Electronic Supplementary Information

8-Aminoquinoline as Bidentate Traceless Directing Group for Cu-Catalyzed/Mediated Selective B(4,5)−H Disulfenylation of *o*-Carboranes

Yu Chen, Yangjian Quan* and Zuowei Xie*

Department of Chemistry and State Key Laboratory of Synthetic Chemistry, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China

E-mail: yjquan@cuhk.edu.hk; zxie@cuhk.edu.hk

Table of Contents

General Procedures S2

Optimization of Reaction Conditions S3

Experimental Section S4

Preliminary Mechanistic Study S20

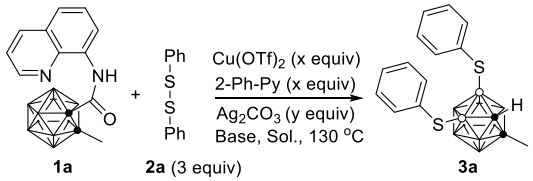
NMR Spectra S25

References S171

General Procedures. All reactions were carried out in flame-dried glassware under an atmosphere of dry argon with the exclusion of air and moisture using standard Schlenk techniques or in drybox. All organic solvents were dried and distilled by standard methods prior to use. ^{1}H, ^{13}C, ^{11}B and ^{19}F NMR spectra were recorded on Bruker DPX 400/500 spectrometer at 400/500, 100/125, 128/160 and 376/470 MHz, respectively. All chemical shifts were reported in δ units with references to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, to external $BF_3 \cdot OEt_2$ (0.00 ppm) for boron chemical shifts, and to external $CFCl_3$ (0.00) for fluorine chemical shifts. High Resolution Mass Spectra (HRMS) were obtained on a Thermo Q Exactive™ Focus Hybrid Quadrupole-Orbitrap™ Mass Spectrometer. GC-MS analyses were performed on Agilent GC-MS 6890N. Melting points were measured using a Nikon Polarizing Microscope ECLIPSE 50i POL equipped with an INTEC HCS302 heating stage without calibration. Carboranyl amides (**1a**-**1f**) was prepared according to literature method.[1] All other chemicals were purchased from either Aldrich or Acros Chemical Co. and used as received unless otherwise specified.

Optimization of Reaction Conditions

Table S1 Optimization of reaction conditions.[a]



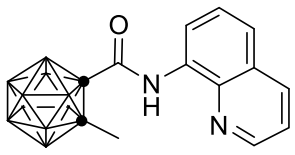
1a **2a** (3 equiv) **3a**

Entry	x	y	Base (equiv)	Sol.	Time (h)	Yield (%)[b]
1	0.2	2.0	Li_2CO_3 (2)	DCE	12	22
2[c]	0.2	2.0	Li_2CO_3 (2)	DCE	12	5[c]
3[d]	0.2	2.0	Li_2CO_3 (2)	DCE	12	12
4	0.6	2.0	Li_2CO_3 (2)	DCE	12	44
5	0.6	2.0	K_2CO_3 (2)	DCE	12	24
6	0.6	2.0	^{t}BuOLi (2)	DCE	12	60
7	0.6	2.0	^{t}BuOLi (3)	DCE	12	74
8	0.6	2.0	^{t}BuOLi (4)	DCE	12	80
9	**0.6**	**2.0**	**^{t}BuOLi** (4)	DCE	**48**	**93**
10[e]	0.6	0	^{t}BuOLi (4)	DCE	48	0
11	0.6	0	^{t}BuOLi (4)	DCE	48	66
12	0.8	0	^{t}BuOLi (4)	DCE	48	85
13	**1.0**	**0**	**^{t}BuOLi** (4)	DCE	**48**	**92 (86)[f]**
14[g]	1.0	0	^{t}BuOLi (4)	THF	48	0
15	1.0	0	^{t}BuOLi (4)	Tol	48	32
16	1.0	0	^{t}BuOLi (4)	DME	48	0
17[h]	1.0	0	^{t}BuOLi (4)	DCE	48	78
18[i]	1.0	0	^{t}BuOLi (4)	DCE	48	89
19[j]	1.0	0	^{t}BuOLi (4)	DCE	48	80
20[k]	1.0	0	^{t}BuOLi (4)	DCE	48	56

[a]Reactions were conducted on 0.05 mmol scale in 3.0 mL of solvent in a closed flask; DCE = 1,2-dichloroethane; THF = tetrahydrofuran; Tol = toluene; DME = 1,2-dimethoxyethane; 2-Ph-Py = 2-phenylpyridine. [b]GC yield. [c]$Cu(NTf_2)_2$ (20 mol%) was used in place of $Cu(OTf)_2$. [d]Without addition of 2-Ph-Py. [e]1 atm O_2 gas was filled in the sealed tube. [f]Isolated yield in the parentheses. [g]Reaction was carried out in THF at 100 °C. [h]Reaction was carried out in DCE at 110 °C. [i]2.5 equiv. of **2a** were utilized. [j]2.0 equiv. of **2a** were utilized. [k]1.0 equiv. of **2a** were utilized.

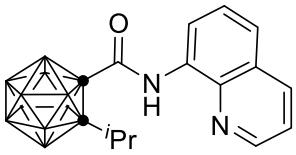
Preparation of 8-aminoquinoline carboranyl amides (1)

A representative procedure. A dichloromethane solution (10 mL) of *o*-carboranyl monocarboxylic acid (404.0 mg, 2.0 mmol) and DMF (0.1 mL) was cooled to 0 ºC, to which was slowly added oxalyl chloride (0.51 mL, 6.0 mmol). The resulting solution was stirred for 1 h at room temperature, followed by removal of the solvent and excess oxalyl chloride in vacuo. The resultant acid chloride was dissolved in dichloromethane (5 mL) and cooled to 0 ºC, to which was added dropwise another dichloromethane solution (10 mL) of 8-aminoquinoline (374.8 mg, 2.6 mmol) and triethylamine (0.84 mL, 6.0 mmol). The reaction mixture was stirred for 12 h at room temperature and then quenched with water (15 mL). The organic layer was separated, and the aqueous layer was extracted with dichloromethane (15 mL x 2). The organic solutions were combined and dried over anhydrous Na_2SO_4. After removal of solvent, the residue was submitted to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (100/1 in v/v) as eluent to give **1a** (610.0 mg, 93%).

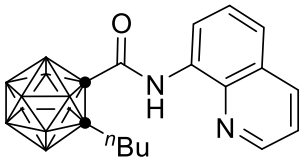


1a: Yield 93%. White solid. Mp: 167−168 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.99 (s, 1H) (N*H*), 8.90 (s, 1H), 8.62 (d, *J* = 6.1 Hz, 1H), 8.20 (d, *J* = 7.1 Hz, 1H), 7.56 (m, 3H) (Aryl C*H*), 2.23 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.9 (*C*=O), 149.1, 138.7, 136.5, 133.3, 128.0,

127.0, 123.5, 122.3, 117.0 (Aryl *C*), 76.5, 76.4 (Cage *C*), 24.5 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, CDCl$_3$): δ -2.11 (1B), -5.84 (1B), -10.8 (8B). HRMS (APCI pos): *m/z* calcd for $C_{13}H_{20}{}^{10}B_2{}^{11}B_8N_2O$ $[M+H]^+$: 329.2649. Found: 329.2658.

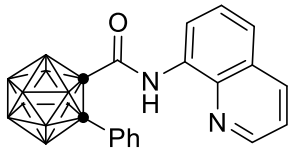


1b: Yield 82%. White solid. Mp: 160−161 °C. ^{1}H NMR (400 MHz, CDCl$_3$): δ 10.96 (s, 1H) (N*H*), 8.90 (dd, *J* = 1.6, 4.2 Hz, 1H), 8.62 (dd, *J* = 1.1, 7.6 Hz, 1H), 8.20 (dd, *J* = 1.5, 8.3 Hz, 1H), 7.62 (dd, *J* = 1.2, 8.3 Hz, 1H), 7.54 (m, 2H) (Aryl C*H*), 2.60 (m, 1H) (^{i}Pr), 1.24 (d, *J* = 8.0 Hz, 6H) (^{i}Pr). ^{13}C NMR (100 MHz, CDCl$_3$): δ 155.4 (*C*=O), 149.2, 138.8, 136.5, 133.3, 128.0, 127.1, 123.5, 122.3, 117.0 (Aryl *C*), 88.2, 80.5 (Cage *C*), 33.0, 24.4 (^{i}Pr). ^{11}B{^{1}H} NMR (128 MHz, CDCl$_3$): δ -3.13 (1B), -4.08 (1B), -10.04 (2B), -11.70 (6B). HRMS (APCI pos): *m/z* calcd for $C_{15}H_{24}{}^{10}B_2{}^{11}B_8N_2O$ $[M+H]^+$: 357.2961. Found: 357.2972.

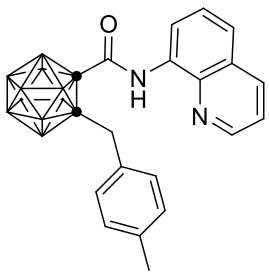


1c: Yield 90%. White solid. Mp: 153−154 °C. ^{1}H NMR (400 MHz, CDCl$_3$): δ 10.98 (s, 1H) (N*H*), 8.90 (dd, *J* = 1.4, 4.2 Hz, 1H), 8.64 (d, *J* = 7.5 Hz, 1H), 8.19 (dd, *J* = 1.3, 8.3 Hz, 1H), 7.56 (m, 3H) (Aryl C*H*), 2.43 (m, 2H), 1.58 (m, 2H), 1.29 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H) (^{n}Bu). ^{13}C NMR (100 MHz, CDCl$_3$): δ 155.5 (*C*=O), 149.1, 138.7, 136.4, 133.3, 127.9, 127.0, 123.4, 122.2, 116.9 (Aryl *C*), 81.8, 78.2 (Cage *C*), 35.8, 31.9, 22.3, 13.7 (^{n}Bu). ^{11}B{^{1}H} NMR (128 MHz, CDCl$_3$): δ -2.53 (1B), -4.88 (1B), -10.40 (8B). HRMS (APCI

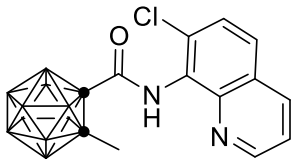
pos): *m/z* calcd for $C_{16}H_{26}{}^{10}B_2{}^{11}B_8N_2O$ $[M+H]^+$: 371.3125. Found: 371.3129.



1d: Yield 77%. White solid. Mp: 173–174 °C. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 10.77 (s, 1H) (N*H*), 8.89 (dd, *J* = 1.6, 4.2 Hz, 1H), 8.28 (d, *J* = 7.7 Hz, 1H), 8.19 (d, *J* = 8.3 Hz, 1H), 7.74 (d, *J* = 7.9 Hz, 2H), 7.53 (m, 2H) 7.42 (dd, *J* = 8.0, 8.0 Hz, 1H), 7.31 (m, 3H) (Aryl C*H*). ^{13}C NMR (125 MHz, CD_2Cl_2): δ 154.0 (*C*=O), 148.7, 138.2, 136.1, 132.7, 130.5, 130.4, 130.3, 128.2, 127.5, 126.5, 122.9, 121.9, 116.2 (Aryl *C*), 83.7, 80.3 (Cage *C*). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.64 (1B), -3.64 (1B), -10.34 (8B). HRMS (APCI neg): *m/z* calcd for $C_{18}H_{22}{}^{10}B_2{}^{11}B_8N_2O$ $[M]^-$: 390.2750. Found: 390.2748.



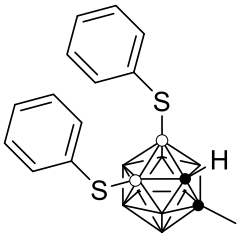
1e: Yield 85%. White solid. Mp: 117–118 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.98 (s, 1H) (N*H*), 8.88 (d, *J* = 2.9 Hz, 1H), 8.72 (d, *J* = 7.2 Hz, 1H), 8.22 (d, *J* = 8.2 Hz, 1H), 7.62 (m, 2H), 7.53 (dd, *J* = 4.2, 8.2 Hz, 1H), 7.10 (dd, *J* = 7.5, 7.5 Hz, 1H), 6.98 (m, 3H) (Aryl C*H*), 3.69 (s, 2H) (C*H*$_2$), 2.11 (s, 3H) (C*H*$_3$). ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.7 (*C*=O), 149.2, 138.8, 138.2, 136.5, 135.3, 133.4, 131.1, 128.7, 128.4, 128.0, 127.5, 127.2, 123.6, 122.3, 117.1 (Aryl *C*), 81.6, 78.1 (Cage *C*), 41.5 (*C*H$_2$), 21.2 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.86 (1B), -3.97 (1B), -9.62 (8B). HRMS (APCI neg): *m/z* calcd for $C_{20}H_{26}{}^{10}B_2{}^{11}B_8N_2O$ $[M]^-$: 418.3064. Found: 418.3060.



1f: Yield 79%. Light brown solid. Mp: 171–173 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.01 (s, 1H) (N*H*), 8.90 (d, *J* = 2.9 Hz, 1H), 8.16 (d, *J* = 8.1 Hz, 1H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.57 (d, *J* = 8.9 Hz, 1H), 7.48 (dd, *J* = 4.1, 8.1 Hz, 1H) (Aryl C*H*), 2.26 (s, 3H) (C*H*$_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.9 (*C*=O), 151.0, 143.4, 136.2, 131.0, 130.2, 128.5, 127.3, 127.0, 122.2 (Aryl *C*), 76.7, 75.9 (Cage *C*), 24.4 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.12 (1B), -5.87 (1B), -10.8 (8B). HRMS (APCI pos): *m/z* calcd for $C_{13}H_{19}{}^{10}B_2{}^{11}B_8N_2OCl$ $[M+Na]^+$: 385.2091. Found: 385.2088.

Synthesis of cage B(4,5)-disulfenylated *o*-carborane derivatives (3)

A representative procedure. 8-Aminoquinoline carboranyl amide (**1a**; 32.8 mg, 0.10 mmol), diphenyl disulfide (**2a**; 65.5 mg, 0.30 mmol), $Cu(OTf)_2$ (36.3 mg, 0.10 mmol), 2-phenylpyridine (15.5 mg, 0.10 mmol) and ^{t}BuOLi (32.0 mg, 0.40 mmol) were mixed in dry DCE (5 mL) in a closed flask. The reaction mixture was heated at 130 °C (bath temperature) for 48 h under argon. The resulting reaction solution was cooled to room temperature. After filtration, the solid was washed with dichloromethane (5 mL x 3). The organic portions were combined and concentrated under reduced pressure. The residue was then subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (100/1 to 10/1 in V/V) as eluent to give **3a** (32.2 mg, 86%) and N,N'-di-8-quinolinyl-urea **5** (12.6 mg, 40%).



3a: Yield 86%. Colorless crystals. Mp: 210–211 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (m, 4H), 7.32 (m, 6H) (Aryl C*H*), 3.81 (s, 1H) (Cage C*H*), 1.91 (s, 3H) (C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.6, 133.2, 129.1, 127.9 (Aryl *C*), 70.2, 65.5 (Cage *C*), 25.8 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.22 (2B) (*B*–S), -2.94 (1B), -4.97 (1B), -9.51 (2B), -11.41 (2B), -14.98 (2B). HRMS (APCI neg): *m/z* calcd for $C_{15}H_{22}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 373.2102. Found: 373.2097.

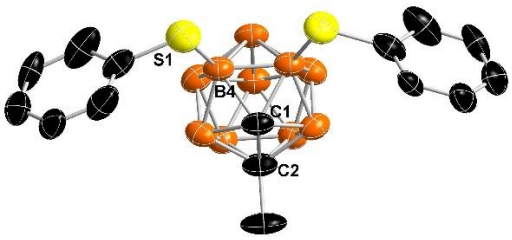
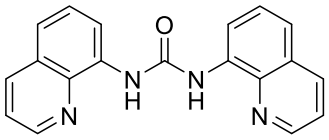
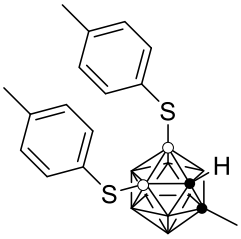


Figure S1 Molecular Structure of **3a**.

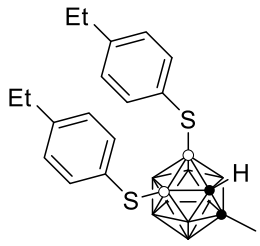


5: Yield 40%. Light brown solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.47 (s, 2H) (N*H*), 8.86 (d, *J* = 4.8 Hz, 2H), 8.70 (d, *J* = 8.8 Hz, 2H), 8.19 (d, *J* = 8.8 Hz, 2H), 7.58 (dd, *J* = 7.8, 7.8 Hz, 2H), 7.48 (m, 4H) (Aryl C*H*). HRMS (APCI pos): *m/z* calcd for $C_{19}H_{14}N_4O$ [M+Na]$^+$: 337.1060. Found: 337.1058. This is a known compound and these data are very similar to the reported one.[2]

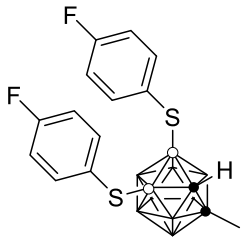


3b: Yield 88%. White solid. Mp: 183–184 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 (d, *J* = 7.9 Hz, 4H), 7.12 (d, *J* = 7.9 Hz, 4H) (Aryl C*H*), 3.78 (s, 1H) (Cage C*H*), 2.35 (s, 6H) (C*H*$_3$), 1.91 (s, 3H) (Cage C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 137.9, 135.4, 129.9, 129.6 (Aryl *C*), 70.1, 65.4 (Cage *C*), 25.8 (Cage *C*H$_3$), 21.3 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.16 (2B) (*B*–S), -3.05 (1B), -4.94 (1B), -9.50 (2B), -11.44 (2B), -14.94 (2B).

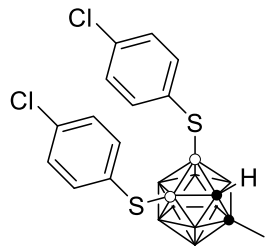
HRMS (APCI neg): *m/z* calcd for $C_{17}H_{26}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 401.2416. Found: 401.2405.



3c: Yield 85%. White solid. Mp: 170–172 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (d, *J* = 8.1 Hz, 4H), 7.15 (d, *J* = 8.0 Hz, 4H) (Aryl C*H*), 3.79 (s, 1H) (Cage C*H*), 2.65 (q, *J* = 7.6 Hz, 4H) (CH_2CH_3), 1.91 (s, 3H) (Cage CH_3), 1.24 (t, *J* = 7.6 Hz, 6H) (CH_2CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.2, 135.5, 129.8, 128.7 (Aryl *C*), 70.1, 65.5 (Cage *C*), 28.6 (CH_2CH_3), 25.8 (Cage CH_3), 15.5 (CH_2CH_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.98 (2B) (*B*–S), -2.91 (1B), -4.81 (1B), -9.33 (2B), -11.27 (2B), -14.80 (2B). HRMS (APCI neg): *m/z* calcd for $C_{19}H_{30}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 429.2730. Found: 429.2713.



3d: Yield 81%. White solid. Mp: 194–195 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (m, 4H), 7.02 (m, 4H) (Aryl C*H*), 3.81 (s, 1H) (Cage C*H*), 1.94 (s, 3H) (CH_3). ^{13}C NMR (126 MHz, $CDCl_3$): δ 162.8 (d, *J* = 248.2 Hz), 137.3 (d, *J* = 7.6 Hz), 128.1 (d, *J* = 3.8 Hz), 116.2 (d, *J* = 21.4 Hz) (Aryl *C*), 70.4, 65.3 (Cage *C*), 25.8 (CH_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.88 (3B) (*B*–S), -4.50 (1B), -9.02 (2B), -10.88 (2B), -14.32 (2B). ^{19}F NMR (471 MHz, $CDCl_3$): δ -113.81 (s, 1F). HRMS (APCI neg): *m/z* calcd for $C_{17}H_{20}{}^{10}B_2{}^{11}B_8F_2S_2$ [M-H]$^-$: 409.1913. Found: 409.1904.



3e: Yield 81%. Colorless crystals. Mp: 172–173 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 (d, *J* = 8.4 Hz, 4H), 7.29 (d, *J* = 8.4 Hz, 4H) (Aryl C*H*), 3.82 (s, 1H) (Cage C*H*), 1.95 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.8, 134.4, 131.5, 129.3 (Aryl *C*), 70.4, 65.3 (Cage *C*), 25.8 (CH_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.57 (2B) (*B*–S), -2.58 (1B), -5.03 (1B), -9.52 (2B), -11.37 (2B), -14.73 (2B). HRMS (APCI neg): *m/z* calcd for $C_{15}H_{22}{}^{10}B_2{}^{11}B_8Cl_2S_2$ [M-H]$^-$: 442.1302. Found: 442.1285.

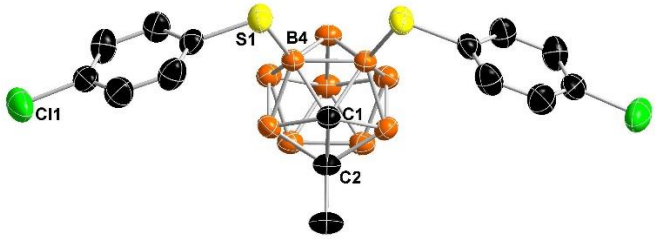
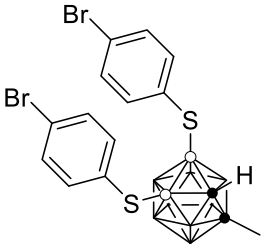


Figure S2 Molecular Structure of **3e**.



3f: Yield 82%. Colorless crystals. Mp: 198–199 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 (m, 8H) (Aryl C*H*), 3.82 (s, 1H) (Cage C*H*), 1.95 (s, 3H) (CH_3). ^{13}C NMR (126 MHz, $CDCl_3$): δ 137.0, 132.3, 132.1, 122.5 (Aryl *C*), 70.4, 65.3 (Cage *C*), 25.8 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.53 (2B) (*B*–S), -2.54 (1B), -4.92 (1B), -9.36 (2B), -11.25 (2B), -14.57 (2B). HRMS (APCI neg): *m/z* calcd for $C_{15}H_{20}{}^{10}B_2{}^{11}B_8Br_2S_2$ [M-H]$^-$: 531.0289. Found: 531.0286.

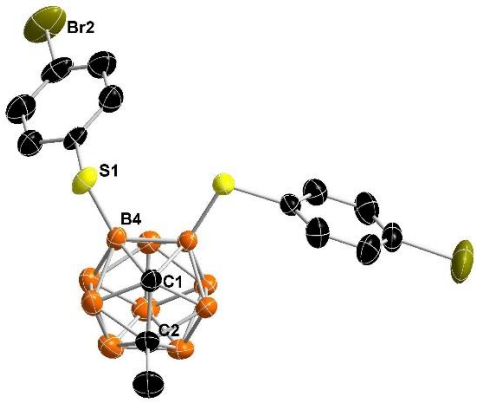
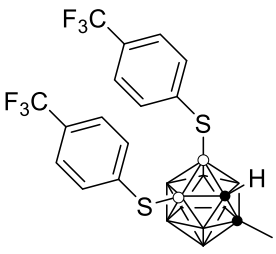
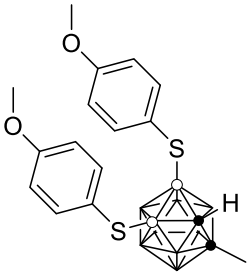


Figure S3 Molecular Structure of **3f**.

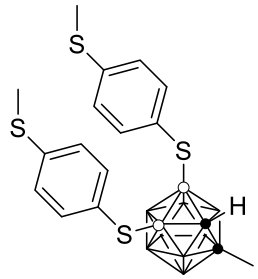


3g: Yield 76%. White solid. Mp: 156–157 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.1 Hz, 4H), 7.57 (d, *J* = 8.1 Hz, 4H) (Aryl C*H*), 3.90 (s, 1H) (Cage C*H*), 1.97 (s, 3H) (CH_3). ^{13}C NMR (126 MHz, $CDCl_3$): δ 137.9, 135.6, 130.2 (q, *J* = 32.8 Hz), 125.9 (q, *J* = 3.8 Hz), 124.1 (q, *J* = 273.0 Hz) (Aryl *C*), 70.7, 65.5 (Cage *C*), 25.8 (*C*H$_3$). ^{11}B{^{1}H} NMR

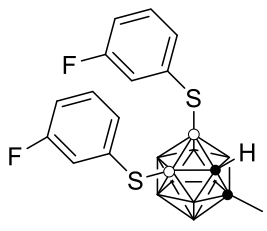
(128 MHz, $CDCl_3$): δ -2.25 (2B) (*B*–S), -2.26 (1B), -4.53 (1B), -8.97 (2B), -10.81 (2B), -13.96 (2B). ^{19}F NMR (377 MHz, $CDCl_3$): δ -62.73 (s, 1F). HRMS (APCI neg): *m/z* calcd for $C_{17}H_{20}{}^{10}B_2{}^{11}B_8F_6S_2$ $[M-H]^-$: 509.1850. Found: 509.1833.



3h: Yield 71%. White solid. Mp: 204–206 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 7.48 (d, *J* = 8.4 Hz, 4H), 6.85 (d, *J* = 8.4 Hz, 4H) (Aryl C*H*), 3.81 (s, 6H) (OC*H*$_3$), 3.75 (s, 1H) (Cage C*H*), 1.91 (s, 3H) (Cage C*H*$_3$). ^{13}C NMR (126 MHz, $CDCl_3$): δ 159.6, 136.8, 123.8, 114.7 (Aryl *C*), 70.1, 65.3 (Cage *C*), 55.4 (O*C*H$_3$), 25.8 (Cage *C*H$_3$). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.07 (2B) (*B*–S), -3.13 (1B), -5.05 (1B), -9.52 (2B), -11.48 (2B), -15.02 (2B). HRMS (APCI neg): *m/z* calcd for $C_{17}H_{26}{}^{10}B_2{}^{11}B_8O_2S_2$ $[M-H]^-$: 433.2314. Found: 433.2303.



3i: Yield 65%. White solid. Mp: 187–188 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 7.47 (m, 4H), 7.18 (m, 4H) (Aryl C*H*), 3.79 (s, 1H) (Cage C*H*), 2.49 (s, 6H) (SC*H*$_3$), 1.92 (s, 3H) (Cage C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.8, 135.8, 129.1, 126.7 (Aryl *C*), 70.3, 65.3 (Cage *C*), 25.8 (Cage *C*H$_3$), 15.6 (S*C*H$_3$). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -1.61 (2B) (*B*–S), -1.62 (1B), -4.29 (1B), -8.78 (2B), -10.62 (2B), -14.09 (2B). HRMS (APCI neg): *m/z* calcd for $C_{17}H_{26}{}^{10}B_2{}^{11}B_8S_4$ $[M-H]^-$: 465.1858. Found: 465.1843.



3j: Yield 80%. Colorless crystals. Mp: 147–148 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 7.35 (m, 2H), 7.29 (m, 4H), 7.02 (m, 2H) (Aryl C*H*), 3.85 (s, 1H) (Cage C*H*), 1.96 (s, 3H) (C*H*$_3$). ^{13}C NMR (126 MHz, $CDCl_3$): δ 162.5 (d, *J* = 249.5 Hz), 134.9 (d, *J* = 8.8 Hz), 131.3 (d, *J* = 2.5 Hz), 130.3 (d, *J* = 8.8 Hz), 122.3 (d, *J* = 22.7 Hz), 115.3 (d, *J* = 20.2 Hz) (Aryl *C*), 70.5, 65.5 (Cage *C*), 25.8 (*C*H$_3$). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.57 (2B) (*B*–S),

-2.58 (1B), -4.93 (1B), -9.42 (2B), -11.30 (2B), -14.60 (2B). ^{19}F NMR (377 MHz, $CDCl_3$): δ -112.02 (s, 1F). HRMS (APCI neg): *m/z* calcd for $C_{15}H_{22}{}^{10}B_2{}^{11}B_8F_2S_2$ [M-H]$^-$: 409.1913. Found: 409.1905.

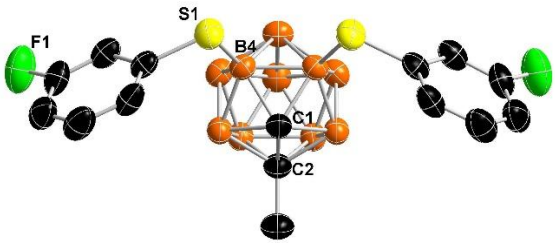
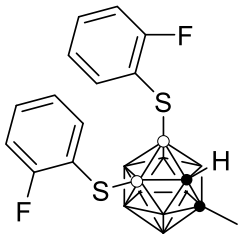
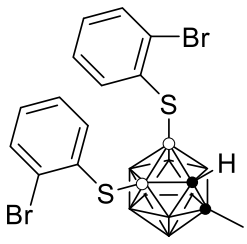


Figure S4 Molecular Structure of **3j**.

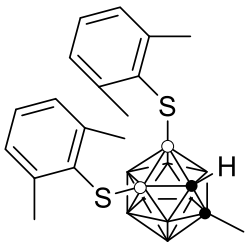


3k: Yield 79%. White solid. Mp: 192–193 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.33 (m, 2H), 7.12 (dd, *J* = 7.9, 7.9 Hz, 4H) (Aryl C*H*), 4.06 (s, 1H) (Cage C*H*), 1.95 (s, 3H) (C*H*$_3$). ^{13}C NMR (126 MHz, $CDCl_3$): δ 163.3 (d, *J* = 245.7 Hz), 138.2, 130.5 (d, *J* = 7.6 Hz), 124.7 (d, *J* = 3.8 Hz), 120.2 (d, *J* = 18.9 Hz), 116.1 (d, *J* = 23.9 Hz) (Aryl *C*), 70.7, 66.0 (Cage *C*), 25.9 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.87 (2B) (*B*–S), -2.88 (1B), -4.56 (1B), -9.58 (2B), -11.37 (2B), -14.89 (2B). ^{19}F NMR (377 MHz, $CDCl_3$): δ -105.62 (s, 1F). HRMS (APCI neg): *m/z* calcd for $C_{15}H_{20}{}^{10}B_2{}^{11}B_8F_2S_2$ [M-H]$^-$: 409.1913. Found: 409.1907.

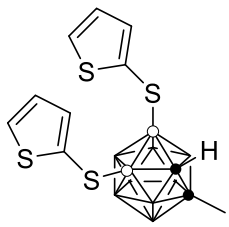


3l: Yield 78%. White solid. Mp: 220–221 °C. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.76 (dd, *J* = 1.4, 7.7 Hz, 2H), 7.68 (dd, *J* = 1.0, 8.0 Hz, 2H), 7.31 (dd, *J* = 7.5, 7.5 Hz, 2H), 7.22 (dd, *J* = 7.7, 7.7 Hz, 2H) (Aryl C*H*), 4.34 (s, 1H) (Cage C*H*), 1.95 (s, 3H) (C*H*$_3$). ^{13}C NMR (126 MHz, CD_2Cl_2): δ 138.5, 135.0, 133.7, 131.0, 130.1, 128.4 (Aryl *C*), 71.2, 66.3 (Cage *C*), 26.0 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2): δ -2.79 (2B) (*B*–S), -2.80 (1B), -4.55 (1B), -10.10 (2B), -11.37 (2B), -14.83 (2B). HRMS (APCI neg): *m/z* calcd for

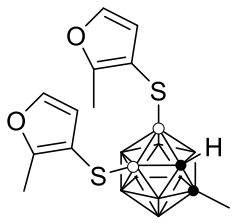
$C_{15}H_{20}{}^{10}B_2{}^{11}B_8Br_2S_2$ [M-H]$^-$: 531.0289. Found: 531.0283.



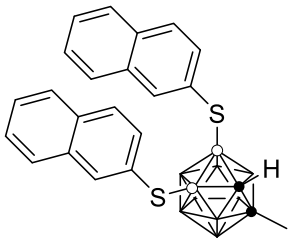
3m: Yield 77%. White solid. Mp: 246–248 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.13 (m, 6H) (Aryl C*H*), 3.92 (s, 1H) (Cage C*H*), 2.60 (s, 12H) (C*H*$_3$), 1.95 (s, 3H) (Cage C*H*$_3$). ^{13}C NMR (126 MHz, $CDCl_3$): δ 133.0, 128.3, 128.2, 128.0 (Aryl *C*), 70.3, 66.4 (Cage *C*), 26.0 (Cage *C*H$_3$), 23.0 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.81 (2B) (*B*–S), -2.82 (1B), -3.89 (1B), -10.20 (2B), -11.83 (2B), -15.22 (2B). HRMS (APCI neg): *m/z* calcd for $C_{19}H_{30}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 429.2730. Found: 429.2714.



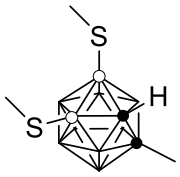
3n: Yield 69%. White solid. Mp: 133–135 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32 (m, 2H), 7.19 (m, 2H), 7.00 (m, 2H) (Aryl C*H*), 3.80 (s, 1H) (Cage C*H*), 1.93 (s, 3H) (C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.1, 131.0, 129.4, 127.8 (Aryl *C*), 70.3, 64.9 (Cage *C*), 25.9 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.39 (2B) (*B*–S), -2.40 (1B), -5.02 (1B), -8.79 (2B), -10.97 (2B), -14.28 (2B). HRMS (ESI neg): *m/z* calcd for $C_{11}H_{18}{}^{10}B_2{}^{11}B_8S_4$ [M-H]$^-$: 385.1222. Found: 385.1227.



3o: Yield 71%. White solid. Mp: 124–126 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29 (d, *J* = 1.7 Hz, 2H), 6.40 (d, *J* = 1.7 Hz, 2H) (Aryl C*H*), 3.78 (s, 1H) (Cage C*H*), 2.38 (s, 6H) (C*H*$_3$), 1.99 (s, 3H) (Cage C*H*$_3$). ^{13}C NMR (126 MHz, $CDCl_3$): δ 155.4, 140.4, 116.2, 108.1 (Aryl *C*), 70.4, 65.3 (Cage *C*), 25.9 (Cage *C*H$_3$), 12.2 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.68 (2B) (*B*–S), -2.69 (1B), -5.13 (1B), -9.35 (2B), -11.47 (2B), -14.95 (2B). HRMS (ESI neg): *m/z* calcd for $C_{13}H_{22}{}^{10}B_2{}^{11}B_8O_2S_2$ [M-H]$^-$: 381.1992. Found: 381.1994.



3p: Yield 72%. White solid. Mp: 250–252 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ 8.13 (s, 2H), 7.93 (m, 6H), 7.63 (dd, *J* = 1.5, 8.5 Hz, 2H), 7.56 (m, 4H) (Aryl C*H*), 5.91 (s, 1H) (Cage C*H*), 1.93 (s, 3H) (C*H*$_3$). ^{13}C NMR (126 MHz, THF-d$_8$): δ 135.1, 134.7, 133.5, 133.3, 131.7, 128.9, 128.3, 128.1, 127.0, 126.9 (Aryl *C*), 71.7, 67.7 (Cage *C*), 30.5 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, THF-d$_8$): δ -2.10 (2B) (*B*–S), -3.48 (1B), -4.98 (1B), -9.74 (2B), -11.01 (2B), -14.83 (2B). HRMS (APCI neg): *m/z* calcd for $C_{23}H_{26}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 473.2418. Found: 473.2394.



3q: Yield 66%. Colorless crystals. Mp: 191–192 °C. ^{1}H NMR (400 MHz, CDCl$_3$): δ 3.86 (s, 1H) (Cage C*H*), 2.20 (s, 6H) (SC*H*$_3$), 2.06 (s, 3H) (Cage C*H*$_3$). ^{13}C NMR (126 MHz, CDCl$_3$): δ 69.9, 66.7 (Cage *C*), 25.9 (Cage *C*H$_3$), 14.6 (S*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, CDCl$_3$): δ -1.30 (2B) (*B*–S), -2.71 (1B), -4.36 (1B), -9.39 (2B), -10.92 (2B), -14.26 (2B). HRMS (APCI neg): *m/z* calcd for $C_5H_{18}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 249.1784. Found: 249.1783.

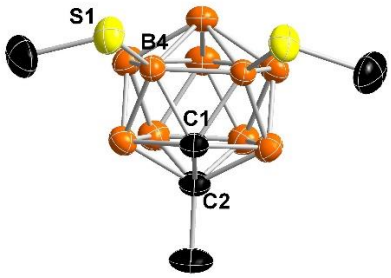
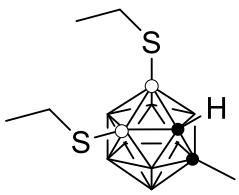
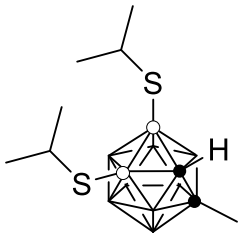


Figure S5 Molecular Structure of **3q**.

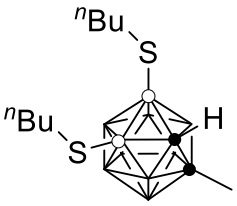


3r: Yield 64%. White solid. Mp: 137–139 °C. ^{1}H NMR (400 MHz, CDCl$_3$): δ 3.82 (s, 1H) (Cage C*H*), 2.74 (m, 4H) (SC*H*$_2$CH$_3$), 2.06 (s, 3H) (Cage C*H*$_3$), 1.32 (t, *J* = 7.4 Hz, 6H) (SCH$_2$C*H*$_3$). ^{13}C NMR (126 MHz, CDCl$_3$): δ 70.1, 66.7 (Cage *C*), 26.7 (*C*H$_2$CH$_3$), 25.9 (Cage *C*H$_3$), 17.1 (CH$_2$*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, CDCl$_3$): δ -1.93 (2B) (*B*–S), -2.96 (1B),

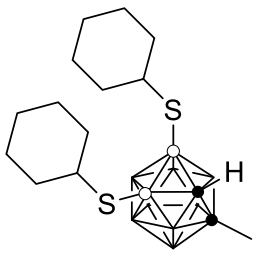
-4.54 (1B), -9.73 (2B), -11.31 (2B), -14.66 (2B). HRMS (APCI neg): *m/z* calcd for $C_7H_{22}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 277.2098. Found: 277.2095.



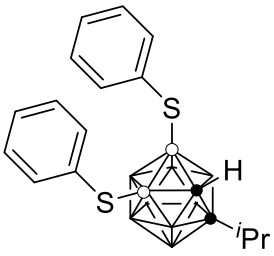
3s: Yield 51%. White solid. Mp: 143–145 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.79 (s, 1H) (Cage C*H*), 3.20 (m, 2H) (^{i}Pr), 2.06 (s, 3H) (Cage CH_3), 1.37 (d, *J* = 2.5 Hz, 6H), 1.35 (d, *J* = 2.5 Hz, 6H) (^{i}Pr). ^{13}C NMR (126 MHz, $CDCl_3$): δ 70.2, 66.8 (Cage *C*), 37.7, 26.6, 26.5 (^{i}Pr), 25.9 (Cage *C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -0.78 (2B) (*B*–S), -2.61 (1B), -4.53 (1B), -8.65 (2B), -10.70 (2B), -14.04 (2B). HRMS (APCI neg): *m/z* calcd for $C_9H_{26}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 305.2412. Found: 305.2409.



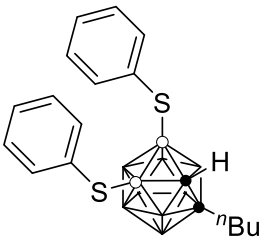
3t: Yield 71%. White solid. Mp: 120–122 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.83 (s, 1H) (Cage C*H*), 2.71 (m, 4H) (^{n}Bu), 2.06 (s, 3H) (Cage CH_3), 1.63 (m, 4H), 1.42 (m, 4H), 0.91 (t, *J* = 7.3 Hz, 6H) (^{n}Bu). ^{13}C NMR (126 MHz, $CDCl_3$): δ 70.0, 66.8 (Cage *C*), 33.8, 32.3 (^{n}Bu), 25.9 (Cage *C*H$_3$), 22.1, 13.8 (^{n}Bu). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.06 (2B) (*B*–S), -3.34 (1B), -4.82 (1B), -10.00 (2B), -11.58 (2B), -14.99 (2B). HRMS (APCI neg): *m/z* calcd for $C_{11}H_{30}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 333.2726. Found: 333.2723.



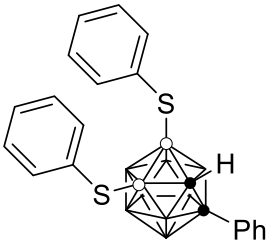
3u: Yield 63%. White solid. Mp: 168–170 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.77 (s, 1H) (Cage C*H*), 2.93 (m, 2H), 2.06 (m, 4H) (Cy), 2.05 (s, 3H) (CH_3), 1.74 (m, 4H), 1.56 (m, 2H), 1.33 (m, 10H) (Cy). ^{13}C NMR (126 MHz, $CDCl_3$): δ 70.2, 66.7 (Cage *C*), 45.9, 36.5, 26.5 (Cy), 25.9 (*C*H$_3$), 25.6 (Cy). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.66 (2B) (*B*–S), -2.86 (1B), -4.40 (1B), -9.45 (2B), -11.17 (2B), -14.59 (2B). HRMS (APCI neg): *m/z* calcd for $C_{15}H_{34}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 385.3041. Found: 385.3033.



3v: Yield 55%. White solid. Mp: 137–138 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (m, 4H), 7.31 (m, 6H) (Aryl C*H*), 3.83 (s, 1H) (Cage C*H*), 2.37 (m, 1H), 0.99 (d, *J* = 6.9 Hz, 6H) (*i*Pr). ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.6, 133.2, 129.1, 128.0 (Aryl *C*), 81.3, 64.0 (Cage *C*), 34.8, 31.1, 22.8 (*i*Pr). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.09 (2B) (*B*–S), -3.10 (1B), -4.37 (1B), -9.61 (2B), -13.40 (2B), -15.71 (2B). HRMS (APCI neg): *m/z* calcd for $C_{17}H_{26}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 401.2416. Found: 401.2407.



3w: Yield 84%. White solid. Mp: 97–99 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (m, 4H), 7.32 (m, 6H) (Aryl C*H*), 3.80 (s, 1H) (Cage C*H*), 2.08 (m, 2H), 1.24 (m, 4H), 0.84 (t, *J* = 7.1 Hz, 3H) (*n*Bu). ^{13}C NMR (126 MHz, $CDCl_3$): δ 135.6, 133.2, 129.1, 127.9 (Aryl *C*), 75.5, 64.9 (Cage *C*), 37.7, 31.2, 22.1, 13.7 (*n*Bu). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.60 (2B) (*B*–S), -2.61 (1B), -3.65 (1B), -9.52 (2B), -12.11 (2B), -15.48 (2B). HRMS (APCI neg): *m/z* calcd for $C_{18}H_{28}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 415.2573. Found: 415.2564.



3x: Yield 50%. Colorless crystals. Mp: 107–109 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (m, 4H), 7.32 (m, 7H), 7.30 (m, 4H) (Aryl C*H*), 4.19 (s, 1H) (Cage C*H*). ^{13}C NMR (126 MHz, $CDCl_3$): δ 135.6, 133.1, 132.8, 130.2, 129.2, 129.1, 128.0, 127.5 (Aryl *C*), 76.6, 64.2 (Cage *C*). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.00 (2B) (*B*–S), -2.01 (1B), -3.06 (1B), -9.00 (2B), -11.03 (2B), -14.76 (2B). HRMS (APCI neg): *m/z* calcd for $C_{20}H_{24}{}^{10}B_2{}^{11}B_8S_2$ [M]$^-$: 436.2339. Found: 436.2331.

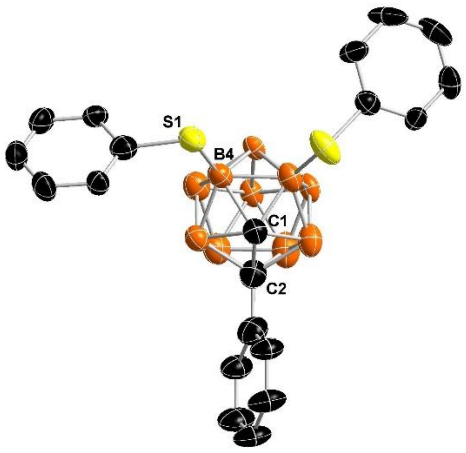
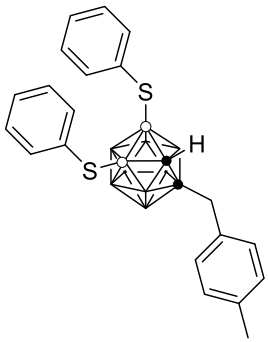
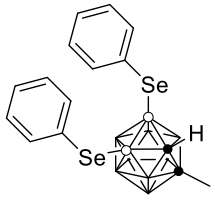


Figure S6 Molecular Structure of **3x**.



3y: Yield 71%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 (m, 4H), 7.29 (m, 6H), 7.10 (d, *J* = 7.8 Hz, 2H), 6.79 (d, *J* = 8.0 Hz, 2H) (Aryl C*H*), 3.29 (s, 1H) (Cage C*H*), 3.29 (s, 2H) (CH_2), 2.40 (s, 3H) (CH_3). ^{13}C NMR (126 MHz, $CDCl_3$): δ 138.5, 135.6, 133.1, 130.8, 129.9, 129.5, 129.1, 127.9 (Aryl *C*), 74.6, 62.5 (Cage *C*), 42.8 (*C*H_2), 21.3 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.92 (2B) (*B*–S), -3.43 (2B), -8.48 (2B), -12.33 (2B), -14.18 (2B). HRMS (APCI neg): *m/z* calcd for $C_{22}H_{28}{}^{10}B_2{}^{11}B_8S_2$ $[M]^-$: 464.2653. Found: 464.2641.



3z: Yield 66%. Colorless crystals. Mp: 207–208 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 6.9 Hz, 4H) 7.30 (m, 6H) (Aryl C*H*), 3.82 (s, 1H) (Cage C*H*), 1.90 (s, 3H) (CH_3). ^{13}C NMR (126 MHz, $CDCl_3$): δ 136.8, 129.2, 128.0, 127.5 (Aryl *C*), 72.7, 66.1 (Cage *C*), 25.8 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.79 (1B), -4.25 (1B), -6.19 (2B) (*B*–Se), -8.63 (2B), -10.88 (2B), -13.52 (2B). HRMS (APCI neg): *m/z* calcd for $C_{15}H_{22}{}^{10}B_2{}^{11}B_8Se_2$ $[M-H]^-$: 467.1003. Found: 467.0993.

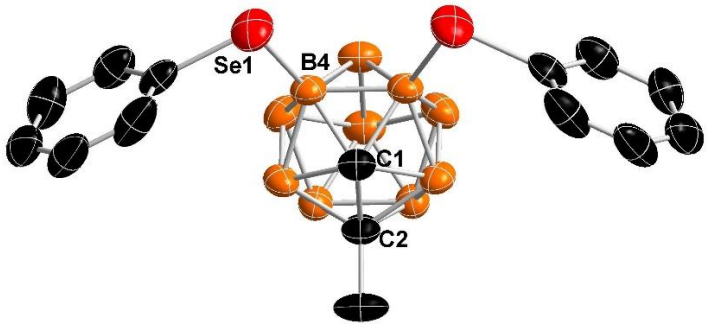
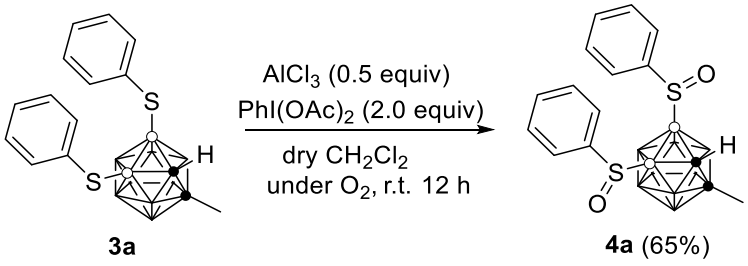
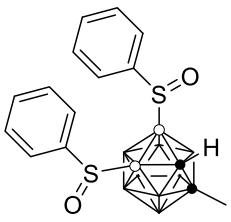


Figure S7 Molecular Structure of **3z**.

Oxidation of 3a. Disulfenylated *o*-carborane (**3a**; 37.4 mg, 0.10 mmol), $AlCl_3$ (6.7 mg, 0.05 mmol) and $PhI(OAc)_2$ (64.4 mg, 0.20 mmol) were mixed in dry DCM (5 mL) in a closed flask filled with oxygen (1 atm). The reaction mixture was stirred for 12 h at room temperature. After filtration, the solid was washed with dichloromethane (5 mL x 3). The organic portions were combined and concentrated under reduced pressure. The residue was then subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (10/1 to 5/1 in V/V) as eluent to give **4a** (26.4 mg, 65%).

Scheme S1 Oxidation of **3a**.





4a: Yield 65%. Colorless crystals. Mp: 270–272 °C. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.97 (d, *J* = 7.6 Hz, 2H), 7.69 (dd, *J* = 7.4, 7.4 Hz, 1H), 7.60 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.50 (m, 2H), 7.33 (m, 3H) (Aryl C*H*), 4.63 (s, 1H) (Cage C*H*), 2.01 (s, 3H) (C*H*$_3$). ^{13}C NMR (126 MHz, CD_2Cl_2): δ 135.8, 133.4, 129.4, 128.3 (Aryl *C*), 71.0, 66.1 (Cage *C*), 25.9 (*C*H$_3$). ^{11}B{^{1}H}

NMR (160 MHz, CD_2Cl_2): δ -1.96 (2B) (*B*–S), -2.91 (1B), -4.69 (1B), -9.34 (2B), -10.99 (2B), -14.54 (2B). HRMS (APCI neg): *m/z* calcd for $C_{15}H_{22}{}^{10}B_2{}^{11}B_8O_2S_2$ $[M-H]^-$: 405.2000. Found: 405.1993.

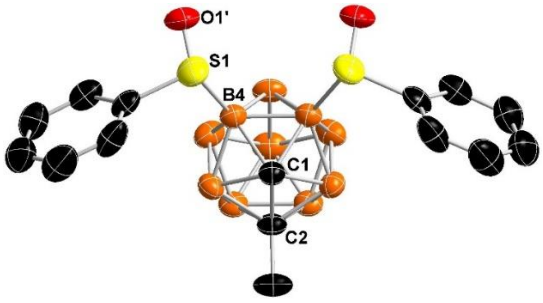
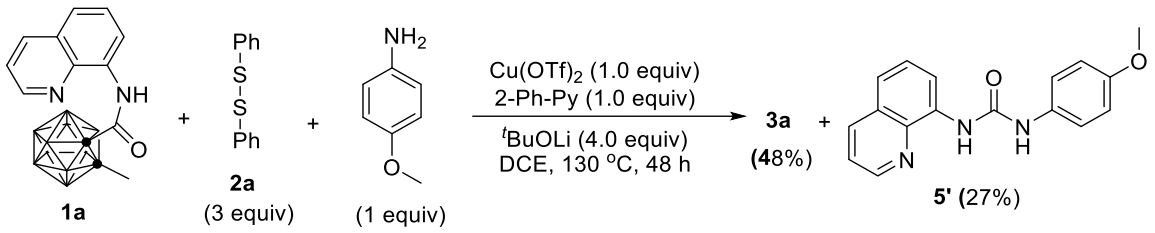


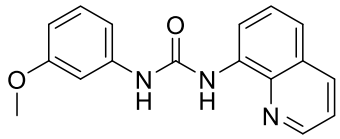
Figure S8 Molecular Structure of **4a**.

Preliminary mechanistic study

Control experiment for directing group removal. 8-Aminoquinoline carboranyl amide (**1a**; 32.8 mg, 0.10 mmol), diphenyl disulfide (**2a**; 65.5 mg, 0.30 mmol), $Cu(OTf)_2$ (36.3 mg, 0.10 mmol), 2-phenylpyridine (15.5 mg, 0.10 mmol), ^{t}BuOLi (24.0 mg, 0.30 mmol) and *p*-anisidine (12.3 mg, 0.10 mmol) were mixed in dry DCE (5 mL) in a closed flask. The reaction mixture was heated at 130 ^{o}C (bath temperature) for 48 h under argon. The resulting reaction mixture was cooled to room temperature. After filtration, the solid was washed with dichloromethane (5 mL x 3). The organic portions were combined and concentrated under reduced pressure. The residue was then subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (100/1 to 5/1 in V/V) as eluent to give **3a** (18.0 mg, 48%) and N-(4-methoxyphenyl)-N'-8-quinolinyl-urea **5'** (8.0 mg, 27%).

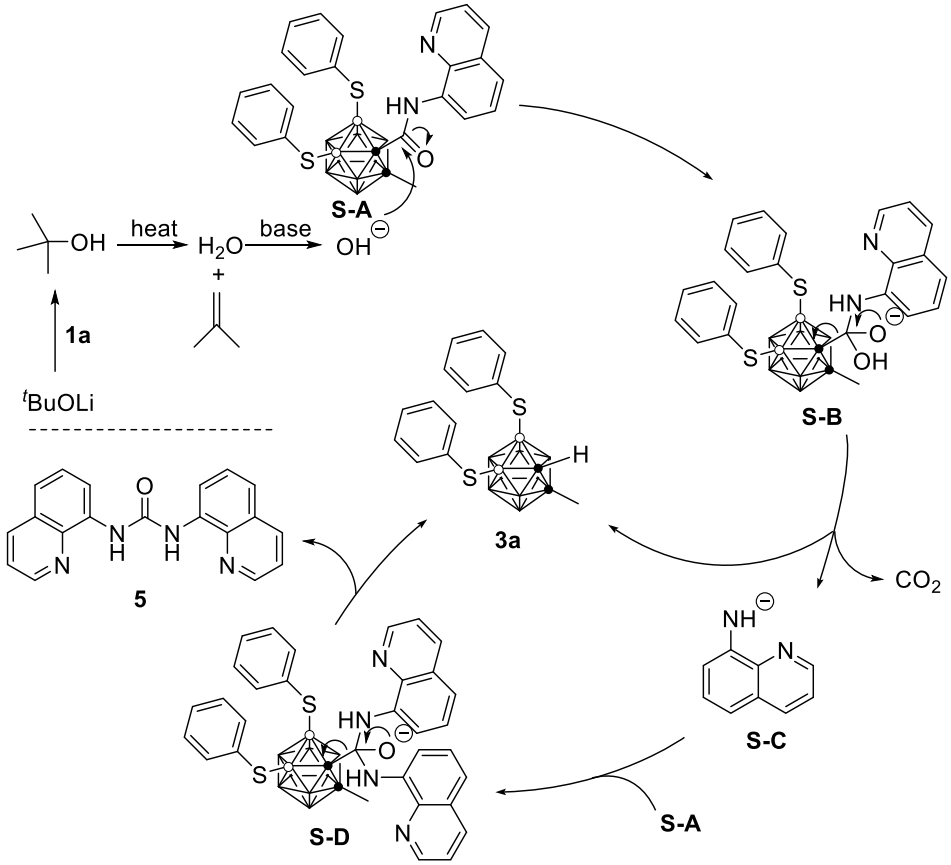
Scheme S2 Isolation of urea **5'**.





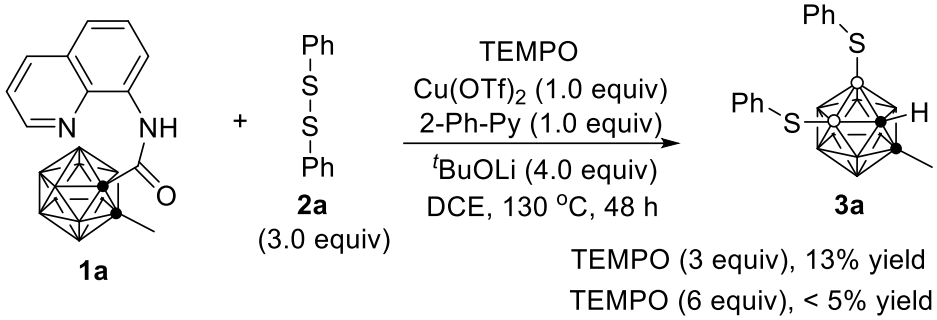
5': Yield 27%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.31 (s, 1H) (N*H*), 8.68 (dd, *J* = 1.6, 4.2 Hz, 1H), 8.61 (d, *J* = 7.7 Hz, 1H), 8.14 (dd, *J* = 1.8, 8.3 Hz, 1H), 7.53 (dd, *J* = 8.1, 8.1 Hz, 1H), 7.39 (m, 4H), 6.93 (m, 3H) (Aryl C*H* and N*H*). This is a known compound and these data are very similar to the reported one.[3]

Scheme S3 Plausible pathway for the directing group removal.



Radical trapping experiment. 8-Aminoquinoline carboranyl amide (**1a**; 32.8 mg, 0.10 mmol), diphenyl disulfide (**2a**; 65.5 mg, 0.30 mmol), $Cu(OTf)_2$ (36.3 mg, 0.10 mmol), 2-phenylpyridine (15.5 mg, 0.10 mmol), ^{t}BuOLi (24.0 mg, 0.30 mmol) and TEMPO (2,2,6,6-tetramethylpiperidine-1-oxyl; 46.9/93.8 mg, 0.30/0.60 mmol) were mixed in dry DCE (5 mL) in a closed flask. The reaction mixture was heated at 130 ^{o}C (bath temperature) for 48 h under argon. The resulting reaction mixture was cooled to room temperature, and then filtered through Celite and subjected to GC-MS analysis. 13% yield and trace amount (< 5%) of product **3a** were detected, respectively (Scheme S4).

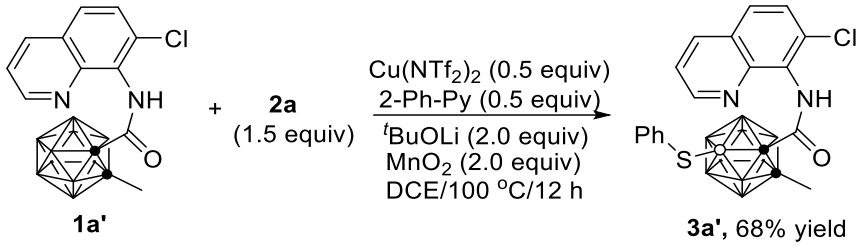
Scheme S4 Radical trapping experiment.

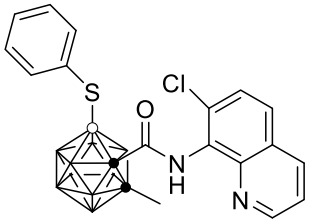


Synthesis of B(4)–sulfenylated *o*-carborane derivative (3a'). 7-Cl-*N*-8-aminoquinoline carboranyl amide (**1a'**; 36.3 mg, 0.10 mmol), diphenyl disulfide (**2a**; 32.8 mg, 0.15 mmol), $Cu(NTf_2)_2$ (31.2 mg, 0.05 mmol), 2-phenylpyridine (7.8 mg, 0.05 mmol), ^{t}BuOLi (16.0 mg, 0.20 mmol) and MnO_2 (17.4 mg, 0.20 mmol) were mixed in dry DCE (5 mL) in a closed flask. The reaction mixture was heated at 100 ^{o}C (bath temperature) for 12 h under argon. The resulting reaction mixture was cooled to room temperature. After filtration, the solid was washed with dichloromethane (5 mL x 3). The organic portions were combined and concentrated under reduced pressure. The residue was then subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate

(100/1 in V/V) as eluent to give **3a'** (32.1 mg, 68%).

Scheme S5 Synthesis of **3a'**.

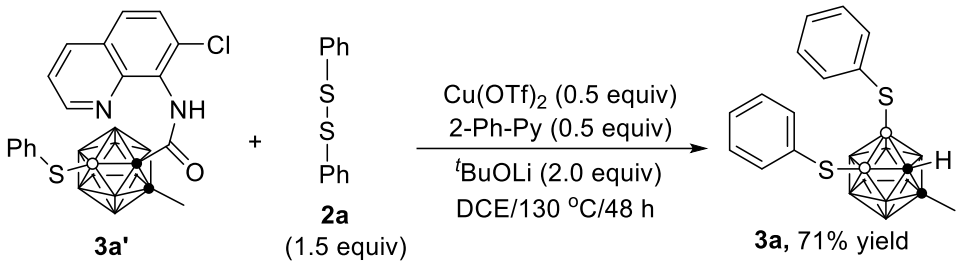




3a': Yield 68%. Colorless oil. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 9.43 (s, 1H) (N*H*), 8.93 (dd, *J* = 1.6, 4.2 Hz, 1H), 8.25 (dd, *J* = 1.6, 8.3 Hz, 1H), 7.81 (d, *J* = 8.9 Hz, 1H), 7.66 (d, *J* = 8.9 Hz, 1H), 7.60 (m, 2H), 7.53 (dd, *J* = 4.2, 8.3 Hz, 1H), 7.28 (m, 3H) (Aryl C*H*), 2.21 (s, 3H) (CH_3). ^{13}C NMR (126 MHz, CD_2Cl_2): δ 154.7, 151.3, 143.8, 136.6, 135.8, 133.8, 131.2, 130.8, 129.1, 128.8, 128.2, 127.8, 127.5, 122.6 (Aryl *C*), 78.2, 77.9 (Cage *C*), 24.7 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2): δ 0.21 (1B) (*B*–S), -1.55 (1B), -4.29 (1B), -12.08 (7B). HRMS (APCI pos): *m/z* calcd for $C_{19}H_{23}{}^{10}B_2{}^{11}B_8N_2OClS$ $[M+H]^+$: 472.2281. Found: 472.2273.

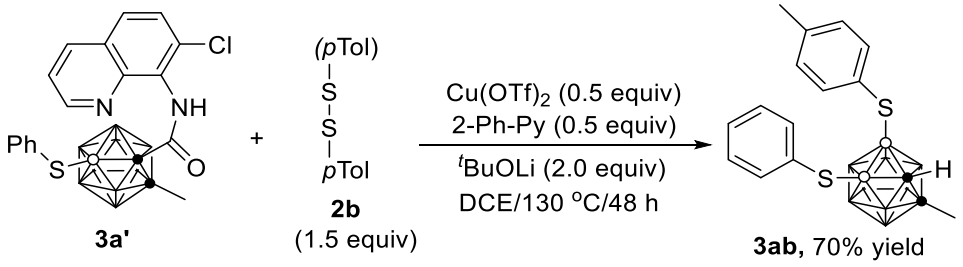
Stepwise cage B–H sulfenylation for the synthesis of 3a. Compound **3a'** (47.1 mg, 0.10 mmol), diphenyl disulfide (**2a**; 32.8 mg, 0.15 mmol), $Cu(OTf)_2$ (18.2 mg, 0.05 mmol), 2-phenylpyridine (7.8 mg, 0.05 mmol) and ^{t}BuOLi (16.0 mg, 0.20 mmol) were mixed in dry DCE (5 mL) in a closed flask. The reaction mixture was heated at 130 °C (bath temperature) for 48 h under argon. The resulting reaction mixture was cooled to room temperature. After filtration, the solid was washed with dichloromethane (5 mL x 3). The organic portions were combined and concentrated under reduced pressure. The residue was then subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (100/1 to 50/1 in V/V) as eluent to give **3a** (26.5 mg, 71%).

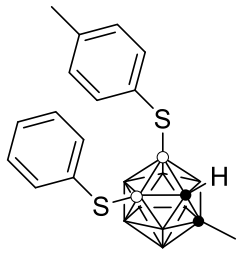
Scheme S6 Synthesis of **3a** from **3a'**.



Stepwise cage B–H sulfenylation for the synthesis of 3ab. Compound **3a'** (47.1 mg, 0.10 mmol), bis(4-methylphenyl)-disulfide, (**2b**; 37.0 mg, 0.15 mmol), $Cu(OTf)_2$ (18.2 mg, 0.05 mmol), 2-phenylpyridine (7.8 mg, 0.05 mmol) and ^{t}BuOLi (16.0 mg, 0.20 mmol) were mixed in dry DCE (5 mL) in a closed flask. The reaction mixture was heated at 130 °C (bath temperature) for 48 h under argon. The resulting reaction mixture was cooled to room temperature. After filtration, the solid was washed with dichloromethane (5 mL x 3). The organic portions were combined and concentrated under reduced pressure. The residue was then subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (100/1 to 50/1 in V/V) as eluent to give **3ab** (27.2 mg, 70%).

Scheme S7 Synthesis of **3ab** from **3a'**.





3ab: Yield 70%. White solid. Mp: 163–165 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (m, 2H), 7.46 (d, J = 8.0 Hz, 2H), 7.31 (m, 3H), 7.12 (d, J = 7.8 Hz, 2H) (Aryl C*H*), 3.79 (s, 1H) (Cage C*H*), 2.35 (s, 3H) (CH_3), 1.91 (s, 3H) (Cage CH_3). ^{13}C NMR (126 MHz, $CDCl_3$): δ 137.9, 135.6, 135.4, 133.3, 129.9, 129.6, 129.1, 127.9 (Aryl *C*), 70.2, 65.5 (Cage *C*), 25.8 (Cage

*C*H$_3$), 21.3(*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, CDCl$_3$): δ -1.72 (2B) (*B*–S), -2.54 (1B), -4.45 (1B), -9.02 (2B), -10.99 (2B), -14.44 (2B). HRMS (APCI neg): *m/z* calcd for $C_{16}H_{24}{}^{10}B_2{}^{11}B_8S_2$ [M-H]$^-$: 387.2259. Found: 387.2250.

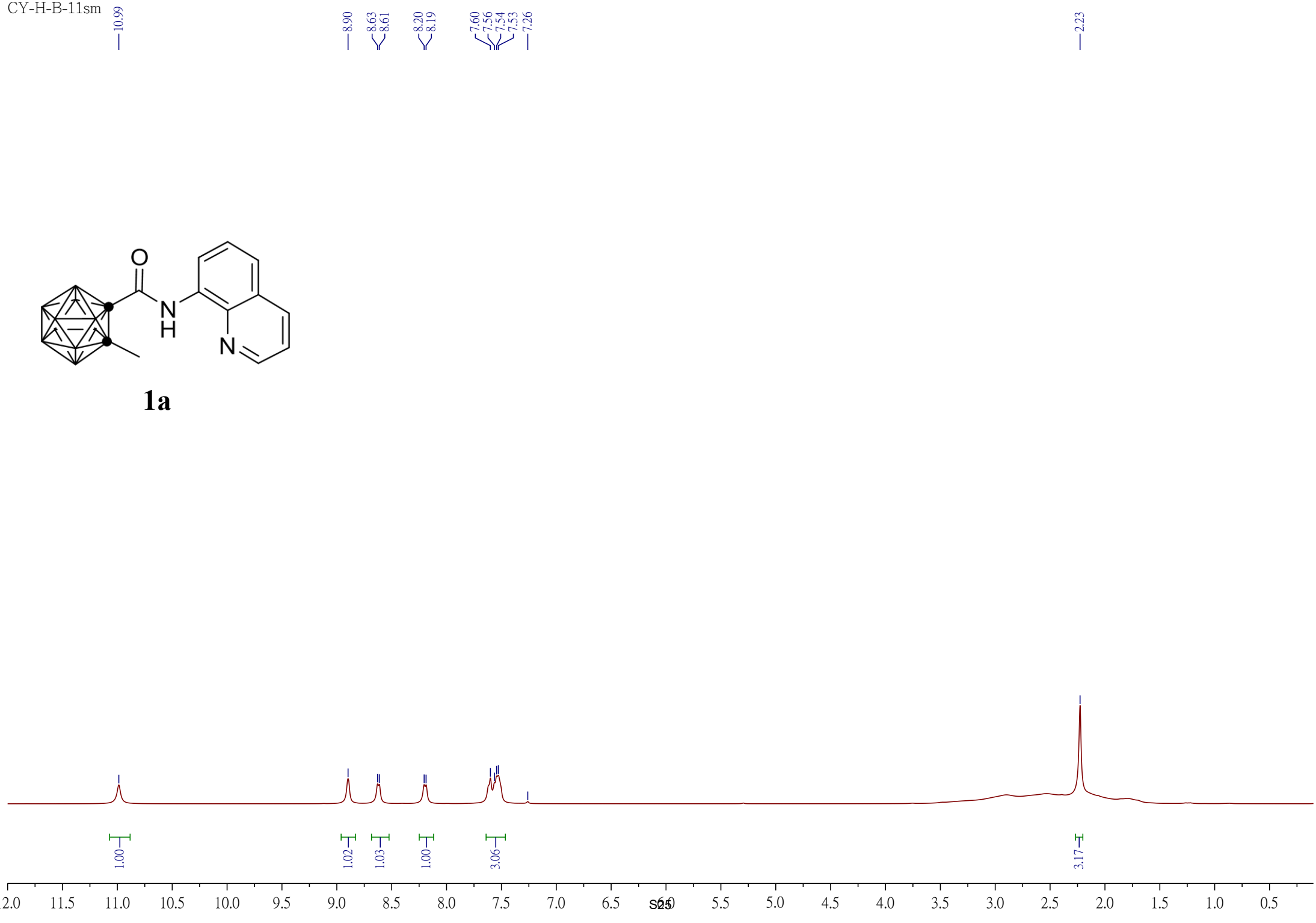
X-ray Structure Determination. Single crystal X-ray data of **3a**, **3e**, **3f**, **3j**, **3q**, **3x**, **3z** and **4a** were collected at 293 K on a Bruker SMART 1000 CCD diffractometer using Mo-Kα radiation. An empirical absorption correction was applied using the SADABS program.[4] All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-hydrogen atoms by full-matrix least squares calculations on F^2 using the SHELXTL program package.[5] All hydrogen atoms were geometrically fixed using the riding model.

