Electronic Supplementary Information

Dehydrogenative Cross-Coupling of *o*-Carborane with Thiophenes via Ir-Catalyzed Regioselective Cage B-H and C(sp^2)-H Activation

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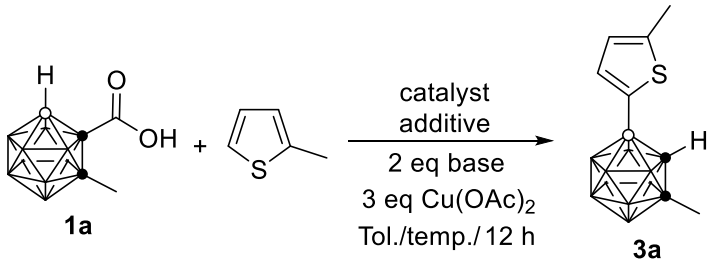
General Procedures. All reactions were carried out in flame-dried glassware using standard Schlenk techniques. DMF (dimethylformamide), DMSO (dimethyl sulfoxide) and PhCl were dried with 4A molecular sieves for a week before distillation under reduced pressure. Other solvents were freshly distilled from sodium benzophenone ketyl immediately prior to use. ^{1}H, ^{13}C, and ^{11}B NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400, 100 and 128 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, and to external $BF_3 \cdot OEt_2$ (0.00 ppm) for boron chemical shifts. High resolution mass spectra (HRMS) were obtained on a Thermo Finnigan MAT 95 XL spectrometer. Carboranyl carboxylic acids **1**[1] and **A'**[2] were prepared according to literature methods. All other chemicals were purchased from either Aldrich or Acros Chemical Co. and used as received unless otherwise specified.

Detailed Optimization Experiments.

Table S1 Optimization of reaction conditions[a]



1a **3a**

entry	catalyst (%)	additive (%)	base	temp. (^{o}C)	**3a** (%)[b]
1	$Pd(OAc)_2$ (10)	-	K_2HPO_4	110	messy

2[c]	$Pd(OAc)_2$ (10)	-	K_2HPO_4	110	messy
3	$[Cp^*RhCl_2]_2$ (5)	-	K_2HPO_4	110	trace
4	$[Cp^*RhCl_2]_2$ (5)	-	K_2HPO_4	130	trace
5	$[Cp^*RhCl_2]_2$ (5)	-	K_2HPO_4	150	11
6[c]	$[Cp^*RhCl_2]_2$ (5)	-	K_2HPO_4	150	-
7[d]	$[Cp^*RhCl_2]_2$ (5)	-	K_2HPO_4	150	-
8	$[Cp^*RhCl_2]_2$ (5)	$AgSbF_6$ (20)	K_2HPO_4	150	22
9	$[Cp^*RhCl_2]_2$ (5)	$AgNTf_2$ (20)	K_2HPO_4	150	40
10	$[Cp^*RhCl_2]_2$ (5)	AgOAc (20)	K_2HPO_4	150	15
11	$[Cp^*IrCl_2]_2$ (5)	-	K_2HPO_4	150	12
12	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	K_2HPO_4	150	56
13	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	K_2HPO_4	140	60
14	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	K_2HPO_4	130	55
15	$[Cp^*IrCl_2]_2$ (5)	AgOAc (20)	K_2HPO_4	140	20
16	$[Cp^*IrCl_2]_2$ (5)	$AgSbF_6$ (20)	K_2HPO_4	140	48
17	$[Cp^*IrCl_2]_2$ (5)	$AgBF_4$ (20)	K_2HPO_4	140	57
18	$[Cp^*IrCl_2]_2$ (5)	$AgPF_6$ (20)	K_2HPO_4	140	43
19	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	Li_2CO_3	140	68
20	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	Na_2CO_3	140	64
21	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	K_2CO_3	140	55
22	$[Cp^*IrCl_2]_2$ (5)	$Zn(NTf_2)_2$ (20)	Li_2CO_3	140	32

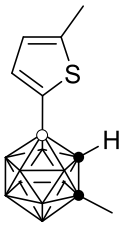
23[c]	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	Li_2CO_3	140	trace
24[d]	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	Li_2CO_3	140	-
25[e]	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	Li_2CO_3	140	-
26[f]	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20)	Li_2CO_3	140	51
27	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (10) + AgOAc (10)	Li_2CO_3	140	79
28	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (20) + AgOAc (20)	Li_2CO_3	140	72
29[g]	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (10) + AgOAc (10)	Li_2CO_3	130	86
30[g,h]	$[Cp^*IrCl_2]_2$ (5)	$AgNTf_2$ (5) + AgOAc (5)	Li_2CO_3	130	65

[a] Reactions were conducted using 0.05 mmol of **1a** and 1.00 mmol of 2-methylthiophene in 2 mL of toluene in a closed flask; $AgNTf_2$ = silver bis(trifluoromethanesulfonyl)imide, $Zn(NTf_2)_2$ = zinc di[bis(trifluoromethylsulfonyl)imide]. [b] GC yield. [c] 2 equiv of Ag_2CO_3 was used as the oxidant. [d] DMF was used as the solvent. [e] DMSO was used as the solvent. [f] PhCl was used as the solvent. [g] Reaction time was 24 h. [h] 2.5 mol% $[Cp^*IrCl_2]_2$ was used.

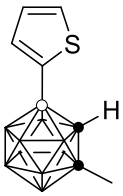
Preparation of B(4)-Thienylated-*o*-Carboranes (3). A Representative Procedure. *o*-Carborane monocarboxylic acid **1** (0.10 mmol), $[Cp^*IrCl_2]_2$ (0.005 mmol), $AgNTf_2$ (0.01 mmol), AgOAc (0.01 mmol), Li_2CO_3 (0.20 mmol), $Cu(OAc)_2$ (0.30 mmol), and thiophene (0.20-2.00 mmol) were mixed in toluene (5 mL) under Ar. The resulting mixture was heated in a closed flask at 130-160 ^oC for 24 h. After hydrolysis with water (10 mL) and extraction with diethyl ether (10 mL x 3), the ether solutions were combined and concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel

(230-400 mesh) using *n*-hexane and ethyl acetate (100/1 in v/v) as eluent to give the product **3**.

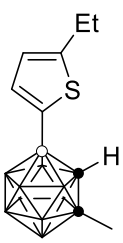
The B(4)-selectivity in **3o** was unambiguously confirmed by single-crystal X-ray analyses. The B(4)-selectivity for other products was inferred from the similarity of ^{11}B NMR spectra. It was noted that the relative integration of the cage C*H*$_3$ peak was higher than 3 because of the overlap with broad B-H resonances.



3a: Yield 81%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02 (d, *J* = 3.2 Hz, 1H), 6.72 (d, *J* = 3.2 Hz, 1H) (thienyl *H*), 3.74 (s, 1H) (cage *H*), 2.48 (s, 3H), 2.08 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 144.2, 134.0, 126.8 (thienyl *C*), 71.2, 63.0 (cage *C*), 26.1, 15.3 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.1 (1B), -5.4 (1B) (*B*-C), -6.1 (1B), -9.0 (1B), -10.3 (1B), -11.7 (4B), -14.0 (1B). HRMS: *m*/*z* calcd for $C_8H_{18}B_{10}S$ $[M]^+$: 254.2127. Found: 254.2129.

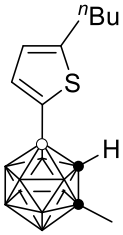


3b: Yield 62%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (d, *J* = 4.8 Hz, 1H), 7.24 (d, *J* = 3.2 Hz, 1H), 7.08 (dd, *J* = 3.2, 4.8 Hz, 1H) (thienyl *H*), 3.78 (s, 1H) (cage *H*), 2.09 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 133.9, 129.4, 128.3 (thienyl *C*), 71.4, 63.0 (cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.0 (1B), -5.4 (1B) (*B*-C), -6.1 (1B), -9.0 (1B), -10.2 (1B), -11.5 (4B), -13.8 (1B). HRMS: *m*/*z* calcd for $C_7H_{16}B_{10}S$ $[M]^+$: 240.1970. Found: 240.1972.

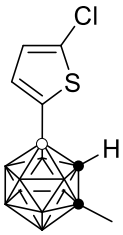


3c: Yield 92%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.05 (d, *J* = 3.2 Hz, 1H), 6.76 (d, *J* = 2.4 Hz, 1H) (thienyl *H*), 3.75 (s, 1H) (cage *H*), 2.84 (q, *J* = 7.6 Hz, 2H) (Et), 2.08 (s, 3H) (C*H*$_3$), 1.31 (t, *J* = 7.6 Hz, 3H) (Et). ^{13}C{^{1}H} NMR

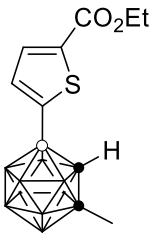
(100 MHz, $CDCl_3$): δ 152.0, 133.8, 124.9 (thienyl *C*), 71.2, 63.0 (cage *C*), 26.1 (*C*H_3), 23.5, 16.1 (Et). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -1.7 (1B), -4.9 (1B) (*B*-C), -5.8 (1B), -8.7 (1B), -9.9 (1B), -11.3 (4B), -13.6 (1B). HRMS: *m*/*z* calcd for $C_9H_{20}B_{10}S$ $[M]^+$: 268.2283. Found: 268.2281.



3d: Yield 86%. Colorless oil. ^1H NMR (400 MHz, $CDCl_3$): δ 7.04 (d, *J* = 3.6 Hz, 1H), 6.74 (d, *J* = 3.2 Hz, 1H) (thienyl *H*), 3.75 (s, 1H) (cage *H*), 2.80 (t, *J* = 7.6 Hz, 2H) (^{n}Bu), 2.08 (s, 3H) (CH_3) 1.65 (m, 2H), 1.40 (m, 2H), 0.94 (t, *J* = 7.6 Hz, 3H) (^{n}Bu). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 150.4, 133.8, 125.5 (thienyl *C*), 71.2, 63.0 (cage *C*), 34.0, 29.8, 26.1, 22.4, 14.0 (*C*H_3 & ^{n}Bu). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.1 (1B), -5.3 (1B) (*B*-C), -6.1 (1B), -9.0 (1B), -10.3 (1B), -11.7 (4B), -14.0 (1B). HRMS: *m*/*z* calcd for $C_{11}H_{24}B_{10}S$ $[M]^+$: 296.2602. Found: 296.2605.

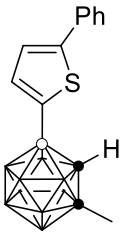


3e: Yield 70%. Colorless oil. ^1H NMR (400 MHz, $CDCl_3$): δ 6.99 (d, *J* = 3.6 Hz, 1H), 6.86 (d, *J* = 3.2 Hz, 1H) (thienyl *H*), 3.75 (s, 1H) (cage *H*), 2.09 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 133.3, 133.2, 127.5 (thienyl *C*), 71.2, 62.8 (cage *C*), 26.1 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -1.8 (1B), -6.1 (2B) (*B*-C & *B*-H), -9.1 (1B), -10.1 (1B), -11.5 (4B), -13.6 (1B). HRMS: *m*/*z* calcd for $C_7H_{15}B_{10}SCl$ $[M]^+$: 275.1558. Found: 275.1559.

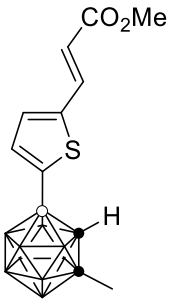


3f: Yield 76%. Colorless oil. ^1H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 3.6 Hz, 1H), 7.18 (d, *J* = 3.6 Hz, 1H) (thienyl *H*), 4.33 (q, *J* = 7.2 Hz, 2H) (Et), 3.82 (s, 1H) (cage *H*), 2.10 (s, 3H) (CH_3), 1.36 (t, *J* = 7.2 Hz, 3H) (Et). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 162.2 (*C*=O), 137.4, 134.2, 134.0 (thienyl *C*), 71.6, 62.8 (cage

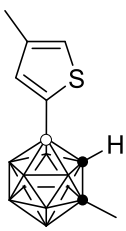
C), 61.3 (Et), 26.1 (*C*H_3), 14.5 (Et). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -1.8 (1B), -6.2 (2B) (*B*-C & *B*-H), -8.9 (1B), -9.9 (1B), -11.4 (4B), -13.3 (1B). HRMS: *m*/*z* calcd for $C_{10}H_{20}B_{10}SO_2$ $[M]^+$: 312.2182. Found: 312.2184.



3g: Yield 90%. White solid. ^1H NMR (400 MHz, $CDCl_3$): δ 7.59 (m, 2H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.27 (m, 2H), 7.19 (d, *J* = 3.2 Hz, 1H) (aryl *H*), 3.79 (s, 1H) (cage *H*), 2.09 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 148.5, 134.8, 134.4, 129.0, 127.7, 126.0, 124.4 (aryl *C*), 71.4, 62.9 (cage *C*), 26.0 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.0 (1B), -6.1 (2B) (*B*-C & *B*-H), -9.0 (1B), -10.1 (1B), -11.5 (4B), -13.7 (1B). HRMS: *m*/*z* calcd for $C_{13}H_{20}B_{10}S$ $[M]^+$: 316.2289. Found: 316.2292.

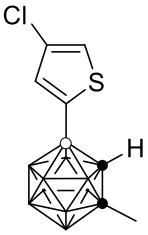


3h: Yield 38%. Colorless oil. ^1H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 15.6 Hz, 1H) (alkenyl *H*), 7.19 (d, *J* = 3.2 Hz, 1H), 7.15 (d, *J* = 3.2 Hz, 1H) (thienyl *H*), 6.22 (d, *J* = 16.0 Hz, 1H) (alkenyl *H*), 3.78 (m, 4H) (cage *H* & C*H*$_3$), 2.10 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 167.5 (*C*=O), 143.2, 137.1, 134.6, 132.1, 116.8 (thienyl & alkenyl *C*), 71.5, 62.8 (cage *C*), 51.8, 26.1 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -1.9 (1B), -6.2 (2B) (*B*-C & *B*-H), -9.1 (1B), -10.1 (1B), -11.5 (5B). HRMS: *m*/*z* calcd for $C_{11}H_{20}B_{10}SO_2$ $[M]^+$: 324.2187. Found: 324.2186.

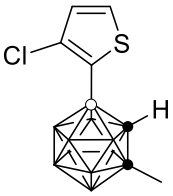


3i: Yield 76%. Colorless oil. ^1H NMR (400 MHz, $CDCl_3$): δ 7.04 (s, 1H), 6.98 (s, 1H) (thienyl *H*), 3.76 (s, 1H) (cage *H*), 2.25 (s, 3H), 2.08 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 139.1, 136.4, 124.9 (thienyl *C*), 71.3, 62.9 (cage *C*), 26.1, 15.4 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.1 (1B), -5.4 (1B) (*B*-C), -6.1 (1B),

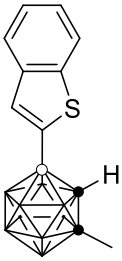
-9.0 (1B), -10.2 (1B), -11.6 (4B), -13.9 (1B). HRMS: *m*/*z* calcd for $C_8H_{18}B_{10}S$ $[M]^+$: 254.2127. Found: 254.2128.



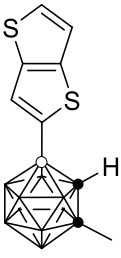
3j: Yield 66%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.17 (s, 1H), 7.07 (s, 1H) (thienyl *H*), 3.77 (s, 1H) (cage *H*), 2.09 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 133.7, 123.9 (thienyl *C*), 71.6, 62.8 (cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.6 (1B), -6.0 (2B) (*B*-C & *B*-H), -8.9 (1B), -9.8 (1B), -11.3 (4B), -13.3 (1B). HRMS: *m*/*z* calcd for $C_7H_{15}B_{10}SCl$ $[M]^+$: 275.1558. Found: 275.1556.



3j': Yield 16%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (d, *J* = 4.8 Hz, 1H), 6.94 (d, *J* = 4.8 Hz, 1H) (thienyl *H*), 4.27 (s, 1H) (cage *H*), 2.10 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 129.5, 129.1, 128.4 (thienyl *C*), 70.9, 61.9 (cage *C*), 26.2 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.4 (1B), -5.9 (1B), -6.6 (1B) (*B*-C), -8.5 (1B), -9.6 (1B), -11.1 (2B), -11.9 (2B), -12.6 (1B). HRMS: *m*/*z* calcd for $C_7H_{15}B_{10}SCl$ $[M]^+$: 275.1558. Found: 275.1560.

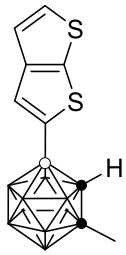


3k: Yield 65%. Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.6 Hz, 1H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.46 (s, 1H), 7.32 (m, 2H) (aryl *H*), 3.85 (s, 1H) (cage *H*), 2.11 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 142.7, 141.1, 130.8, 124.5, 124.4, 123.6, 122.2 (aryl *C*), 71.4, 62.8 (cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.6 (1B), -6.7 (2B) (*B*-C & *B*-H), -9.6 (1B), -10.6 (1B), -12.0 (4B), -14.1 (1B). HRMS: *m*/*z* calcd for $C_{11}H_{18}B_{10}S$ $[M]^+$: 290.2133. Found: 290.2136.

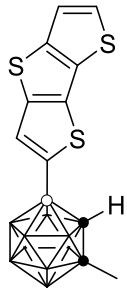


3l: Yield 66%. Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 (m, 2H), 7.21

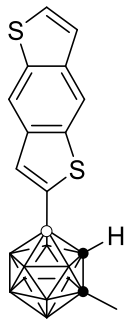
(d, J = 5.2 Hz, 1H) (aryl *H*), 3.81 (s, 1H) (cage *H*), 2.10 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 143.2, 141.0, 128.1, 125.7, 119.3 (aryl *C*), 71.5, 62.9 (cage *C*), 26.1 (*C*H$_3$). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -1.9 (1B), -6.0 (2B) (*B*-C & *B*-H), -9.0 (1B), -10.1 (1B), -11.5 (4B), -13.6 (1B). HRMS: *m*/*z* calcd for $C_9H_{16}B_{10}S_2$ $[M]^+$: 296.1691. Found: 296.1693.



3m: Yield 40%. Yellow solid. ^1H NMR (400 MHz, $CDCl_3$): δ 7.34 (m, 2H), 7.17 (d, J = 5.2 Hz, 1H) (aryl *H*), 3.81 (s, 1H) (cage *H*), 2.10 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 148.9, 140.9, 128.6, 126.4, 119.6 (aryl *C*), 71.4, 62.9 (cage *C*), 26.1 (*C*H$_3$). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -1.2 (1B), -5.4 (2B) (*B*-C & *B*-H), -8.4 (1B), -9.6 (1B), -11.0 (4B), -13.1 (1B). HRMS: *m*/*z* calcd for $C_9H_{16}B_{10}S_2$ $[M]^+$: 296.1691. Found: 296.1689.



3n: Yield 54%. Yellow solid. ^1H NMR (400 MHz, $CDCl_3$): δ 7.38 (s, 1H), 7.35 (d, J = 5.2 Hz, 1H), 7.28 (m, 1H) (aryl *H*), 3.83 (s, 1H) (cage *H*), 2.11 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 142.1, 134.5, 130.7, 127.0, 126.2, 126.0, 121.0 (aryl *C*), 71.5, 62.9 (cage *C*), 26.1 (*C*H$_3$). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -1.6 (1B), -5.8 (2B) (*B*-C & *B*-H), -8.8 (1B), -10.0 (1B), -11.3 (4B), -13.3 (1B). HRMS: *m*/*z* calcd for $C_{11}H_{16}B_{10}S_3$ $[M]^+$: 352.1417. Found: 352.1418.



3o: Yield 60%. Yellow crystals. ^1H NMR (400 MHz, $CDCl_3$): δ 8.24 (s, 2H), 7.48 (s, 1H), 7.46 (d, J = 5.6 Hz, 1H), 7.34 (d, J = 5.6 Hz, 1H) (aryl *H*), 3.87 (s, 1H) (cage *H*), 2.11 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 139.9, 139.1, 137.7, 137.3, 129.8, 127.4, 123.1, 116.7, 116.4 (aryl *C*), 71.4, 62.8 (cage *C*), 26.1 (*C*H$_3$). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.0 (1B), -6.1 (2B) (*B*-C & *B*-H), -9.0

(1B), -9.9 (1B), -11.4 (4B), -13.3 (1B). HRMS: *m/z* calcd for $C_{13}H_{18}B_{10}S_2$ $[M]^+$: 346.1853. Found: 346.1859.

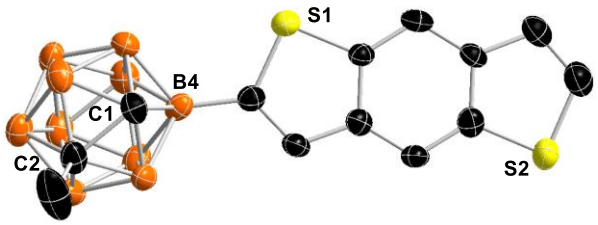
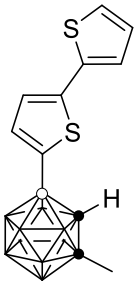
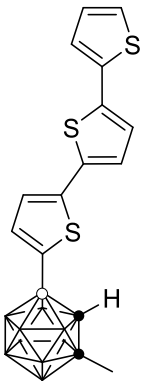


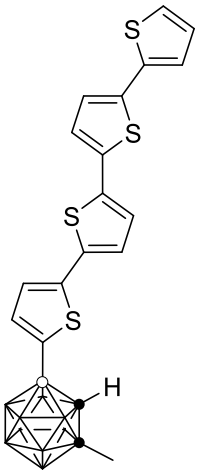
Figure S1 Molecular structure of **3o**.



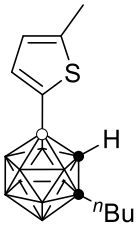
3p: Yield 90%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21 (dd, *J* = 1.2, 4.8 Hz, 1H), 7.17 (dd, *J* = 0.8, 3.6 Hz, 1H), 7.12 (m, 2H), 7.01 (dd, *J* = 3.6, 4.8 Hz, 1H) (aryl *H*), 3.78 (s, 1H) (cage *H*), 2.09 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 141.3, 137.3, 134.6, 128.0, 125.0, 124.6, 123.9 (aryl *C*), 71.4, 62.9 (cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.9 (1B), -6.0 (2B) (*B*-C & *B*-H), -8.9 (1B), -10.0 (1B), -11.5 (4B), -13.7 (1B). HRMS: *m/z* calcd for $C_{11}H_{18}B_{10}S_2$ $[M]^+$: 322.1854. Found: 322.1853.



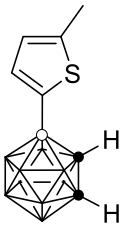
3q: Yield 86%. Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.22 (d, *J* = 4.8 Hz, 1H), 7.17 (d, *J* = 3.6 Hz, 1H), 7.12 (m, 2H), 7.07 (m, 2H), 7.02 (dd, *J* = 3.6, 4.8 Hz, 1H) (aryl *H*), 3.79 (s, 1H) (cage *H*), 2.09 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 141.0, 137.2, 136.4, 136.1, 134.6, 128.0, 125.0, 124.6, 124.5, 124.4, 123.8 (aryl *C*), 71.4, 62.9 (cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.8 (1B), -6.0 (2B) (*B*-C & *B*-H), -8.9 (1B), -10.0 (1B), -11.4 (4B), -13.5 (1B). HRMS: *m/z* calcd for $C_{15}H_{20}B_{10}S_3$ $[M]^+$: 405.1694. Found: 405.1693.



