, 68.1, 32.8, 23.6, 21.5. QEFMS calcd for $[C_{12}H_{16}O_2Na]^+$: 215.10425, found: 215.10431.



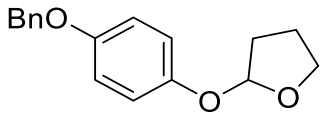
5r

Colorless liquid. 97% Isolated yield, 31% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.85 (s, 1H), 6.67 (s, 1H), 5.79 (d, J = 4.7 Hz, 1H), 4.09 (q, J = 6.0 Hz, 1H), 3.97 (q, J = 6.2 Hz, 1H) 2.30 (s, 3H), 2.25-2.11 (m, 9H), 1.99-1.96 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.1, 137.7, 135.6, 124.1, 123.0, 113.5, 102.8, 68.0, 32.9, 23.7, 21.4, 20.2, 11.7. QEFMS calcd for $[C_{13}H_{18}O_2Na]^+$: 229.11990, found: 229.11983.



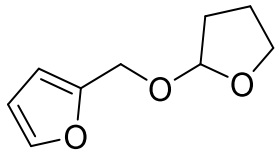
5s

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.97 (dd, J = 6.7 Hz, 2.3 Hz, 2H), 6.82 (dd, J = 6.7 Hz, 2.3 Hz, 2H), 5.70 (t, J = 4.8 Hz, 1H), 4.07-4.03 (m, 1H), 3.96-3.90 (m, 1H), 3.76 (s, 3H), 2.18-1.90 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.7, 151.2, 118.0, 114.7, 103.3, 68.0, 55.8, 32.8, 23.6. QEFMS calcd for $[C_{11}H_{14}O_3Na]^+$: 217.08352, found: 217.08356.



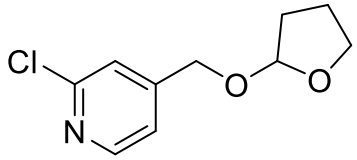
5t

Colorless liquid. 89% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.45 (d, J = 7.1 Hz, 2H), 7.40 (t, J = 7.2 Hz, 2H), 7.34 (t, J = 7.2 Hz, 1H), 7.00 (dd, J = 6.7 Hz, 2.35 Hz, 2H), 6.92 (dd, J = 6.7 Hz, 2.35 Hz, 2H), 5.73 (d, J = 4.8 Hz, 1H), 5.03 (s, 2H), 4.10-4.05 (m, 1H), 3.98-3.94 (m, 1H), 2.20-1.91 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.8, 151.5, 137.4, 128.6, 128.6, 127.9, 127.6, 118.0, 115.8, 70.6, 67.9, 32.7, 23.5. QEFMS calcd for $[C_{17}H_{18}O_3Na]^+$: 293.11482, found: 293.11440.



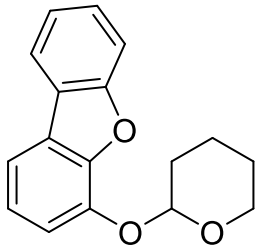
5u

Colorless liquid. 70% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.40 (s, 1H), 6.32 (m, 2H), 5.21 (t, J = 3.0 Hz, 1H), 4.60 (d, J = 12.8 Hz, 1H), 4.46 (d, J = 12.8 Hz, 1H), 3.92 (m,2H), 2.05-1.97 (m, 1H), 1.95-1.91 (m, 2H), 1.87-1.79 (m, 1H) . ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.9, 142.9, 110.4, 109.3, 102.8, 67.2, 60.7, 32.4, 25.5. QEFMS calcd for $[C_9H_{12}O_3Na]^+$: 191.06787, found: 191.06778.



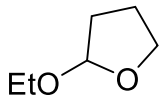
5v

Colorless liquid. 65% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.33 (d, J = 1.9 Hz, 1H), 7.61 (dd, J = 8.2, 2.2 Hz, 1H), 7.28 (d, J = 8.1 Hz, 1H), 5.18 (t, J = 2.8 Hz, 1H), 4.67 (d, J = 12.2 Hz, 1H), 4.45 (d, J = 12.2 Hz, 1H), 3.89 (t, J = 6.3 Hz, 2H), 2.05-1.80 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.6, 149.1, 138.4, 133.1, 124.1, 103.6, 67.4, 65.5, 32.5, 23.5. QEFMS calcd for $[C_{10}H_{12}NO_2Cl+H]^+$: 214.06293, found: 214.06257.



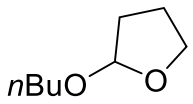
5w

Colorless liquid. 69% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93 (d, J = 7.7 Hz, 1H), 7.63-7.59 (m, 2H), 7.45 (t, J = 8.2 Hz, 1H), 7.34 (t, J = 7.2 Hz, 1H), 7.28-7.26 (m, 2H), 6.10 (d, J = 4.8 Hz, 1H), 4.17 (q, J = 8.0 Hz, 1H), 4.03 (q, J = 7.7 Hz, 1H), 2.49-2.40 (m, 1H), 2.35-2.10 (m, 2H), 2.08-1.96 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.2, 146.2, 142.8, 127.2, 126.1, 124.6, 123.5, 122.8, 120.8, 114.6, 114.0, 112.0, 103.6, 68.5, 32.9, 23.5. QEFMS calcd for $[C_{16}H_{14}O_3Na]^+$: 277.08352, found: 277.08289.



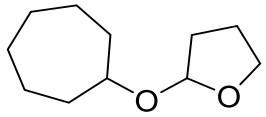
5x

Colorless liquid. 95% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.07 (q, J = 3.3 Hz, 1H), 3.87-3.78 (m, 2H), 3.69-3.62 (m, 1H), 3.41-3.35 (m, 1H), 1.99-1.73 (m, 4H), 1.14 (t, J = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 103.8, 67.0, 62.8, 32.5, 23.7, 15.4. QEFMS calcd for $[C_6H_{12}O_2Na]^+$: 139.07295, found: 139.07284.



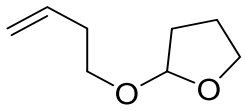
5y

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.1 (dd, J = 4.8 Hz, 1.6 Hz, 1H), 3.90-3.82 (m, 2H), 3.65 (dt, J = 9.6 Hz, 6.8 Hz, 1H), 3.36 (dt, J = 9.6 Hz, 6.7 Hz, 1H), 2.03-1.77 (m, 4H) , 1.56-1.51, (m, 2H), 1.39-1.31(m, 2H), 0.91 (t, J = 7.4 Hz 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 103.9, 67.1, 66.9, 32.5, 32.0, 23.7, 19.5, 14.0. QEFMS calcd for $[C_8H_{16}O_2Na]^+$: 167.10425, found: 167.10419.



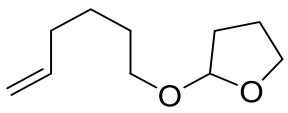
5z

Colorless liquid. 92% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.20 (d, J = 4.8 1H), 3.89-3.79 (m, 2H), 3.69 (sept, J = 4.3, 1H), 2.02-1.93 (m, 1H), 1.92-1.74 (m, 5H), 1.64-1.46 (m, 8H), 1.40-1.33 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 102.0, 76.9, 66.6, 35.9, 33.8, 32.7, 28.4, 28.2, 23.7, 23.2, 23.0. QEFMS calcd for $[C_{11}H_{20}O_2Na]^+$: 207.13555, found: 207.13549.



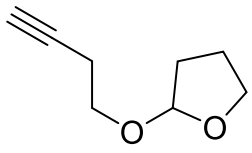
5aa

Colorless liquid. 94% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.85-5.77 (m, 1H), 5.12-5.07 (m, 2H), 5.03-5.01 (m, 1H), 3.87 (dq, J = 18.5 Hz, 7.9 Hz, 2H), 3.87 (dt, J = 13.9 Hz, 6.9 Hz, 1H), 3.43 (dt, J = 9.6 Hz, 6.9 Hz, 1H), 2.32 (q, J = 6.8 Hz, 2H), 2.02-1.78 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.5, 116.3, 103.9, 67.0, 66.6, 34.3, 32.5, 23.6. QEFMS calcd for $[C_8H_{14}O_2Na]^+$: 165.08860, found: 165.08851.



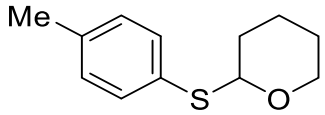
5ab

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.84-5.75 (m, 1H), 5.09 (dd, J = 1.5 Hz, 4.7 Hz, 1H), 5.01-4.97 (m, 1H), 4.94-4.91 (m, 1H), 3.90-3.82 (m, 2H), 3.64 (dt, J = 6.8 Hz, 9.6 Hz, 1H), 3.36 (dt, J = 6.8 Hz, 9.6 Hz, 1H), 2.06 (q, J = 7.3 Hz, 2H), 2.01-1.81 (m, 4H), 1.57 (quin, J = 6.6 Hz, 2H), 1.42 (quin, J = 7.3 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 138.9, 114.6, 103.9, 67.1, 66.9, 33.6, 32.4, 29.3, 25.6, 23.6. QEFMS calcd for $[C_{10}H_{18}O_2Na]^+$: 193.11990, found: 193.11995.



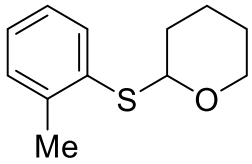
5ac

Colorless liquid. 97% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.14 (t, J = 2.8 Hz, 1H), 3.92-3.83 (m, 2H), 3.77-3.72 (m, 1H), 3.56-3.51 (m, 1H), 2.44 (sext, J = 2.5 Hz, 2H), 2.03-1.95 (m, 2H), 1.93-1.89 (m, 2H), 1.85-1.77 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 104.0, 81.6, 69.2, 67.1, 65.3, 32.4, 23.5, 20.1. QEFMS calcd for $[C_8H_{12}O_2Na]^+$: 163.07295, found: 163.07270.



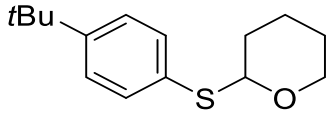
6a

Colorless liquid. 88% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 7.9 Hz, 2H), 5.14 (dd, J = 6.1, 2.1 Hz, 1H), 4.20-4.15(m, 1H), 3.59-3.54 (m, 1H), 2.32 (s, 3H), 2.05-1.98 (m, 1H), 1.90-1.77 (m, 2H), 1.68-1.58 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 137.1, 131.8, 131.5, 129.7, 85.8, 64.7, 31.7, 25.7, 21.8, 21.2. QEFMS calcd for $[C_{12}H_{16}OSNa]^+$: 231.08141, found: 231.08107.



6b

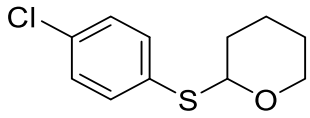
Colorless liquid. 89% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56-7.54 (m, 1H), 7.18-7.10 (m, 3H), 5.21 (dd, J = 5.6 Hz, 1.8 Hz, 1H), 4.20-4.14 (m, 1H), 3.63-3.58 (m, 1H), 2.40 (s, 3H), 2.09-2.02 (m, 1H), 1.95-1.84 (m, 2H), 1.71-1.59 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.3, 135.1, 130.4, 130.1, 126.6, 126.5, 84.6, 64.7, 31.9, 25.7, 21.8, 20.9. QEFMS calcd for $[C_{12}H_{16}OSNa]^+$: 231.08141, found: 231.08113.



6c

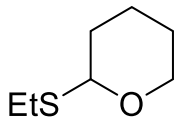
Colorless liquid. 96% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (d, J = 8.5 Hz, 2H), 7.31 (d, J = 8.5 Hz, 2H), 5.17 (d, J = 9.6 Hz, 1H), 4.21-4.16 (m, 1H), 3.61-

3.55 (m, 1H), 2.06-1.99 (m, 1H), 1.91-1.79 (m, 2H), 1.68-1.58 (m, 3H), 1.30 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.1, 131.8, 131.2, 126.0, 85.7, 64.6, 34.6, 31.7, 31.4, 25.7, 21.8. QEFMS calcd for $[C_{15}H_{22}OSNa]^+$: 273.12836, found: 273.12806.



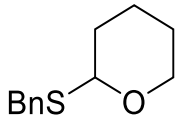
6d

Colorless liquid. 79% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.40 (d, J = 8.5 Hz, 2H), 7.25 (d, J = 8.6 Hz, 2H), 5.17 (t, J = 5.8 Hz, 1H), 4.17-4.13 (m, 1H), 3.60-3.56 (m, 1H), 2.05-1.99 (m, 1H), 1.88-1.78 (m, 2H), 1.68-1.60 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 134.0, 132.9, 132.3, 129.0, 85.4, 64.6, 31.6, 25.6, 21.7. QEFMS calcd for $[C_{11}H_{13}ClOSNa]^+$: 251.02678, found: 251.02649.



6e

Colorless liquid. 99% Isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.87 (dd, J = 6.7 Hz, 3.1 Hz, 1H), 4.11-4.07 (m, 1H), 3.53-3.48 (m, 1H), 2.72-2.54 (m, 2H), 1.95-1.90 (m, 1H), 1.85-1.80 (m, 1H), 1.71-1.65 (m, 1H), 1.61-1.53 (m, 3H), 1.28 (t, J = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 82.1, 64.9, 31.6, 25.8, 24.5, 22.0, 15.2. QEFMS calcd for $[C_7H_{14}SONa]^+$: 169.06576, found: 169.06565.



6f

Colorless liquid. 97% Isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26-7.21 (m, 4H), 7.18-7.14 (m, 1H), 4.63 (dd, J = 6.4 Hz, 2.7 Hz, 1H), 4.07-4.02 (m, 1H), 3.78 (d, J = 13.2 Hz, 1H), 3.64 (d, J = 13.2 Hz, 1H), 3.46-3.40 (m, 1H), 1.82-1.68 (m, 2H), 1.60-1.41 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.7, 129.1, 128.6, 126.9, 80.6, 64.4, 34.0, 30.9, 25.8, 21.7. QEFMS calcd for $[C_{12}H_{16}OSNa]^+$: 231.08141, found: 231.08119.

3. Catalyst stability test

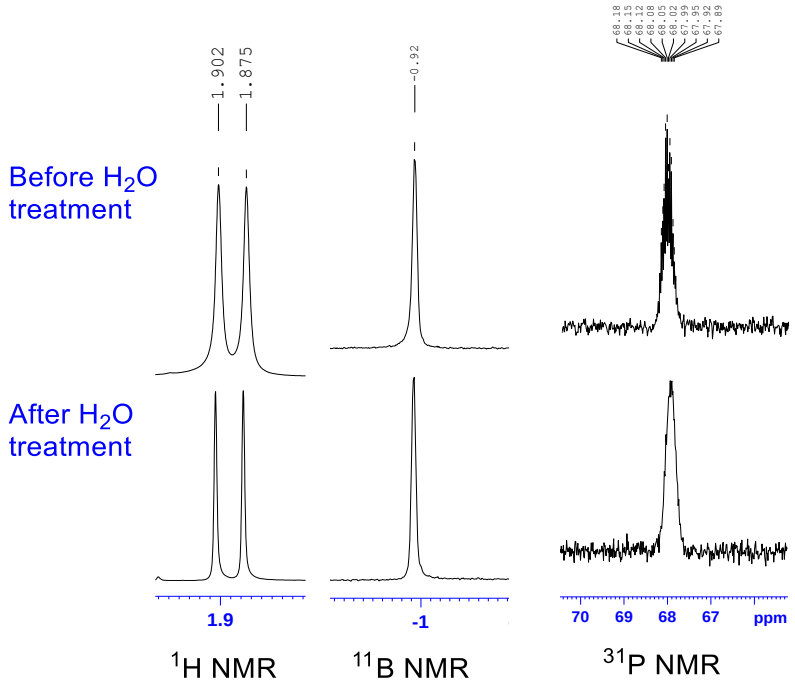
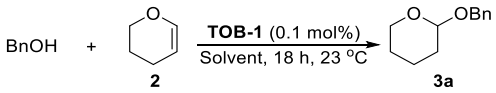


Figure S1. NMR experiments of **TOB-1** before and after treatment with water

*Note: **TOB-1** catalyst (0.1 mmol) was dissolved in H_2O (0.1 mL) and the solution was stirred at 23 ^oC for 12 h. Water was then removed under reduced pressure and the residue was dissolved in $CDCl_3$ for ^1H, ^{11}B, and ^{31}P NMR experiments.*

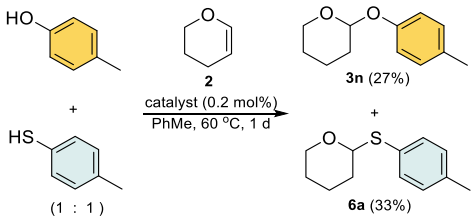
4. Solvent screening and temperature effect on the chemoselectivity

Table S1. Solvent screening[a]



Entry	Solvent	Yield [%]
1	$CHCl_3$ (no catalyst)	0
2	$CHCl_3$	93
3	CH_2Cl_2	40
4	$(CH_2Cl)_2$	50
5	THF	0
6	Acetone	14
7	MeCN	49
8	*n*-Hexane	17
9	PhMe	30

[a]Reaction were carried out with benzyl alcohols (0.20 mmol), 3,4-dihydro-2H-pyran (**2**) (0.24 mmol) and **TOB-1** (0.1 mol%) in solvent (0.4 mL) at 23 °C for 18 h. The yields were measured in NMR with dibromomethane as the internal standard.



Scheme S1. Study on the temperature effect on the chemoselective acetalization

5. NMR titration experiment with TOB-1 and benzyl alcohol

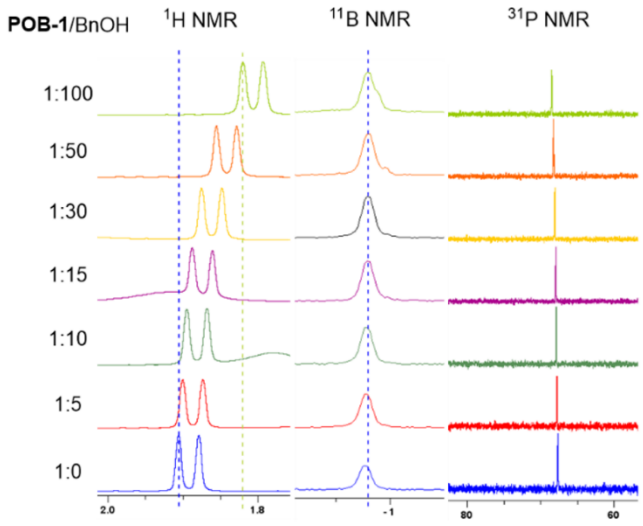


Figure S2. NMR titration experiment with **TOB-1** and benzyl alcohol

*Note: **TOB-1** catalyst (8.0 mg, 0.05 mmol, 1 equiv) was dissolved in $CDCl_3$ (0.4 mL) and the ^{1}H, ^{11}B and ^{31}P NMR spectra were obtained. Different amount of benzyl alcohol was then added and the ^{1}H, ^{11}B and ^{31}P NMR were obtained after each addition.*

6. Comparison of the chemical shift of alcohols and thiols

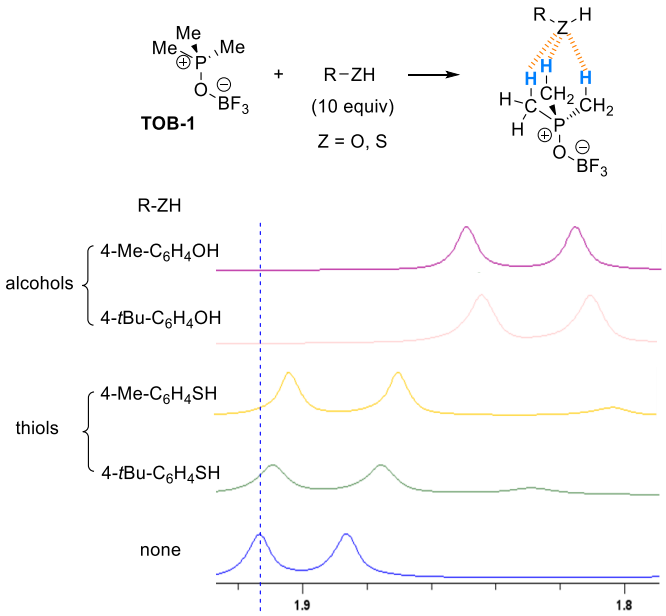


Figure S3. Comparison of the chemical shift of alcohols and thiols in the presence of **TOB-1**

*Note: **TOB-1** catalyst (8.0 mg, 0.05 mmol, 1 equiv) was dissolved in $CDCl_3$ (0.4 mL) and alcohol or thiol (0.5 mmol, 10 equiv) was added. ^1H NMR experiments were then carried out on these samples.*

7. X-ray crystal data of TOB-2

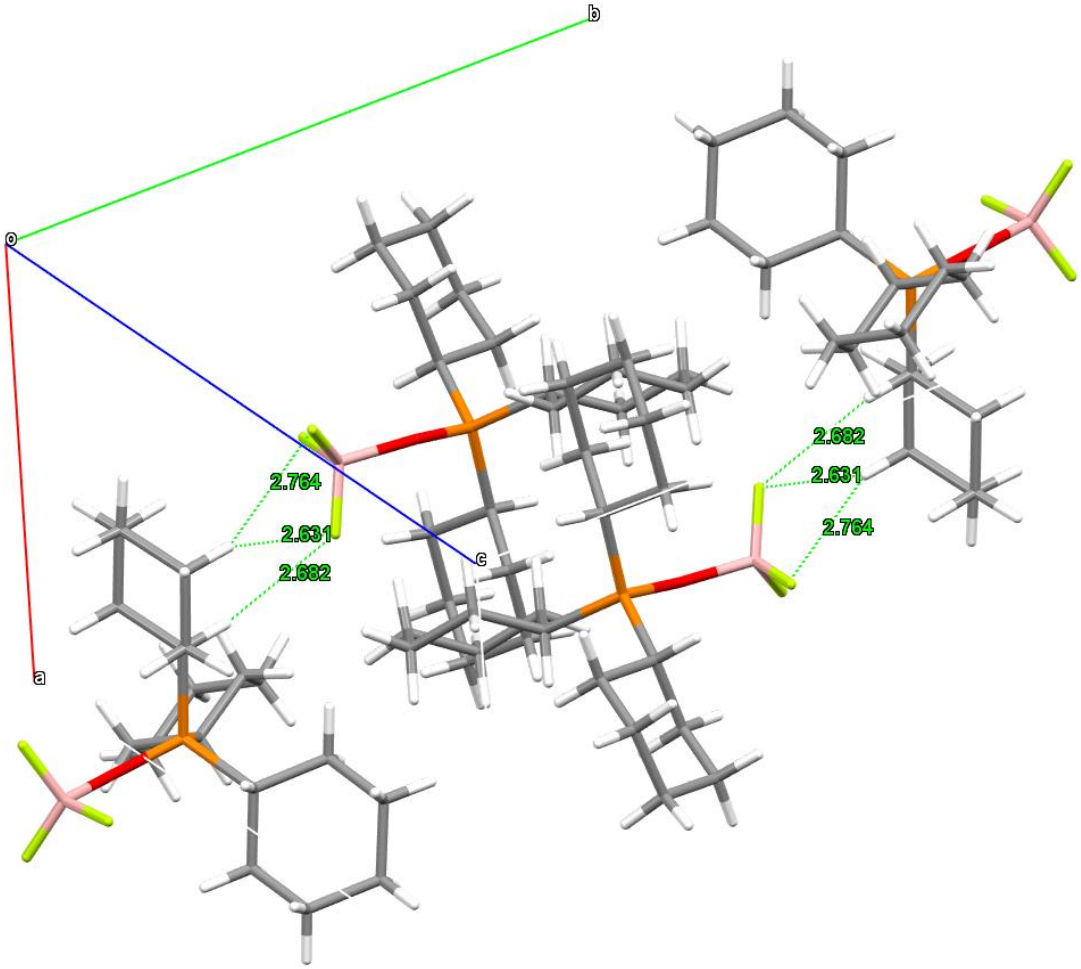


Figure S4. X-ray crystal packing of **TOB-2** (CCDC 2209696)

Crystal data and structure refinement for **TOB-2**.

Identification code	vinn1173pcy3obf3	
Empirical formula	C18 H33 B F3 O P	
Formula weight	364.22	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.9919(7) Å	α= 90°.
	b = 13.6548(12) Å	β= 94.856(3)°.
	c = 18.5379(18) Å	γ = 90°.
Volume	2015.7(3) $Å^3$	
Z	4	
Density (calculated)	1.200 Mg/m^3	
Absorption coefficient	0.165 mm^{-1}	
F(000)	784	
Crystal size	0.400 x 0.300 x 0.200 mm^3	
Theta range for data collection	2.662 to 25.248°.	
Index ranges	-9<=h<=8, -16<=k<=16, -22<=l<=22	
Reflections collected	20181	
Independent reflections	3631 [R(int) = 0.0290]	
Completeness to theta = 25.242°	99.3 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.7456 and 0.6570	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3631 / 0 / 245	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0469, wR2 = 0.1258	
R indices (all data)	R1 = 0.0610, wR2 = 0.1410	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.374 and -0.189 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **TOB-2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	6916(4)	3907(3)	3335(2)	92(1)
O(1)	5534(2)	4635(1)	3382(1)	64(1)
P(1)	3688(1)	4789(1)	3121(1)	41(1)
C(1)	3164(3)	6029(2)	3379(1)	53(1)
C(2)	4279(4)	6443(2)	3993(2)	83(1)
C(3)	3945(4)	7523(2)	4102(2)	90(1)
C(4)	2090(5)	7714(2)	4178(2)	101(1)
C(5)	983(4)	7291(2)	3588(2)	77(1)
C(6)	1318(3)	6209(2)	3472(1)	59(1)
C(7)	2363(2)	3908(1)	3522(1)	45(1)
C(8)	2498(3)	2874(2)	3215(1)	59(1)
C(9)	1327(3)	2175(2)	3571(2)	74(1)
C(10)	1648(4)	2176(2)	4389(2)	86(1)
C(11)	1546(3)	3193(2)	4695(1)	77(1)
C(12)	2726(3)	3893(2)	4348(1)	63(1)
C(13)	3405(3)	4703(1)	2146(1)	46(1)
C(14)	4599(3)	5383(2)	1778(1)	73(1)
C(15)	4412(4)	5244(2)	961(2)	85(1)
C(16)	2623(5)	5378(2)	656(1)	86(1)
C(17)	1449(4)	4715(2)	1018(1)	80(1)
C(18)	1598(3)	4857(2)	1834(1)	57(1)
F(1)	6354(5)	3245(4)	2780(2)	105(2)
F(2)	8272(6)	4347(5)	3165(6)	154(4)
F(3)	7084(11)	3387(6)	3951(3)	146(4)
F(1')	6682(18)	3102(8)	3440(30)	298(18)
F(2')	7850(20)	4271(15)	2848(12)	205(9)
F(3')	8027(18)	4318(18)	3929(9)	202(8)

Bond lengths [Å] and angles [°] for **TOB-2**.

B(1)-F(1')	1.134(10)
B(1)-F(2)	1.302(6)
B(1)-F(2')	1.317(16)
B(1)-F(3)	1.341(6)
B(1)-F(1)	1.414(6)
B(1)-F(3')	1.466(13)
B(1)-O(1)	1.494(4)
O(1)-P(1)	1.5275(14)
P(1)-C(7)	1.8045(19)
P(1)-C(13)	1.805(2)
P(1)-C(1)	1.819(2)
C(1)-C(2)	1.496(3)
C(1)-C(6)	1.520(3)
C(2)-C(3)	1.515(4)
C(3)-C(4)	1.524(5)
C(4)-C(5)	1.466(4)
C(5)-C(6)	1.520(3)
C(7)-C(8)	1.529(3)
C(7)-C(12)	1.534(3)
C(8)-C(9)	1.526(3)
C(9)-C(10)	1.516(4)
C(10)-C(11)	1.506(4)
C(11)-C(12)	1.522(3)
C(13)-C(18)	1.524(3)
C(13)-C(14)	1.533(3)
C(14)-C(15)	1.520(4)
C(15)-C(16)	1.503(4)
C(16)-C(17)	1.502(4)
C(17)-C(18)	1.521(3)
F(1')-B(1)-F(2')	126.4(18)
F(2)-B(1)-F(3)	115.2(5)
F(2)-B(1)-F(1)	109.8(6)
F(3)-B(1)-F(1)	106.5(5)
F(1')-B(1)-F(3')	110.0(16)
F(2')-B(1)-F(3')	91.6(10)
F(1')-B(1)-O(1)	120.1(7)

F(2)-B(1)-O(1)	110.0(4)
F(2')-B(1)-O(1)	104.6(8)
F(3)-B(1)-O(1)	108.9(4)
F(1)-B(1)-O(1)	106.1(3)
F(3')-B(1)-O(1)	96.0(6)
B(1)-O(1)-P(1)	140.5(2)
O(1)-P(1)-C(7)	111.21(9)
O(1)-P(1)-C(13)	110.18(10)
C(7)-P(1)-C(13)	109.96(9)
O(1)-P(1)-C(1)	106.40(9)
C(7)-P(1)-C(1)	110.83(10)
C(13)-P(1)-C(1)	108.17(10)
C(2)-C(1)-C(6)	112.0(2)
C(2)-C(1)-P(1)	114.62(17)
C(6)-C(1)-P(1)	115.34(15)
C(1)-C(2)-C(3)	111.6(2)
C(2)-C(3)-C(4)	111.3(3)
C(5)-C(4)-C(3)	113.1(3)
C(4)-C(5)-C(6)	112.8(2)
C(5)-C(6)-C(1)	110.9(2)
C(8)-C(7)-C(12)	110.24(17)
C(8)-C(7)-P(1)	113.54(14)
C(12)-C(7)-P(1)	110.66(14)
C(9)-C(8)-C(7)	110.6(2)
C(10)-C(9)-C(8)	112.0(2)
C(11)-C(10)-C(9)	111.5(2)
C(10)-C(11)-C(12)	111.4(2)
C(11)-C(12)-C(7)	111.00(19)
C(18)-C(13)-C(14)	110.66(19)
C(18)-C(13)-P(1)	113.92(14)
C(14)-C(13)-P(1)	112.13(16)
C(15)-C(14)-C(13)	110.8(2)
C(16)-C(15)-C(14)	111.7(2)
C(17)-C(16)-C(15)	111.6(2)
C(16)-C(17)-C(18)	111.6(2)
C(17)-C(18)-C(13)	110.6(2)

Symmetry transformations used to generate equivalent atoms:

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **TOB-2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	43(2)	115(3)	117(3)	22(3)	8(2)	24(2)
O(1)	33(1)	78(1)	81(1)	3(1)	-3(1)	5(1)
P(1)	31(1)	45(1)	46(1)	1(1)	2(1)	0(1)
C(1)	50(1)	48(1)	61(1)	-6(1)	5(1)	-5(1)
C(2)	76(2)	75(2)	92(2)	-24(2)	-21(2)	-8(1)
C(3)	116(3)	64(2)	86(2)	-25(2)	-11(2)	-20(2)
C(4)	136(3)	72(2)	93(2)	-32(2)	5(2)	12(2)
C(5)	85(2)	62(2)	86(2)	-12(1)	18(2)	16(1)
C(6)	56(1)	60(1)	63(1)	-13(1)	7(1)	9(1)
C(7)	36(1)	49(1)	48(1)	8(1)	1(1)	1(1)
C(8)	58(1)	49(1)	70(1)	4(1)	3(1)	-3(1)
C(9)	65(2)	56(1)	102(2)	17(1)	2(1)	-12(1)
C(10)	69(2)	85(2)	102(2)	46(2)	2(2)	-9(1)
C(11)	68(2)	100(2)	62(2)	31(1)	8(1)	-6(1)
C(12)	64(1)	76(2)	49(1)	14(1)	1(1)	-6(1)
C(13)	50(1)	45(1)	46(1)	1(1)	10(1)	2(1)
C(14)	70(2)	86(2)	67(2)	14(1)	22(1)	-15(1)
C(15)	115(3)	80(2)	66(2)	15(1)	43(2)	-1(2)
C(16)	132(3)	77(2)	48(1)	13(1)	10(2)	12(2)
C(17)	99(2)	88(2)	50(1)	2(1)	-9(1)	-6(2)
C(18)	58(1)	65(1)	47(1)	2(1)	-1(1)	-2(1)
F(1)	89(2)	108(3)	119(3)	-24(2)	16(2)	41(2)
F(2)	31(2)	138(4)	295(11)	28(5)	26(3)	-8(2)
F(3)	147(5)	176(8)	111(3)	55(3)	-11(3)	76(5)
F(1')	116(10)	57(5)	730(50)	71(18)	90(20)	8(5)
F(2')	121(11)	309(19)	200(13)	-16(11)	104(11)	67(12)
F(3')	115(8)	270(20)	203(12)	-2(12)	-84(8)	58(11)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for **TOB-2**.

	x	y	z	U(eq)
H(1A)	3396	6431	2961	63
H(2A)	5443	6352	3897	99
H(2B)	4095	6090	4434	99
H(3A)	4295	7889	3692	108
H(3B)	4602	7750	4533	108
H(4A)	1796	7444	4634	121
H(4B)	1904	8416	4192	121
H(5A)	1136	7643	3144	92
H(5B)	-175	7375	3695	92
H(6A)	644	5982	3045	71
H(6B)	992	5839	3884	71
H(7A)	1198	4123	3417	54
H(8A)	2206	2886	2697	71
H(8B)	3646	2644	3300	71
H(9A)	172	2365	3439	89
H(9B)	1482	1517	3391	89
H(10A)	827	1760	4595	103
H(10B)	2753	1906	4524	103
H(11A)	1836	3173	5213	92
H(11B)	403	3432	4612	92
H(12A)	3879	3691	4471	75
H(12B)	2591	4547	4538	75
H(13A)	3708	4033	2021	56
H(14A)	4355	6058	1893	88
H(14B)	5748	5245	1960	88
H(15A)	5120	5713	738	102
H(15B)	4787	4592	845	102
H(16A)	2291	6054	721	103
H(16B)	2540	5242	141	103
H(17A)	1702	4039	908	96
H(17B)	304	4848	827	96
H(18A)	870	4395	2053	68
H(18B)	1238	5514	1948	68

8. Kinetic Study of the Acetalization Reaction

Four NMR tubes charged with $CDCl_3$ (0.4 mL) and internal standard mesitylene (27.8 μL, 0.2 mmol, 1 equiv). Different amounts of benzyl alcohol, 3,4-dihydropyran **2** and **TOB-1** were added to the four NMR tubes according to the following table.

Entry	Benzyl alcohol	3,4-Dihydropyran	TOB-1
I	20.7 μL(1 equiv.)	18.2 μL (1 equiv.)	1 mol %
II	10.4 μL (0.5 equiv.)	18.2 μL (1 equiv.)	1 mol %
III	20.7 μL (1 equiv.)	9.1 μL (0.5 equiv.)	1 mol %
IV	20.7 μL (1 equiv.)	18.2 μL (1 equiv.)	0.5 mol %

The reactions were monitored by ^{1}H NMR experiments in 1.5 hour. The NMR yield of the product were recorded and the curves of the amount of acetal product against time were plotted. A polynomial trendline of the graph was obtained and the initial rates were determined (Figure S5-S7). The rate orders of different reactants are summarized in Table S2.

Table S2. Rate order of different Reactants

Reactants	Rate Order
Benzyl alcohol	1.048
3,4-Dihydropyran **2**	1.034
TOB-1	1.040

(i) Kinetic study of benzyl alcohol

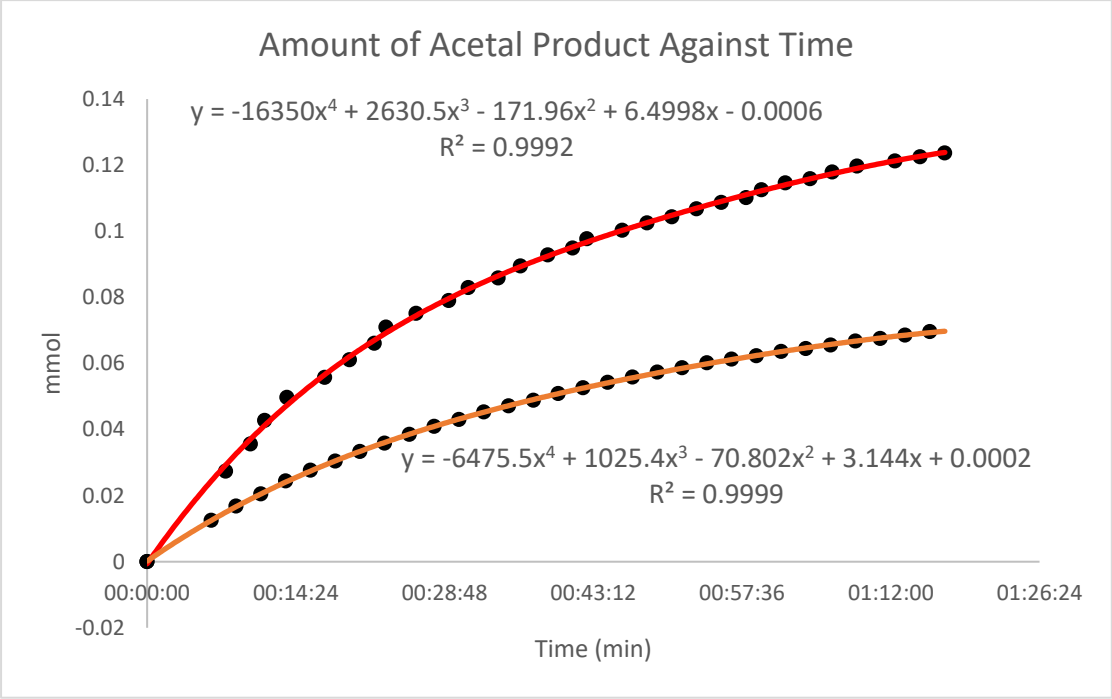


Figure S5. Kinetic study of benzyl alcohol

Rate I = $k[BnOH]^x[3,4\text{-Dihydropyran}]^y[\mathbf{TOB\text{-}1}]^z$

= $\frac{dy}{dt}$ (at t=0)

= 6.4998

Rate II = $k\frac{1}{2^x}[BnOH]^x[3,4\text{-Dihydropyran}]^y[\mathbf{TOB\text{-}1}]^z$

= $\frac{dy}{dt}$ (at t=0)

= 3.144

$\frac{Rate\ I}{Rate\ II} = 2^x$

x = 1.048

Rate Order of benzyl alcohol = 1.048

(ii) Kinetic study of 3,4-dihydropyran **2**

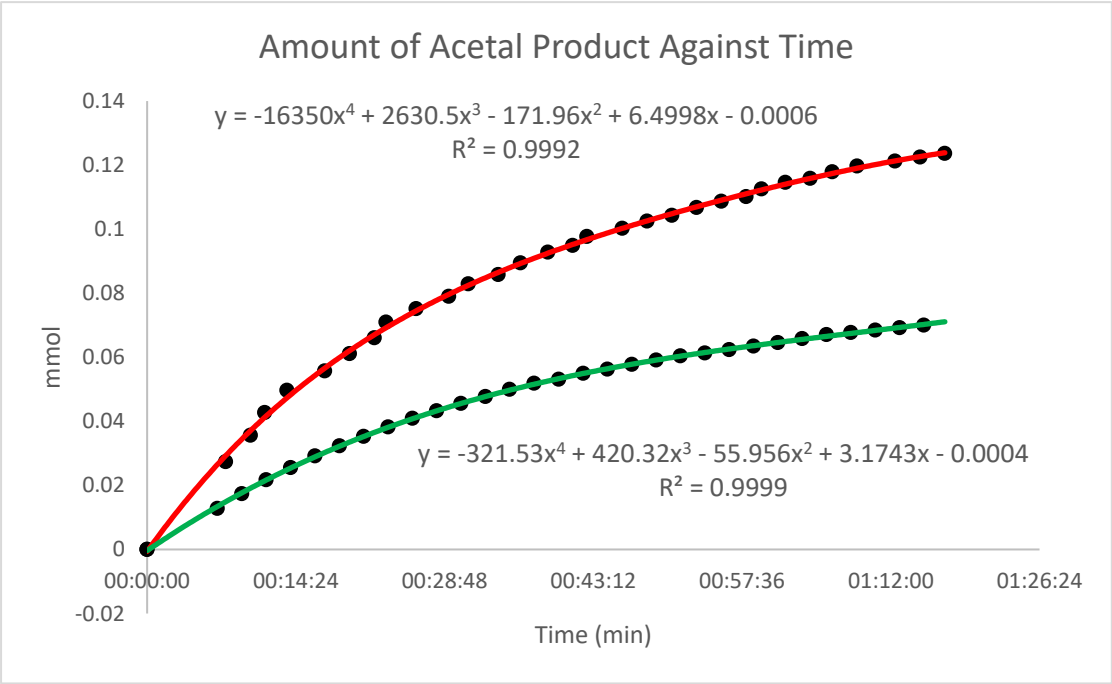


Figure S6. Kinetic study of 3,4-dihydropyran **2**

Rate I = $k[BnOH]^x[3,4\text{-Dihydropyran}]^y[\mathbf{TOB\text{-}1}]^z$

= $\frac{dy}{dt}$ (at t=0)

= 6.4998

Rate III = $k[BnOH]^x \frac{1}{2^y}[3,4\text{-Dihydropyran}]^y[\mathbf{TOB\text{-}1}.]^z$

= $\frac{dy}{dt}$ (at t=0)

= 3.1743

$\frac{Rate\ I}{Rate\ III} = 2^y$

y = 1.034

Kinetic Order of 3,4-dihydropyran **2** = 1.034

(iii) Kinetic study of catalyst **TOB-1**

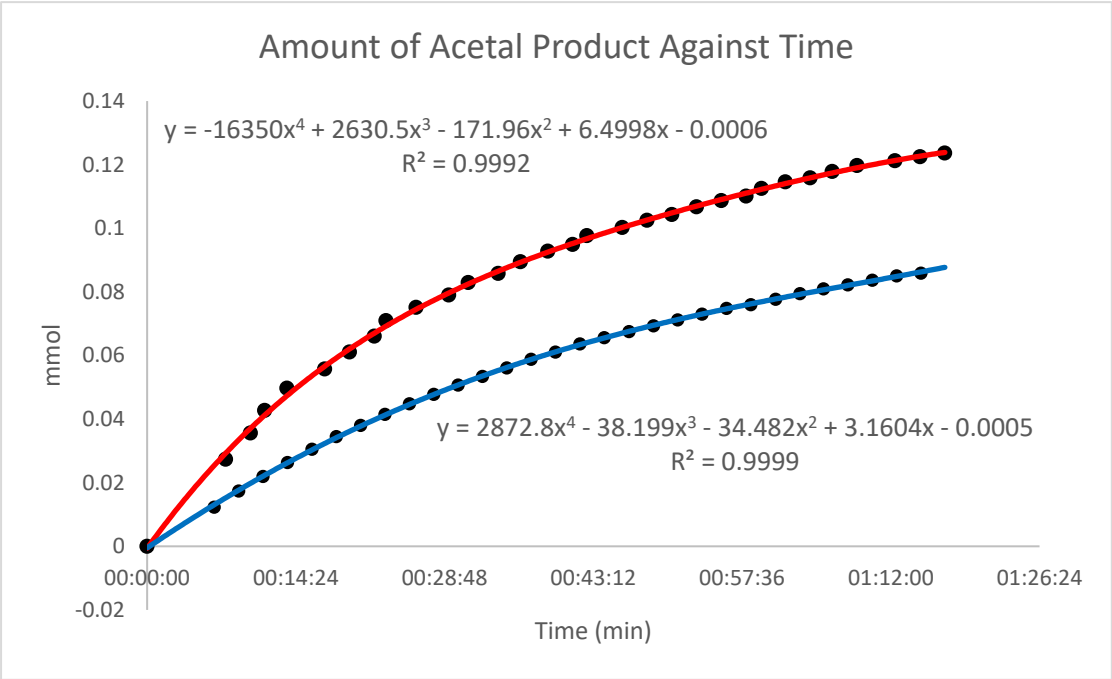


Figure S7. Kinetic study of catalyst **TOB-1**

Rate I = $k[\text{BnOH}]^x[\text{3,4-Dihydropyran}]^y[\textbf{TOB-1}]^z$

= $\frac{dy}{dt}$ (at t=0)

= 6.4998

Rate IV = $k[\text{BnOH}]^x[\text{3,4-Dihydropyran}]^y \frac{1}{2^z}[\textbf{TOB-1}]^z$

= $\frac{dy}{dt}$ (at t=0)

= 3.1604

$$\frac{Rate\ I}{Rate\ IV} = 2^z$$

z = 1.040

Kinetic Order of **TOB-1** = 1.040

9. Computational studies

All Density Functional Theory (DFT) calculations were carried out using M06-2X hybrid functional[2] with Grimme D3 dispersion correction.[3] These systems were studied in SMD solvents (chloroform and toluene)[4] with Gaussian 16 (ver. C.02).[5] Their geometries were optimized with 6-311G(d) basis set, while the single-point energies, electrostatic potential calculations, and NBO analyses were performed with aug-cc-pVTZ basis set. For binding energy calculations, basis set superposition errors (BSSE) were handled by a counterpoise procedure.[6] Based on the electrostatic potential (ESP) map of **TOB-1**, positive charges are shown to be localized at the methyl groups and phosphonium centre, suggesting that these positions are potential active sites of the catalyst. To investigate the interactions of the trilateral complexes formed between **2**, **TOB-1**, and the alcohol/thiol, configurational searches were performed by initially placing **2** and the alcohol/thiol near the potential active sites at methyl groups and phosphonium centre of **TOB-1**. Several optimized configurations were obtained, and the one with strongest binding between **2** and the complex of the other two species was selected for further study. Additional optimizations of the complexes were done with different implicit SMD solvents to study the solvent effect on the O/S chemoselectivity in the acetalization. The E(2) stabilization energies were computed with second order perturbation theory analysis in NBO basis.[7] Atoms In Molecules (AIM)[8] analysis and electrostatic potential (ESP) map generation was done by Multiwfn 3.8.[9]

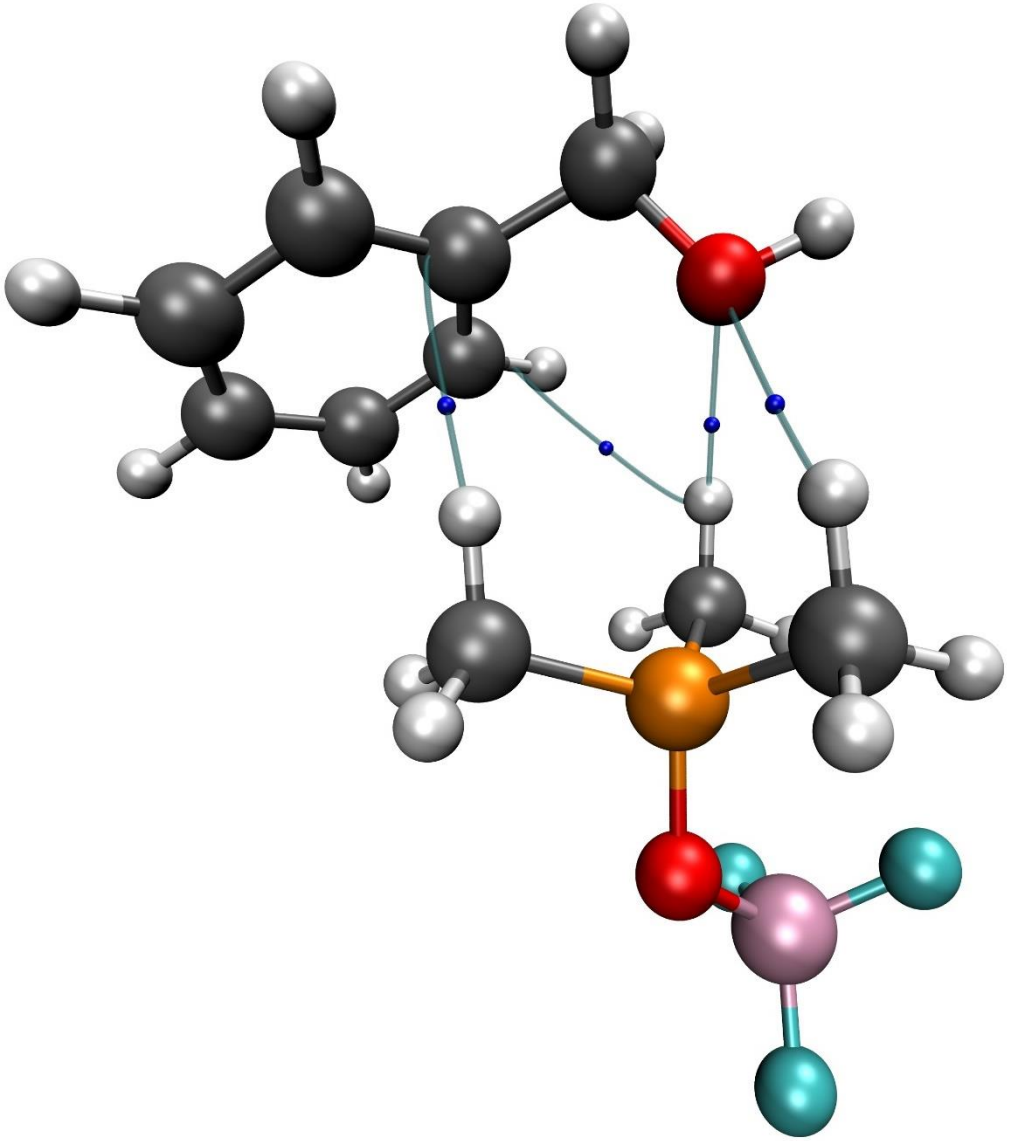


Figure S8. AIM bond paths in complex **A**

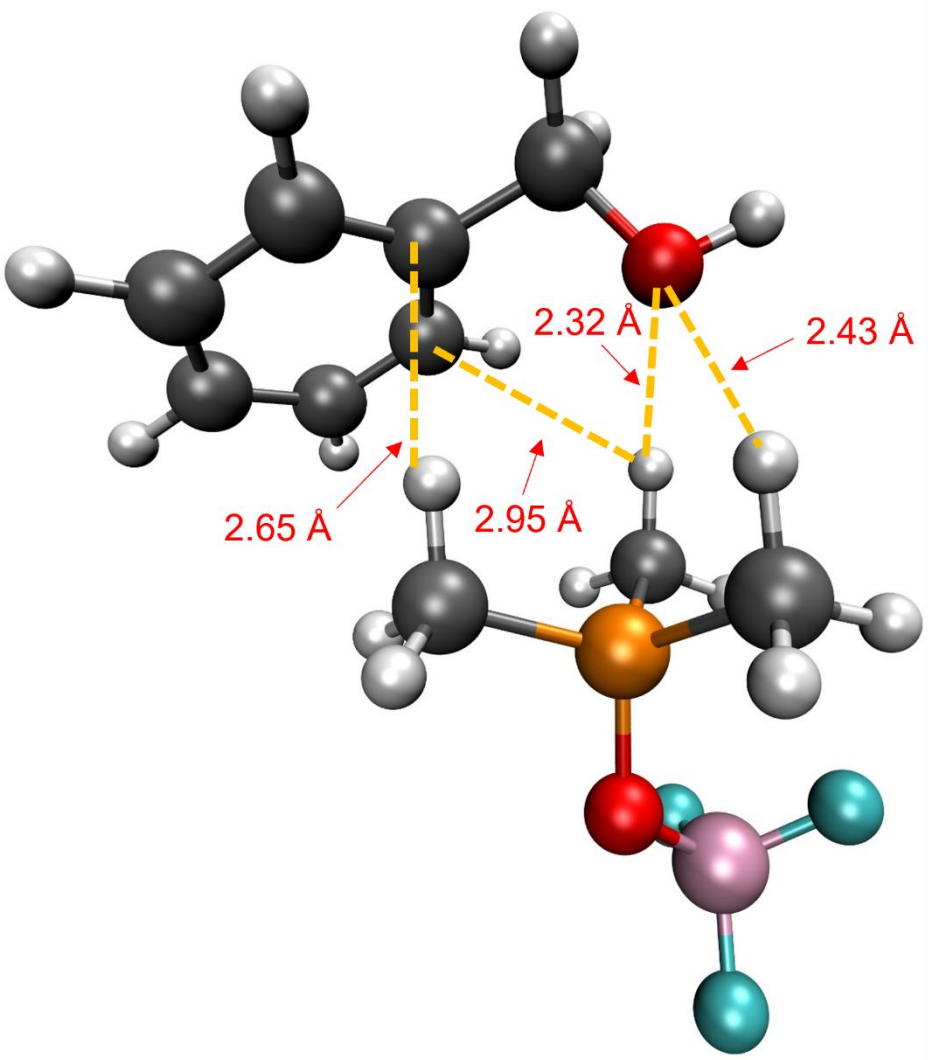


Figure S9. Snapshot of the optimized structure of complex **A**

*Note: Binding energy between **TOB-1** and BnOH (M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(chloroform)) = -5.12 kcal/mol*

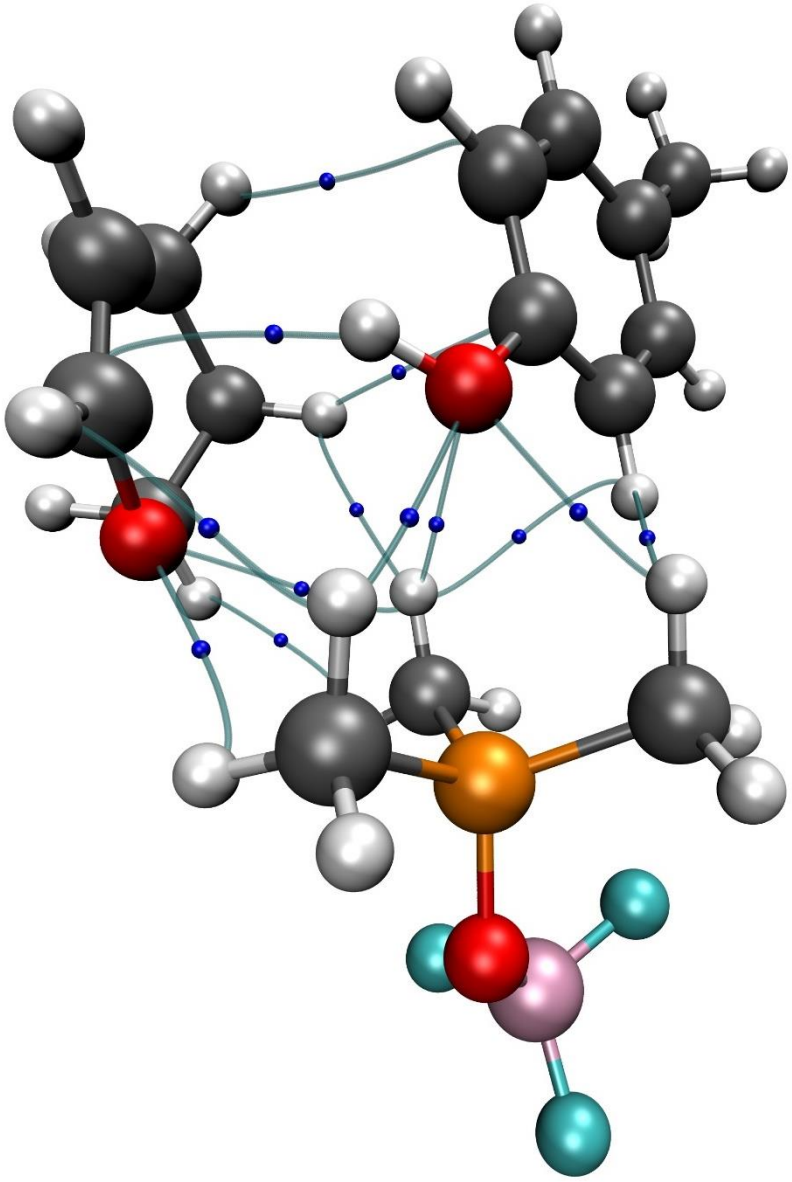


Figure S10. AIM bond paths in complex **B**

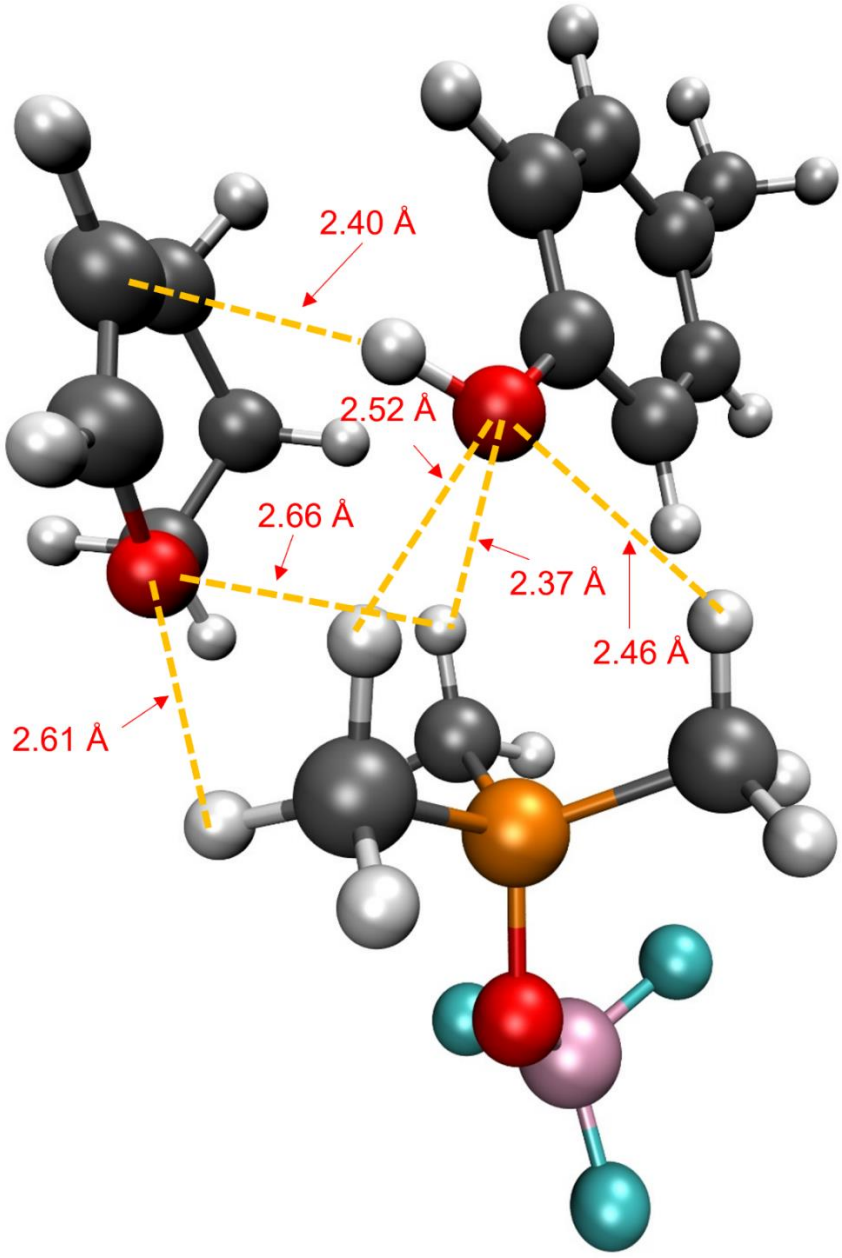


Figure S11. Snapshot of the optimized structure of complex **B**

*Note: Binding energy between **2** and the complex of **TOB-1** and 4-Me-C_6H_4-OH (M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -7.97 kcal/mol*

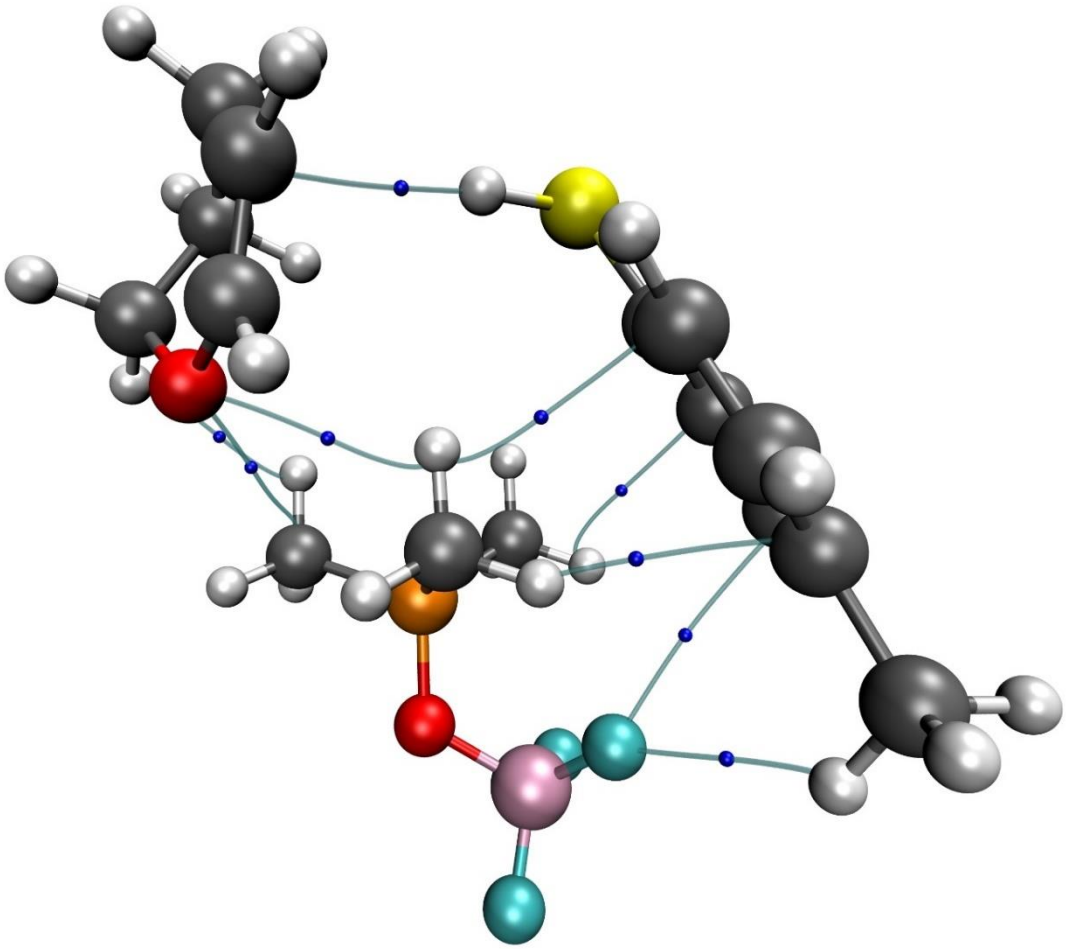


Figure S12. AIM bond paths in complex **C**

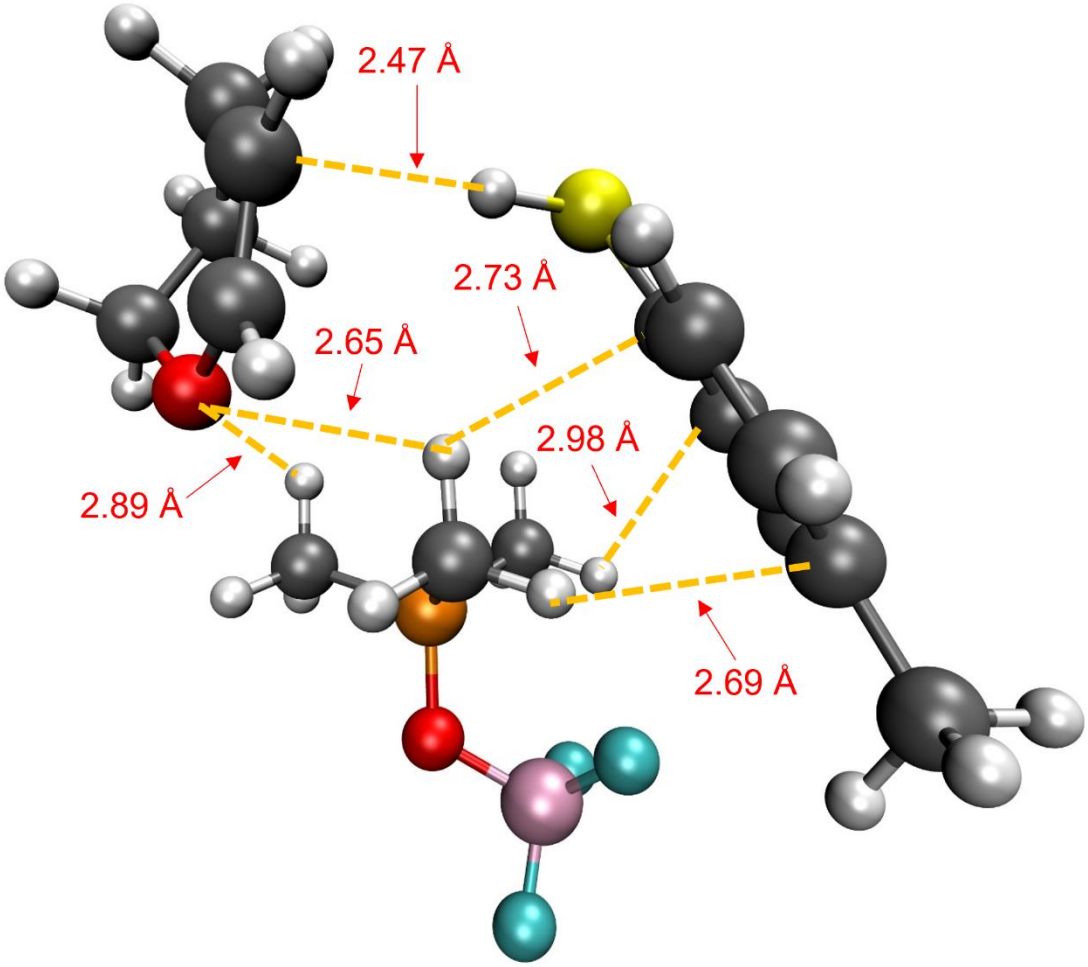


Figure S13. Snapshot of the optimized structure of complex **C**

*Note: Binding energy between **2** and the complex of **TOB-1** and 4-Me-C_6H_4-SH (M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -5.64 kcal/mol*

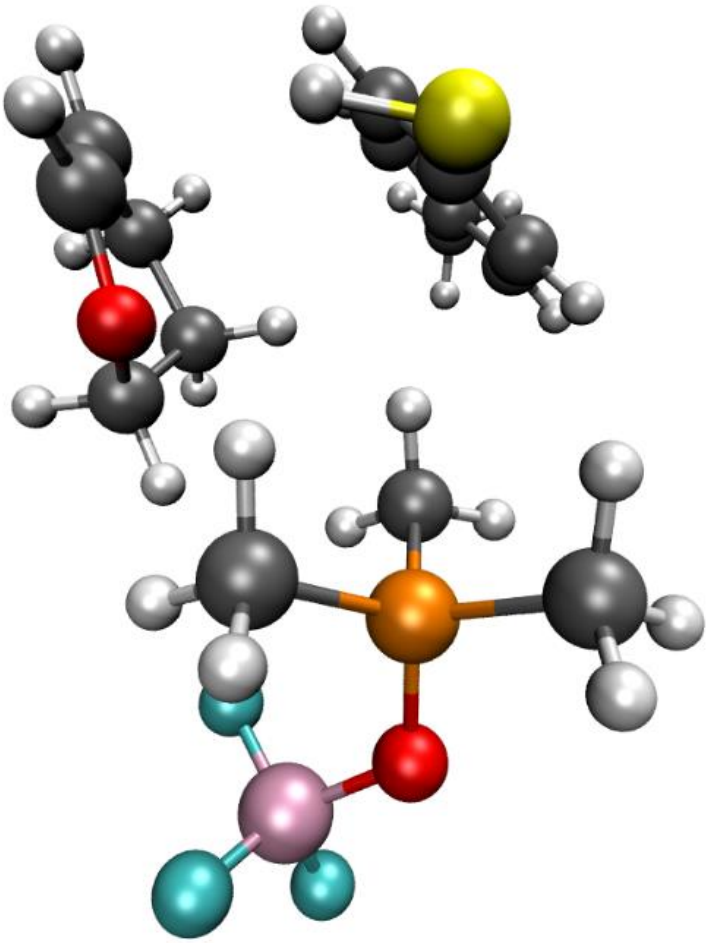
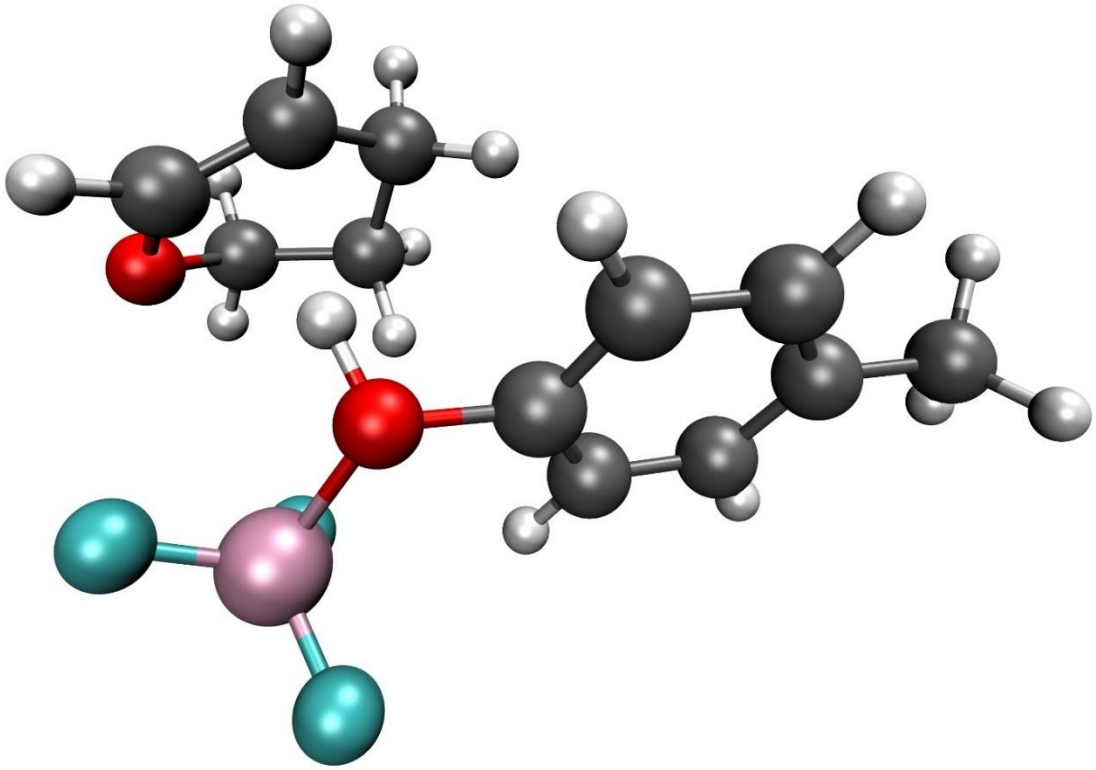
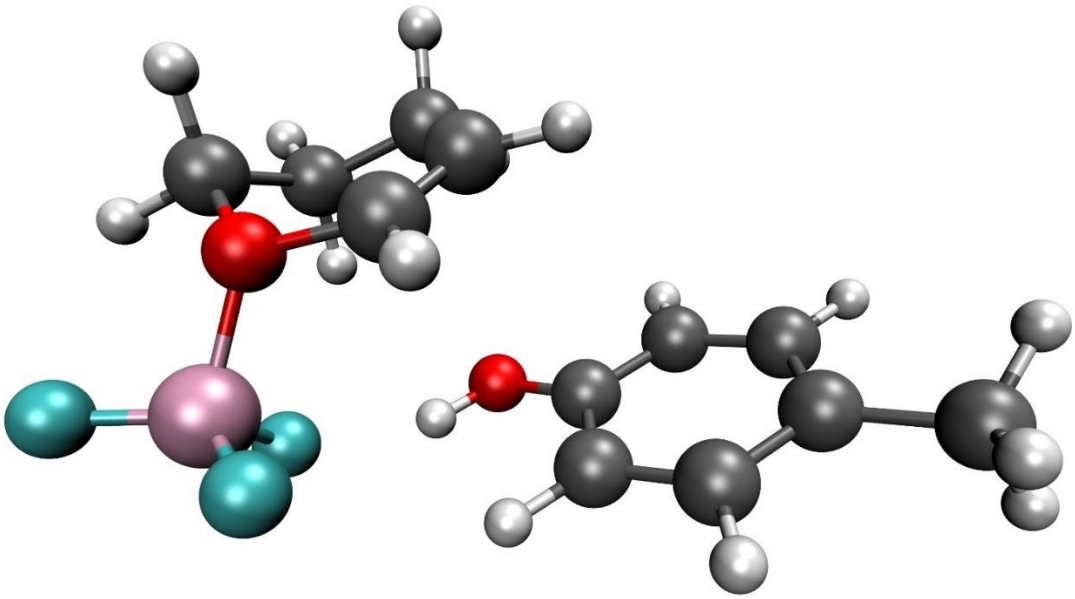


Figure S14. Snapshot of complex **C'** with sulfur positioned close to the C(sp^3)-H

*Note: Binding energy between **2** and the complex of **TOB-1** and 4-Me-C_6H_4-SH (M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -4.30 kcal/mol*



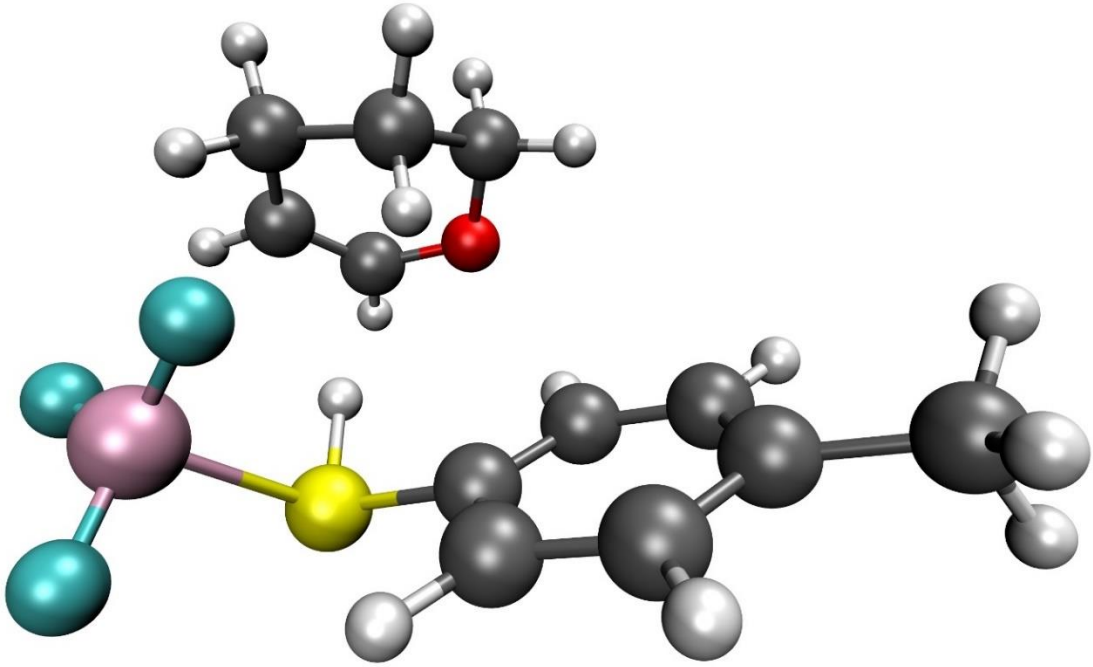
(D)



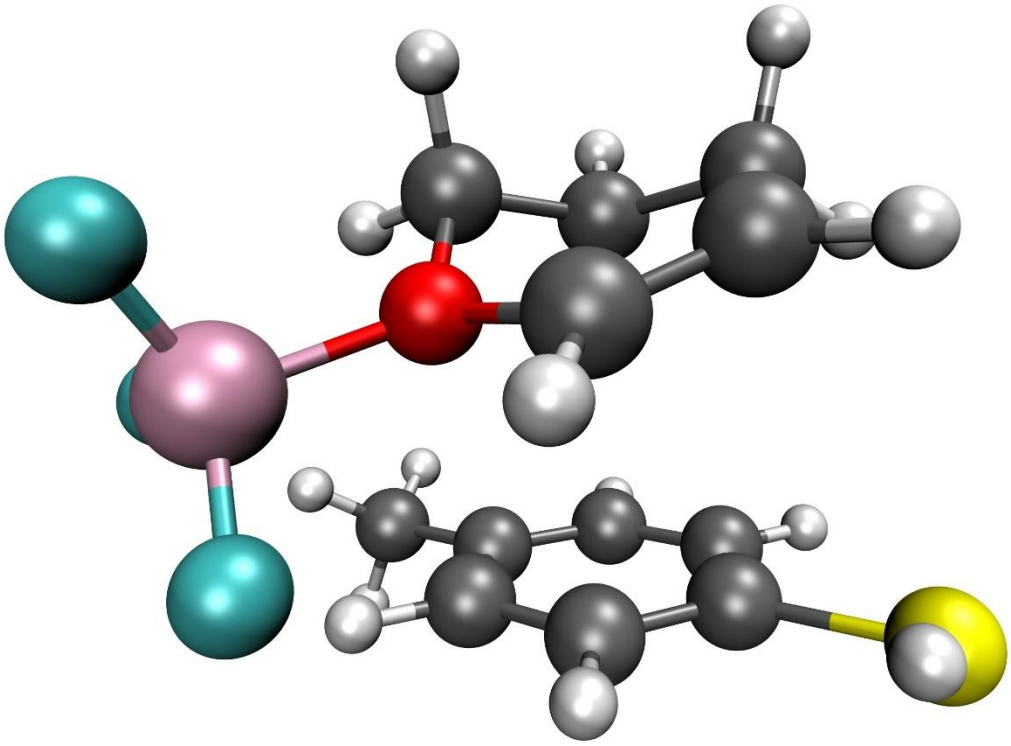
(D')

Figure S15. Snapshots of complexes **D** and **D'**

*Note: In the calculation, bilateral complexes **D** (BF_3 complexed with 4-Me-C_6H_4-OH) and **D'** (BF_3 complexed with **2**) were found but no trilateral complex was identified.*



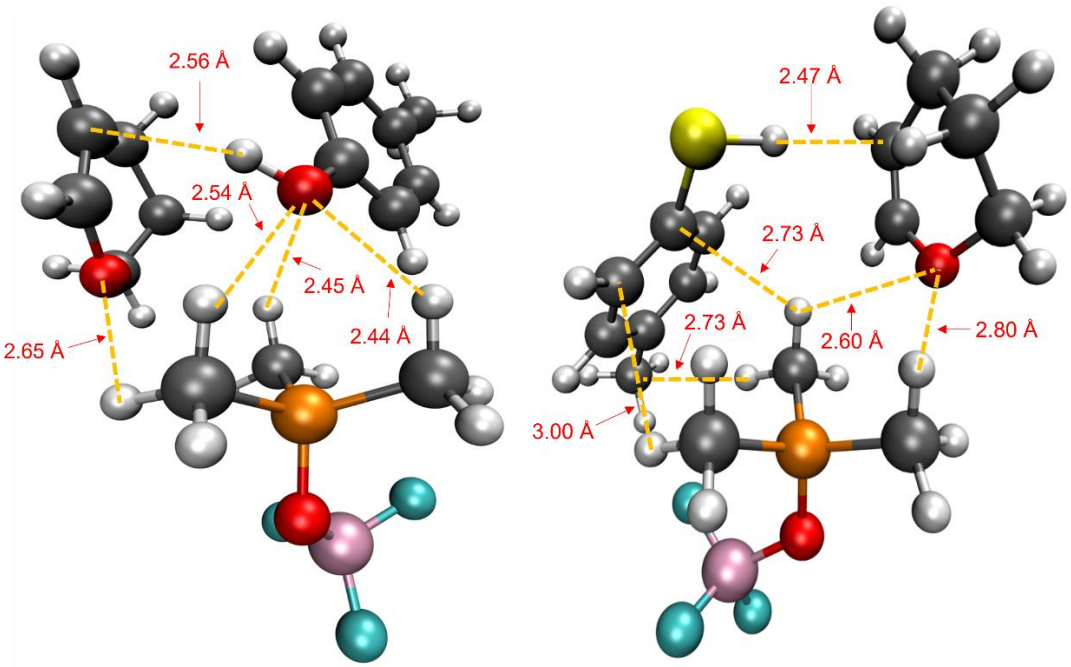
(E)



(E')

Figure S16. Snapshots of complexes **E** and **E'**.