CCDC 2018134−2018141 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

CY-H-B-11sm

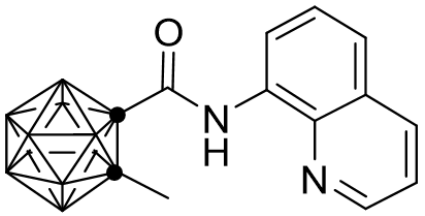
O
N
H
N

1a

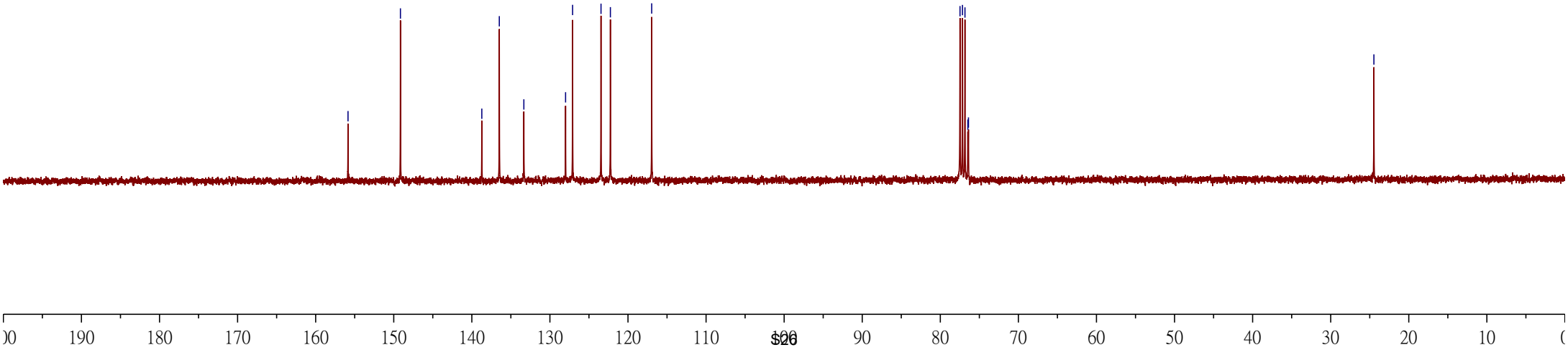

10.99
8.90
8.63
8.61
8.20
8.19
7.60
7.56
7.54
7.53
7.26
2.23
1.00
1.02
1.03
1.00
3.06
3.17
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

CY-C-B-11sm

155.86
149.14
138.72
136.48
133.34
127.99
127.09
123.46
122.25
116.96
77.48
77.16
76.84
76.47
76.39
24.47

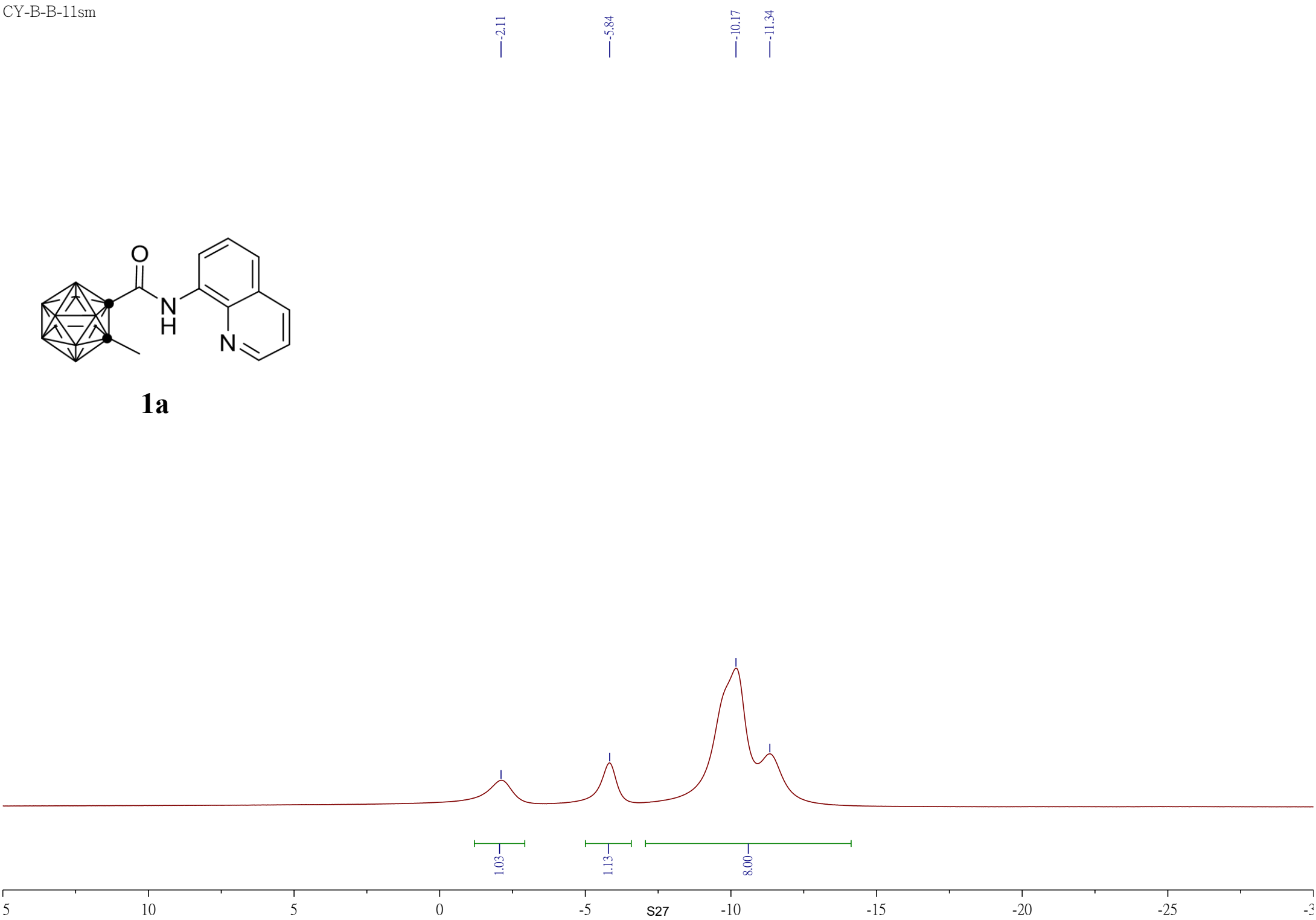


1a



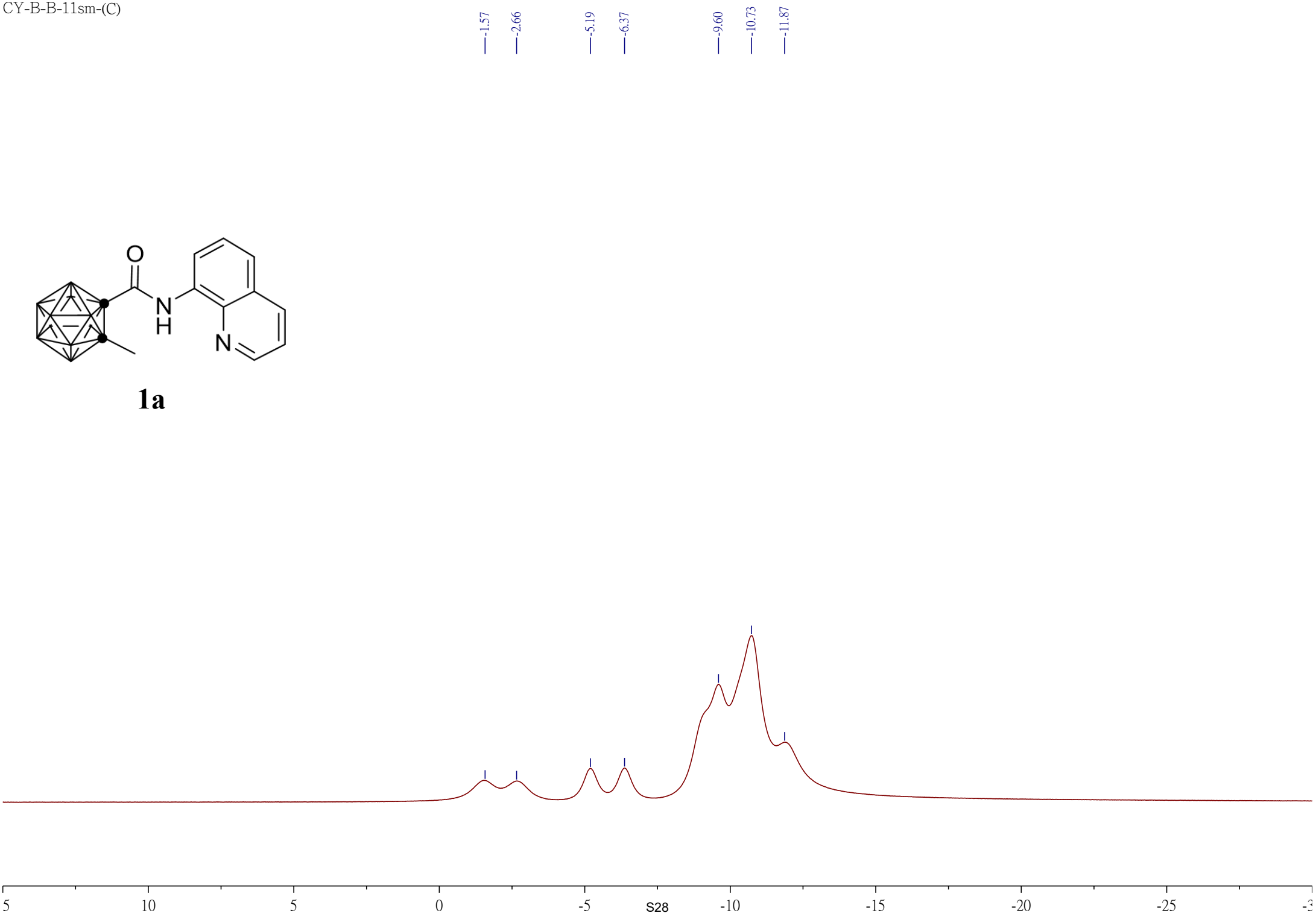
CY-B-B-11sm

1a

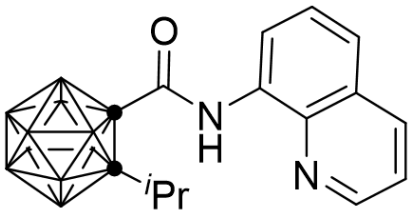


CY-B-B-11sm-(C)

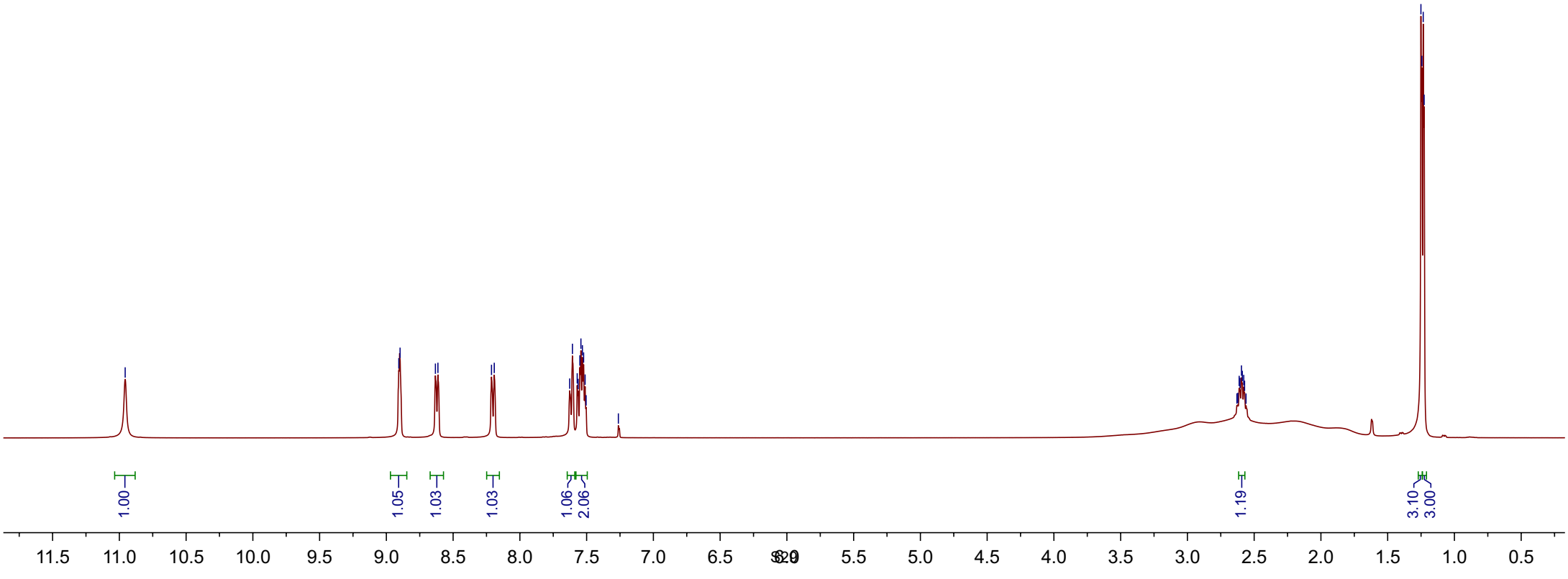
1a



CY-H-B-43SM


O
N
H
N
iPr

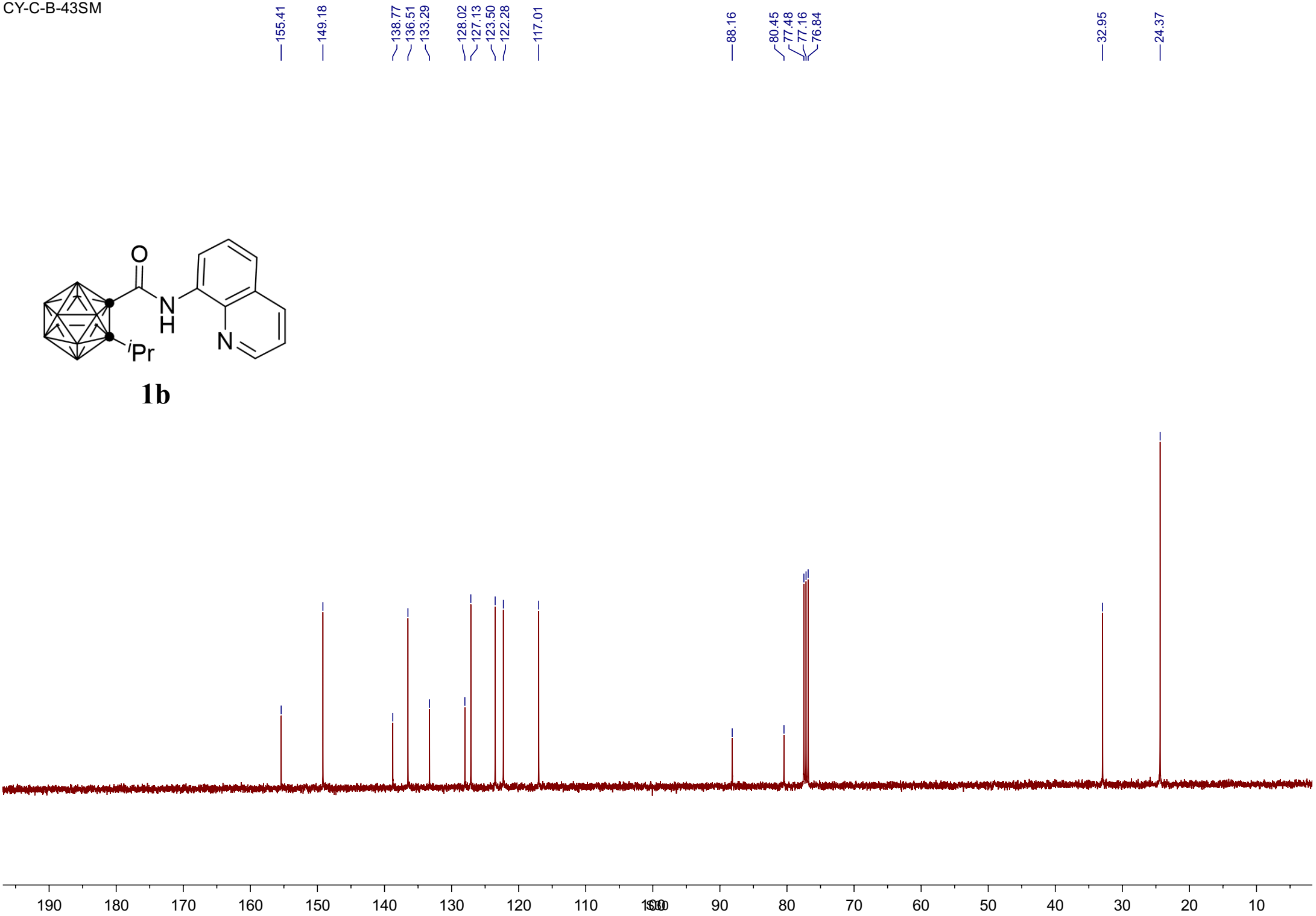
1b


10.96
8.91
8.90
8.63
8.61
8.21
8.19
7.63
7.61
7.57
7.56
7.55
7.54
7.53
7.52
7.51
7.50
7.26
2.63
2.62
2.61
2.61
2.60
2.59
2.58
2.57
2.56
1.25
1.24
1.23
1.23
1.00
1.05
1.03
1.03
1.06
2.06
1.19
3.10
3.00
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

CY-C-B-43SM

O
N
H
N
iPr

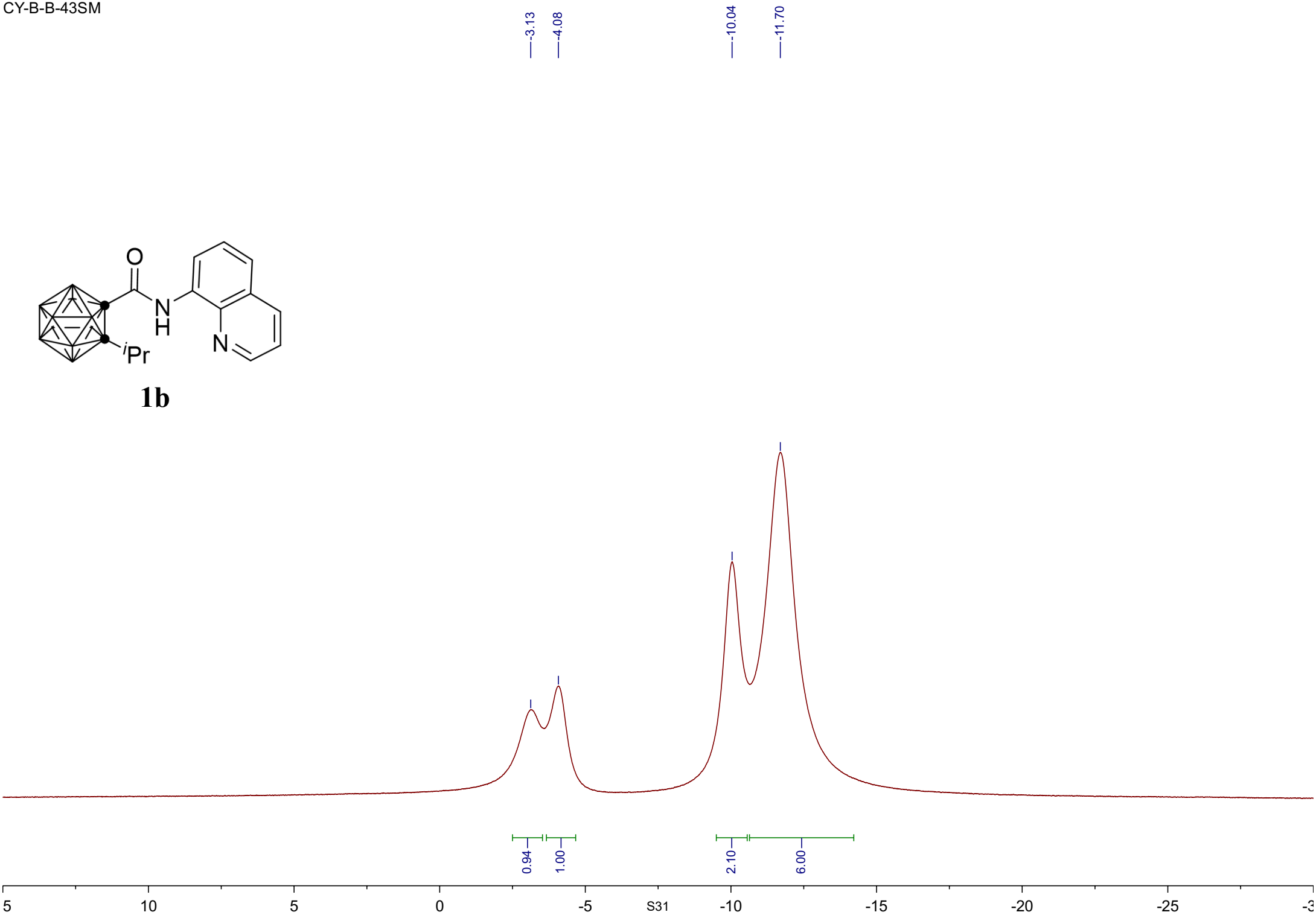
1b


155.41
149.18
138.77
136.51
133.29
128.02
127.13
123.50
122.28
117.01
88.16
80.45
77.48
77.16
76.84
32.95
24.37
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

CY-B-B-43SM

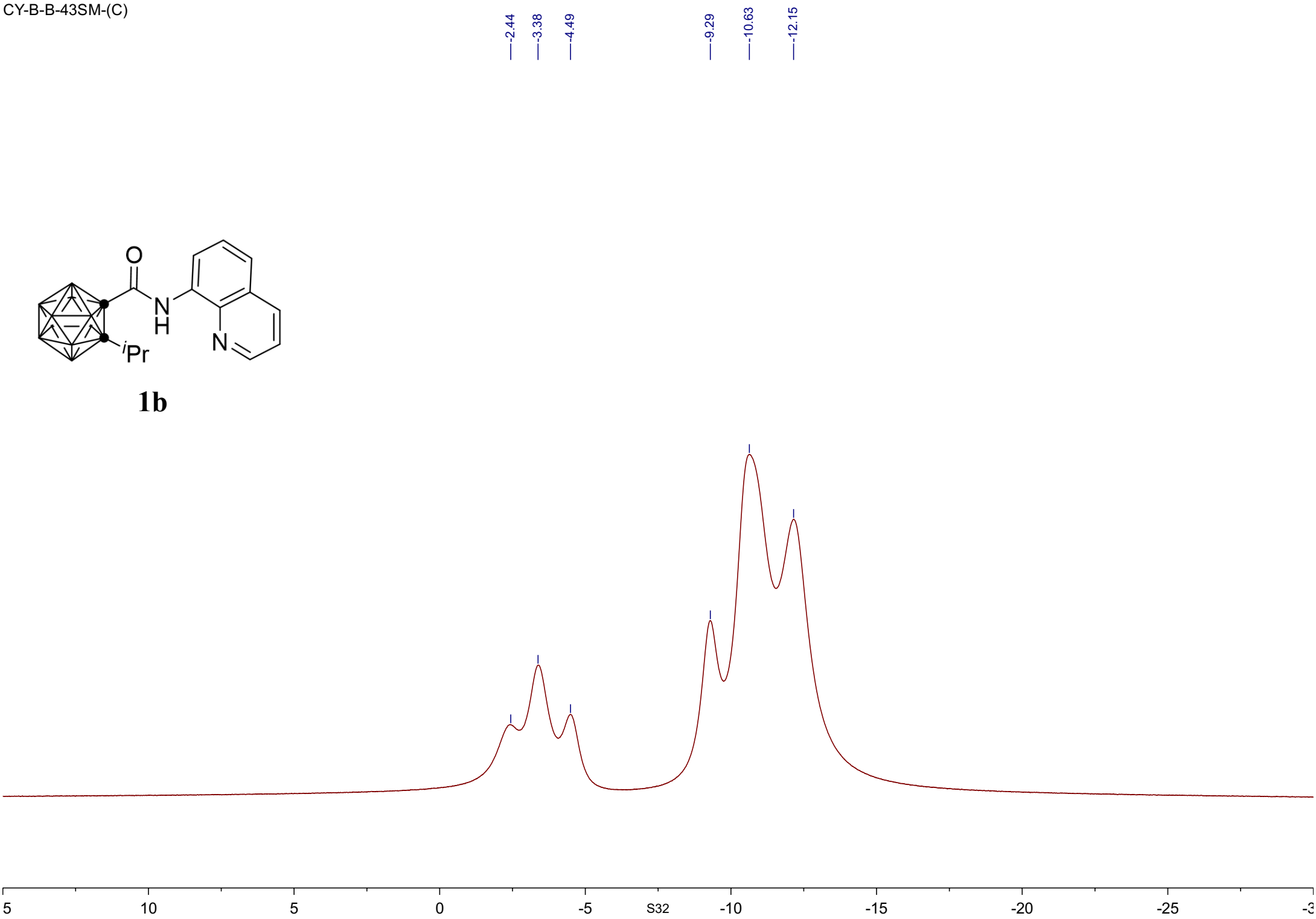
O
N
H
N
iPr

1b

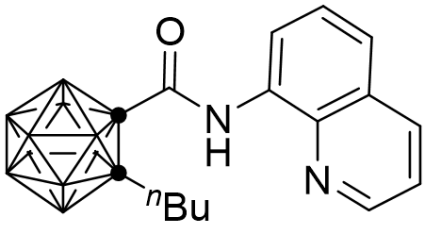

-3.13
-4.08
-10.04
-11.70
0.94
1.00
2.10
6.00
5
10
5
0
-5
S31
-10
-15
-20
-25

CY-B-B-43SM-(C)

1b



CY-H-B-35sm

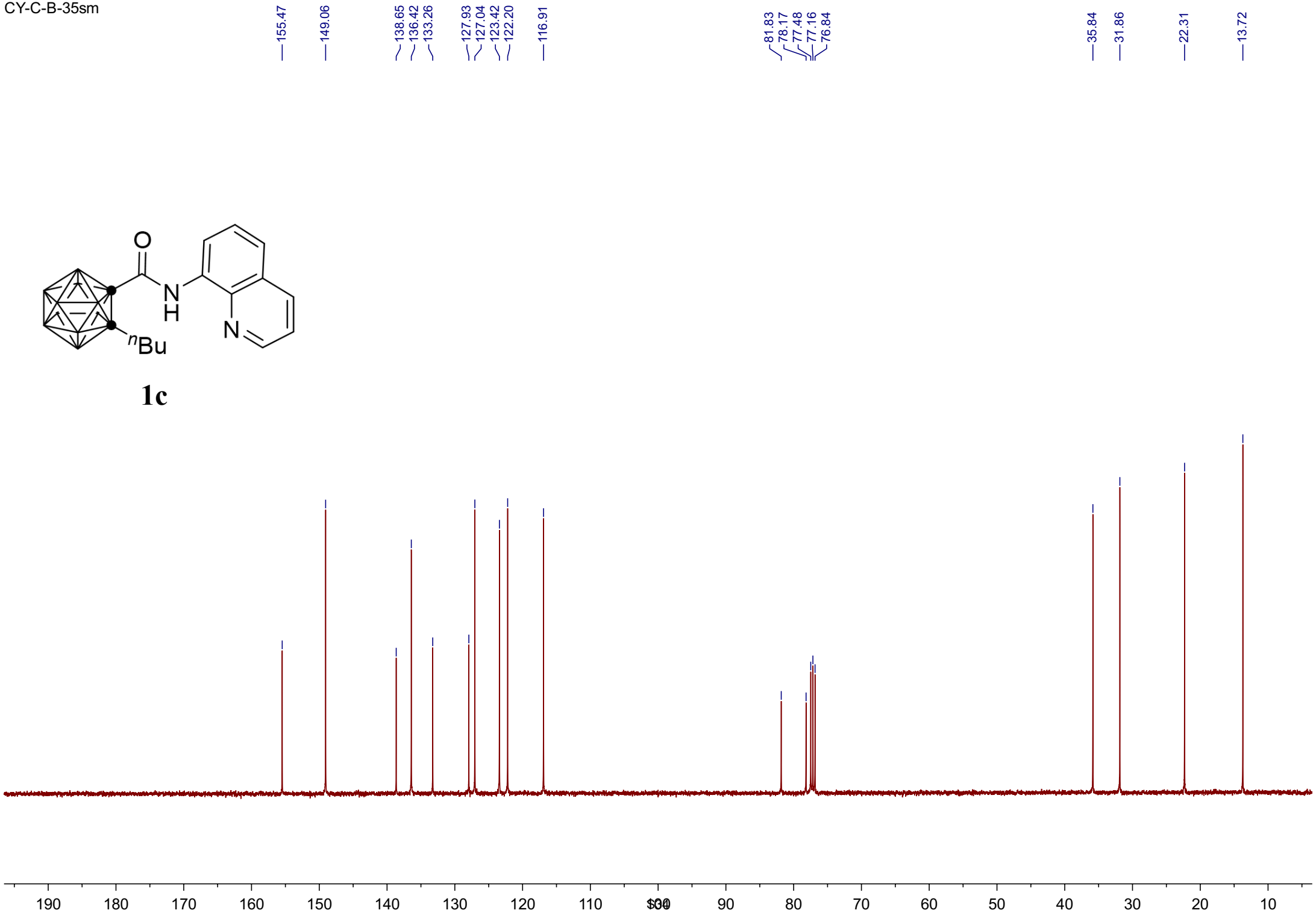


1c

CY-C-B-35sm

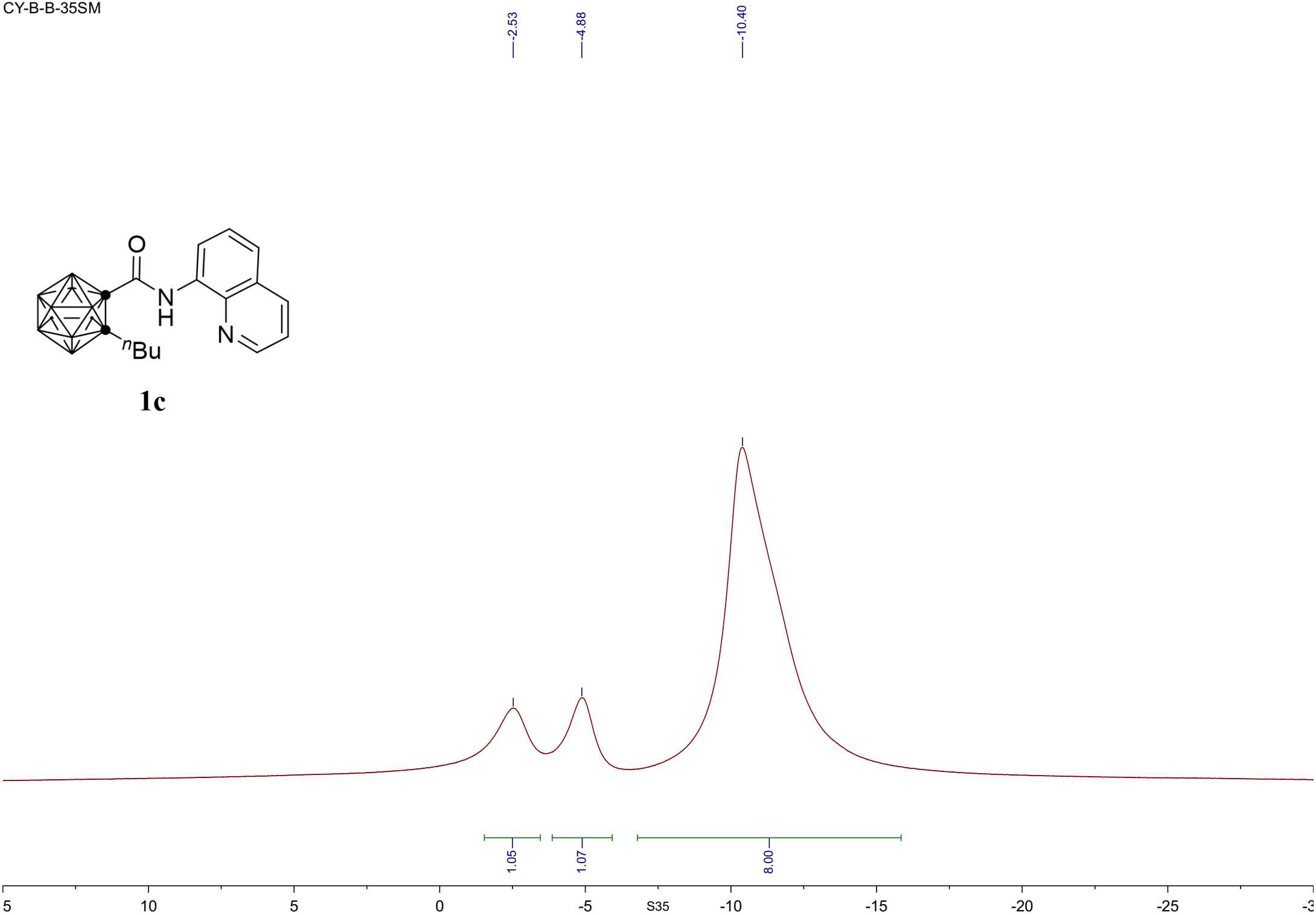
O
N
H
N
nBu

1c


155.47
149.06
138.65
136.42
133.26
127.93
127.04
123.42
122.20
116.91
81.83
78.17
77.48
77.16
76.84
35.84
31.86
22.31
13.72
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

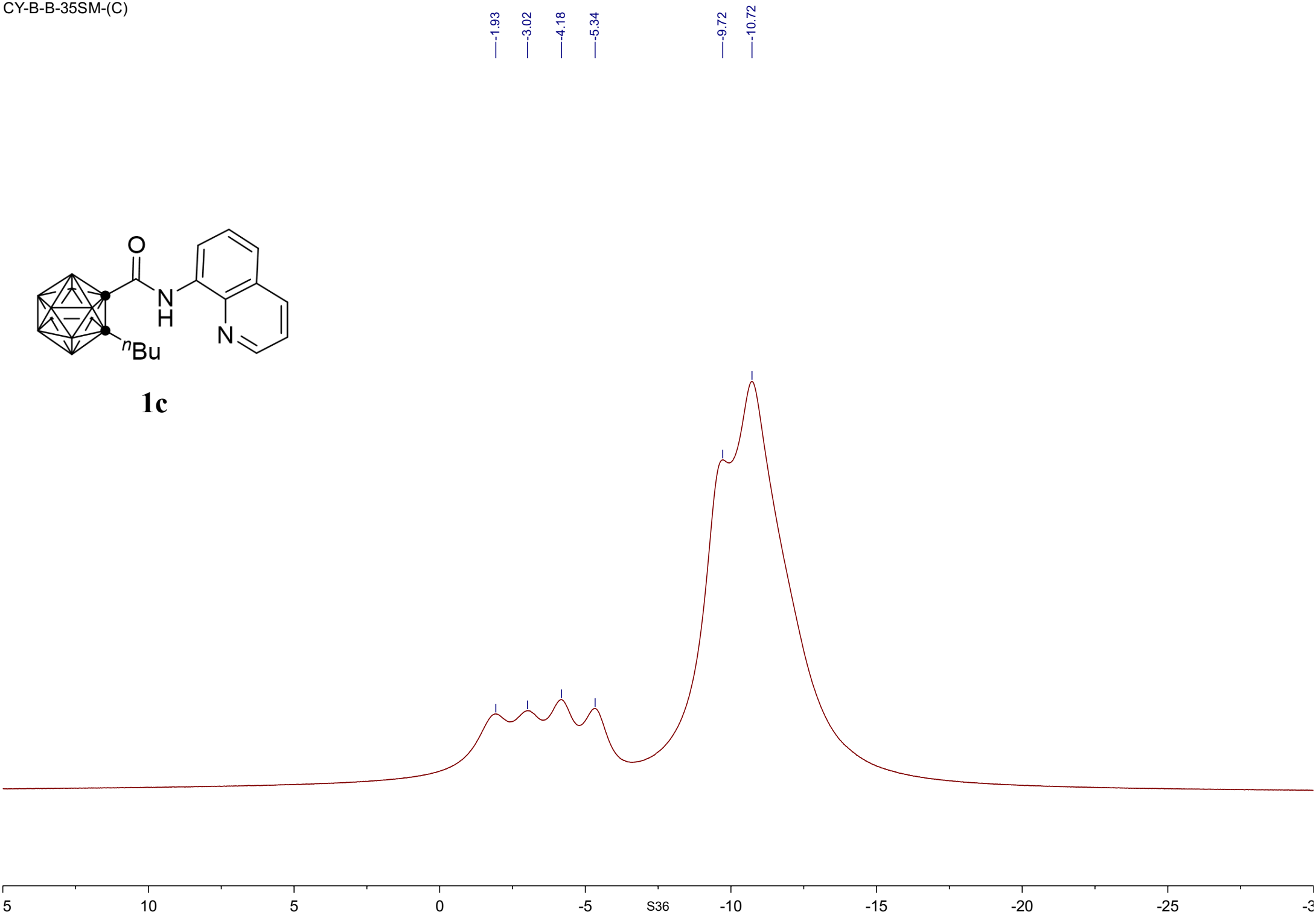
CY-B-B-35SM

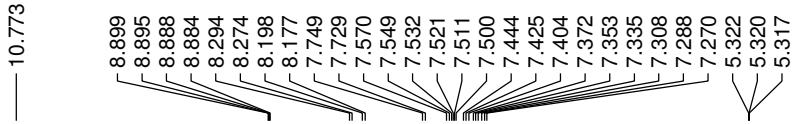
1c



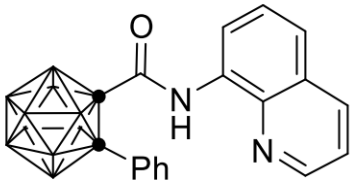
CY-B-B-35SM-(C)

1c





CY-H-A-168sm-C-Ph

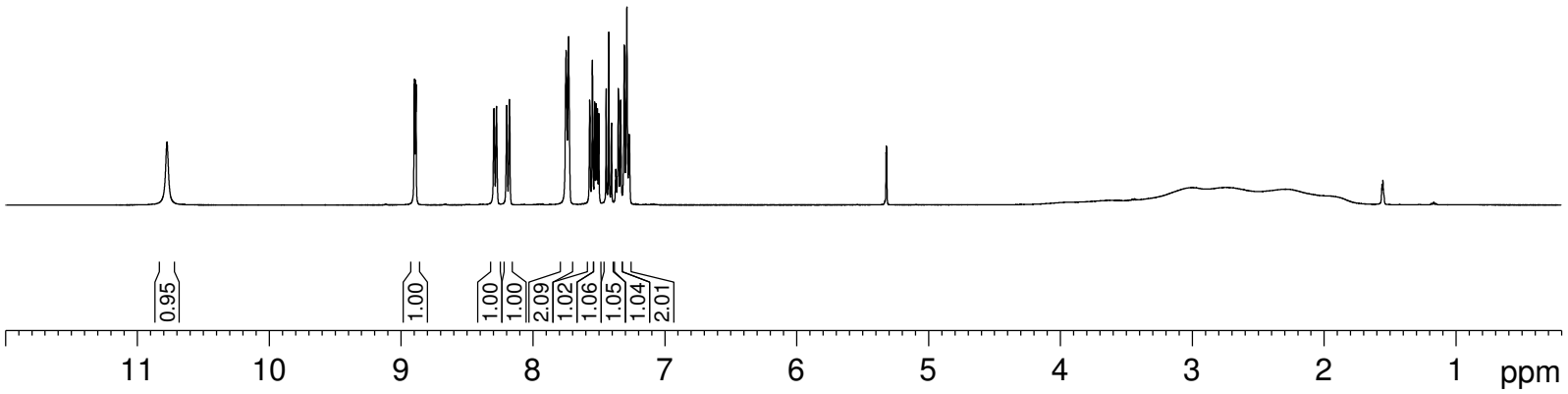


1d

Current Data Parameters
NAME CY-H-A-168sm-C-Ph
EXPNO 1
PROCNO 1

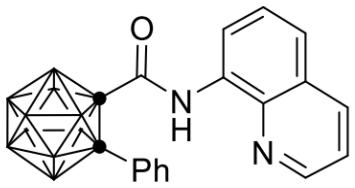
F2 - Acquisition Parameters
Date_ 20190621
Time 17.24 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 14.50 usec
PLW1 8.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2300156 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

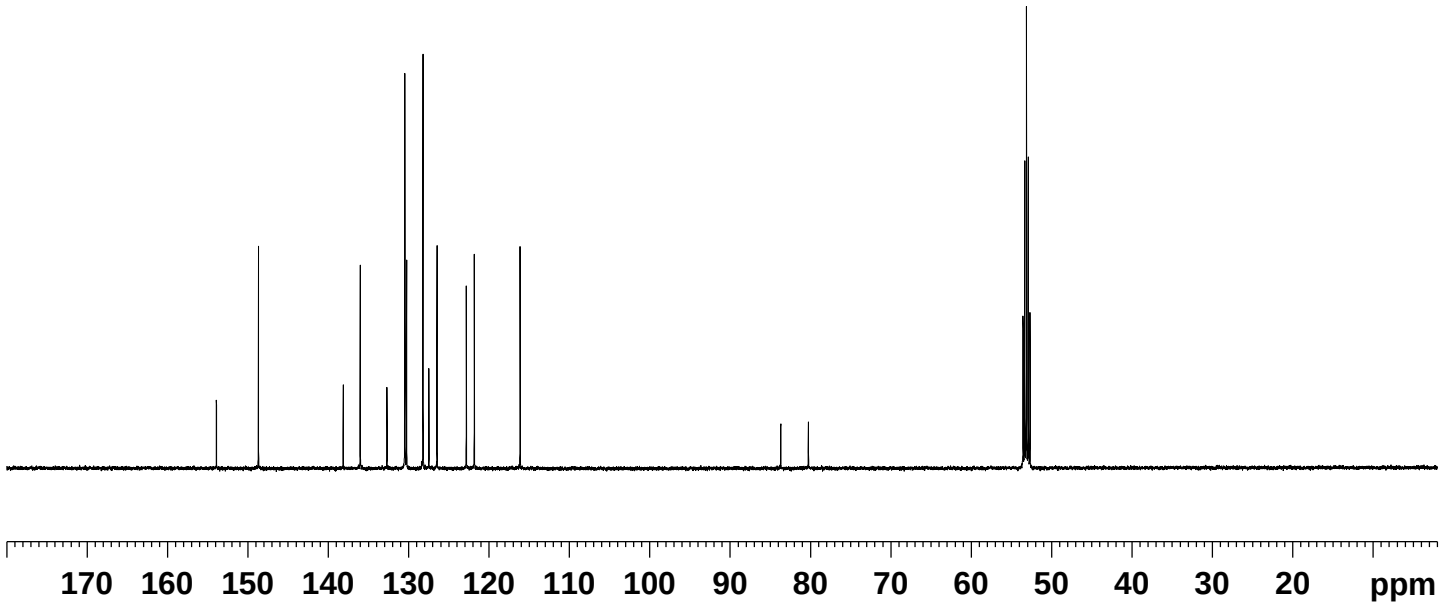


CY-C-A-168sm-C-Ph

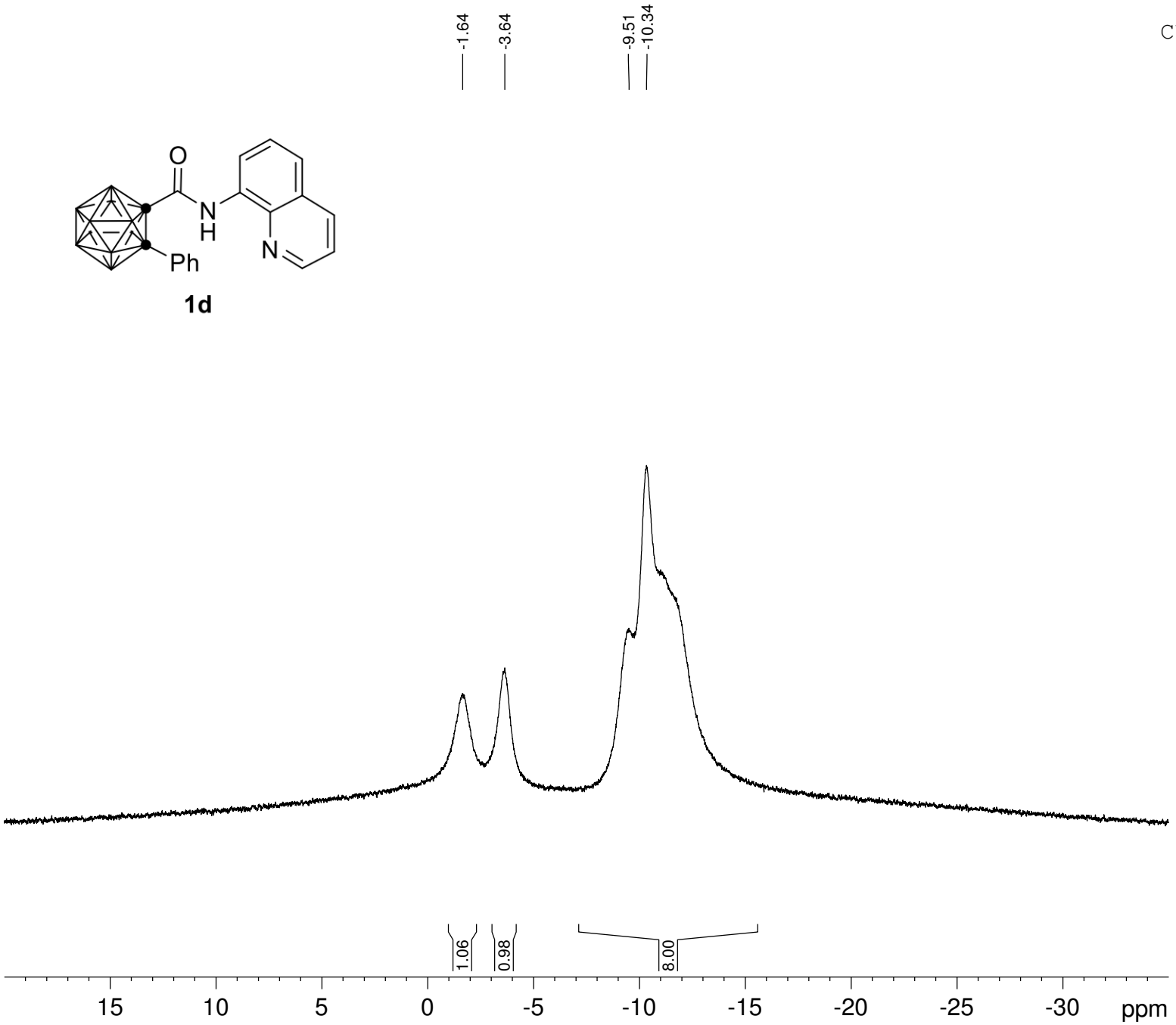
153.95
148.73
138.17
136.06
132.73
130.51
130.47
130.29
128.24
127.52
126.50
122.86
121.87
116.16
83.73
80.29
53.58
53.36
53.14
52.93
52.71



1d

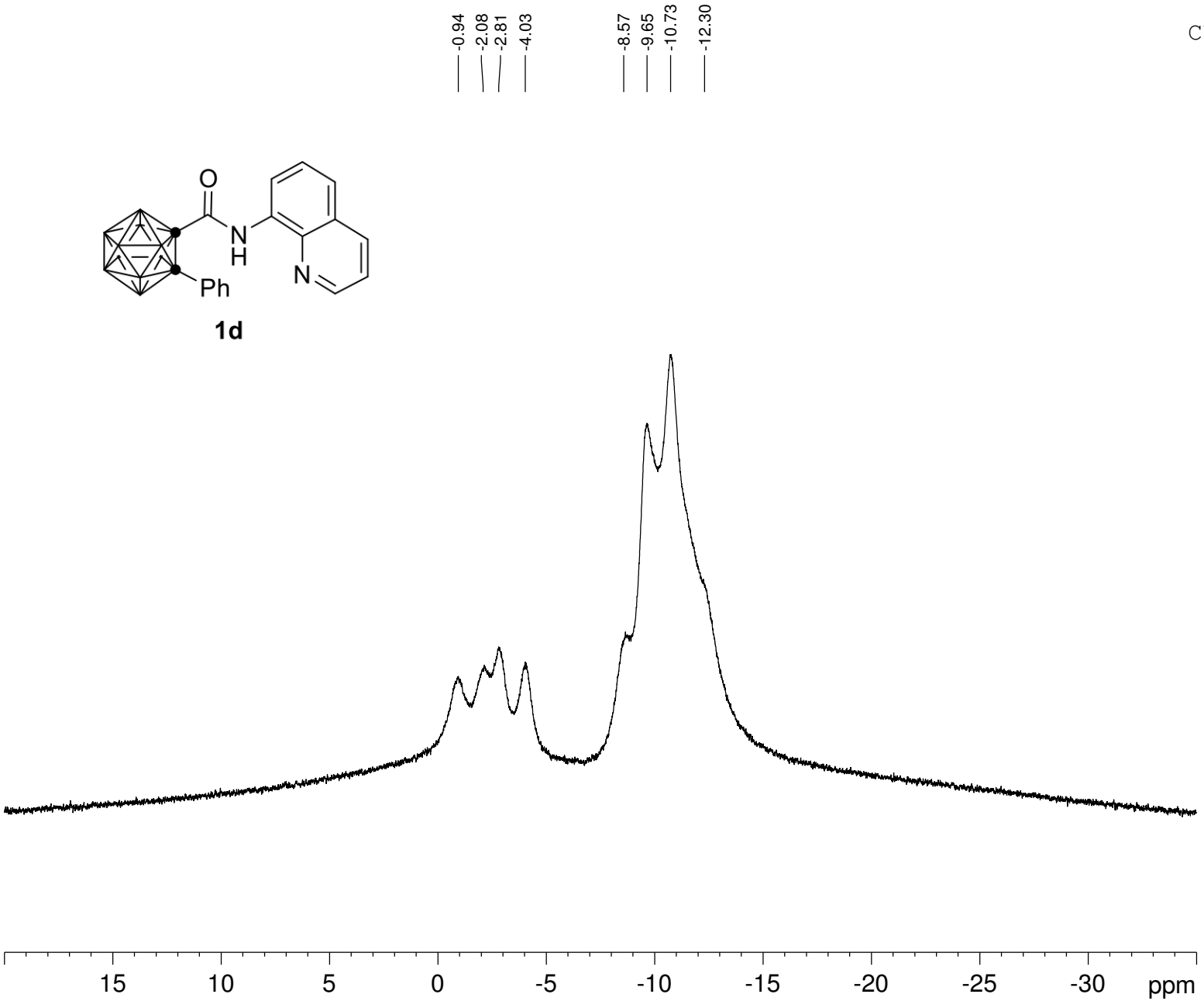



```
Current Data Parameters
NAME      CY-C-A-168sm-C-Ph
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190621
Time              19.37 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CD2Cl2
NS                   72
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7578275 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



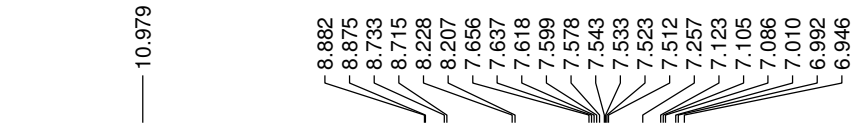
CY-B-A-168sm

```
Current Data Parameters
NAME        CY-B-A-168sm
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171009
Time               21.43 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   406
DW                20.800 usec
DE                 6.50 usec
TE                298.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

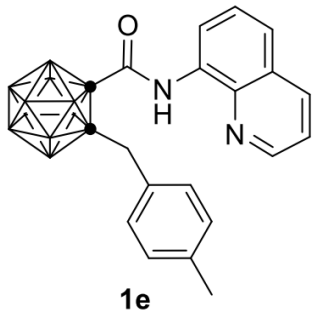


CY-B-A-168sm-(C)

```
Current Data Parameters
NAME      CY-B-A-168sm-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171009
Time               21.47 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                   48
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  406
DW                20.800 usec
DE                 6.50 usec
TE                297.5 K
D1           2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



CY-H-B-44sm-4-Me-Bn

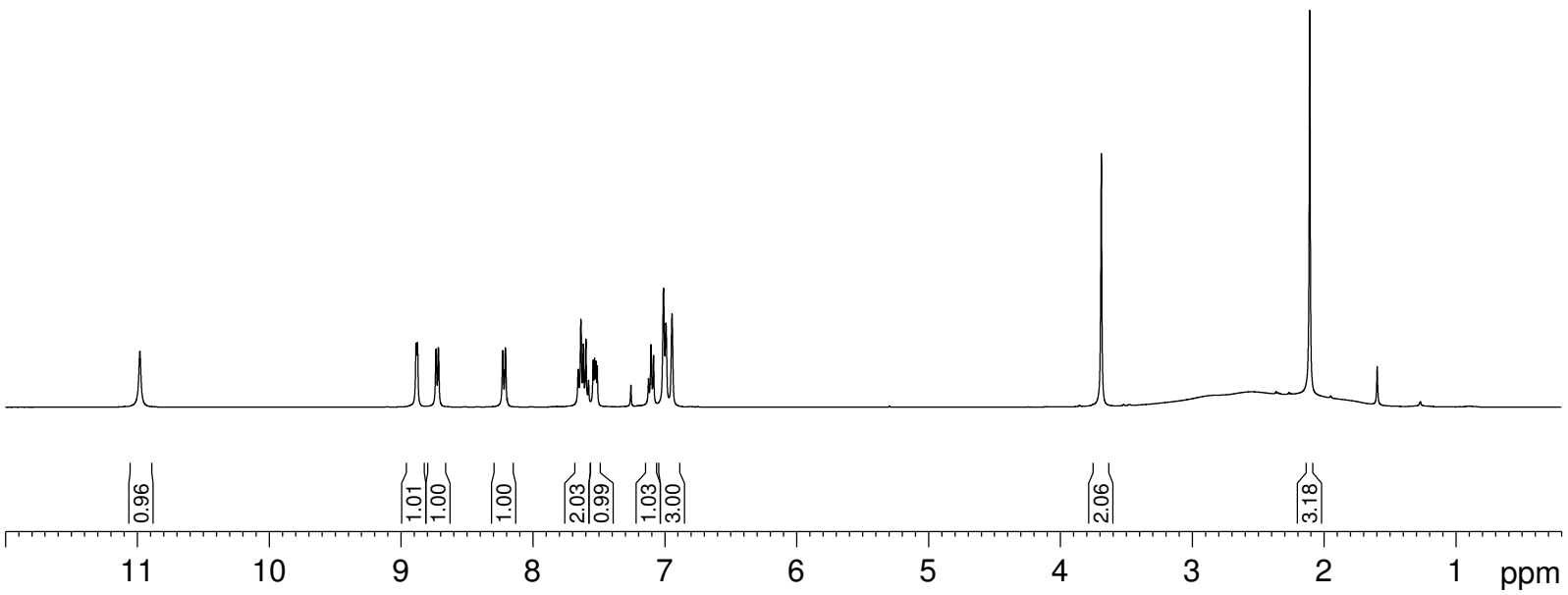


1e

Current Data Parameters
NAME CY-H-B-44sm-4-Me-Bn
EXPNO 1
PROCNO 1

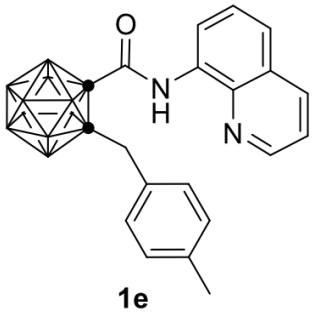
F2 - Acquisition Parameters
Date_ 20190621
Time 16.57 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 52
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 14.50 usec
PLW1 8.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

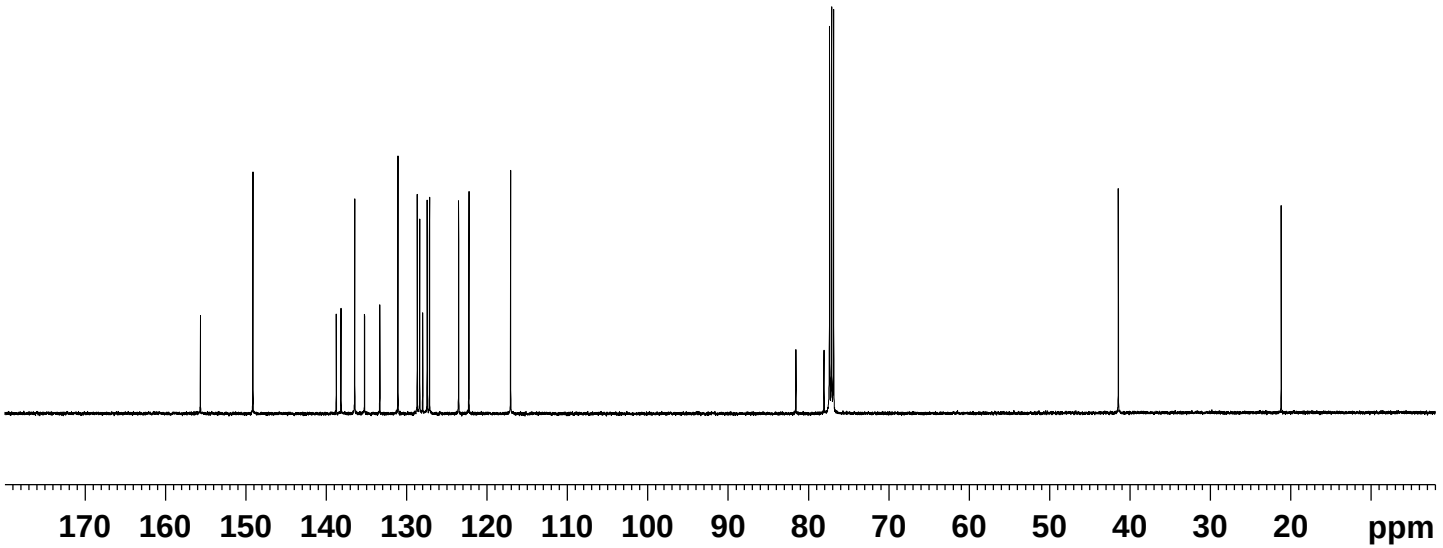


CY-C-B-44sm-4-Me-Bn

155.69
149.16
138.79
138.20
136.49
135.27
133.37
131.11
128.72
128.40
128.04
127.48
127.18
123.56
122.28
117.09
81.59
78.09
77.41
77.15
76.90
41.47
21.21



1e

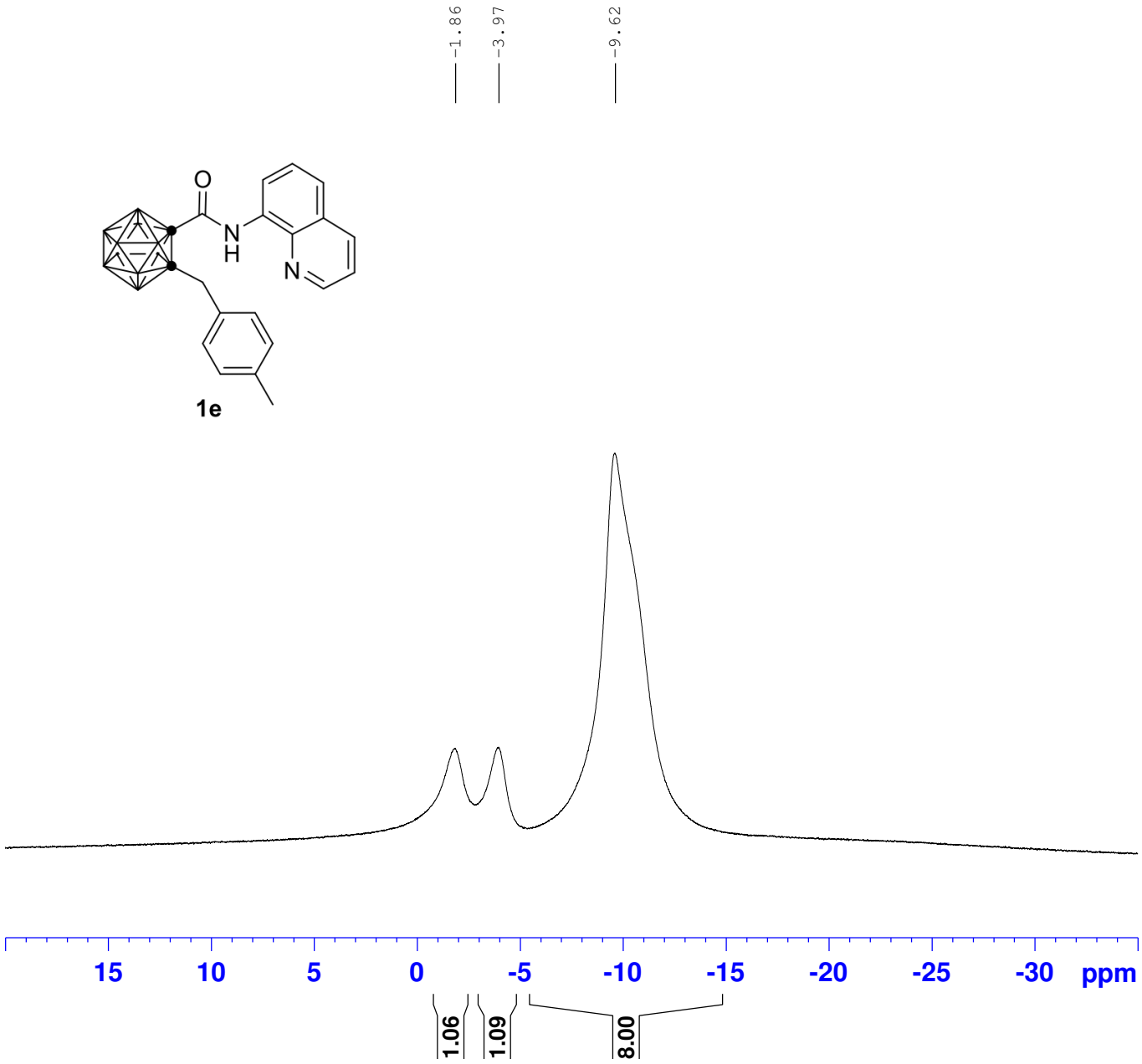


Current Data Parameters
NAME CY-C-B-44sm-4-Me-Bn
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190621
Time 17.43 h
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 160
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 206.72
DW 16.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 10.00 usec
PLW1 61.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.29663000 W
PLW13 0.14920001 W

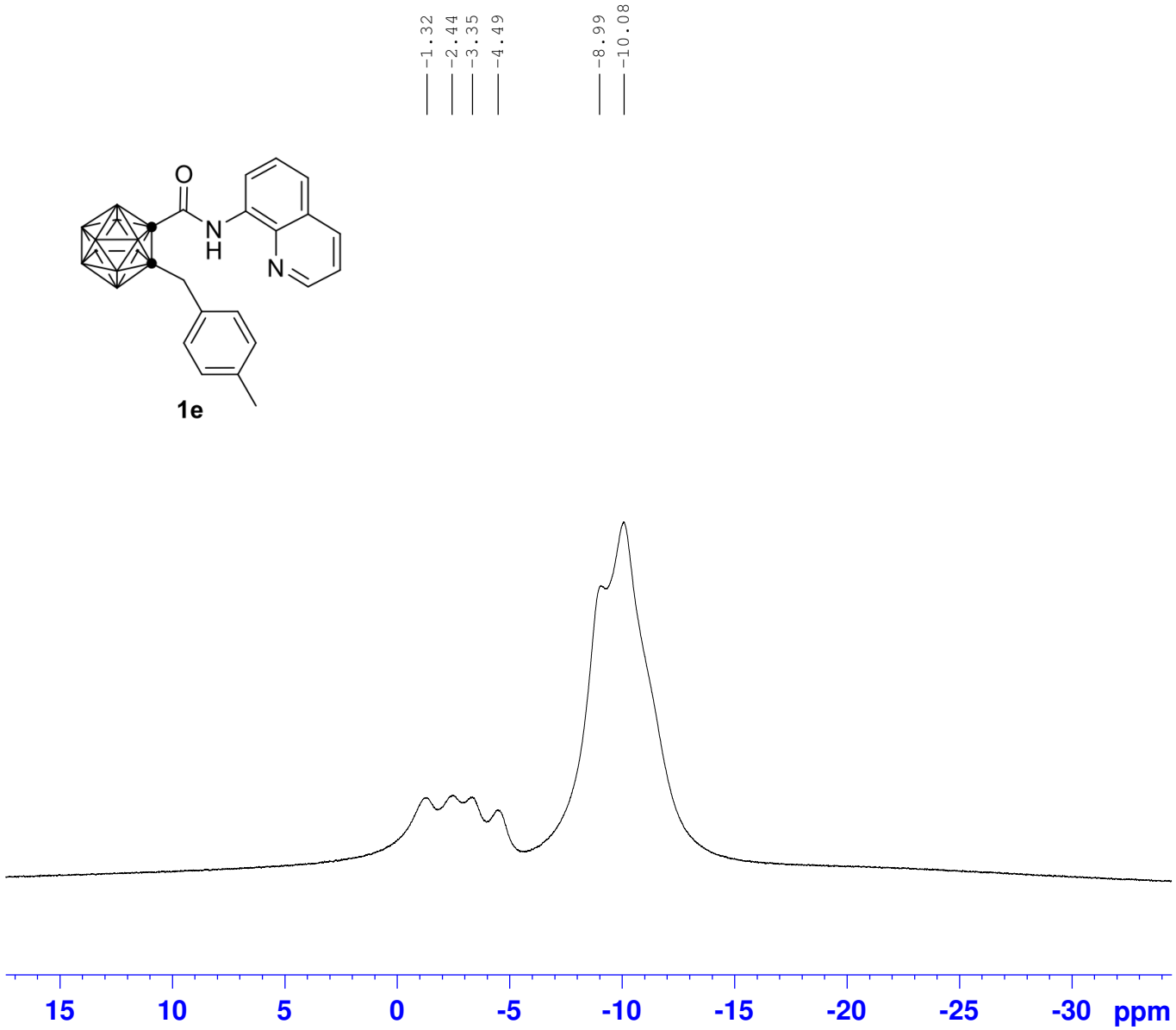
F2 - Processing parameters
SI 32768
SF 125.7577776 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CY-B-B-44sm-4-MeBn




```
Current Data Parameters
NAME      CY-B-B-44sm-4-MeBn
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190621
Time              19.01 h
INSTRUM             spect
PROBHD   Z820201_0170 (
PULPROG             zgig
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            25510.203 Hz
FIDRES          0.778510 Hz
AQ              1.2845056 sec
RG                   181
DW                19.600 usec
DE                 6.50 usec
TE                295.9 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.3776050 MHz
NUC1                  11B
P1                 28.50 usec
PLW1         14.79100037 W
SFO2         400.1324710 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.17000008 W
PLW12         0.07408100 W

F2 - Processing parameters
SI                 32768
SF           128.3776052 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

CY-B-B-44sm-4-MeBn-(C)



Current Data Parameters
NAME CY-B-B-44sm-4-MeBn-(C)
EXPNO 1
PROCNO 1

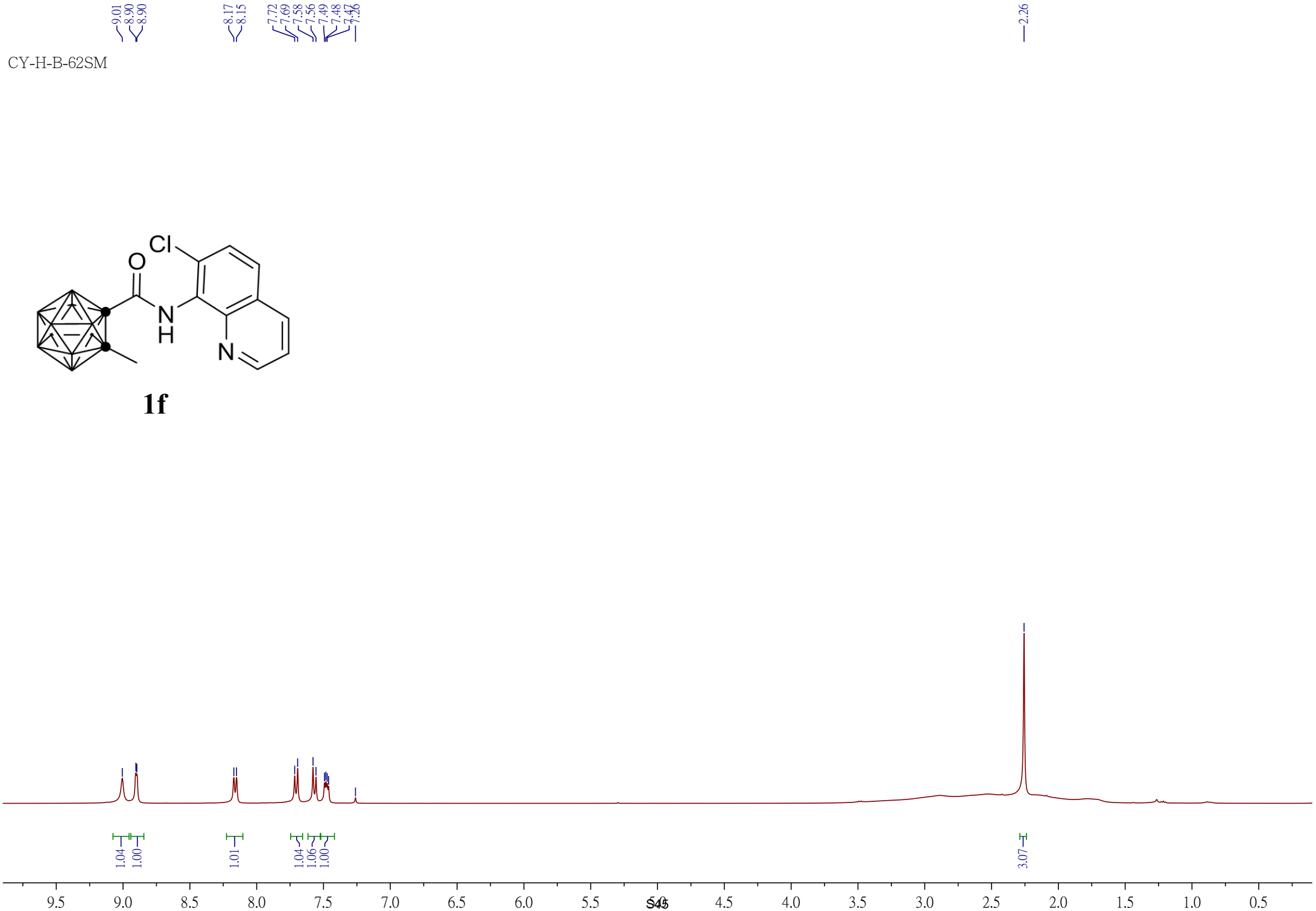
F2 - Acquisition Parameters
Date_ 20190621
Time 19.04 h
INSTRUM spect
PROBHD Z820201_0170 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 44
DS 4
SWH 25510.203 Hz
FIDRES 0.778510 Hz
AQ 1.2845056 sec
RG 181
DW 19.600 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
SFO1 128.3776050 MHz
NUC1 11B
P1 28.50 usec
PLW1 14.79100037 W

F2 - Processing parameters
SI 32768
SF 128.3776052 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CY-H-B-62SM

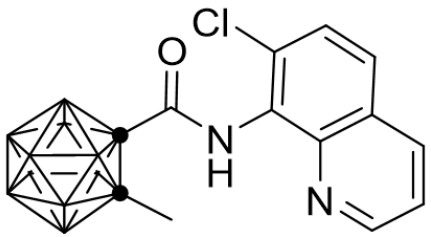
Cl
O
N
H
N

1f

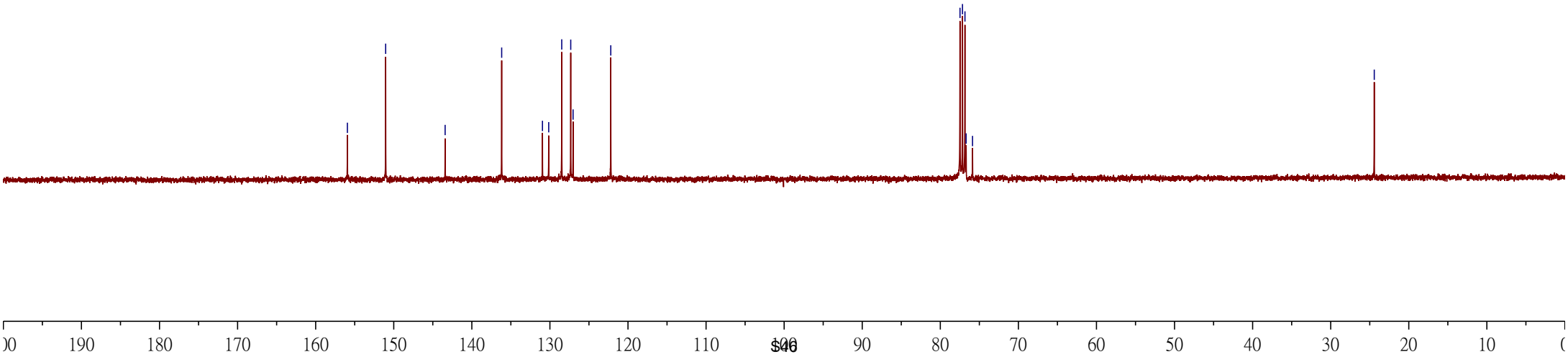

9.01
8.90
8.90
8.17
8.15
7.72
7.69
7.58
7.56
7.49
7.48
7.47
7.26
2.26
1.04
1.00
1.01
1.04
1.06
1.00
3.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

155.94
151.04
143.42
136.18
130.95
130.15
128.48
127.33
127.03
122.20
77.48
77.16
76.84
76.69
75.87
24.42

CY-C-B-62SM

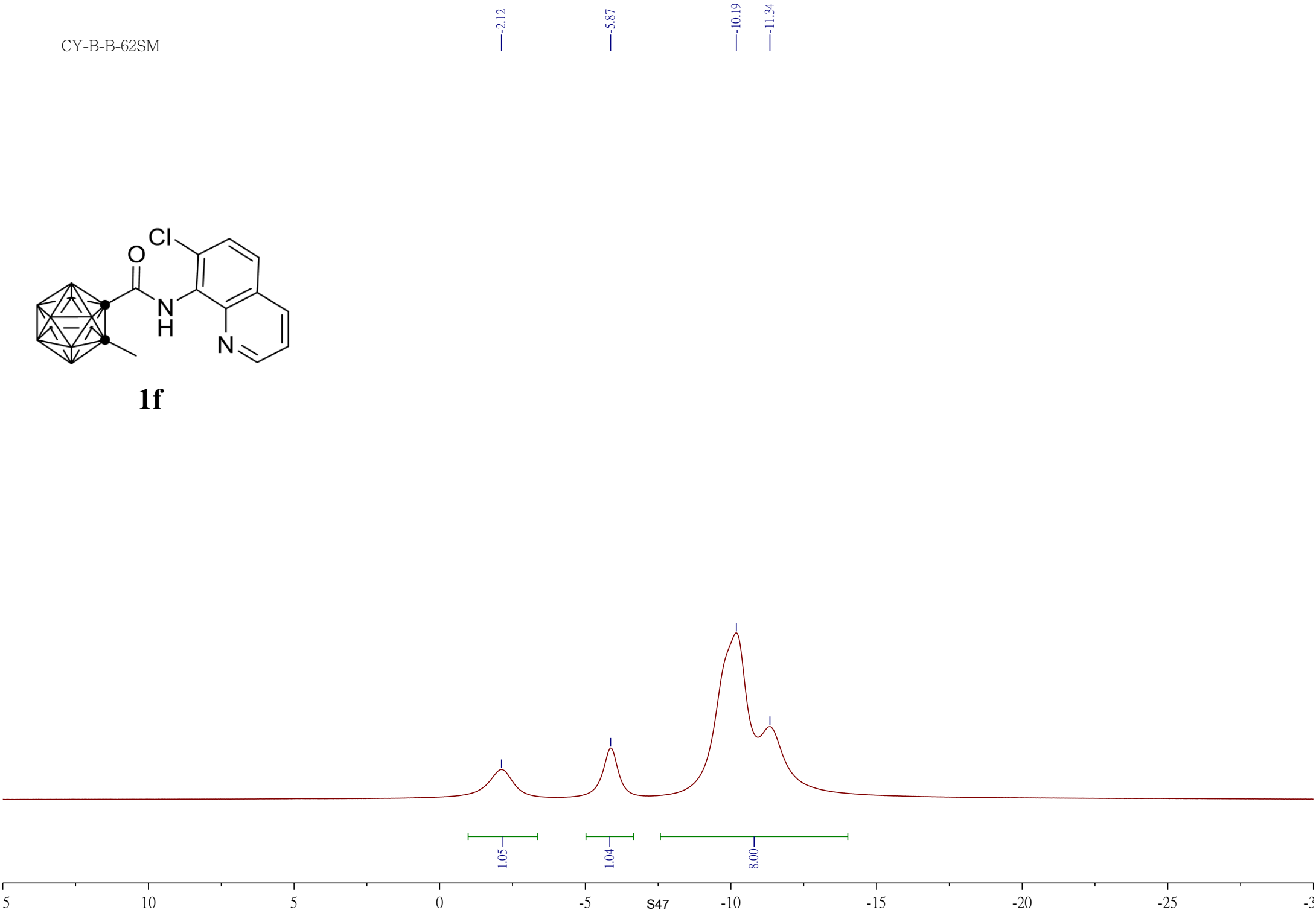


1f



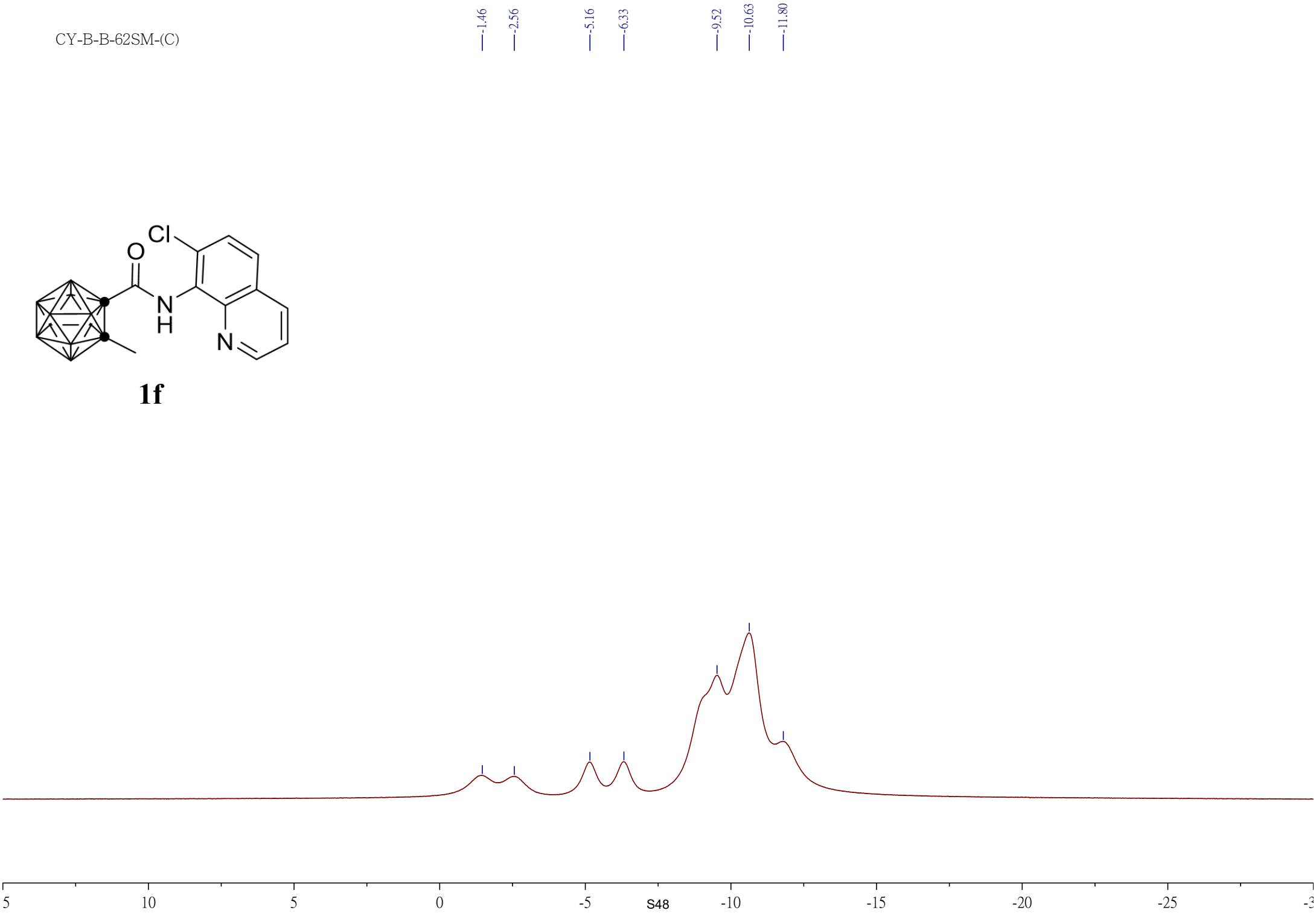
CY-B-B-62SM

1f



CY-B-B-62SM-(C)