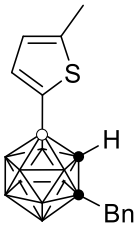
3r: Yield 72%. Yellow solid. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.26 (d, *J* = 5.2 Hz, 1H), 7.21 (d, *J* = 3.2 Hz, 1H), 7.16 (m, 2H), 7.11 (m, 4H), 7.05 (dd, *J* = 3.6, 4.8 Hz, 1H) (aryl *H*), 3.92 (s, 1H) (cage *H*), 2.10 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, CD_2Cl_2): δ 141.2, 137.3, 136.8, 136.5, 136.3, 135.6, 134.9, 128.8, 128.4, 125.3, 125.1, 124.9, 124.8, 124.7, 124.2 (aryl *C*), 72.2, 63.5 (cage *C*), 26.2 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, CD_2Cl_2): δ -2.1 (1B), -6.2 (2B) (*B*-C & *B*-H), -9.1 (1B), -10.2 (1B), -11.5 (4B), -13.4 (1B). HRMS: *m*/*z* calcd for $C_{19}H_{22}B_{10}S_4$ $[M]^+$: 487.1584. Found: 487.1582.



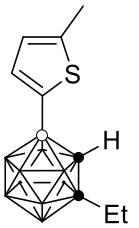
3s: Yield 72%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02 (d, *J* = 3.2 Hz, 1H), 6.72 (d, *J* = 3.2 Hz, 1H) (thienyl *H*), 3.73 (s, 1H) (cage *H*), 2.48 (s, 3H) (C*H*$_3$), 2.24 (m, 2H), 1.45 (m, 2H), 1.30 (m, 2H), 0.90 (t, *J* = 7.2 Hz, 3H) (^{n}Bu). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 144.2, 134.0, 126.8 (thienyl *C*), 76.4, 62.3 (cage *C*), 38.0, 31.4, 22.3, 15.3, 13.8 (*C*H$_3$ & ^{n}Bu). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.8 (1B), -5.5 (2B) (*B*-C & *B*-H), -9.2 (1B), -10.5 (1B), -12.7 (4B), -14.6 (1B). HRMS: *m*/*z* calcd for $C_{11}H_{24}B_{10}S$ $[M]^+$: 296.2602. Found: 296.2601.



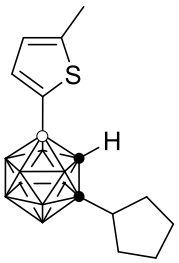
3t: Yield 49%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.03 (d, *J* = 3.2 Hz, 1H), 6.72 (dd, *J* = 1.2, 3.2 Hz, 1H) (thienyl *H*), 3.72 (s, 2H) (cage *H*), 2.48 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 144.3, 134.1, 126.8 (thienyl *C*), 55.7, 55.1 (cage *C*), 15.3 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.9 (1B), -2.7 (1B), -6.1 (1B) (*B*-C), -9.0 (1B), -10.4 (1B), -13.1 (1B), -14.8 (3B), -17.1 (1B). HRMS: *m*/*z* calcd for $C_7H_{16}B_{10}S$ $[M]^+$: 240.1970. Found: 240.1969.



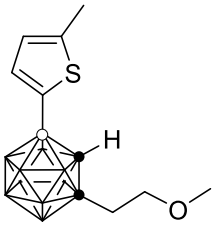
3u: Yield 70%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (m, 3H), 7.14 (m, 2H), 6.93 (d, *J* = 3.2 Hz, 1H), 6.69 (dd, *J* = 1.2, 3.6 Hz, 1H) (aryl *H*), 3.56 (s, 2H) (Bn), 3.41 (s, 1H) (cage *H*), 2.45 (s, 3H) (C*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 144.2, 134.4, 133.9, 129.9, 129.2, 128.7, 126.8 (aryl *C*), 75.4, 60.7 (cage *C*), 43.8 (Bn), 15.2 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.7 (1B), -5.1 (2B) (*B*-C & *B*-H), -8.7 (1B), -10.1 (1B), -12.7 (5B). HRMS: *m*/*z* calcd for $C_{14}H_{22}B_{10}S$ $[M]^+$: 330.2447. Found: 330.2441.



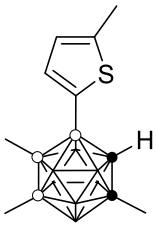
3v: Yield 73%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02 (d, *J* = 3.2 Hz, 1H), 6.72 (m, 1H) (thienyl *H*), 3.73 (s, 1H) (cage *H*), 2.48 (s, 3H) (C*H*$_3$), 2.33 (q, *J* = 7.6 Hz, 2H) (Et), 1.11 (t, *J* = 7.6 Hz, 3H) (Et). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 144.2, 134.0, 126.8 (thienyl *C*), 62.2 (cage *C*), 31.8, 15.2, 13.7 (*C*H$_3$ & Et). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.8 (1B), -5.6 (2B) (*B*-C & *B*-H), -9.2 (1B), -10.5 (1B), -12.7 (4B), -14.8 (1B). HRMS: *m*/*z* calcd for $C_9H_{20}B_{10}S$ $[M]^+$: 268.2283. Found: 268.2280.



3w: Yield 70%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02 (d, *J* = 3.2 Hz, 1H), 6.72 (d, *J* = 2.4 Hz, 1H) (thienyl *H*), 3.78 (s, 1H) (cage *H*), 2.50 (m, 1H), 2.48 (s, 3H) (C*H*$_3$), 1.89 (m, 2H), 1.75 (m, 2H), 1.57 (m, 2H), 1.42 (m, 2H) (alkyl *H*). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 144.1, 133.9, 126.8 (thienyl *C*), 76.8, 62.7 (cage *C*), 47.2, 33.9, 33.8, 24.0, 15.3 (alkyl *C*). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.3 (1B), -4.8 (1B), -6.2 (1B) (*B*-C), -9.3 (1B), -10.5 (1B), -13.1 (4B), -14.7 (1B). HRMS: *m*/*z* calcd for $C_{12}H_{24}B_{10}S$ $[M]^+$: 308.2602. Found: 308.2605.

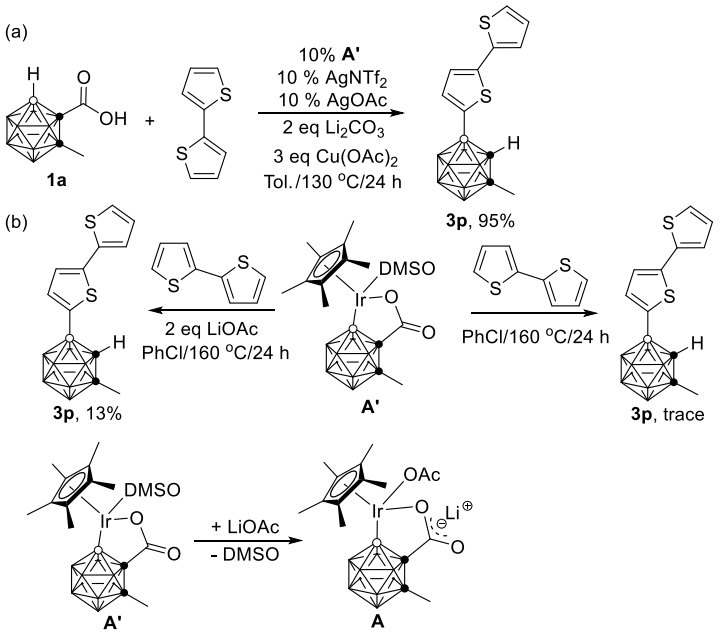


3x: Yield 48%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02 (d, *J* = 3.2 Hz, 1H), 6.72 (d, *J* = 2.4 Hz, 1H) (thienyl *H*), 4.09 (s, 1H) (cage *H*), 3.48 (t, *J* = 6.0 Hz, 2H) (OCH_2), 3.29 (s, 3H) (OCH_3), 2.53 (t, *J* = 5.6 Hz, 2H) (CH_2), 2.48 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 144.1, 133.8 126.8 (thienyl *C*), 74.1, 61.5 (cage *C*), 70.2, 58.8, 37.6, 15.3 (*C*H_2 & *C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -0.4 (1B), -3.1 (2B) (*B*-C & *B*-H), -7.6 (1B), -8.9 (1B), -10.3 (4B), -12.2 (1B). HRMS: *m*/*z* calcd for $C_{10}H_{22}B_{10}OS$ $[M]^+$: 298.2395. Found: 298.2395.



3y: Yield 34%. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02 (d, *J* = 3.2 Hz, 1H), 6.76 (d, *J* = 3.2 Hz, 1H) (thienyl *H*), 3.54 (s, 1H) (cage *H*), 2.51 (s, 3H), 2.08 (s, 3H) (CH_3), 0.26 (s, 3H), 0.17 (s, 3H) (B-CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 144.0, 134.0, 126.8 (thienyl *C*), 65.2, 56.5 (cage *C*), 25.3, 15.3 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ 8.0 (1B) (*B*-CH_3), 3.4 (1B) (*B*-CH_3), -6.0 (1B) (*B*-C), -7.2 (1B), -8.1 (1B), -12.6 (3B), -13.6 (2B). HRMS: *m*/*z* calcd for $C_{10}H_{22}B_{10}S$ $[M]^+$: 282.2445. Found: 282.2446.

Control Experiments.



Scheme S1 Control experiments.

Dehydrogenative cage B-H and thienyl C-H cross-coupling catalyzed by 1,4-[Cp*Ir(DMSO)OCO]-2-Me-$C_2B_{10}H_9$ (A'). 1-COOH-2-Me-$C_2B_{10}H_{10}$ (**1a**) (20.2 mg, 0.10 mmol), **A'** (6.1 mg, 0.01 mmol), $AgNTf_2$ (3.9 mg, 0.01 mmol), AgOAc (1.7 mg, 0.01 mmol), Li_2CO_3 (14.8 mg, 0.20 mmol), $Cu(OAc)_2$ (54.5 mg, 0.30 mmol), and 2,2'-bithiophene (83.1 mg, 0.50 mmol) were mixed in toluene (5 mL) under Ar. The resulting mixture was heated in a closed flask at 130 ^oC for 24 h. After hydrolysis with water, the organic portion was sent for GC-MS analyses. Product **3p** was obtained in 95% GC yield.

Reaction of A' with 2,2'-bithiophene. Compound **A'** (12.1 mg, 0.02 mmol) and 2,2'-bithiophene (16.6 mg, 0.10 mmol) were heated in PhCl (1 mL) at 160 ^oC for 24 h. After hydrolysis with water, the organic portion was sent for GC-MS analyses. Only trace amount of target product **3p** was observed from GC-MS. However, reaction of **A'** (12.1 mg, 0.02 mmol), 2,2'-bithiophene (16.6 mg, 0.10 mmol) and LiOAc (2.6 mg, 0.04 mmol) in PhCl at

160 ^{o}C for 24 h gave **3p** in 13% GC yield.[3]

X-ray Structure Determination. X-ray data of **3o** were collected at 293 K on a Bruker SMART 1000 CCD diffractometer using Cu-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 1526066 (**3o**) 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.

References

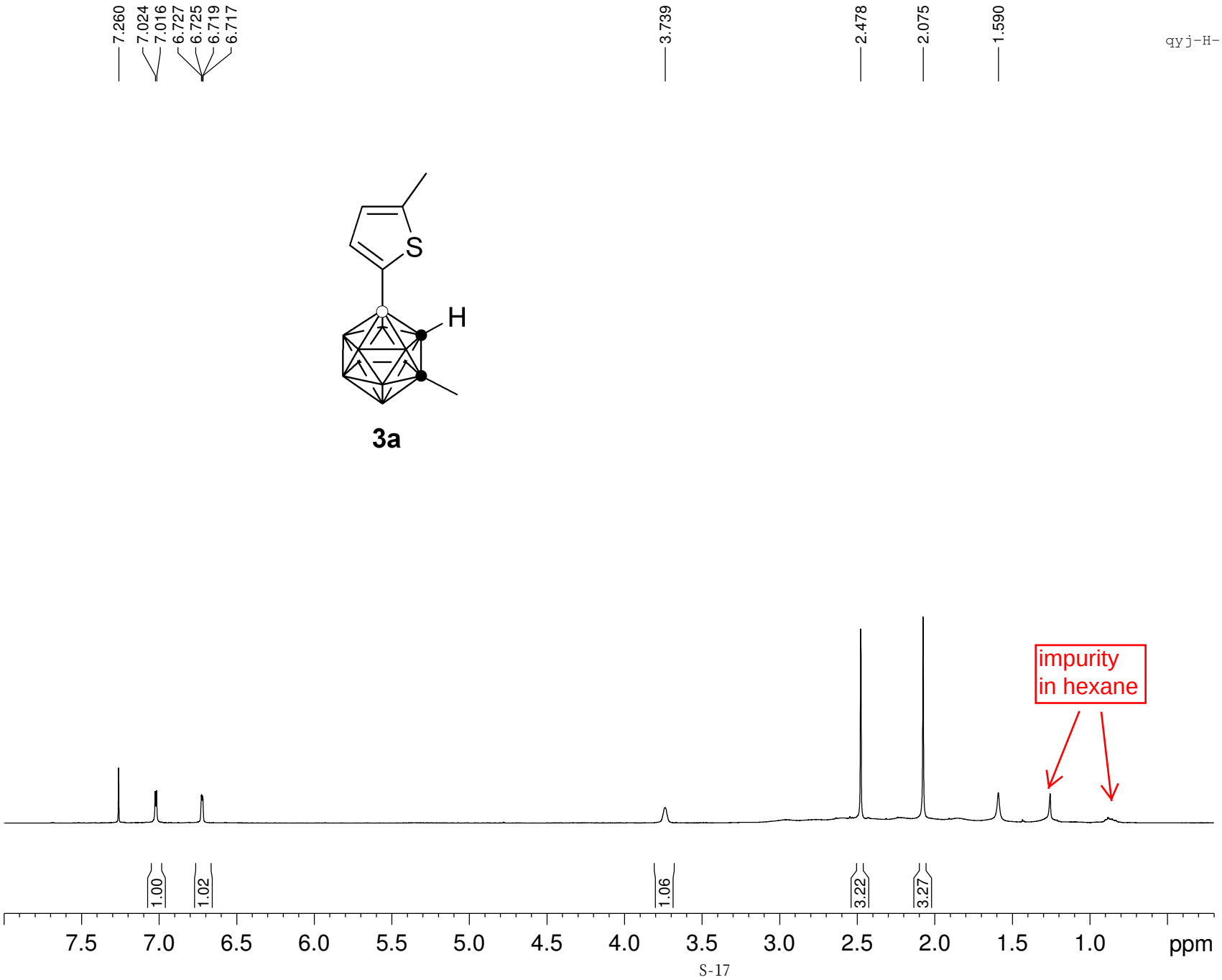
1 (*a*) R. A. Kasar, G. M. Knudsen and S. B. Kahl, *Inorg. Chem.*, 1999, **38**, 2936; (*b*) H. Lyu, Y. Quan and Z. Xie, *Angew. Chem., Int. Ed.*, 2016, **55**, 11840.

2 Y. Quan and Z. Xie, *J. Am. Chem. Soc.*, 2014, **136**, 15513.

3 It has been documented that OAc^- plays an important role in $C(sp^2)$-H activation: D. L. Davies, S. M. A. Donald, O. Al-Duaij, S. A. Macgregor and M. Pölleth, *J. Am. Chem. Soc.*, 2006, **128**, 4210.