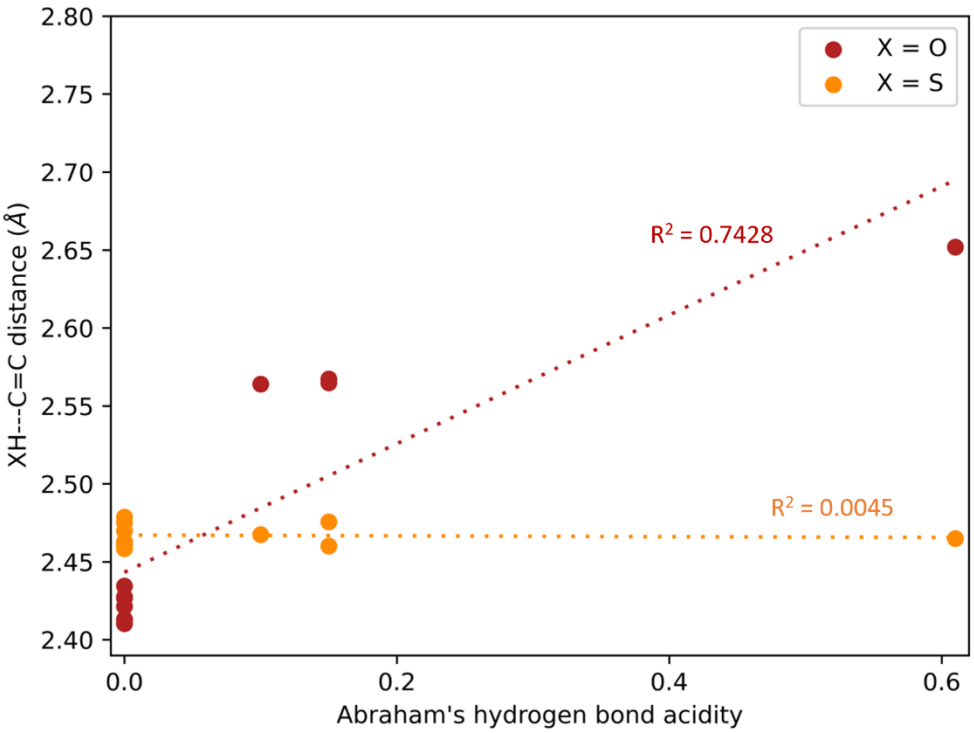
*Note: In the calculation, bilateral complexes **E** (BF_3 complexed with 4-Me-C_6H_4-SH) and **E'** (BF_3 complexed with **2**) were found but no trilateral complex was identified.*



(Complex B in SMD chloroform) **(Complex C in SMD chloroform)**

Figure S17. Snapshots of complexes **B** and **C** in SMD chloroform

*Note: Implicit SMD solvent model investigation was conducted to get a better understanding on the solvent effect. It was observed that the interactions in trilateral complex **B** was considerably interrupted when changing the solvent from toluene to chloroform. In particular, the OH-C(pyran) bond length significantly elongated from 2.40 to 2.56 Å. In contrast, the bond lengths in the trilateral complex **C** are consistent in toluene and chloroform.*



SMD solvent	Abraham's hydrogen bond acidity	OH---C=C (Å)	SH---C=C (Å)
hexane	0.00	2.41	2.48
toluene	0.00	2.41	2.47
chlorobenzene	0.00	2.43	2.46
dibutylether	0.00	2.42	2.46
tetrachloromethane	0.00	2.41	2.48
dichlormethane	0.10	2.56	2.47
chloroform	0.15	2.57	2.48
bromoform	0.15	2.56	2.46
acetic acid	0.61	2.65	2.46

Figure S18. Correlation between Abraham's hydrogen bond acidity[10] of some selected SMD solvents and the intermolecular distances between the 4-Me-C_6H_4-OH/4-Me-C_6H_4-SH and dihydropyran in their trilateral complexes with **TOB-1**

Cartesian coordinates

Complex A

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(chloroform)) = -1207.79728075

C	3.39670700	-2.23936500	-0.04561900
H	3.44743900	-3.31432400	-0.17469000
C	2.84969000	-1.70157400	1.11866300
H	2.47797000	-2.35806700	1.89723000
C	3.88229800	-1.39445200	-1.03738000
H	4.31231600	-1.80890900	-1.94182100
C	3.81331500	-0.01267900	-0.87048700
H	4.18313100	0.64779400	-1.64822800
C	3.26272900	0.53259700	0.28697200
C	2.78532500	-0.32331500	1.28266100
H	2.36147500	0.09782900	2.18909700
C	3.10253300	2.01919600	0.44314200
H	3.44933500	2.33257100	1.43340600
H	3.69160400	2.54250300	-0.31606300
O	1.71258400	2.32223600	0.29464900
H	1.58479600	3.25131800	0.51846500
P	-1.10850100	0.15685400	-0.45226700
C	-0.75975200	0.37963500	1.28975700
H	-0.61097000	-0.59422400	1.75894900
H	0.14042000	0.99169400	1.37511100
H	-1.60584900	0.88505900	1.75772500
C	0.20006300	-0.78445300	-1.22183500
H	0.26823000	-1.76132300	-0.74114900
H	-0.03348800	-0.91179400	-2.28061700
H	1.14347600	-0.24662000	-1.11147700
C	-1.20577300	1.76417000	-1.23837400
H	-1.48686000	1.62835600	-2.28435400
H	-1.96233400	2.36573600	-0.73391800
H	-0.22794300	2.24501800	-1.17121400
O	-2.42908900	-0.65462100	-0.67227200
B	-3.66866000	-0.41708700	0.14627200
F	-3.78850900	0.96985900	0.35103900
F	-4.74202000	-0.91853400	-0.55966100
F	-3.51310500	-1.05571300	1.37553000

Complex B

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -1478.34109403

C	-4.04898080	-2.44064538	0.27616579
C	-2.68236883	-2.71134249	0.38759531
H	-2.35871816	-3.61297490	0.89770295
C	-4.42938244	-1.27396617	-0.38319905
H	-5.48349079	-1.04002328	-0.48918146
C	-3.48506440	-0.40227138	-0.91858805
H	-3.79628141	0.49602654	-1.44312566
C	-2.13114352	-0.68814577	-0.78603593
C	-1.72690419	-1.84925389	-0.13078435
H	-0.66920182	-2.06273834	-0.02653048
C	-5.06758307	-3.39375640	0.84505396
H	-6.07820051	-2.99489355	0.74772147
H	-5.03457663	-4.35627397	0.32775431
H	-4.87911778	-3.58450766	1.90435328
O	-1.16345340	0.14363826	-1.28273085
H	-1.54063311	1.02760783	-1.40918514
P	2.22828799	-0.02266272	-0.74470573
C	1.33536590	0.03699121	0.80922316
H	1.75745313	0.84389304	1.40969570
H	0.28109599	0.22265464	0.60615405
H	1.47862600	-0.90695298	1.33678546
C	1.89690882	1.44814552	-1.71068539
H	2.05708373	2.33191971	-1.09288115
H	2.58072820	1.45868132	-2.56160190
H	0.86673951	1.42049073	-2.06569402
C	1.71426849	-1.45012444	-1.70351962
H	2.33859121	-1.50219154	-2.59806650
H	1.86791917	-2.35401259	-1.11371127
H	0.66746641	-1.34497532	-1.99156422
O	3.76822759	-0.05104644	-0.49870237
B	4.37225649	-0.90405369	0.60232699
F	3.63619585	-2.10490032	0.63640927
F	5.69119115	-1.11798187	0.29139337
F	4.20991660	-0.22586006	1.80565181
C	-0.99247708	3.16010268	-0.69024905
H	-0.48964188	3.44349432	-1.60937898

C	-2.32309788	3.14413920	-0.56368703
H	-2.91638367	3.46730834	-1.41128347
C	-2.99824964	2.72950609	0.71765496
H	-3.84114718	2.06680136	0.50618675
H	-3.41358107	3.61068610	1.21858737
C	-1.98761870	2.02859648	1.62763625
H	-2.35264460	1.97387855	2.65481895
H	-1.82174382	1.00213067	1.28563911
C	-0.67036266	2.78655259	1.60349696
H	0.08674231	2.31677772	2.22958338
H	-0.81778362	3.81850756	1.94172919
O	-0.10858599	2.83370918	0.28429394

Complex C

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -1801.30294136

C	-1.64849295	2.99880782	-0.65918862
C	-1.68829436	2.63671442	0.68971572
H	-2.64908257	2.54774245	1.18630468
C	-0.39960635	3.09910150	-1.27276629
H	-0.34105828	3.38837655	-2.31692596
C	0.77447433	2.83234577	-0.57489474
H	1.73390863	2.92343888	-1.07200738
C	0.71299864	2.43457329	0.75805761
C	-0.52560019	2.35230103	1.39357407
H	-0.58134860	2.04876683	2.43318544
C	-2.92627302	3.23285063	-1.41780877
H	-2.72737252	3.53332212	-2.44723202
H	-3.52509276	2.31866448	-1.43333876
H	-3.52643684	4.01298728	-0.94327154
S	2.18175754	2.01236596	1.68299873
H	2.83343839	1.44682472	0.64917196
P	-0.93167475	-1.69229246	0.30436035
C	-1.18650434	-1.04310763	1.95815273
H	-1.56911612	-1.83812787	2.60016477
H	-0.23826314	-0.66855654	2.35105292
H	-1.91847652	-0.23631545	1.91297850
C	0.20687868	-3.07140245	0.40911047
H	-0.25870002	-3.87537597	0.98132347

H	0.44550118	-3.42226275	-0.59585833
H	1.11929669	-2.74163913	0.90903179
C	-0.21066843	-0.42067213	-0.72299208
H	-0.03341825	-0.83600260	-1.71651859
H	-0.91119095	0.41267436	-0.78561307
H	0.73363472	-0.09545418	-0.28459341
O	-2.25885725	-2.23018998	-0.30807589
B	-3.56437558	-1.46470107	-0.16177374
F	-3.25522775	-0.09462837	-0.29664096
F	-4.41582914	-1.89688433	-1.14507247
F	-4.05212360	-1.70339435	1.11745097
C	3.01036762	-0.39039002	-1.64420464
H	2.35795678	0.03474950	-2.39894137
C	4.05930674	0.26011958	-1.13649802
H	4.28618602	1.24400012	-1.53044930
C	4.90571301	-0.32052506	-0.03387048
H	5.08389319	0.43200750	0.74058388
H	5.89189944	-0.60133279	-0.41847420
C	4.19868434	-1.54164616	0.55835529
H	4.88124605	-2.14769917	1.15679400
H	3.37876922	-1.21950844	1.20993370
C	3.62223830	-2.37818620	-0.57274453
H	3.12819843	-3.28136008	-0.21578642
H	4.41517682	-2.66574719	-1.27314779
O	2.62843499	-1.64921982	-1.29898751

Complex C'

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -1801.29901922

C	3.95670455	-1.43757971	-1.41485646
C	2.56330351	-1.51431793	-1.46440481
H	2.06980547	-1.68057778	-2.41653748
C	4.56253577	-1.22527045	-0.17525924
H	5.64395034	-1.16540808	-0.11312139
C	3.80413648	-1.09161355	0.98244465
H	4.28890848	-0.93443107	1.93871335
C	2.41436848	-1.15820953	0.91620503
C	1.79651814	-1.38263612	-0.31277883
H	0.71643318	-1.45420552	-0.37266953

C	4.77745104	-1.60447210	-2.66529488
H	5.79423989	-1.23658779	-2.52319677
H	4.83812001	-2.65965401	-2.94630079
H	4.32962642	-1.06655918	-3.50316796
P	-2.61923107	-0.70563886	0.86922269
C	-1.45585550	0.54179785	0.31953071
H	-1.83945337	1.53215237	0.56626608
H	-0.49569236	0.38962955	0.81663381
H	-1.34235558	0.46350355	-0.76287995
C	-2.85239460	-0.54587443	2.63732090
H	-3.22119734	0.45670283	2.85929855
H	-3.58485148	-1.28263192	2.97097923
H	-1.90423837	-0.71366698	3.15177902
C	-1.95492297	-2.33748574	0.52813334
H	-2.68898454	-3.08480622	0.83654900
H	-1.78292211	-2.43310728	-0.54435133
H	-1.02637003	-2.48643201	1.08291893
O	-4.01524166	-0.52185770	0.20502077
B	-4.13476017	-0.17215469	-1.27192655
F	-3.12669560	-0.89673108	-1.93945700
F	-5.38993215	-0.53269163	-1.68614598
F	-3.89141496	1.18919046	-1.40646469
C	1.20756033	2.78874023	1.35537092
H	0.96117684	2.90851258	2.40556133
C	2.39490706	2.35189279	0.93063848
H	3.15187178	2.12922154	1.67421127
C	2.69372732	2.14934620	-0.53019808
H	3.22393452	1.20428647	-0.67431747
H	3.35719007	2.94121203	-0.89557597
C	1.38294321	2.14616160	-1.31701501
H	1.55808771	2.26585002	-2.38822922
H	0.87323545	1.19006645	-1.17089314
C	0.48243498	3.27066525	-0.82897128
H	-0.47665501	3.28206161	-1.34664699
H	0.97545749	4.23919378	-0.97510873
O	0.16624195	3.14275319	0.56151254
S	1.43706346	-1.01275860	2.41496044
H	1.37380930	0.33322912	2.40316142

Complex D

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -941.949174058

C	3.62474421	-0.36020727	0.12917177
C	3.07150927	-0.55711869	-1.13886150
H	3.66211643	-1.03639894	-1.91223590
C	2.84681202	0.26842050	1.10018001
H	3.25857624	0.43399265	2.08938170
C	1.54510136	0.68341219	0.83527963
H	0.94063416	1.15901939	1.59660064
C	1.03593858	0.46906968	-0.43246359
C	1.78225870	-0.13522036	-1.43192107
H	1.35654046	-0.26500142	-2.42017307
C	5.03614811	-0.79593871	0.42045108
H	5.25094985	-0.74946374	1.48856285
H	5.20951125	-1.81904184	0.08006181
H	5.75278272	-0.15105290	-0.09528066
O	-0.27717259	0.86044353	-0.74664388
H	-0.84138307	0.08758136	-1.02178053
C	-2.66013274	-0.99755268	-1.05260787
H	-3.15514842	-0.48124151	-1.86855478
C	-1.57244229	-1.76663595	-1.23178047
H	-1.23064981	-1.92957146	-2.24771347
C	-0.87780229	-2.43831294	-0.07290924
H	0.20764389	-2.36382810	-0.18502083
H	-1.11810711	-3.50671326	-0.06269495
C	-1.32459185	-1.77706150	1.23285873
H	-1.05380990	-2.38662106	2.09683119
H	-0.84336338	-0.80356608	1.35254567
C	-2.82983448	-1.57141619	1.21947114
H	-3.17789528	-1.05861093	2.11404660
H	-3.34782819	-2.53333075	1.13185647
O	-3.25380302	-0.74803586	0.12353388
B	-1.12252672	2.00879596	0.03717962
F	-2.23347956	2.10588801	-0.74743078
F	-1.37023057	1.51063533	1.29227991
F	-0.29366574	3.08702986	0.03307725

Complex D'

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -941.955591108

C	-3.69058176	-0.43482359	-0.32111001
C	-3.58265415	0.84702026	0.22157844
H	-4.38255396	1.56252797	0.05859876
C	-2.64492871	-1.32841552	-0.08567702
H	-2.69928763	-2.33265616	-0.49393559
C	-1.52939453	-0.96401397	0.65888307
H	-0.71770407	-1.66804126	0.81354316
C	-1.43835972	0.32443748	1.18246870
C	-2.47452884	1.22960377	0.96716030
H	-2.39532573	2.22651223	1.38531653
C	-4.91243926	-0.84942577	-1.09994140
H	-4.67812366	-1.64703890	-1.80733104
H	-5.69611044	-1.22001508	-0.43239839
H	-5.32814849	-0.00966966	-1.66046909
O	-0.35817295	0.74955473	1.88820530
H	0.32255022	0.06370455	1.87531931
C	0.90762774	0.12649352	-1.40929849
H	0.49294775	-0.75488542	-1.87322698
C	0.34818038	1.31930975	-1.32249186
H	-0.62786530	1.42841483	-1.78206471
C	0.95740307	2.48848140	-0.60729405
H	0.21116091	2.91136121	0.06988756
H	1.20150284	3.26757308	-1.33714111
C	2.19875013	2.06673774	0.17892705
H	2.83974580	2.92377893	0.39342337
H	1.90592616	1.62329711	1.13093546
C	3.00345120	1.05601451	-0.60981216
H	3.87672105	0.68552135	-0.07934677
H	3.29584150	1.43195062	-1.59153923
O	2.19190819	-0.13319349	-0.88086158
B	2.32308331	-1.36871150	0.13751660
F	1.53950207	-2.34099308	-0.40661821
F	3.65476269	-1.63743625	0.17798787
F	1.83220983	-0.89581348	1.34682375

Complex E

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -1264.89587822

C	-3.56633095	-0.47433782	0.17425216
C	-3.21128550	0.86172740	0.35379508
H	-3.88860303	1.53028770	0.87375792
C	-2.66721984	-1.31507811	-0.48649392
H	-2.92021504	-2.36045329	-0.63054237
C	-1.45424115	-0.84032722	-0.96686036
H	-0.76217098	-1.51039022	-1.46500055
C	-1.12407131	0.49736114	-0.76774871
C	-1.99564332	1.35417659	-0.10735029
H	-1.72754754	2.39103477	0.05967659
C	-4.89073101	-0.99933166	0.65945052
H	-4.78714474	-2.00280168	1.07652643
H	-5.31601059	-0.35022425	1.42584290
H	-5.60632002	-1.05696079	-0.16576935
S	0.41796124	1.16215251	-1.39124798
H	1.19629901	0.08340753	-1.14894771
C	2.45167018	-1.92123203	-1.05112078
H	2.74225523	-1.98264760	-2.09426410
C	3.10978227	-1.18919310	-0.15018725
H	3.99227264	-0.65326337	-0.47839097
C	2.65111766	-1.07007884	1.27836660
H	2.68920454	-0.02454428	1.59236059
H	3.33298655	-1.62005445	1.93615037
C	1.22548480	-1.61016216	1.41049346
H	0.97833381	-1.82248187	2.45261779
H	0.50589818	-0.86603444	1.05831863
C	1.07518302	-2.88162831	0.59083855
H	0.06215615	-3.28079300	0.63797445
H	1.77564008	-3.64784797	0.94390603
O	1.33572183	-2.65718043	-0.80044233
B	1.19119974	2.30505676	0.35681174
F	2.51633296	2.21904264	0.10545176
F	0.73693389	1.58616696	1.40671299
F	0.61134686	3.51035833	0.17457087

Complex E'

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(toluene)) = -1264.91626130

C	1.30753368	2.31388544	0.14828778
C	2.47310331	1.76522846	0.68562424
H	3.03162798	2.32186559	1.43125698
C	0.61407359	1.56917323	-0.80745108
H	-0.29805363	1.96610171	-1.23968628
C	1.06401791	0.32053444	-1.21604771
H	0.50169085	-0.22786185	-1.96349655
C	2.21721502	-0.22418634	-0.65316924
C	2.92547834	0.50803528	0.29891112
H	3.82169661	0.09369969	0.74754323
C	0.81218737	3.67333194	0.56532558
H	-0.27936268	3.70095005	0.58043738
H	1.18040477	3.94334836	1.55652561
H	1.15068638	4.44130099	-0.13622888
S	2.83600955	-1.82658699	-1.12655154
H	1.68046058	-2.27617003	-1.64086834
C	-1.17835123	-1.78506593	-0.15655149
H	-1.59183857	-2.04755164	-1.11921498
C	-0.39657796	-2.53695548	0.60020982
H	-0.16111333	-3.52768659	0.22987842
C	0.17041803	-2.08882303	1.91645347
H	1.24811674	-2.27369371	1.92371258
H	-0.25791771	-2.70223376	2.71610927
C	-0.10961019	-0.60418438	2.15789638
H	-0.03597313	-0.35717489	3.21856296
H	0.61426183	0.01123413	1.62055050
C	-1.49451135	-0.23501386	1.67426380
H	-1.70845622	0.82506129	1.77648384
H	-2.28179923	-0.83117940	2.14289891
O	-1.56585193	-0.49932949	0.24088253
B	-2.62968340	0.30182718	-0.68127437
F	-2.13000834	0.13654598	-1.94437919
F	-2.57170584	1.58302778	-0.21083249
F	-3.82553144	-0.32011563	-0.46954881

Complex B (in SMD chloroform)

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(chloroform)) = -1478.35127719

C	-3.88022703	-2.44556144	0.30159579
C	-2.50982491	-2.72332360	0.30080941
H	-2.14801320	-3.61634612	0.80077244
C	-4.31081791	-1.29465713	-0.35557744
H	-5.36956814	-1.05793262	-0.37976022
C	-3.41140414	-0.44057440	-0.98886132
H	-3.76116262	0.44875274	-1.50399202
C	-2.05120080	-0.72706083	-0.95798634
C	-1.59801304	-1.87890488	-0.31682557
H	-0.53652038	-2.09876846	-0.30173683
C	-4.84932828	-3.37058595	0.99114960
H	-5.87495413	-3.01380854	0.88686607
H	-4.79640084	-4.37839414	0.57131409
H	-4.62461259	-3.44861855	2.05812268
O	-1.12455999	0.09450072	-1.54044510
H	-1.53198669	0.95994470	-1.69505960
P	2.23217246	0.07488150	-0.74390444
C	1.25216223	0.01517795	0.75479124
H	1.61313430	0.79839280	1.42305089
H	0.20683000	0.19198647	0.50171093
H	1.38156606	-0.95611325	1.23420588
C	1.90615196	1.58485686	-1.64419642
H	2.00172525	2.43672227	-0.97053269
H	2.63230588	1.66281987	-2.45567781
H	0.89771197	1.54407796	-2.05550789
C	1.85347939	-1.31970669	-1.80506182
H	2.54317703	-1.29807102	-2.65163320
H	1.99683060	-2.24728143	-1.25056205
H	0.82656733	-1.23795302	-2.16337168
O	3.76010852	0.09395558	-0.39814398
B	4.35996604	-0.79607275	0.65492090
F	3.71771613	-2.04616535	0.57693464
F	5.71030593	-0.90512370	0.39530939
F	4.11934305	-0.22874529	1.90527876
C	-1.17029816	3.06137969	-0.62299170

H	-0.66892702	3.37474248	-1.53340784
C	-2.49956923	3.01401431	-0.50042645
H	-3.09810043	3.33674193	-1.34472850
C	-3.16831536	2.54749556	0.76605049
H	-3.99634517	1.87439801	0.53010222
H	-3.60232648	3.40272637	1.29572098
C	-2.14314528	1.84017603	1.65387176
H	-2.50918811	1.73562118	2.67699136
H	-1.94294904	0.83453239	1.26889507
C	-0.84883331	2.63650251	1.66338002
H	-0.08308728	2.17055600	2.28179352
H	-1.02999876	3.65335001	2.03026173
O	-0.28046195	2.73779424	0.35035059

Complex C (in SMD chloroform)

E(M06-2X/aug-cc-pVTZ, Grimme D3 dispersion, SMD(chloroform)) = -1801.31262297

C	-1.46626012	3.12721199	-0.63537426
C	-1.55121837	2.73975233	0.70453702
H	-2.52118495	2.71869159	1.19138067
C	-0.20591828	3.14062609	-1.23406967
H	-0.11193225	3.44531919	-2.27133480
C	0.93571124	2.77246793	-0.52832588
H	1.90519193	2.79946456	-1.01368166
C	0.82749321	2.35794869	0.79708296
C	-0.42243989	2.35302331	1.41598323
H	-0.51577651	2.03342043	2.44818082
C	-2.70927472	3.48973463	-1.40237660
H	-2.46990734	3.79103100	-2.42291667
H	-3.39061410	2.63612356	-1.44618897
H	-3.24258651	4.31120115	-0.91759036
S	2.25069020	1.82546516	1.73542625
H	2.90661814	1.28300543	0.69150334
P	-1.03044199	-1.67406473	0.28262904
C	-1.26165973	-1.02503492	1.93816111
H	-1.66628383	-1.81189230	2.57695881
H	-0.29697965	-0.69074996	2.32701792
H	-1.95956372	-0.18798782	1.90401865

C	0.06753265	-3.08260745	0.36813060
H	-0.40864680	-3.86990444	0.95467728
H	0.27638154	-3.44180357	-0.64055356
H	0.99806579	-2.77217081	0.84647919
C	-0.29537227	-0.41561422	-0.75009872
H	-0.14108189	-0.82897285	-1.74852204
H	-0.96841406	0.44120913	-0.79701780
H	0.66311000	-0.12507169	-0.31894790
O	-2.38336043	-2.17639728	-0.32059513
B	-3.66561038	-1.39764038	-0.17950252
F	-3.35696783	-0.02941133	-0.31600991
F	-4.52652794	-1.82196773	-1.16797750
F	-4.17987407	-1.62889755	1.09412784
C	2.96469532	-0.43955079	-1.60992521
H	2.28288938	0.00269838	-2.32824191
C	4.07252799	0.17042839	-1.18274696
H	4.31297636	1.13958131	-1.60461190
C	4.96491897	-0.43185908	-0.12894061
H	5.22046259	0.32298270	0.62140635
H	5.91266203	-0.75480871	-0.57270237
C	4.25285364	-1.61832123	0.52498419
H	4.95223459	-2.24774203	1.07820395
H	3.49563026	-1.25992343	1.23049840
C	3.56248074	-2.44094793	-0.55054108
H	3.05453184	-3.31517706	-0.14478004
H	4.29022666	-2.77130173	-1.30087435
O	2.55205235	-1.67567131	-1.21706095

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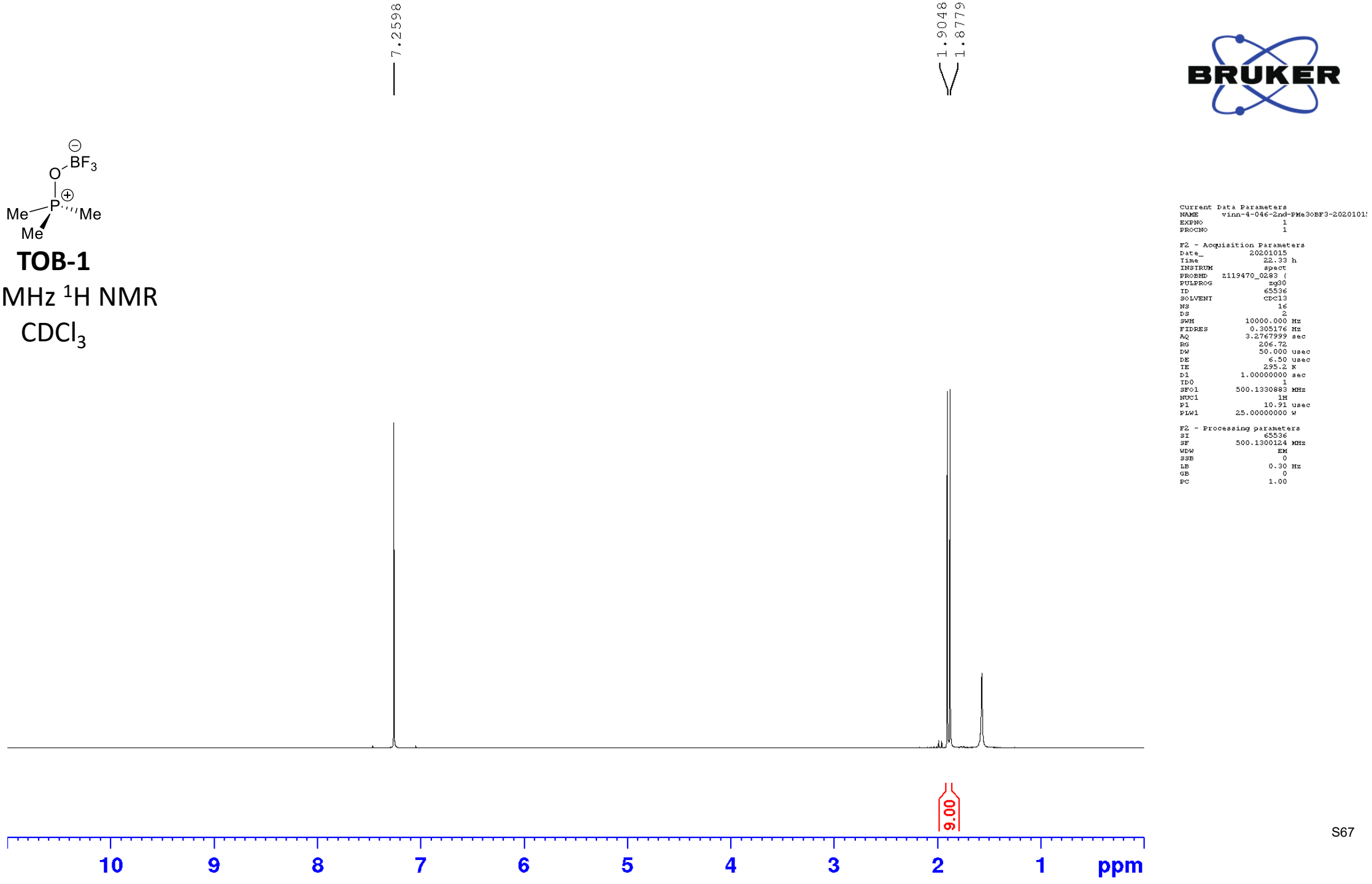
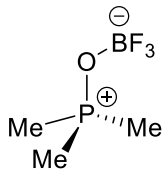
TOB-1

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME        vinn-4-046-2nd-PMe3oBF3-20201015
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201015
Time              22.33 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ                3.2767999 sec
RG                   206.72
DW                  50.000 usec
DE                   6.50 usec
TE                  295.2 K
D1            1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                  10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300124 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



TOB-1

125 MHz ^{13}C NMR

$CDCl_3$

77.41
77.16
76.90
15.12
14.55

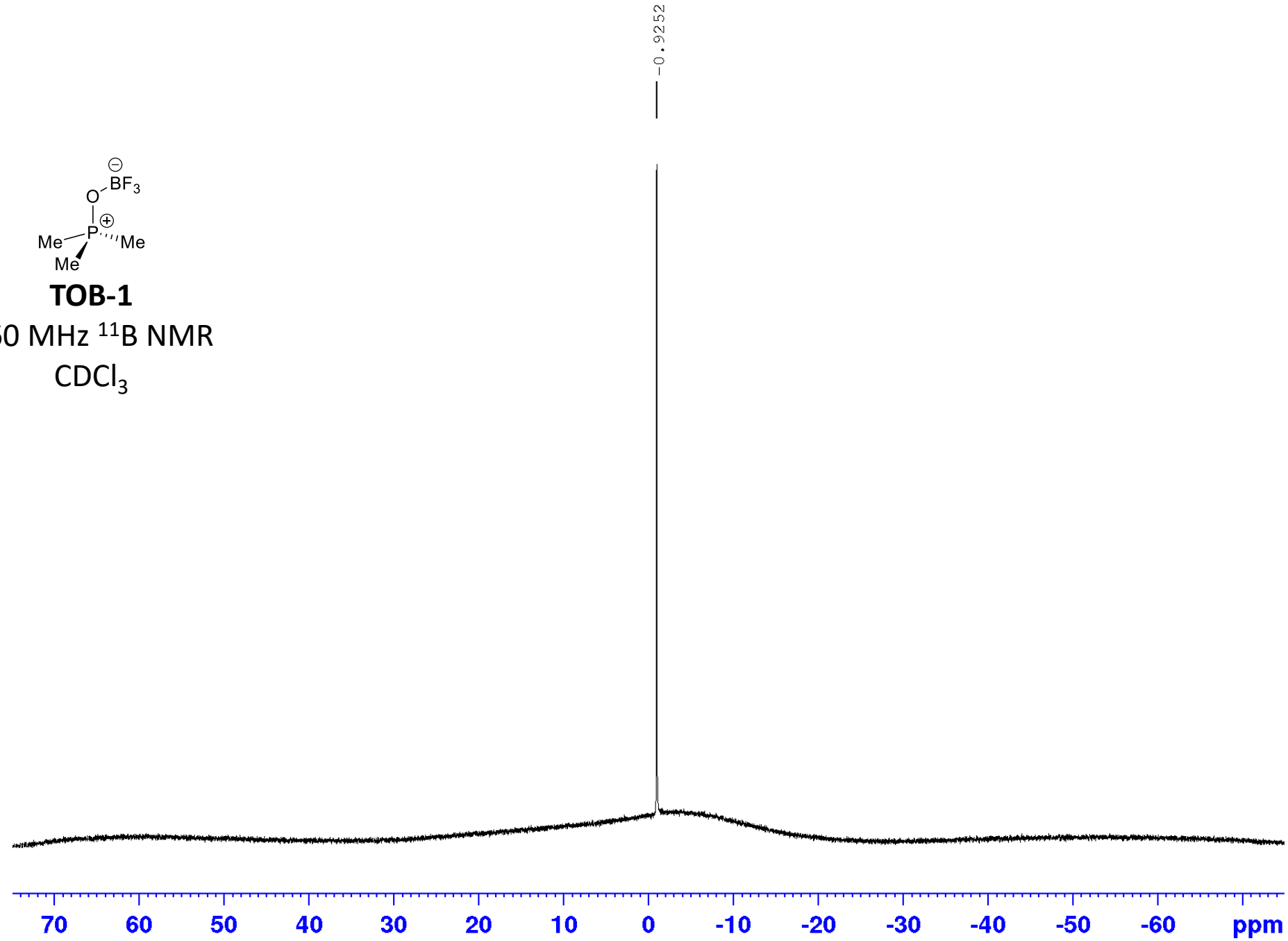
```
Current Data Parameters
NAME      vinn-4-046-2nd-PMe3OBF3-2021
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201015
Time              23.28 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                 6.50 usec
TE                295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                 32768
SF          125.7577726 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

200 180 160 140 120 100 80 60 40 20 0 ppm

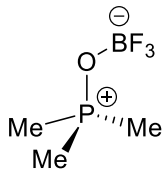
TOB-1

160 MHz ^{11}B NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-046-2nd-PMe3OBF3-20201015
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201015
Time              23.29 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zgig
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                206.72
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        160.4615790 MHz
NUC1                11B
P1                16.00 usec
PLW1        50.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W

F2 - Processing parameters
SI                 16384
SF          160.4615792 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



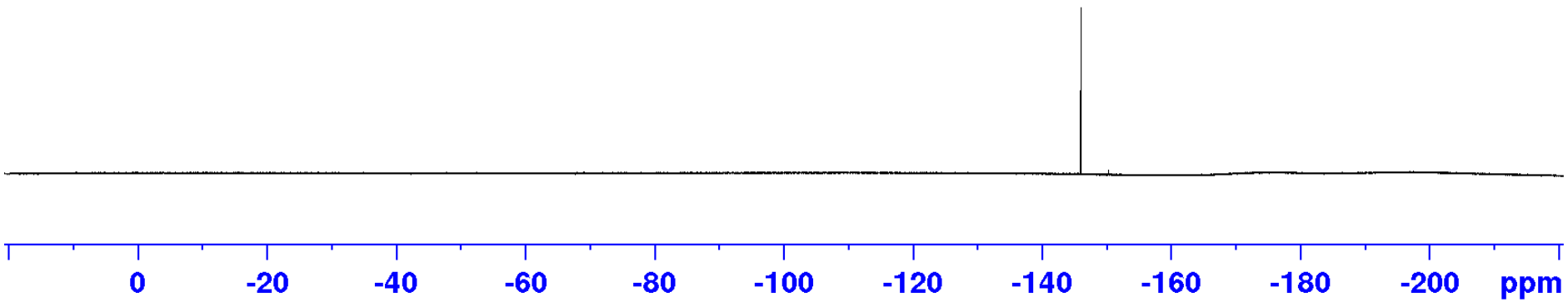
TOB-1

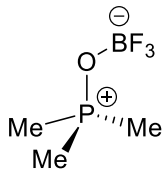
470 MHz ^{19}F NMR

$CDCl_3$

-146.0408

```
Current Data Parameters
NAME      vinn-4-046-2nd-PMe3OBF3-20201015
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20201015
Time              23.31 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgflqn
TD               131072
SOLVENT            CDCl3
NS                    32
DS                     4
SWH          113636.367 Hz
FIDRES         1.733953 Hz
AQ             0.5767168 sec
RG                206.72
DW                 4.400 usec
DE                 6.50 usec
TE                295.2 K
D1           1.00000000 sec
TD0                   1
SFO1         470.5453180 MHz
NUC1                19F
P1                15.00 usec
PLW1         47.23500061 W

F2 - Processing parameters
SI                65536
SF           470.5923772 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```





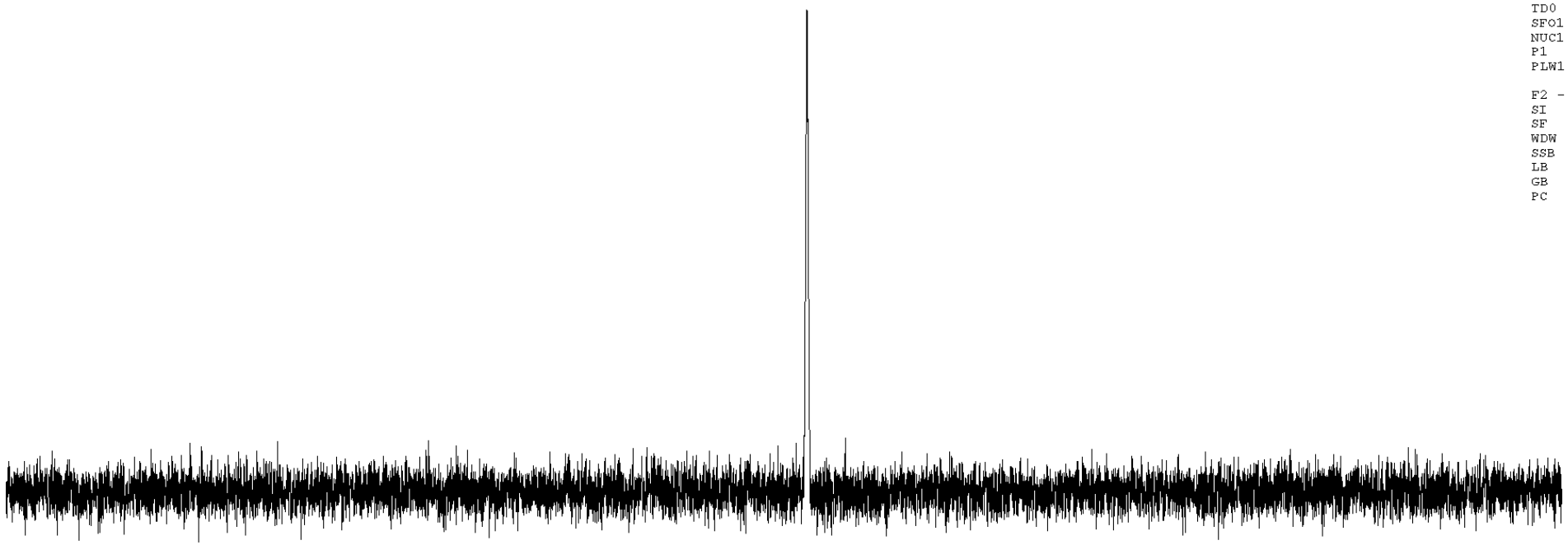
TOB-1

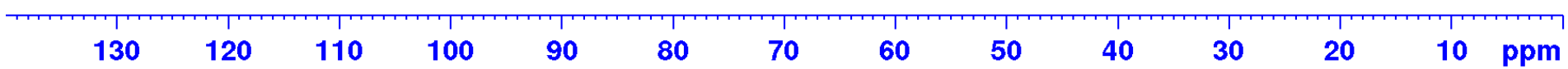
200 MHz ^{31}P NMR

$CDCl_3$

67.94

```
Current Data Parameters
NAME      vinn-4-046-2nd-PMe3OBF3-2021
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201015
Time              23.35 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    64
DS                     4
SWH           81521.742 Hz
FIDRES         2.487846 Hz
AQ             0.4019541 sec
RG                206.72
DW                6.133 usec
DE                 6.50 usec
TE                295.1 K
D1            2.00000000 sec
TD0                    1
SFO1        202.4462121 MHz
NUC1                 31P
P1                14.00 usec
PLW1        54.00000000 W

F2 - Processing parameters
SI                 32768
SF          202.4563350 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

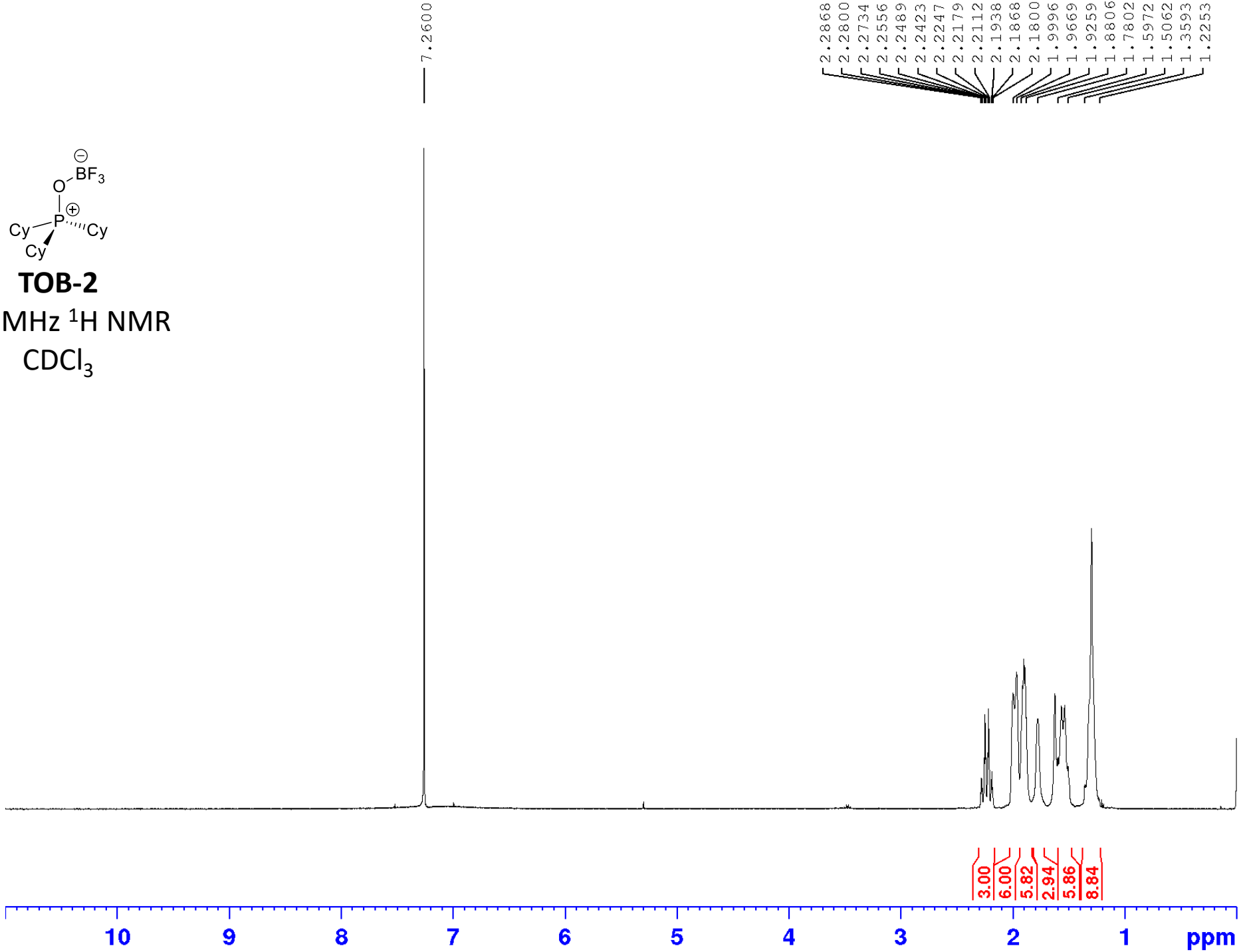




TOB-2

400 MHz ^{1}H NMR

$CDCl_3$

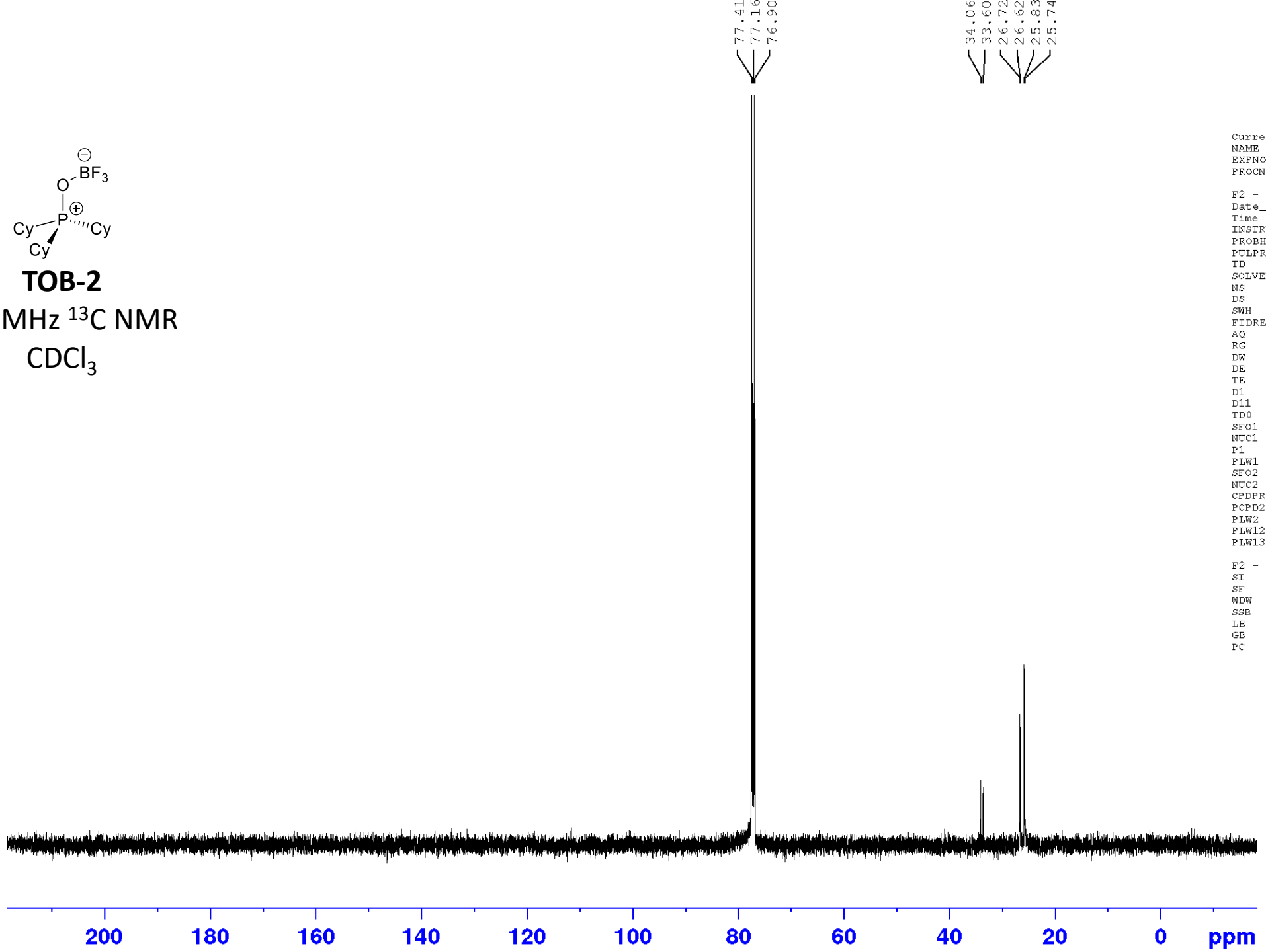



```
Current Data Parameters
NAME      vinn-1-173-PCy3OBF3-20191211
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20191211
Time              11.34 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                   161
DW                62.400 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.2324714 MHz
NUC1                  1H
P1                12.80 usec
PLW1         13.56000042 W

F2 - Processing parameters
SI                 65536
SF          400.2300100 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

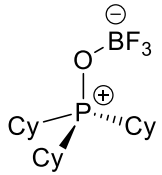
TOB-2

125 MHz ^{13}C NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-026-PCy3OBF3-2020082:
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20200823
Time              18.53 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT         CDCl3
NS                400
DS                  4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1              13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.39063001 W
PLW13         0.19648001 W

F2 - Processing parameters
SI               32768
SF          125.7577735 MHz
WDW                EM
SSB                0
LB              1.00 Hz
GB                 0
PC              1.40
```



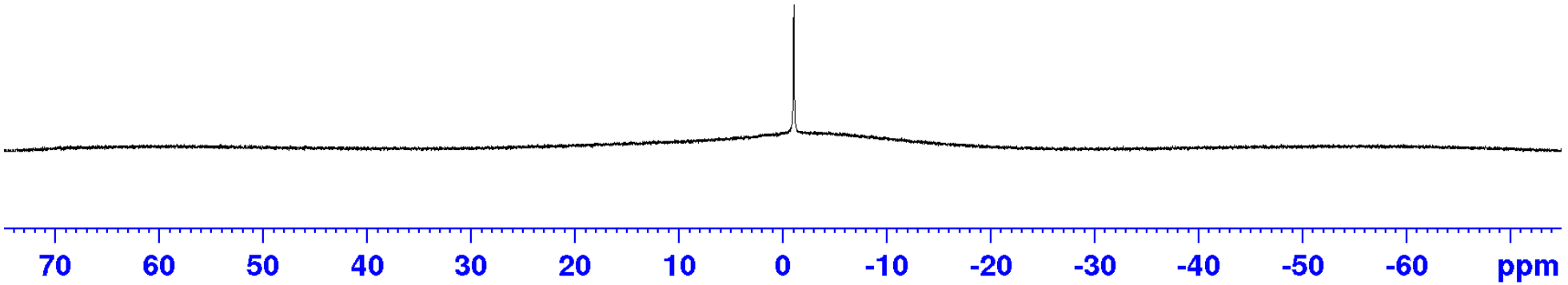
TOB-2

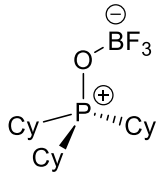
160 MHz ^{11}B NMR

$CDCl_3$

-1.0258

```
Current Data Parameters
NAME      vinn-4-026-PCy3OBF3-20200822
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20200823
Time              18.55 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zgig
TD                 32768
SOLVENT             CDCl3
NS                    16
DS                     4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ             0.6815744 sec
RG                206.72
DW               20.800 usec
DE                6.50 usec
TE               295.2 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         160.4615790 MHz
NUC1                 11B
P1                16.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.39063001 W

F2 - Processing parameters
SI                 16384
SF           160.4615792 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```





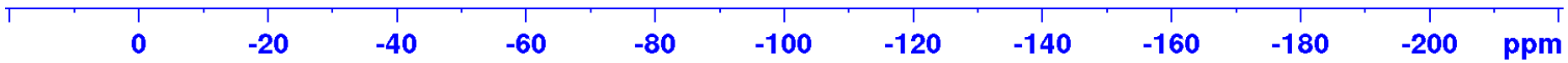
TOB-2

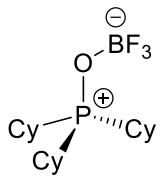
470 MHz ^{19}F NMR

$CDCl_3$

-145.92

```
Current Data Parameters
NAME      vinn-4-026-PCy3OBF3-2020082
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20200823
Time             18.56 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG          zgflqn
TD               131072
SOLVENT            CDCl3
NS                    16
DS                     4
SWH          113636.367 Hz
FIDRES         1.733953 Hz
AQ             0.5767168 sec
RG                206.72
DW                 4.400 usec
DE                 6.50 usec
TE                295.2 K
D1           1.00000000 sec
TD0                   1
SFO1         470.5453180 MHz
NUC1                19F
P1                15.00 usec
PLW1         47.23500061 W

F2 - Processing parameters
SI                65536
SF           470.5923772 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```





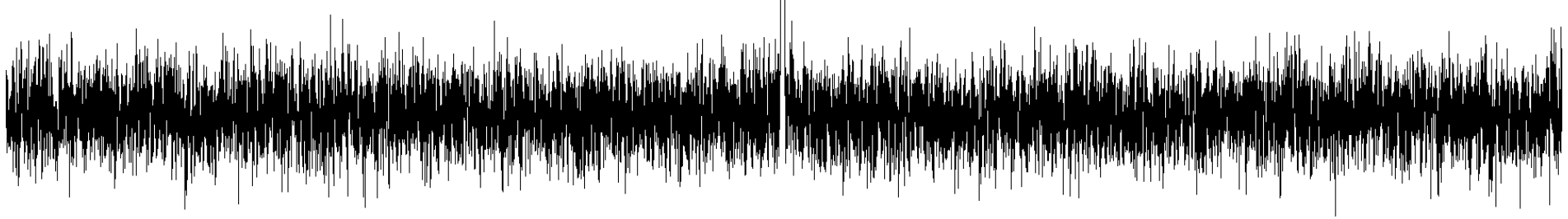
TOB-2

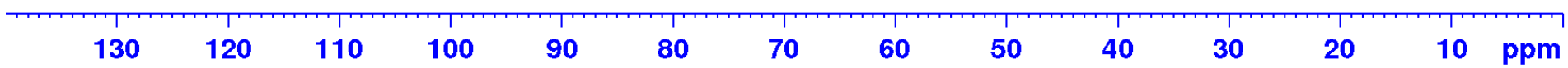
200 MHz ^{31}P NMR

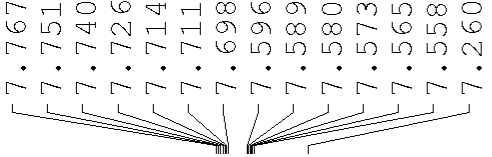
$CDCl_3$

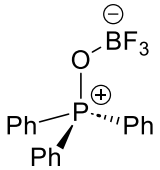
70.09

```
Current Data Parameters
NAME      vinn-4-026-PCy3OBF3-2020082:
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_           20200823
Time              18.58 h
INSTRUM             spect
PROBHD    Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            81521.742 Hz
FIDRES          2.487846 Hz
AQ              0.4019541 sec
RG                206.72
DW                6.133 usec
DE                6.50 usec
TE                295.1 K
D1             2.00000000 sec
TD0                    1
SFO1         202.4462121 MHz
NUC1                 31P
P1                14.00 usec
PLW1         54.00000000 W

F2 - Processing parameters
SI                 32768
SF           202.4563350 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```







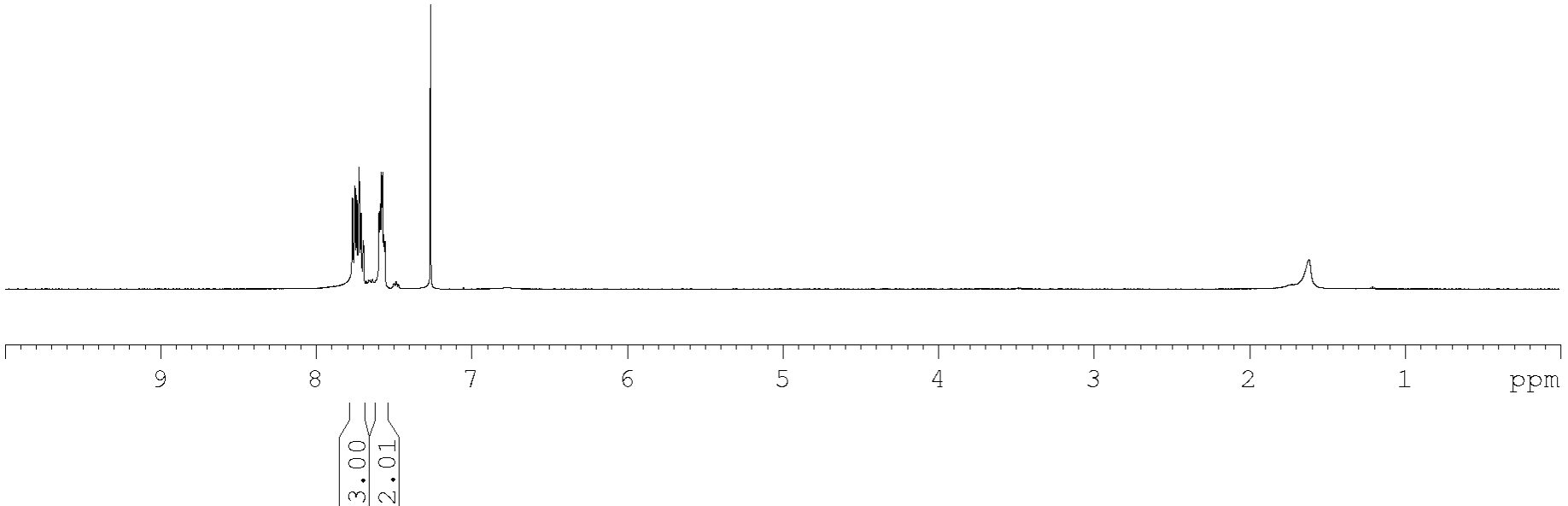


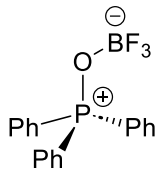
TOB-3

500 MHz ^{1}H NMR

$CDCl_3$

```
Current Data Parameters
NAME      vinn-3-102-PPh3OBF3-CDCl3-20201111
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20201114
Time              12.09 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                142.5
DW                50.000 usec
DE                 6.50 usec
TE                295.2 K
D1            1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300127 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```





TOB-3

125 MHz ^{13}C NMR

$CDCl_3$

134.406
134.384
133.242
133.149
129.440
129.334
125.370
124.484
77.411
77.157
76.903

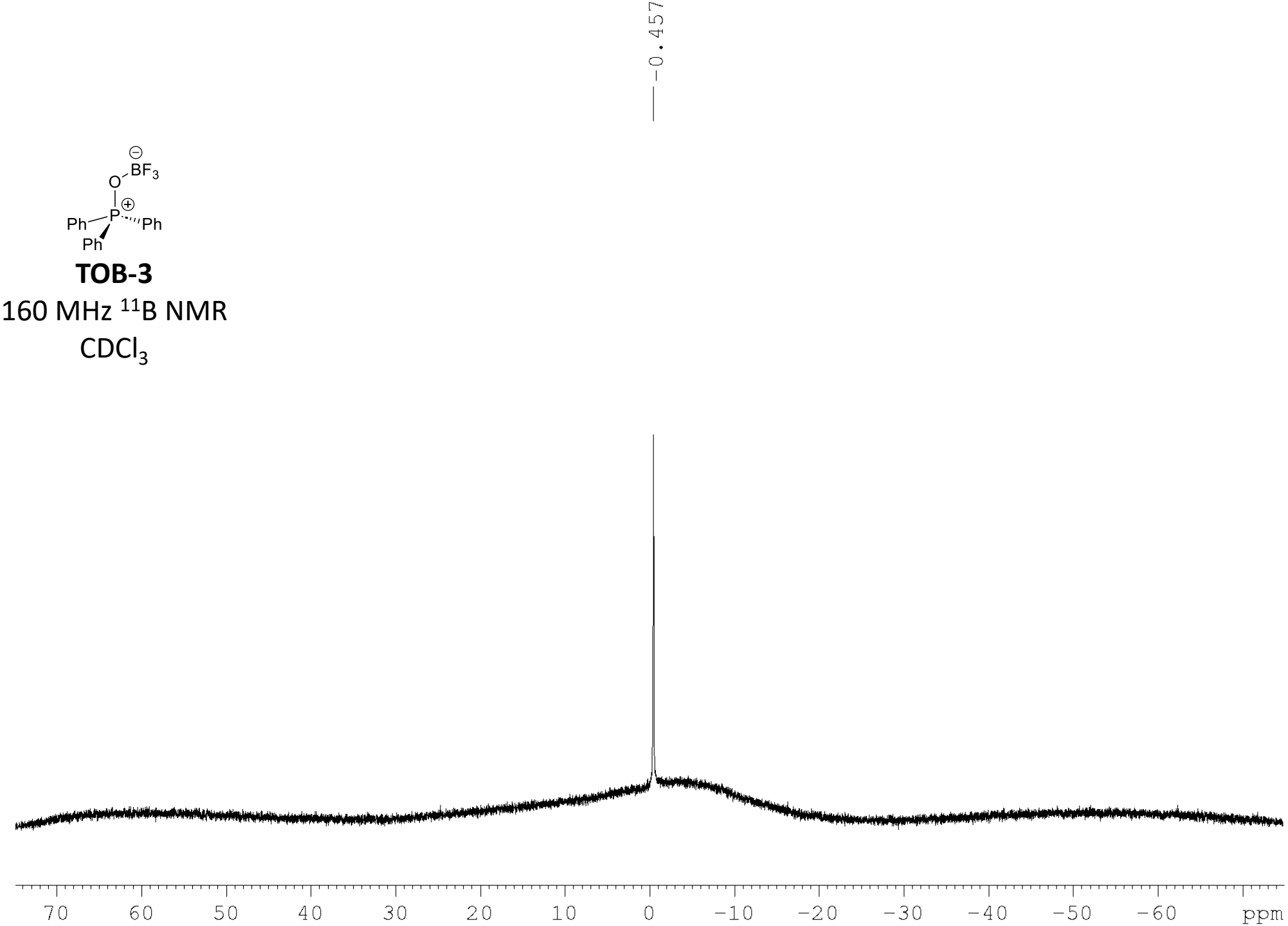
```
Current Data Parameters
NAME      vinn-3-102-PPh3OBF3-CDCl3-20201114
EXPNO                 6
PROCNO                1

F2 - Acquisition Parameters
Date_          20201114
Time              12.31 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577729 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

200 180 160 140 120 100 80 60 40 20 0 ppm

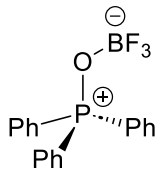
TOB-3

160 MHz ^{11}B NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-3-102-PPh3OBF3-CDCl3-2020111
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20201114
Time              12.11 h
INSTRUM             spect
PROBHD    Z119470_0283 (
PULPROG             zgig
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ             0.6815744 sec
RG                206.72
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         160.4615790 MHz
NUC1                11B
P1                16.00 usec
PLW1          50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          25.00000000 W
PLW12          0.46495000 W