1f



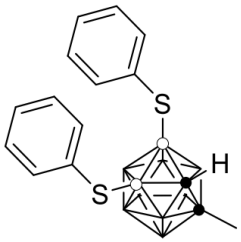
CY-H-B-11P

7.596 7.587 7.584 7.578 7.572 7.332 7.326 7.320 7.316 7.309 7.300 7.260

3.809

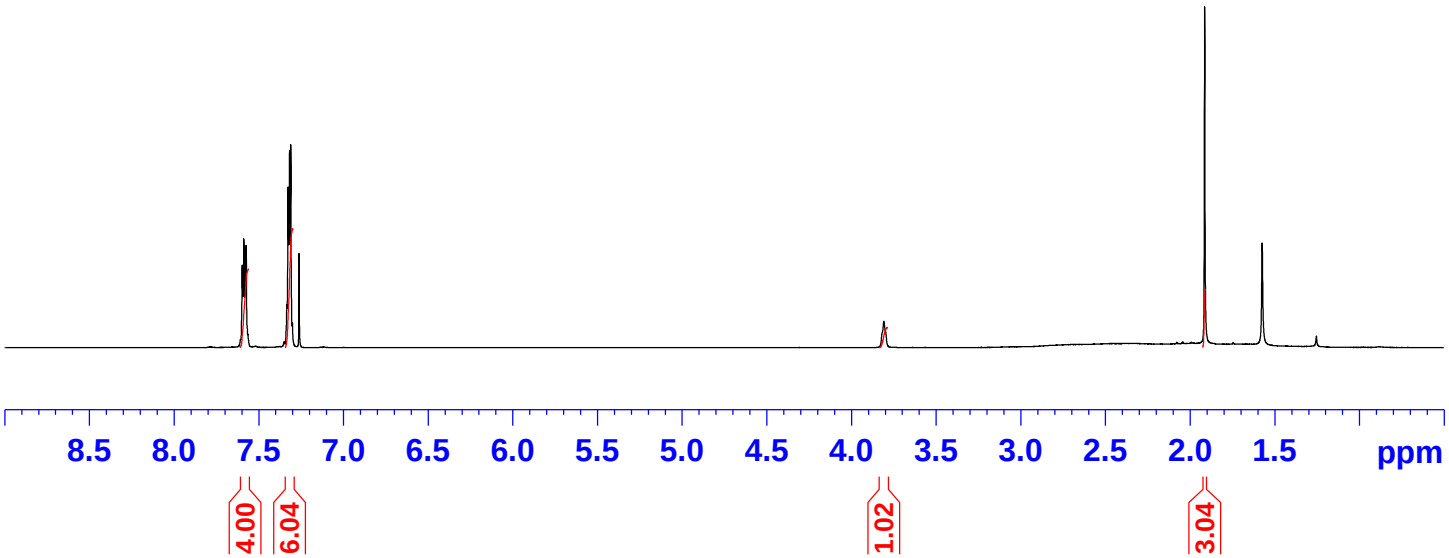
1.914

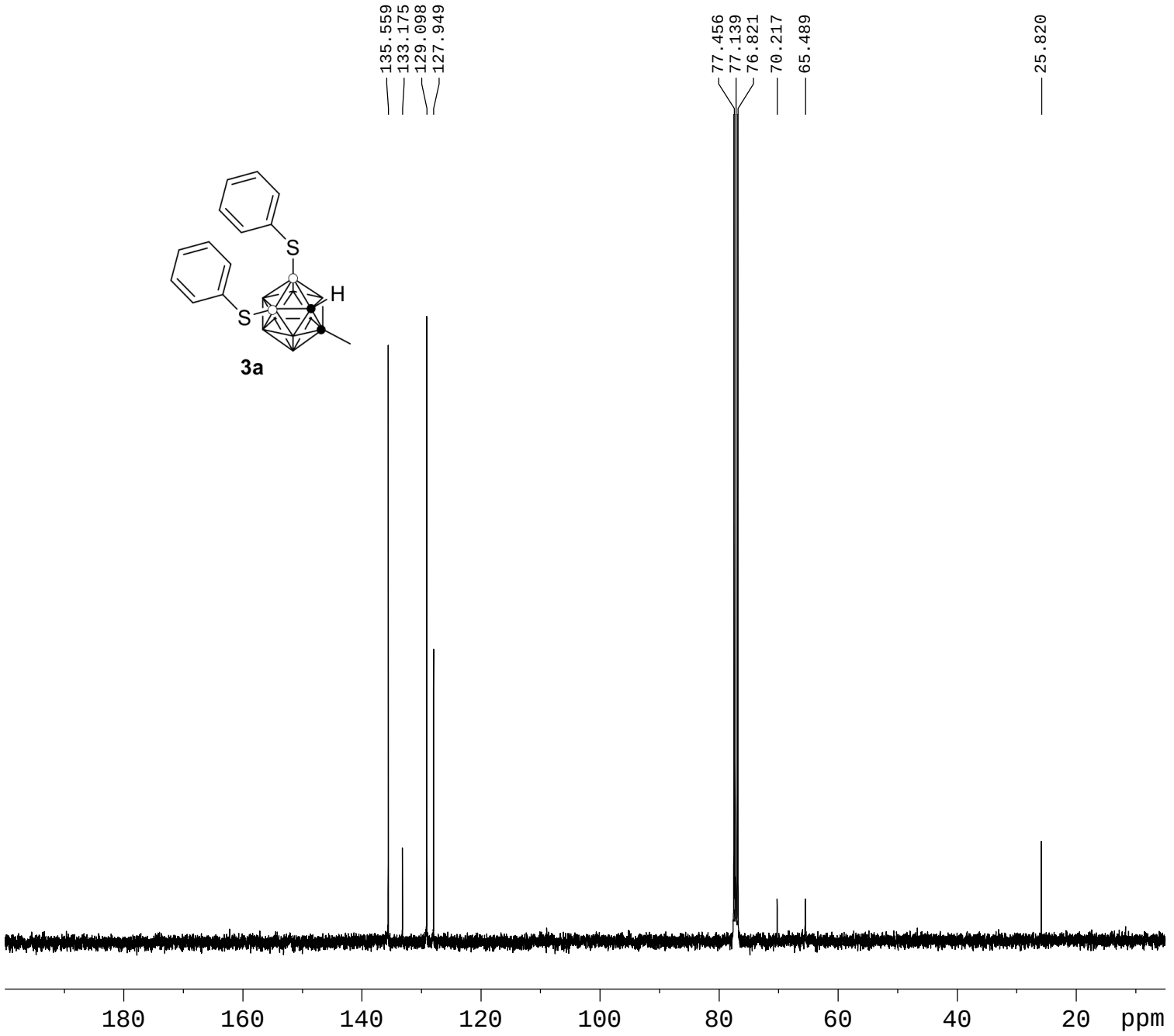
1.574



3a

```
Current Data Parameters
NAME          CY-H-B-11P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180108
Time               9.46 h
INSTRUM           spect
PROBHD   Z824601_0021 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   12
DS                    2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                  203
DW                62.400 usec
DE                 6.50 usec
TE                295.6 K
D1            1.00000000 sec
TD0                   1
SFO1        400.1324708 MHz
NUC1                1H
P1                15.00 usec
PLW1          8.31000042 W

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





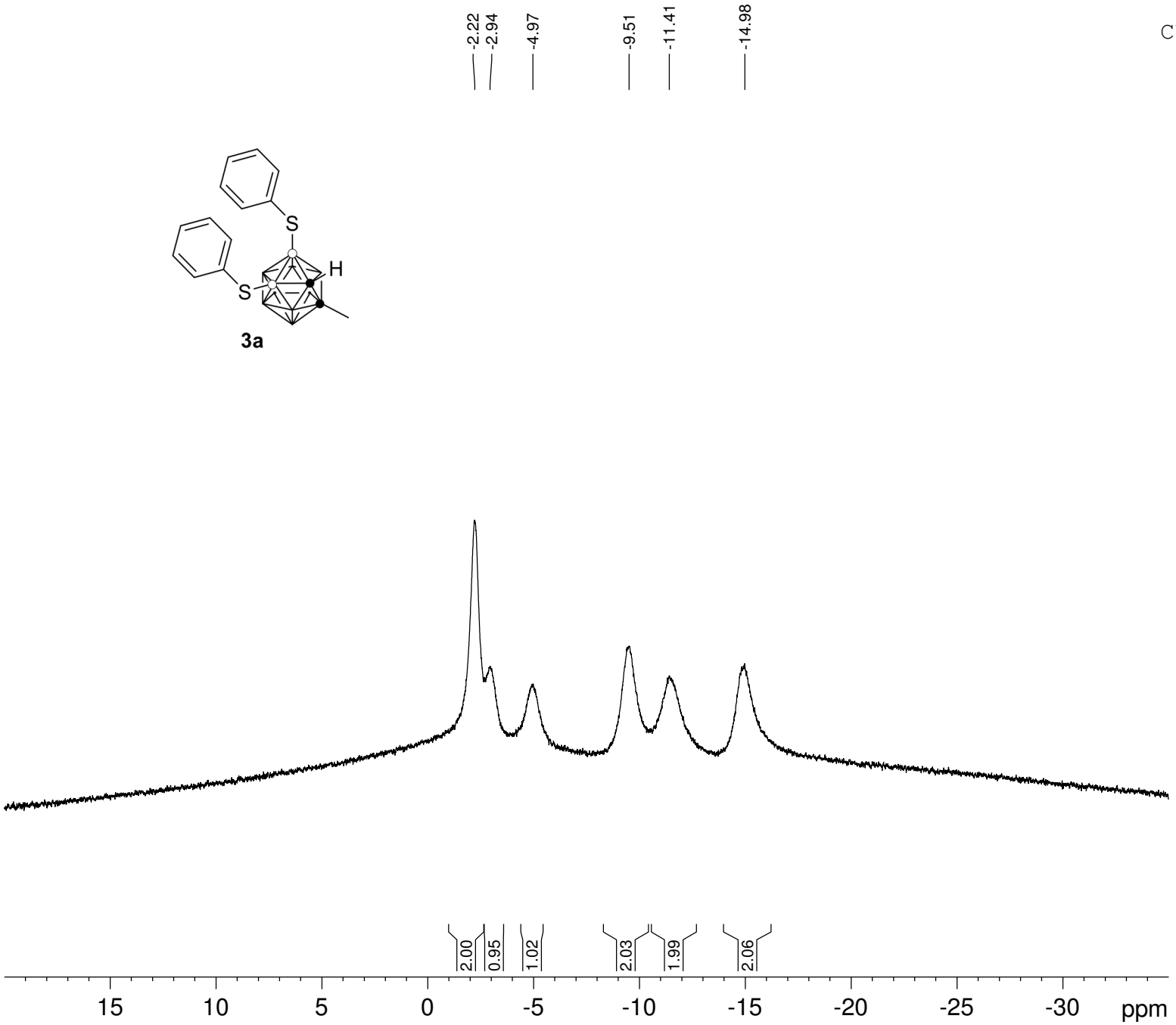
CY-C-B-11P

Bruker Advance III 400

Current Data Parameters
NAME CY-C-B-11P
EXPNO 2
PROCNO 1

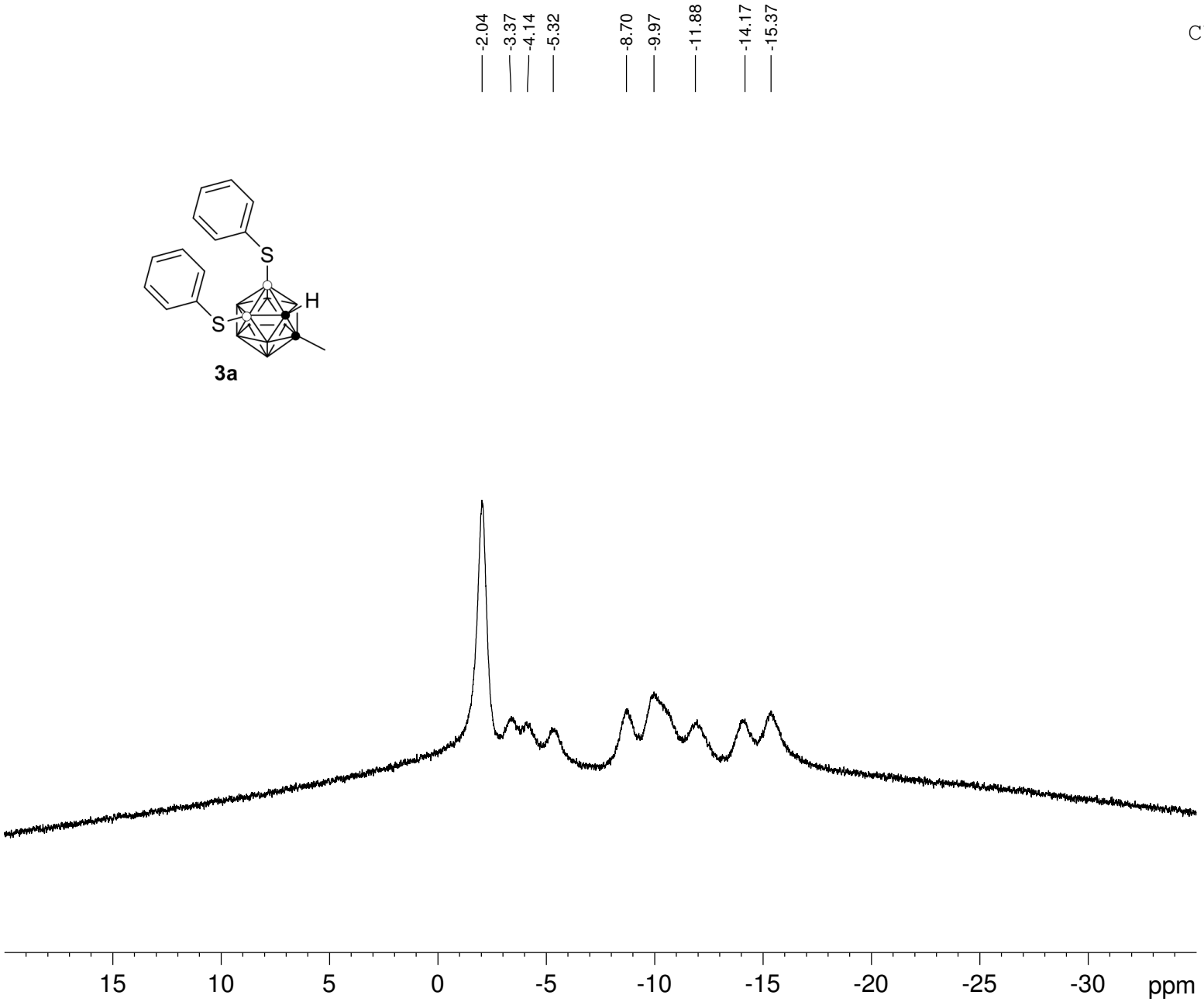
F2 - Acquisition Parameters
Date_ 20180108
Time 10.32 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 794
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W

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



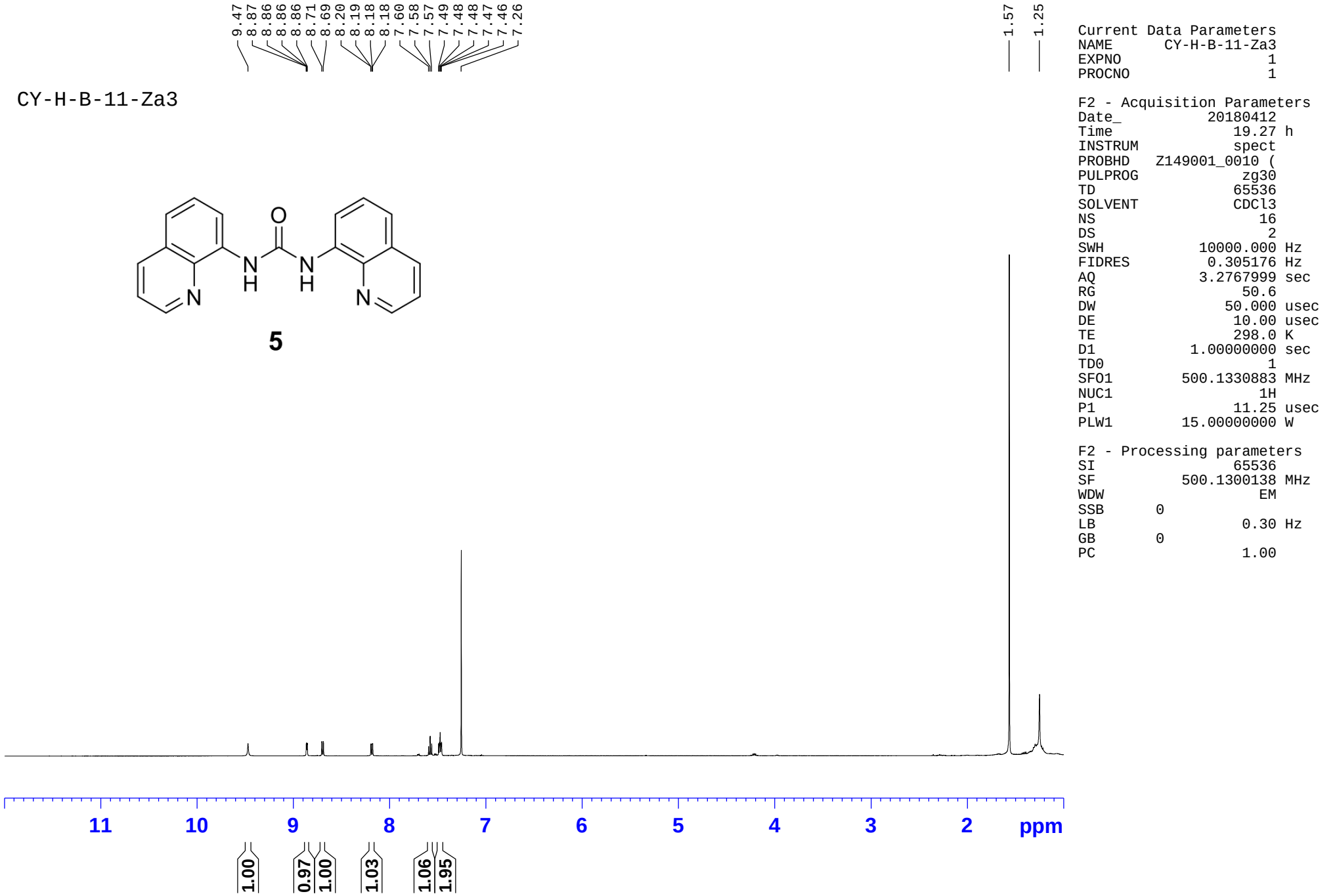
CY-B-B-11p-1

```
Current Data Parameters
NAME        CY-B-B-11p-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171227
Time               19.40 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    57
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   362
DW                20.800 usec
DE                 6.50 usec
TE                295.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

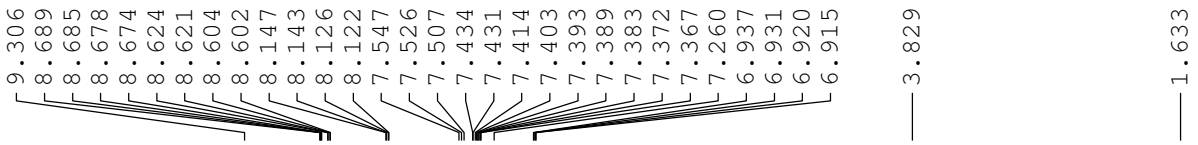


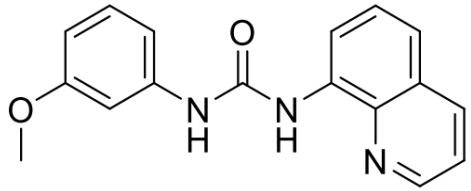
CY-B-B-11p-1-(C)

```
Current Data Parameters
NAME      CY-B-B-11p-1-(C)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171227
Time               19.43 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     40
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    322
DW                20.800 usec
DE                 6.50 usec
TE                295.3 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                 7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

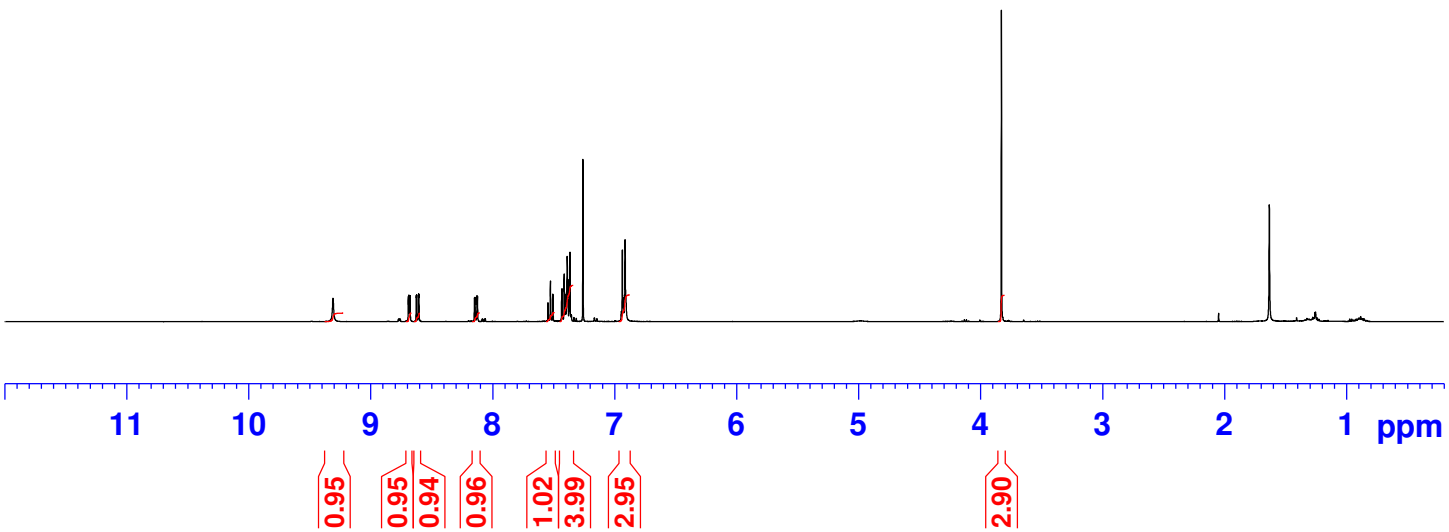



```
Current Data Parameters
NAME       CY-H-B-11-Za3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180412
Time              19.27 h
INSTRUM            spect
PROBHD    Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                  50.6
DW                50.000 usec
DE                10.00 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         500.1330883 MHz
NUC1                  1H
P1                 11.25 usec
PLW1        15.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.1300138 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



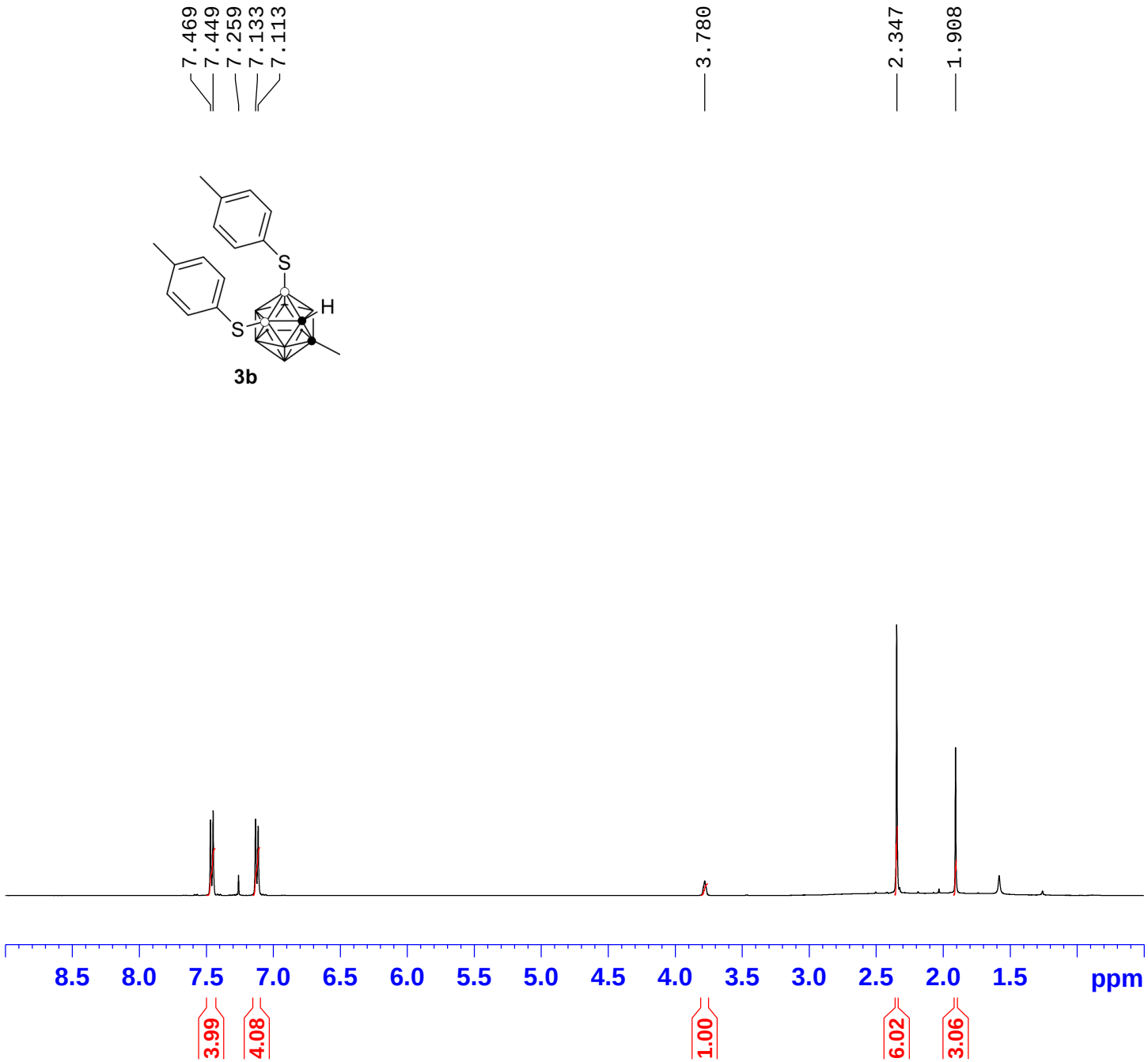


5'

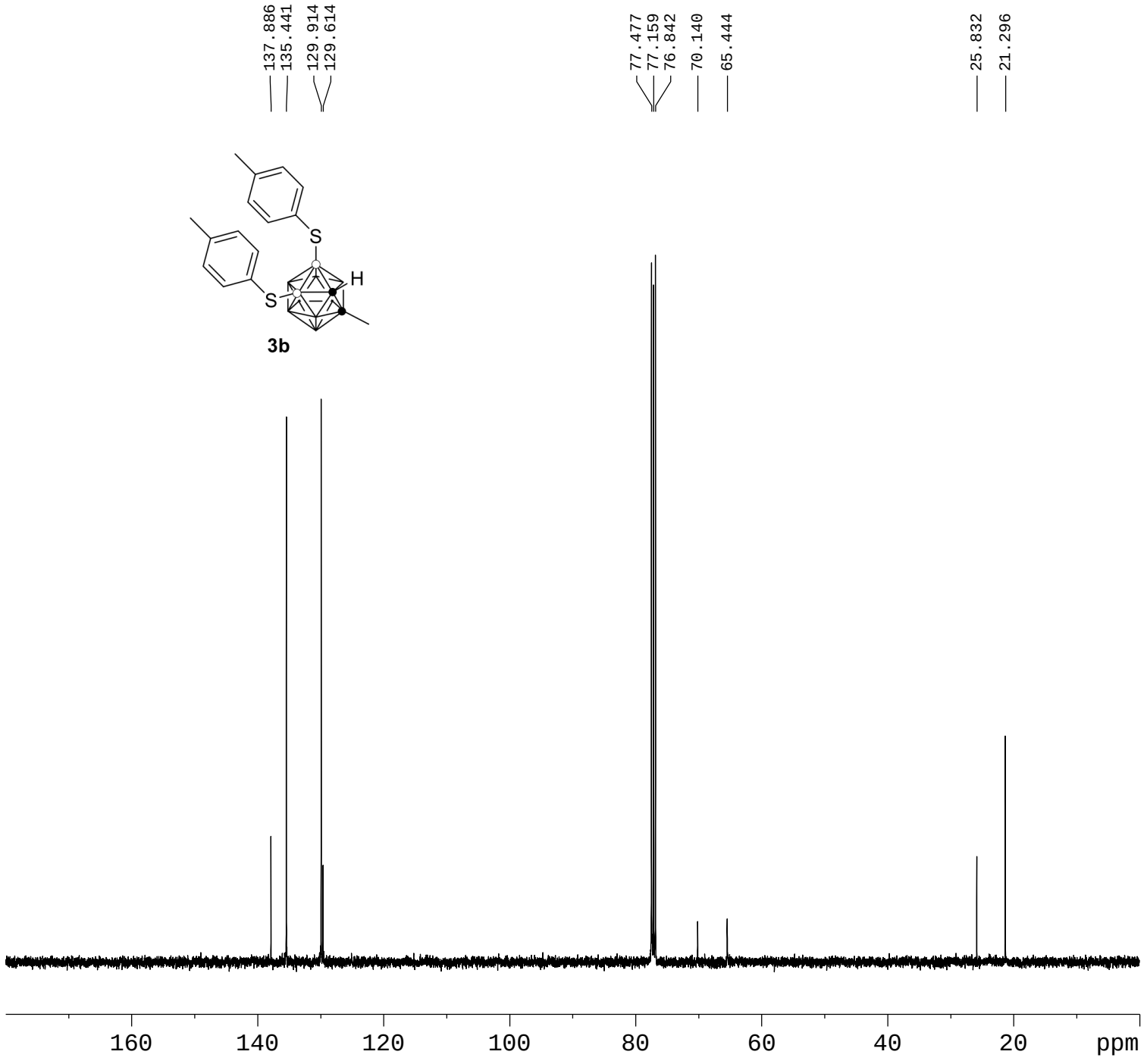



```
Current Data Parameters
NAME      CY-H-B-11-NH2C6H4OMe
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20200723
Time                  12.08 h
INSTRUM               spect
PROBHD    Z820201_0170 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       12
DS                        2
SWH                8012.820 Hz
FIDRES             0.244532 Hz
AQ                 4.0894465 sec
RG                       203
DW                    62.400 usec
DE                     6.50 usec
TE                    296.6 K
D1              1.00000000 sec
TD0                      1
SFO1           400.1324708 MHz
NUC1                    1H
P1                    6.75 usec
PLW1           13.17700005 W

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

CY-H-B-21p-CH3




```
Current Data Parameters
NAME      CY-H-B-21p-CH3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180123
Time              20.11 h
INSTRUM            spect
PROBHD    Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    11
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                   203
DW                62.400 usec
DE                 6.50 usec
TE                296.9 K
D1           1.00000000 sec
TD0                    1
SFO1        400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1          8.31000042 W

F2 - Processing parameters
SI                 65536
SF          400.1300100 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



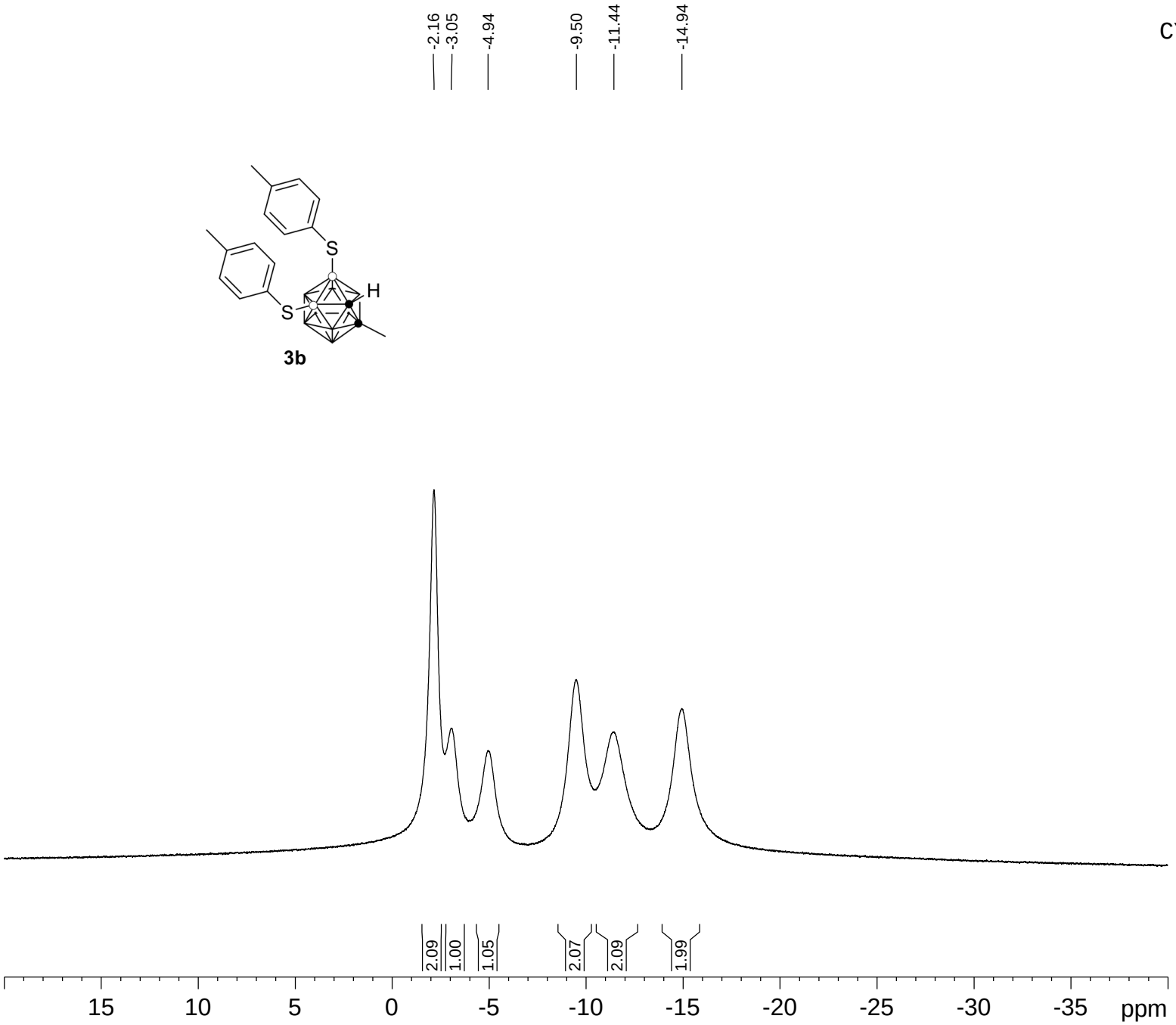
CY-C-B-21p-CH3

Bruker Advance III 400

Current Data Parameters
NAME CY-C-B-21p-CH3
EXPNO 3
PROCNO 1

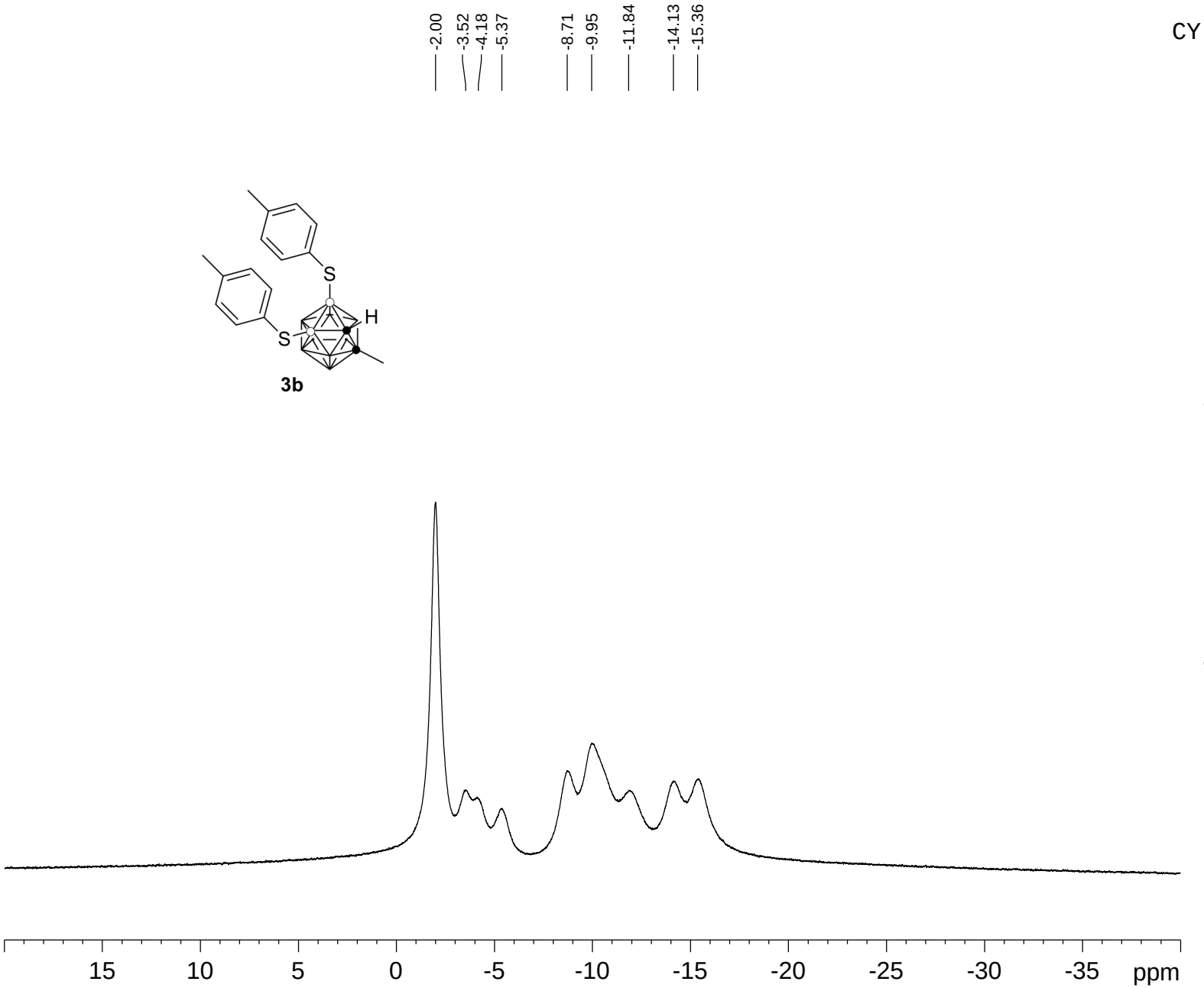
F2 - Acquisition Parameters
Date_ 20180123
Time 20.37 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 432
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W

F2 - Processing parameters
SI 32768
SF 100.6127565 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



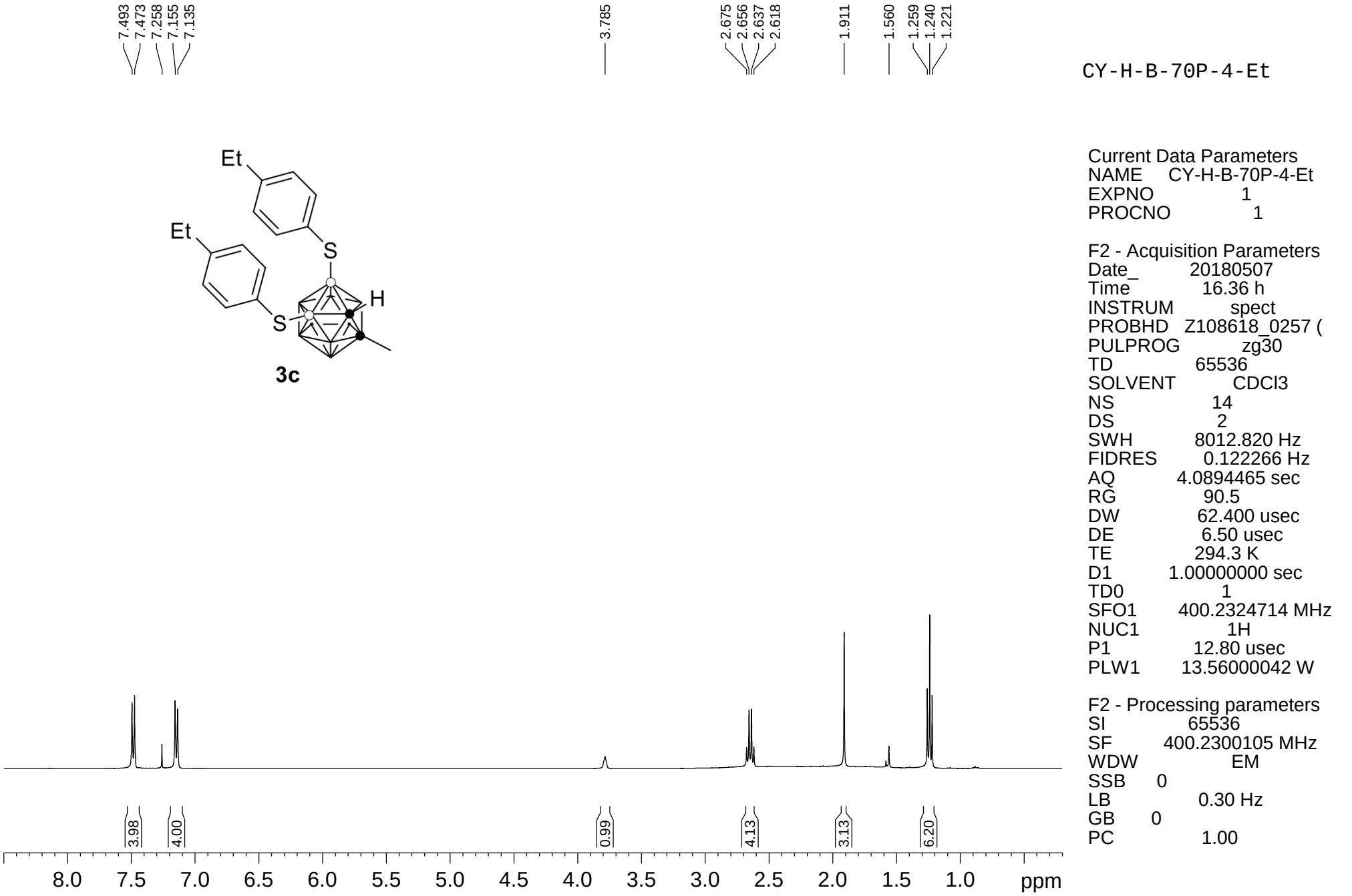
CY-B-B-21p-CH3

```
Current Data Parameters
NAME      CY-B-B-21p-CH3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180123
Time                9.47 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    35
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   362
DW                20.800 usec
DE                 6.50 usec
TE                295.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

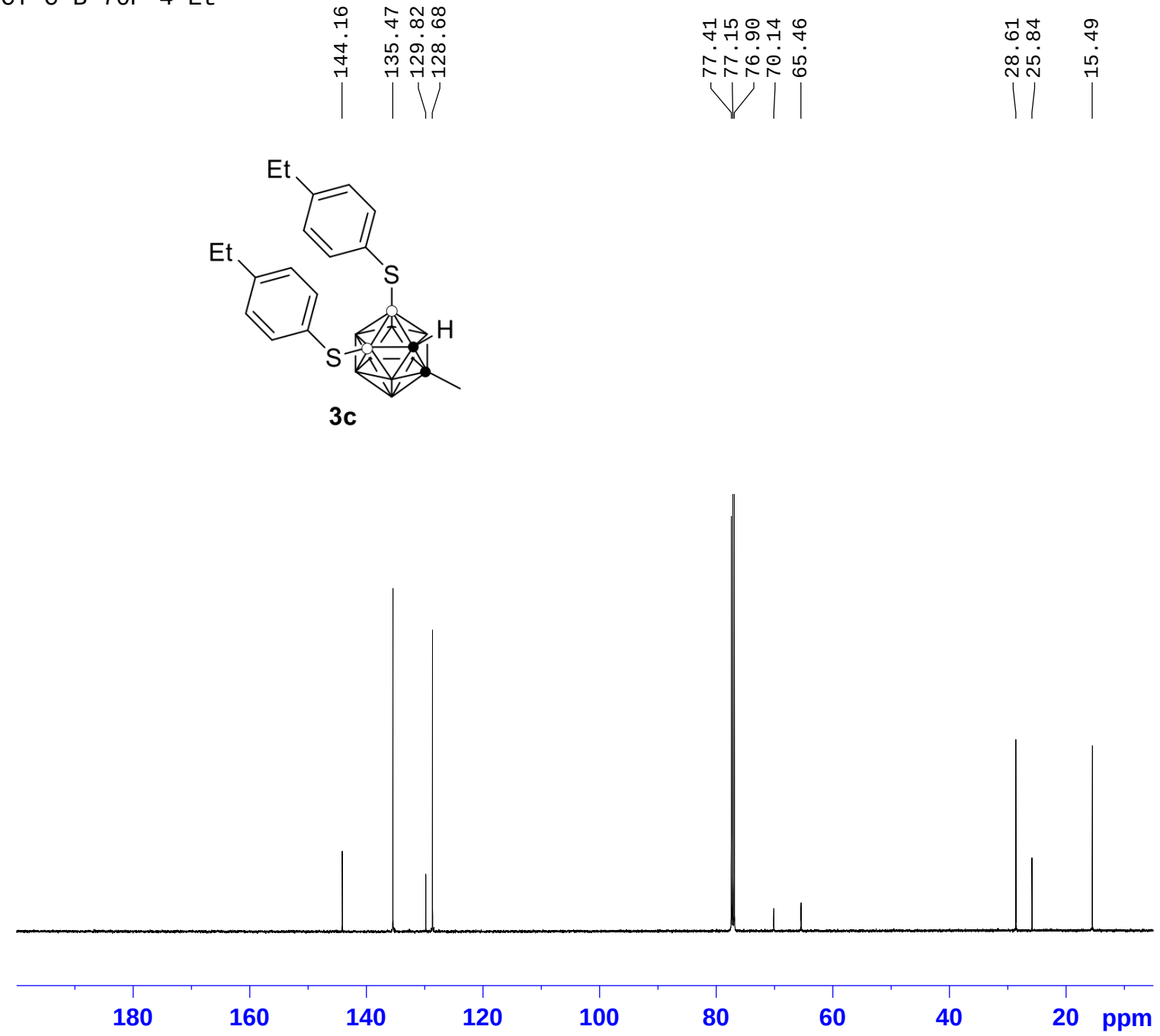


CY-B-B-21p-CH3-(C)

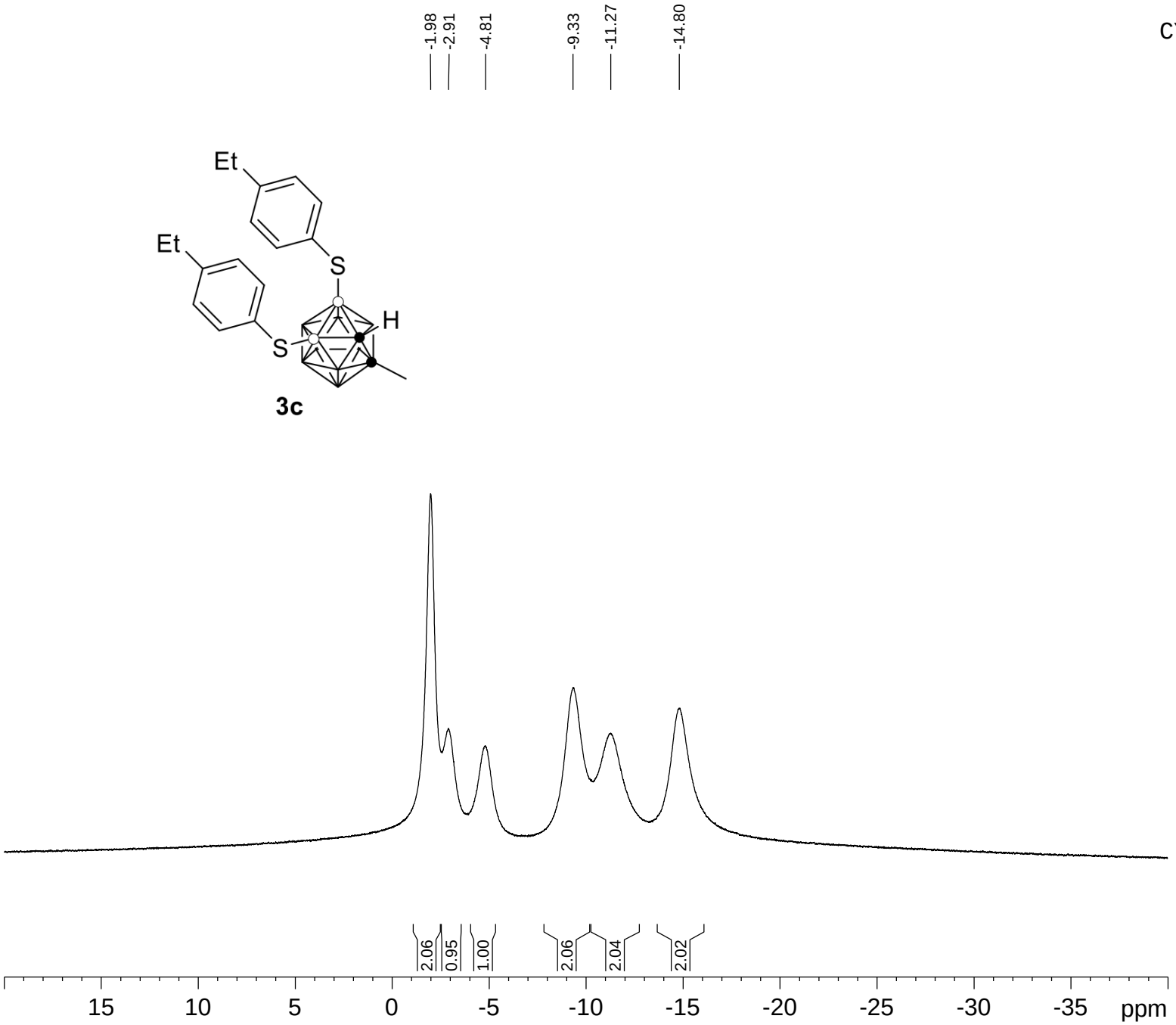
```
Current Data Parameters
NAME      CY-B-B-21p-CH3-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180123
Time                   9.49 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                       26
DS                        2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                      362
DW                  20.800 usec
DE                   6.50 usec
TE                  295.3 K
D1              2.00000000 sec
TD0                       1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                    32768
SF             128.4097430 MHz
WDW                      EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```


7.493
7.473
7.258
7.155
7.135
3.785
2.675
2.656
2.637
2.618
1.911
1.560
1.259
1.240
1.221
CY-H-B-70P-4-Et
Et
Et
S
S
H
3c
Current Data Parameters
NAME CY-H-B-70P-4-Et
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180507
Time 16.36 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 14
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 90.5
DW 62.400 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
3.98
4.00
0.99
4.13
3.13
6.20
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

CY-C-B-70P-4-Et

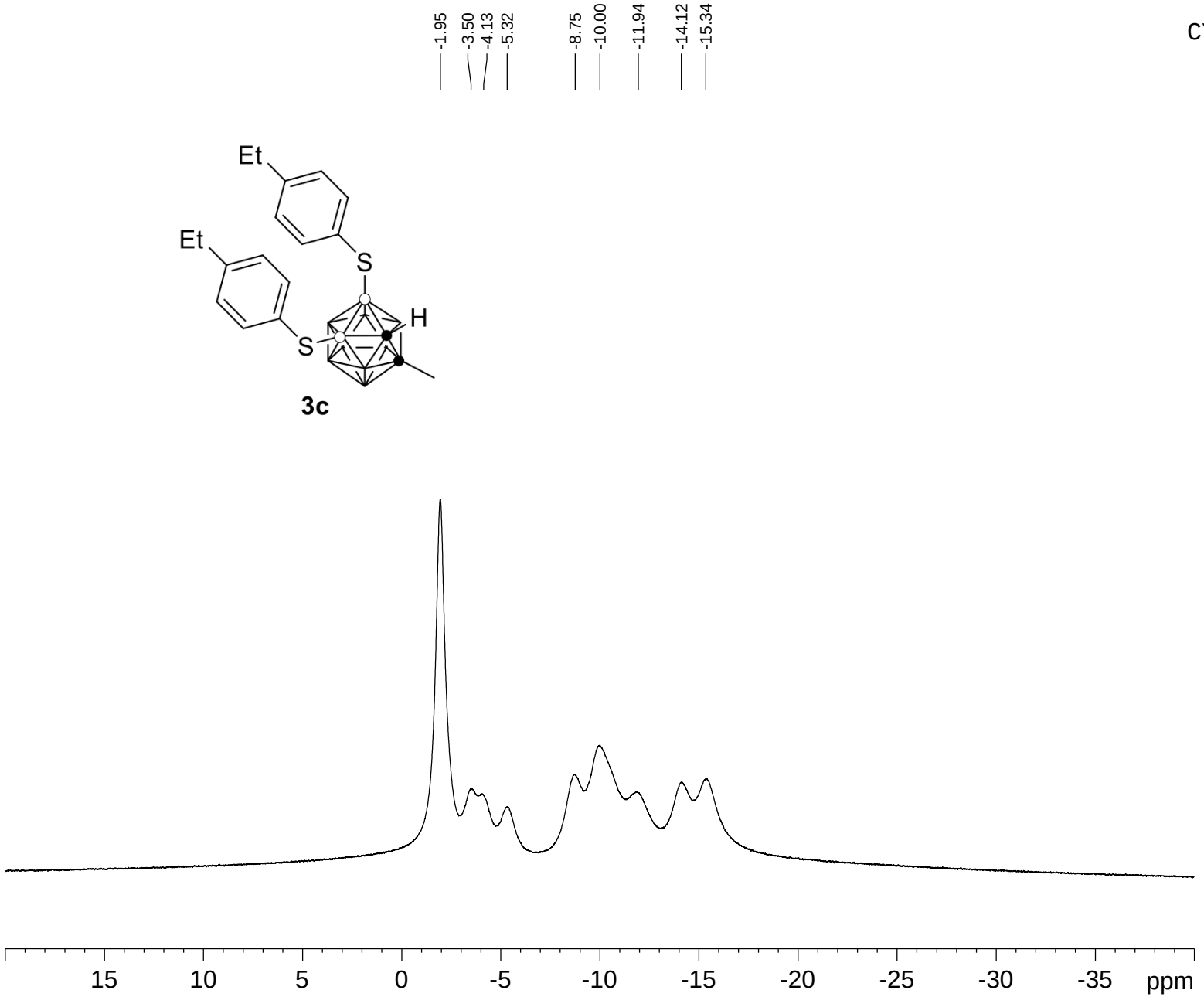



```
Current Data Parameters
NAME      CY-C-B-70P-4-Et
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180507
Time              19.09 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  240
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7577739 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```



CY-B-B-70P-4-Et

```
Current Data Parameters
NAME      CY-B-B-70P-4-Et
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180507
Time                16.38 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     60
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    362
DW                 20.800 usec
DE                  6.50 usec
TE                 294.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1          55.09999847 W
SFO2          400.2316009 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          13.56000042 W
PLW12          0.27428001 W

F2 - Processing parameters
SI                  32768
SF            128.4097418 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



CY-B-B-70P-4-Et-(C)

```
Current Data Parameters
NAME      CY-B-B-70P-4-Et-(C)
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180507
Time                  16.43 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT               CDCl3
NS                        76
DS                         2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                       287
DW                  20.800 usec
DE                   6.50 usec
TE                   294.7 K
D1              2.00000000 sec
TD0                        1
SFO1           128.4096890 MHz
NUC1                    11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                     32768
SF             128.4097430 MHz
WDW                       EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

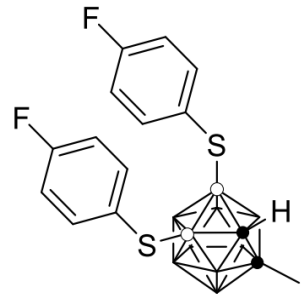
CY-H-B-50p-4-F

7.551 7.544 7.538 7.530 7.522 7.514 7.508 7.501 7.259 7.042 7.035 7.029 7.013 6.996 6.991 6.983

3.808

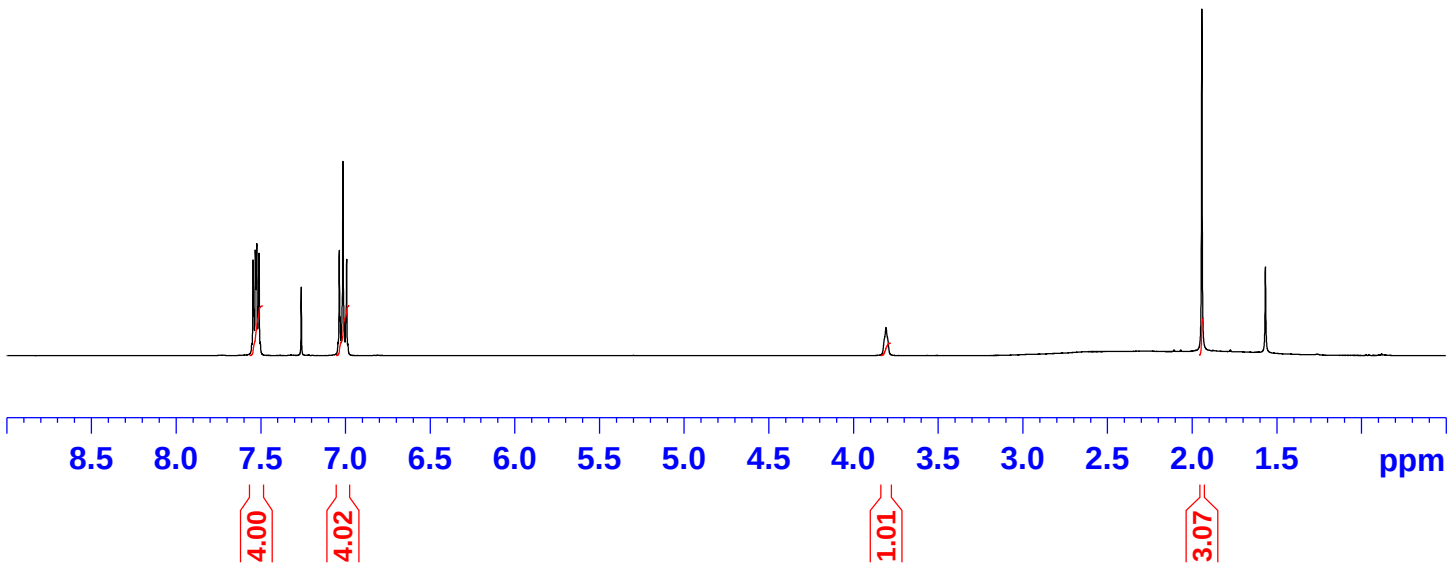
1.942

1.567

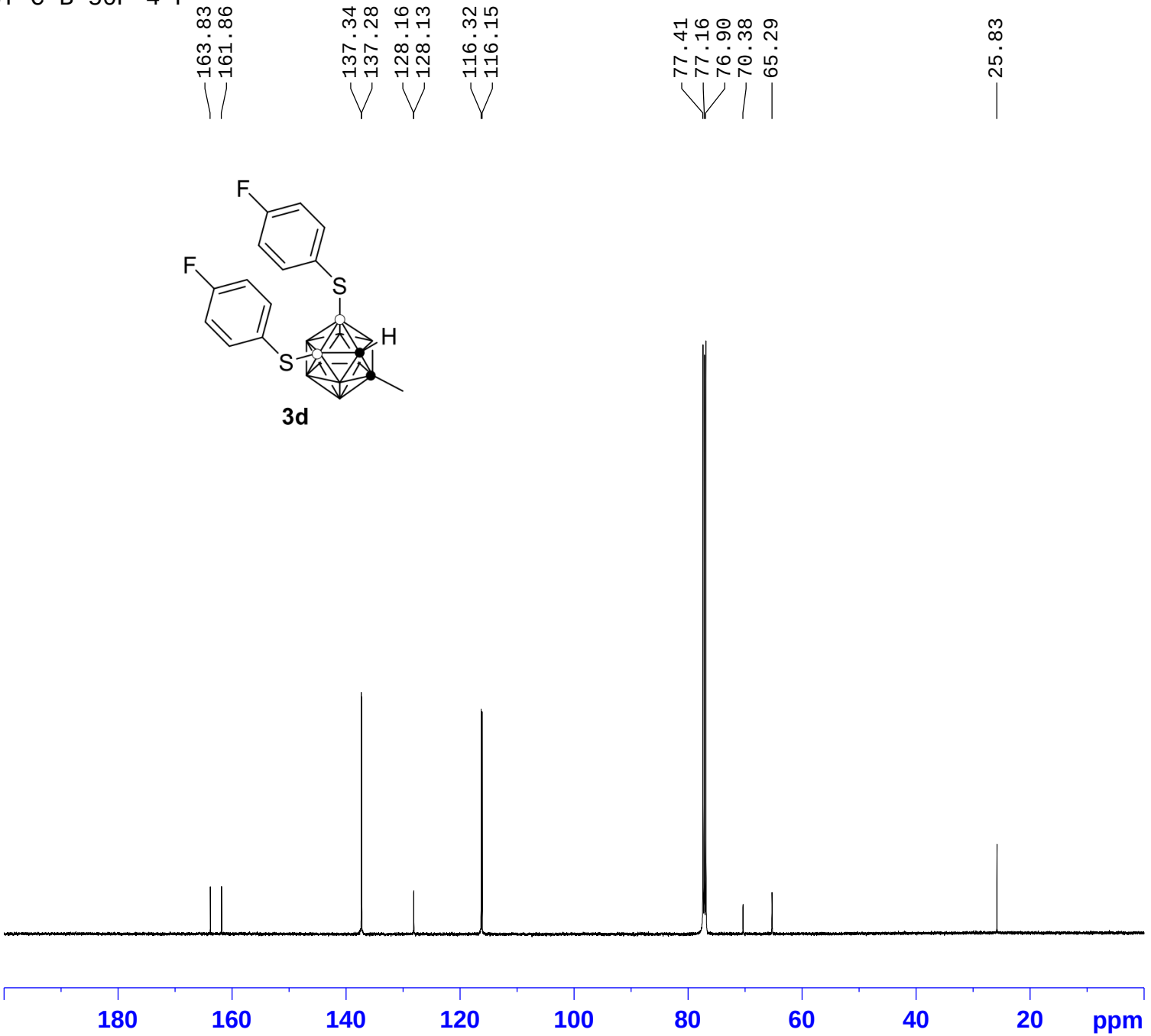


3d

```
Current Data Parameters
NAME      CY-H-B-50p-4-F
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180322
Time              14.35 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    11
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                   203
DW                62.400 usec
DE                 6.50 usec
TE                295.9 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1           8.31000042 W

F2 - Processing parameters
SI                 65536
SF           400.1300102 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

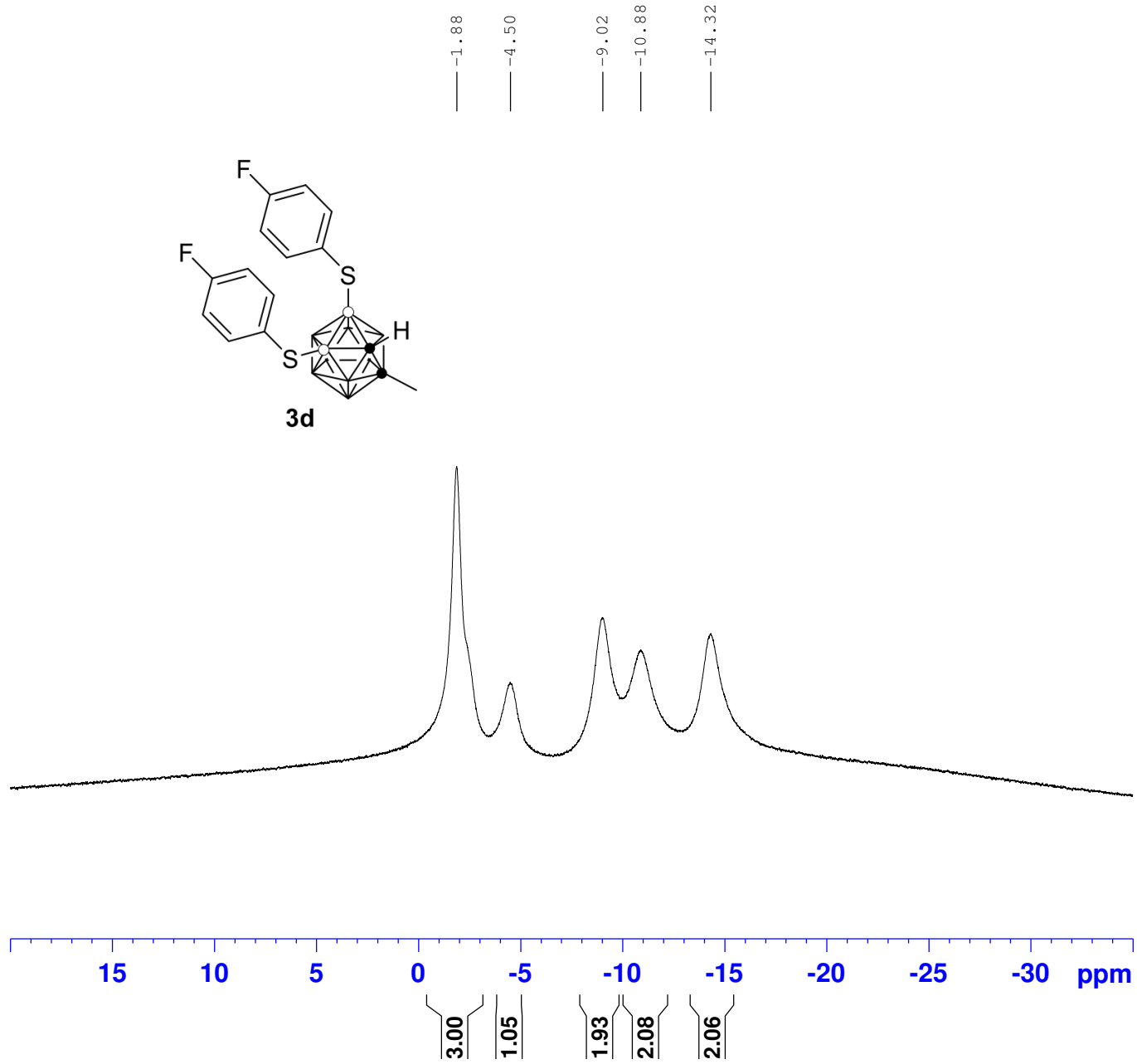


CY-C-B-50P-4-F



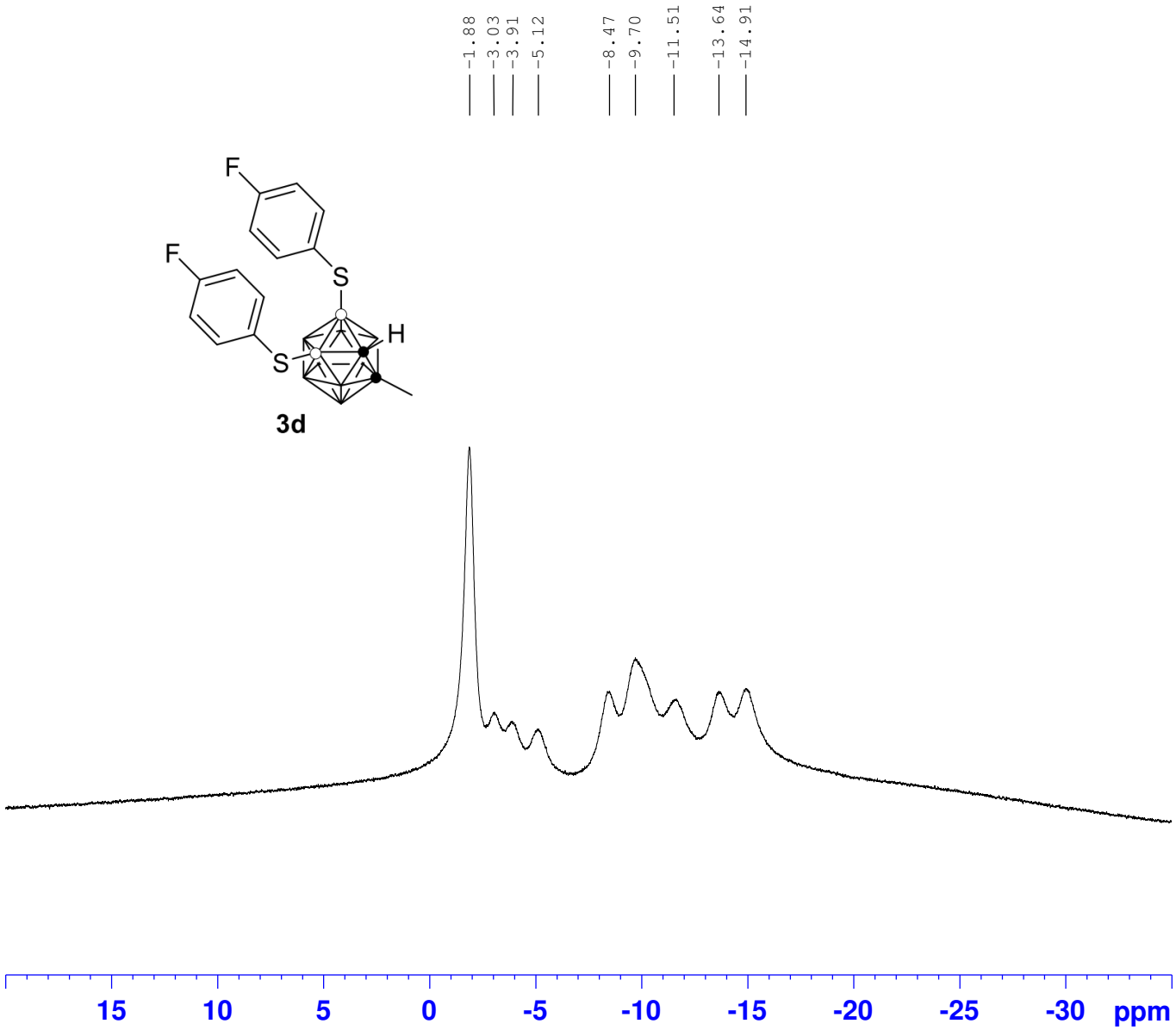

```
Current Data Parameters
NAME      CY-C-B-50P-4-F
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180322
Time              19.04 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  500
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

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

CY-B-B-50P-4-F




```
Current Data Parameters
NAME      CY-B-B-50P-4-F
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20190620
Time              11.05 h
INSTRUM            spect
PROBHD   Z820201_0170 (
PULPROG            zgig
TD                65536
SOLVENT           CDCl3
NS                  106
DS                    4
SWH           25510.203 Hz
FIDRES         0.778510 Hz
AQ             1.2845056 sec
RG                  181
DW                19.600 usec
DE                 6.50 usec
TE                296.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        128.3776050 MHz
NUC1                11B
P1                28.50 usec
PLW1        14.79100037 W
SFO2        400.1324710 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.17000008 W
PLW12        0.07408100 W

F2 - Processing parameters
SI                32768
SF          128.3776052 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

CY-B-B-50P-4-F-(C)

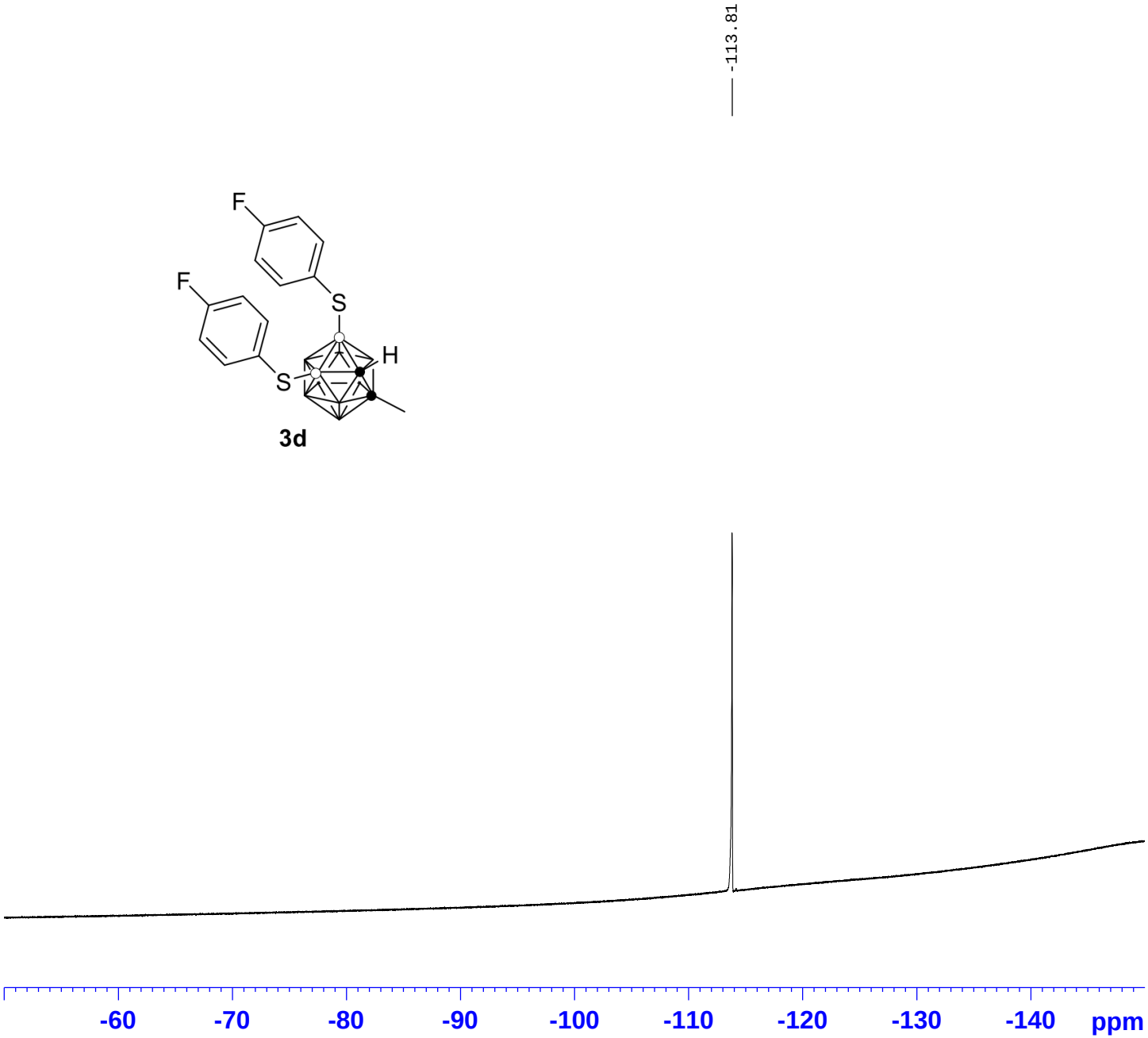


Current Data Parameters
NAME CY-B-B-50P-4-F-(C)
EXPNO 1
PROCNO 1

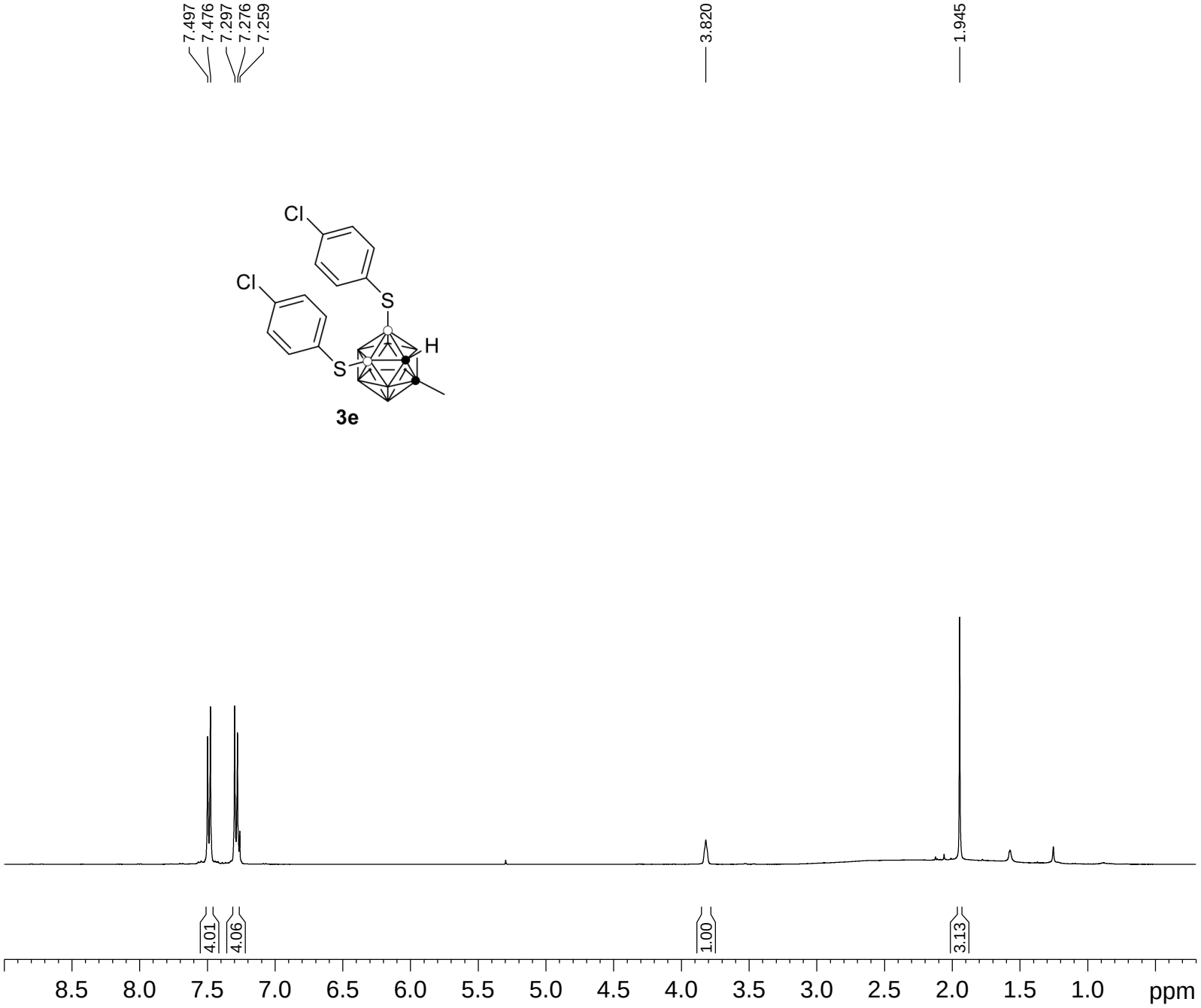
F2 - Acquisition Parameters
Date_ 20190620
Time 11.10 h
INSTRUM spect
PROBHD Z820201_0170 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 25510.203 Hz
FIDRES 0.778510 Hz
AQ 1.2845056 sec
RG 203
DW 19.600 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1
SFO1 128.3776050 MHz
NUC1 11B
P1 28.50 usec
PLW1 14.79100037 W

F2 - Processing parameters
SI 32768
SF 128.3776052 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3d




```
Current Data Parameters
NAME      CY-F-B-50P-4-F
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190620
Time              11.17 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG            zgflqn
TD                 131072
SOLVENT              None
NS                     16
DS                      4
SWH           113636.367 Hz
FIDRES          1.733953 Hz
AQ             0.5767168 sec
RG                  7.38
DW                 4.400 usec
DE                 18.00 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         470.5453180 MHz
NUC1                 19F
P1                 15.00 usec
PLW1         15.23299980 W

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

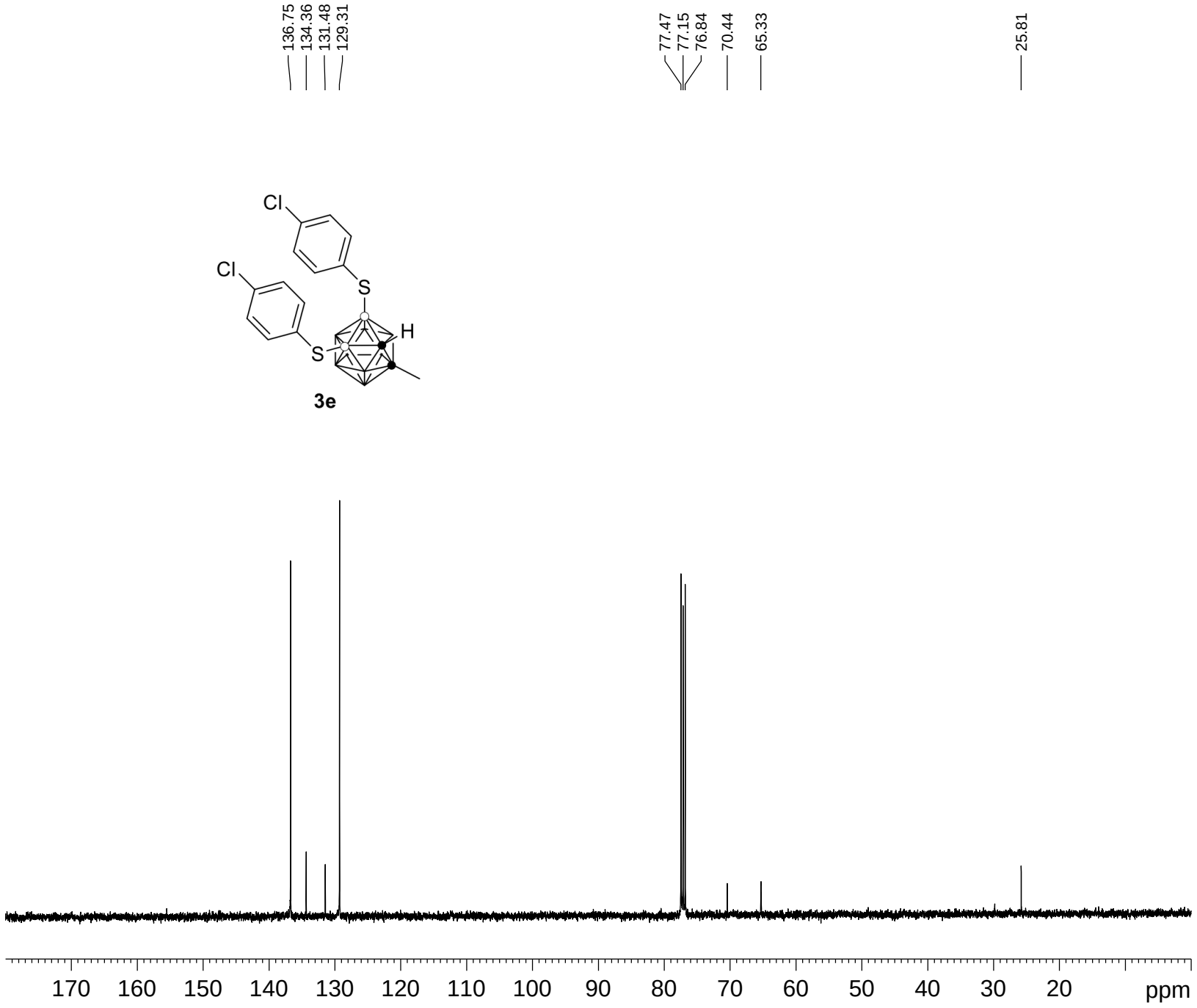


CY-H-B-18p-4-Cl

Current Data Parameters
NAME CY-H-B-18p-4-Cl
EXPNO 1
PROCNO 1

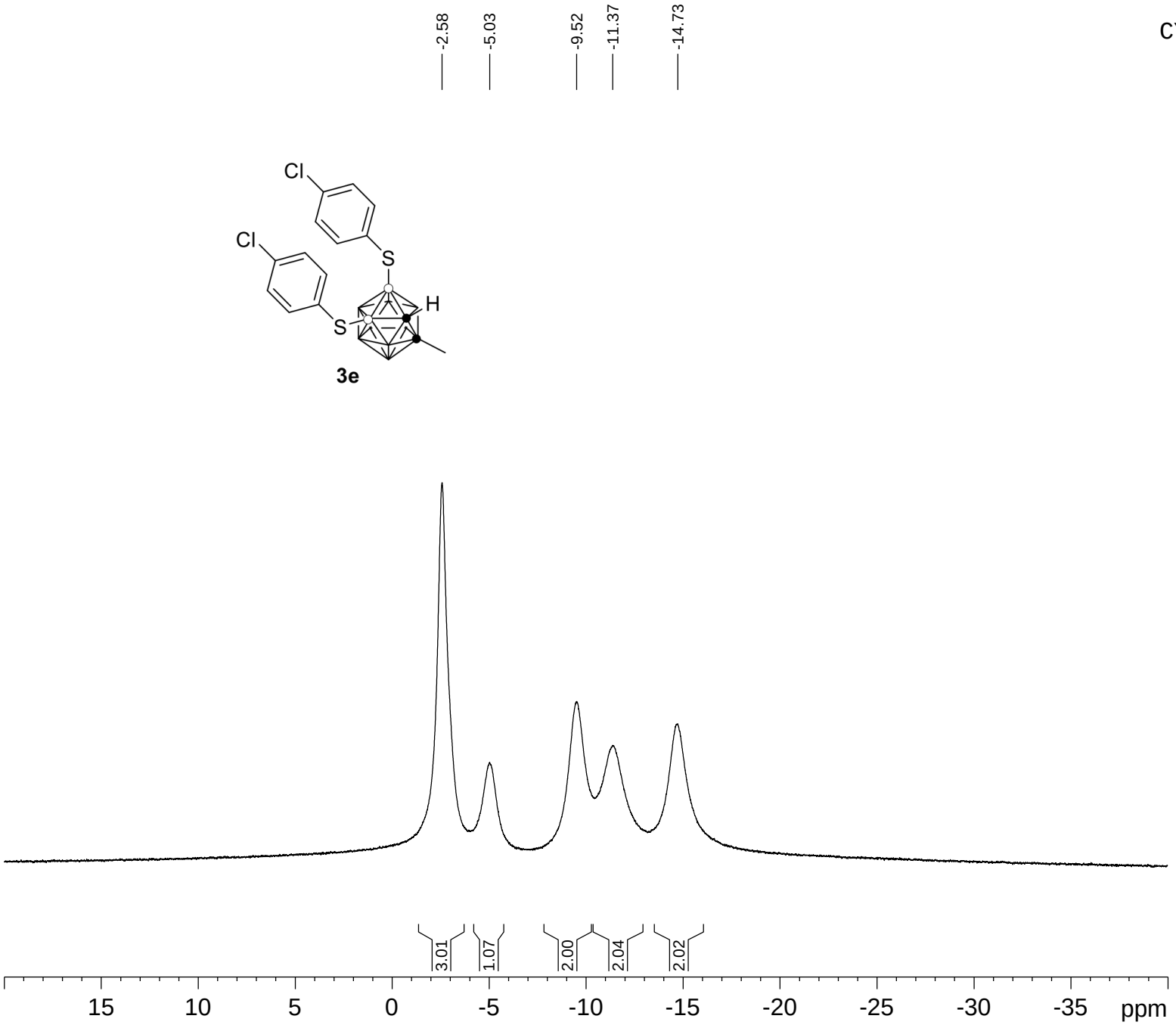
F2 - Acquisition Parameters
Date_ 20180119
Time 13.19 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



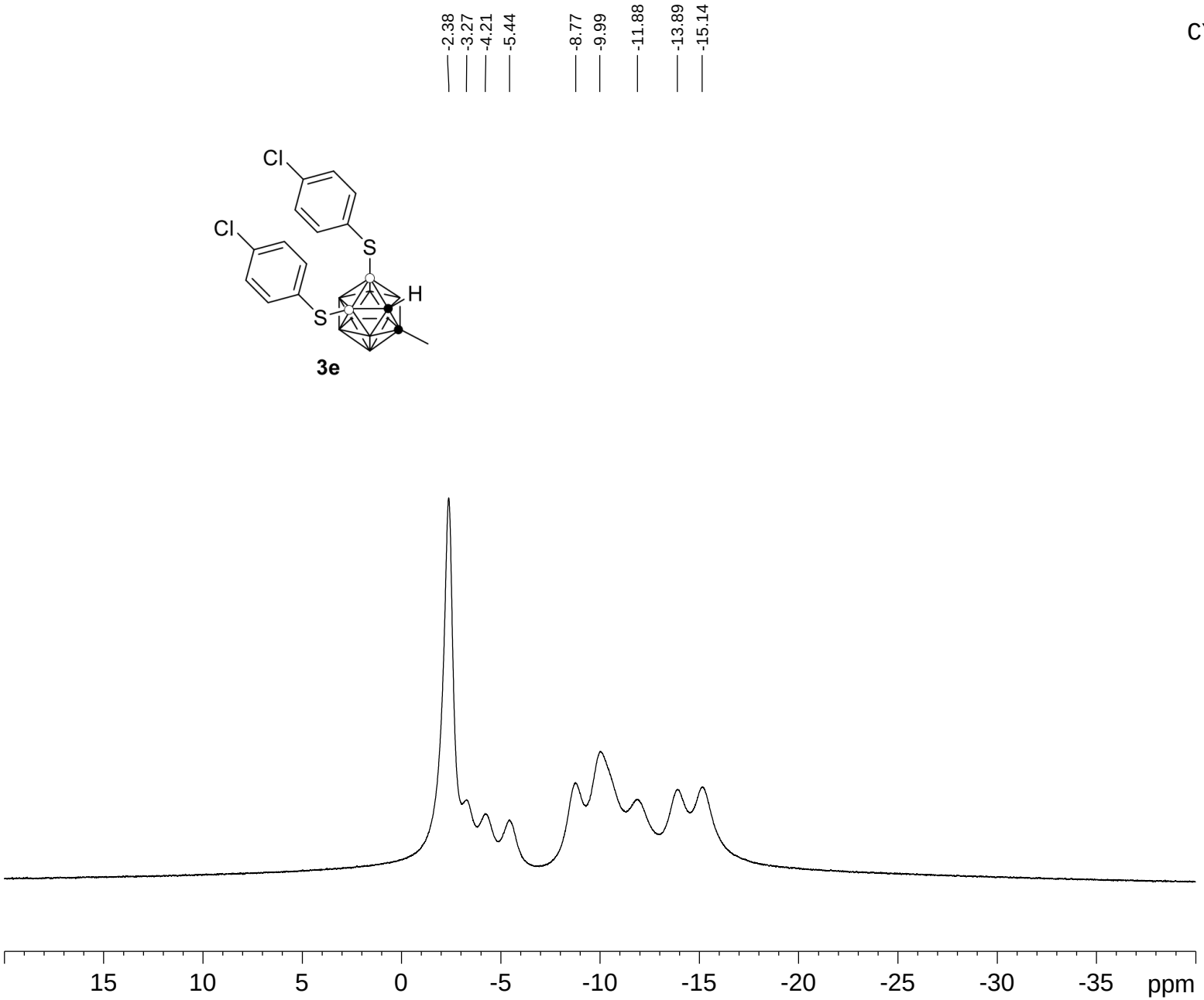
CY-C-B-18p-4-Cl

