Supporting information

Triethyl Amine as an Effective Reducing Agent for Sulfoxide Deoxygenation

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Content

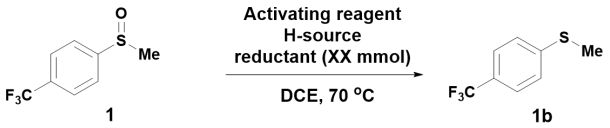
1. Materials and Methods

All reactions were carried out under an argon atmosphere with dry solvents under anhydrous conditions, unless otherwise noted. All the chemicals were purchased commercially, and used without further purification. Anhydrous Et_3N were distilled from calcium hydride. Extra dry 1,2-dichloroethane (DCE), dichloromethane (DCM) and acetonitrile (MeCN) were purchased from J&K Scientific. Thin-layer chromatography (TLC) was conducted with 0.25 mm Tsingdao silica gel plates (60F-254) and visualized by exposure to UV light (254 nm). Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.0400.063 mm). Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. ^1H NMR (400 MHz, and 600 MHz) and ^{13}C NMR (101 MHz, 151 MHz) spectra were recorded on a Bruker AV III HD spectrometer, and were reported in terms of chemical shift relative to residual $CDCl_3$ (δ 7.26 and δ 77.0 ppm, respectively). Data for ^1H NMR spectra are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Abbreviations are used as follows: s = singlet, bs = broad singlet, d = doublet, t = triplet, q = quartet, m = complex multiplet. Data for ^{13}C NMR spectra are reported in terms of chemical shift. All GC analyses were performed on Agilent 7980A gas chromatograph equipped with (30 m×320 μm×0.25 μm) HP-5 column and a flame-ionization detector. GC yields were determined using standard curves with dodecane as internal standard. High-resolution mass spectra (HRMS) data was obtained by using Thermo Scientific™ Q Exactive™ Quadrupole-Orbitrap Mass Spectrometer.

2. General Procedure for Identifying the Optimal Reaction Condition for Sulfoxide Deoxygenation

To a solution of sulfoxide **1** (1.0 mmol) in dry DCE (2 mL), the reductant (1.0-2.0 mmol) and H-source (1.1 mmol or 0 mmol) were added and stirred for 10 minutes under an argon atmosphere. Then the activating reagent (1.05 mmol) was added slowly. The mixture was stirred at 70 °C for 8 h. After cooling to room temperature, phenyltrimethylsilican (50 mg, 0.33 mmol) was added into the mixture as the internal standard to determine yield by ^{1}H NMR. The results were showed in **Table S1.**

Table S1. Searching for optimal reaction condition.[a]



entry	activating reagent	H-source	reductant (X mmol)	yield
1	$SOCl_2$	HCOOH	-	4%
2	$SOCl_2$	HCOOH	Et_3N (1.0 mmol)	72%
3	-	HCOOH	Et_3N (1.0 mmol)	0%
4	$SOCl_2$	-	Et_3N (1.0 mmol)	83%
5	$SOCl_2$	-	Et_3N (1.5 mmol)	90%
6	$SOCl_2$	-	Et_3N (2.0 mmol)	99%
7	$(COCl)_2$	-	Et_3N (2.0 mmol)	99%
8	TFAA	-	Et_3N (2.0 mmol)	5%
9	Tf_2O	-	Et_3N (2.0 mmol)	40%
10	Bz_2O	-	Et_3N (2.0 mmol)	0%
11	$SOCl_2$	-	TMEDA (2.0 mmol)	90%
12	$SOCl_2$	-	DBU (2.0 mmol)	78%
13	$SOCl_2$	-	DIPEA (2.0 mmol)	88%
14	$SOCl_2$	-	DMAP (2.0 mmol)	97%
15	$SOCl_2$	-	Et_2NH (2.0 mmol)	70%
16	$SOCl_2$	-	pyridine (2.0 mmol)	2%
17	$SOCl_2$	-	sodium phenolate (4.0 mmol)	34%
18	$SOCl_2$	-	K_2CO_3 (2.0 mmol)	8%

[a]General condition: sulfoxide **1** (1.0 mmol), activating agent (1.05 mmol), reductant (1.0-2.0 mmol), HCOOH (1.1 mmol or 0 mmol), 1,2-dichloroethane (DCE, 2 mL), 70 °C, 8 h. Yields of products were based on a phenyltrimethylsilane internal standard. 1,2-Dichloroethane, DCE; trifluoroacetic anhydride, TFAA; trifluoromethanesulfonic anhydride, Tf_2O; benzoic anhydride, Bz_2O; *N*, *N*, *N'*, *N'*-tetramethylethylenediamine, TMEDA.

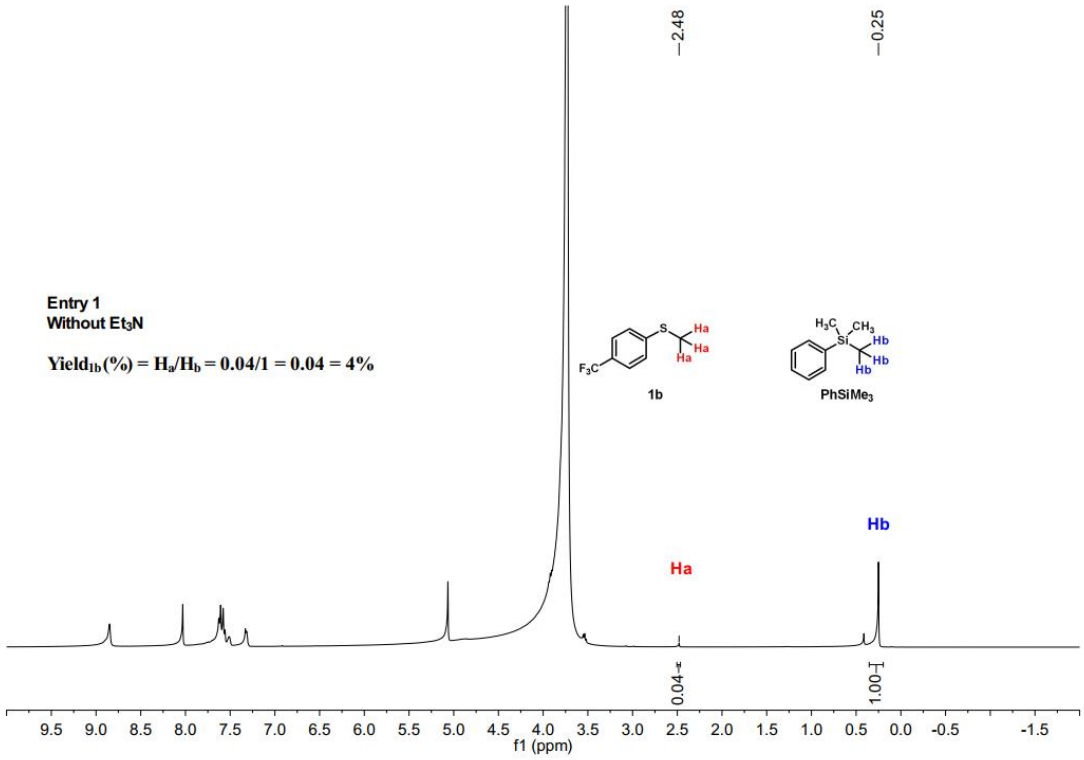


Figure S1. Crude ^{1}H NMR spectrum for the mixture of **entry 1** without Et_3N.

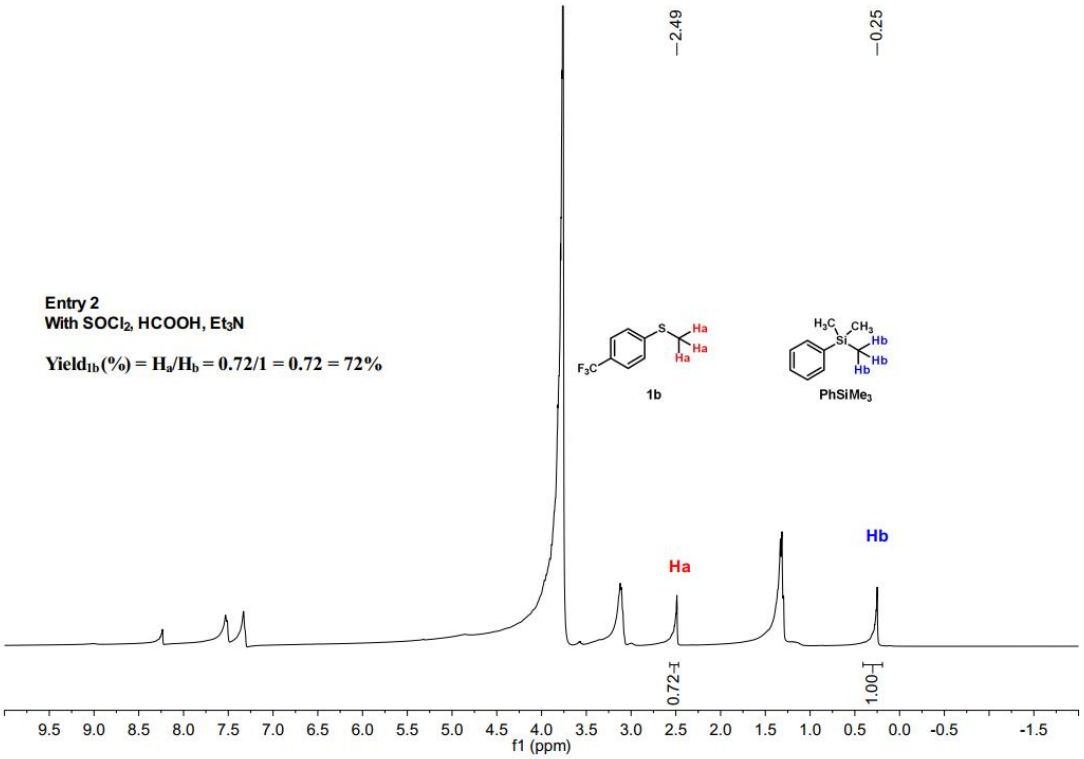


Figure S2. Crude ^{1}H NMR spectrum for the mixture of **entry 2** with Et_3N, $SOCl_2$ and HCOOH.

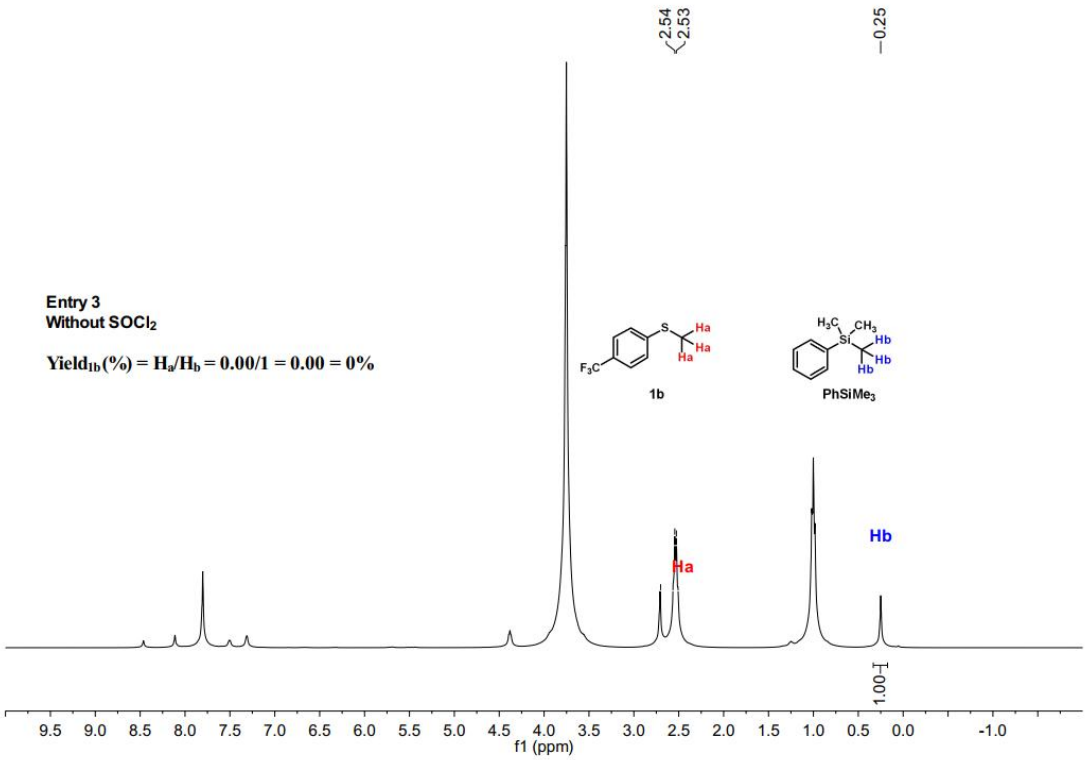


Figure S3. Crude ^{1}H NMR spectrum for the mixture of **entry 3** without $SOCl_2$.

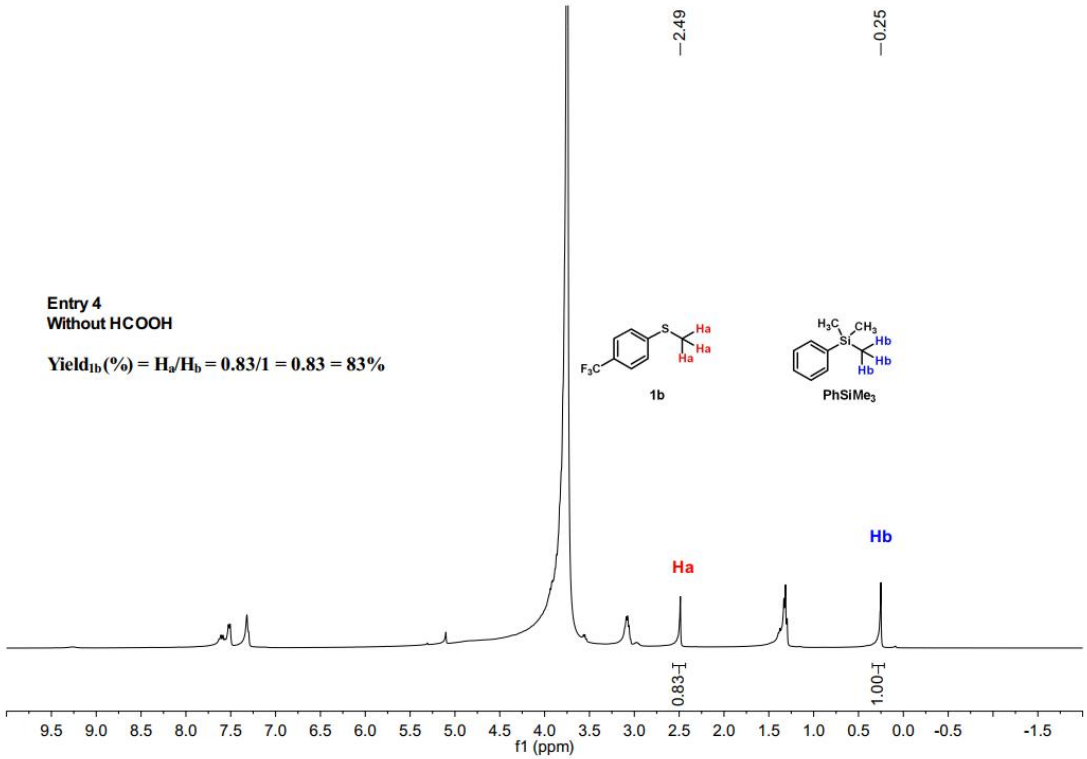


Figure S4. Crude ^{1}H NMR spectrum for the mixture of **entry 4** without HCOOH.

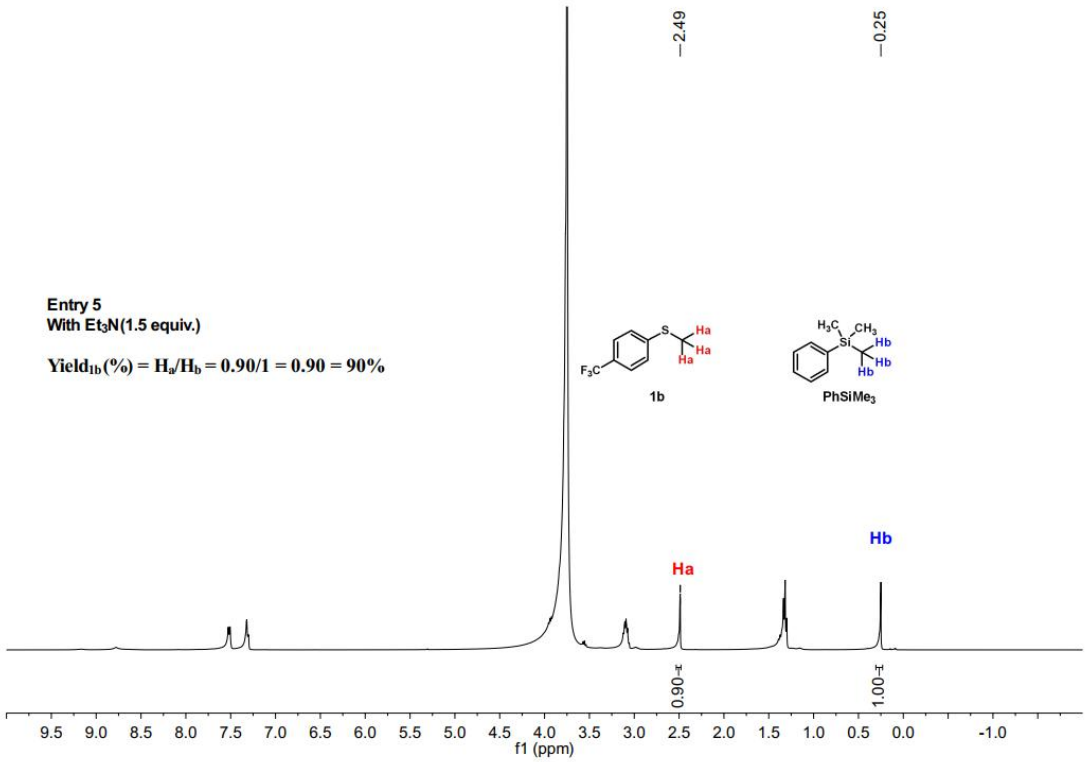


Figure S5. Crude ^{1}H NMR spectrum for the mixture of **entry 5** with Et_3N (1.5 equiv.).

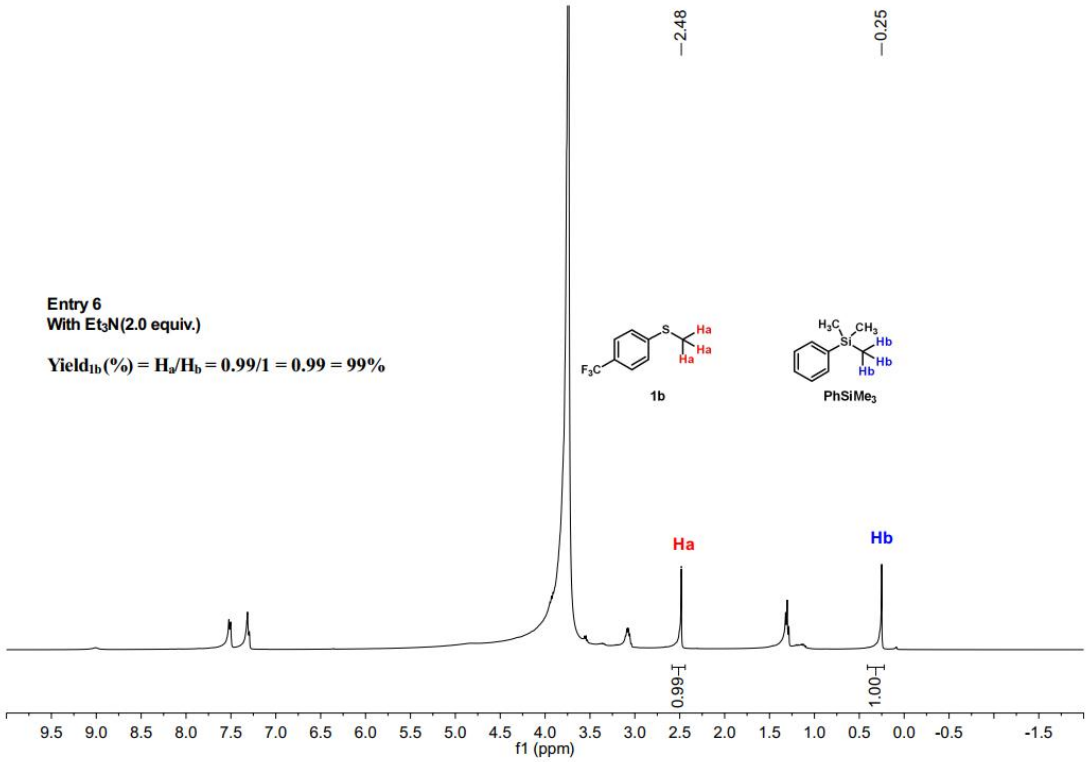


Figure S6. Crude ^{1}H NMR spectrum for the mixture of **entry 6** with Et_3N (2.0 equiv.).

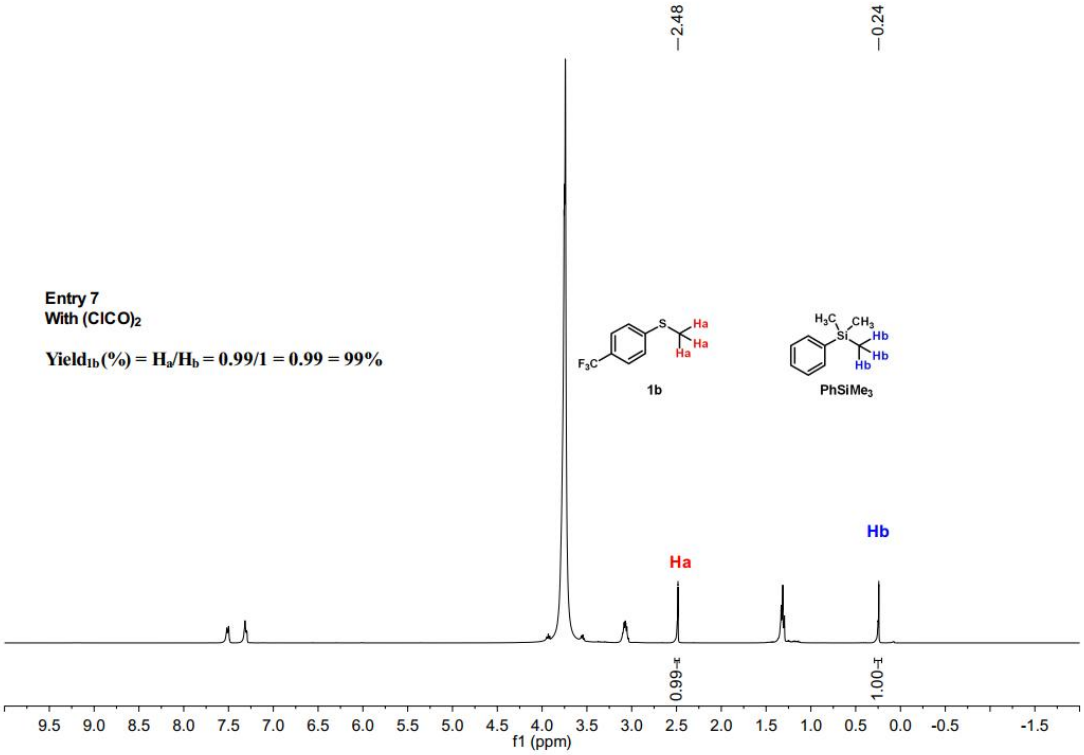


Figure S7. Crude ^{1}H NMR spectrum for the mixture of **entry 7** with $(ClCO)_2$.

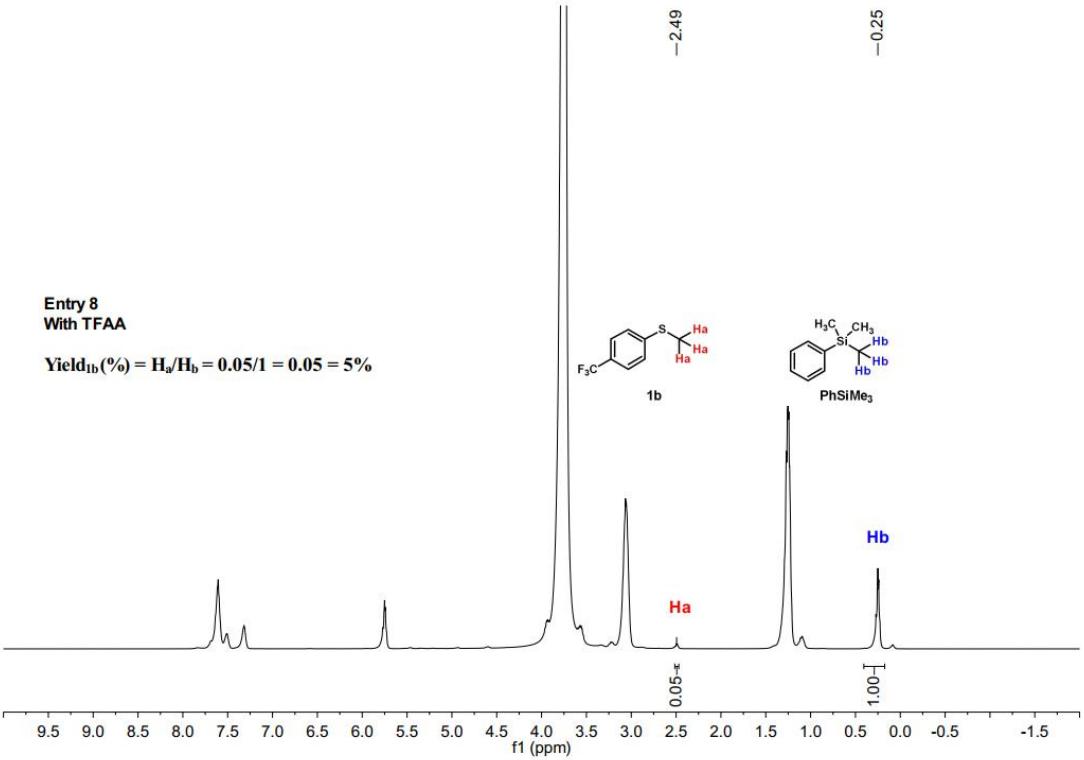


Figure S8. Crude ^{1}H NMR spectrum for the mixture of **entry 8** with TFAA.

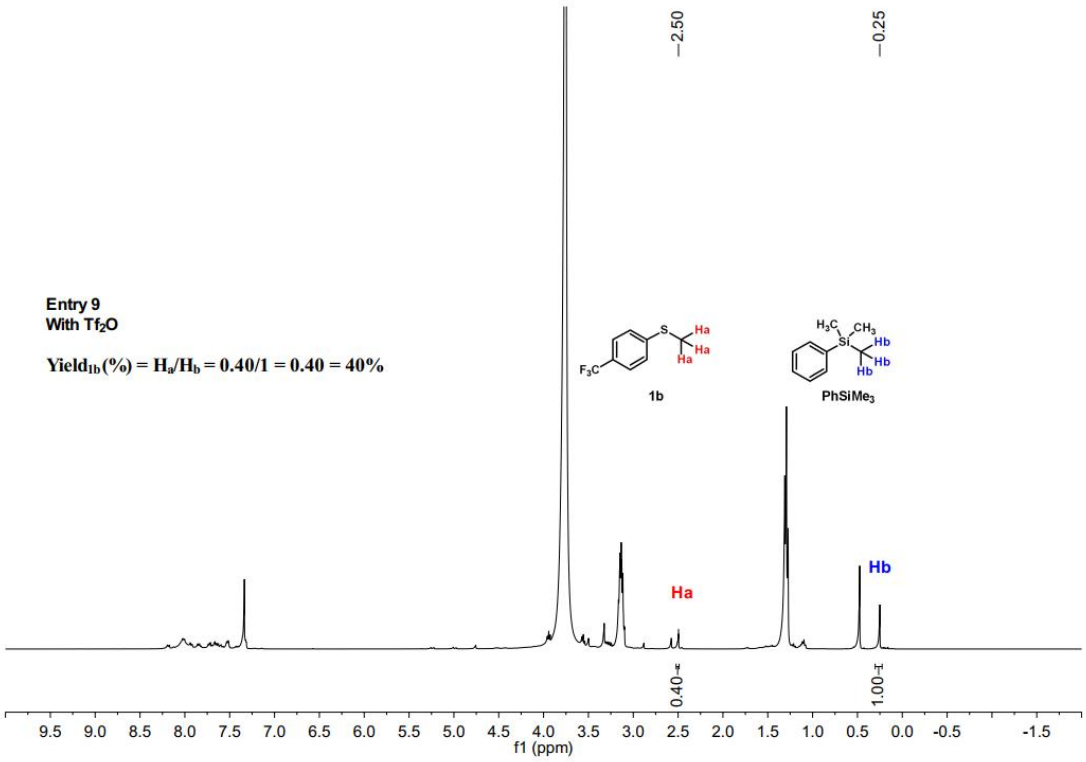


Figure S9. Crude ^{1}H NMR spectrum for the mixture of **entry 9** with Tf_2O.

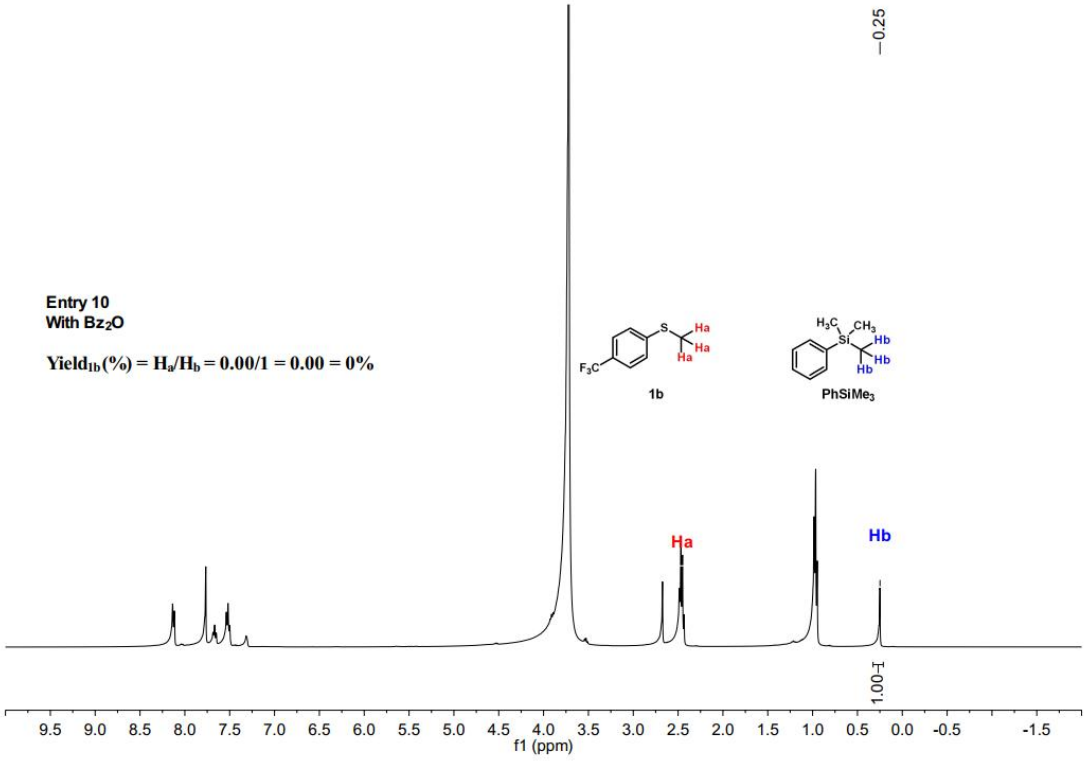


Figure S10. Crude ^{1}H NMR spectrum for the mixture of **entry 10** with Bz_2O.

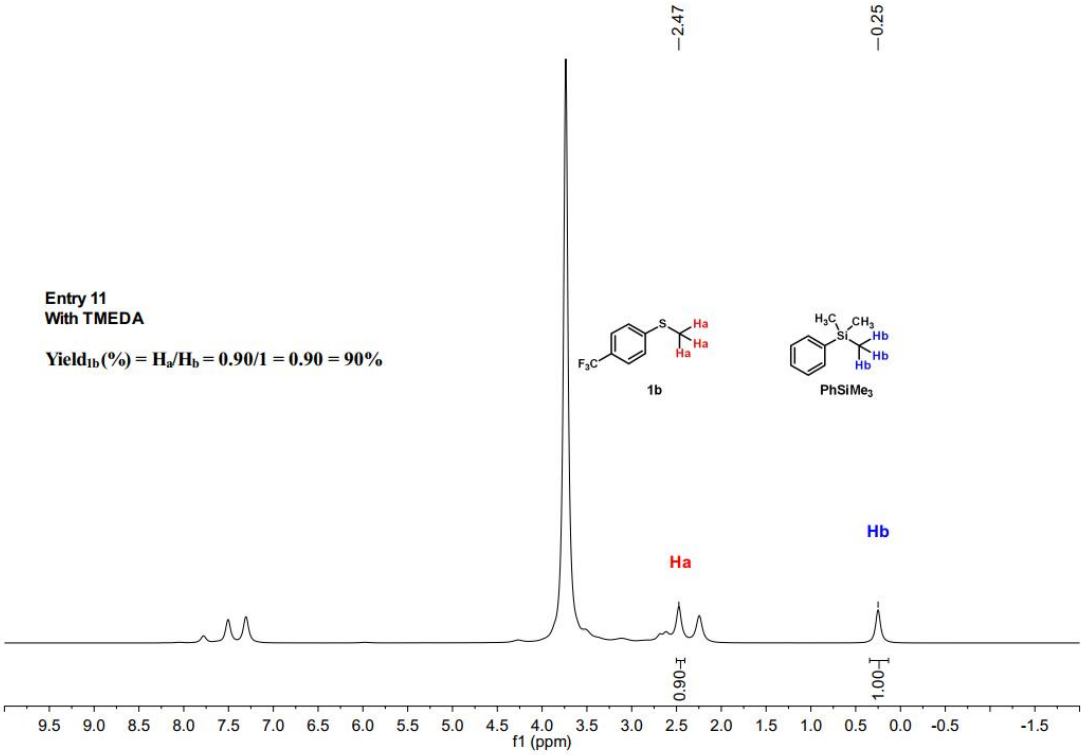


Figure S11. Crude ^{1}H NMR spectrum for the mixture of **entry 11** with TMEDA.

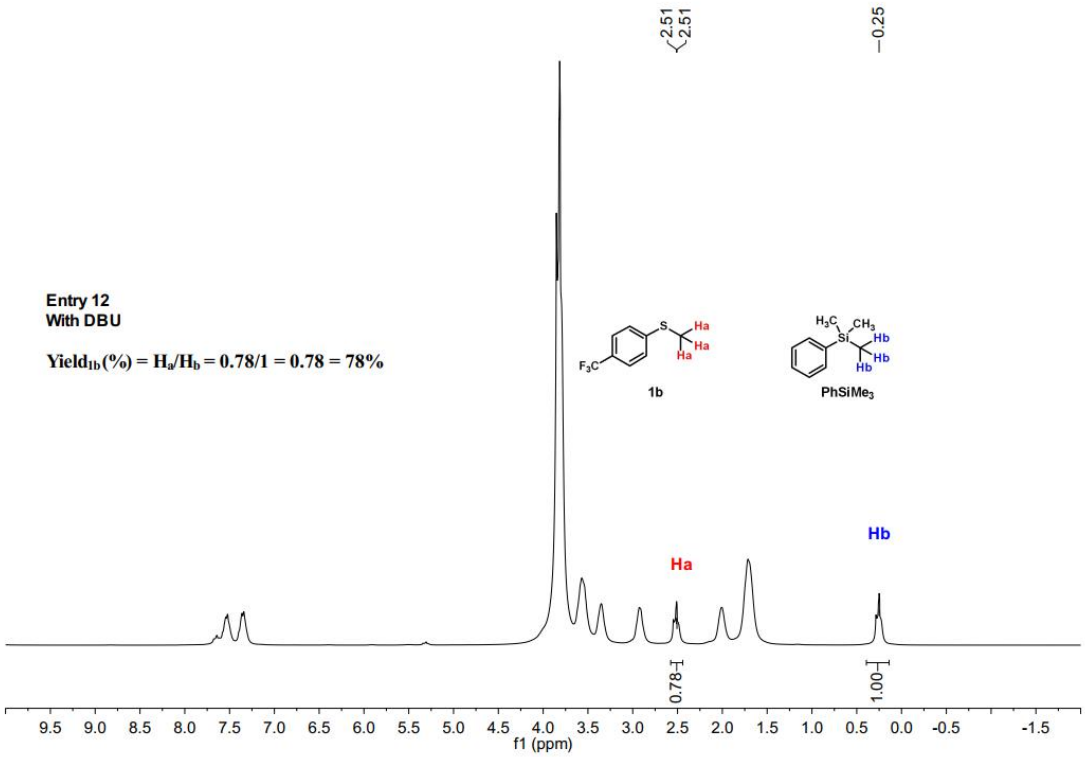


Figure S12. Crude ^{1}H NMR spectrum for the mixture of **entry 12** with DUB.

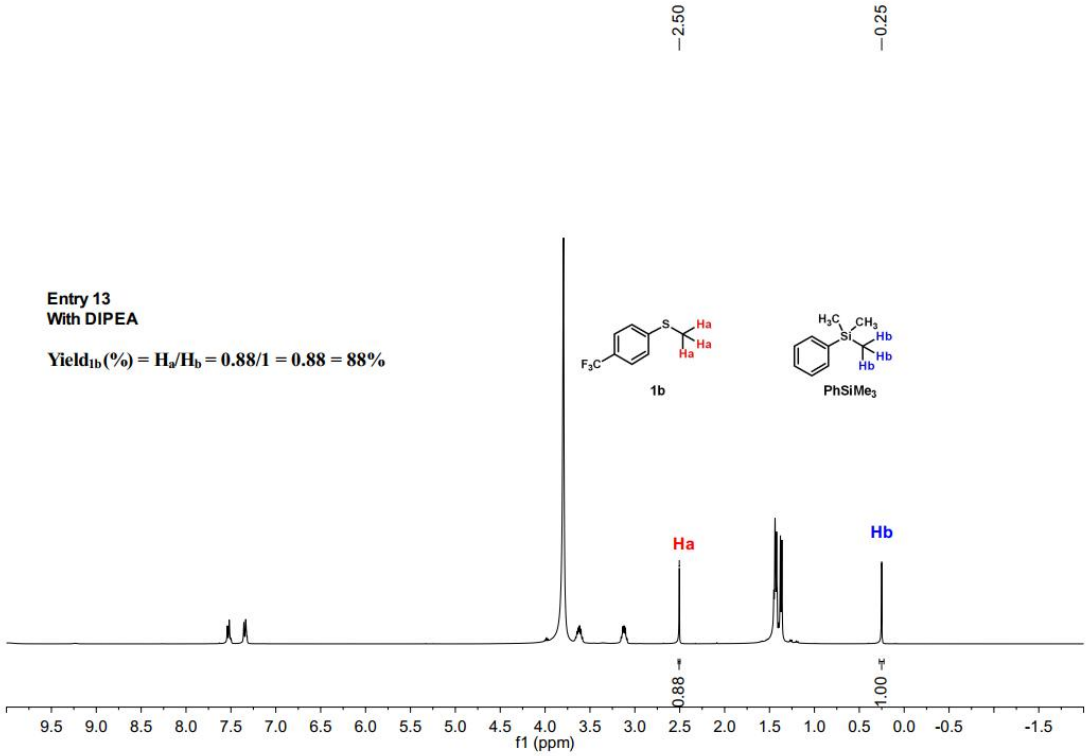


Figure S13. Crude ^{1}H NMR spectrum for the mixture of **entry 13** with DUB.

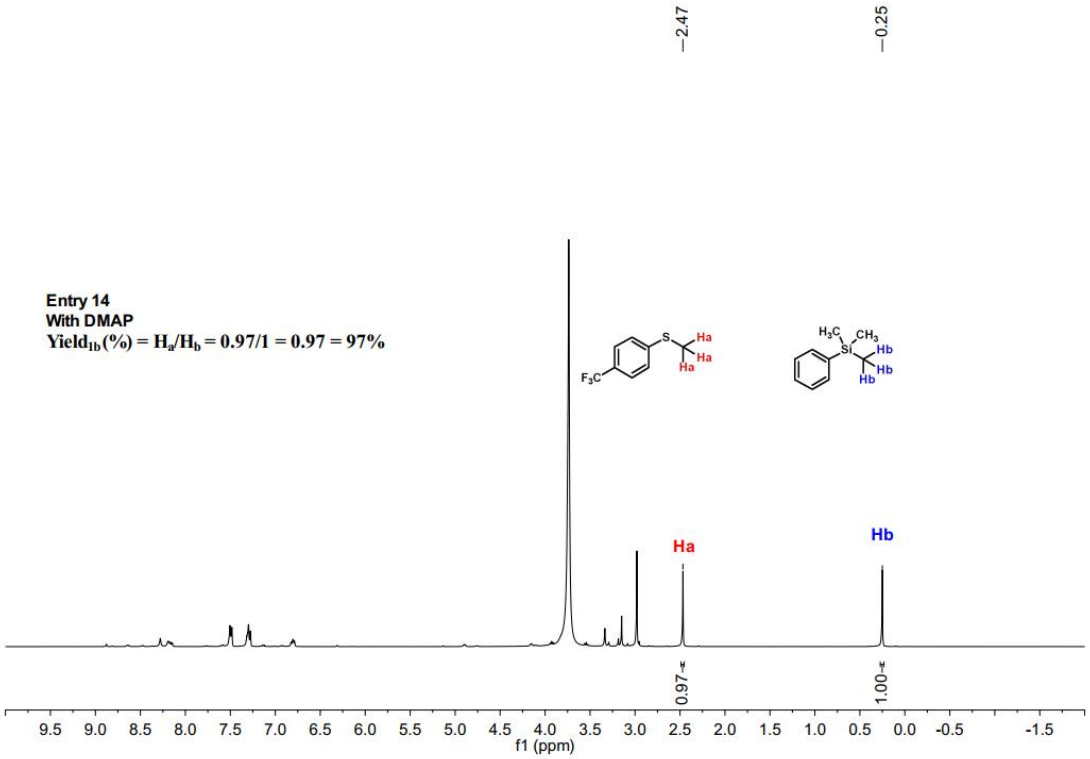


Figure S14. Crude ^{1}H NMR spectrum for the mixture of **entry 14** with DMAP.

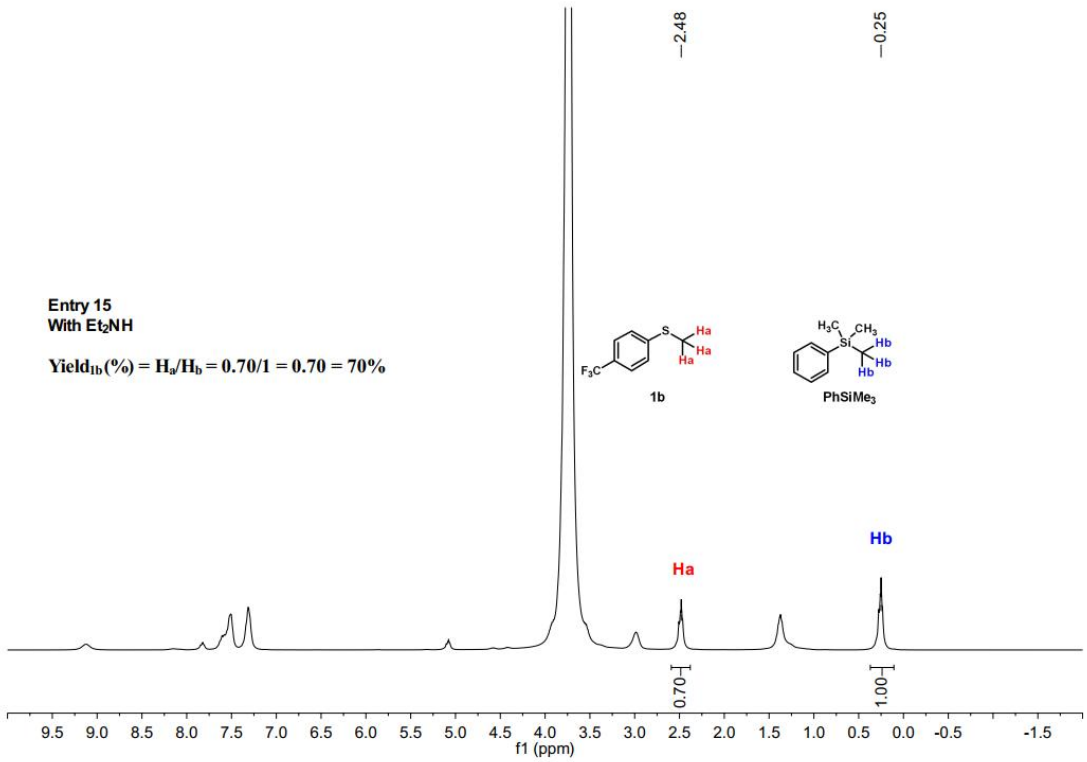


Figure S15. Crude ^{1}H NMR spectrum for the mixture of **entry 15** with Et_2NH.