F2 - Processing parameters
SI                 16384
SF           160.4615792 MHz
WDW                   EM
```



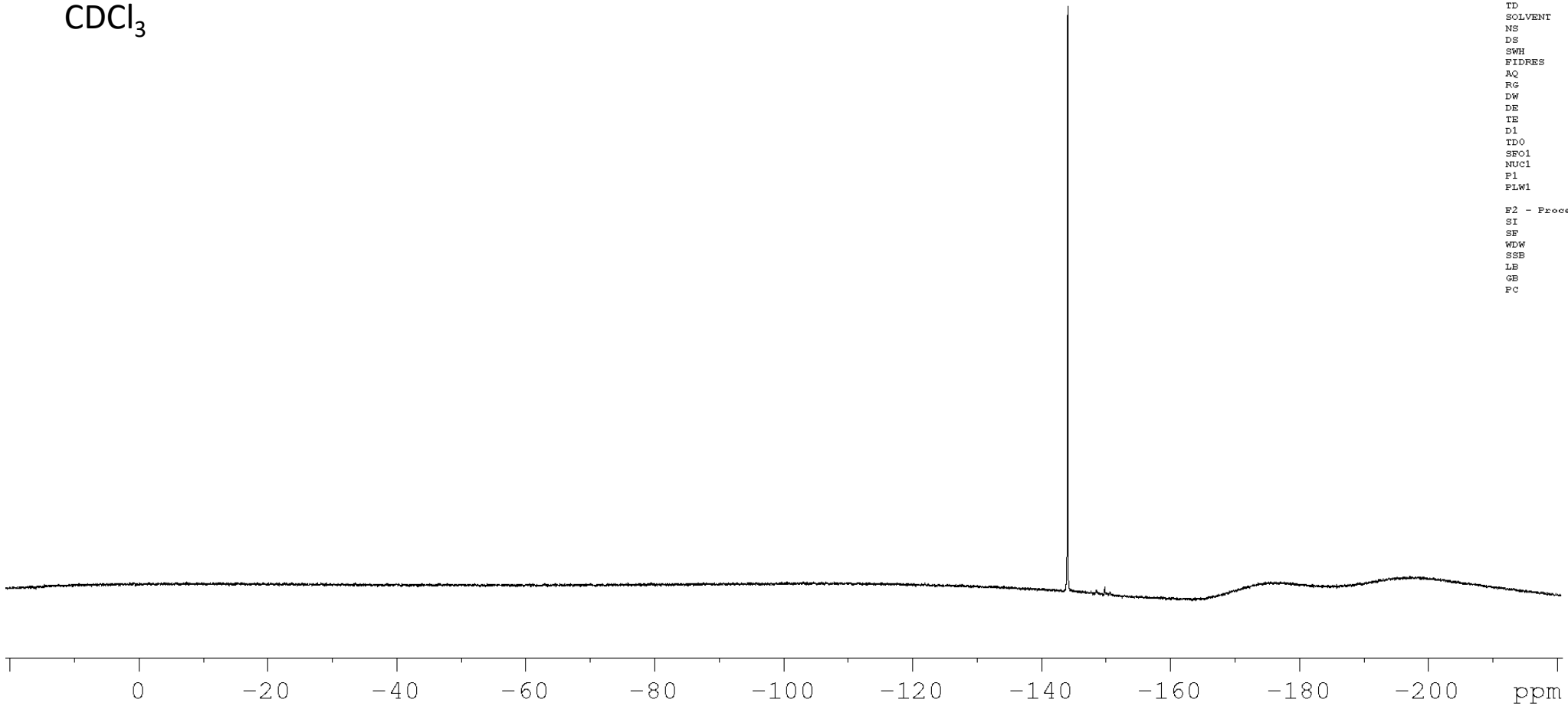
TOB-3

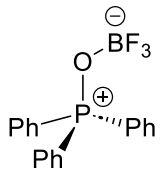
470 MHz ^{19}F NMR

$CDCl_3$

-144.056

```
Current Data Parameters
NAME      vinn-3-102-PPh3OBF3-CDCl3-20201114
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201114
Time              12.12 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG          zgflqn
TD               131072
SOLVENT            CDCl3
NS                    16
DS                     4
SWH          113636.367 Hz
FIDRES         1.733953 Hz
AQ             0.5767168 sec
RG                206.72
DW                 4.400 usec
DE                 6.50 usec
TE                295.2 K
D1            1.00000000 sec
TD0                    1
SFO1         470.5453180 MHz
NUC1                 19F
P1                15.00 usec
PLW1         47.23500061 W

F2 - Processing parameters
SI                 65536
SF           470.5923772 MHz
WDW                   EM
SSB                    0
LB                10.00 Hz
GB                     0
PC                 1.00
```





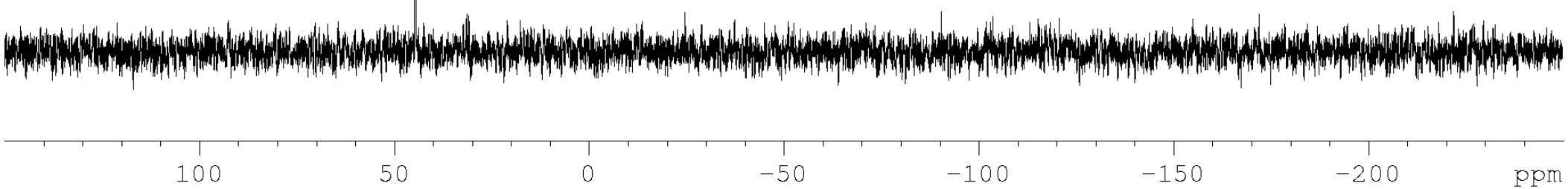
TOB-3

200 MHz ^{31}P NMR

$CDCl_3$

44.451

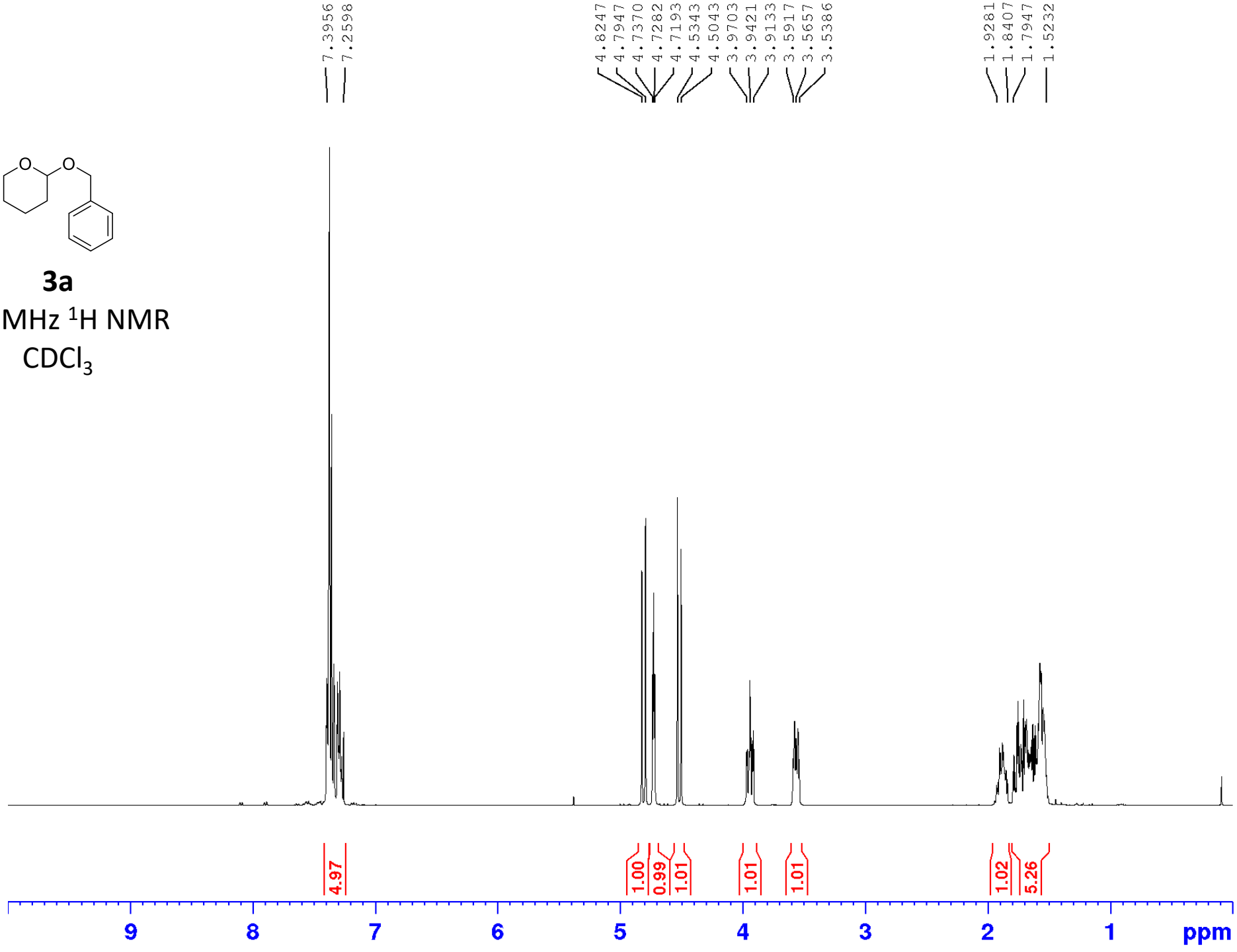
```
Current Data Parameters
NAME      vinn-3-102-PPh3OBF3-CDCl3-20201114
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20201114
Time              12.16 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   4
SWH          81521.742 Hz
FIDRES        2.487846 Hz
AQ            0.4019541 sec
RG               206.72
DW                6.133 usec
DE                6.50 usec
TE               295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1       202.4462121 MHz
NUC1               31P
P1               14.00 usec
PLW1        54.00000000 W
SFO2       500.1320005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI               32768
SF         202.4563350 MHz
WDW                EM
SSB                 0
LB              10.00 Hz
GB                  0
PC               1.40
```



3a

400 MHz ^{1}H NMR

$CDCl_3$

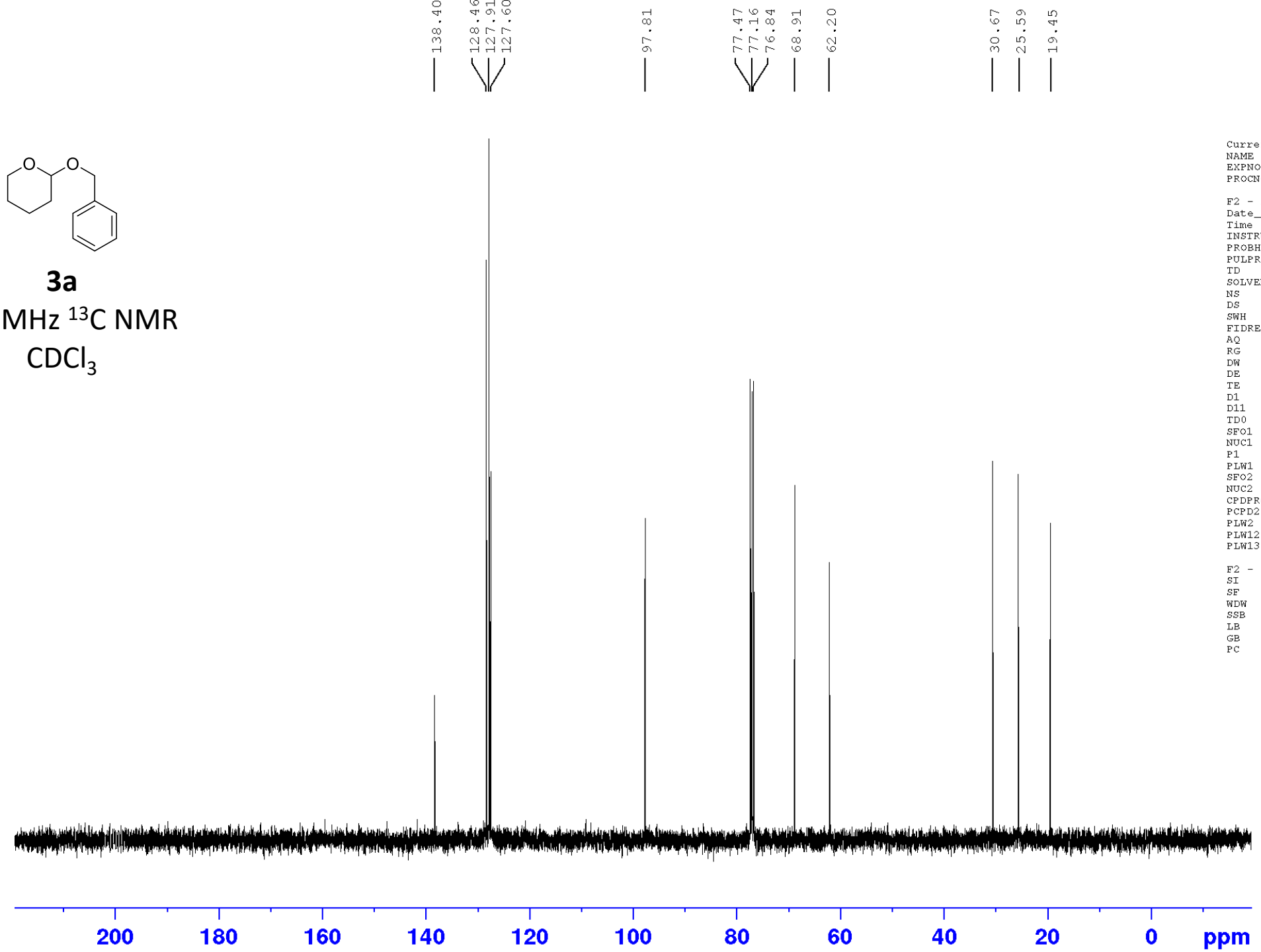



```
Current Data Parameters
NAME      vinn-4-127-islt-20201124
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20201124
Time              12.05 h
INSTRUM           spect
PROBHD   Z820201_0170 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                  32
DW               62.400 usec
DE                6.50 usec
TE               295.6 K
D1            1.00000000 sec
TD0                  1
SFO1         400.1324708 MHz
NUC1                 1H
P1                6.75 usec
PLW1         13.17700005 W

F2 - Processing parameters
SI               65536
SF           400.1300098 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

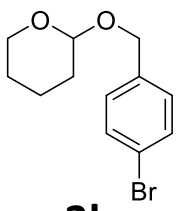
3a

100 MHz ^{13}C NMR

$CDCl_3$



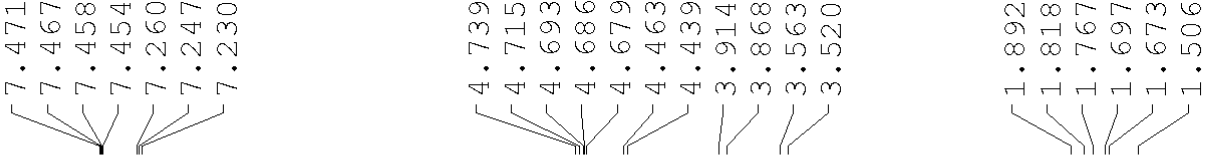

```
Current Data Parameters
NAME      vinn-4-127-islt-20201124
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20201124
Time             12.11 h
INSTRUM            spect
PROBHD   Z820201_0170 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   60
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               295.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1        100.6228298 MHz
NUC1               13C
P1               28.00 usec
PLW1        14.80000019 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        13.17000008 W
PLW12        0.07408100 W
PLW13        0.03726200 W

F2 - Processing parameters
SI                32768
SF          100.6127610 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```

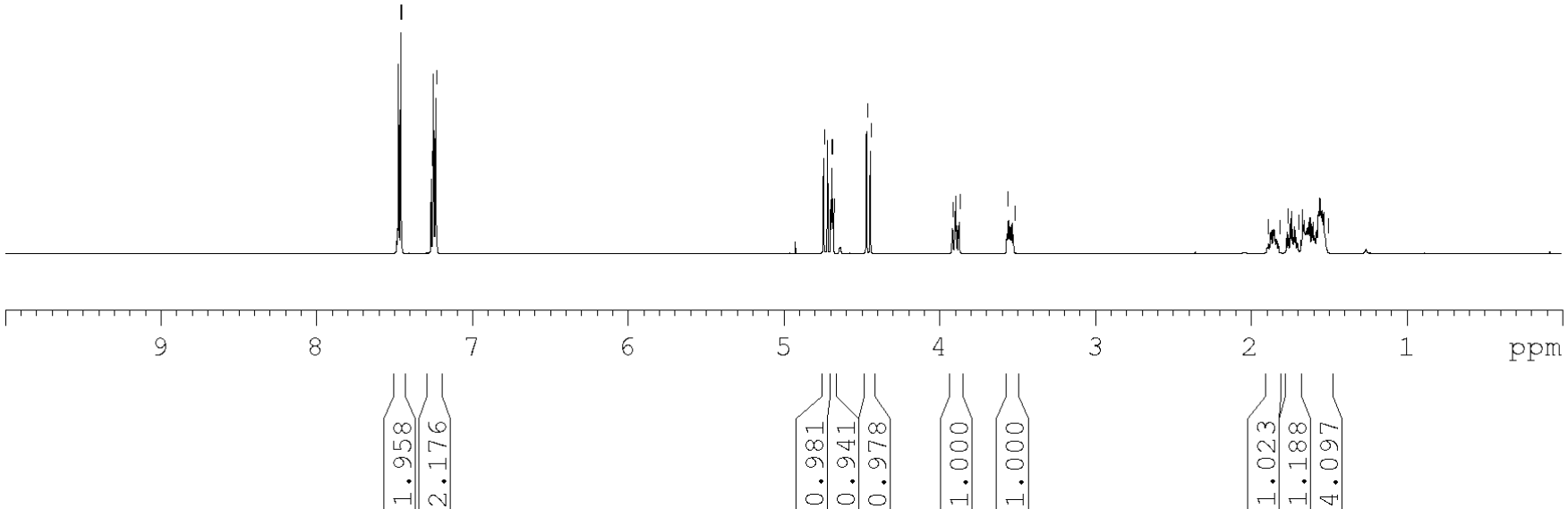


3b

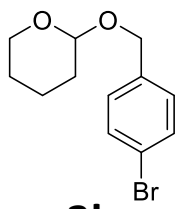
500 MHz ^{1}H NMR

$CDCl_3$






```
Current Data Parameters
NAME      vinn-4-137-1-islt-20201207
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20201207
Time              18.39 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                   1
SFO1          500.1330883 MHz
NUC1                 1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300122 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



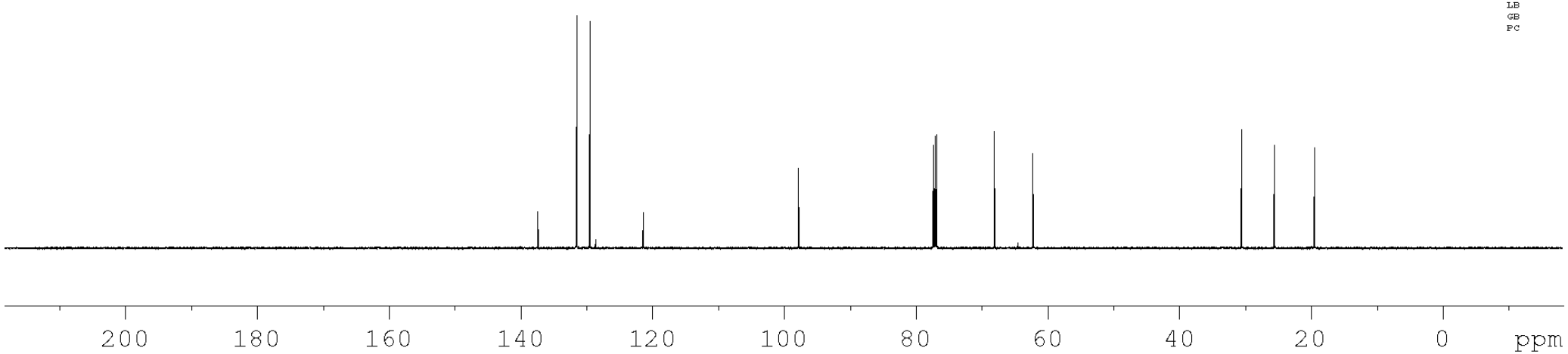
3b

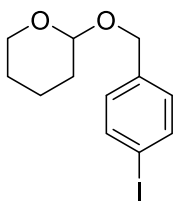
125 MHz ^{13}C NMR

$CDCl_3$

137.438
131.546
129.524
121.448
97.900
77.411
77.156
76.903
68.149
62.271
30.615
25.524
19.419

```
Current Data Parameters
NAME      vinn-4-137-1-islt-20201207
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20201207
Time              18.45 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW              16.800 usec
DE               6.50 usec
TE               295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1               9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2           80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577782 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```

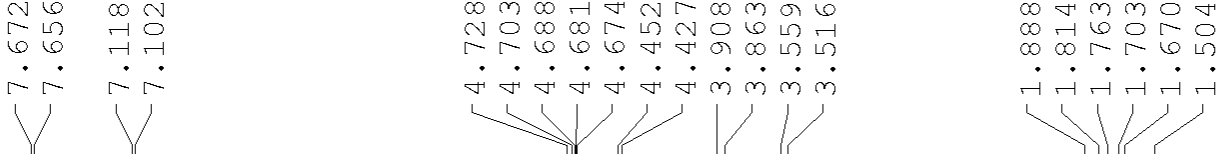




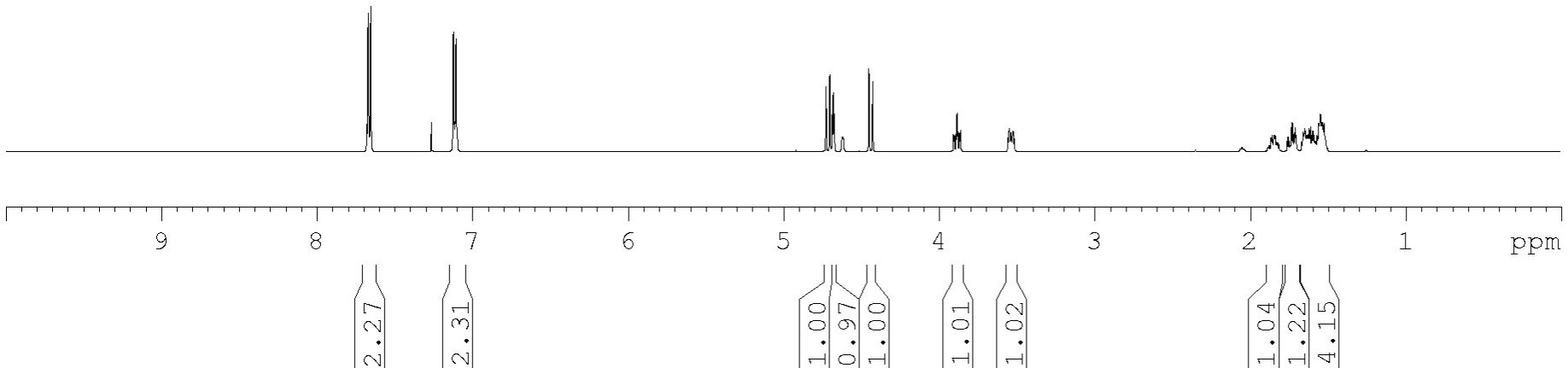
3c

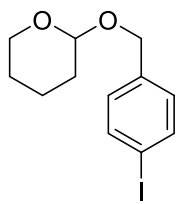
500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-2-islt-20201207
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20201207
Time              18.49 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1            1.00000000 sec
TD0                    1
SFO1        500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI                 65536
SF          500.1300122 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```





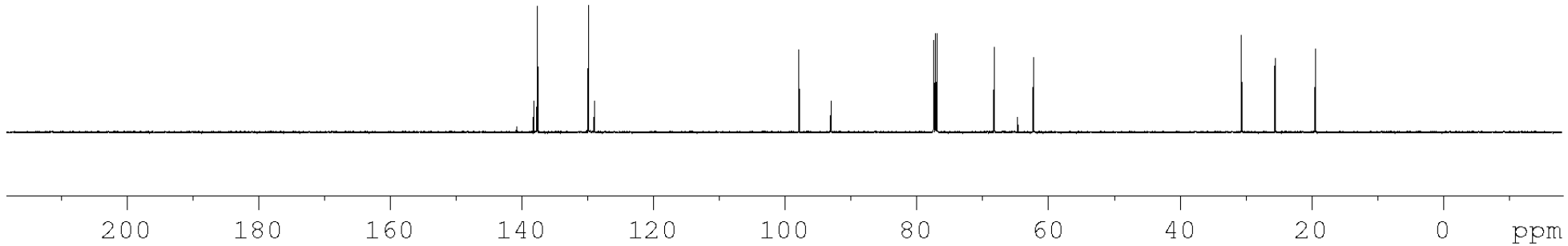
3c

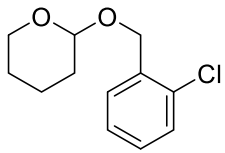
125 MHz ^{13}C NMR

$CDCl_3$

138.089
137.511
129.759
128.861
97.884
77.412
77.157
76.904
68.201
62.258
30.601
25.512
19.399

```
Current Data Parameters
NAME      vinn-4-137-2-ialt-20201207
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20201207
Time              18.55 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                 6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577798 MHz
```





3d

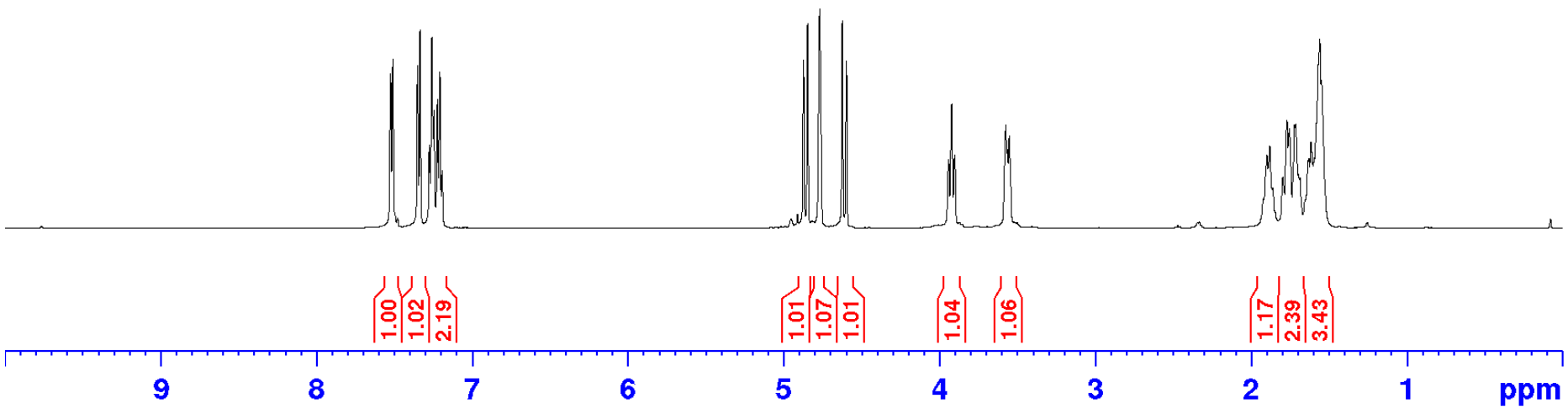
500 MHz ^{1}H NMR

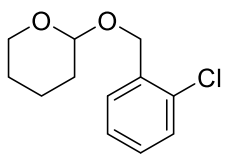
$CDCl_3$

7.5254
7.5104
7.3513
7.3357
7.2751
7.1936
4.8737
4.8473
4.7698
4.6247
4.5983
3.9434
3.9223
3.9034
3.5748
3.5525
1.9206
1.8607
1.7962
1.6865
1.6340
1.6275
1.5478

BRUKER

```
Current Data Parameters
NAME      vinn-4-137-16-islt-2020121
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20201211
Time               6.34 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ                3.2767999 sec
RG                   30.85
DW                  50.000 usec
DE                   6.50 usec
TE                  295.1 K
D1             1.00000000 sec
TD0                   1
SFO1          500.1330883 MHz
NUC1                  1H
P1                  10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                65536
SF            500.1300150 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



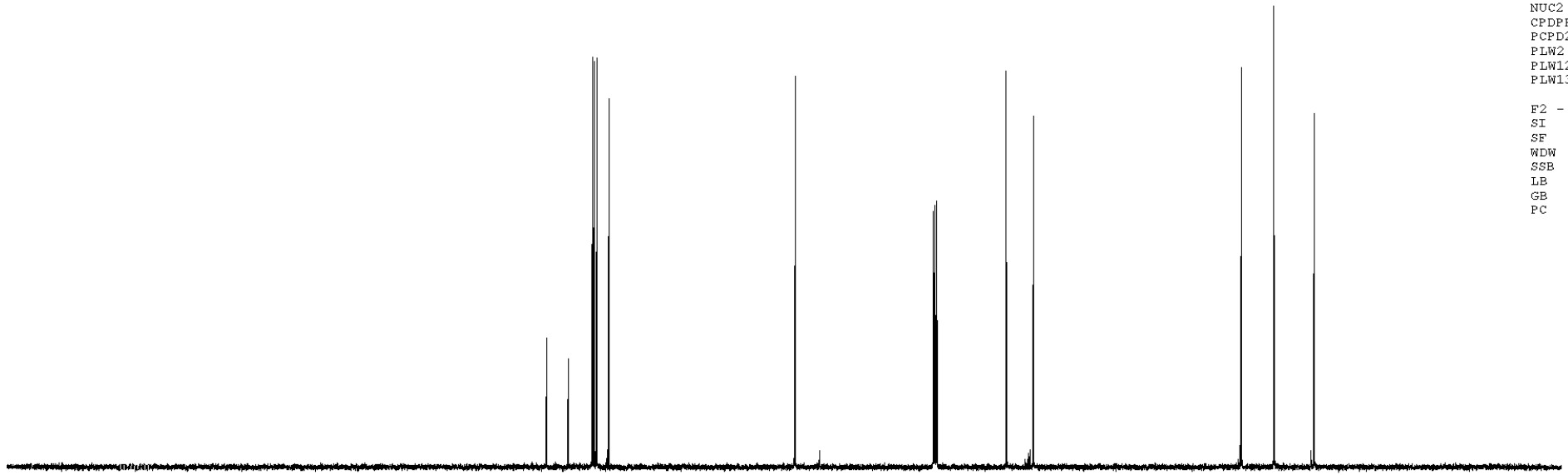


3d

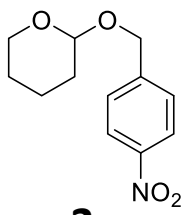
125 MHz ^{13}C NMR

$CDCl_3$

136.28
133.00
129.30
129.04
128.60
126.81
98.44
77.41
77.15
76.90
66.36
62.21
30.60
25.54
19.40



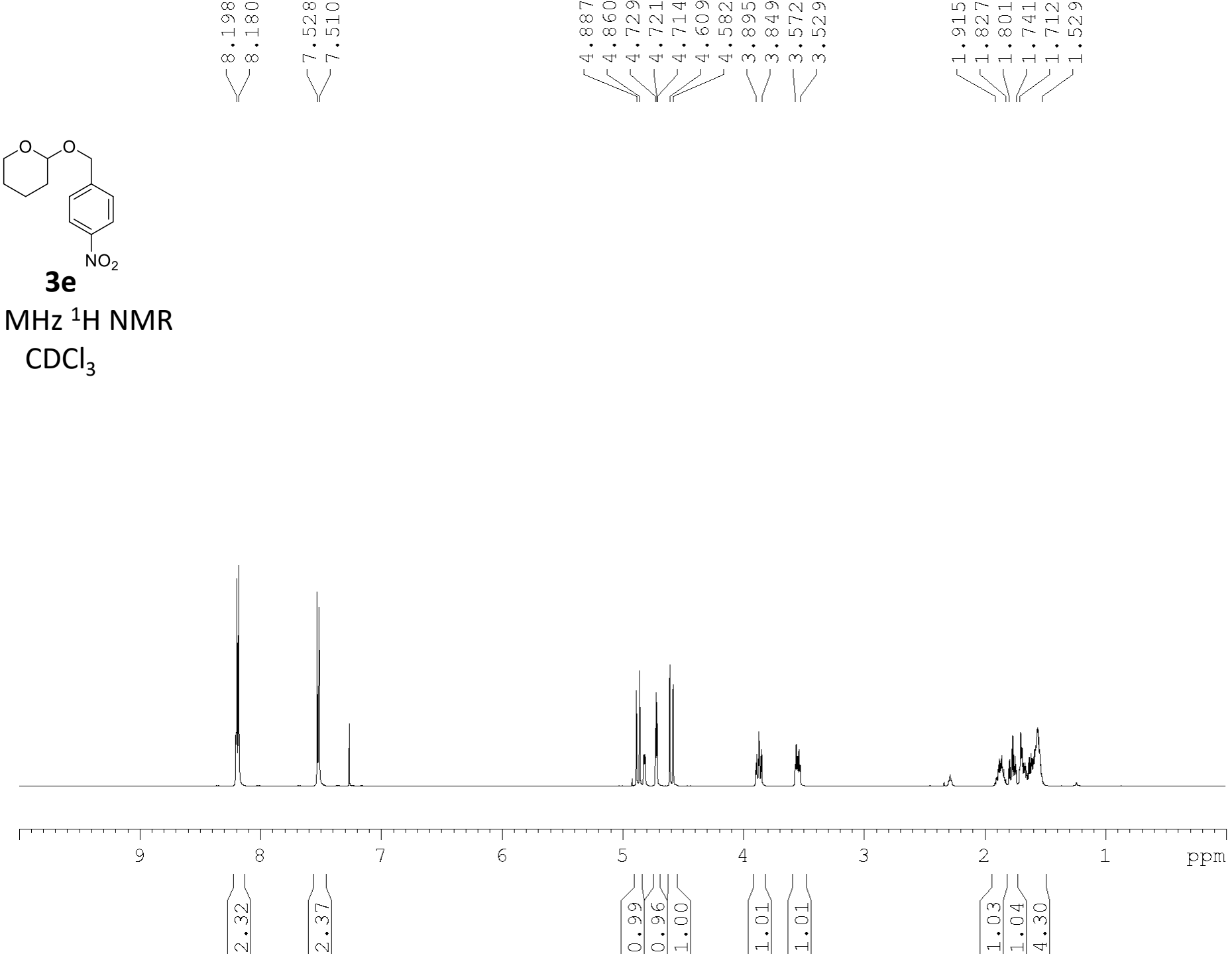

```
Current Data Parameters
NAME      vinn-4-137-16-islt-20201210
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20201211
Time                6.39 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577804 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



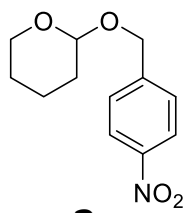
3e

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-4-islt-20201207
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_              20201207
Time                 19.08 h
INSTRUM              spect
PROBHD    Z119470_0283 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10000.000 Hz
FIDRES              0.305176 Hz
AQ                3.2767999 sec
RG                     50.6
DW                  50.000 usec
DE                   6.50 usec
TE                  295.2 K
D1              1.00000000 sec
TD0                     1
SFO1            500.1330883 MHz
NUC1                   1H
P1                  10.91 usec
PLW1           25.00000000 W

F2 - Processing parameters
SI                  65536
SF              500.1300122 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



3e

125 MHz ^{13}C NMR

$CDCl_3$

146.219
127.858
127.057
123.685
98.399
77.411
77.156
76.901
67.724
62.393
30.540
25.434
19.353

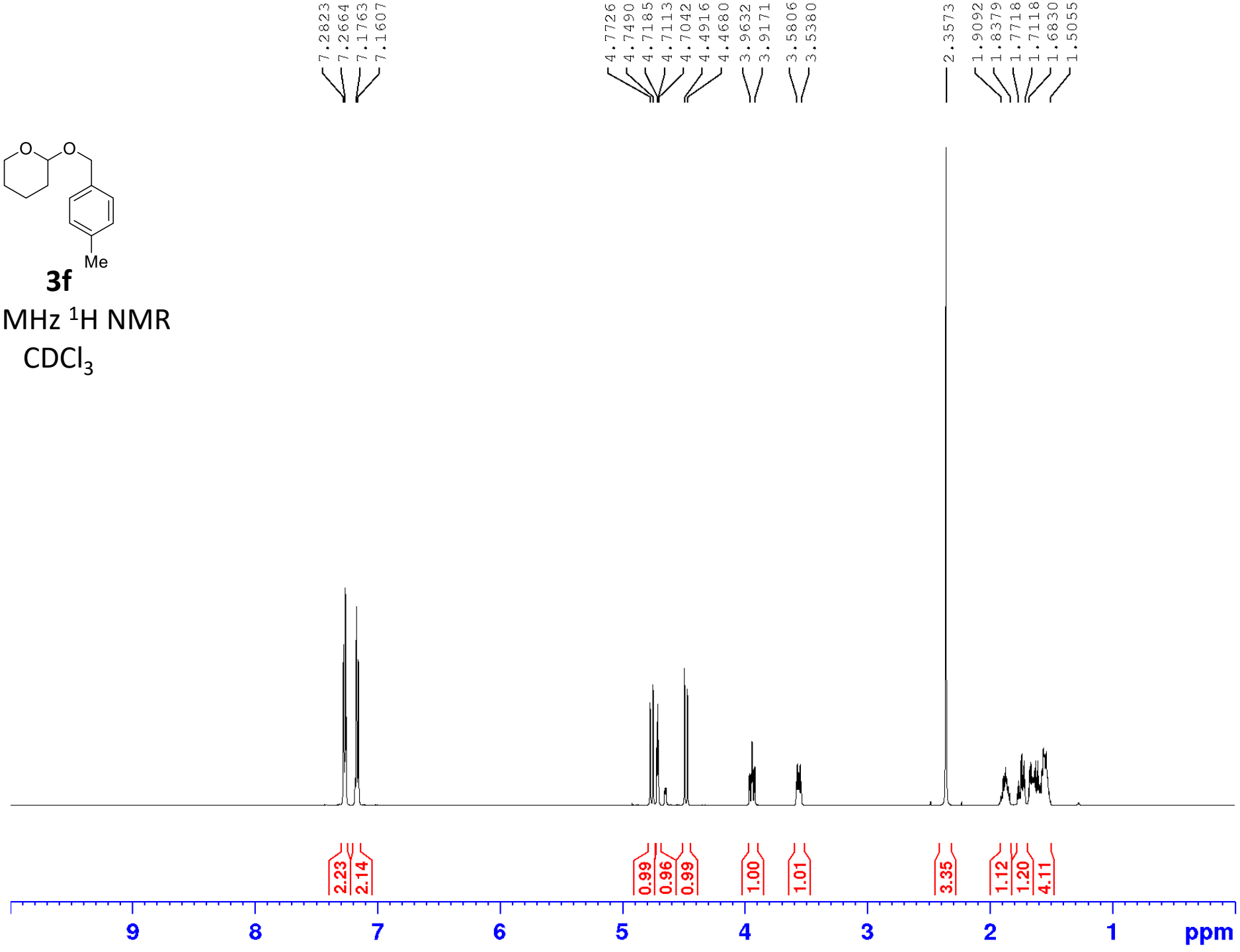
```
Current Data Parameters
NAME      vinn-4-137-4-islt-20201207
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20201207
Time              19.14 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW              16.800 usec
DE               6.50 usec
TE               295.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577777 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

200 180 160 140 120 100 80 60 40 20 0 ppm

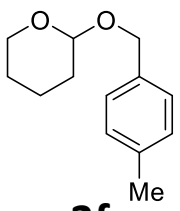
3f

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-3-islt-20201207
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20201207
Time              18.58 h
INSTRUM             spect
PROBHD    Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300121 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



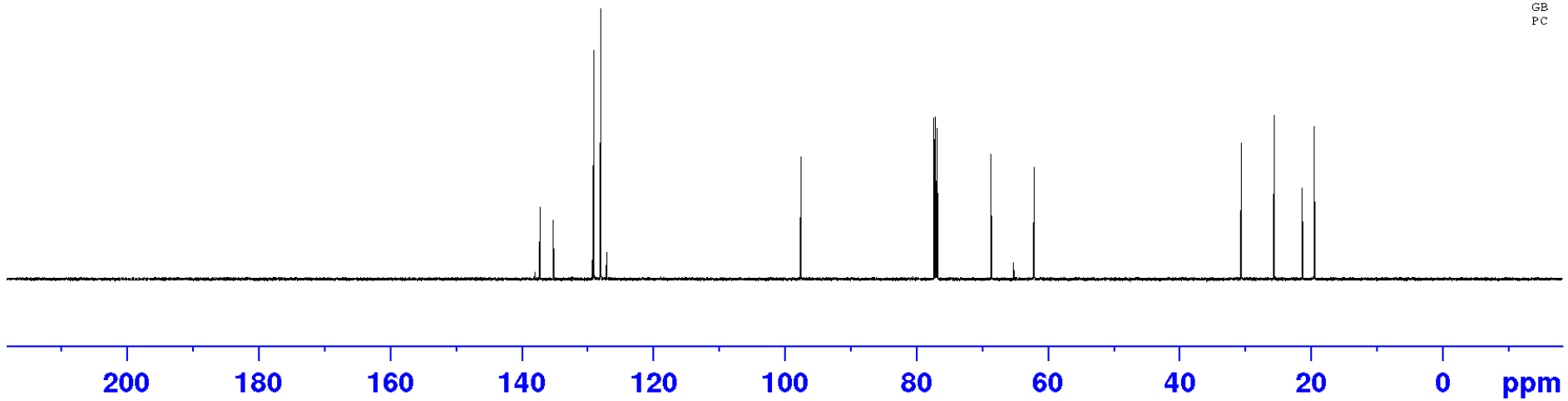
3f

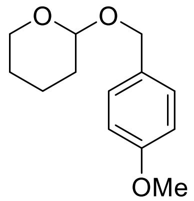
125 MHz ^{13}C NMR

$CDCl_3$

137.30
135.29
129.14
128.08
97.64
77.41
77.16
76.90
68.76
62.19
30.69
25.60
21.27
19.47

```
Current Data Parameters
NAME      vinn-4-137-3-islt-20201207
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20201207
Time              19.04 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW               16.800 usec
DE                6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577796 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

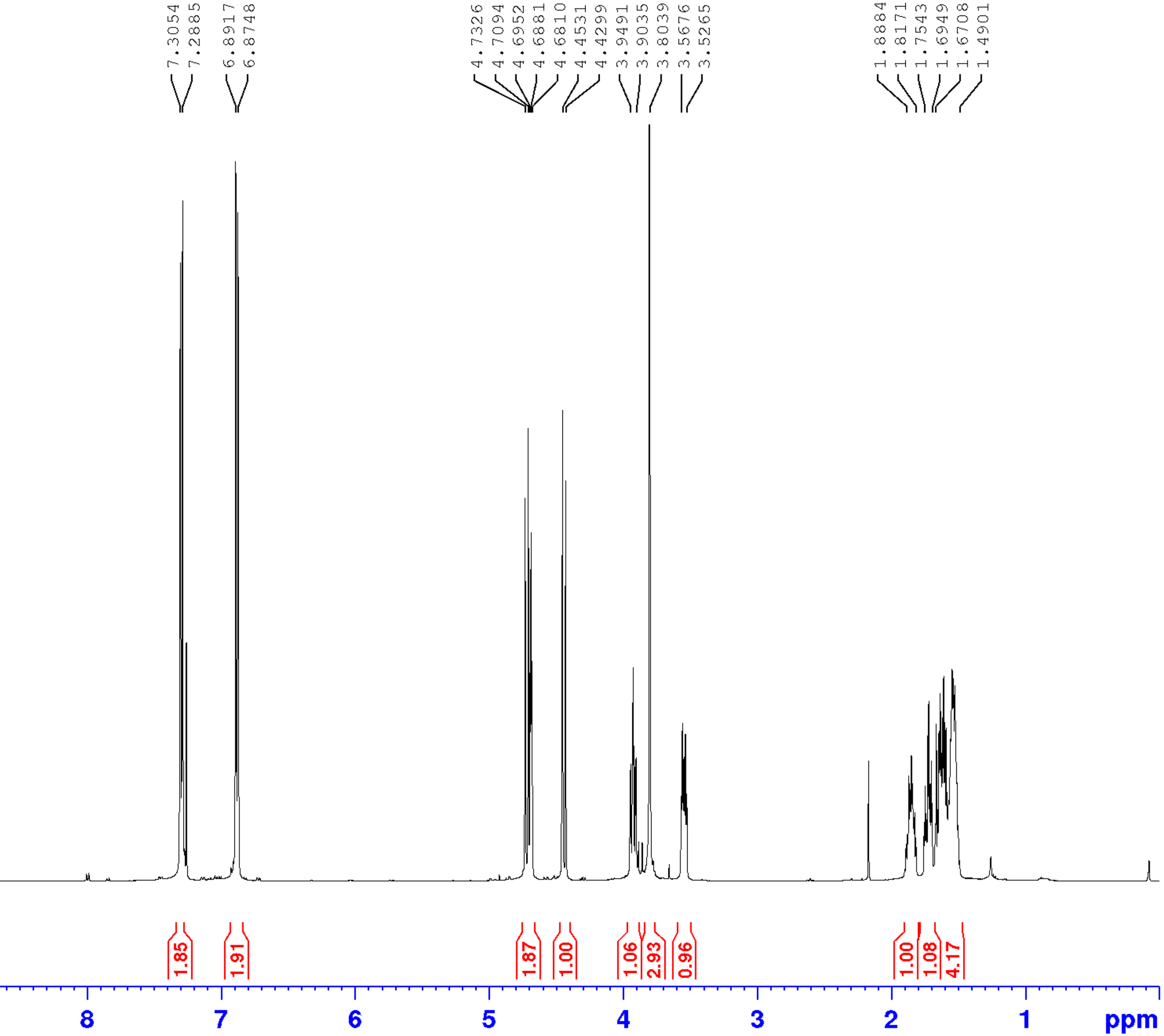




3g

500 MHz ^{1}H NMR

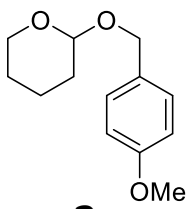
$CDCl_3$



Current Data Parameters
NAME vinn-4-137-7-islt2-2020012
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210121
Time 8.38 h
INSTRUM spect
PROBHD Z119470_0283 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 56.83
DW 50.000 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330883 MHz
NUC1 1H
P1 10.91 usec
PLW1 25.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



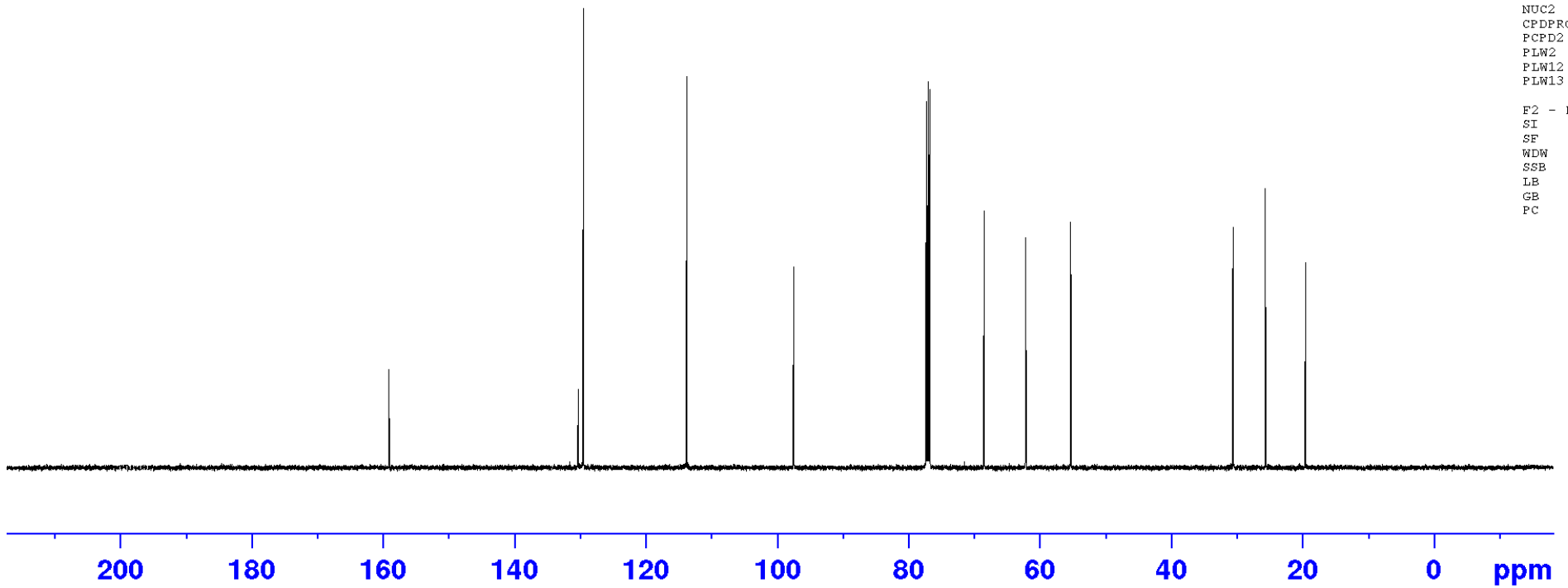
3g

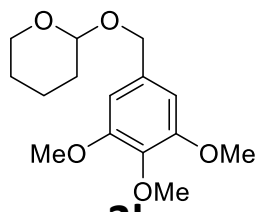
125 MHz ^{13}C NMR

$CDCl_3$

159.24
130.42
129.62
113.88
97.58
77.41
77.15
76.90
68.60
62.27
55.39
30.71
25.61
19.53

```
Current Data Parameters
NAME      vinn-4-137-7-islt2-20200120
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time               8.52 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW               16.800 usec
DE                6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577765 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

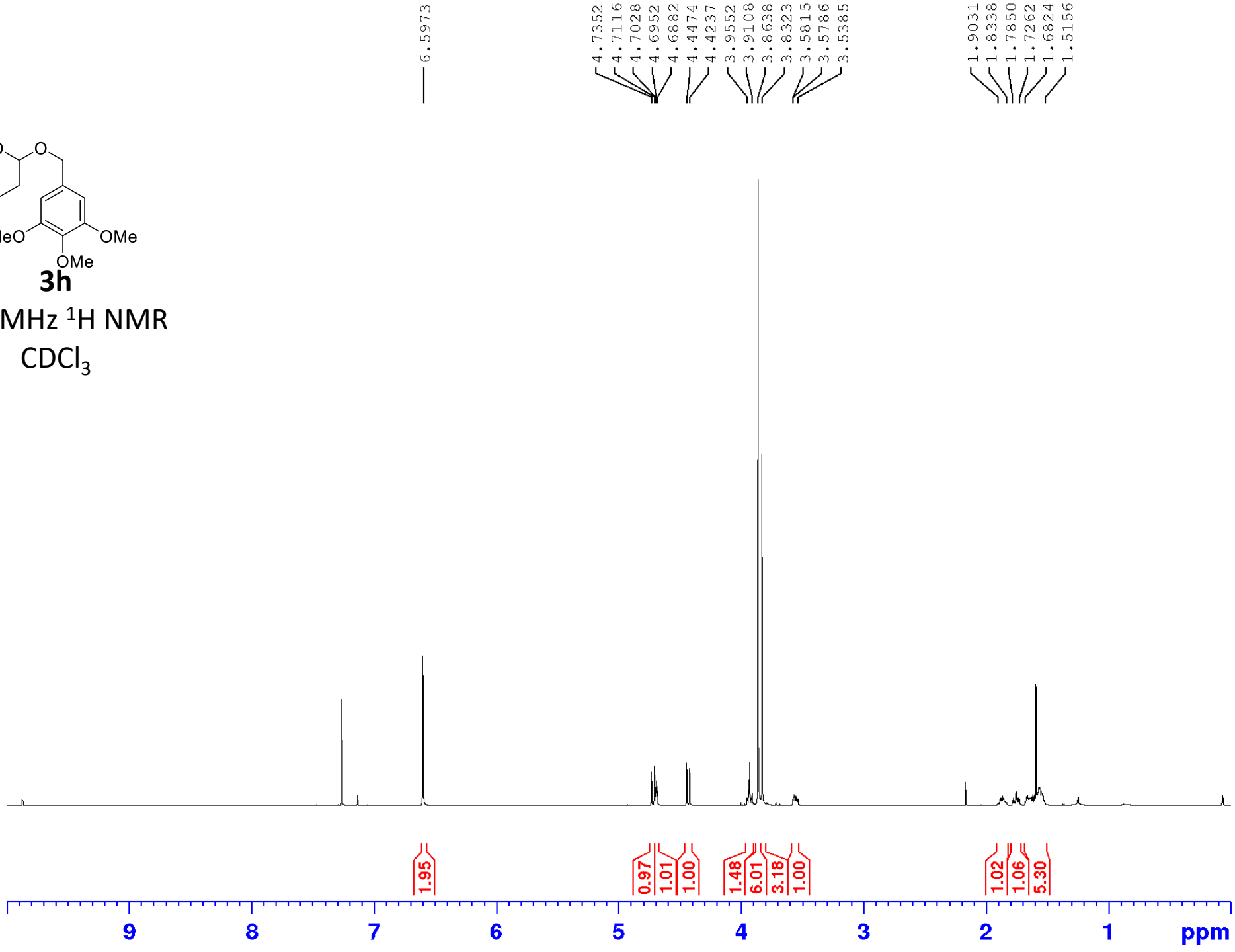




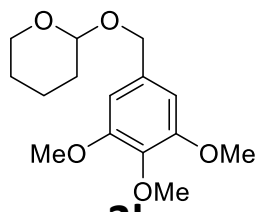
3h

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-6-islt2-2020012
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_              20210121
Time                  8.20 h
INSTRUM              spect
PROBHD    Z119470_0283 (
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ                3.2767999 sec
RG                     102.6
DW                    50.000 usec
DE                     6.50 usec
TE                    295.1 K
D1             1.00000000 sec
TD0                      1
SFO1           500.1330883 MHz
NUC1                    1H
P1                    10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                   65536
SF             500.1300123 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



3h

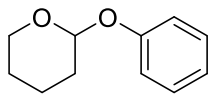
125 MHz ^{13}C NMR

$CDCl_3$

153.36
137.44
133.97
105.01
97.92
77.41
77.16
76.90
69.23
62.53
60.97
56.21
30.75
25.58
19.65

```
Current Data Parameters
NAME      vinn-4-137-6-islt2-20200120
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time               8.34 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 256
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1       125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1       94.00000000 W
SFO2       500.1320005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2            80.00 usec
PLW2       25.00000000 W
PLW12       0.46495000 W
PLW13       0.23387000 W

F2 - Processing parameters
SI               32768
SF         125.7577734 MHz
WDW                EM
SSB                 0
LB              1.00 Hz
GB                  0
PC              1.40
```

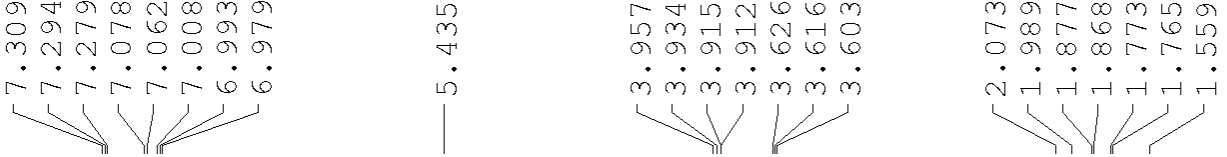
200 180 160 140 120 100 80 60 40 20 0 ppm



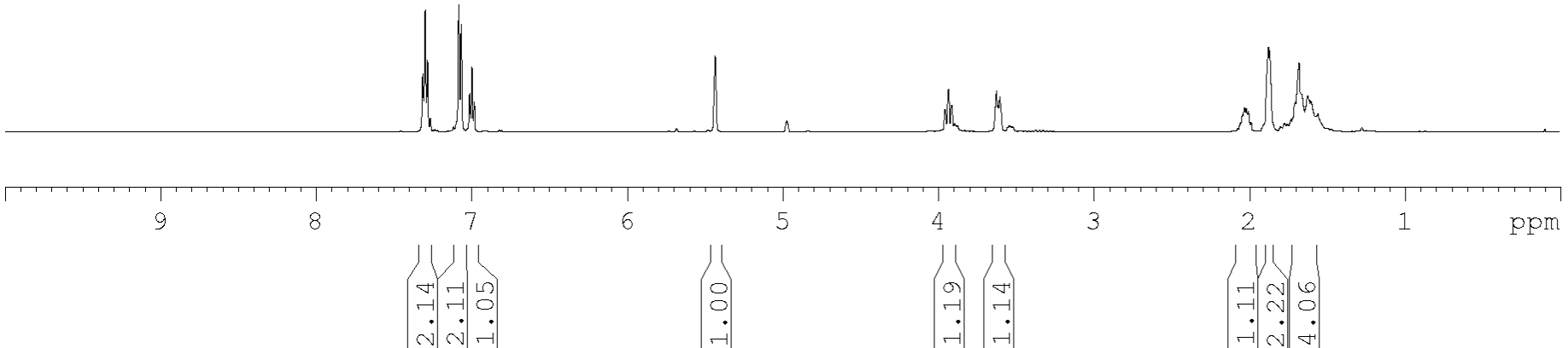
3i

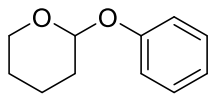
500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-139-1-islt-20201222
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201223
Time               8.33 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW               50.000 usec
DE                6.50 usec
TE               295.2 K
D1            1.00000000 sec
TD0                   1
SFO1        500.1330883 MHz
NUC1                 1H
P1                10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI                65536
SF          500.1300123 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```





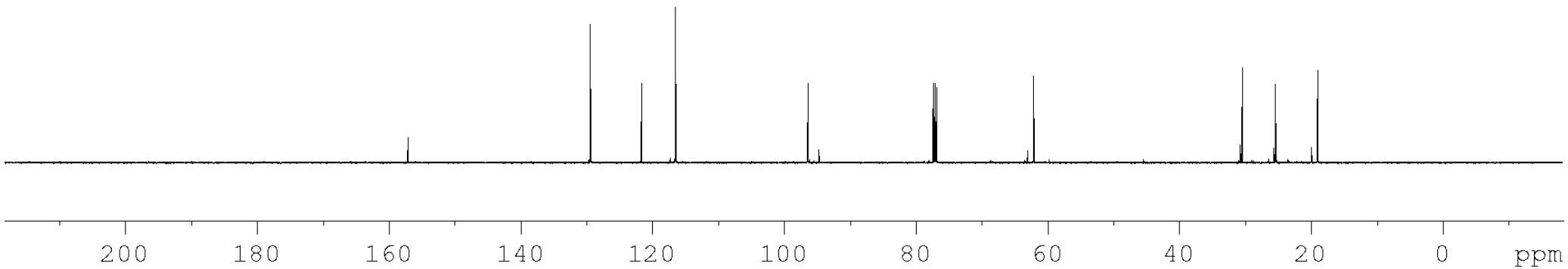
3i

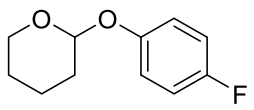
125 MHz ^{13}C NMR

$CDCl_3$

157.155
129.467
121.671
116.550
96.414
77.411
77.157
76.903
62.150
30.503
25.328
18.939

```
Current Data Parameters
NAME      vinn-4-139-1-islt-20201222
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20201223
Time               8.41 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW              16.800 usec
DE               6.50 usec
TE               295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1       125.7703643 MHz
NUC1                13C
P1               9.75 usec
PLW1        94.00000000 W
SFO2       500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2           80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF         125.7577796 MHz
WDW                EM
SSB                 0
LB              1.00 Hz
GB                  0
PC              1.40
```



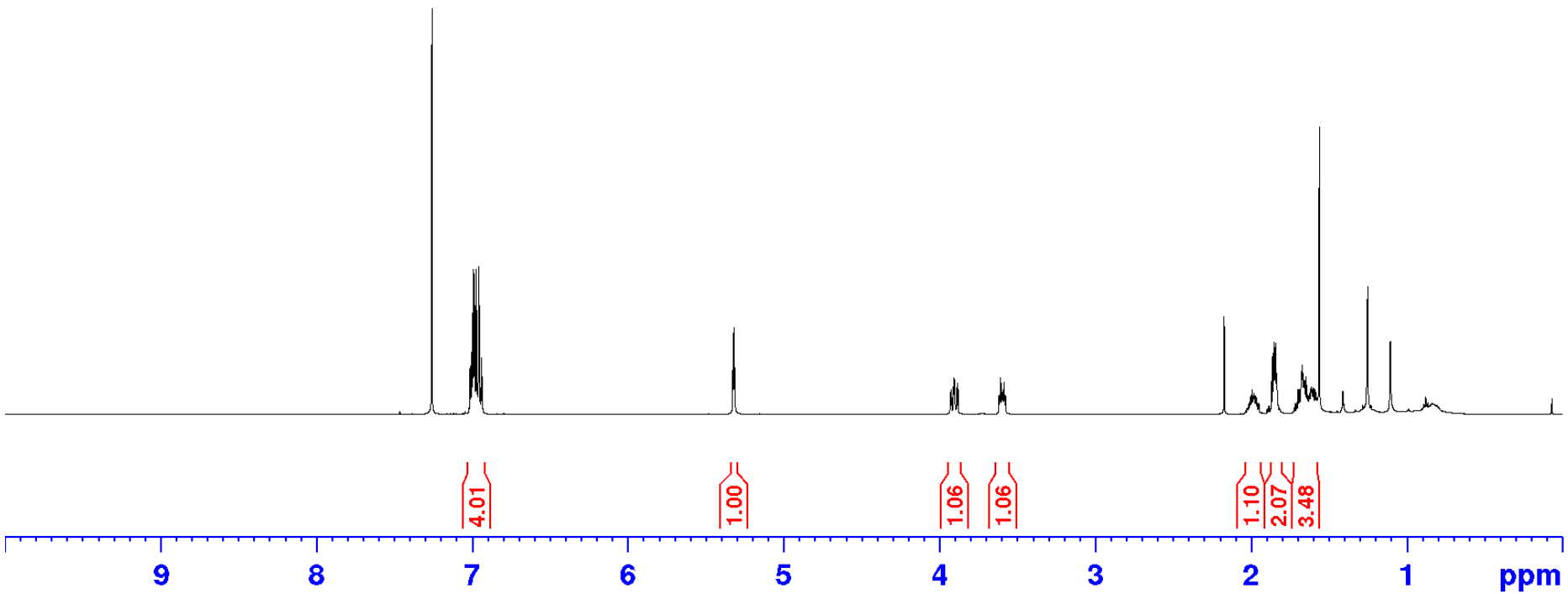


3j

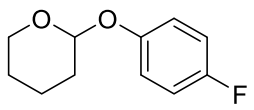
500 MHz ^{1}H NMR

$CDCl_3$

7.0139
6.9393
5.3277
5.3211
5.3146
3.9310
3.8829
3.6186
3.5766
2.0355
1.9505
1.8961
1.8067
1.7244
1.5769



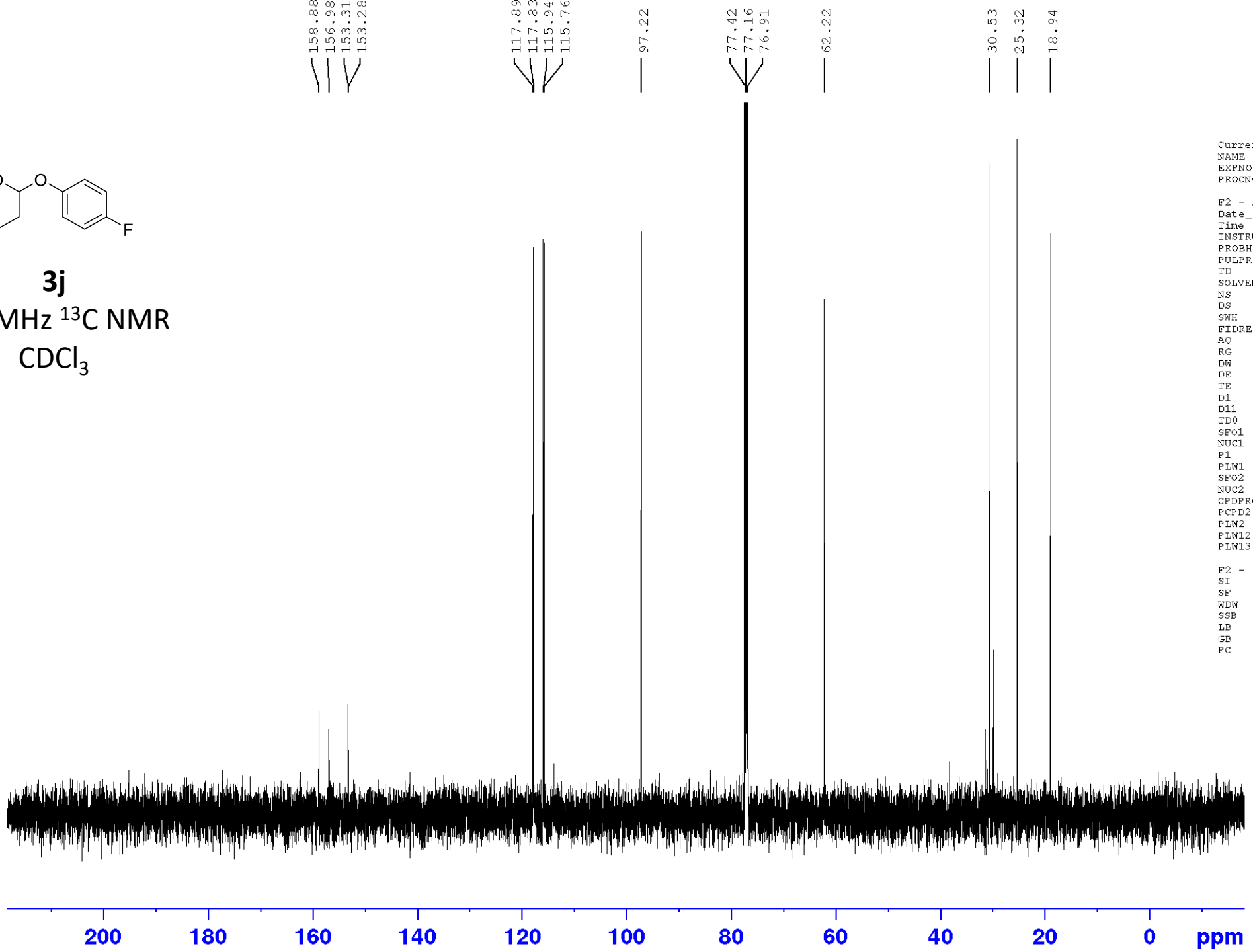

```
Current Data Parameters
NAME      vinn-4-139-4-2-islt2-20200120
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20210121
Time               9.14 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                117.01
DW               50.000 usec
DE                6.50 usec
TE                295.1 K
D1           1.00000000 sec
TD0                   1
SFO1        500.1330883 MHz
NUC1                  1H
P1               10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI                65536
SF          500.1300124 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



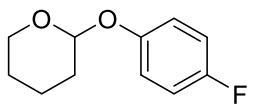
3j

125 MHz ^{13}C NMR

$CDCl_3$



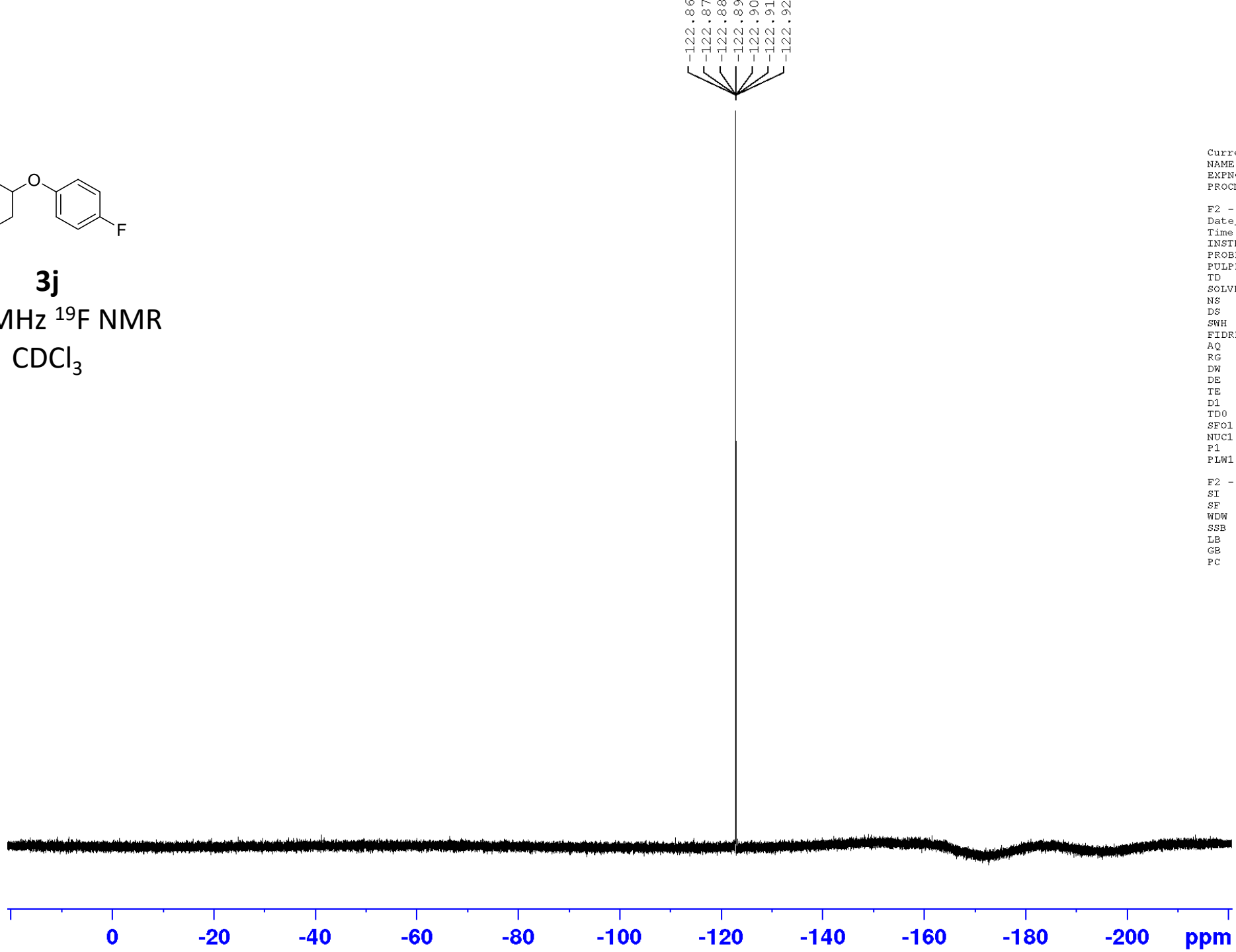

```
Current Data Parameters
NAME      vinn-4-139-4-2-islt2-2020012
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20210121
Time                9.28 h
INSTRUM            spect
PROBHD    Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7665629 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