```
Current Data Parameters
NAME      CY-C-B-18p-4-Cl
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180119
Time               13.28 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   160
DS                     4
SWH            40760.871 Hz
FIDRES          0.621962 Hz
AQ              0.8039083 sec
RG                   203
DW                12.267 usec
DE                 6.50 usec
TE                 295.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         100.6479773 MHz
NUC1                13C
P1                 9.50 usec
PLW1         55.34000015 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                 32768
SF           100.6379028 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



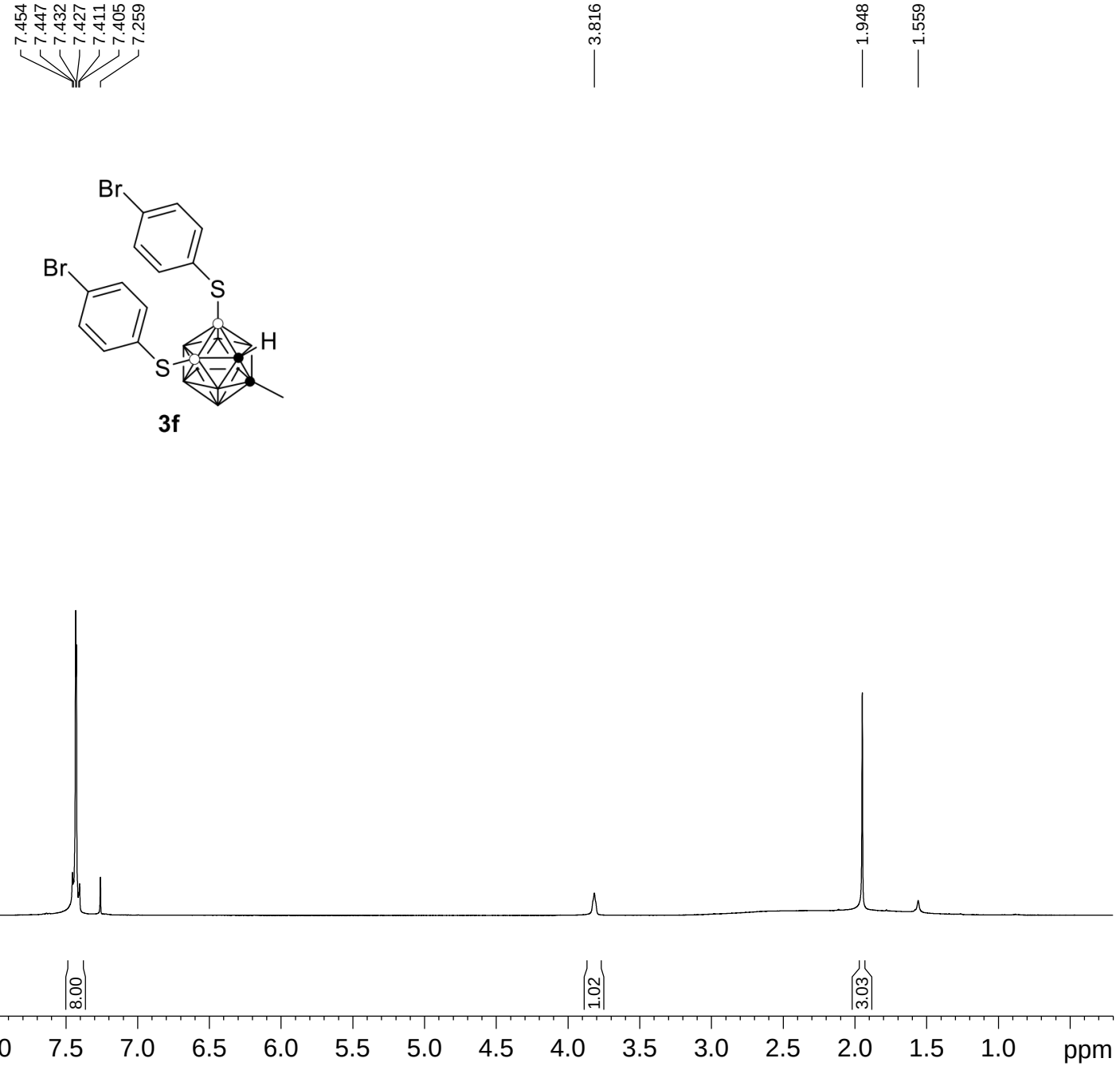
CY-B-B-18p-4-Cl

```
Current Data Parameters
NAME      CY-B-B-18p-4-Cl
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180119
Time                13.38 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     18
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    362
DW                 20.800 usec
DE                  6.50 usec
TE                 295.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                11B
P1                  7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                  32768
SF           128.4097615 MHz
WDW                 EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



CY-B-B-18p-4-Cl-(C)

```
Current Data Parameters
NAME      CY-B-B-18p-4-Cl-(C)
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20180119
Time                  13.41 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      44
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                     322
DW                  20.800 usec
DE                   6.50 usec
TE                  295.3 K
D1              2.00000000 sec
TD0                      1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                   32768
SF             128.4097430 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



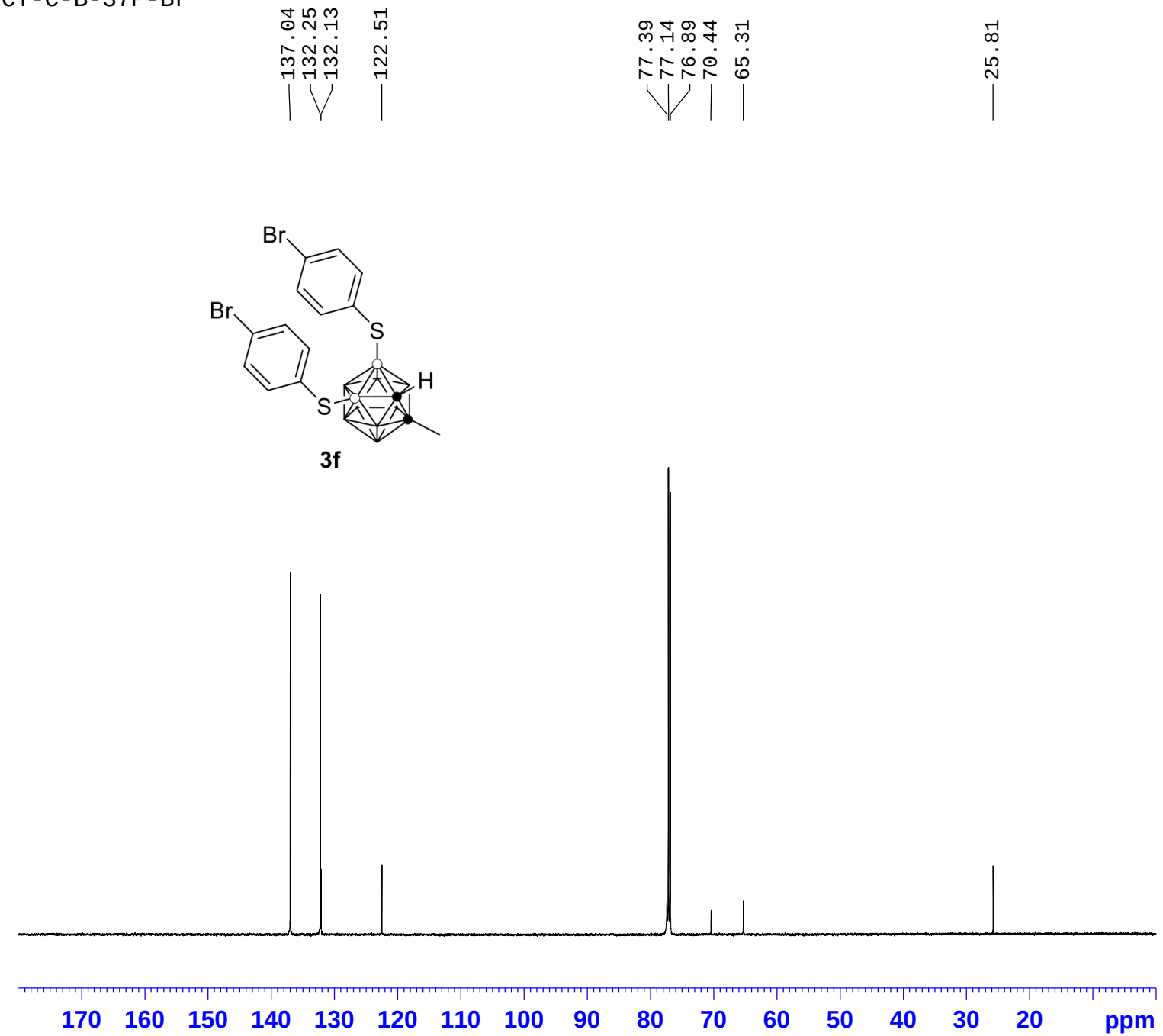
CY-H-B-37p-Br

Current Data Parameters
NAME CY-H-B-37p-Br
EXPNO 1
PROCNO 1

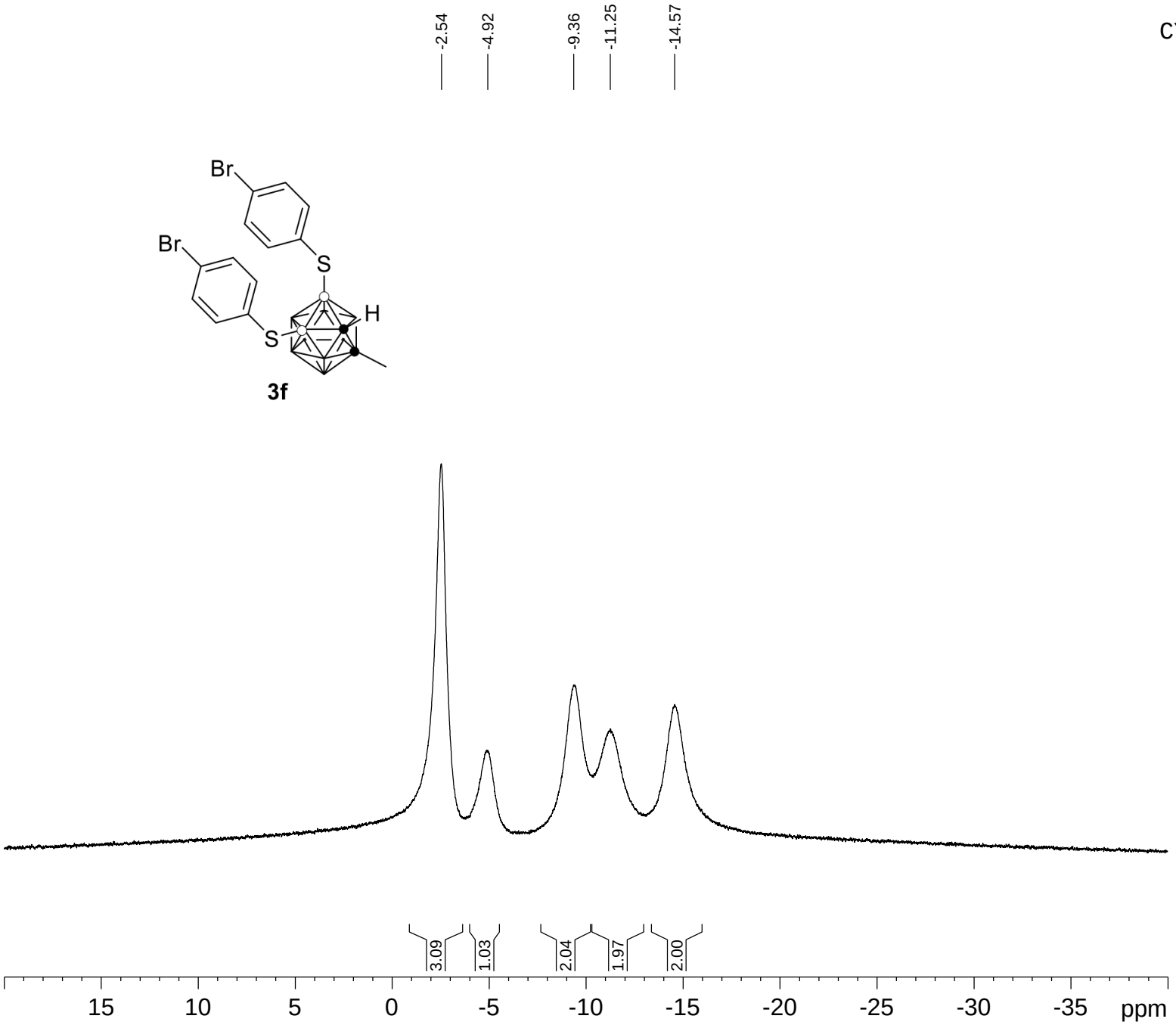
F2 - Acquisition Parameters
Date_ 20180308
Time 19.30 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-37P-Br

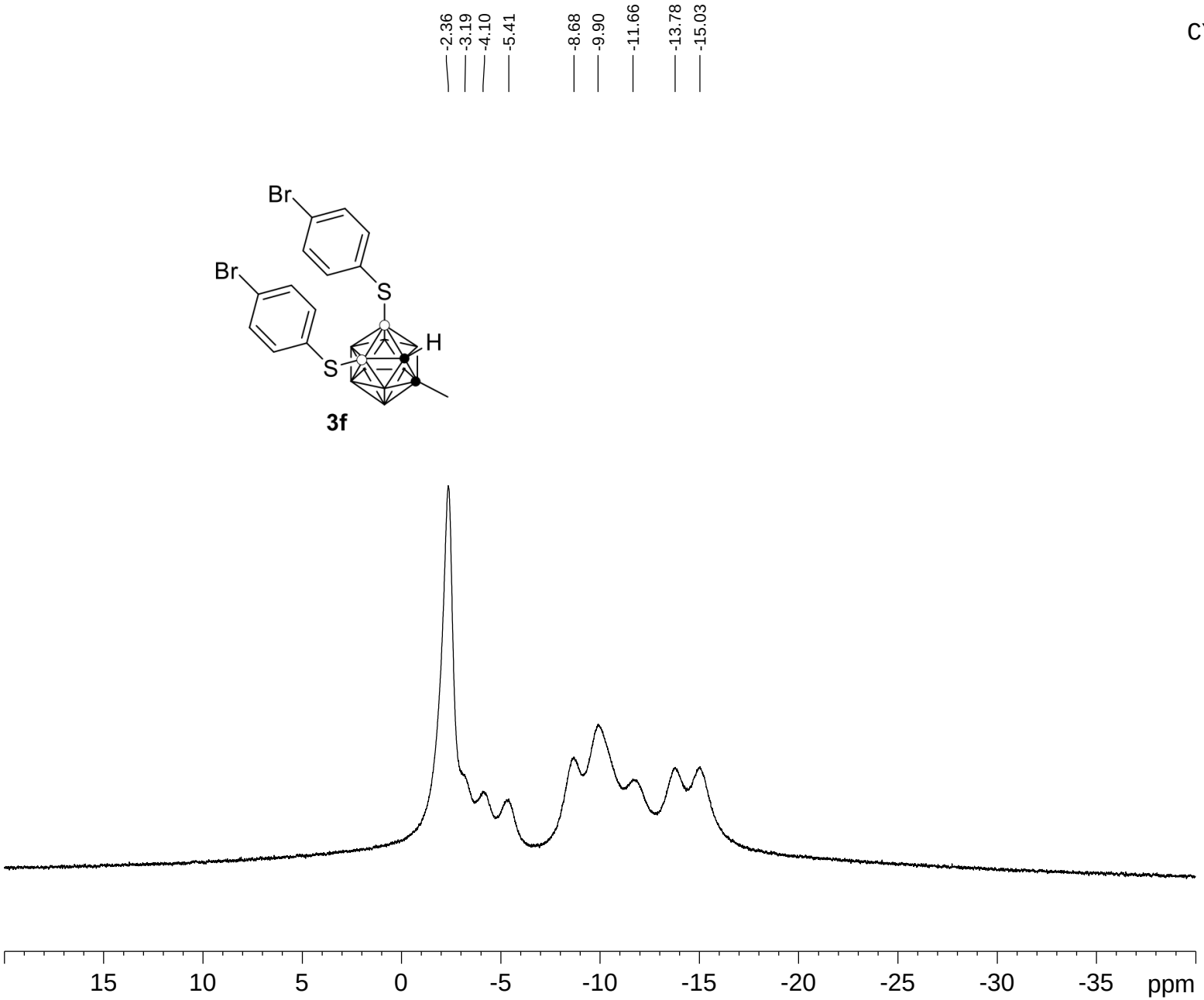



```
Current Data Parameters
NAME       CY-C-B-37P-Br
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180309
Time              19.05 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   360
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ              1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P1                10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

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



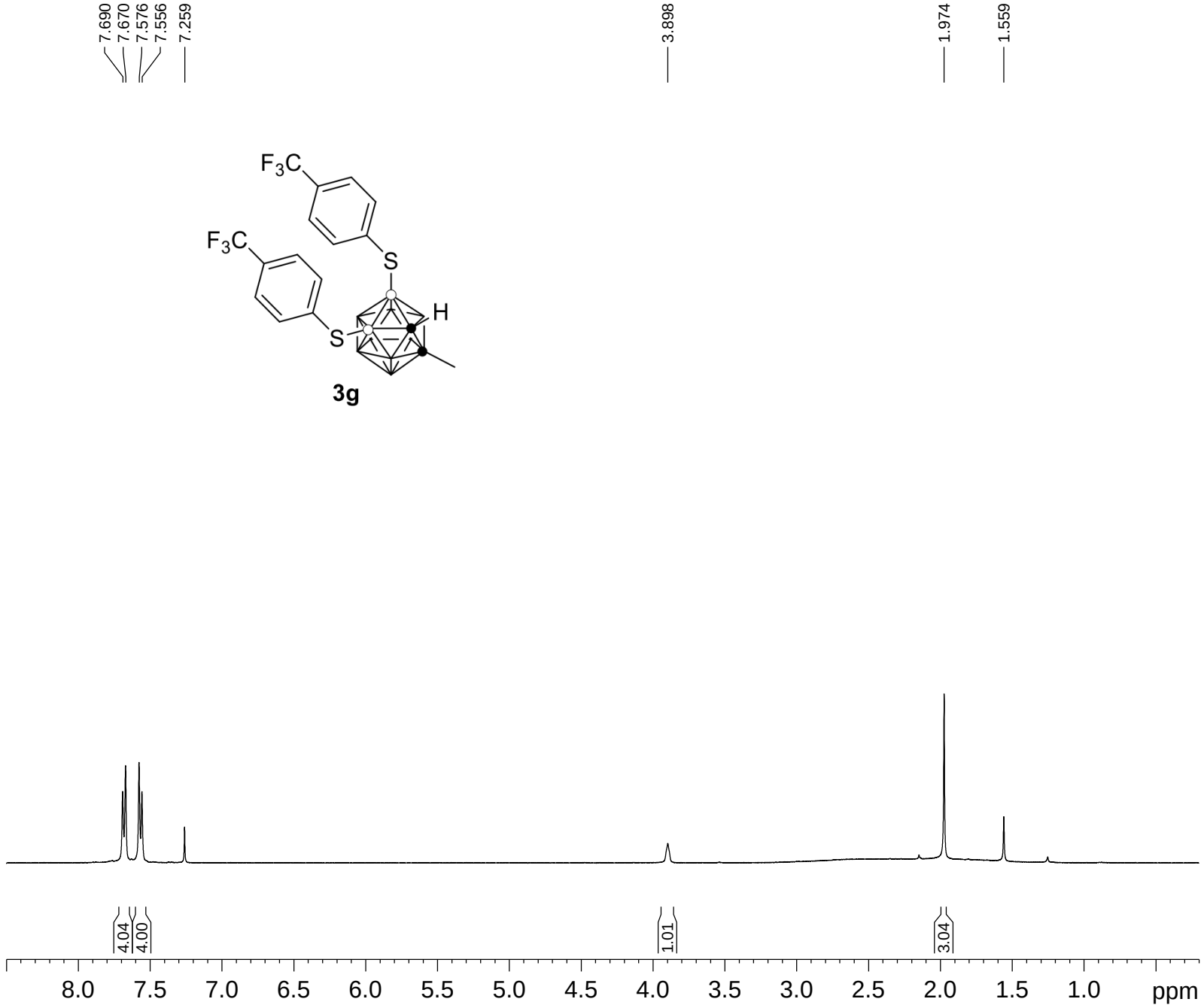
CY-B-B-37p-Br

```
Current Data Parameters
NAME       CY-B-B-37p-Br
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180308
Time               19.41 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    18
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   406
DW                20.800 usec
DE                 6.50 usec
TE                295.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

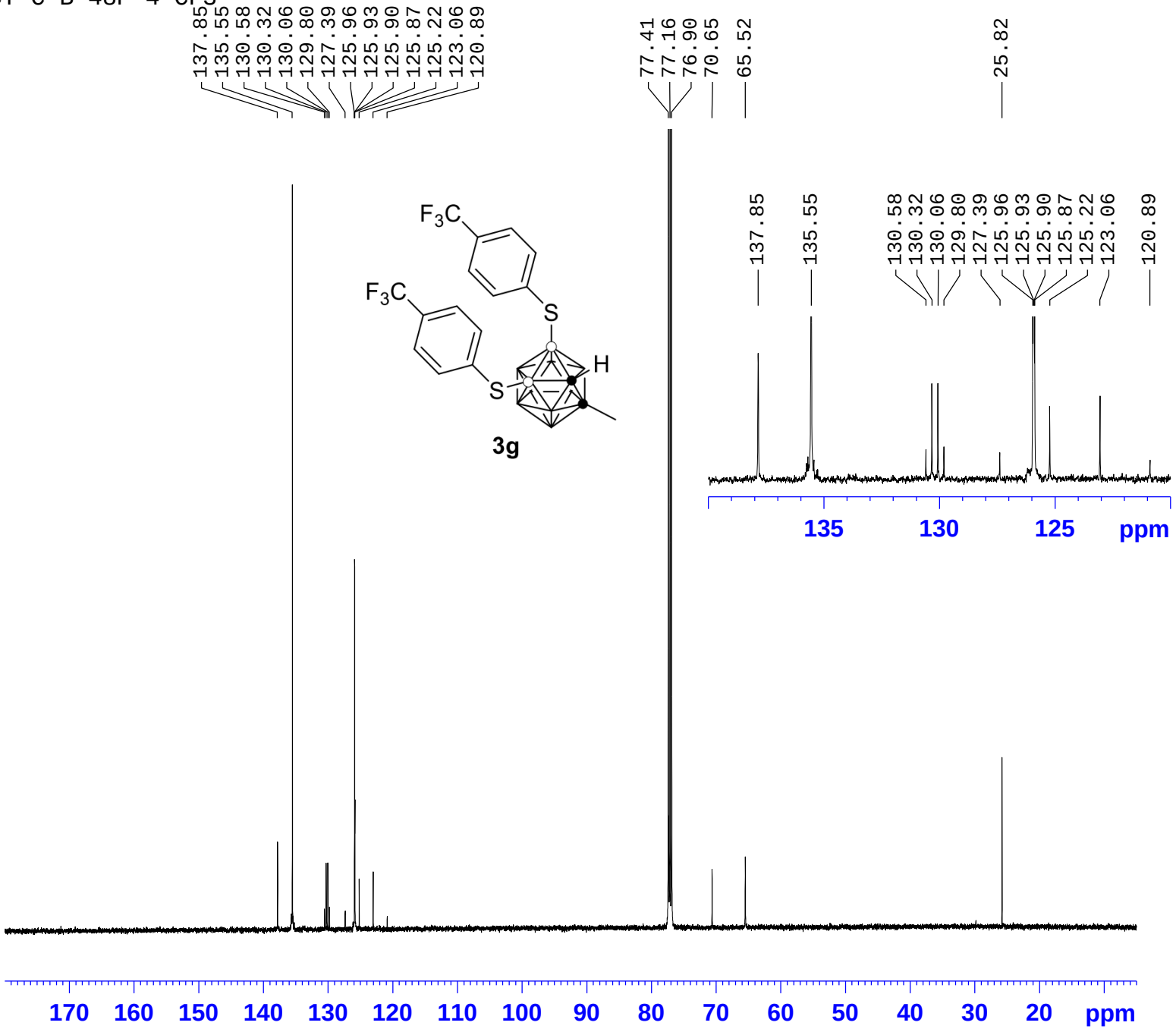


CY-B-B-37p-Br-(C)

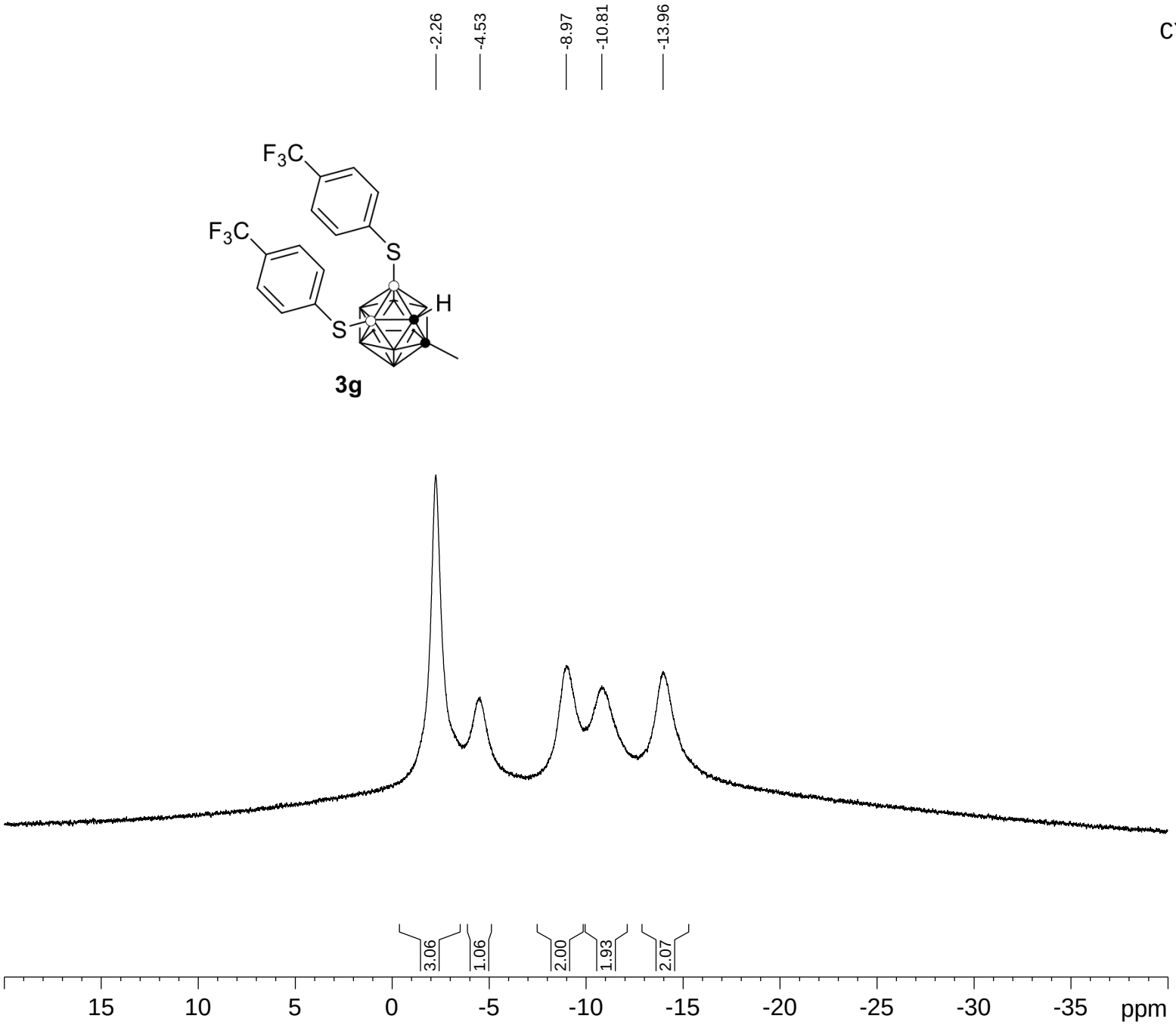
```
Current Data Parameters
NAME      CY-B-B-37p-Br-(C)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180308
Time                19.43 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      22
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     406
DW                  20.800 usec
DE                   6.50 usec
TE                  295.1 K
D1             2.00000000 sec
TD0                      1
SFO1          128.4096890 MHz
NUC1                  11B
P1                   7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                   32768
SF            128.4097430 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```


7.690
7.670
7.576
7.556
7.259
3.898
1.974
1.559
CY-H-B-48p-4-CF3
F3C
F3C
S
S
H
3g
Current Data Parameters
NAME CY-H-B-48p-4-CF3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180409
Time 14.58 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 1
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
4.04
4.00
1.01
3.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

CY-C-B-48P-4-CF3

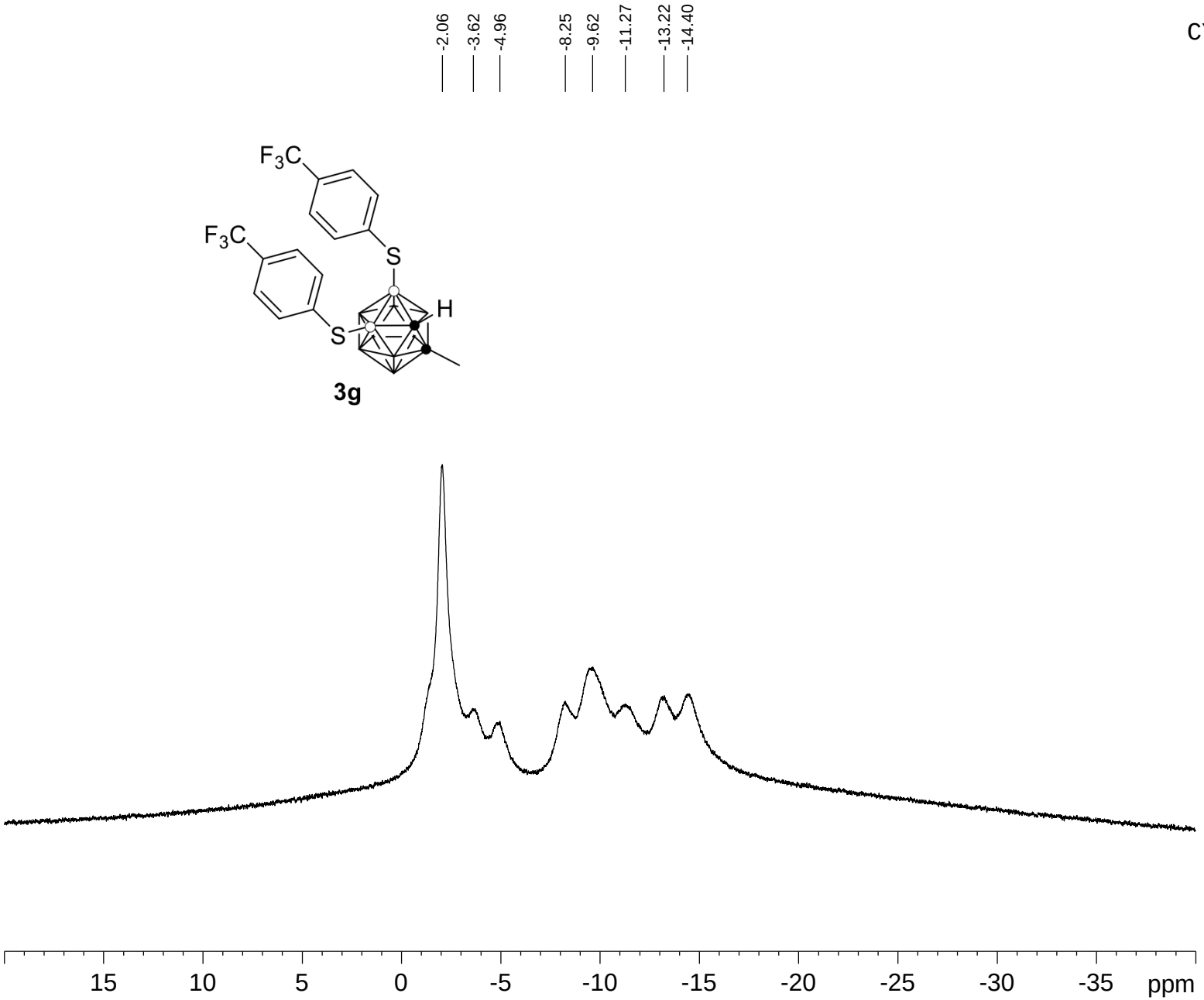



```
Current Data Parameters
NAME      CY-C-B-48P-4-CF3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180409
Time              19.21 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  600
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7577722 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



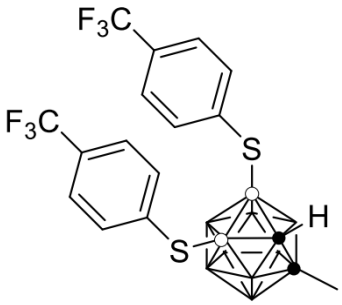
CY-B-B-48p-4-CF3

```
Current Data Parameters
NAME      CY-B-B-48p-4-CF3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180406
Time                 20.31 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT              C6D6
NS                     64
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                    406
DW                 20.800 usec
DE                  6.50 usec
TE                 297.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1          55.09999847 W
SFO2          400.2316009 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          13.56000042 W
PLW12          0.27428001 W

F2 - Processing parameters
SI                   32768
SF            128.4097615 MHz
WDW                  EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



CY-B-B-48p-CF3-(C)

```
Current Data Parameters
NAME      CY-B-B-48p-CF3-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180406
Time                  20.37 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                  zg
TD                    65536
SOLVENT                C6D6
NS                       83
DS                        2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                      406
DW                   20.800 usec
DE                    6.50 usec
TE                   297.8 K
D1             2.00000000 sec
TD0                       1
SFO1           128.4096890 MHz
NUC1                   11B
P1                    7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                    32768
SF             128.4097430 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



3g

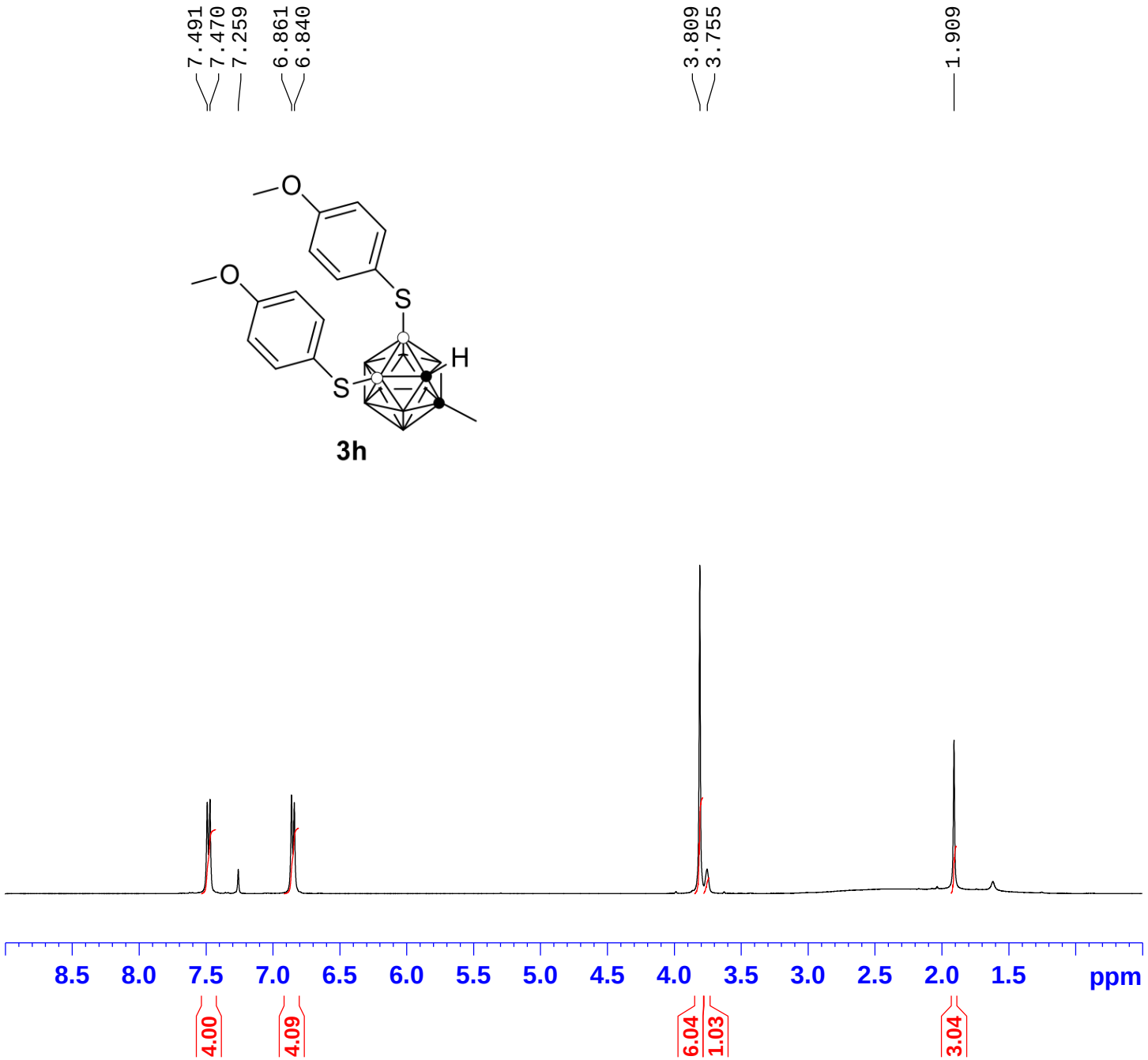
-62.73

CY-F-B-48P

```
Current Data Parameters
NAME          CY-F-B-48P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180413
Time              15.01 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     13
DS                      4
SWH            89285.711 Hz
FIDRES          0.681196 Hz
AQ             0.7340032 sec
RG                   645
DW                 5.600 usec
DE                 6.50 usec
TE                 295.1 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1
SFO1         376.5548010 MHz
NUC1                 19F
P1                14.70 usec
PLW1         18.36000061 W
SFO2         400.2316009 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                   65536
SF           376.5924602 MHz
WDW                     EM
SSB      0
LB                  0.30 Hz
GB       0
PC                  1.00
```

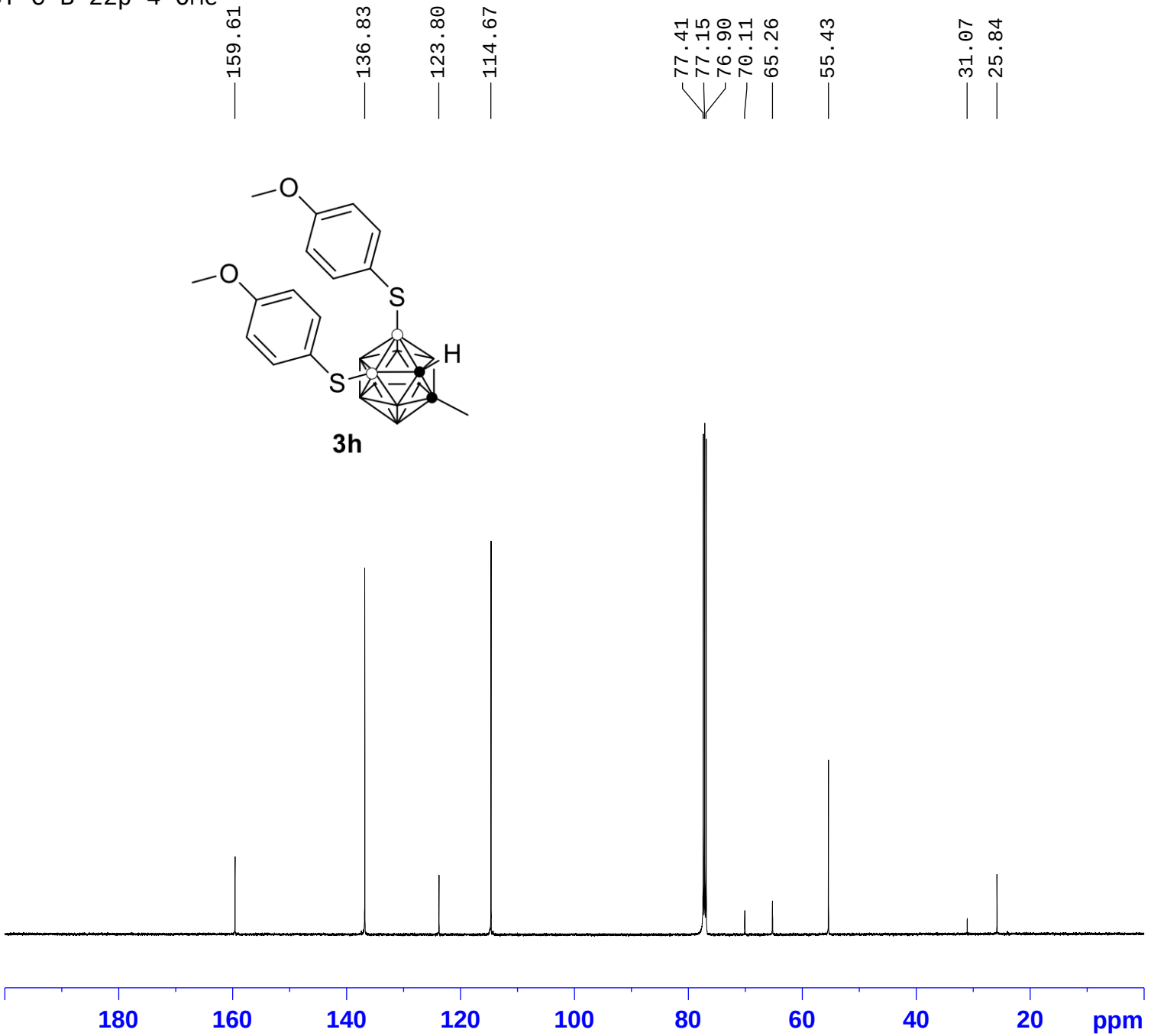
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 ppm

CY-H-B-22p-4-OMe-re

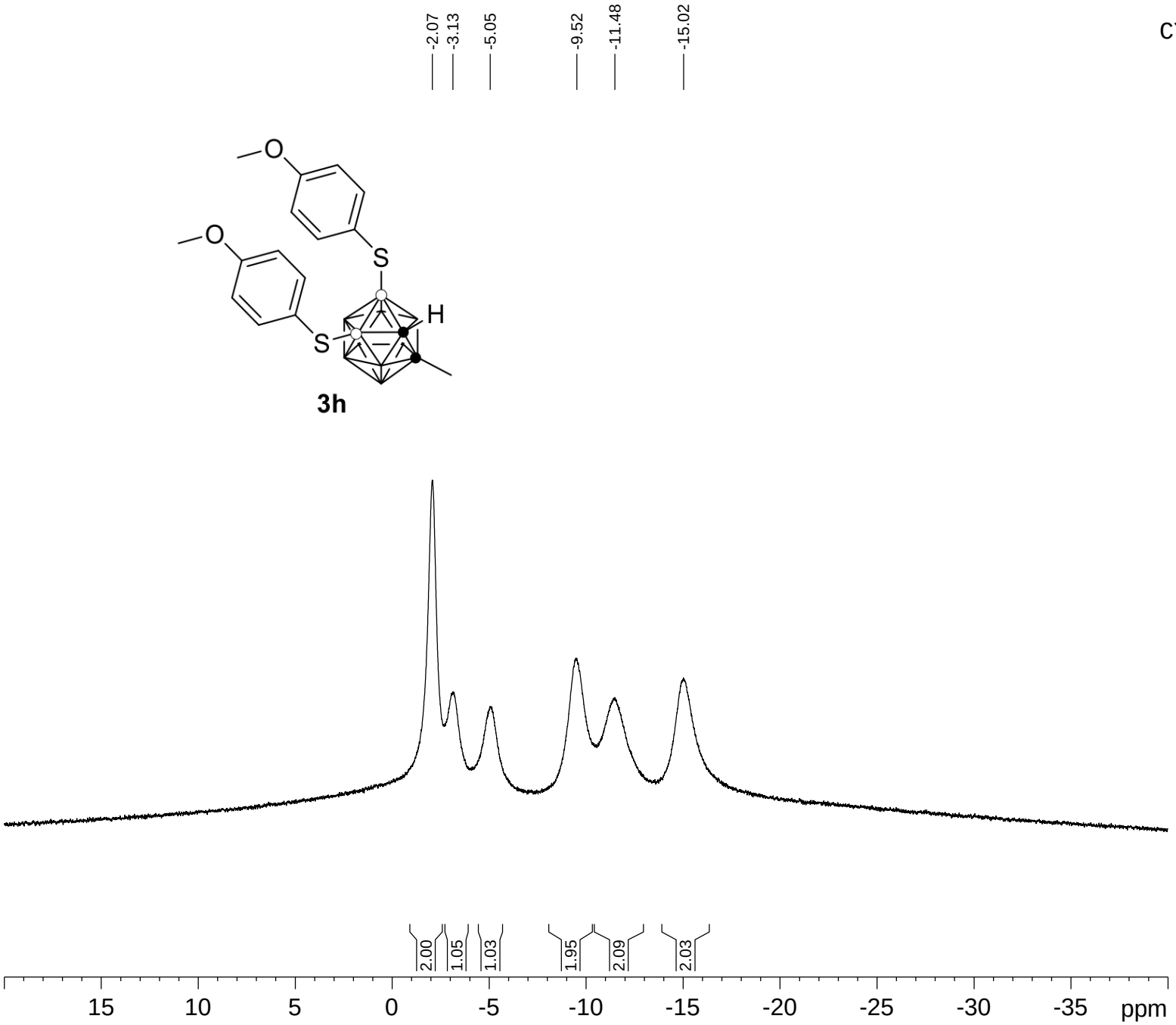



```
Current Data Parameters
NAME      CY-H-B-22p-4-OMe-re
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_            20180201
Time                20.58 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                    203
DW                 62.400 usec
DE                  6.50 usec
TE                 295.0 K
D1            1.00000000 sec
TD0                     1
SFO1         400.1324708 MHz
NUC1                   1H
P1                 15.00 usec
PLW1          8.31000042 W

F2 - Processing parameters
SI                  65536
SF           400.1300100 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

CY-C-B-22p-4-OMe

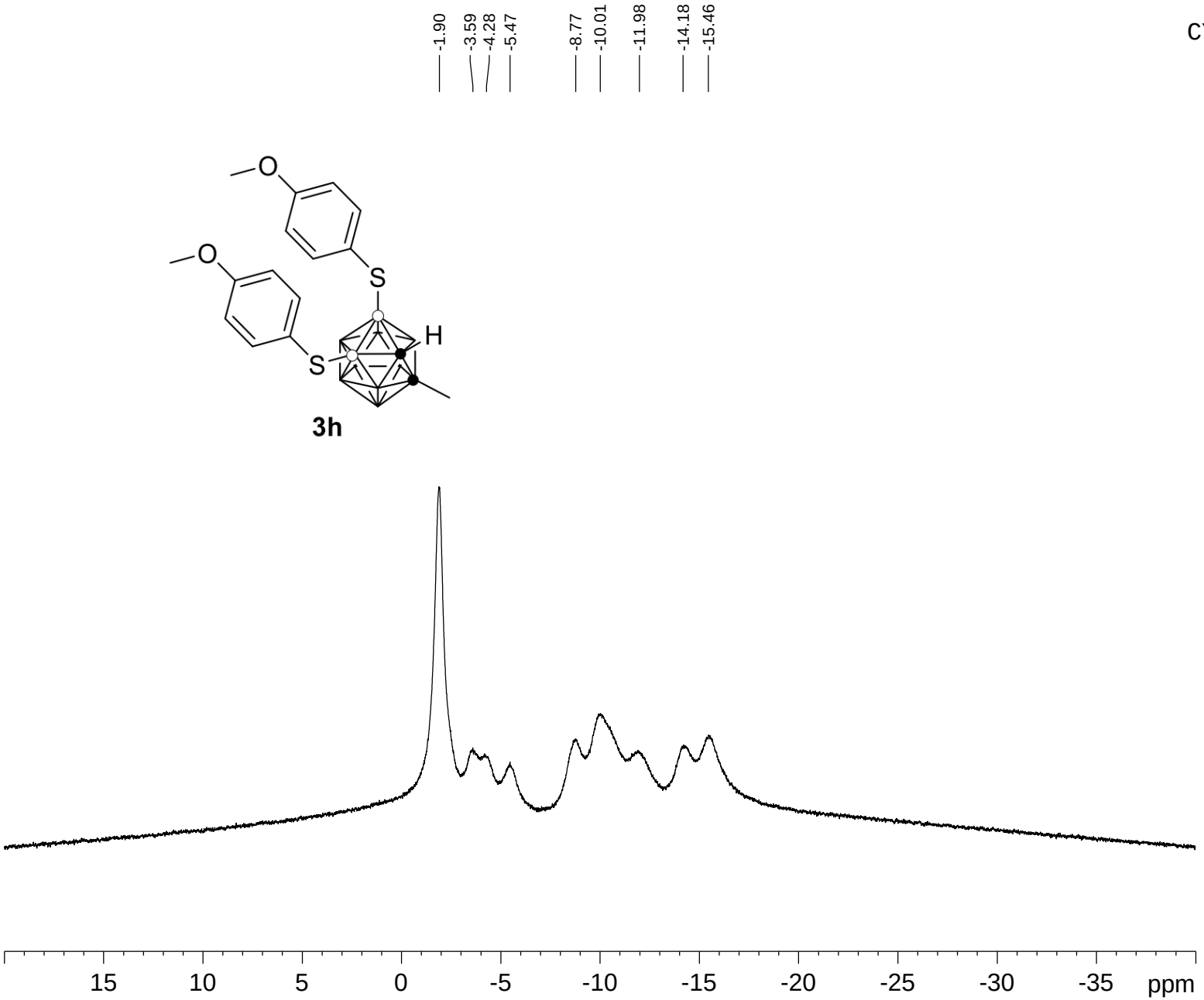



```
Current Data Parameters
NAME      CY-C-B-22p-4-OMe
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180202
Time               18.55 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   400
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P1                10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

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



CY-B-B-22p-4-OMe

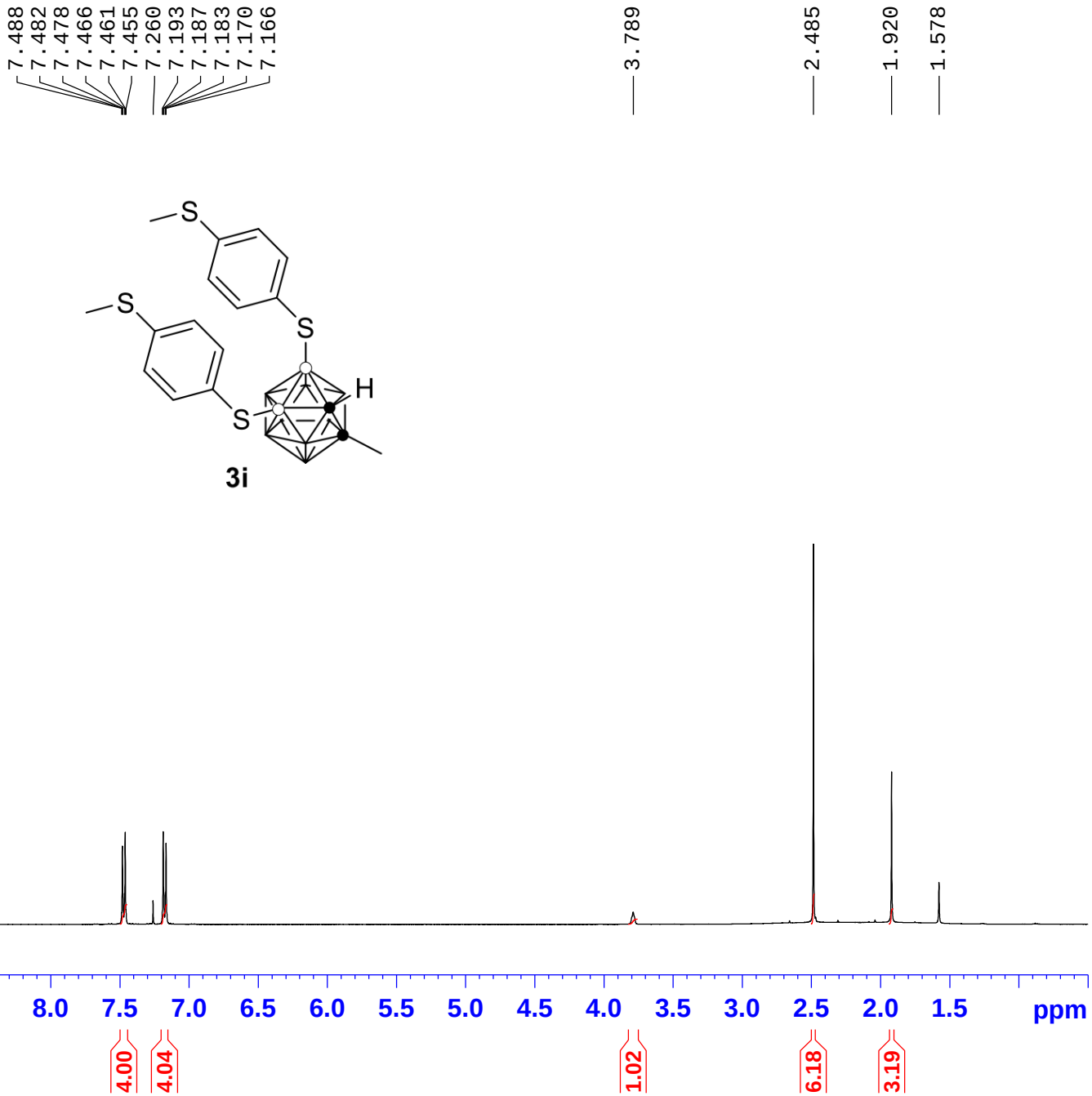
```
Current Data Parameters
NAME      CY-B-B-22p-4-OMe
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180129
Time                 21.56 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG               zgdc
TD                   65536
SOLVENT              CDCl3
NS                      51
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                     362
DW                  20.800 usec
DE                   6.50 usec
TE                  295.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1
SFO1           128.4096890 MHz
NUC1                  11B
P1                   7.50 usec
PLW1           55.09999847 W
SFO2           400.2316009 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           13.56000042 W
PLW12           0.27428001 W

F2 - Processing parameters
SI                   32768
SF             128.4097615 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



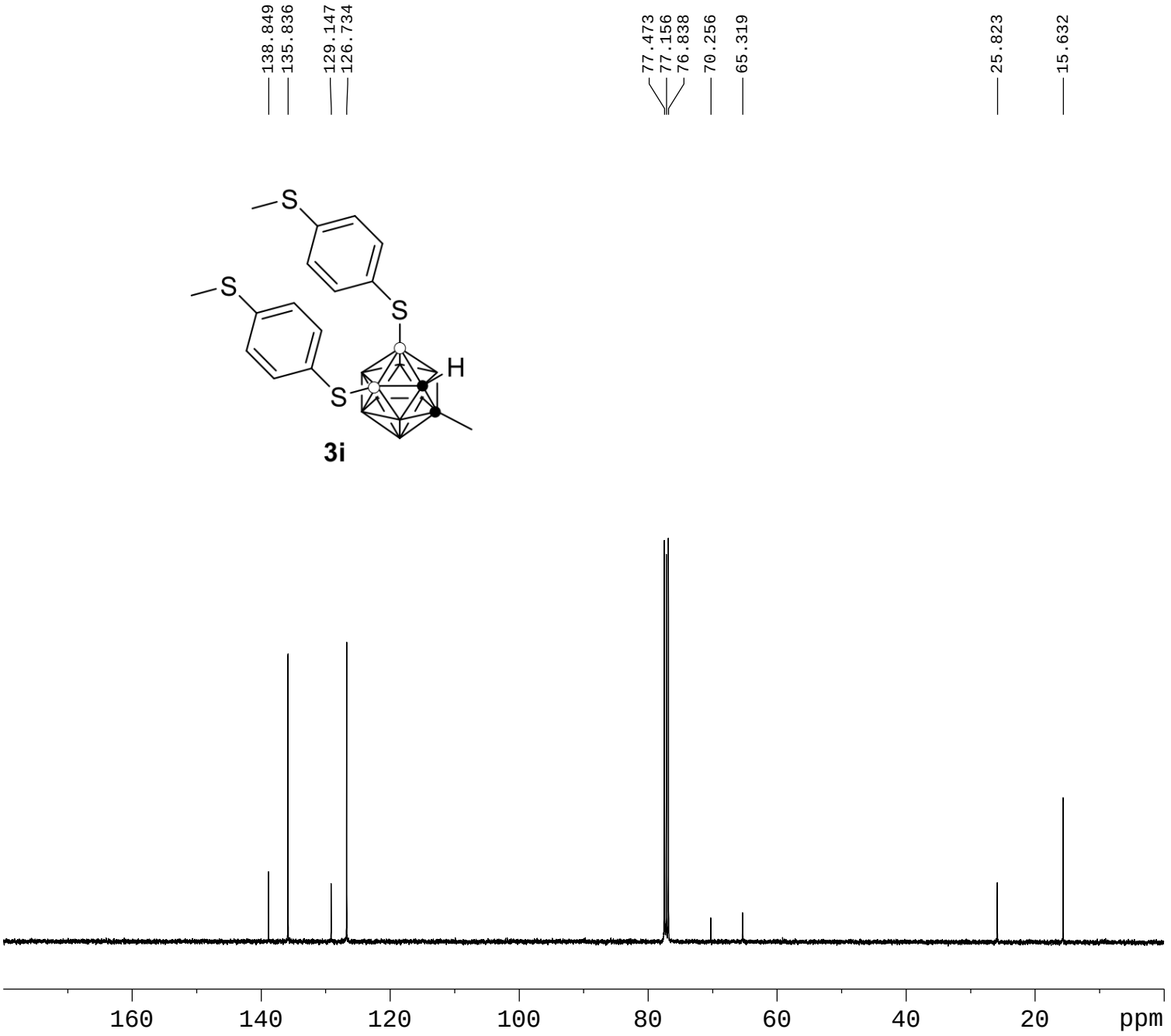
CY-B-B-22p-4-OMe-(C)

```
Current Data Parameters
NAME     CY-B-B-22p-4-OMe-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180129
Time              22.01 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                  65536
SOLVENT             CDCl3
NS                     48
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    406
DW                20.800 usec
DE                 6.50 usec
TE                 295.2 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

CY-H-B-54p-SMe



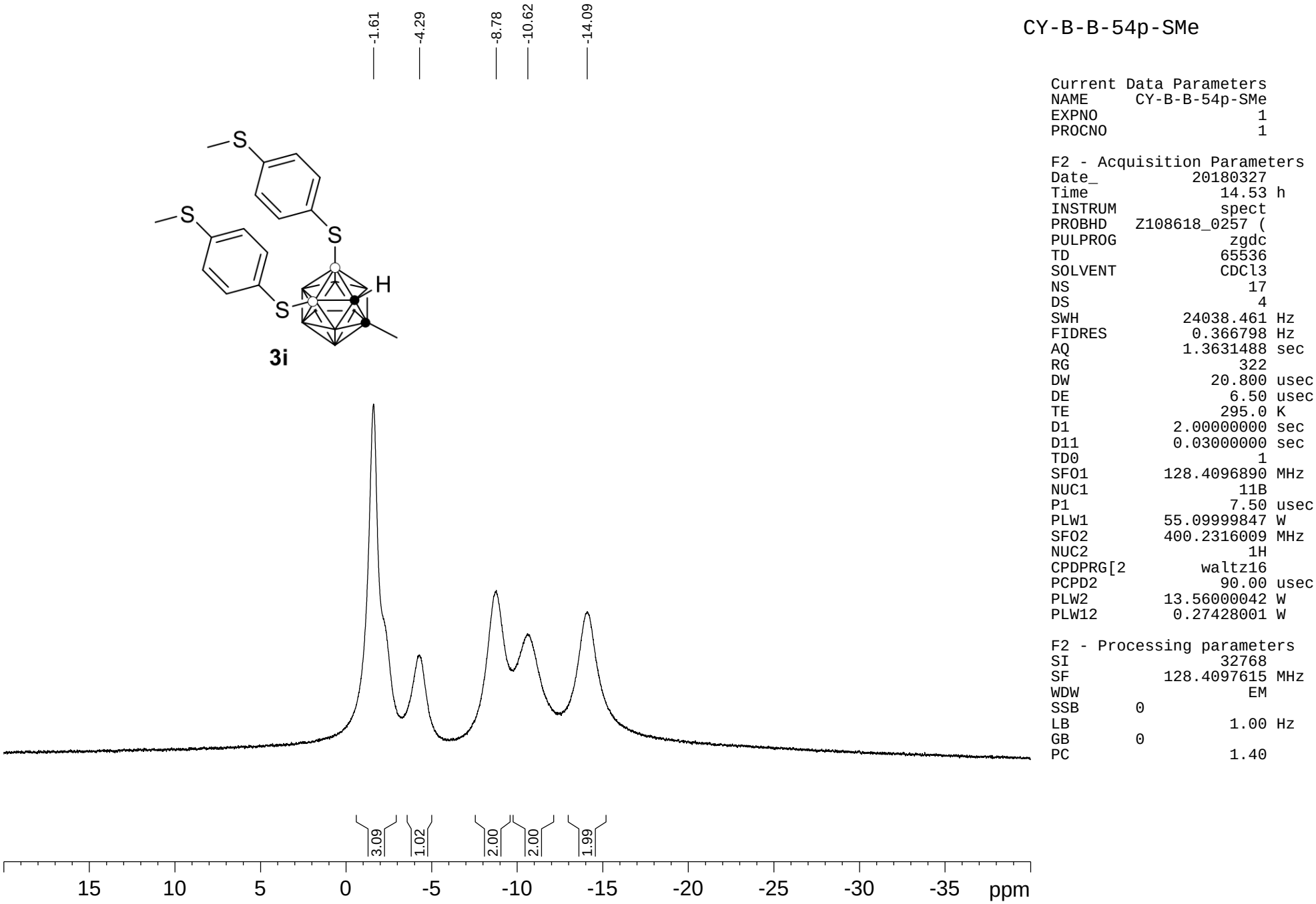

```
Current Data Parameters
NAME      CY-H-B-54p-SMe
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180327
Time               9.39 h
INSTRUM            spect
PROBHD   Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                   203
DW                62.400 usec
DE                 6.50 usec
TE                297.3 K
D1           1.00000000 sec
TD0                    1
SFO1        400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1         8.31000042 W

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



CY-C-B-54p-SMe

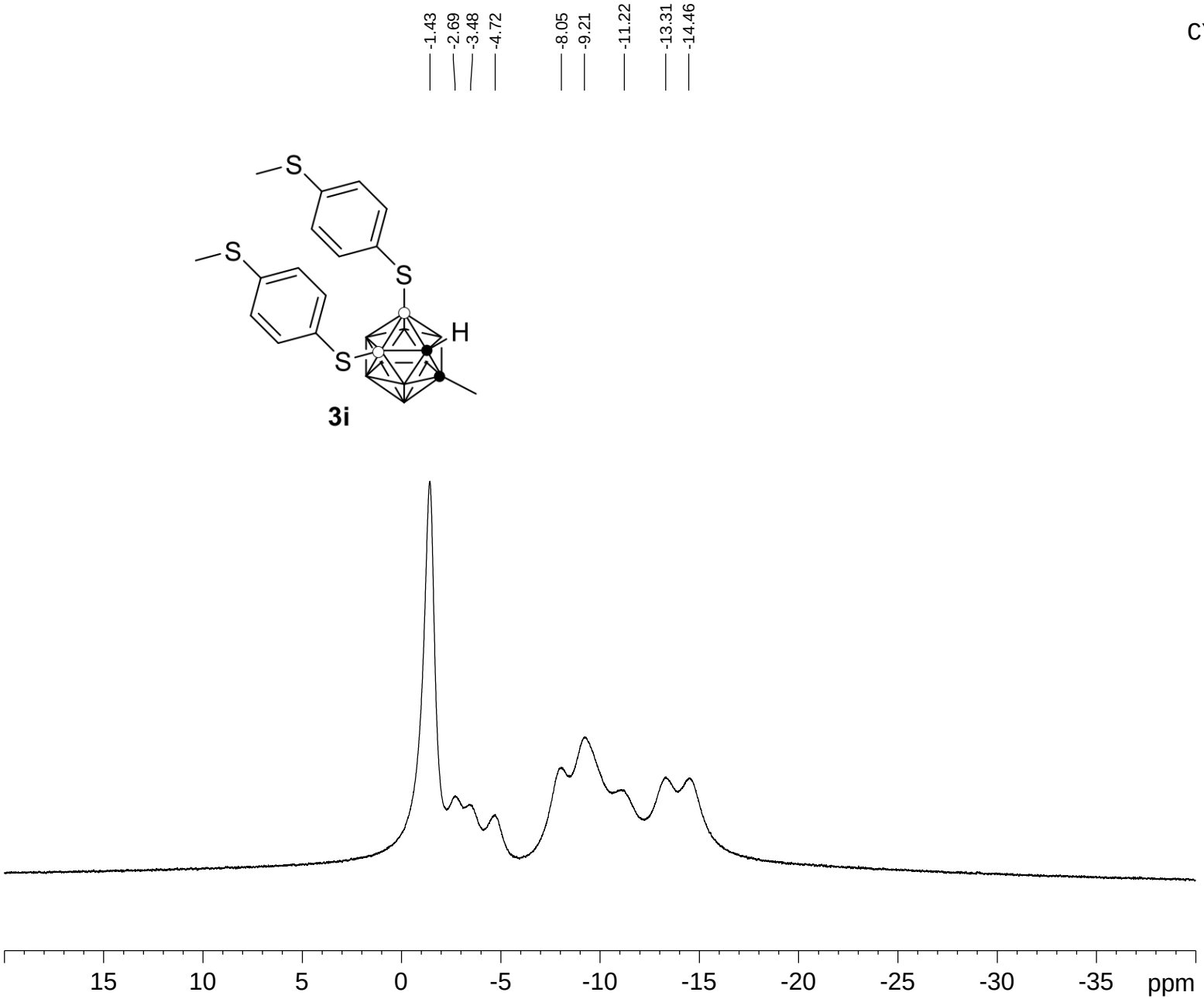
Bruker Advance III 400

```
Current Data Parameters
NAME     CY-C-B-54p-SMe
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20180327
Time              10.15 h
INSTRUM            spect
PROBHD   Z824601_0021 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  600
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                  203
DW                20.800 usec
DE                 6.50 usec
TE                297.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.50 usec
PLW1        41.25000000 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         8.31000042 W
PLW12        0.23083000 W
PLW13        0.11611000 W

F2 - Processing parameters
SI                32768
SF          100.6127576 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```



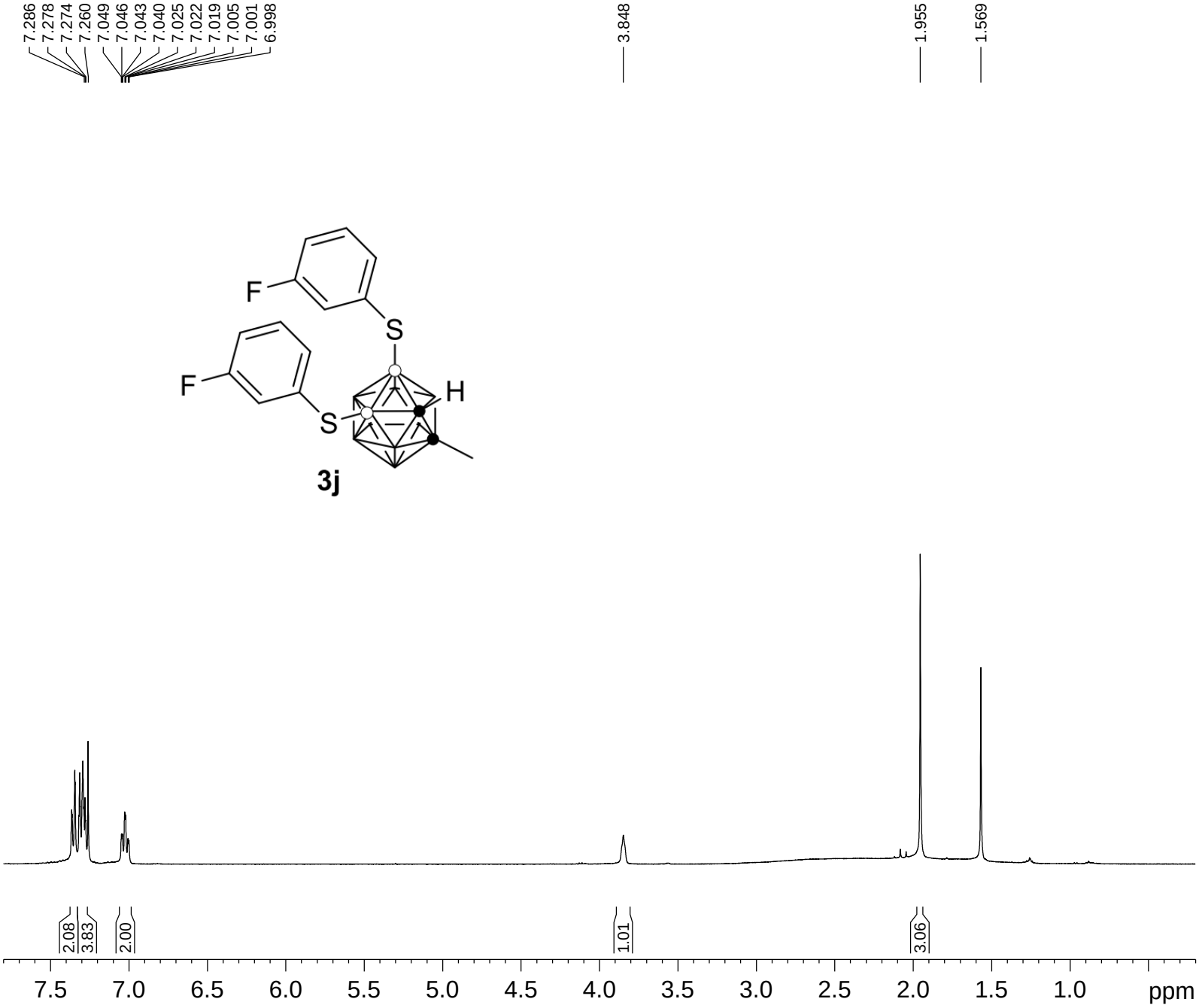
CY-B-B-54p-SMe

```
Current Data Parameters
NAME      CY-B-B-54p-SMe
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180327
Time               14.53 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    17
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   322
DW                20.800 usec
DE                 6.50 usec
TE                295.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1          128.4096890 MHz
NUC1                 11B
P1                 7.50 usec
PLW1          55.09999847 W
SFO2          400.2316009 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          13.56000042 W
PLW12          0.27428001 W

F2 - Processing parameters
SI                 32768
SF            128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



CY-B-B-54p-SMe-(C)

```
Current Data Parameters
NAME      CY-B-B-54p-SMe-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180327
Time                  14.55 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                       30
DS                        2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                      406
DW                   20.800 usec
DE                    6.50 usec
TE                   294.6 K
D1             2.00000000 sec
TD0                       1
SFO1          128.4096890 MHz
NUC1                   11B
P1                    7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                    32768
SF            128.4097430 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