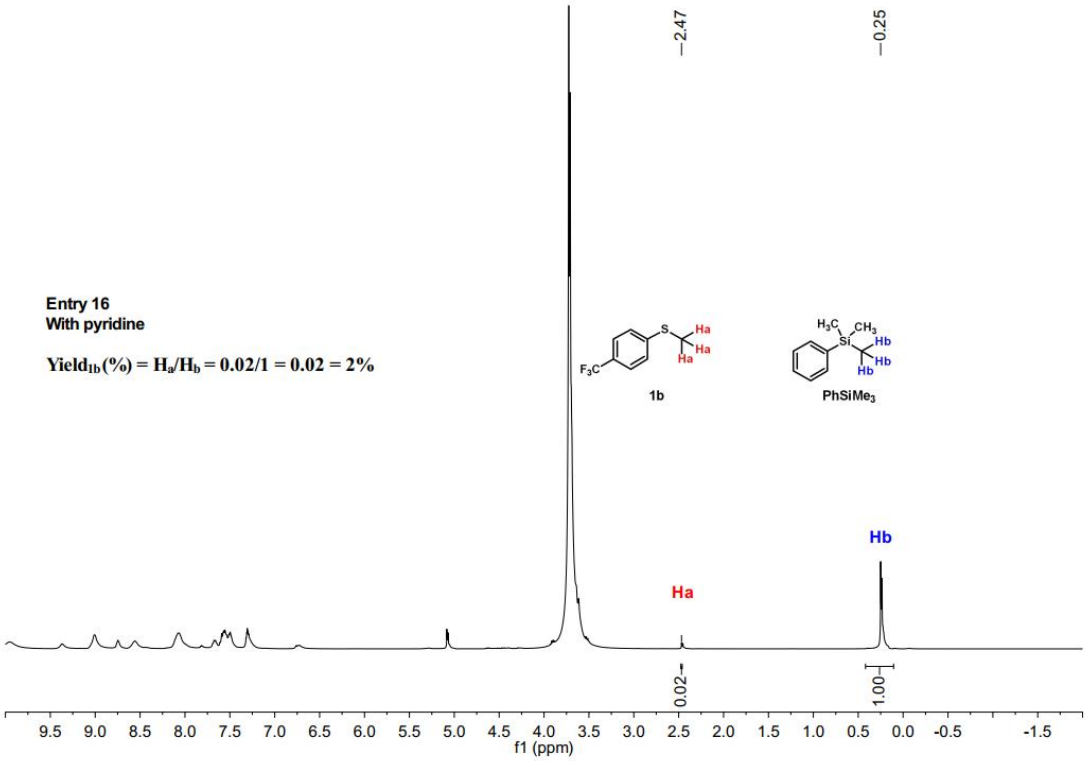


Figure S16. Crude ^{1}H NMR spectrum for the mixture of **entry 16** with pyridine.

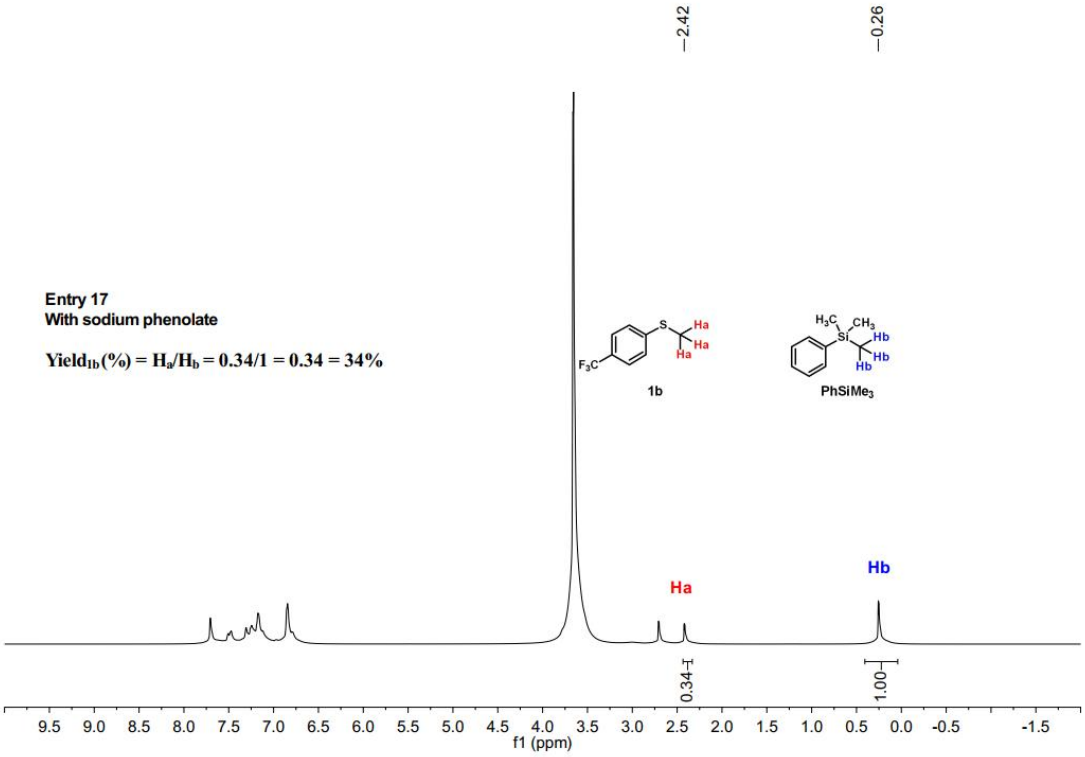


Figure S17. Crude ^{1}H NMR spectrum for the mixture of **entry 17** with sodium phenolate.

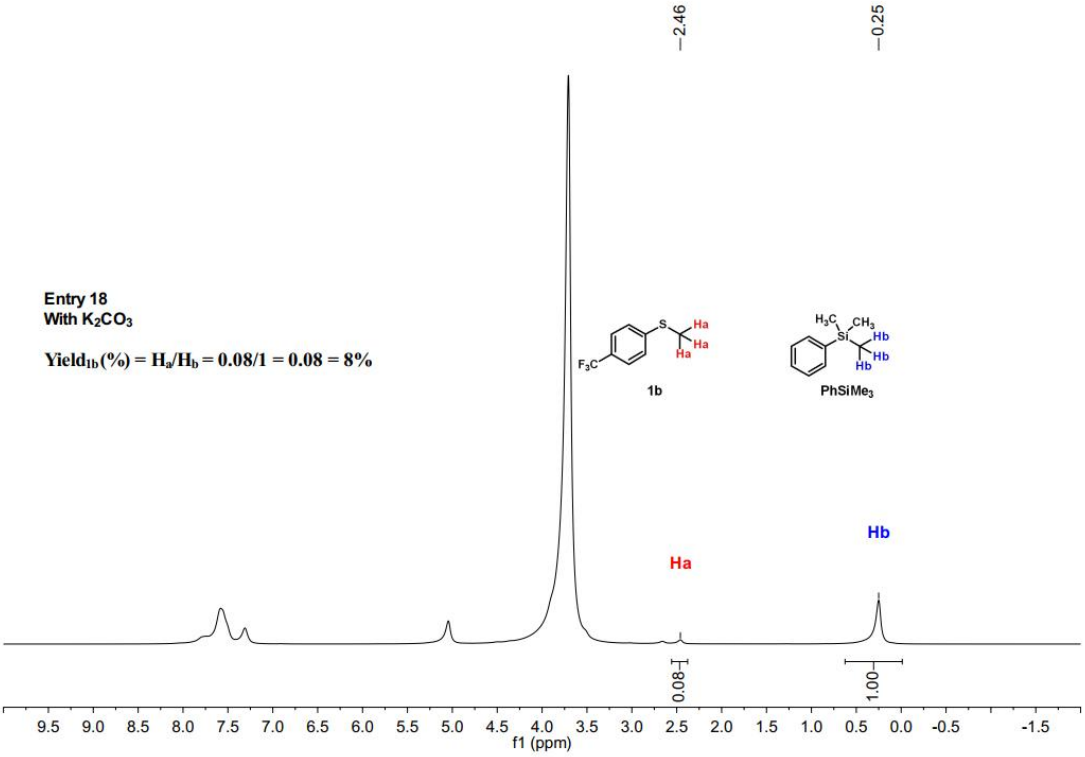
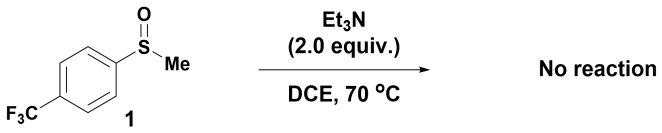


Figure S18. Crude ^{1}H NMR spectrum for the mixture of **entry 18** with K_2CO_3.

3. Mechanism for this Sulfoxide Deoxygenation Reaction

3.1 Control experiments



To a solution of sulfoxide **1** (208.2 mg, 1.0 mmol) in extra dry DCE (2 mL), Et_3N (2.0 mmol) was added and stirred for 10 minutes under an argon atmosphere. Then the mixture was stirred at 70 °C for 3 h. After cooling to room temperature, phenyltrimethylsilican (50 mg, 0.33 mmol) was added into the mixture as the internal standard to give the NMR yield of **1b** with 0% yield (**Figure S19**).

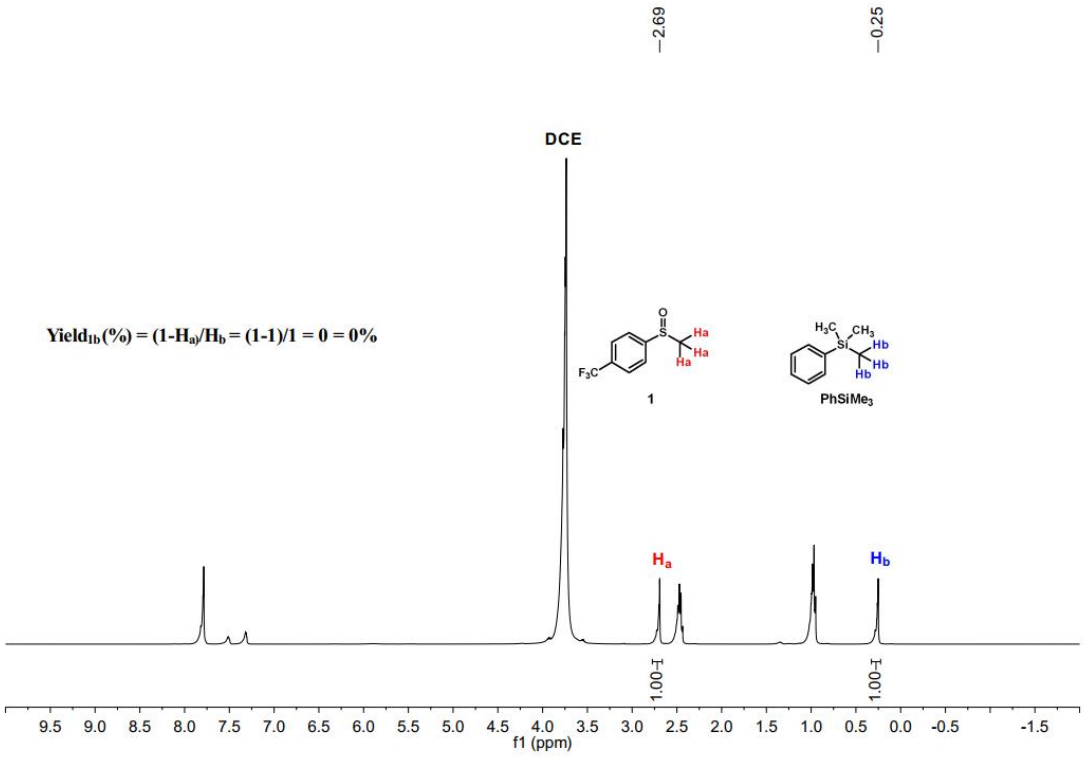
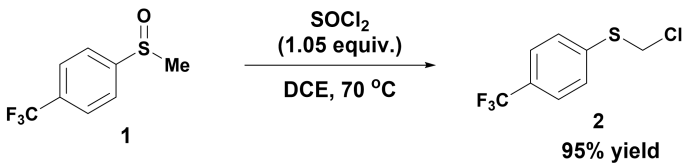


Figure S19. Crude ^1H NMR spectrum for control experiment with Et_3N.



To a solution of sulfoxide **1** (208.2 mg, 1.0 mmol) in extra dry DCE (2 mL), $SOCl_2$ (1.05 mmol) was added slowly. Then the mixture was stirred at 70 °C for 3 h. After cooling to room temperature, phenyltrimethylsilican (50 mg, 0.33 mmol) was added into the mixture as the internal standard to give the NMR yield of **2** with 95% yield (**Figure S20**).

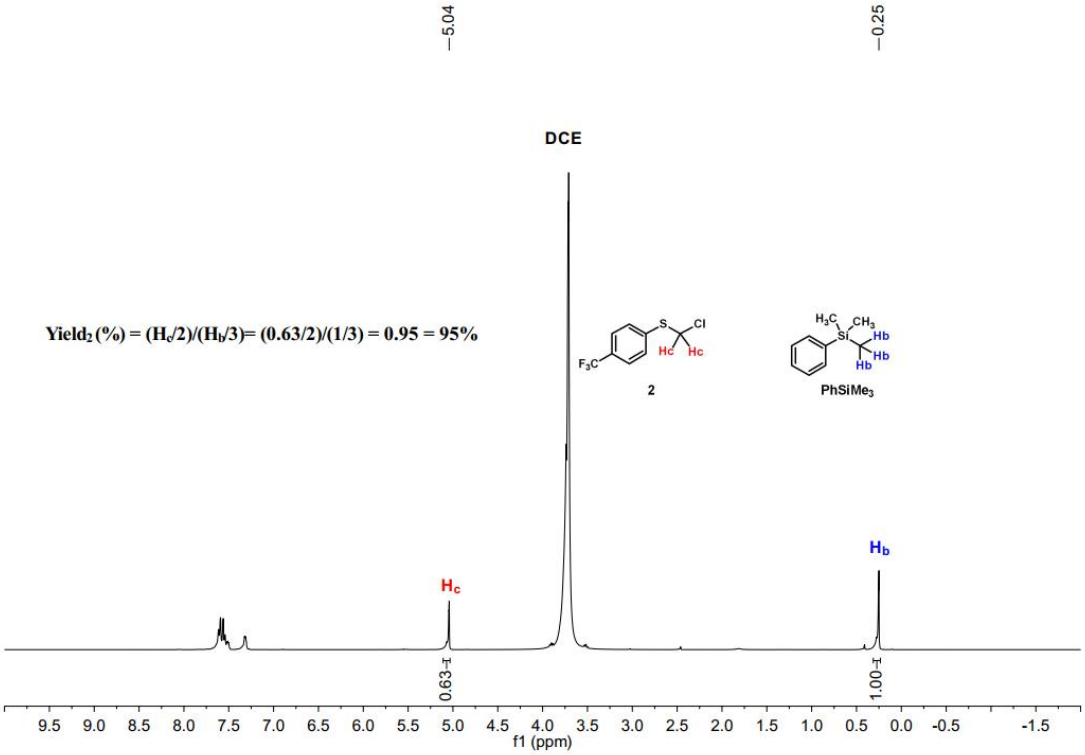
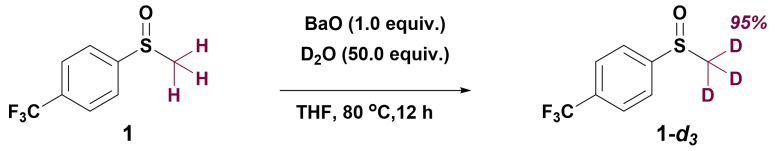


Figure S20. Crude ^{1}H NMR spectrum for control experiment with $SOCl_2$.

3.2 Deuterium labeling experiments

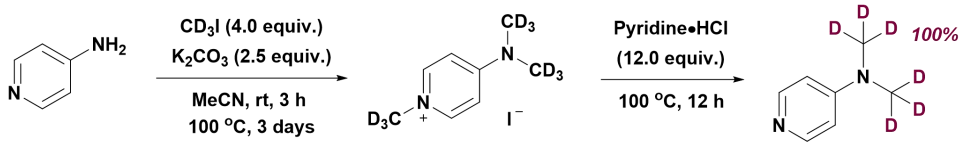
Synthesis and Characterization of **1-*d*$_3$**[1]



To a 25 mL bottle, sulfoxide **1** (208.2 mg, 1.0 mmol) and BaO (153.3 mg, 1 mmol) were added. Then D_2O (1.0 mL, 50 mmol) and THF (0.25 mL) was added. The mixture was stirred at 80 °C for 12 h. After cooling to room temperature, the mixture was concentrated under reduce pressure. The crude product was purified by silica flash chromatography (eluted with hexane/EtOAc = 1:1) to give the product **1-*d*$_3$**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 – 7.74 (m, 4H) ppm.
^{13}C NMR (101 MHz, $CDCl_3$): δ 150.0, 133.00 (q, *J* = 32.9 Hz), 126.33 (q, *J* = 3.7 Hz), 124.0, 123.43 (q, *J* = 272.6 Hz), 44.17 – 42.30 (m) ppm.
^{19}F NMR (377 MHz, $CDCl_3$): δ -62.84 ppm.

Synthesis and Characterization of **DMAP-*d*$_6$** [2]

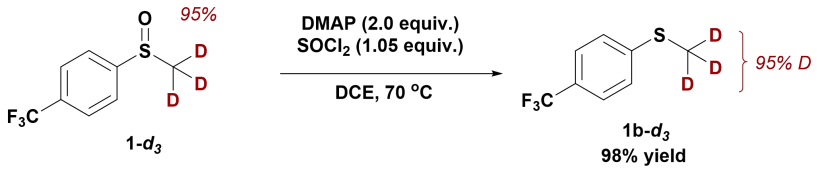


Step 1: To a 50 mL bottle, 4-aminopyridine (1.6 g, 17.2 mmol), K_2CO_3 (5.9 g, 43.1 mmol), CD_3I (10 g, 69.0 mmol) and MeCN (30 mL) was added. The mixture was stirred at rt for 3 h and then at 100 °C for 3 days. The mixture was cooled to room temperature and filtered. Then the residue was washed with hot MeCN. *N*-(trideuteriomethyl)-4-bis(trideuteriomethyl)amino pyridinium iodide (white solid) was obtained by evaporation of filtrate.

Step 2: To a 50 mL bottom, *N*-(trideuteriomethyl)-4-bis(trideuteriomethyl)amino pyridinium iodide (1.0 g, 3.7 mmol) and pyridinium hydrochloride (5.1 g, 44 mmol.) was added. The mixture was refluxed for 12 h. Then cooled to room temperature, and washed by sat. aq. NH_4OH. The volatiles were evaporated. The resulting residue was washed with CH_2Cl_2 and the CH_2Cl_2 washings were combined and solvent was evaporated under reduce pressure. The crude product was purified by silica flash chromatography (CH_2Cl_2/MeOH = 9:1) to give the final product **DMAP-*d*$_6$**.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29 (d, *J* = 7.4 Hz, 2H), 6.84 (d, *J* = 7.4 Hz, 2H) ppm.
^{13}C NMR (101 MHz, $CDCl_3$): δ 155.7, 142.7, 107.9, 47.84 – 42.48 (m), 42.21 – 37.61 (m) ppm.

Procedure for Deuterium Labeling Experiments



To a solution of sulfoxide **1-*d*$_3$** (42.2 mg, 0.2 mmol) in dry DCE (0.5 mL), DMAP (48.9 mg, 0.4 mmol) was added and stirred for 10 minutes. Then $SOCl_2$ (25.0 mg, 0.21 mmol) was added slowly. The mixture was stirred at 70 °C for 8 h. After cooling to room temperature, phenyltrimethylsilane (10 mg, 0.07 mmol) was added into the mixture as the internal standard to give the NMR yield of **1b-*d*$_3$** with 98% yield.

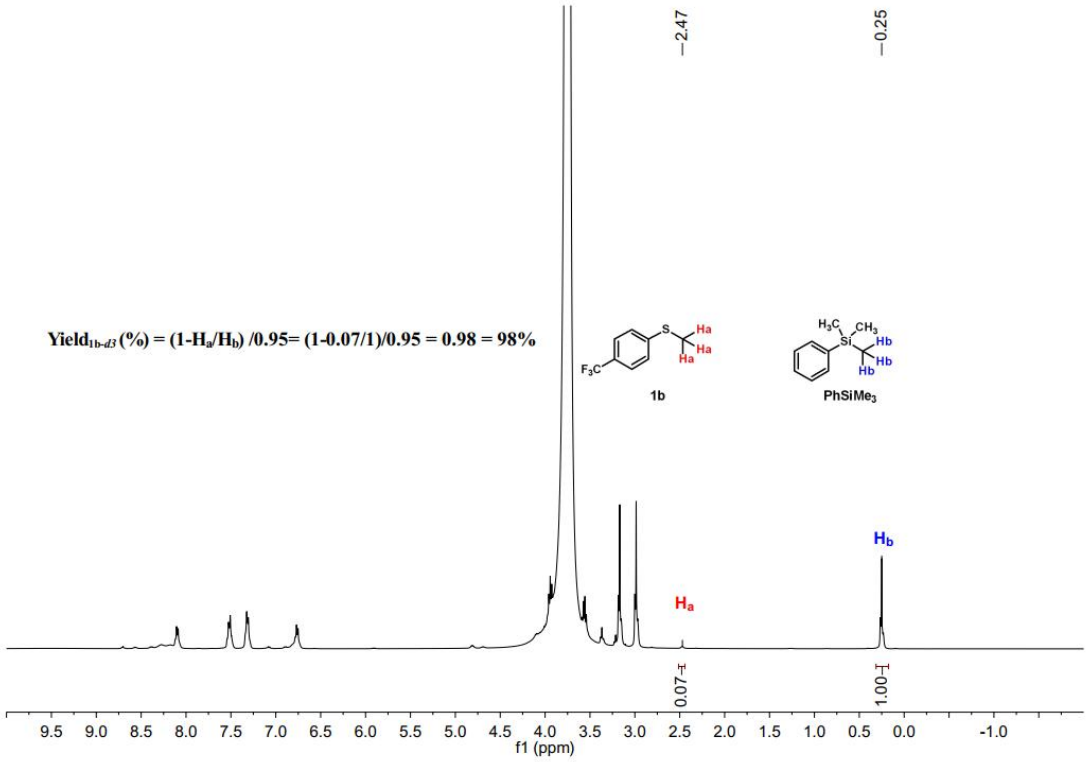
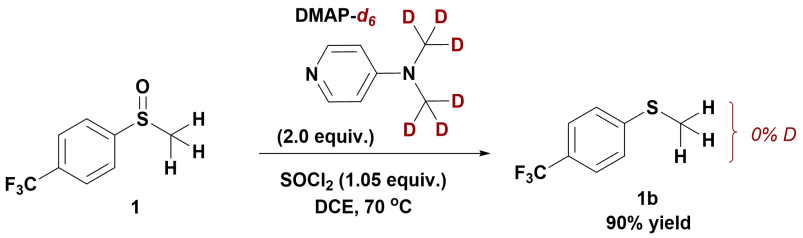


Figure S21. Crude ^{1}H NMR spectrum for deuterium labeling experiment with sulfoxide **1-*d*$_3$**.



To a solution of sulfoxide **1** (41.6mg, 0.2 mmol) in extra dry DCE (0.5 mL), DMAP-d_6 (51.3 mg, 0.4 mmol) was added and stirred for 10 minutes. Then $SOCl_2$ (25.0 mg, 0.21 mmol) was added dropwise slowly. The mixture was stirred at 70 ℃ for 8 h. After cooling to room temperature, phenyltrimethylsilane (10 mg, 0.07 mmol) was added into the mixture as the internal standard to give the NMR yield of **1b** with 90% yield.

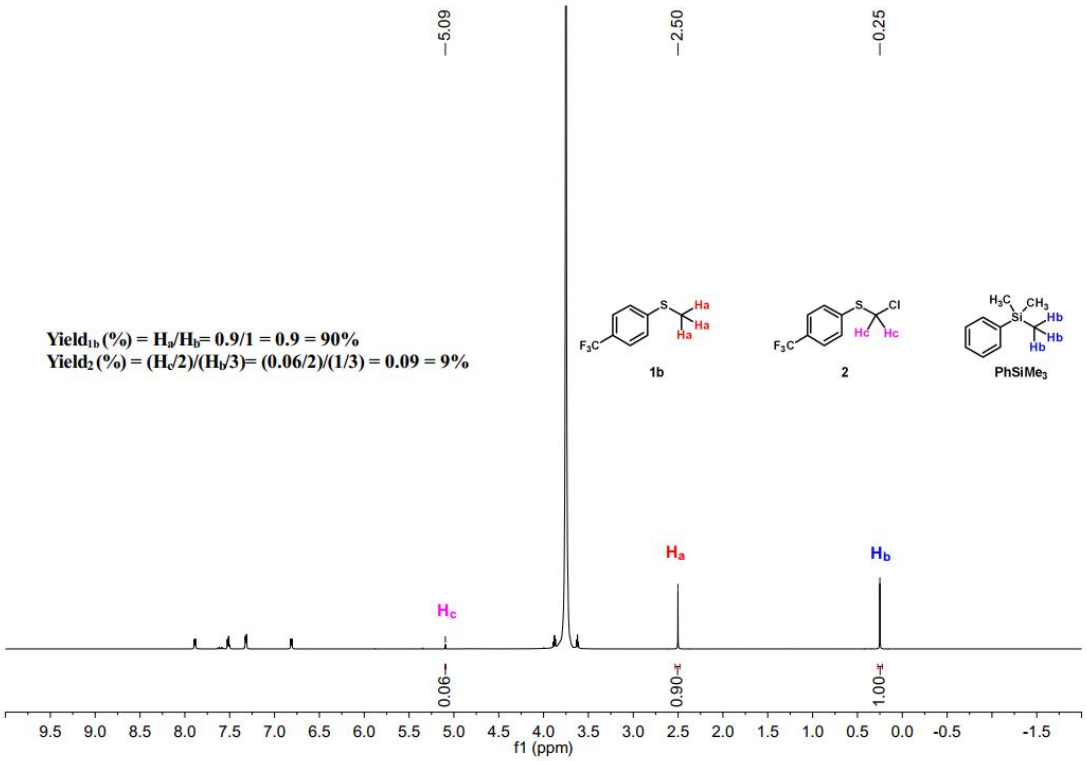
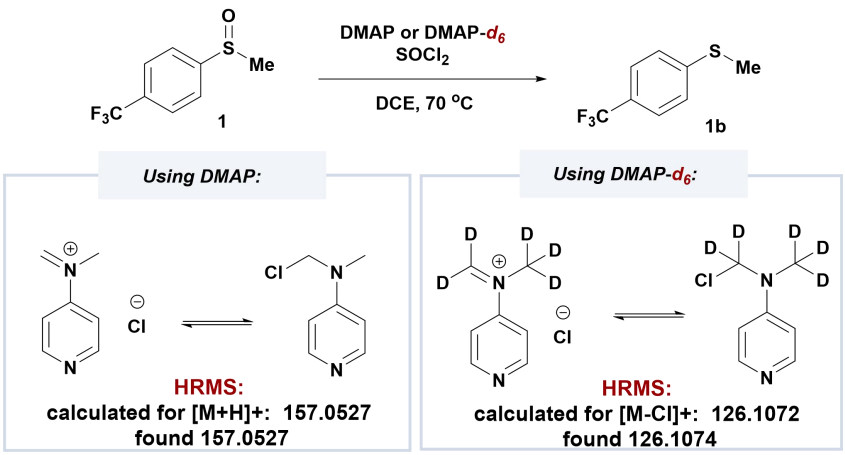


Figure S22. Crude ^{1}H NMR spectrum for deuterium labeling experiment with DMAP-d_6.

3.3 HRMS experiments



To a solution of sulfoxide **1** (208.2 mg, 1.0 mmol) in extra dry DCE (2 mL), DMAP (122.2 mg, 2.0 mmol) or DMAP-d_6 (128.2 mg, 2.0 mmol) was added and stirred for 10 minutes. Then $SOCl_2$ (124.9 mg, 1.05 mmol) was added slowly. The mixture was stirred at 70 ℃ for 8 h. After cooling to room temperature, an appropriate amount of sample was tested by high-resolution mass spectrometry.

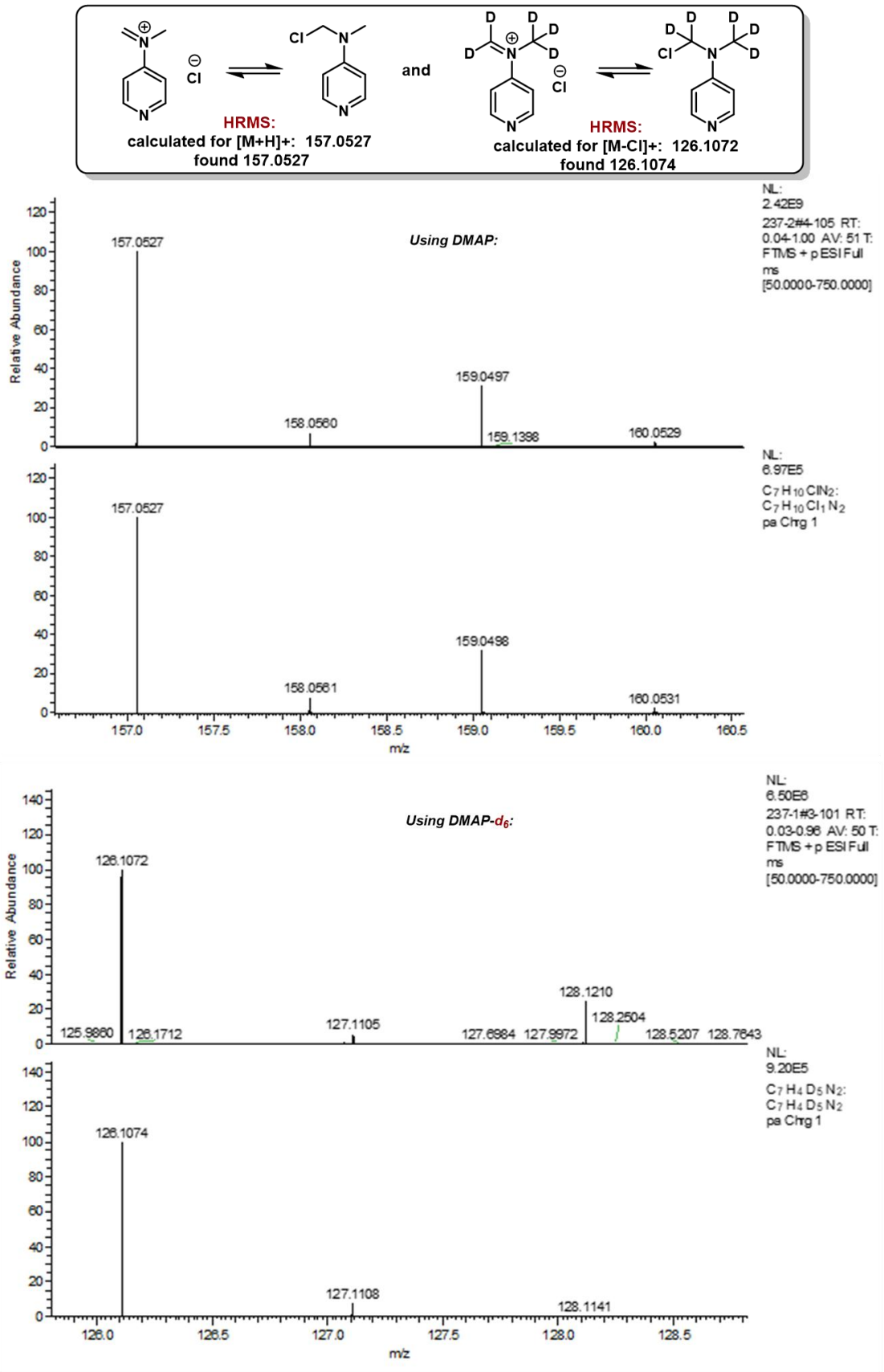
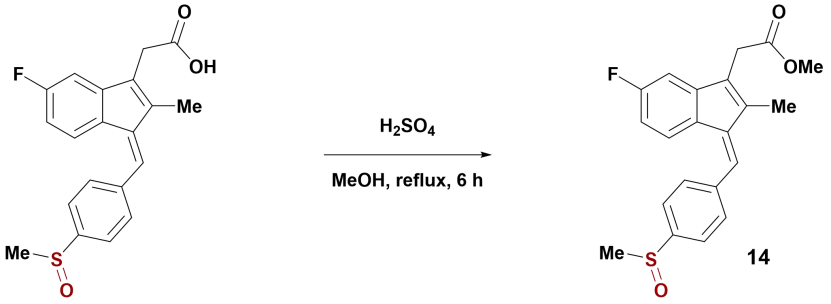


Figure S23. HRMS for the mixture.

4. General Procedure for Reduction of Sulfoxides

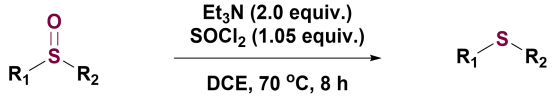
Synthesis and Characterization of the Sulfoxide 14



To a solution of sulindac (10 mmol, 3.56 g) in anhydrous CH_2Cl_2 (30 mL), methanol (100 mL) and sulfuric acid (0.2 mL) were added. The mixture was refluxed for 6 hours. After cooling to room temperature, the mixture was quenched with water and extracted with CH_2Cl_2 (3×50 mL). The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. dried and concentrated under reduce pressure. The crude product was purified by flash chromatography (eluted with hexane/EtOAc = 1:1) to give the corresponding product sulfoxide **14** (3.44 g, 93% yield).

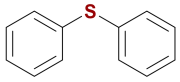
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.2 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.16 – 7.11 (m, 2H), 6.86 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.55 (td, *J* = 8.9, 2.4 Hz, 1H), 3.70 (s, 3H), 3.56 (s, 2H), 2.80 (s, 3H), 2.20 (s, 3H)ppm. **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 170.7, 163.28 (d, *J* = 246.5 Hz), 146.63 (d, *J* = 9.2 Hz), 145.3, 141.6, 139.6, 138.1, 131.68 (d, *J* = 2.7 Hz), 130.2, 129.42 (d, *J* = 3.4 Hz), 128.17 (d, *J* = 2.0 Hz), 123.7, 123.58 (d, *J* = 9.3 Hz), 110.72 (d, *J* = 22.6 Hz), 106.04 (d, *J* = 23.7 Hz), 52.2, 43.8, 31.5, 10.5 ppm. **^{19}F NMR (376 MHz, $CDCl_3$):** δ -112.89 ppm.

General Procedure for Reduction of Sulfoxides

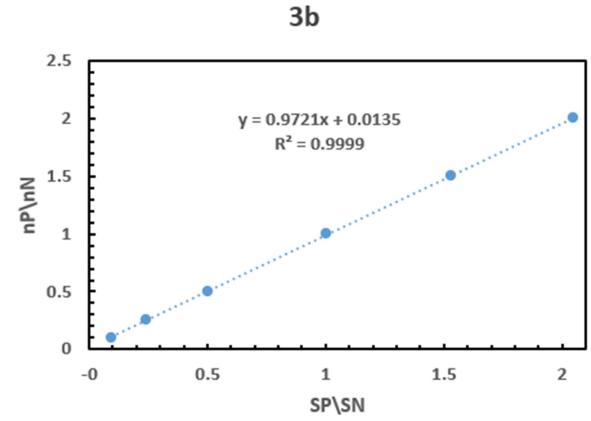


To a solution of sulfoxides (1.0 mmol) in dry DCE (2 mL), Et_3N (2.0 mmol) was added and stirred for 10 minutes. Then $SOCl_2$ (1.05 mmol) was added slowly. Then the mixture was stirred at 70 ℃ for 8 h. After cooling to room temperature, phenyltrimethylsilane (50 mg, 0.33 mmol) was added into the mixture as the internal standard to determine yield by ^{1}H NMR or dodecane (170.3 mg, 1.0 mmol) was added into the mixture as the internal standard to determine yield by GC. Then the mixture was concentrated in vacuo and the residue was subjected to column chromatography with only hexane as eluent to afford the corresponding sulfide.

Diphenylsulfane (3b)



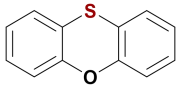
The general procedure was followed and dodecane (170.3 mg, 1.0 mmol) was added into the crude residue as the internal standard. The conversion of **3b** was determined by GC (99% yield) **(Figure S24)**. The desired product **3b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.34 – 7.19 (m, 10H) ppm. **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 135.7, 131.0, 129.2, 127.0 ppm.



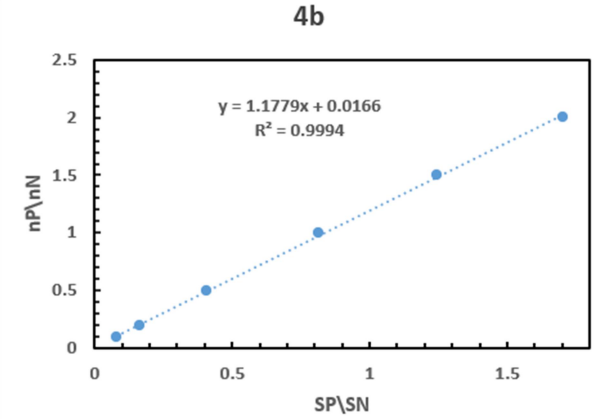
$yield_{3b}$ = nP/nN = 0.9721 × (SP/SN) + 0.0135
= 0.9721 × (50.705/49.295) + 0.0135 = 0.99 = 99%

Figure S24. GC standard cure of **3b** to dodecane and the GC yield of **3b**.

Phenoxathiine (4b)



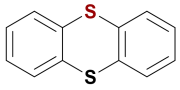
The general procedure was followed and phenyltrimethylsilane (50 mg, 0.33 mmol) was added into the crude residue as the internal standard. The conversion of **4b** was determined by GC (99% yield) (**Figure S25**). The desired product **4b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.15 – 7.10 (m, 4H), 7.03 – 7.00 (m, 4H) ppm. **^{13}C NMR (151 MHz, $CDCl_3$)**: δ 152.1, 127.6, 126.7, 124.5, 120.1, 117.7 ppm.



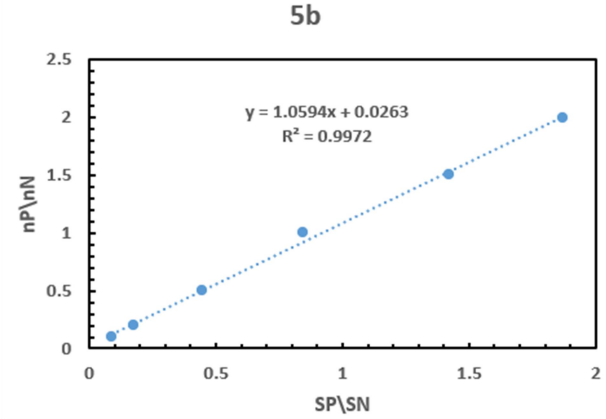
$yield_{4b}$ = nP/nN = 1.1779 × (SP/SN) + 0.0166
= 1.1779 × (45.829/54.171)+ 0.0166 = 0.99 = 99%

Figure S25. GC standard cure of **4b** to dodecane and the GC yield of **4b**.

Thianthrene (5b)



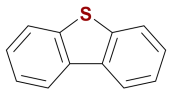
The general procedure was followed and dodecane (170.3 mg, 1.0 mmol) was added into the crude residue as the internal standard. The conversion of **5b** was determined by GC (99% yield) (**Figure S26**). The desired product **5b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.53 – 7.50 (m, 4H), 7.28 – 7.25 (m, 4H) ppm. **^{13}C NMR (151 MHz, $CDCl_3$)**: δ 135.5, 128.7, 127.6 ppm.



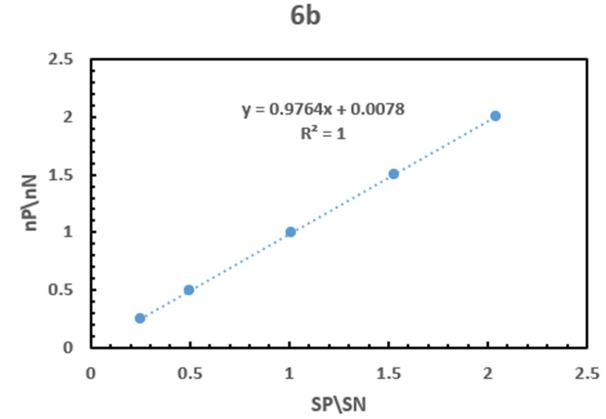
$yield_{5b}$ = nP/nN = 1.0594 × (SP/SN) + 0.0263
= 1.0594 ×(48.599/51.401) + 0.0263 = 0.99 = 99%

Figure S26. GC standard cure of **5b** to dodecane and the GC yield of **5b**.

Dibenzo[b,d]thiophene (6b)



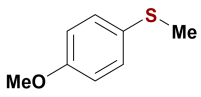
The general procedure was followed and dodecane (170.3 mg, 1.0 mmol) was added into the crude residue as the internal standard. The conversion of **6b** was determined by GC (96% yield) (**Figure S27**). The desired product **6b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 8.20 – 8.14 (m, 2H), 7.90 – 7.83 (m, 2H), 7.50 – 7.44 (m, 4H) ppm. **^{13}C NMR (151 MHz, $CDCl_3$)**: δ 139.4, 135.5, 126.7, 124.3, 122.8, 121.5 ppm.



$yield_{6b}$ = nP/nN = 0.9764 × (SP/SN) + 0.0078
= 0.9764 ×(49.293/50.707) + 0.0078 = 0.96 = 96%

Figure S27. GC standard cure of **6b** to dodecane and the GC yield of **6b**.

(4-Methoxyphenyl)(methyl)sulfane (7b)



The general procedure was followed and phenyltrimethylsilane (50 mg, 0.33 mmol) was added into the crude residue as the internal standard. The conversion of **7b** was determined by ^{1}H NMR (77% yield) (**Figure S28**). The desired product **7b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.27 (d, *J* = 7.7 Hz, 2H), 6.85 (d, *J* = 7.7 Hz, 2H), 3.78 (s, 3H), 2.44 (s, 3H) ppm. **^{13}C NMR (151 MHz, $CDCl_3$)**: δ 158.1, 130.1, 128.7, 114.5, 55.3, 18.0 ppm.

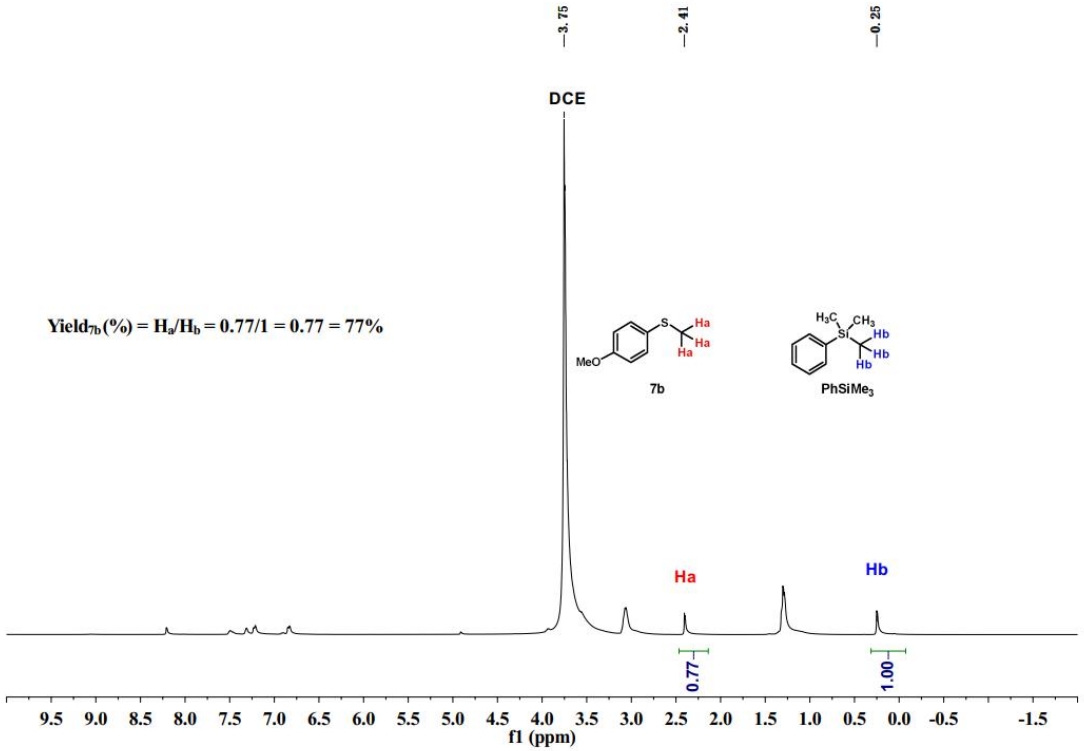
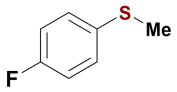


Figure S28. Crude ^{1}H NMR spectrum for the mixture of **7b**.

(4-Fluorophenyl)(methyl)sulfane (8b)



The general procedure was followed and phenyltrimethylsilane (50 mg, 0.33 mmol) was added into the crude residue as the internal standard. The conversion of **8b** was determined by ^{1}H NMR (95% yield) (**Figure S29**). The desired product **8b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.24 – 7.20 (m, 2H), 6.96 (t, *J* = 8.0 Hz, 2H), 2.43 (s, 3H) ppm. **^{13}C NMR (151 MHz, $CDCl_3$)**: δ 161.13 (d, *J* = 245.0 Hz), 133.27 (d, *J* = 3.3 Hz), 129.25 (d, *J* = 8.1 Hz), 115.91 (d, *J* = 21.9 Hz), 17.1 ppm. **^{19}F NMR (376 MHz, $CDCl_3$)**: δ -117.34 ppm.