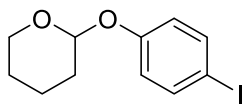
3j

470 MHz ^{19}F NMR

$CDCl_3$



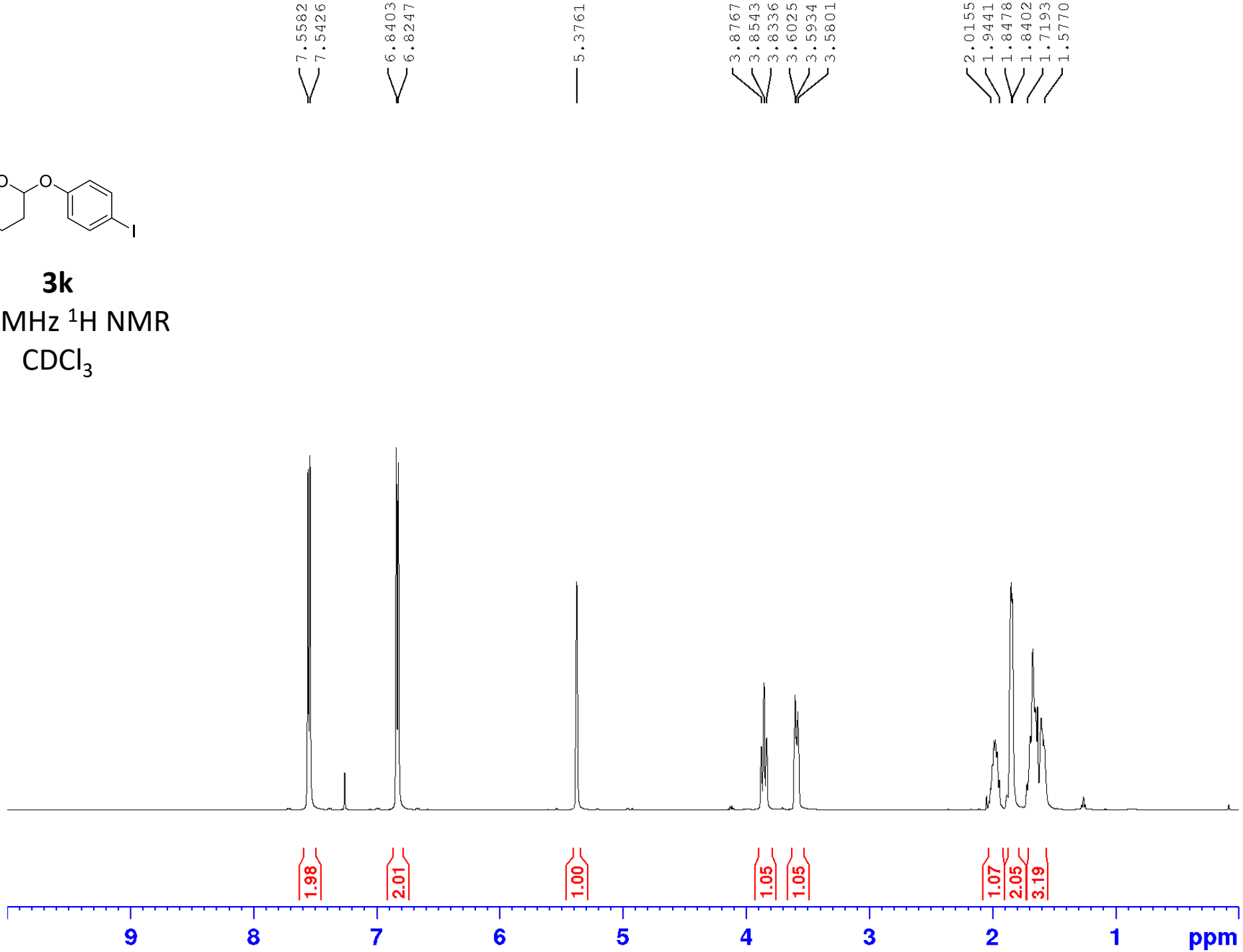

```
Current Data Parameters
NAME      vinn-4-139-4-2-islt2-2020012
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time              9.30 h
INSTRUM          spect
PROBHD   Z119470_0283 (
PULPROG         zgflqn
TD              131072
SOLVENT           CDCl3
NS                   16
DS                    4
SWH          113636.367 Hz
FIDRES         1.733953 Hz
AQ             0.5767168 sec
RG                206.72
DW                4.400 usec
DE                6.50 usec
TE                295.2 K
D1           1.00000000 sec
TD0                   1
SFO1         470.5453180 MHz
NUC1                19F
P1                15.00 usec
PLW1         47.23500061 W

F2 - Processing parameters
SI                65536
SF           470.5923772 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



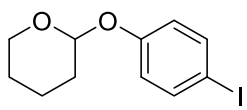
3k

500 MHz ^{1}H NMR

$CDCl_3$



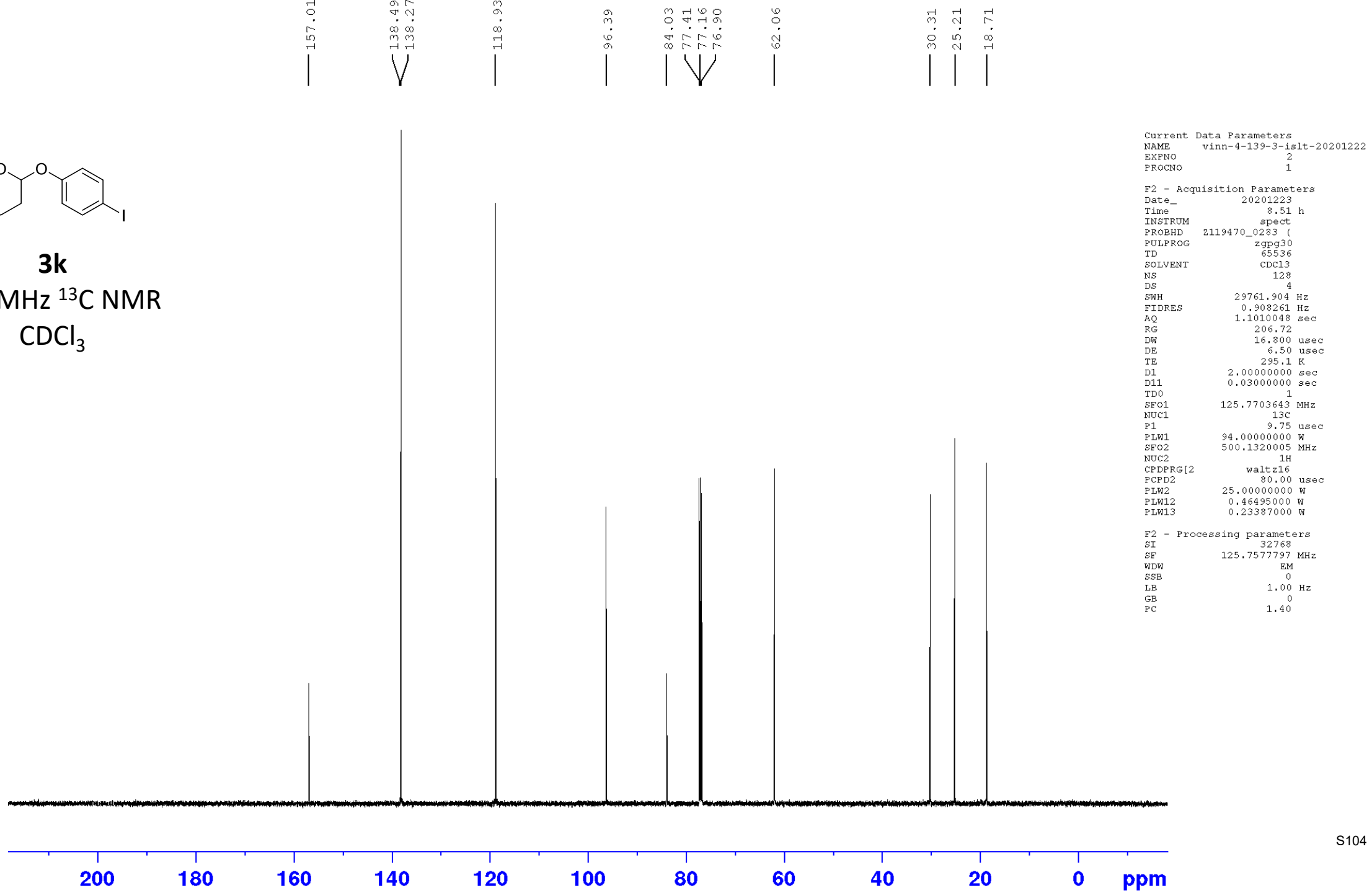

```
Current Data Parameters
NAME      vinn-4-139-3-islt-20201222
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201223
Time                8.44 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.2 K
D1             1.00000000 sec
TD0                   1
SFO1          500.1330883 MHz
NUC1                 1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                65536
SF            500.1300120 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



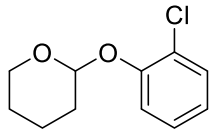
3k

125 MHz ^{13}C NMR

$CDCl_3$



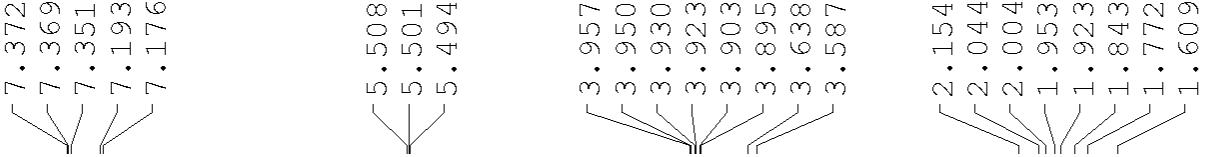

```
Current Data Parameters
NAME      vinn-4-139-3-islt-20201222
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201223
Time               8.51 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW              16.800 usec
DE               6.50 usec
TE              295.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577797 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```



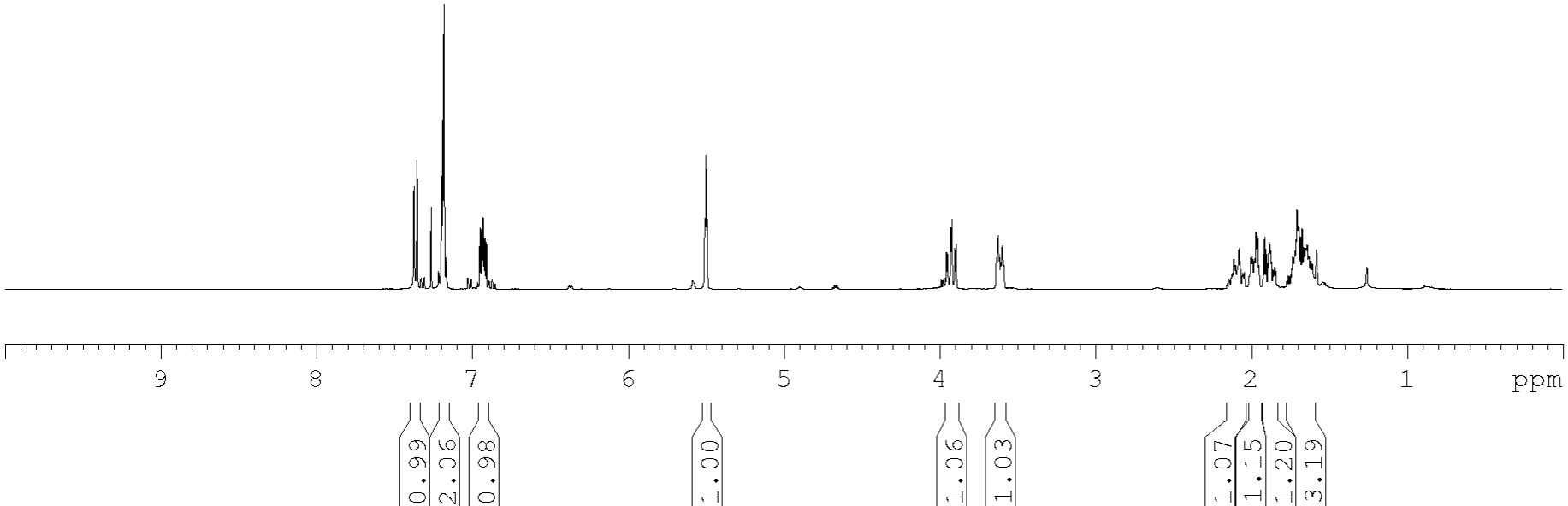
3l

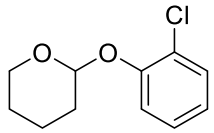
400 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      Andy-1-180-3-islt-20220817
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20220819
Time              17.55 h
INSTRUM           spect
PROBHD    Z108618_0257 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                   203
DW                62.400 usec
DE                 6.50 usec
TE                296.2 K
D1            1.00000000 sec
TD0                    1
SFO1          400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1          12.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300098 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```





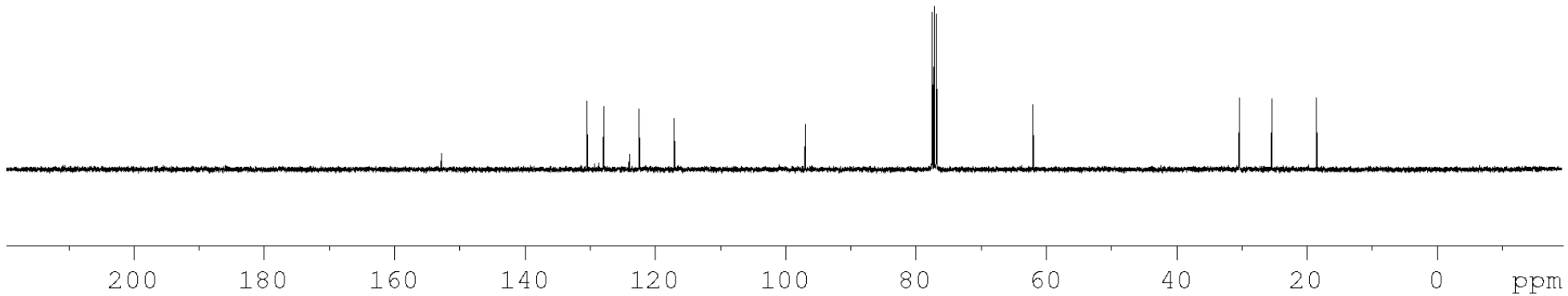
3l

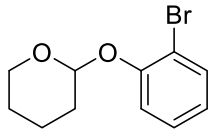
100 MHz ^{13}C NMR

$CDCl_3$

152.664
130.324
127.727
123.957
122.455
117.059
96.919
77.475
77.157
76.840
61.984
30.317
25.345
18.483

```
Current Data Parameters
NAME      Andy-1-180-3-islt-20220817
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20220819
Time              18.00 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG         zgpg30
TD              65536
SOLVENT           CDCl3
NS                   62
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                  203
DW                20.800 usec
DE                 6.50 usec
TE                296.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         51.00000000 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.17465000 W

F2 - Processing parameters
SI                32768
SF          100.6127565 MHz
```



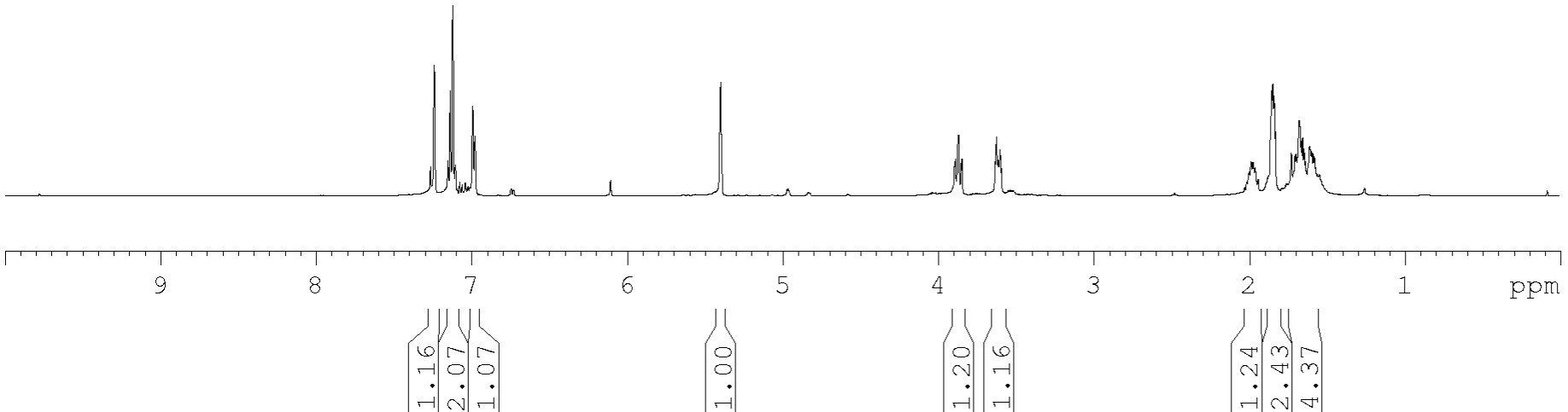


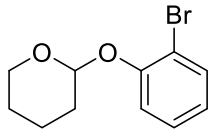
3m

500 MHz ^{1}H NMR

$CDCl_3$


```
Current Data Parameters
NAME      vinn-4-139-2-2-iselt2-20210111
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210111
Time              18.36 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1            1.00000000 sec
TD0                    1
SFO1        500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI                 65536
SF          500.1300128 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```





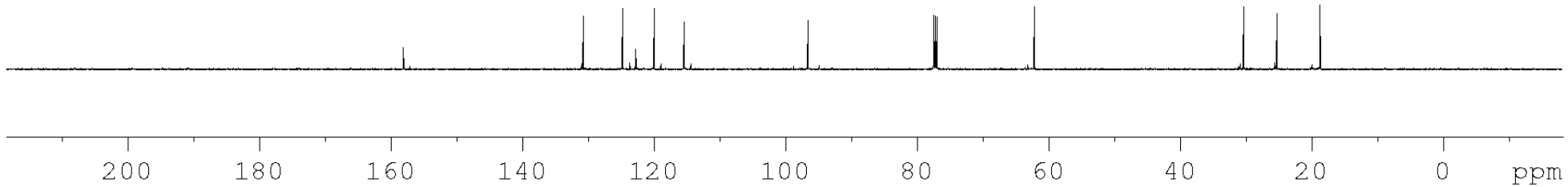
3m

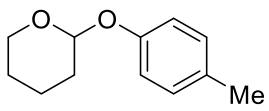
125 MHz ^{13}C NMR

$CDCl_3$

157.962
130.588
124.769
122.748
119.958
115.368
96.561
77.447
77.193
76.938
62.137
30.345
25.240
18.709

```
Current Data Parameters
NAME      vinn-4-139-2-2-islt2-20210111
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20210111
Time              18.43 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG                117.01
DW                16.800 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577740 MHz
```

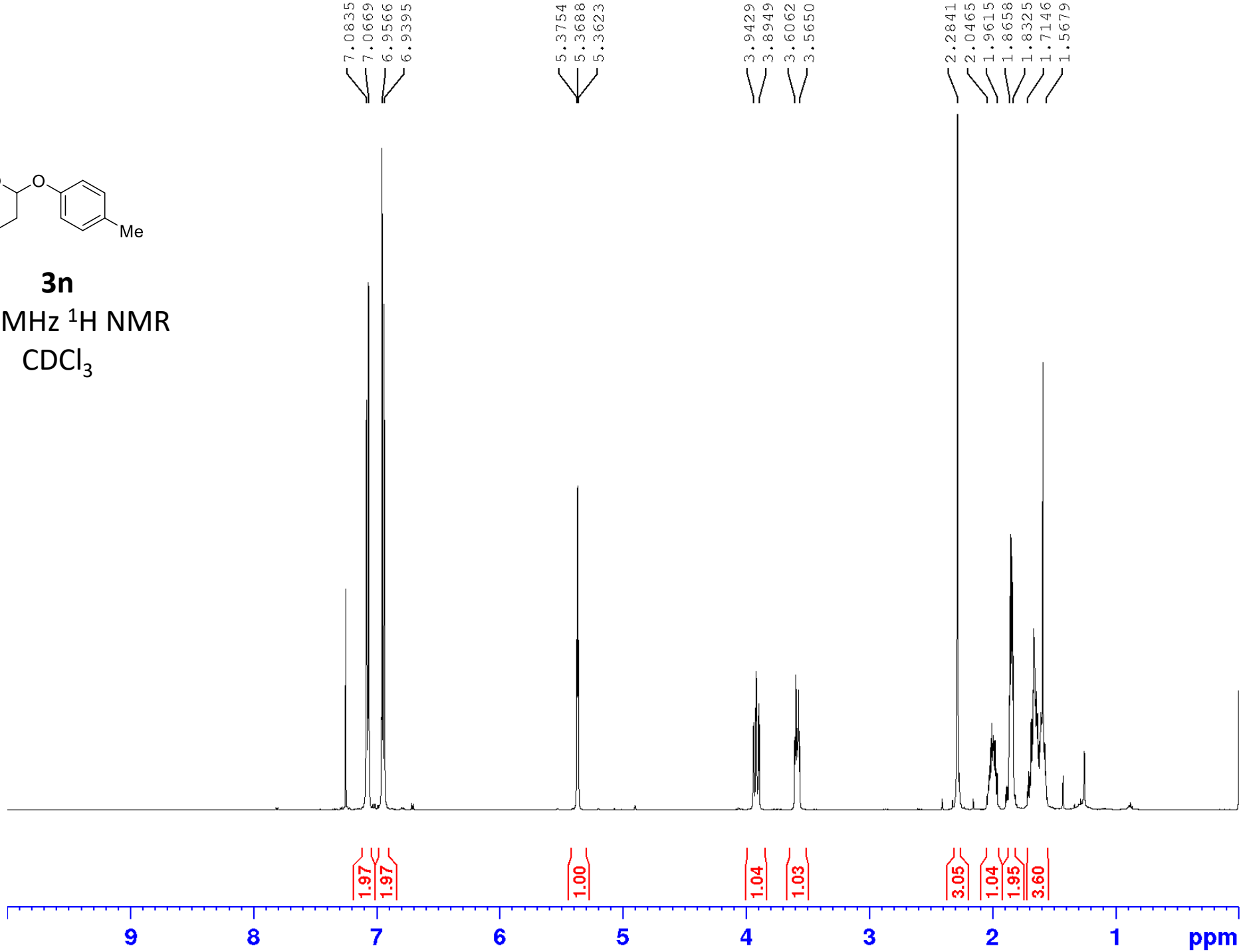




3n

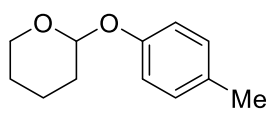
500 MHz ^{1}H NMR

$CDCl_3$



BRUKER

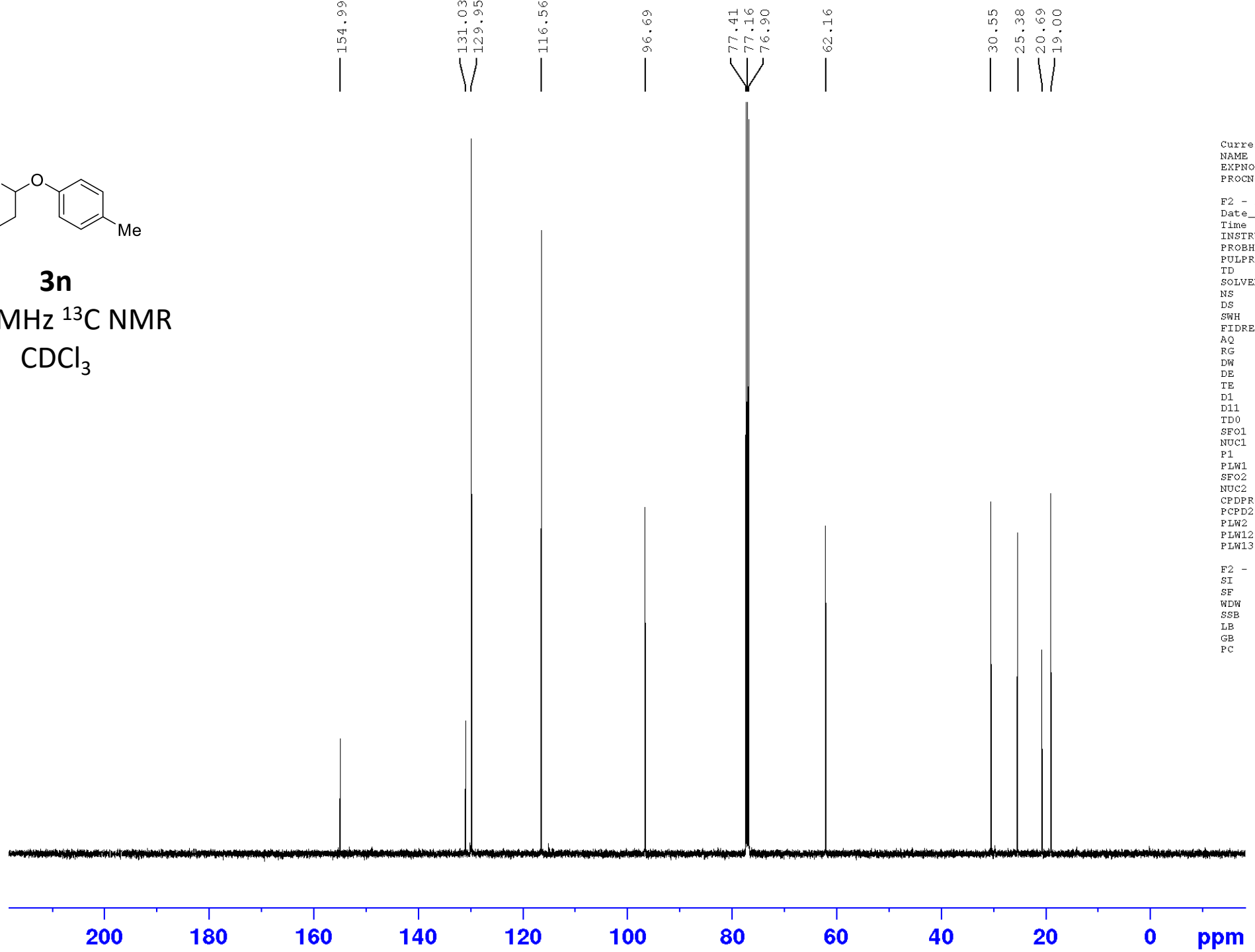
```
Current Data Parameters
NAME      vinn-4-190-3-clm9-20230103
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20230103
Time              17.02 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 93.28
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300163 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



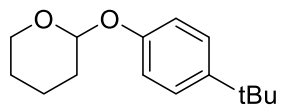
3n

125 MHz ^{13}C NMR

$CDCl_3$



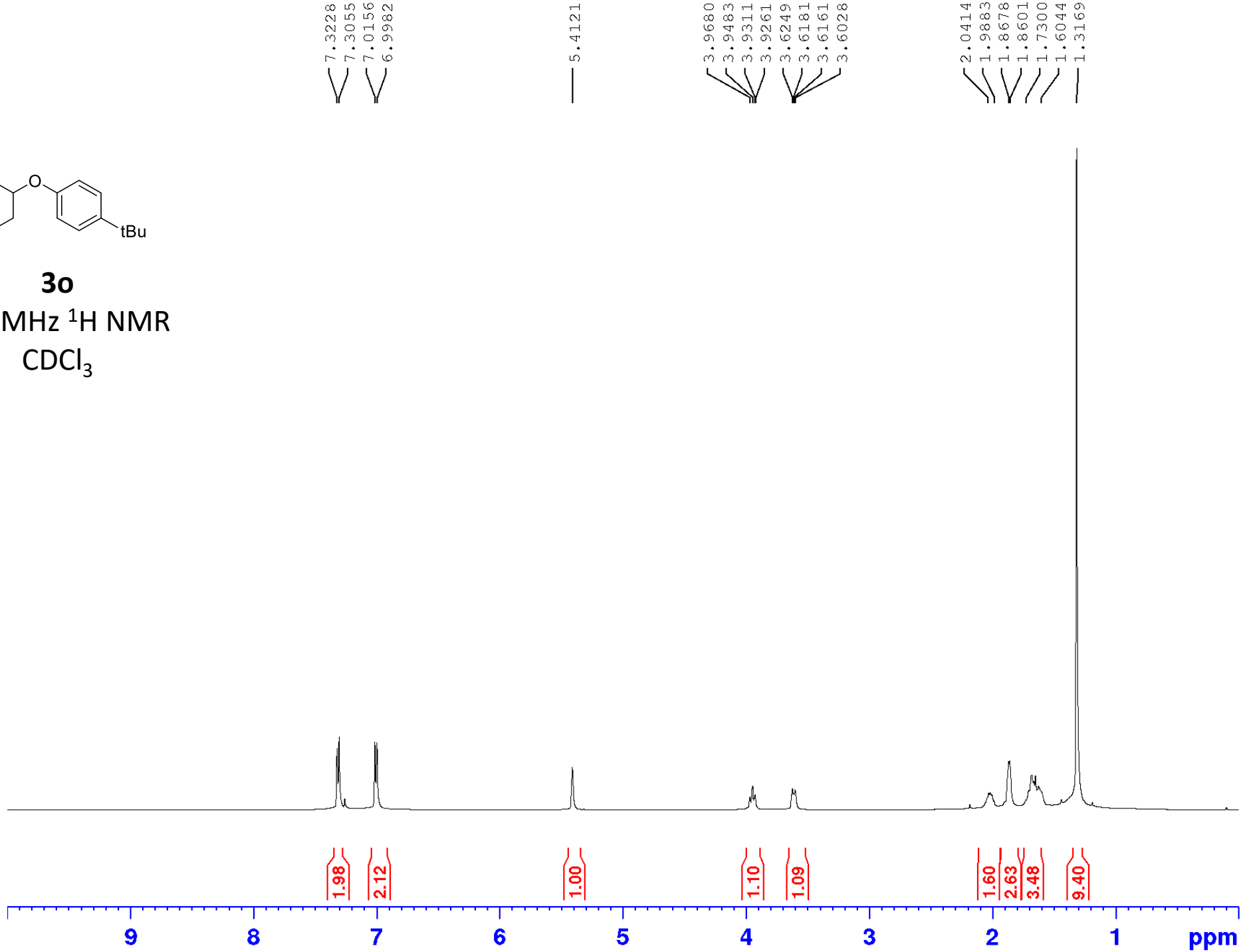

```
Current Data Parameters
NAME      vinn-4-190-3-clm9-20230103
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20230103
Time              18.26 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                163.99
DW                16.800 usec
DE                 6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577750 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



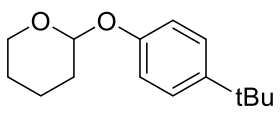
3o

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-139-8-islt2-2020012
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time               7.42 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW              50.000 usec
DE               6.50 usec
TE              295.2 K
D1           1.00000000 sec
TD0                  1
SFO1       500.1330883 MHz
NUC1               1H
P1              10.91 usec
PLW1       25.00000000 W

F2 - Processing parameters
SI               65536
SF         500.1300131 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



3o

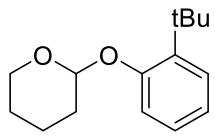
125 MHz ^{13}C NMR

$CDCl_3$

154.91
144.33
126.27
116.00
96.54
77.41
77.16
76.90
62.13
34.22
31.64
30.56
25.39
18.98

```
Current Data Parameters
NAME      vinn-4-139-8-islt2-20200120
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time               7.56 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577780 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

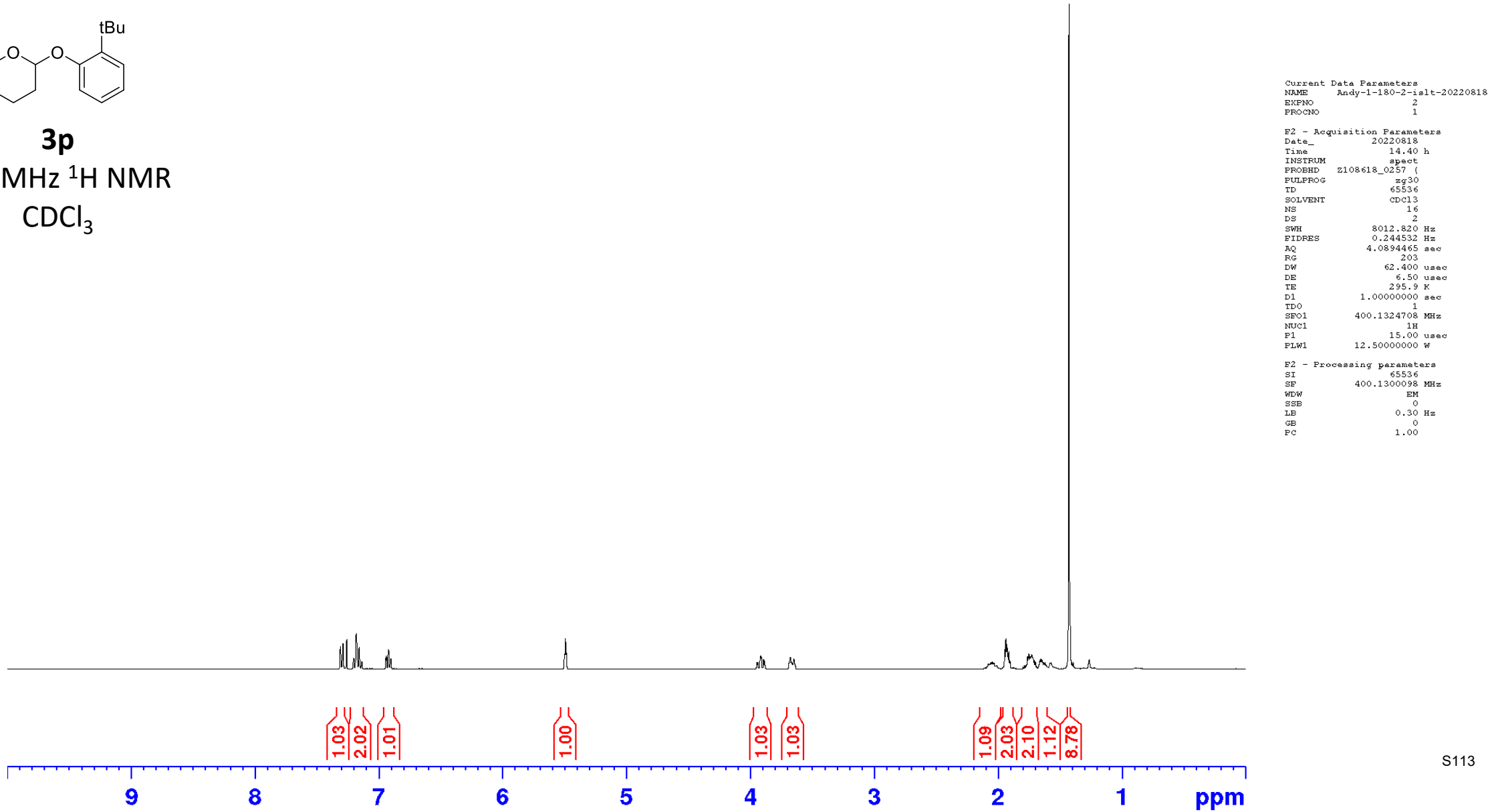
200 180 160 140 120 100 80 60 40 20 ppm



3p

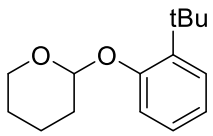
400 MHz ^{1}H NMR

$CDCl_3$



BRUKER

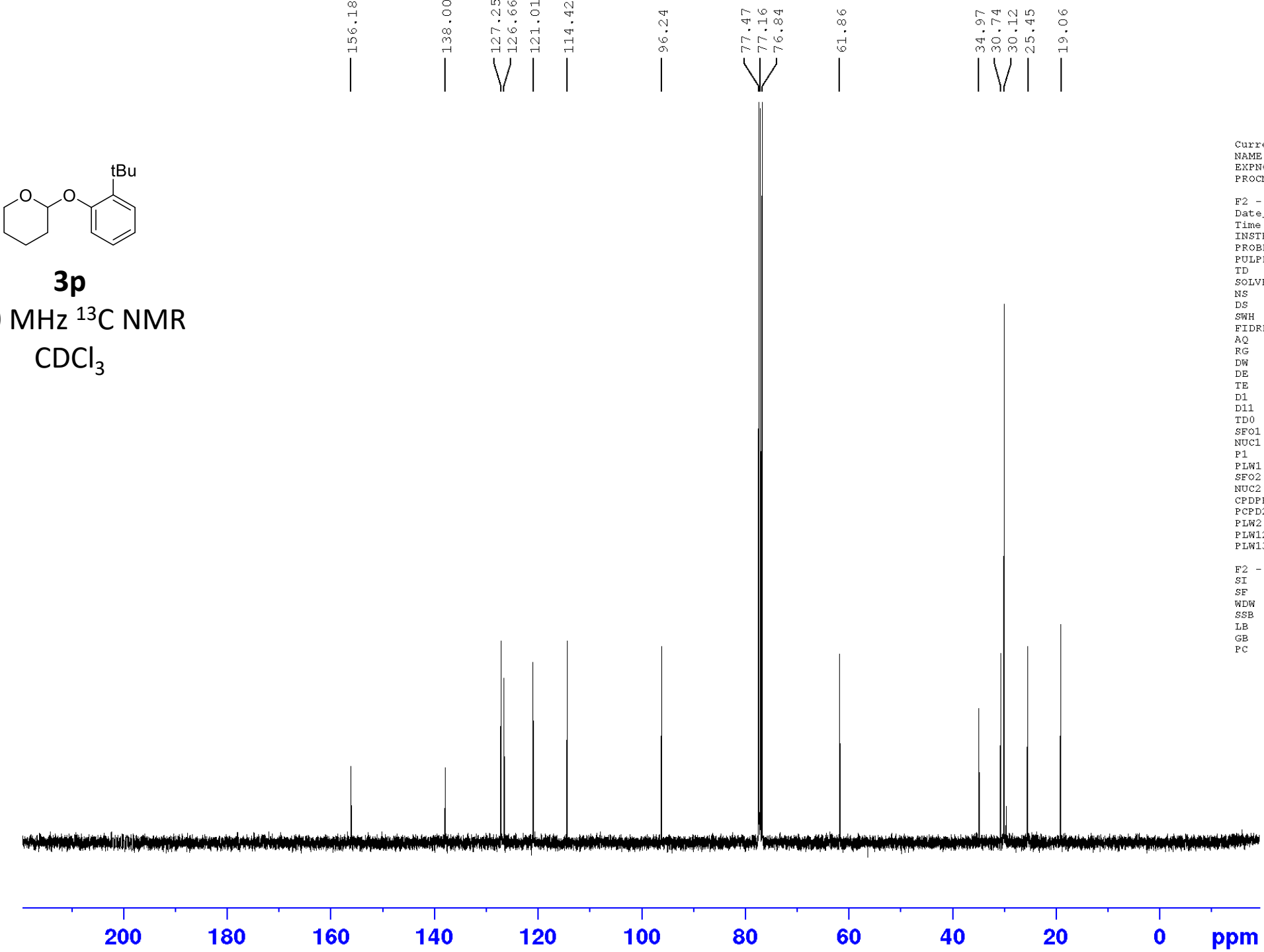
```
Current Data Parameters
NAME      Andy-1-180-2-islt-20220818
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20220818
Time              14.40 h
INSTRUM           spect
PROBHD    Z108618_0257 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                 203
DW              62.400 usec
DE               6.50 usec
TE              295.9 K
D1          1.00000000 sec
TD0                  1
SFO1       400.1324708 MHz
NUC1               1H
P1              15.00 usec
PLW1       12.50000000 W

F2 - Processing parameters
SI               65536
SF         400.1300098 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



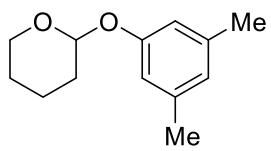
3p

100 MHz ^{13}C NMR

$CDCl_3$



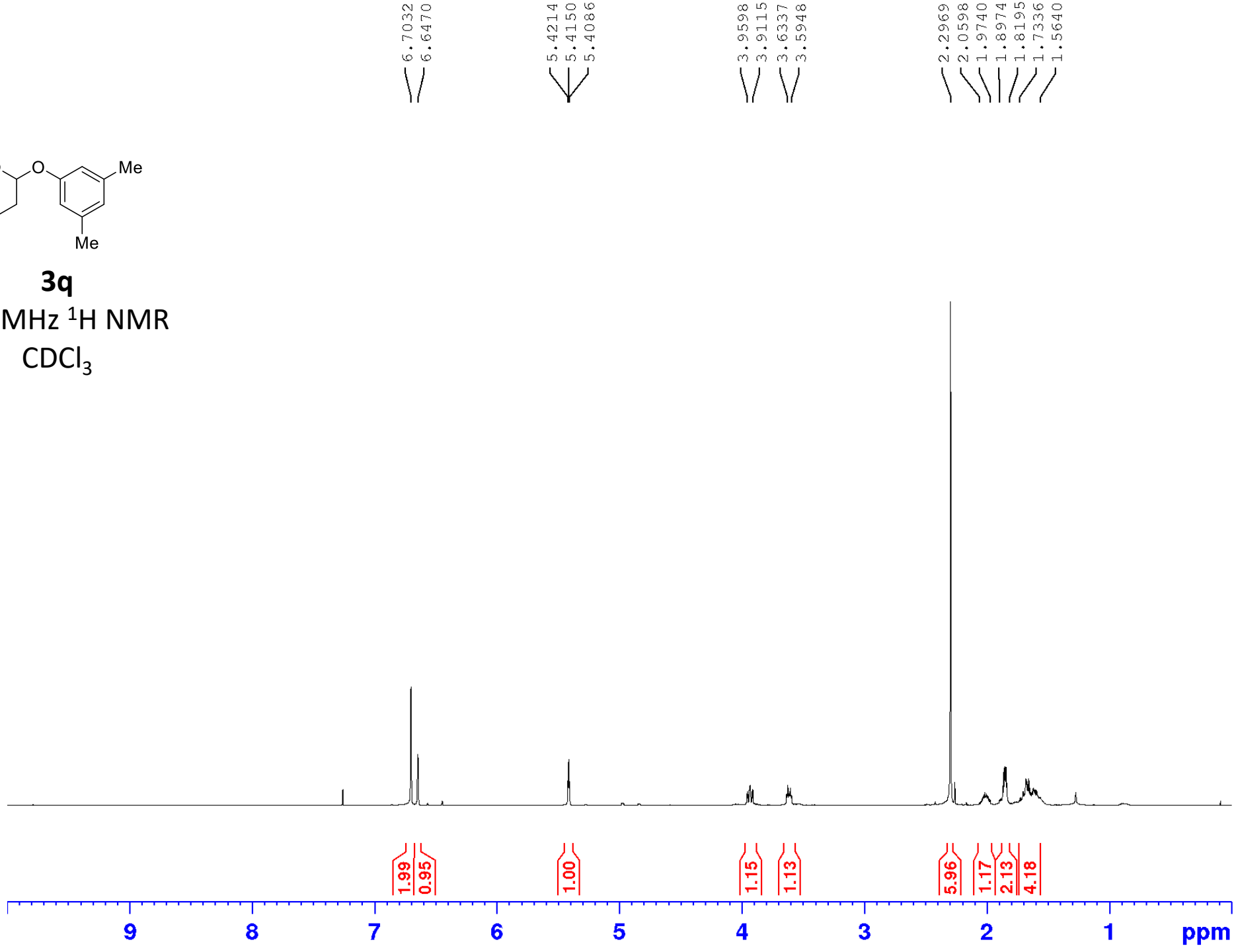

```
Current Data Parameters
NAME      Andy-1-180-2-islt-20220818
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20220818
Time              14.54 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE                296.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1               13C
P1               10.00 usec
PLW1        51.00000000 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.17465000 W

F2 - Processing parameters
SI                32768
SF          100.6127560 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



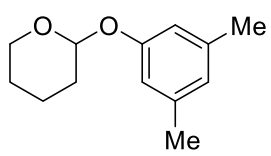
3q

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-139-9-islt-20210111
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20210111
Time              18.58 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300125 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



3q

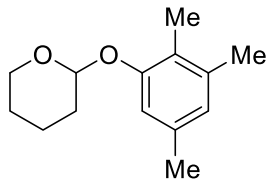
125 MHz ^{13}C NMR

$CDCl_3$

157.16
139.19
123.50
114.28
96.27
77.41
77.16
76.90
62.08
30.55
25.39
21.53
18.91

```
Current Data Parameters
NAME      vinn-4-139-9-islt-20210111
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210111
Time             19.03 h
INSTRUM          spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 100
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1       125.7703643 MHz
NUC1              13C
P1                9.75 usec
PLW1       94.00000000 W
SFO2       500.1320005 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2            80.00 usec
PLW2       25.00000000 W
PLW12       0.46495000 W
PLW13       0.23387000 W

F2 - Processing parameters
SI               32768
SF         125.7577784 MHz
WDW                EM
SSB                 0
LB              1.00 Hz
GB                  0
PC              1.40
```

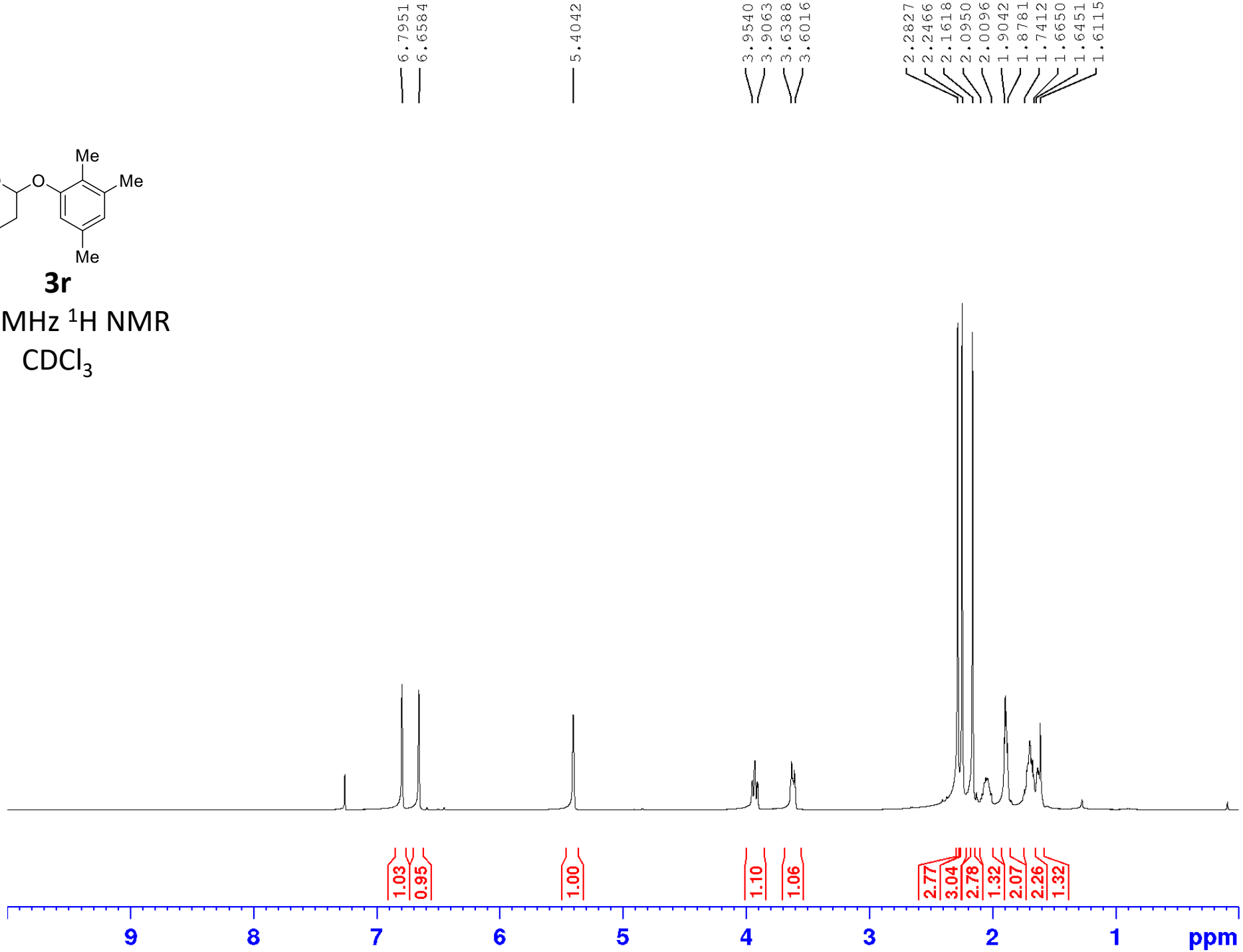
200 180 160 140 120 100 80 60 40 20 0 ppm



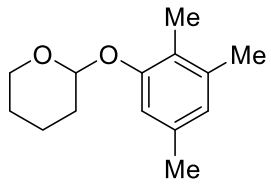
3r

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-139-10-islt2-20200120
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time               8.02 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES           0.305176 Hz
AQ            3.2767999 sec
RG                50.6
DW              50.000 usec
DE               6.50 usec
TE              295.1 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P1                10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300128 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



3r

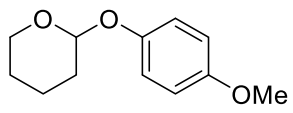
125 MHz ^{13}C NMR

$CDCl_3$

154.91
137.65
135.59
124.02
122.74
112.93
96.41
77.41
77.16
76.90
62.10
30.78
25.50
21.40
20.20
19.09
11.63

```
Current Data Parameters
NAME      vinn-4-139-10-islt2-20200120
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time              8.16 h
INSTRUM          spect
PROBHD   Z119470_0283 (
PULPROG        zgpg30
TD              65536
SOLVENT         CDCl3
NS                256
DS                  4
SWH         29761.904 Hz
FIDRES       0.908261 Hz
AQ           1.1010048 sec
RG              206.72
DW              16.800 usec
DE               6.50 usec
TE              295.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                 1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1       94.00000000 W
SFO2       500.1320005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2            80.00 usec
PLW2       25.00000000 W
PLW12       0.46495000 W
PLW13       0.23387000 W

F2 - Processing parameters
SI                32768
SF         125.7577766 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

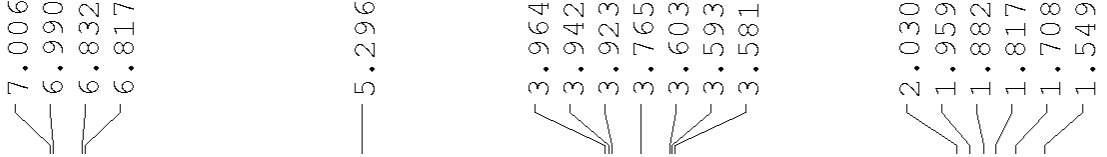
200 180 160 140 120 100 80 60 40 20 0 ppm



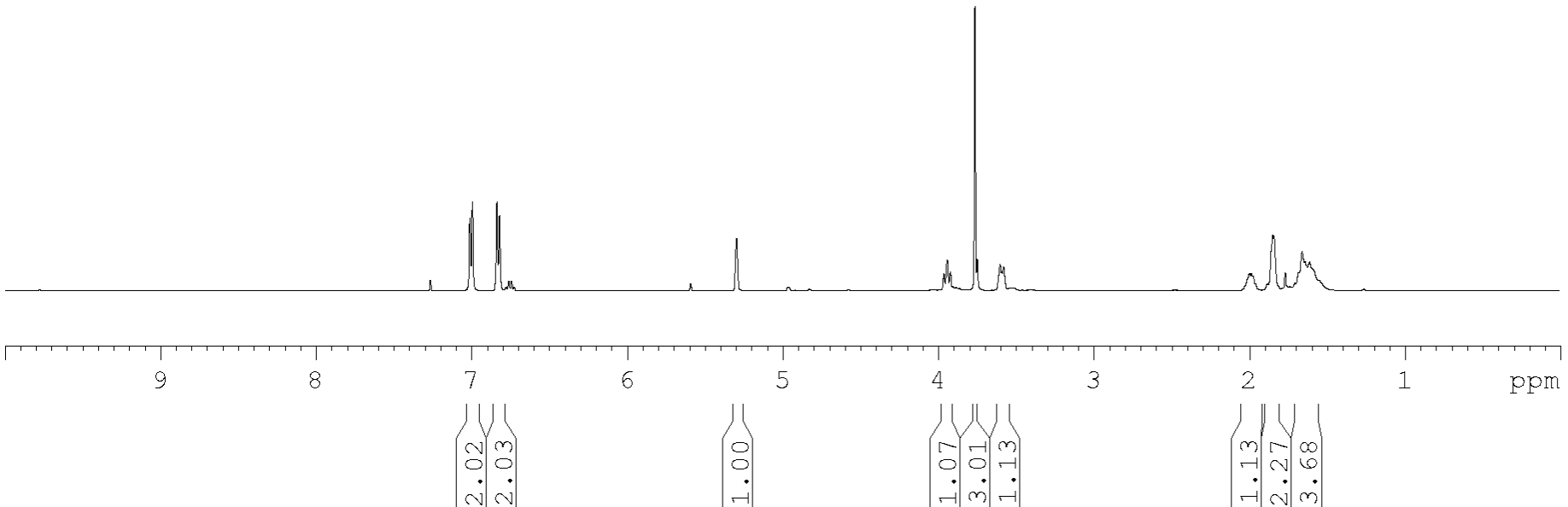
3s

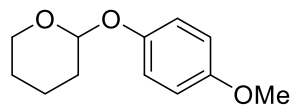
500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-139-5-2-islt-20201216
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201216
Time              19.13 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1            1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300121 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```





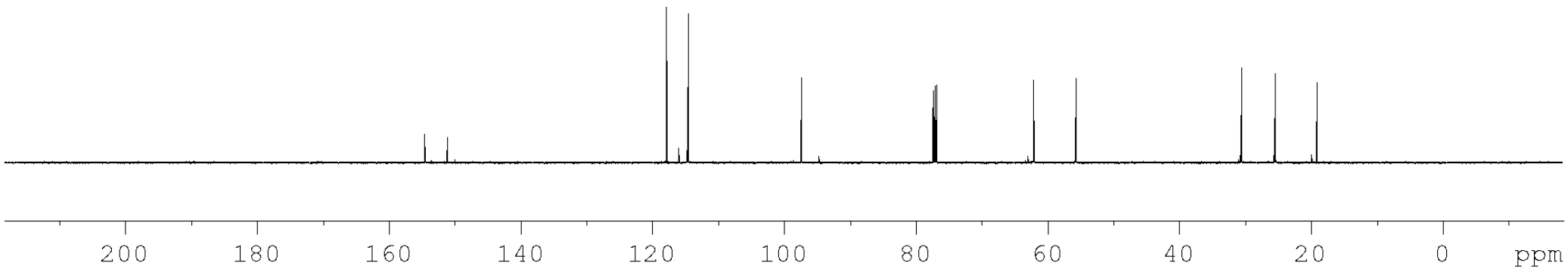
3s

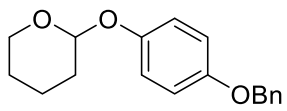
125 MHz ^{13}C NMR

$CDCl_3$

154.584
151.174
117.870
114.577
97.406
77.412
77.157
76.903
62.171
55.727
30.579
25.344
19.019

```
Current Data Parameters
NAME      vinn-4-139-5-2-islt-20201216
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20201216
Time              19.18 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW               16.800 usec
DE                6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577799 MHz
WDW                 EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

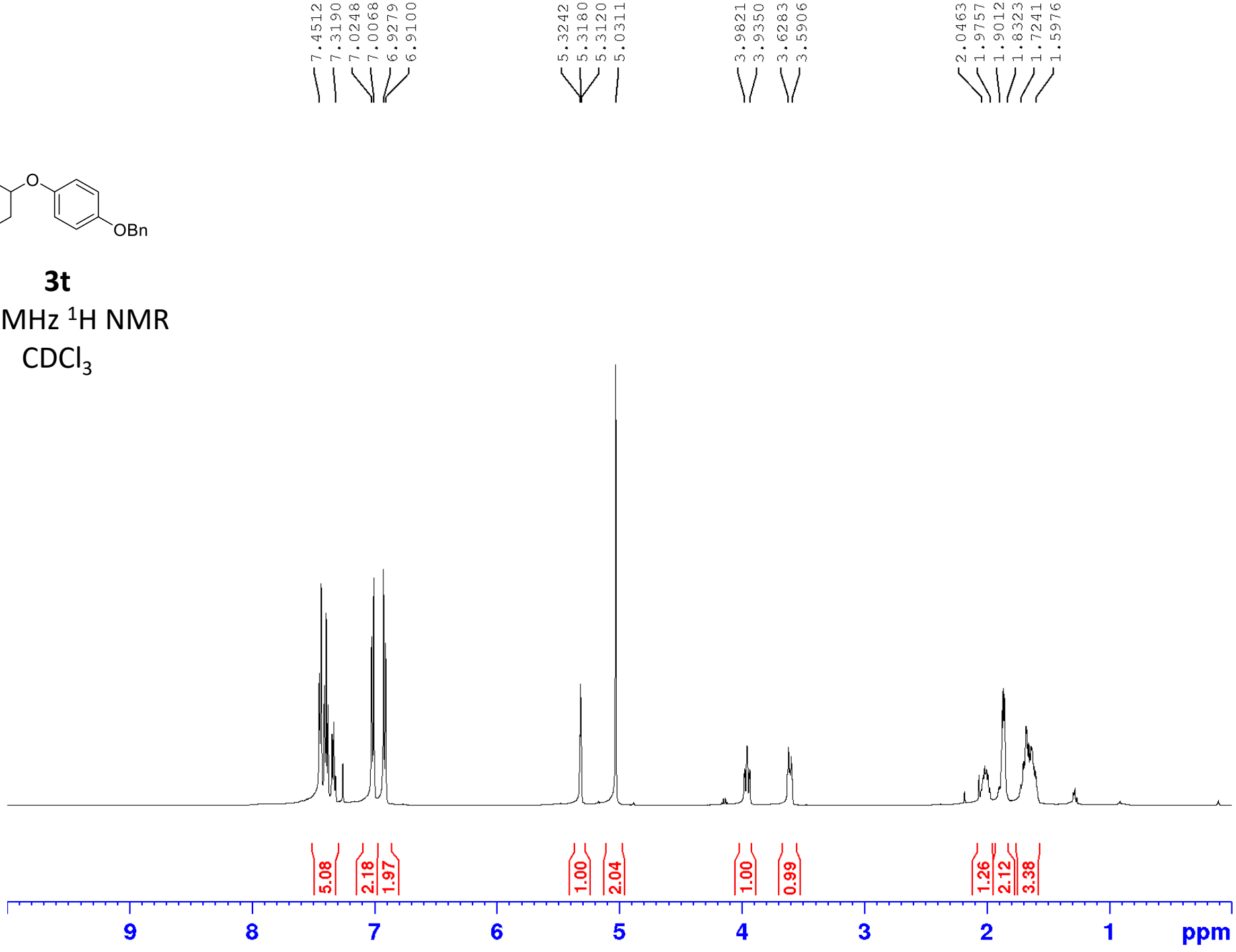




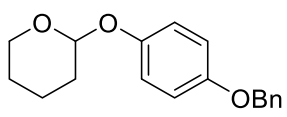
3t

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-139-6-2-islt2-20200120
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time              9.35 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW               50.000 usec
DE                6.50 usec
TE               295.1 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P1                10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300127 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



3t

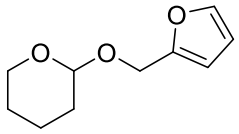
125 MHz ^{13}C NMR

$CDCl_3$

153.80
151.41
137.37
128.64
127.97
127.58
117.83
115.72
97.35
77.41
77.16
76.90
70.64
62.18
30.59
25.35
19.03

```
Current Data Parameters
NAME      vinn-4-139-6-2-islt2-2020012
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time               9.50 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                 6.50 usec
TE                295.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1
SFO1         125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1          94.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          25.00000000 W
PLW12          0.46495000 W
PLW13          0.23387000 W

F2 - Processing parameters
SI                32768
SF           125.7577812 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

200 180 160 140 120 100 80 60 40 20 ppm

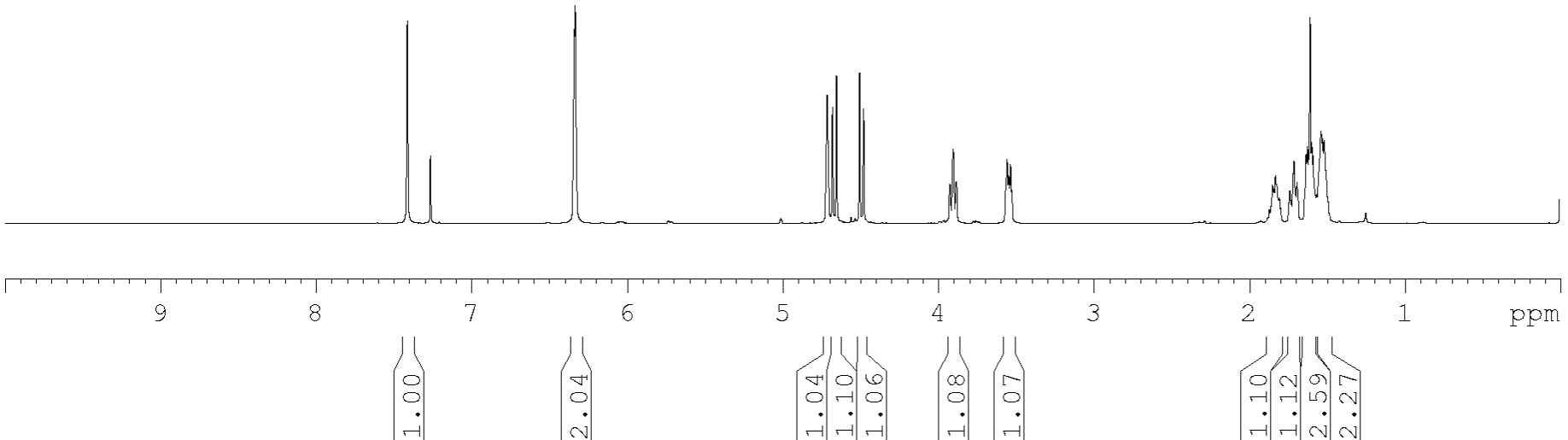


3u

500 MHz ^{1}H NMR

$CDCl_3$

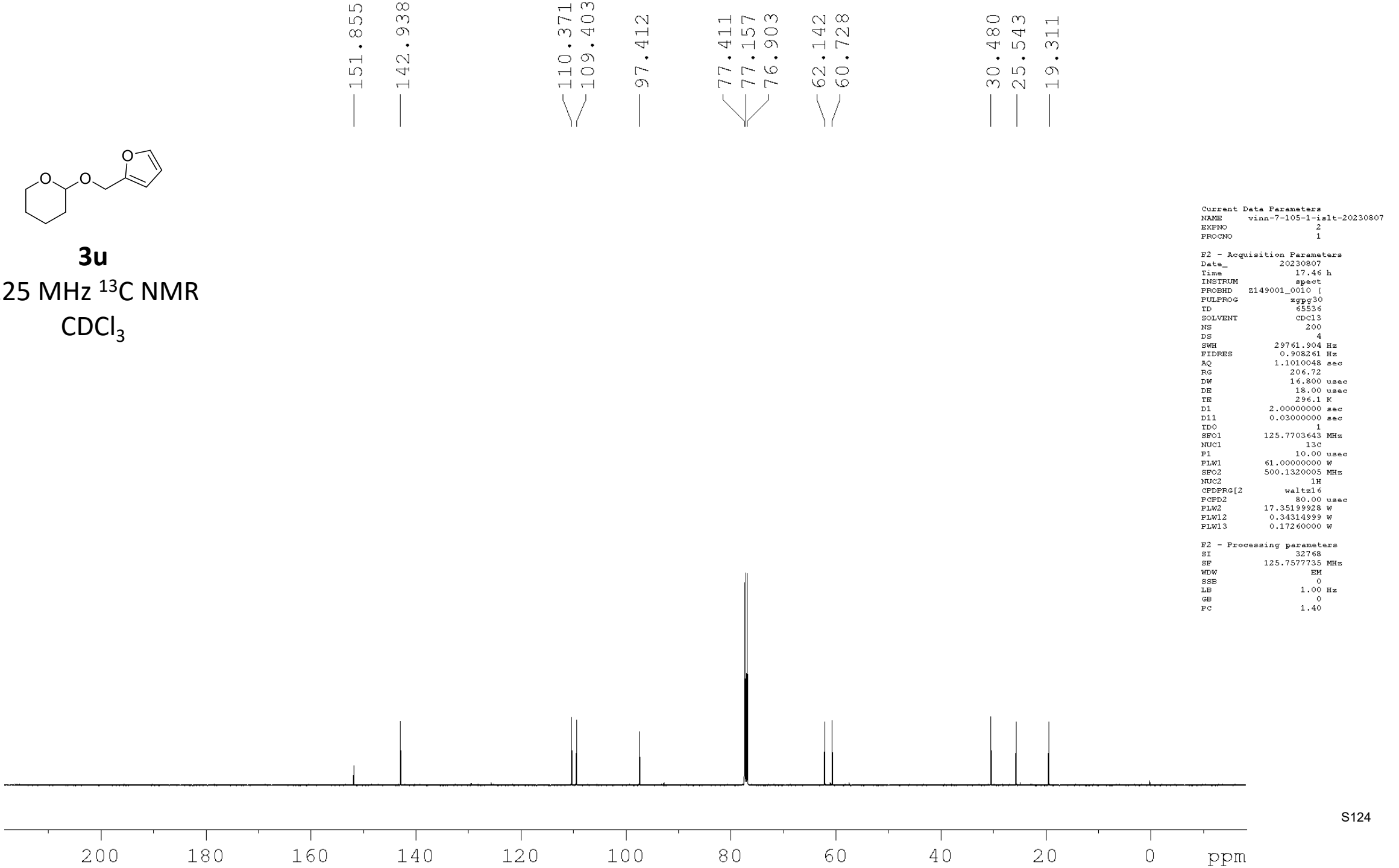
```
Current Data Parameters
NAME      vinn-7-105-1-islt-20230807
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20230807
Time              17.34 h
INSTRUM           spect
PROBHD    Z149001_0010 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW               50.000 usec
DE               10.00 usec
TE               296.2 K
D1            1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P1               11.25 usec
PLW1        17.35199928 W

F2 - Processing parameters
SI               65536
SF          500.1300130 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



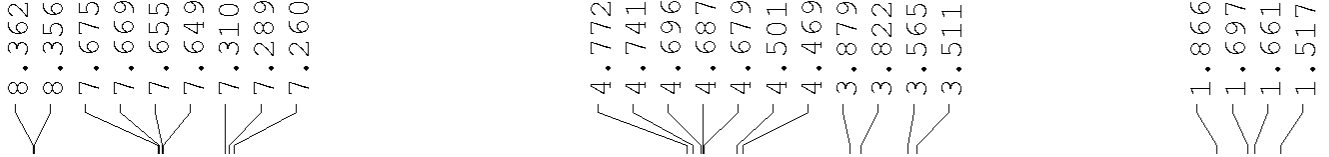
3u

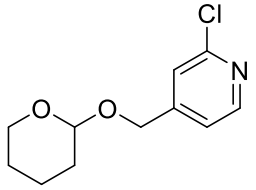
125 MHz ^{13}C NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-7-105-1-islt-20230807
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230807
Time              17.46 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW              16.800 usec
DE              18.00 usec
TE              296.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1              10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2           80.00 usec
PLW2        17.35199928 W
PLW12        0.34314999 W
PLW13        0.17260000 W

F2 - Processing parameters
SI                32768
SF          125.7577735 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



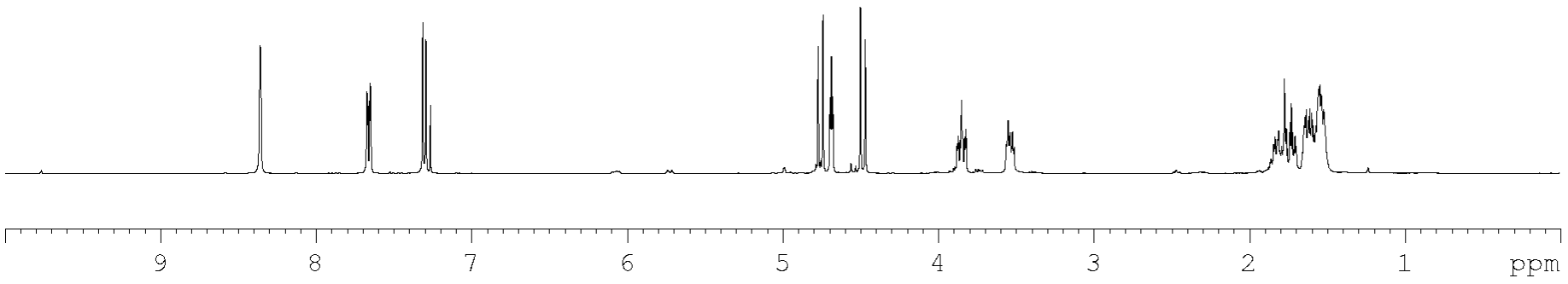


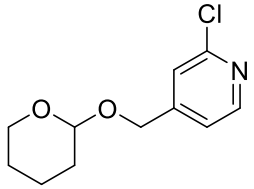
3v

400 MHz ^{1}H NMR

$CDCl_3$

```
Current Data Parameters
NAME      vinn-7-110-1-islt-20230810
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20230810
Time              17.08 h
INSTRUM           spect
PROBHD    Z108618_0257 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                   101
DW                62.400 usec
DE                 6.50 usec
TE                295.8 K
D1            1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300097 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```





3v

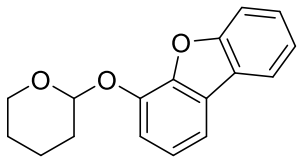
100 MHz ^{13}C NMR

$CDCl_3$

150.712
149.101
138.469
132.922
124.136
98.250
77.473
77.156
76.838
65.657
62.388
30.515
25.428
19.347

```
Current Data Parameters
NAME      vinn-7-110-1-ialt-20230810
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20230810
Time              17.12 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               296.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6228298 MHz
NUC1                13C
P1               10.00 usec
PLW1         51.00000000 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.17465000 W

F2 - Processing parameters
SI                32768
SF           100.6127586 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

200 180 160 140 120 100 80 60 40 20 0 ppm

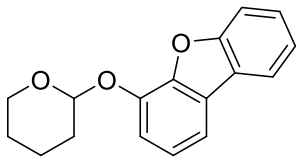


3w

400 MHz ^{1}H NMR

$CDCl_3$

```
Current Data Parameters
NAME      vinn-7-110-3-islt-20230810
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20230810
Time              17.17 h
INSTRUM           spect
PROBHD    Z108618_0257 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                90.5
DW              62.400 usec
DE               6.50 usec
TE              295.8 K
D1          1.00000000 sec
TD0                  1
SFO1       400.1324708 MHz
NUC1                 1H
P1              15.00 usec
PLW1       12.50000000 W

F2 - Processing parameters
SI               65536
SF          400.1300168 MHz
WDW                 EM
SSB                  0
LB              0.30 Hz
GB                   0
PC                1.00
```



3w

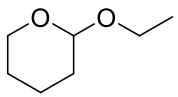
100 MHz ^{13}C NMR

$CDCl_3$

156.251
146.172
142.725
127.212
126.158
124.561
123.491
122.841
120.834
114.687
113.995
112.059
97.517
77.473
77.155
76.838
62.195
30.366
25.321
18.738

```
Current Data Parameters
NAME      vinn-7-110-3-ialt-20230810
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20230810
Time              17.22 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   60
DS                    4
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               296.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6228298 MHz
NUC1                 13C
P1                10.00 usec
PLW1         51.00000000 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.17465000 W

F2 - Processing parameters
SI                32768
SF           100.6127596 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

200 180 160 140 120 100 80 60 40 20 0 ppm

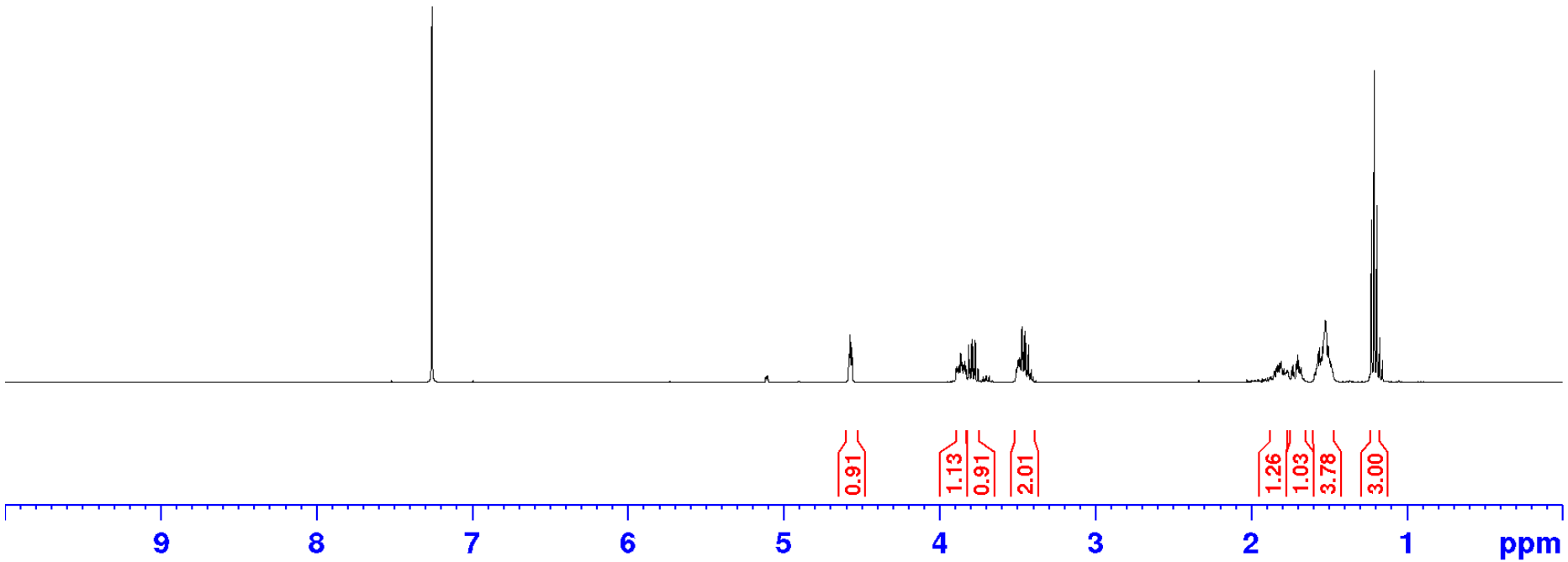


3x

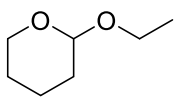
400 MHz ^{1}H NMR

$CDCl_3$

7.2598
4.5817
4.5750
4.5705
4.5633
3.8920
3.8306
3.8128
3.7709
3.5098
3.3996
1.8845
1.7646
1.7400
1.6640
1.5990
1.4775
1.2279
1.2102
1.1924




```
Current Data Parameters
NAME      vinn-4-183-5-islt-20230320
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230320
Time              12.52 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                  71.8
DW                62.400 usec
DE                 6.50 usec
TE                295.4 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300101 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```



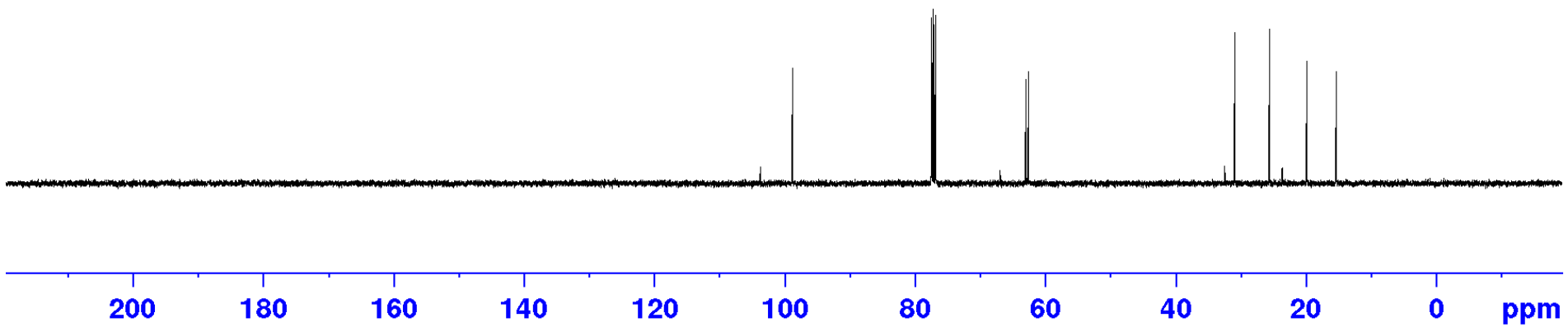
3x

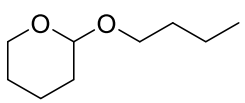
100 MHz ^{13}C NMR

$CDCl_3$

98.84
77.47
77.36
77.16
76.84
63.00
62.58
30.94
25.59
19.89
15.32