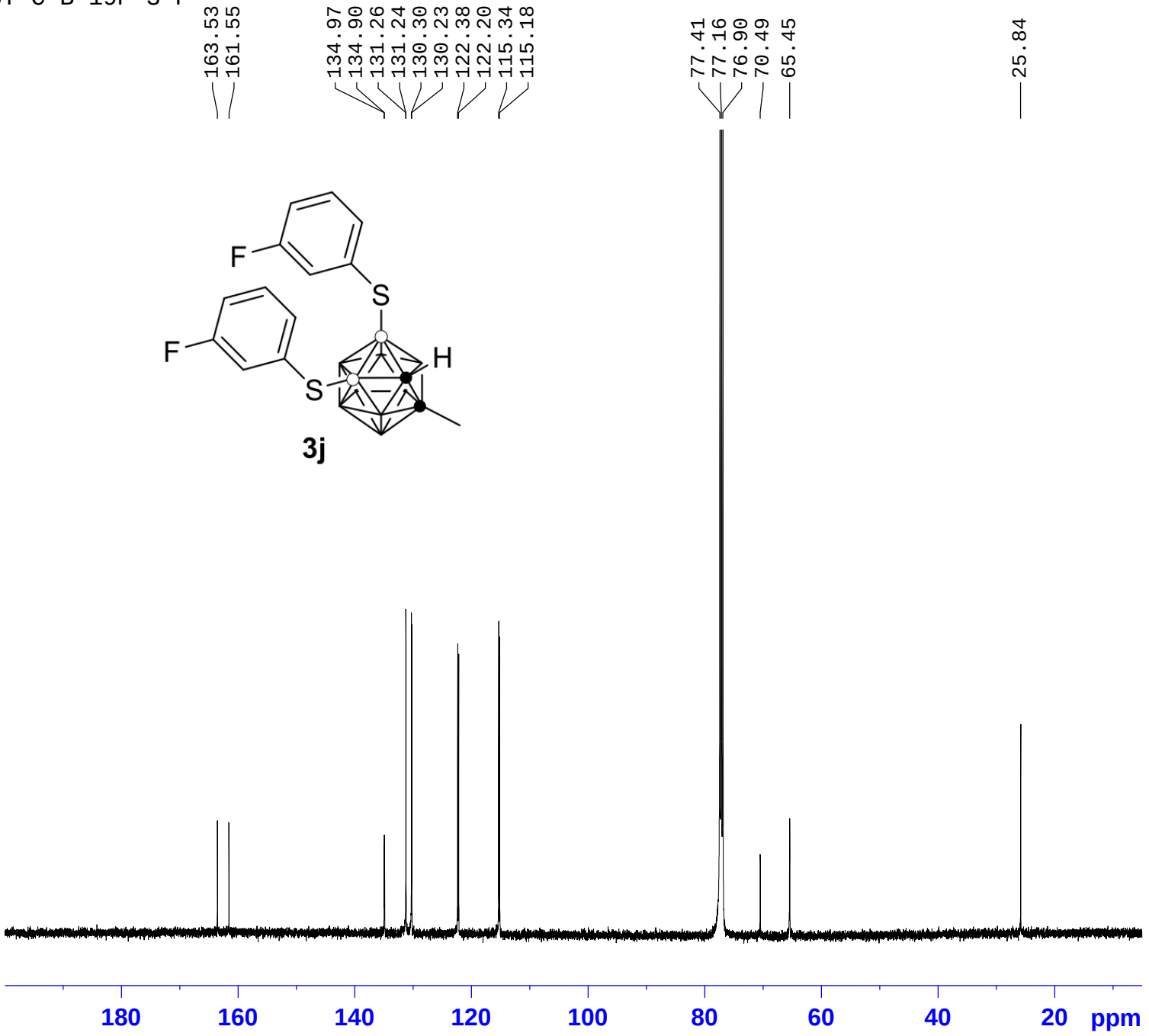
CY-H-B-19p-3-F-p

Current Data Parameters
NAME CY-H-B-19p-3-F-p
EXPNO 1
PROCNO 1

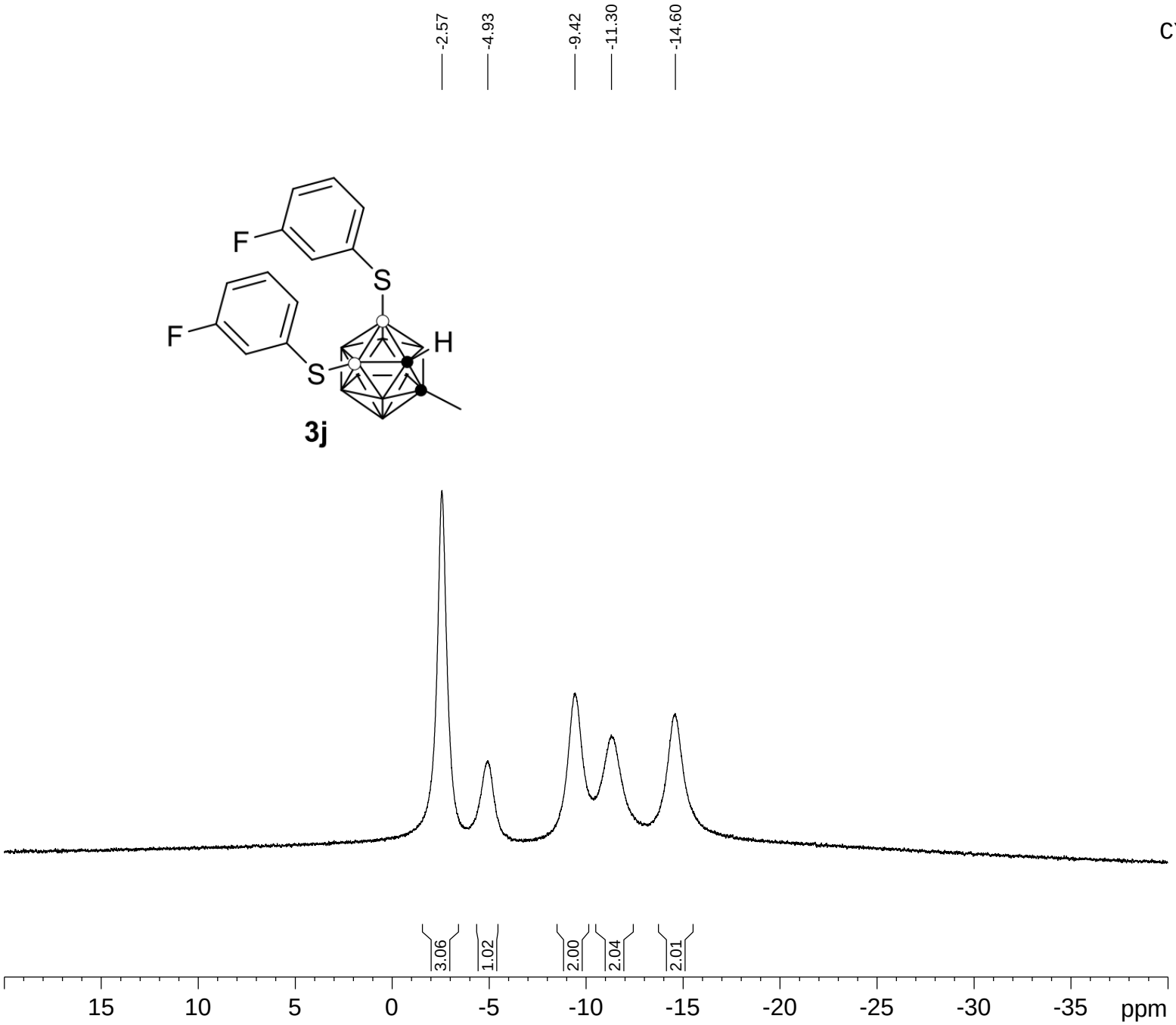
F2 - Acquisition Parameters
Date_ 20180120
Time 17.11 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-19P-3-F

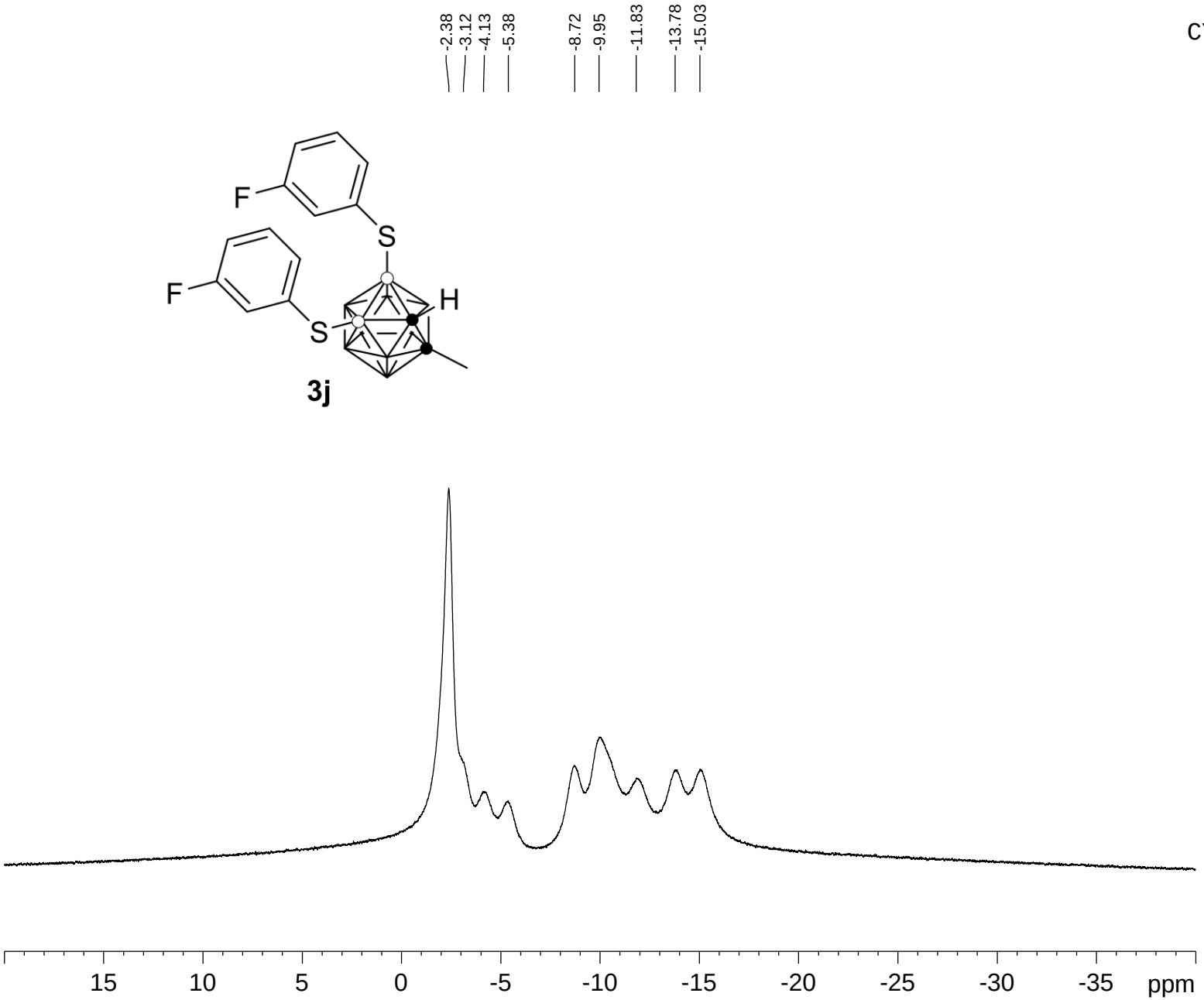



```
Current Data Parameters
NAME      CY-C-B-19P-3-F
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20180122
Time              20.18 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  857
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

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



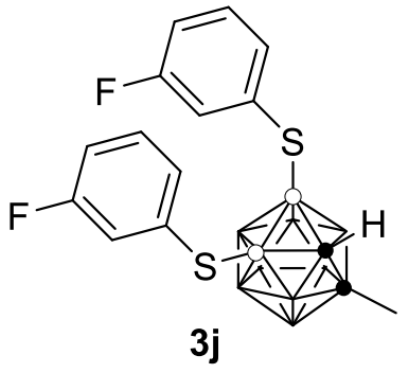
CY-B-B-19p-3-F

```
Current Data Parameters
NAME      CY-B-B-19p-3-F
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180120
Time               17.24 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    24
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   362
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```



CY-B-B-19p-3-F-(C)

```
Current Data Parameters
NAME      CY-B-B-19p-3-F-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180119
Time                  22.29 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                       40
DS                        2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                      362
DW                  20.800 usec
DE                   6.50 usec
TE                  295.2 K
D1              2.00000000 sec
TD0                       1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                    32768
SF             128.4097430 MHz
WDW                      EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

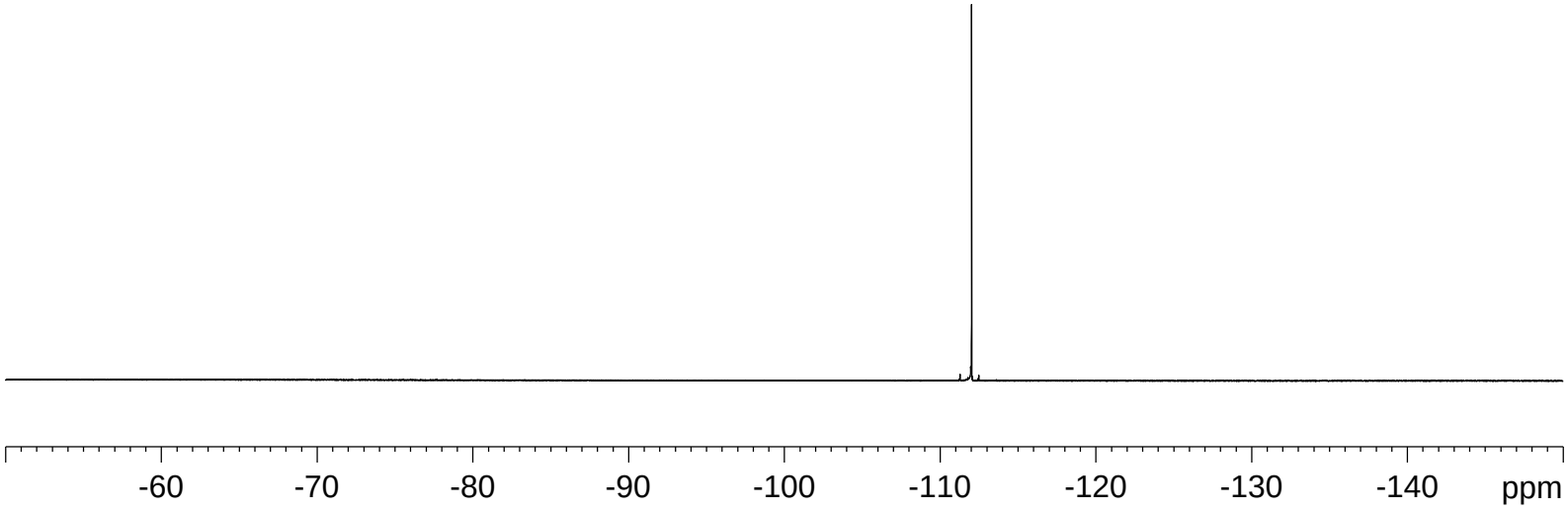


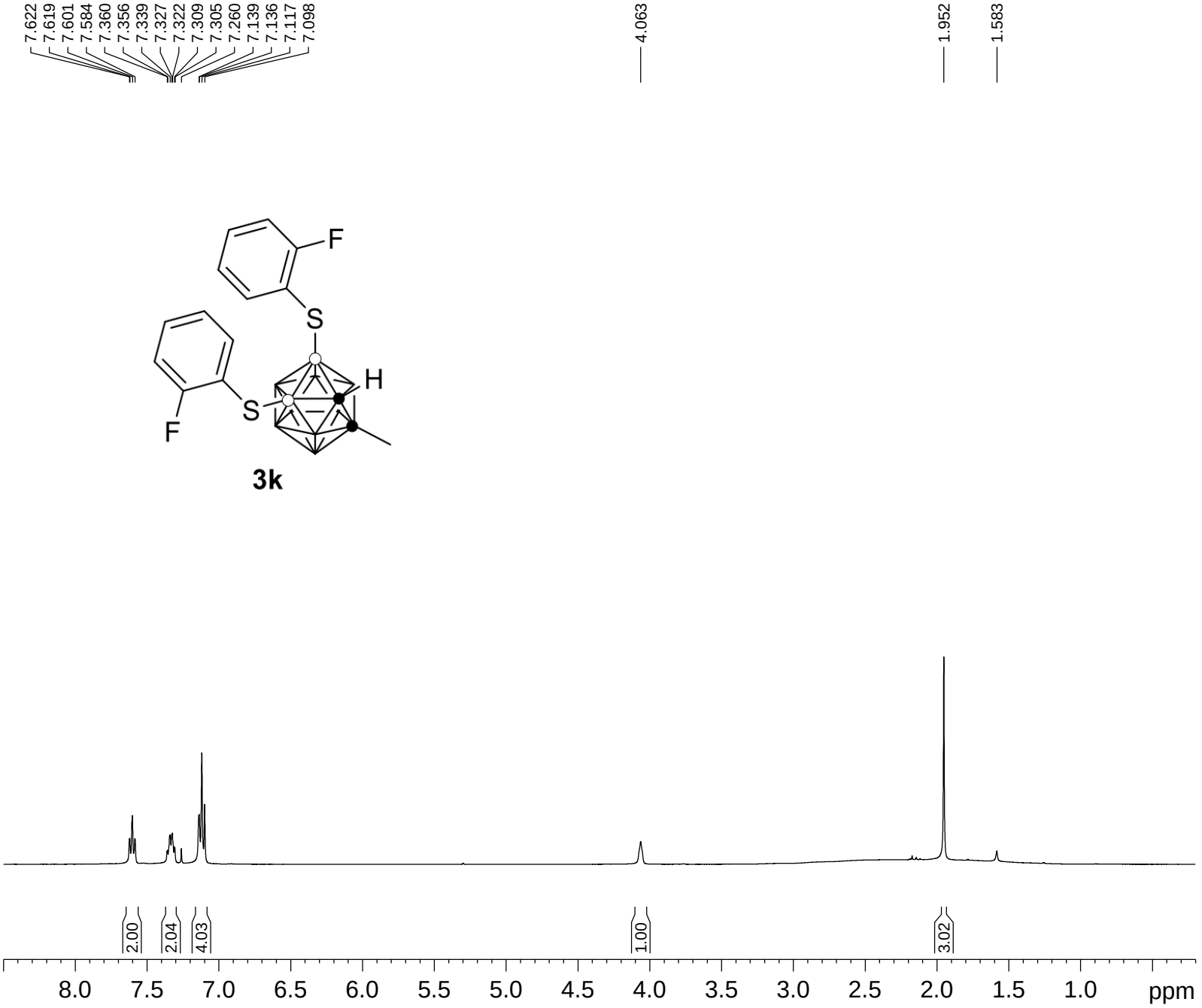
3j

-112.02

CY-F-B-19p-3-F

```
Current Data Parameters
NAME      CY-F-B-19p-3-F
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180120
Time              17.21 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     26
DS                      4
SWH             89285.711 Hz
FIDRES          0.681196 Hz
AQ              0.7340032 sec
RG                    645
DW                5.600 usec
DE                6.50 usec
TE                295.4 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                     1
SFO1         376.5548010 MHz
NUC1                  19F
P1                14.70 usec
PLW1         18.36000061 W
SFO2         400.2316009 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                    65536
SF           376.5924602 MHz
WDW                      EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



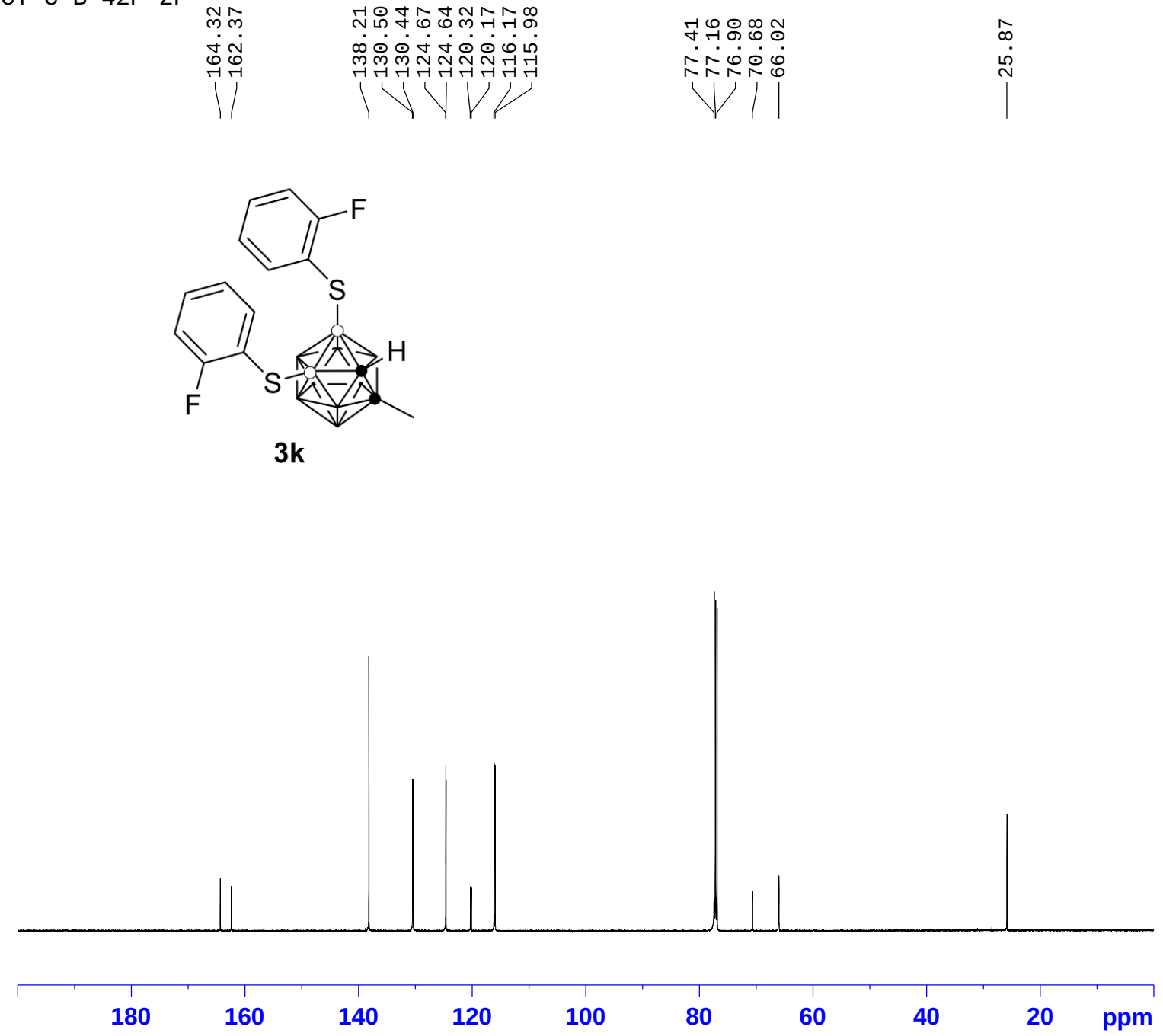


Current Data Parameters
NAME CY-H-B-42p-2F
EXPNO 1
PROCNO 1

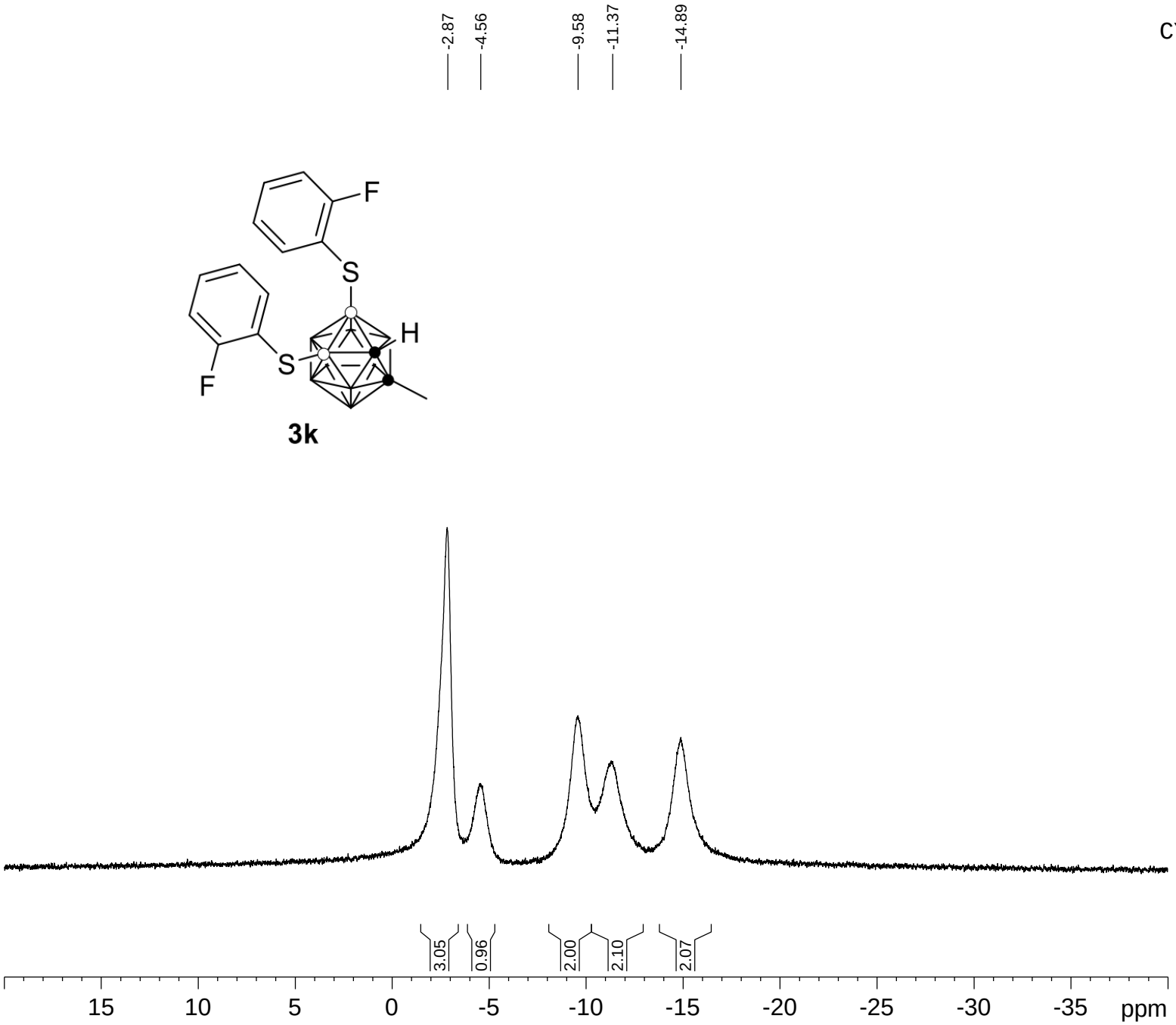
F2 - Acquisition Parameters
Date_ 20180309
Time 15.50 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-42P-2F

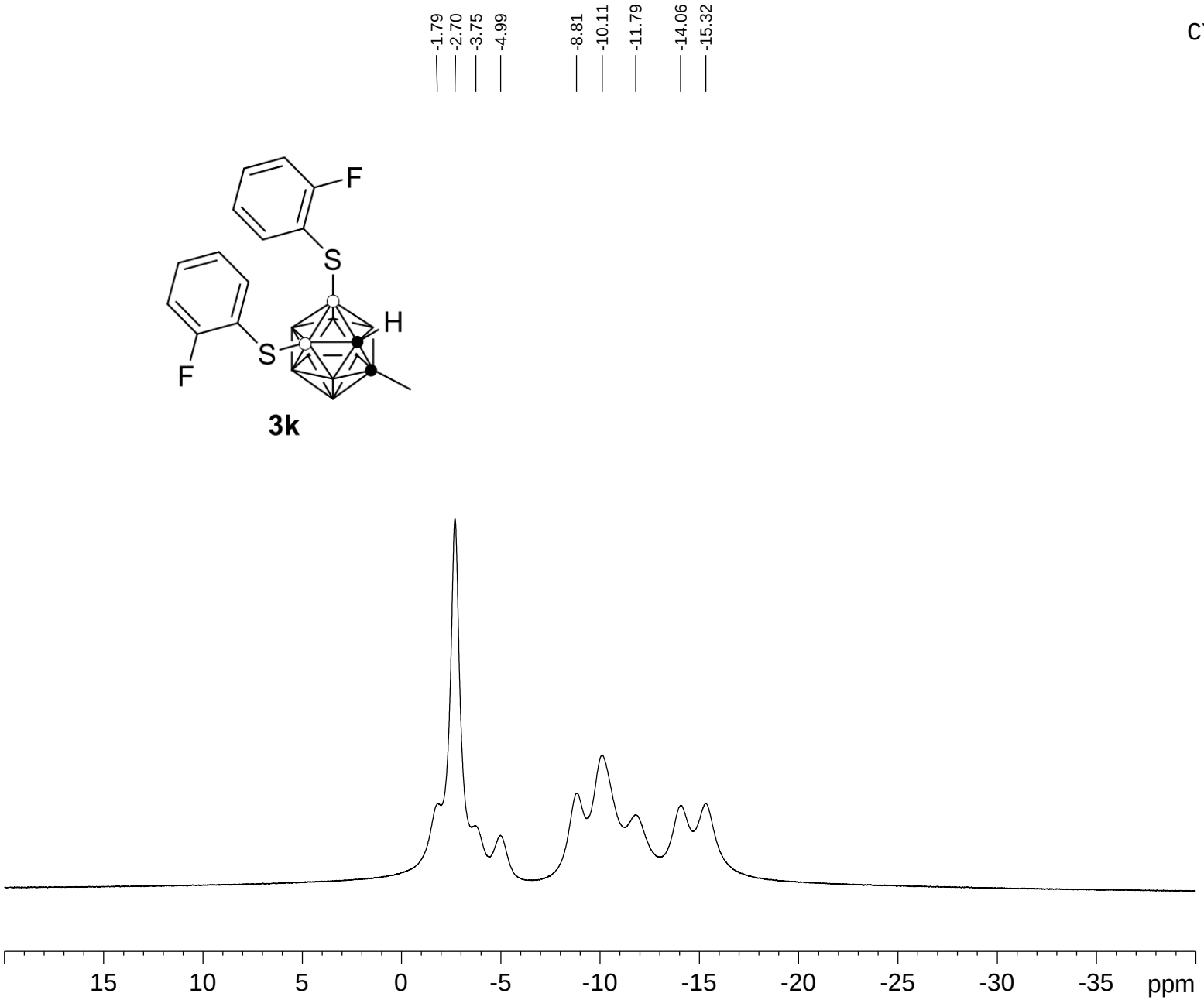



```
Current Data Parameters
NAME      CY-C-B-42P-2F
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20180309
Time             19.30 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7577759 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



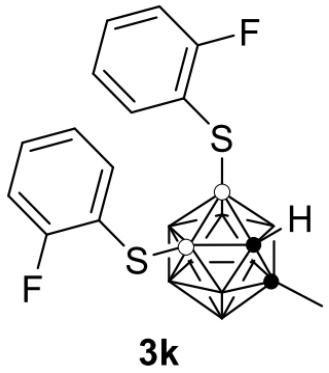
CY-B-B-42p-2F

```
Current Data Parameters
NAME       CY-B-B-42p-2F
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180309
Time               15.53 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    22
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                     1
DW                20.800 usec
DE                 6.50 usec
TE                295.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



CY-B-B-42p-2F-(C)

```
Current Data Parameters
NAME      CY-B-B-42p-2F-(C)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180309
Time                 15.56 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      37
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                     256
DW                  20.800 usec
DE                   6.50 usec
TE                  295.0 K
D1              2.00000000 sec
TD0                      1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                   32768
SF             128.4097430 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

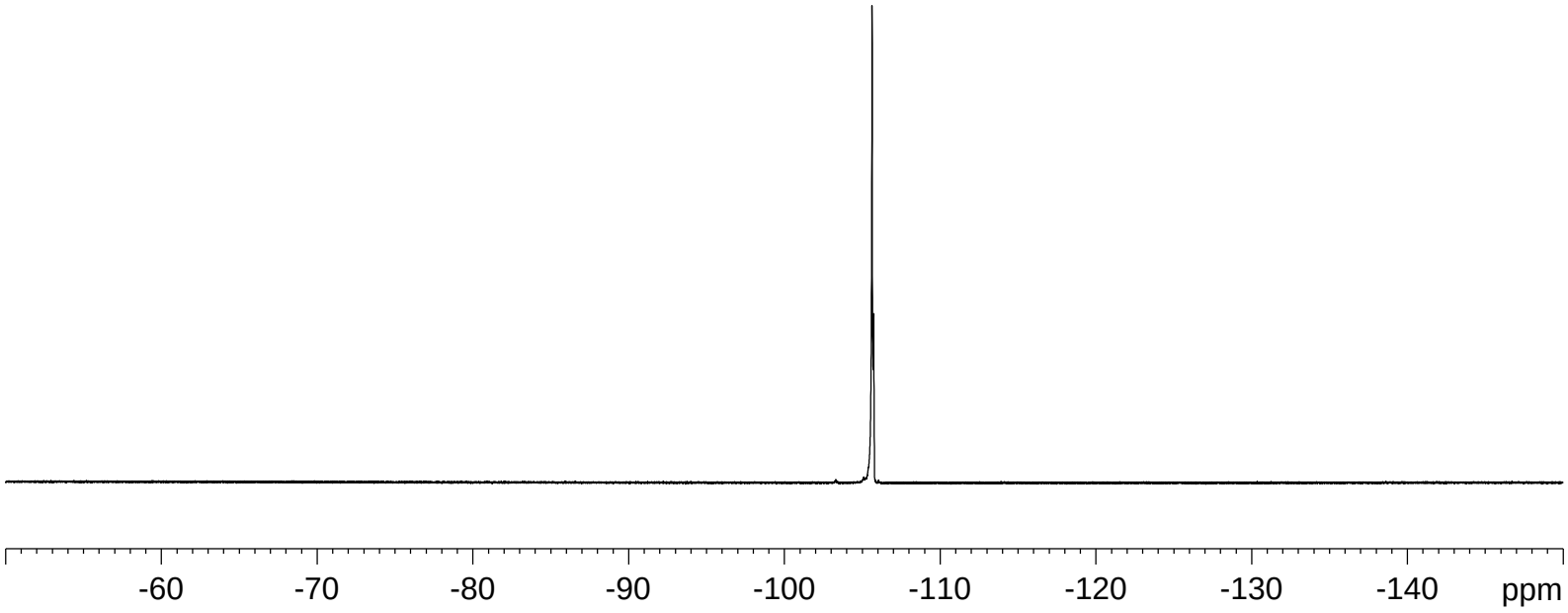


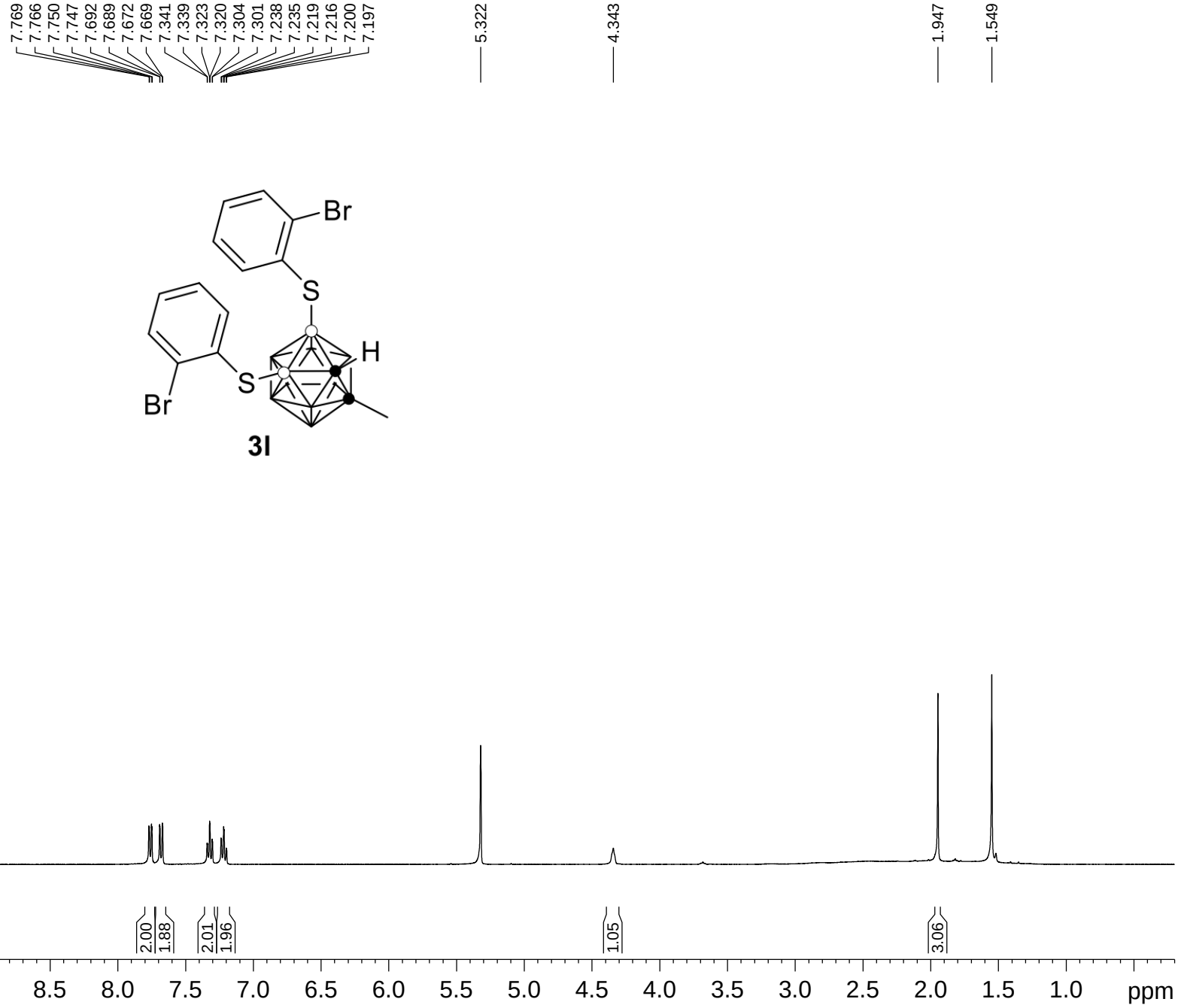
3k

-105.62

CY-F-B-42P-2F

```
Current Data Parameters
NAME      CY-F-B-42P-2F
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20180309
Time             16.01 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG      zgfhigqn.2
TD               131072
SOLVENT            CDCl3
NS                    12
DS                     4
SWH            89285.711 Hz
FIDRES         0.681196 Hz
AQ             0.7340032 sec
RG                   645
DW                 5.600 usec
DE                 6.50 usec
TE                 295.0 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1
SFO1         376.5548010 MHz
NUC1                 19F
P1                14.70 usec
PLW1         18.36000061 W
SFO2         400.2316009 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 65536
SF           376.5924602 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```



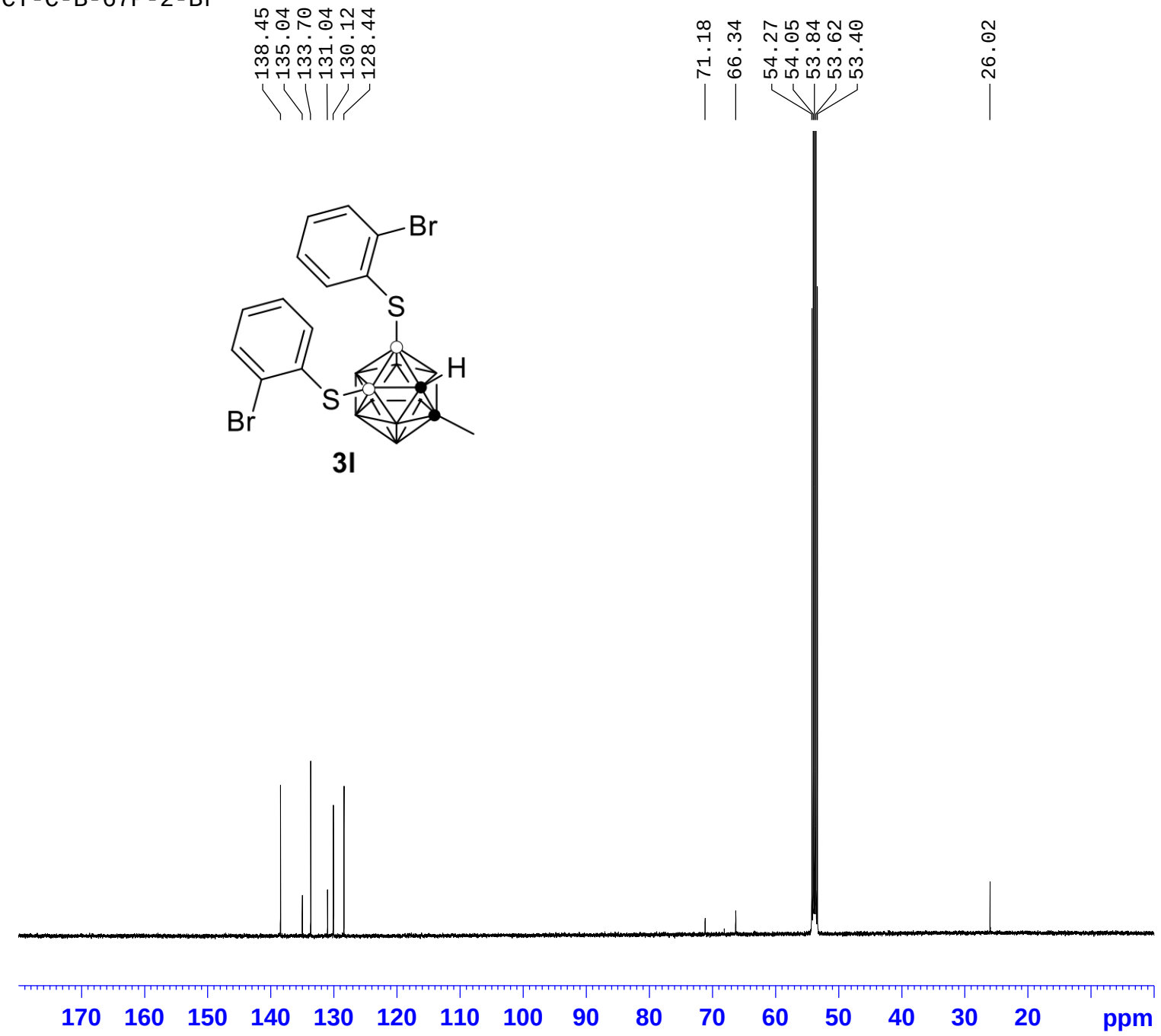


Current Data Parameters
NAME CY-H-B-67p-2-Br-re
EXPNO 1
PROCNO 1

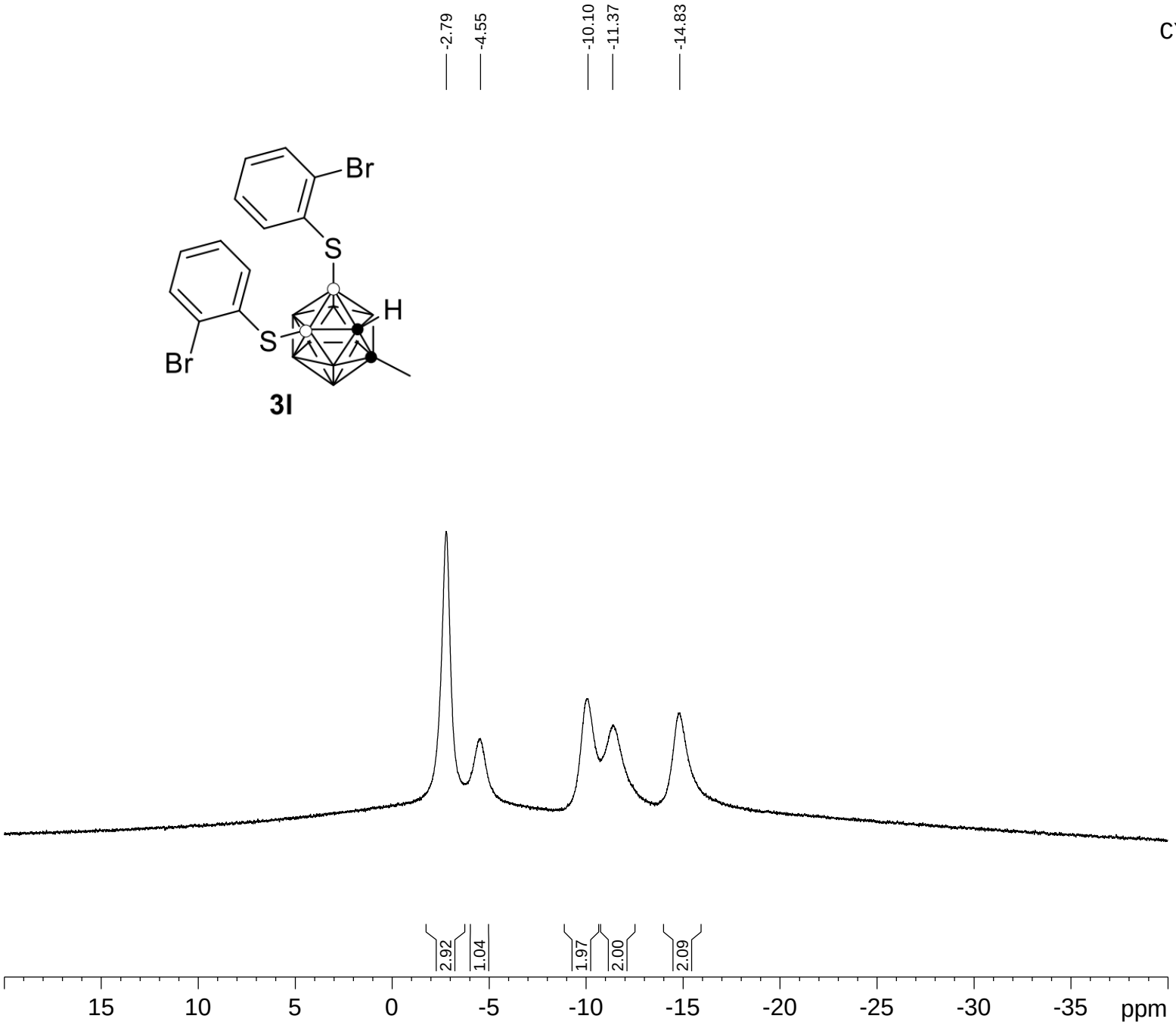
F2 - Acquisition Parameters
Date_ 20180503
Time 14.29 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 17
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300147 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-67P-2-Br

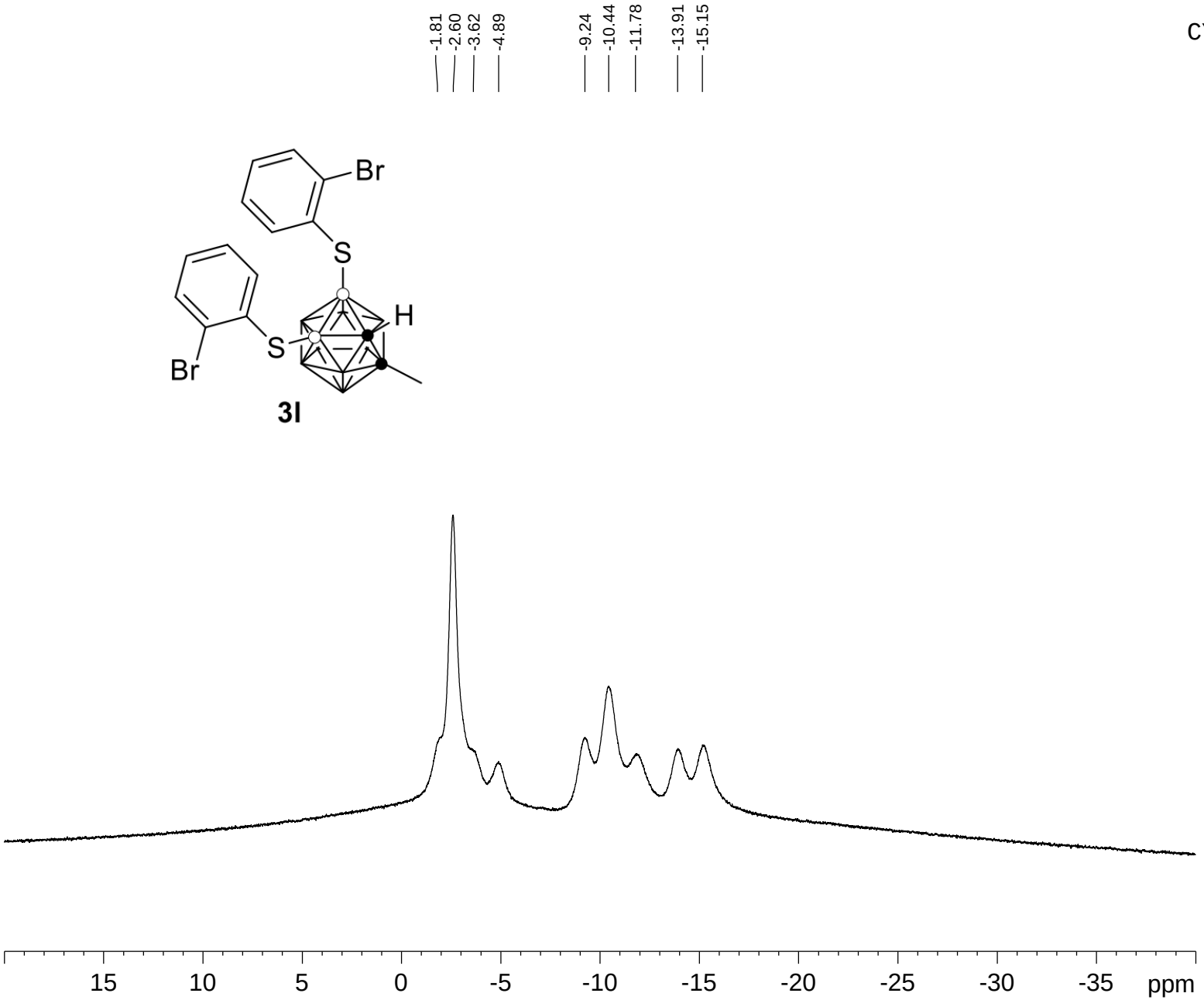



```
Current Data Parameters
NAME      CY-C-B-67P-2-Br
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180503
Time              18.27 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT           CD2Cl2
NS                   800
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

F2 - Processing parameters
SI                 32768
SF           125.7577379 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



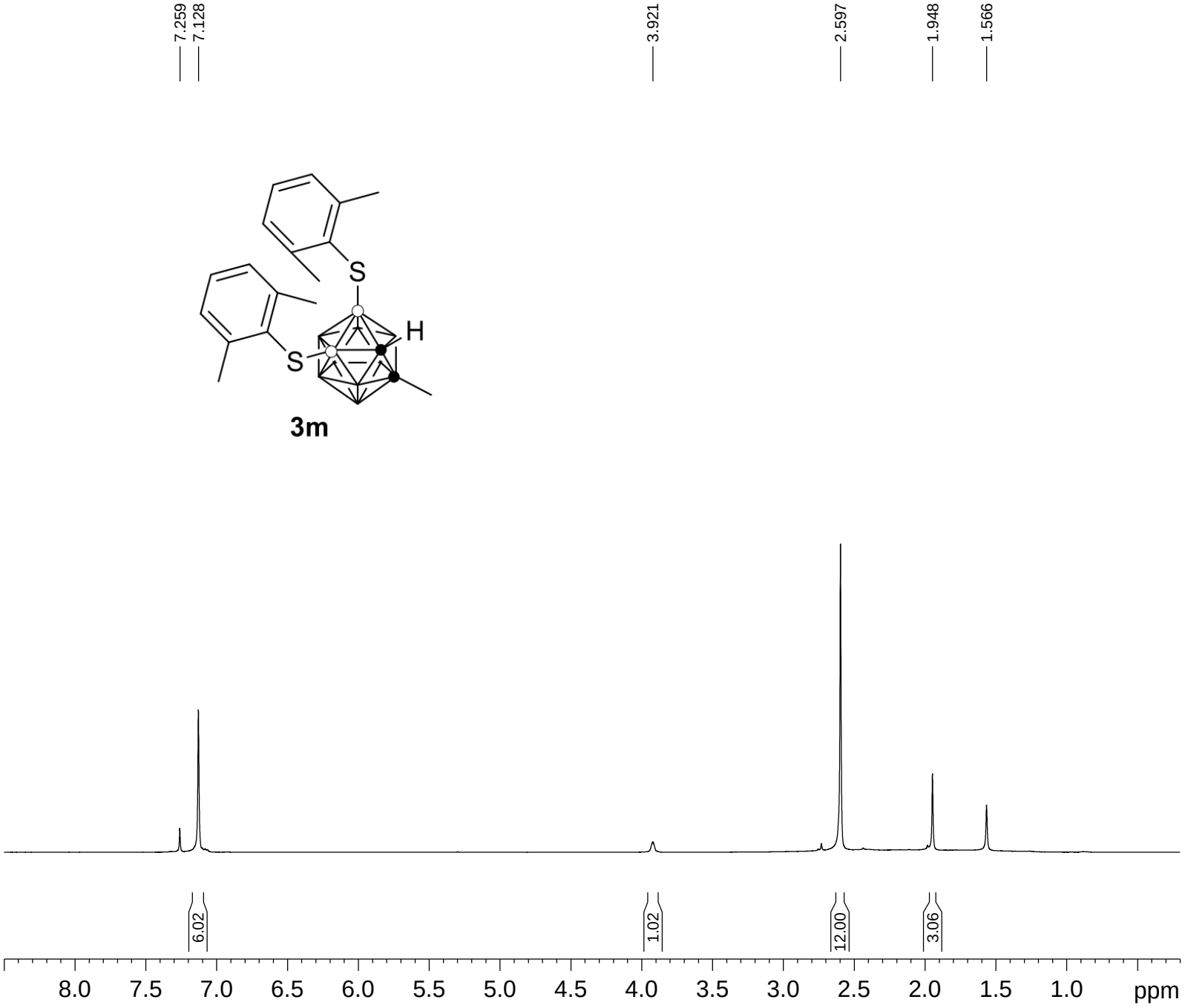
CY-B-B-67p-2-Br

```
Current Data Parameters
NAME      CY-B-B-67p-2-Br
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180503
Time                14.35 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT           CD2Cl2
NS                     64
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                    512
DW                 20.800 usec
DE                  6.50 usec
TE                 295.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1          55.09999847 W
SFO2          400.2316009 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          13.56000042 W
PLW12          0.27428001 W

F2 - Processing parameters
SI                  32768
SF            128.4097615 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



CY-B-B-67p-2-Br-(C)

```
Current Data Parameters
NAME      CY-B-B-67p-2-Br-(C)
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20180503
Time                  14.38 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                  zg
TD                    65536
SOLVENT              CD2Cl2
NS                      126
DS                        2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                      287
DW                  20.800 usec
DE                   6.50 usec
TE                  294.6 K
D1              2.00000000 sec
TD0                       1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                    32768
SF             128.4097430 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



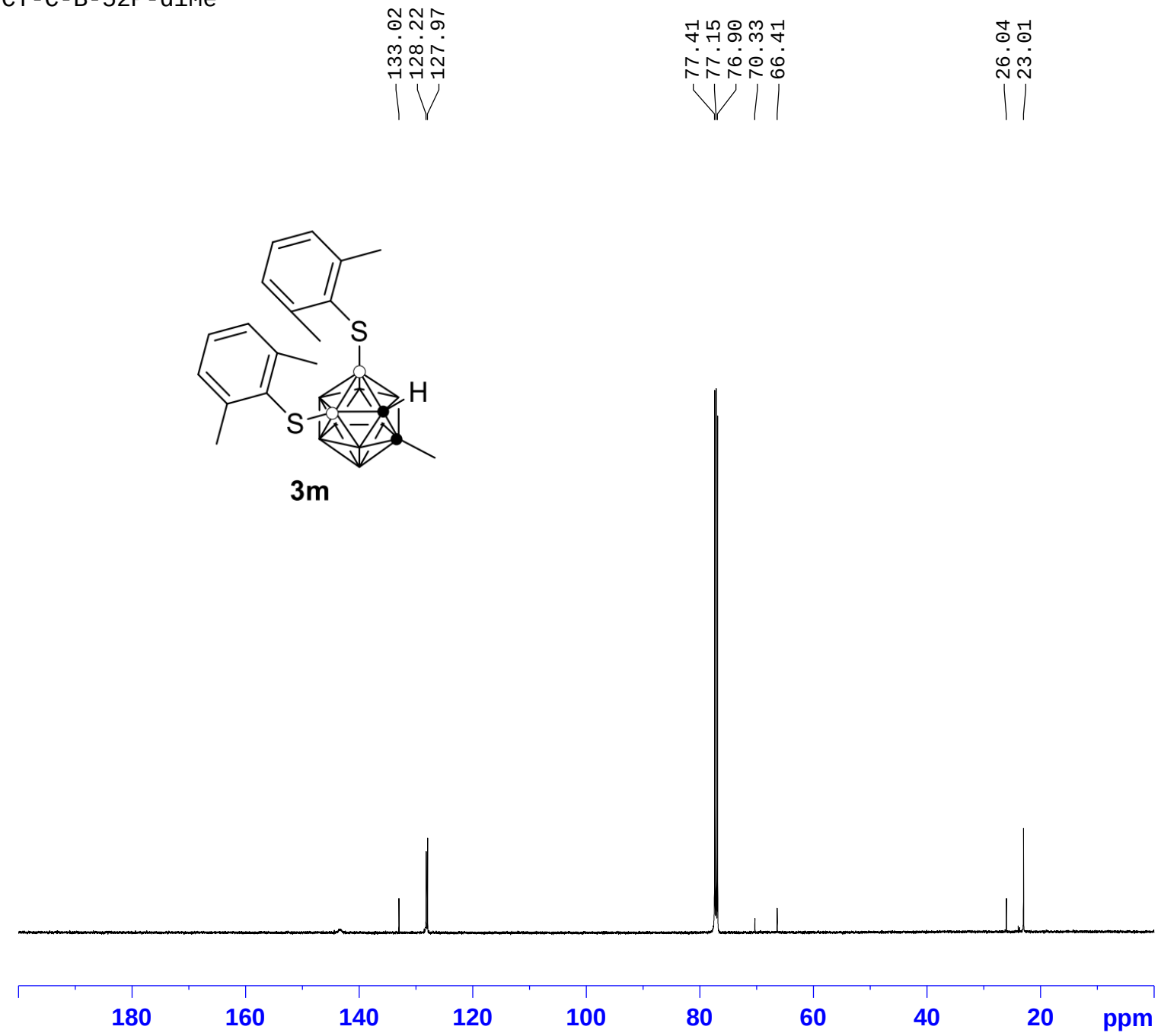
CY-H-B-52p-diMe

Current Data Parameters
NAME CY-H-B-52p-diMe
EXPNO 1
PROCNO 1

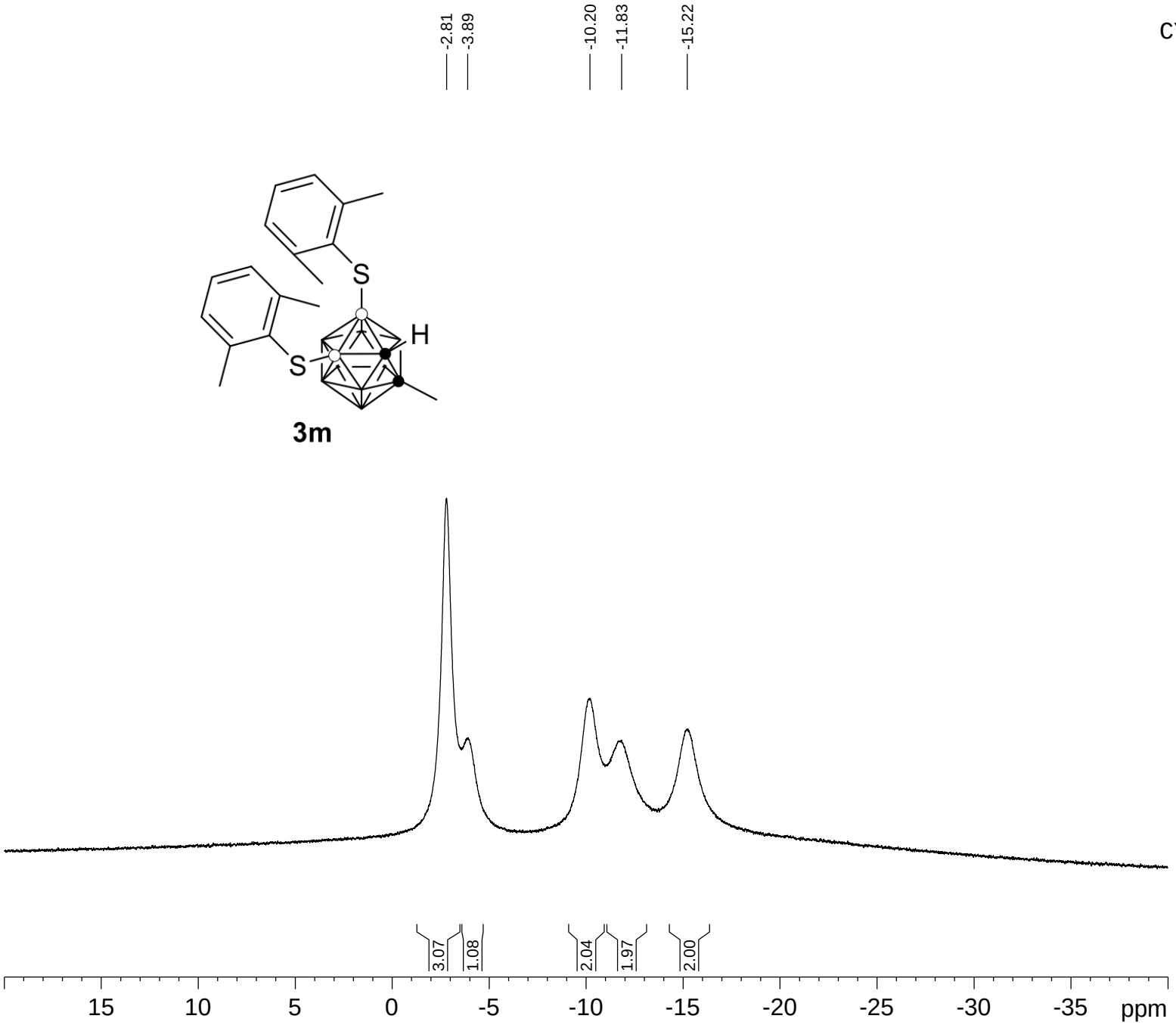
F2 - Acquisition Parameters
Date_ 20180326
Time 21.06 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 11
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-52P-diMe

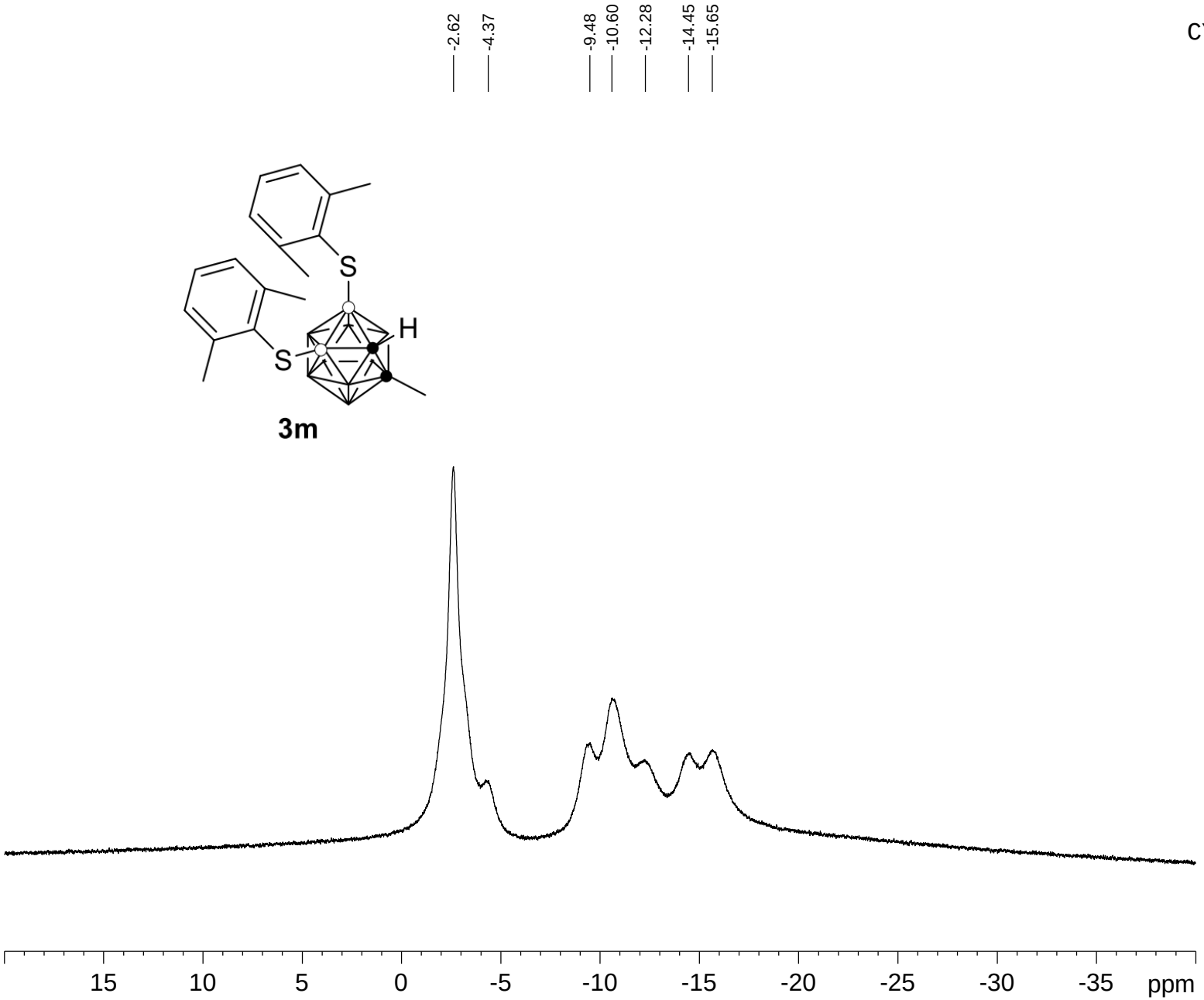



```
Current Data Parameters
NAME      CY-C-B-52P-diMe
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180327
Time               16.16 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   400
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P1                10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

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



CY-B-B-52p-diMe

```
Current Data Parameters
NAME      CY-B-B-52p-diMe
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180326
Time                21.11 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     46
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    456
DW                 20.800 usec
DE                  6.50 usec
TE                 294.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1          55.09999847 W
SFO2          400.2316009 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          13.56000042 W
PLW12          0.27428001 W

F2 - Processing parameters
SI                  32768
SF            128.4097615 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



CY-B-B-52p-diMe-(C)

```
Current Data Parameters
NAME      CY-B-B-52p-diMe-(C)
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180326
Time                  21.14 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      41
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                     406
DW                  20.800 usec
DE                   6.50 usec
TE                  294.4 K
D1              2.00000000 sec
TD0                      1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                   32768
SF             128.4097430 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

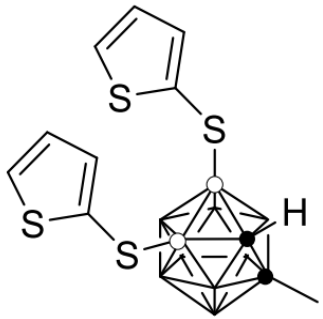
CY-H-B-23p-thio

7.331 7.329 7.317 7.315 7.259 7.197 7.195 7.189 7.187 7.013 7.004 7.000 6.991

3.805

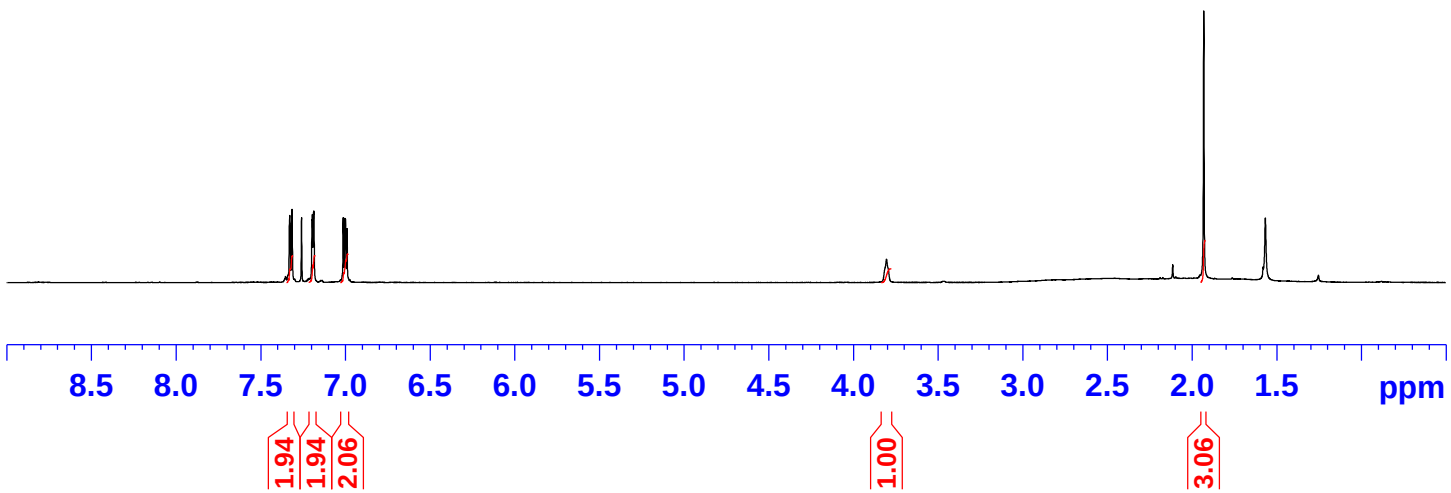
1.931

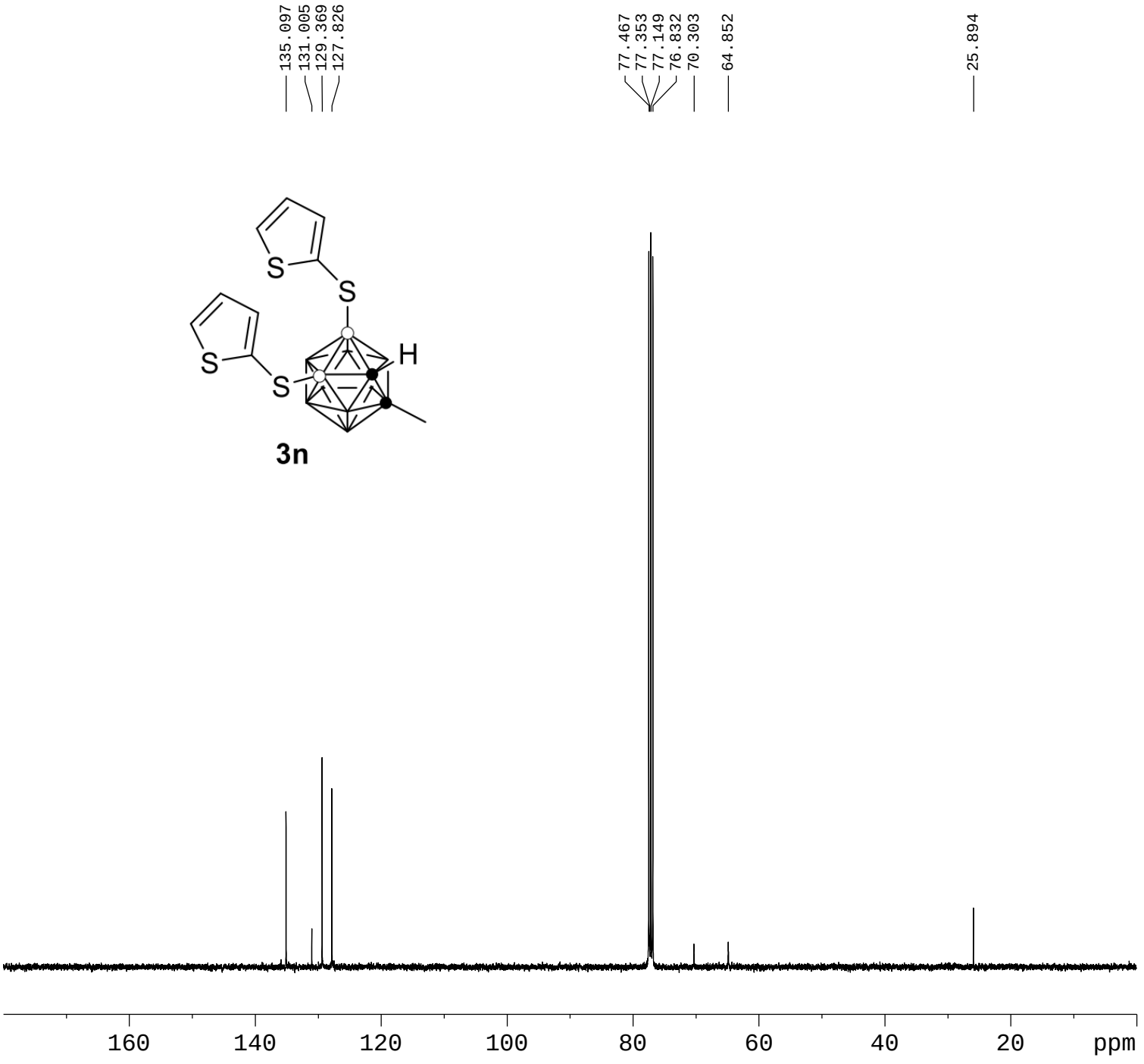
1.567



3n

```
Current Data Parameters
NAME      CY-H-B-23p-thio
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180123
Time                12.45 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                    203
DW                 62.400 usec
DE                  6.50 usec
TE                 296.6 K
D1              1.00000000 sec
TD0                     1
SFO1          400.1324708 MHz
NUC1                   1H
P1                 15.00 usec
PLW1           8.31000042 W

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





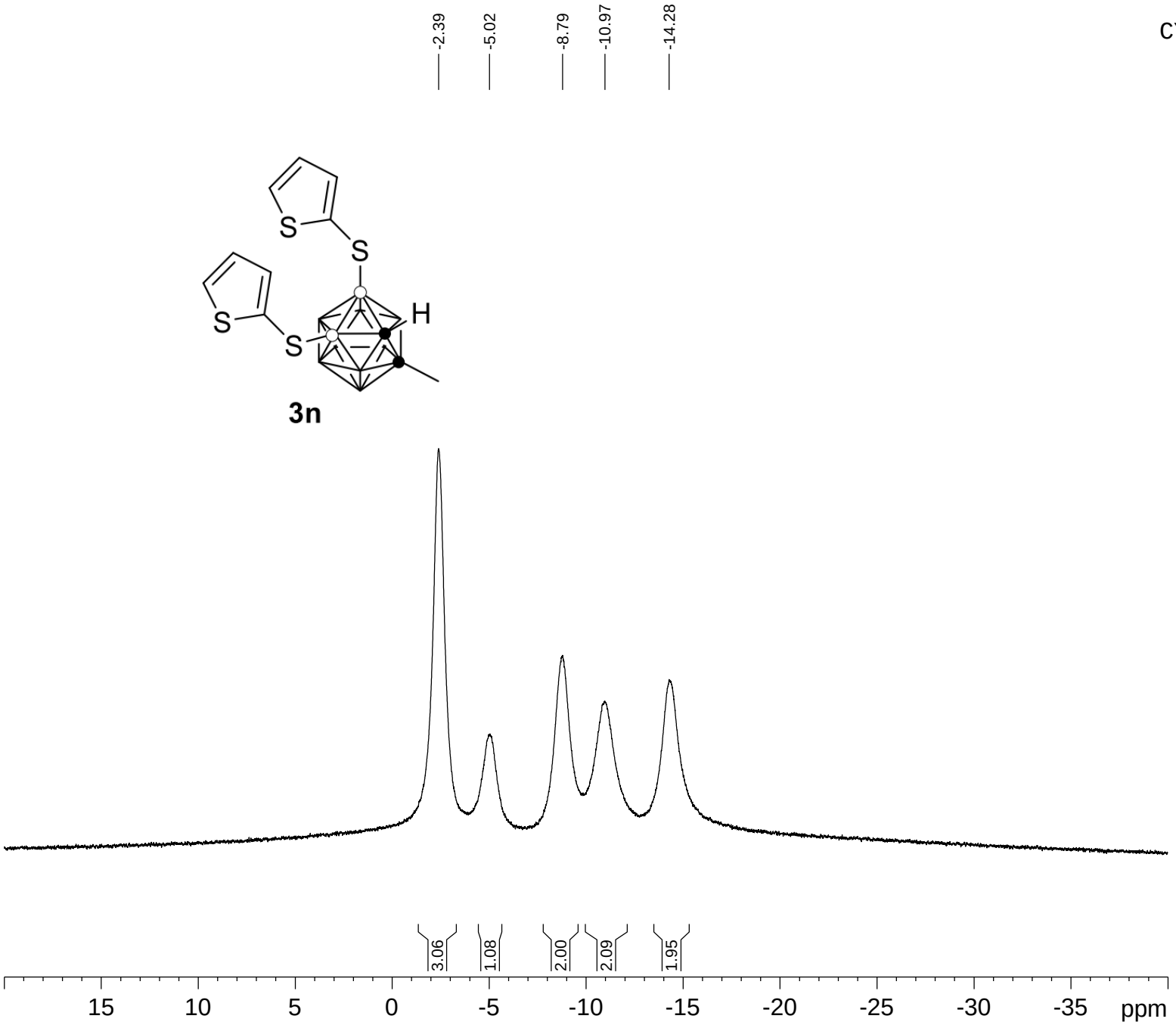
CY-C-B-23p-thio

Bruker Advance III 400

Current Data Parameters
NAME CY-C-B-23p-thio
EXPNO 4
PROCNO 1

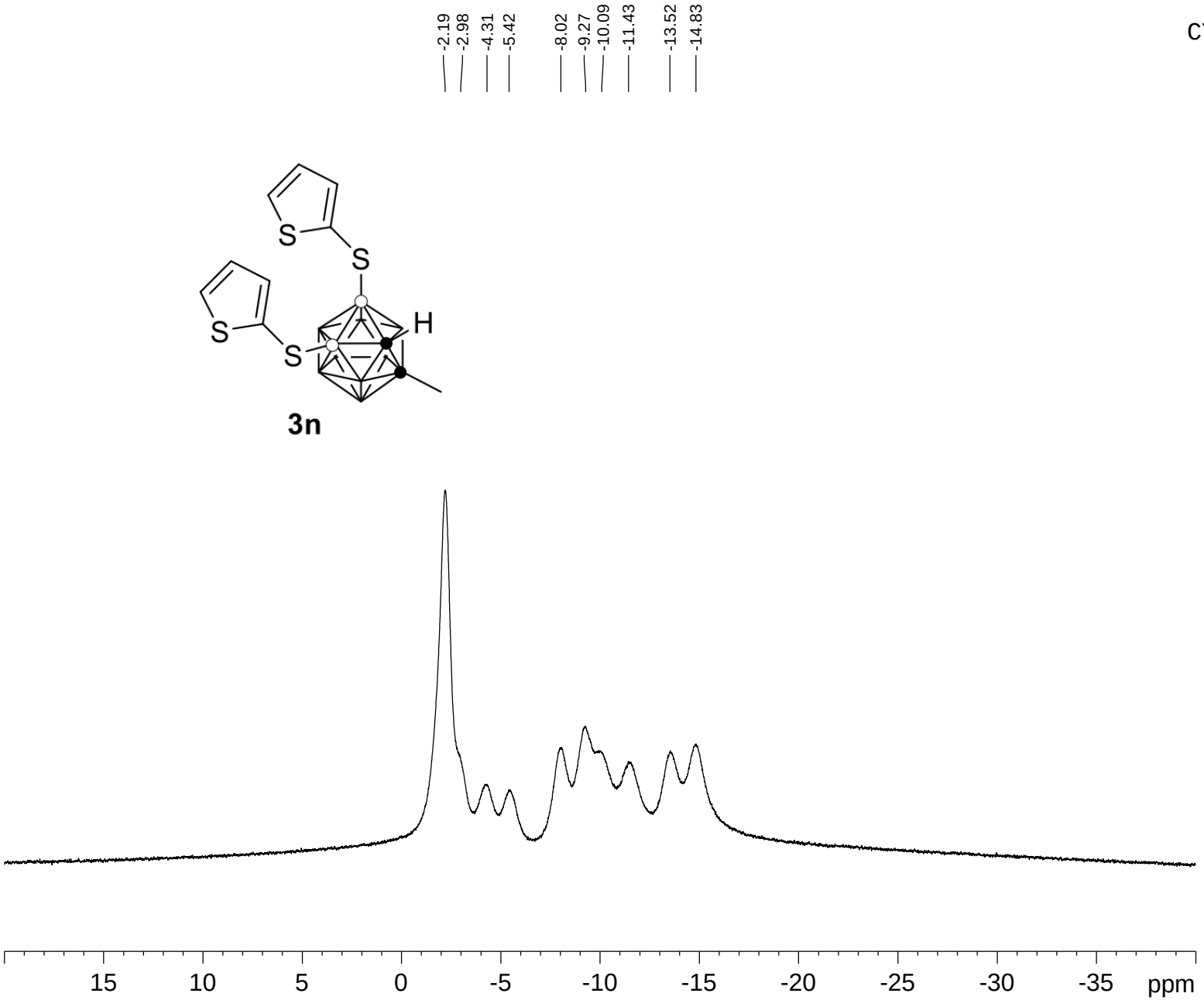
F2 - Acquisition Parameters
Date_ 20180123
Time 23.15 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1397
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W

F2 - Processing parameters
SI 32768
SF 100.6127565 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



CY-B-B-23p-thio

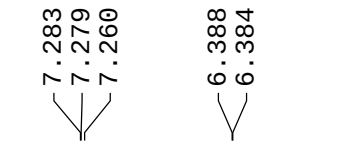
```
Current Data Parameters
NAME      CY-B-B-23p-thio
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180123
Time                23.15 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     19
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    362
DW                 20.800 usec
DE                  6.50 usec
TE                 296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                  32768
SF           128.4097615 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