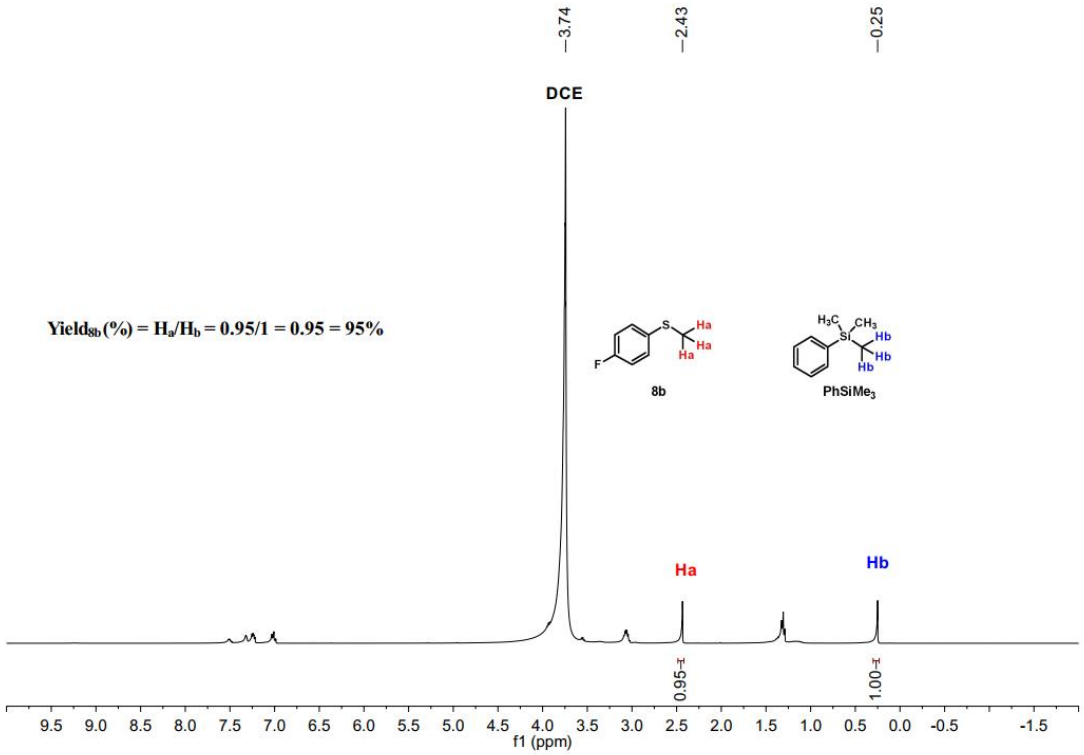
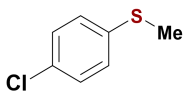


Figure S29. Crude ^{1}H NMR spectrum for the mixture of **8b**.

(4-Chlorophenyl)(methyl)sulfane (9b)



The general procedure was followed and phenyltrimethylsilane (50 mg, 0.33 mmol) was added into the crude residue as the internal standard. The conversion of **9b** was determined by ^{1}H NMR (97% yield) (**Figure S30**). The desired product **9b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.27 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 2.48 (s, 3H) ppm. **^{13}C NMR (151 MHz, $CDCl_3$)**: δ 136.9, 130.8, 128.8, 127.8, 16.0 ppm.

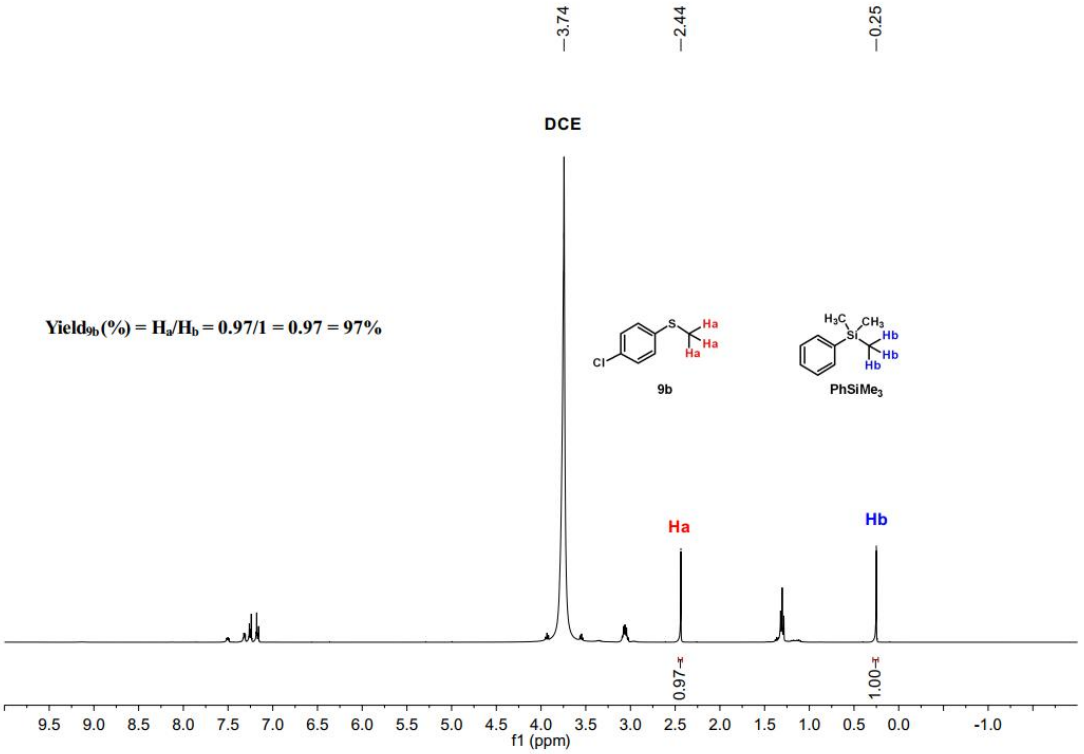
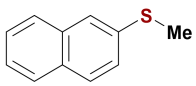


Figure S30. Crude ^{1}H NMR spectrum for the mixture of **9b**.

Methyl(naphthalen-2-yl)sulfane (10b)



The general procedure was followed and phenyltrimethylsilane (50 mg, 0.33 mmol) was added into the crude residue as the internal standard. The conversion of **10b** was determined by ^{1}H NMR (96% yield) (**Figure S31**). The desired product **10b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (600 MHz, $CDCl_3$)**: δ 7.78 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.61 (s, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 2.59 (s, 3H) ppm. **^{13}C NMR (151 MHz, $CDCl_3$)**: δ 136.1, 133.9, 131.3, 128.2, 127.7, 126.8, 126.5, 125.7, 125.2, 123.4, 15.8 ppm.

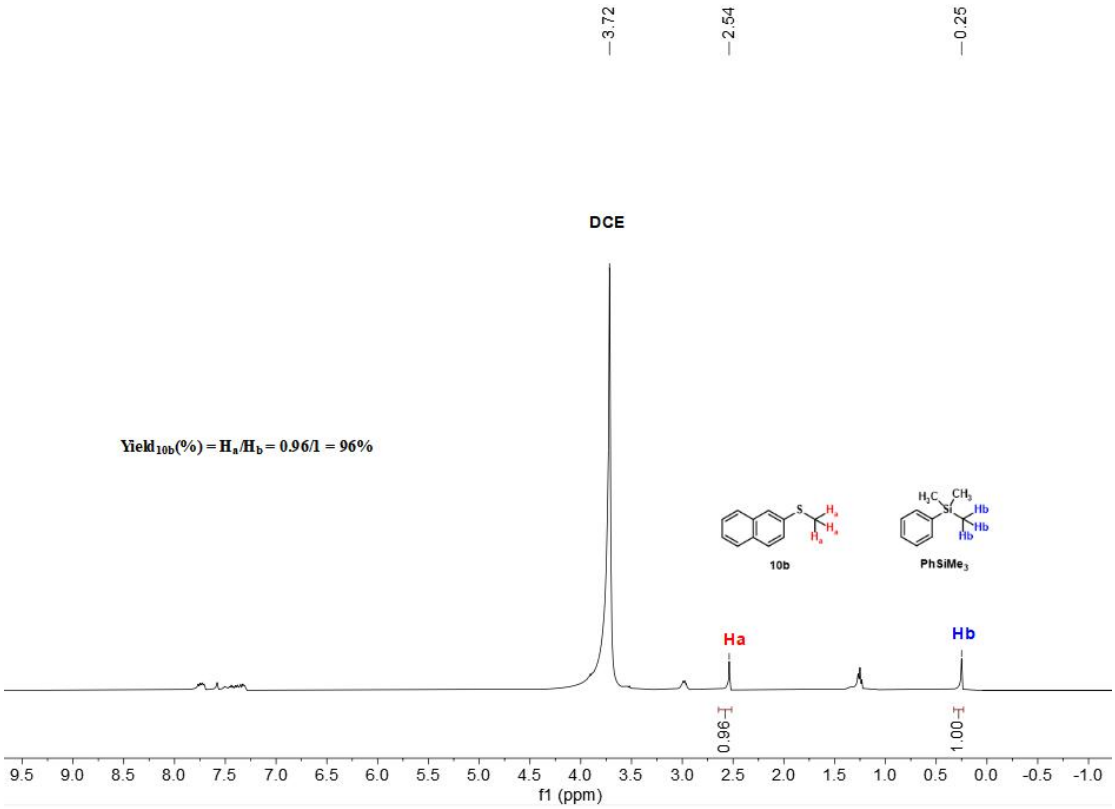
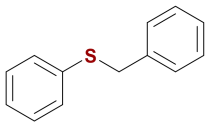
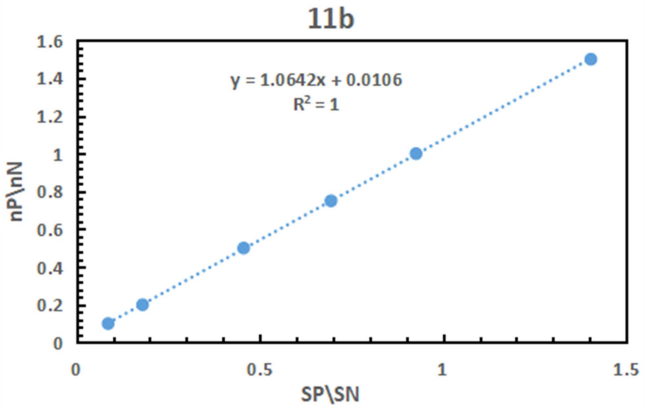


Figure S31. Crude ^{1}H NMR spectrum for the mixture of **10b**.

Benzyl(phenyl)sulfane (11b)



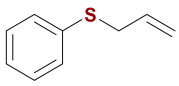
The general procedure was followed and dodecane (170.3 mg, 1.0 mmol) was added into the crude residue as the internal standard. The conversion of **11b** was determined by GC (83% yield) (**Figure S32**). The desired product **11b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.27 – 7.07 (m, 10H), 4.05 (s, 2H).**^{13}C NMR (151 MHz, $CDCl_3$)**: δ 137.3, 136.3, 129.7, 128.7, 128.4, 127.1, 126.2, 38.9 ppm.



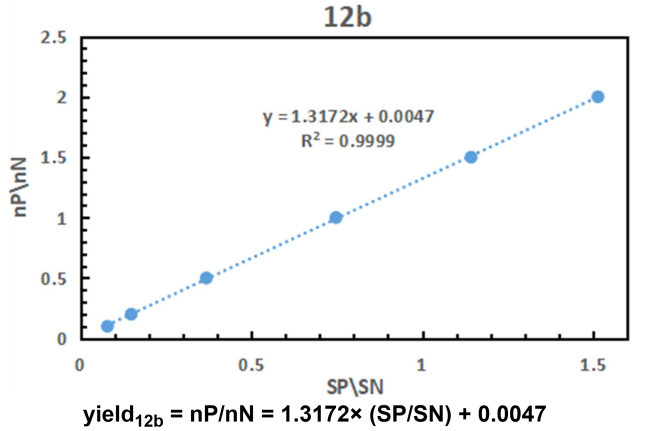
$yield_{11b}$ = nP/nN = 1.0642× (SP/SN) + 0.0106
= 1.0642× (43.5/56.5) + 0.0106 = 0.83 = 83%

Figure S32. GC standard cure of **11b** to dodecane and the GC yield of **11b**.

Allyl(phenyl)sulfane (12b)



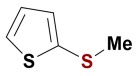
The general procedure was followed and dodecane (170.3 mg, 1.0 mmol) was added into the crude residue as the internal standard. The conversion of **12b** was determined by GC (65% yield) (**Figure S33**). The desired product **12b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.39 – 7.32 (m, 2H), 7.32 – 7.26 (m, 2H), 7.23 – 7.15 (m, 1H), 5.96 – 5.83 (m, 1H), 5.15 (dd, *J* = 17.0, 1.4 Hz, 1H), 5.08 (d, *J* = 10.0 Hz, 1H), 3.56 (d, *J* = 6.9 Hz, 2H) ppm. **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 135.9, 133.5, 129.8, 128.7, 126.2, 117.6, 37.1 ppm.



$yield_{12b}$ = nP/nN = 1.3172× (SP/SN) + 0.0047
= 1.3172× (27.68/72.32) + 0.0047 = 0.65 = 65%

Figure S33. GC standard cure of 1**2b** to dodecane and the GC yield of 1**2b**.

2-(Methylthio)thiophene (13b)



The general procedure was followed and phenyltrimethylsilane (50 mg, 0.33 mmol) was added into the crude residue as the internal standard. The conversion of **13b** was determined by ^{1}H NMR (80% yield) (**Figure S34**). The desired product **13b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.30 (d, *J* = 5.3 Hz, 1H), 7.08 (d, *J* = 3.6 Hz, 1H), 6.96 (dd, *J* = 5.3, 3.6 Hz, 1H), 2.49 (s, 3H) ppm. **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 137.1, 131.0, 127.9, 127.4, 22.2 ppm.

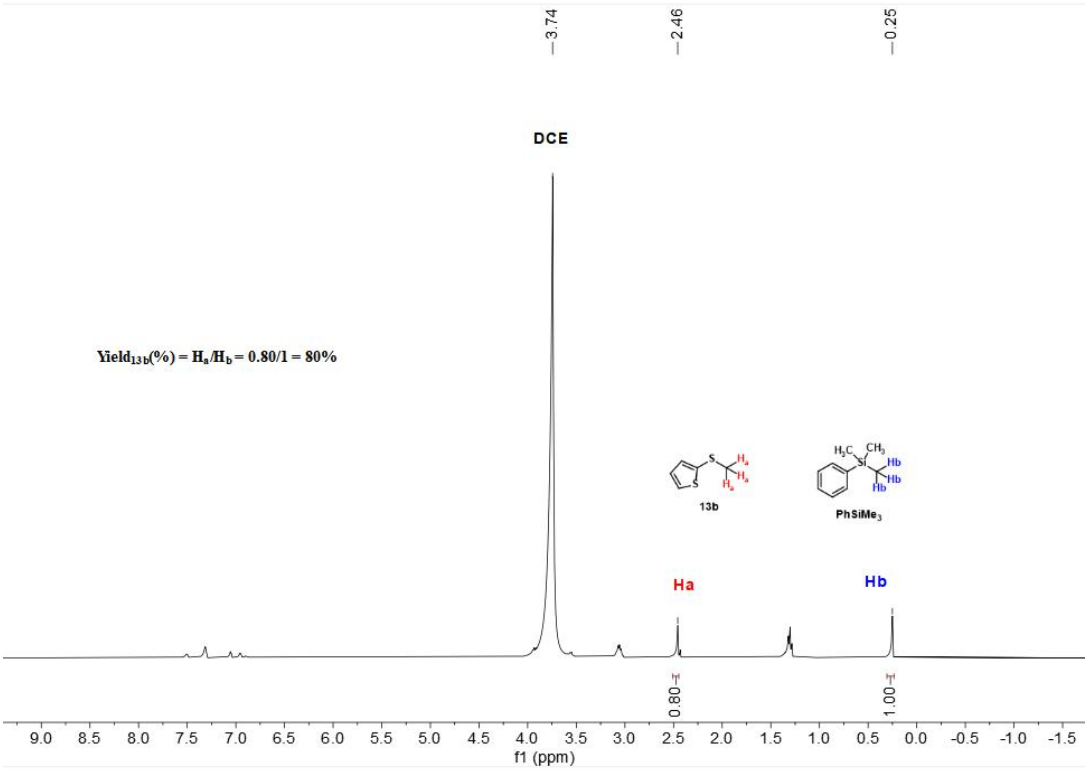
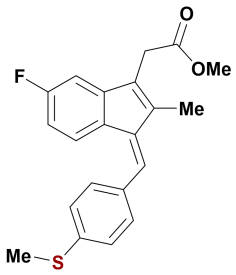


Figure S34. Crude ^{1}H NMR spectrum for the mixture of **13b**.

Methyl (Z)-2-(5-fluoro-2-methyl-1-(4-(methylthio)benzylidene)-1H-inden-3-yl)acetate (14b)



The general procedure was followed and phenyltrimethylsilane (50 mg, 0.33 mmol) was added into the crude residue as the internal standard. The conversion of **14b** was determined by ^{1}H NMR (95% yield) (**Figure S35**). The desired product **14b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.2 Hz, 1H), 7.37 (dd, *J* = 8.4, 5.2 Hz, 1H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.14 (s, 1H), 6.88 (d, *J* = 8.8 Hz, 1H), 6.59 (t, *J* = 8.8 Hz, 1H), 3.70 (s, 3H), 3.57 (s, 2H), 2.54 (s, 3H), 2.20 (s, 3H) ppm. **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 170.8, 163.03 (d, *J* = 245.7 Hz), 146.39 (d, *J* = 8.8 Hz), 140.0 , 139.1, 138.4, 132.9, 130.60 (d, *J* = 2.7 Hz), 129.8, 129.71 (d, *J* = 2.8 Hz), 125.8, 125.5, 123.59 (d, *J* = 9.1 Hz), 110.47 (d, *J* = 22.7 Hz), 105.67 (d, *J* = 23.9 Hz), 52.1, 31.5, 15.3, 10.5 ppm. **^{19}F NMR (376 MHz, $CDCl_3$)**: δ -113.74 ppm.

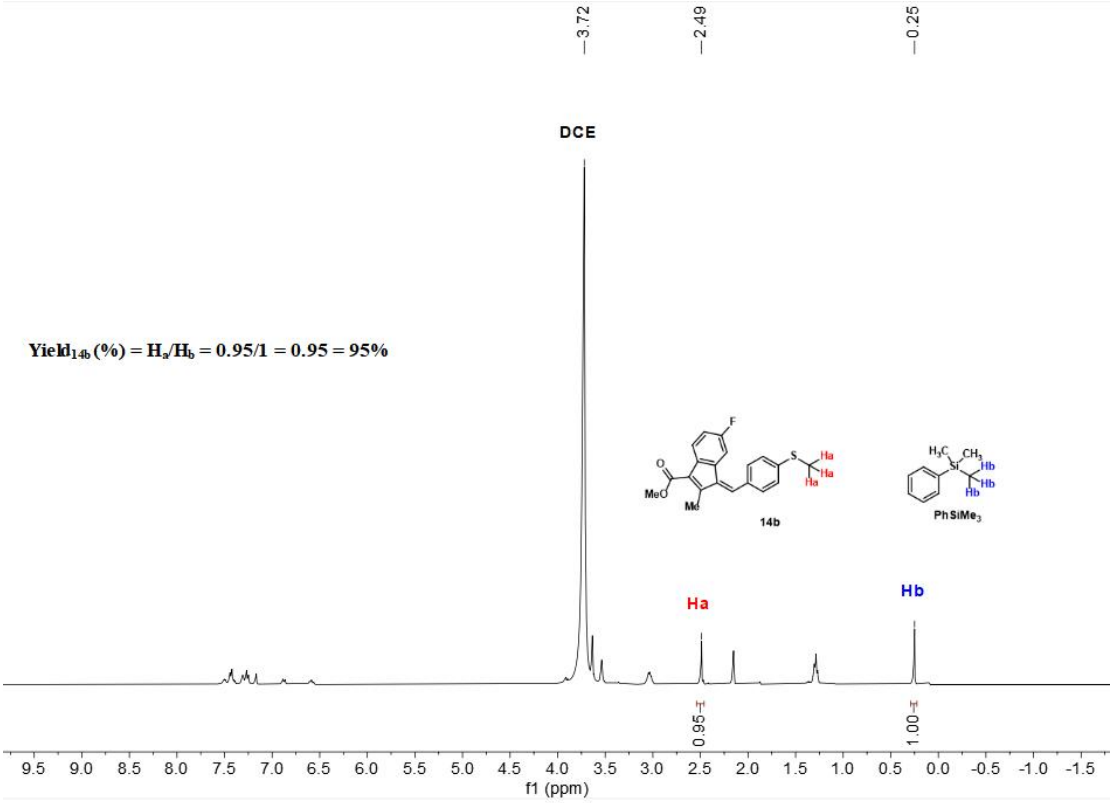
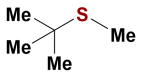
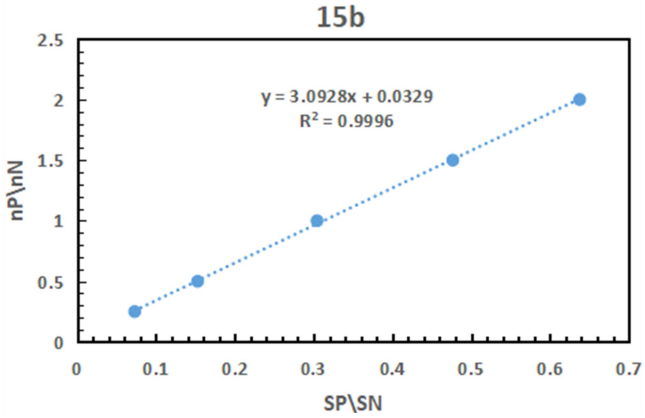


Figure S35. Crude ^{1}H NMR spectrum for the mixture of **14b**.

Tert-butyl(methyl)sulfane (15b)



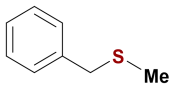
The general procedure was followed and dodecane (170.3 mg, 1.0 mmol) was added into the crude residue as the internal standard. The conversion of **15b** was determined by GC (66% yield) (**Figure S36**). The desired product **15b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (600 MHz, $CDCl_3$):** δ 1.94 (s, 3H), 1.20 (s, 9H) ppm. **^{13}C NMR (151 MHz, $CDCl_3$):** δ 39.9, 29.7, 10.7 ppm.



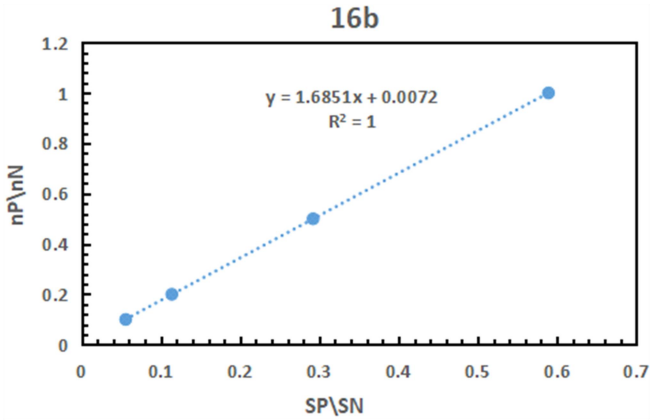
$yield_{15b}$ = nP/nN = 3.0928× (SP/SN) + 0.0329
= 3.0928× (16.815/83.185) + 0.0329 = 0.66 = 66%

Figure S36. GC standard cure of **15b** to dodecane and the GC yield of **15b**.

Benzyl(methyl)sulfane (16b)



The general procedure was followed and dodecane (170.3 mg, 1.0 mmol) was added into the crude residue as the internal standard. The conversion of **16b** was determined by GC (59% yield) (**Figure S37**). The desired product **16b** was also purified by silica gel column chromatography using petroleum ethe as eluent. **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 7.41 – 7.20 (m, 5H), 3.71 (s, 2H), 2.03 (s, 3H) ppm. **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 138.2, 128.8, 128.4, 126.9, 38.3, 14.9 ppm.



$yield_{16b}$ = nP/nN = 1.6851× (SP/SN) + 0.0072
= 1.6851× (25.613/74.387) + 0.0072 = 0.59 = 59%

Figure S37. GC standard cure of **16b** to dodecane and the GC yield of **16b**.

5. References

[1] Hui-ke Fan, Yang S ,Jun-hua Li,et al.BaO-Catalyzed α-Deuteration of Ketones, Sulfones, Sulfoxides, and Nitriles. *Eur. J. Org. Chem*. **2022**, e202201218

[2] Korvinson K , Akula H , Malinchak C ,et al. Catalytic Reductions Without External Hydrogen Gas: Broad Scope Hydrogenations with Tetrahydroxydiboron and a Tertiary Amine. *Adv. Synth. Catal*. **2020**, 166 – 176.

6. NMR date

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5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	295.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
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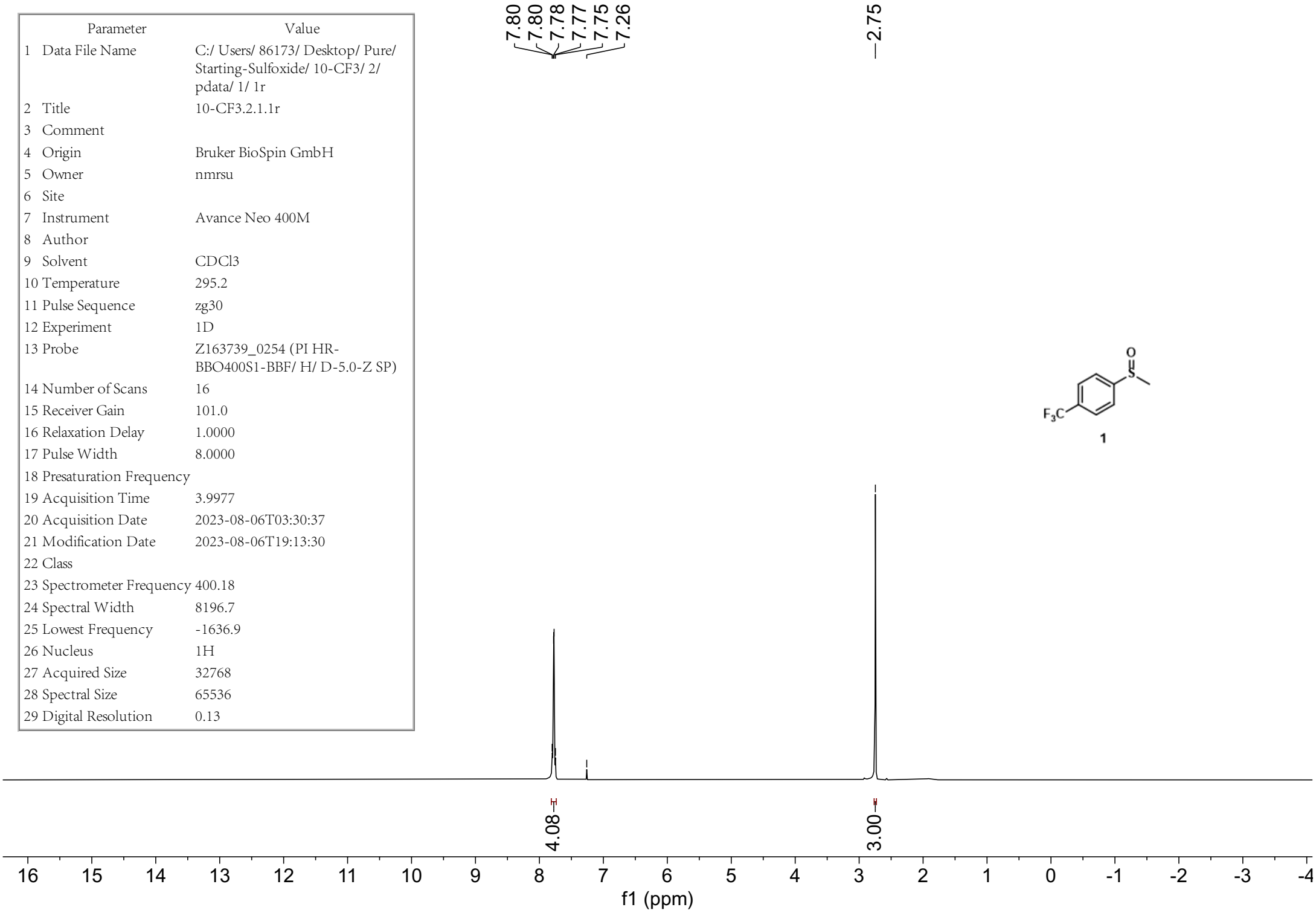
25 Lowest Frequency	-1636.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



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6	Site	
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8	Author	
9	Solvent	CDCl3
10	Temperature	296.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
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18	Presaturation Frequency	
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21	Modification Date	2023-08-06T19:13:32
22	Class	
23	Spectrometer Frequency	100.64
24	Spectral Width	23809.5
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26	Nucleus	13C
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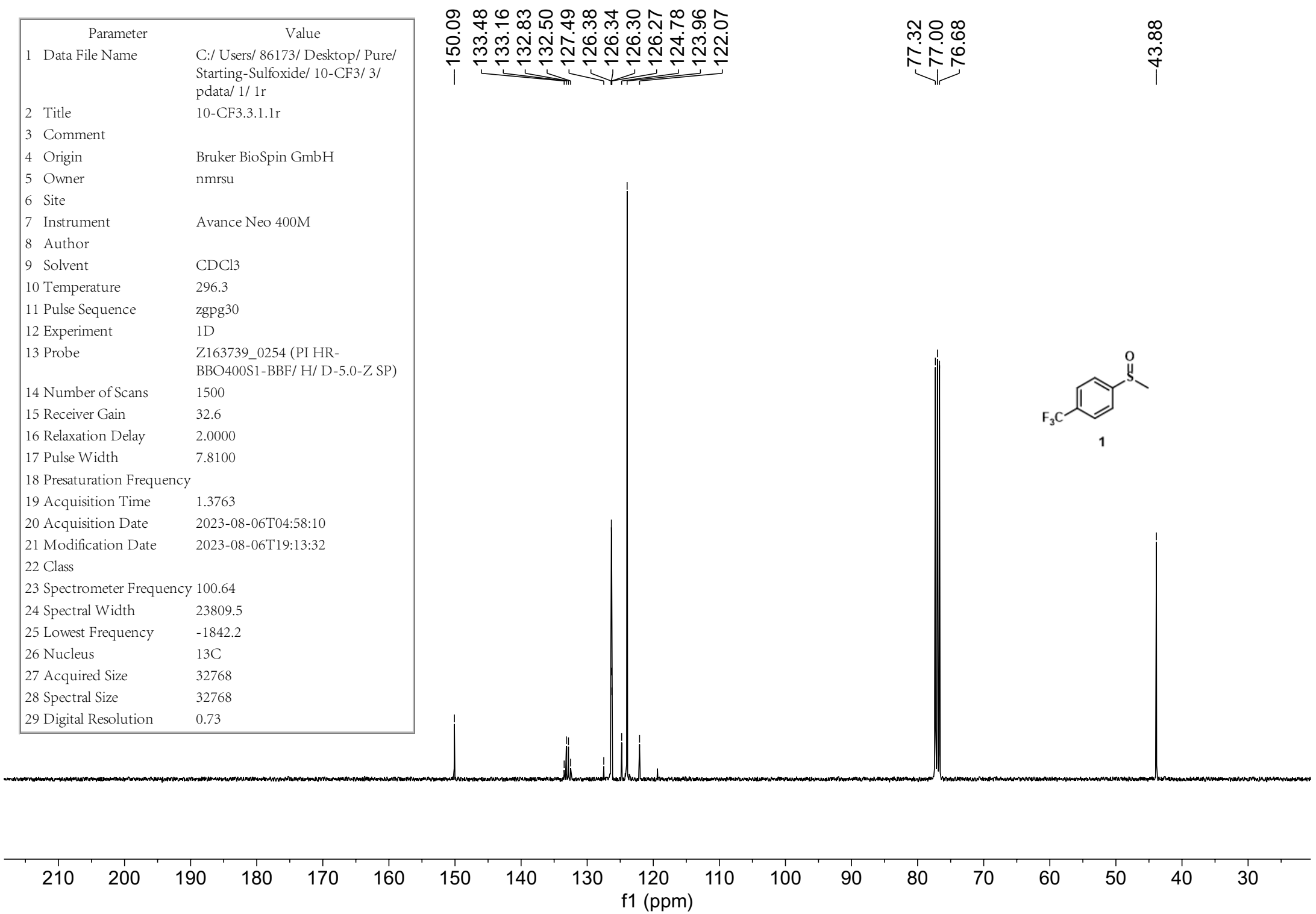
28	Spectral Size	32768
29	Digital Resolution	0.73



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5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	295.8
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	11.7400
18 Presaturation Frequency	
19 Acquisition Time	0.7209
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22 Class	
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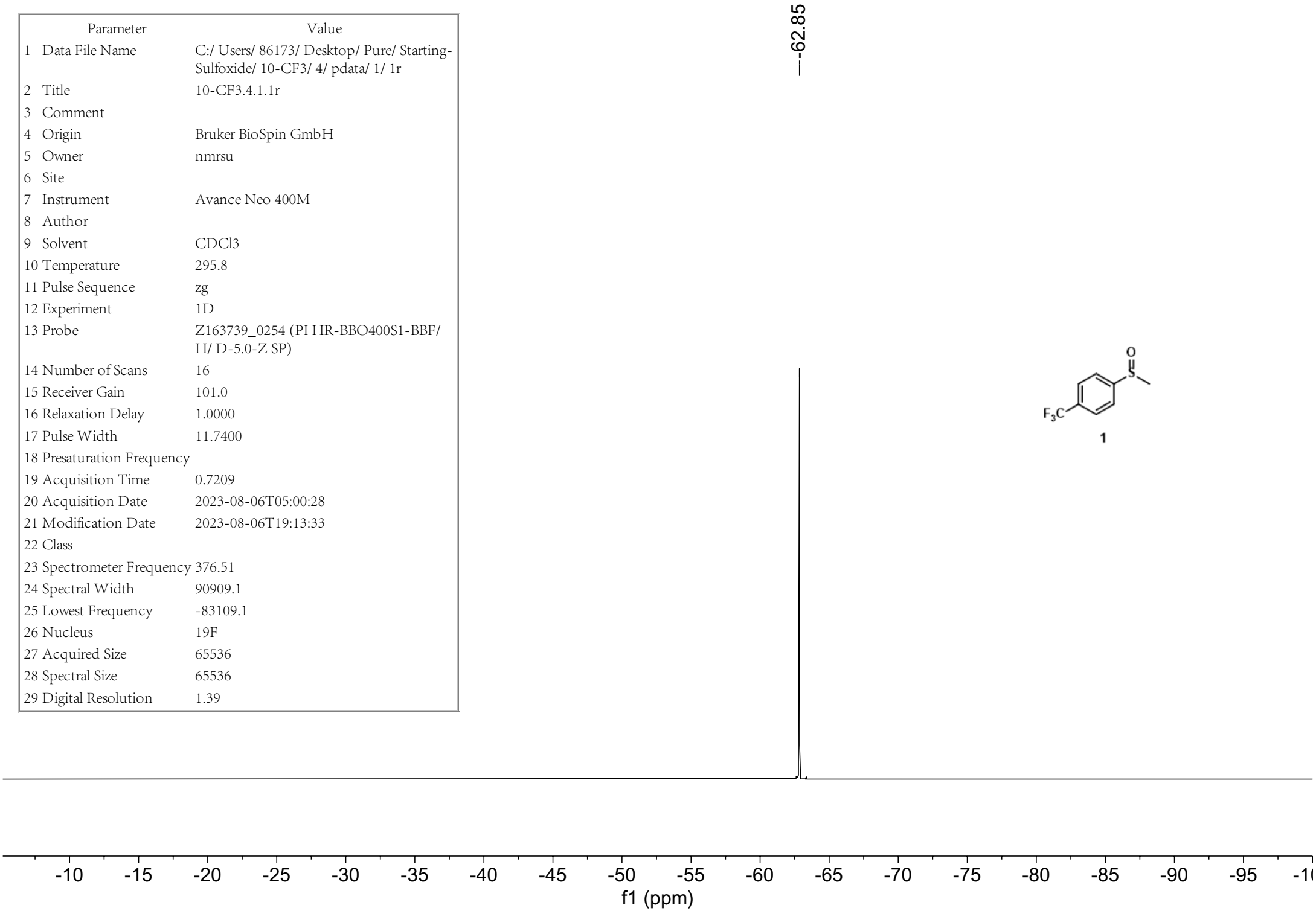

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5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	294.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
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18 Presaturation Frequency	
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26 Nucleus	1H
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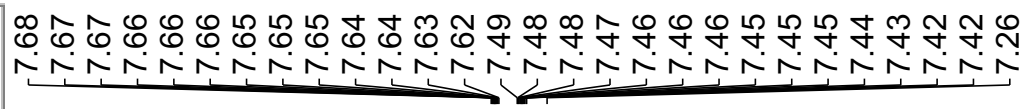

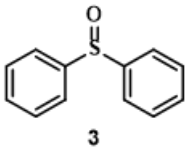

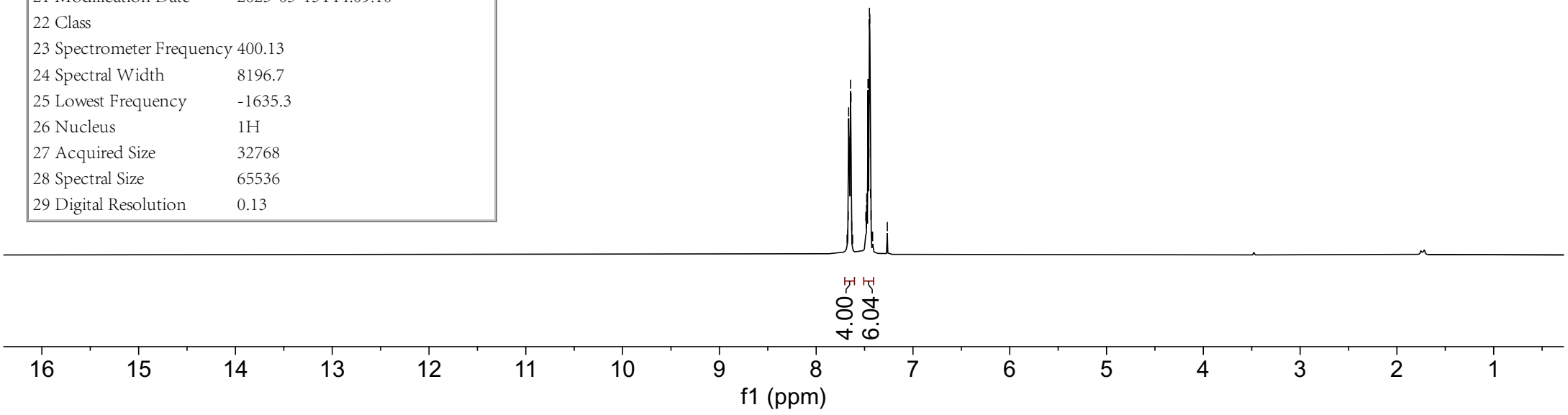

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6 Site	
7 Instrument	Avance Neo 400M
8 Author	
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10 Temperature	297.1
11 Pulse Sequence	zgpg30
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14 Number of Scans	1024
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19 Acquisition Time	1.3763
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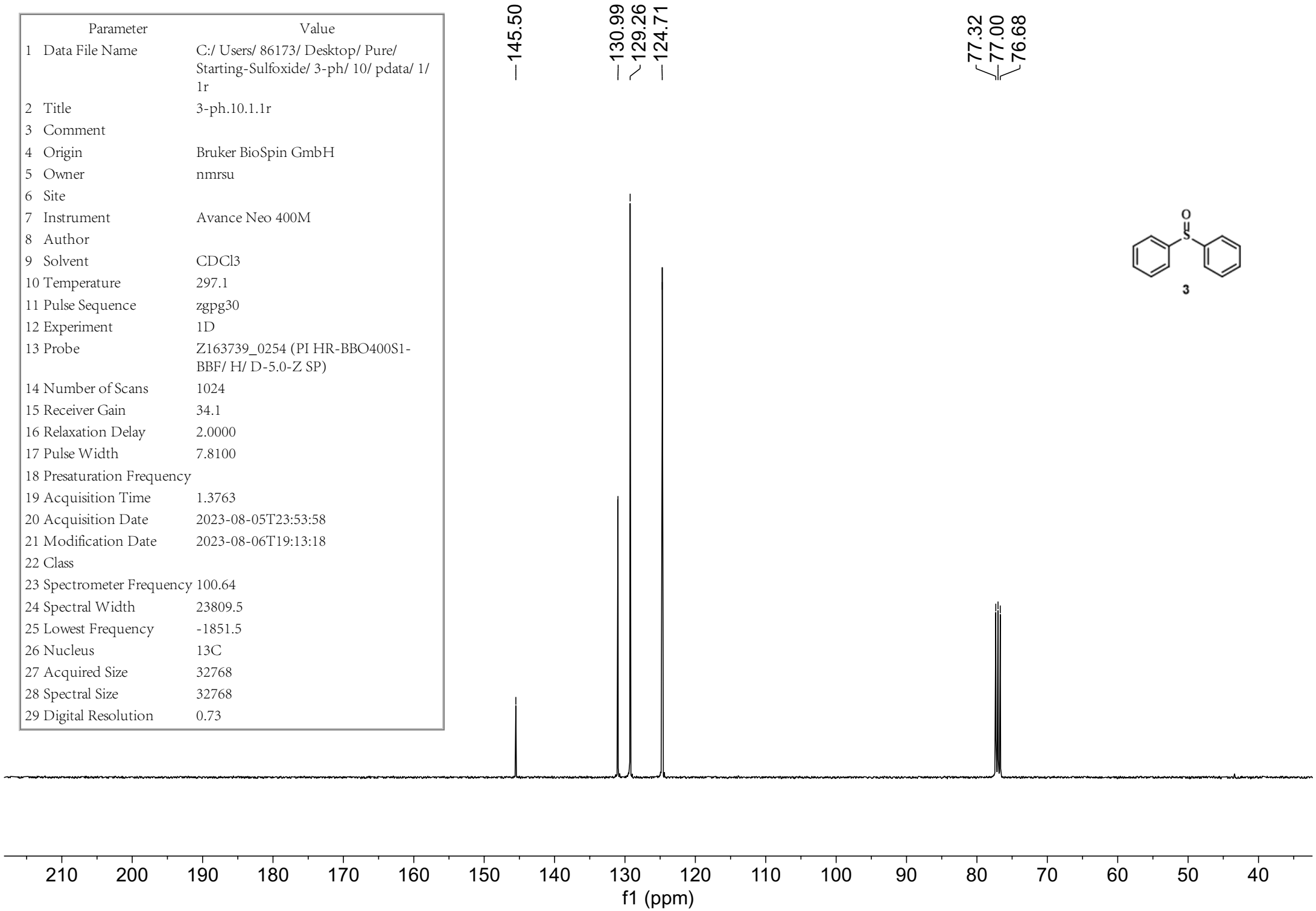
29 Digital Resolution	0.73



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5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
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11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
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18 Presaturation Frequency	
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22 Class	
23 Spectrometer Frequency	400.18
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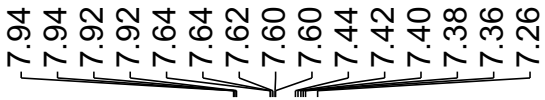

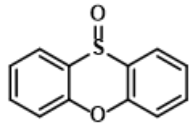

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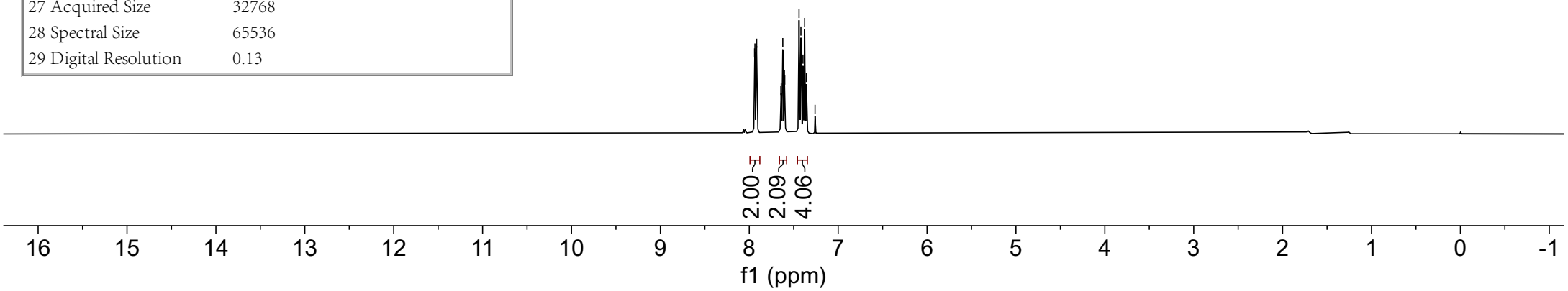