4 G. M. Sheldrick, SADABS: 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.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6.725
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3.739
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1.590
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S
H
3a
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PROCNO 1
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DE 6.50 usec
TE 294.6 K
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NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
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LB 0.30 Hz
GB 0
PC 1.00
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in hexane
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1.02
1.06
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7.0
6.5
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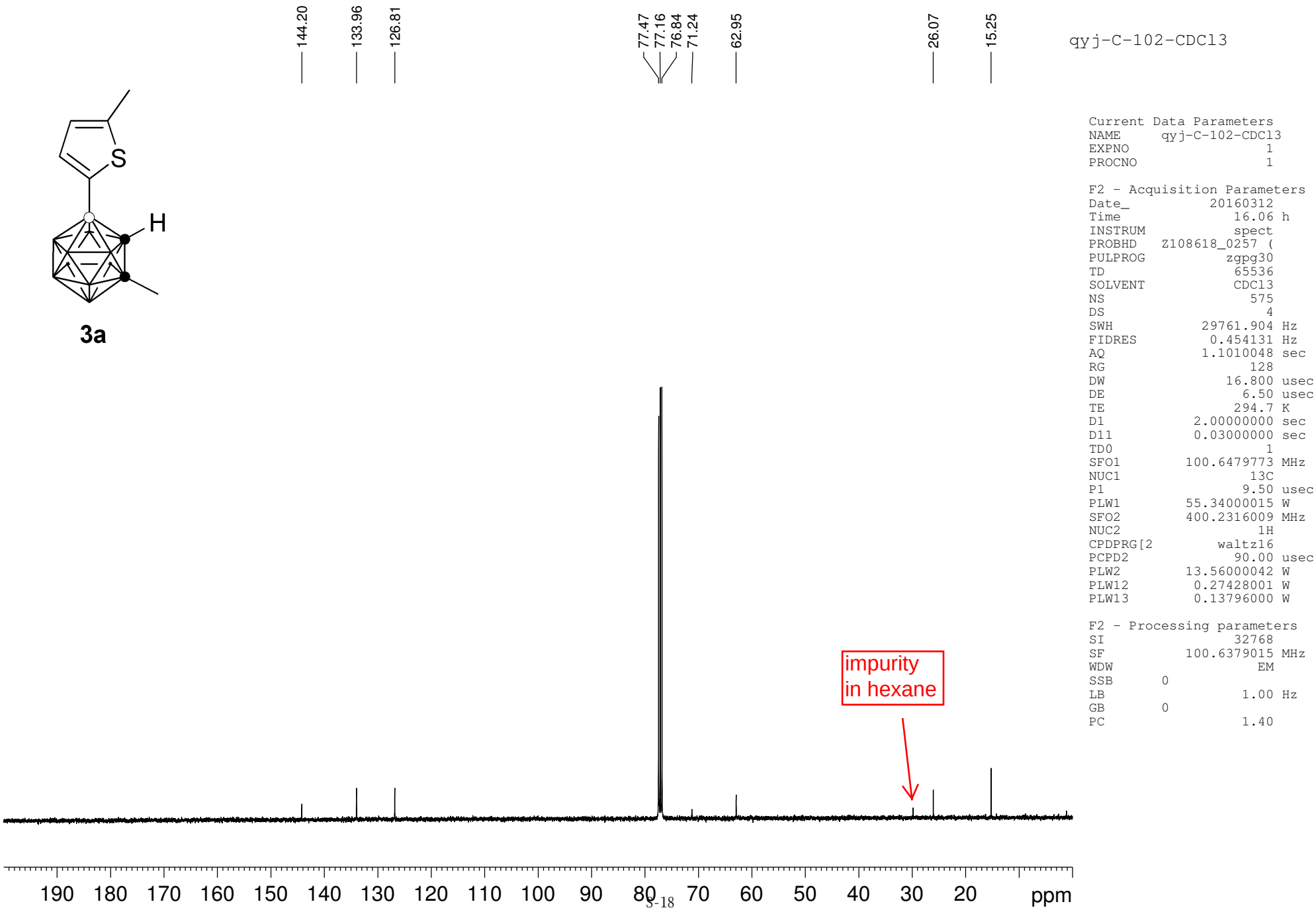
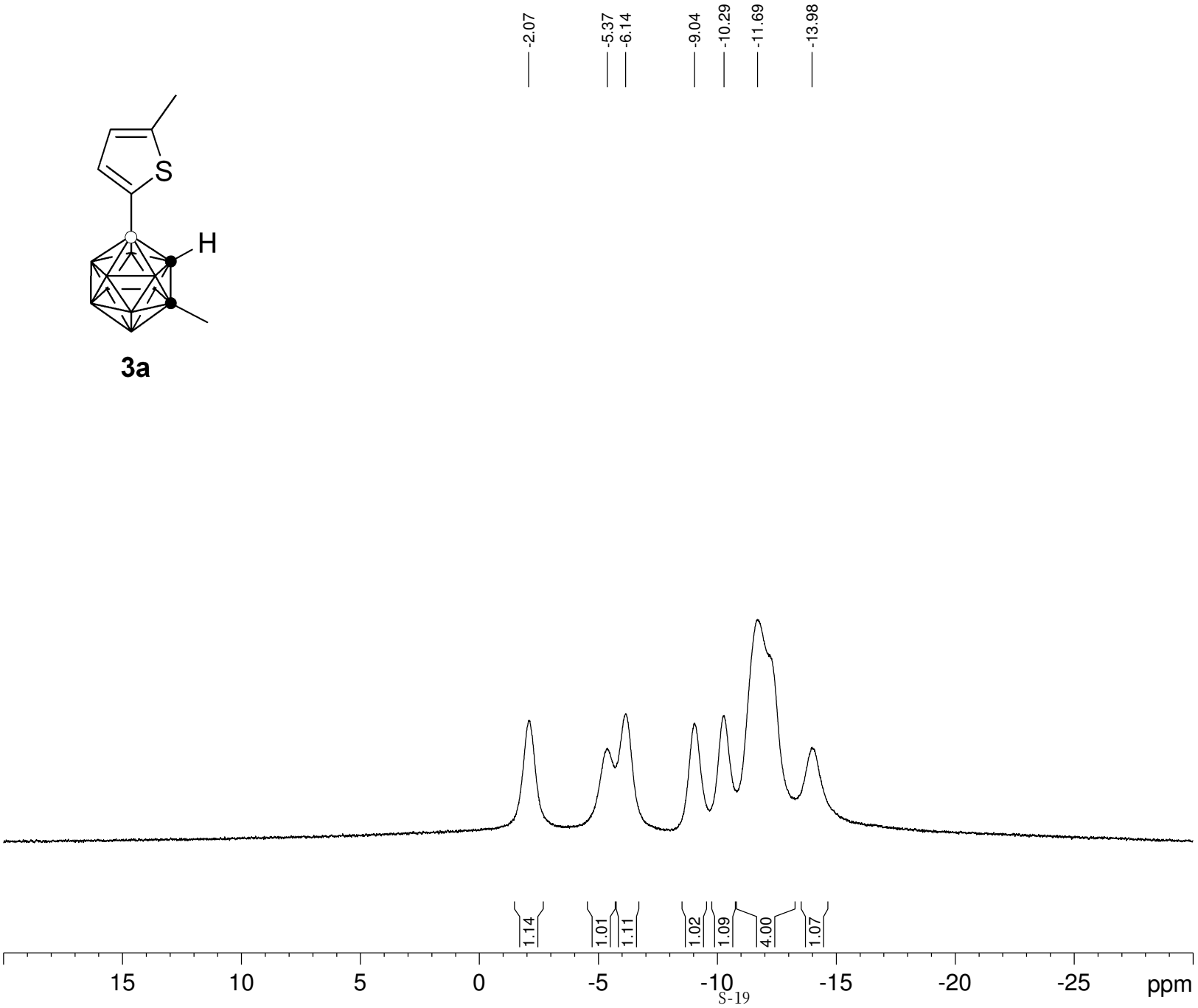
1.0
ppm




```
Current Data Parameters
NAME      qyj-C-102-CDCl3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160312
Time              16.06 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  575
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  128
DW                16.800 usec
DE                 6.50 usec
TE                294.7 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           100.6379015 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

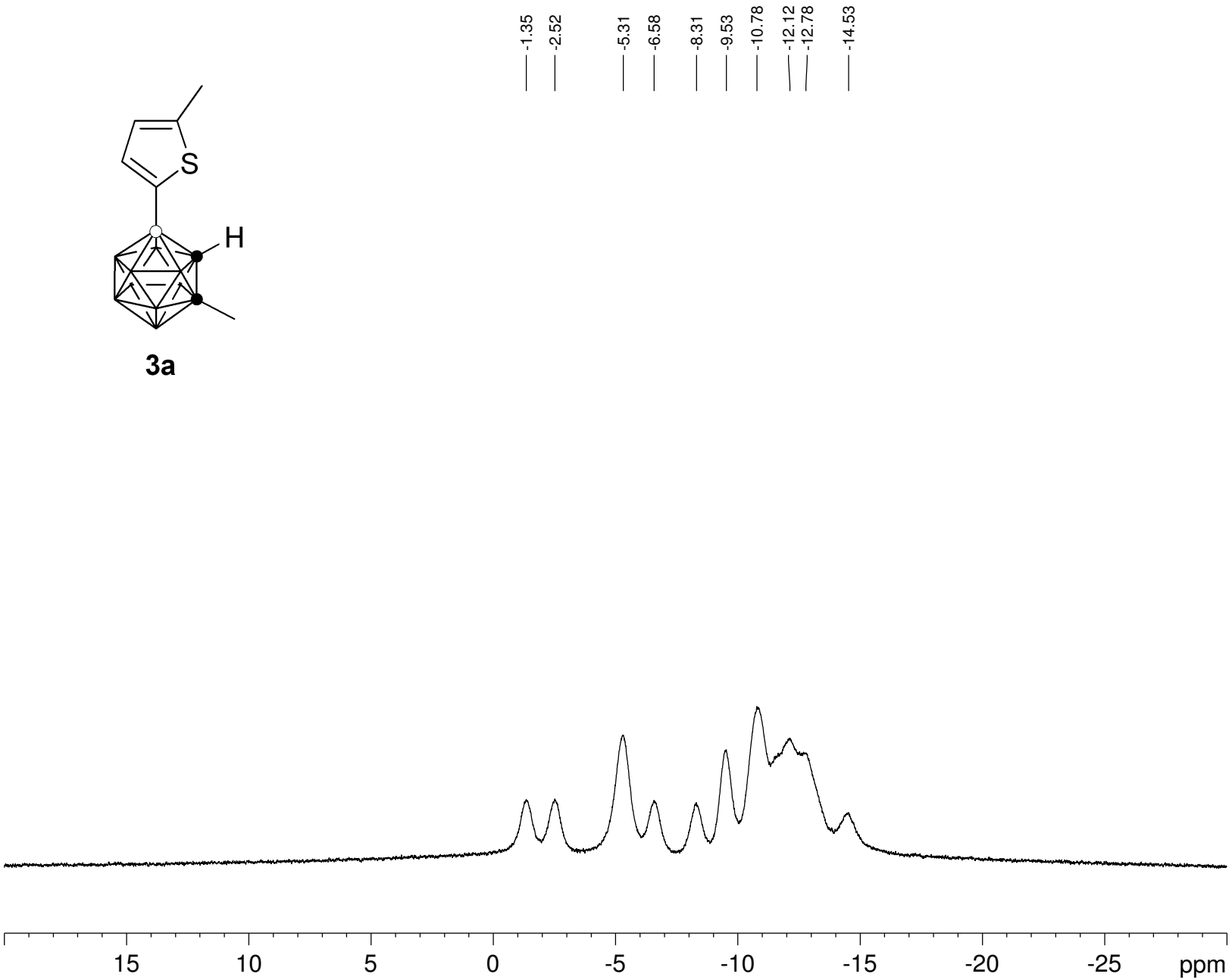
3a



qyj-B-102-CDCl3

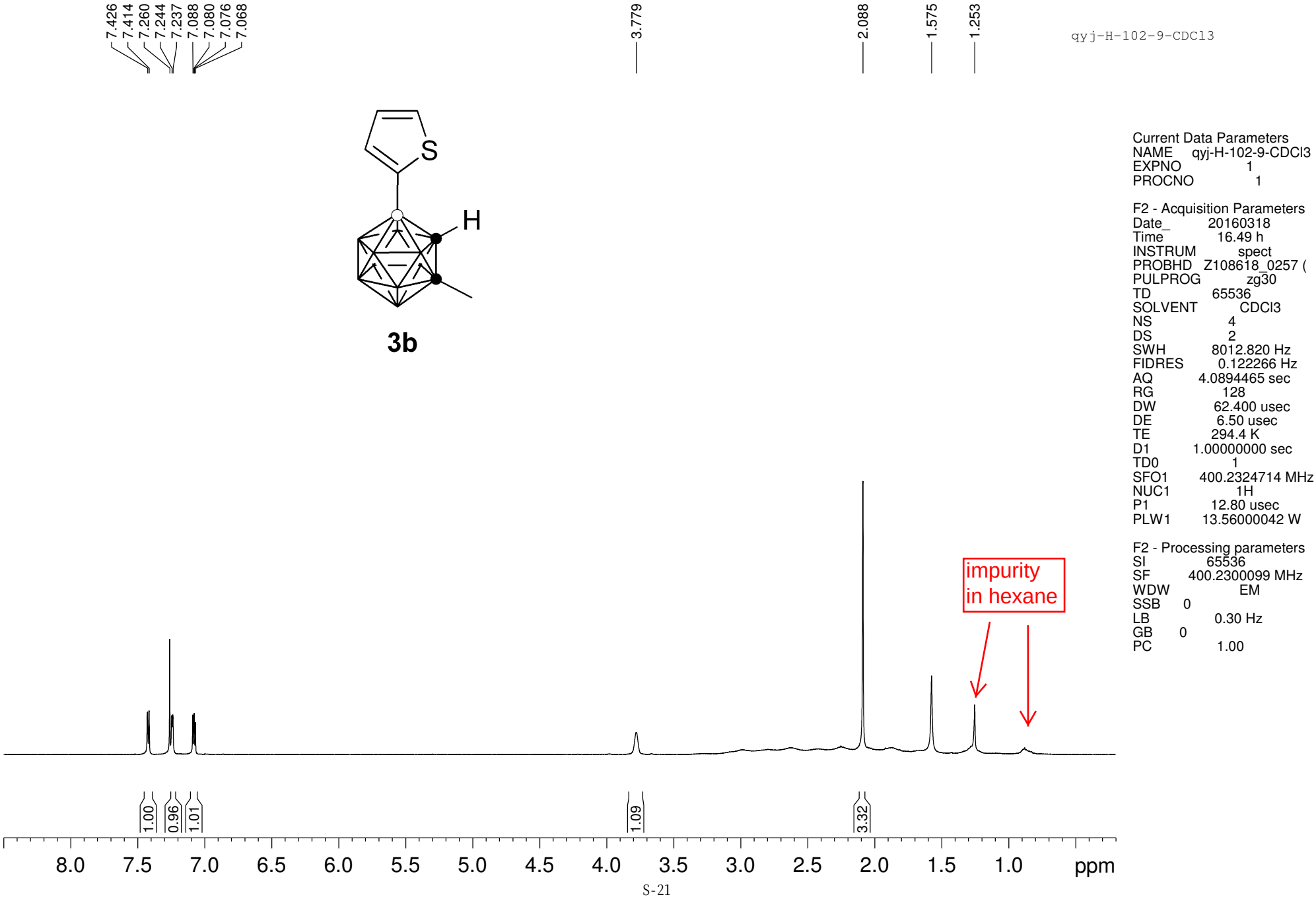
```
Current Data Parameters
NAME      qyj-B-102-CDCl3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160312
Time               15.35 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG            zgdc
TD                65536
SOLVENT           CDCl3
NS                   16
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                295.1 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
```

3a

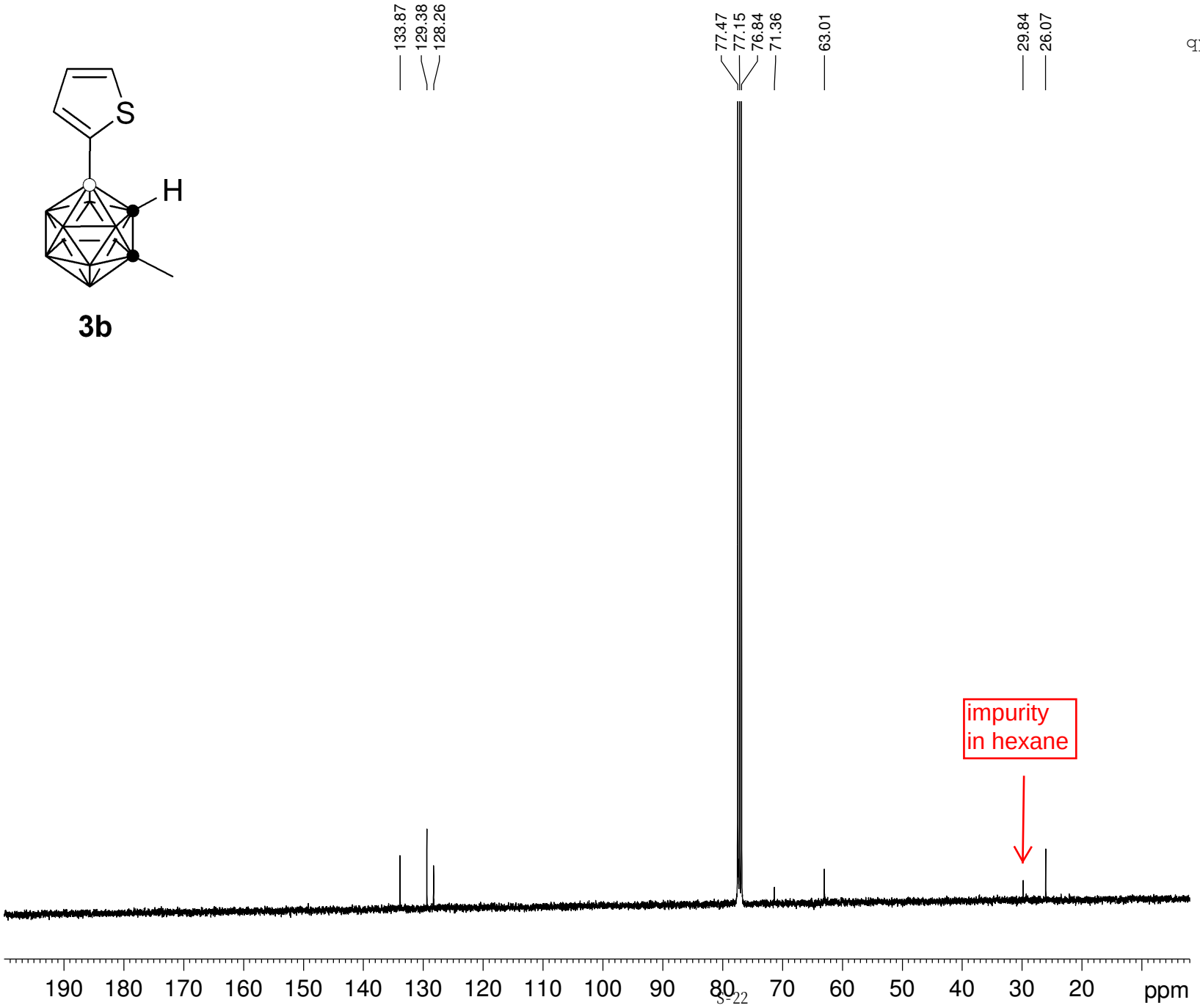


qyj-B-102-CDCl3(c)

```
Current Data Parameters
NAME      qyj-B-102-CDCl3(c)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160312
Time               15.36 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                      8
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                 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
```


7.426
7.414
7.260
7.244
7.237
7.088
7.080
7.076
7.068
3.779
2.088
1.575
1.253
qyj-H-102-9-CDCl3
S
H
3b
Current Data Parameters
NAME qyj-H-102-9-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160318
Time 16.49 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
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 294.4 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 400.2300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
impurity
in hexane
1.00
0.96
1.01
1.09
3.32
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

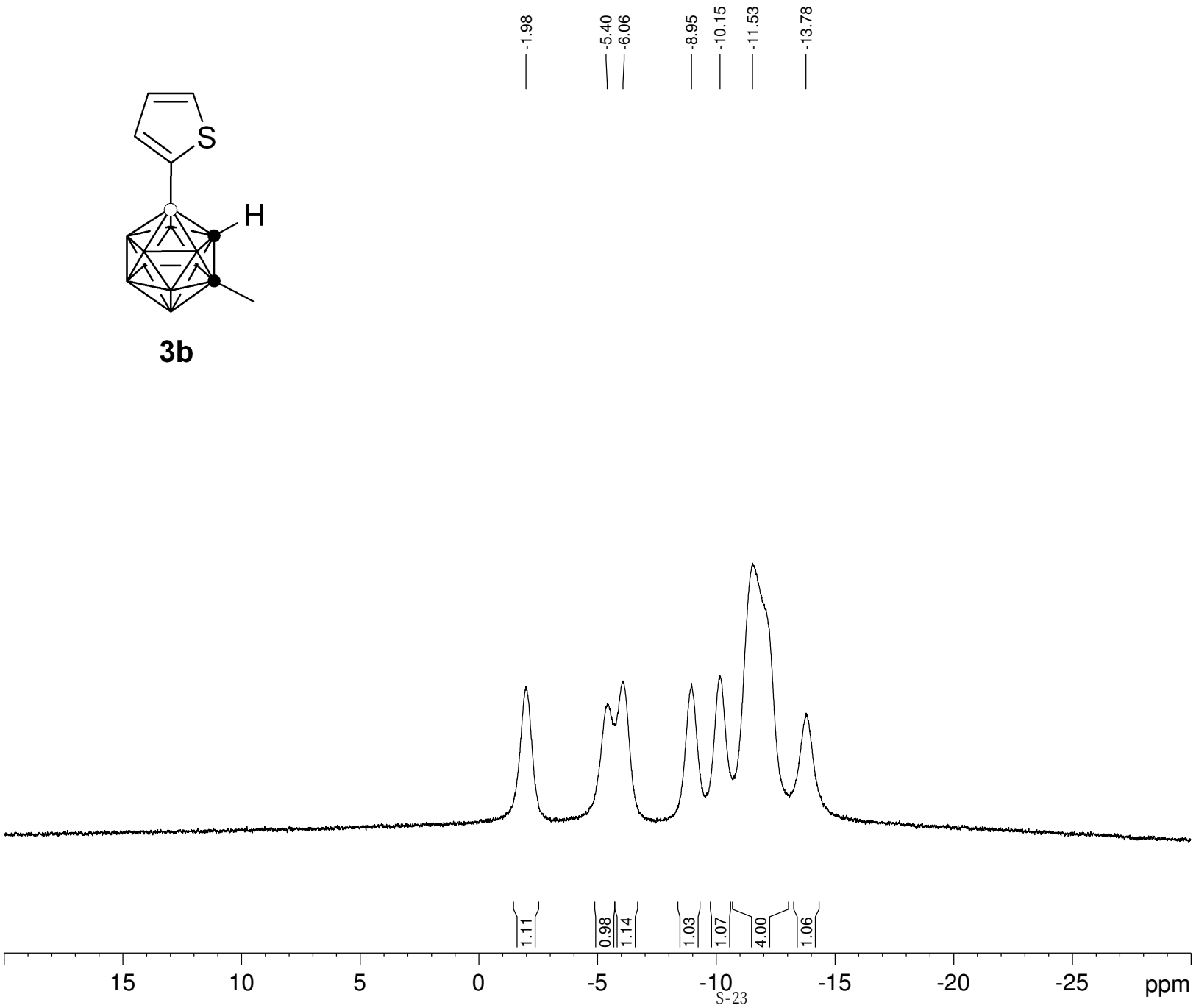
3b



qyj-C-102-13-CDCl3

```
Current Data Parameters
NAME      qyj-C-102-13-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160318
Time              17.11 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  999
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  161
DW               16.800 usec
DE                6.50 usec
TE                294.9 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          100.6379015 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

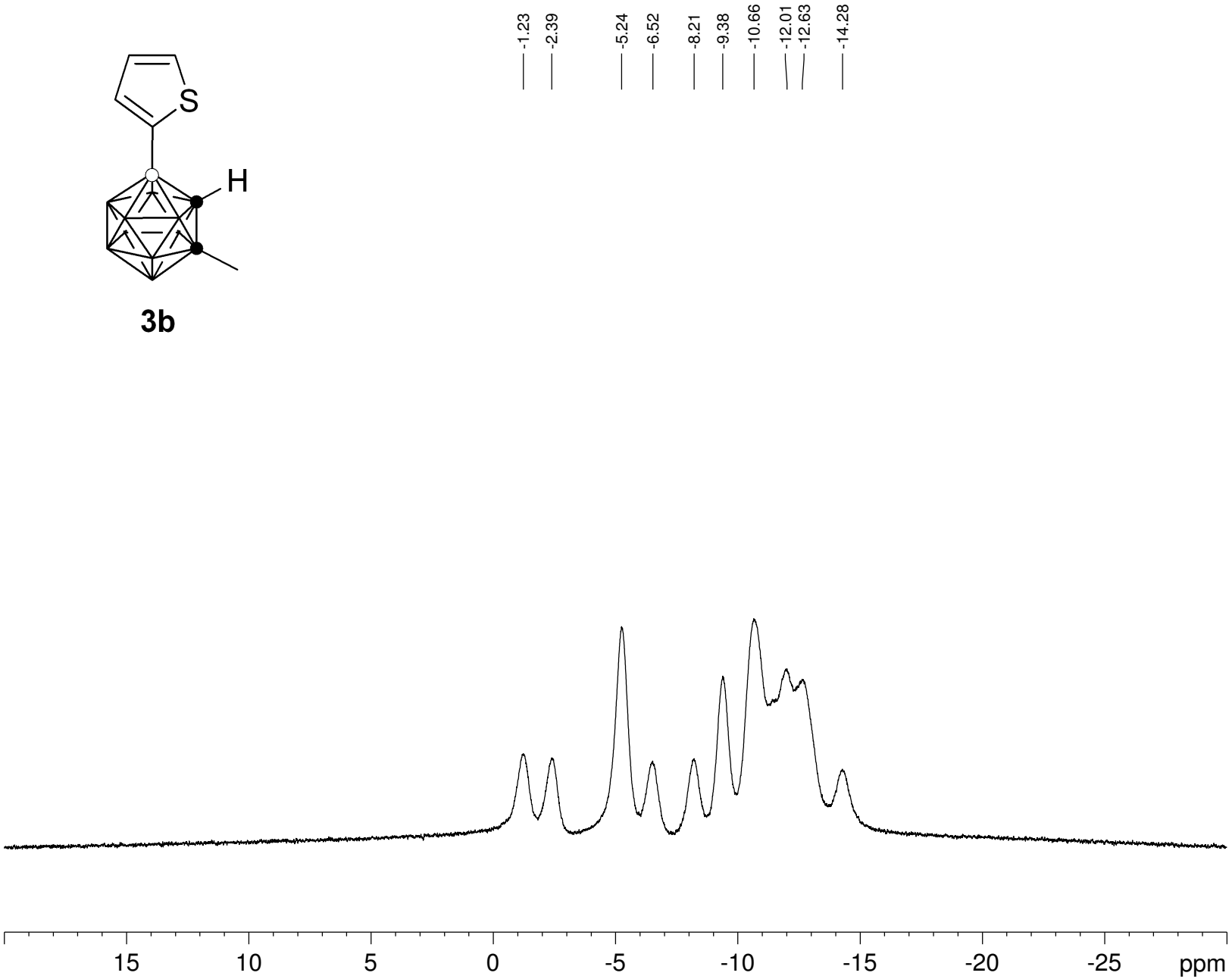
3b



qyj-B-102-9-CDCl3

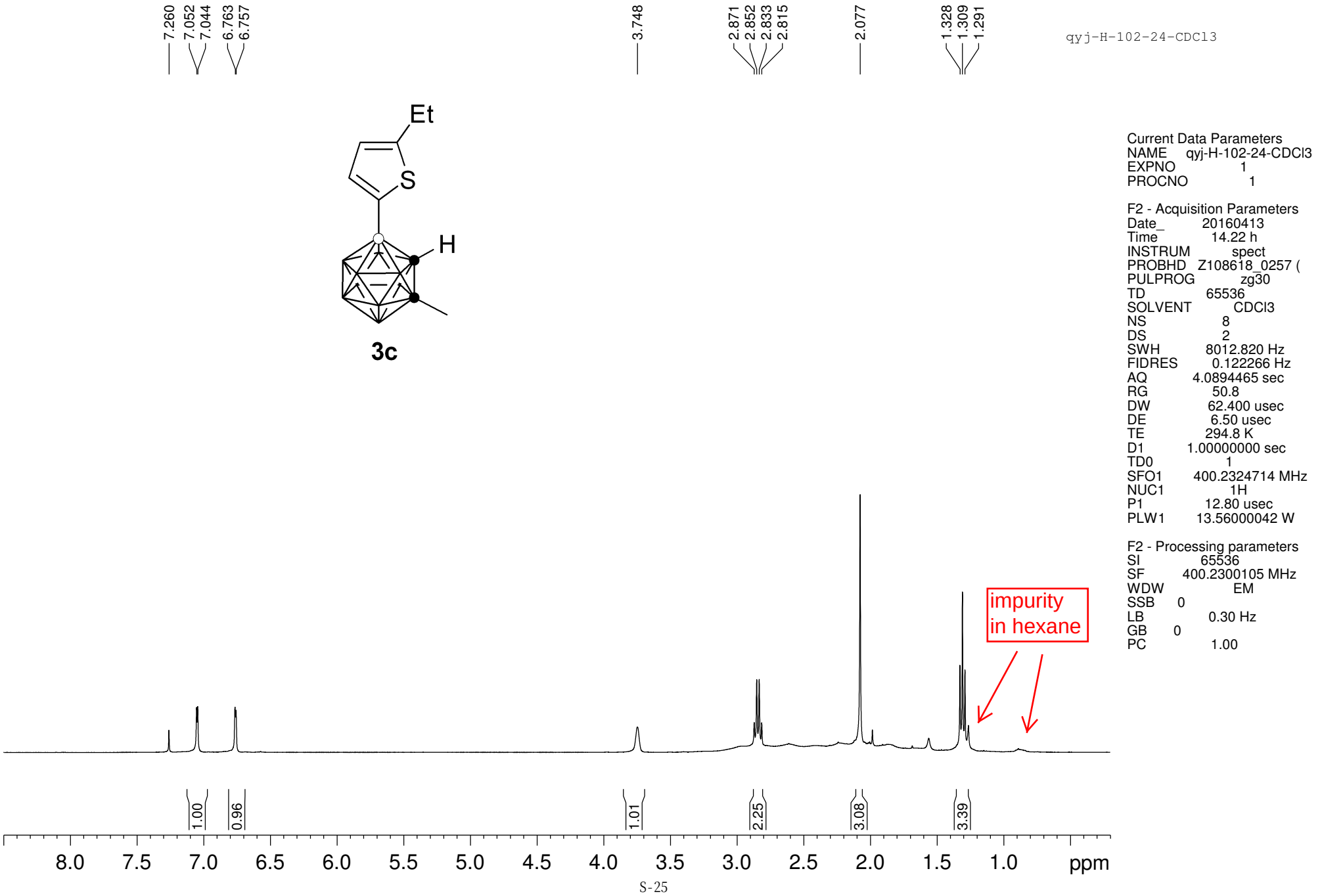
```
Current Data Parameters
NAME      qyj-B-102-9-CDCl3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160318
Time              16.51 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG           zgdc
TD                65536
SOLVENT           CDCl3
NS                   16
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               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
```

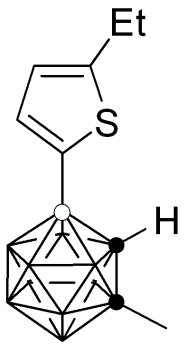
3b



qyj-B-102-9-CDCl3(c)

```
Current Data Parameters
NAME      qyj-B-102-9-CDCl3(c)
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20160318
Time                16.53 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      24
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                  294.5 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
```