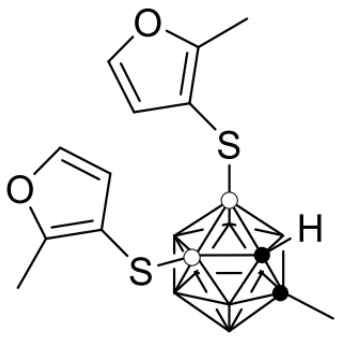


CY-B-B-23p-thio-(C)

```
Current Data Parameters
NAME      CY-B-B-23p-thio-(C)
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180123
Time                  23.18 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT               CDCl3
NS                        32
DS                         2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                       362
DW                  20.800 usec
DE                   6.50 usec
TE                   295.6 K
D1              2.00000000 sec
TD0                        1
SFO1           128.4096890 MHz
NUC1                    11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                     32768
SF             128.4097430 MHz
WDW                       EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

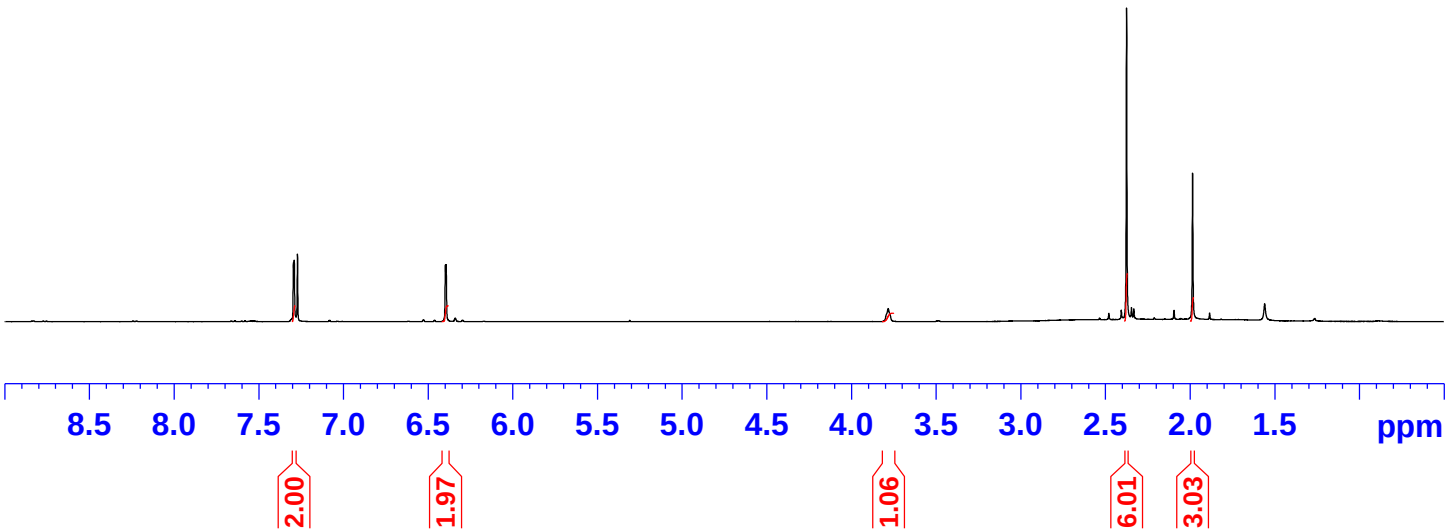
CY-H-B-24p-furan



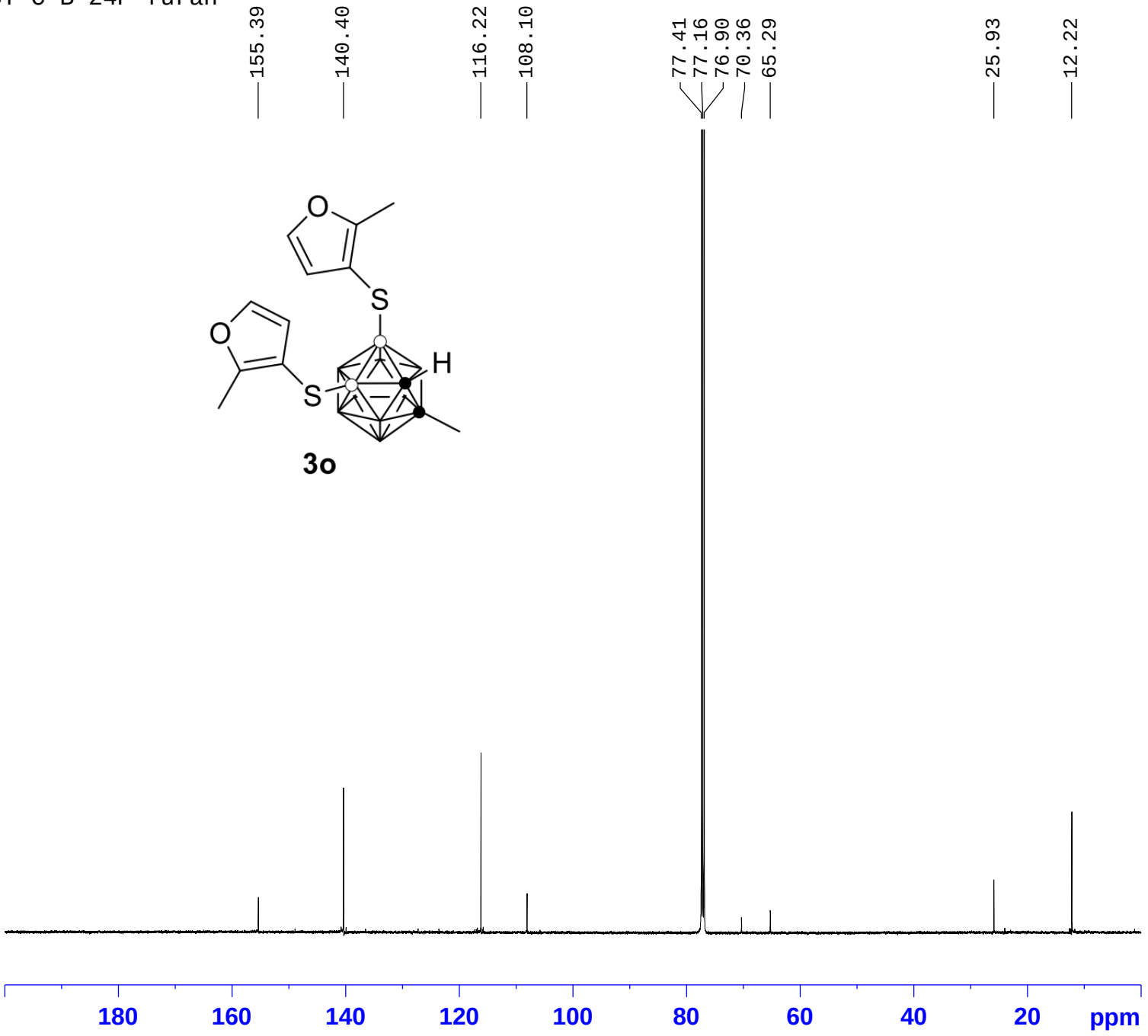


3o

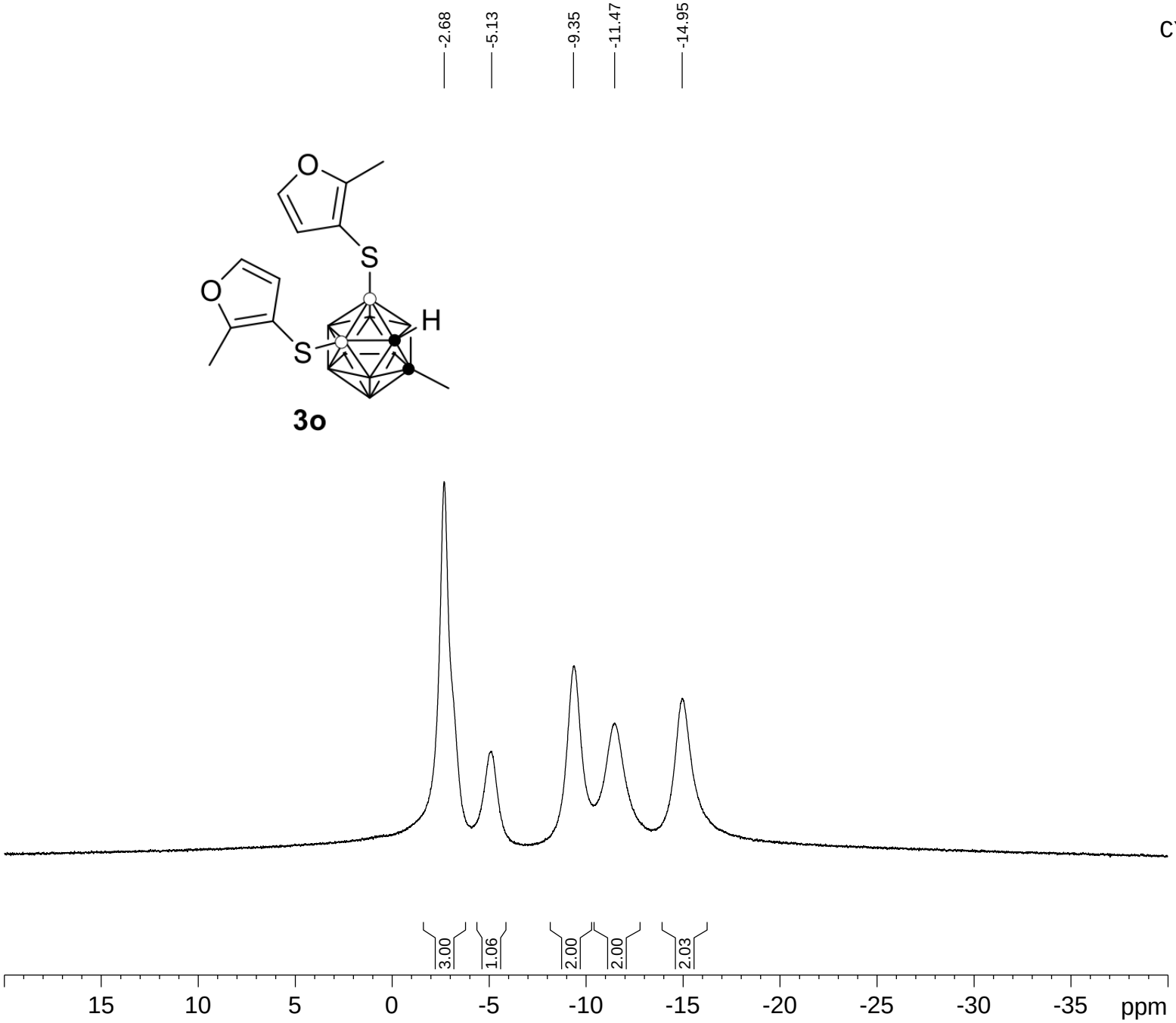
```
Current Data Parameters
NAME      CY-H-B-24p-furan
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180127
Time                14.19 h
INSTRUM              spect
PROBHD    Z824601_0021 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        9
DS                        2
SWH                8012.820 Hz
FIDRES                0.244532 Hz
AQ                 4.0894465 sec
RG                      203
DW                   62.400 usec
DE                    6.50 usec
TE                   296.5 K
D1              1.00000000 sec
TD0                       1
SFO1           400.1324708 MHz
NUC1                     1H
P1                   15.00 usec
PLW1            8.31000042 W

F2 - Processing parameters
SI                    65536
SF             400.1300059 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```



CY-C-B-24P-furan

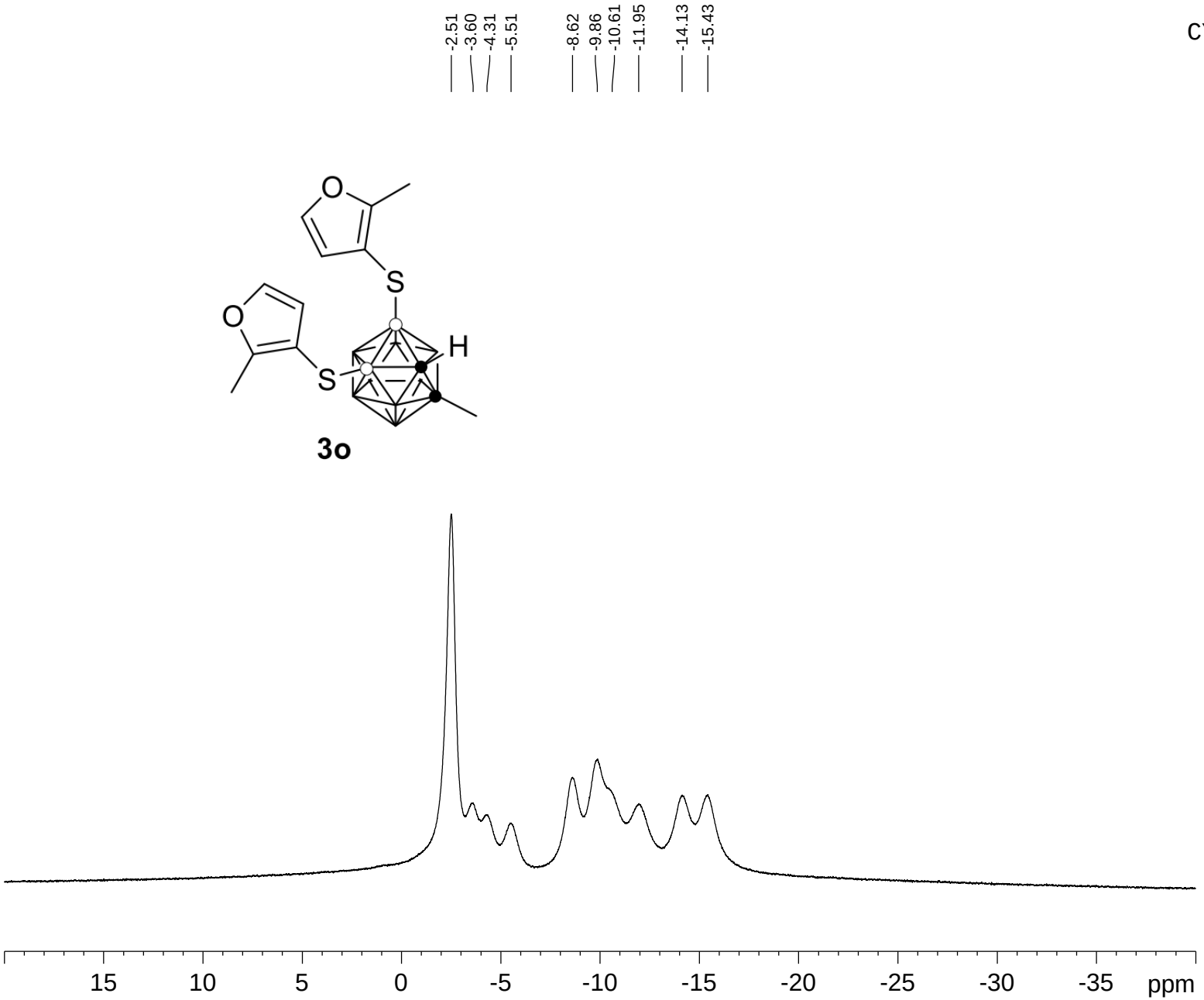



```
Current Data Parameters
NAME      CY-C-B-24P-furan
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180128
Time                5.27 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P1                10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

F2 - Processing parameters
SI                 32768
SF           125.7577717 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



CY-B-B-24p-furan

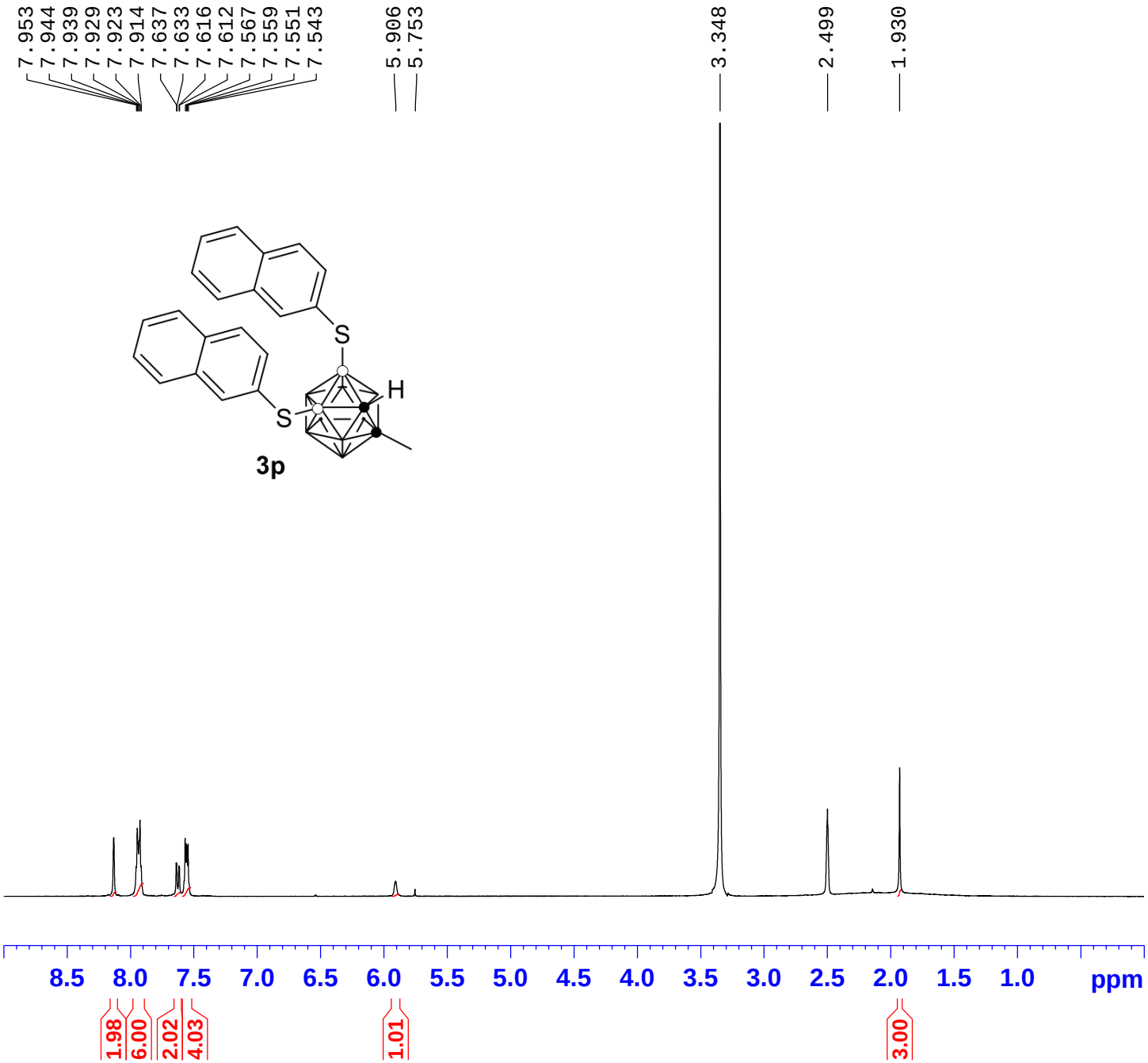
```
Current Data Parameters
NAME      CY-B-B-24p-furan
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180126
Time                19.37 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     19
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                    228
DW                 20.800 usec
DE                  6.50 usec
TE                 295.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1          55.09999847 W
SFO2          400.2316009 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          13.56000042 W
PLW12          0.27428001 W

F2 - Processing parameters
SI                   32768
SF            128.4097615 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



CY-B-B-24p-furan-(C)

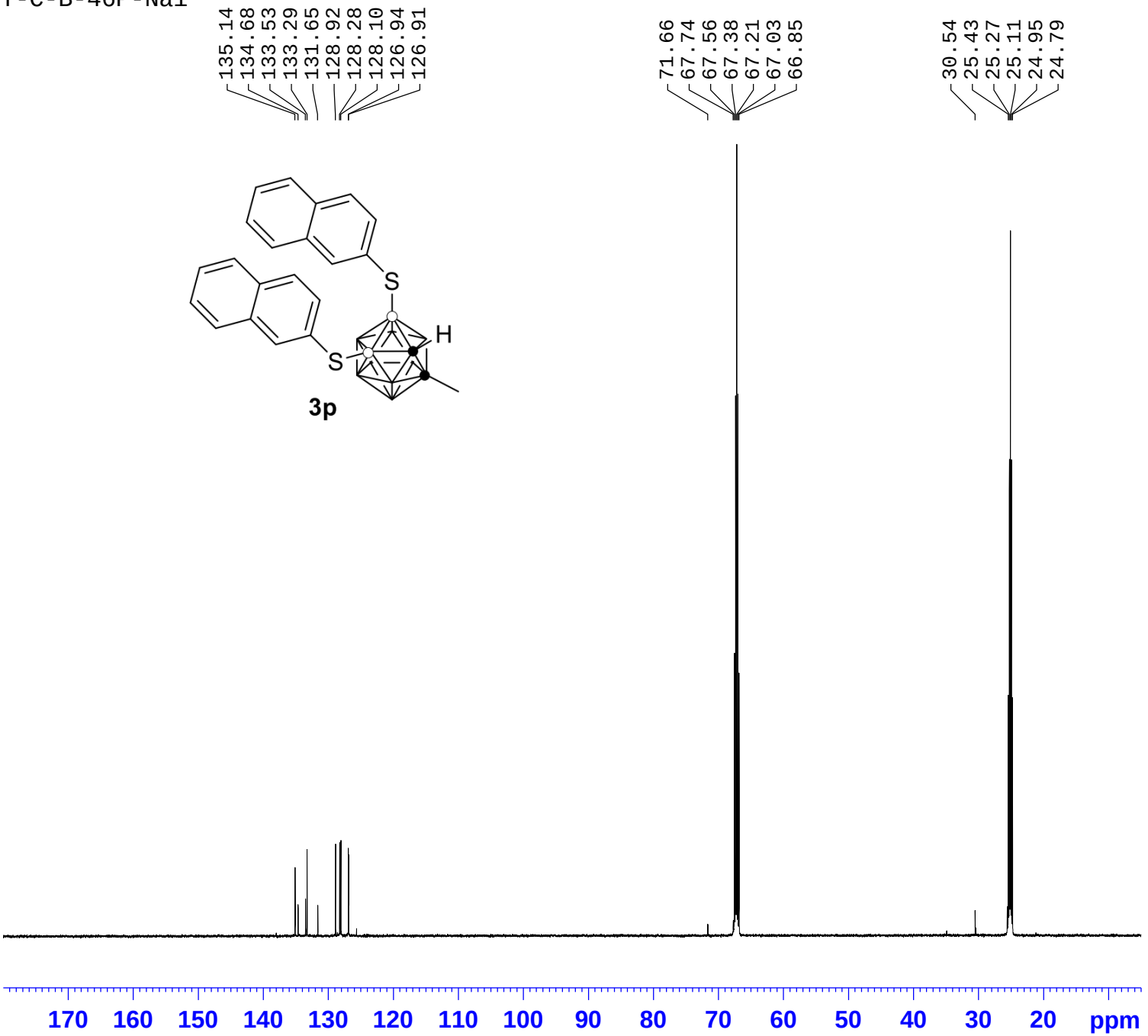
```
Current Data Parameters
NAME     CY-B-B-24p-furan-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180126
Time              19.39 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     26
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    228
DW                20.800 usec
DE                 6.50 usec
TE                 295.5 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

CY-H-B-46p

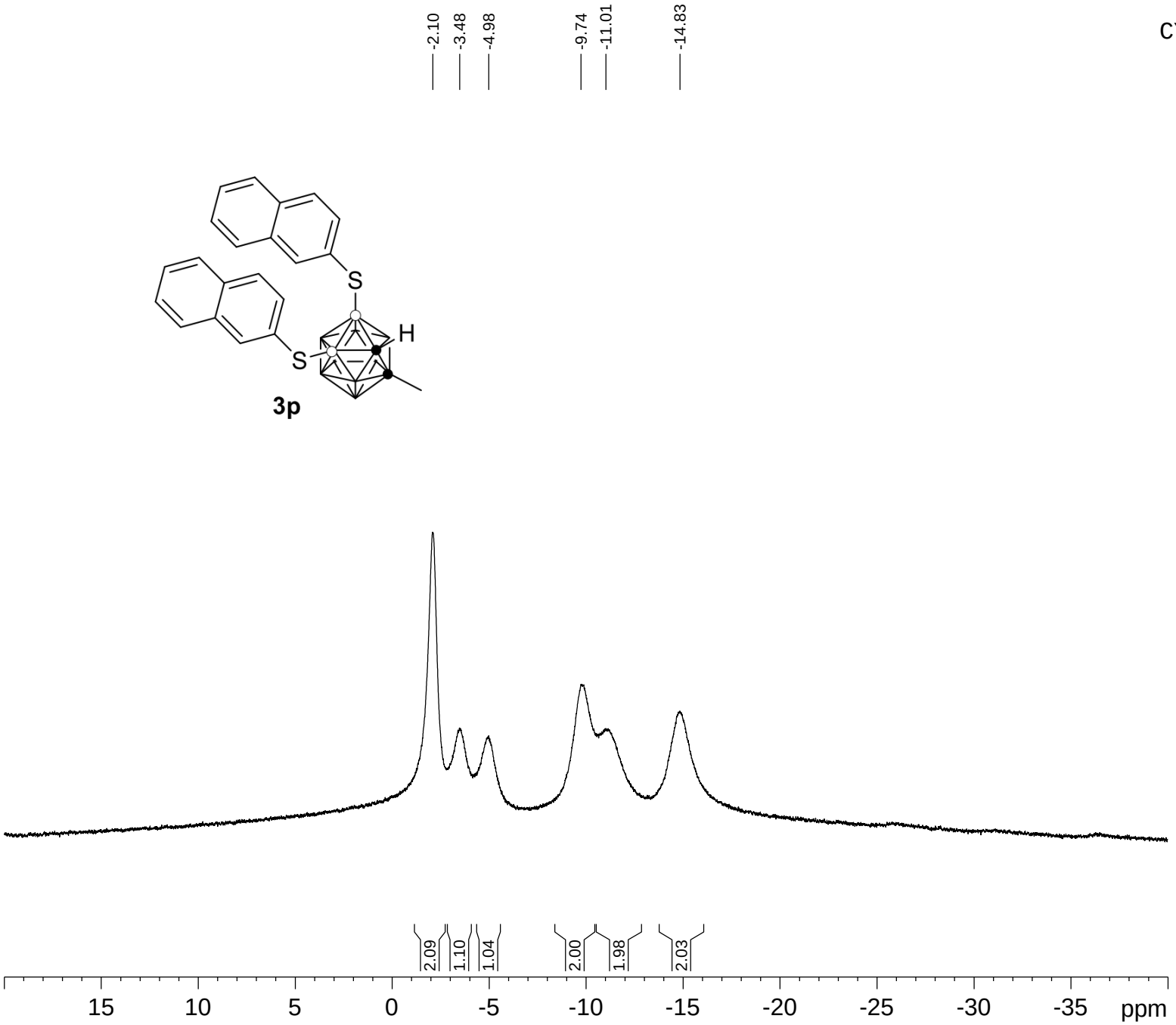



```
Current Data Parameters
NAME          CY-H-B-46p
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180411
Time              10.09 h
INSTRUM           spect
PROBHD   Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                   203
DW                62.400 usec
DE                 6.50 usec
TE                297.0 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1           8.31000042 W

F2 - Processing parameters
SI                 65536
SF           400.1300034 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

CY-C-B-46P-Nai

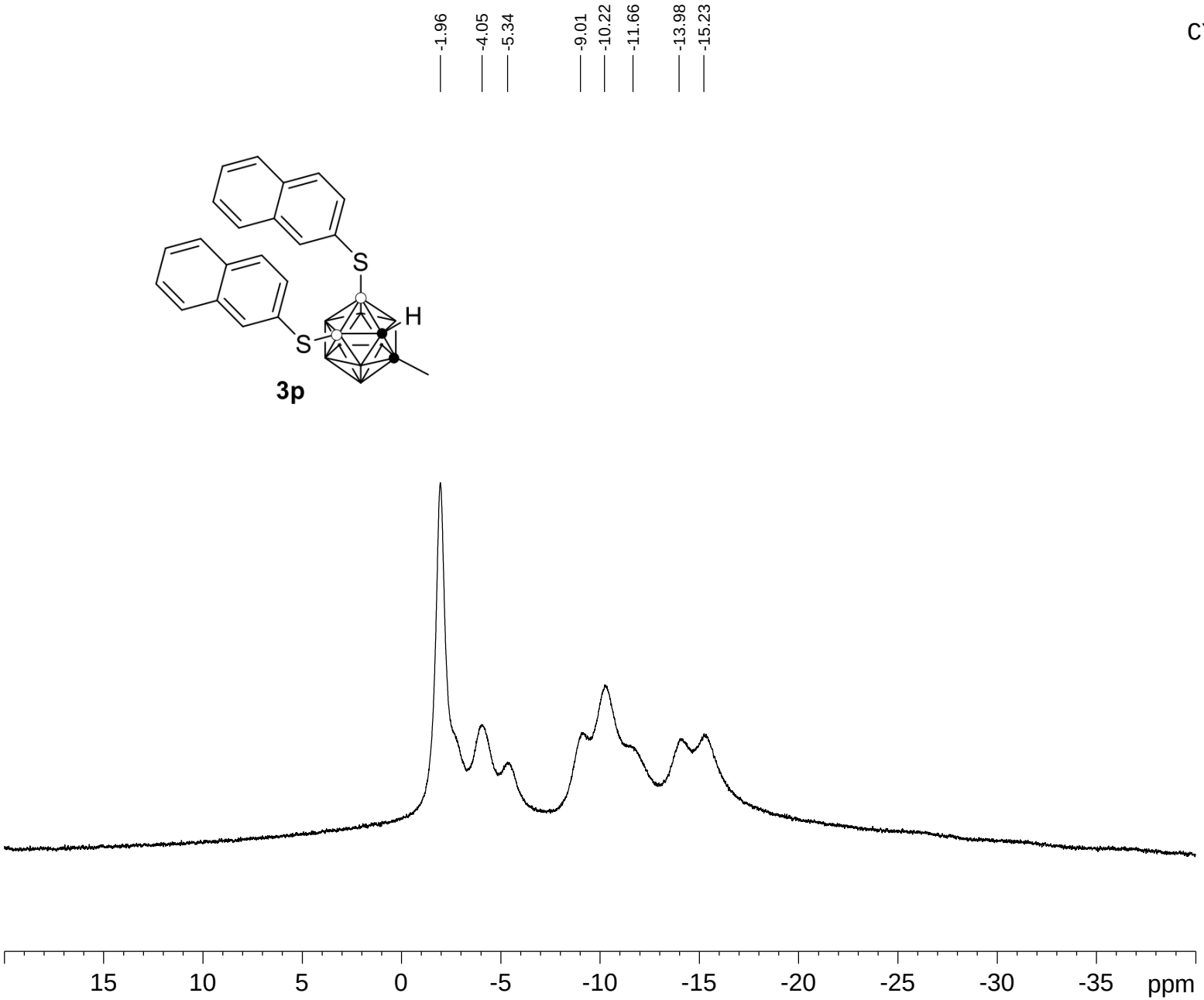



```
Current Data Parameters
NAME      CY-C-B-46P-Nai
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180416
Time               14.50 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT              THF
NS                   160
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ              1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P1                10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

F2 - Processing parameters
SI                 32768
SF           125.7576918 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



CY-B-B-46p-Nai

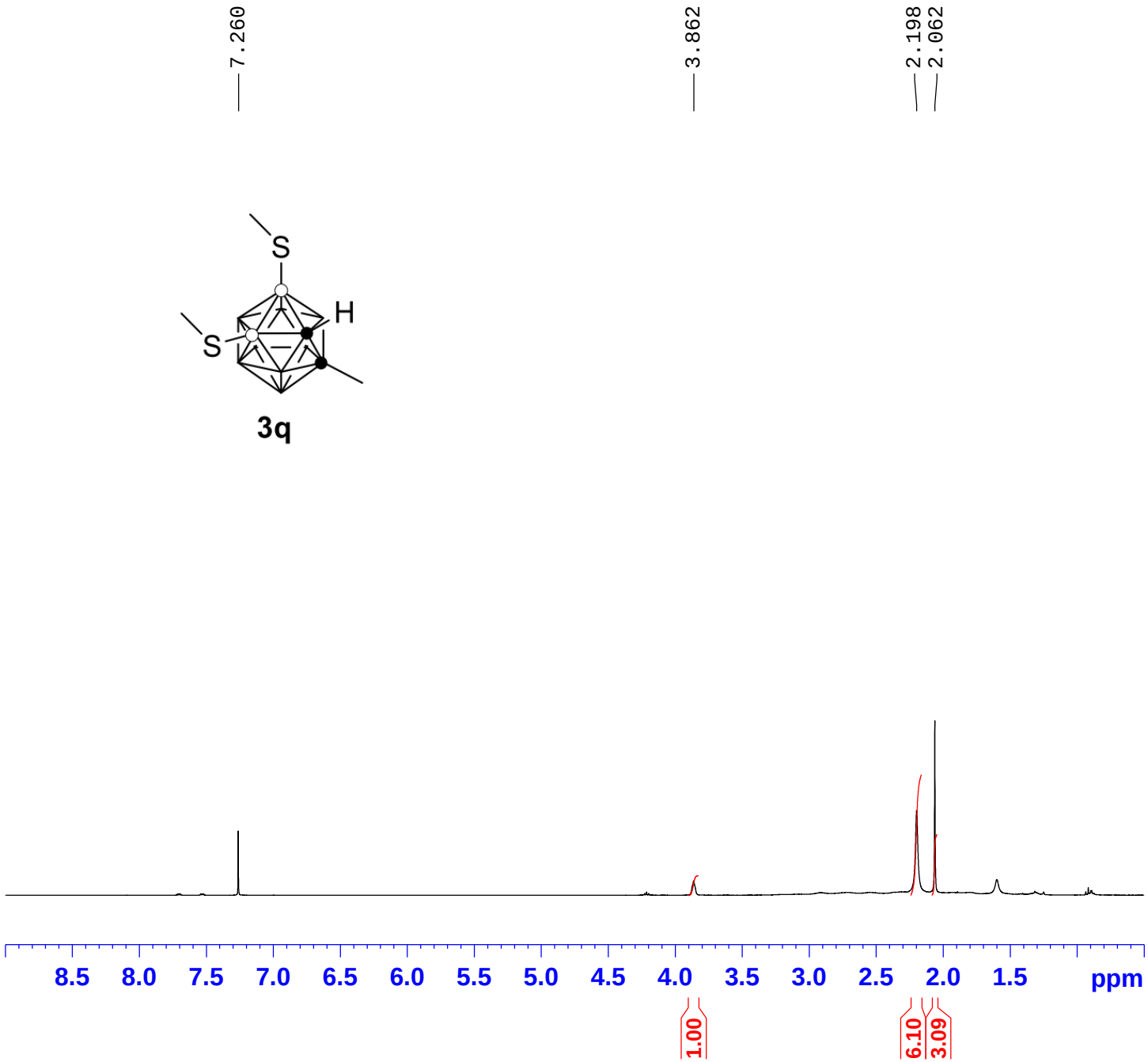
```
Current Data Parameters
NAME      CY-B-B-46p-Nai
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180413
Time               21.04 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG            zgdc
TD                65536
SOLVENT             THF
NS                   32
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  406
DW               20.800 usec
DE                6.50 usec
TE               295.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1               11B
P1                7.50 usec
PLW1         55.09999847 W
SFO2        400.2316009 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                32768
SF          128.4097615 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



CY-B-B-46p-Nai-(C)

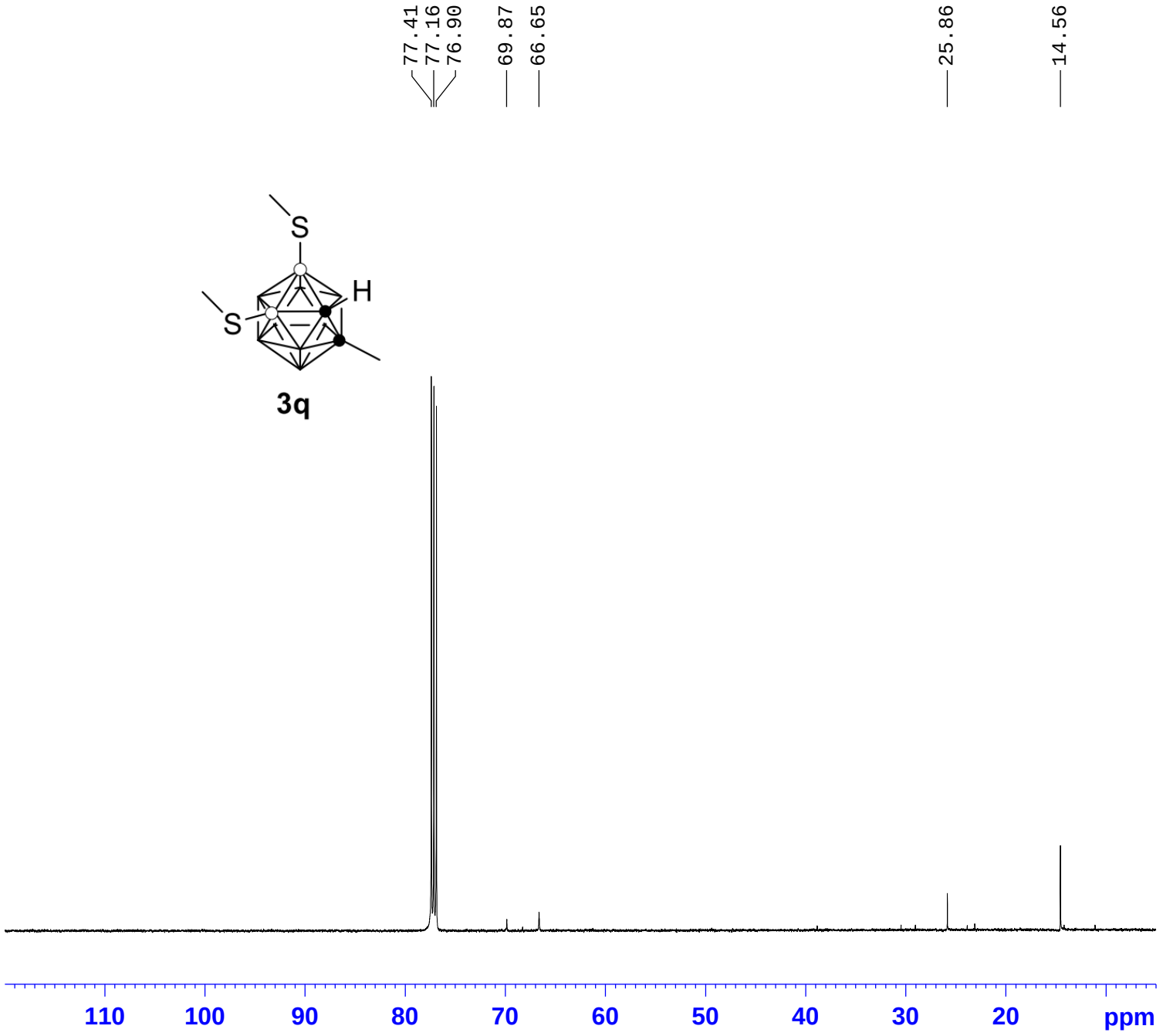
```
Current Data Parameters
NAME      CY-B-B-46p-Nai-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180413
Time                  21.08 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT                THF
NS                      52
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                     406
DW                  20.800 usec
DE                   6.50 usec
TE                  294.8 K
D1              2.00000000 sec
TD0                      1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                   32768
SF             128.4097430 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

CY-H-B-27p-Me

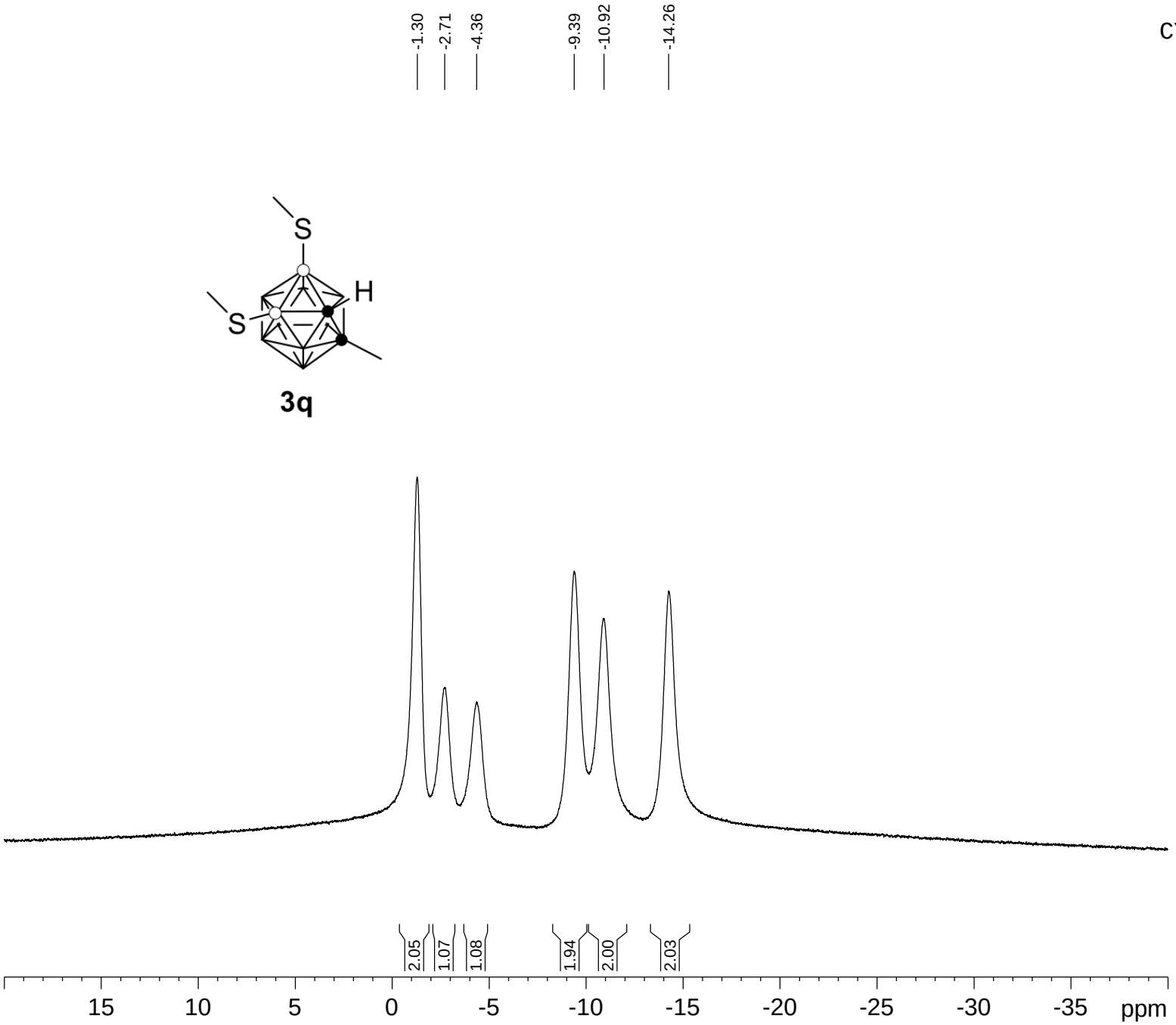



```
Current Data Parameters
NAME      CY-H-B-27p-Me
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20180226
Time             11.05 h
INSTRUM           spect
PROBHD   Z824601_0021 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            4.0894465 sec
RG                 203
DW               62.400 usec
DE                6.50 usec
TE               296.9 K
D1            1.00000000 sec
TD0                  1
SFO1        400.1324708 MHz
NUC1                1H
P1               15.00 usec
PLW1          8.31000042 W

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

CY-C-B-27P-Me

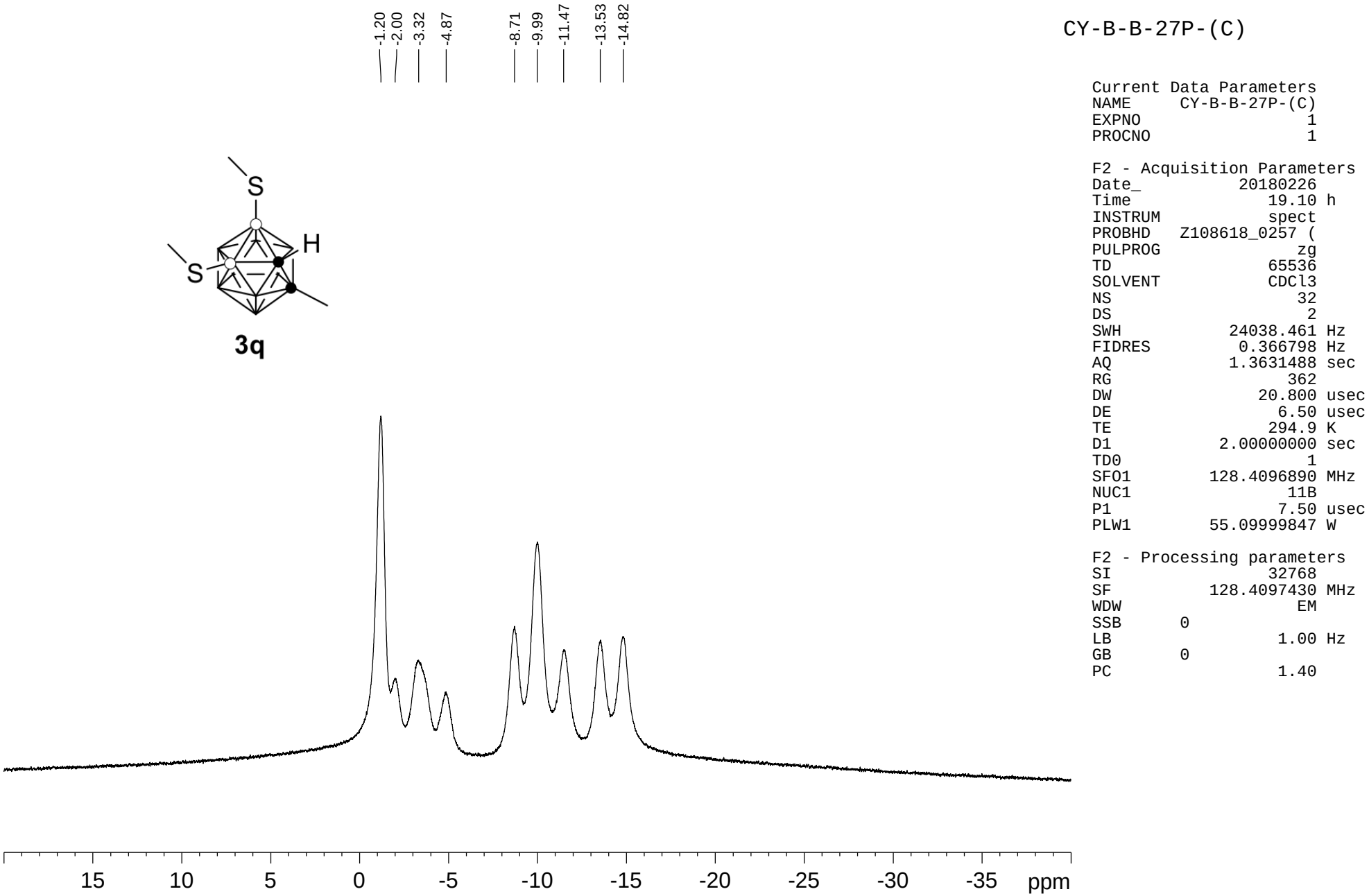



```
Current Data Parameters
NAME      CY-C-B-27P-Me
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20180226
Time              18.56 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

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



CY-B-B-27P

```
Current Data Parameters
NAME          CY-B-B-27P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180226
Time               19.15 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    52
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   362
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



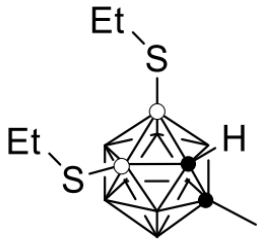
CY-B-B-27P-(C)

```
Current Data Parameters
NAME      CY-B-B-27P-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180226
Time                19.10 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    362
DW                 20.800 usec
DE                  6.50 usec
TE                 294.9 K
D1              2.00000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                  11B
P1                  7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                  32768
SF            128.4097430 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

CY-H-B-28p-Et

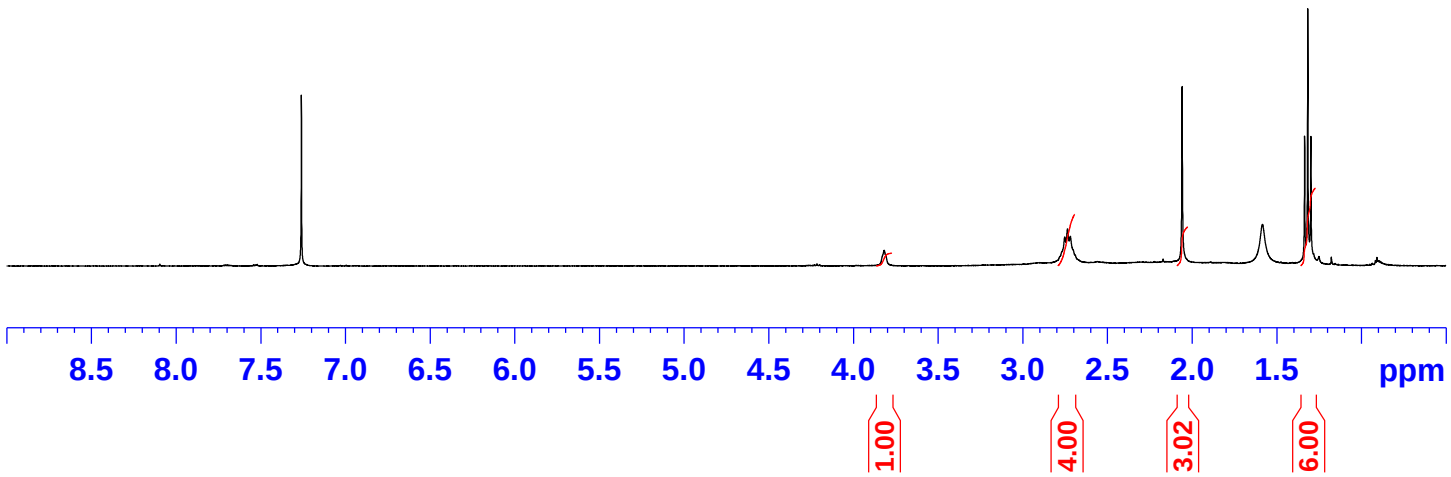
7.260

3.819
2.800
2.782
2.772
2.752
2.735
2.719
2.702
2.690
2.672
2.059
1.584
1.336
1.317
1.299

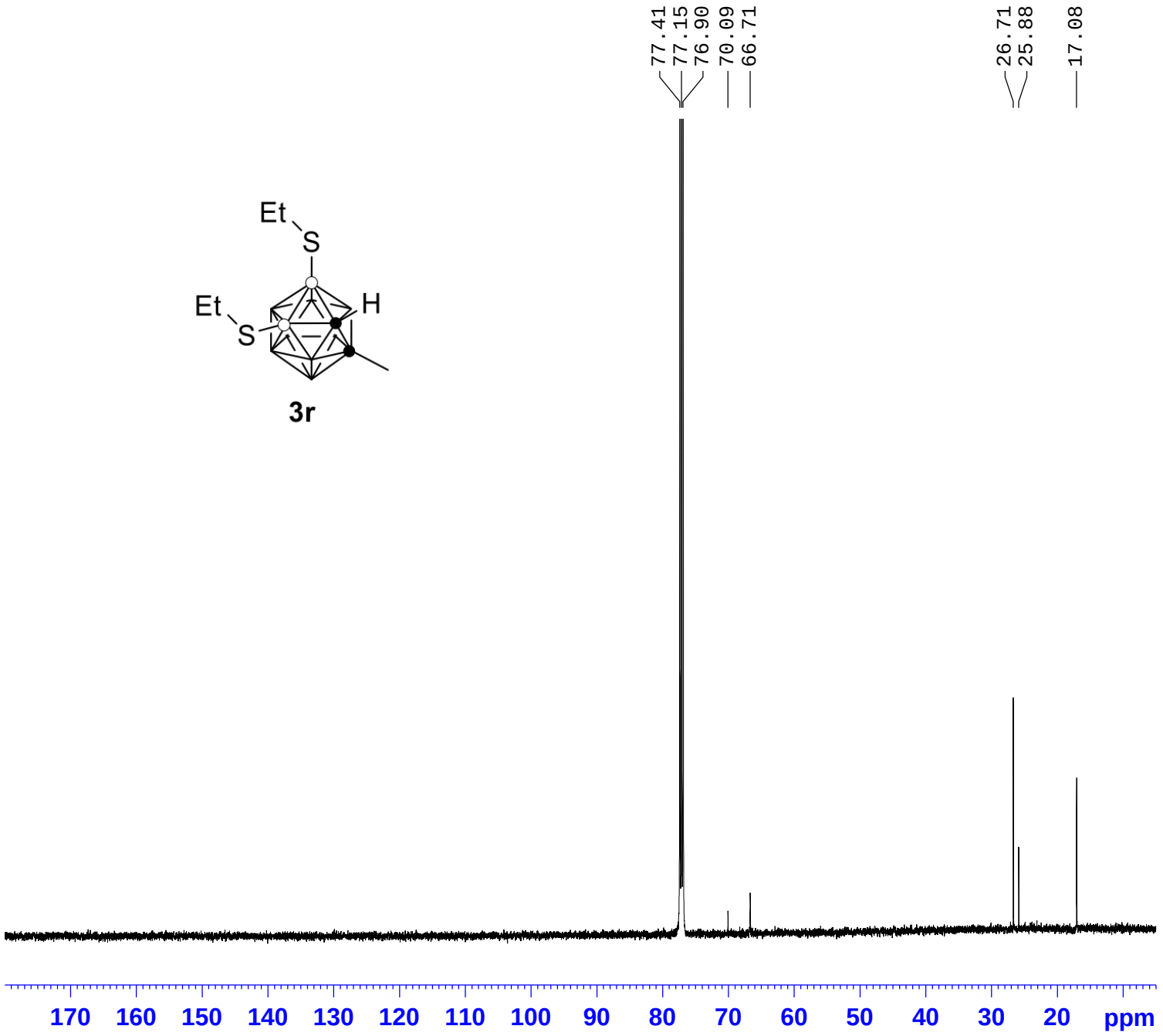


3r

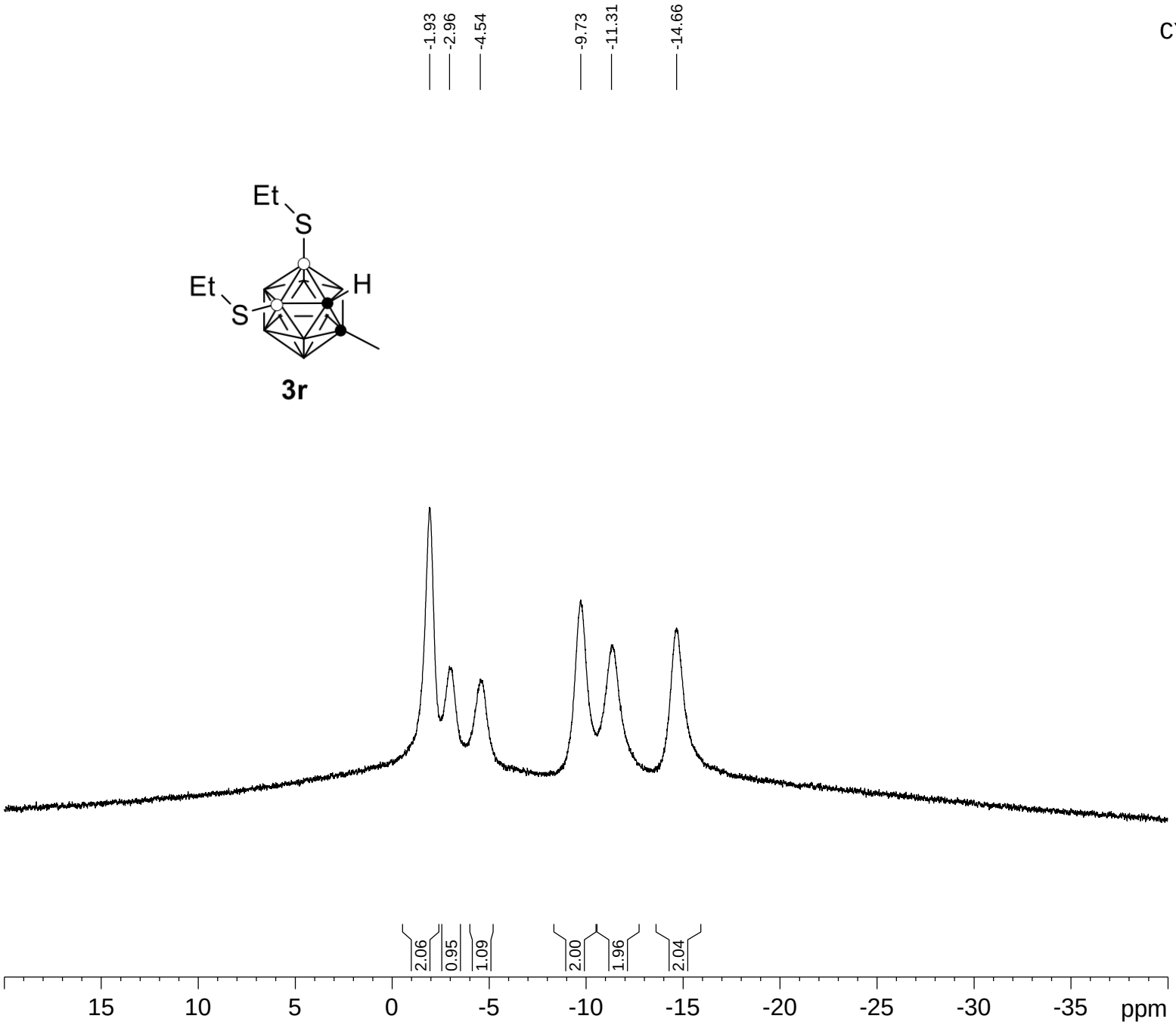
```
Current Data Parameters
NAME      CY-H-B-28p-Et
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20180228
Time               9.53 h
INSTRUM           spect
PROBHD   Z824601_0021 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  12
DS                   2
SWH           8012.820 Hz
FIDRES        0.244532 Hz
AQ            4.0894465 sec
RG                 203
DW               62.400 usec
DE                6.50 usec
TE               296.6 K
D1            1.00000000 sec
TD0                  1
SFO1        400.1324708 MHz
NUC1               1H
P1               15.00 usec
PLW1          8.31000042 W

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



CY-C-B-28P-Et

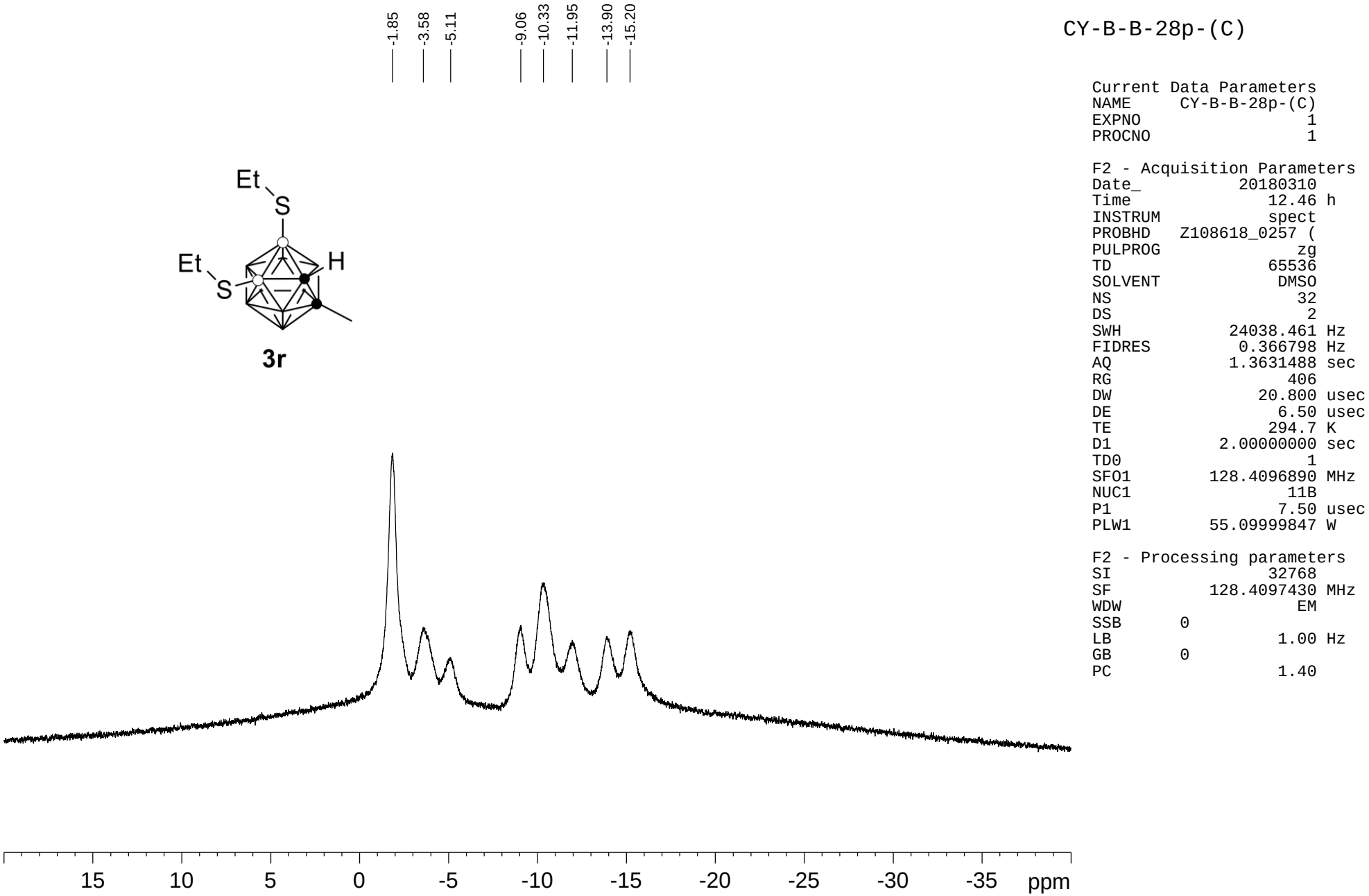



```
Current Data Parameters
NAME      CY-C-B-28P-Et
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20180306
Time              23.32 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7577722 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```



CY-B-B-28p

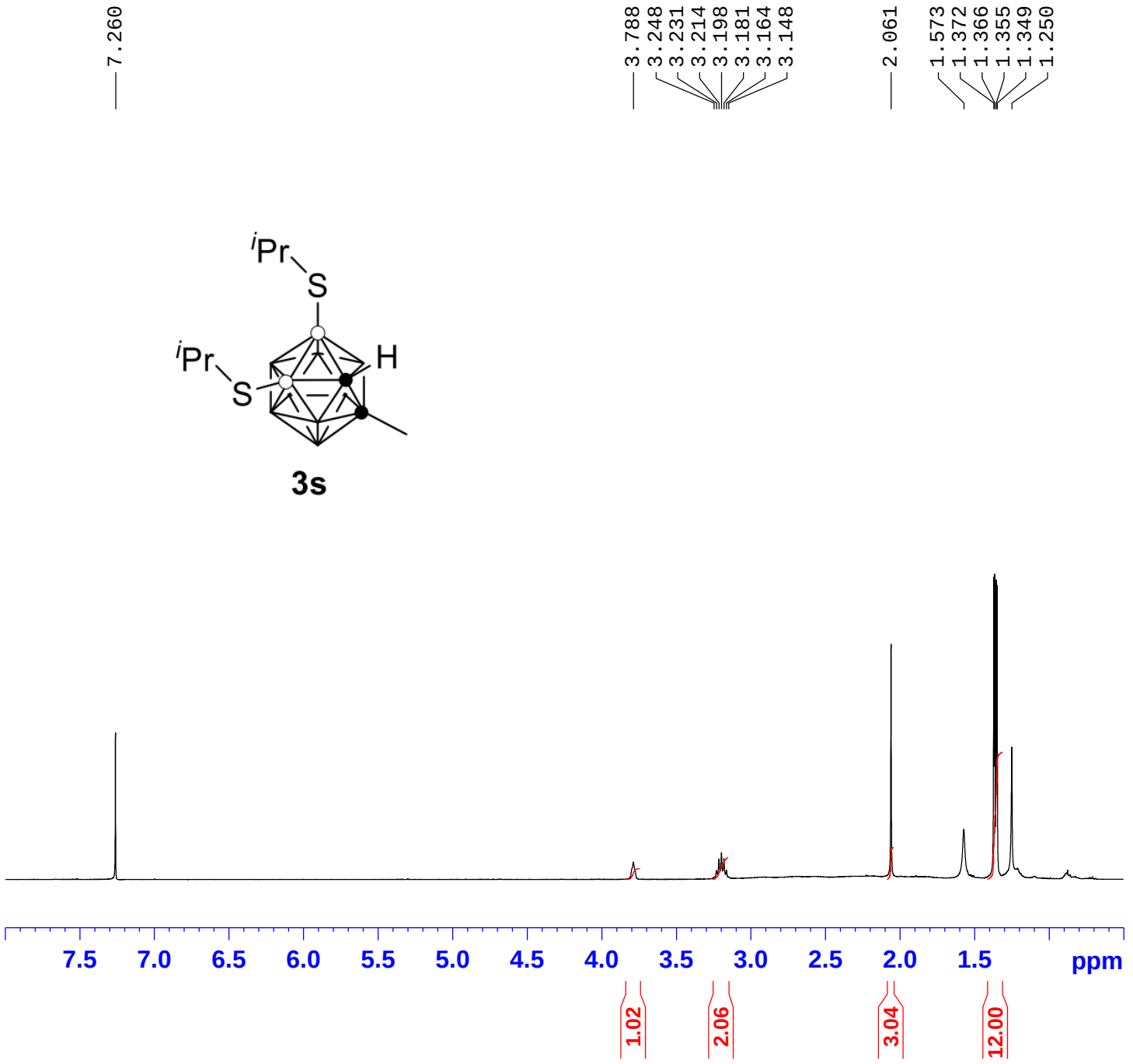
```
Current Data Parameters
NAME          CY-B-B-28p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180310
Time               12.49 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT             DMSO
NS                    40
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   406
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```



CY-B-B-28p-(C)

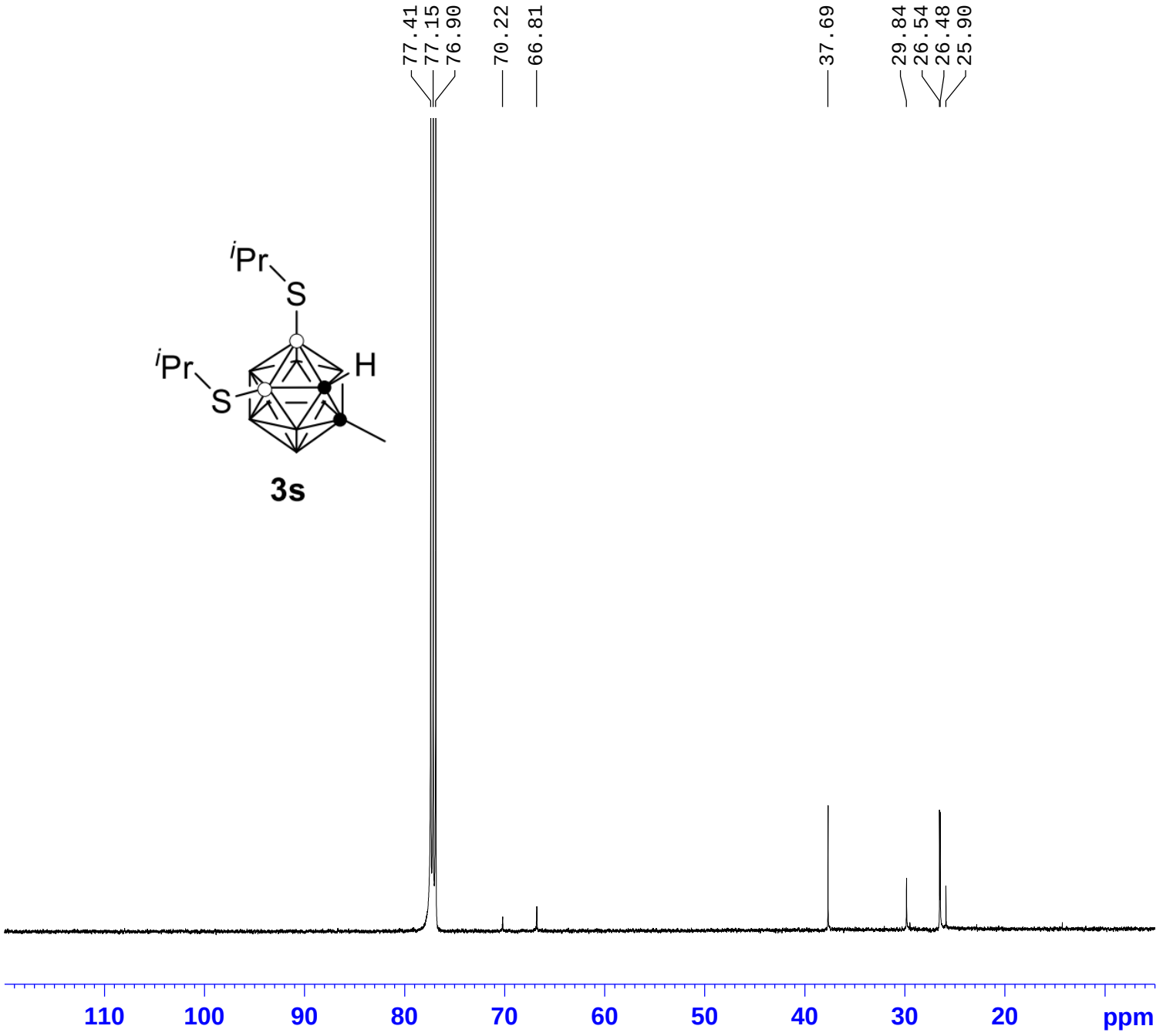
```
Current Data Parameters
NAME      CY-B-B-28p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180310
Time                12.46 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT              DMSO
NS                     32
DS                      2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                    406
DW                20.800 usec
DE                 6.50 usec
TE                294.7 K
D1             2.00000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                  11B
P1                 7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                  32768
SF            128.4097430 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

CY-H-B-33p-iPr

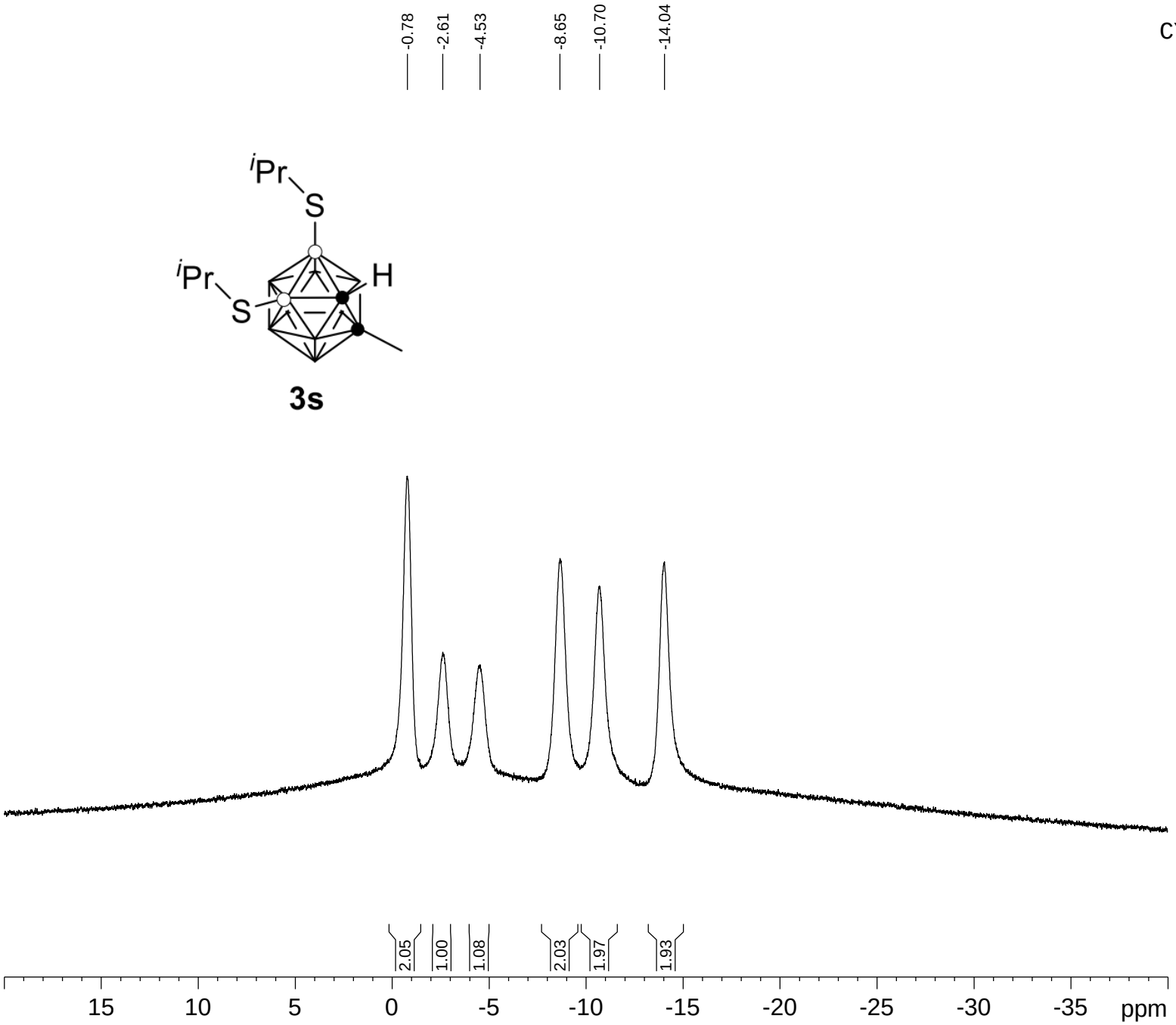



```
Current Data Parameters
NAME      CY-H-B-33p-iPr
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180303
Time                14.25 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ               4.0894465 sec
RG                    203
DW                 62.400 usec
DE                  6.50 usec
TE                 297.0 K
D1            1.00000000 sec
TD0                     1
SFO1         400.1324708 MHz
NUC1                   1H
P1                 15.00 usec
PLW1          8.31000042 W

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

CY-C-B-33P-iPr

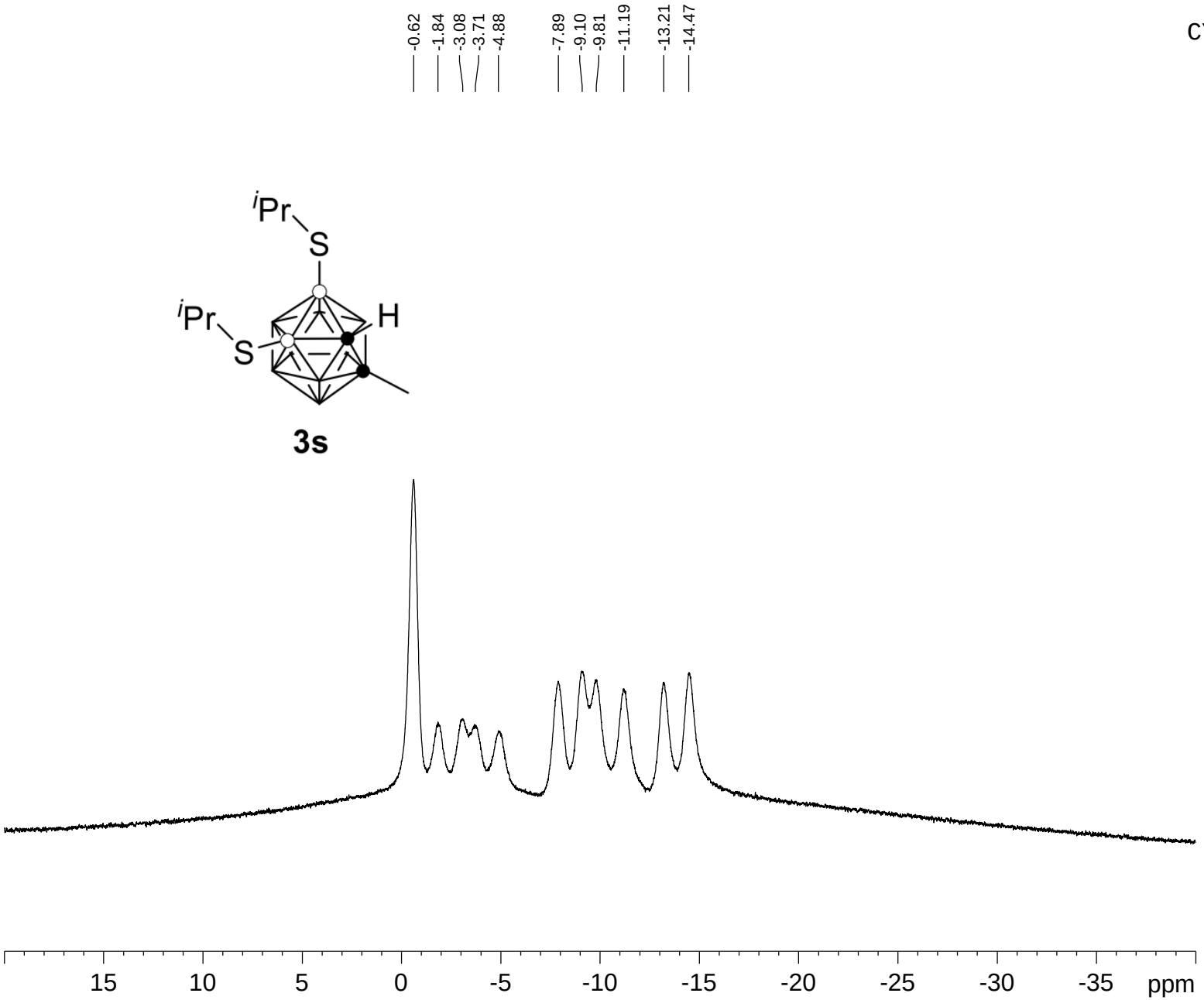



```
Current Data Parameters
NAME      CY-C-B-33P-iPr
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180303
Time              16.31 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  900
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

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



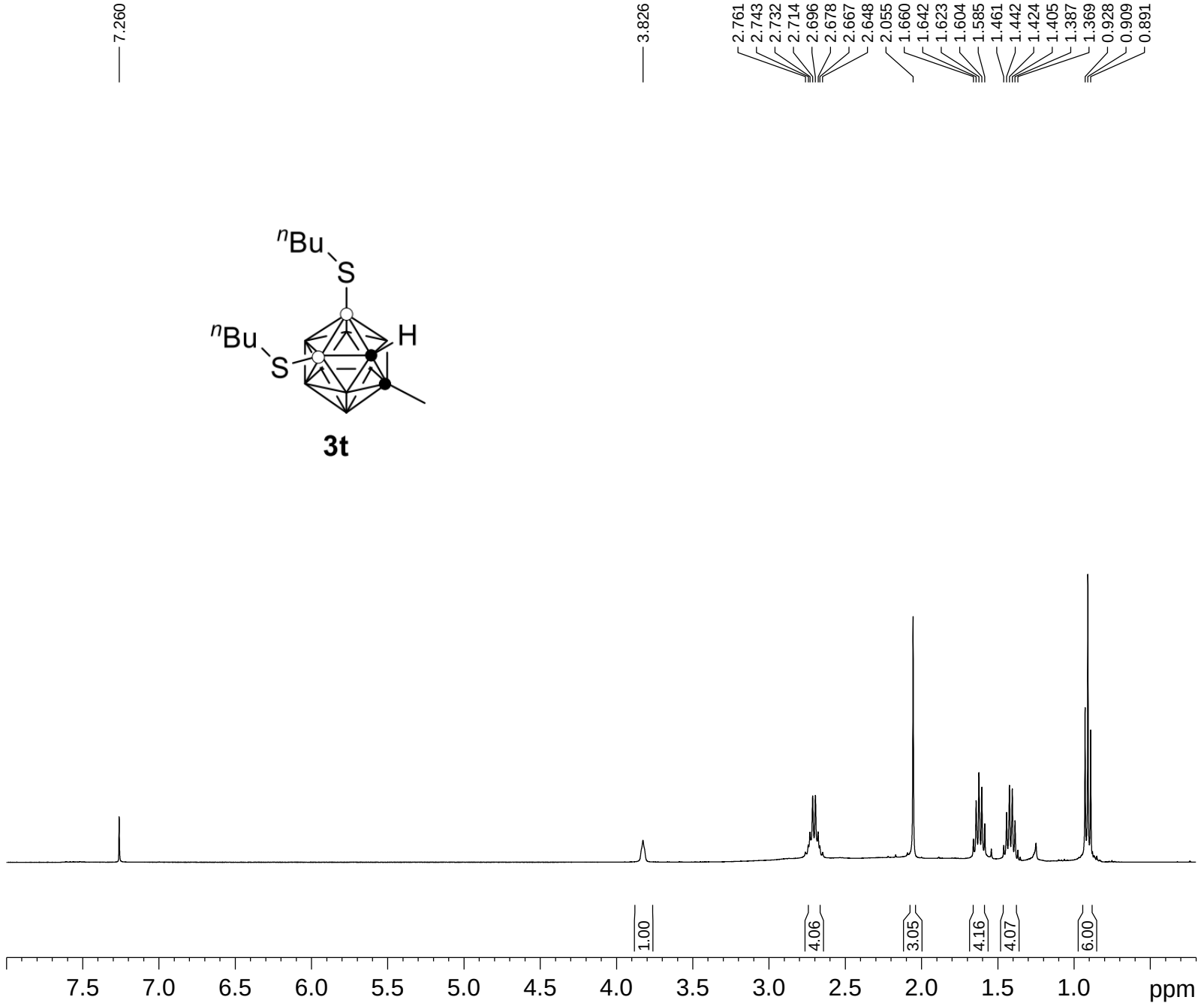
CY-B-B-33p-iPr