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5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	296.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
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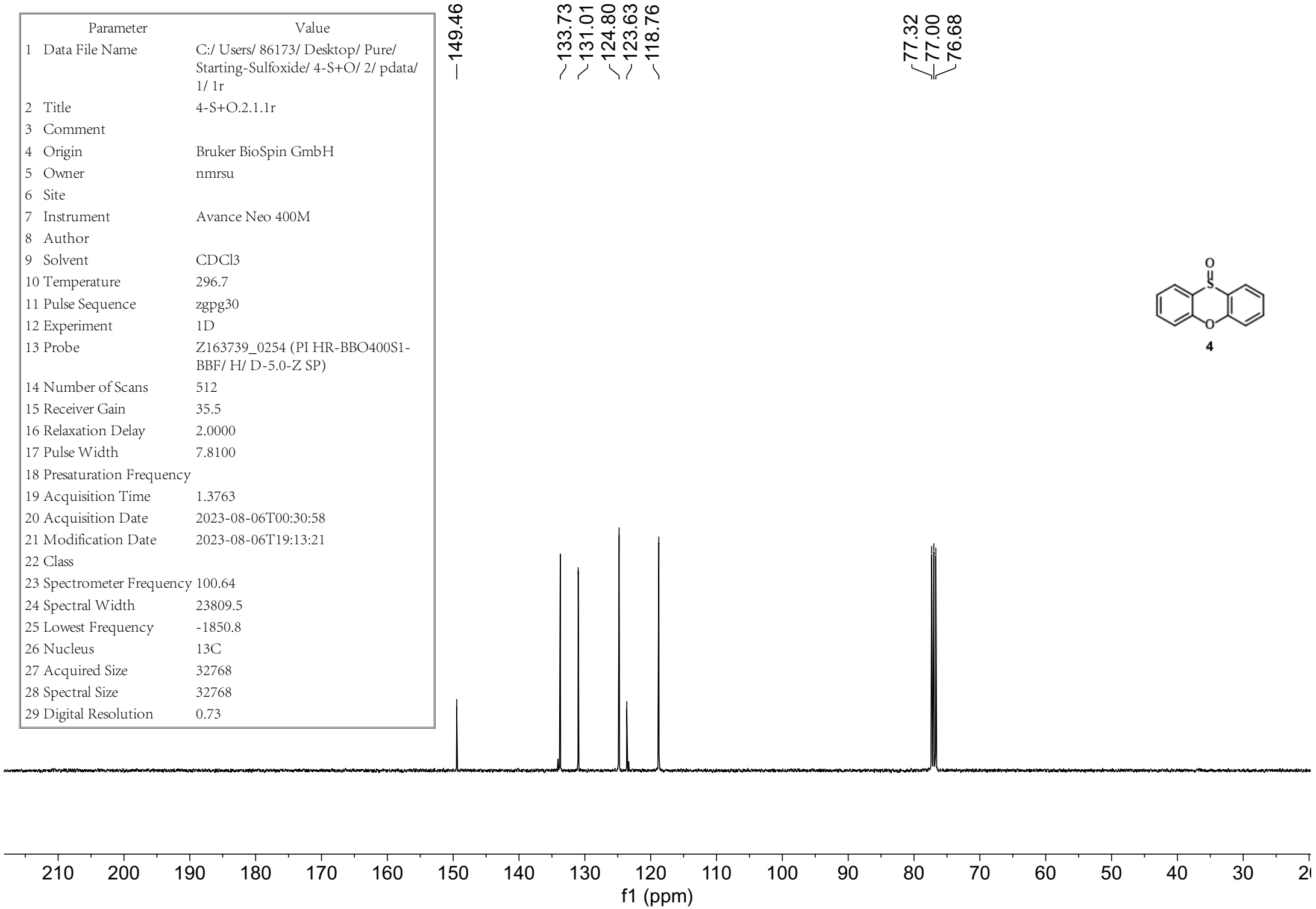

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6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	296.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	16
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25 Lowest Frequency	-1636.0
26 Nucleus	1H
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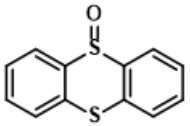

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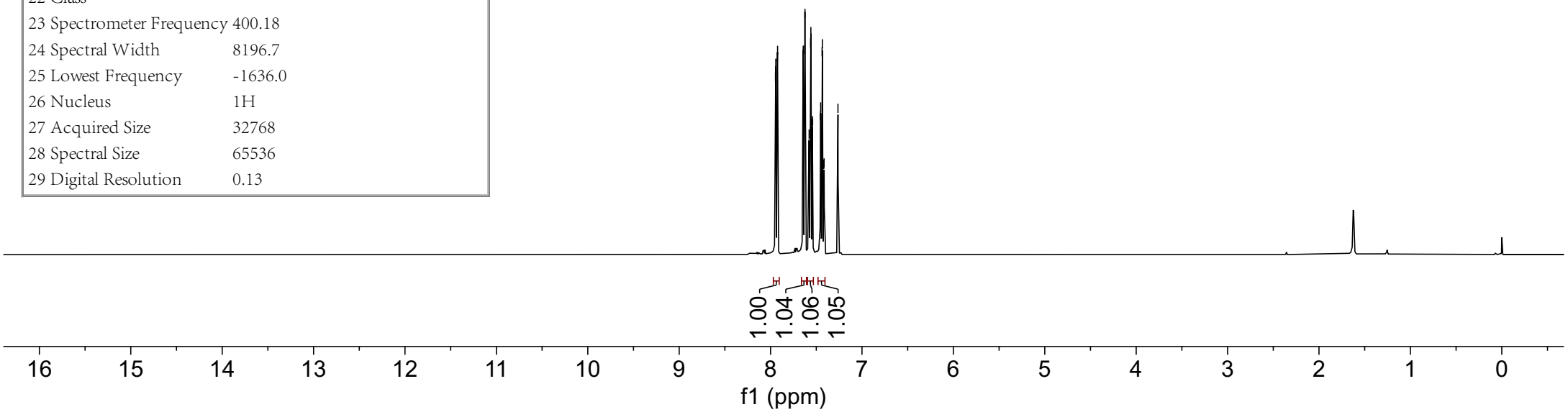

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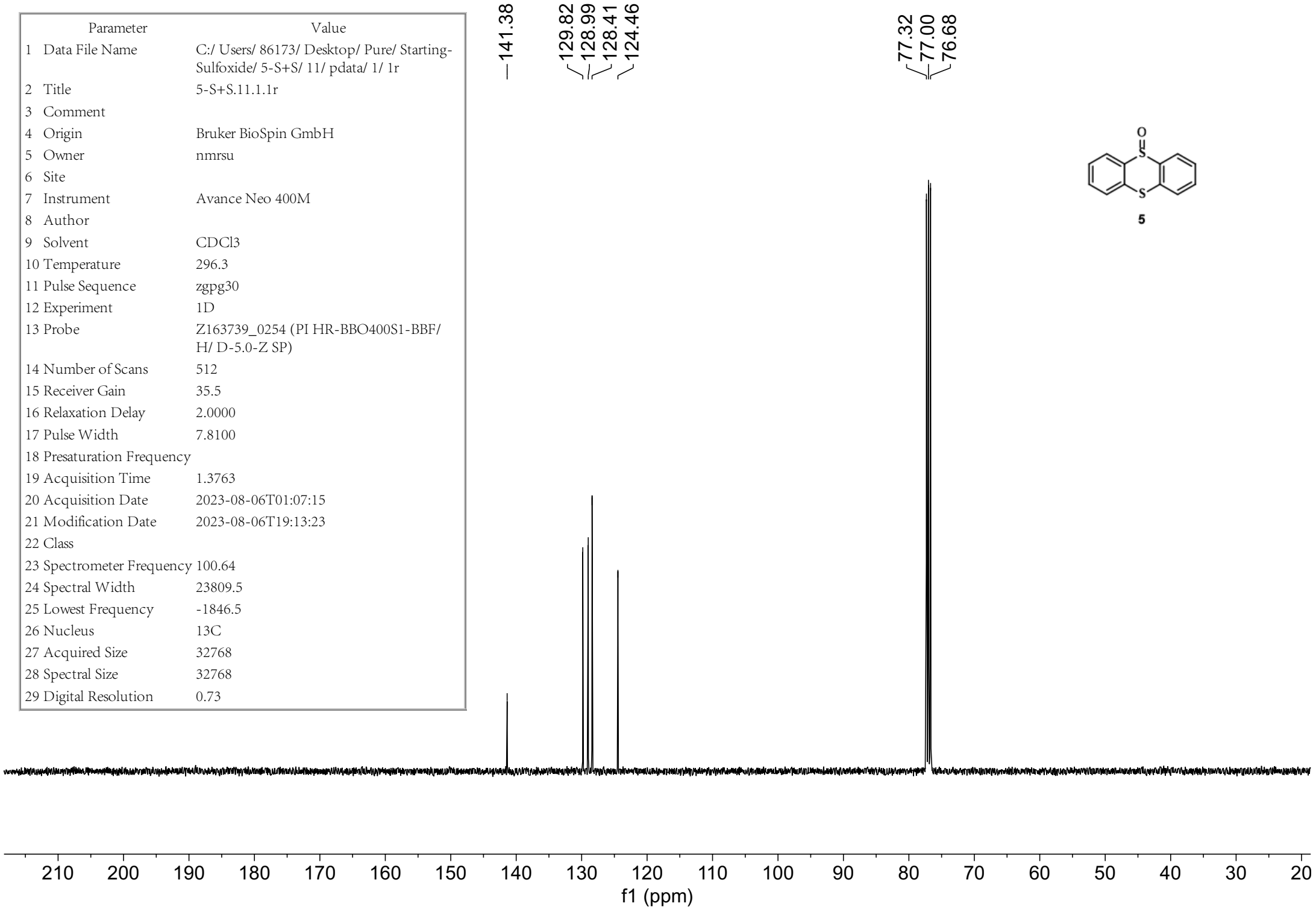

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5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	71.8
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.7525
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21 Modification Date	2023-08-07T14:18:52
22 Class	
23 Spectrometer Frequency	600.15
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26 Nucleus	1H
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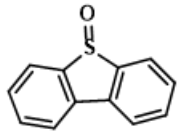

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10 Temperature	298.2
11 Pulse Sequence	zgpg30
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132.46
129.44
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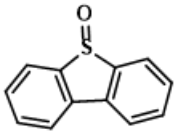

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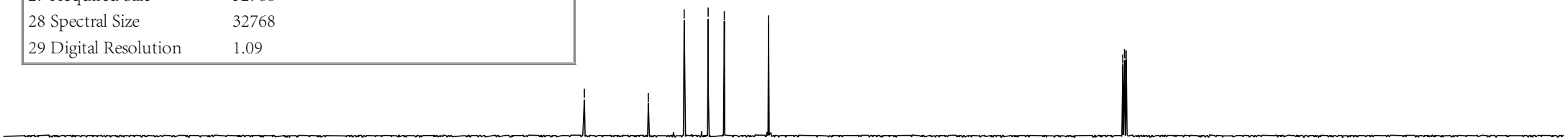

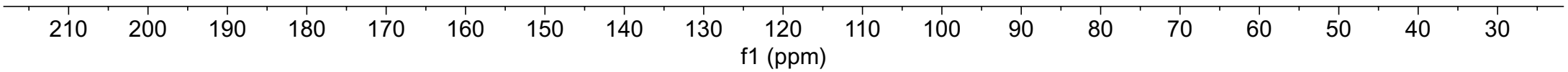

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5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
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14 Number of Scans	8
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17 Pulse Width	10.0000
18 Presaturation Frequency	
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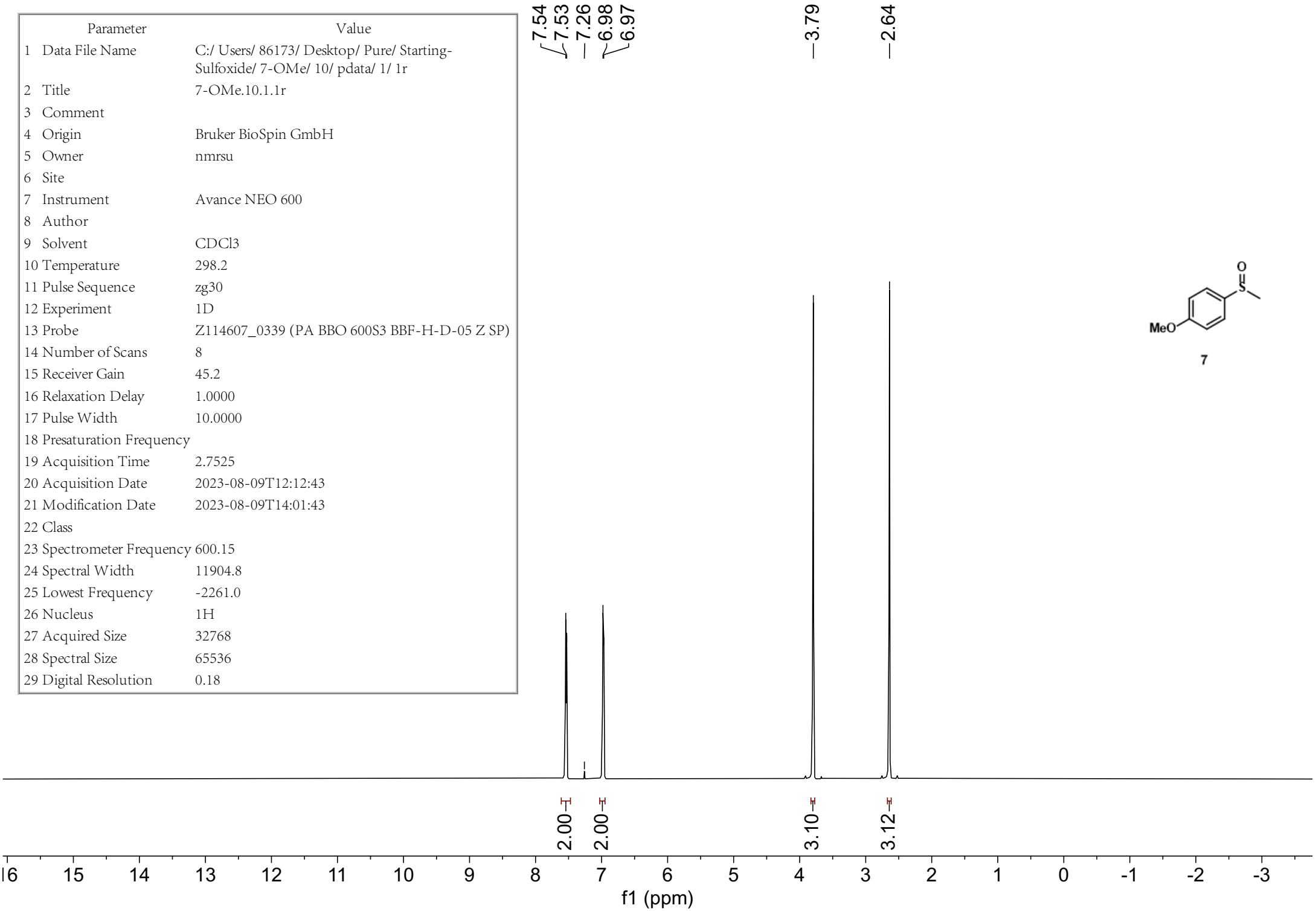
28 Spectral Size	65536
29 Digital Resolution	0.18



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5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
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11 Pulse Sequence	zgpg30
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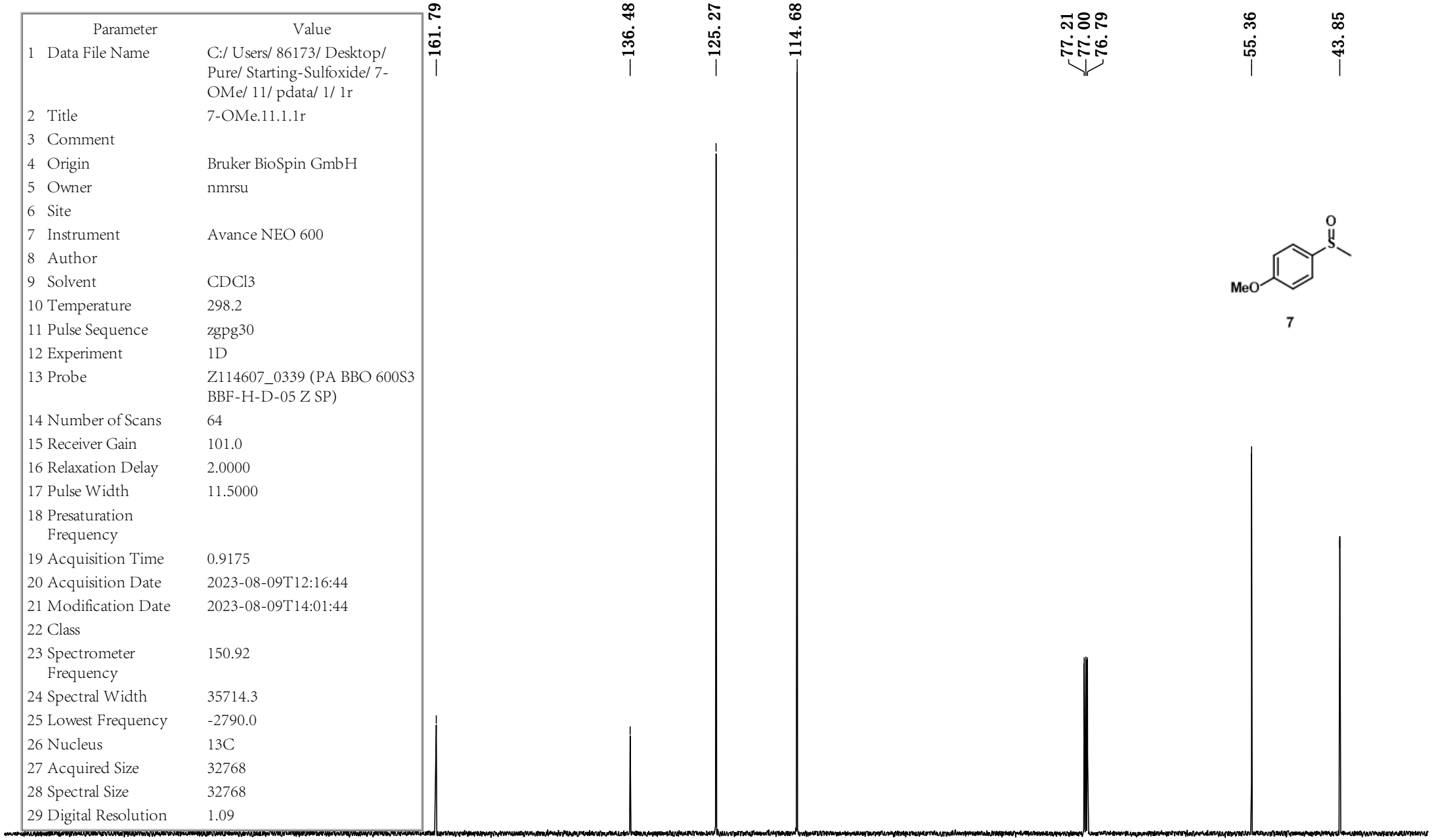
28 Spectral Size	32768
29 Digital Resolution	1.09



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6	Site	
7	Instrument	Avance NEO 600
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zg30
12	Experiment	1D
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17	Pulse Width	10.0000
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21	Modification Date	2023-08-07T14:18:48
22	Class	
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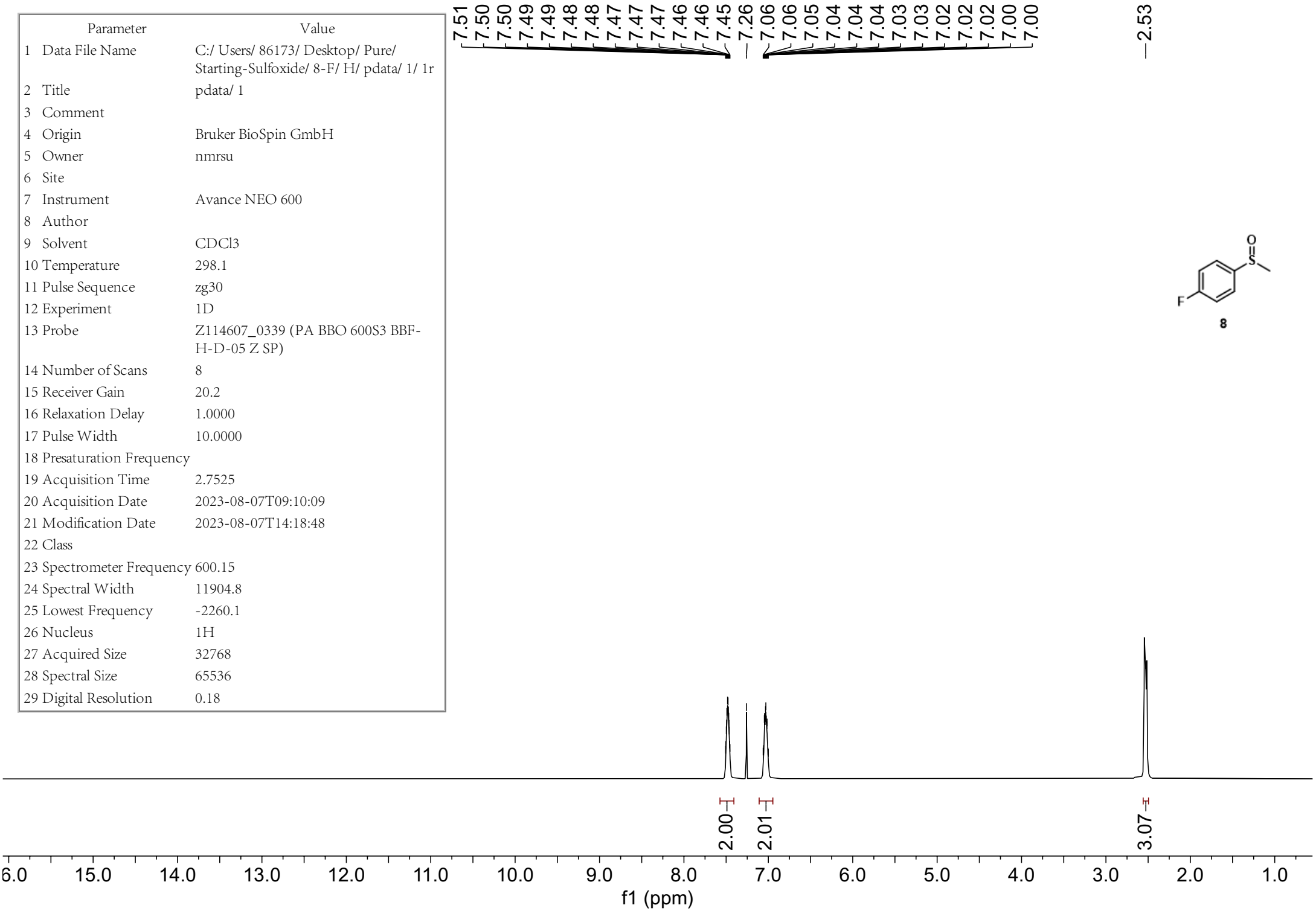
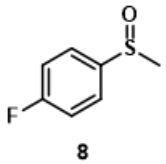
24	Spectral Width	11904.8
25	Lowest Frequency	-2260.1
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536
29	Digital Resolution	0.18



Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 8-F/ F/ pdata/ 1/ 1r
2 Title	8-F.11.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	296.0
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	11.7400
18 Presaturation Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2023-08-06T01:56:33
21 Modification Date	2023-08-06T19:13:27
22 Class	
23 Spectrometer Frequency	376.51
24 Spectral Width	90909.1
25 Lowest Frequency	-83109.1
26 Nucleus	19F
27 Acquired Size	65536
28 Spectral Size	65536
29 Digital Resolution	1.39



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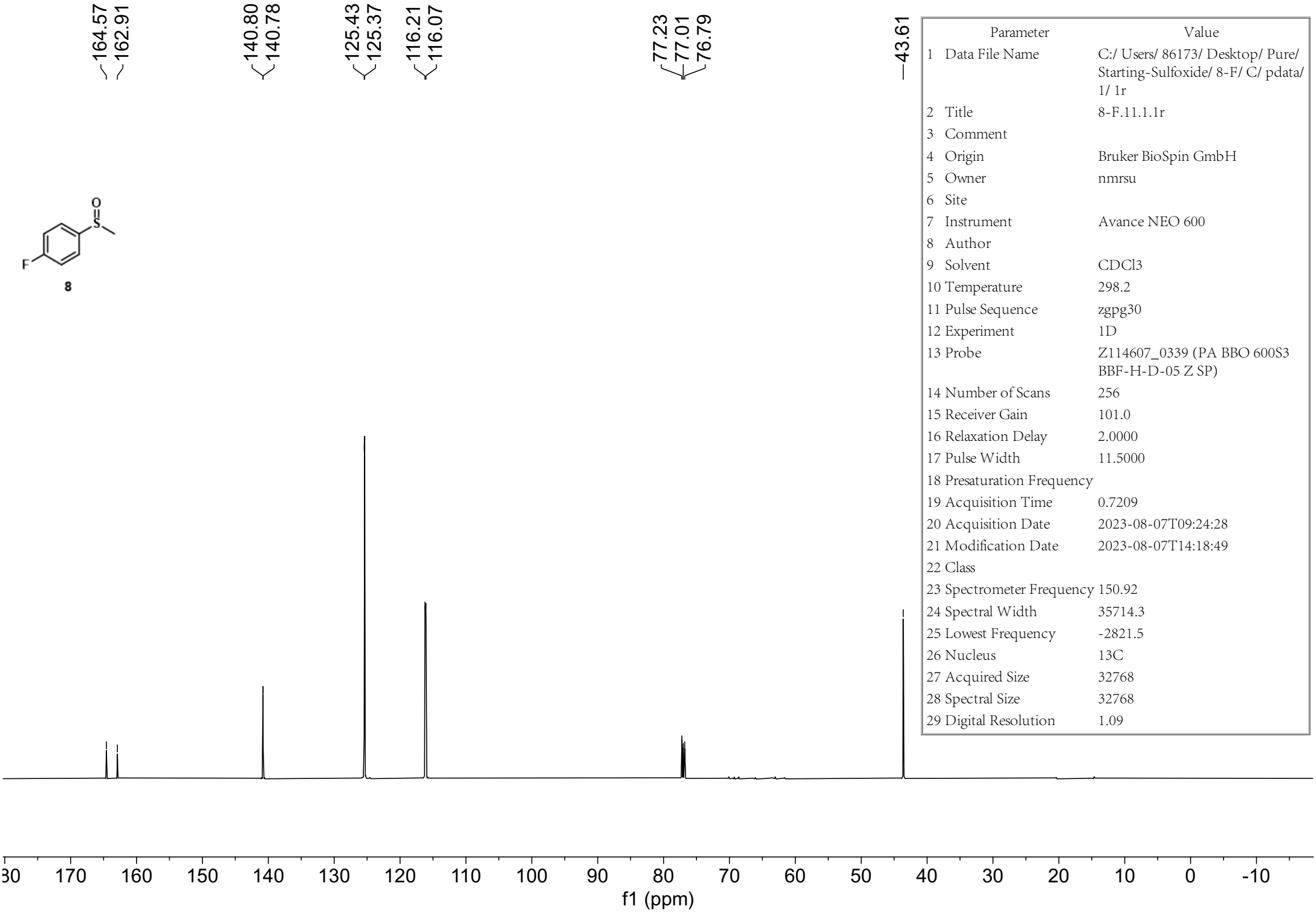
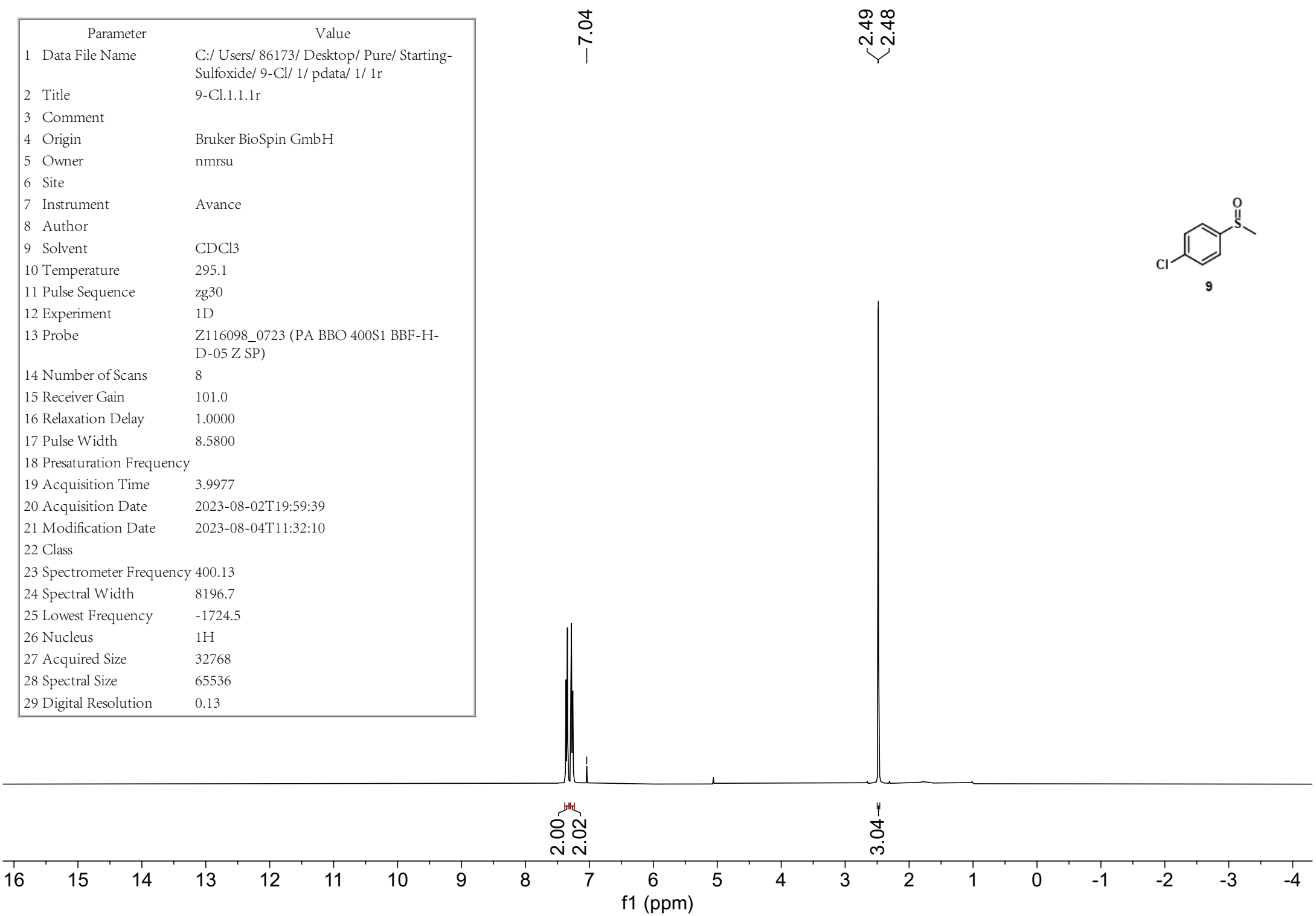


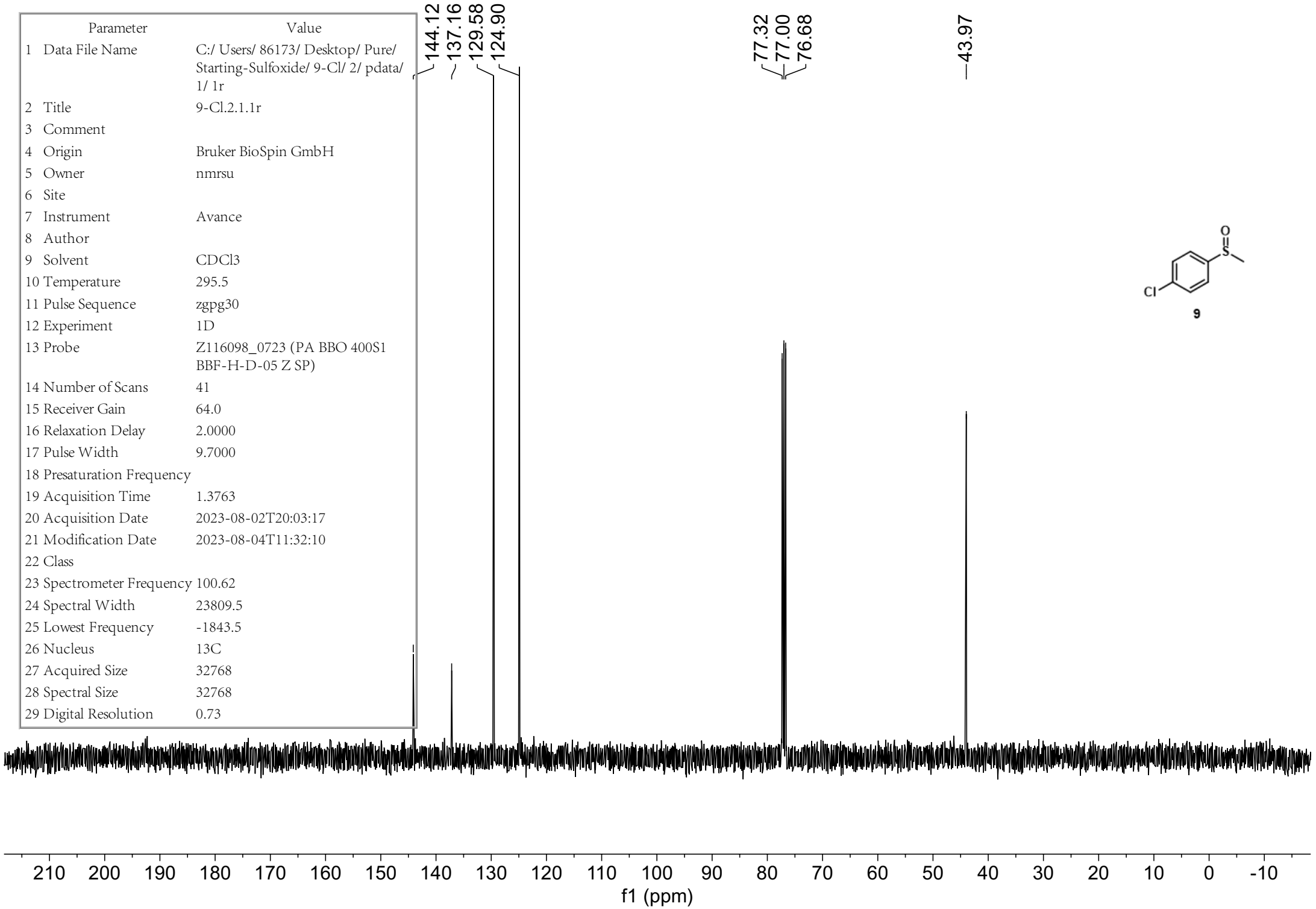
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 8-F/ C/ pdata/ 1/ 1r
2 Title	8-F.11.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	256
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	11.5000
18 Presaturation Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2023-08-07T09:24:28
21 Modification Date	2023-08-07T14:18:49
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2821.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09

Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 9-Cl/ 1/ pdata/ 1/ 1r
2 Title	9-Cl.1.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.5800
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-08-02T19:59:39
21 Modification Date	2023-08-04T11:32:10
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1724.5
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

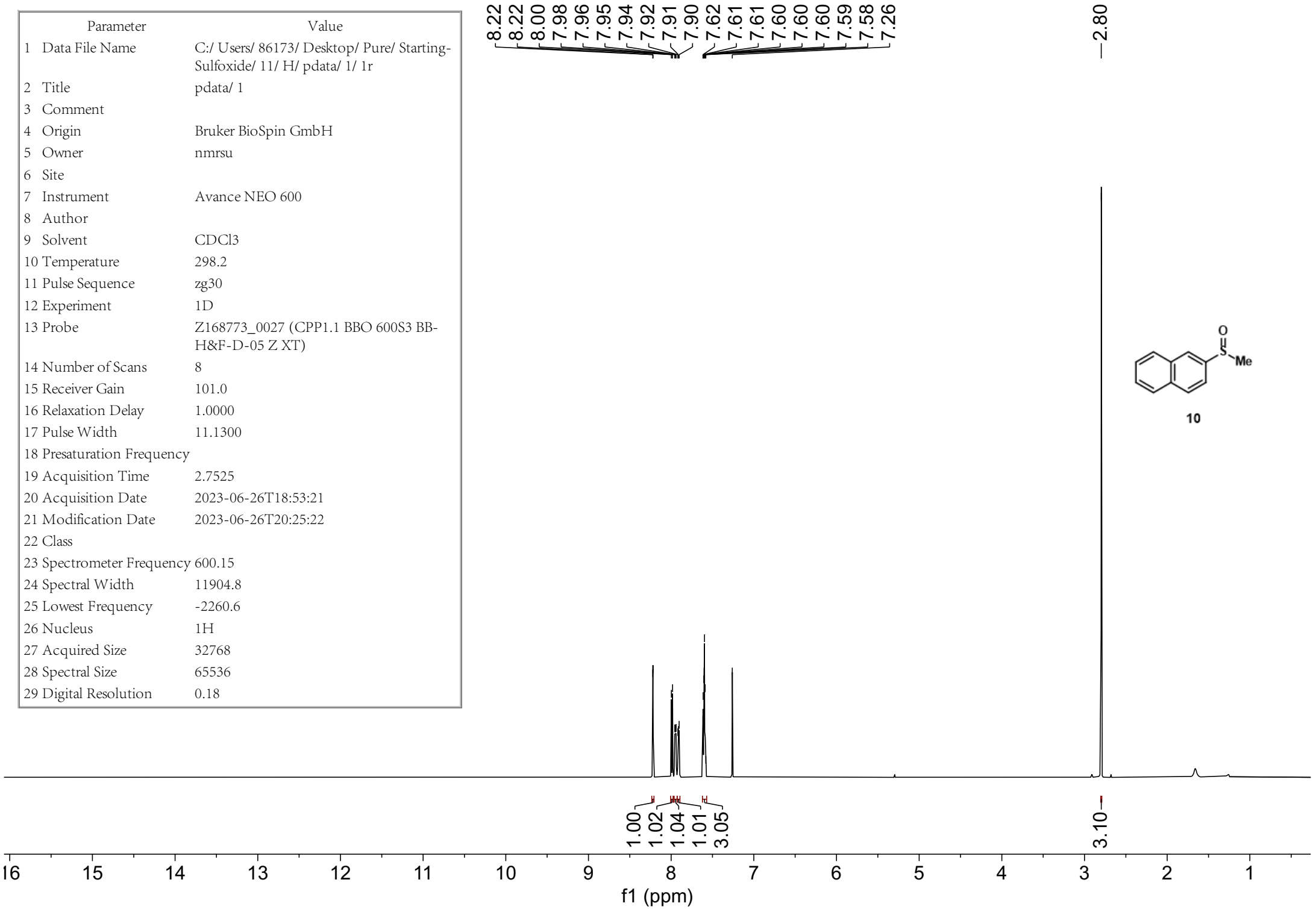


9

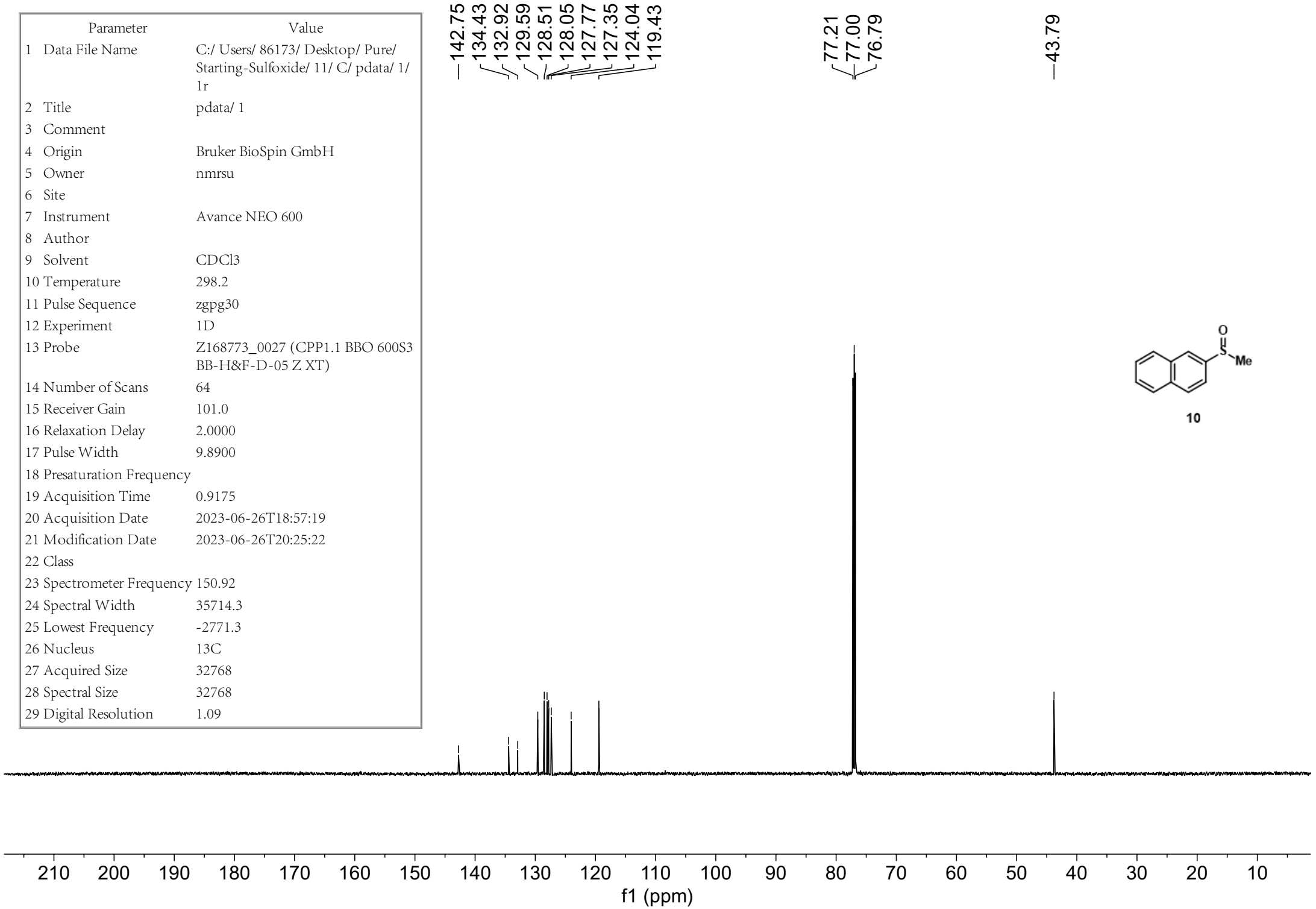
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 9-Cl/ 2/ pdata/ 1/ 1r
2 Title	9-Cl.2.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	295.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	41
15 Receiver Gain	64.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.7000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-08-02T20:03:17
21 Modification Date	2023-08-04T11:32:10
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73

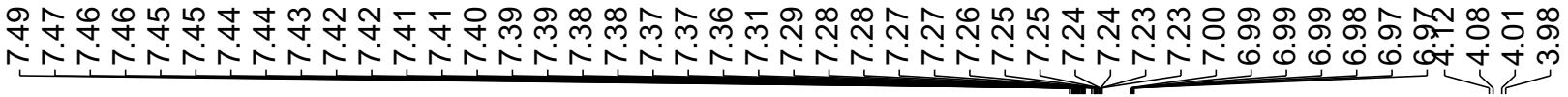


Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 11/ H/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	11.1300
18 Presaturation Frequency	
19 Acquisition Time	2.7525
20 Acquisition Date	2023-06-26T18:53:21
21 Modification Date	2023-06-26T20:25:22
22 Class	
23 Spectrometer Frequency	600.15
24 Spectral Width	11904.8
25 Lowest Frequency	-2260.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.18

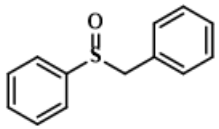


Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 11/ C/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans	64
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.8900
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-06-26T18:57:19
21 Modification Date	2023-06-26T20:25:22
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2771.3
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09





Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 12/ 1/ pdata/ 1/ 1r
2 Title	12.1.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	295.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.5800
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-08-09T21:42:24
21 Modification Date	2023-08-10T14:01:18
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1636.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