```
Current Data Parameters
NAME      vinn-4-183-5-islt-20230320
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20230320
Time              12.56 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                   37
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                  203
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         51.00000000 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.17465000 W

F2 - Processing parameters
SI                32768
SF           100.6127571 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

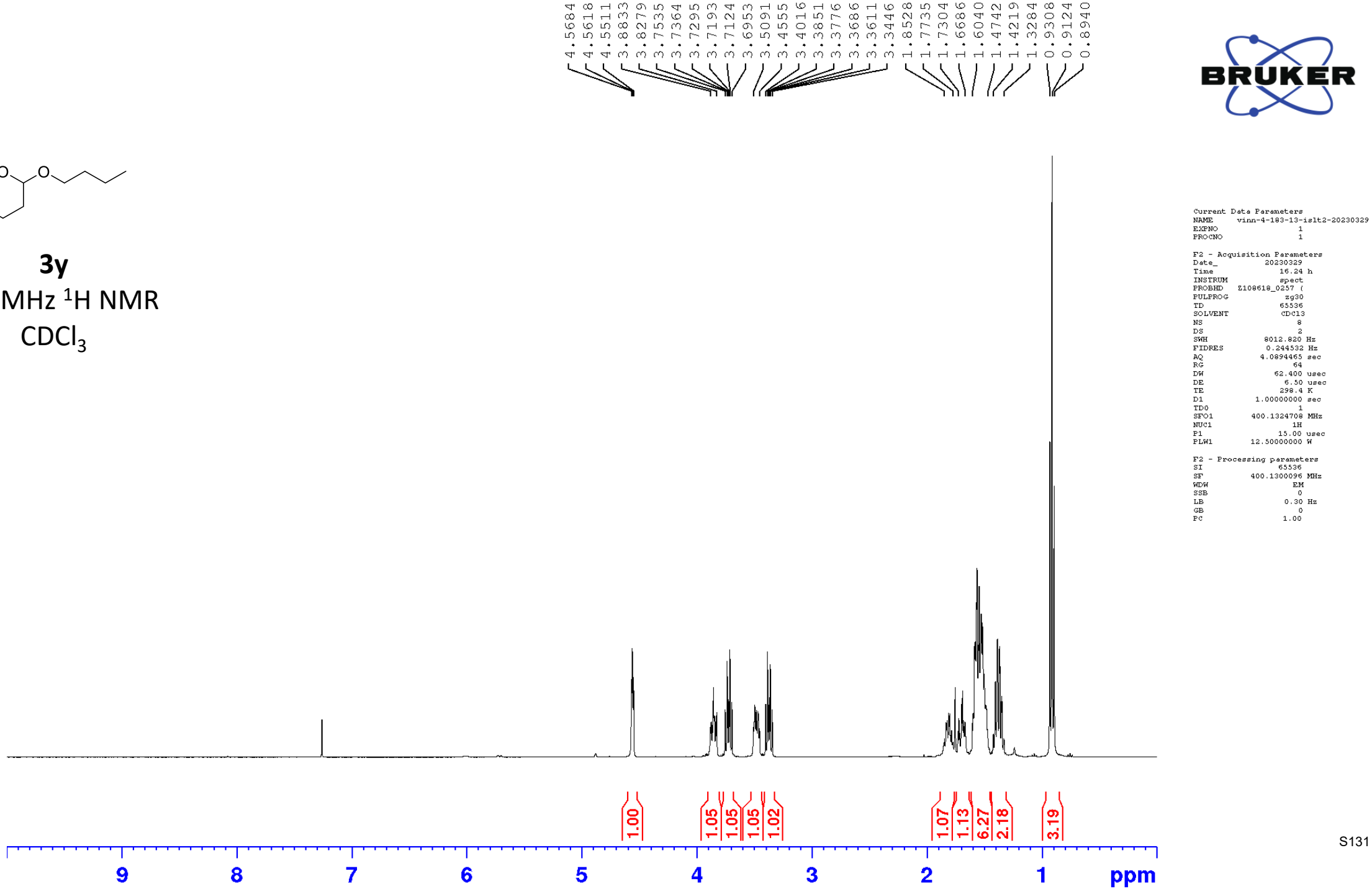




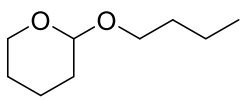
3y

400 MHz ^{1}H NMR

$CDCl_3$



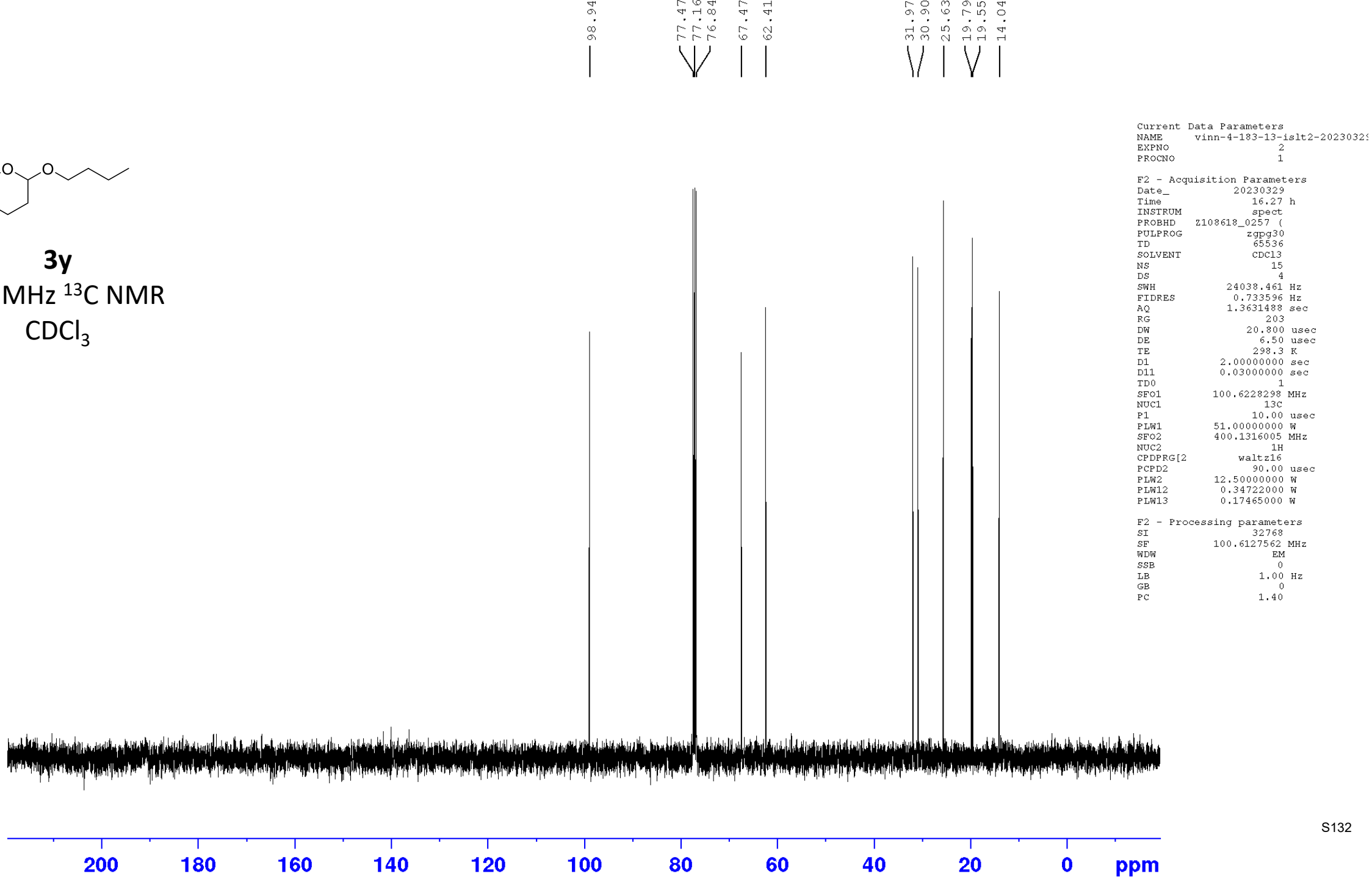

```
Current Data Parameters
NAME      vinn-4-183-13-islt2-20230329
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20230329
Time             16.24 h
INSTRUM           spect
PROBHD    5108618_0257 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            4.0894465 sec
RG                  64
DW               62.400 usec
DE                6.50 usec
TE              298.4 K
D1            1.00000000 sec
TD0                  1
SFO1        400.1324708 MHz
NUC1               1H
P1               15.00 usec
PLW1        12.50000000 W

F2 - Processing parameters
SI               65536
SF          400.1300096 MHz
WDW                EM
SSB                 0
LB              0.30 Hz
GB                  0
PC              1.00
```



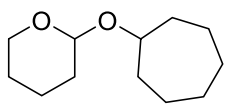
3y

100 MHz ^{13}C NMR

$CDCl_3$



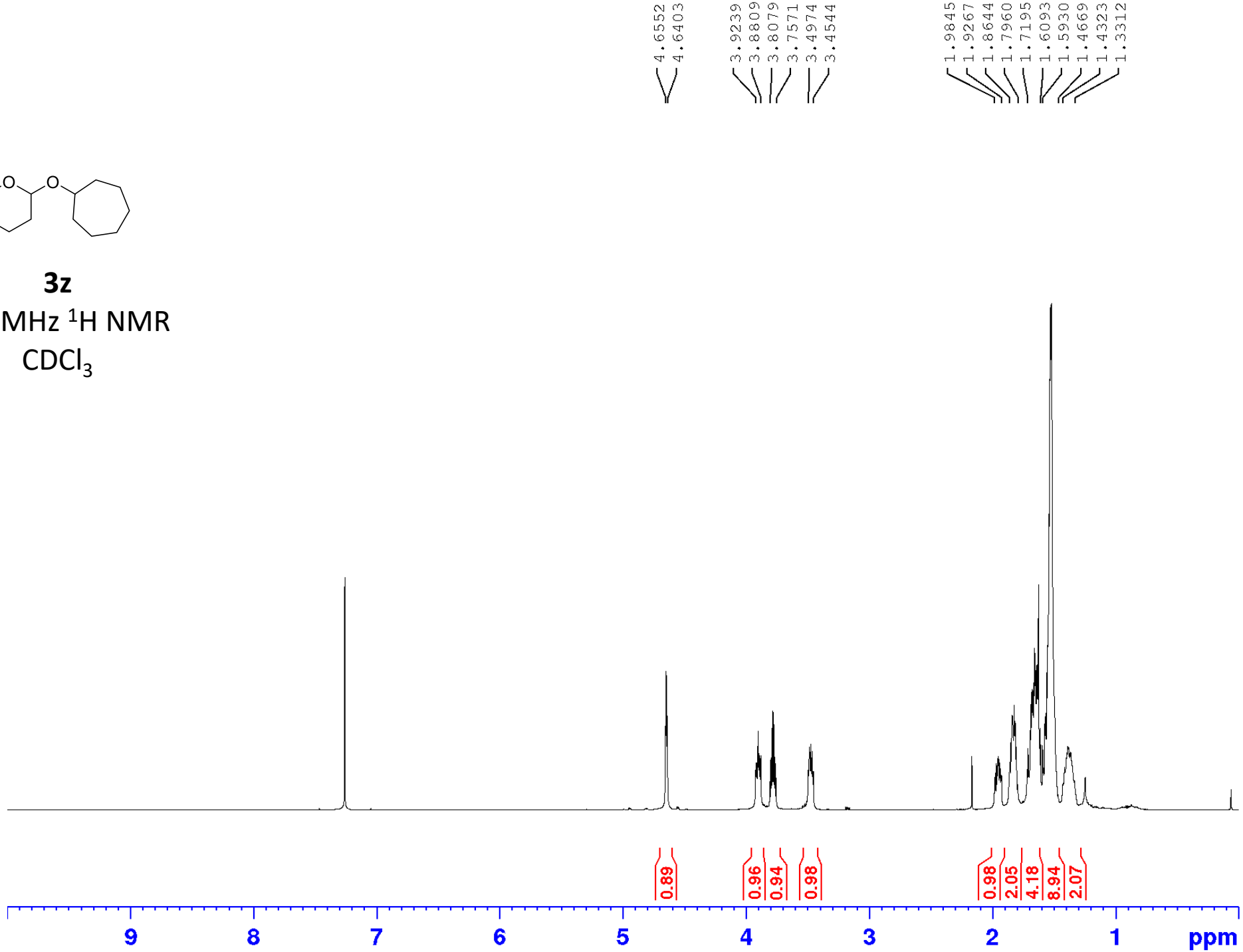

```
Current Data Parameters
NAME      vinn-4-183-13-islt2-2023032
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230329
Time              16.27 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   15
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                  203
DW                20.800 usec
DE                 6.50 usec
TE                298.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        51.00000000 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.17465000 W

F2 - Processing parameters
SI                32768
SF          100.6127562 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```



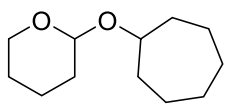
3z

500 MHz ^{1}H NMR

$CDCl_3$



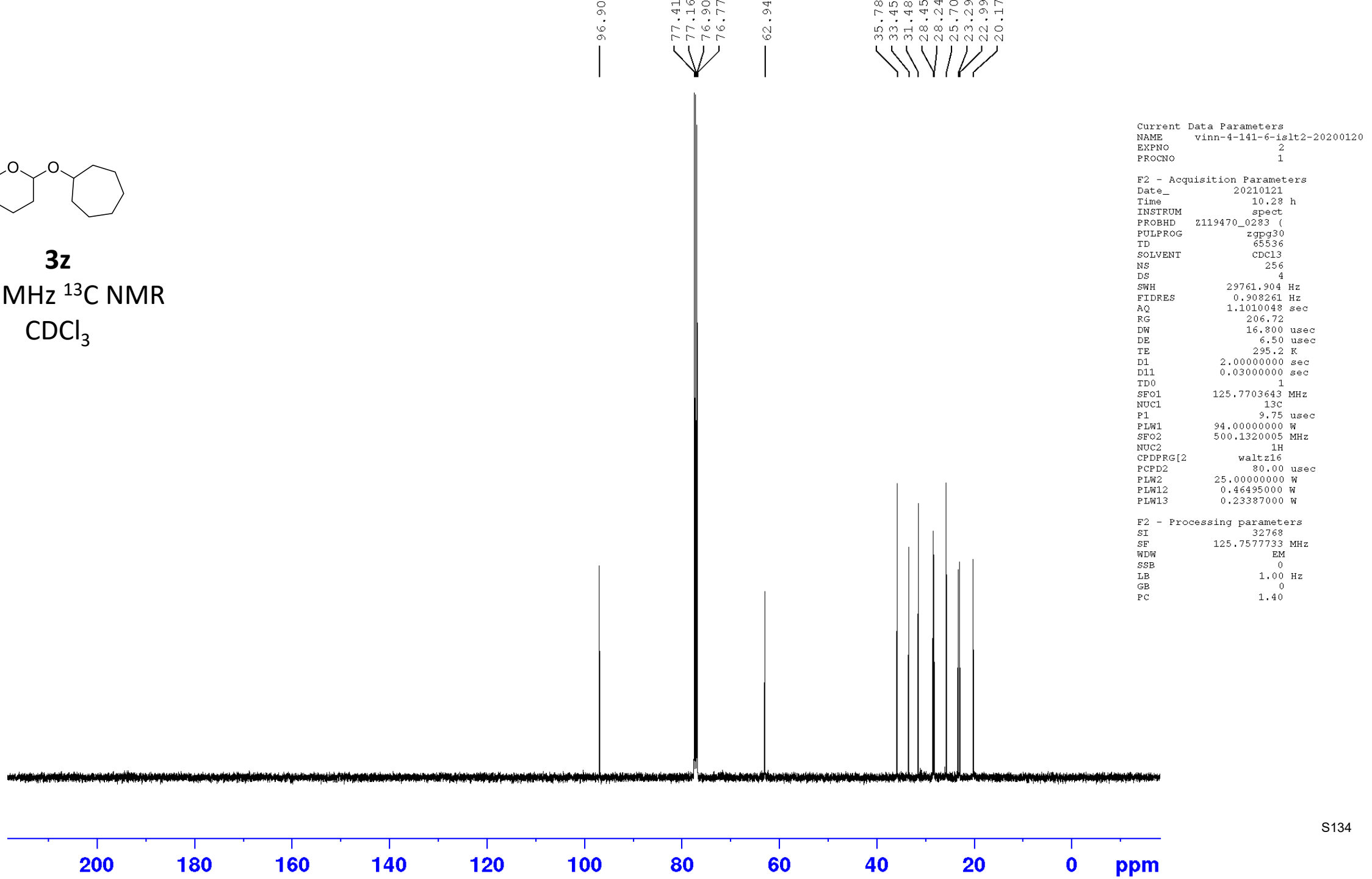

```
Current Data Parameters
NAME      vinn-4-141-6-islt2-2020012
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20210121
Time                         10.14 h
INSTRUM                       spect
PROBHD    Z119470_0283 (
PULPROG                       zg30
TD                           65536
SOLVENT                      CDCl3
NS                              16
DS                               2
SWH                      10000.000 Hz
FIDRES                       0.305176 Hz
AQ                        3.2767999 sec
RG                           63.76
DW                           50.000 usec
DE                            6.50 usec
TE                           295.1 K
D1                     1.00000000 sec
TD0                              1
SFO1                  500.1330883 MHz
NUC1                          1H
P1                           10.91 usec
PLW1                  25.00000000 W

F2 - Processing parameters
SI                           65536
SF                    500.1300126 MHz
WDW                             EM
SSB                              0
LB                            0.30 Hz
GB                               0
PC                            1.00
```



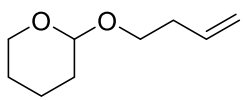
3z

125 MHz ^{13}C NMR

$CDCl_3$



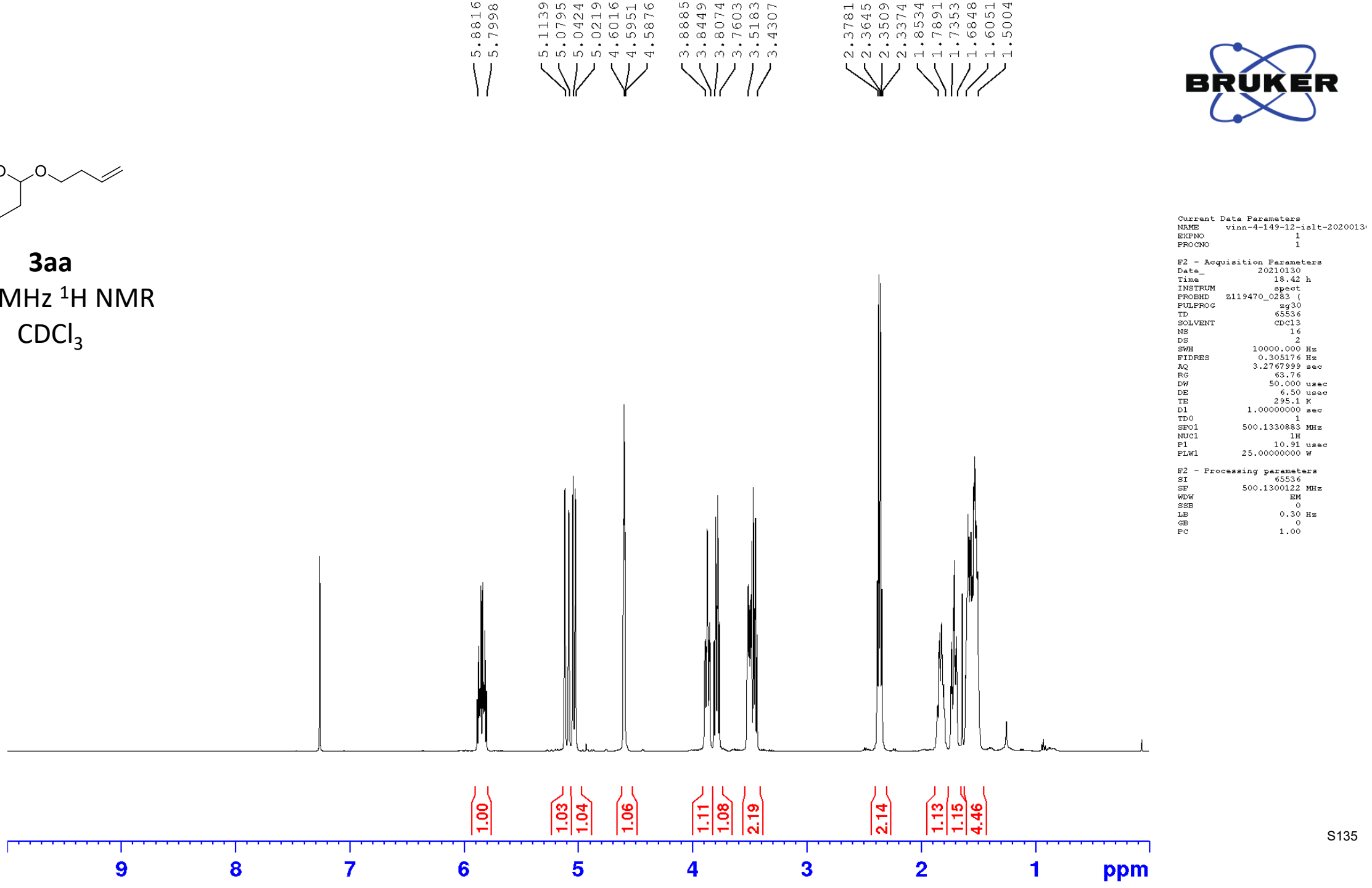

```
Current Data Parameters
NAME      vinn-4-141-6-islt2-20200120
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210121
Time              10.28 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                 6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577733 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```



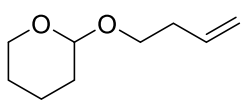
3aa

500 MHz ^{1}H NMR

$CDCl_3$



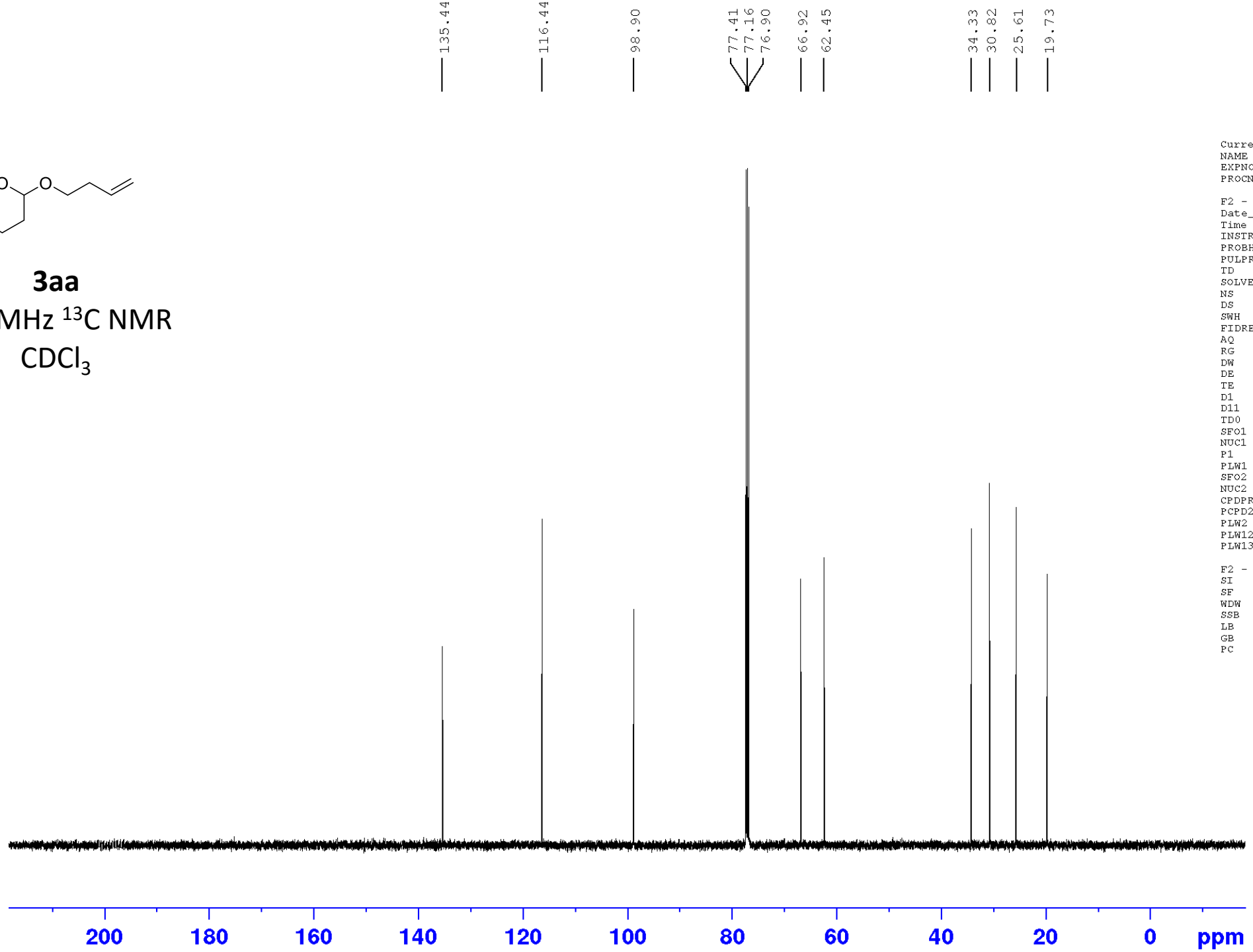

```
Current Data Parameters
NAME      vinn-4-149-12-islt-2020013
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210130
Time              18.42 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                63.76
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                  1
SFO1          500.1330883 MHz
NUC1                 1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI               65536
SF            500.1300122 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



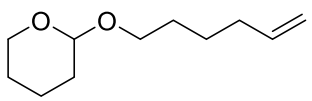
3aa

125 MHz ^{13}C NMR

$CDCl_3$



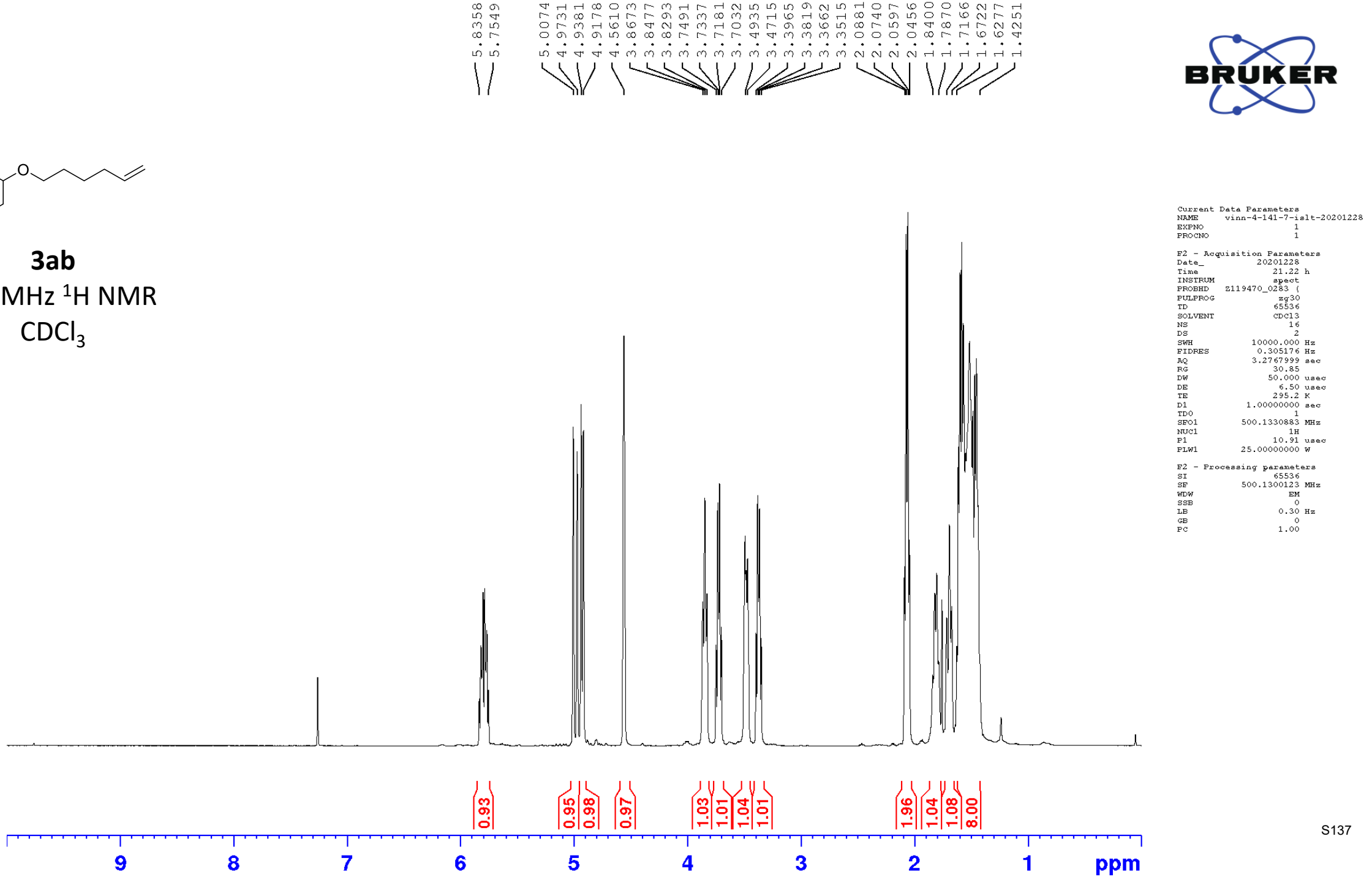

```
Current Data Parameters
NAME      vinn-4-149-12-islt-20200130
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210130
Time              18.49 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577732 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



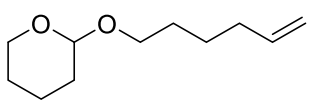
3ab

500 MHz ^{1}H NMR

$CDCl_3$



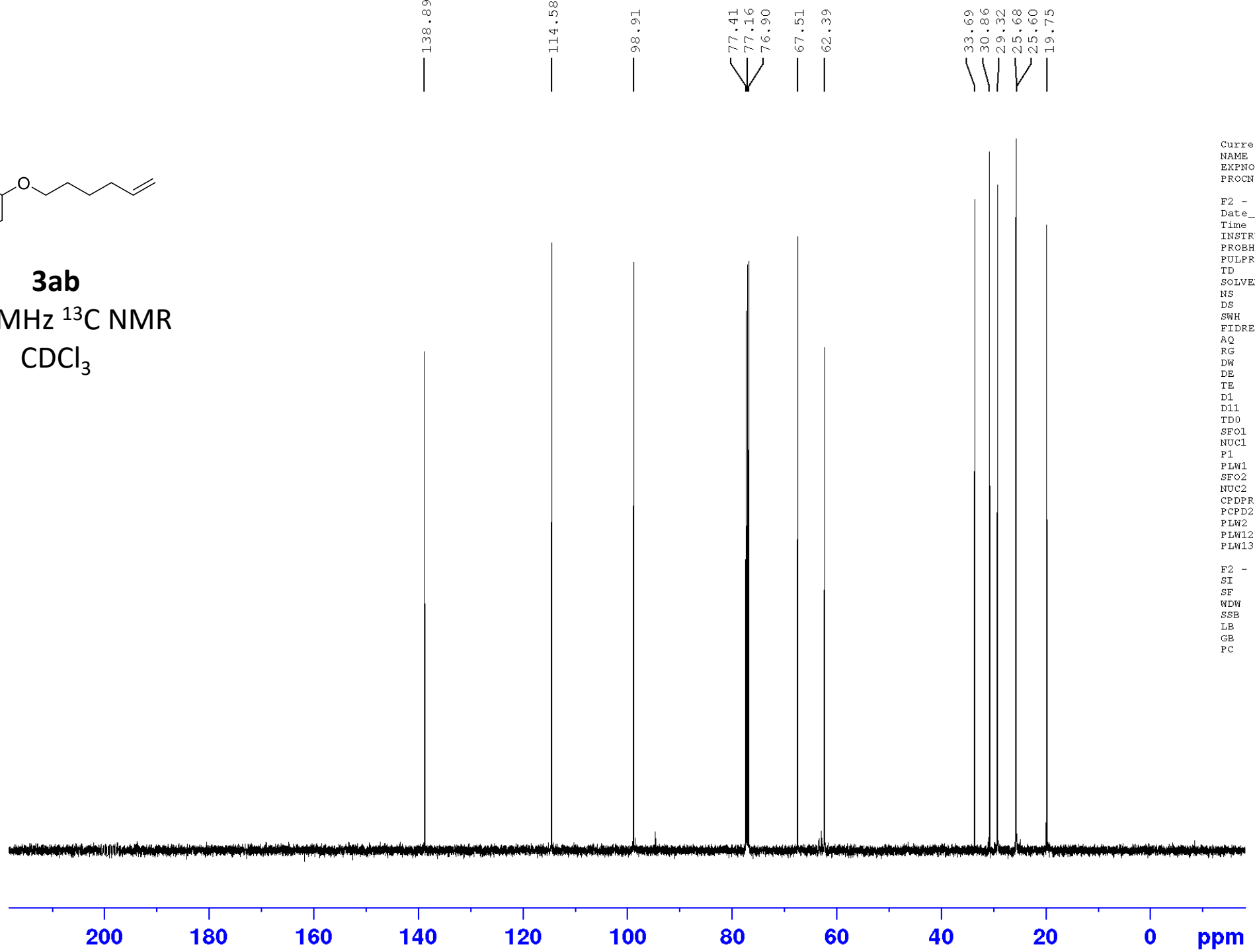

```
Current Data Parameters
NAME      vinn-4-141-7-islt-20201228
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201228
Time              21.22 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ              3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.2 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300123 MHz
WDW                  EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```



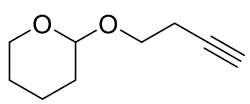
3ab

125 MHz ^{13}C NMR

$CDCl_3$



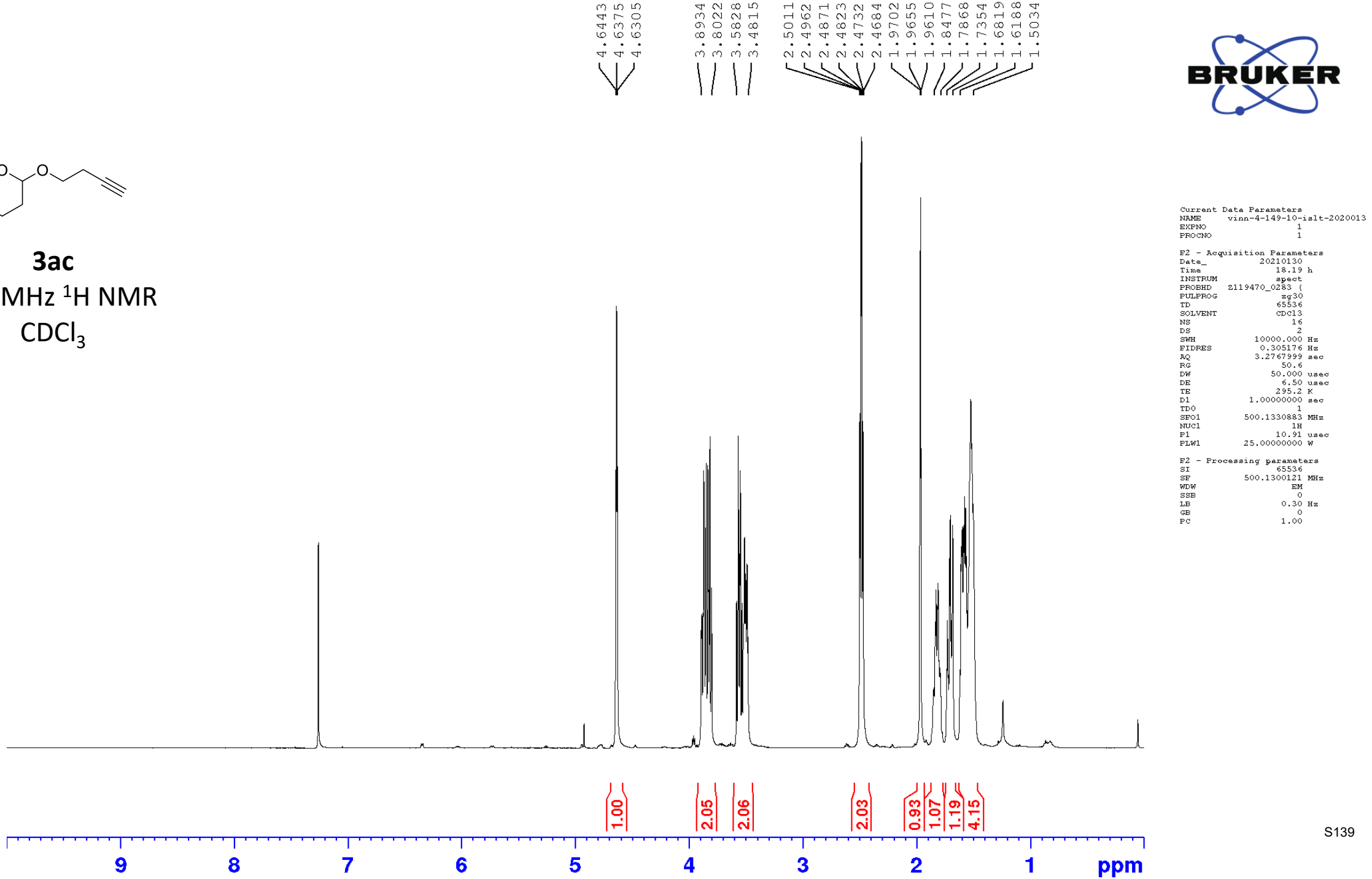

```
Current Data Parameters
NAME      vinn-4-141-7-islt-20201228
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20201228
Time             21.28 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW              16.800 usec
DE               6.50 usec
TE              295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577754 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



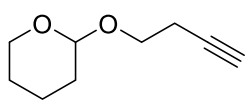
3ac

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-149-10-islt-2020013
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210130
Time              18.19 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                50.6
DW              50.000 usec
DE               6.50 usec
TE              295.2 K
D1           1.00000000 sec
TD0                  1
SFO1       500.1330883 MHz
NUC1               1H
P1               10.91 usec
PLW1       25.00000000 W

F2 - Processing parameters
SI               65536
SF         500.1300121 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



3ac

125 MHz ^{13}C NMR

$CDCl_3$

98.89
81.55
77.41
77.16
76.90
69.30
65.62
62.35
30.64
25.52
20.05
19.51

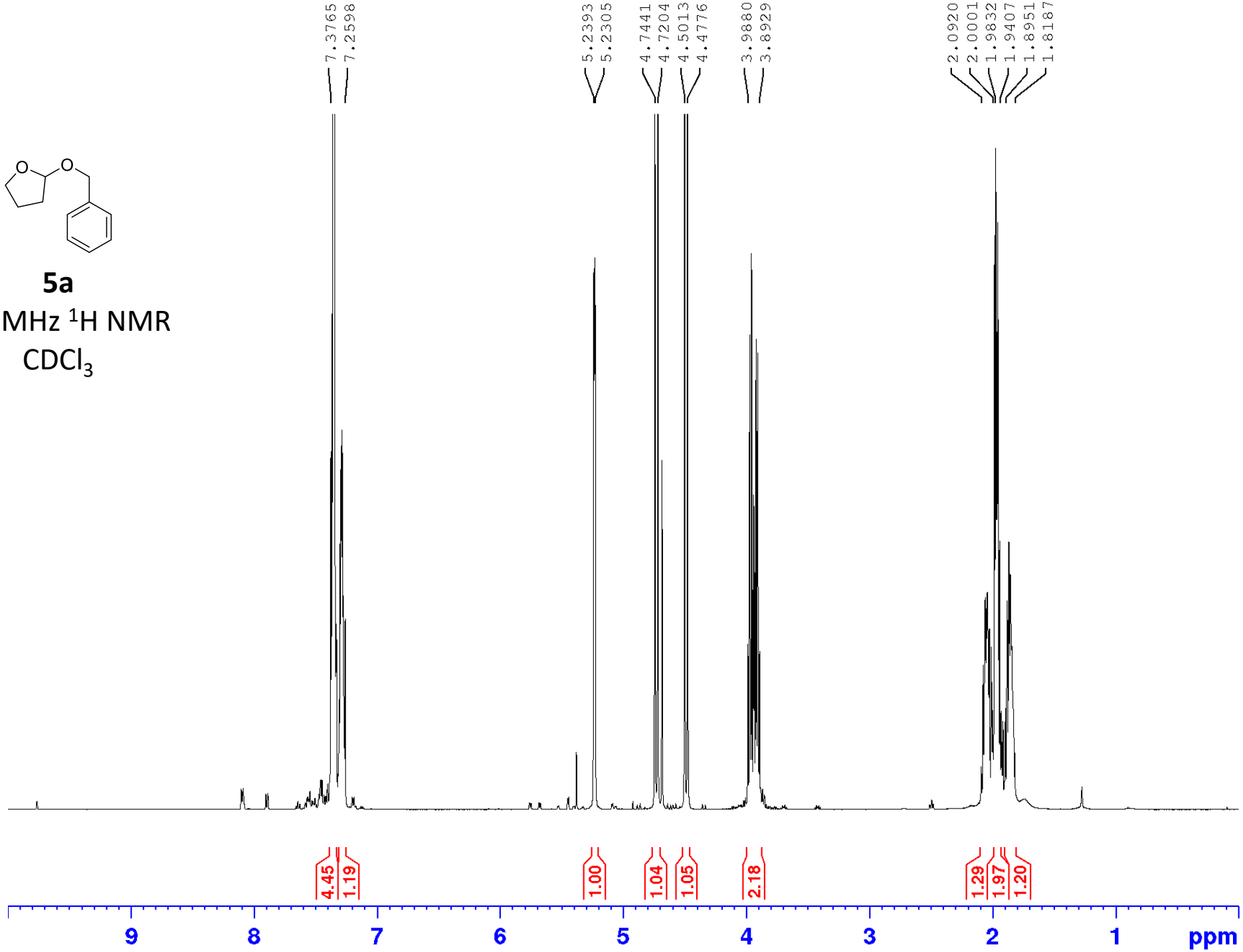
```
Current Data Parameters
NAME      vinn-4-149-10-islt-20200130
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210130
Time              18.27 h
INSTRUM             spect
PROBHD    Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                 6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF         125.7577746 MHz
WDW                 EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

200 180 160 140 120 100 80 60 40 20 0 ppm

5a

500 MHz ^{1}H NMR

$CDCl_3$



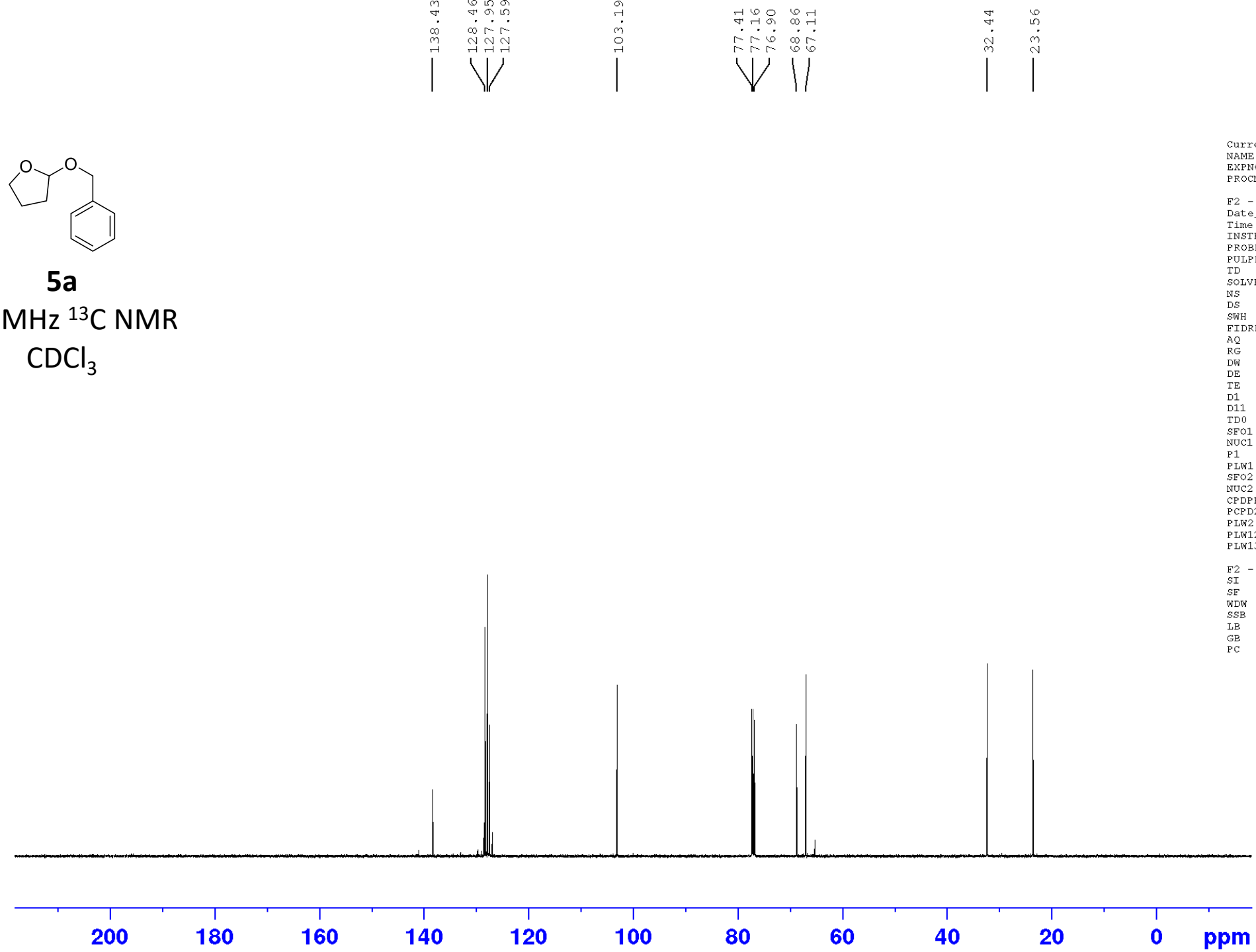
BRUKER

```
Current Data Parameters
NAME      vinn-4-131-2-islt-20201130
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20201130
Time              16.28 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300121 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

5a

125 MHz ^{13}C NMR

$CDCl_3$

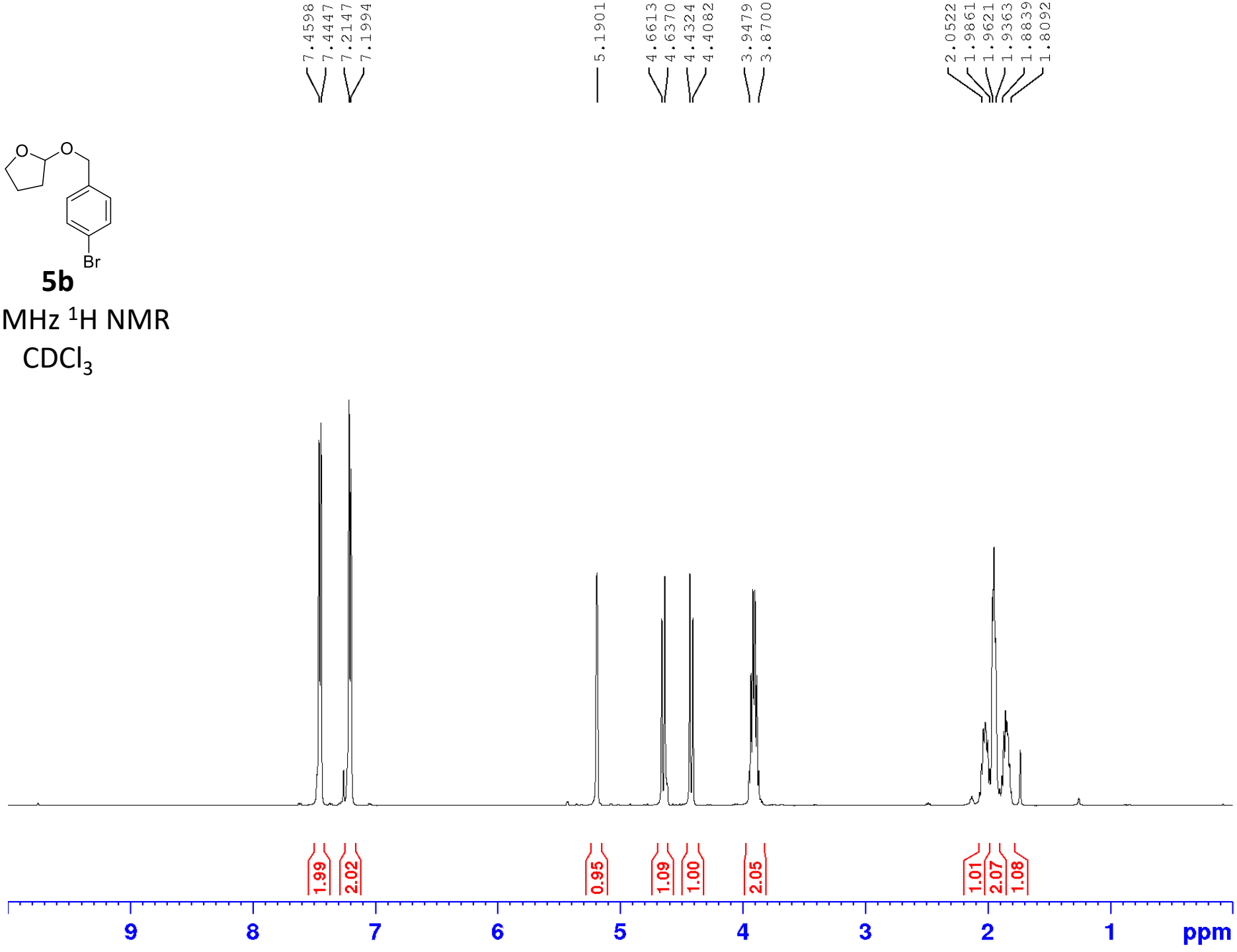



```
Current Data Parameters
NAME      vinn-4-131-2-islt-20201130
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20201130
Time             16.35 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 115
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ           1.1010048 sec
RG              206.72
DW              16.800 usec
DE               6.50 usec
TE              295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI               32768
SF          125.7577804 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

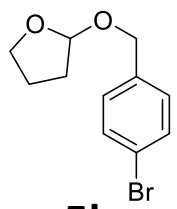
5b

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-8-islt-20201210
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201211
Time               5.37 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                30.85
DW               50.000 usec
DE                6.50 usec
TE               295.1 K
D1            1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P1                10.91 usec
PLW1         25.00000000 W

F2 - Processing parameters
SI               65536
SF           500.1300122 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



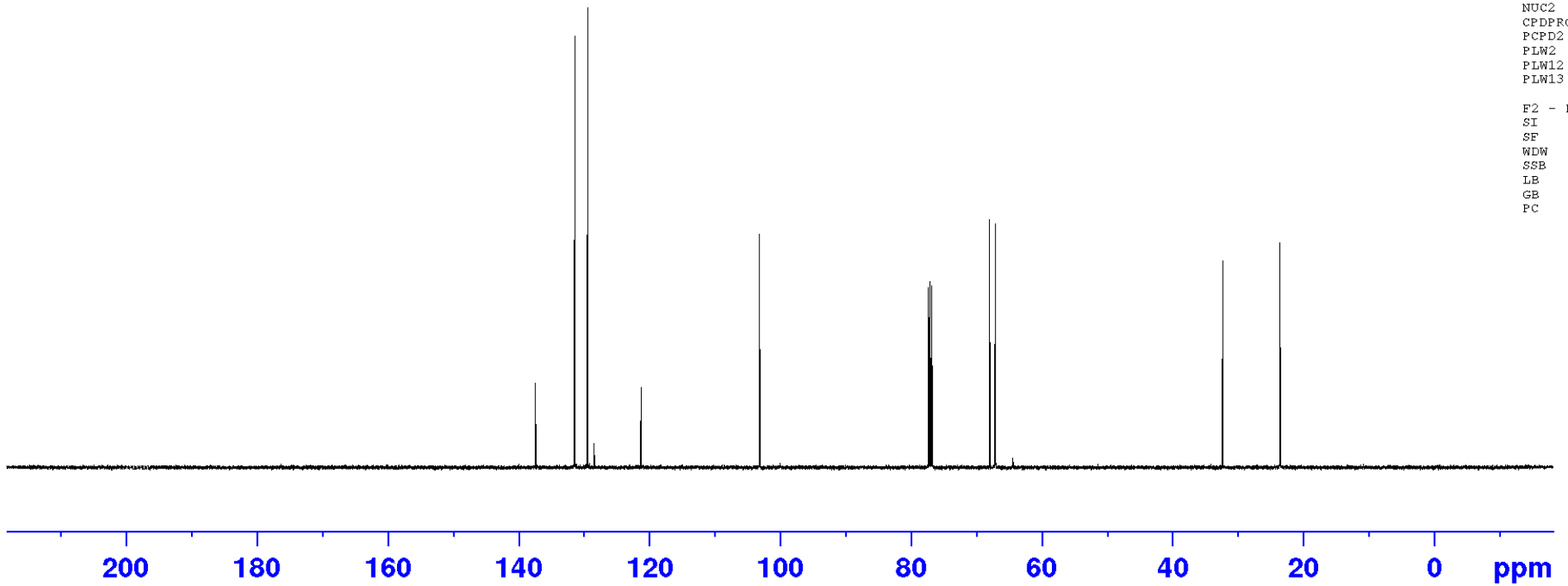
5b

125 MHz ^{13}C NMR

$CDCl_3$

137.52
131.52
129.54
121.41
103.27
77.41
77.16
76.90
68.08
67.20
32.45
23.53

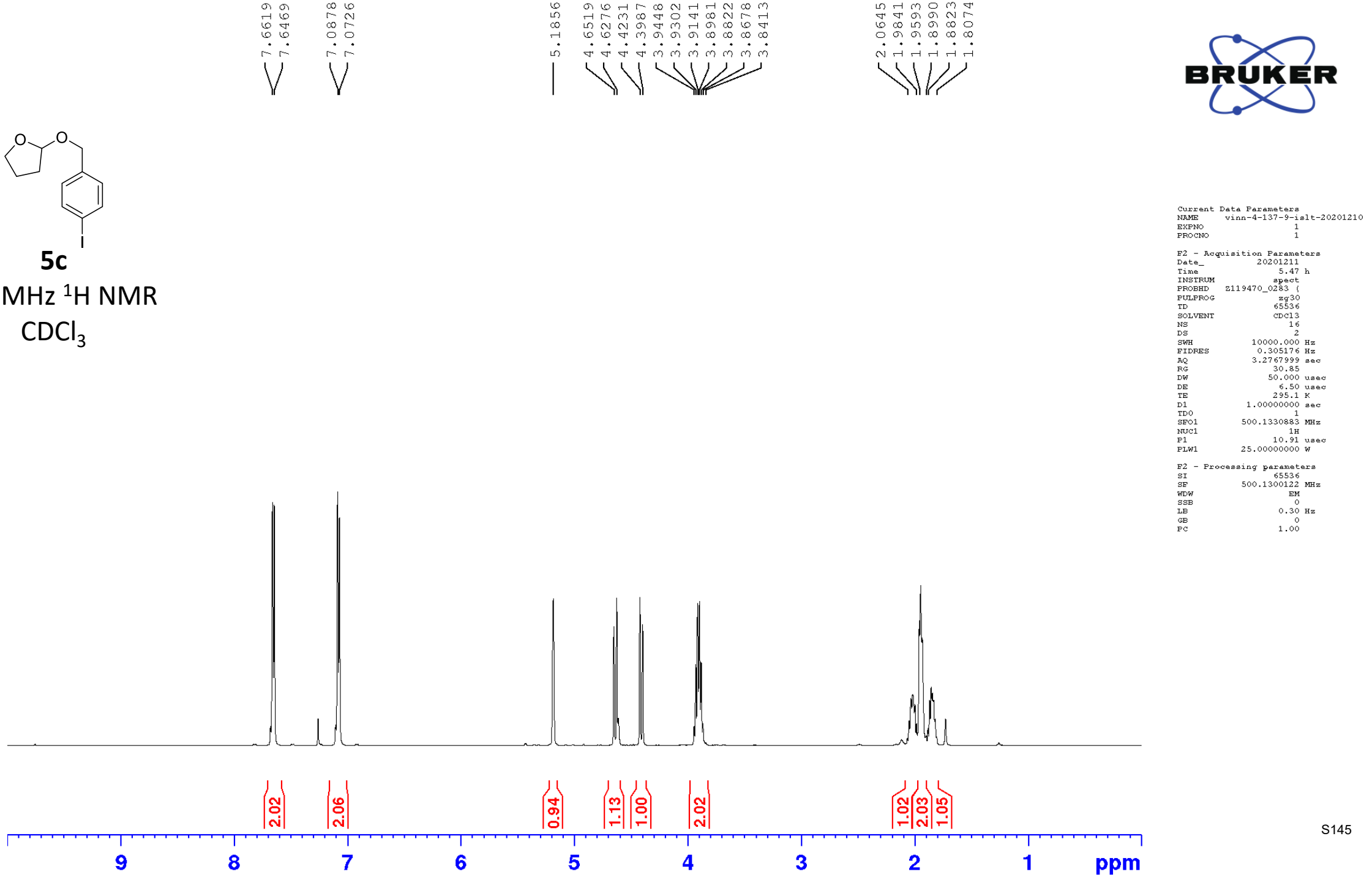
```
Current Data Parameters
NAME      vinn-4-137-8-islt-20201210
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20201211
Time                5.43 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577798 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



5c

500 MHz ^{1}H NMR

$CDCl_3$

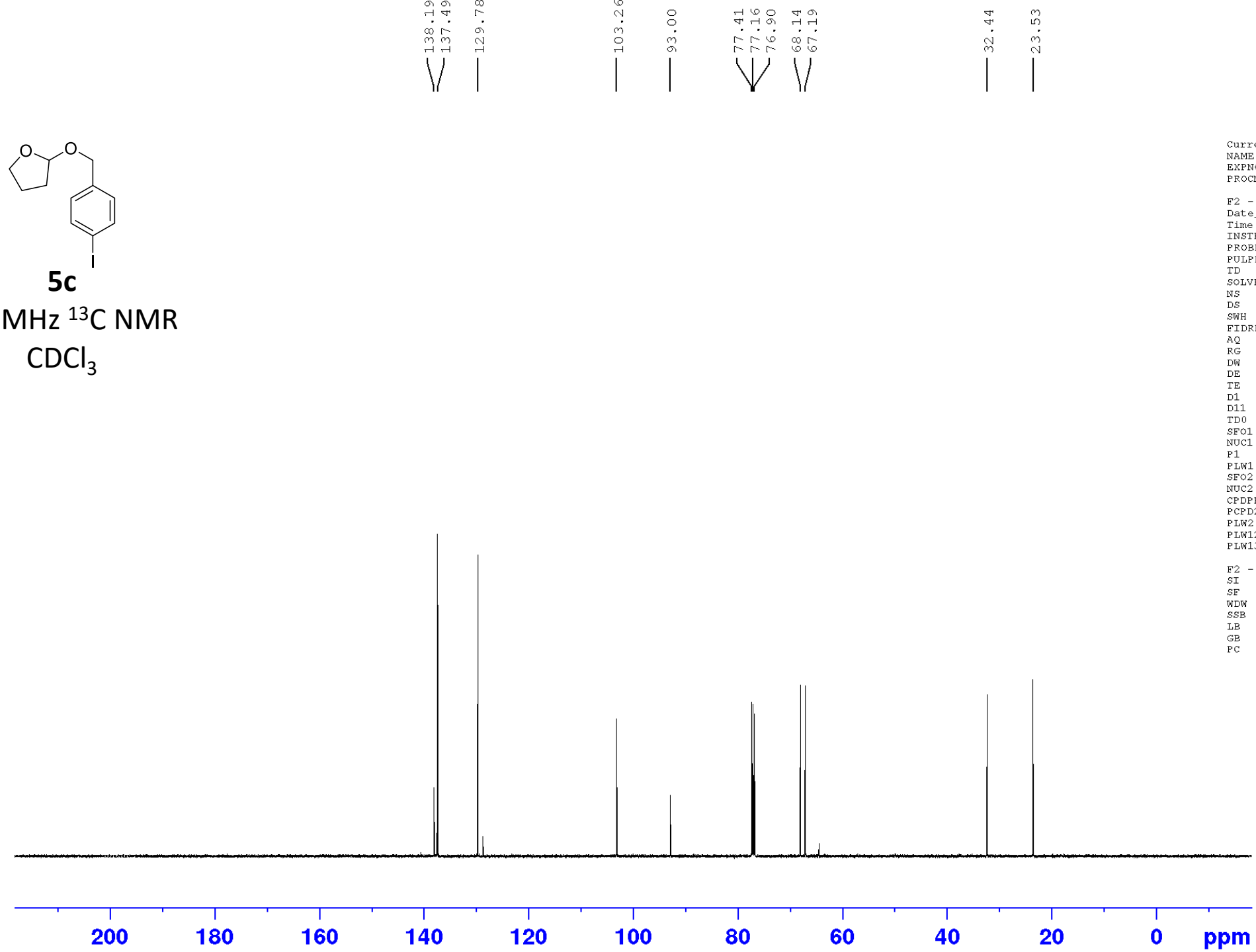



```
Current Data Parameters
NAME      vinn-4-137-9-islt-20201210
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20201211
Time               5.47 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW               50.000 usec
DE                6.50 usec
TE               295.1 K
D1            1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P1                10.91 usec
PLW1         25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300122 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

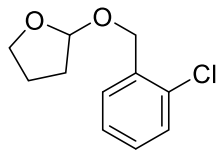
5c

125 MHz ^{13}C NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-9-islt-20201210
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20201211
Time               5.52 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                 6.50 usec
TE                295.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1
SFO1         125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF           125.7577813 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

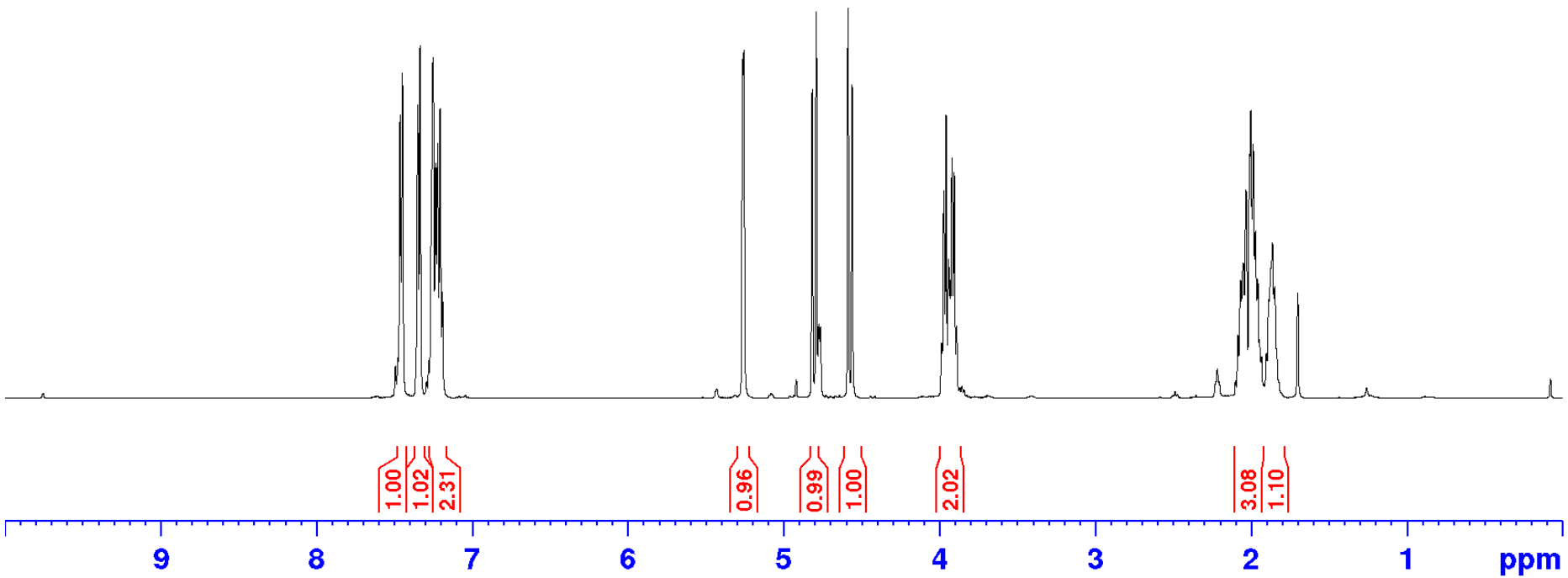


5d

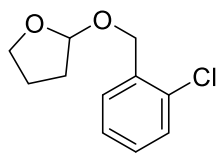
500 MHz ^{1}H NMR

$CDCl_3$

7.4638
7.4490
7.3505
7.3355
7.2541
7.2506
7.1922
5.2647
5.2566
4.8178
4.7919
4.5874
4.5615
3.9865
3.8908
2.0992
1.9324
1.9012
1.8215




```
Current Data Parameters
NAME      vinn-4-137-17-islt-2020121
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20201211
Time               6.43 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW              50.000 usec
DE               6.50 usec
TE              295.2 K
D1           1.00000000 sec
TD0                  1
SFO1       500.1330883 MHz
NUC1               1H
P1              10.91 usec
PLW1       25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300133 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



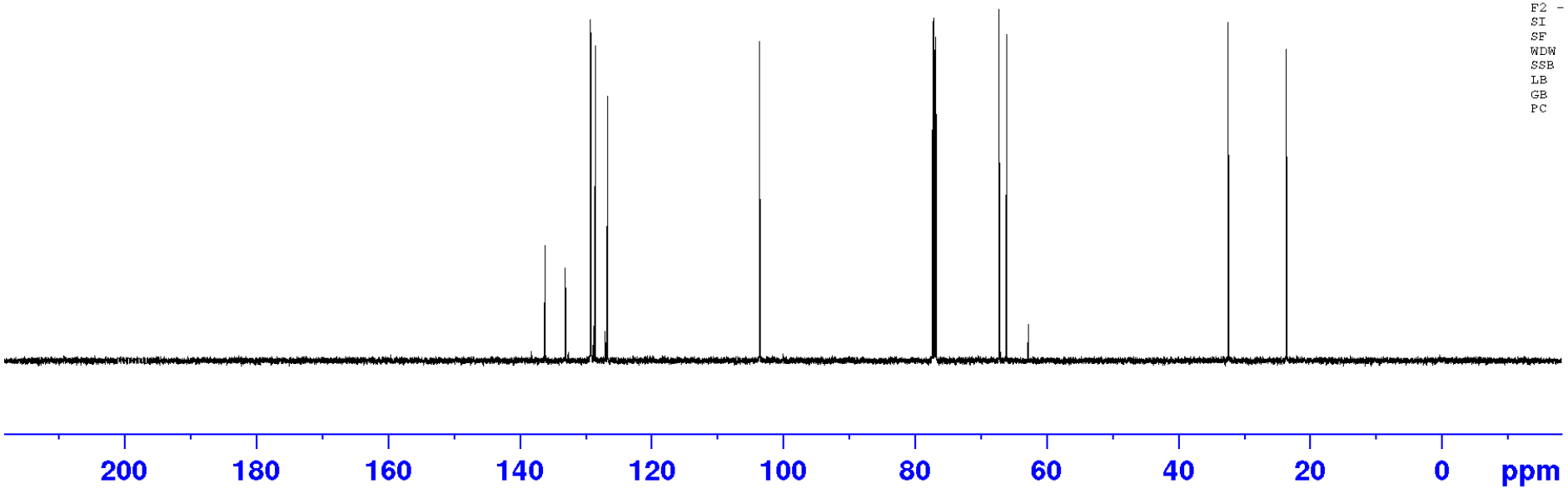
5d

125 MHz ^{13}C NMR

$CDCl_3$

136.27
133.16
129.37
129.27
128.67
126.79
103.71
77.41
77.16
76.90
67.29
66.17
32.49
23.54

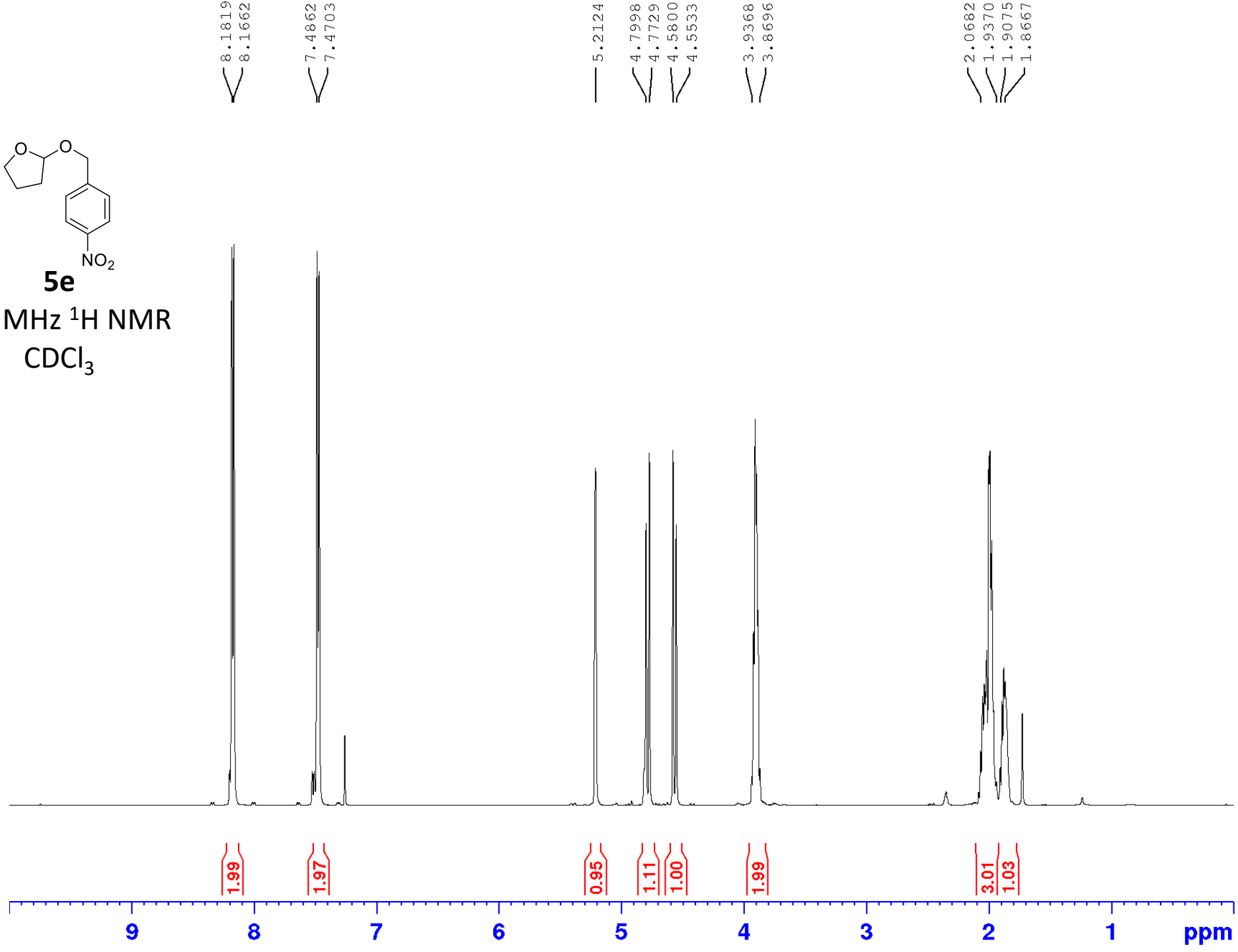
```
Current Data Parameters
NAME      vinn-4-137-17-islt-20201210
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201211
Time               6.49 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577777 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



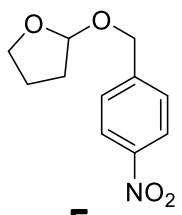
5e

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-11-islt-2020121
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20201211
Time                           6.05 h
INSTRUM                       spect
PROBHD    Z119470_0283 (
PULPROG                       zg30
TD                           65536
SOLVENT                      CDCl3
NS                              16
DS                               2
SWH                      10000.000 Hz
FIDRES                       0.305176 Hz
AQ                       3.2767999 sec
RG                              30.85
DW                          50.000 usec
DE                           6.50 usec
TE                           295.1 K
D1                     1.00000000 sec
TD0                              1
SFO1                 500.1330883 MHz
NUC1                            1H
P1                          10.91 usec
PLW1                25.00000000 W

F2 - Processing parameters
SI                           65536
SF                   500.1300121 MHz
WDW                             EM
SSB                              0
LB                           0.30 Hz
GB                               0
PC                            1.00
```