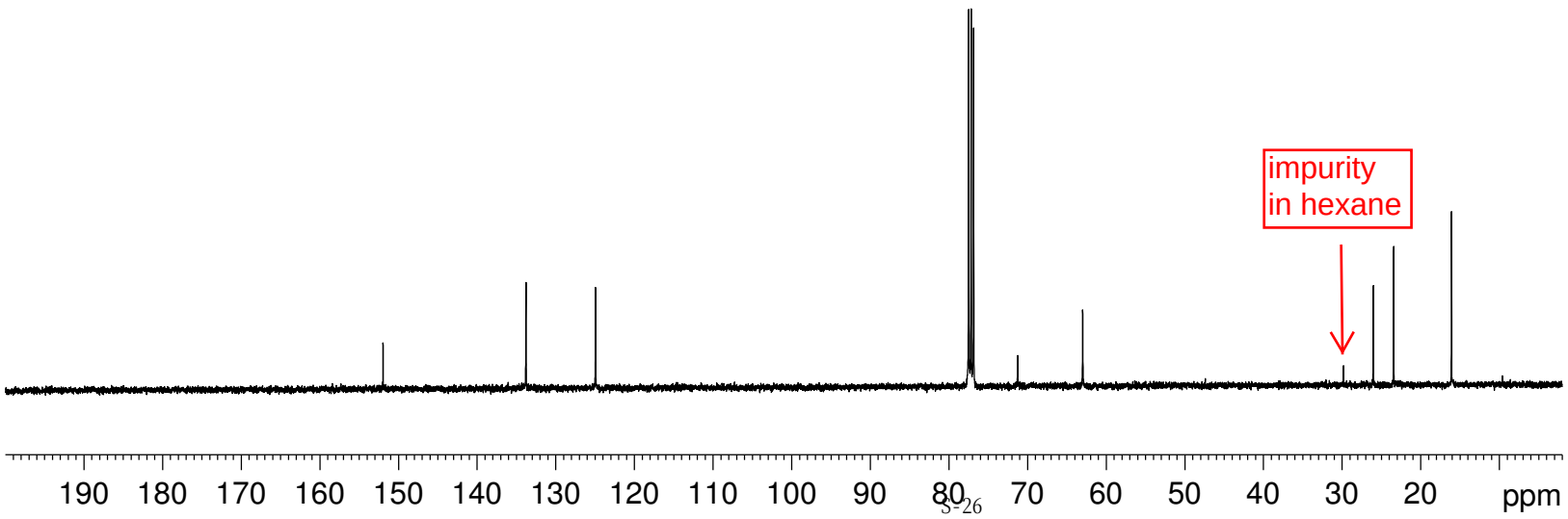

7.260
7.052
7.044
6.763
6.757
3.748
2.871
2.852
2.833
2.815
2.077
1.328
1.309
1.291
qyj-H-102-24-CDCl3
Et
S
H
3c
Current Data Parameters
NAME qyj-H-102-24-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160413
Time 14.22 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 50.8
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 400.2300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
impurity
in hexane
1.00
0.96
1.01
2.25
3.08
3.39
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



3c

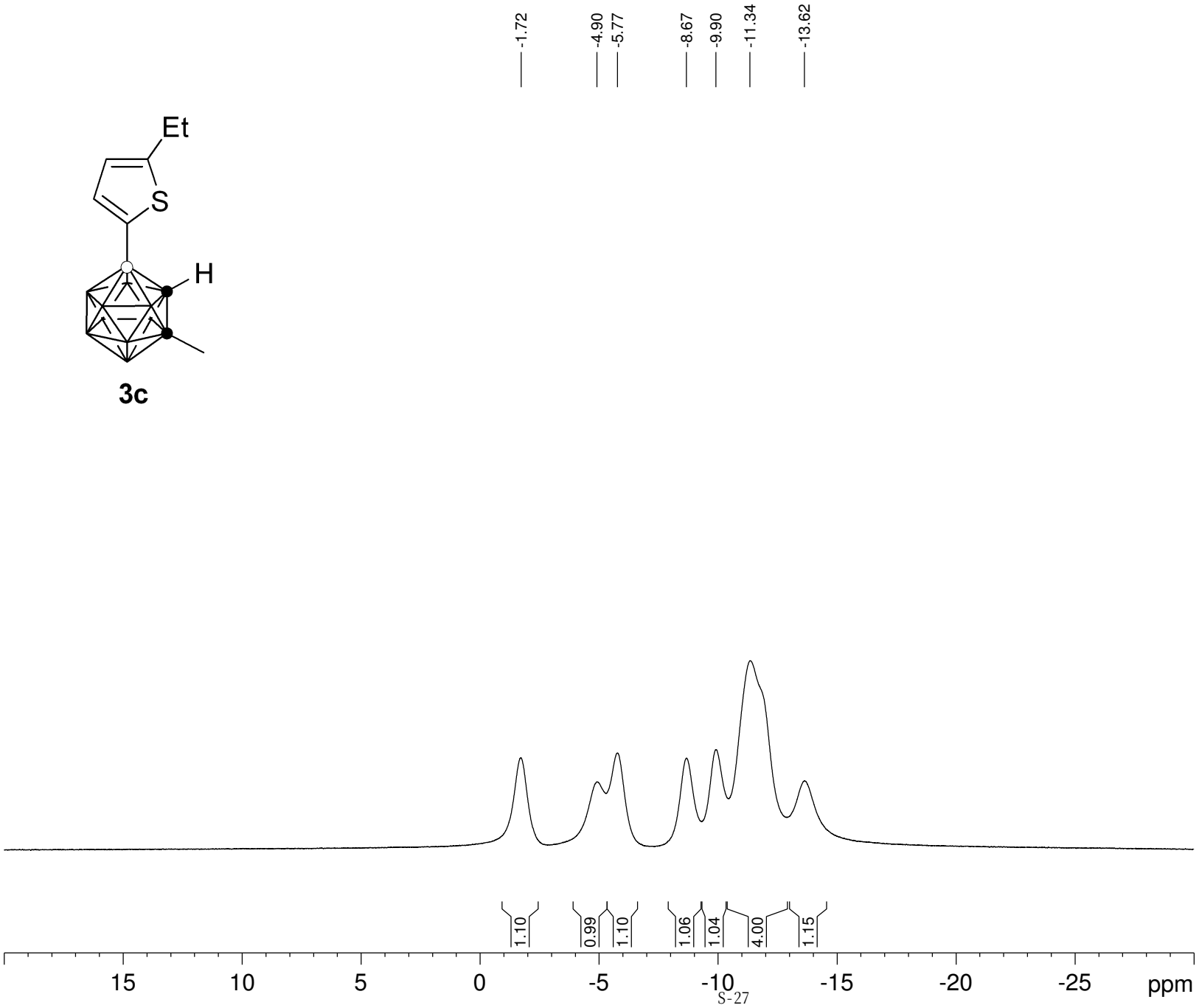
151.95 133.77 124.92 77.47 77.15 76.84 71.24 62.97 29.84 26.05 23.46 16.09

qyj-C-102-24-CDCl3



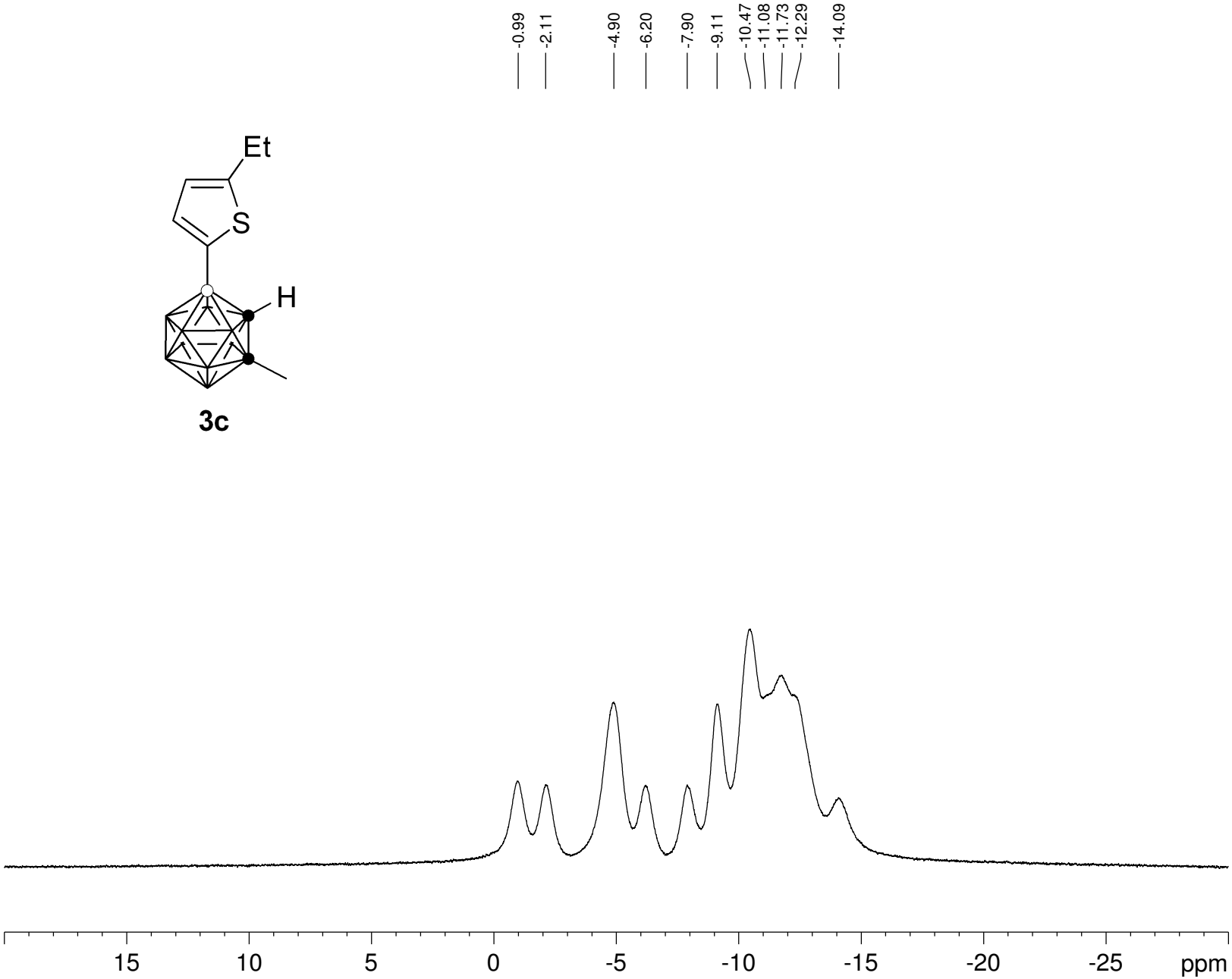

```
Current Data Parameters
NAME      qyj-C-102-24-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160413
Time              14.37 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   389
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                   128
DW                16.800 usec
DE                 6.50 usec
TE                295.0 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           100.6379033 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

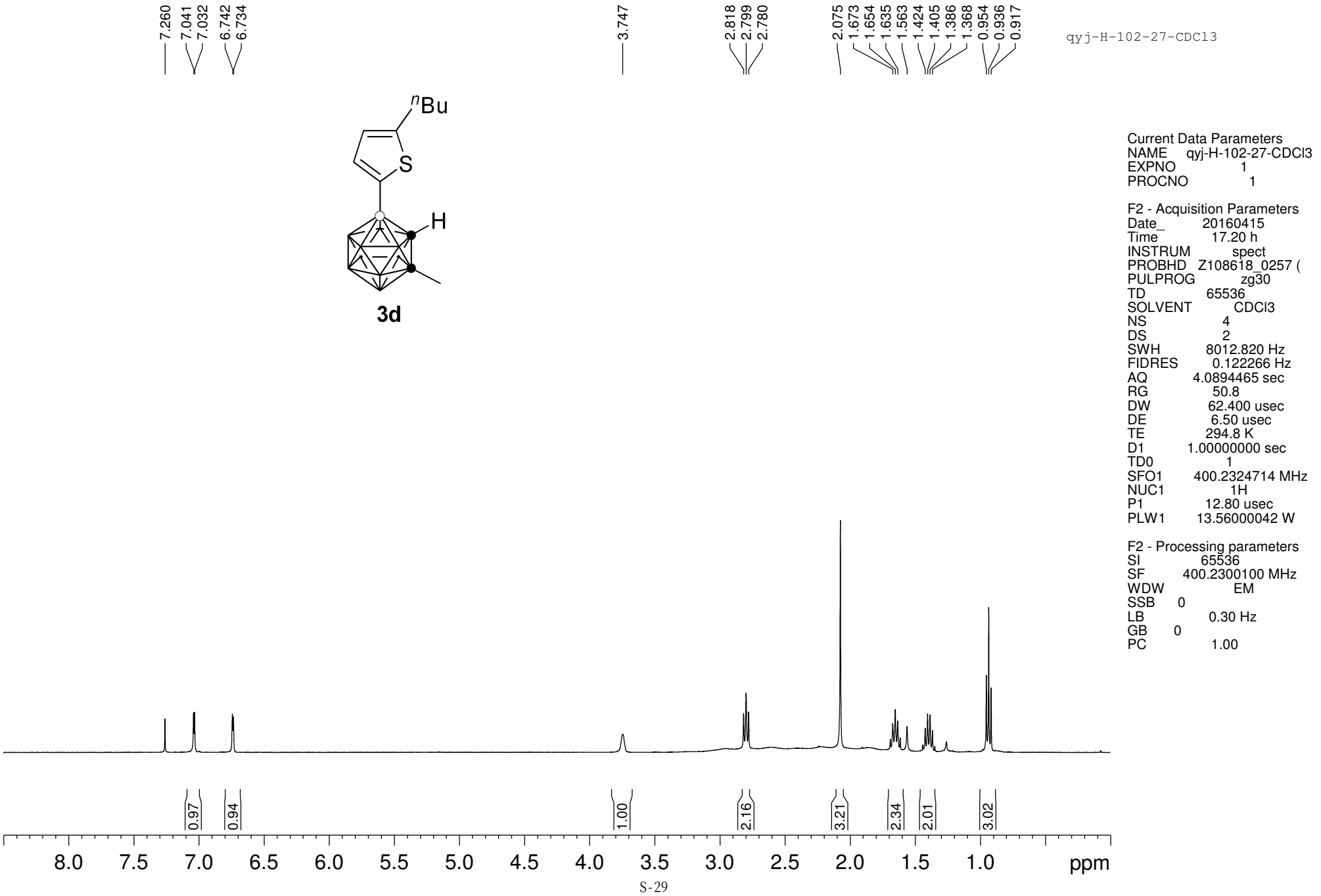
3c

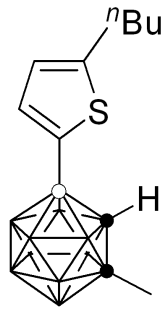


qyj-B-102-24-CDCl3

```
Current Data Parameters
NAME      qyj-B-102-24-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20160413
Time                14.07 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     33
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                 295.4 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
```


-0.99
-2.11
-4.90
-6.20
-7.90
-9.11
-10.47
-11.08
-11.73
-12.29
-14.09
qyj-B-102-24-CDCl3(c)
Et
S
H
3c
Current Data Parameters
NAME qyj-B-102-24-CDCl3(c)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160413
Time 14.08 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 8
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 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
15
10
5
0
-5
-10
-15
-20
-25
ppm


7.260
7.041
7.032
6.742
6.734
3.747
2.818
2.799
2.780
2.075
1.673
1.654
1.635
1.563
1.424
1.405
1.386
1.368
0.954
0.936
0.917
qyj-H-102-27-CDCl3
nBu
S
H
3d
Current Data Parameters
NAME qyj-H-102-27-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160415
Time 17.20 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 50.8
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 400.2300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0.97
0.94
1.00
2.16
3.21
2.34
2.01
3.02
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

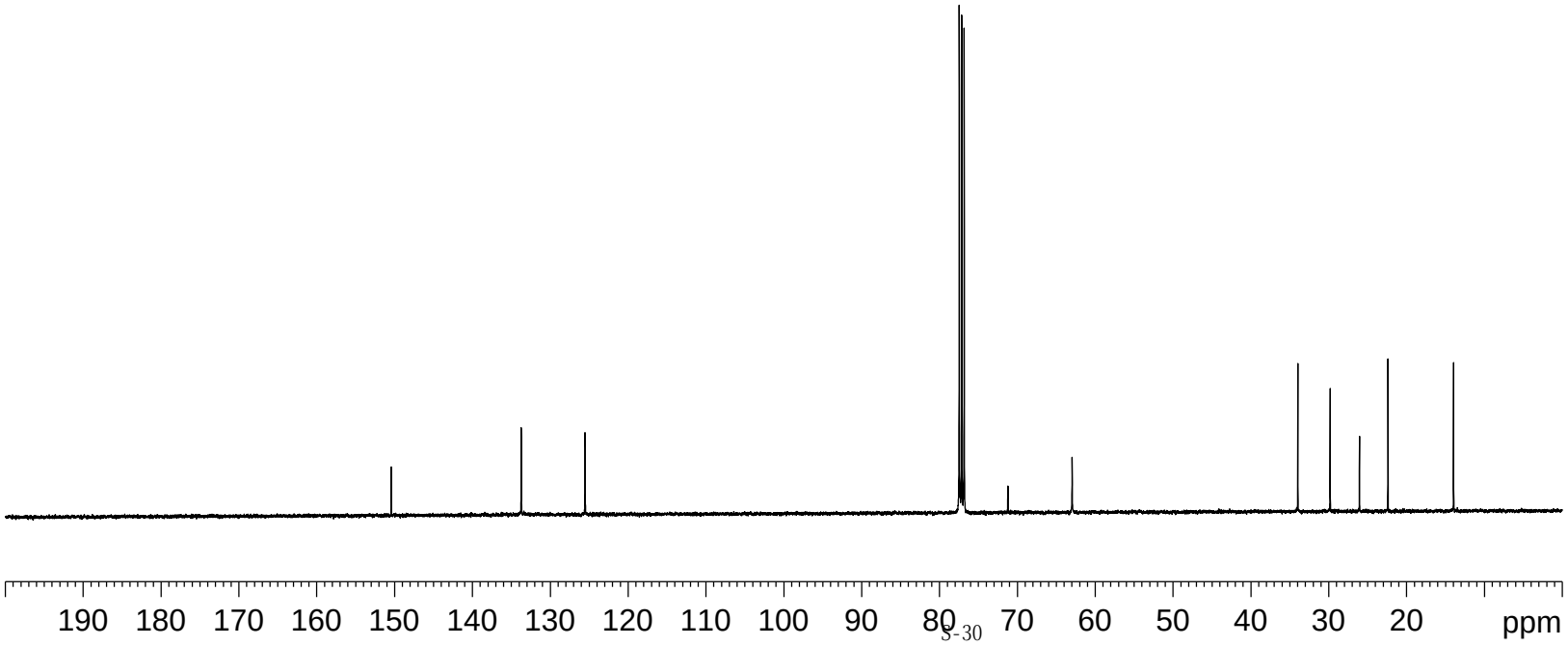


3d

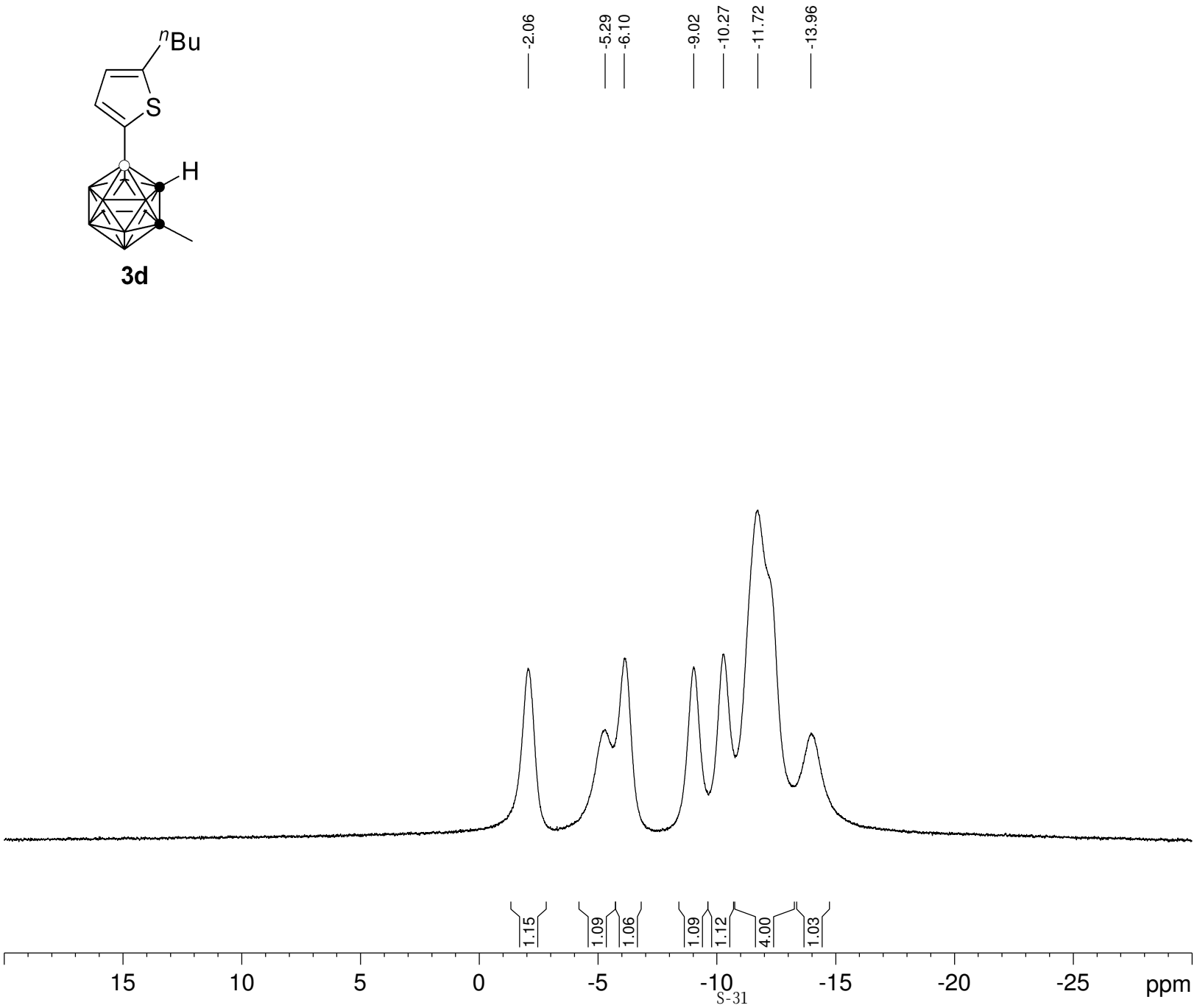
150.40
133.75
125.54
77.47
77.36
77.16
76.84
71.22
62.98
33.98
29.82
26.06
22.40
13.97

qyj-C-102-27-CDCl3

```
Current Data Parameters
NAME      qyj-C-102-27-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20160415
Time                17.37 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1433
DS                      4
SWH             29761.904 Hz
FIDRES           0.454131 Hz
AQ              1.1010048 sec
RG                    128
DW                 16.800 usec
DE                  6.50 usec
TE                  295.1 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            100.6379019 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