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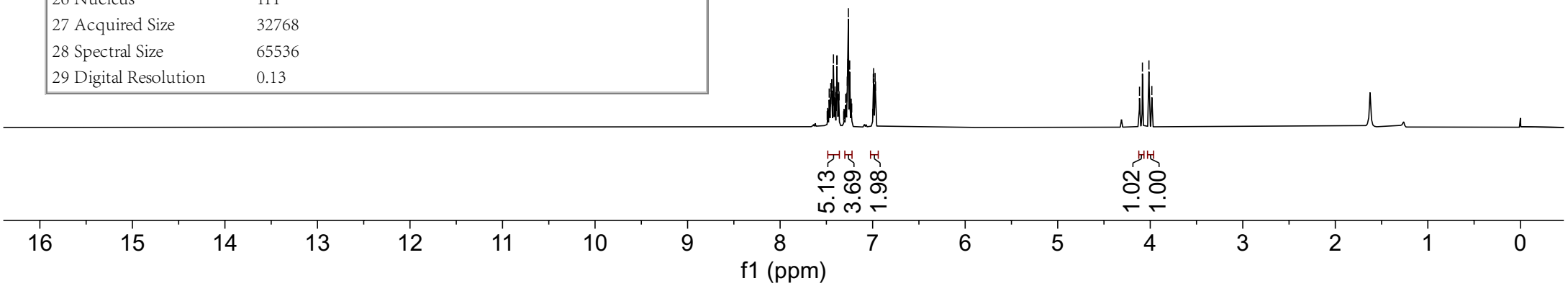
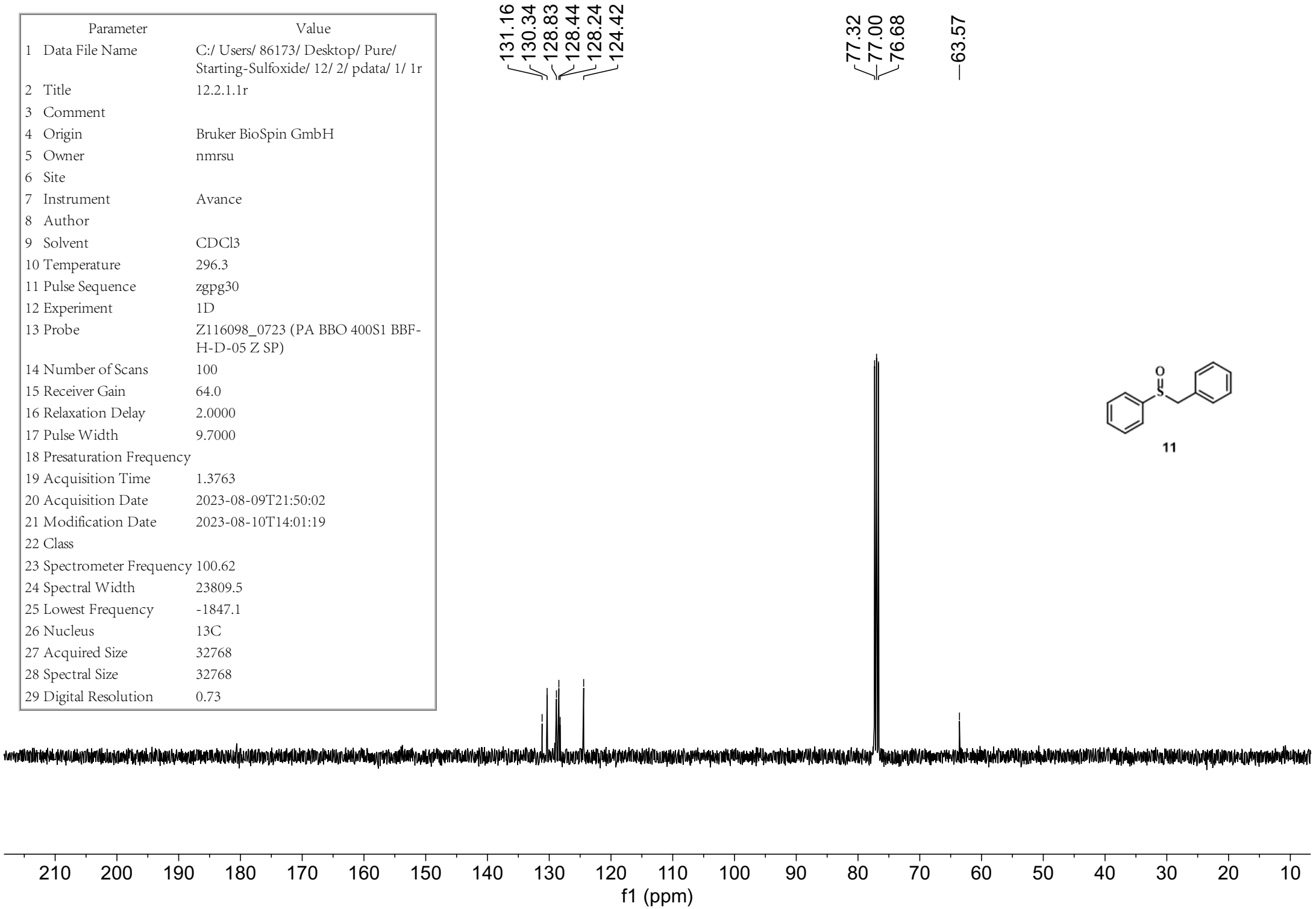
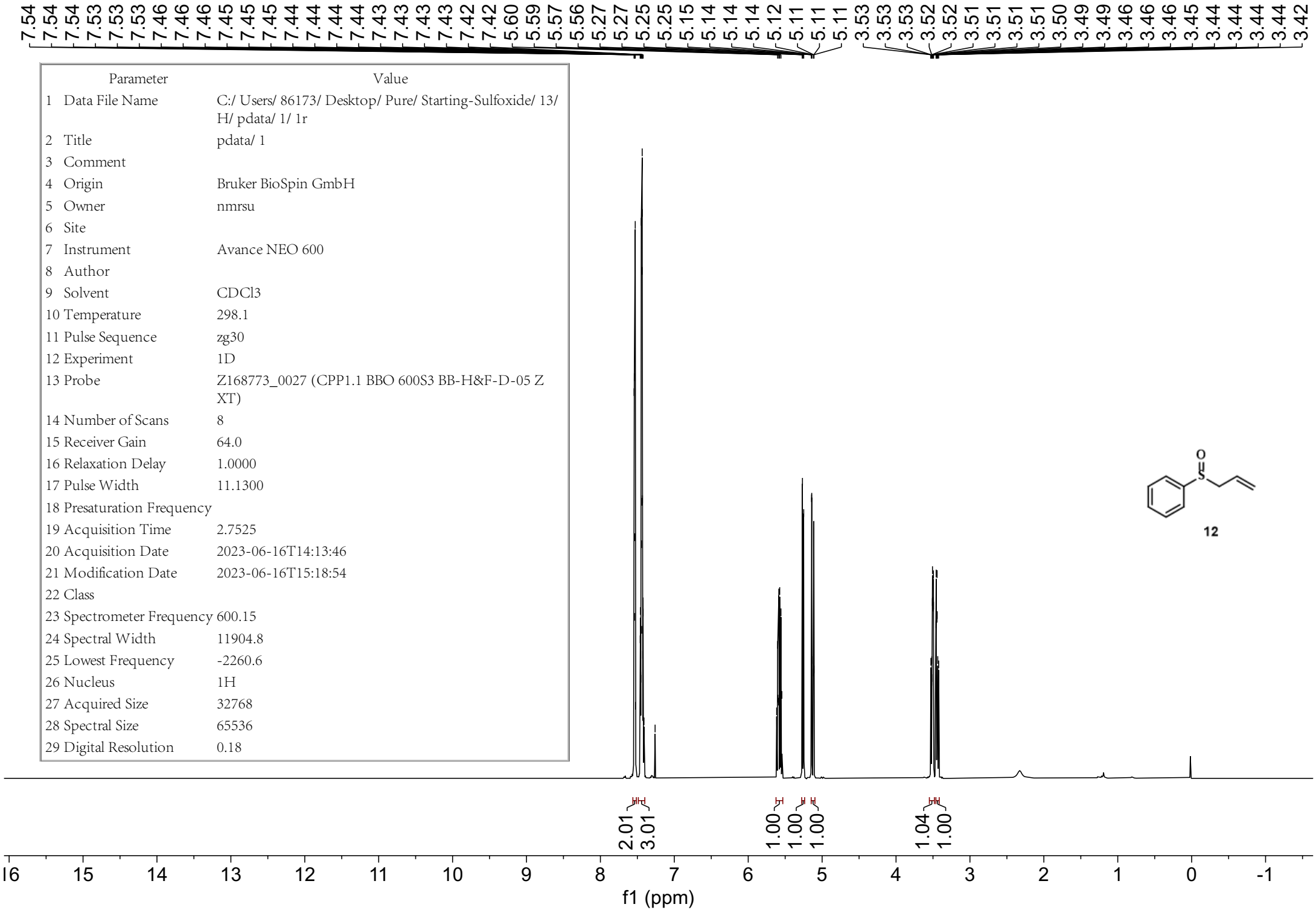
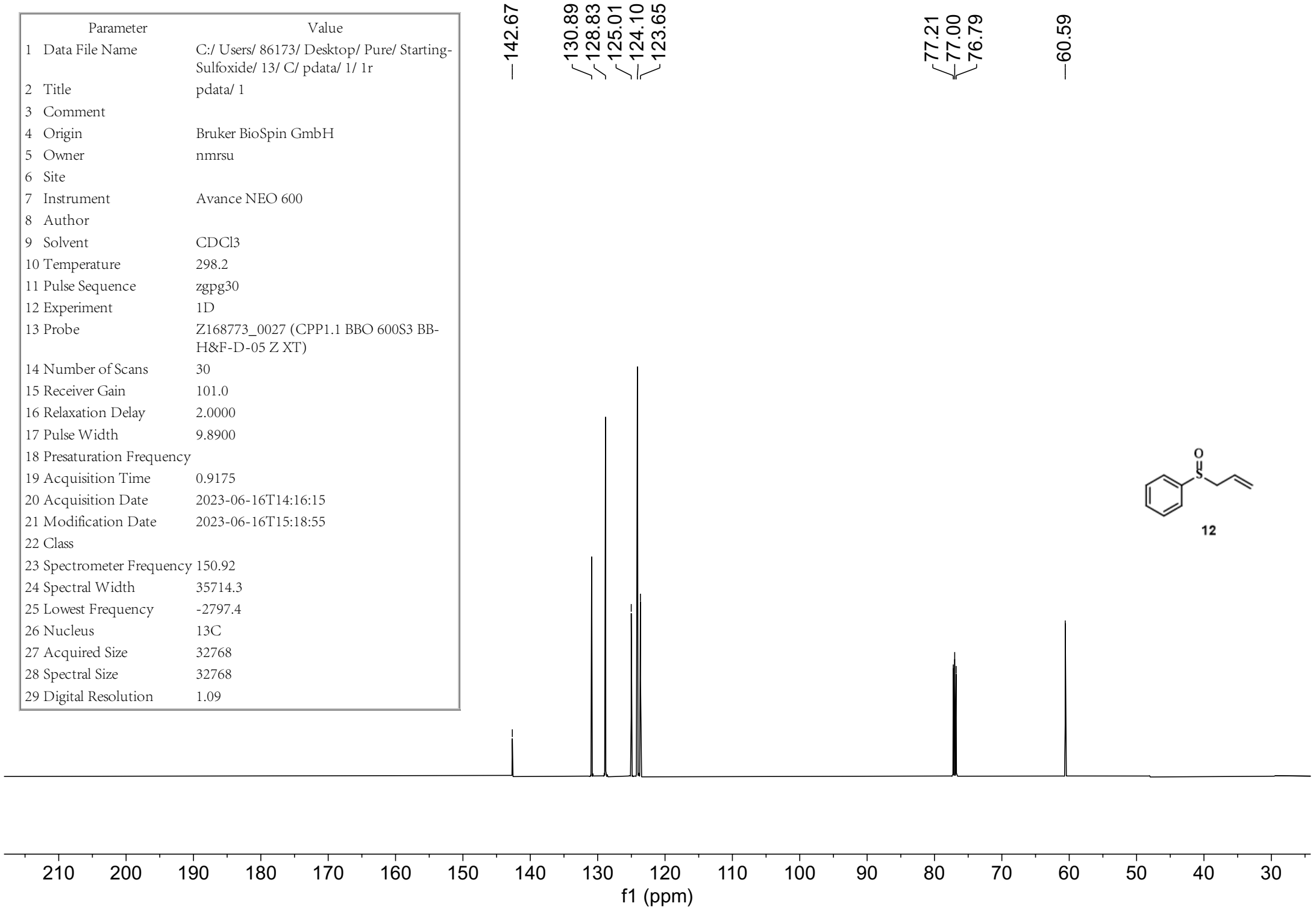


Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 12/ 2/ pdata/ 1/ 1r
2 Title	12.2.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	296.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	100
15 Receiver Gain	64.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.7000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-08-09T21:50:02
21 Modification Date	2023-08-10T14:01:19
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1847.1
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73

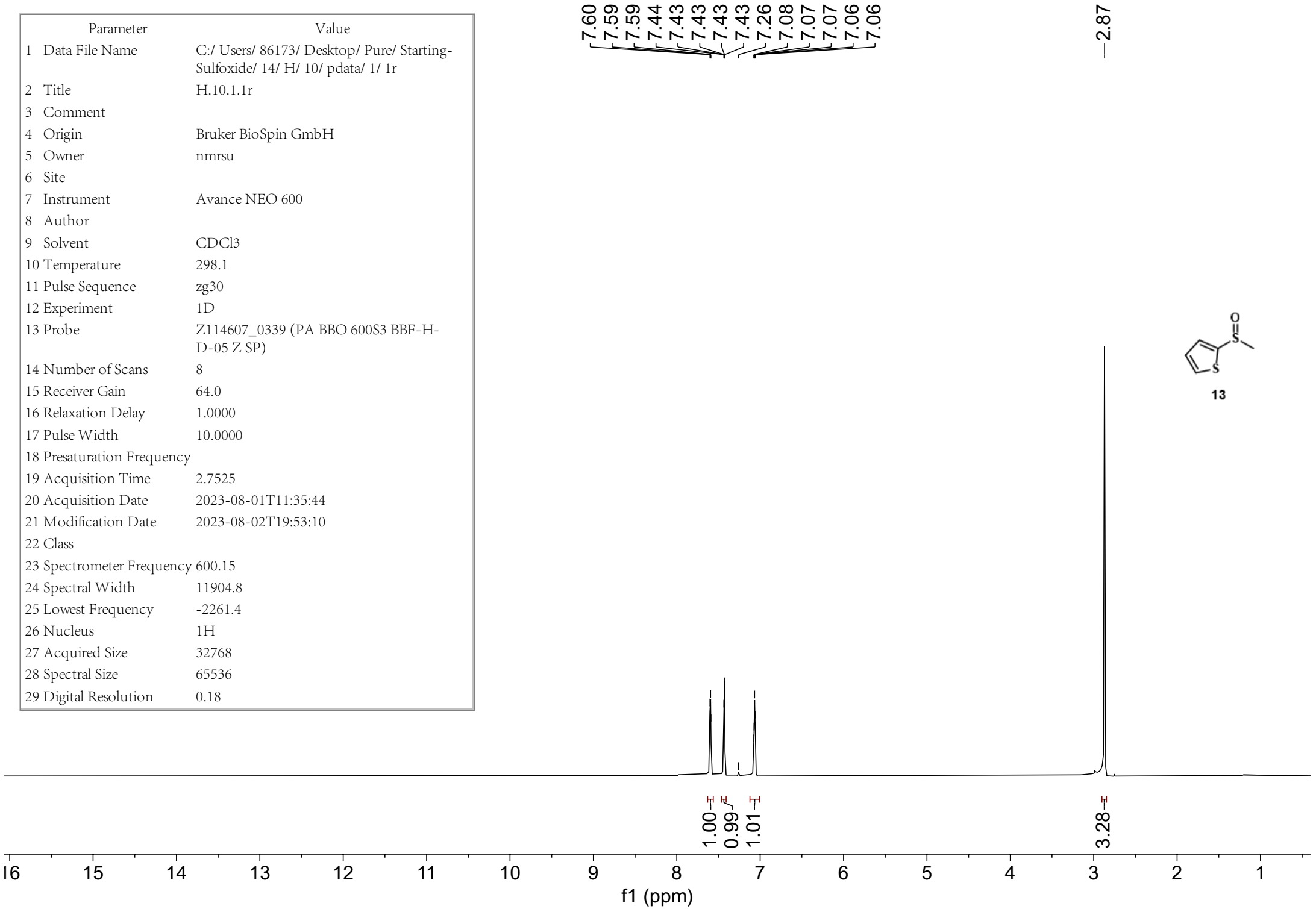



7.54 7.54 7.54 7.53 7.53 7.53 7.46 7.46 7.46 7.45 7.45 7.45 7.44 7.44 7.44 7.44 7.43 7.43 7.43 7.43 7.42 7.42 5.60 5.59 5.57 5.56 5.27 5.27 5.25 5.25 5.15 5.14 5.14 5.14 5.12 5.11 5.11 5.11 3.53 3.53 3.53 3.52 3.52 3.51 3.51 3.51 3.51 3.50 3.49 3.49 3.46 3.46 3.46 3.45 3.44 3.44 3.44 3.44 3.42
Parameter Value
1 Data File Name C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 13/ H/ pdata/ 1/ 1r
2 Title pdata/ 1
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Instrument Avance NEO 600
8 Author
9 Solvent CDCl3
10 Temperature 298.1
11 Pulse Sequence zg30
12 Experiment 1D
13 Probe Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans 8
15 Receiver Gain 64.0
16 Relaxation Delay 1.0000
17 Pulse Width 11.1300
18 Presaturation Frequency
19 Acquisition Time 2.7525
20 Acquisition Date 2023-06-16T14:13:46
21 Modification Date 2023-06-16T15:18:54
22 Class
23 Spectrometer Frequency 600.15
24 Spectral Width 11904.8
25 Lowest Frequency -2260.6
26 Nucleus 1H
27 Acquired Size 32768
28 Spectral Size 65536
29 Digital Resolution 0.18
O
S
12
2.01
3.01
1.00
1.00
1.00
1.04
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 13/ C/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans	30
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.8900
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-06-16T14:16:15
21 Modification Date	2023-06-16T15:18:55
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2797.4
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09

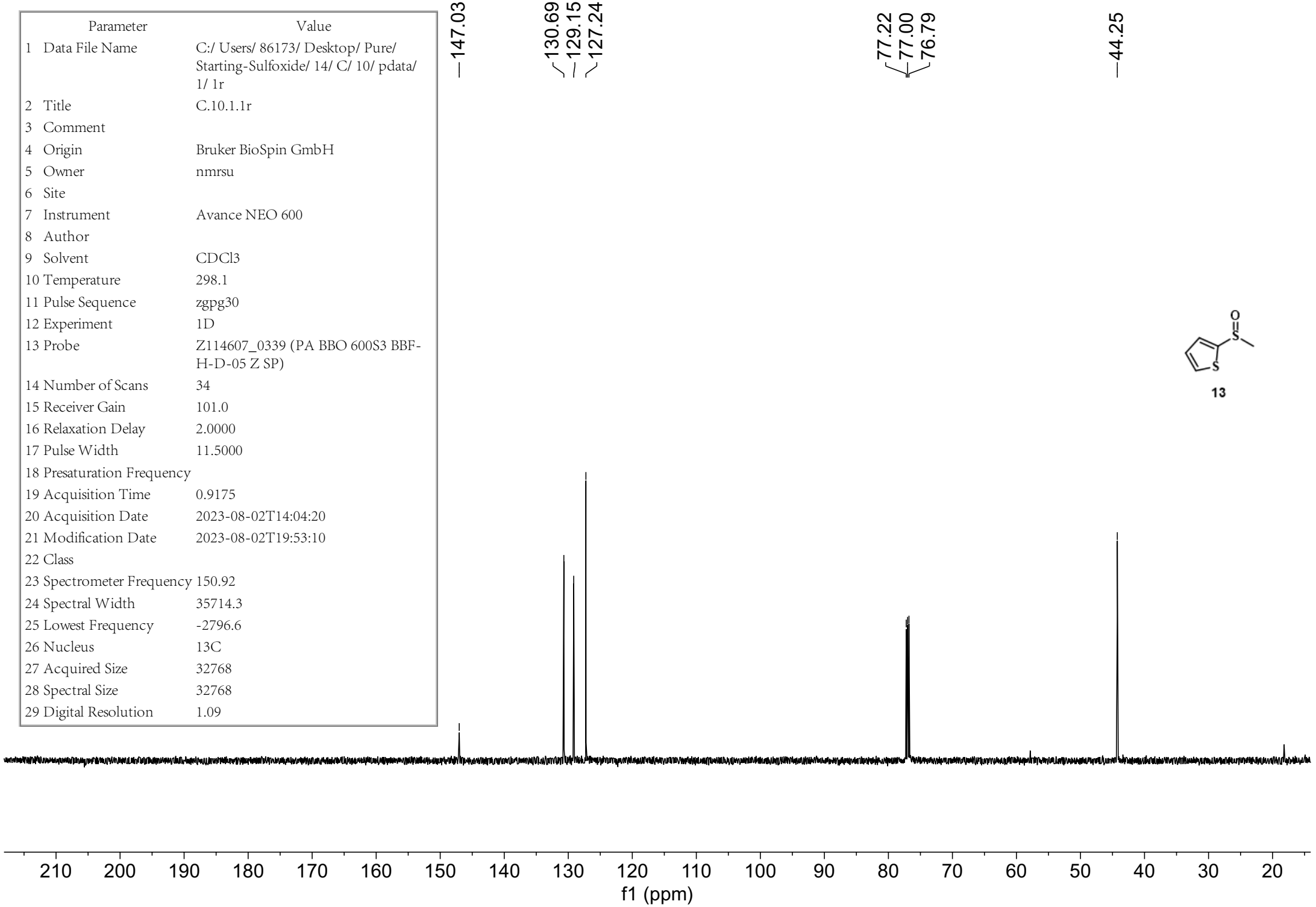


Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 14/ H/ 10/ pdata/ 1/ 1r
2 Title	H.10.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	64.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.7525
20 Acquisition Date	2023-08-01T11:35:44
21 Modification Date	2023-08-02T19:53:10
22 Class	
23 Spectrometer Frequency	600.15
24 Spectral Width	11904.8
25 Lowest Frequency	-2261.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.18

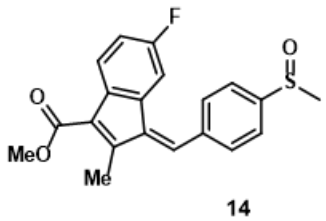


13

Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 14/ C/ 10/ pdata/ 1/ 1r
2 Title	C.10.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	34
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	11.5000
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-08-02T14:04:20
21 Modification Date	2023-08-02T19:53:10
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2796.6
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09



Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 15/ H/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	294.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.5800
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-07-22T10:05:22
21 Modification Date	2023-07-22T12:39:05
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



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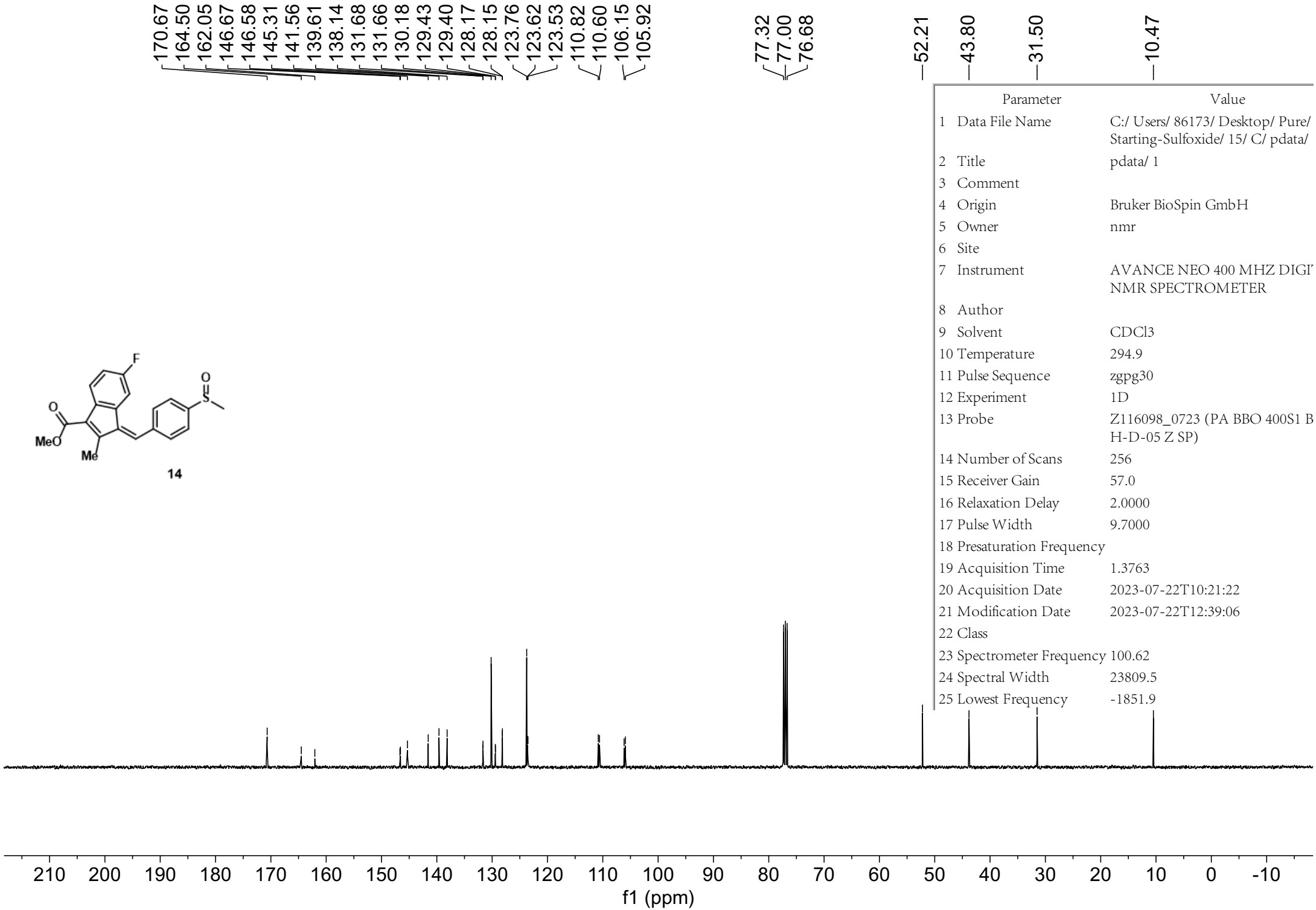
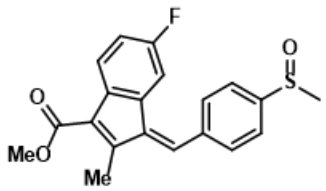
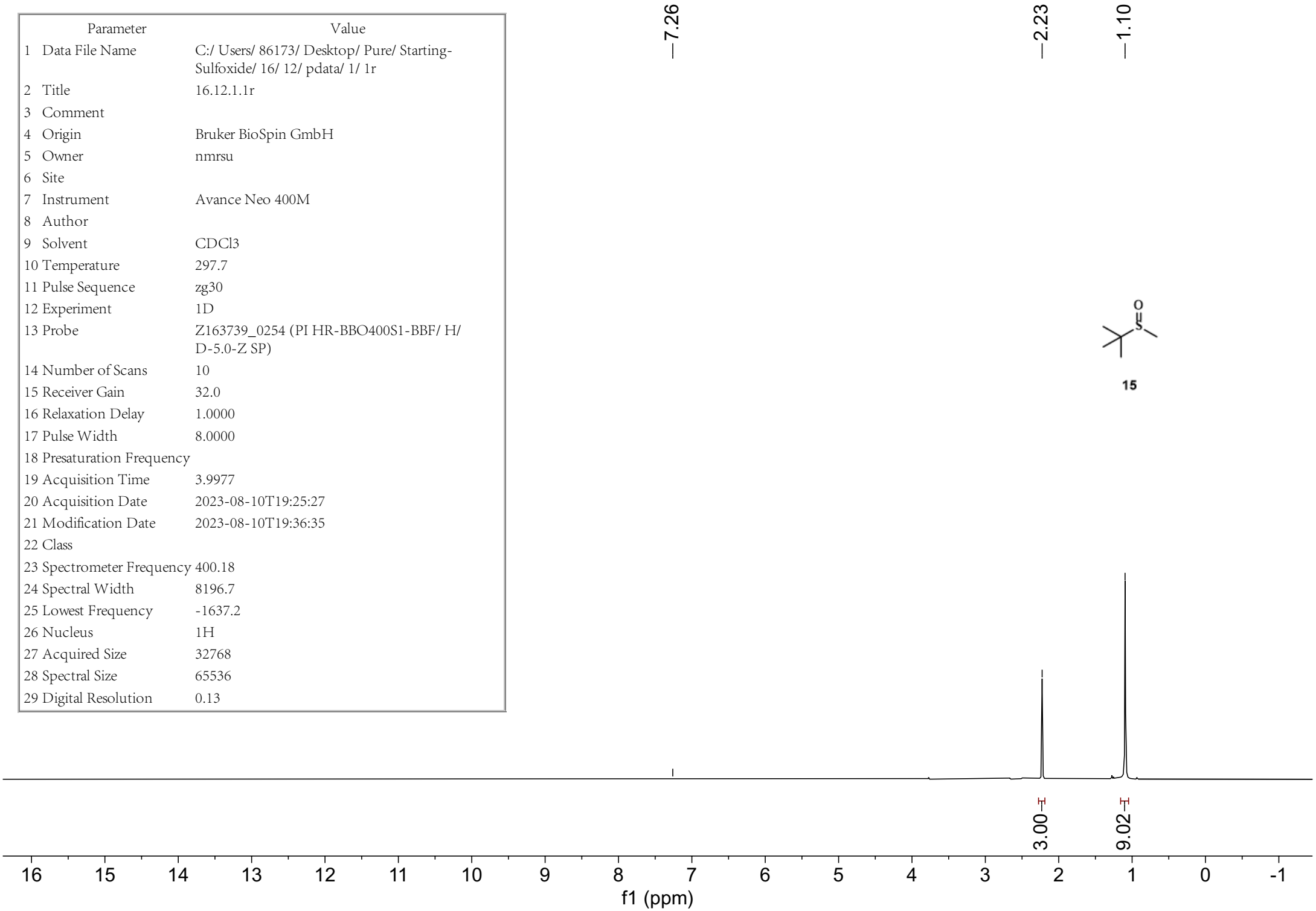

170.67
164.50
162.05
146.67
146.58
145.31
141.56
139.61
138.14
131.68
131.66
130.18
129.43
129.40
128.17
128.15
123.76
123.62
123.53
110.82
110.60
106.15
105.92
77.32
77.00
76.68
52.21
43.80
31.50
10.47
F
O
O
MeO
Me
S
14
Parameter Value
1 Data File Name C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 15/ C/ pdata/
2 Title pdata/ 1
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmr
6 Site
7 Instrument AVANCE NEO 400 MHZ DIGI NMR SPECTROMETER
8 Author
9 Solvent CDCl3
10 Temperature 294.9
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Probe Z116098_0723 (PA BBO 400S1 B H-D-05 Z SP)
14 Number of Scans 256
15 Receiver Gain 57.0
16 Relaxation Delay 2.0000
17 Pulse Width 9.7000
18 Presaturation Frequency
19 Acquisition Time 1.3763
20 Acquisition Date 2023-07-22T10:21:22
21 Modification Date 2023-07-22T12:39:06
22 Class
23 Spectrometer Frequency 100.62
24 Spectral Width 23809.5
25 Lowest Frequency -1851.9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ 15/ F/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	10
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	17.8500
18 Presaturation Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2023-08-28T11:23:03
21 Modification Date	2023-08-28T14:08:44
22 Class	
23 Spectrometer Frequency	376.46
24 Spectral Width	90909.1
25 Lowest Frequency	-83104.4
26 Nucleus	19F
27 Acquired Size	65536
28 Spectral Size	65536
29 Digital Resolution	1.39

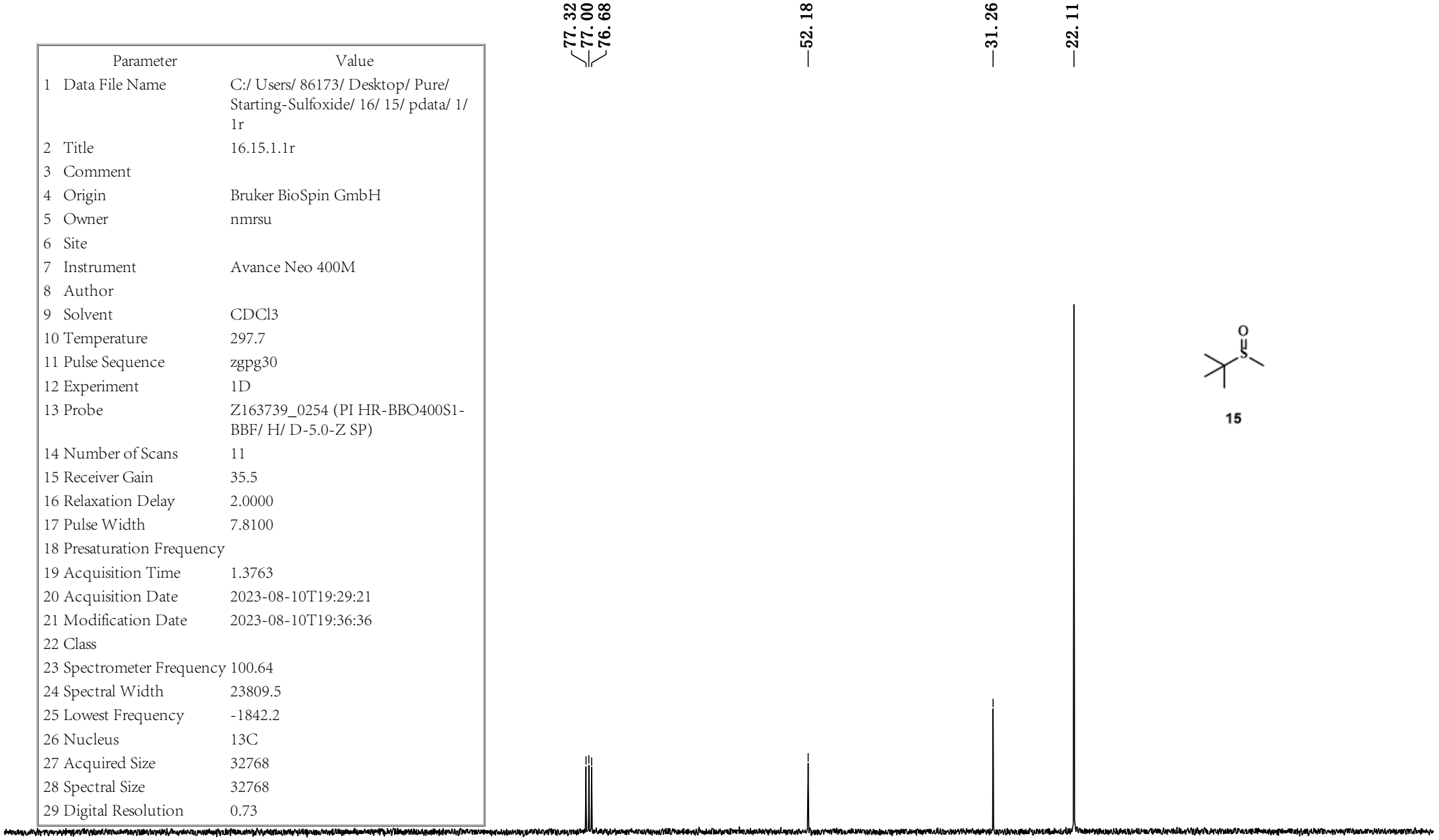


14

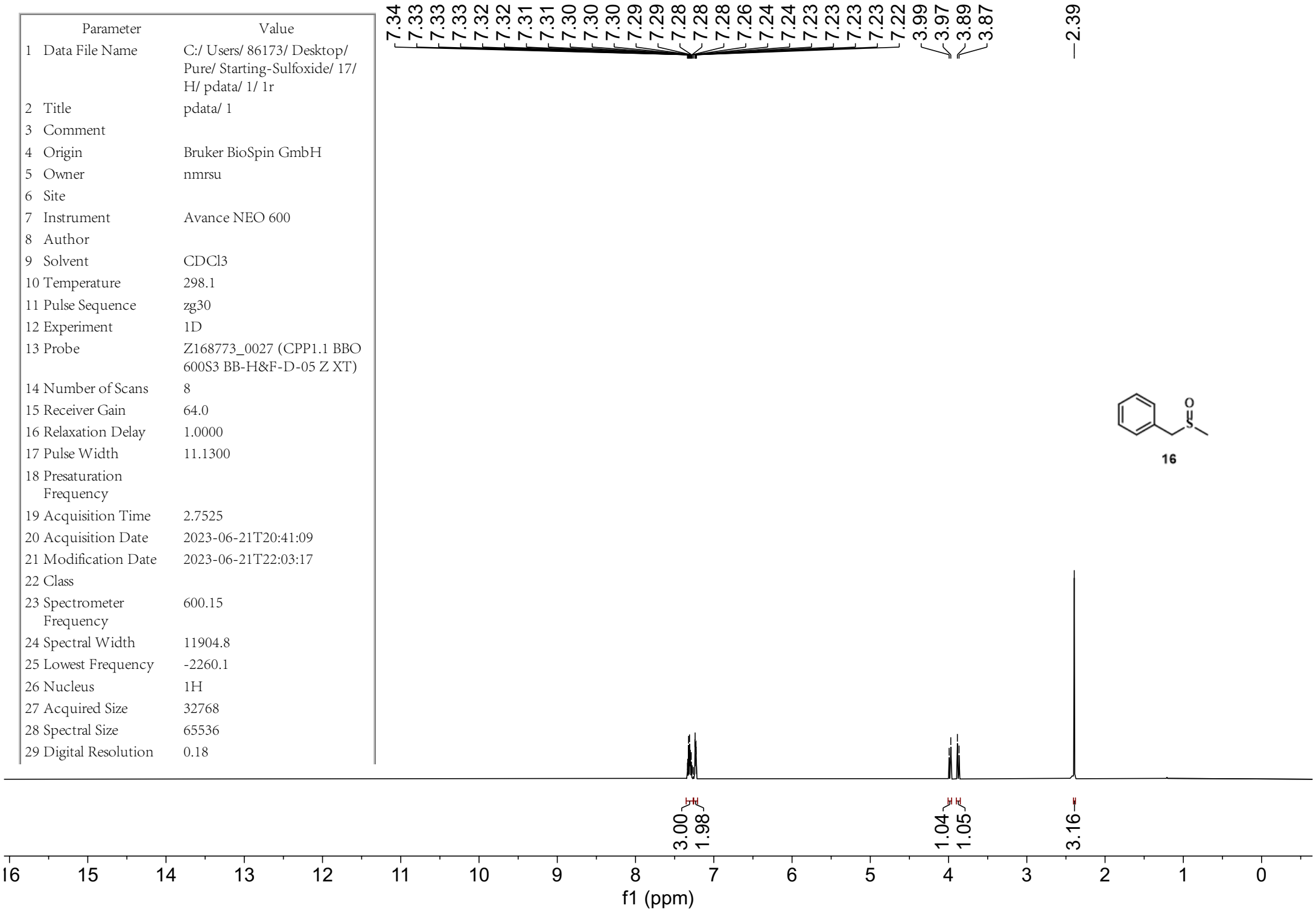
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 16/ 12/ pdata/ 1/ 1r
2 Title	16.12.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	297.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	10
15 Receiver Gain	32.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-08-10T19:25:27
21 Modification Date	2023-08-10T19:36:35
22 Class	
23 Spectrometer Frequency	400.18
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



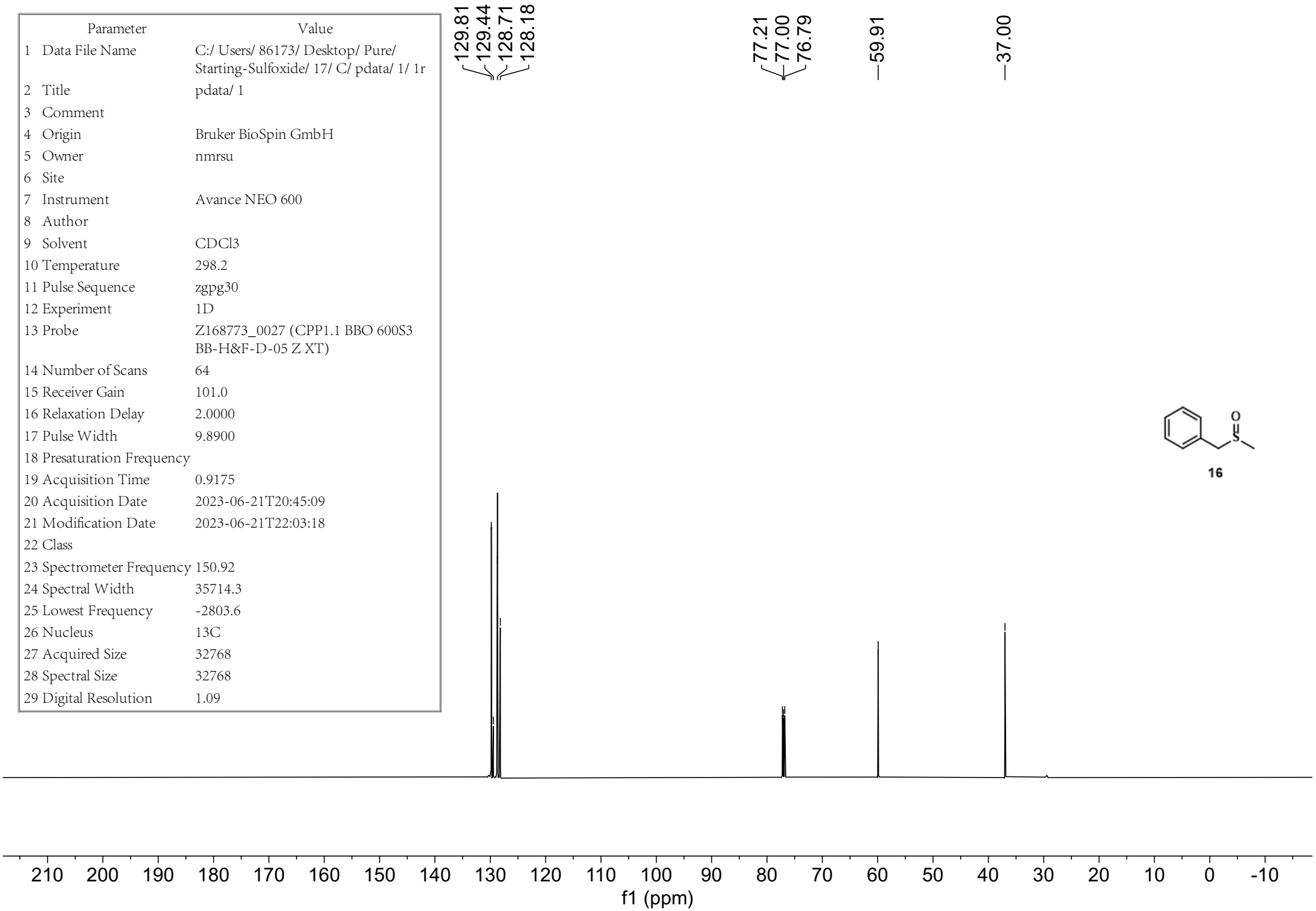
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 16/ 15/ pdata/ 1/ 1r
2 Title	16.15.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	297.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	11
15 Receiver Gain	35.5
16 Relaxation Delay	2.0000
17 Pulse Width	7.8100
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-08-10T19:29:21
21 Modification Date	2023-08-10T19:36:36
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	23809.5
25 Lowest Frequency	-1842.2
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73



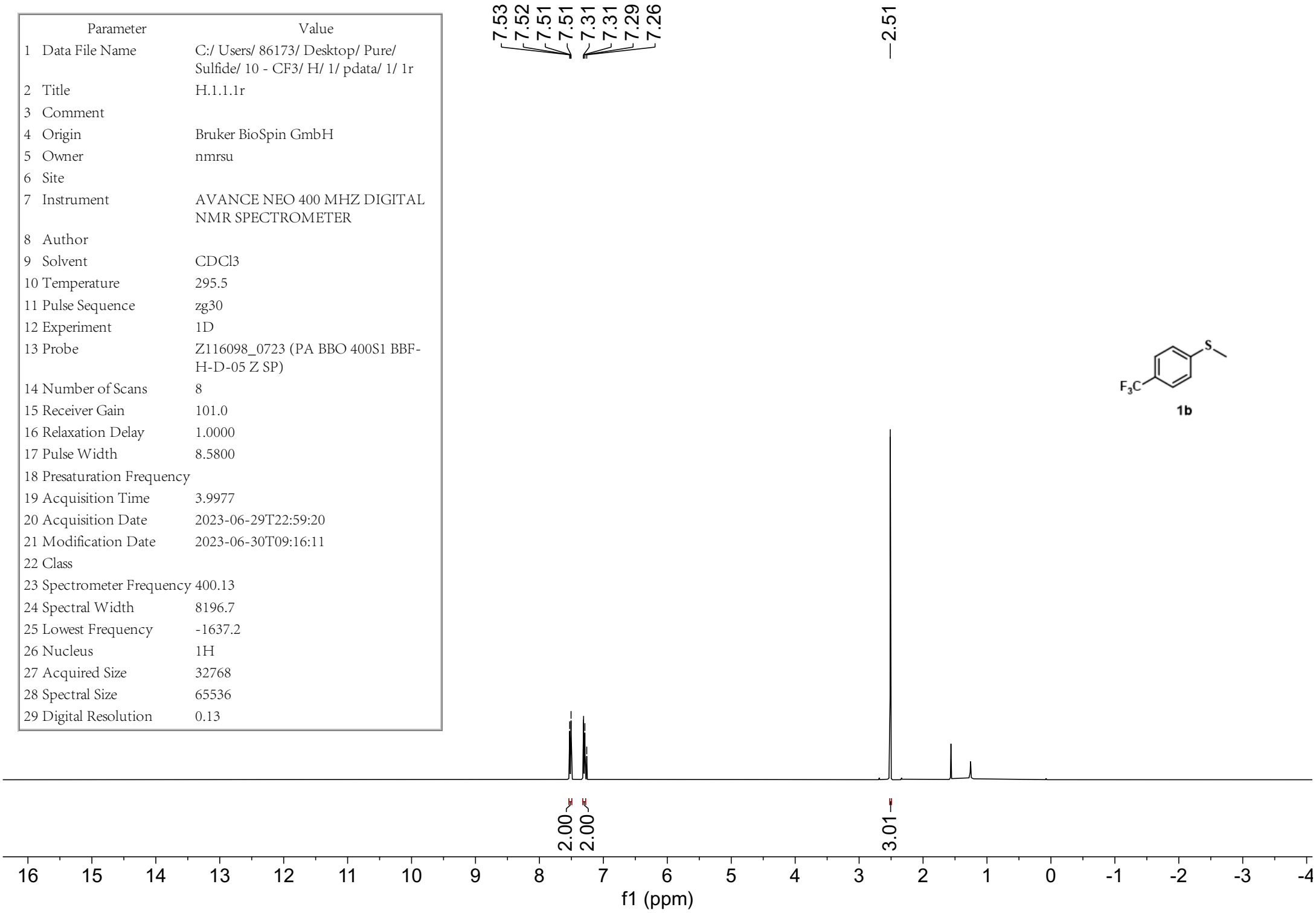
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 17/ H/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans	8
15 Receiver Gain	64.0
16 Relaxation Delay	1.0000
17 Pulse Width	11.1300
18 Presaturation Frequency	
19 Acquisition Time	2.7525
20 Acquisition Date	2023-06-21T20:41:09
21 Modification Date	2023-06-21T22:03:17
22 Class	
23 Spectrometer Frequency	600.15
24 Spectral Width	11904.8
25 Lowest Frequency	-2260.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.18



Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Starting-Sulfoxide/ 17/ C/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans	64
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.8900
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-06-21T20:45:09
21 Modification Date	2023-06-21T22:03:18
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2803.6
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09

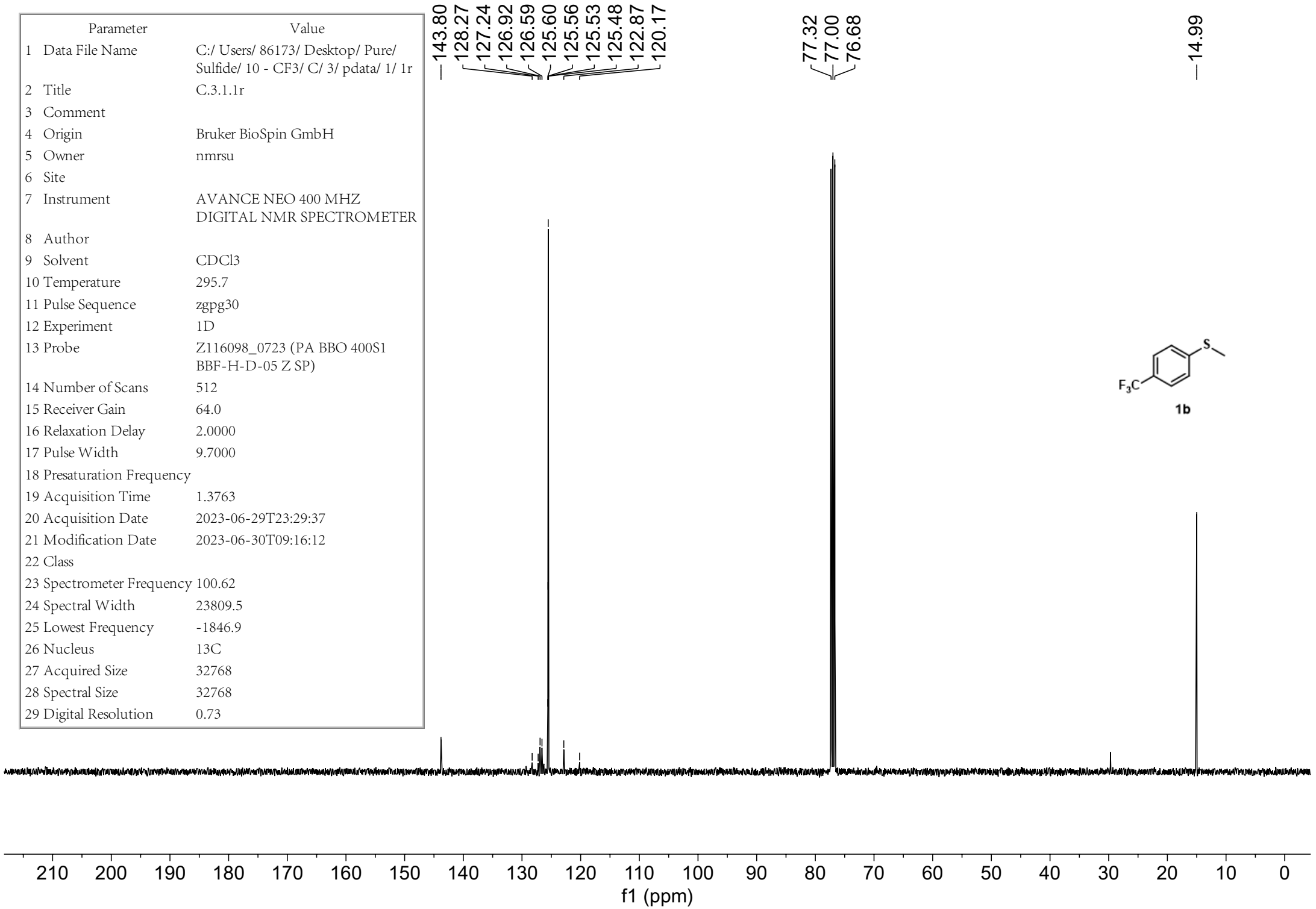


Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 10 - CF3/ H/ 1/ pdata/ 1/ 1r
2 Title	H.1.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	295.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.5800
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-06-29T22:59:20
21 Modification Date	2023-06-30T09:16:11
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

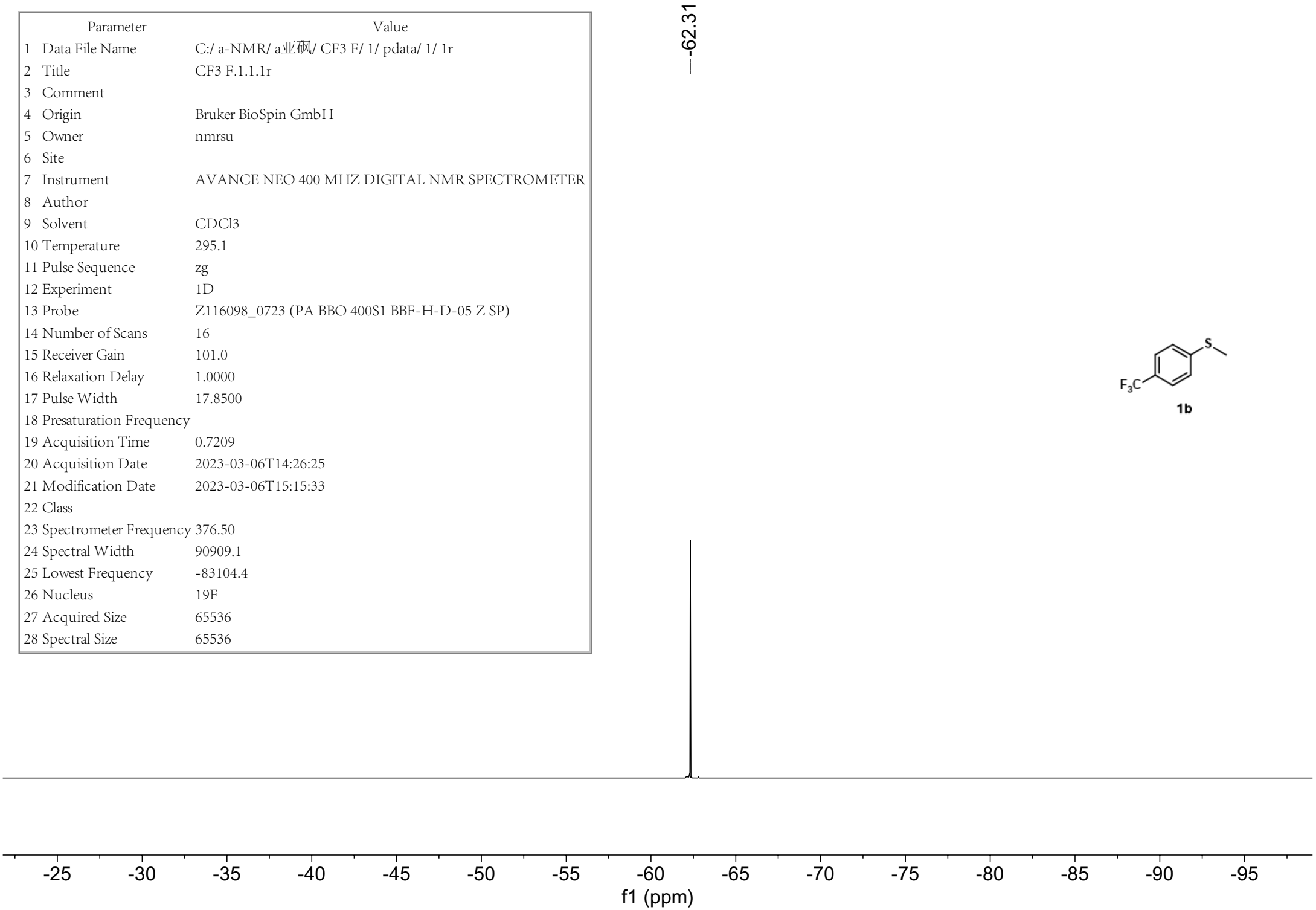


1b

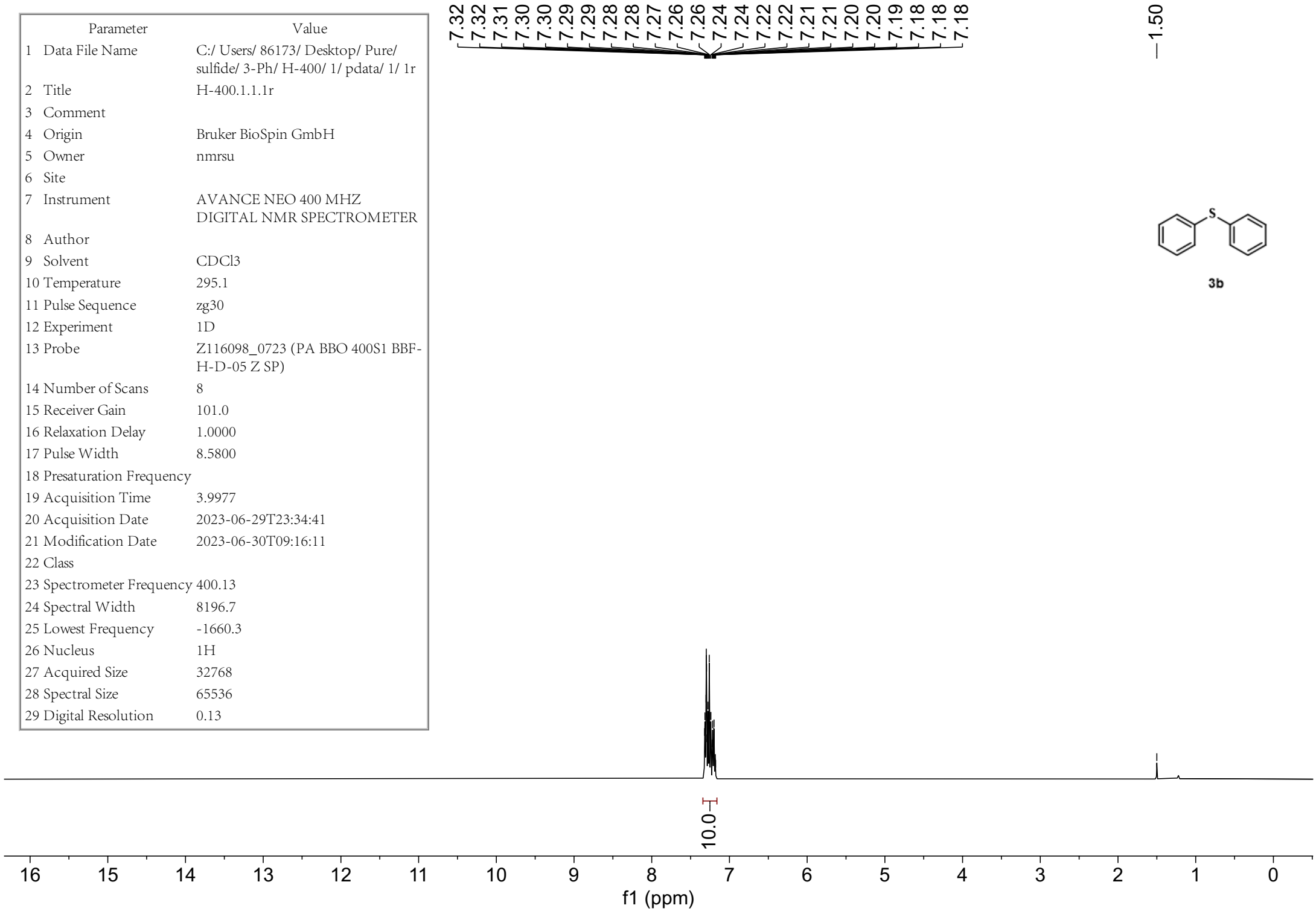
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 10 - CF3/ C/ 3/ pdata/ 1/ 1r
2 Title	C.3.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	295.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	512
15 Receiver Gain	64.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.7000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-06-29T23:29:37
21 Modification Date	2023-06-30T09:16:12
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1846.9
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73



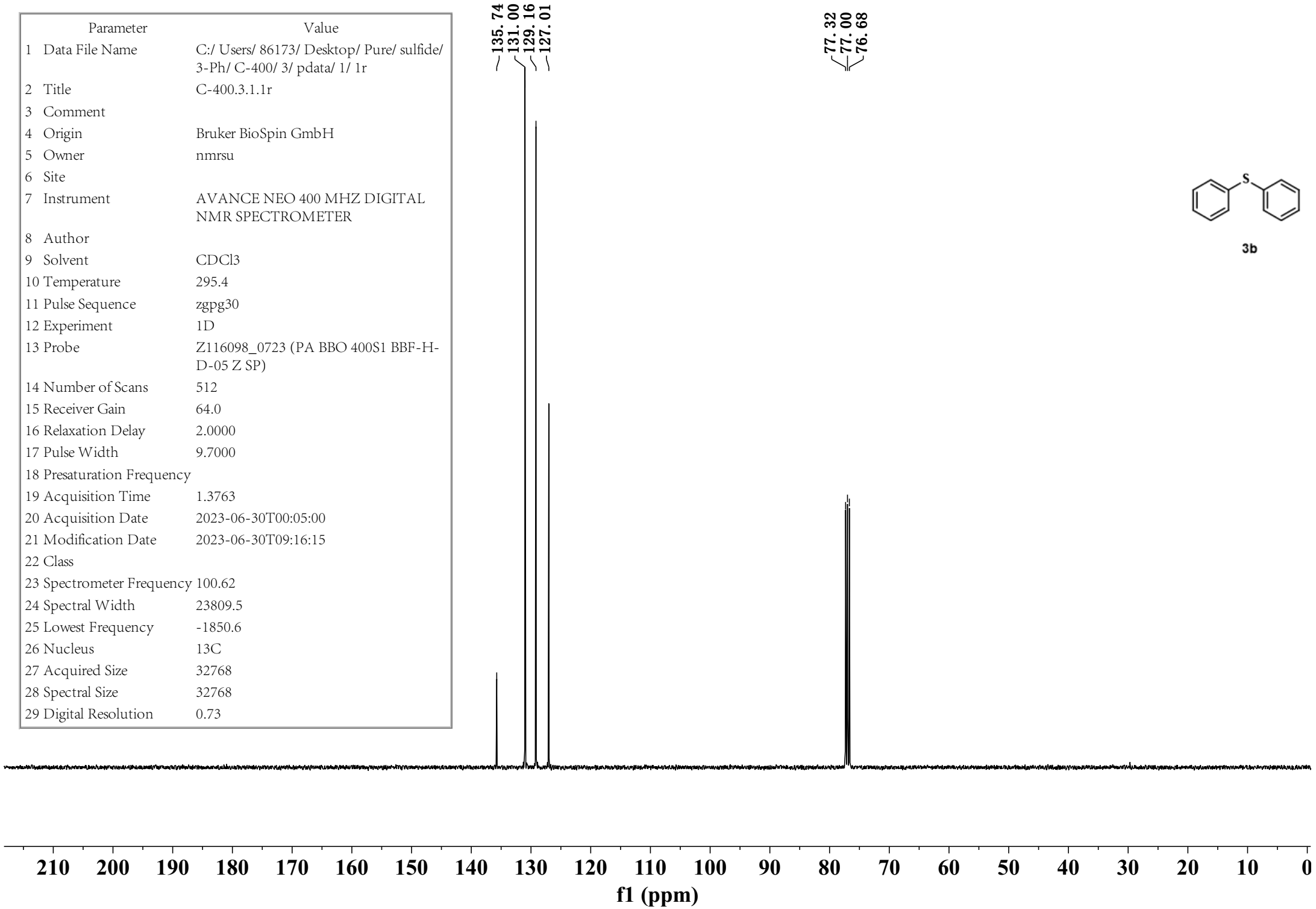
Parameter	Value
1 Data File Name	C:/ a-NMR/ a亚砜/ CF3 F/ 1/ pdata/ 1/ 1r
2 Title	CF3 F.1.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	17.8500
18 Presaturation Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2023-03-06T14:26:25
21 Modification Date	2023-03-06T15:15:33
22 Class	
23 Spectrometer Frequency	376.50
24 Spectral Width	90909.1
25 Lowest Frequency	-83104.4
26 Nucleus	19F
27 Acquired Size	65536
28 Spectral Size	65536



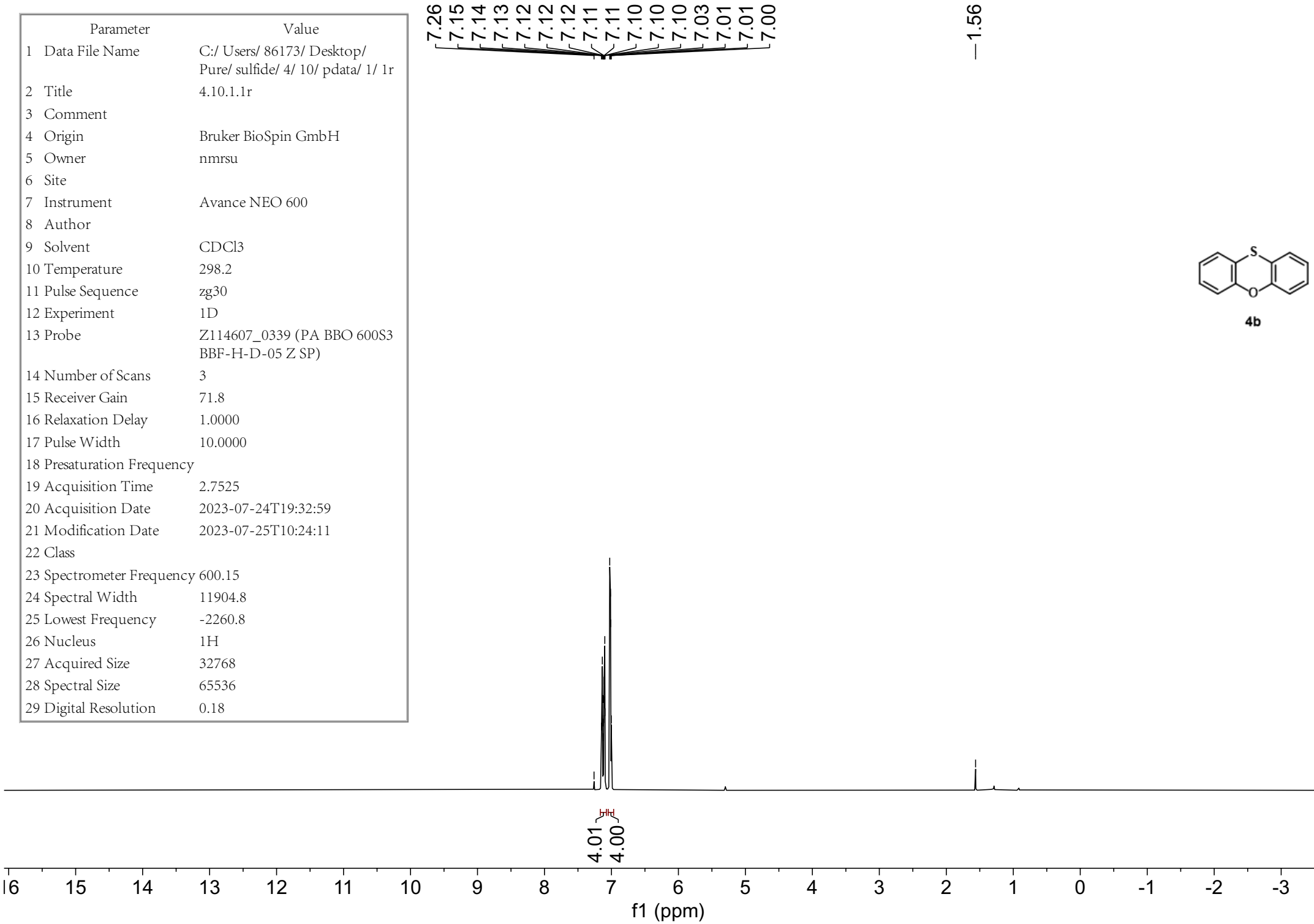
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 3-Ph/ H-400/ 1/ pdata/ 1/ 1r
2 Title	H-400.1.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.5800
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-06-29T23:34:41
21 Modification Date	2023-06-30T09:16:11
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1660.3
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



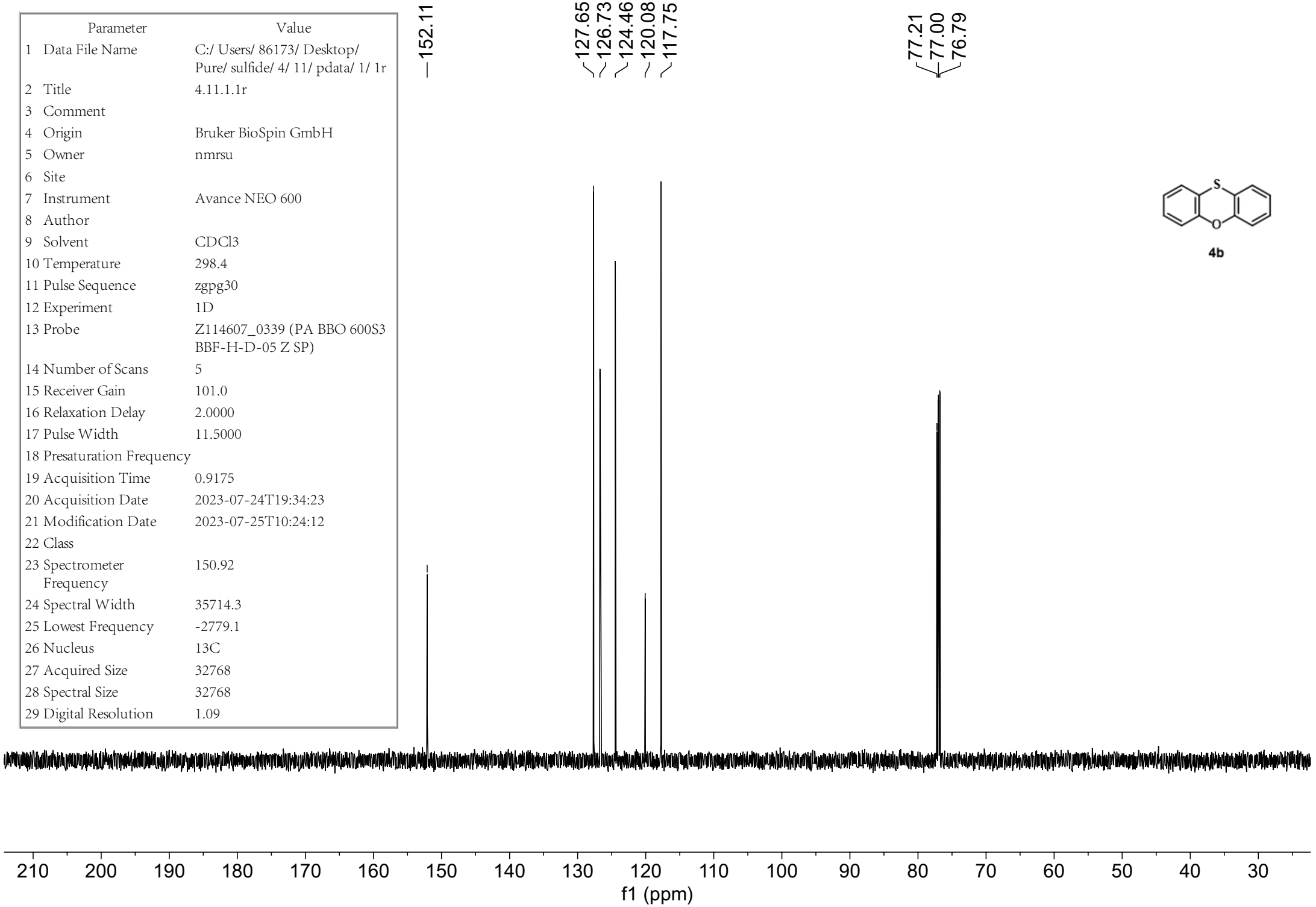
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 3-Ph/ C-400/ 3/ pdata/ 1/ 1r
2 Title	C-400.3.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	295.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	512
15 Receiver Gain	64.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.7000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-06-30T00:05:00
21 Modification Date	2023-06-30T09:16:15
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1850.6
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73



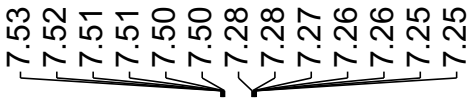
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 4/ 10/ pdata/ 1/ 1r
2 Title	4.10.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	3
15 Receiver Gain	71.8
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.7525
20 Acquisition Date	2023-07-24T19:32:59
21 Modification Date	2023-07-25T10:24:11
22 Class	
23 Spectrometer Frequency	600.15
24 Spectral Width	11904.8
25 Lowest Frequency	-2260.8
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.18

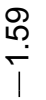


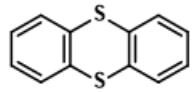
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 4/ 11/ pdata/ 1/ 1r
2 Title	4.11.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	5
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	11.5000
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-07-24T19:34:23
21 Modification Date	2023-07-25T10:24:12
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2779.1
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09



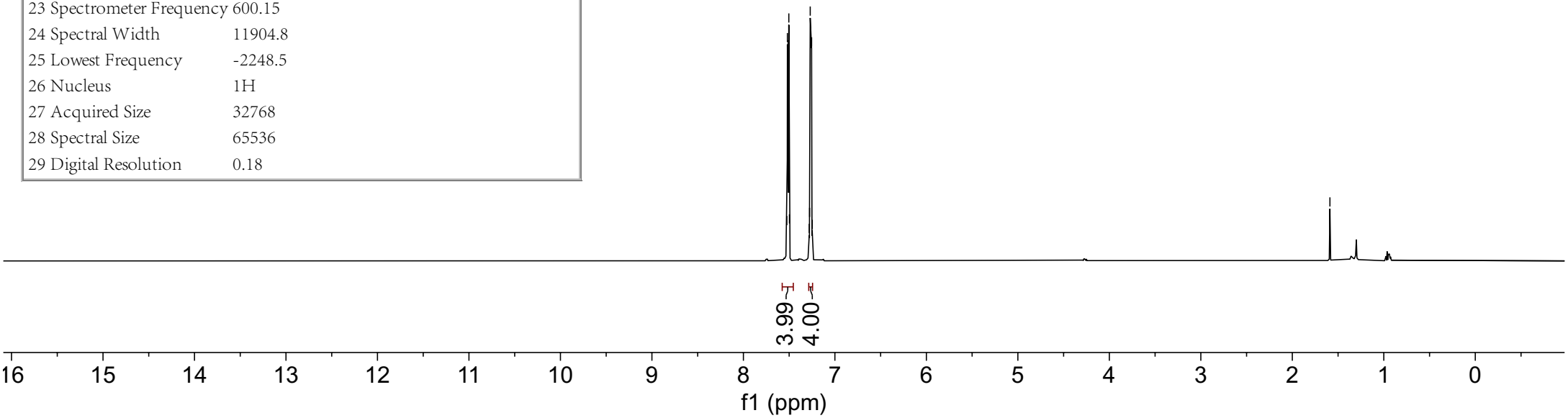
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 5/ H/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	71.8
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.7525
20 Acquisition Date	2023-07-24T19:55:37
21 Modification Date	2023-07-25T10:24:10
22 Class	
23 Spectrometer Frequency	600.15
24 Spectral Width	11904.8
25 Lowest Frequency	-2248.5
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.18



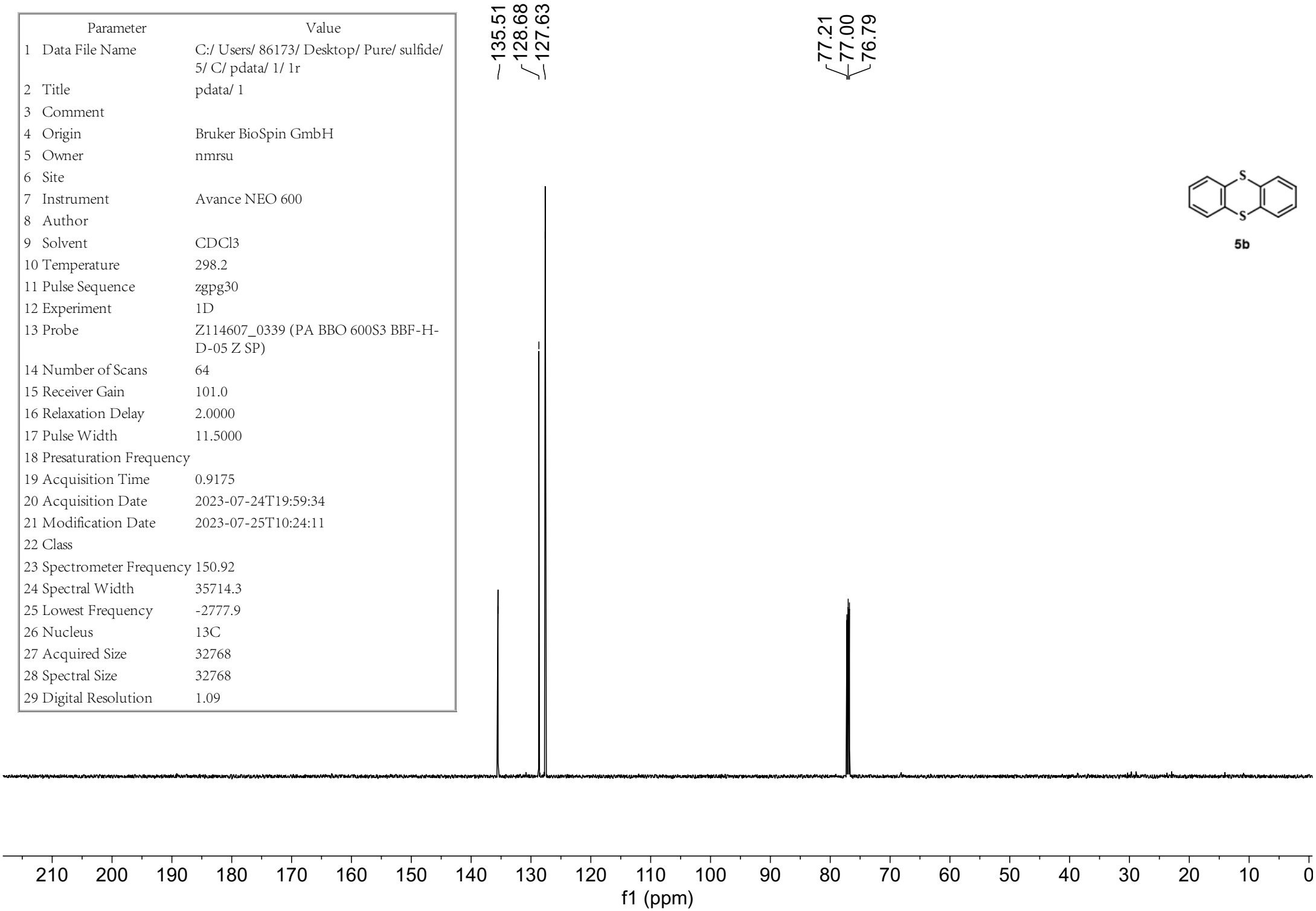




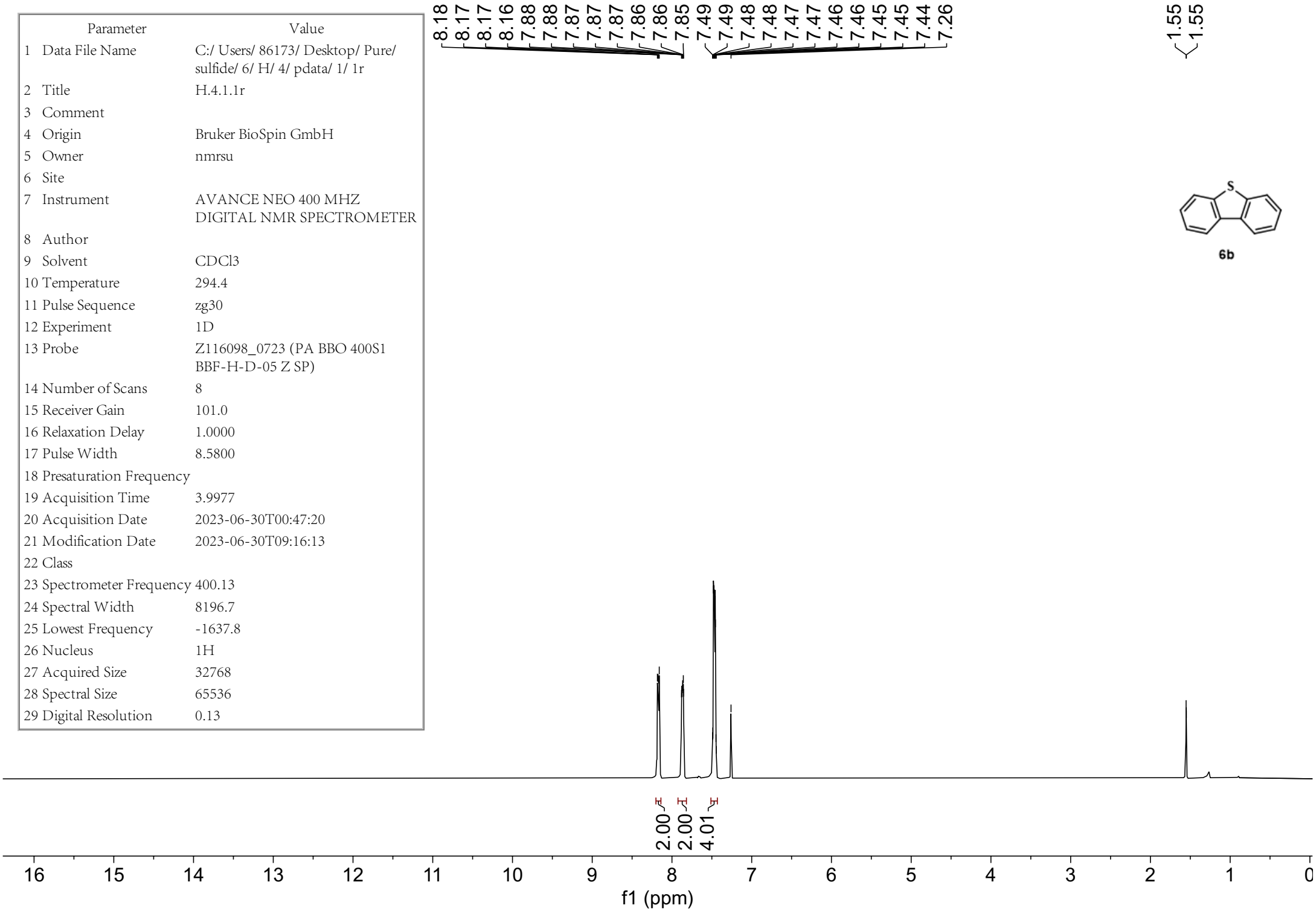
5b



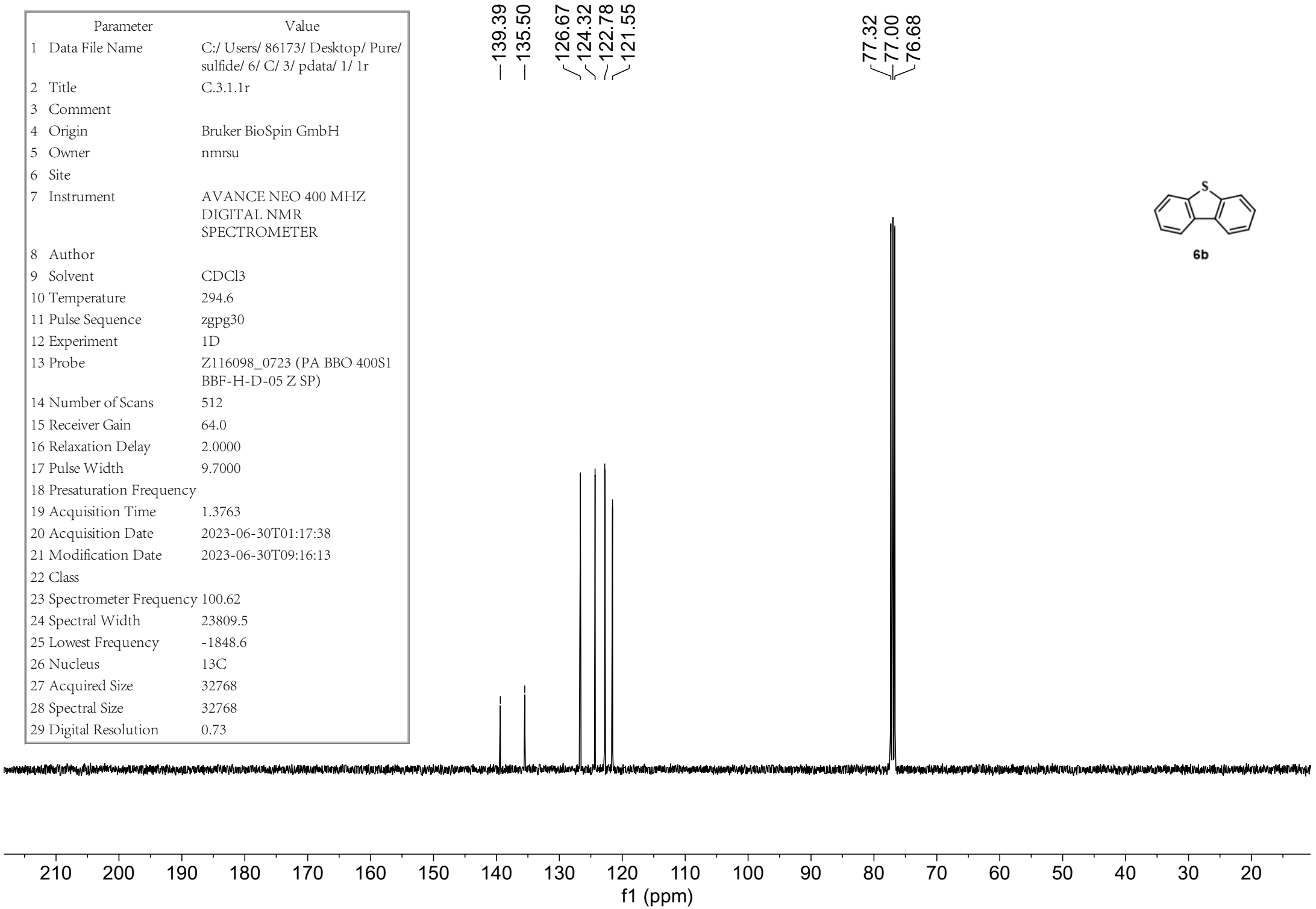
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 5/ C/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	64
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	11.5000
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-07-24T19:59:34
21 Modification Date	2023-07-25T10:24:11
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2777.9
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09



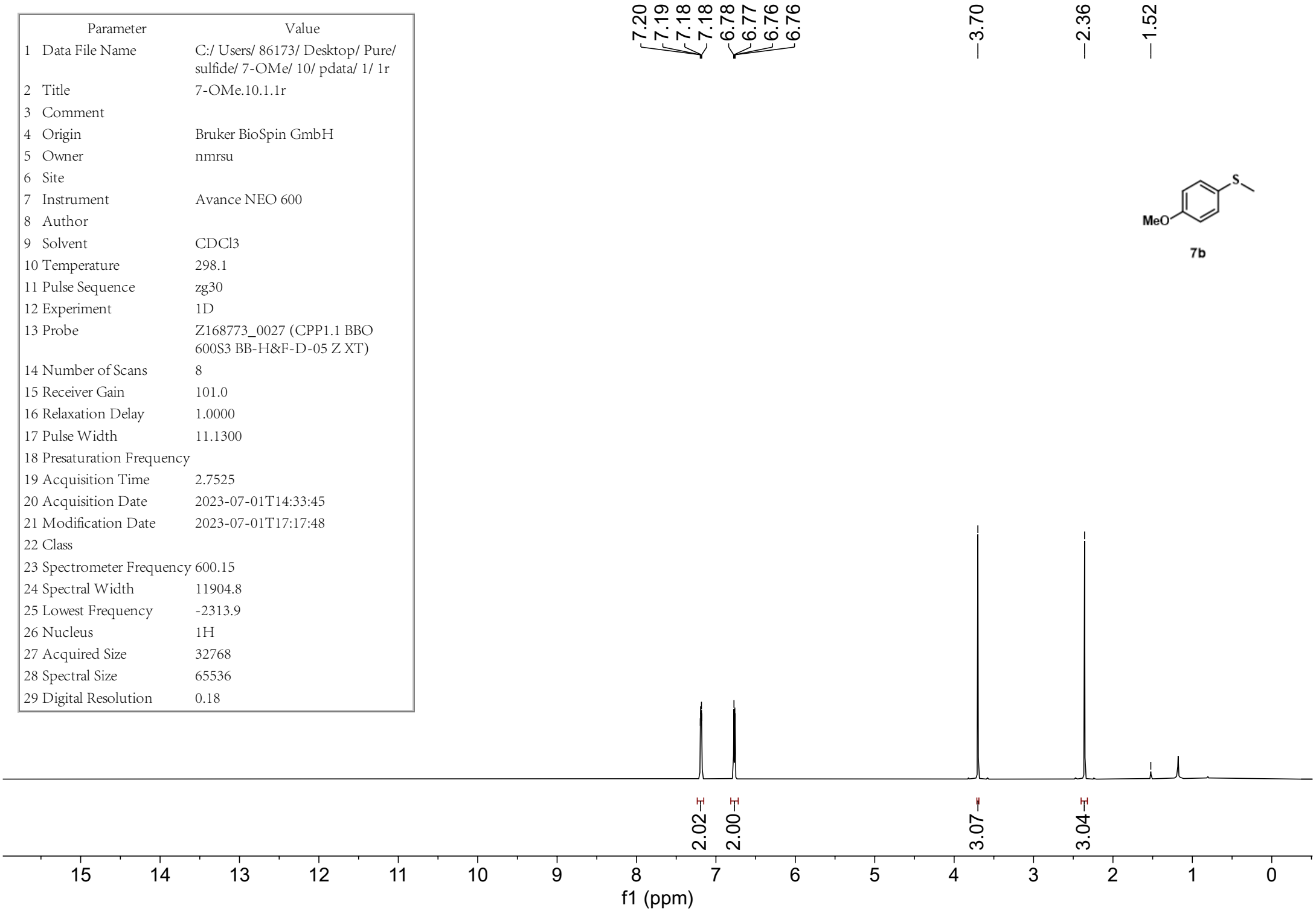
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 6/ H/ 4/ pdata/ 1/ 1r
2 Title	H.4.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	294.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.5800
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-06-30T00:47:20
21 Modification Date	2023-06-30T09:16:13
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.8
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