5e

125 MHz ^{13}C NMR

$CDCl_3$

147.30
146.38
127.88
123.64
103.76
77.41
77.16
76.90
67.65
67.40
32.50
23.51

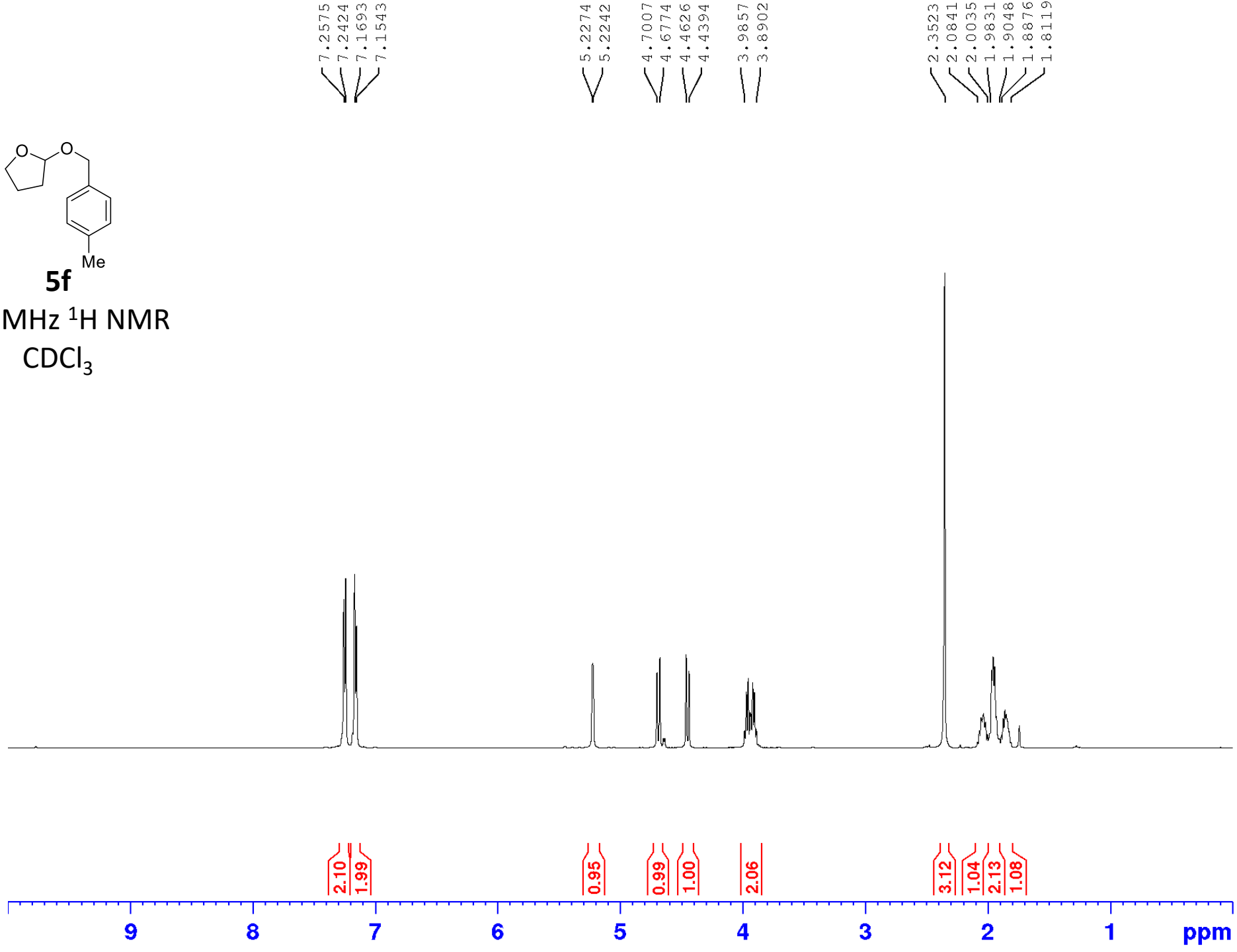
```
Current Data Parameters
NAME      vinn-4-137-11-islt-20201210
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201211
Time                6.11 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577786 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

200 180 160 140 120 100 80 60 40 20 0 ppm

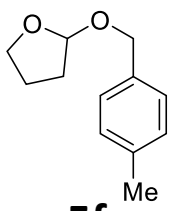
5f

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-10-islt-2020121
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20201211
Time               5.56 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW              50.000 usec
DE               6.50 usec
TE              295.1 K
D1           1.00000000 sec
TD0                  1
SFO1       500.1330883 MHz
NUC1               1H
P1              10.91 usec
PLW1       25.00000000 W

F2 - Processing parameters
SI               65536
SF         500.1300122 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



5f

125 MHz ^{13}C NMR

$CDCl_3$

137.27
135.35
129.14
128.10
103.02
77.41
77.16
76.90
68.73
67.06
32.43
23.57
21.26

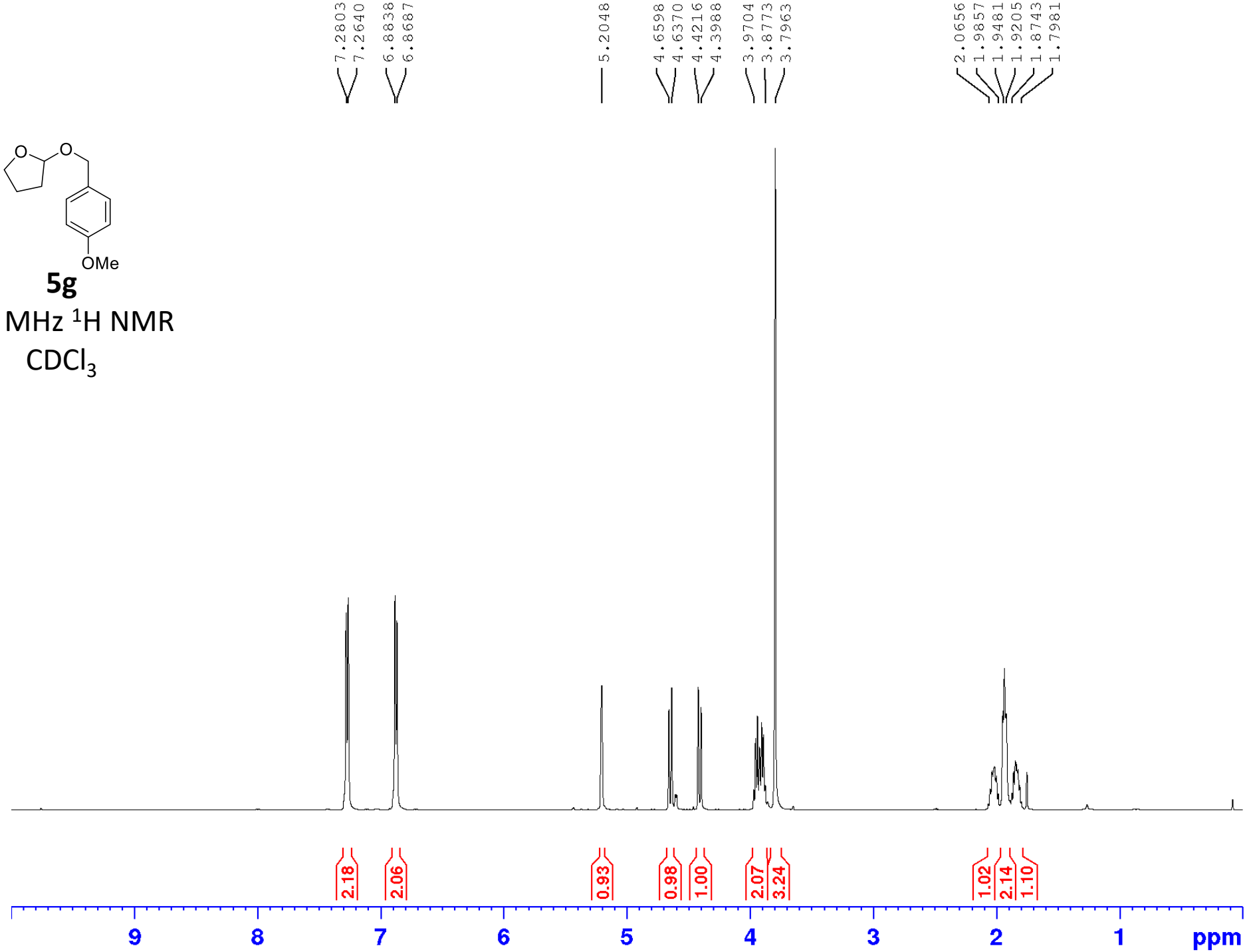
```
Current Data Parameters
NAME      vinn-4-137-10-islt-20201210
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20201211
Time               6.02 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 100
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1       125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1       94.00000000 W
SFO2       500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2       25.00000000 W
PLW12       0.46495000 W
PLW13       0.23387000 W

F2 - Processing parameters
SI                32768
SF         125.7577807 MHz
WDW                EM
SSB                 0
LB              1.00 Hz
GB                  0
PC              1.40
```

200 180 160 140 120 100 80 60 40 20 0 ppm

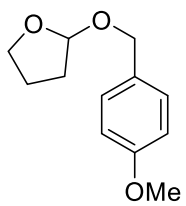
5g

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-13-islt-2020121
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20201211
Time               6.24 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW              50.000 usec
DE               6.50 usec
TE              295.1 K
D1           1.00000000 sec
TD0                  1
SFO1       500.1330883 MHz
NUC1               1H
P1              10.91 usec
PLW1       25.00000000 W

F2 - Processing parameters
SI               65536
SF         500.1300121 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



5g

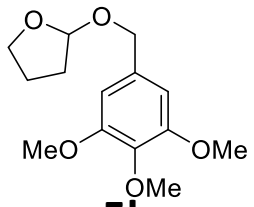
125 MHz ^{13}C NMR

$CDCl_3$

159.20
130.47
129.60
113.87
102.91
77.41
77.16
76.90
68.53
67.05
55.35
32.41
23.57

```
Current Data Parameters
NAME      vinn-4-137-13-islt-20201210
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20201211
Time               6.30 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT         CDCl3
NS                100
DS                  4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW              16.800 usec
DE               6.50 usec
TE              295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                 1
SFO1        125.7703643 MHz
NUC1              13C
P1               9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577796 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

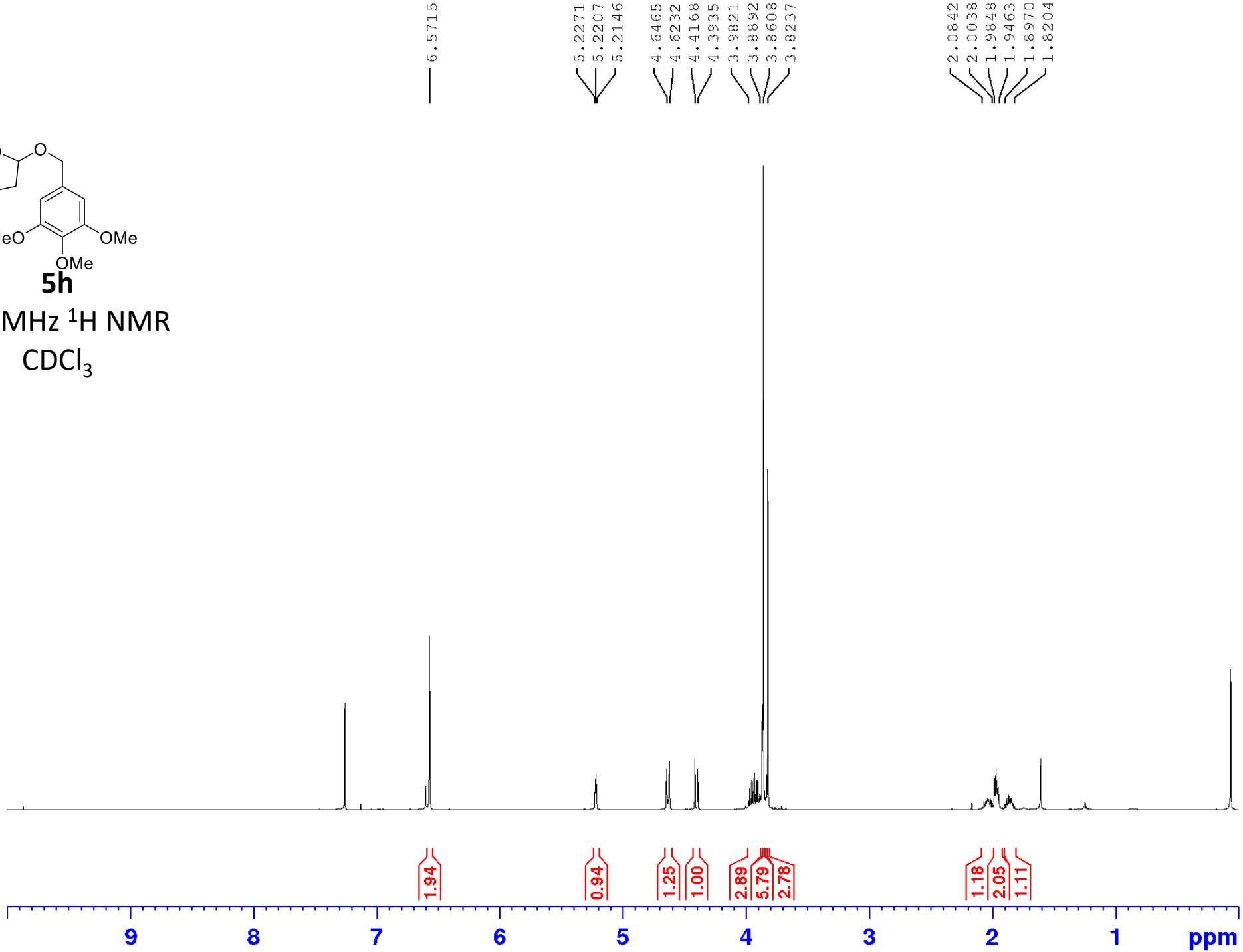
200 180 160 140 120 100 80 60 40 20 0 ppm



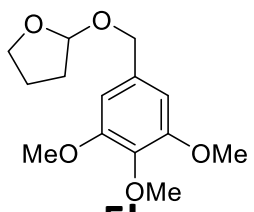
5h

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-137-12-islt2-20200120
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20210121
Time                8.57 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES           0.305176 Hz
AQ             3.2767999 sec
RG                93.28
DW               50.000 usec
DE                6.50 usec
TE               295.1 K
D1            1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P1                10.91 usec
PLW1         25.00000000 W

F2 - Processing parameters
SI               65536
SF           500.1300126 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



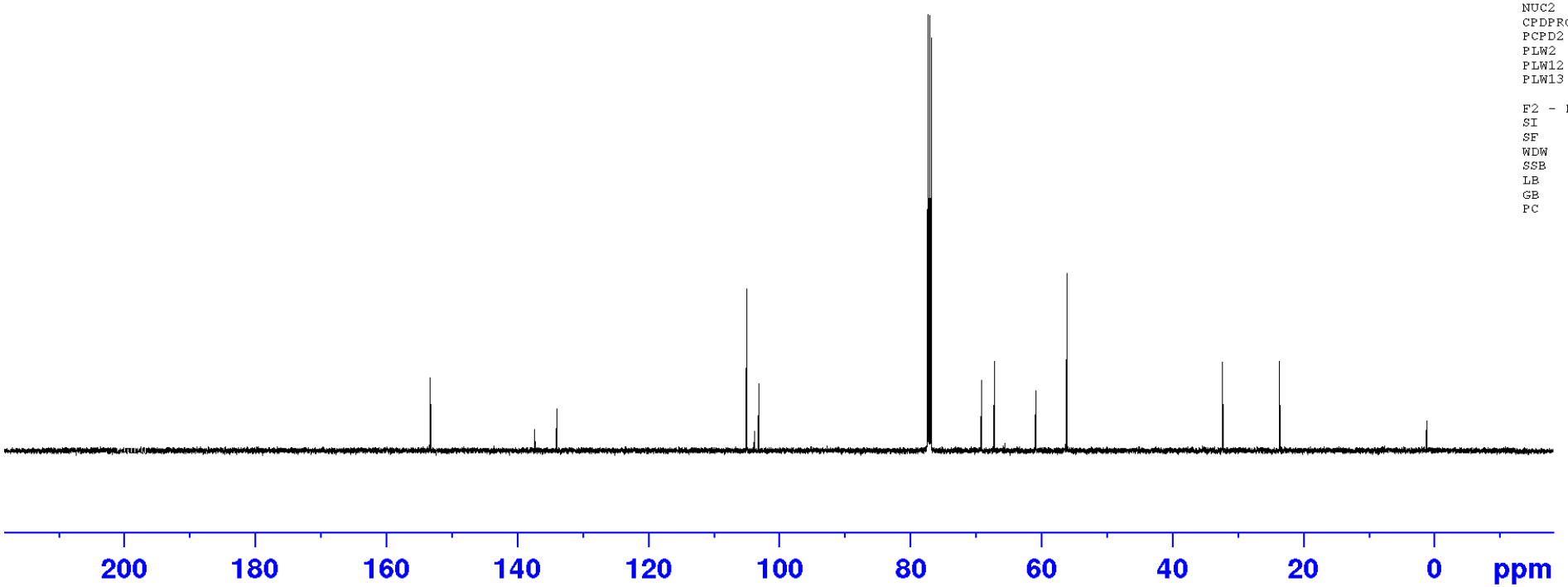
5h

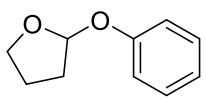
125 MHz ^{13}C NMR

$CDCl_3$

153.35
137.43
134.05
105.04
103.23
77.41
77.16
76.90
69.22
67.24
60.95
56.21
56.19
32.47
23.63

```
Current Data Parameters
NAME      vinn-4-137-12-islt2-20200120
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time               9.10 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT          CDCl3
NS                 256
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577741 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```

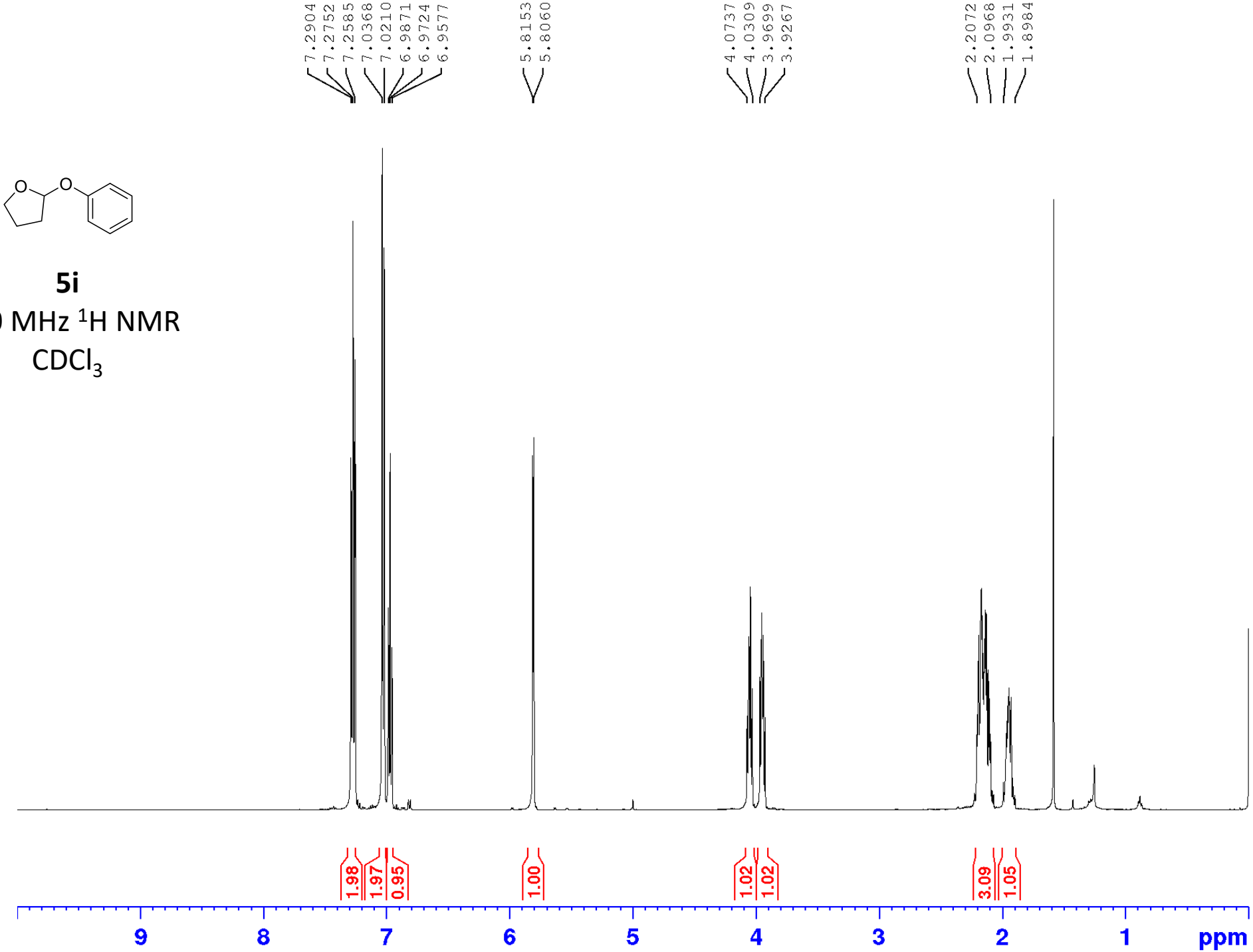




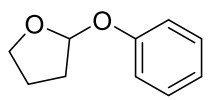
5i

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-193-islt-20230105
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20230105
Time              16.35 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ            3.2767999 sec
RG               117.01
DW               50.000 usec
DE                6.50 usec
TE               295.2 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P1               10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300150 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



5i

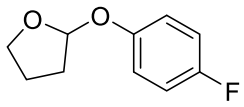
125 MHz ^{13}C NMR

$CDCl_3$

157.27
129.52
121.63
116.63
102.39
77.41
77.16
76.90
68.16
32.83
23.58

```
Current Data Parameters
NAME      vinn-4-193-islt-20230105
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20230105
Time             16.39 h
INSTRUM          spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                  50
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ           1.1010048 sec
RG              206.72
DW              16.800 usec
DE               6.50 usec
TE              295.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

F2 - Processing parameters
SI               32768
SF          125.7577746 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

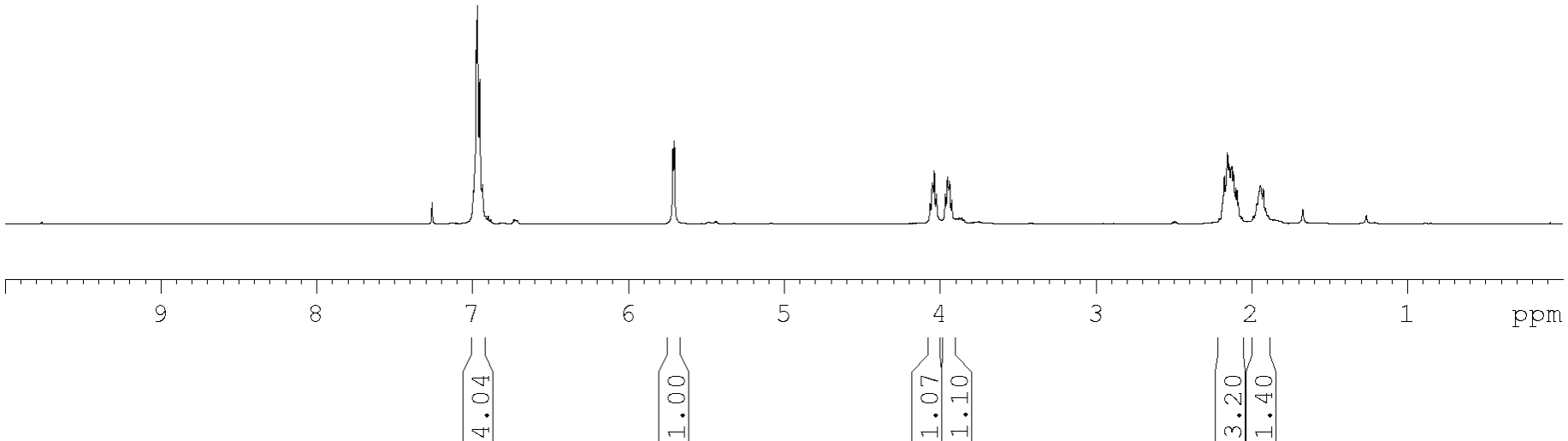
200 180 160 140 120 100 80 60 40 20 0 ppm



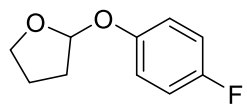
5j

500 MHz ^{1}H NMR

$CDCl_3$



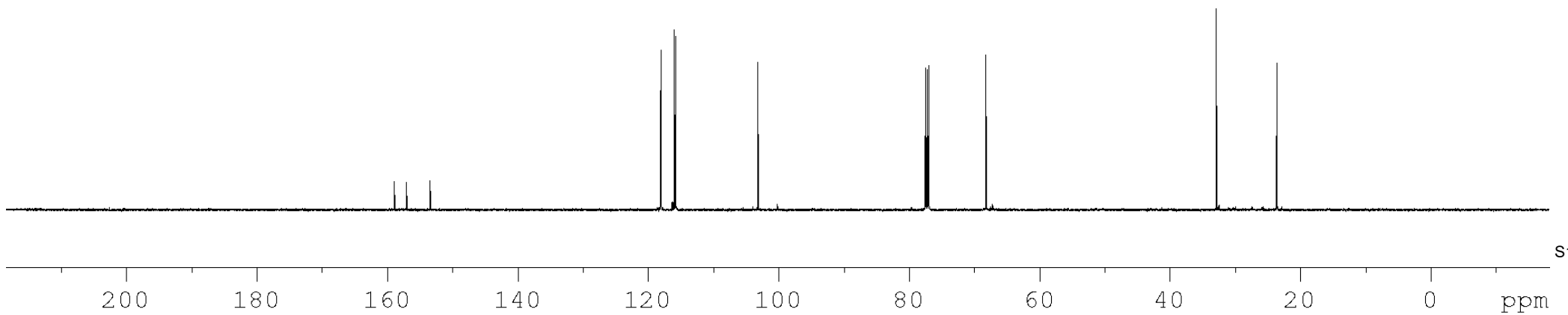
158.901
157.001
153.389
153.370
118.023
117.960
115.935
115.754
103.123
77.416
77.161
76.907
68.136
32.820
23.528

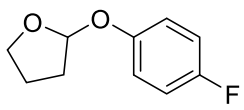


5j

125 MHz ^{13}C NMR

$CDCl_3$





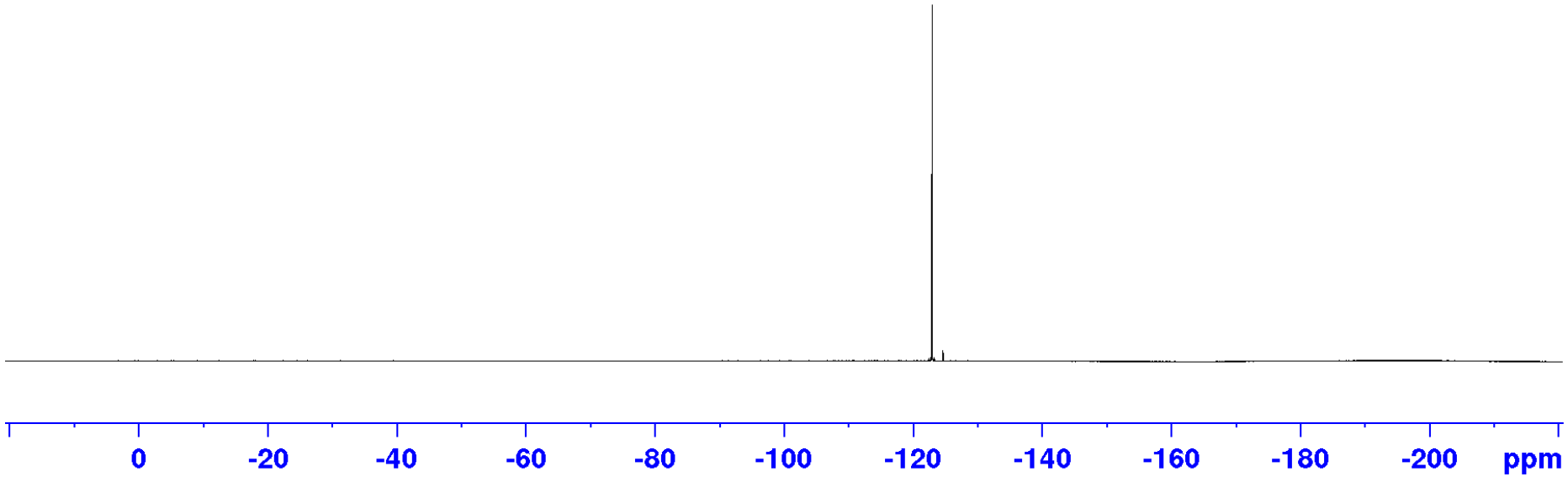
5j

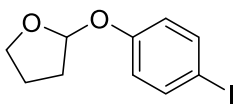
470 MHz ^{1}H NMR

$CDCl_3$

-122.94
-122.95
-122.96
-122.97
-122.98
-122.99

```
Current Data Parameters
NAME      vinn-4-147-3-islt-20200120
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210121
Time              18.34 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgflqn
TD             131072
SOLVENT          CDCl3
NS                  16
DS                   4
SWH          113636.367 Hz
FIDRES         1.733953 Hz
AQ             0.5767168 sec
RG                206.72
DW                 4.400 usec
DE                 6.50 usec
TE                295.1 K
D1           1.00000000 sec
TD0                  1
SFO1         470.5453180 MHz
NUC1               19F
P1                15.00 usec
PLW1         47.23500061 W

F2 - Processing parameters
SI                65536
SF           470.5923772 MHz
WDW                EM
SSB                 0
LB                0.30 Hz
GB                  0
PC                1.00
```

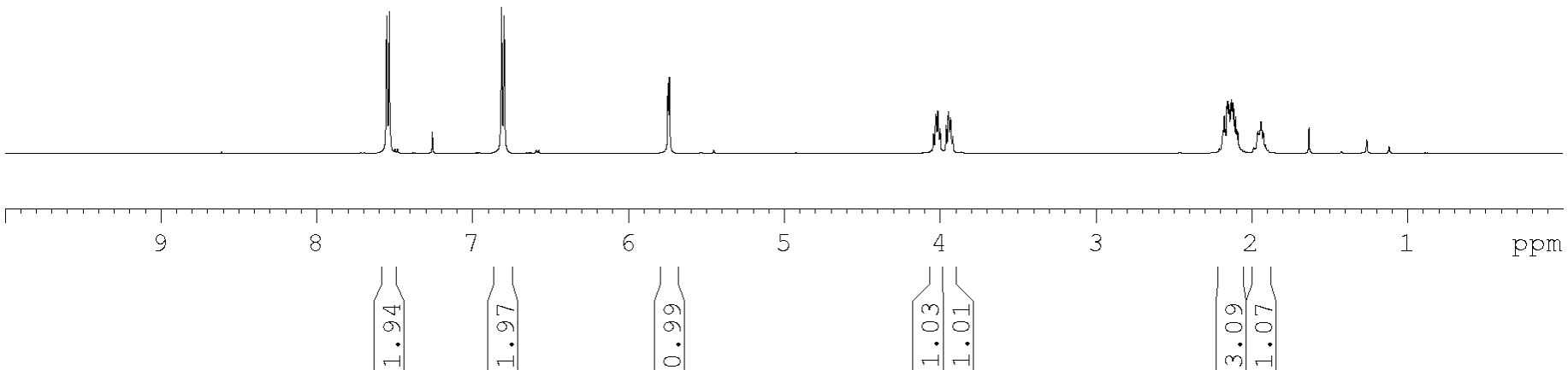


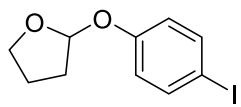


5k

500 MHz ^{1}H NMR

$CDCl_3$



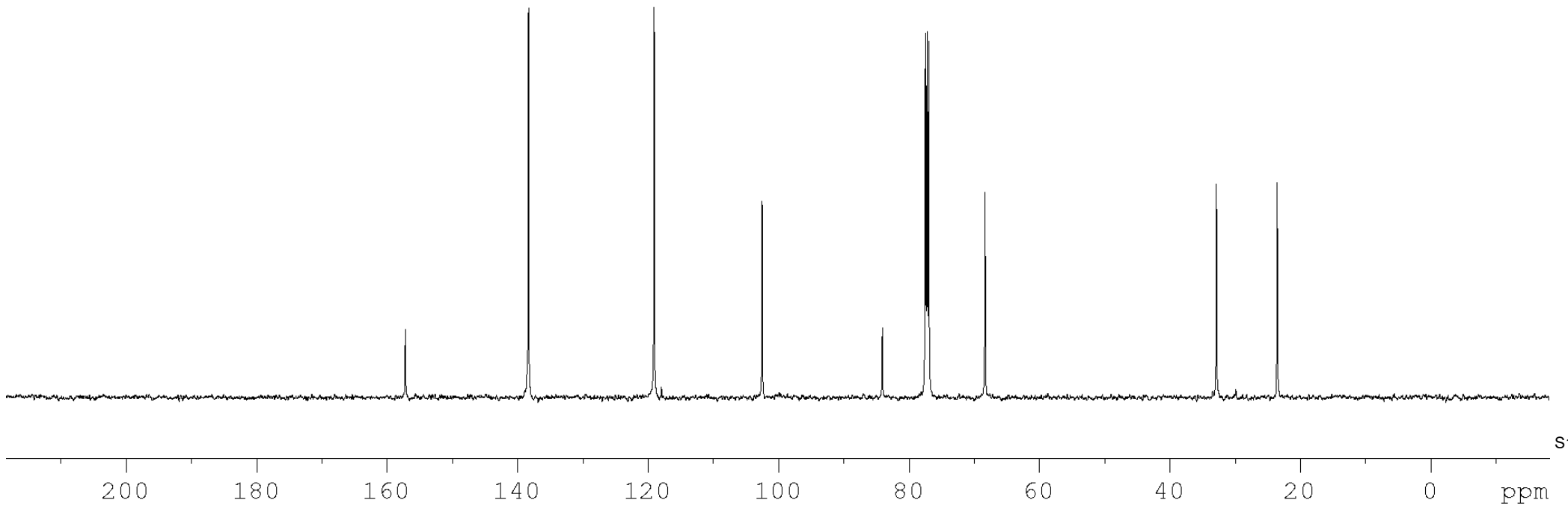


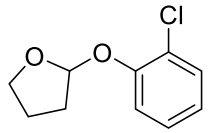
5k

125 MHz ^{13}C NMR

$CDCl_3$

157.143
138.262
118.993
102.433
83.997
77.397
77.143
76.890
68.264
32.773
23.448

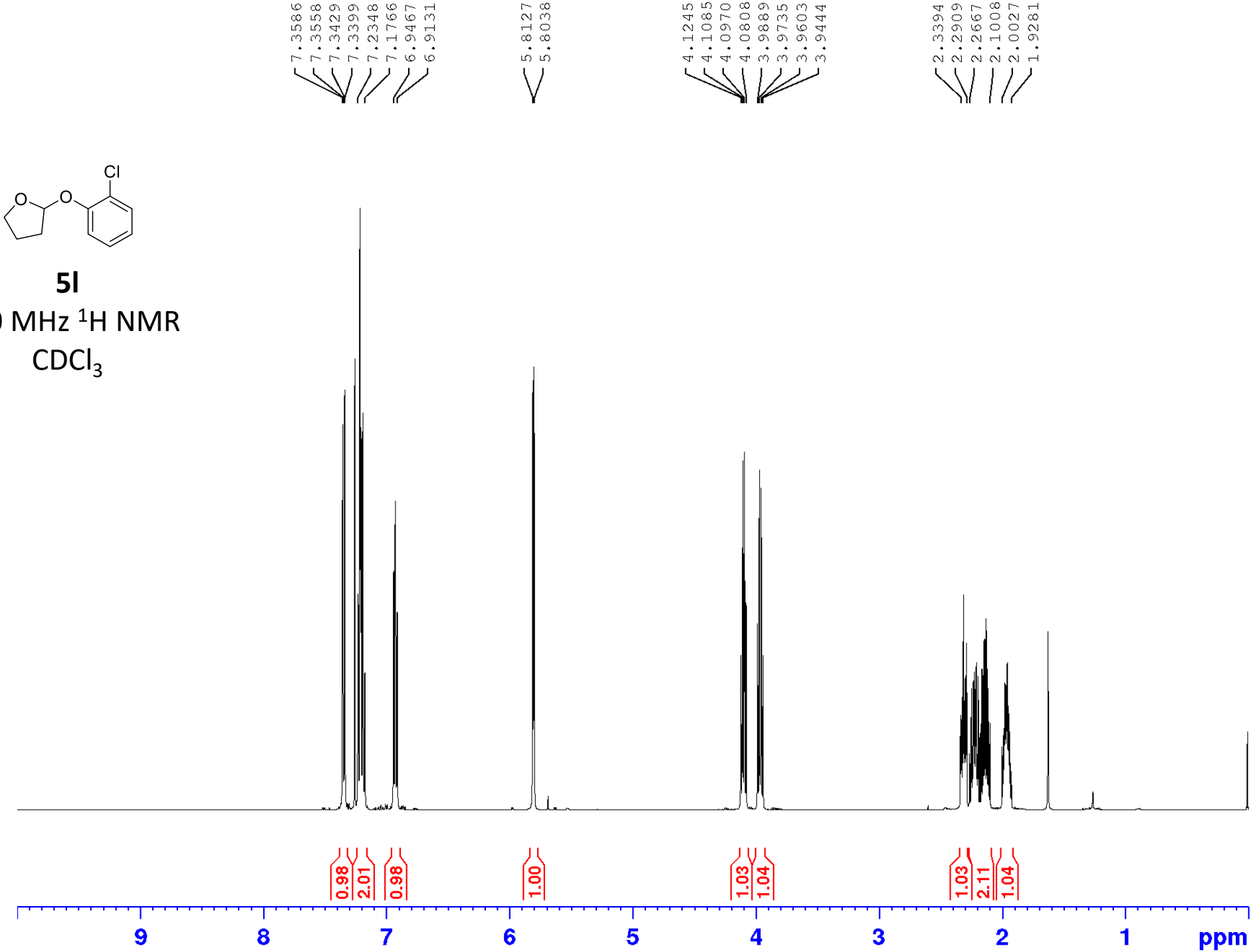




5l

500 MHz ^{1}H NMR

$CDCl_3$

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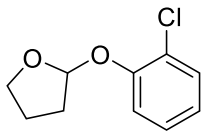
Current Data Parameters
NAME      vinn-4-183-3-islt2-2023032
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20230321
Time              15.51 h
INSTRUM           spect
PROBHD    Z149001_0010 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW              50.000 usec
DE              10.00 usec
TE                296.1 K
D1           1.00000000 sec
TD0                  1
SFO1       500.1330883 MHz
NUC1               1H
P1              11.25 usec
PLW1       17.35199928 W

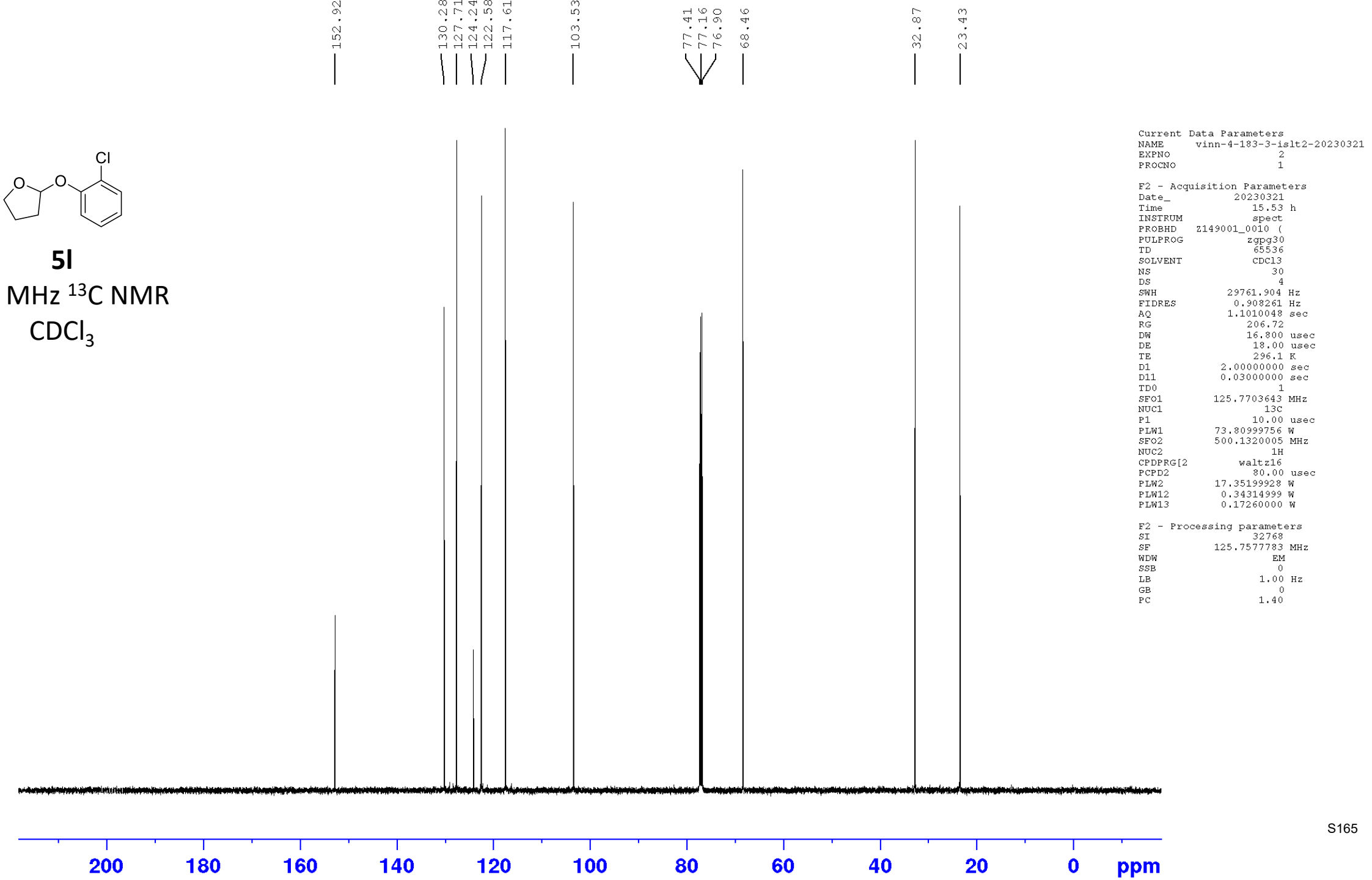
F2 - Processing parameters
SI               65536
SF         500.1300124 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



5l

125 MHz ^{13}C NMR

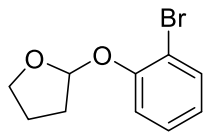
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-183-3-islt2-20230321
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20230321
Time              15.53 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   30
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW              16.800 usec
DE              18.00 usec
TE              296.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1              10.00 usec
PLW1        73.80999756 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2           80.00 usec
PLW2        17.35199928 W
PLW12        0.34314999 W
PLW13        0.17260000 W

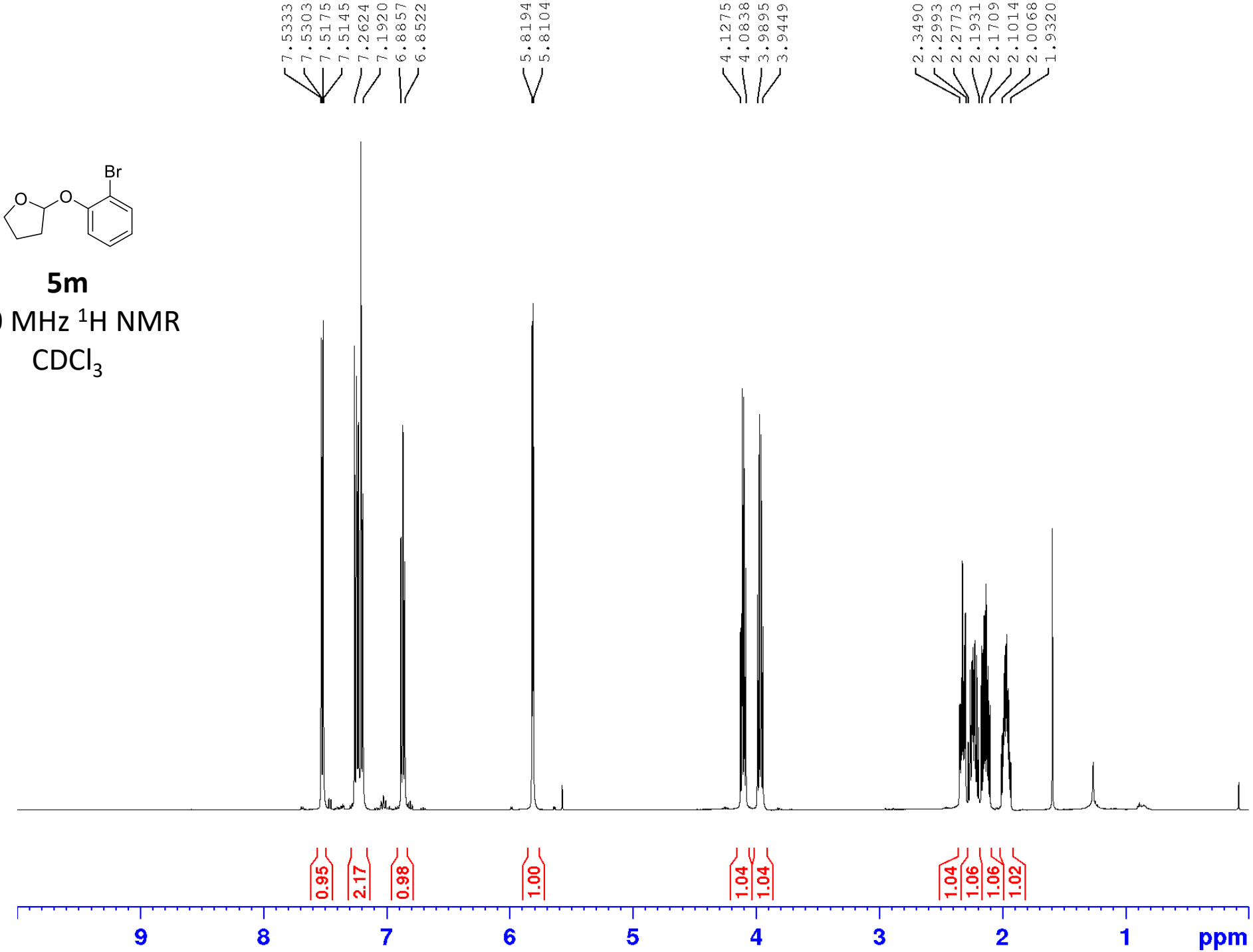
F2 - Processing parameters
SI                32768
SF          125.7577783 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



5m

500 MHz ^{1}H NMR

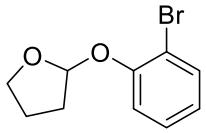
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-147-1-islt-20200121
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210121
Time              19.07 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 63.76
DW                50.000 usec
DE                 6.50 usec
TE                295.2 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300110 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



5m

125 MHz ^{13}C NMR

$CDCl_3$

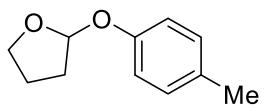
153.87
133.35
128.48
123.03
117.37
113.67
103.52
77.41
77.16
76.90
68.50
32.90
23.44

```
Current Data Parameters
NAME      vinn-4-147-1-islt-20200121
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time              19.21 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577762 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

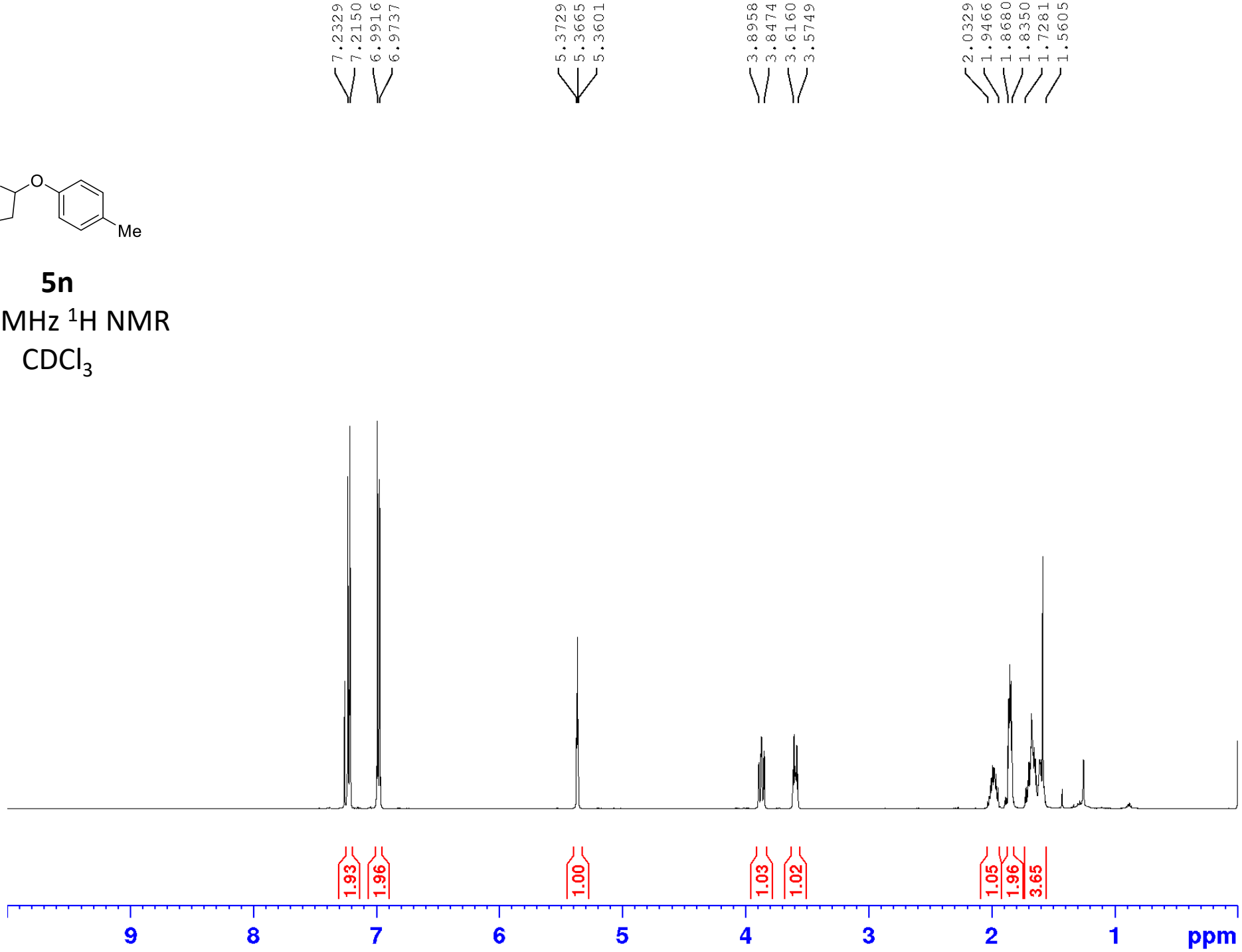
200 180 160 140 120 100 80 60 40 20 0 ppm



5n

500 MHz ^{1}H NMR

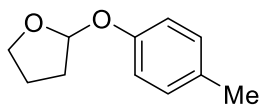
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-190-2-clm8to9-20230103
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20230103
Time              16.58 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                102.6
DW               50.000 usec
DE                6.50 usec
TE                295.1 K
D1           1.00000000 sec
TD0                   1
SFO1        500.1330883 MHz
NUC1                1H
P1                10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300128 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

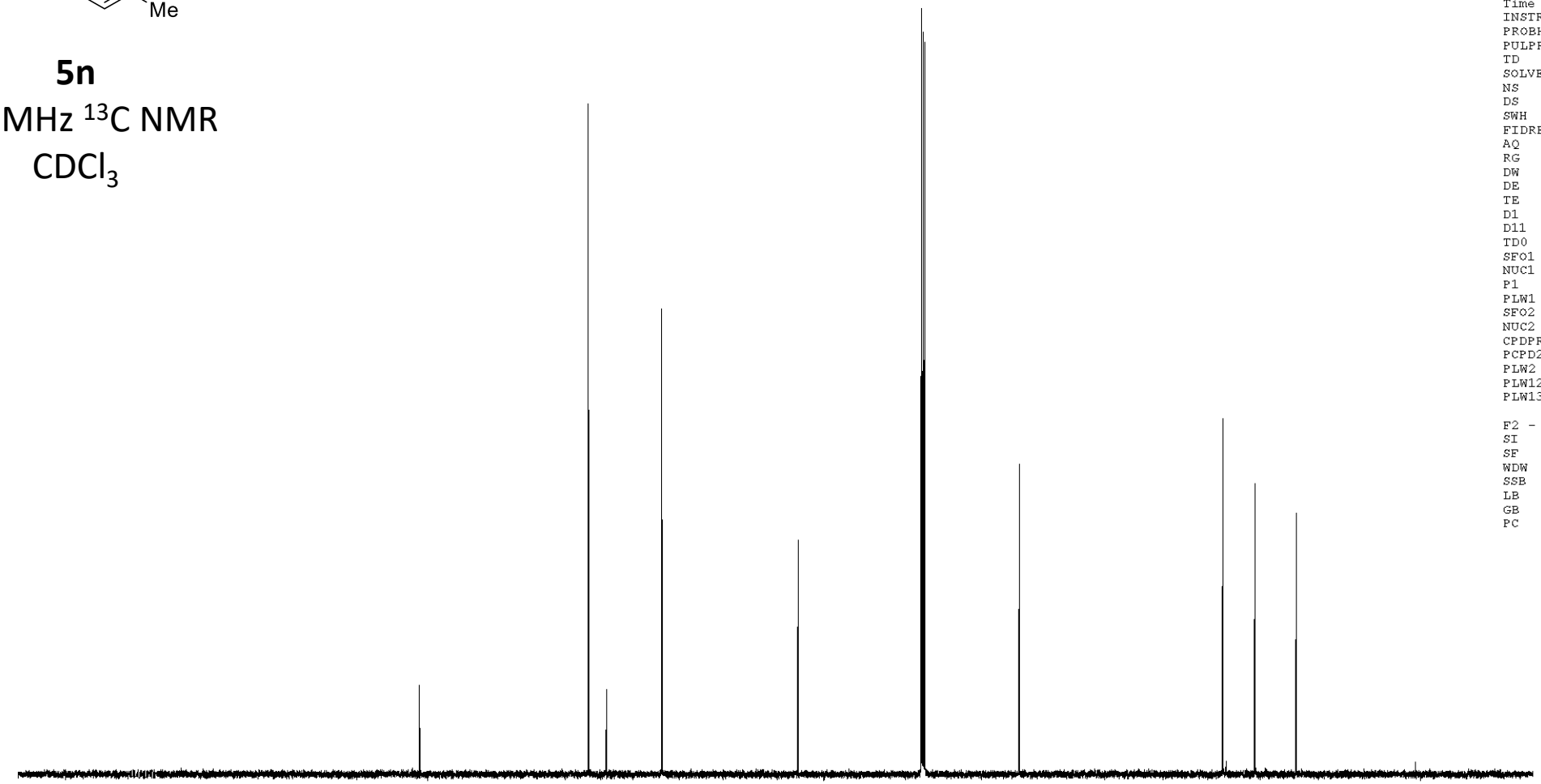


5n

125 MHz ^{13}C NMR

$CDCl_3$

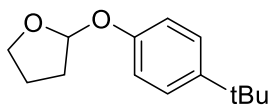
155.77
129.38
126.56
117.92
96.68
77.41
77.16
76.90
62.14
30.39
25.25
18.79




```
Current Data Parameters
NAME      vinn-4-190-2-clm8to9-2023010
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20230103
Time              18.07 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW               16.800 usec
DE                6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

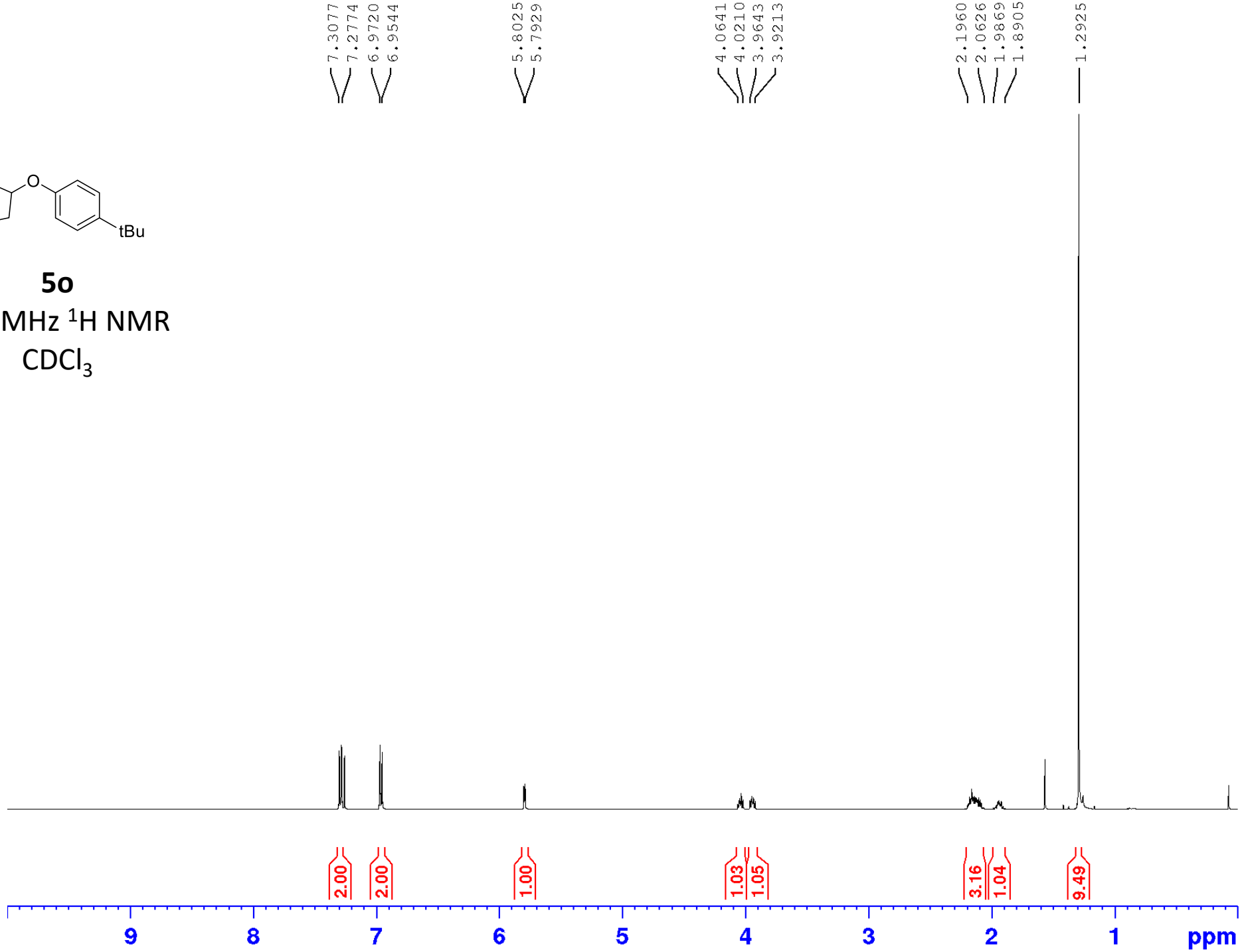
F2 - Processing parameters
SI                32768
SF          125.7577740 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



5o

500 MHz ^{1}H NMR

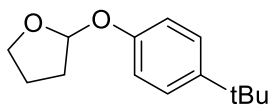
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-147-6-islt2-2020012
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time              19.25 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                93.28
DW              50.000 usec
DE               6.50 usec
TE              295.2 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                1H
P1               10.91 usec
PLW1        25.00000000 W

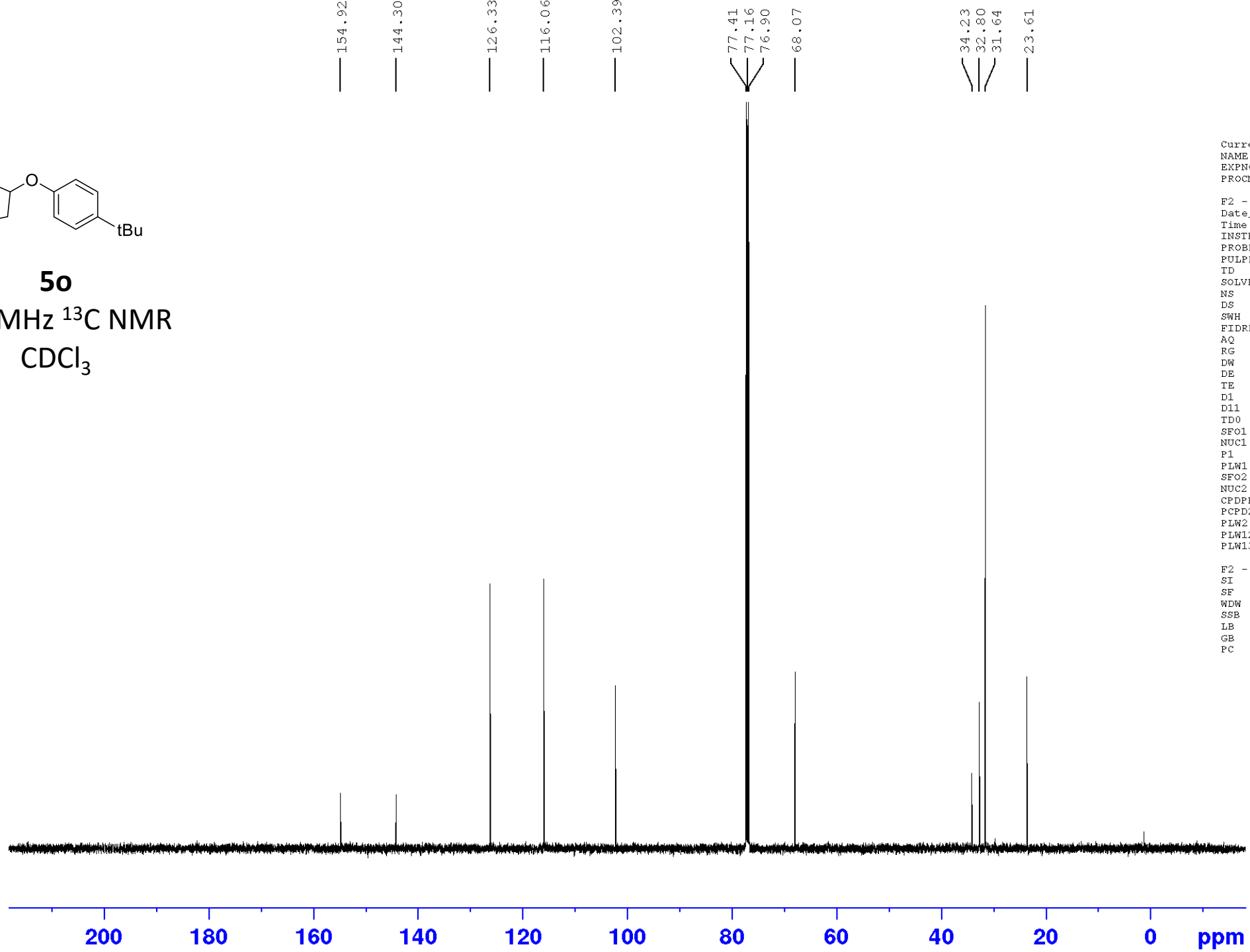
F2 - Processing parameters
SI               65536
SF          500.1300122 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



5o

125 MHz ^{13}C NMR

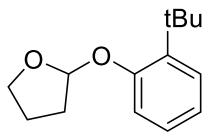
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-147-6-islt2-20200121
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210121
Time              19.39 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577731 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

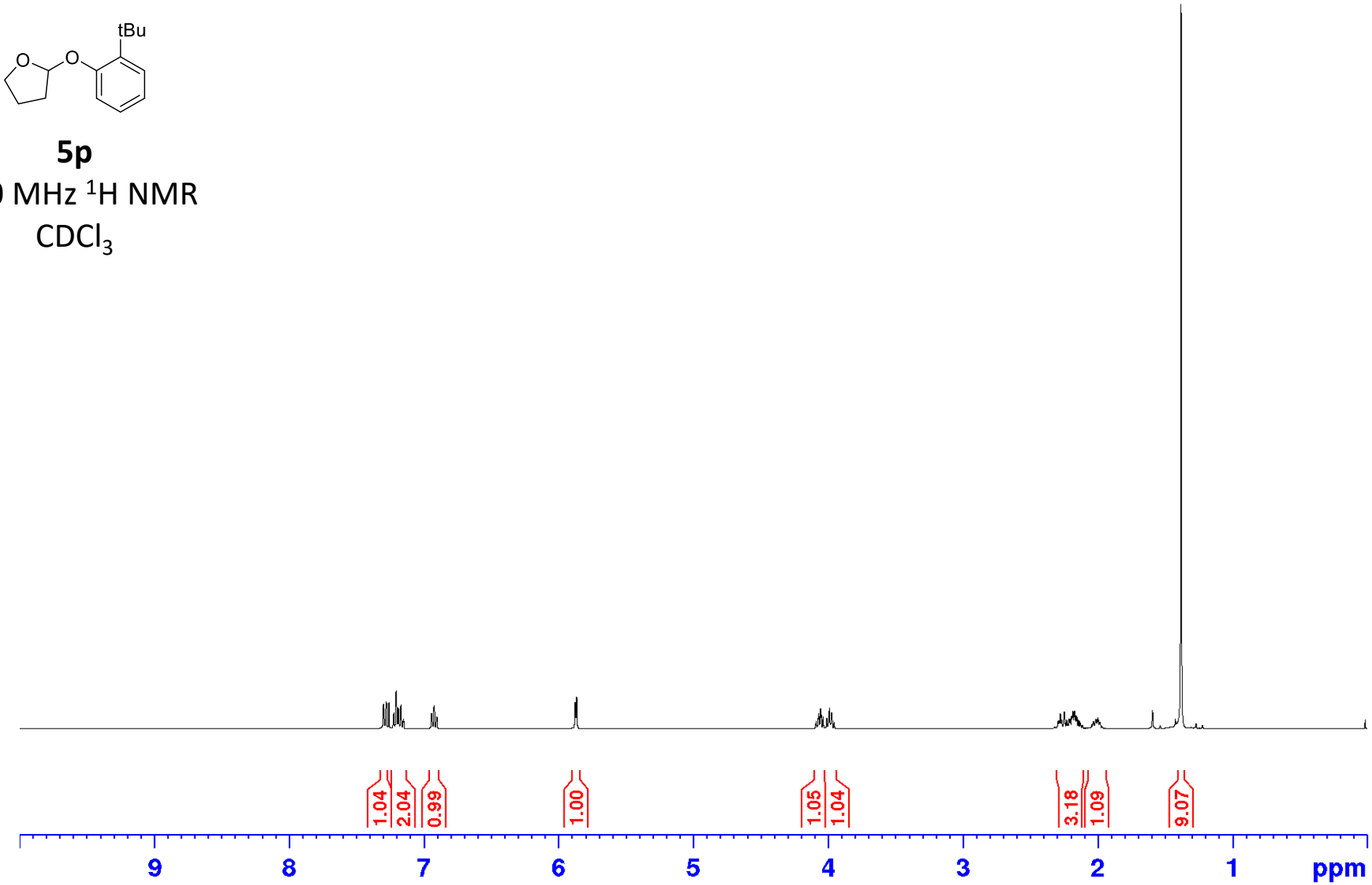


5p

400 MHz ^{1}H NMR

$CDCl_3$

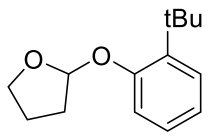
7.3014
7.2599
7.2273
7.1495
6.9440
6.9401
6.9244
6.9070
6.9033
5.8788
5.8672
4.0907
4.0710
4.0573
4.0373
4.0100
3.9911
3.9752
3.9557
2.2953
2.1138
2.0461
1.9688
1.3819




```
Current Data Parameters
NAME      vinn-4-183-4-ialt-20230320
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20230320
Time               18.18 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                 80.6
DW                62.400 usec
DE                 6.50 usec
TE                295.4 K
D1             1.00000000 sec
TD0                   1
SFO1         400.1324708 MHz
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W

F2 - Processing parameters
SI                65536
SF           400.1300101 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



5p

100 MHz ^{13}C NMR

$CDCl_3$

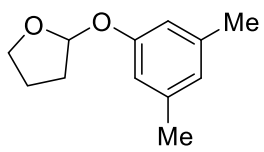
156.04
138.18
127.13
126.74
121.01
114.58
101.80
77.47
77.16
76.84
68.03
34.86
32.93
29.98
23.72

```
Current Data Parameters
NAME      vinn-4-183-4-islt-20230320
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20230320
Time              18.22 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                  40
DS                   4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            1.3631488 sec
RG                 203
DW              20.800 usec
DE               6.50 usec
TE              295.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1       100.6228298 MHz
NUC1               13C
P1              10.00 usec
PLW1       51.00000000 W
SFO2       400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2           90.00 usec
PLW2       12.50000000 W
PLW12       0.34722000 W
PLW13       0.17465000 W

F2 - Processing parameters
SI               32768
SF         100.6127584 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