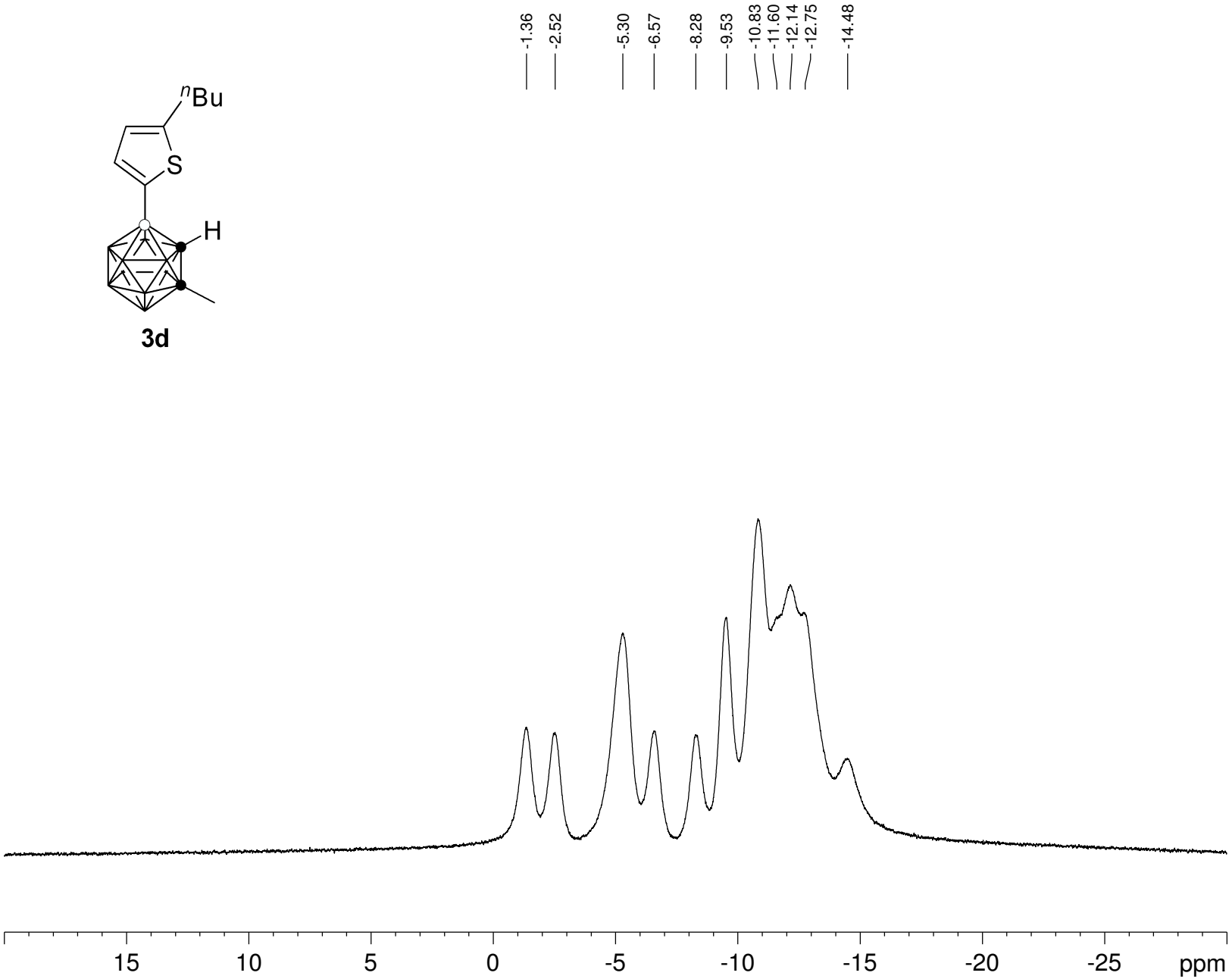


3d



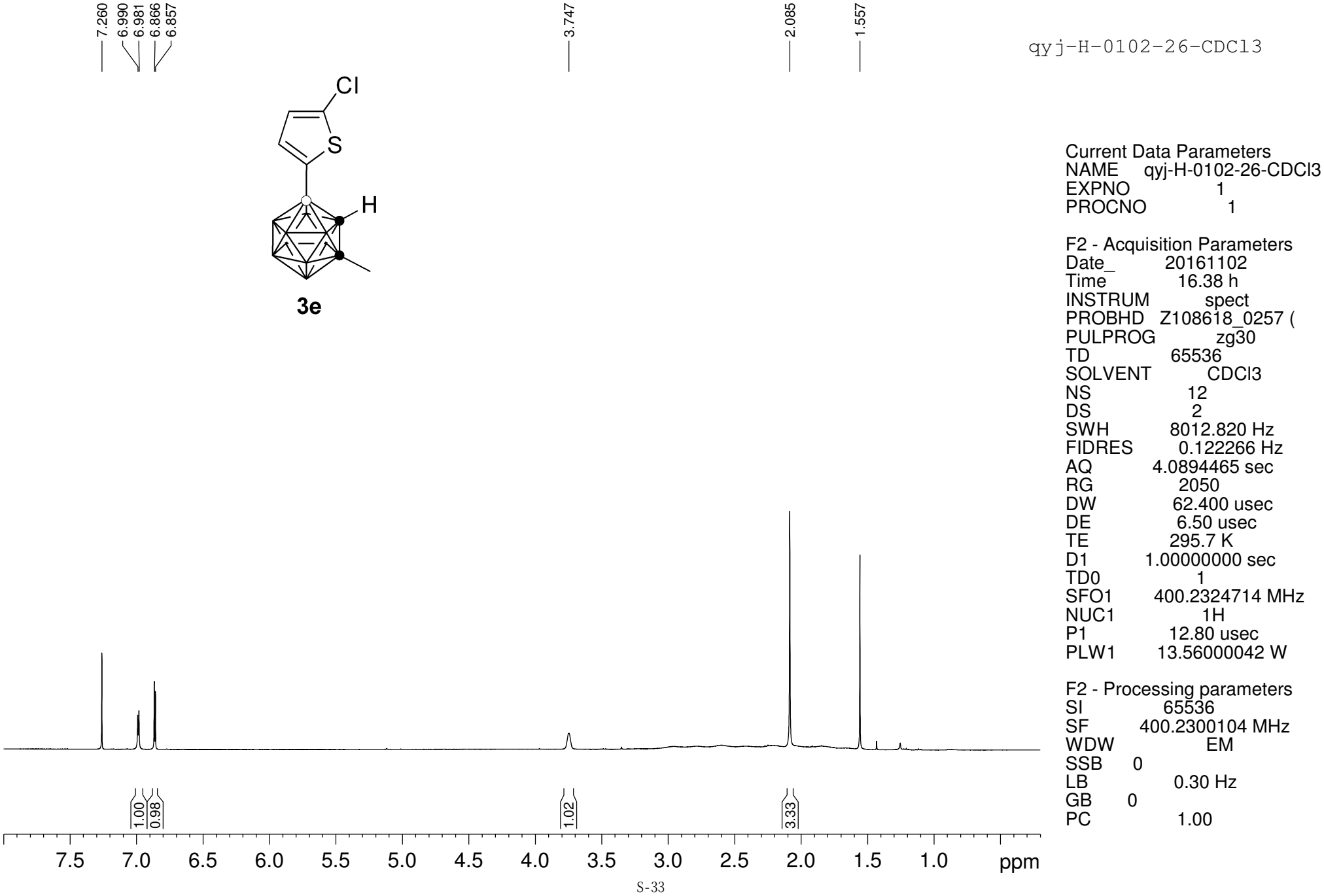
qyj-B-102-27-CDCl3

```
Current Data Parameters
NAME      qyj-B-102-27-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20160415
Time                17.22 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     12
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                 295.1 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
```

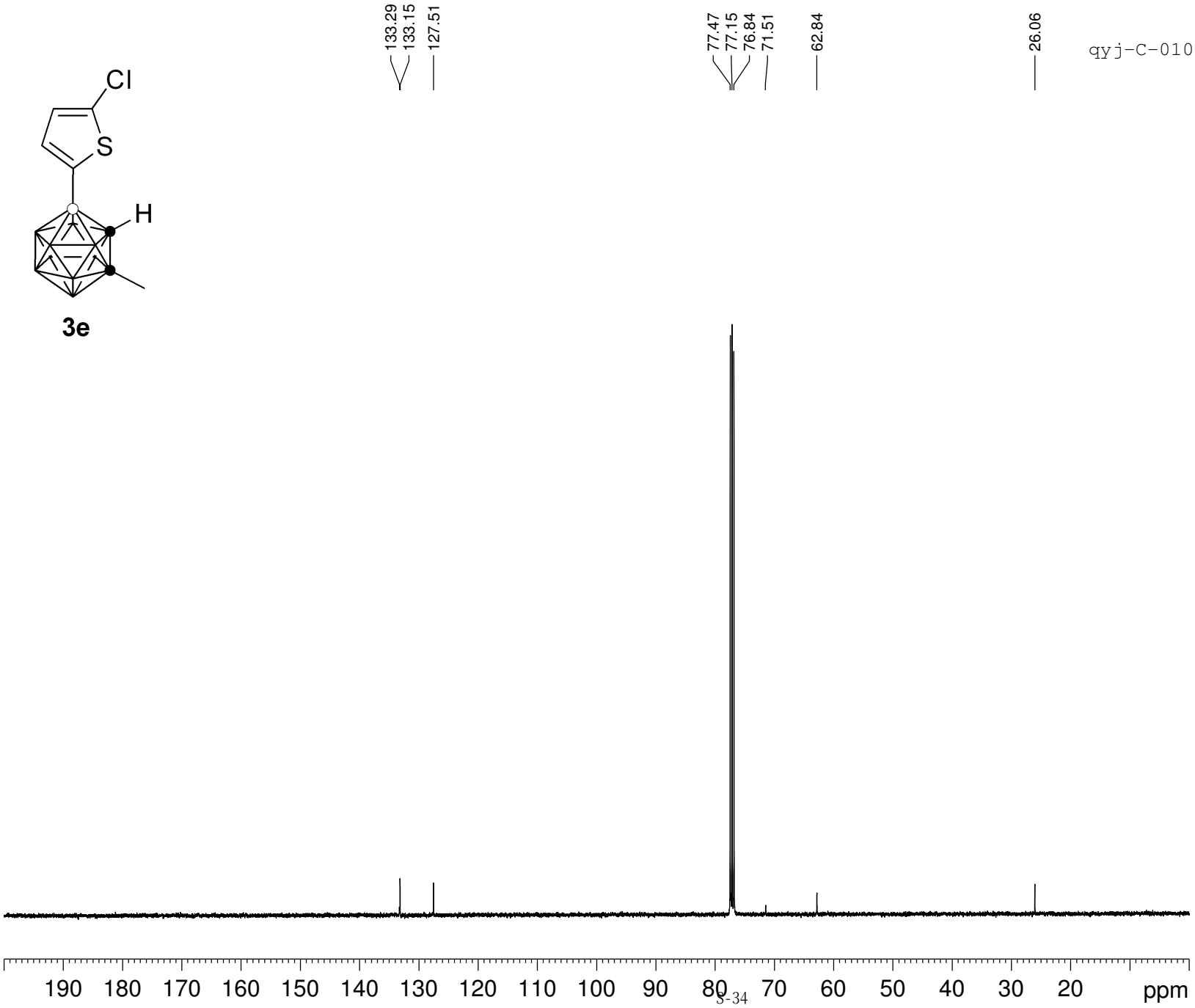


qyj-B-102-27-CDCl3(c)

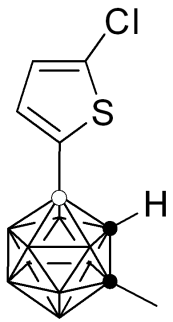
```
Current Data Parameters
NAME      qyj-B-102-27-CDCl3(c)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160415
Time                 17.23 h
INSTRUM              spect
PROBHD    Z108618_0257 (
PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                       16
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                   294.8 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
```


7.260
6.990
6.981
6.866
6.857
3.747
2.085
1.557
qyj-H-0102-26-CDCl3
Cl
S
H
3e
Current Data Parameters
NAME qyj-H-0102-26-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161102
Time 16.38 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 2050
DW 62.400 usec
DE 6.50 usec
TE 295.7 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 400.2300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.00
0.98
1.02
3.33
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

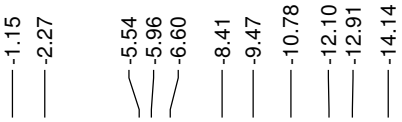
3e




```
Current Data Parameters
NAME      qyj-C-0102-26-CDCl3
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20161102
Time                  19.23 h
INSTRUM               spect
PROBHD    Z108618_0257 (
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1048
DS                        4
SWH               29761.904 Hz
FIDRES             0.454131 Hz
AQ                1.1010048 sec
RG                      161
DW                   16.800 usec
DE                    6.50 usec
TE                   295.9 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              100.6379006 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

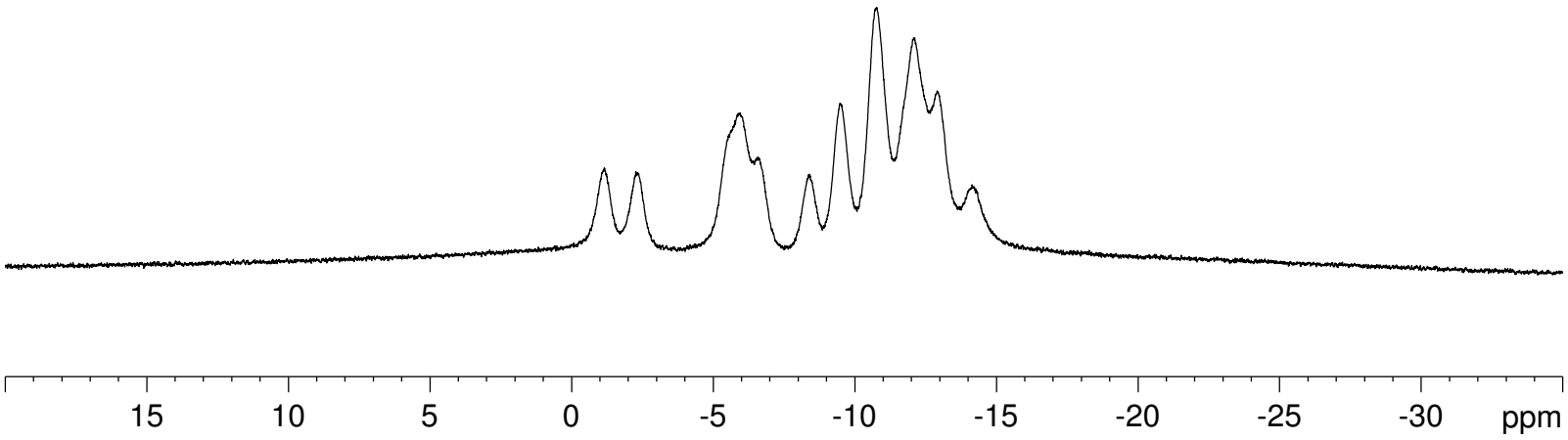


3e

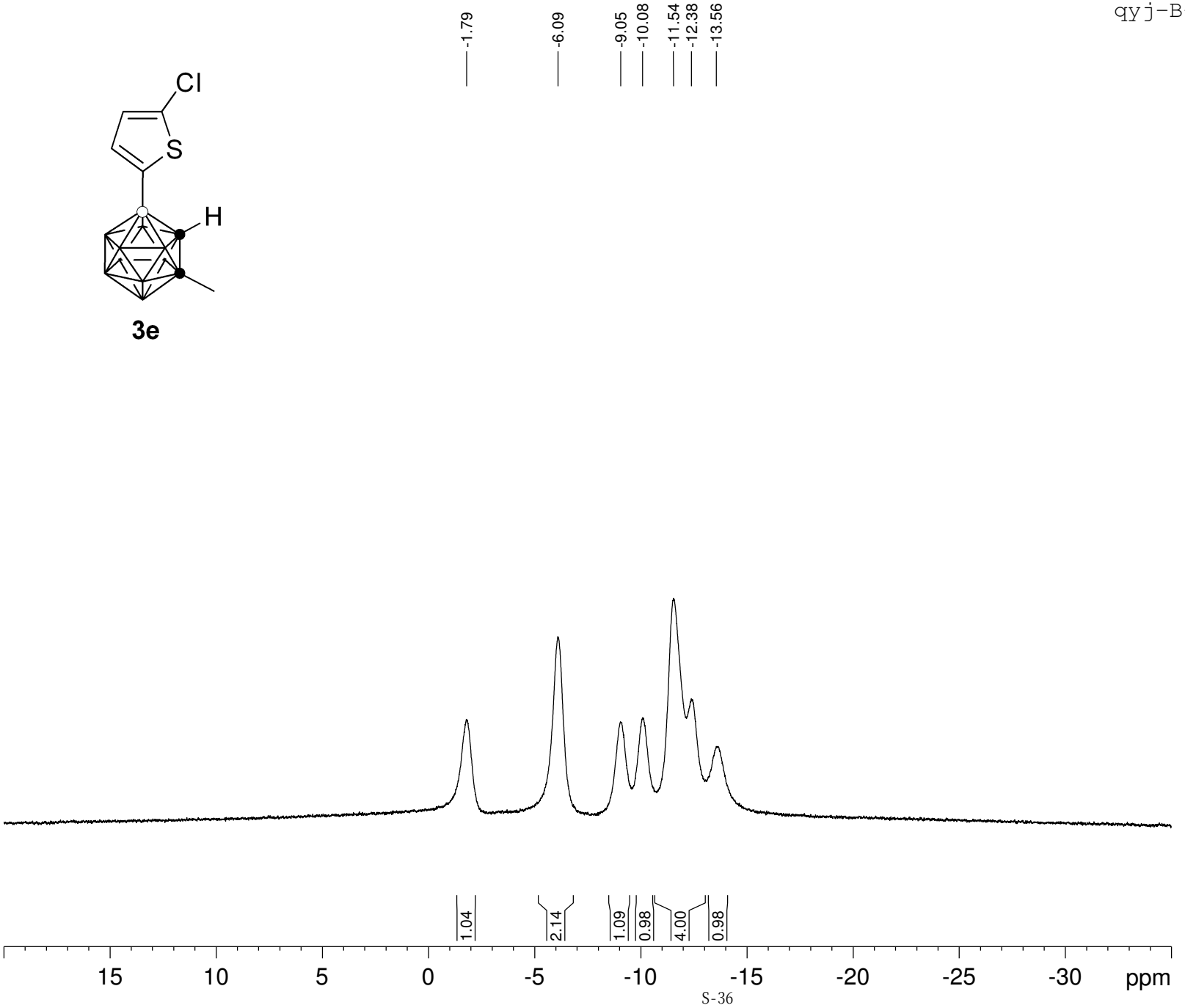


qyj-B-0102-26-CDCl3(c)

```
Current Data Parameters
NAME      qyj-B-0102-26-CDCl3(c)
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20161102
Time                   16.43 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT                CDCl3
NS                        20
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                    295.9 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               128.4097504 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

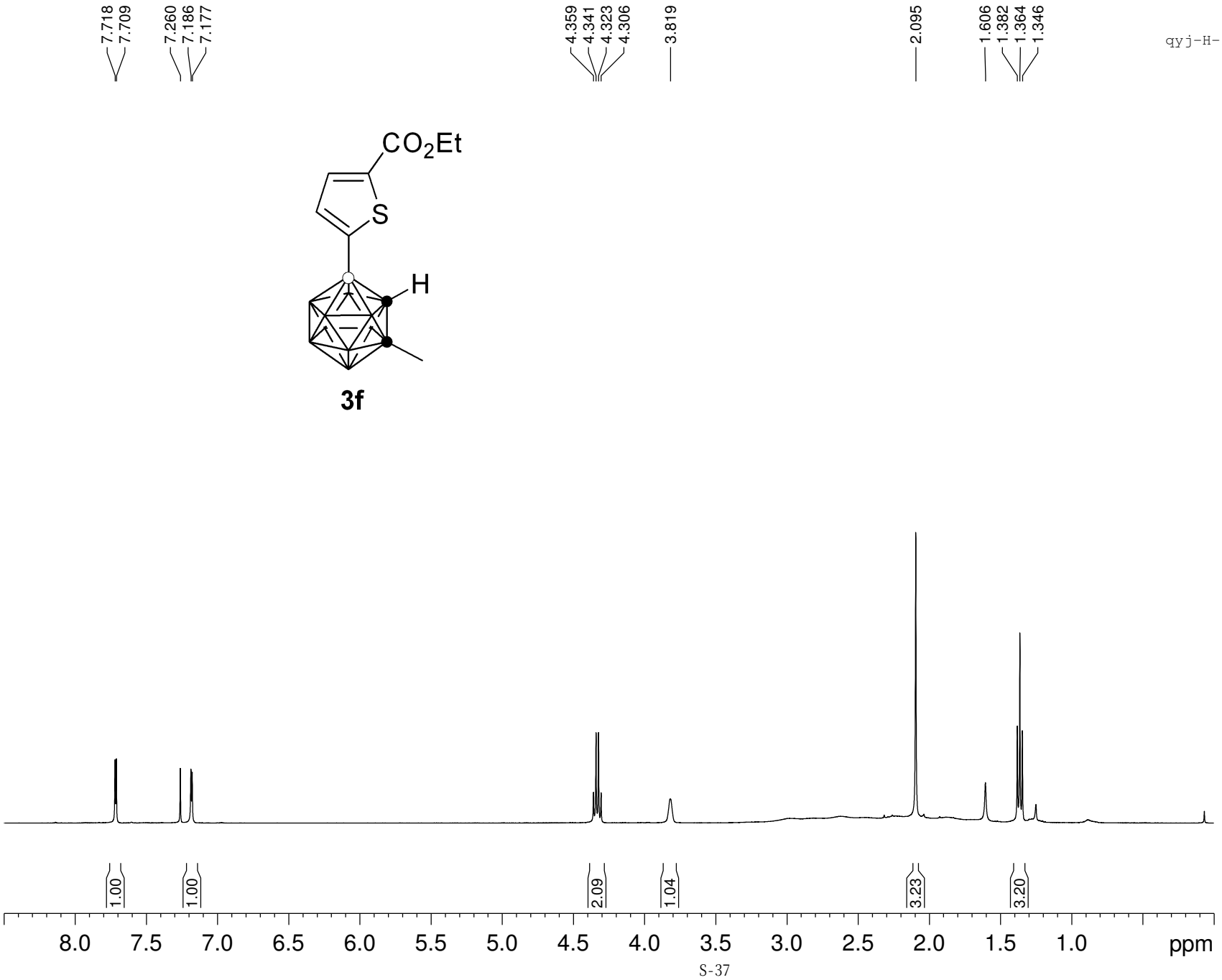


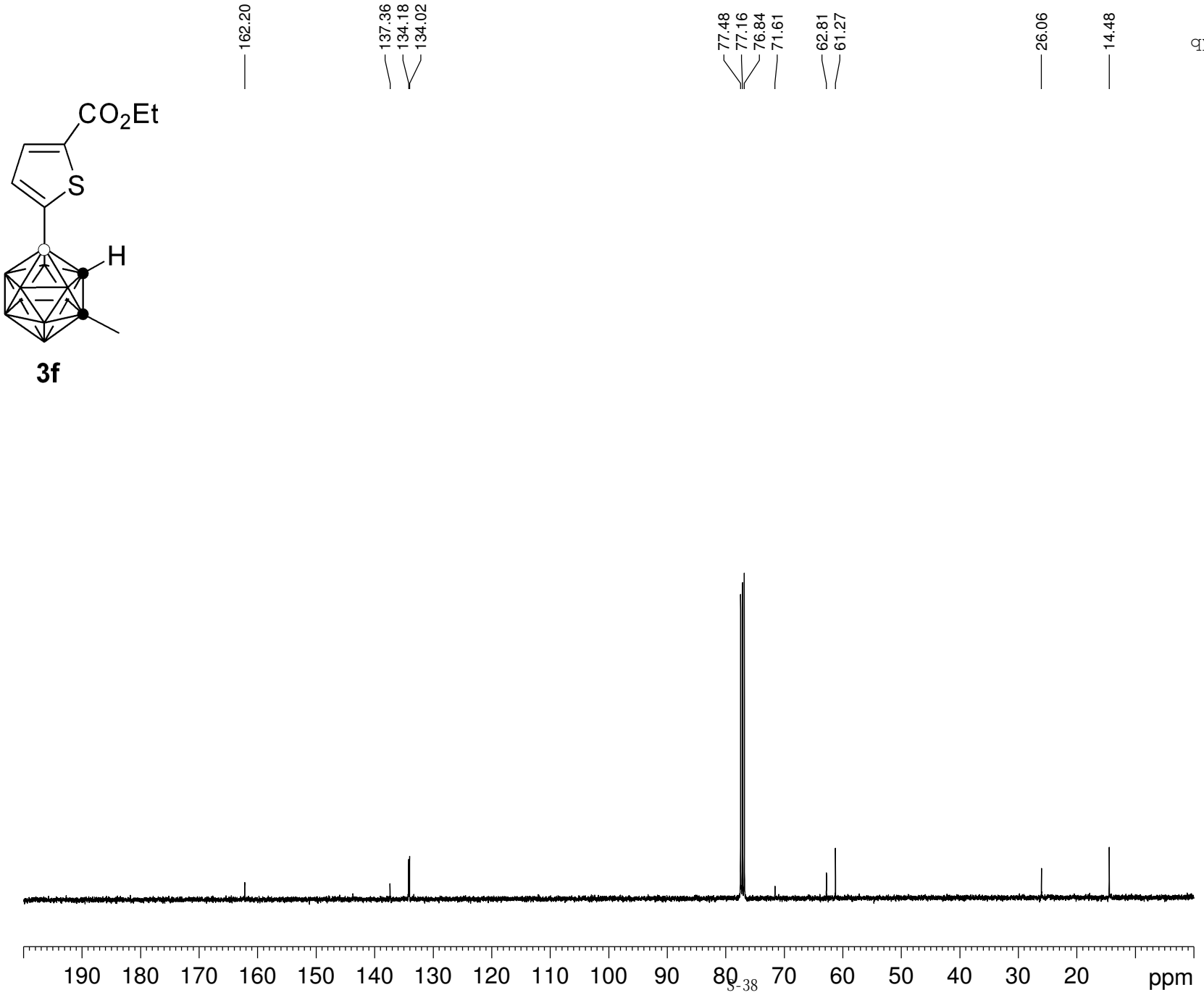
3e



qyj-B-0102-26-CDCl3

```
Current Data Parameters
NAME      qyj-B-0102-26-CDCl3
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20161102
Time                16.41 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    16
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                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
```