```
Current Data Parameters
NAME      CY-B-B-33p-iPr
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180303
Time               10.21 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    48
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   322
DW                20.800 usec
DE                 6.50 usec
TE                295.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



CY-B-B-33p-iPr-(C)

```
Current Data Parameters
NAME      CY-B-B-33p-iPr-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180303
Time                 10.24 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      72
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     322
DW                  20.800 usec
DE                   6.50 usec
TE                  294.9 K
D1             2.00000000 sec
TD0                      1
SFO1          128.4096890 MHz
NUC1                  11B
P1                   7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                   32768
SF            128.4097430 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

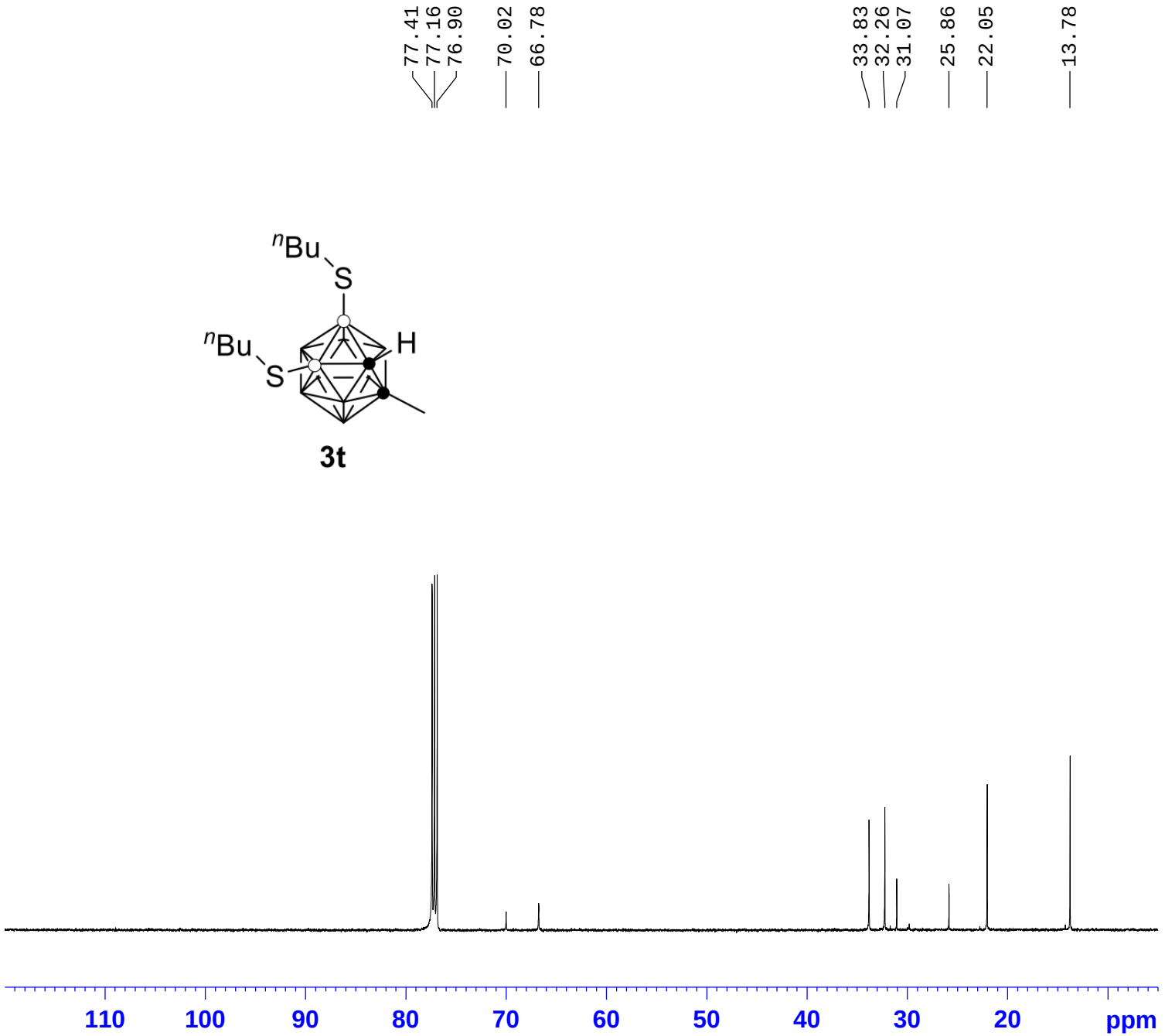


Current Data Parameters
NAME CY-H-B-26p-nBu
EXPNO 1
PROCNO 1

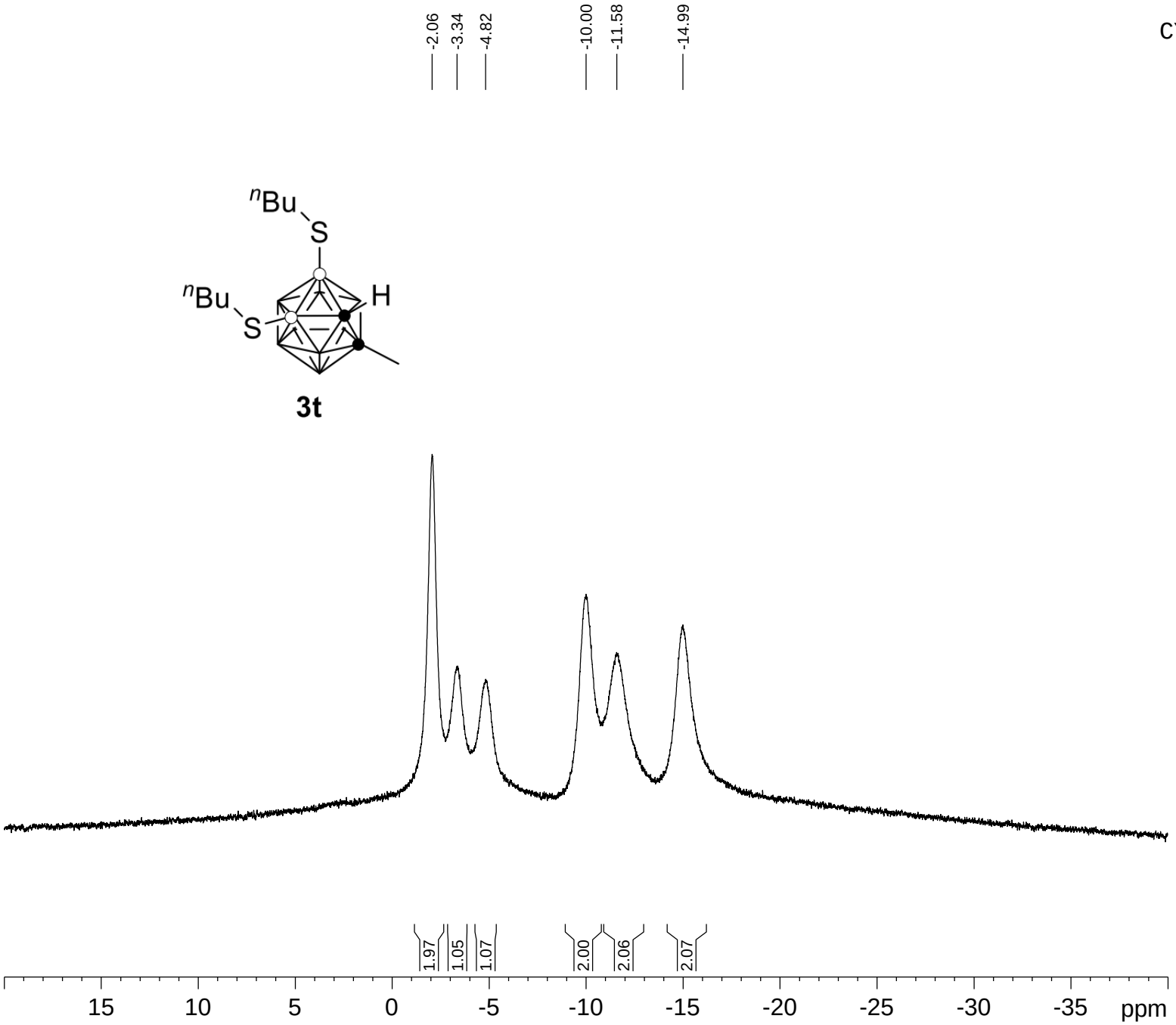
F2 - Acquisition Parameters
Date_ 20180130
Time 19.44 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-26P-nBu

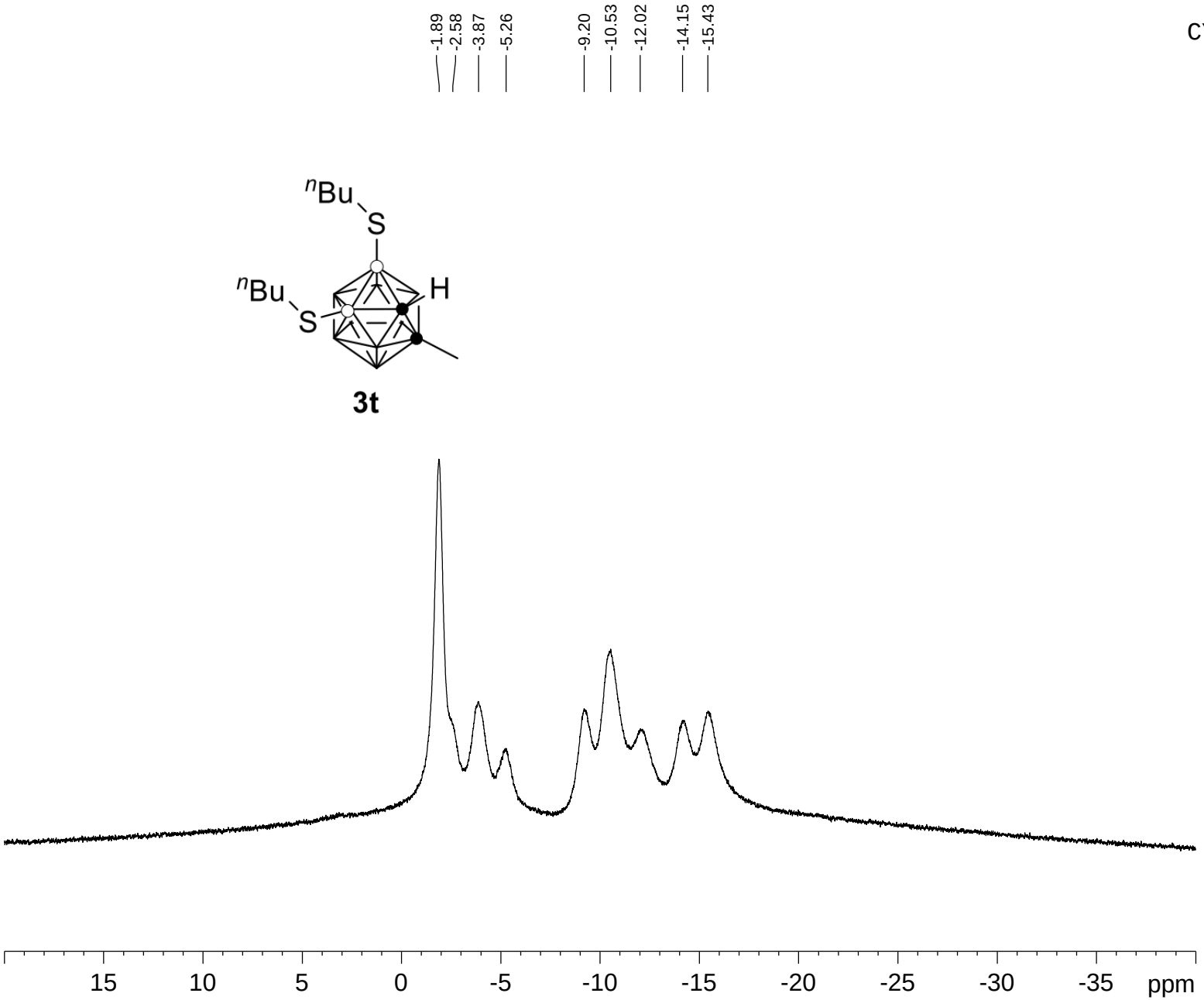



```
Current Data Parameters
NAME      CY-C-B-26P-nBu
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180131
Time               9.52 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  272
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7577739 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```



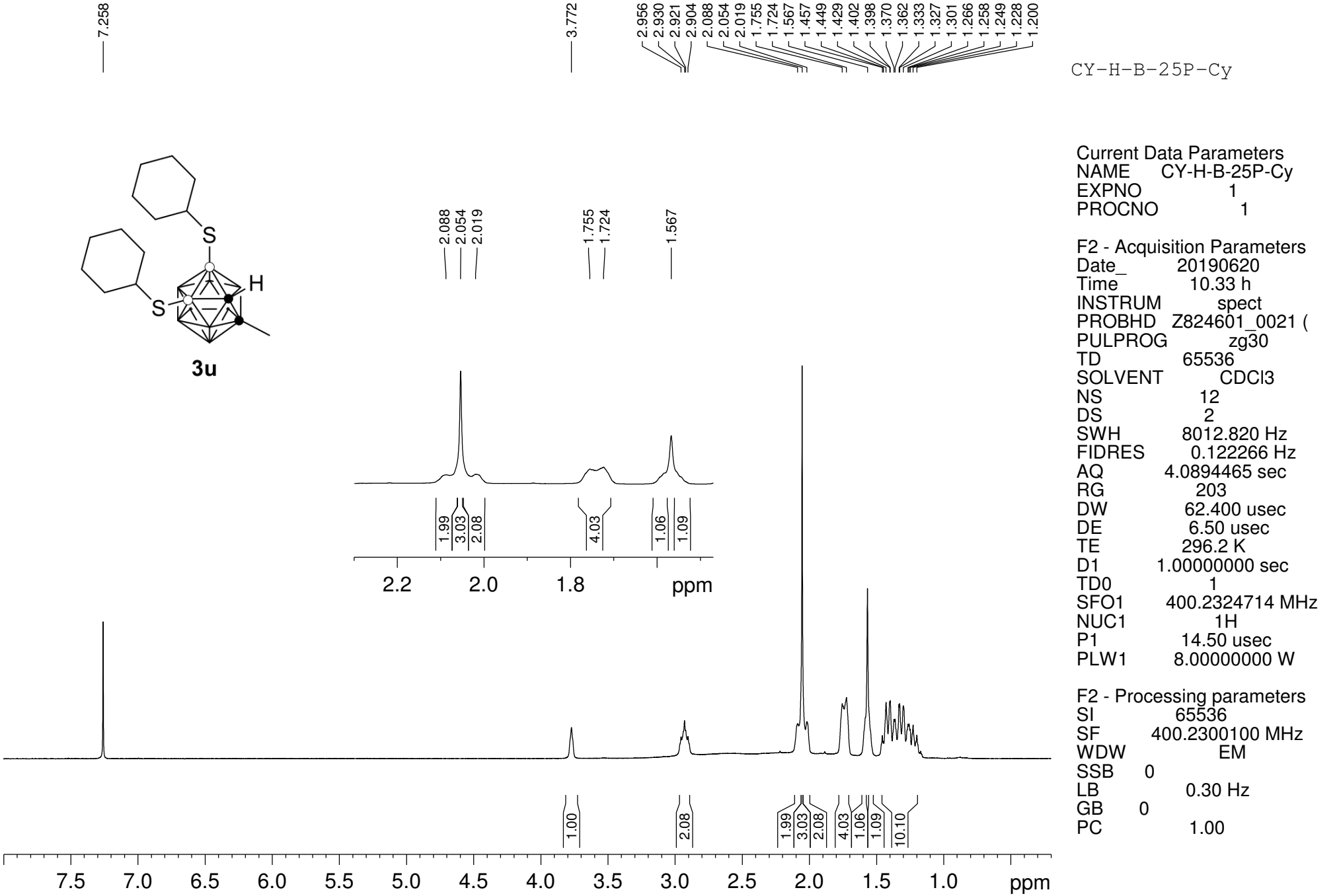
CY-B-B-26p-nBu

```
Current Data Parameters
NAME      CY-B-B-26p-nBu
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180126
Time               22.20 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    19
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   362
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



CY-B-B-26p-nBu-(C)

```
Current Data Parameters
NAME      CY-B-B-26p-nBu-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180126
Time                  22.23 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                       35
DS                        2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                      362
DW                  20.800 usec
DE                   6.50 usec
TE                  295.5 K
D1              2.00000000 sec
TD0                       1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                    32768
SF             128.4097430 MHz
WDW                      EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

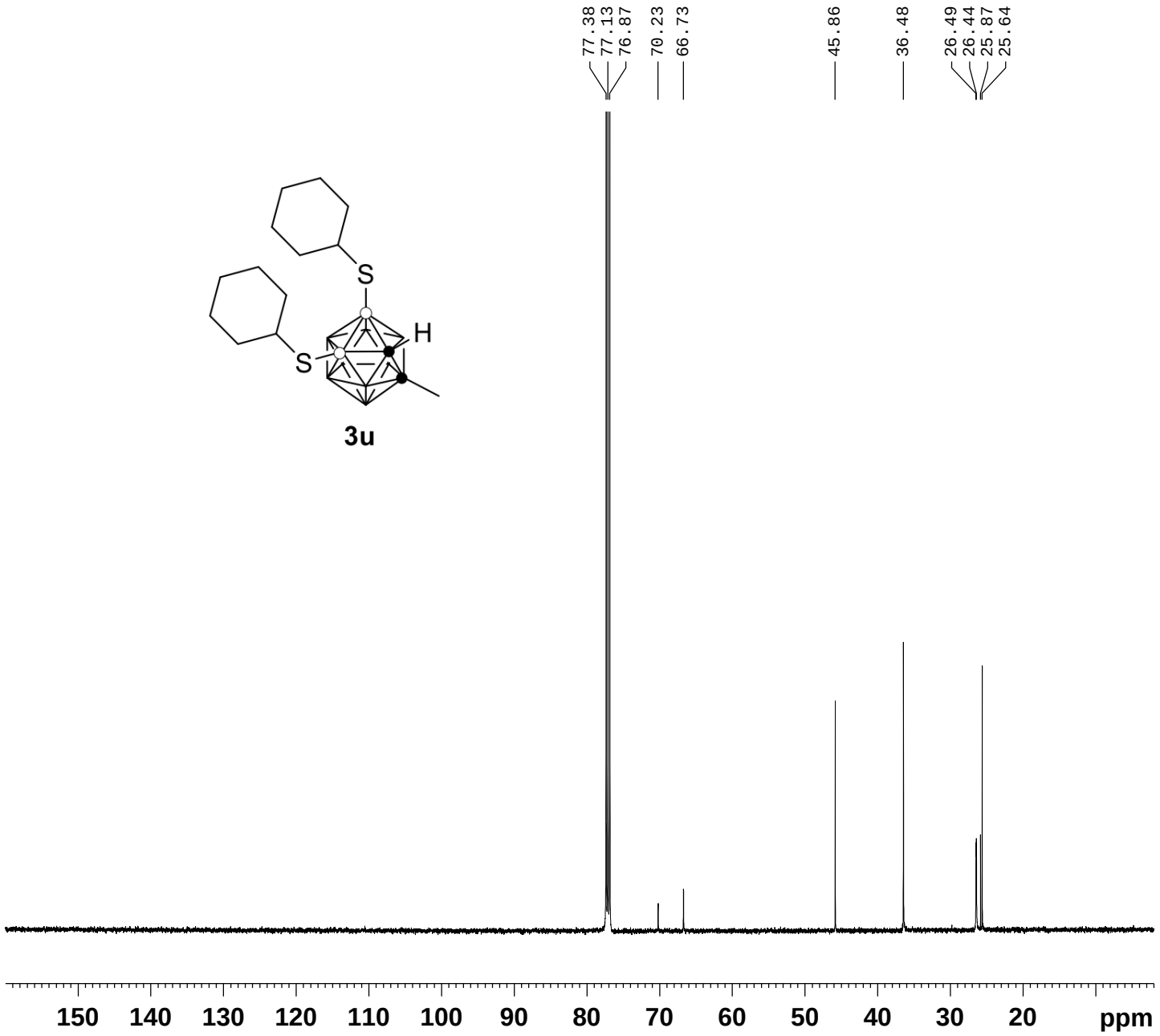


Current Data Parameters
NAME CY-H-B-25P-Cy
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190620
Time 10.33 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 14.50 usec
PLW1 8.00000000 W

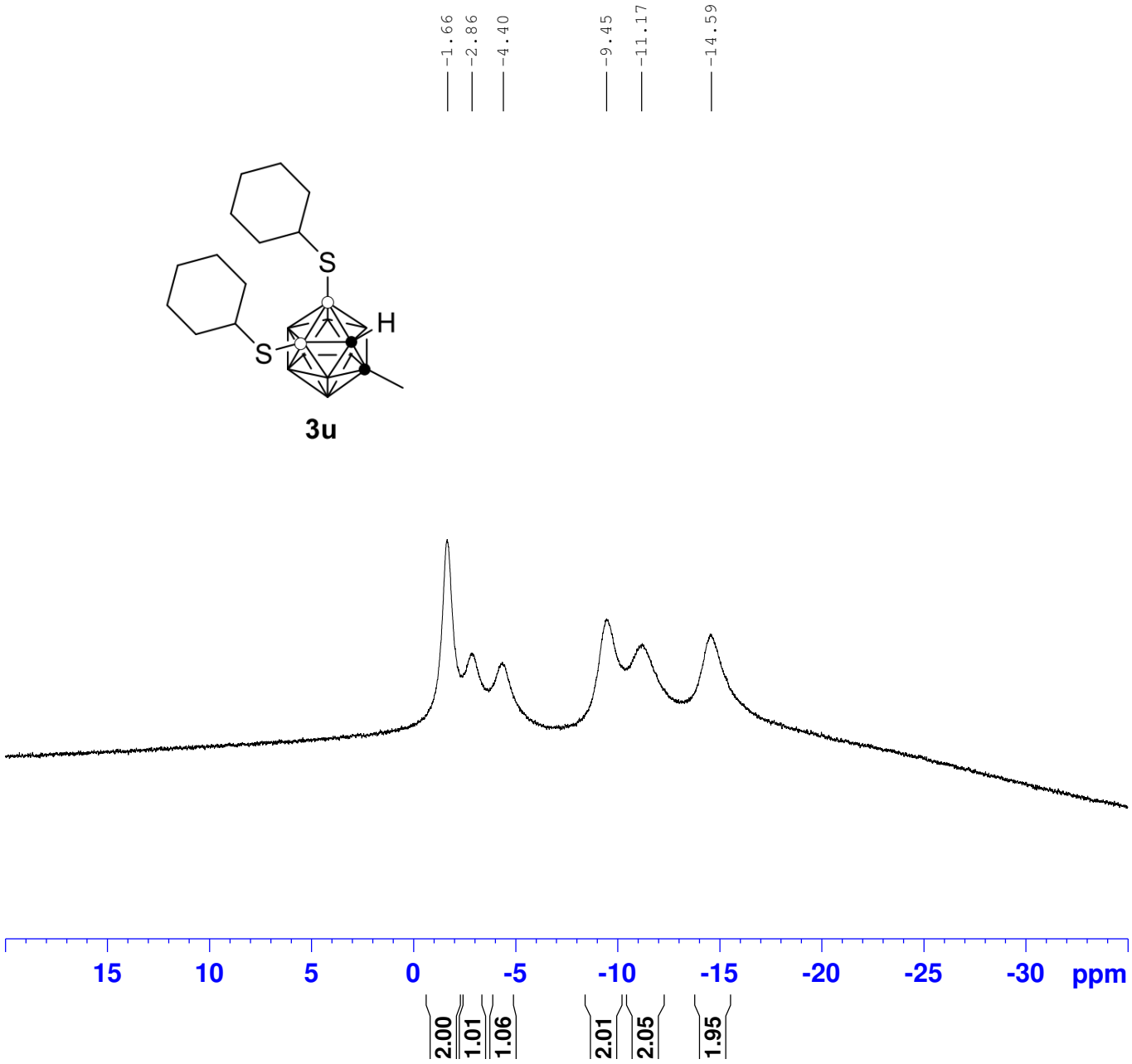
F2 - Processing parameters
SI 65536
SF 400.2300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-25P-Cy



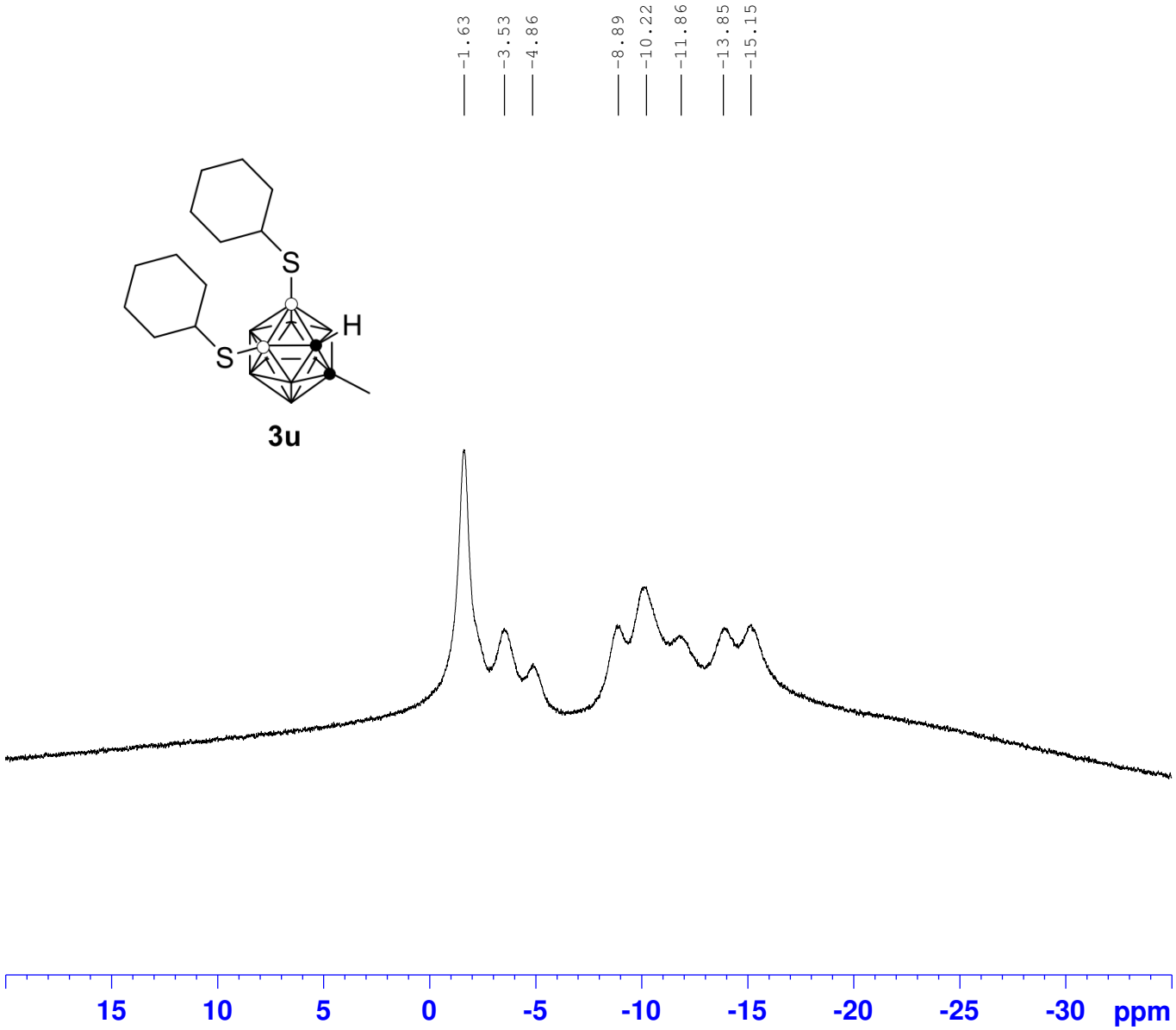

```
Current Data Parameters
NAME      CY-C-B-25P-Cy
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20190620
Time              20.02 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  408
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7577760 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

CY-B-B-25P-Cy

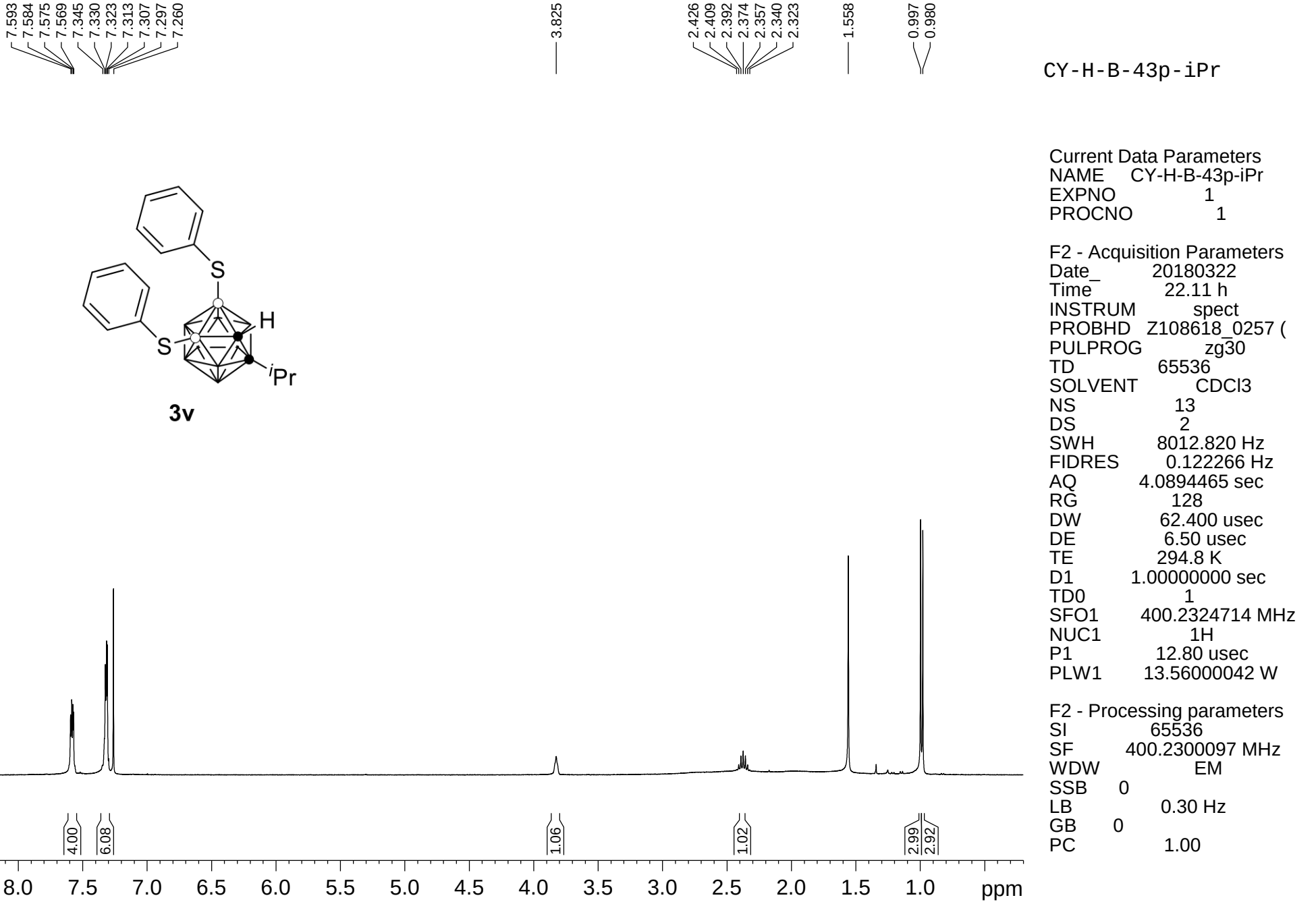



```
Current Data Parameters
NAME      CY-B-B-25P-Cy
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20190620
Time             10.48 h
INSTRUM           spect
PROBHD   Z820201_0170 (
PULPROG           zgig
TD               65536
SOLVENT          CDCl3
NS                  64
DS                   4
SWH          25510.203 Hz
FIDRES        0.778510 Hz
AQ            1.2845056 sec
RG                 181
DW              19.600 usec
DE               6.50 usec
TE              296.5 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1       128.3776050 MHz
NUC1               11B
P1              28.50 usec
PLW1       14.79100037 W
SFO2       400.1324710 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2       13.17000008 W
PLW12       0.07408100 W

F2 - Processing parameters
SI                32768
SF         128.3776052 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

CY-B-B-25P-Cy-(C)



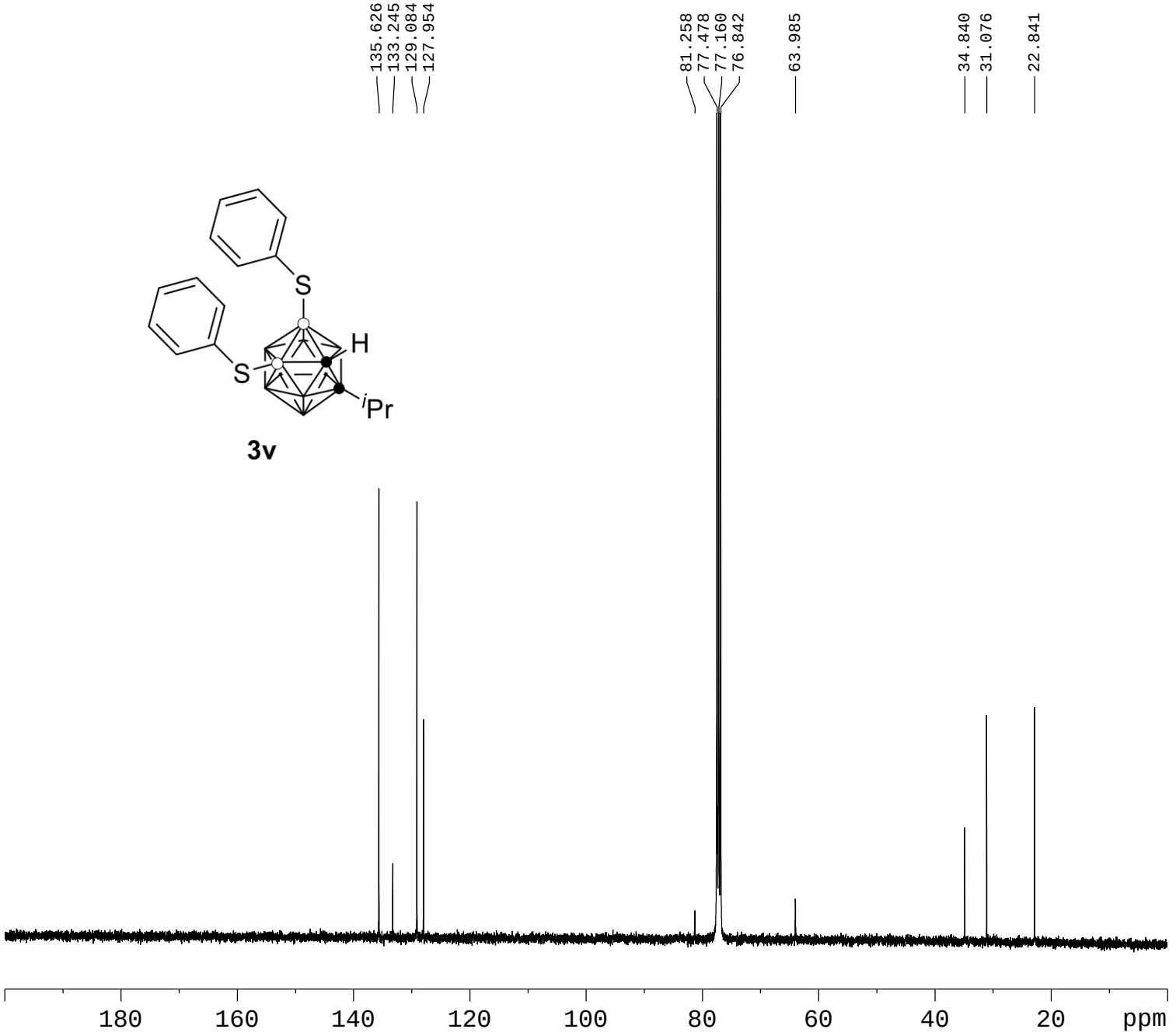

```
Current Data Parameters
NAME      CY-B-B-25P-Cy-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20190620
Time               10.52 h
INSTRUM             spect
PROBHD   Z820201_0170 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     92
DS                      4
SWH            25510.203 Hz
FIDRES          0.778510 Hz
AQ             1.2845056 sec
RG                    203
DW                19.600 usec
DE                 6.50 usec
TE                 296.5 K
D1           1.00000000 sec
TD0                     1
SFO1         128.3776050 MHz
NUC1                  11B
P1                 28.50 usec
PLW1         14.79100037 W

F2 - Processing parameters
SI                  32768
SF           128.3776052 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



Current Data Parameters
NAME CY-H-B-43p-iPr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180322
Time 22.11 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 13
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



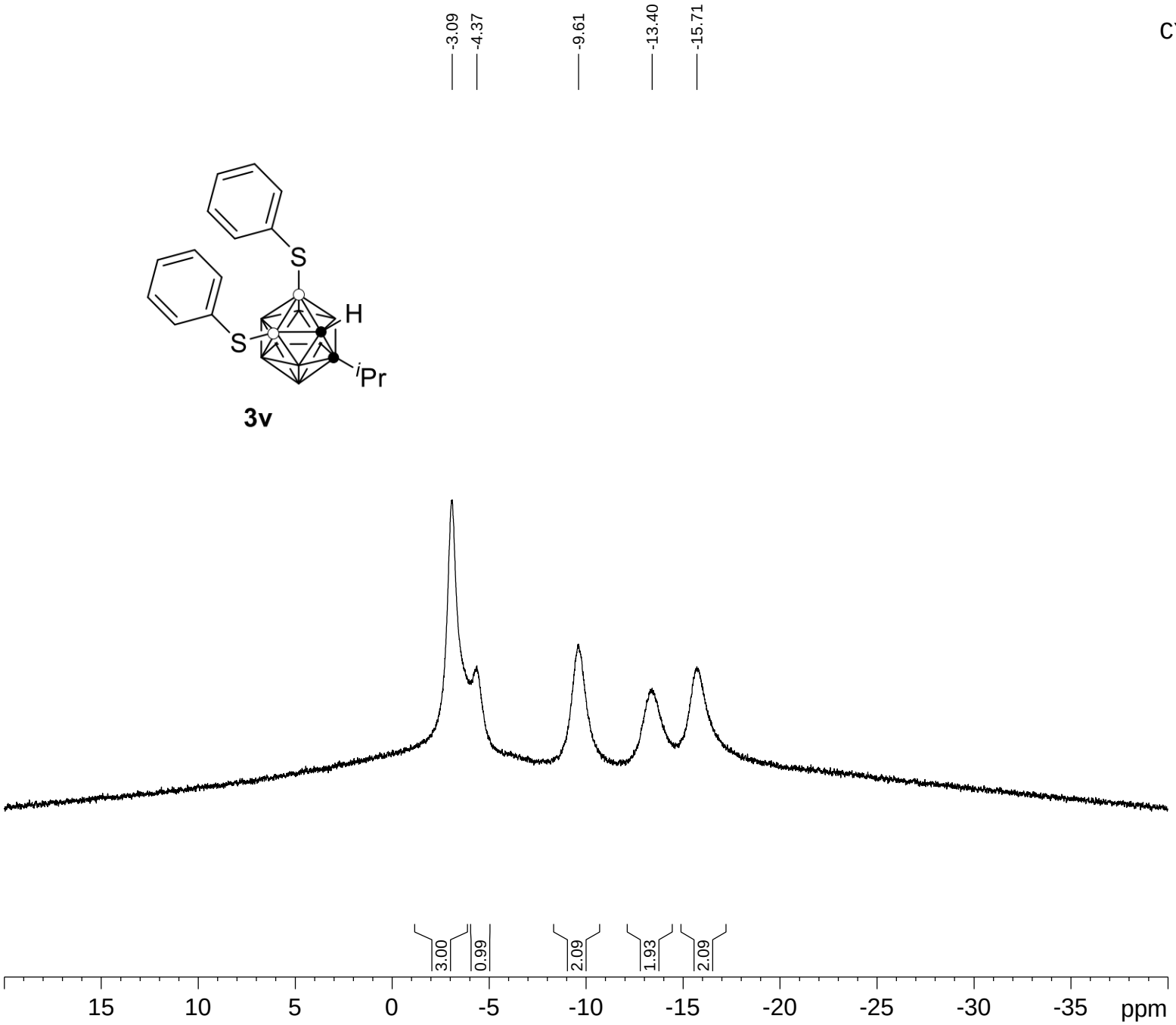
CY-C-B-43P-iPr

Bruker Advance III 400

Current Data Parameters
NAME CY-C-B-43P-iPr
EXPNO 1
PROCNO 1

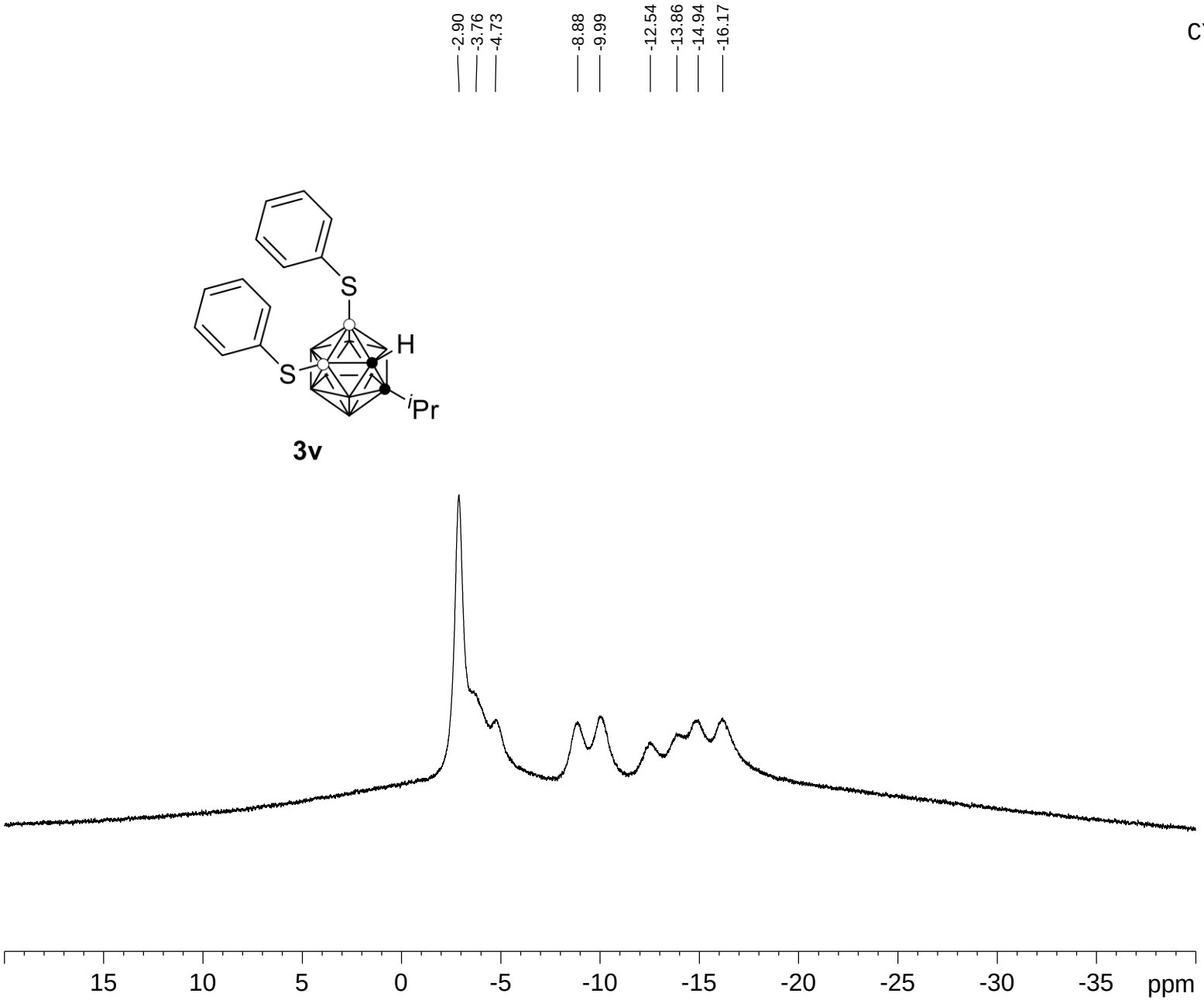
F2 - Acquisition Parameters
Date_ 20180324
Time 8.43 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9435
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W

F2 - Processing parameters
SI 32768
SF 100.6127547 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



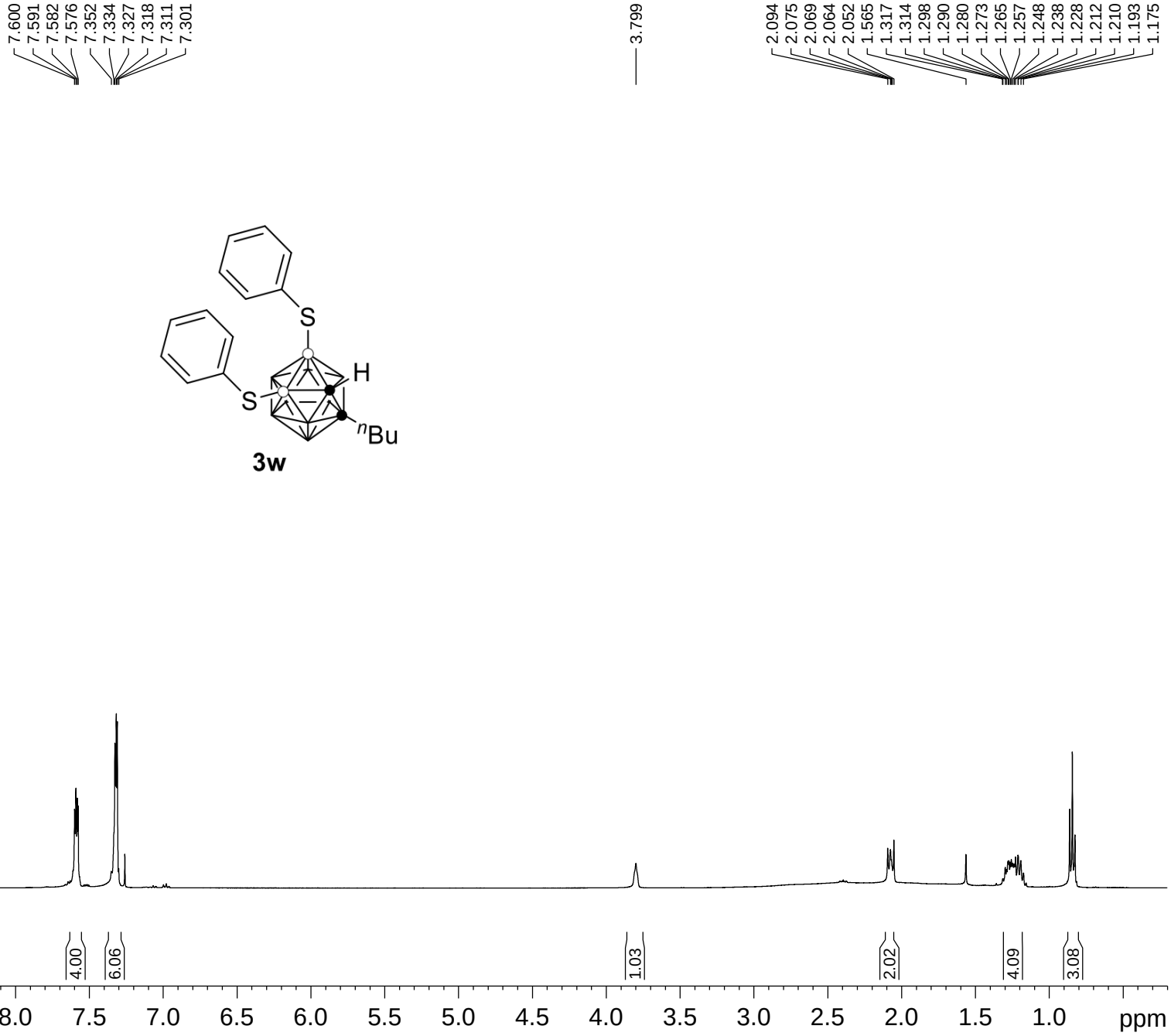
CY-B-B-43p-iPr

```
Current Data Parameters
NAME      CY-B-B-43p-iPr
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180322
Time                22.14 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     46
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    456
DW                 20.800 usec
DE                  6.50 usec
TE                 295.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                11B
P1                  7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                  32768
SF           128.4097615 MHz
WDW                 EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



CY-B-B-43p-iPr-(C)

```
Current Data Parameters
NAME      CY-B-B-43p-iPr-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180322
Time                  22.19 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                       94
DS                        2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                      406
DW                   20.800 usec
DE                    6.50 usec
TE                   295.0 K
D1             2.00000000 sec
TD0                       1
SFO1           128.4096890 MHz
NUC1                   11B
P1                    7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                    32768
SF             128.4097430 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

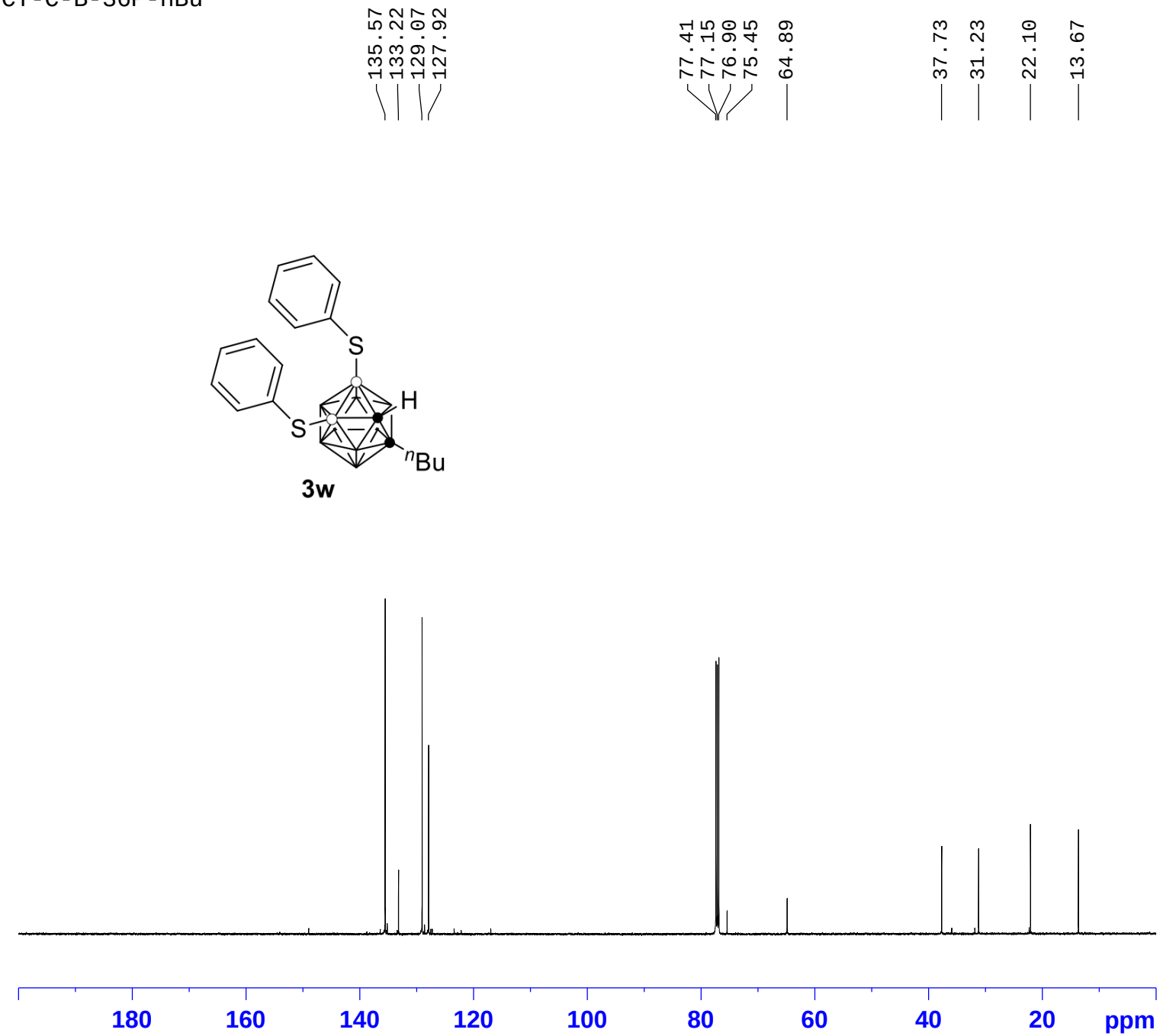


Current Data Parameters
NAME CY-H-B-36p-nBu-re
EXPNO 1
PROCNO 1

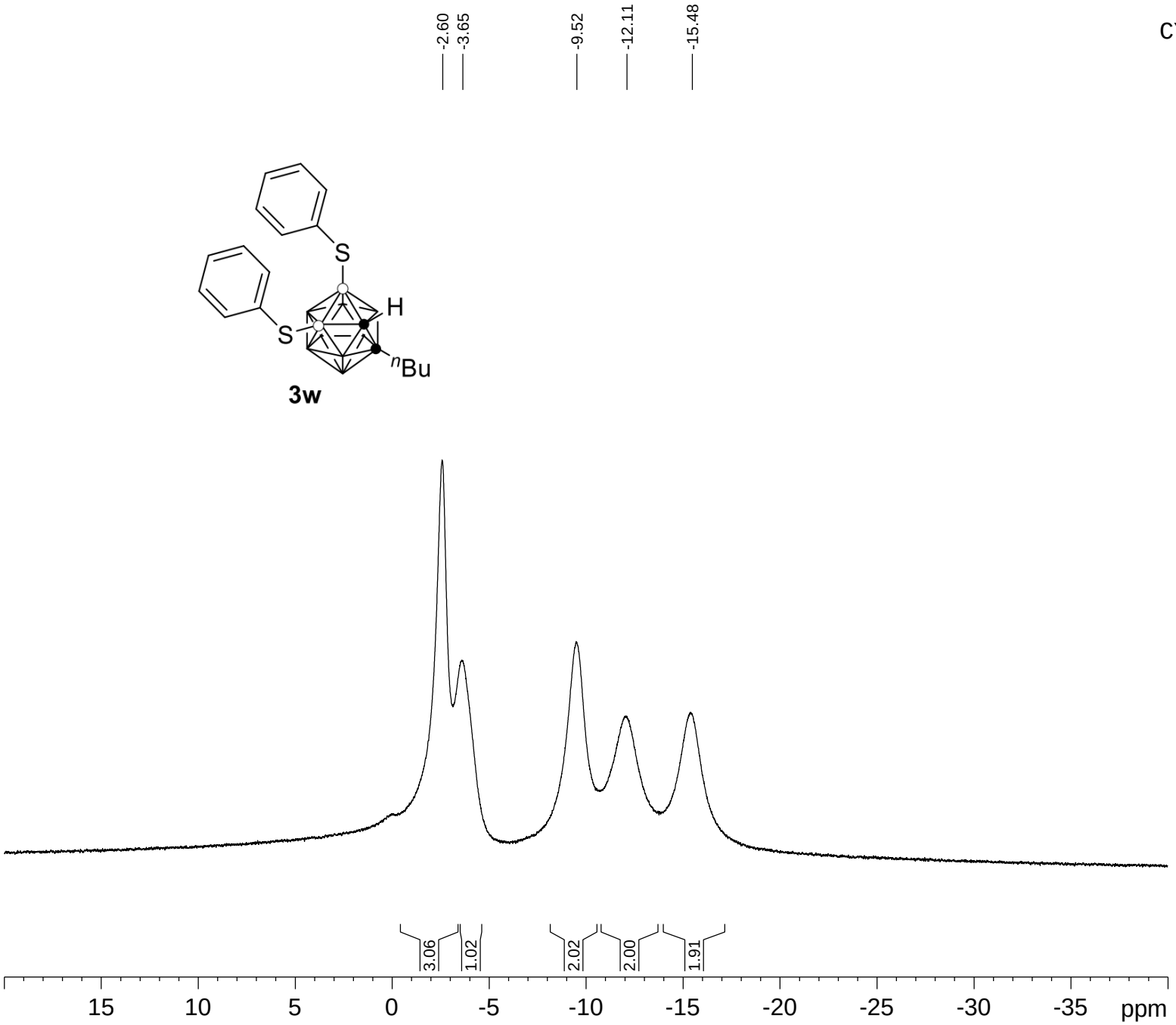
F2 - Acquisition Parameters
Date_ 20180308
Time 19.25 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 11
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-36P-nBu

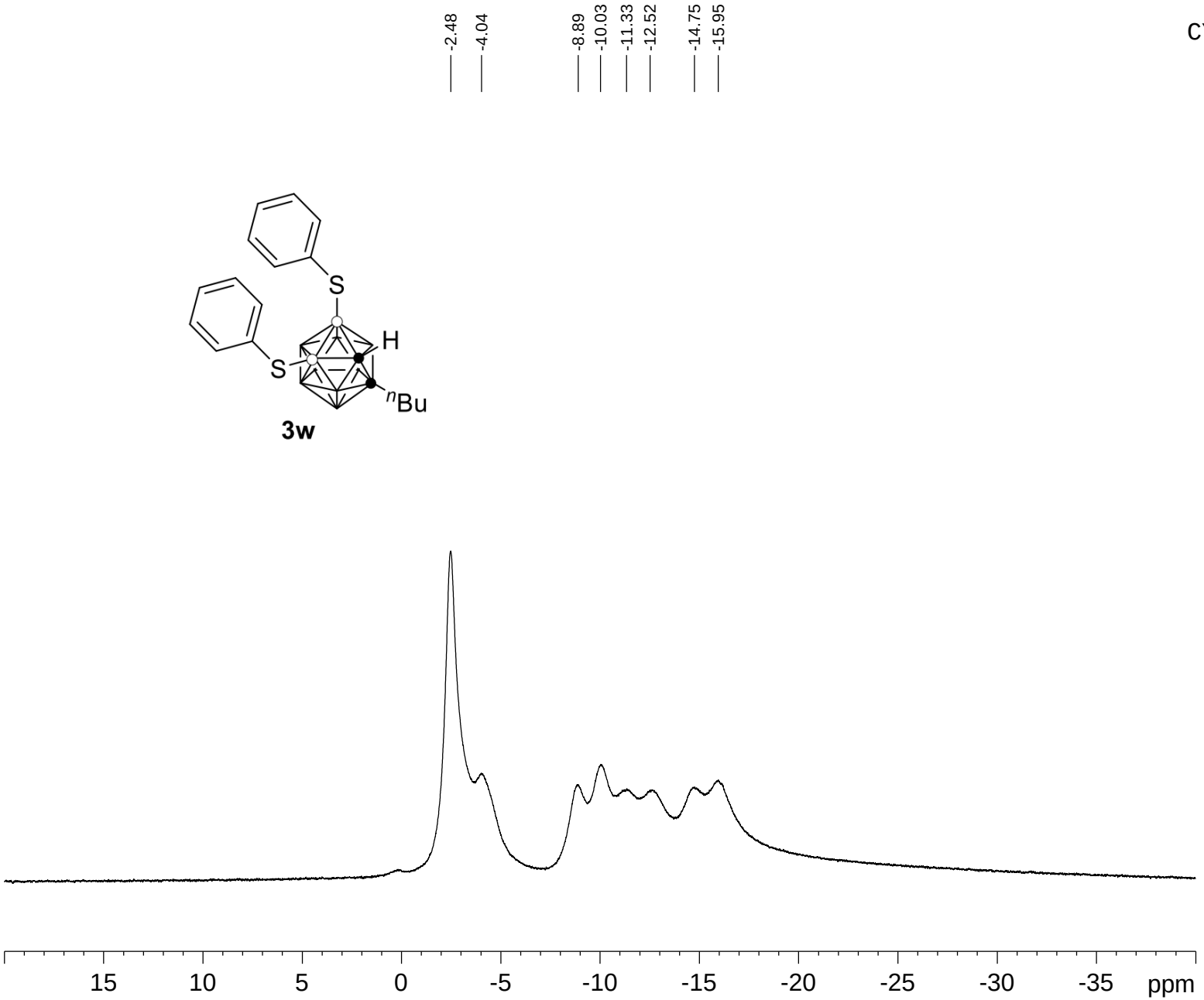



```
Current Data Parameters
NAME      CY-C-B-36P-nBu
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20180309
Time              18.44 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7577760 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



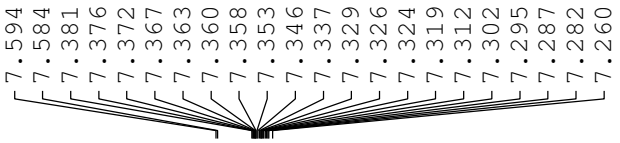
CY-B-B-36p-nBu

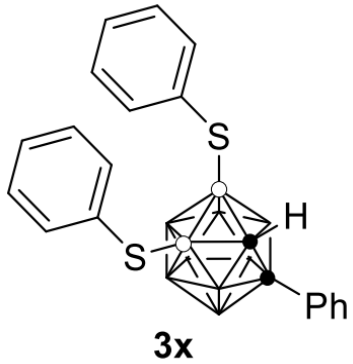
```
Current Data Parameters
NAME      CY-B-B-36p-nBu
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180308
Time               19.47 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    17
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



CY-B-B-36p-nBu-(C)

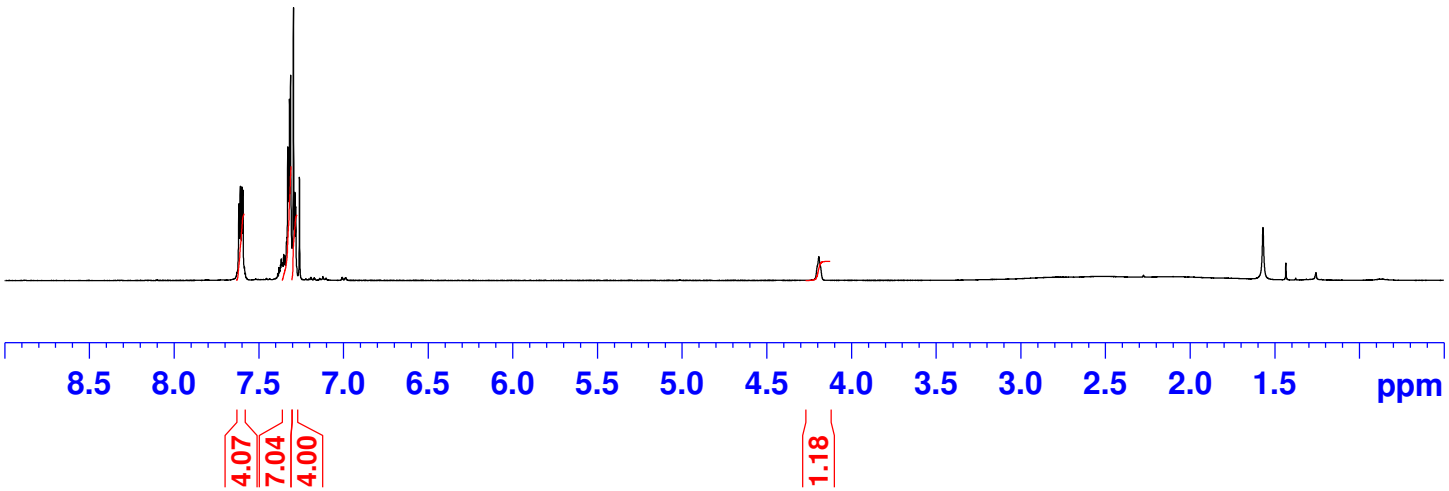
```
Current Data Parameters
NAME      CY-B-B-36p-nBu-(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180308
Time                  19.49 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      19
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                     203
DW                  20.800 usec
DE                   6.50 usec
TE                  295.1 K
D1              2.00000000 sec
TD0                      1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                   32768
SF             128.4097430 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



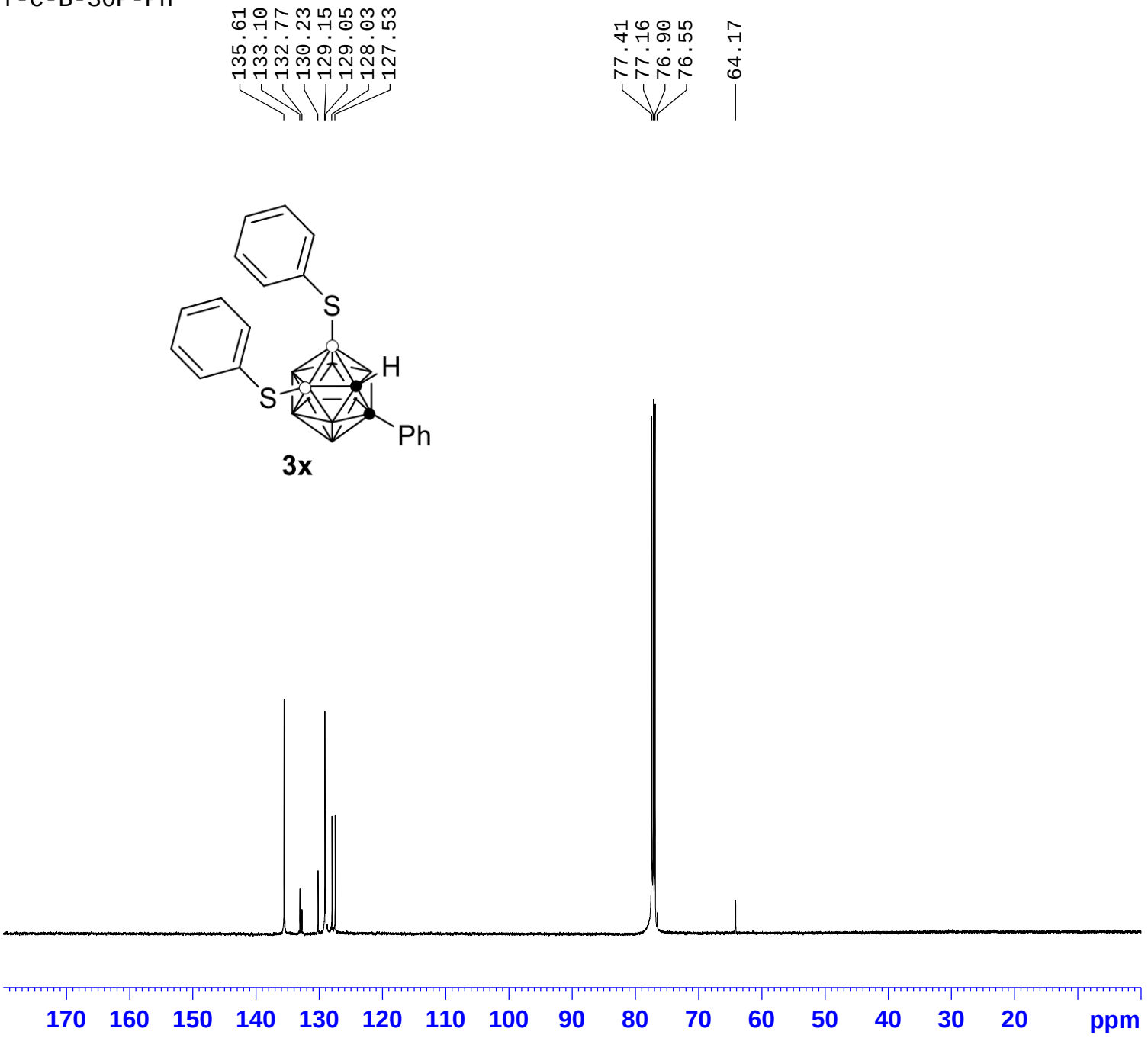


3x

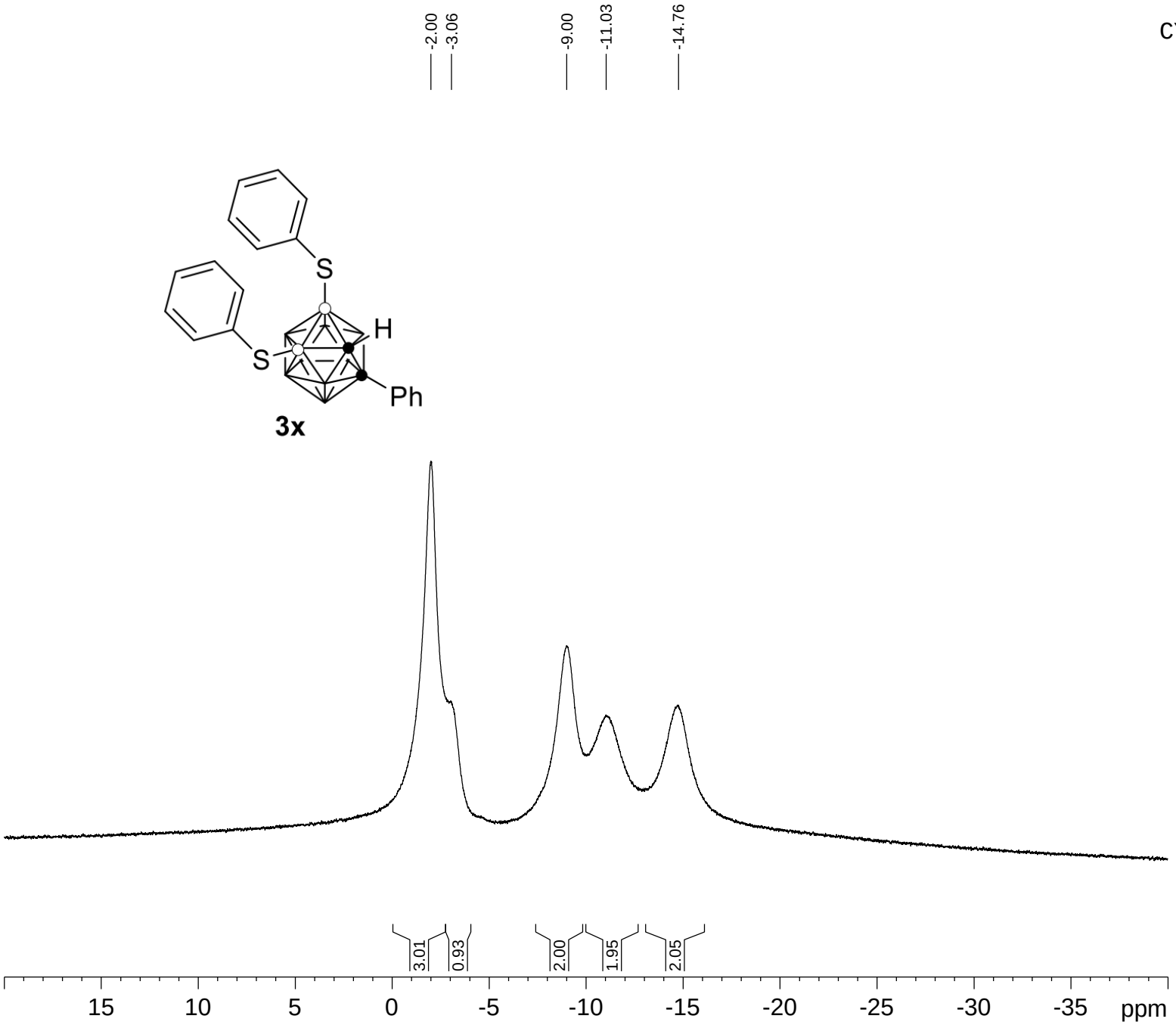
```
Current Data Parameters
NAME       CY-H-B-30p-Ph
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180227
Time               9.53 h
INSTRUM            spect
PROBHD   Z824601_0021 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   11
DS                    2
SWH            8012.820 Hz
FIDRES         0.244532 Hz
AQ             4.0894465 sec
RG                  203
DW                62.400 usec
DE                 6.50 usec
TE                296.4 K
D1            1.00000000 sec
TD0                   1
SFO1         400.1324708 MHz
NUC1                 1H
P1                15.00 usec
PLW1          8.31000042 W

F2 - Processing parameters
SI                65536
SF          400.1300100 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



CY-C-B-30P-Ph

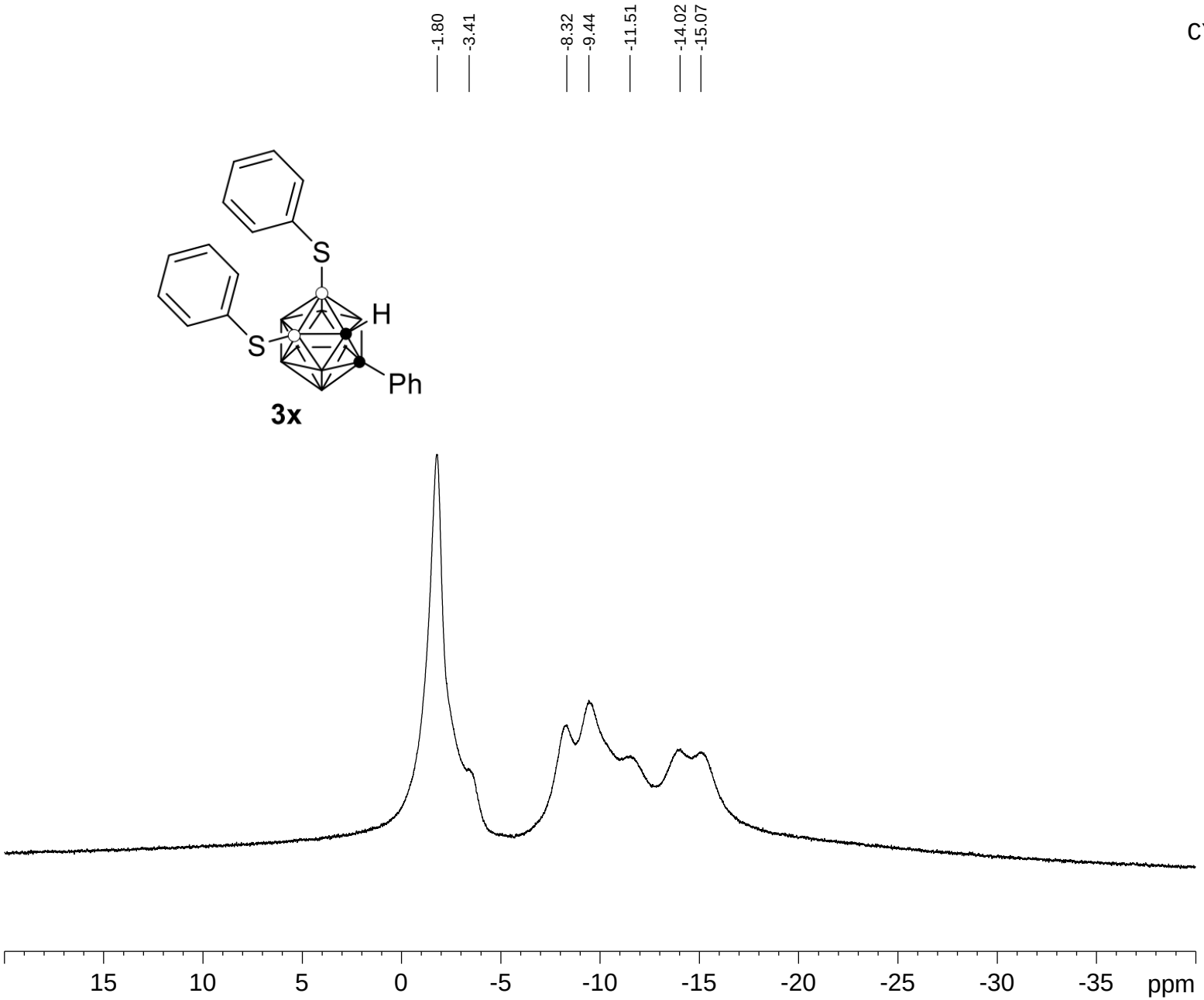



```
Current Data Parameters
NAME      CY-C-B-30P-Ph
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20180227
Time              16.22 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  900
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