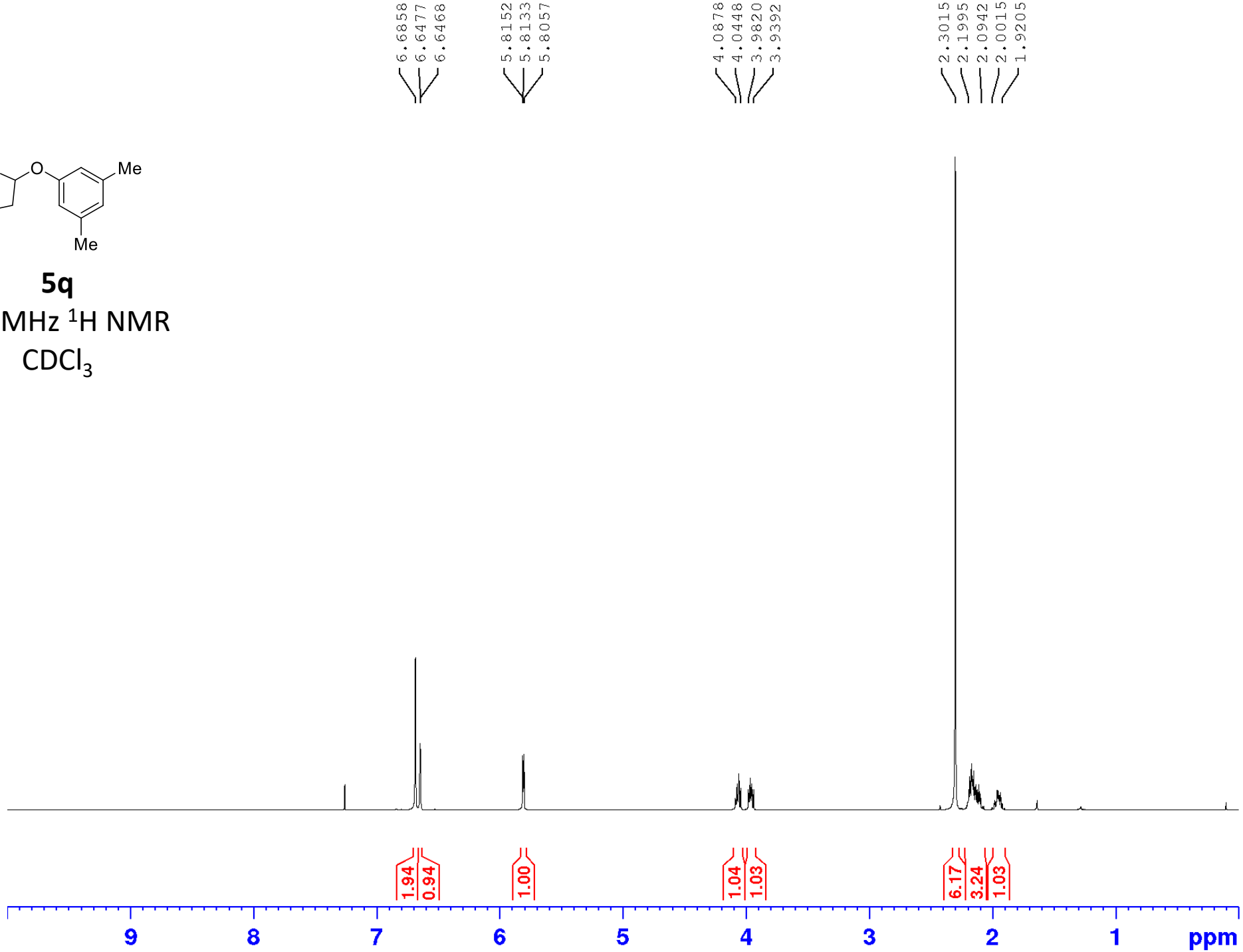
200 180 160 140 120 100 80 60 40 20 0 ppm



5q

500 MHz ^{1}H NMR

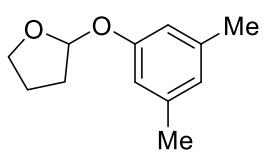
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-147-7-islt-20200120
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210121
Time              18.38 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ               3.2767999 sec
RG                  30.85
DW                 50.000 usec
DE                  6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                 10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300122 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

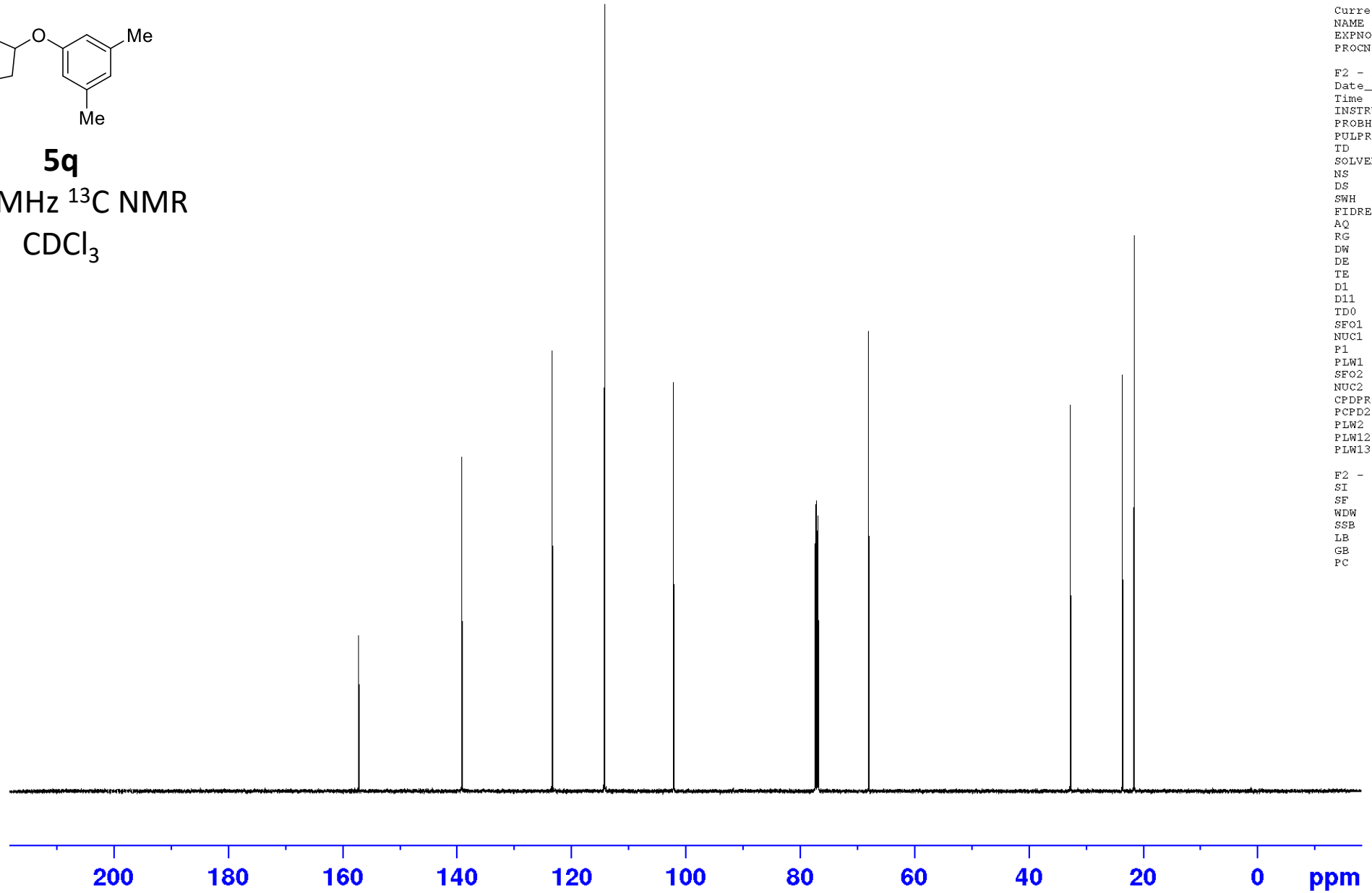


5q

125 MHz ^{13}C NMR

$CDCl_3$

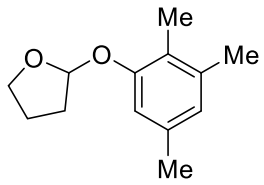
157.25
139.23
123.40
114.27
102.22
77.41
77.16
76.90
68.07
32.80
23.58
21.53




```
Current Data Parameters
NAME      vinn-4-147-7-islt-20200120
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time              18.52 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                 6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                 9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

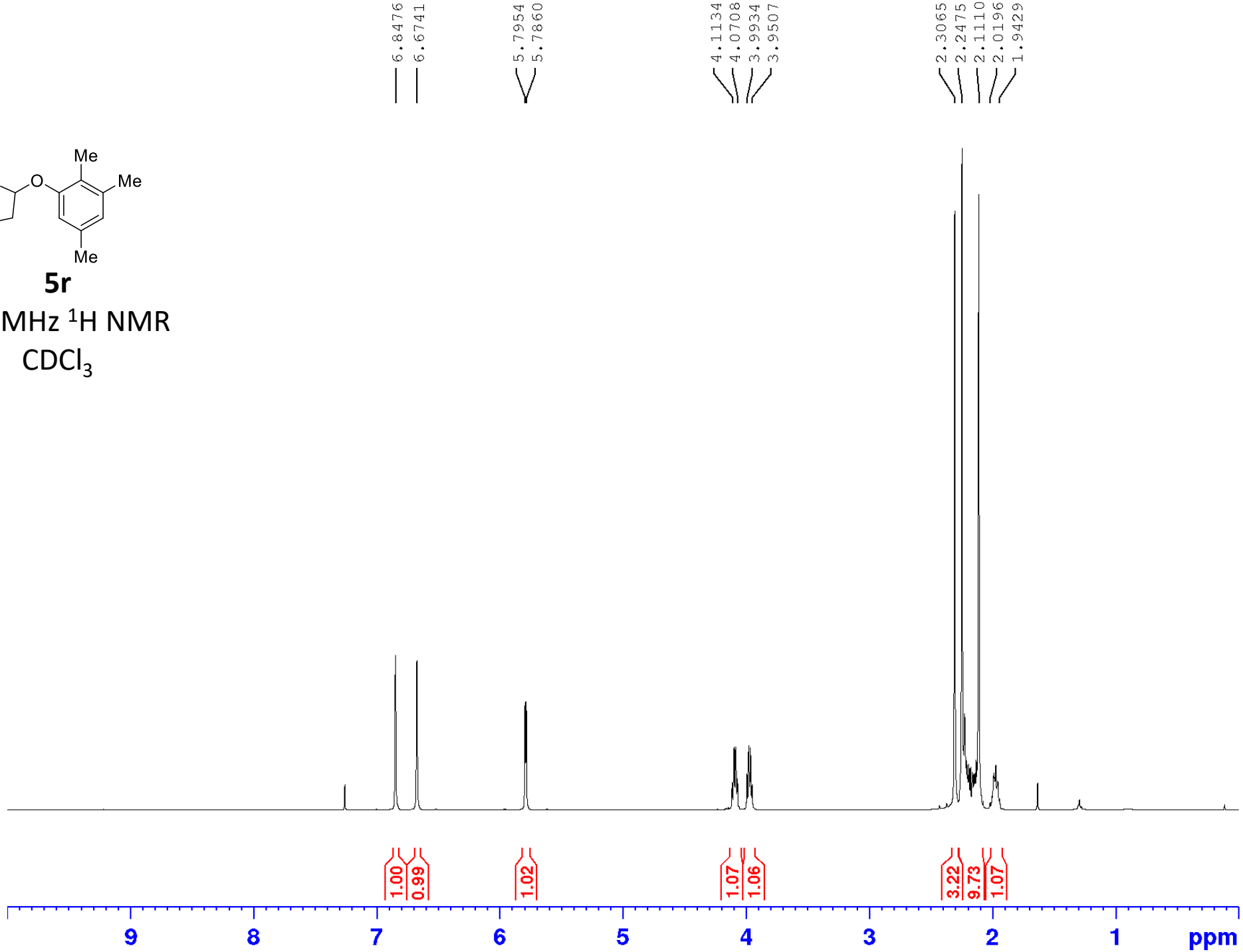
F2 - Processing parameters
SI                32768
SF          125.7577797 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



5r

500 MHz ^{1}H NMR

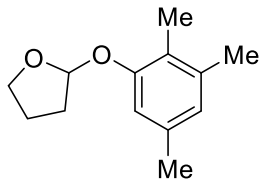
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-147-8-islt-20200120
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210121
Time               7.22 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                30.85
DW               50.000 usec
DE                6.50 usec
TE               295.1 K
D1            1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P1                10.91 usec
PLW1         25.00000000 W

F2 - Processing parameters
SI               65536
SF         500.1300125 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



5r

125 MHz ^{13}C NMR

$CDCl_3$

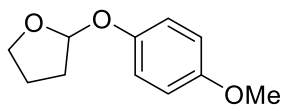
155.10
137.66
135.57
124.14
123.03
113.52
102.80
77.41
77.16
76.90
68.04
32.92
23.72
21.35
20.19
11.67

```
Current Data Parameters
NAME      vinn-4-147-8-islt-20200120
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210121
Time                7.36 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577807 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

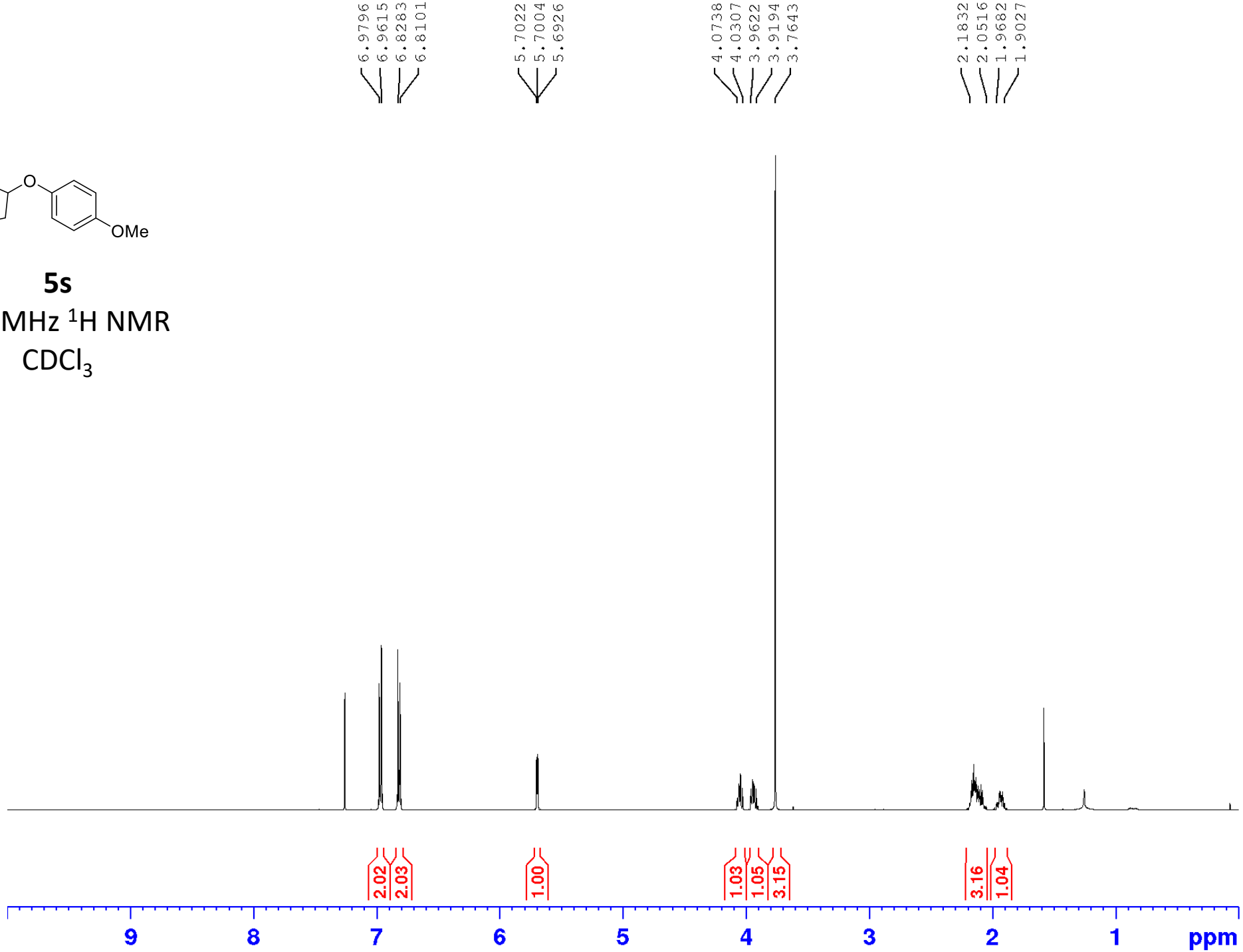
200 180 160 140 120 100 80 60 40 20 0 ppm



5s

500 MHz ^{1}H NMR

$CDCl_3$

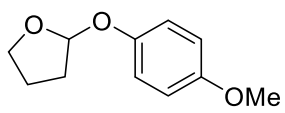


BRUKER

```
Current Data Parameters
NAME      vinn-4-147-4-islt-20200120
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210121
Time                5.27 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 102.6
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

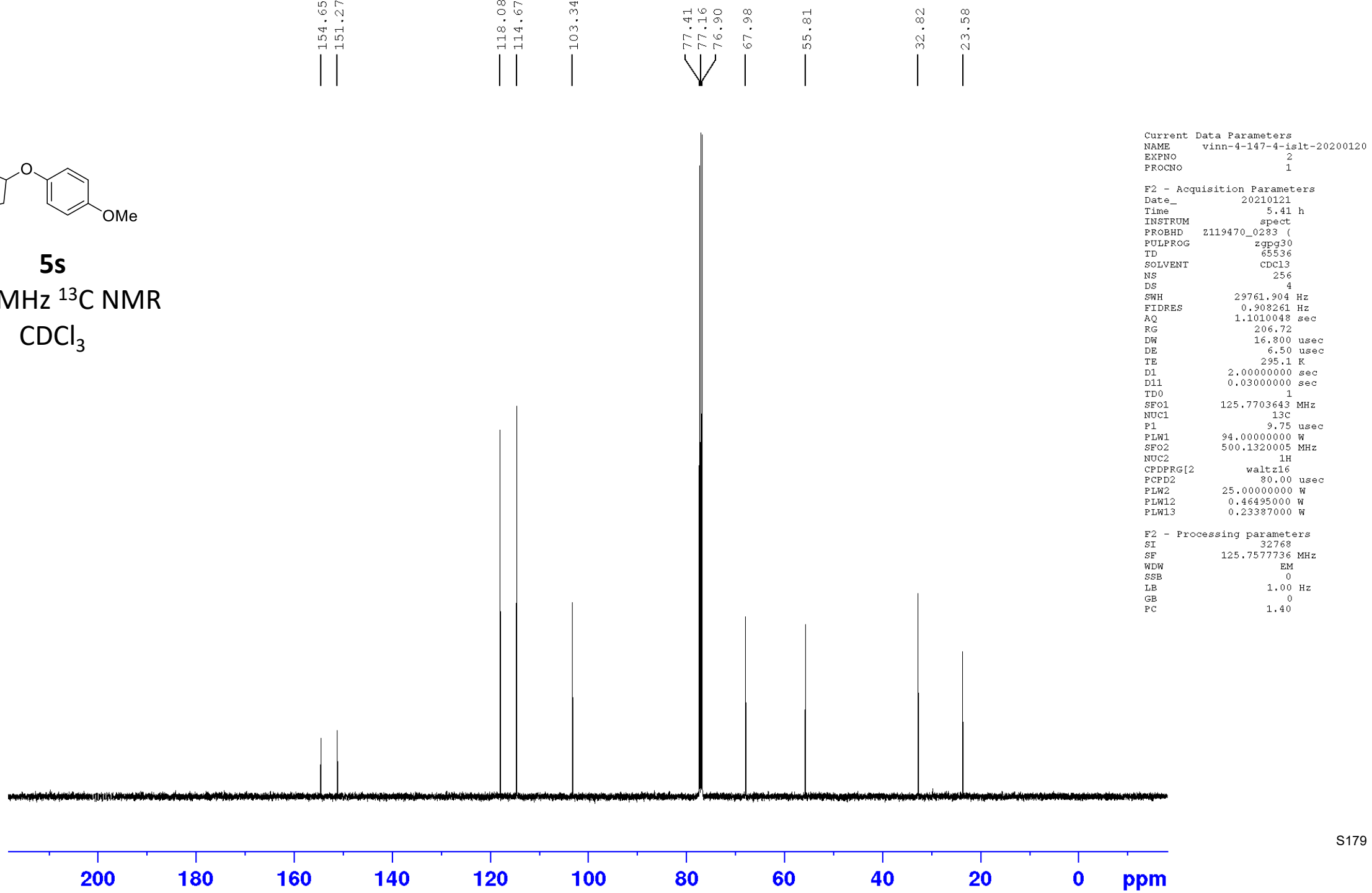
F2 - Processing parameters
SI                65536
SF            500.1300123 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



5s

125 MHz ^{13}C NMR

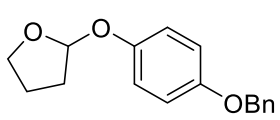
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-147-4-islt-20200120
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time               5.41 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT          CDCl3
NS                 256
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ           1.1010048 sec
RG              206.72
DW              16.800 usec
DE               6.50 usec
TE              295.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

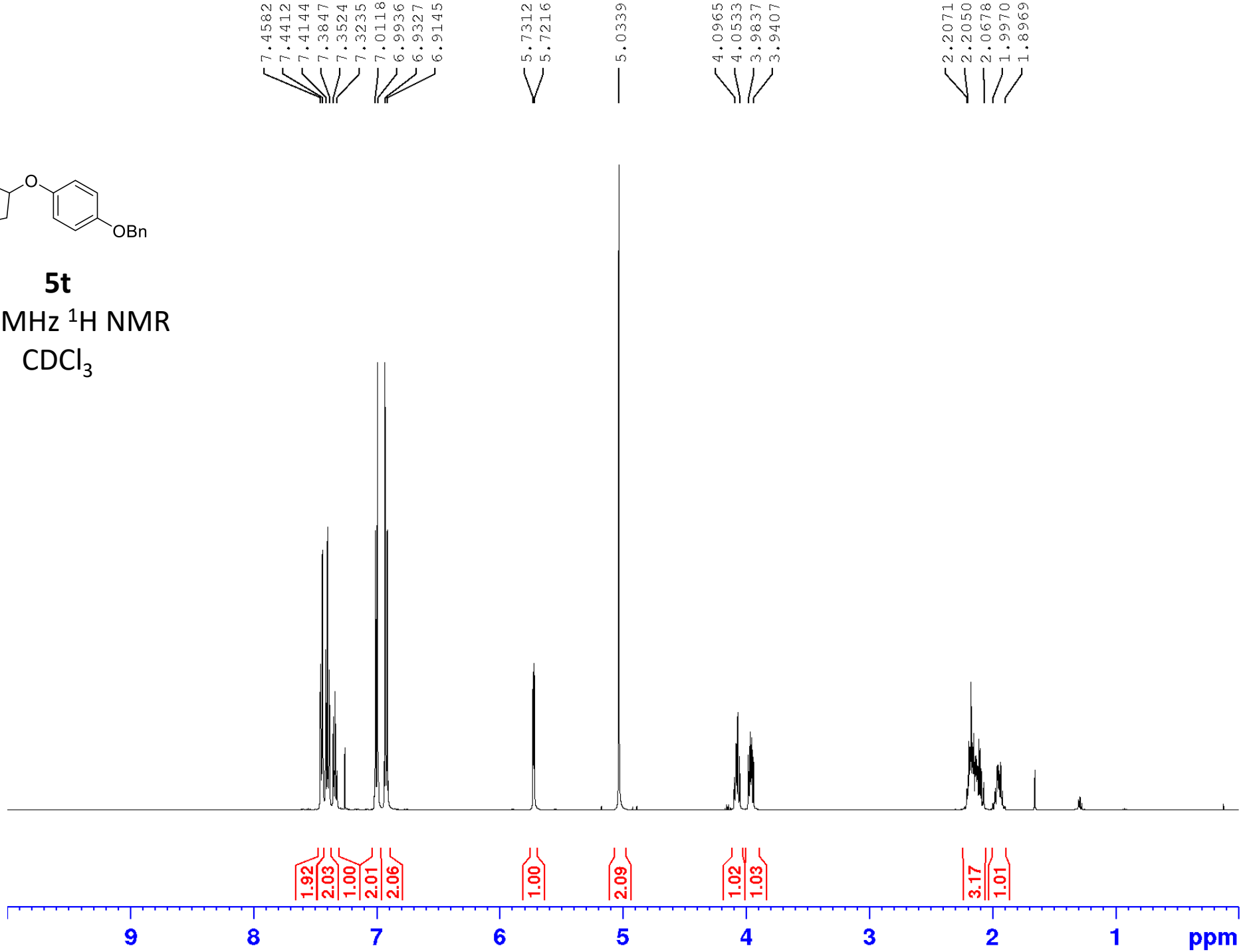
F2 - Processing parameters
SI                32768
SF          125.7577736 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```



5t

500 MHz ^{1}H NMR

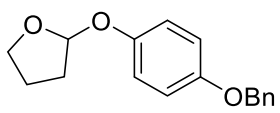
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-147-5-islt-20200120
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210121
Time               5.45 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                30.85
DW               50.000 usec
DE                6.50 usec
TE               295.2 K
D1           1.00000000 sec
TD0                  1
SFO1         500.1330883 MHz
NUC1                 1H
P1                10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300121 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



5t

125 MHz ^{13}C NMR

$CDCl_3$

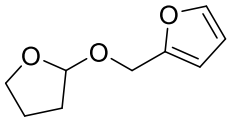
153.78
151.45
137.36
128.62
127.94
127.55
117.95
115.76
103.21
77.41
77.16
76.90
70.62
67.94
32.77
23.54

```
Current Data Parameters
NAME      vinn-4-147-5-islt-20200120
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210121
Time               5.59 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD              65536
SOLVENT          CDCl3
NS                 256
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1
SFO1       125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1       94.00000000 W
SFO2       500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2       25.00000000 W
PLW12       0.46495000 W
PLW13       0.23387000 W

F2 - Processing parameters
SI               32768
SF         125.7577846 MHz
WDW                EM
SSB                 0
LB              1.00 Hz
GB                  0
PC              1.40
```

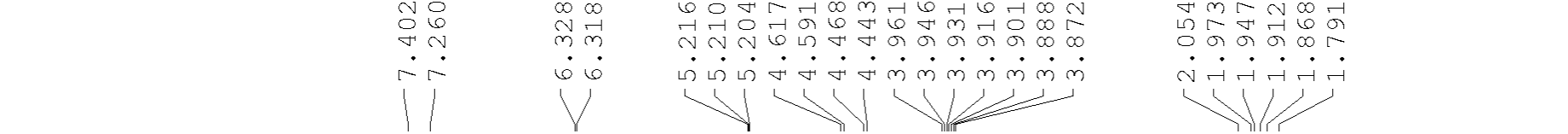
200 180 160 140 120 100 80 60 40 20 0 ppm

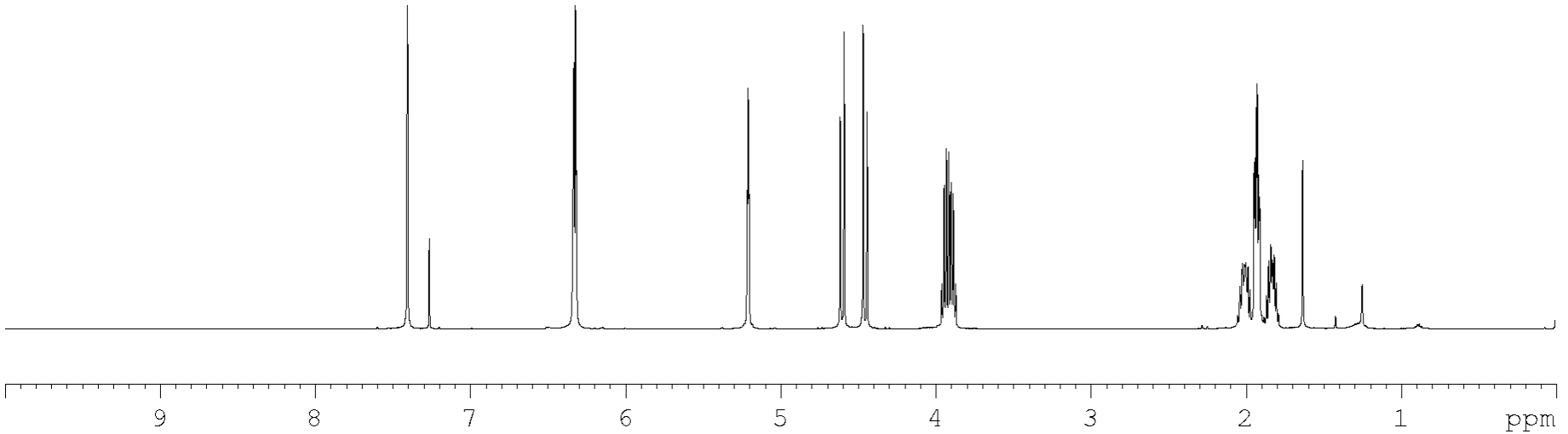


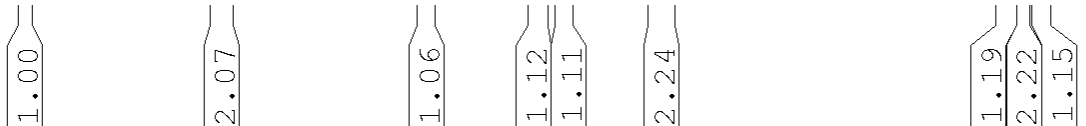
5u

500 MHz ^{1}H NMR

$CDCl_3$








```
Current Data Parameters
NAME      vinn-7-105-2-islt-20230807
EXPNO                 1
PROCNO                1

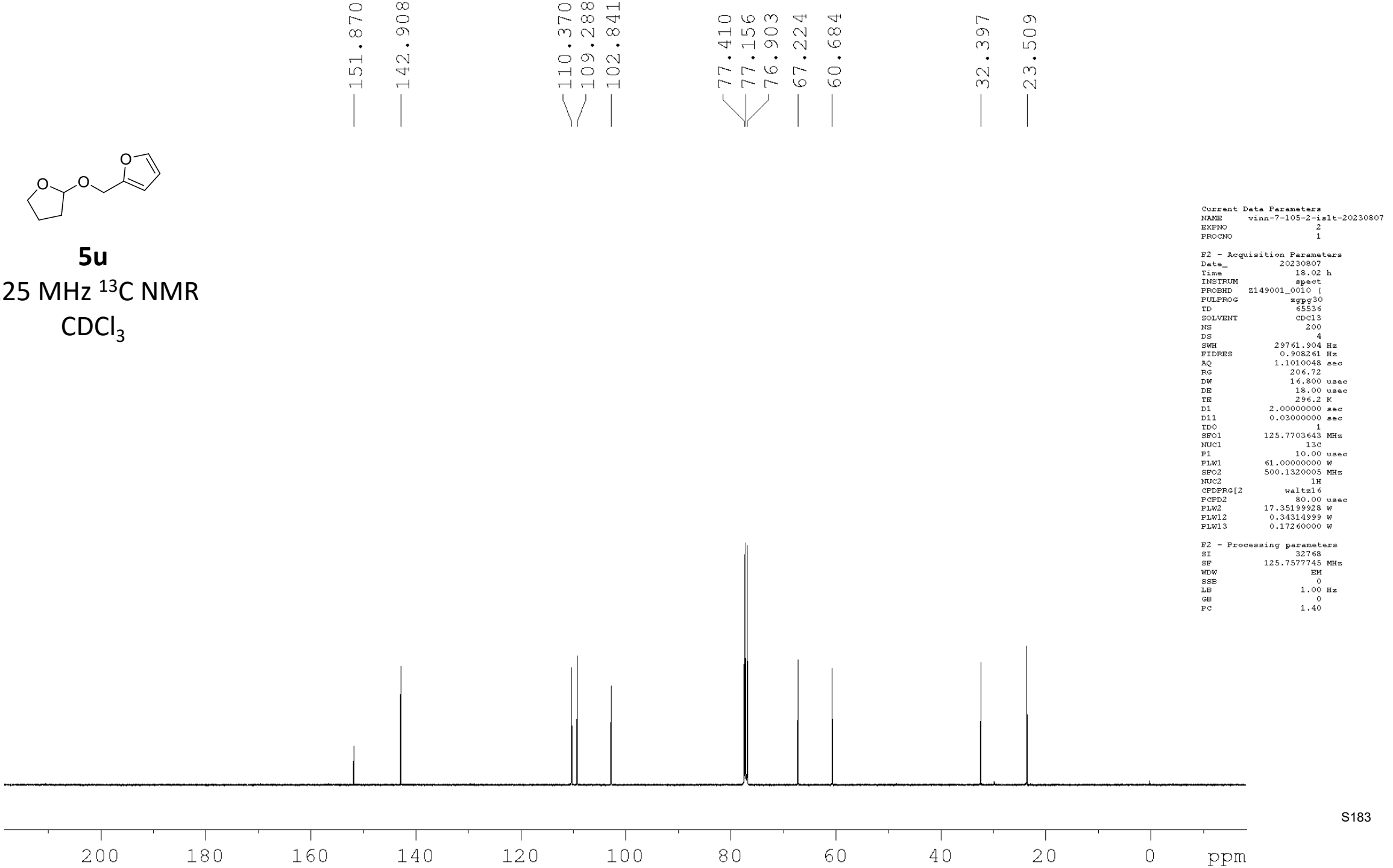
F2 - Acquisition Parameters
Date_           20230807
Time              17.51 h
INSTRUM           spect
PROBHD    Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW               50.000 usec
DE               10.00 usec
TE               296.1 K
D1            1.00000000 sec
TD0                    1
SFO1        500.1330883 MHz
NUC1                  1H
P1               11.25 usec
PLW1        17.35199928 W

F2 - Processing parameters
SI                 65536
SF          500.1300134 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

5u

125 MHz ^{13}C NMR

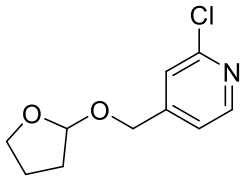
$CDCl_3$




```
Current Data Parameters
NAME      vinn-7-105-2-islt-20230807
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20230807
Time              18.02 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW              16.800 usec
DE              18.00 usec
TE              296.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1              10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2           80.00 usec
PLW2        17.35199928 W
PLW12        0.34314999 W
PLW13        0.17260000 W

F2 - Processing parameters
SI                32768
SF          125.7577745 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```



5v

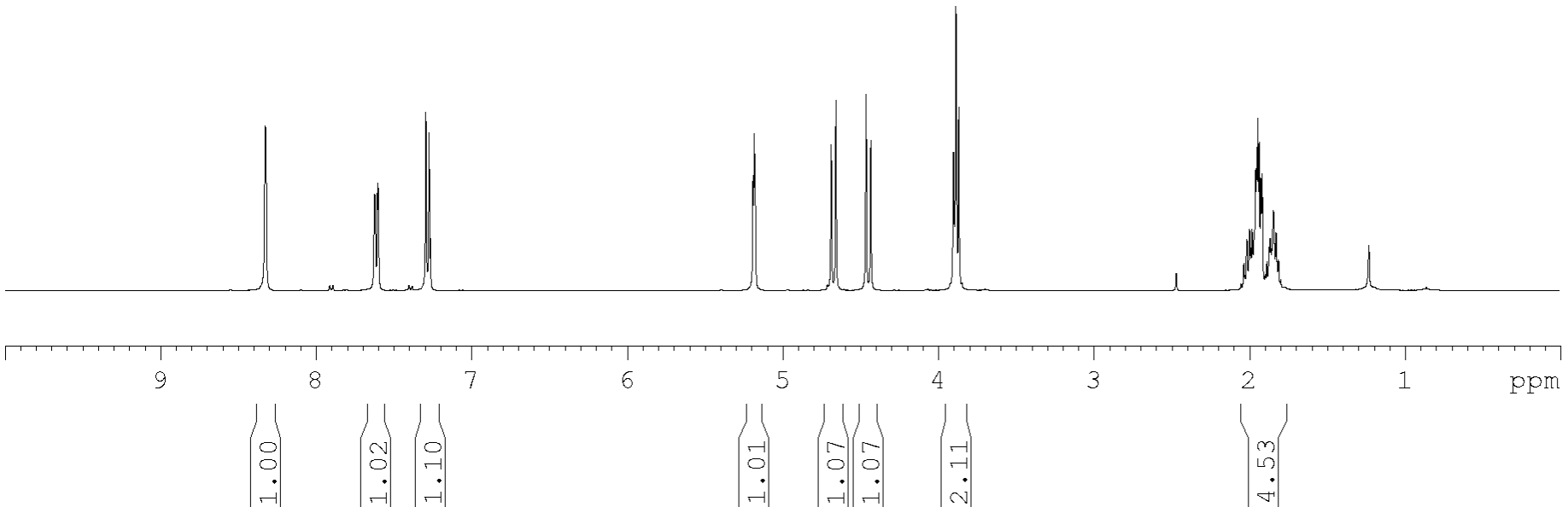
400 MHz ^{1}H NMR

$CDCl_3$


```
Current Data Parameters
NAME      vinn-7-110-2-islt-20230809
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20230809
Time              18.00 h
INSTRUM           spect
PROBHD    Z108618_0257 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                 90.5
DW                62.400 usec
DE                 6.50 usec
TE                295.9 K
D1           1.00000000 sec
TD0                    1
SFO1        400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W

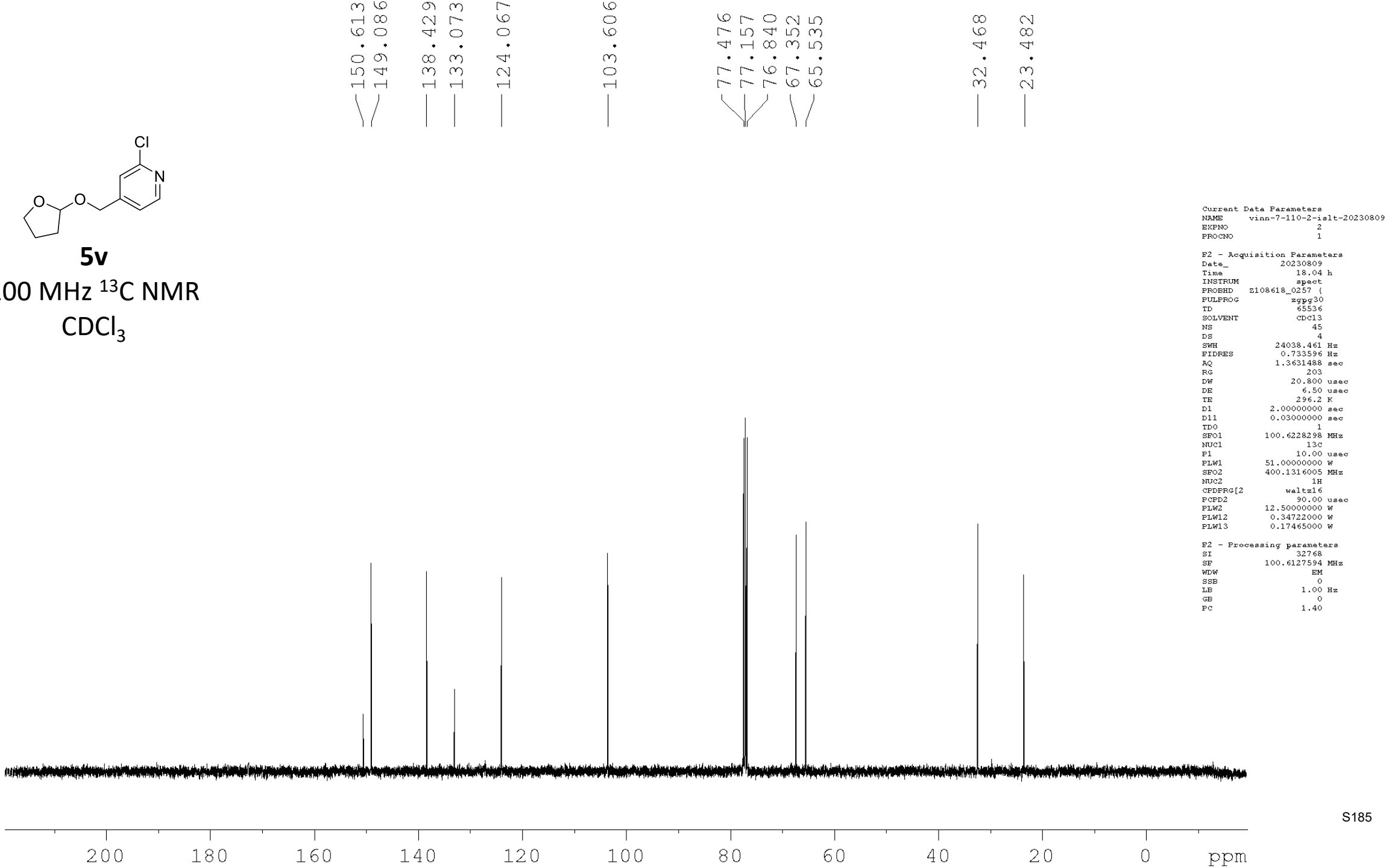
F2 - Processing parameters
SI                 65536
SF          400.1300096 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



5v

100 MHz ^{13}C NMR

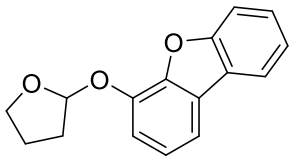
$CDCl_3$




```
Current Data Parameters
NAME      vinn-7-110-2-islt-20230809
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20230809
Time              18.04 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                   45
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               296.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6228298 MHz
NUC1                13C
P1               10.00 usec
PLW1         51.00000000 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.17465000 W

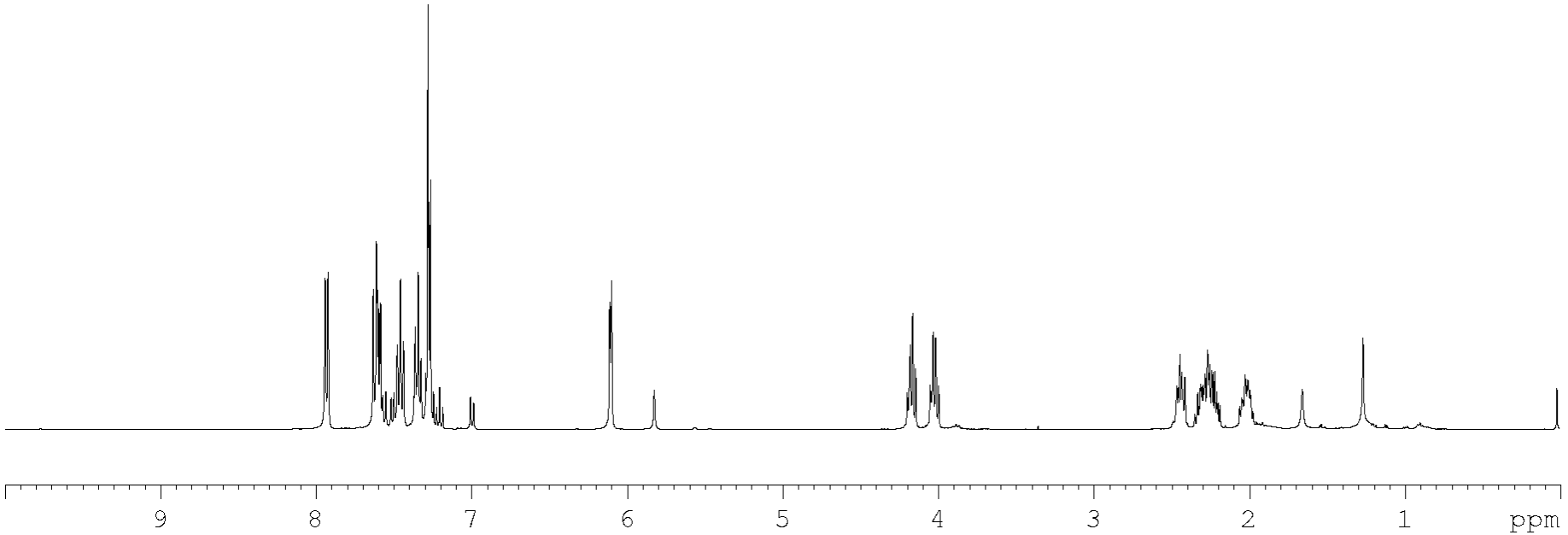
F2 - Processing parameters
SI                32768
SF           100.6127594 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



5w

400 MHz ^{1}H NMR

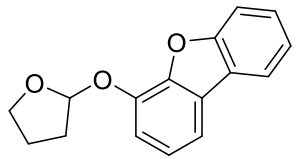
$CDCl_3$




```
Current Data Parameters
NAME      vinn-7-110-4-islt-20230809
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_              20230809
Time                 18.09 h
INSTRUM              spect
PROBHD    Z108618_0257 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES            0.244532 Hz
AQ                4.0894465 sec
RG                     90.5
DW                  62.400 usec
DE                   6.50 usec
TE                  296.1 K
D1             1.00000000 sec
TD0                     1
SFO1          400.1324708 MHz
NUC1                   1H
P1                  15.00 usec
PLW1          12.50000000 W

F2 - Processing parameters
SI                  65536
SF            400.1300099 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



5w

100 MHz ^{13}C NMR

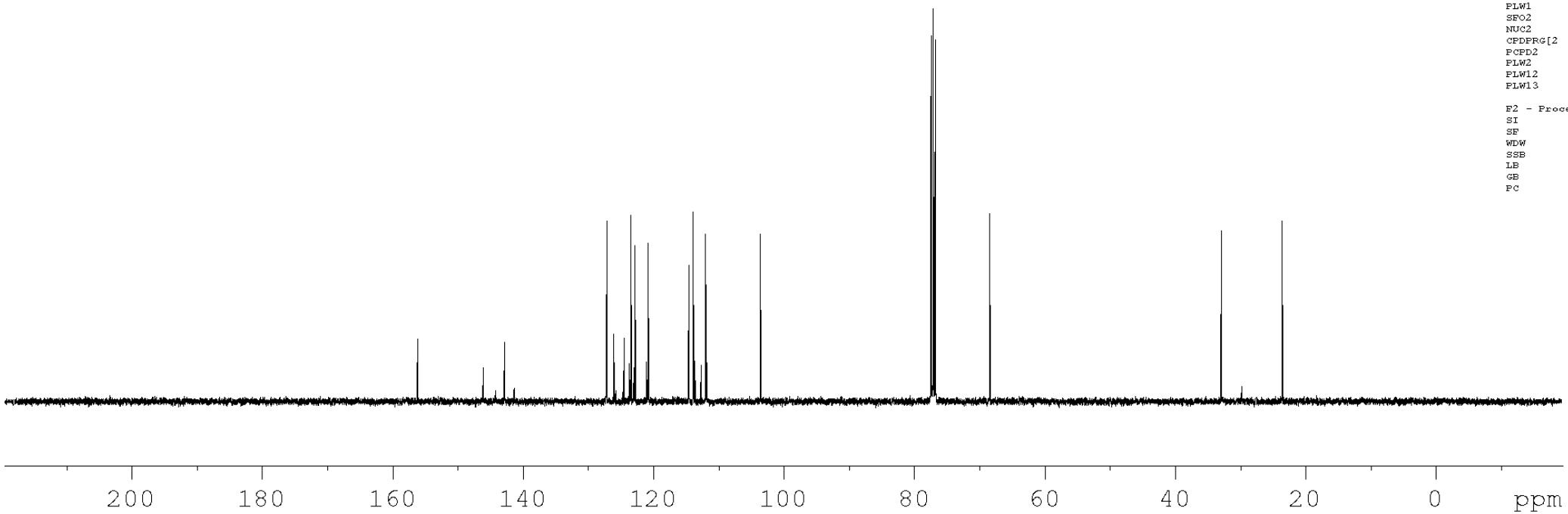
$CDCl_3$

156.226
146.165
142.836
127.204
126.098
124.561
123.501
122.850
120.845
114.617
113.958
112.028
103.624
77.469
77.151
76.834
68.483
32.940
23.489

```
Current Data Parameters
NAME      vinn-7-110-4-ialt-20230809
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20230809
Time              18.21 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  176
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               296.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6228298 MHz
NUC1                13C
P1               10.00 usec
PLW1         51.00000000 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.17465000 W

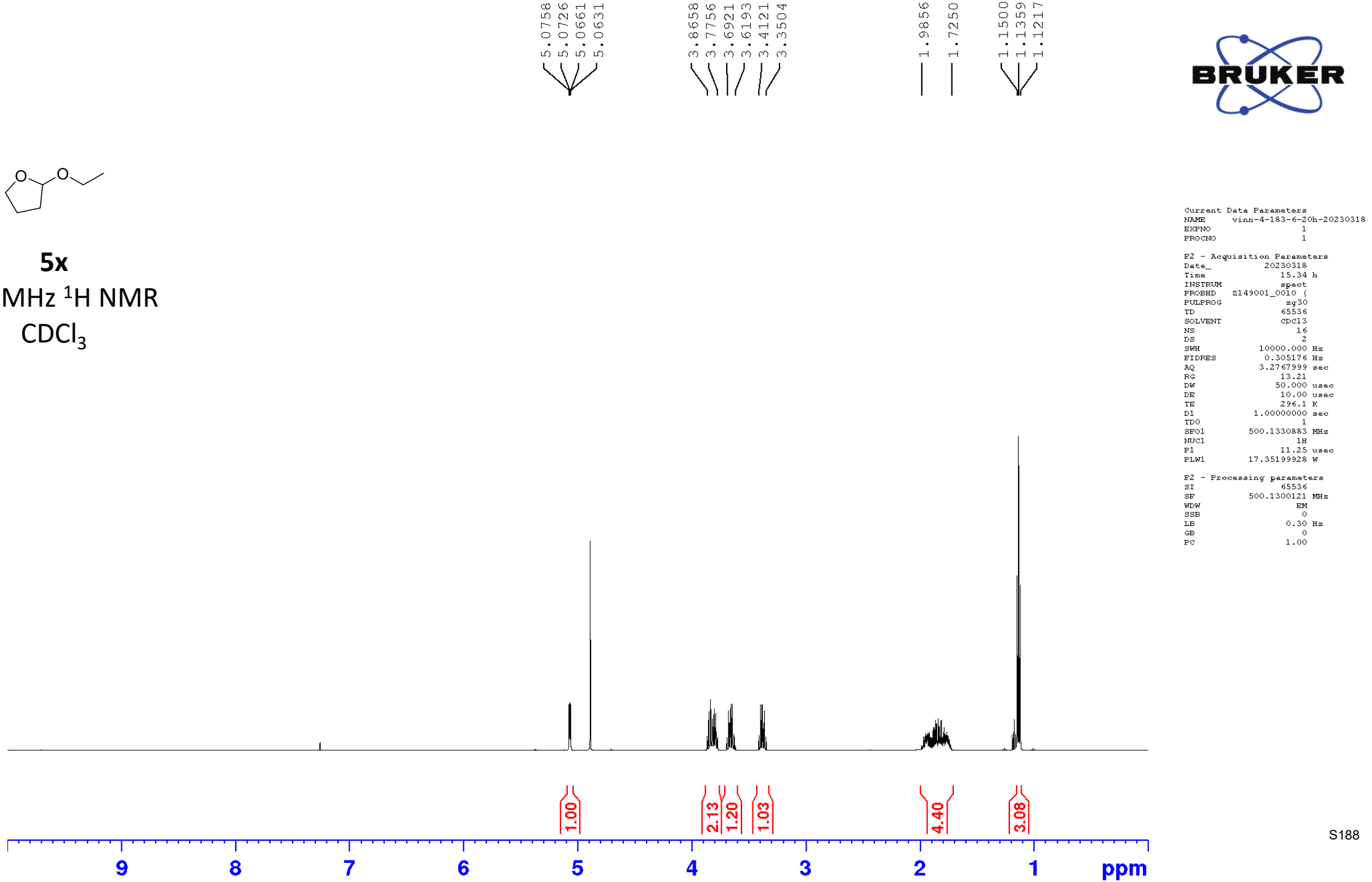
F2 - Processing parameters
SI                32768
SF           100.6127599 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```



5x

500 MHz ^{1}H NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-183-6-20h-20230318
EXPNO                1
PROCNO               1

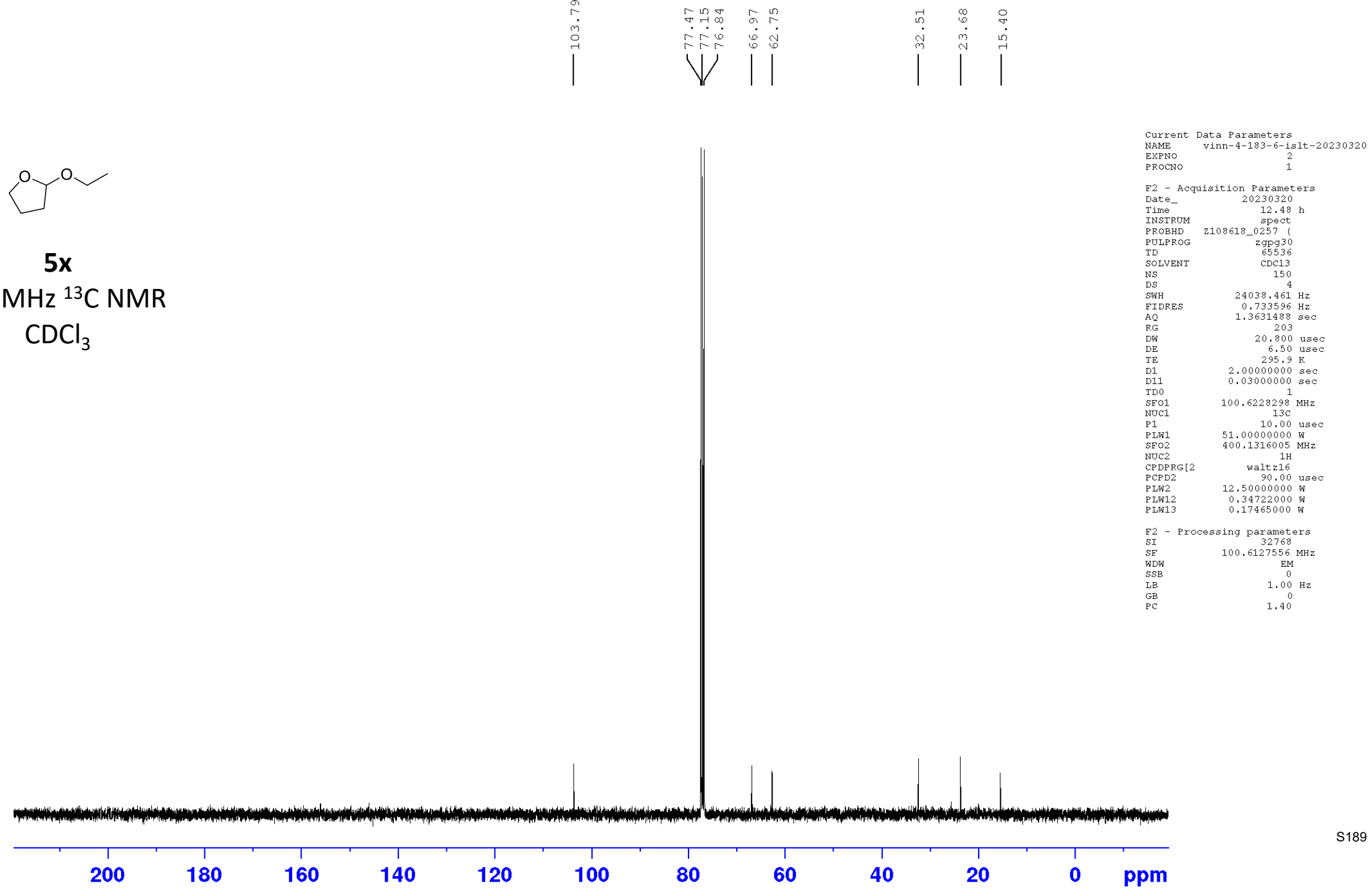
F2 - Acquisition Parameters
Date_          20230318
Time              15.34 h
INSTRUM           spect
PROBHD    Z149001_0010 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                13.21
DW              50.000 usec
DE              10.00 usec
TE              296.1 K
D1           1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                 1H
P1              11.25 usec
PLW1        17.35199928 W

F2 - Processing parameters
SI               65536
SF          500.1300121 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

5x

100 MHz ^{13}C NMR

$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-183-6-islt-20230320
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20230320
Time              12.48 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  150
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               295.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1               13C
P1               10.00 usec
PLW1        51.00000000 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.17465000 W

F2 - Processing parameters
SI                32768
SF          100.6127556 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
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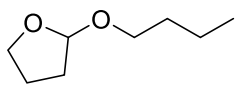
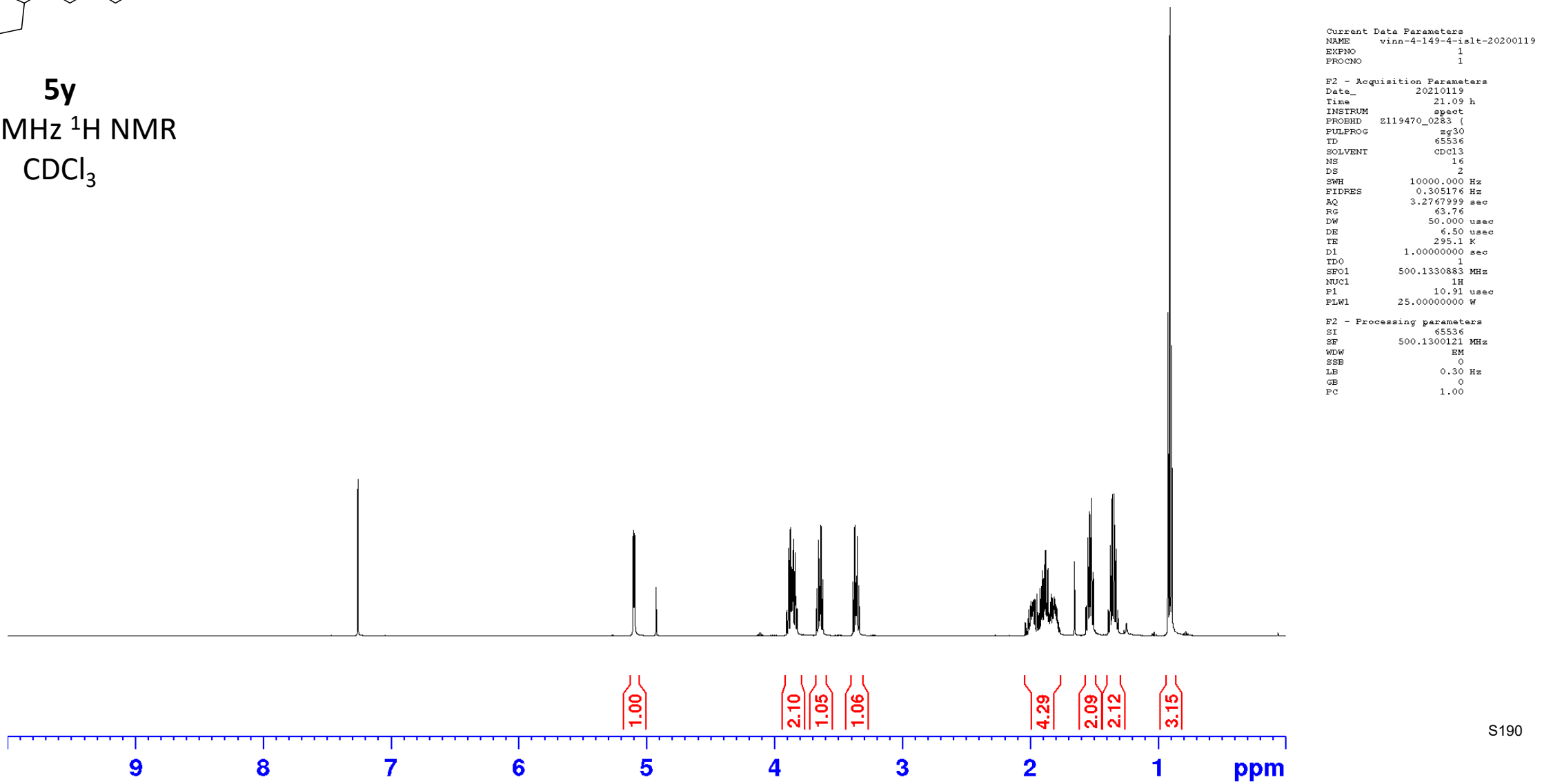


5y

500 MHz ^{1}H NMR

$CDCl_3$

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Current Data Parameters
NAME      vinn-4-149-4-islt-20200119
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210119
Time              21.09 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 63.76
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300121 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
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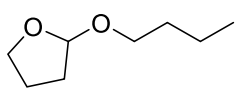
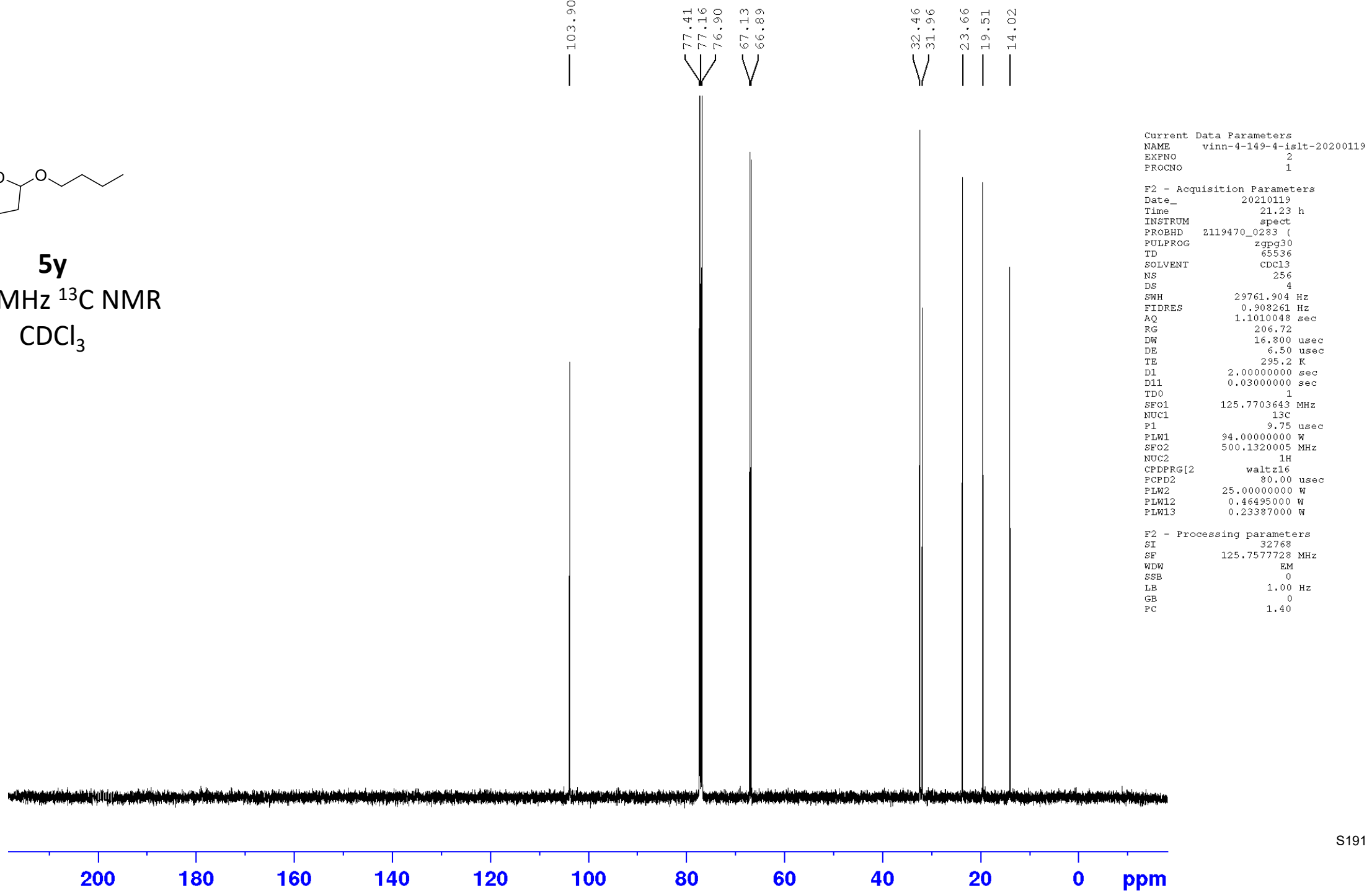


5y

125 MHz ^{13}C NMR

$CDCl_3$

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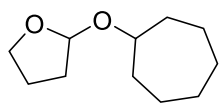
Current Data Parameters
NAME      vinn-4-149-4-islt-20200119
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210119
Time             21.23 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        25.00000000 W
PLW12        0.46495000 W
PLW13        0.23387000 W

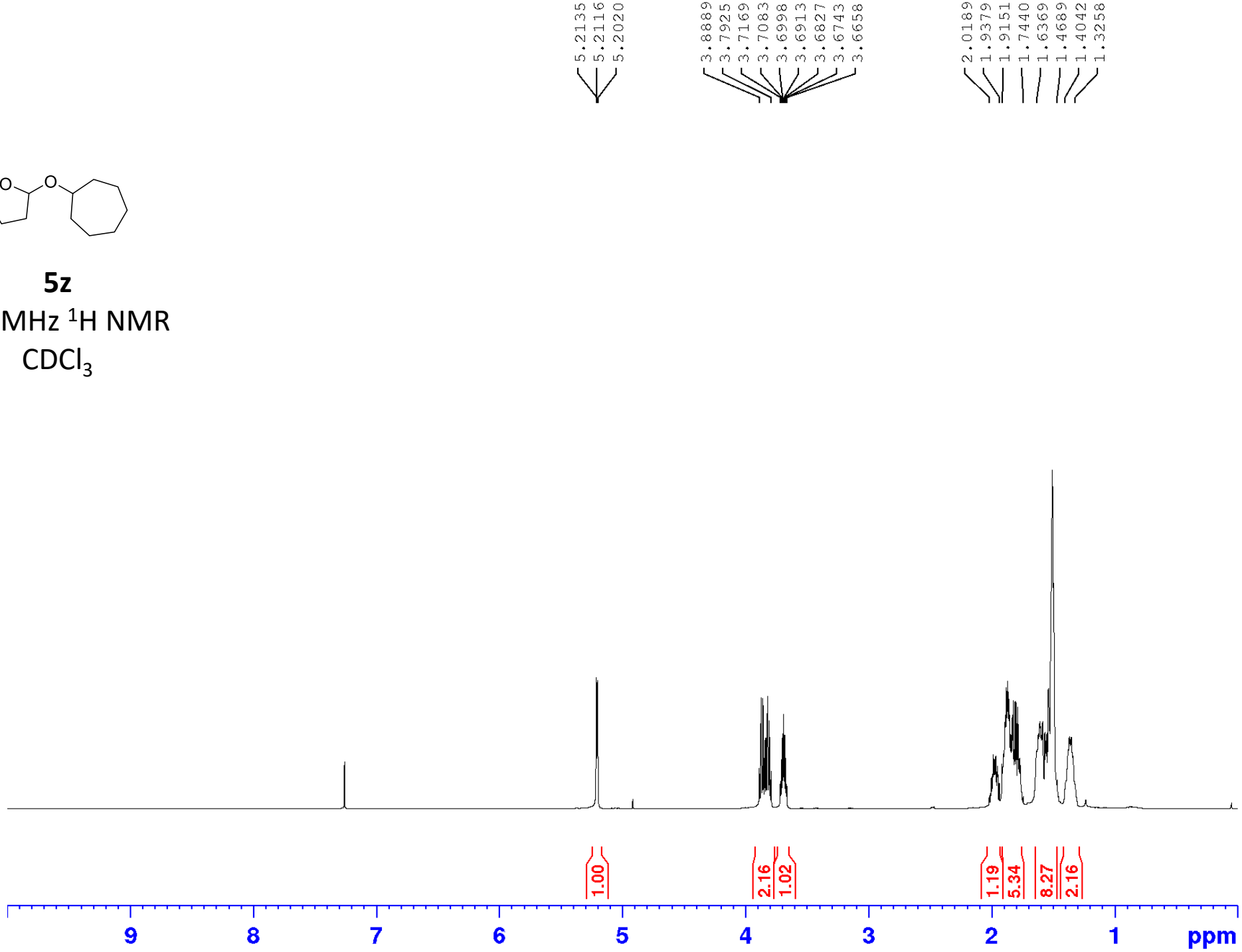
F2 - Processing parameters
SI                32768
SF          125.7577728 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



5z

500 MHz ^{1}H NMR

$CDCl_3$

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Current Data Parameters
NAME      vinn-4-149-8-islt-20200119
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210119
Time              22.02 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES           0.305176 Hz
AQ            3.2767999 sec
RG                30.85
DW               50.000 usec
DE                6.50 usec
TE               295.1 K
D1          1.00000000 sec
TD0                  1
SFO1        500.1330883 MHz
NUC1                 1H
P1               10.91 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300125 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
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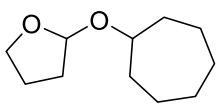
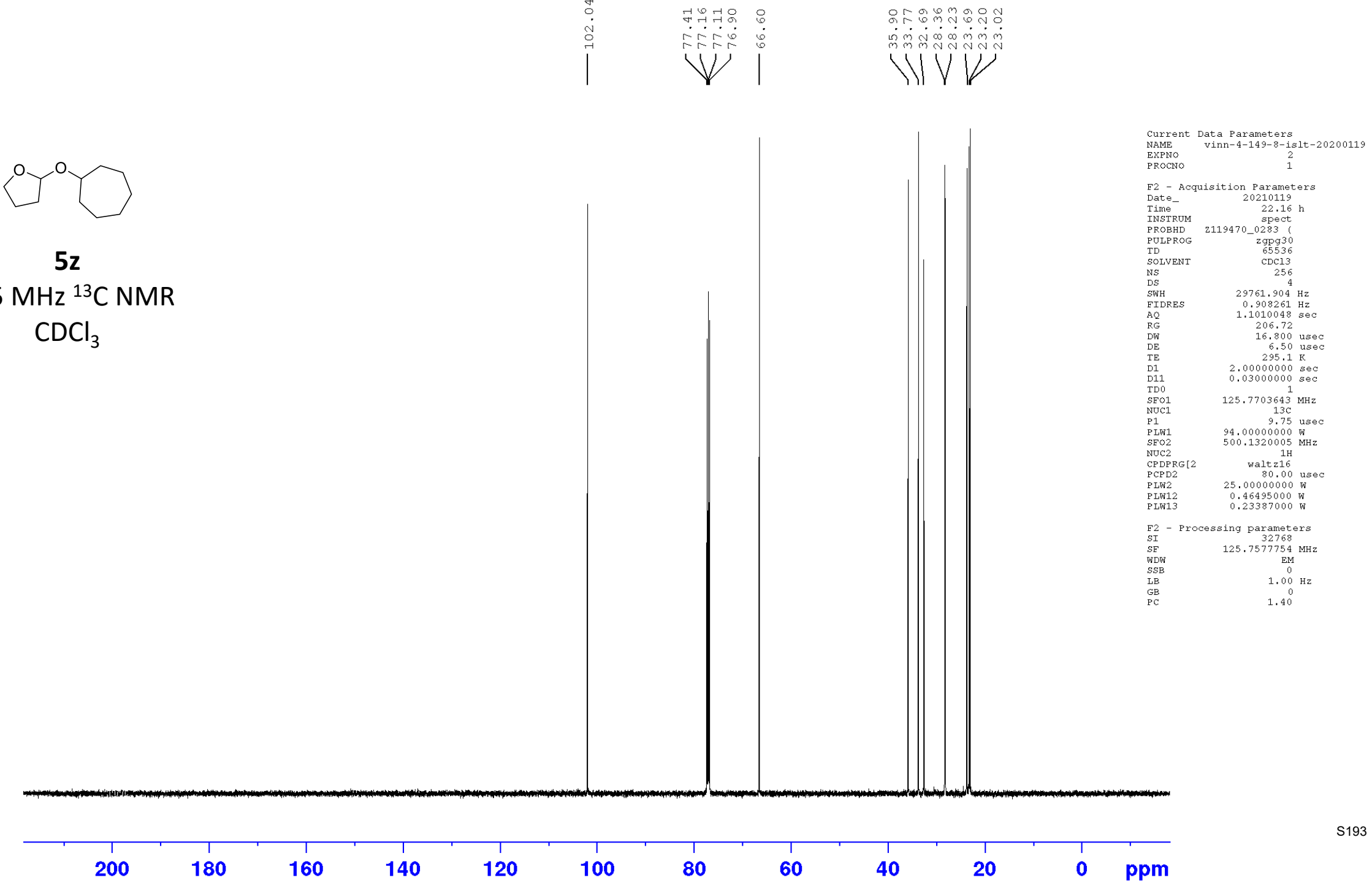


5z

125 MHz ^{13}C NMR

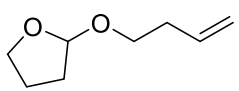
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-149-8-islt-20200119
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210119
Time              22.16 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

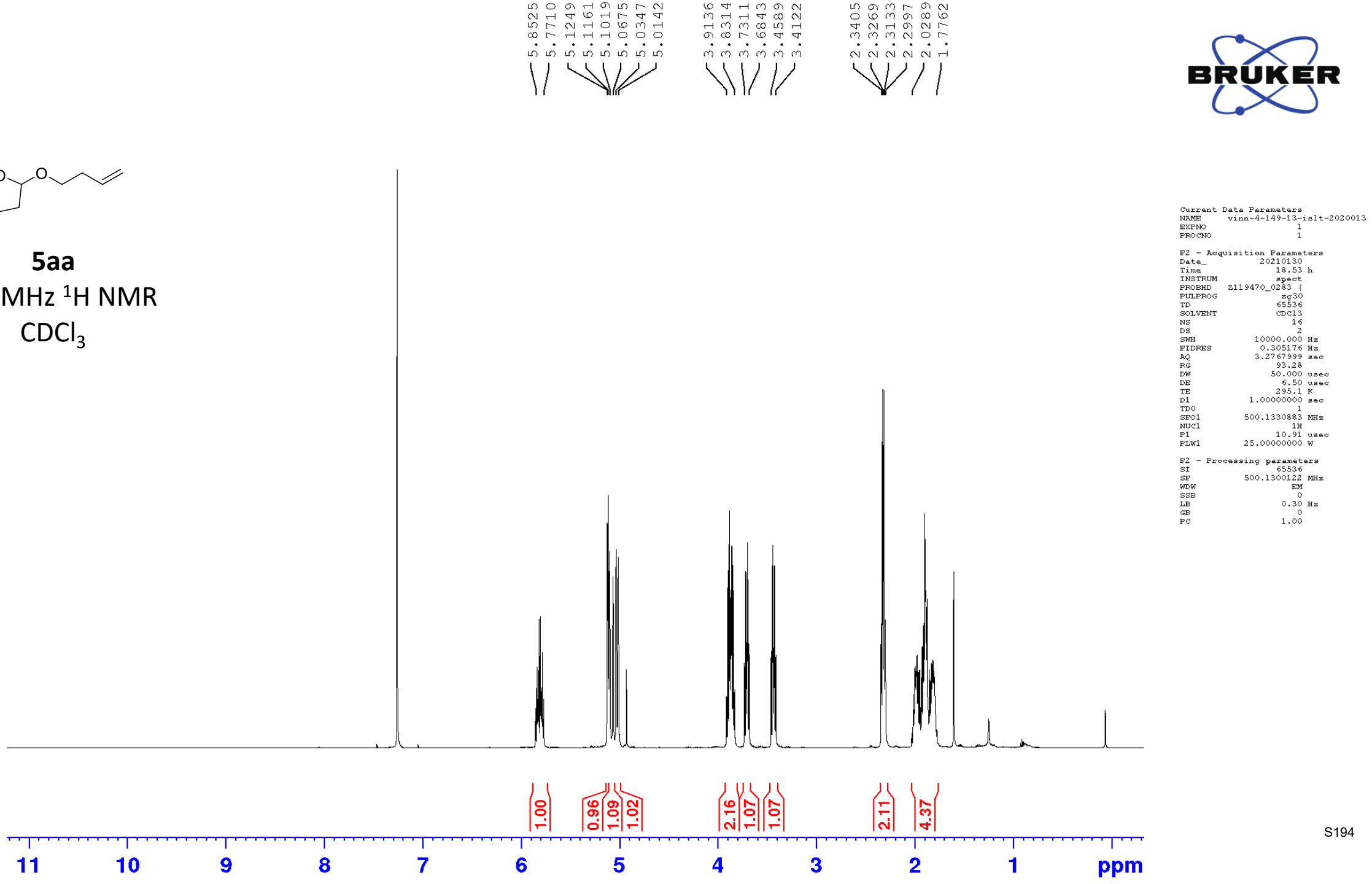
F2 - Processing parameters
SI                32768
SF          125.7577754 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```



5aa

500 MHz ^{1}H NMR

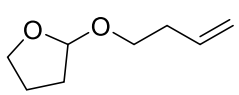
$CDCl_3$