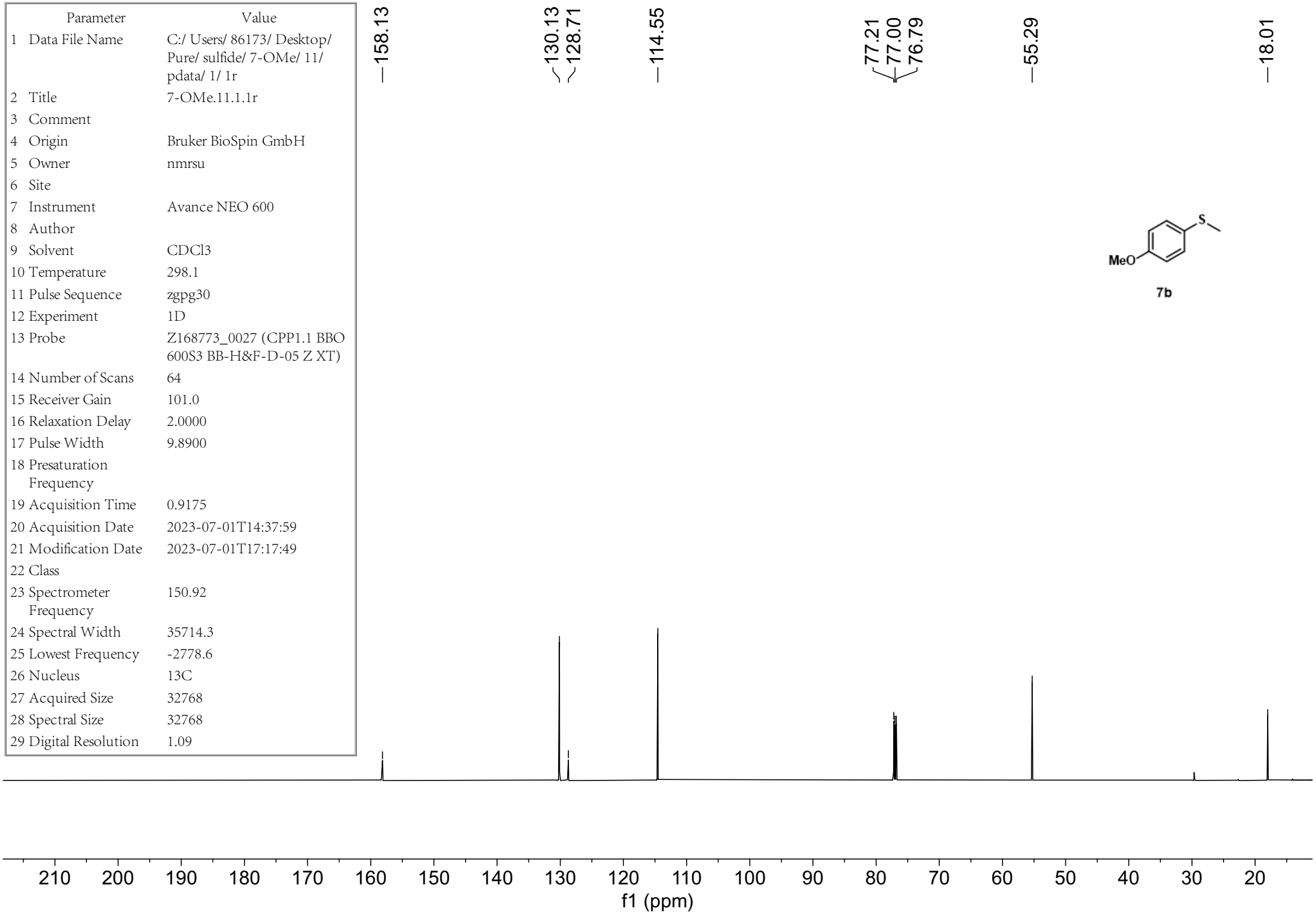
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 6/ C/ 3/ pdata/ 1/ 1r
2 Title	C.3.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	294.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	512
15 Receiver Gain	64.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.7000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-06-30T01:17:38
21 Modification Date	2023-06-30T09:16:13
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1848.6
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73



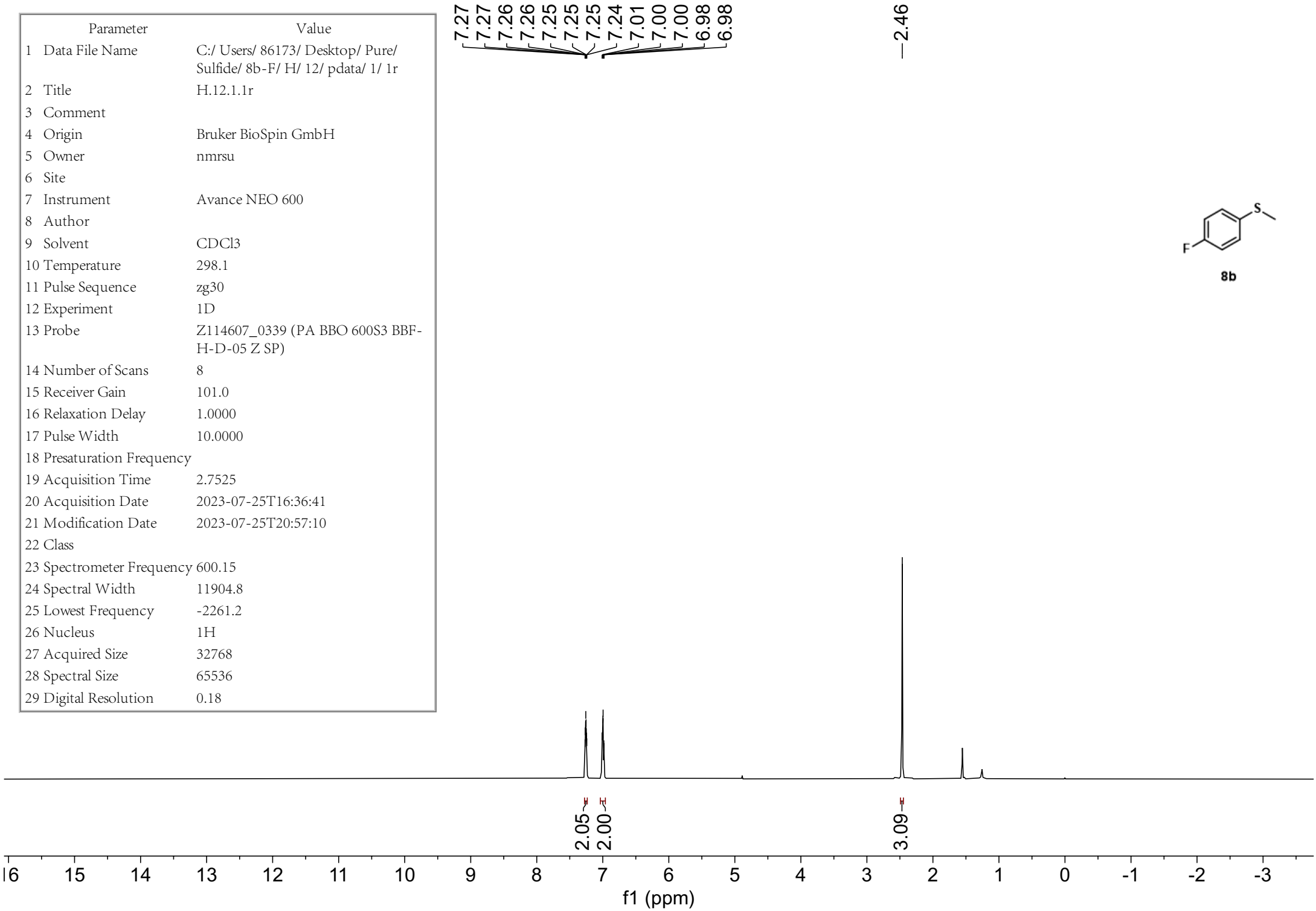
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 7-OMe/ 10/ pdata/ 1/ 1r
2 Title	7-OMe.10.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	11.1300
18 Presaturation Frequency	
19 Acquisition Time	2.7525
20 Acquisition Date	2023-07-01T14:33:45
21 Modification Date	2023-07-01T17:17:48
22 Class	
23 Spectrometer Frequency	600.15
24 Spectral Width	11904.8
25 Lowest Frequency	-2313.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.18



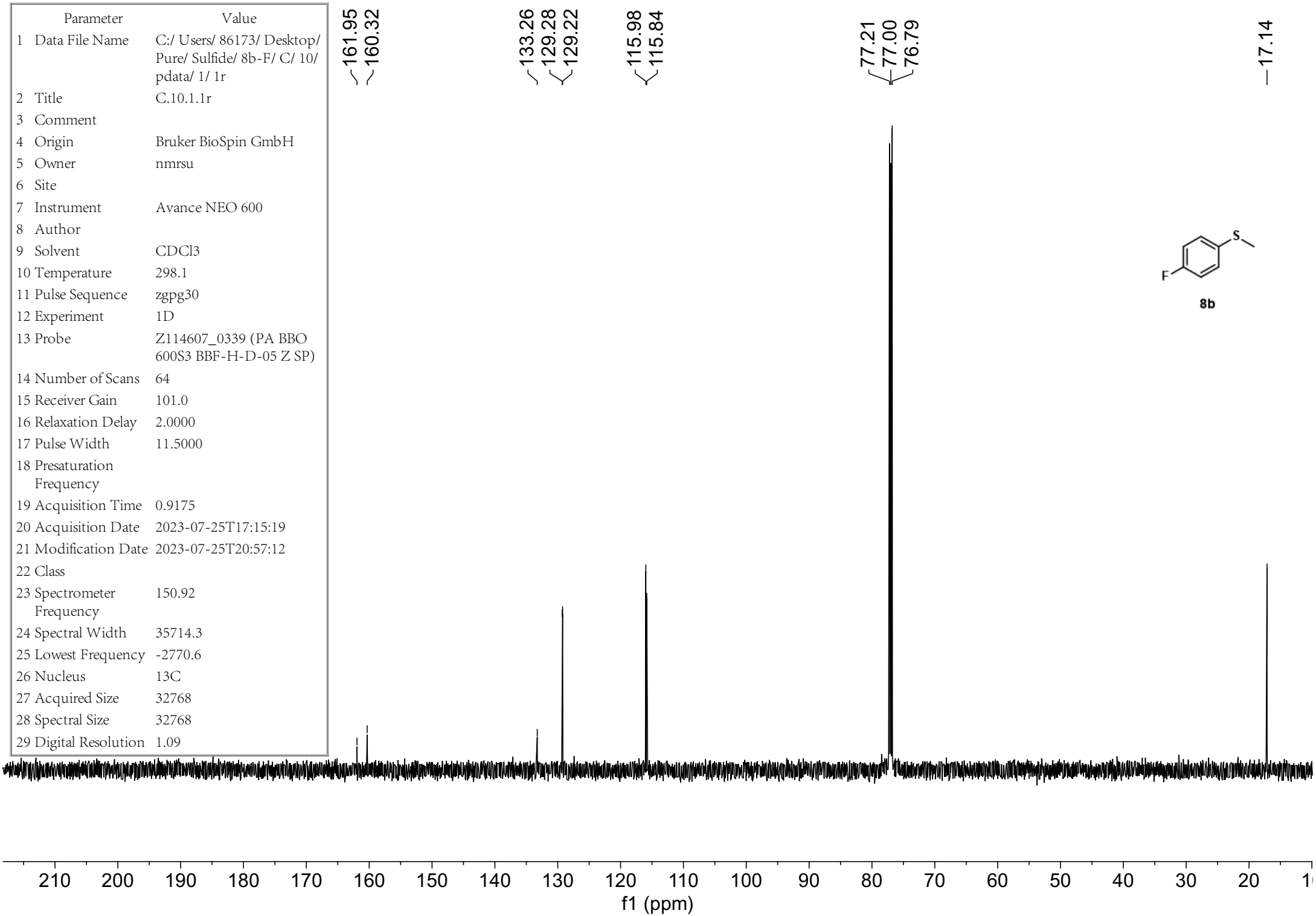
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 7-OMe/ 11/ pdata/ 1/ 1r
2 Title	7-OMe.11.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans	64
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.8900
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-07-01T14:37:59
21 Modification Date	2023-07-01T17:17:49
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2778.6
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09



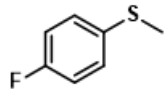
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 8b-F/ H/ 12/ pdata/ 1/ 1r
2 Title	H.12.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	2.7525
20 Acquisition Date	2023-07-25T16:36:41
21 Modification Date	2023-07-25T20:57:10
22 Class	
23 Spectrometer Frequency	600.15
24 Spectral Width	11904.8
25 Lowest Frequency	-2261.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.18



Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 8b-F/ C/ 10/ pdata/ 1/ 1r
2 Title	C.10.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	64
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	11.5000
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-07-25T17:15:19
21 Modification Date	2023-07-25T20:57:12
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2770.6
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09

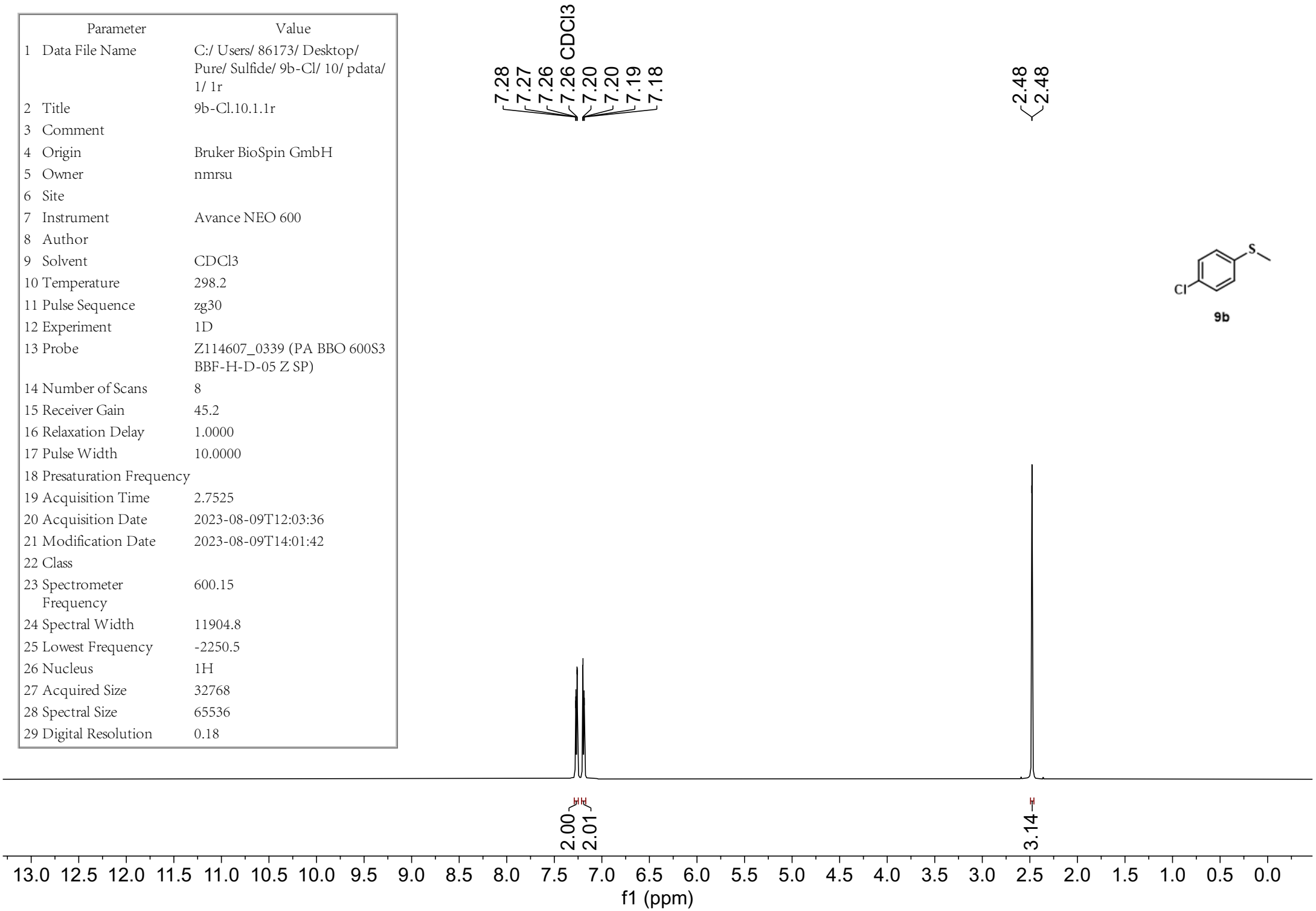


Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 8b-F/ F/ 1/ pdata/ 1/ 1r
2 Title	F.1.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	294.9
11 Pulse Sequence	zg
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	17.8500
18 Presaturation Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2023-06-28T10:58:57
21 Modification Date	2023-06-28T11:15:40
22 Class	
23 Spectrometer Frequency	376.46
24 Spectral Width	90909.1
25 Lowest Frequency	-83104.4
26 Nucleus	19F
27 Acquired Size	65536
28 Spectral Size	65536
29 Digital Resolution	1.39

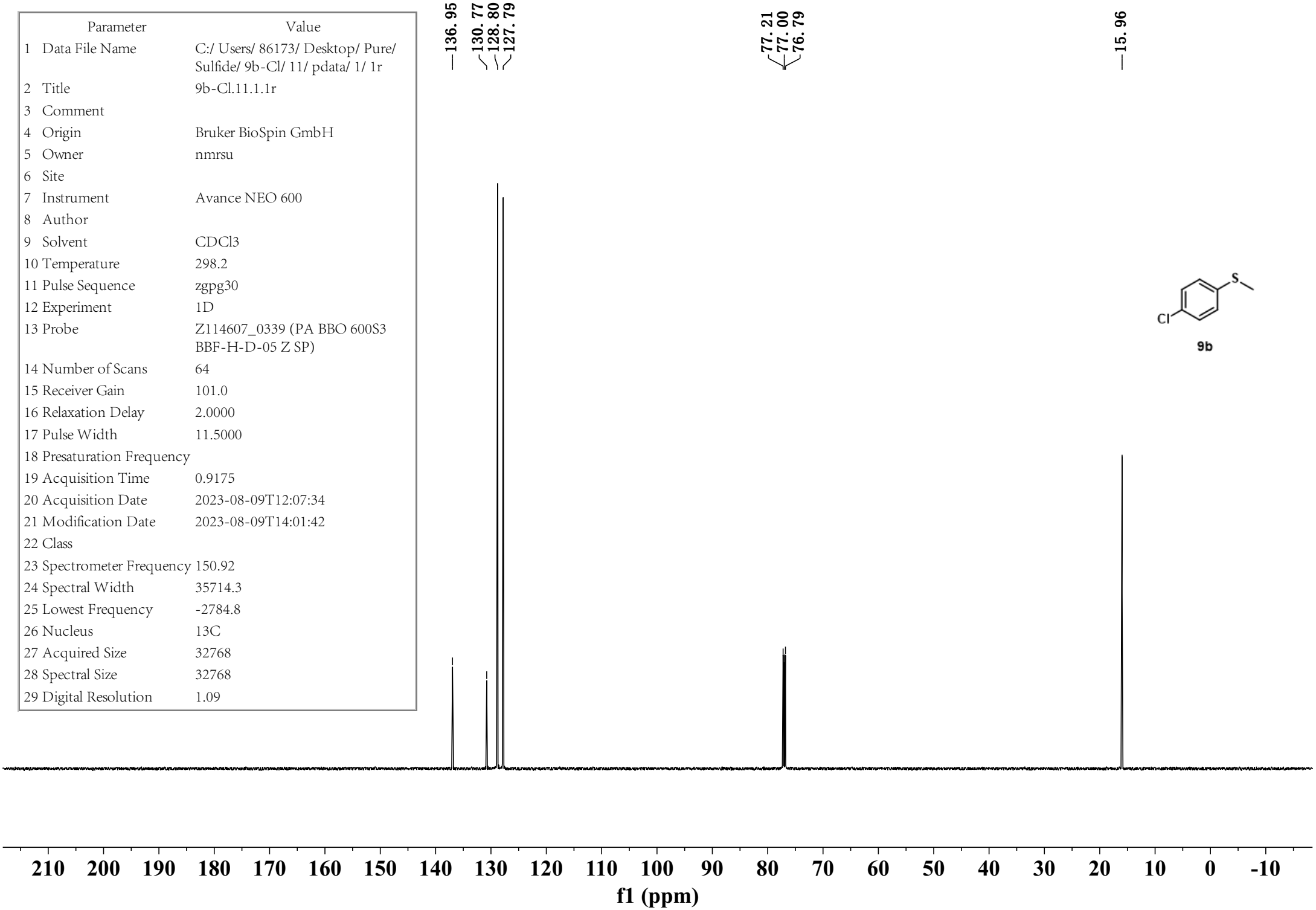


8b

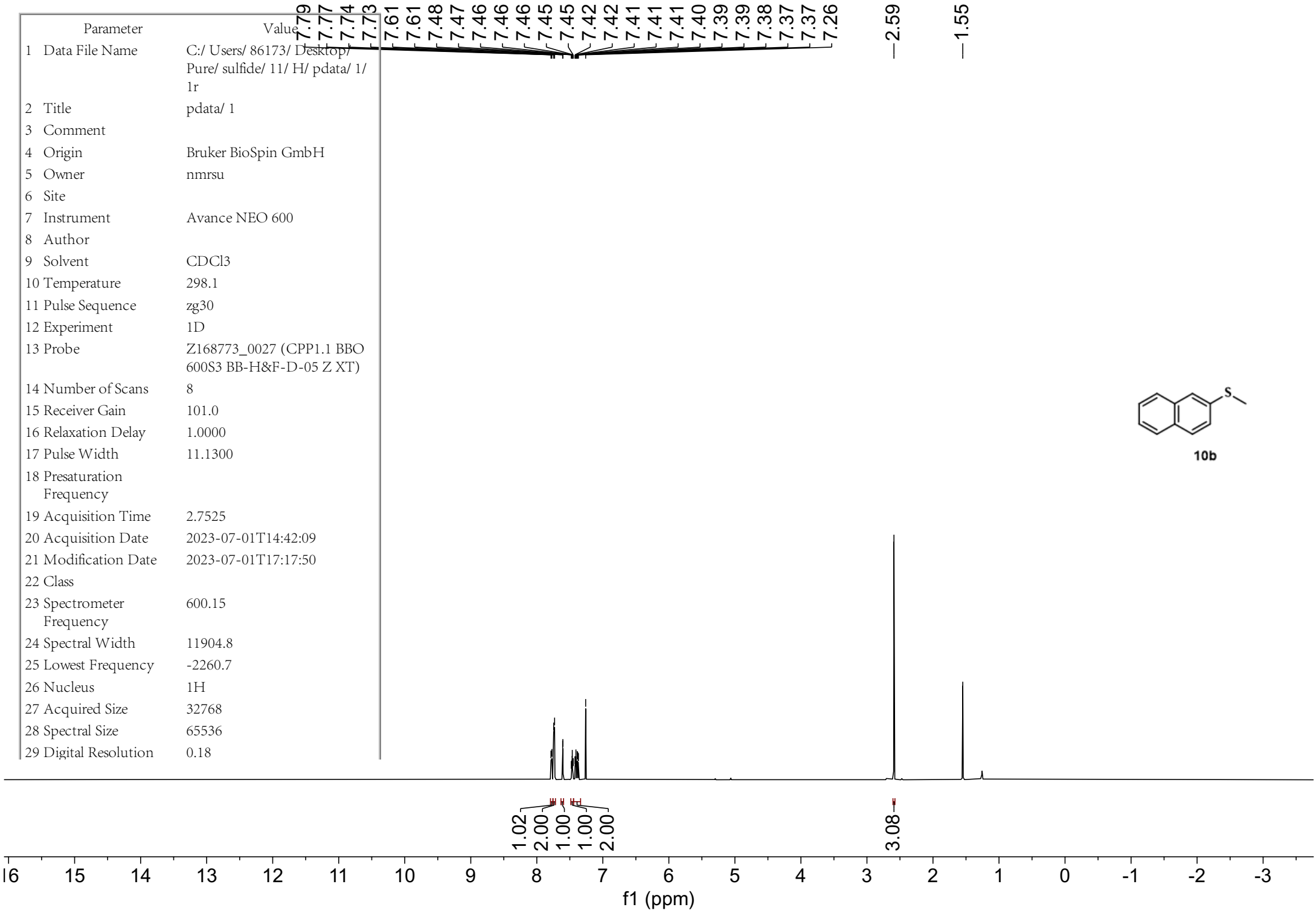
	Parameter	Value
1	Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 9b-Cl/ 10/ pdata/ 1/ 1r
2	Title	9b-Cl.10.1.1r
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance NEO 600
8	Author	
9	Solvent	CDCl3
10	Temperature	298.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14	Number of Scans	8
15	Receiver Gain	45.2
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	2.7525
20	Acquisition Date	2023-08-09T12:03:36
21	Modification Date	2023-08-09T14:01:42
22	Class	
23	Spectrometer Frequency	600.15
24	Spectral Width	11904.8
25	Lowest Frequency	-2250.5
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536
29	Digital Resolution	0.18



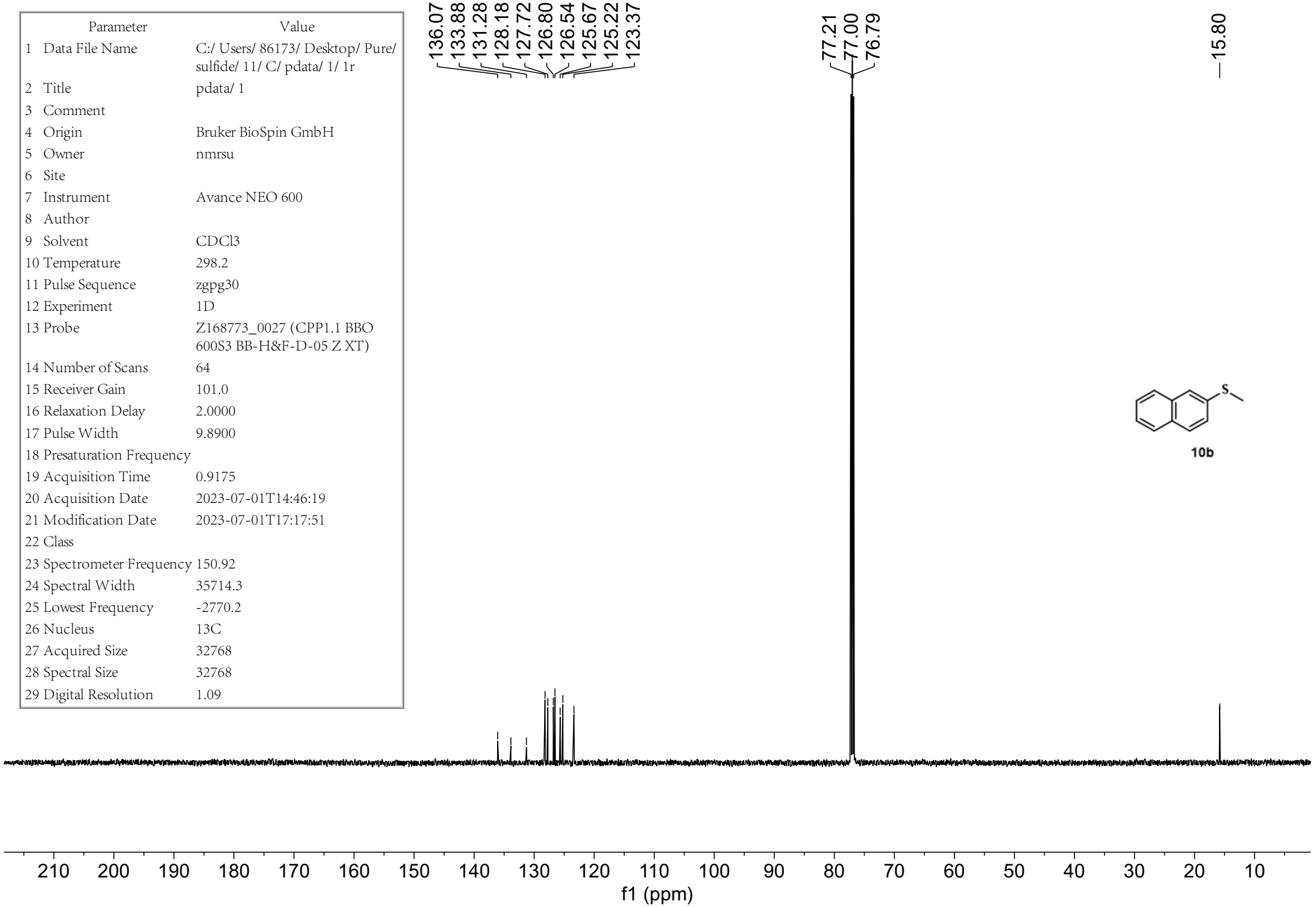
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 9b-Cl/ 11/ pdata/ 1/ 1r
2 Title	9b-Cl.11.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14 Number of Scans	64
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	11.5000
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-08-09T12:07:34
21 Modification Date	2023-08-09T14:01:42
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2784.8
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09



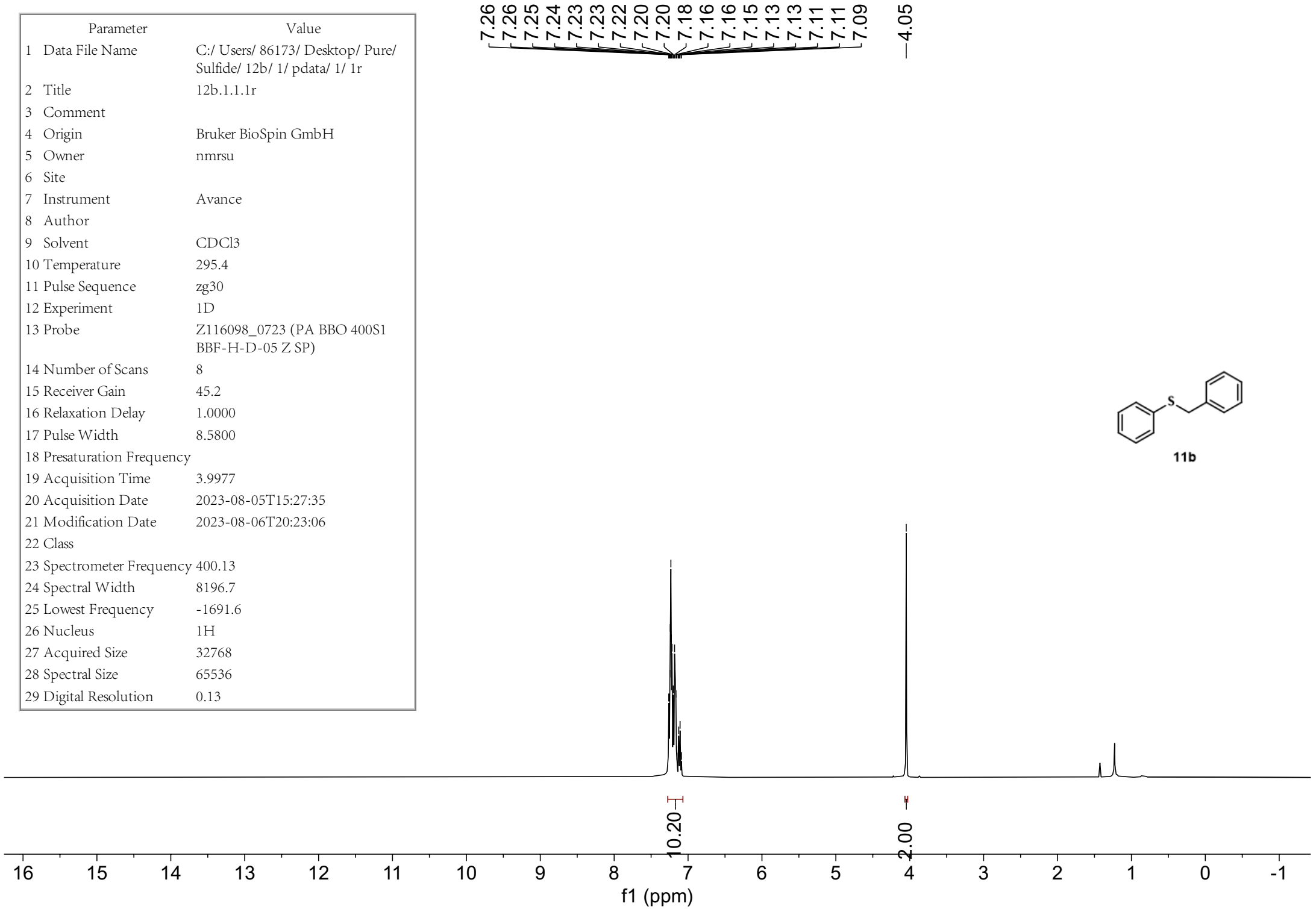
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 11/ H/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	11.1300
18 Presaturation Frequency	
19 Acquisition Time	2.7525
20 Acquisition Date	2023-07-01T14:42:09
21 Modification Date	2023-07-01T17:17:50
22 Class	
23 Spectrometer Frequency	600.15
24 Spectral Width	11904.8
25 Lowest Frequency	-2260.7
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.18



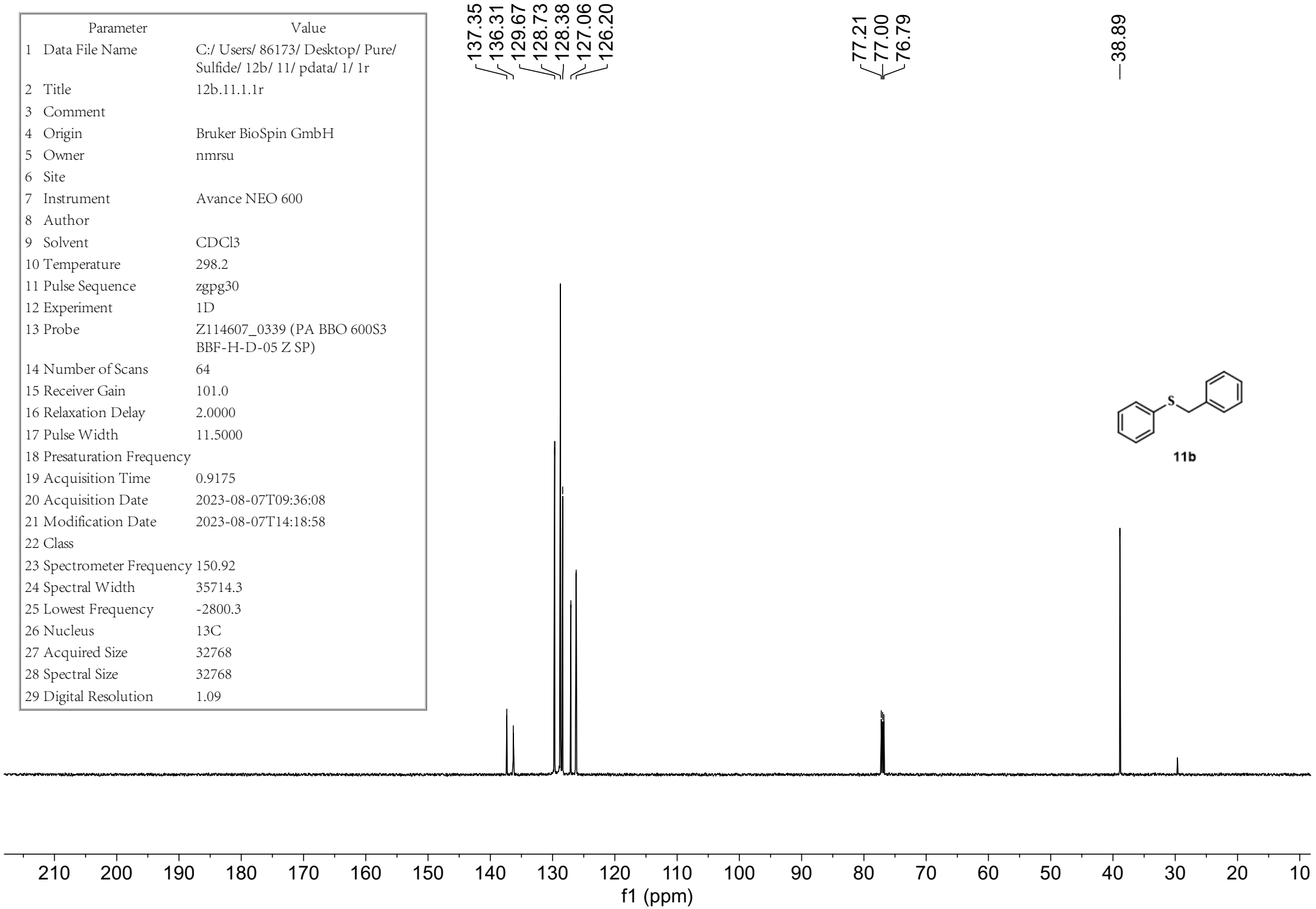
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ sulfide/ 11/ C/ pdata/ 1/ 1r
2 Title	pdata/ 1
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 600
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z168773_0027 (CPP1.1 BBO 600S3 BB-H&F-D-05 Z XT)
14 Number of Scans	64
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.8900
18 Presaturation Frequency	
19 Acquisition Time	0.9175
20 Acquisition Date	2023-07-01T14:46:19
21 Modification Date	2023-07-01T17:17:51
22 Class	
23 Spectrometer Frequency	150.92
24 Spectral Width	35714.3
25 Lowest Frequency	-2770.2
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	1.09

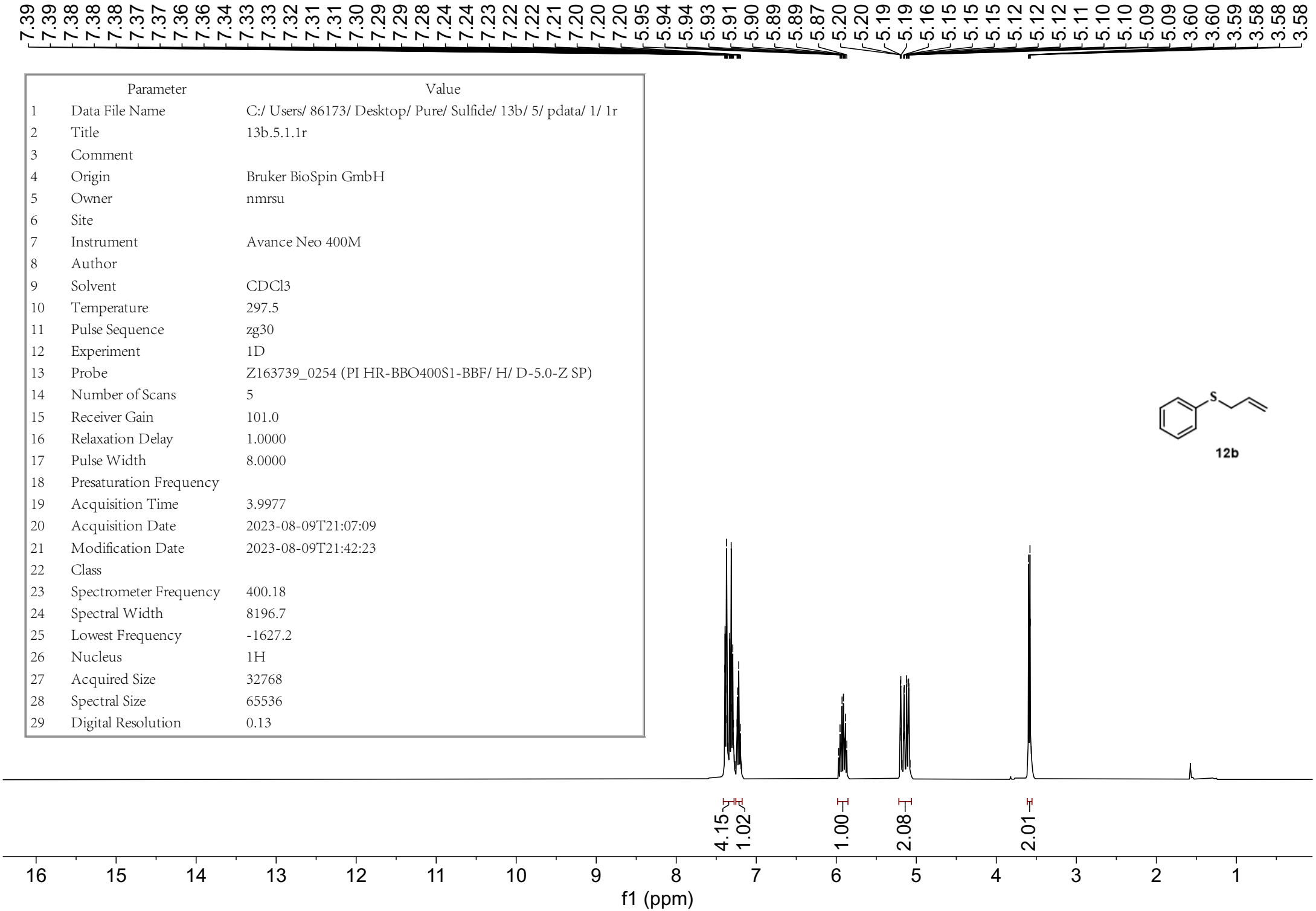


Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 12b/ 1/ pdata/ 1/ 1r
2 Title	12b.1.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	295.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	45.2
16 Relaxation Delay	1.0000
17 Pulse Width	8.5800
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-08-05T15:27:35
21 Modification Date	2023-08-06T20:23:06
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1691.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

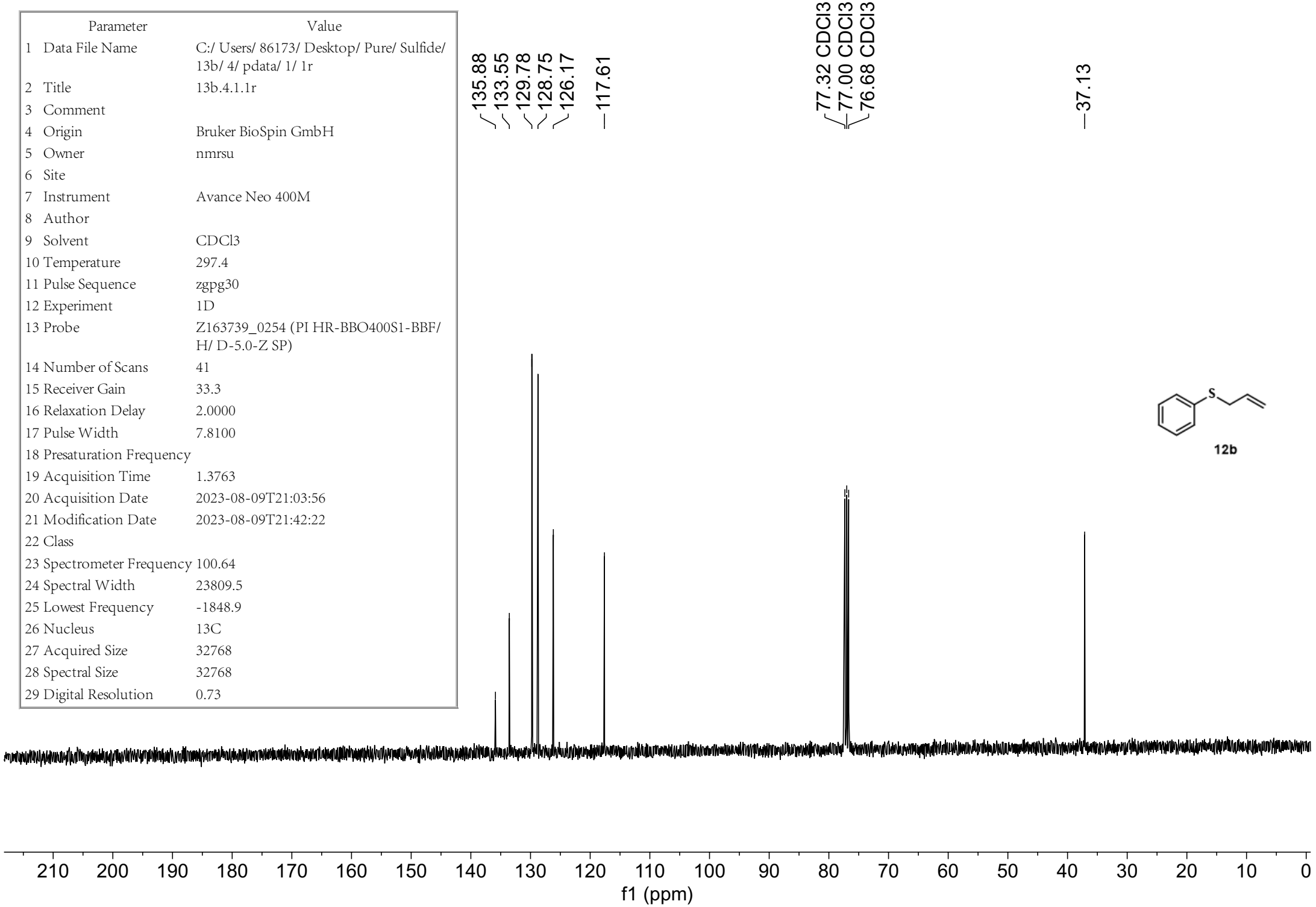


	Parameter	Value
1	Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 12b/ 11/ pdata/ 1/ 1r
2	Title	12b.11.1.1r
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance NEO 600
8	Author	
9	Solvent	CDCl3
10	Temperature	298.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z114607_0339 (PA BBO 600S3 BBF-H-D-05 Z SP)
14	Number of Scans	64
15	Receiver Gain	101.0
16	Relaxation Delay	2.0000
17	Pulse Width	11.5000
18	Presaturation Frequency	
19	Acquisition Time	0.9175
20	Acquisition Date	2023-08-07T09:36:08
21	Modification Date	2023-08-07T14:18:58
22	Class	
23	Spectrometer Frequency	150.92
24	Spectral Width	35714.3
25	Lowest Frequency	-2800.3
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	32768
29	Digital Resolution	1.09