7.718
7.709
7.260
7.186
7.177
4.359
4.341
4.323
4.306
3.819
2.095
1.606
1.382
1.364
1.346
qyj-H-102-29-CDCl3
CO2Et
S
H
3f
Current Data Parameters
NAME qyj-H-102-29-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160416
Time 15.36 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 90.5
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 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
1.00
1.00
2.09
1.04
3.23
3.20
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



Current Data Parameters

NAME	qyj-C-102-29-CDCl3
EXPNO	1
PROCNO	1

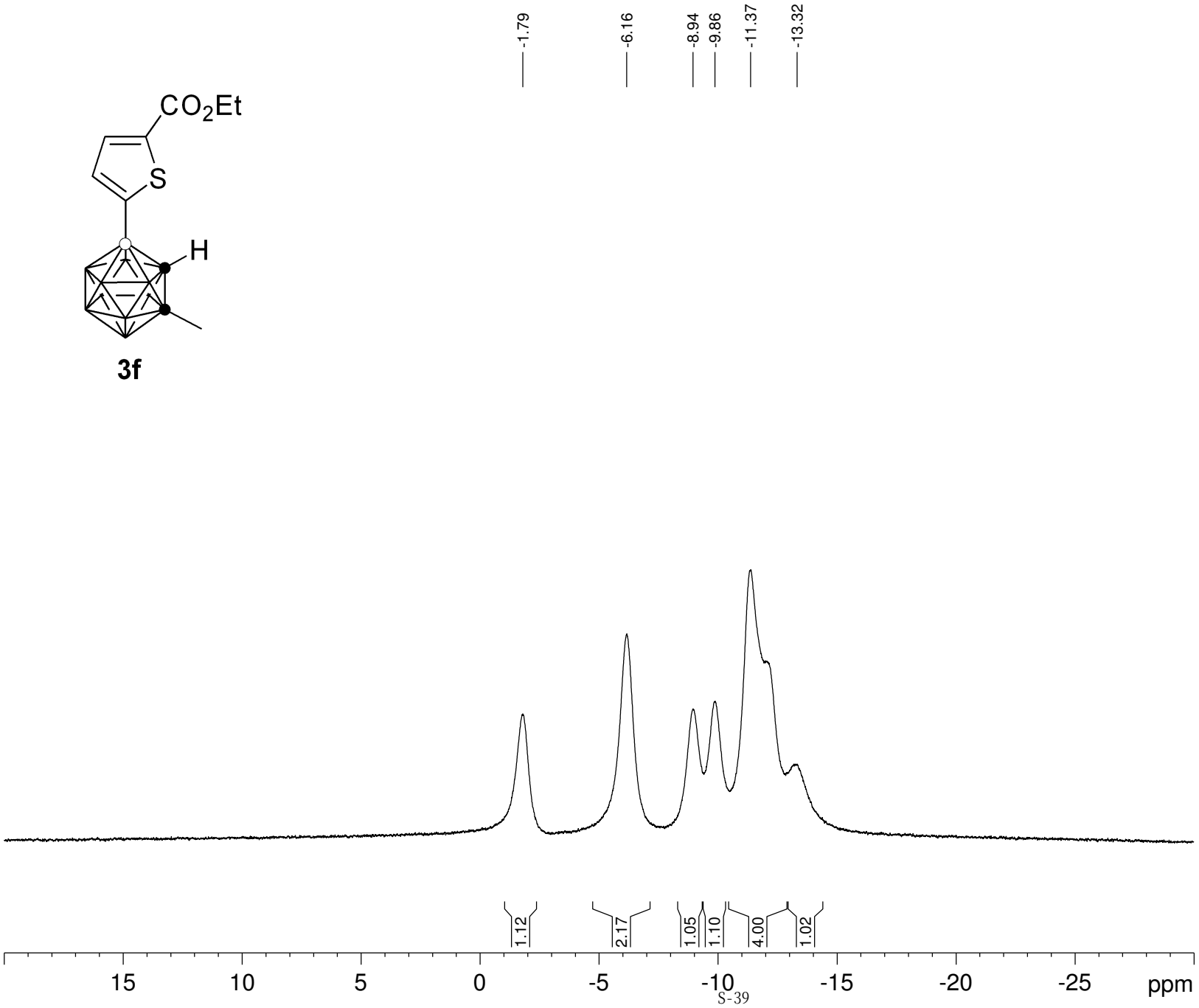
F2 - Acquisition Parameters

Date_	20160416
Time	15.38 h
INSTRUM	spect
PROBHD	Z108618_0257 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	200
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010048 sec
RG	128
DW	16.800 usec
DE	6.50 usec
TE	294.8 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	100.6379015 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

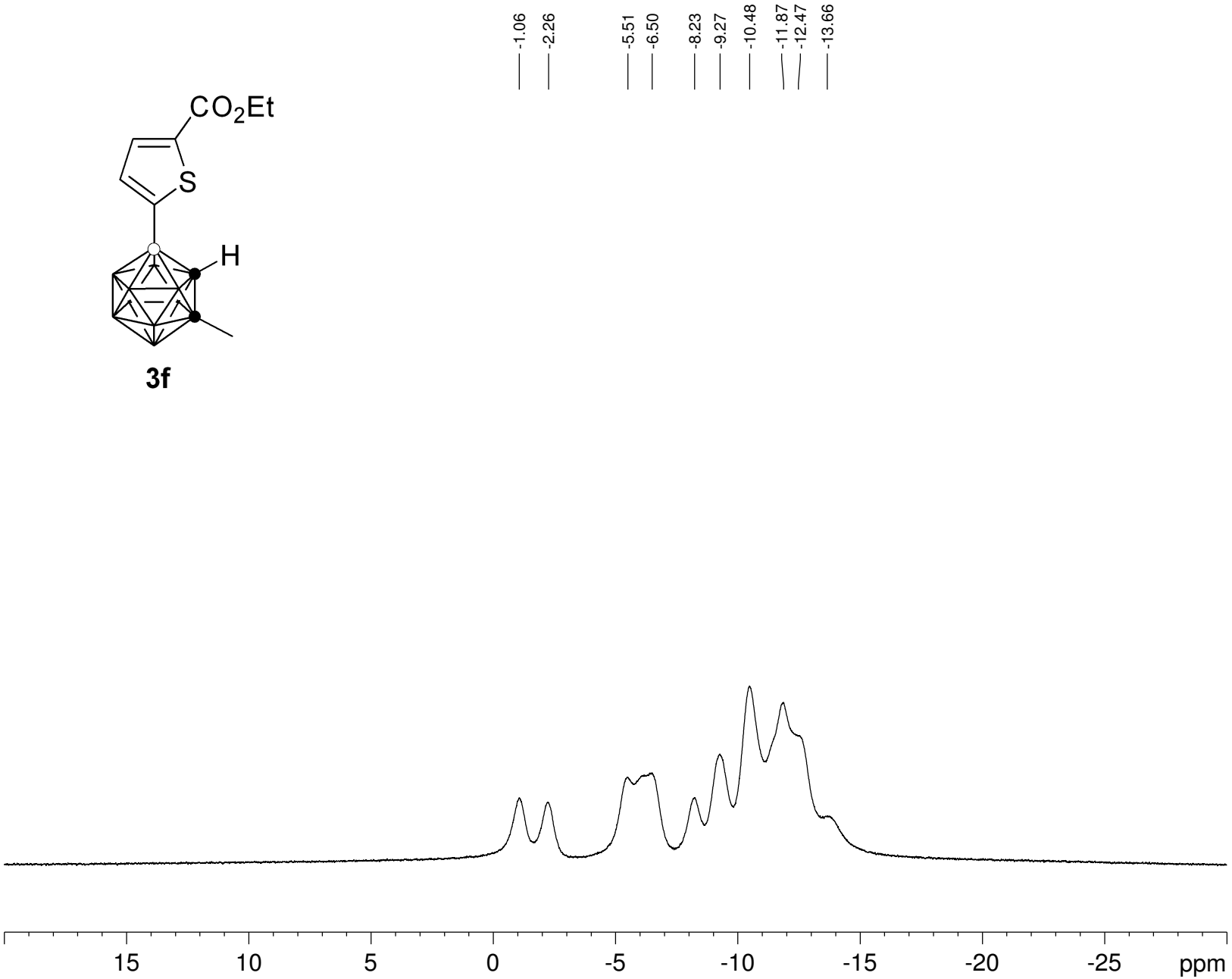
3f



qyj-B-102-29-CDCl3

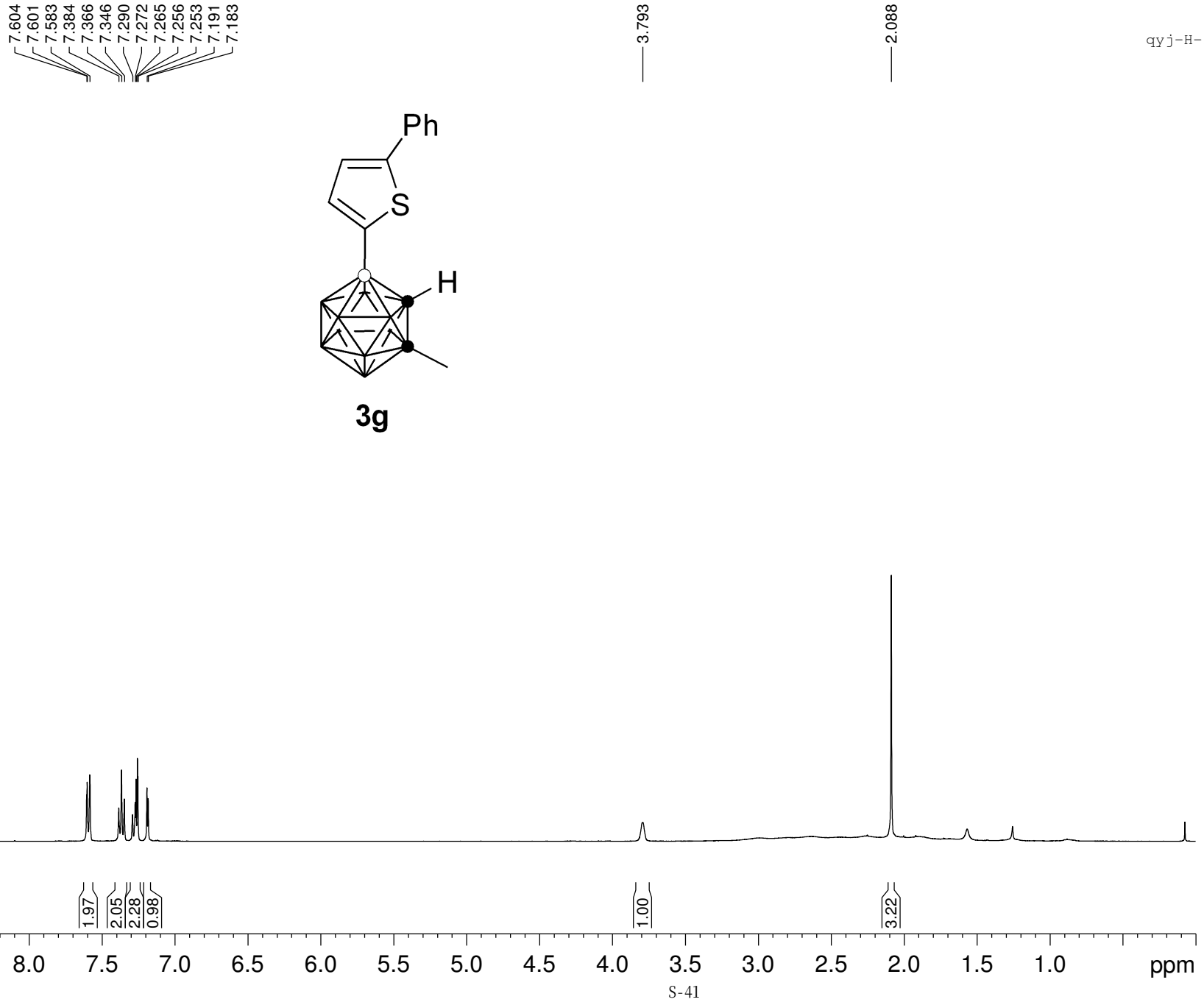
```
Current Data Parameters
NAME      qyj-B-102-29-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160416
Time              15.50 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG           zgdc
TD               65536
SOLVENT          CDCl3
NS                  12
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                294.9 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
```

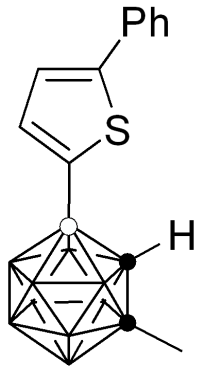
3f



qyj-B-102-29-CDCl3(c)

```
Current Data Parameters
NAME      qyj-B-102-29-CDCl3(c)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160416
Time              15.52 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                  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
```


7.604
7.601
7.583
7.384
7.366
7.346
7.290
7.272
7.265
7.256
7.253
7.191
7.183
3.793
2.088
qyj-H-102-46-CDCl3
Ph
S
H
3g
Current Data Parameters
NAME qyj-H-102-46-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160615
Time 20.55 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 50.8
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 400.2300125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.97
2.05
2.28
0.98
1.00
3.22
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

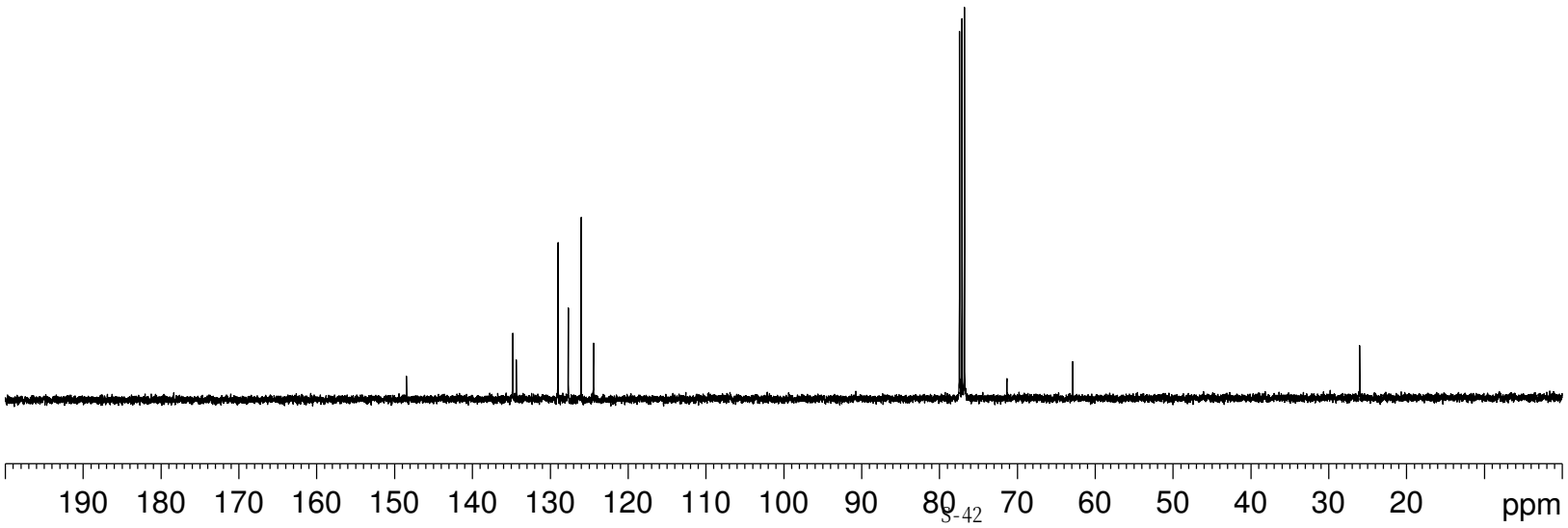


3g

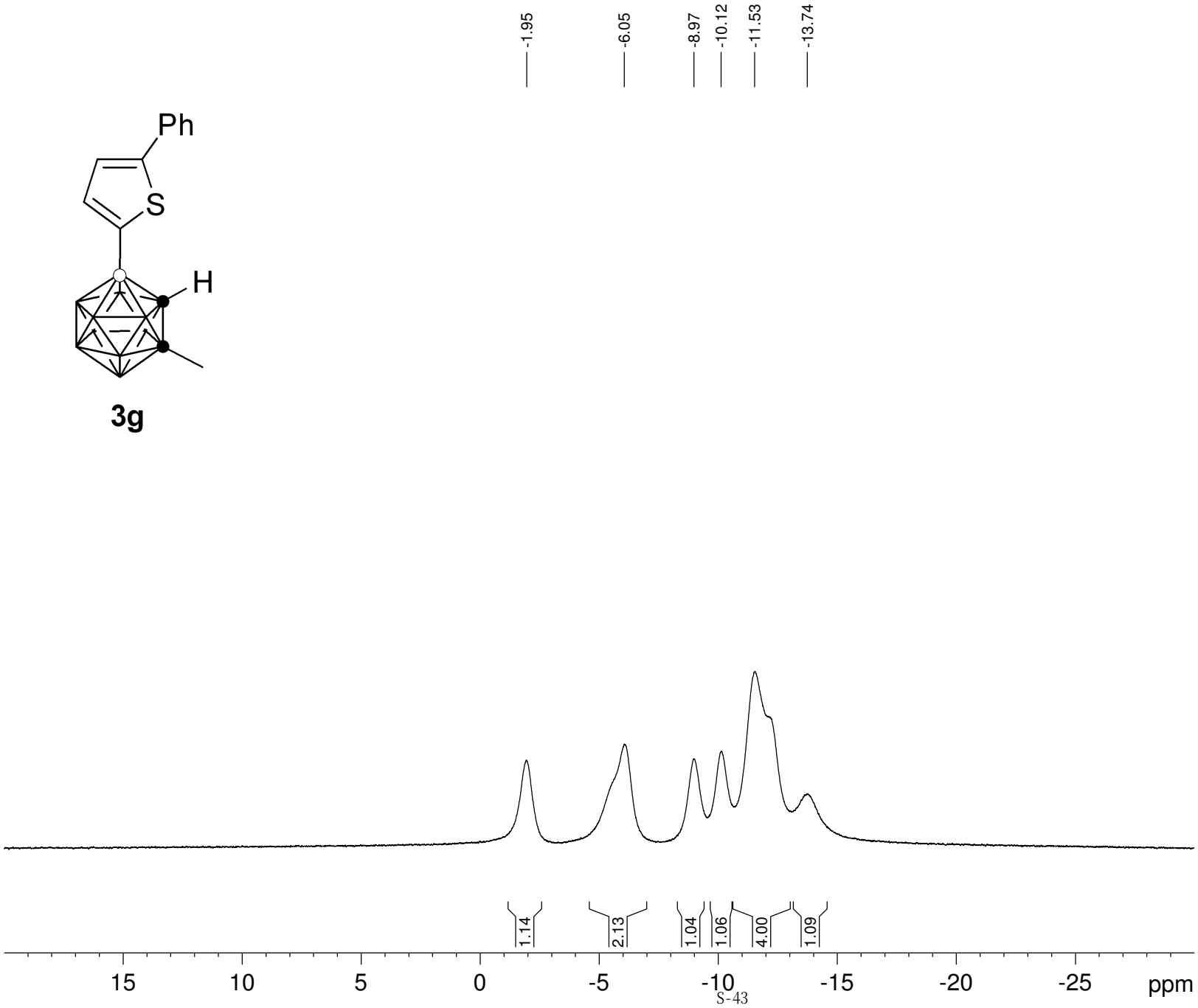
148.46
134.81
134.35
128.98
127.67
126.00
124.42
77.45
77.13
76.81
71.36
62.91
26.04