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



CY-B-B-30P-Ph

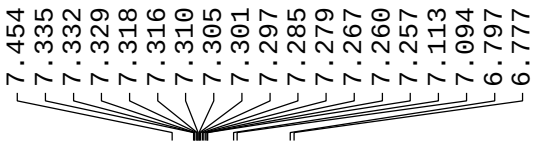
```
Current Data Parameters
NAME       CY-B-B-30P-Ph
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180227
Time               18.31 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    56
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   362
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

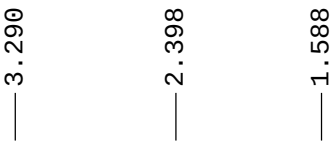


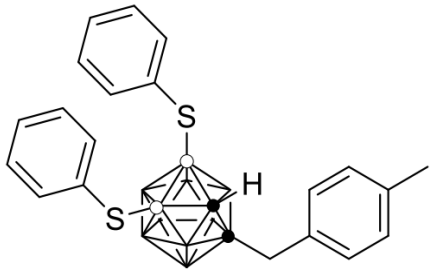
CY-B-B-30P-Ph-(C)

```
Current Data Parameters
NAME      CY-B-B-30P-Ph-(C)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180227
Time                 18.36 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      64
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                     362
DW                  20.800 usec
DE                   6.50 usec
TE                  295.1 K
D1             2.00000000 sec
TD0                      1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                   32768
SF             128.4097430 MHz
WDW                    EM
SSB      0
LB                   1.00 Hz
GB       0
PC                   1.40
```

CY-H-B-44P-MeBn

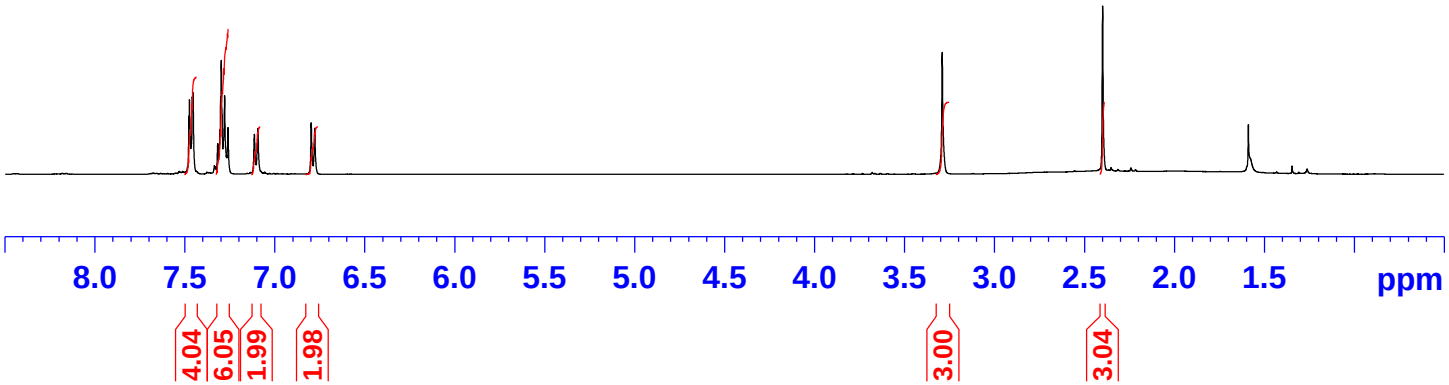




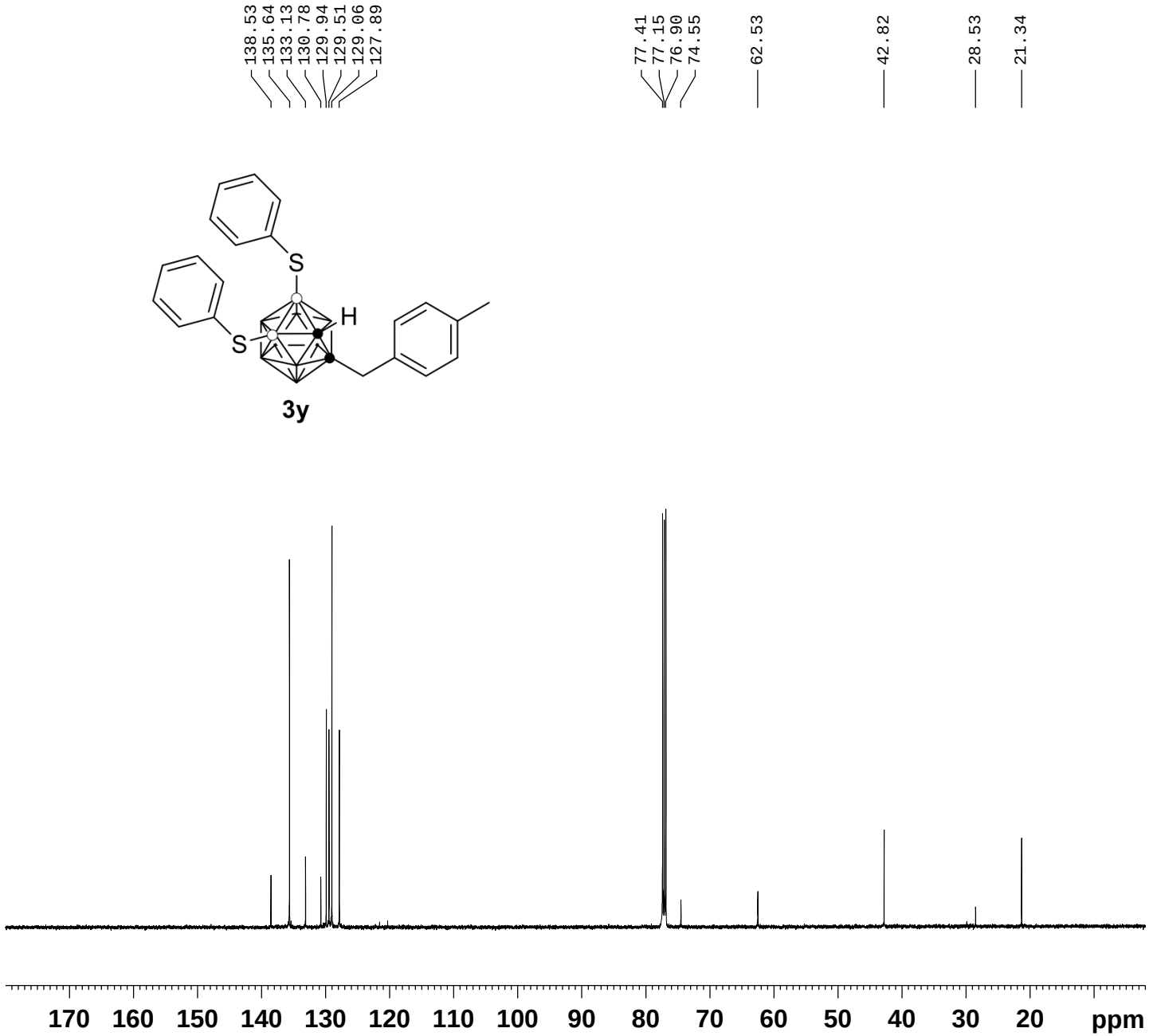


3y

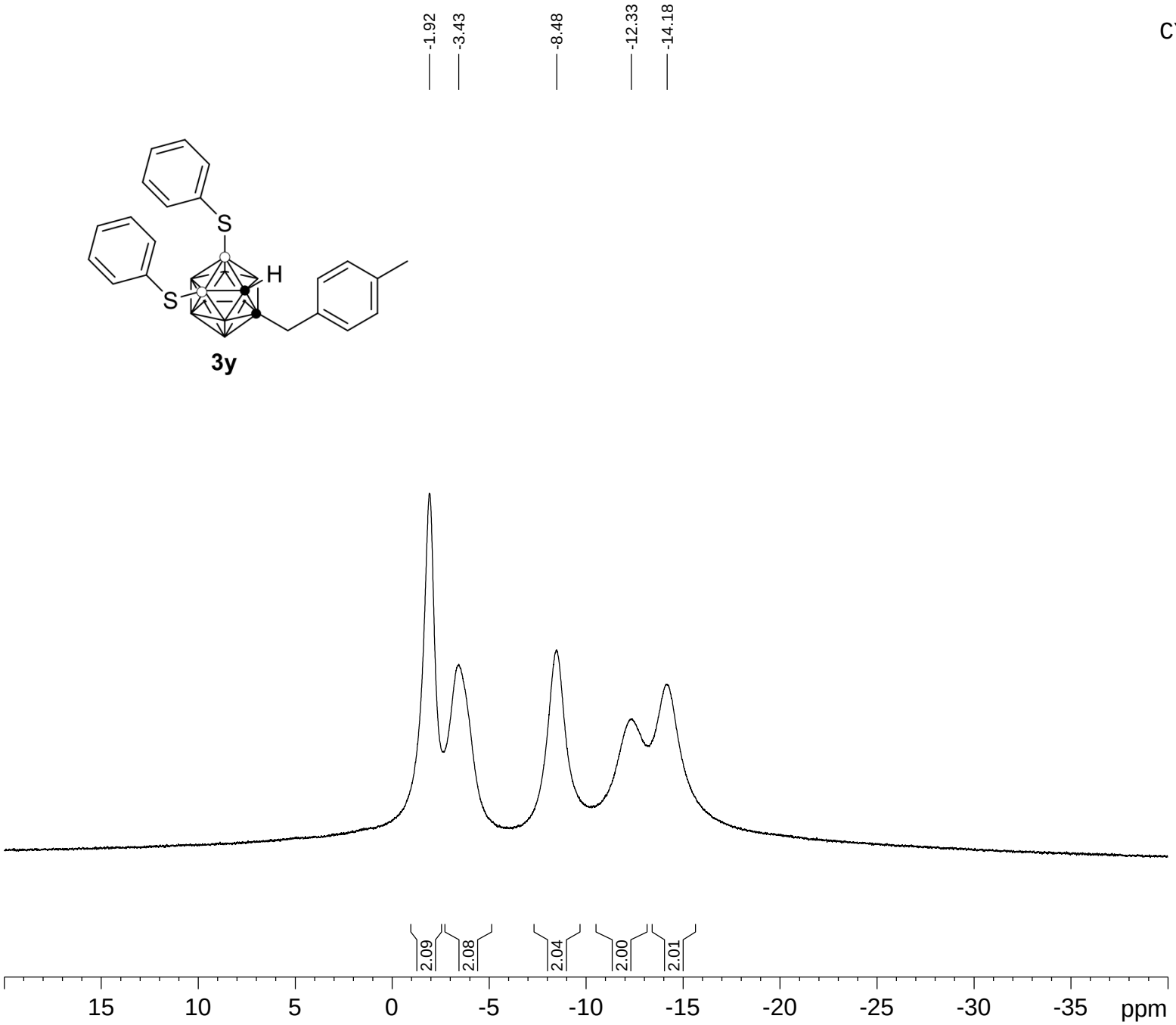
```
Current Data Parameters
NAME      CY-H-B-44P-MeBn
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180315
Time              22.34 h
INSTRUM            spect
PROBHD   Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     9
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                   203
DW                62.400 usec
DE                 6.50 usec
TE                296.7 K
D1           1.00000000 sec
TD0                    1
SFO1        400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1          8.31000042 W

F2 - Processing parameters
SI                 65536
SF          400.1300100 MHz
WDW                   EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```



CY-C-B-44P-MeBn

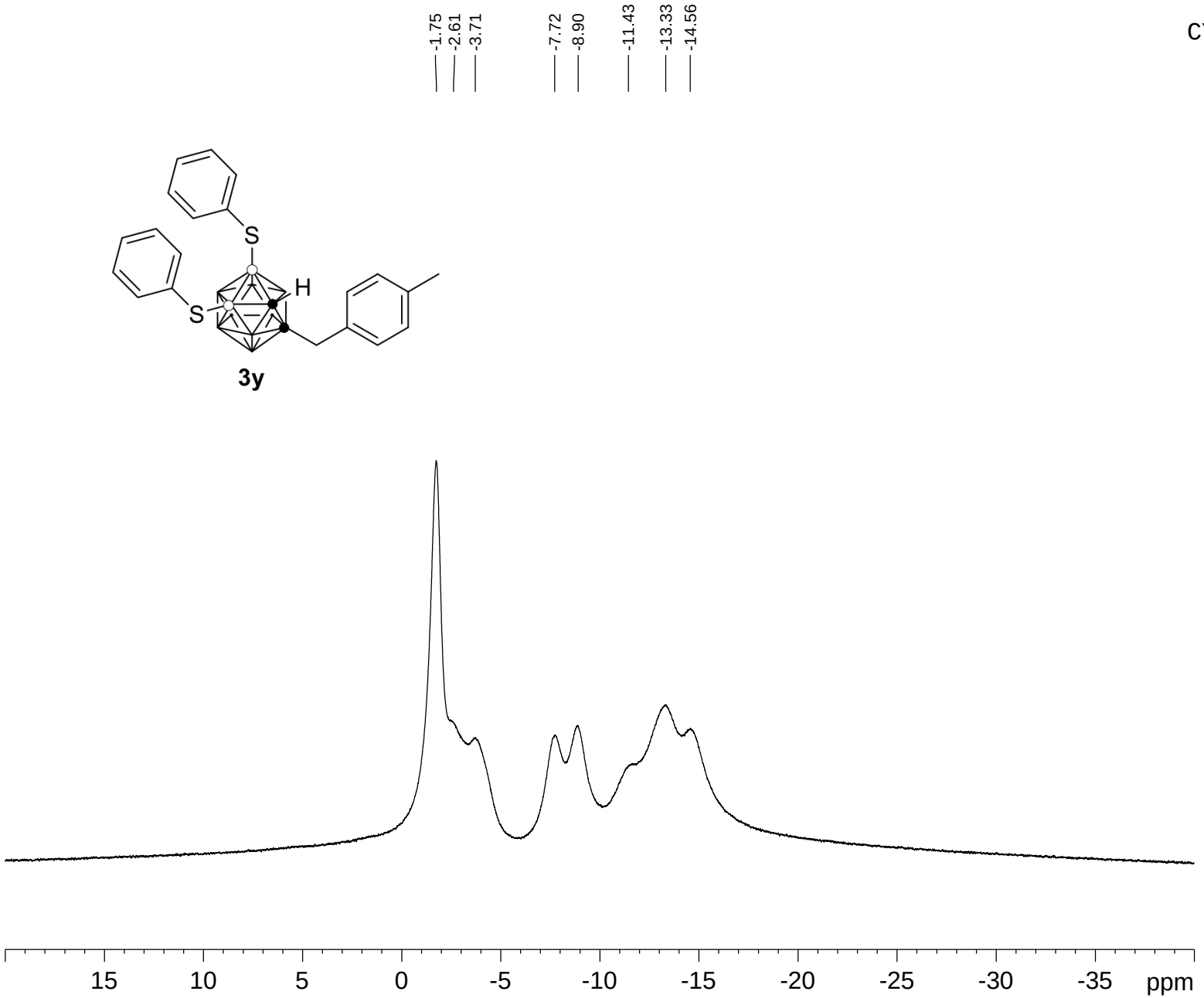



```
Current Data Parameters
NAME      CY-C-B-44P-MeBn
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180316
Time               19.26 h
INSTRUM             spect
PROBHD    Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   120
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

F2 - Processing parameters
SI                 32768
SF           125.7577761 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



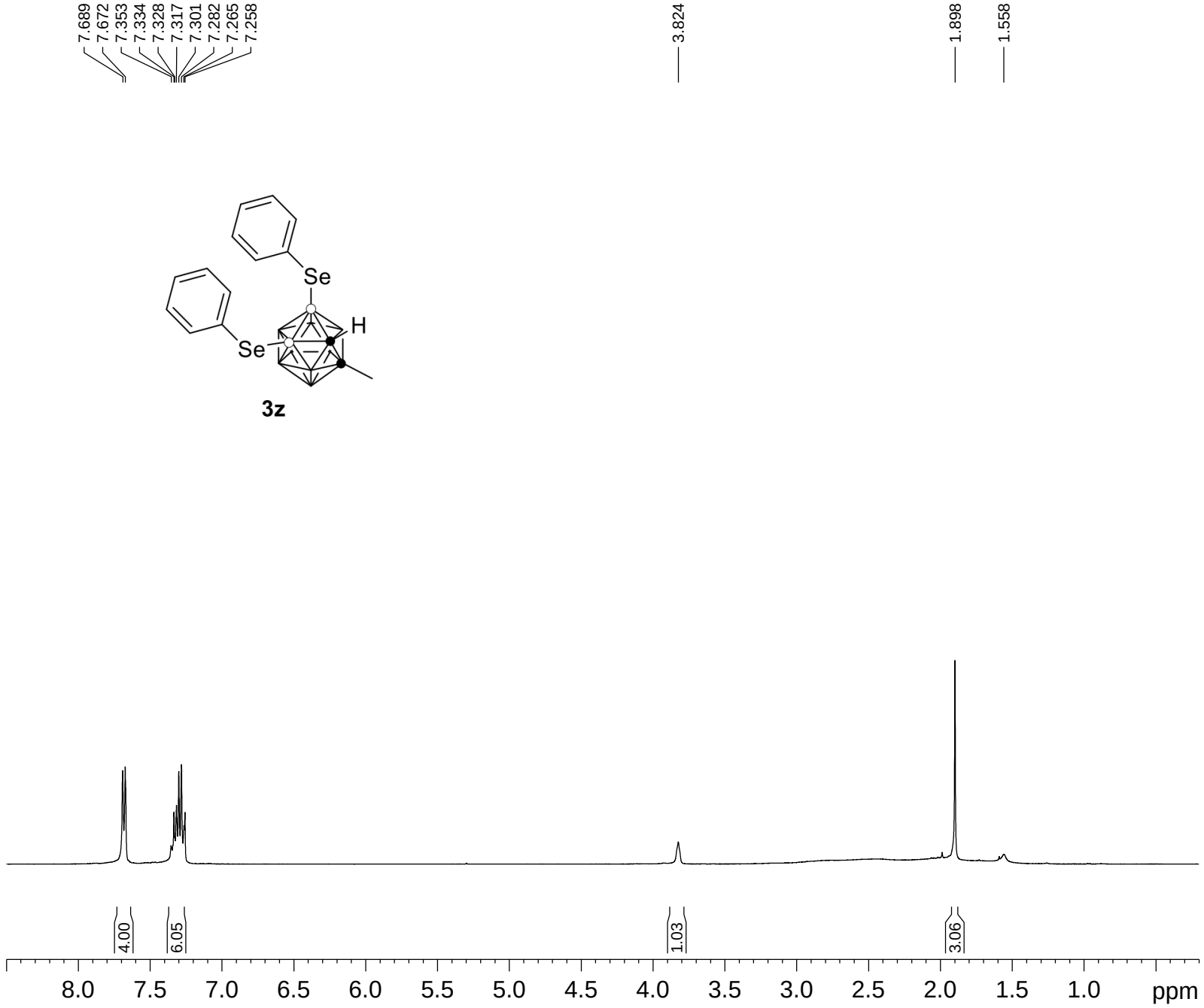
CY-B-B-44P-MeBn

```
Current Data Parameters
NAME      CY-B-B-44p-MeBn
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180316
Time                19.42 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     38
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    287
DW                 20.800 usec
DE                  6.50 usec
TE                 295.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                11B
P1                  7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                  32768
SF           128.4097615 MHz
WDW                 EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



CY-B-B-44P-MeBn-(C)

```
Current Data Parameters
NAME      CY-B-B-44p-MeBn-(C)
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180316
Time                  19.45 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT               CDCl3
NS                        48
DS                         2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                       287
DW                  20.800 usec
DE                   6.50 usec
TE                   294.9 K
D1              2.00000000 sec
TD0                        1
SFO1           128.4096890 MHz
NUC1                    11B
P1                    7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                     32768
SF             128.4097430 MHz
WDW                       EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



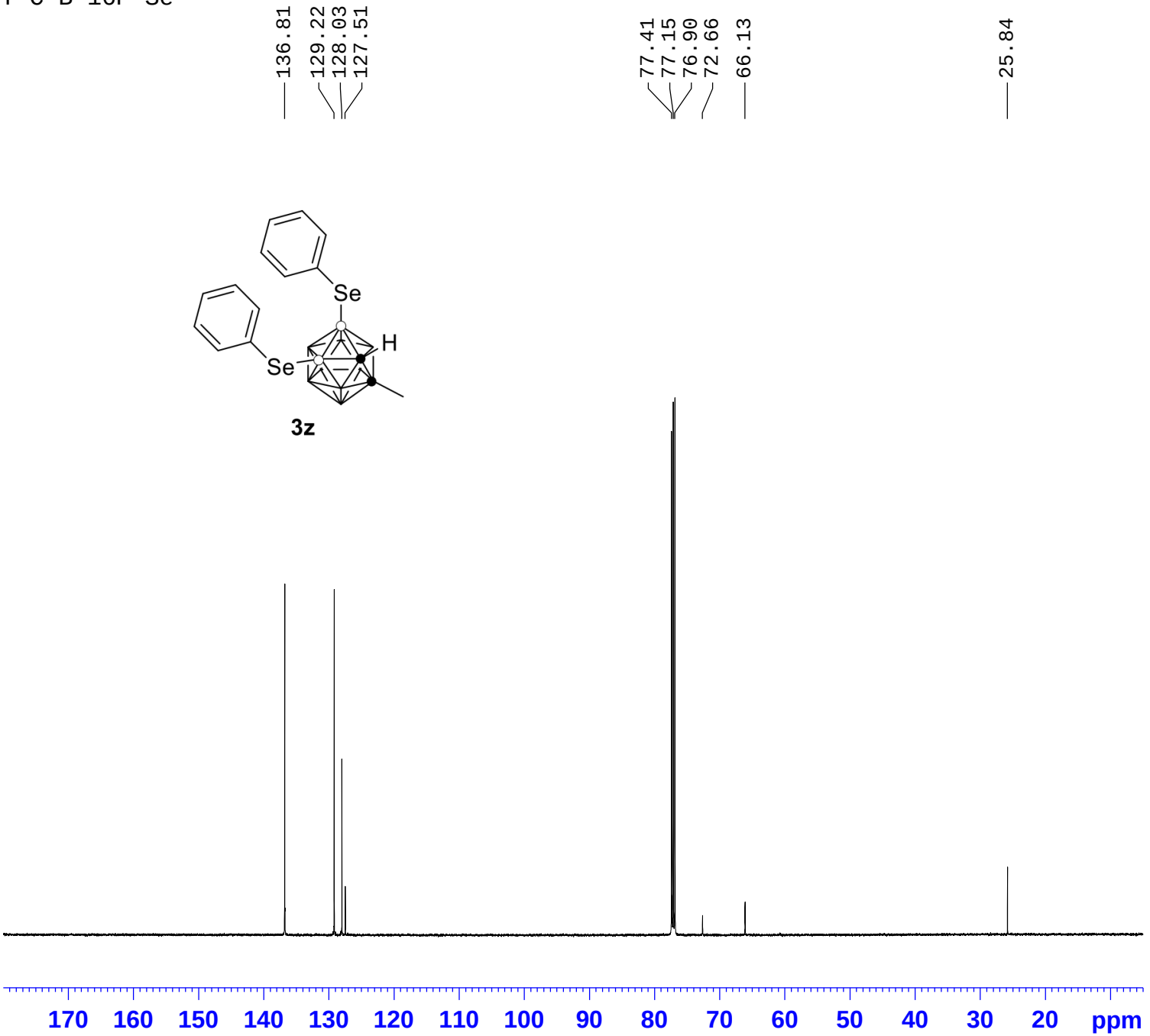
CY-H-B-16P

Current Data Parameters
NAME CY-H-B-16P
EXPNO 1
PROCNO 1

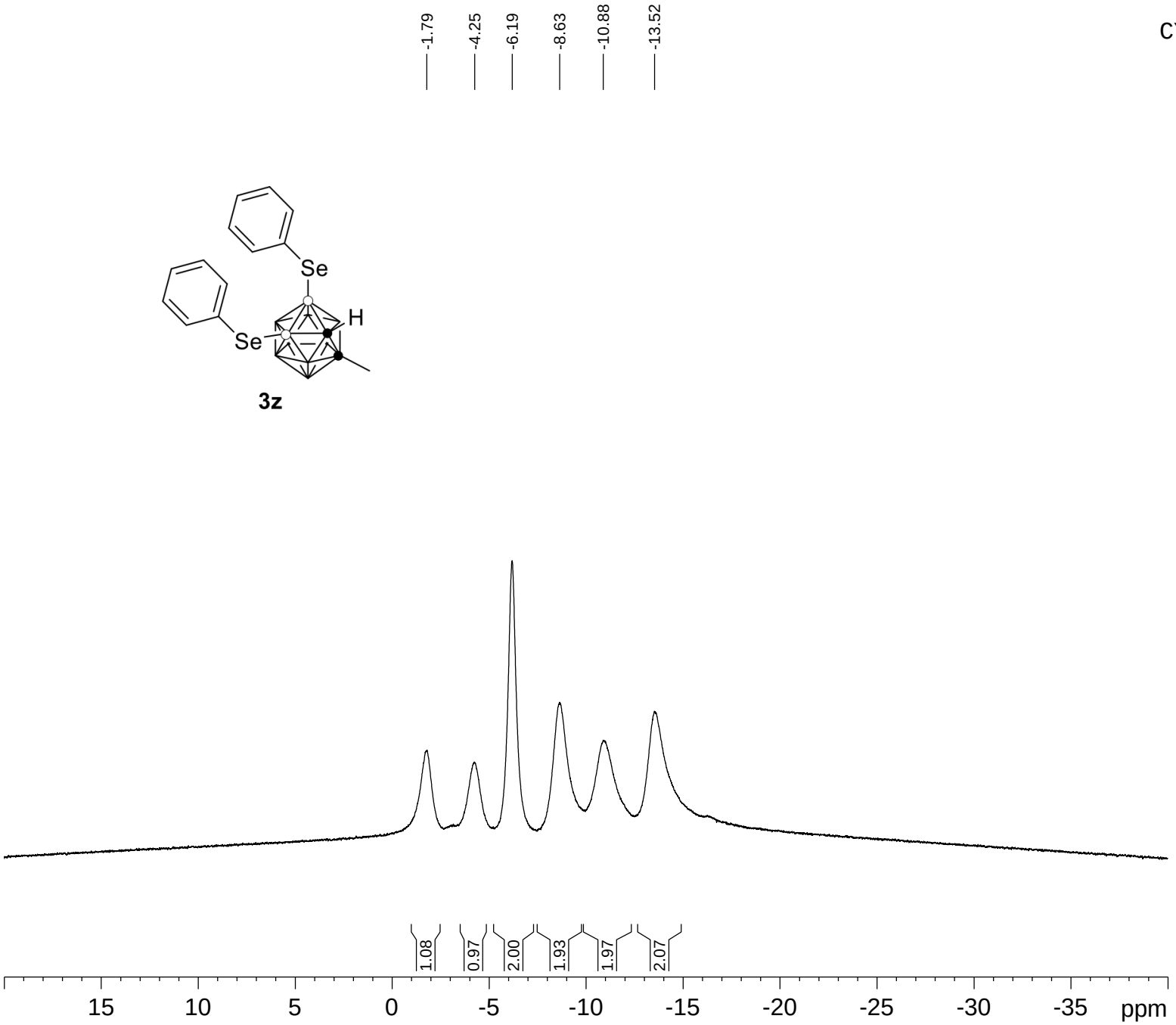
F2 - Acquisition Parameters
Date_ 20180202
Time 16.13 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-16P-Se

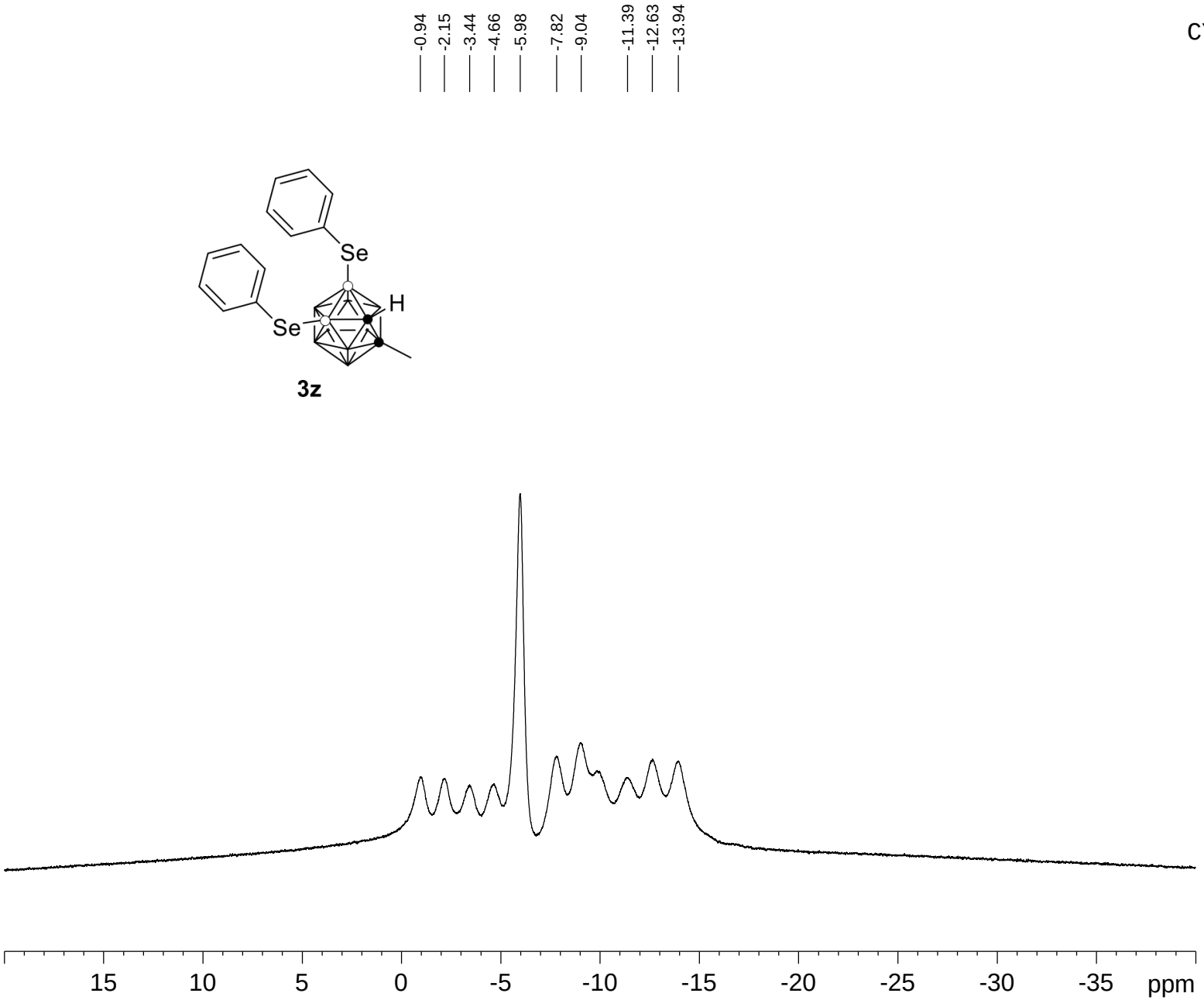



```
Current Data Parameters
NAME      CY-C-B-16P-Se
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20180202
Time              19.18 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7577738 MHz
WDW                EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```



CY-B-B-16p

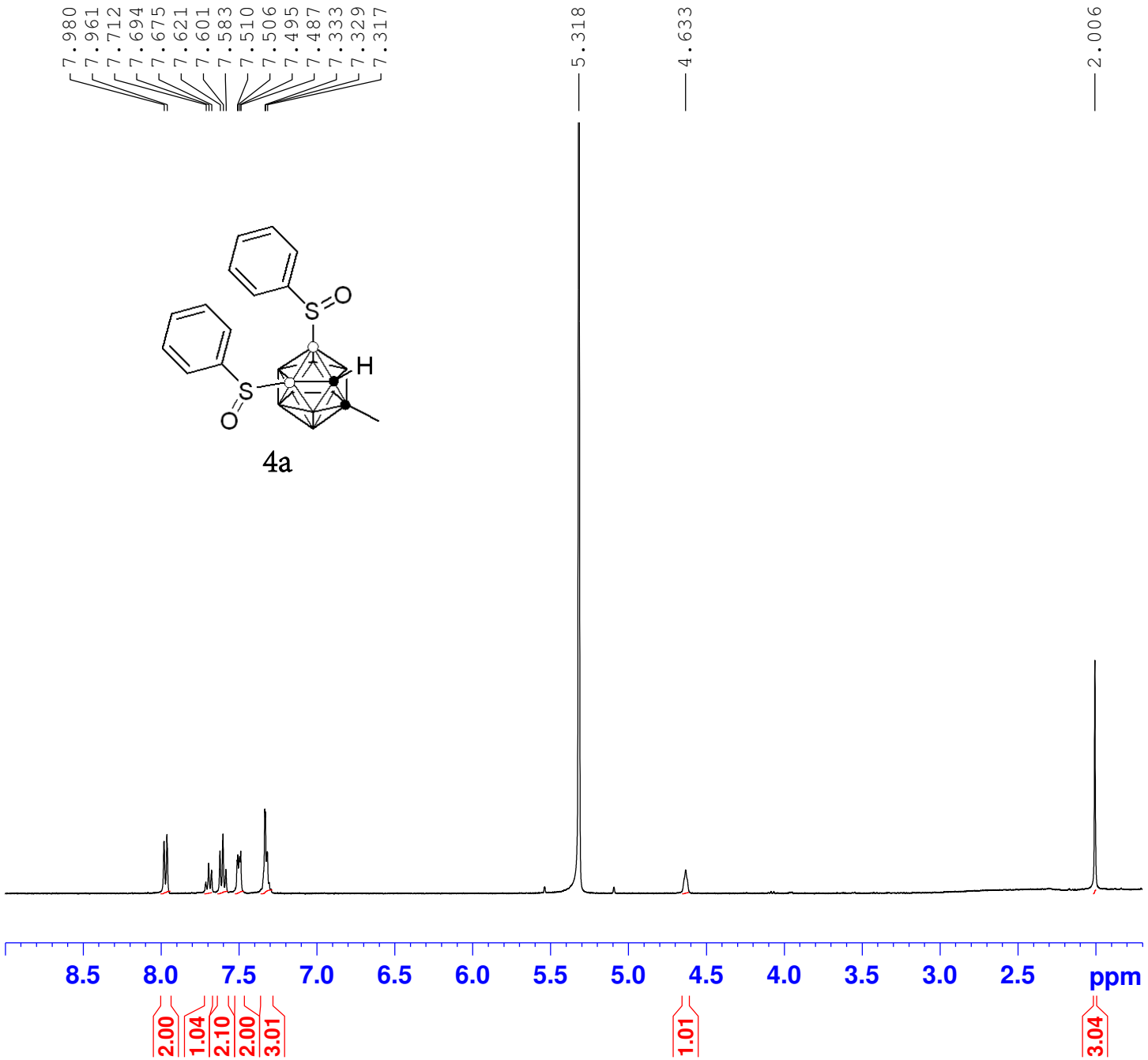
```
Current Data Parameters
NAME          CY-B-B-16p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180202
Time               16.17 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   362
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```



CY-B-B-16p-(C)

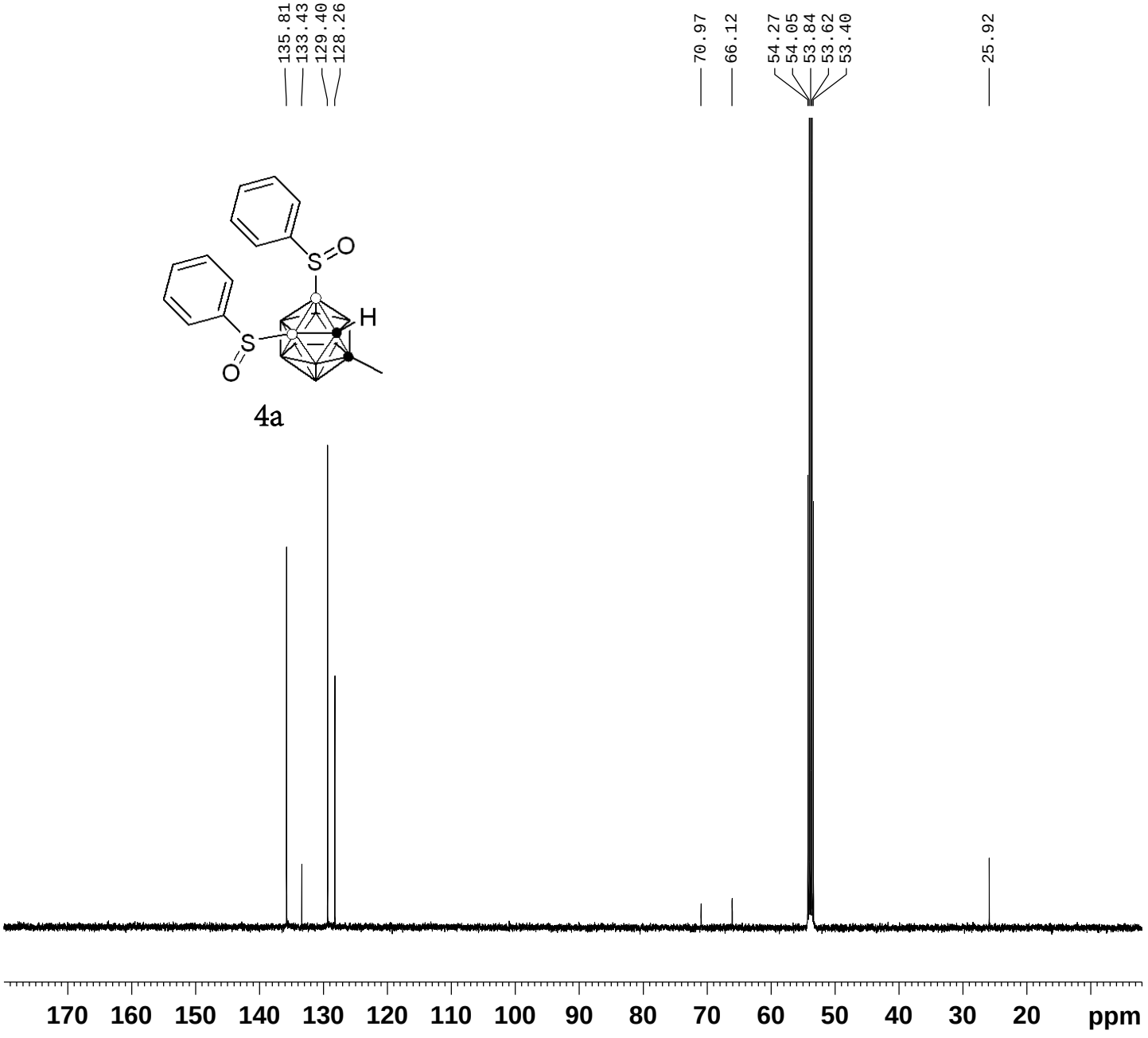
```
Current Data Parameters
NAME      CY-B-B-16p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180202
Time                16.20 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     40
DS                      2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                    362
DW                 20.800 usec
DE                  6.50 usec
TE                 295.1 K
D1            2.00000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                  11B
P1                  7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                  32768
SF            128.4097430 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

CY-H-B-57P-Sulfoxide




```
Current Data Parameters
NAME      CY-H-B-57P-Sulfoxide
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190830
Time              16.14 h
INSTRUM            spect
PROBHD   Z820201_0170 (
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                   203
DW                62.400 usec
DE                 6.50 usec
TE                295.9 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                 6.75 usec
PLW1         13.17700005 W

F2 - Processing parameters
SI                 65536
SF           400.1300161 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

CY-C-B-57P-SO

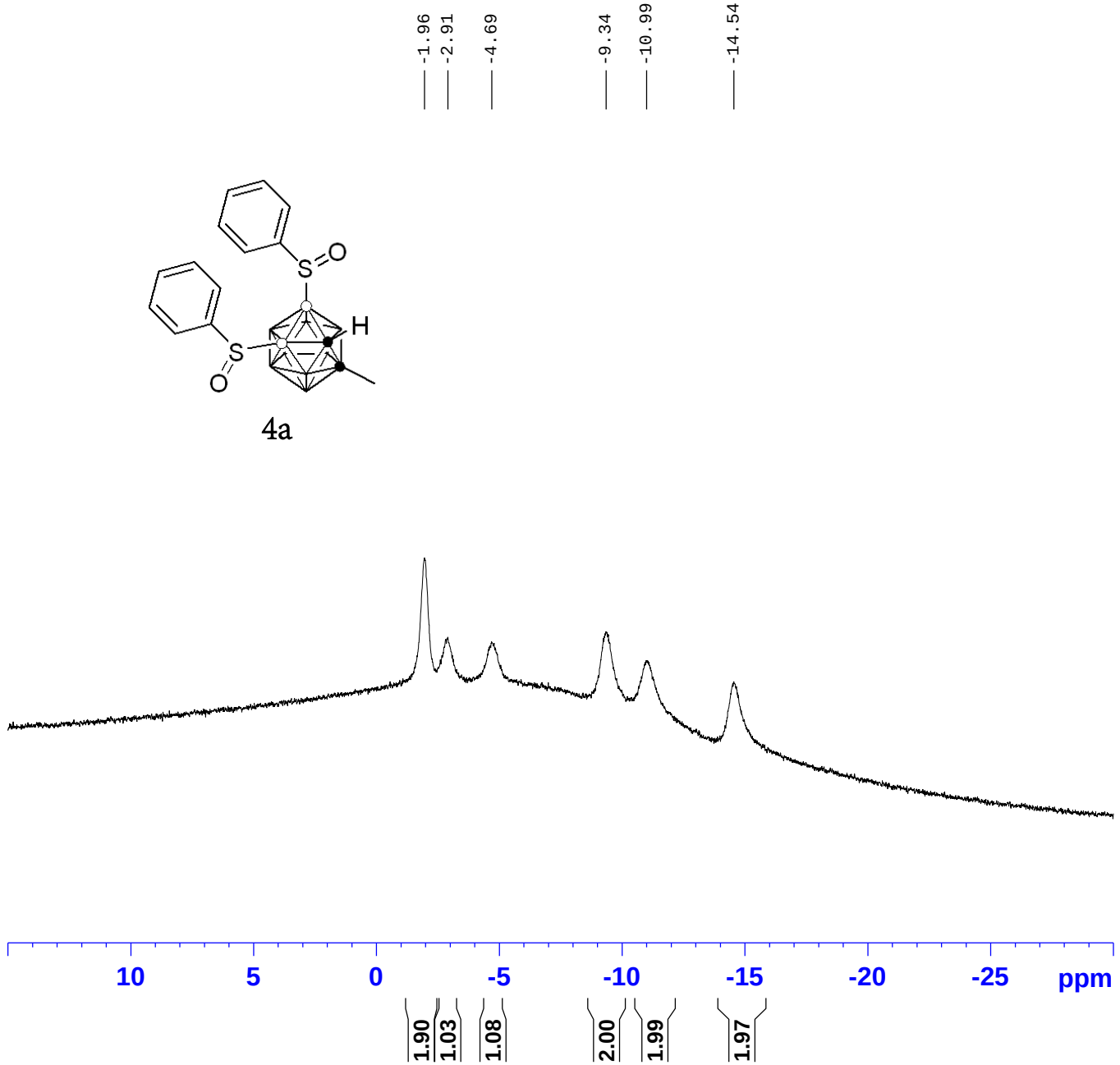


Current Data Parameters
NAME CY-C-B-57P-SO
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181004
Time 16.58 h
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 100
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 206.72
DW 16.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 10.00 usec
PLW1 61.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.29663000 W
PLW13 0.14920001 W

F2 - Processing parameters
SI 32768
SF 125.7577382 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CY-B-B-57P-Sulfoxide

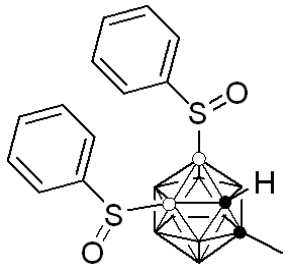


4a

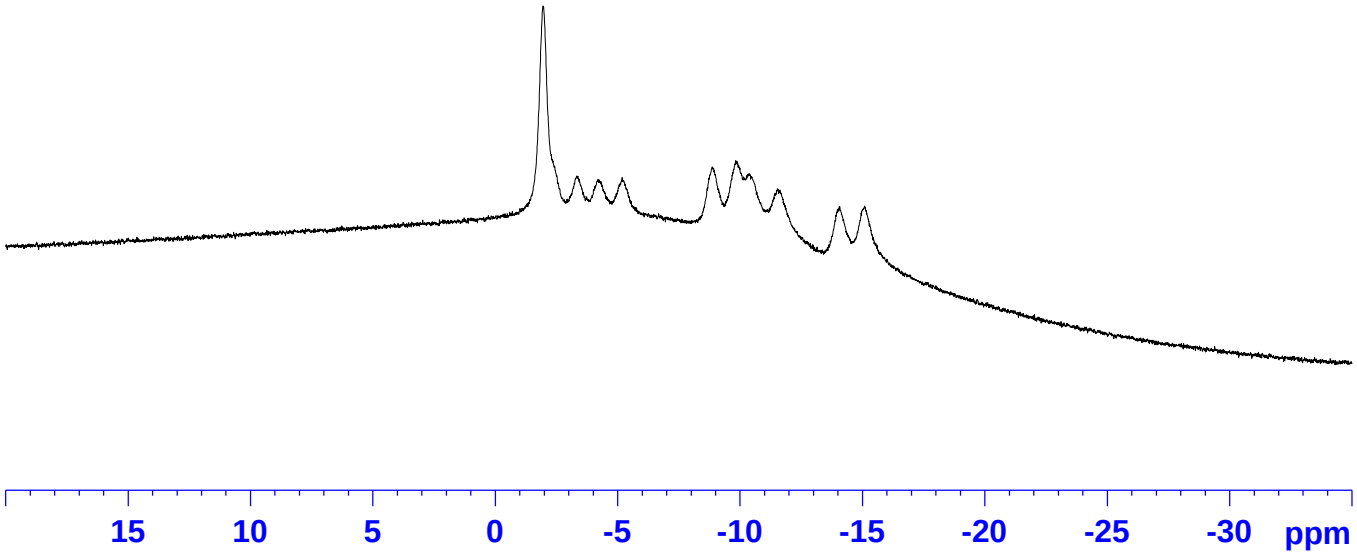
```
Current Data Parameters
NAME      CY-B-B-57P-Sulfoxide
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190905
Time                9.30 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 32768
SOLVENT             None
NS                    32
DS                     4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                206.72
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         160.4615790 MHz
NUC1                11B
P1                15.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

F2 - Processing parameters
SI                 16384
SF           160.4615999 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

CY-B-B-57P-Sulfoxide-(C)

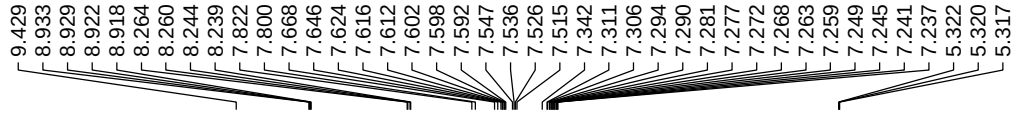
-1.96
-3.28
-4.14
-5.15
-8.78
-9.83
-10.30
-11.59
-14.01
-15.02



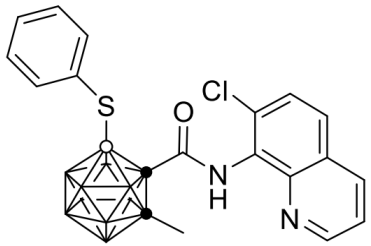
4a



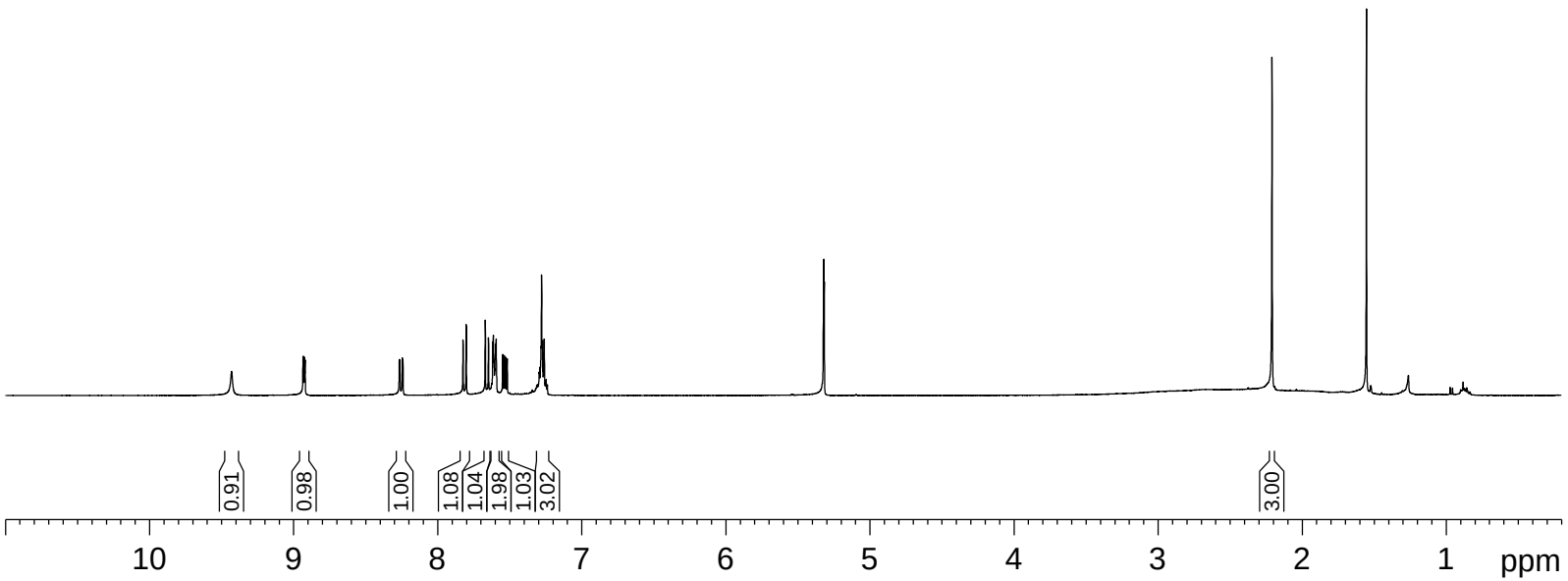

```
Current Data Parameters
NAME      CY-B-B-57P-Sulfoxide-(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190905
Time               9.31 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG              zg
TD                32768
SOLVENT            None
NS                   32
DS                    4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               206.72
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1           1.00000000 sec
TD0                  1
SFO1        160.4615792 MHz
NUC1               11B
P1               15.00 usec
PLW1        50.00000000 W

F2 - Processing parameters
SI                16384
SF          160.4615997 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



CY-H-B-62p



3a'

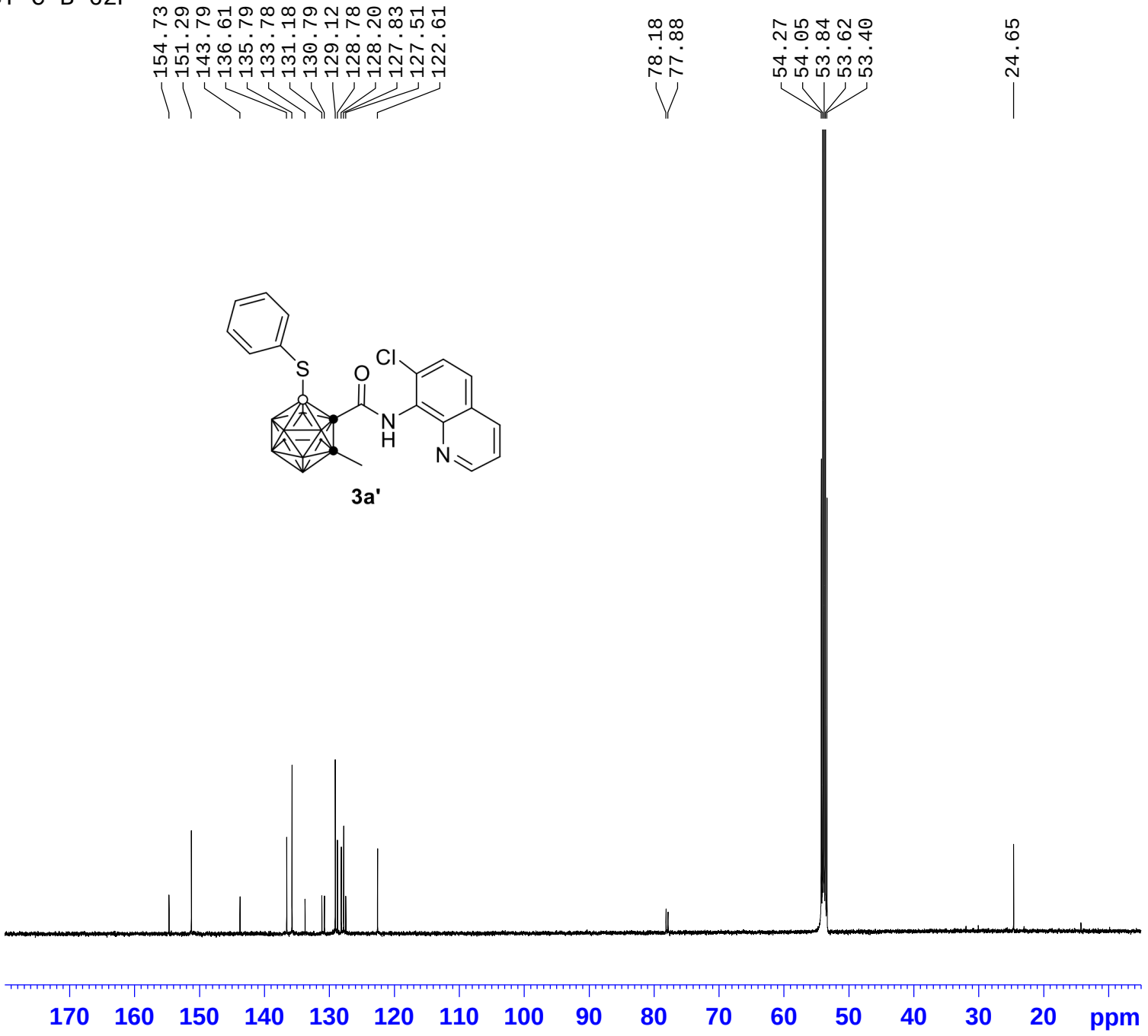


Current Data Parameters
NAME CY-H-B-62p
EXPNO 1
PROCNO 1

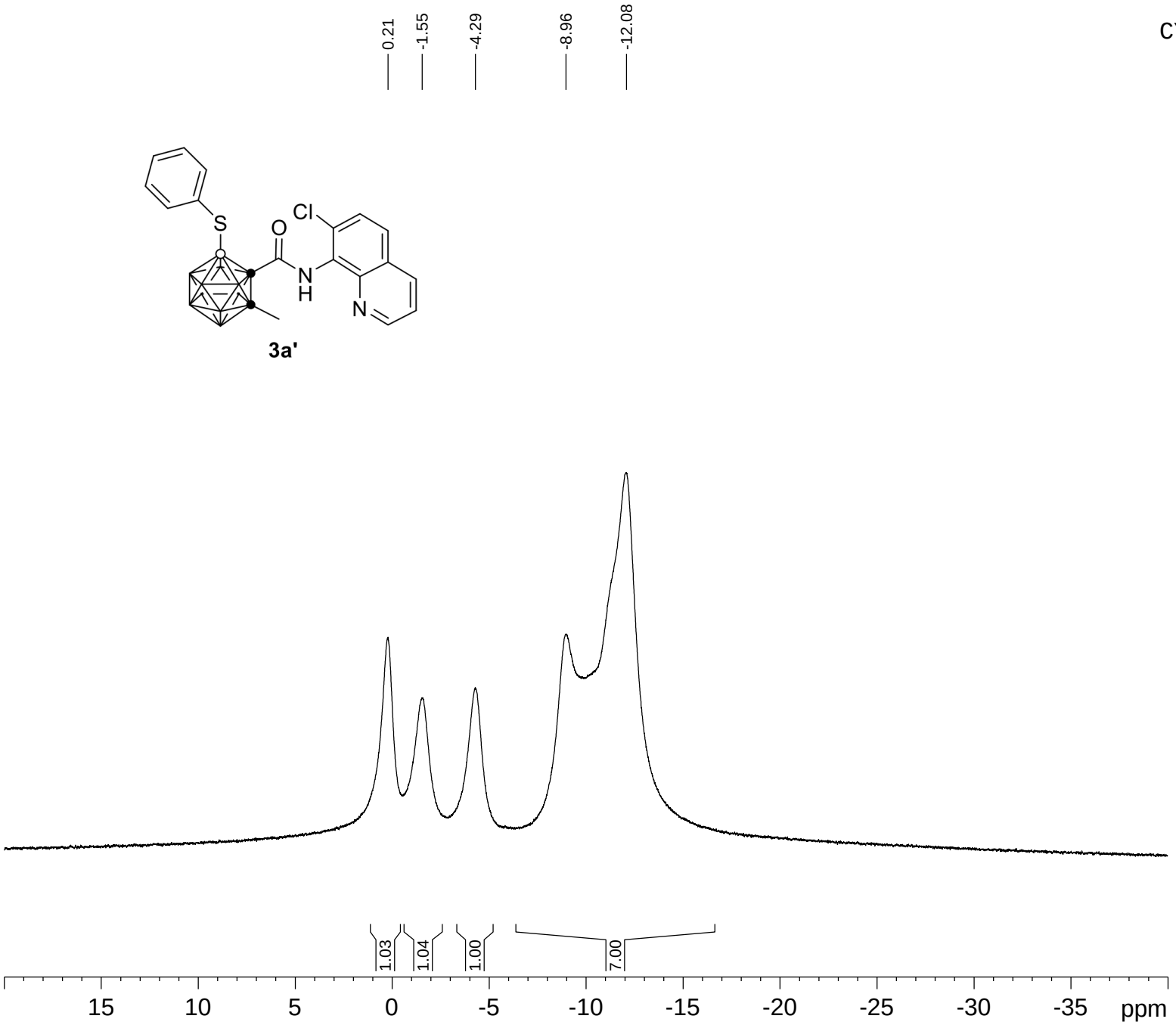
F2 - Acquisition Parameters
Date_ 20180427
Time 22.00 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300156 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-B-62P

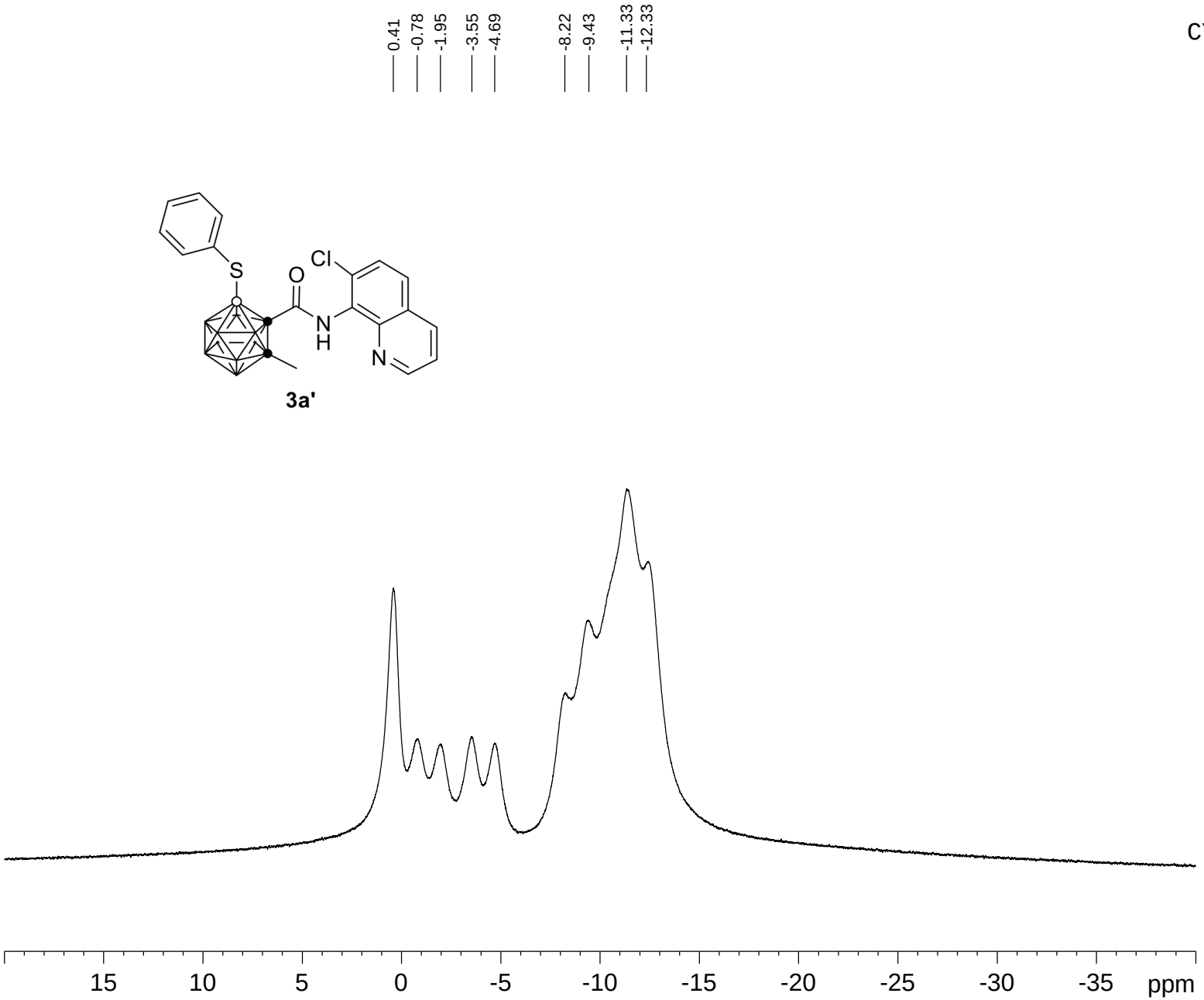



```
Current Data Parameters
NAME          CY-C-B-62P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180430
Time              19.13 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT           CD2Cl2
NS                   700
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ              1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                13C
P1                 10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

F2 - Processing parameters
SI                 32768
SF           125.7577384 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```



CY-B-B-62PP

```
Current Data Parameters
NAME         CY-B-B-62PP
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180427
Time              21.01 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT          CD2Cl2
NS                    24
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   256
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W
SFO2        400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W

F2 - Processing parameters
SI                 32768
SF          128.4097615 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```



CY-B-B-62PP-(C)

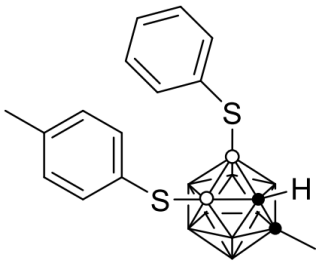
```
Current Data Parameters
NAME      CY-B-B-62PP-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180427
Time                21.03 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT           CD2Cl2
NS                     44
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    256
DW                20.800 usec
DE                 6.50 usec
TE                294.9 K
D1           2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                 7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

CY-H-B-62Q

7.594
7.585
7.576
7.571
7.465
7.446
7.319
7.311
7.305
7.259
7.132
7.112

3.789

2.345
1.910
1.571

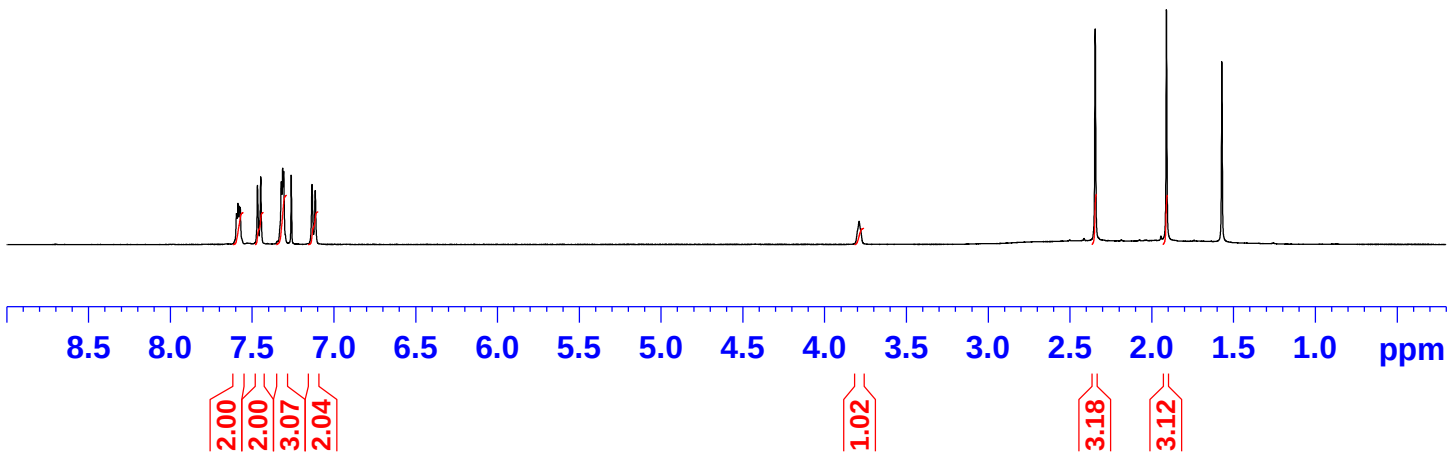


3ab

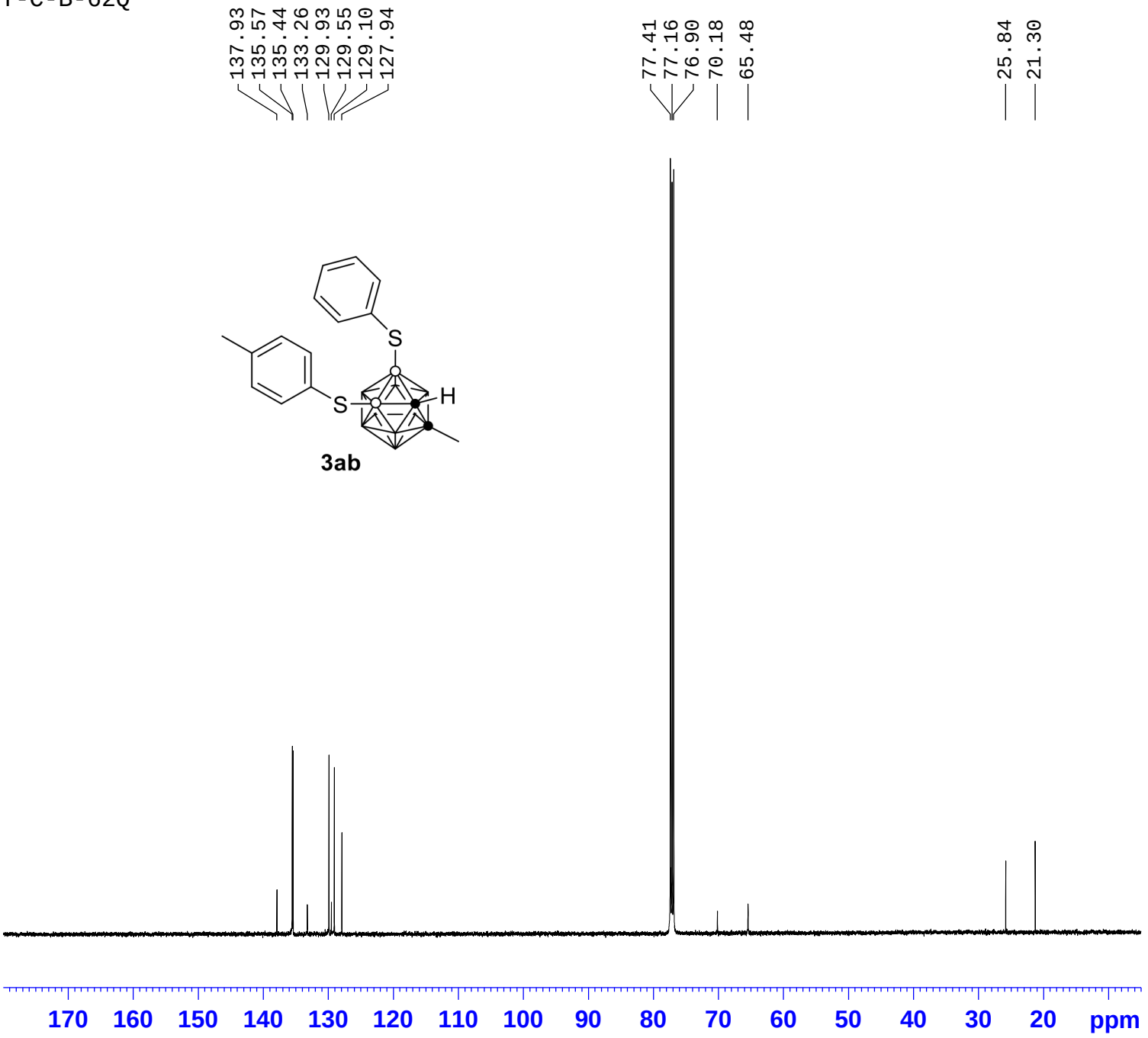
Current Data Parameters
NAME CY-H-B-62Q
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180430
Time 15.43 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 8.31000042 W

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

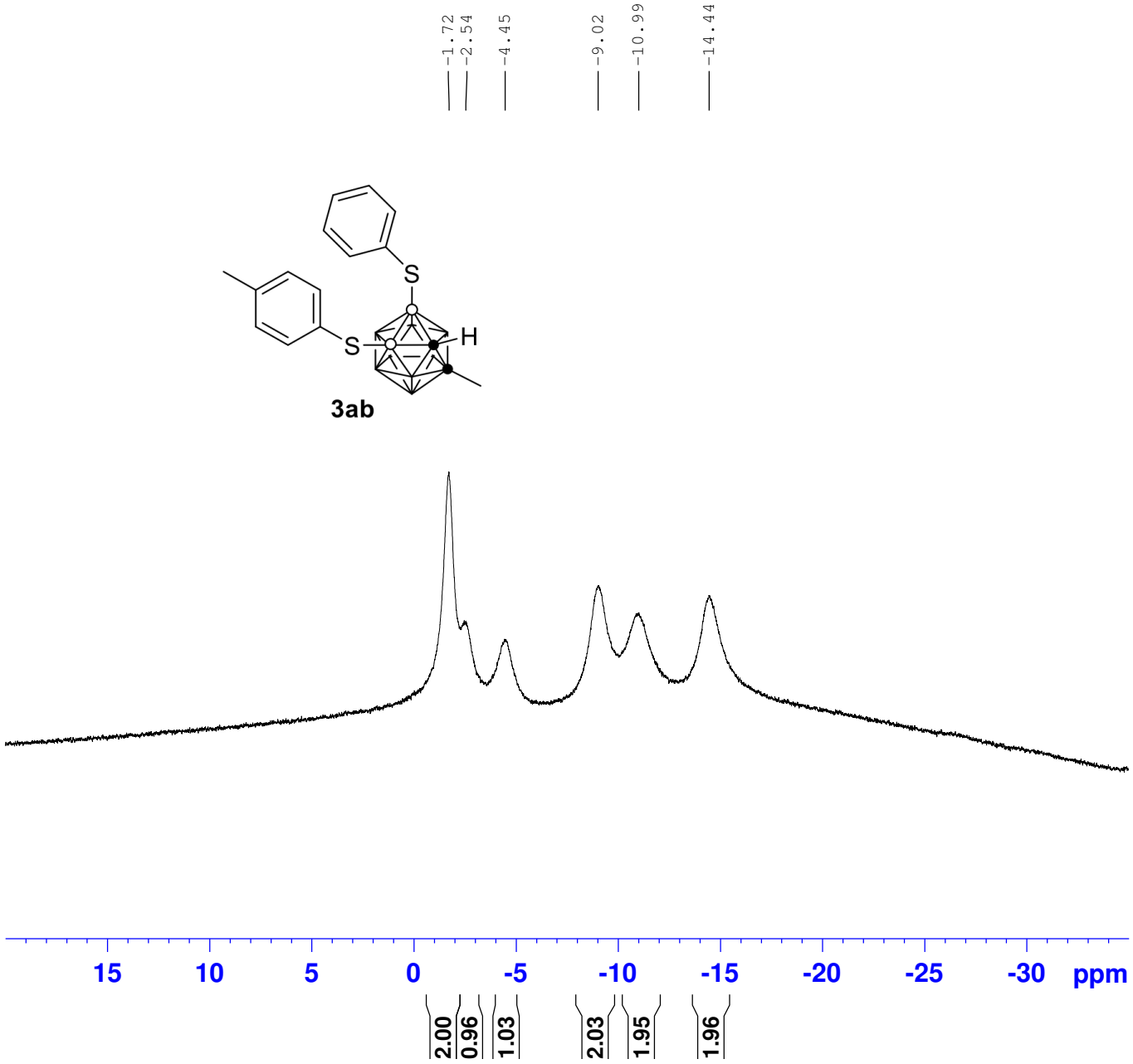


CY-C-B-62Q



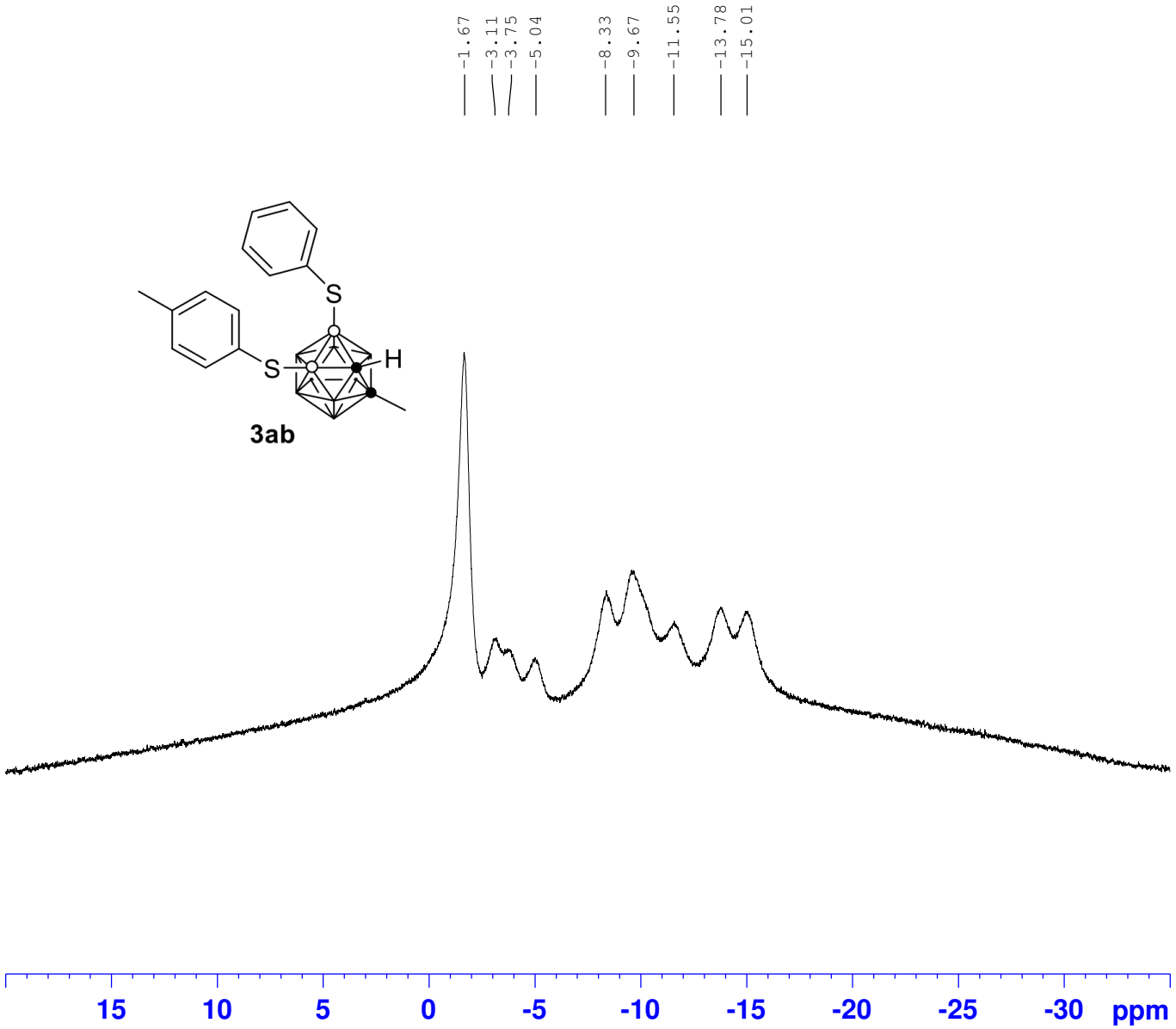

```
Current Data Parameters
NAME          CY-C-B-62Q
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180430
Time              19.32 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

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

CY-B-B-65P-Ph-Tol




```
Current Data Parameters
NAME      CY-B-B-65P-Ph-Tol
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190620
Time              10.56 h
INSTRUM             spect
PROBHD   Z820201_0170 (
PULPROG             zgig
TD                 65536
SOLVENT            CDCl3
NS                    75
DS                     4
SWH            25510.203 Hz
FIDRES          0.778510 Hz
AQ              1.2845056 sec
RG                   181
DW                19.600 usec
DE                 6.50 usec
TE                296.7 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.3776050 MHz
NUC1                11B
P1                 28.50 usec
PLW1         14.79100037 W
SFO2         400.1324710 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.17000008 W
PLW12         0.07408100 W

F2 - Processing parameters
SI                 32768
SF           128.3776052 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

CY-B-B-65P-Ph-Tol-(C)




```
Current Data Parameters
NAME      CY-B-B-65P-Ph-Tol-(C)
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190620
Time                  11.00 h
INSTRUM               spect
PROBHD    Z820201_0170 (
PULPROG                   zg
TD                     65536
SOLVENT                CDCl3
NS                        92
DS                         4
SWH               25510.203 Hz
FIDRES             0.778510 Hz
AQ                1.2845056 sec
RG                       203
DW                   19.600 usec
DE                    6.50 usec
TE                   296.6 K
D1              1.00000000 sec
TD0                        1
SFO1            128.3776050 MHz
NUC1                    11B
P1                   28.50 usec
PLW1           14.79100037 W

F2 - Processing parameters
SI                     32768
SF              128.3776052 MHz
WDW                       EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

References

1. Y. Chen, Y. K. Au, Y. Quan and Z. Xie, *Sci. China Chem.*, 2019, **62**, 74–79.
2. M. Xu, A. R. Jupp, M. S. E. Ong, K. I. Burton, S. S. Chitnis and D. W. Stephan, *Angew. Chem. Int. Ed*., 2019, **58**, 5707–5711.
3. E. V. Vinogradova, B. P. Fors and S. L. Buchwald, *J. Am. Chem. Soc*., 2012, **134**, 11132–11135.
4. G. M. Sheldrick, S*ADABS: Program for Empirical Absorption Correction of Area Detector Data*. (University of Göttingen: Germany, 1996).
5. G. M. Sheldrick, *SHELXTL 5.10 for Windows NT: Structure Determination Software Programs*. (Bruker Analytical X-ray Systems, Inc., Madison, Wisconsin,USA, 1997).