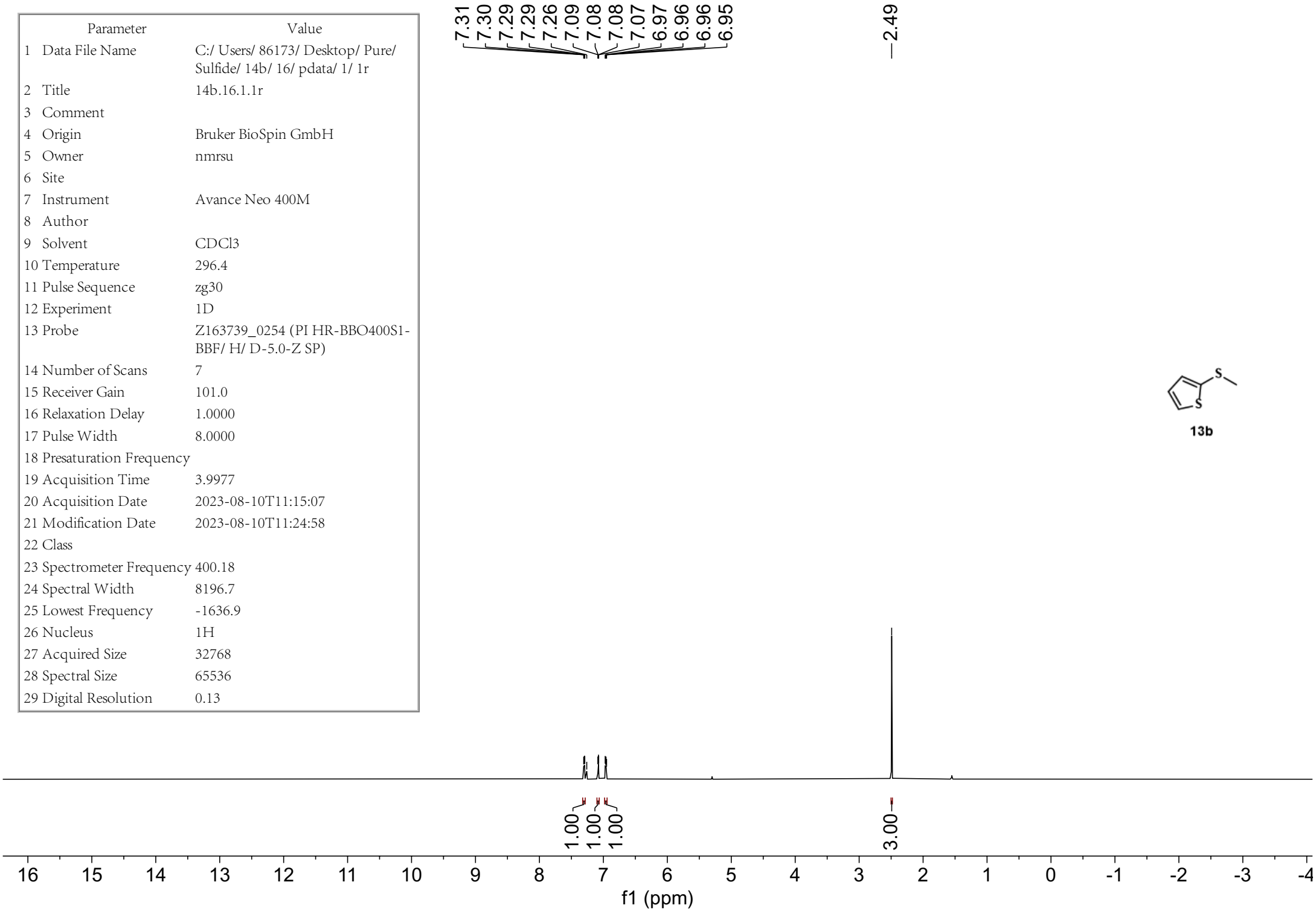



7.39 7.39 7.38 7.38 7.38 7.37 7.37 7.36 7.36 7.34 7.33 7.33 7.32 7.31 7.31 7.30 7.29 7.29 7.28 7.24 7.24 7.23 7.22 7.22 7.21 7.20 7.20 7.20 5.95 5.94 5.94 5.93 5.91 5.90 5.89 5.89 5.87 5.20 5.20 5.19 5.19 5.16 5.15 5.15 5.15 5.12 5.12 5.12 5.11 5.10 5.10 5.09 5.09 3.60 3.60 3.59 3.58 3.58 3.58
Parameter Value
1 Data File Name C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 13b/ 5/ pdata/ 1/ 1r
2 Title 13b.5.1.1r
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Instrument Avance Neo 400M
8 Author
9 Solvent CDCl3
10 Temperature 297.5
11 Pulse Sequence zg30
12 Experiment 1D
13 Probe Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans 5
15 Receiver Gain 101.0
16 Relaxation Delay 1.0000
17 Pulse Width 8.0000
18 Presaturation Frequency
19 Acquisition Time 3.9977
20 Acquisition Date 2023-08-09T21:07:09
21 Modification Date 2023-08-09T21:42:23
22 Class
23 Spectrometer Frequency 400.18
24 Spectral Width 8196.7
25 Lowest Frequency -1627.2
26 Nucleus 1H
27 Acquired Size 32768
28 Spectral Size 65536
29 Digital Resolution 0.13
S
12b
4.15
1.02
1.00
2.08
2.01
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1
f1 (ppm)

Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 13b/ 4/ pdata/ 1/ 1r
2 Title	13b.4.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	297.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	41
15 Receiver Gain	33.3
16 Relaxation Delay	2.0000
17 Pulse Width	7.8100
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-08-09T21:03:56
21 Modification Date	2023-08-09T21:42:22
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	23809.5
25 Lowest Frequency	-1848.9
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73

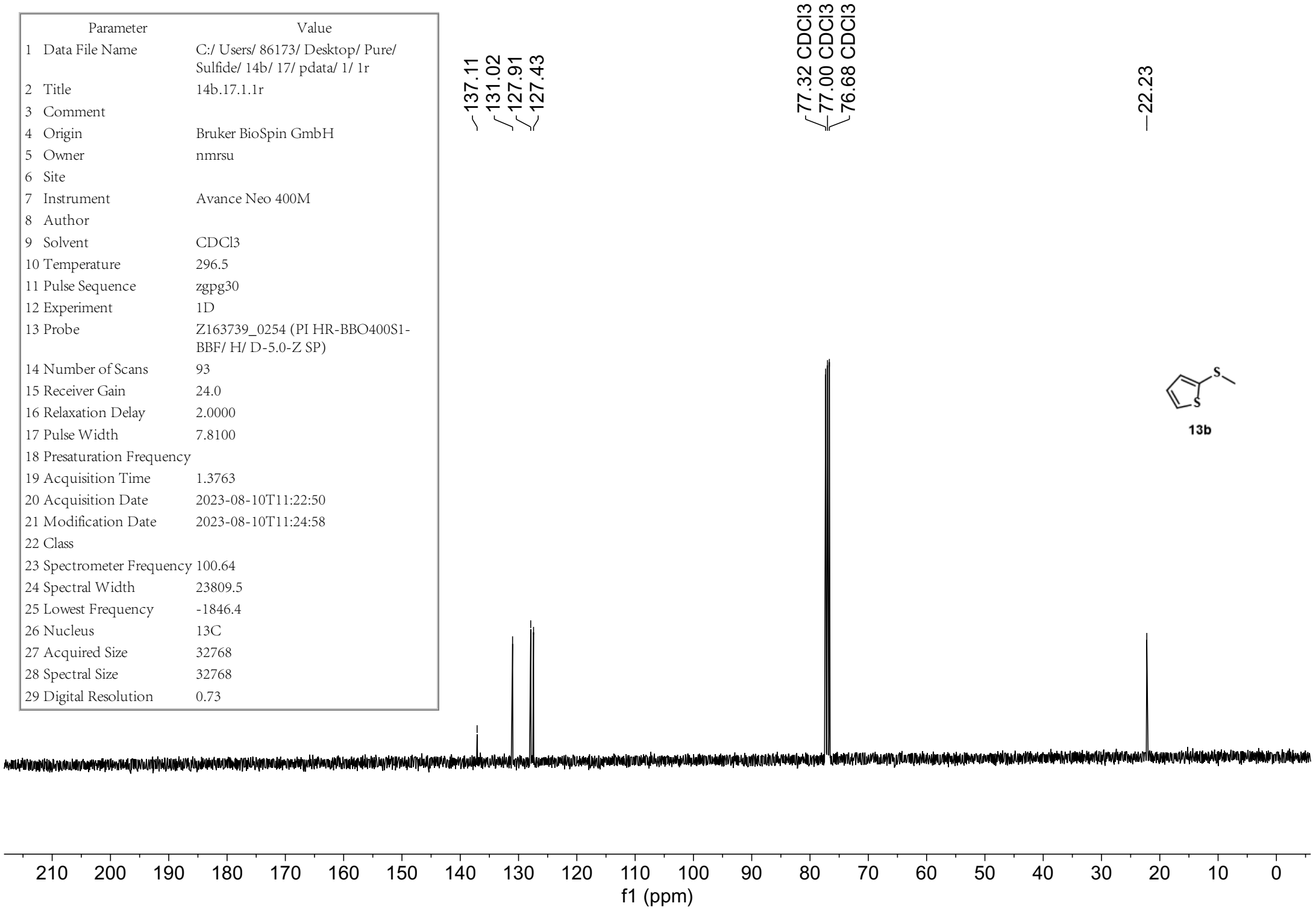


Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 14b/ 16/ pdata/ 1/ 1r
2 Title	14b.16.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	296.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	7
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-08-10T11:15:07
21 Modification Date	2023-08-10T11:24:58
22 Class	
23 Spectrometer Frequency	400.18
24 Spectral Width	8196.7
25 Lowest Frequency	-1636.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

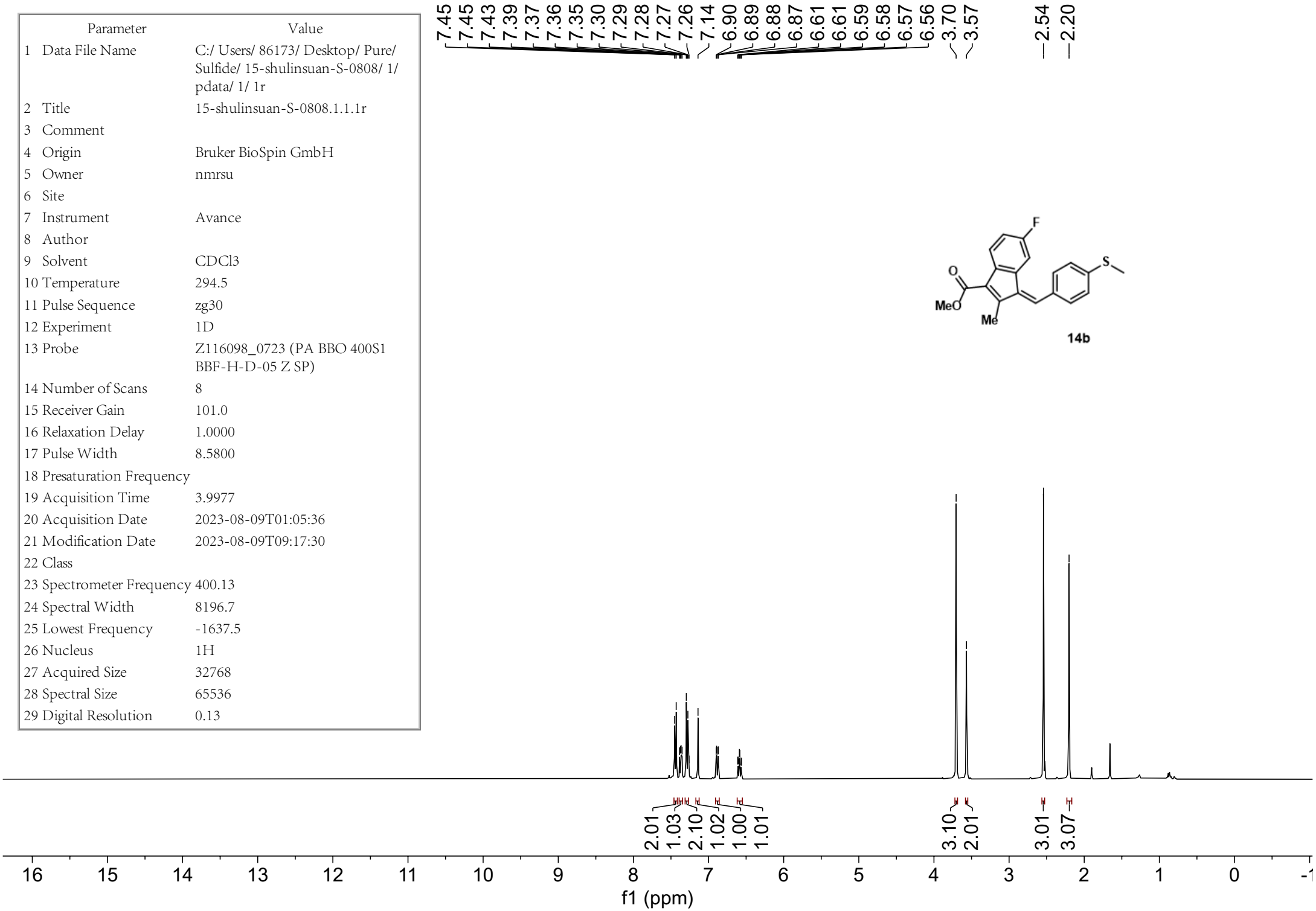


13b

Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 14b/ 17/ pdata/ 1/ 1r
2 Title	14b.17.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	296.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	93
15 Receiver Gain	24.0
16 Relaxation Delay	2.0000
17 Pulse Width	7.8100
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-08-10T11:22:50
21 Modification Date	2023-08-10T11:24:58
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	23809.5
25 Lowest Frequency	-1846.4
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73

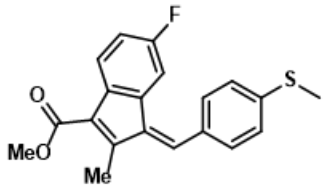


Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 15-shulinsuan-S-0808/ 1/ pdata/ 1/ 1r
2 Title	15-shulinsuan-S-0808.1.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	294.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.5800
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-08-09T01:05:36
21 Modification Date	2023-08-09T09:17:30
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.5
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

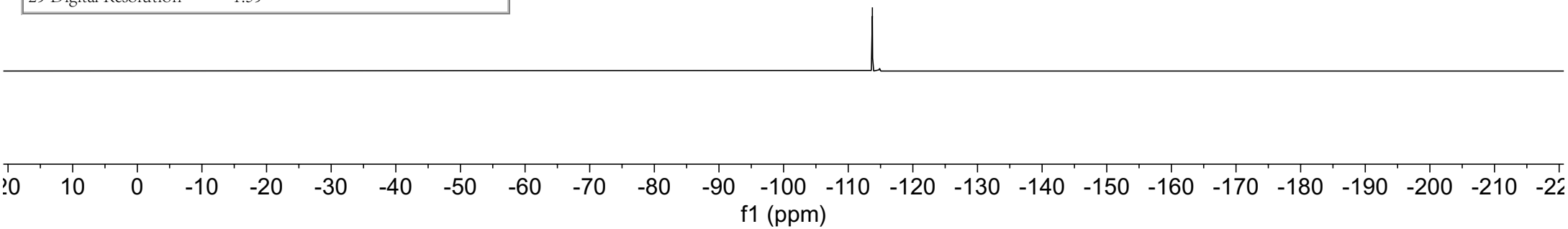


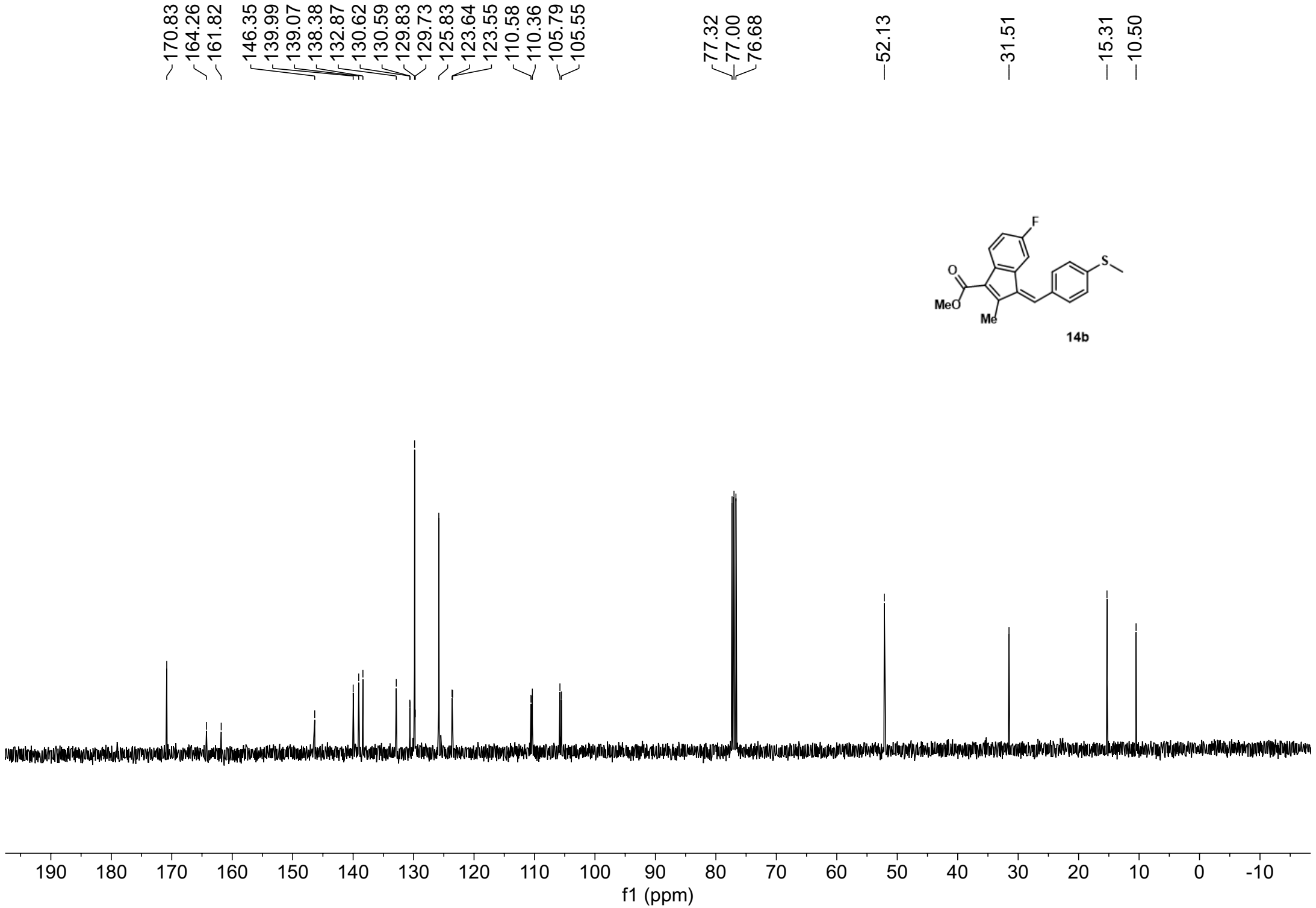
	Parameter	Value
1	Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 15-shulinsuan-S-0808/ 2/ pdata/ 1/ 1r
2	Title	15-shulinsuan-S-0808.2.1.1r
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	294.5
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14	Number of Scans	16
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	17.8500
18	Presaturation Frequency	
19	Acquisition Time	0.7209
20	Acquisition Date	2023-08-09T01:06:59
21	Modification Date	2023-08-09T09:17:31
22	Class	
23	Spectrometer Frequency	376.46
24	Spectral Width	90909.1
25	Lowest Frequency	-83104.4
26	Nucleus	19F
27	Acquired Size	65536
28	Spectral Size	65536
29	Digital Resolution	1.39

-113.74

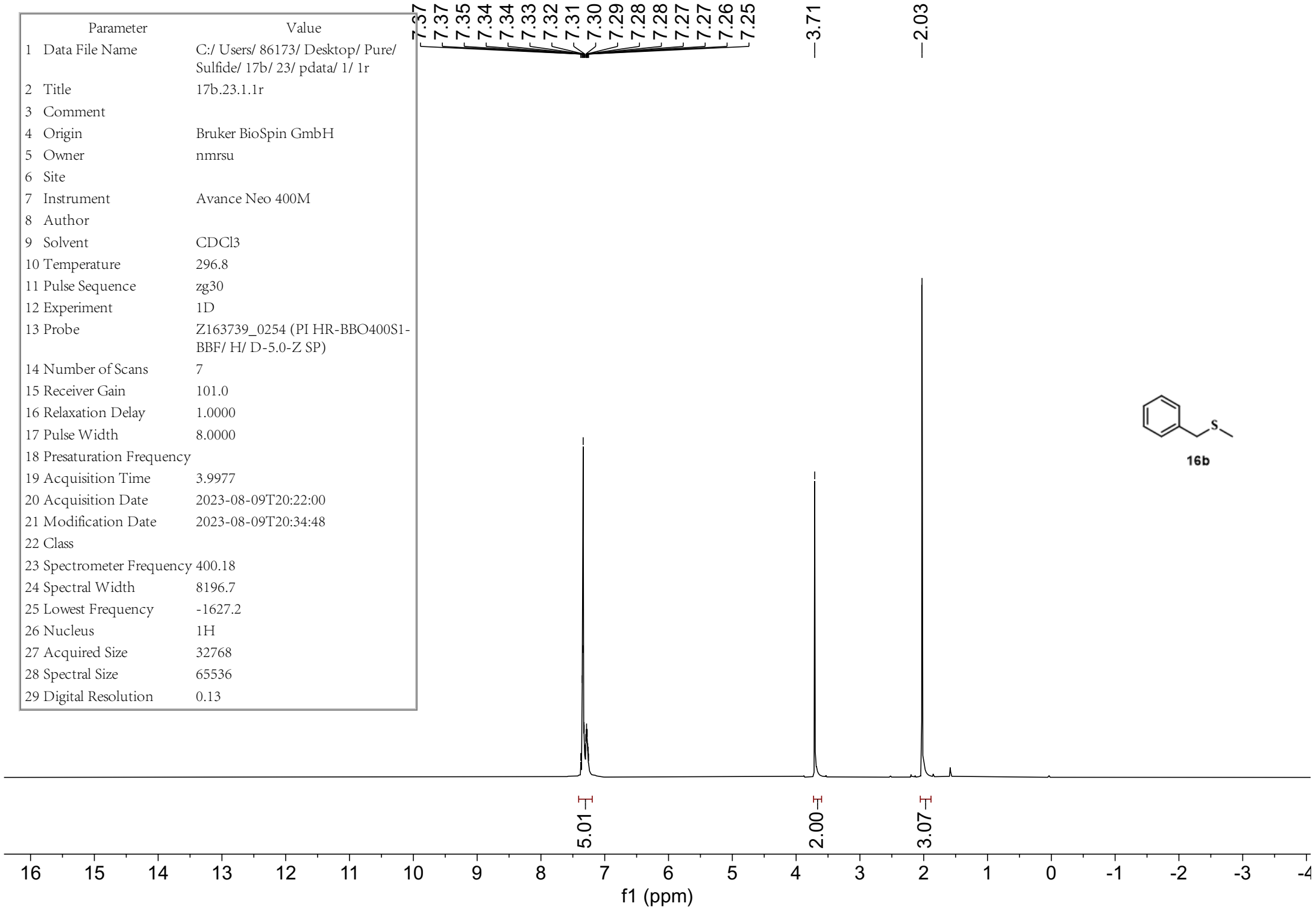


14b

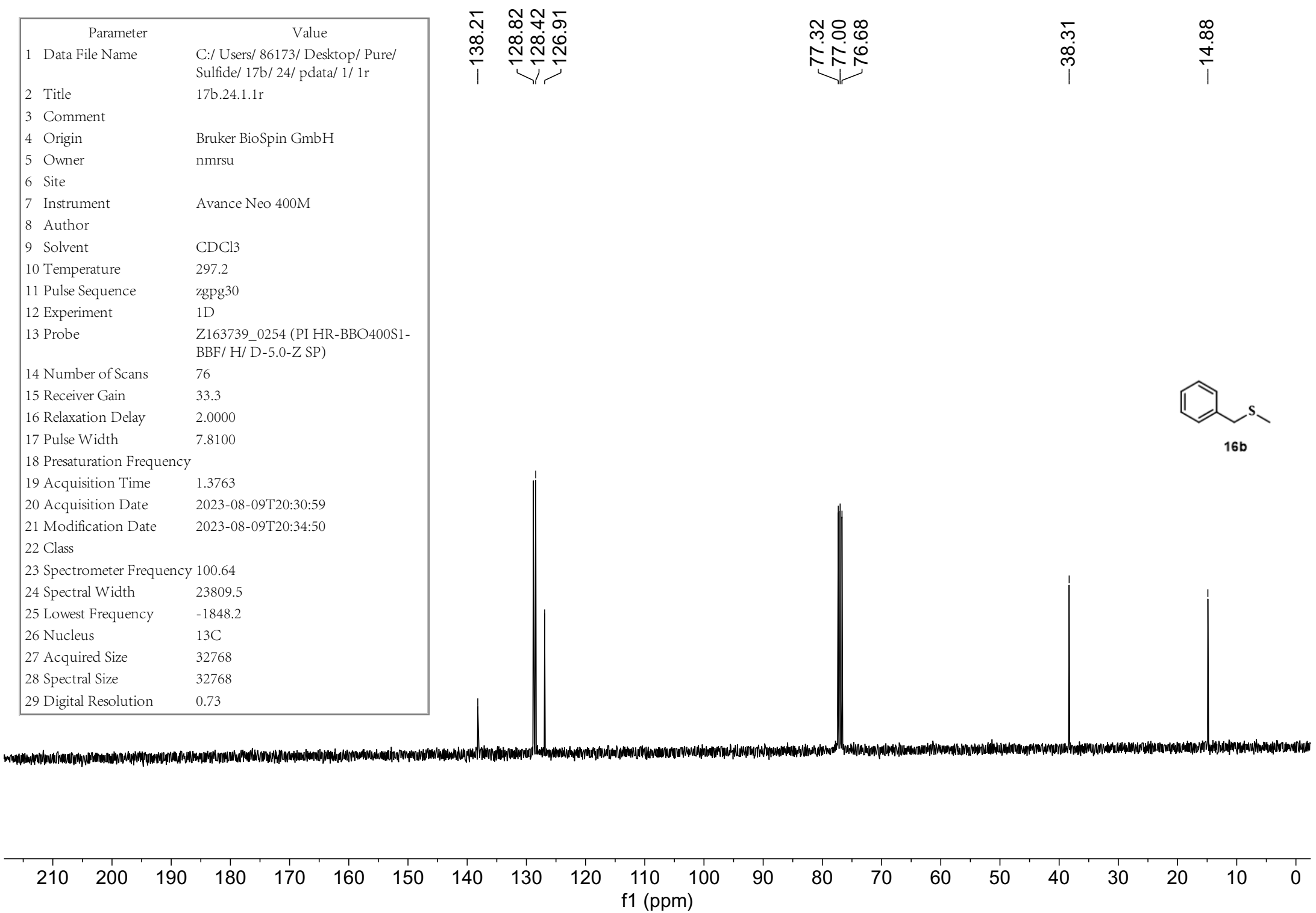



170.83
164.26
161.82
146.35
139.99
139.07
138.38
132.87
130.62
130.59
129.83
129.73
125.83
123.64
123.55
110.58
110.36
105.79
105.55
77.32
77.00
76.68
52.13
31.51
15.31
10.50
F
S
O
MeO
Me
14b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

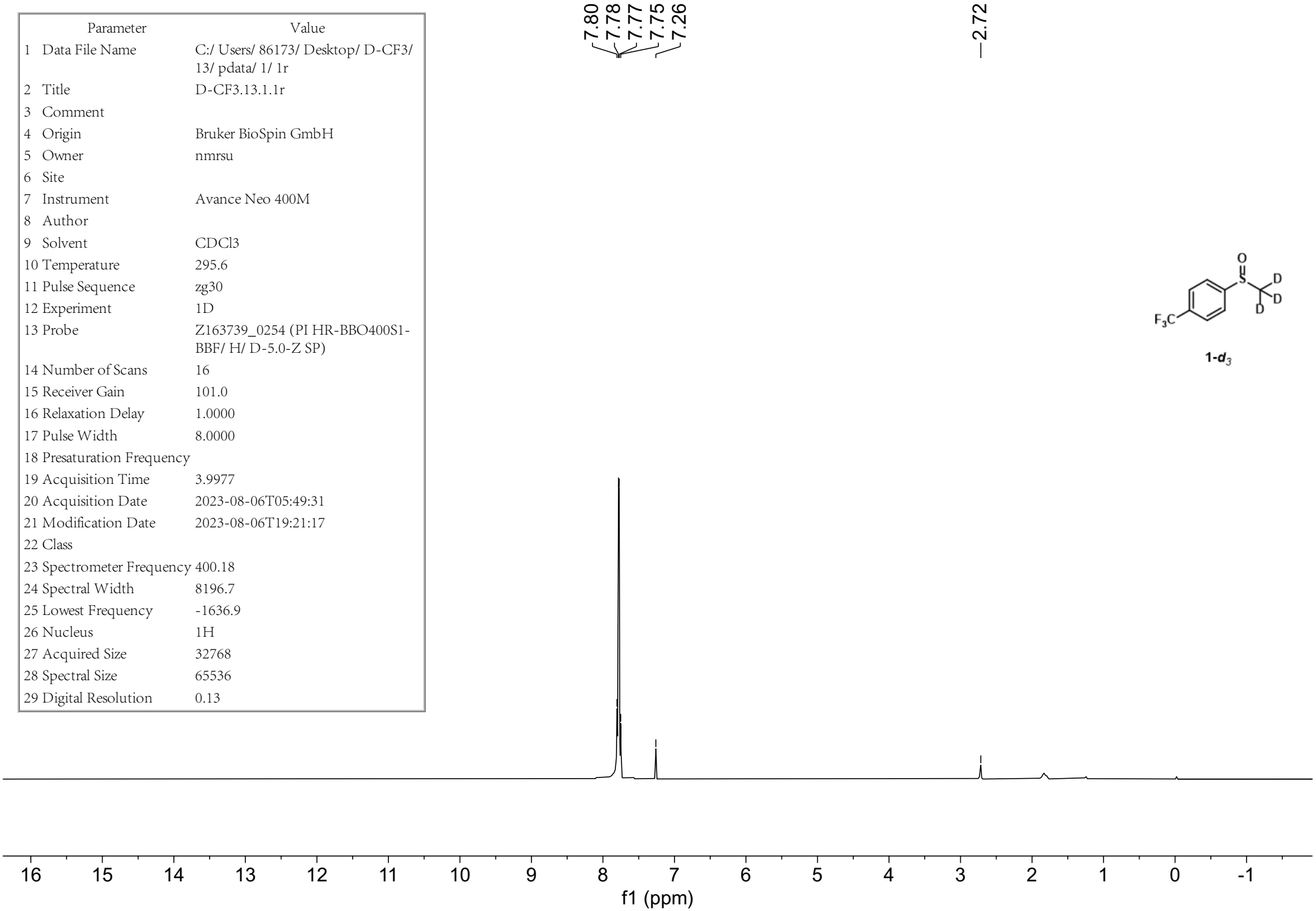
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 17b/ 23/ pdata/ 1/ 1r
2 Title	17b.23.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	296.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	7
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-08-09T20:22:00
21 Modification Date	2023-08-09T20:34:48
22 Class	
23 Spectrometer Frequency	400.18
24 Spectral Width	8196.7
25 Lowest Frequency	-1627.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



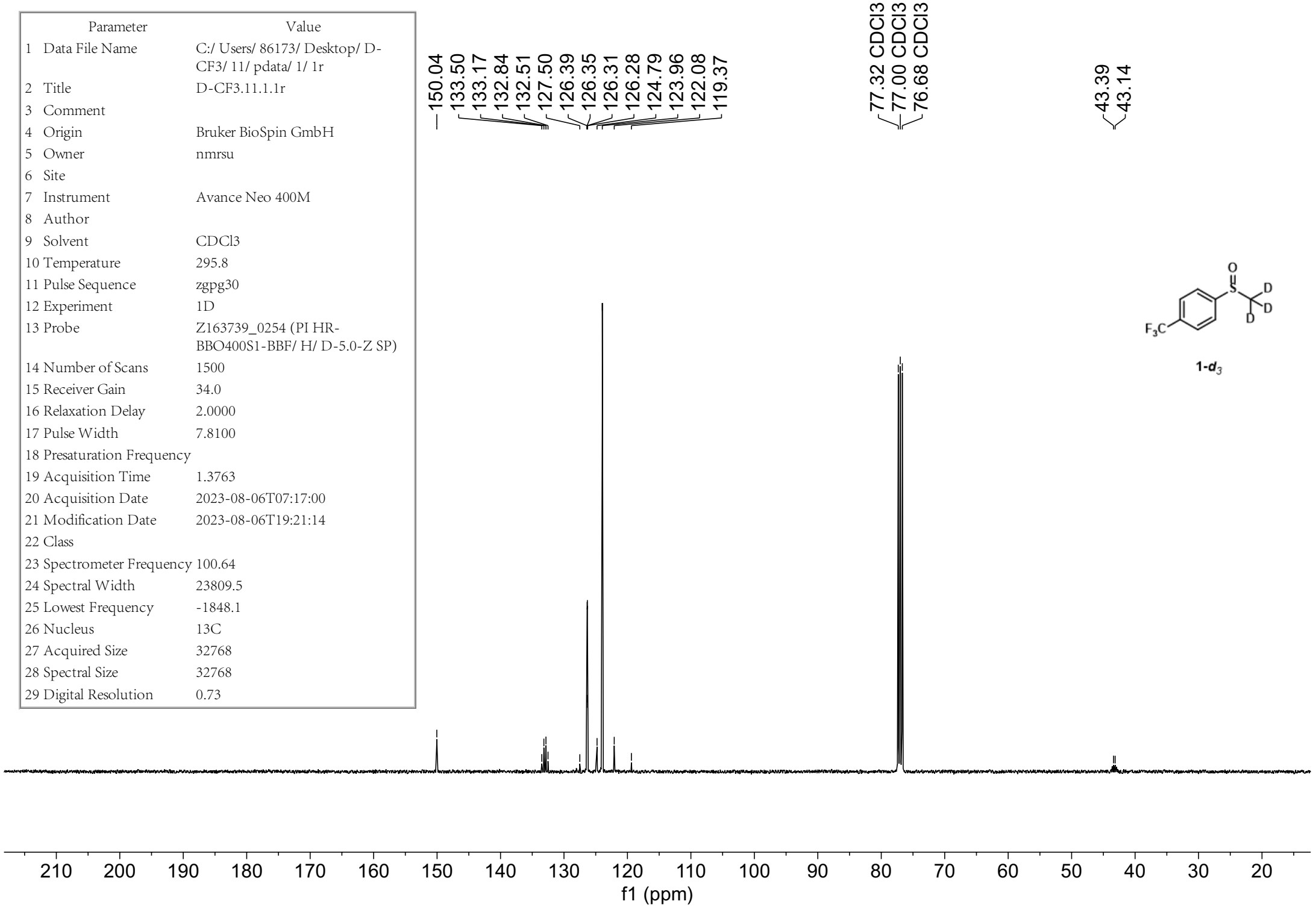
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ Pure/ Sulfide/ 17b/ 24/ pdata/ 1/ 1r
2 Title	17b.24.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	297.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	76
15 Receiver Gain	33.3
16 Relaxation Delay	2.0000
17 Pulse Width	7.8100
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-08-09T20:30:59
21 Modification Date	2023-08-09T20:34:50
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	23809.5
25 Lowest Frequency	-1848.2
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73



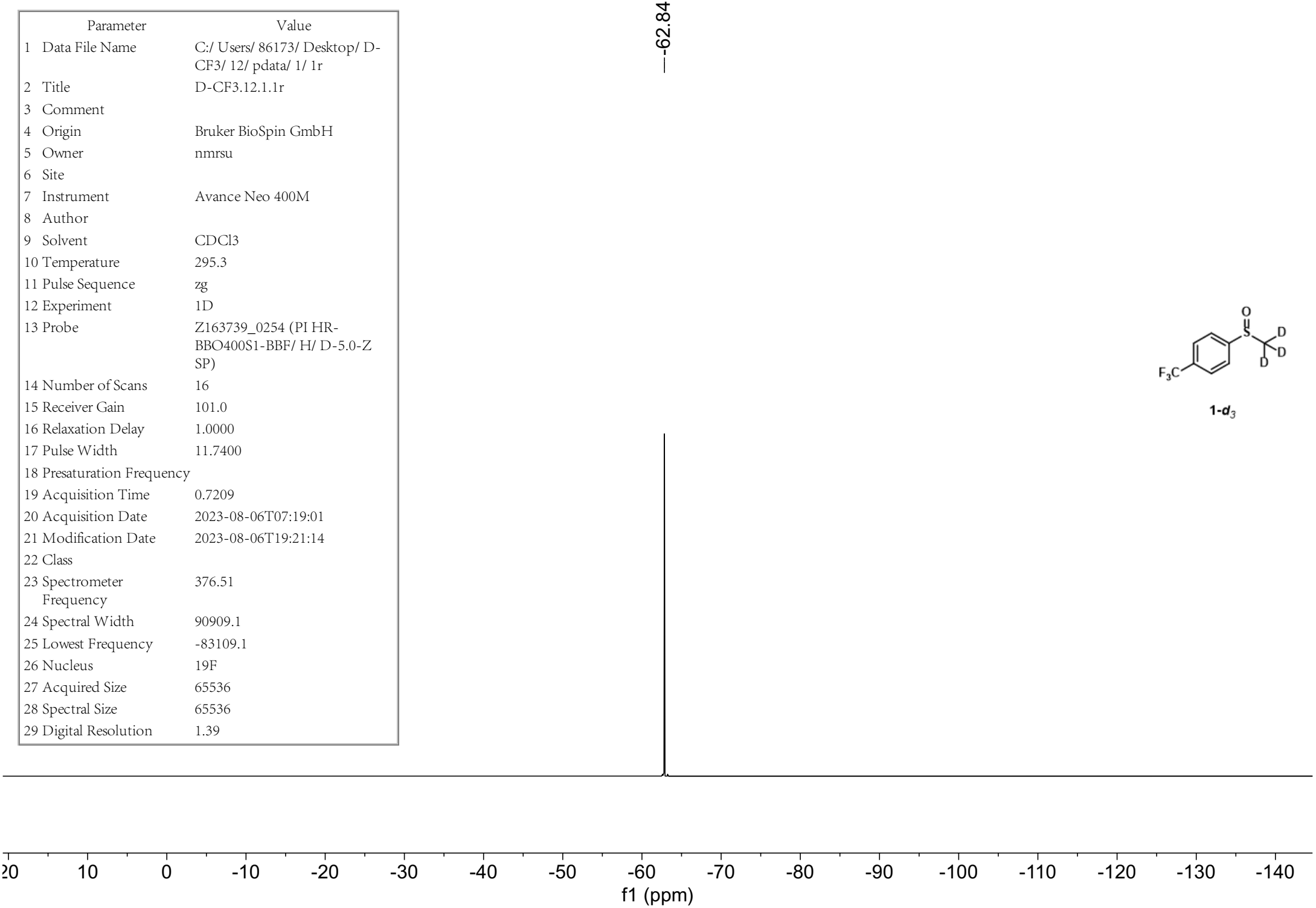
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ D-CF3/ 13/ pdata/ 1/ 1r
2 Title	D-CF3.13.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	295.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-08-06T05:49:31
21 Modification Date	2023-08-06T19:21:17
22 Class	
23 Spectrometer Frequency	400.18
24 Spectral Width	8196.7
25 Lowest Frequency	-1636.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



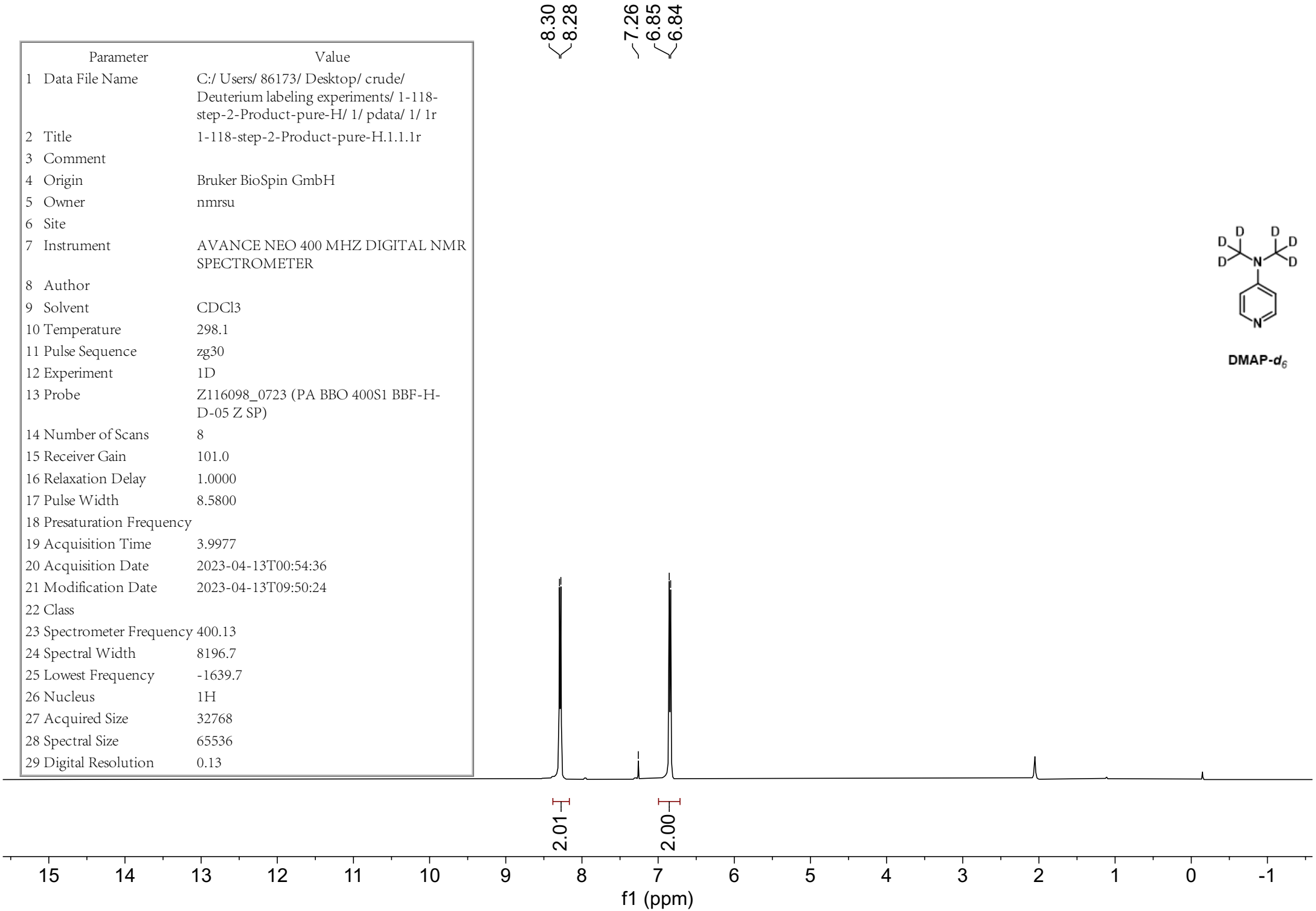
Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ D-CF3/ 11/ pdata/ 1/ 1r
2 Title	D-CF3.11.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance Neo 400M
8 Author	
9 Solvent	CDCl3
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1500
15 Receiver Gain	34.0
16 Relaxation Delay	2.0000
17 Pulse Width	7.8100
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-08-06T07:17:00
21 Modification Date	2023-08-06T19:21:14
22 Class	
23 Spectrometer Frequency	100.64
24 Spectral Width	23809.5
25 Lowest Frequency	-1848.1
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73



	Parameter	Value
1	Data File Name	C:/ Users/ 86173/ Desktop/ D-CF3/ 12/ pdata/ 1/ 1r
2	Title	D-CF3.12.1.1r
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance Neo 400M
8	Author	
9	Solvent	CDCl3
10	Temperature	295.3
11	Pulse Sequence	zg
12	Experiment	1D
13	Probe	Z163739_0254 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14	Number of Scans	16
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	11.7400
18	Presaturation Frequency	
19	Acquisition Time	0.7209
20	Acquisition Date	2023-08-06T07:19:01
21	Modification Date	2023-08-06T19:21:14
22	Class	
23	Spectrometer Frequency	376.51
24	Spectral Width	90909.1
25	Lowest Frequency	-83109.1
26	Nucleus	19F
27	Acquired Size	65536
28	Spectral Size	65536
29	Digital Resolution	1.39



Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ crude/ Deuterium labeling experiments/ 1-118-step-2-Product-pure-H/ 1/ pdata/ 1/ 1r
2 Title	1-118-step-2-Product-pure-H.1.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	8
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.5800
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-04-13T00:54:36
21 Modification Date	2023-04-13T09:50:24
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1639.7
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



DMAP-d_6

Parameter	Value
1 Data File Name	C:/ Users/ 86173/ Desktop/ crude/ Deuterium labeling experiments/ 1-118-step-2-Product-pure-H/ 2/ pdata/ 1/ 1r
2 Title	1-118-step-2-Product-pure-H. 2.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	AVANCE NEO 400 MHZ DIGITAL NMR SPECTROMETER
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0723 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	2048
15 Receiver Gain	64.0
16 Relaxation Delay	2.0000
17 Pulse Width	9.7000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-13T02:53:18
21 Modification Date	2023-04-13T09:50:24
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1880.2
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768
29 Digital Resolution	0.73