qyj-C-102-46-CDCl3

```
Current Data Parameters
NAME      qyj-C-102-46-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160615
Time              20.58 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                    100
DS                      4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                    144
DW                16.800 usec
DE                 6.50 usec
TE                294.9 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           100.6379052 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



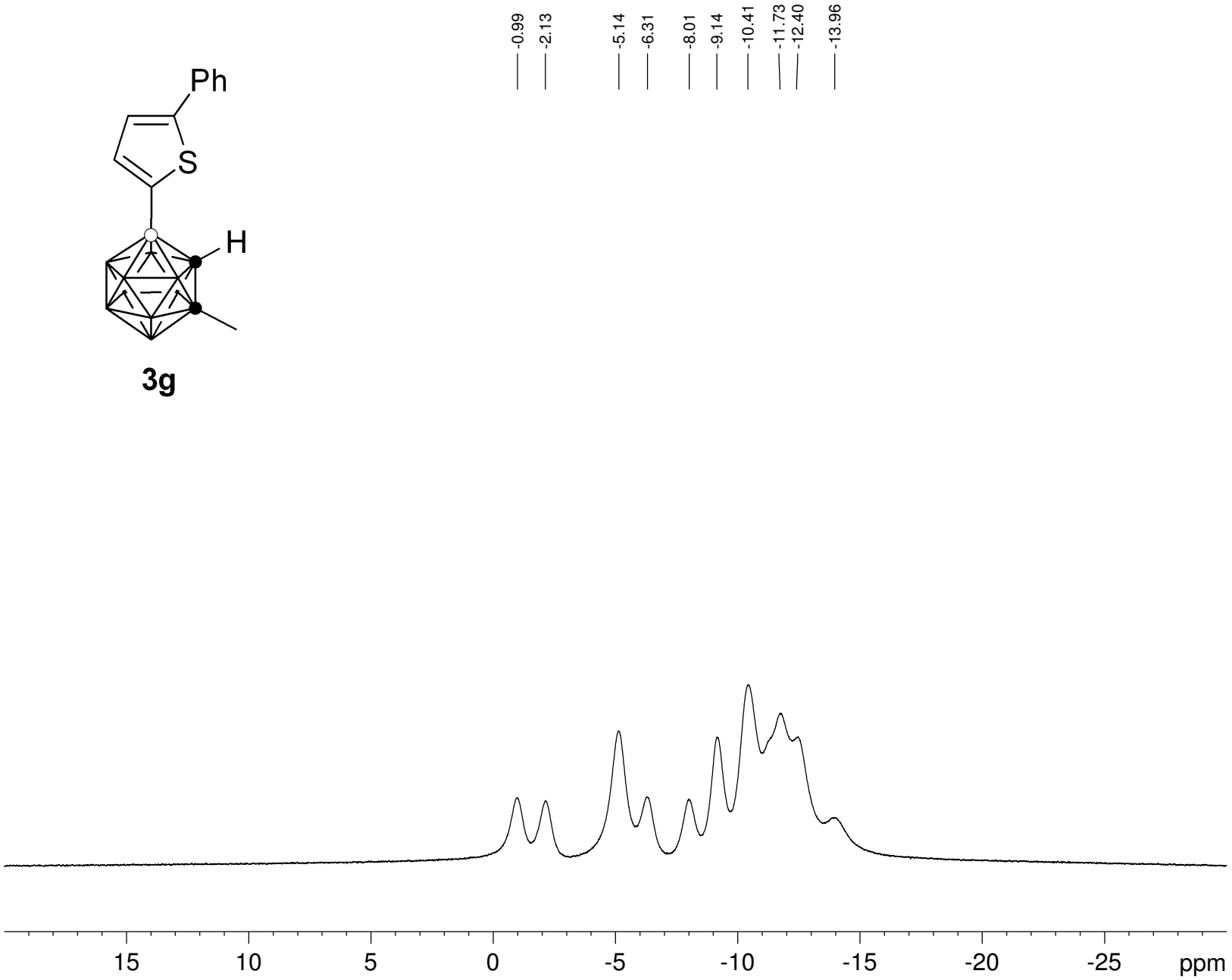
3g



qyj-B-102-46-CDCl3

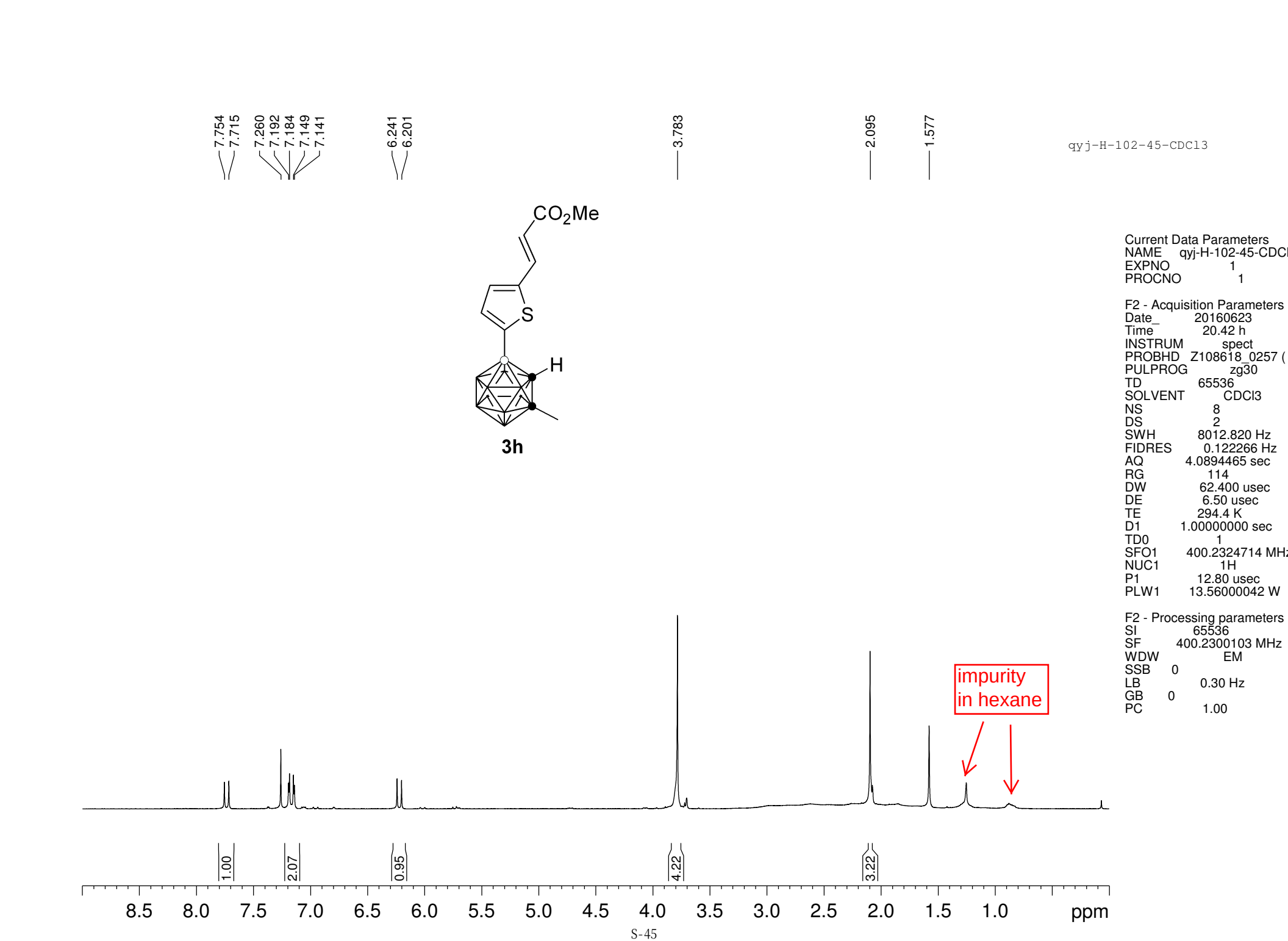
```
Current Data Parameters
NAME      qyj-B-102-46-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20160615
Time                21.05 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     12
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                 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            128.4097615 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

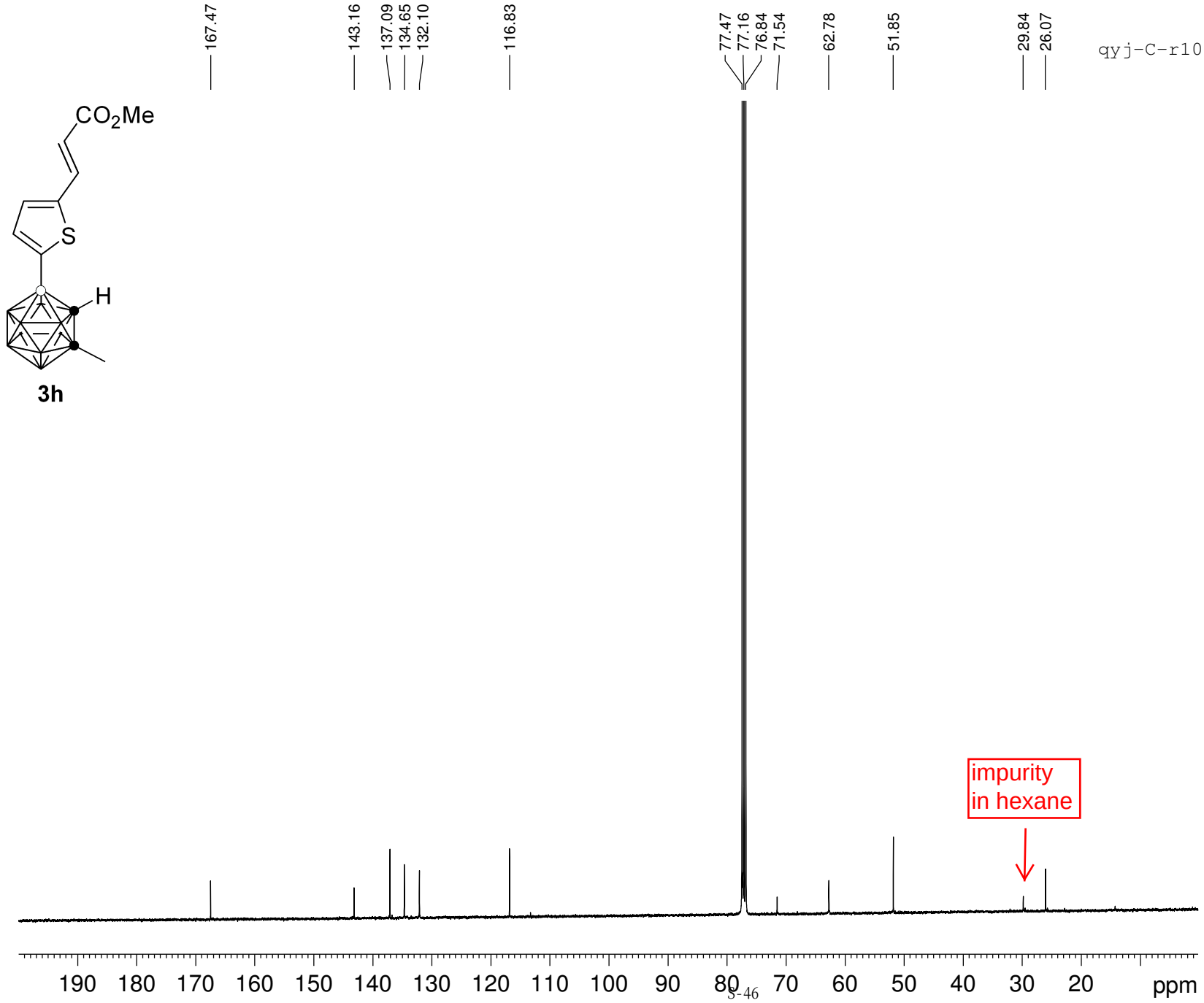
3g



qyj-B-102-46-CDCl3(C)

```
Current Data Parameters
NAME      qyj-B-102-46-CDCl3(C)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160615
Time                 21.07 h
INSTRUM              spect
PROBHD    Z108618_0257 (
PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                       24
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                   294.4 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             128.4097117 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```


7.754
7.715
7.260
7.192
7.184
7.149
7.141
6.241
6.201
3.783
2.095
1.577
qyj-H-102-45-CDCl3
CO2Me
S
H
3h
Current Data Parameters
NAME qyj-H-102-45-CDCl
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160623
Time 20.42 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 294.4 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
impurity
in hexane
1.00
2.07
0.95
4.22
3.22
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
ppm

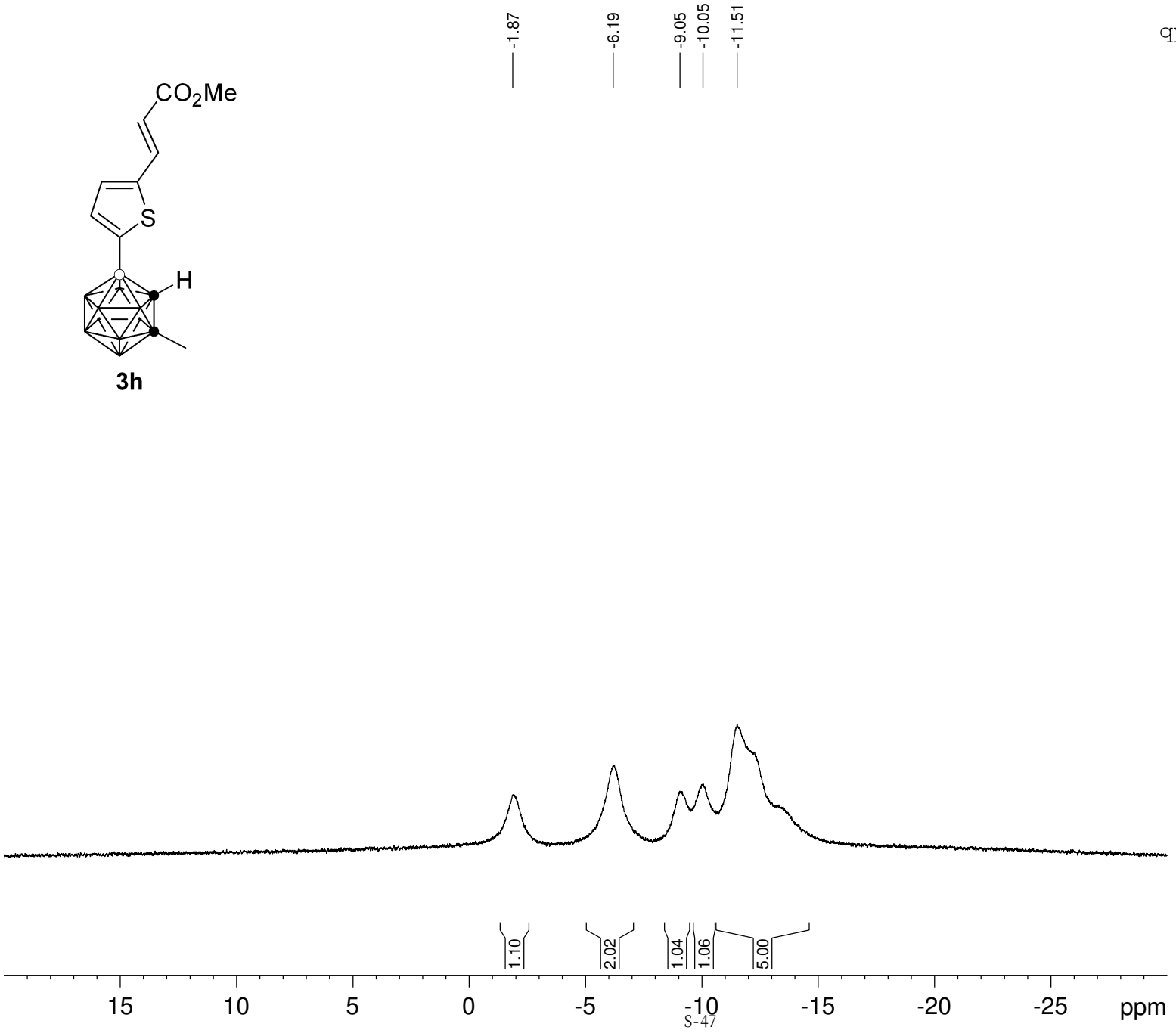


Current Data Parameters
NAME qyj-C-r102-45-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170317
Time 21.58 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9999
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 161
DW 16.800 usec
DE 6.50 usec
TE 295.2 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 100.6379011 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

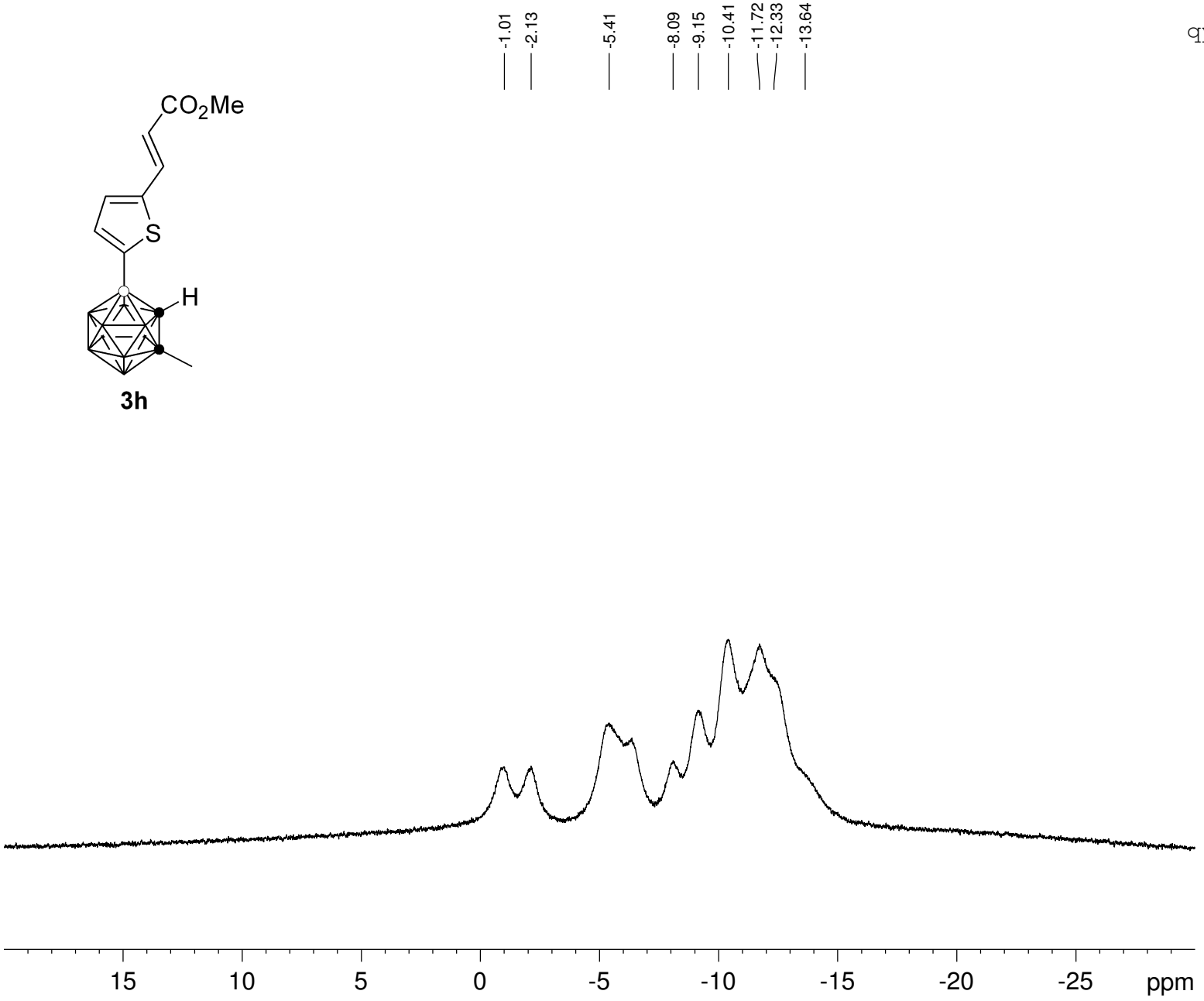
3h



qyj-B-102-45-CDCl3

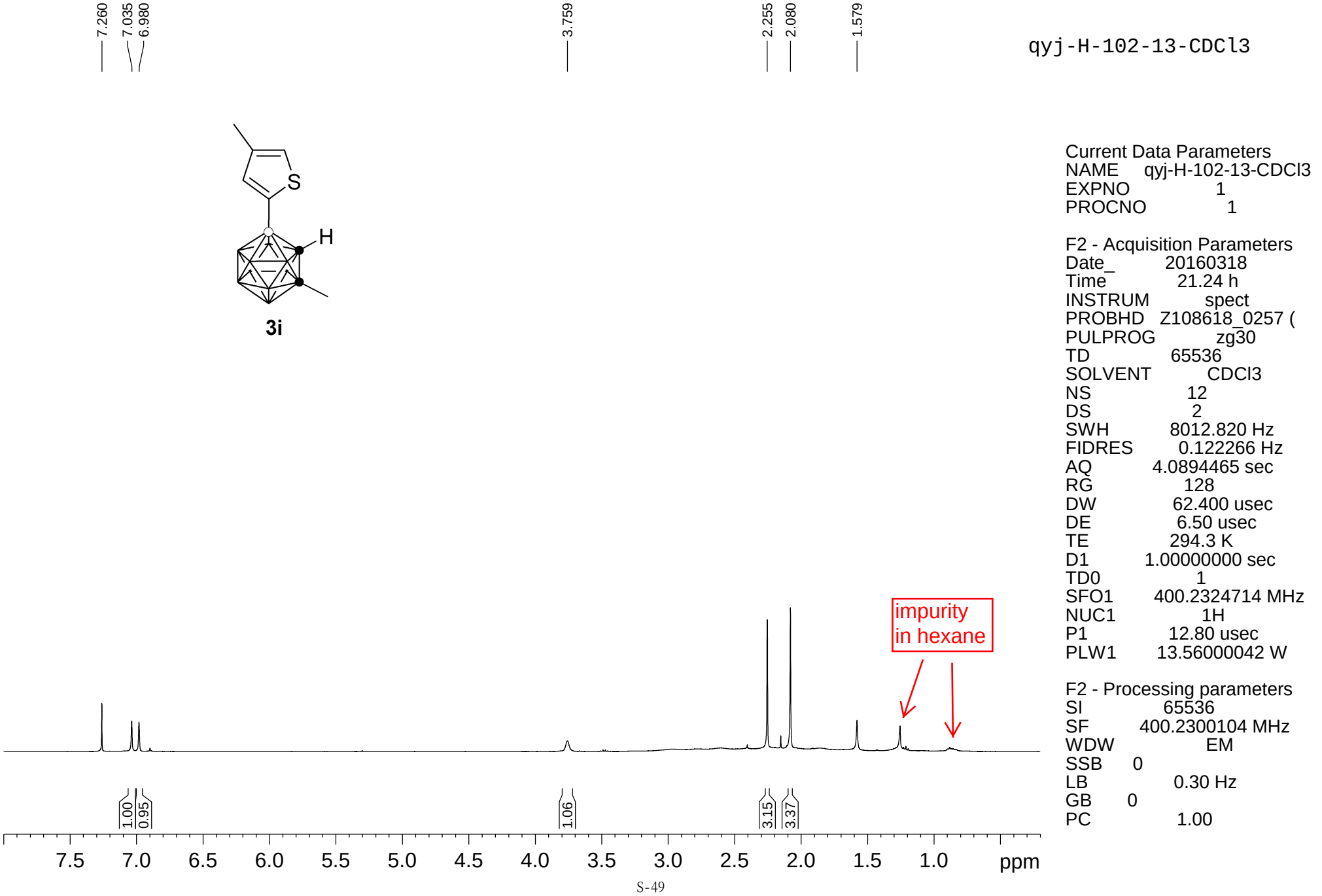
```
Current Data Parameters
NAME      qyj-B-102-45-CDCl3
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20160623
Time                  20.27 h
INSTRUM               spect
PROBHD    Z108618_0257 (
PULPROG                zgdc
TD                     65536
SOLVENT                CDCl3
NS                        12
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                    295.1 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
```

3h



qyj-B-102-45-CDCl3(C)

```
Current Data Parameters
NAME      qyj-B-102-45-CDCl3(C)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160623
Time                  20.29 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                    294.6 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              128.4097117 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