```
Current Data Parameters
NAME      vinn-4-149-13-islt-2020013
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210130
Time              18.53 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG                93.28
DW              50.000 usec
DE               6.50 usec
TE              295.1 K
D1           1.00000000 sec
TD0                  1
SFO1       500.1330883 MHz
NUC1               1H
P1               10.91 usec
PLW1       25.00000000 W

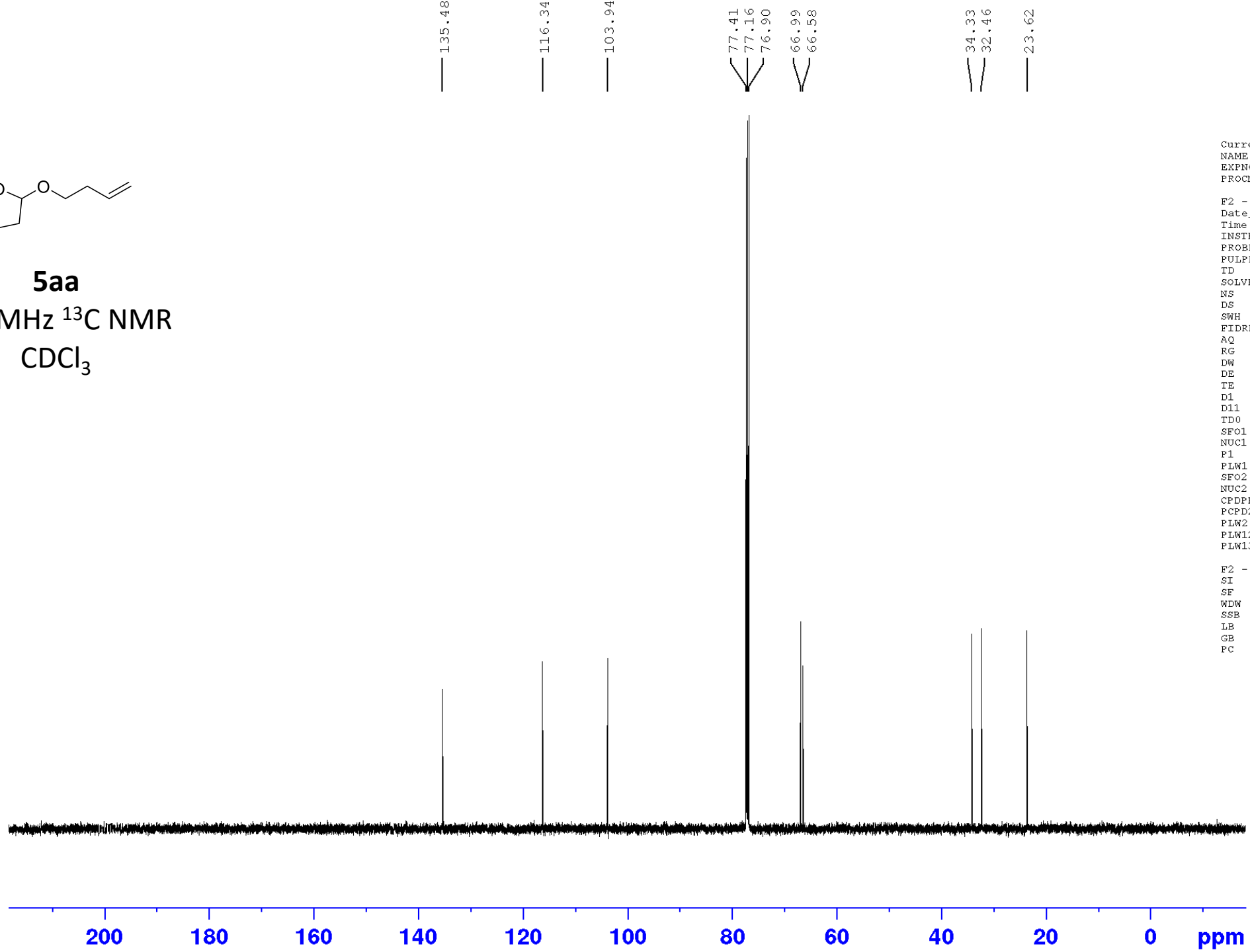
F2 - Processing parameters
SI               65536
SF         500.1300122 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```



5aa

125 MHz ^{13}C NMR

$CDCl_3$

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Current Data Parameters
NAME      vinn-4-149-13-islt-20200130
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210130
Time              19.00 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT             CDCl3
NS                  128
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577727 MHz
WDW                 EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```
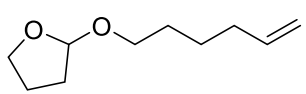
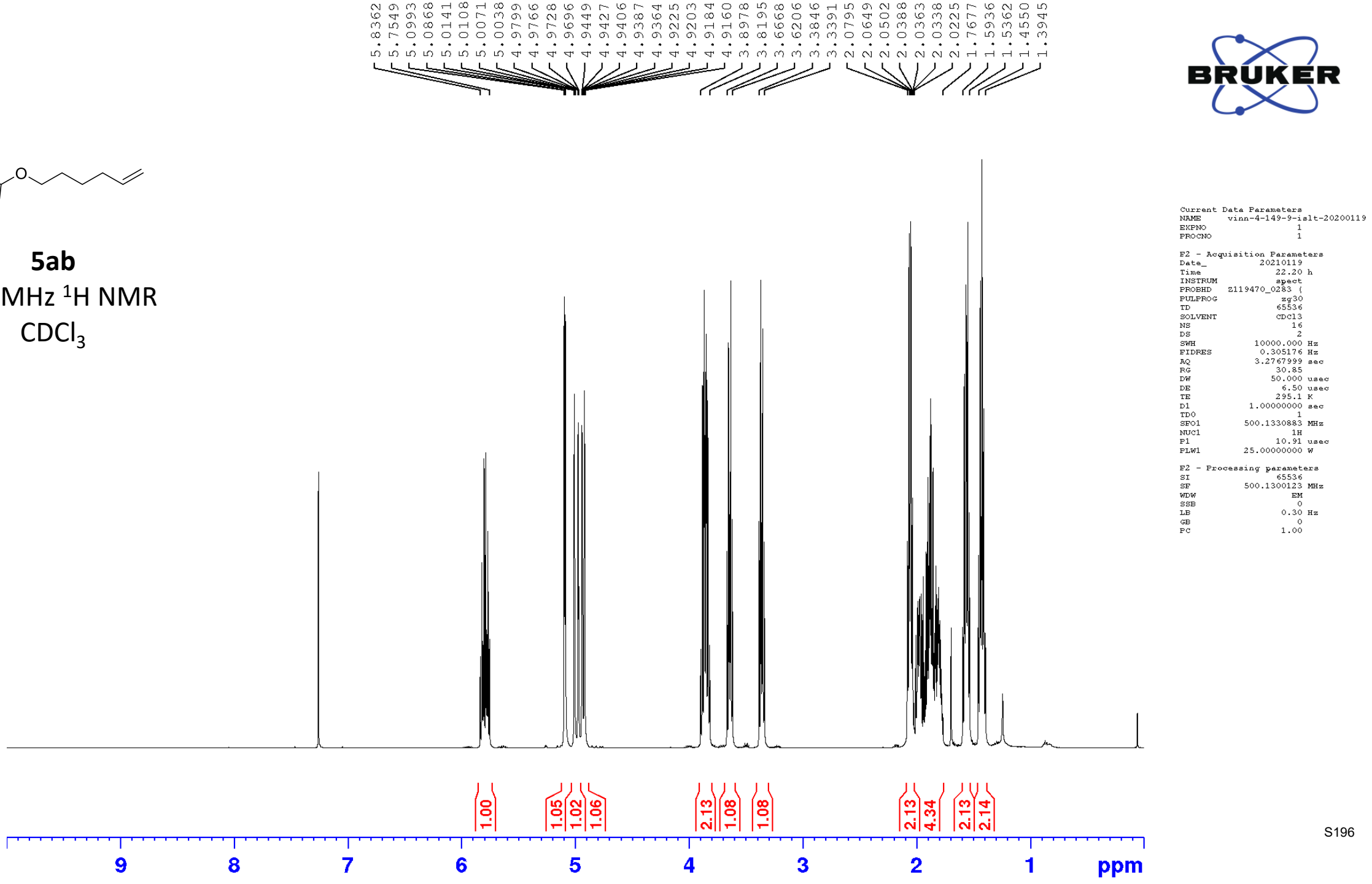



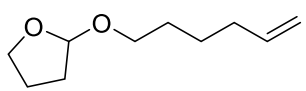
5ab

500 MHz ^{1}H NMR

$CDCl_3$



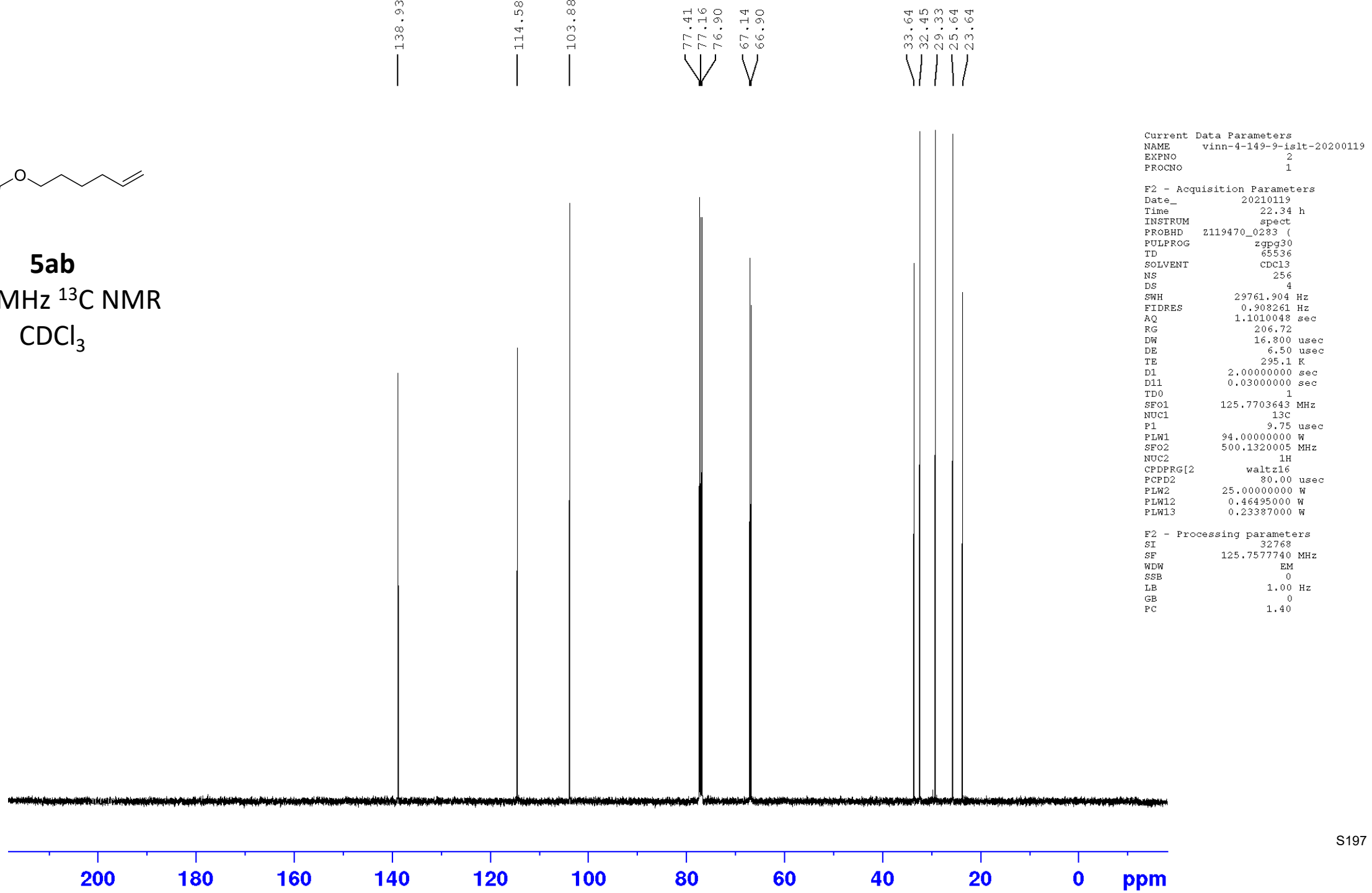

```
Current Data Parameters
NAME      vinn-4-149-9-islt-20200119
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210119
Time              22.20 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ              3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                 6.50 usec
TE                295.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300123 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



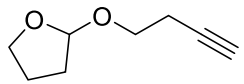
5ab

125 MHz ^{13}C NMR

$CDCl_3$



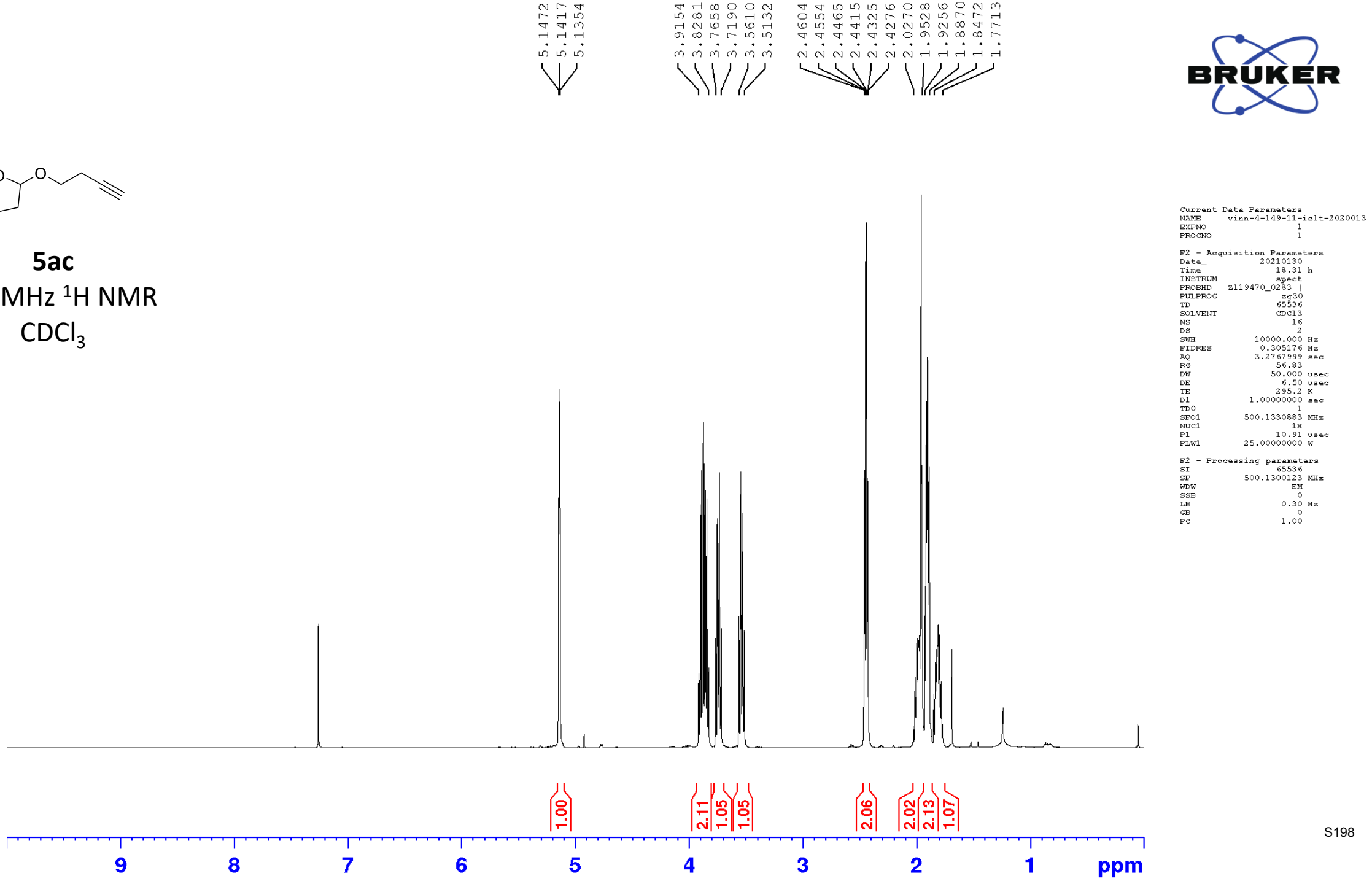

```
Current Data Parameters
NAME      vinn-4-149-9-islt-20200119
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210119
Time              22.34 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577740 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```



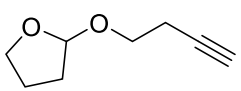
5ac

500 MHz ^{1}H NMR

$CDCl_3$



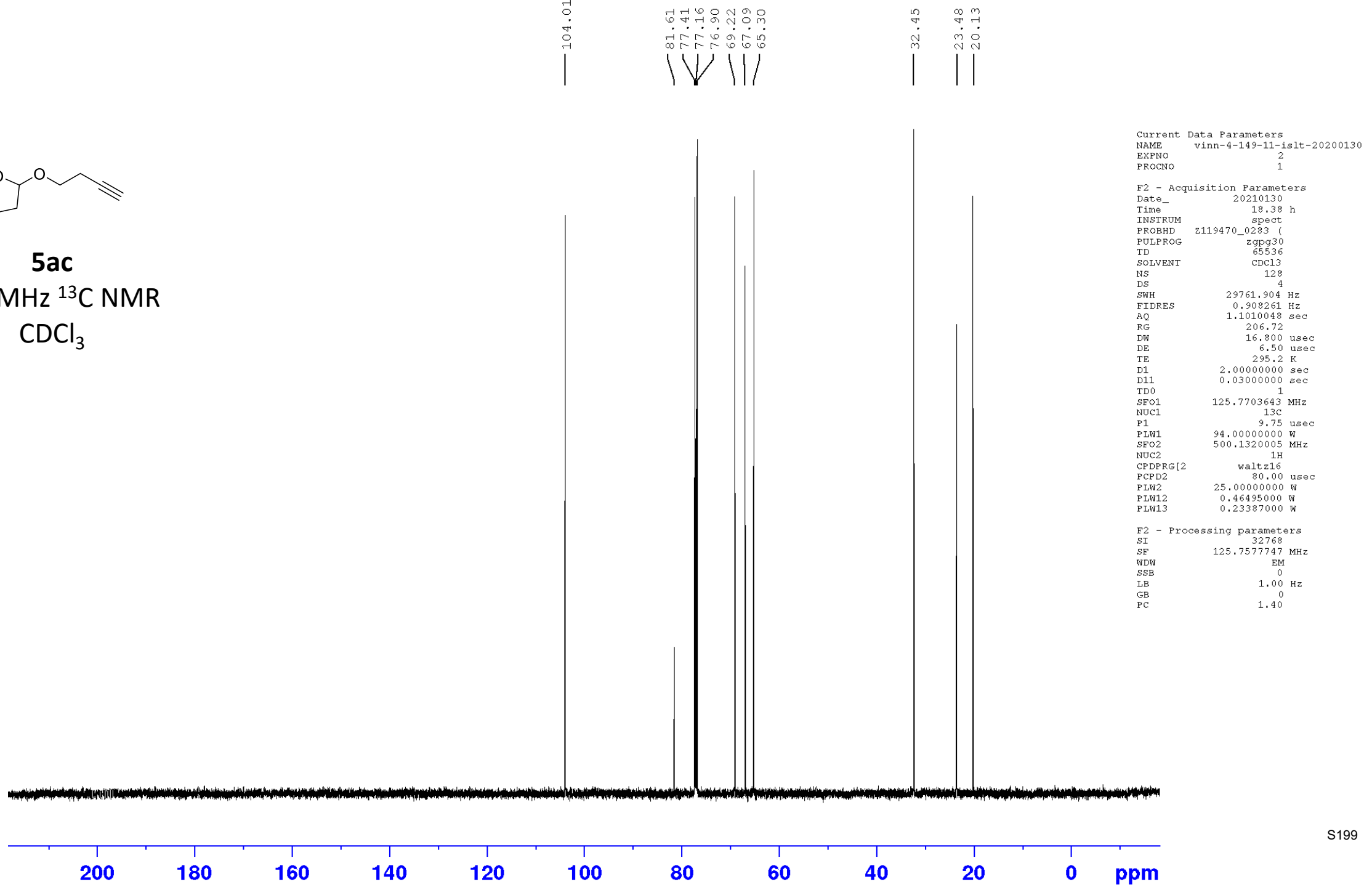

```
Current Data Parameters
NAME      vinn-4-149-11-islt-2020013
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210130
Time              18.31 h
INSTRUM             spect
PROBHD   Z119470_0283 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                 56.83
DW                50.000 usec
DE                 6.50 usec
TE                295.2 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                10.91 usec
PLW1          25.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300123 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



5ac

125 MHz ^{13}C NMR

$CDCl_3$

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Current Data Parameters
NAME      vinn-4-149-11-islt-20200130
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210130
Time              18.38 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  128
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577747 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
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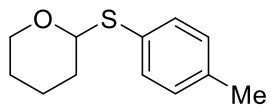
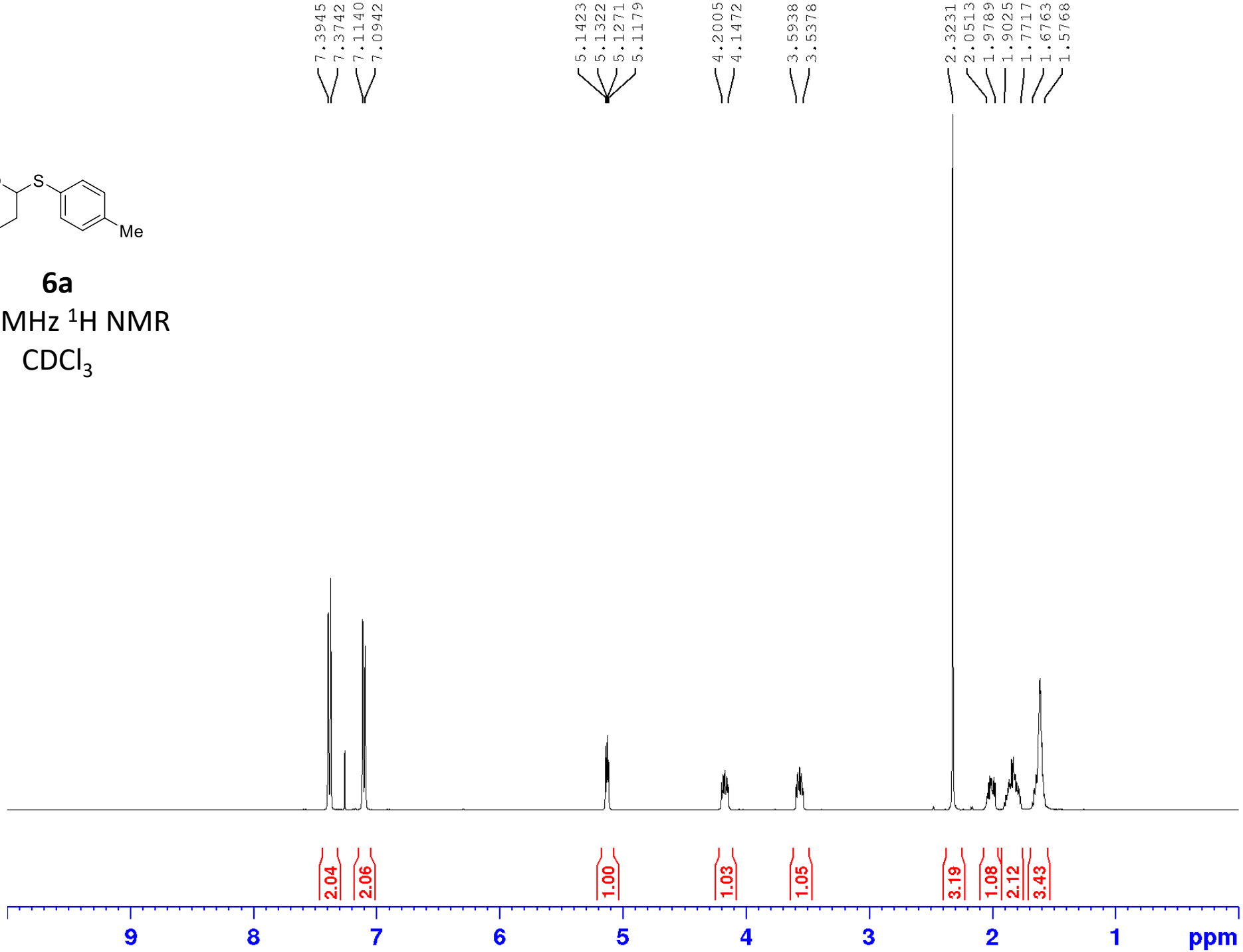


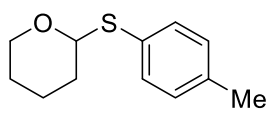
6a

400 MHz ^{1}H NMR

$CDCl_3$



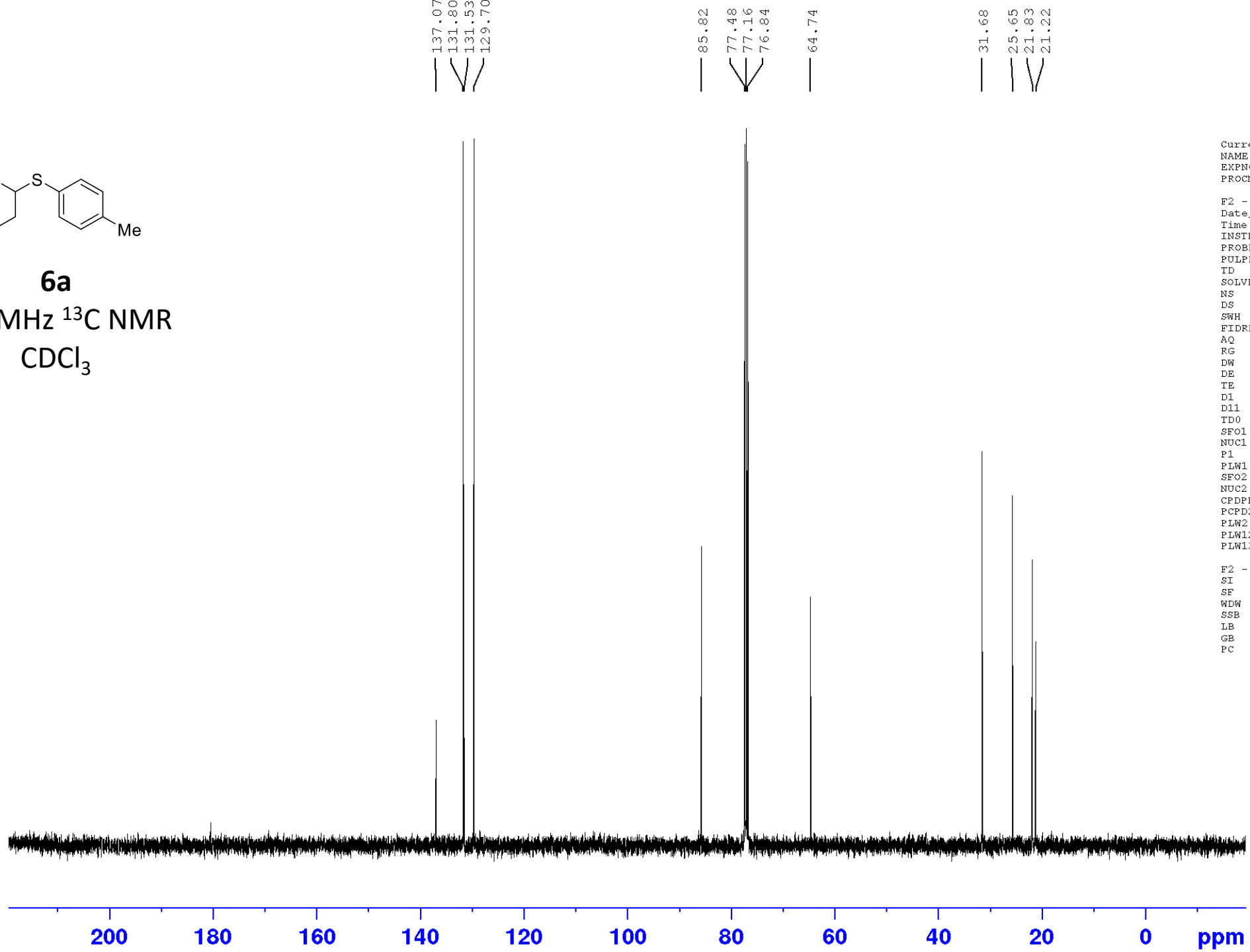

```
Current Data Parameters
NAME      Andy-1-181-1-islt-2-20220812
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220812
Time              18.56 h
INSTRUM             spect
PROBHD   5108618_0257 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.244532 Hz
AQ              4.0894465 sec
RG                   114
DW                62.400 usec
DE                 6.50 usec
TE                295.6 K
D1             1.00000000 sec
TD0                    1
SFO1          400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1          12.50000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300098 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



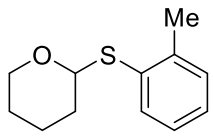
6a

100 MHz ^{13}C NMR

$CDCl_3$



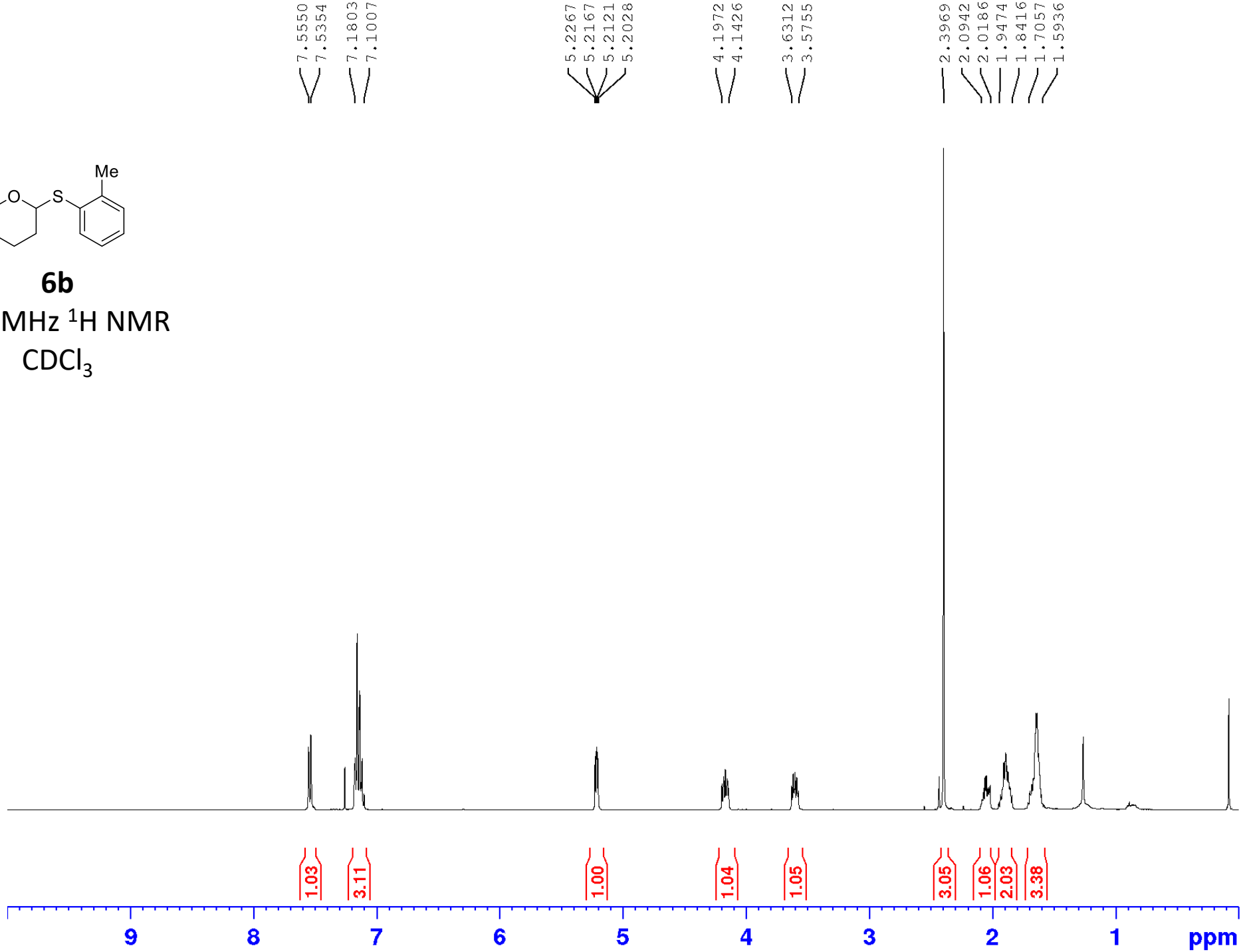

```
Current Data Parameters
NAME      Andy-1-181-1-islt-2-20220812
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220812
Time              19.04 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  102
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1               10.00 usec
PLW1        51.00000000 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.17465000 W

F2 - Processing parameters
SI                32768
SF          100.6127579 MHz
WDW                 EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```



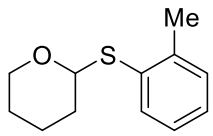
6b

400 MHz ^{1}H NMR

$CDCl_3$



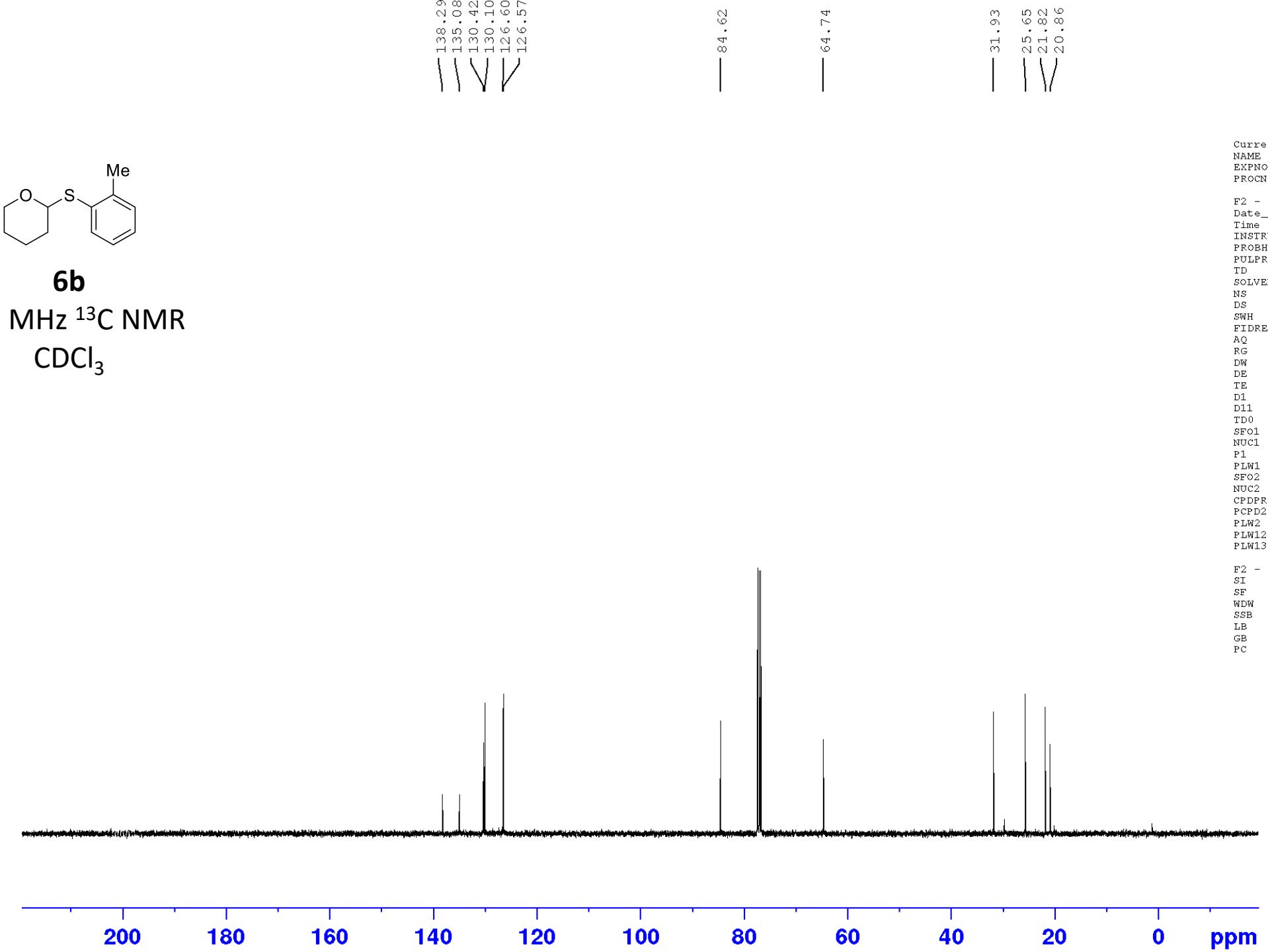

```
Current Data Parameters
NAME      Andy-181-4-islt-20220817
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
Date_          20220817
Time              19.08 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                90.5
DW              62.400 usec
DE               6.50 usec
TE              295.6 K
D1           1.00000000 sec
TD0                  1
SFO1        400.1324708 MHz
NUC1               1H
P1              15.00 usec
PLW1        12.50000000 W

F2 - Processing parameters
SI               65536
SF          400.1300108 MHz
WDW                EM
SSB                 0
LB              0.30 Hz
GB                  0
PC                1.00
```



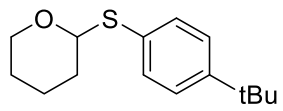
6b

100 MHz ^{13}C NMR

$CDCl_3$



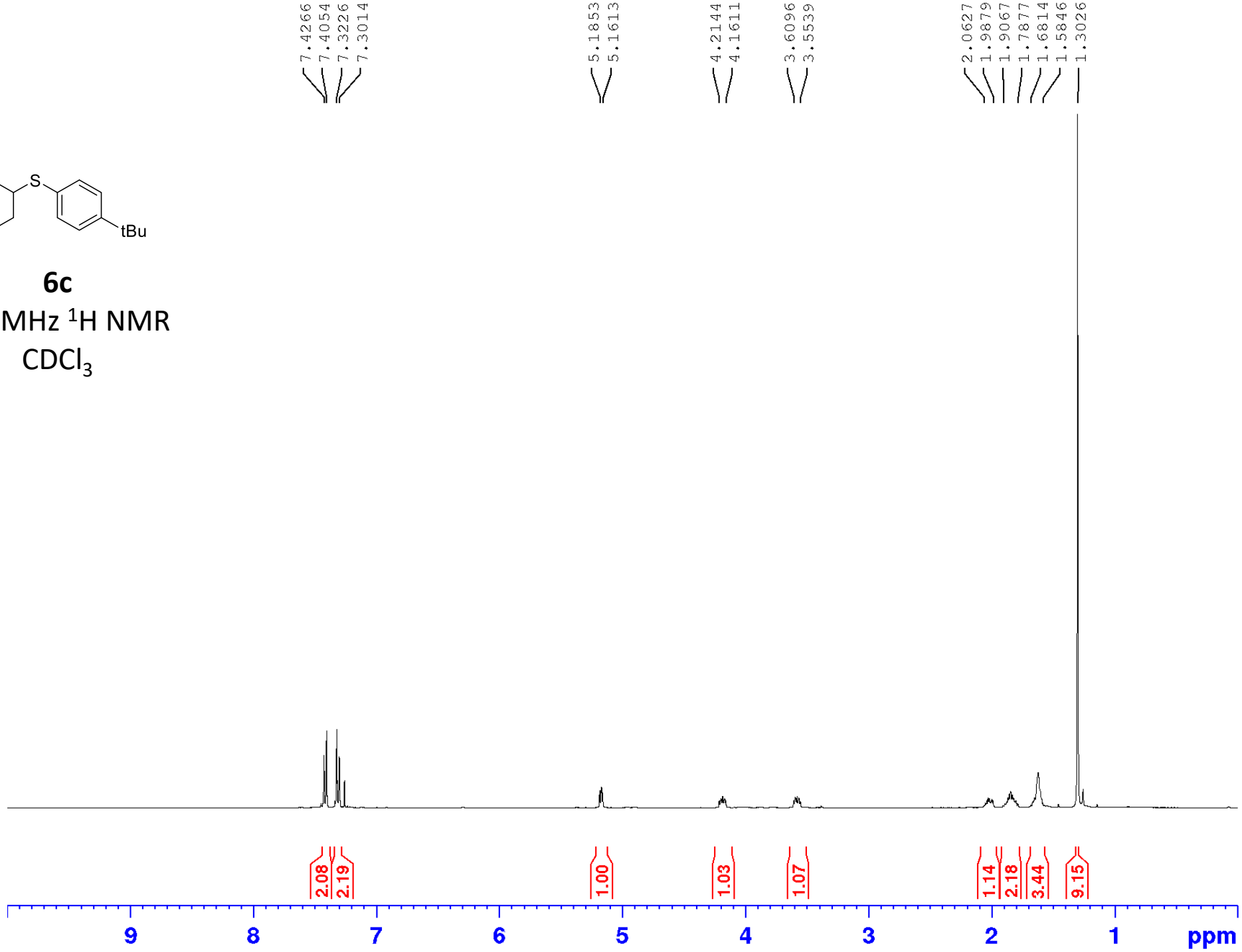

```
Current Data Parameters
NAME      Andy-181-4-islt-20220817
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220817
Time              19.17 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  106
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               296.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1               10.00 usec
PLW1        51.00000000 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.17465000 W

F2 - Processing parameters
SI                32768
SF          100.6127582 MHz
WDW                 EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



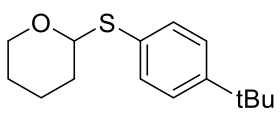
6c

400 MHz ^{1}H NMR

$CDCl_3$



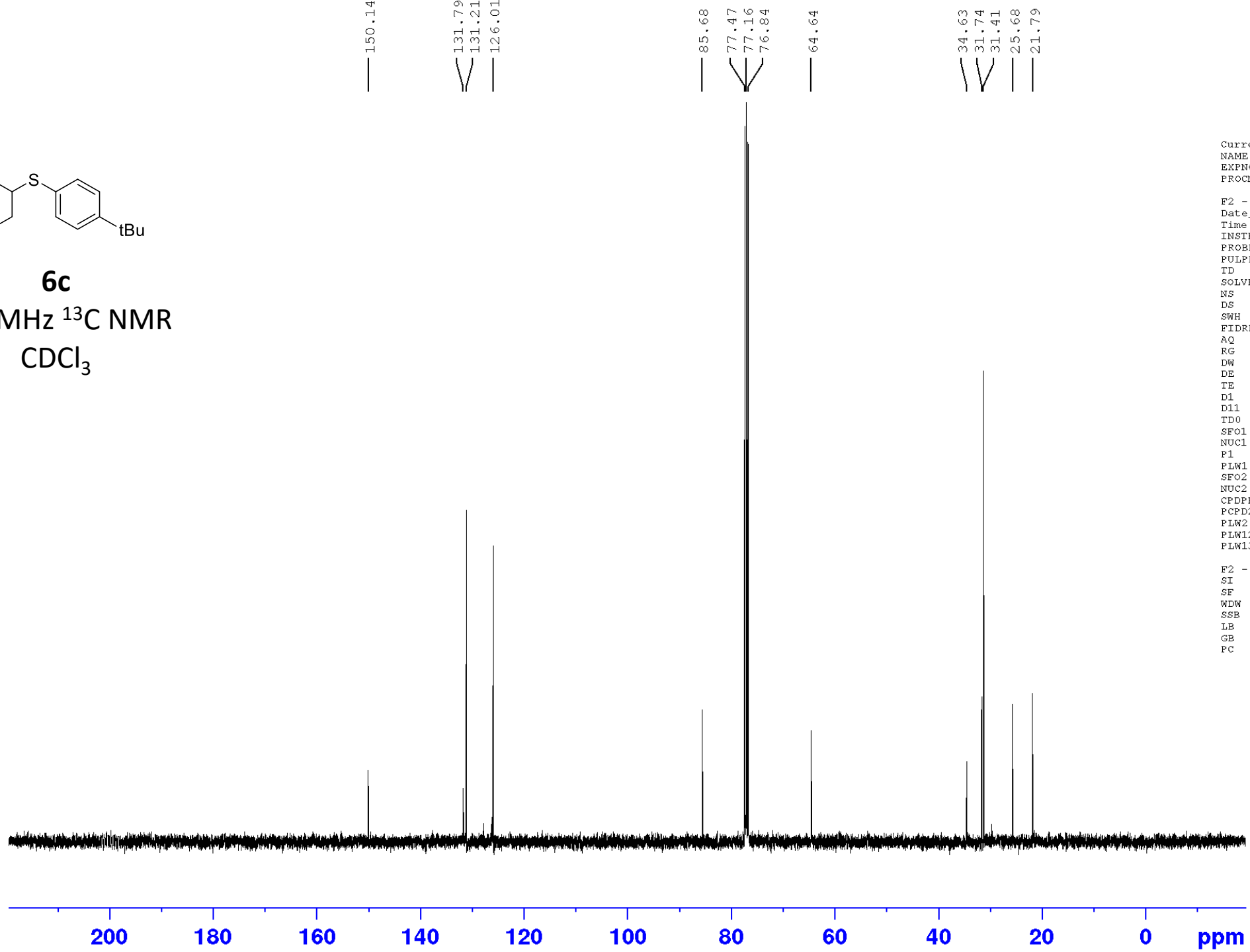

```
Current Data Parameters
NAME      Andy-181-3-islt-20220817
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20220817
Time              18.55 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                 114
DW              62.400 usec
DE               6.50 usec
TE              295.5 K
D1           1.00000000 sec
TD0                  1
SFO1        400.1324708 MHz
NUC1               1H
P1              15.00 usec
PLW1        12.50000000 W

F2 - Processing parameters
SI               65536
SF          400.1300108 MHz
WDW                EM
SSB                 0
LB              0.30 Hz
GB                  0
PC               1.00
```



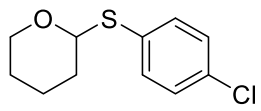
6c

100 MHz ^{13}C NMR

$CDCl_3$



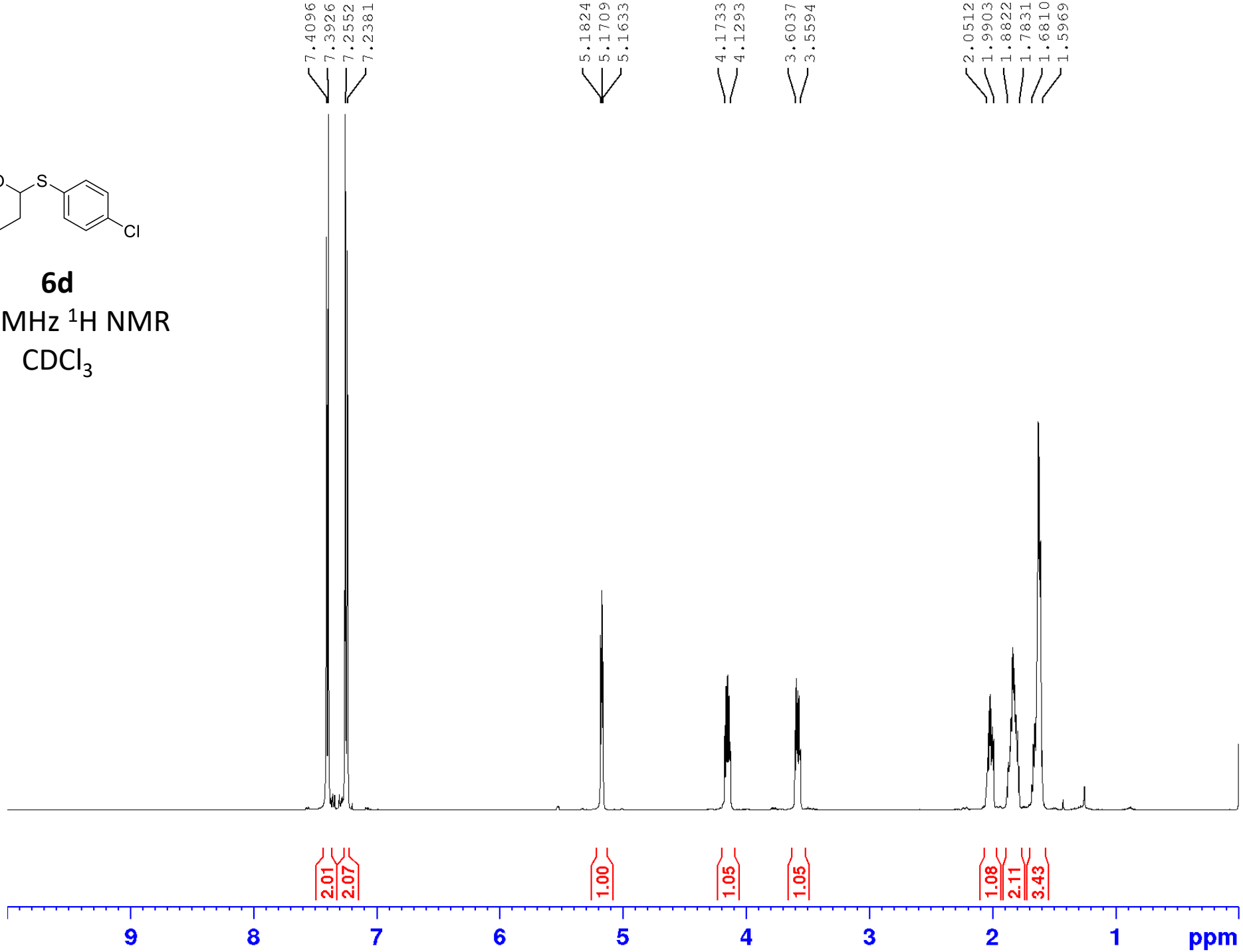

```
Current Data Parameters
NAME      Andy-181-3-islt-20220817
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220817
Time              19.03 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  104
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               296.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1               10.00 usec
PLW1        51.00000000 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.17465000 W

F2 - Processing parameters
SI                32768
SF          100.6127564 MHz
WDW                 EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```



6d

500 MHz ^{1}H NMR

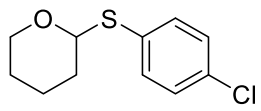
$CDCl_3$



Current Data Parameters
NAME vinn-4-190-4-ialt-20230104
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230104
Time 15.31 h
INSTRUM spect
PROBHD Z119470_0283 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 63.76
DW 50.000 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330883 MHz
NUC1 1H
P1 10.91 usec
PLW1 25.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



6d

125 MHz ^{13}C NMR

$CDCl_3$

133.99
132.92
132.31
129.01
85.44
77.41
77.16
76.90
64.58
31.56
25.56
21.65

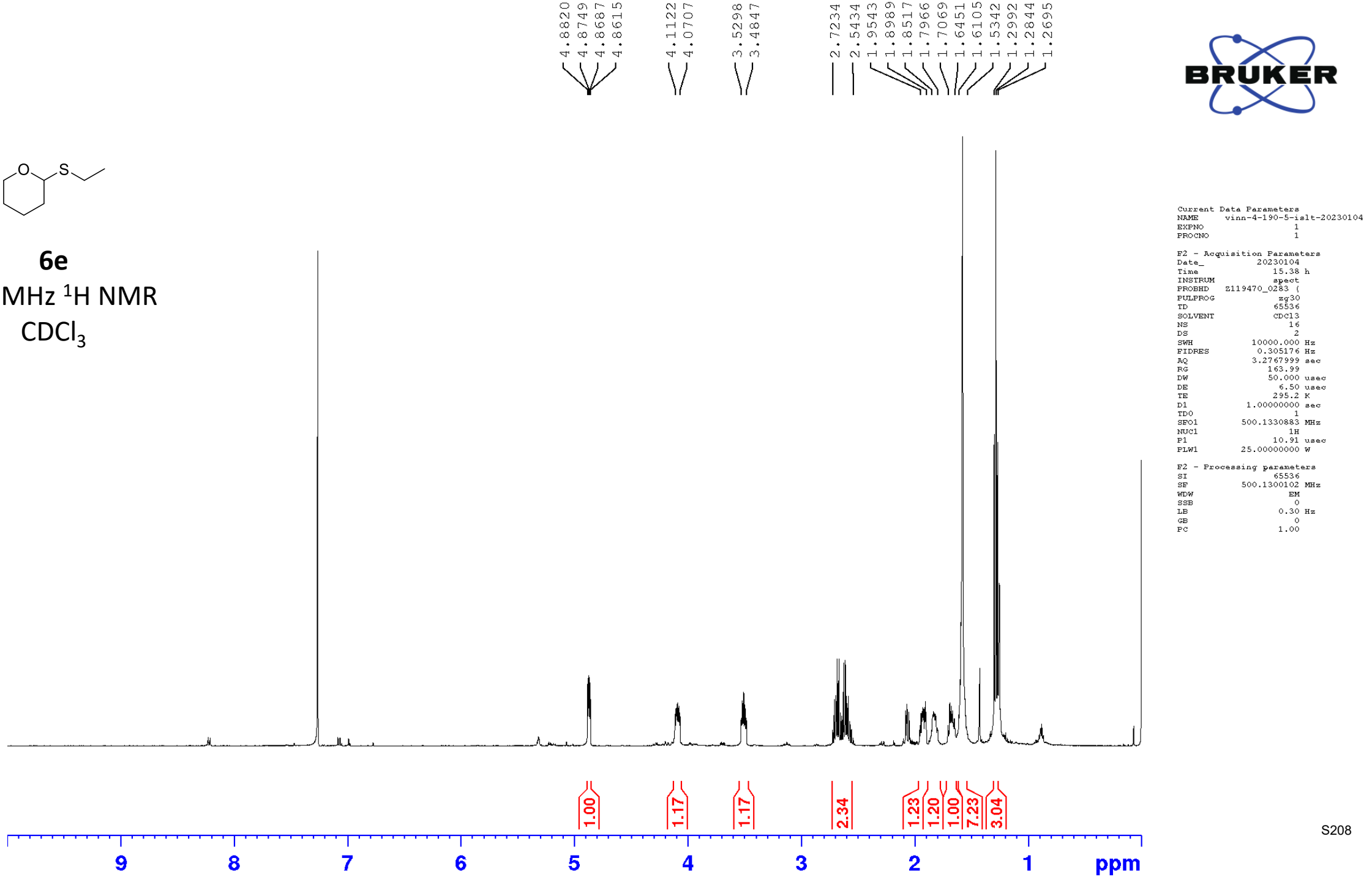
```
Current Data Parameters
NAME      vinn-4-190-4-islt-20230104
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20230104
Time              15.34 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   50
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               186.15
DW               16.800 usec
DE                6.50 usec
TE               295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                9.75 usec
PLW1         94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2         25.00000000 W
PLW12         0.46495000 W
PLW13         0.23387000 W

F2 - Processing parameters
SI                32768
SF          125.7577768 MHz
WDW                EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

200 180 160 140 120 100 80 60 40 20 0 ppm

6e

500 MHz ^{1}H NMR

$CDCl_3$

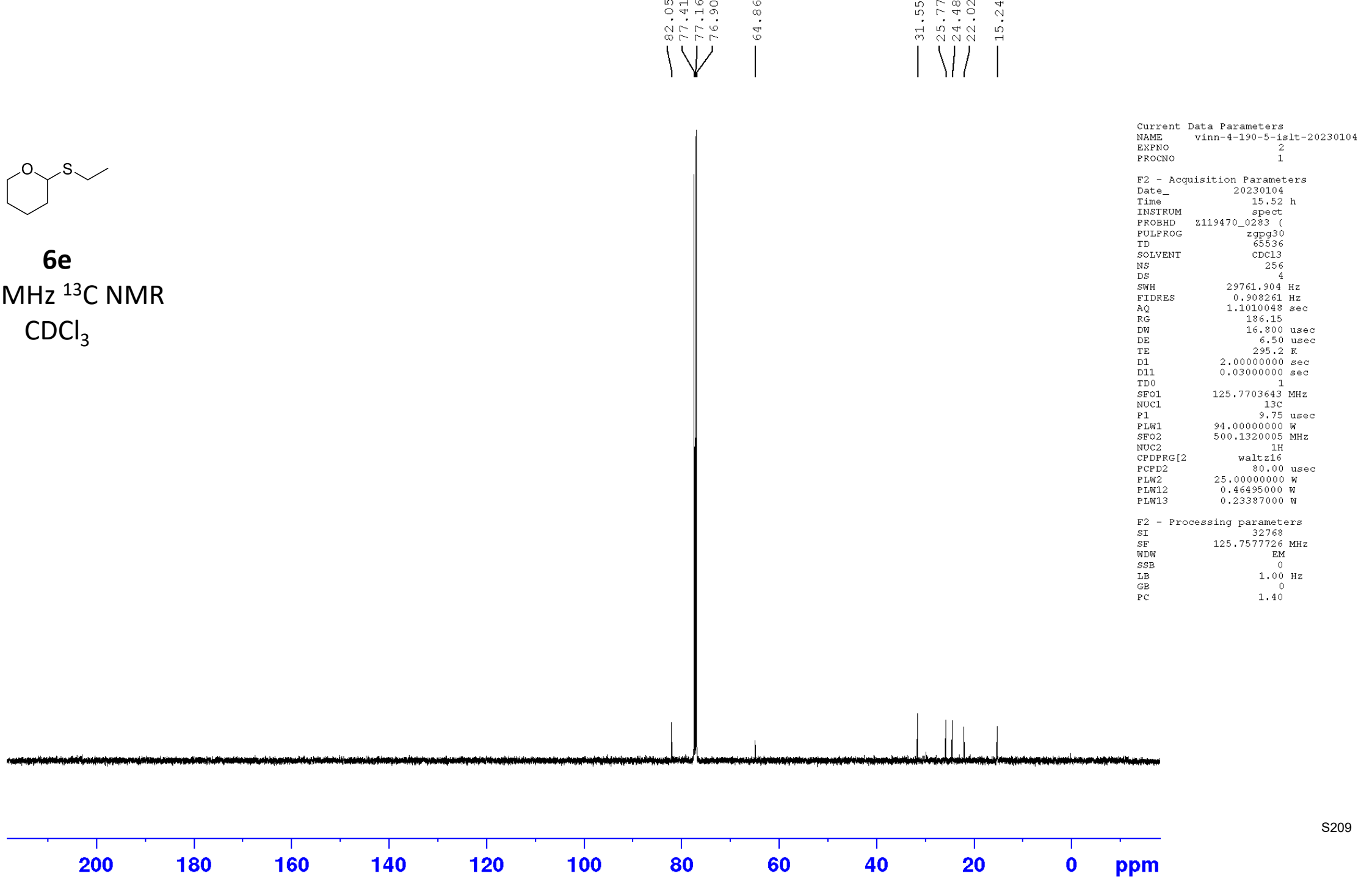


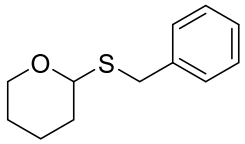

```
Current Data Parameters
NAME      vinn-4-190-5-islt-20230104
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20230104
Time              15.38 h
INSTRUM           spect
PROBHD    Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG               163.99
DW               50.000 usec
DE                6.50 usec
TE               295.2 K
D1            1.00000000 sec
TD0                  1
SFO1          500.1330883 MHz
NUC1                 1H
P1               10.91 usec
PLW1         25.00000000 W

F2 - Processing parameters
SI               65536
SF          500.1300102 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

6e

125 MHz ^{13}C NMR

$CDCl_3$

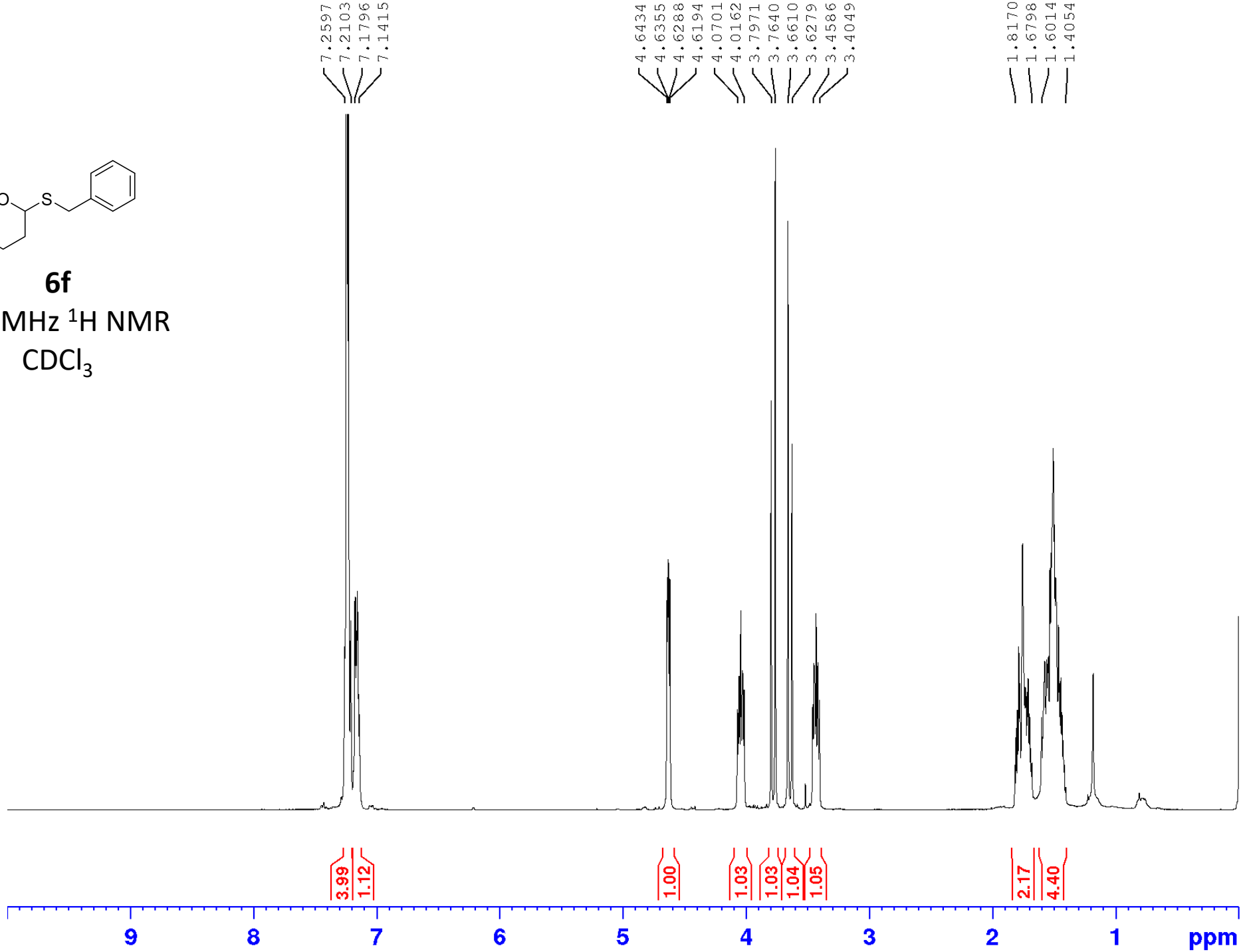




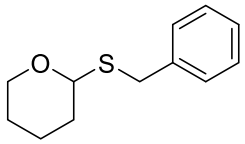
6f

400 MHz ^{1}H NMR

$CDCl_3$



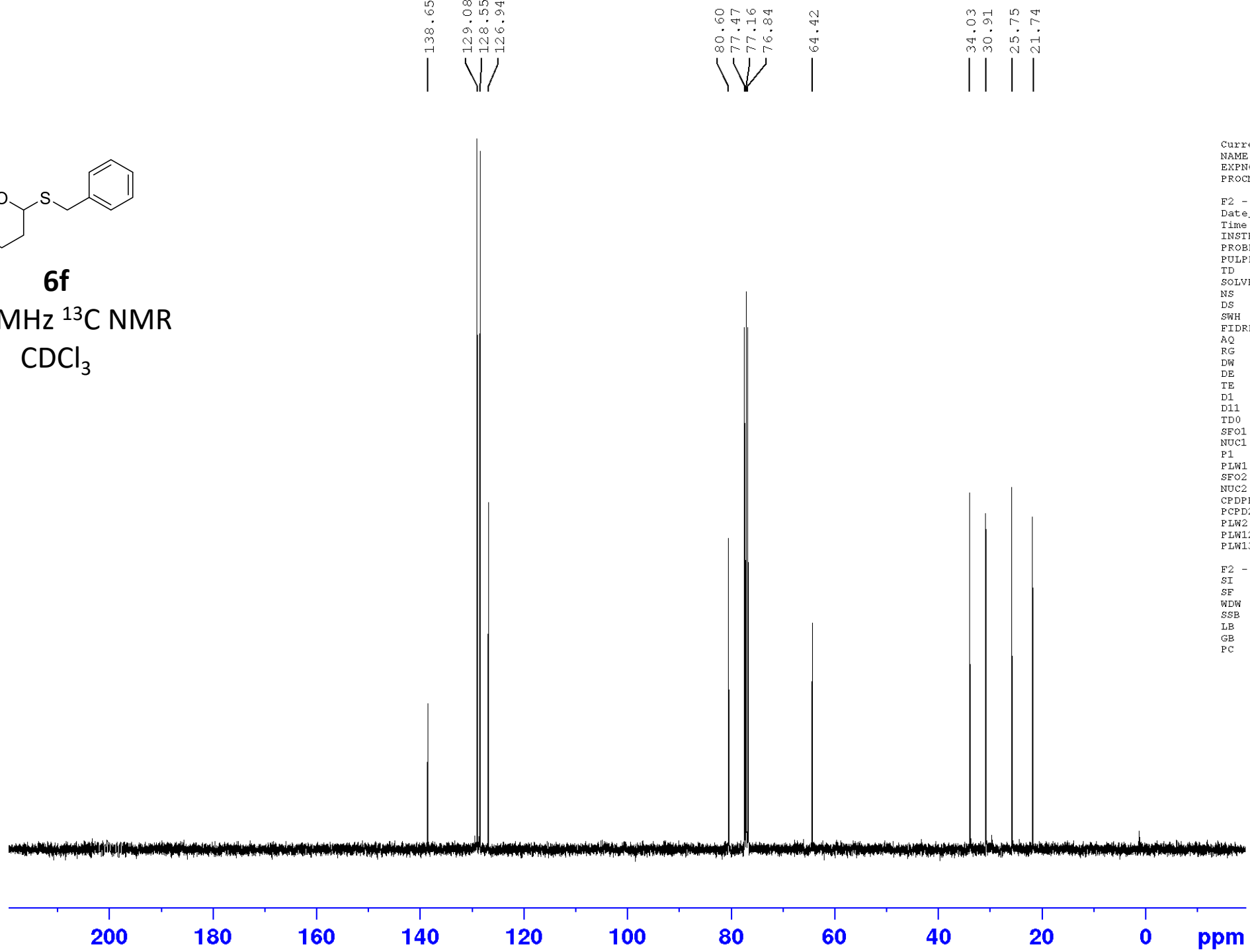

```
Current Data Parameters
NAME      Andy-181-5-islt-20220817
EXPNO                6
PROCNO               1

F2 - Acquisition Parameters
Date_          20220817
Time              19.22 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                80.6
DW              62.400 usec
DE               6.50 usec
TE              295.6 K
D1           1.00000000 sec
TD0                  1
SFO1        400.1324708 MHz
NUC1               1H
P1              15.00 usec
PLW1        12.50000000 W

F2 - Processing parameters
SI               65536
SF          400.1300429 MHz
WDW                EM
SSB                 0
LB              0.30 Hz
GB                  0
PC                1.00
```



6f

100 MHz ^{13}C NMR

$CDCl_3$




```
Current Data Parameters
NAME      Andy-181-5-islt-20220817
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220817
Time              19.30 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   99
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE                296.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1               10.00 usec
PLW1        51.00000000 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.17465000 W

F2 - Processing parameters
SI                32768
SF          100.6127601 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```