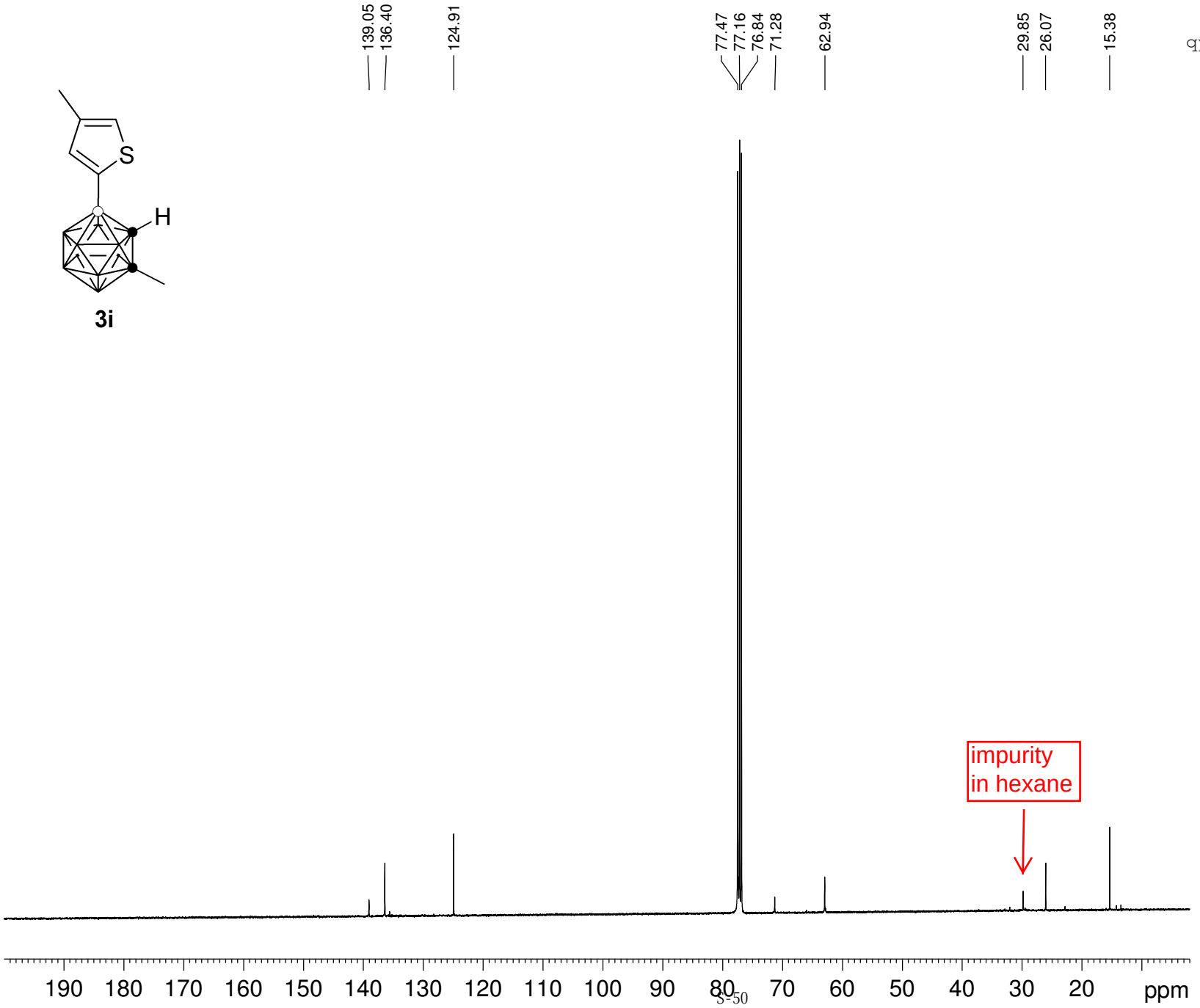


Current Data Parameters
NAME qyj-H-102-13-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160318
Time 21.24 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 128
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

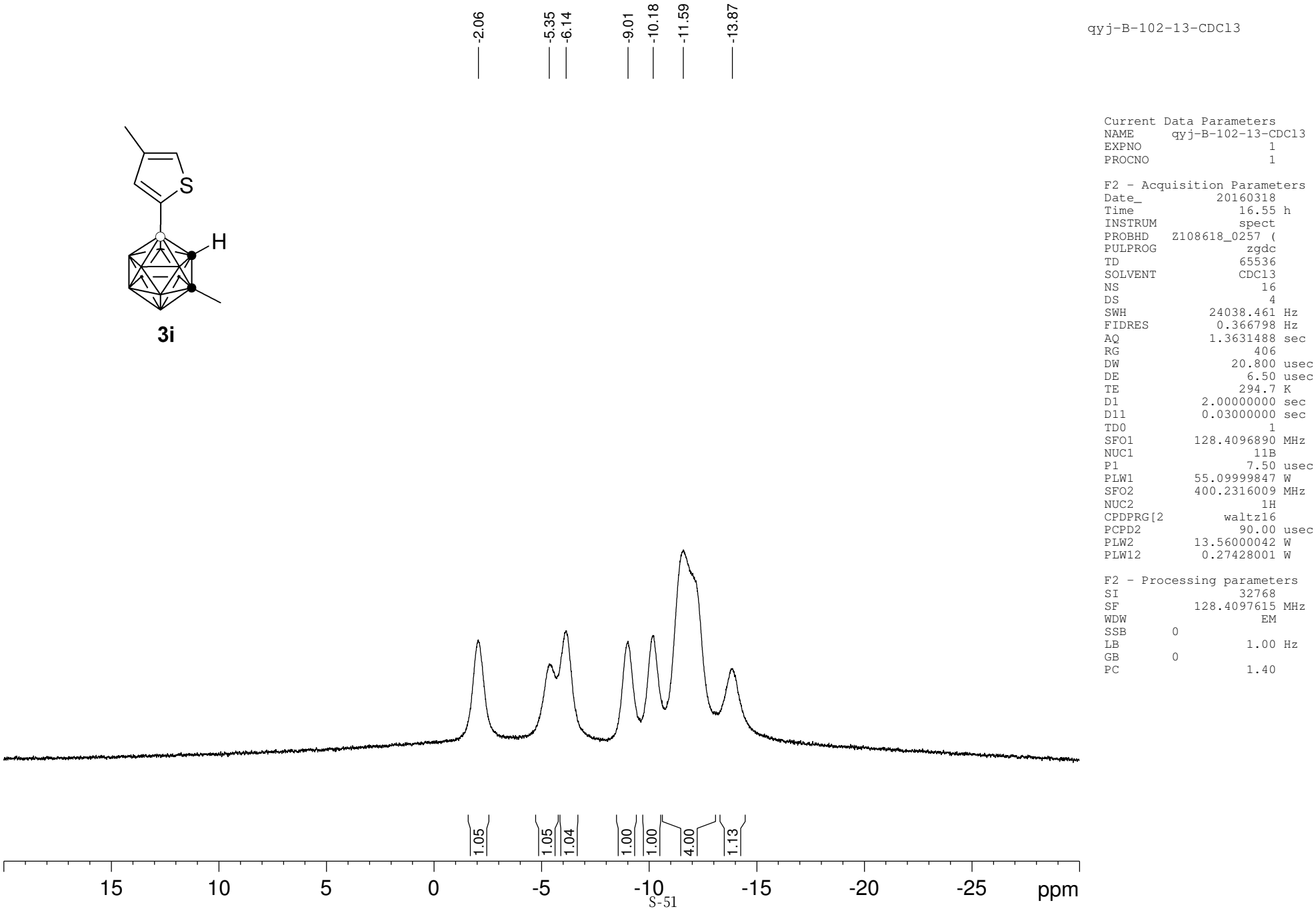
F2 - Processing parameters
SI 65536
SF 400.2300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

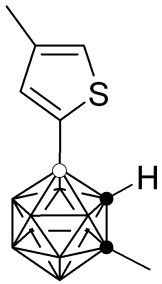
3i



qyj-C-102-13-CDCl3

```
Current Data Parameters
NAME      qyj-C-102-13-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160318
Time              21.27 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                 13945
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                   161
DW                16.800 usec
DE                 6.50 usec
TE                294.4 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            100.6379015 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


-2.06
-5.35
-6.14
-9.01
-10.18
-11.59
-13.87
qyj-B-102-13-CDCl3
S
H
3i
Current Data Parameters
NAME qyj-B-102-13-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160318
Time 16.55 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 16
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 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 128.4097615 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1.05
1.05
1.04
1.00
1.00
4.00
1.13
15
10
5
0
-5
-10
-15
-20
-25
ppm

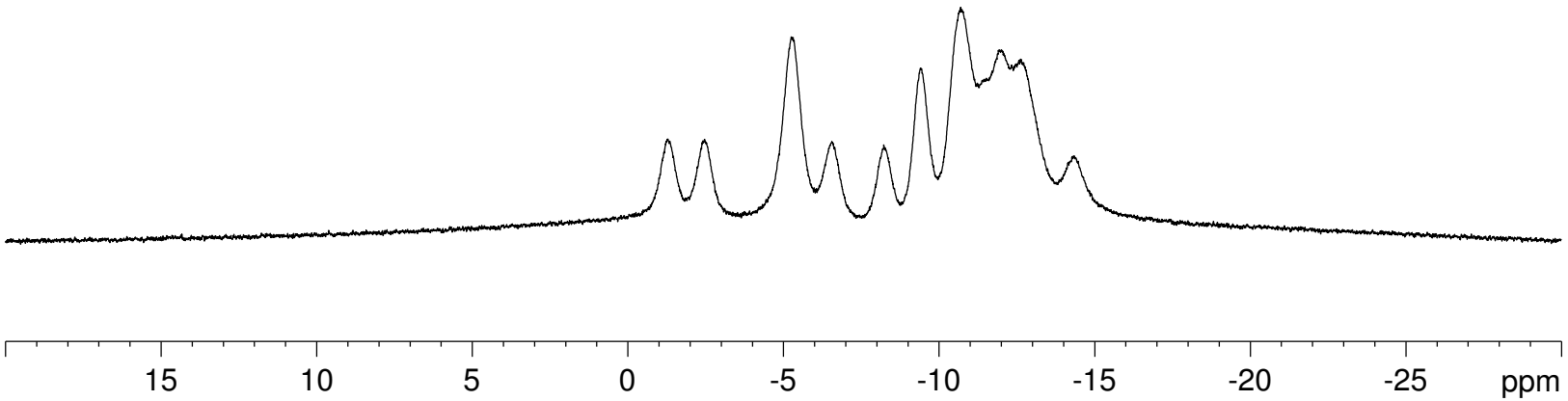


3i

-1.29
-2.47
-5.25
-6.56
-8.23
-9.41
-10.70
-11.93
-14.35

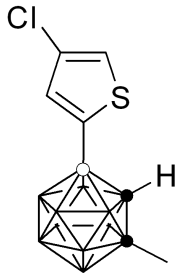
qyj-B-102-13-CDCl3(c)

```
Current Data Parameters
NAME      qyj-B-102-13-CDCl3(c)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160318
Time                  16.56 h
INSTRUM               spect
PROBHD    Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT                CDCl3
NS                        20
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                    294.4 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
```



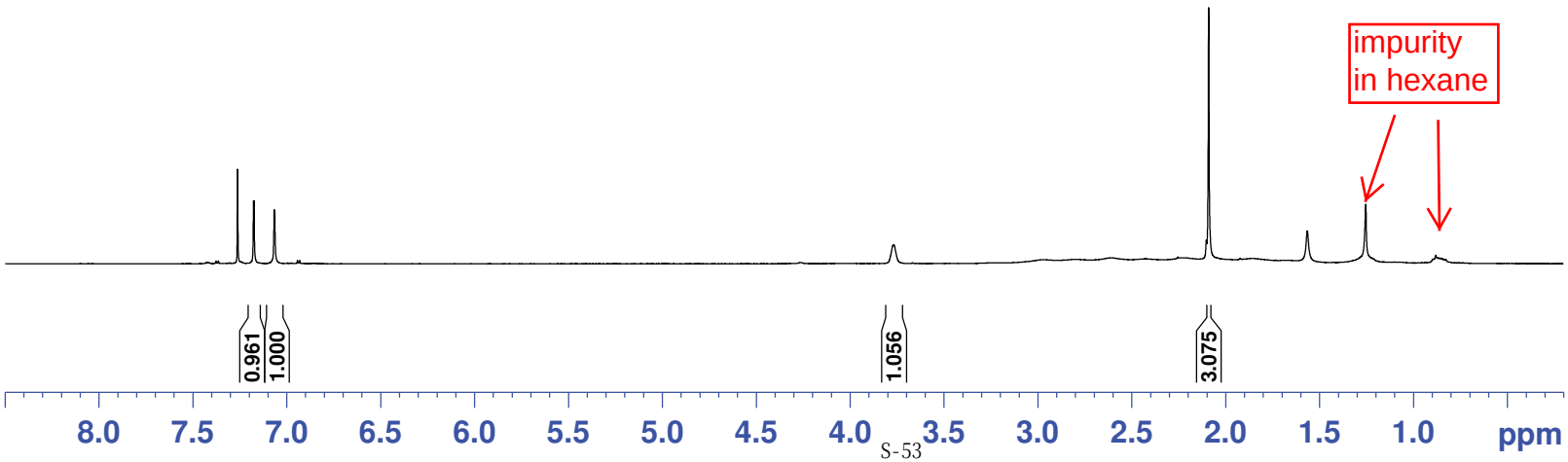
7.260
7.175
7.172
7.065
3.767
2.090
1.565
1.253

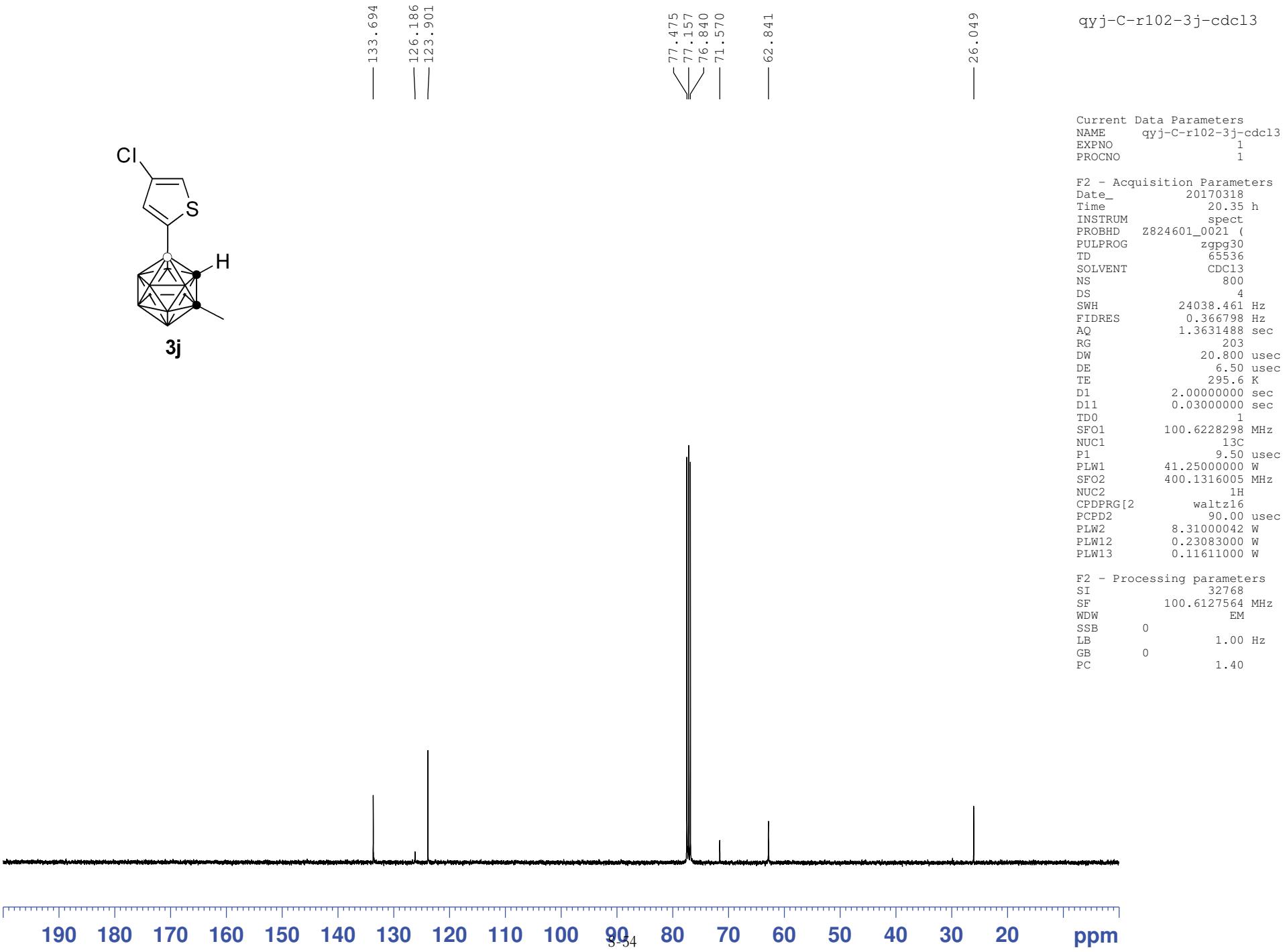
qyj-H-102-18-2-CDCl3

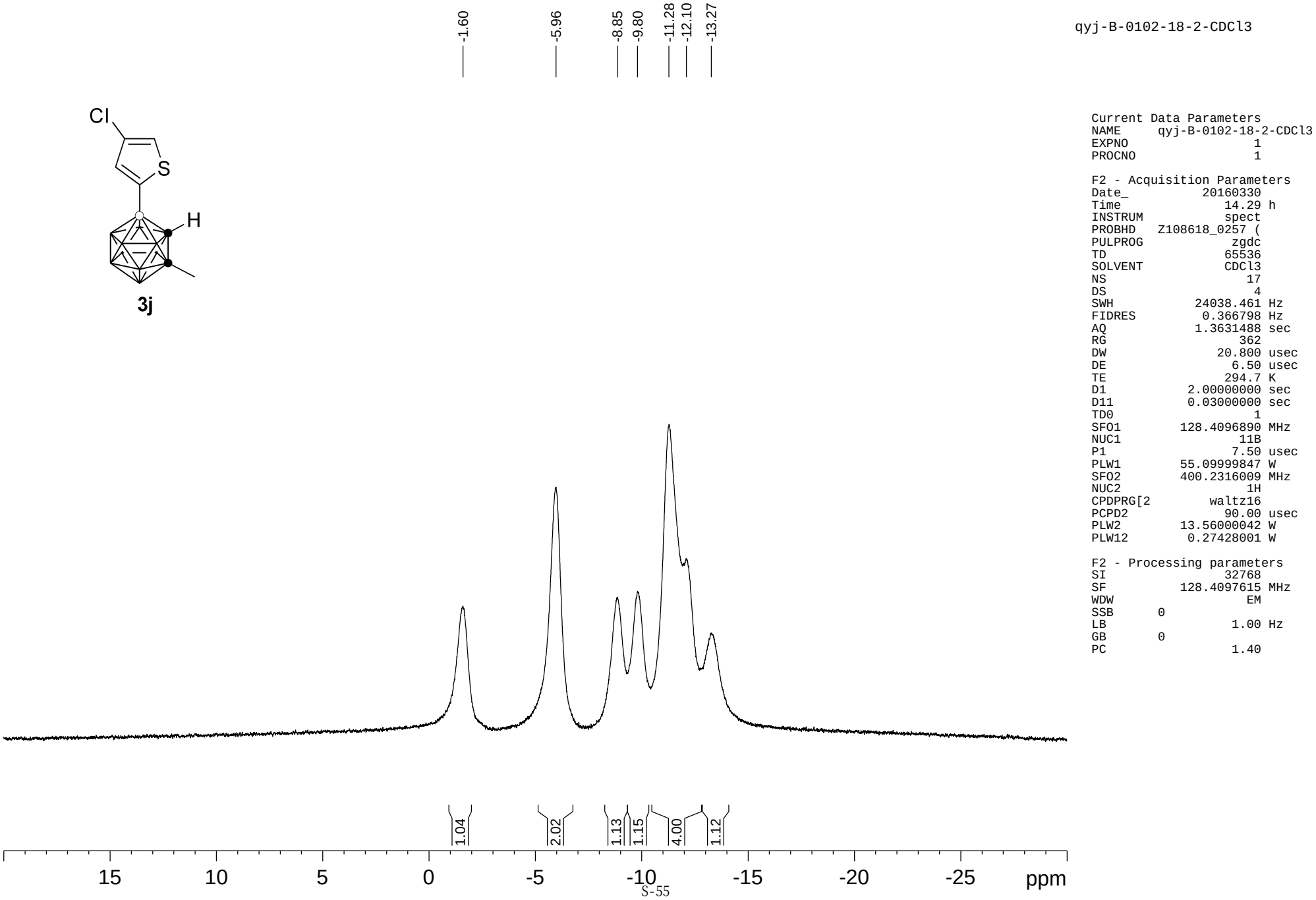


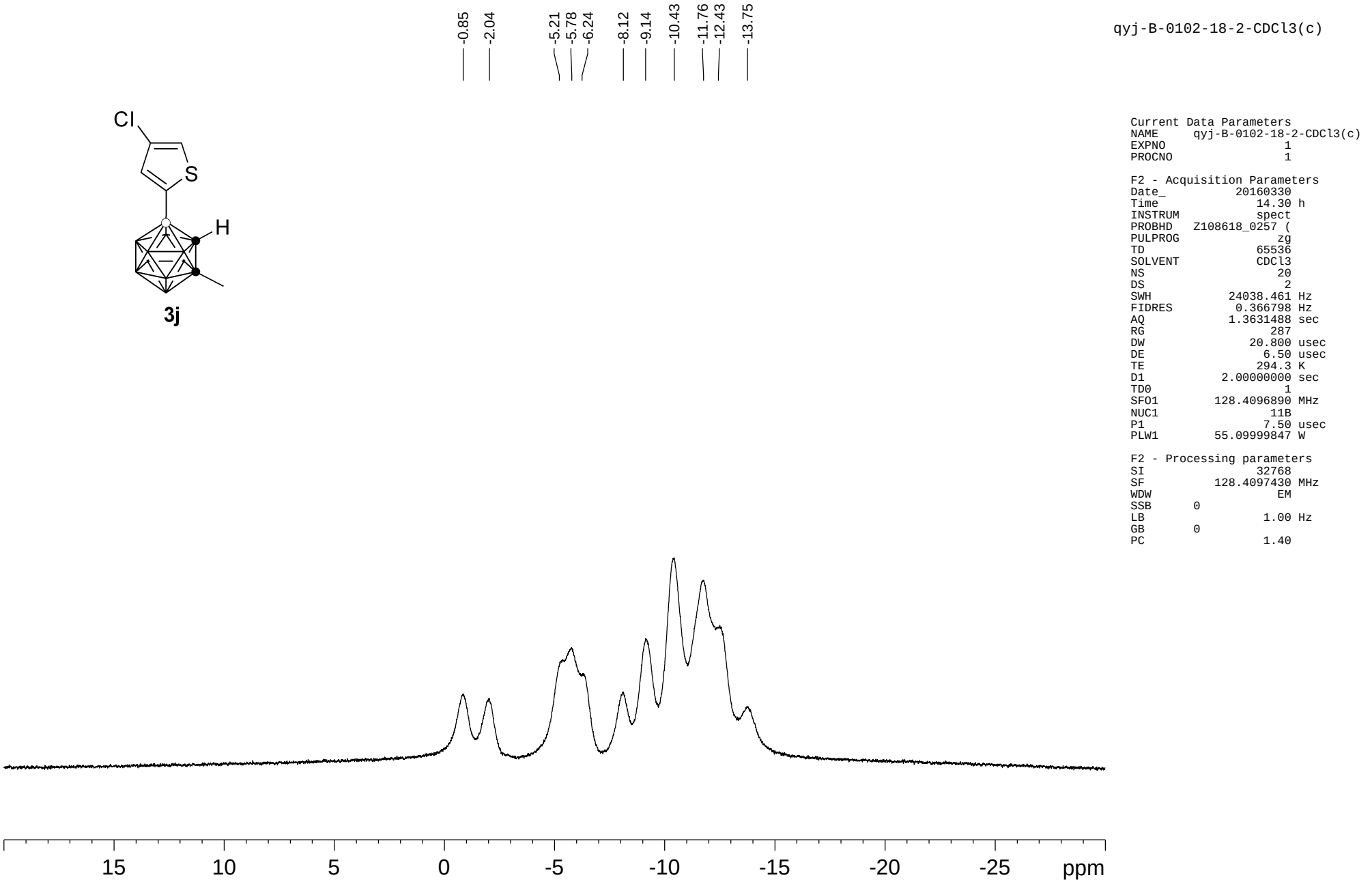
3j

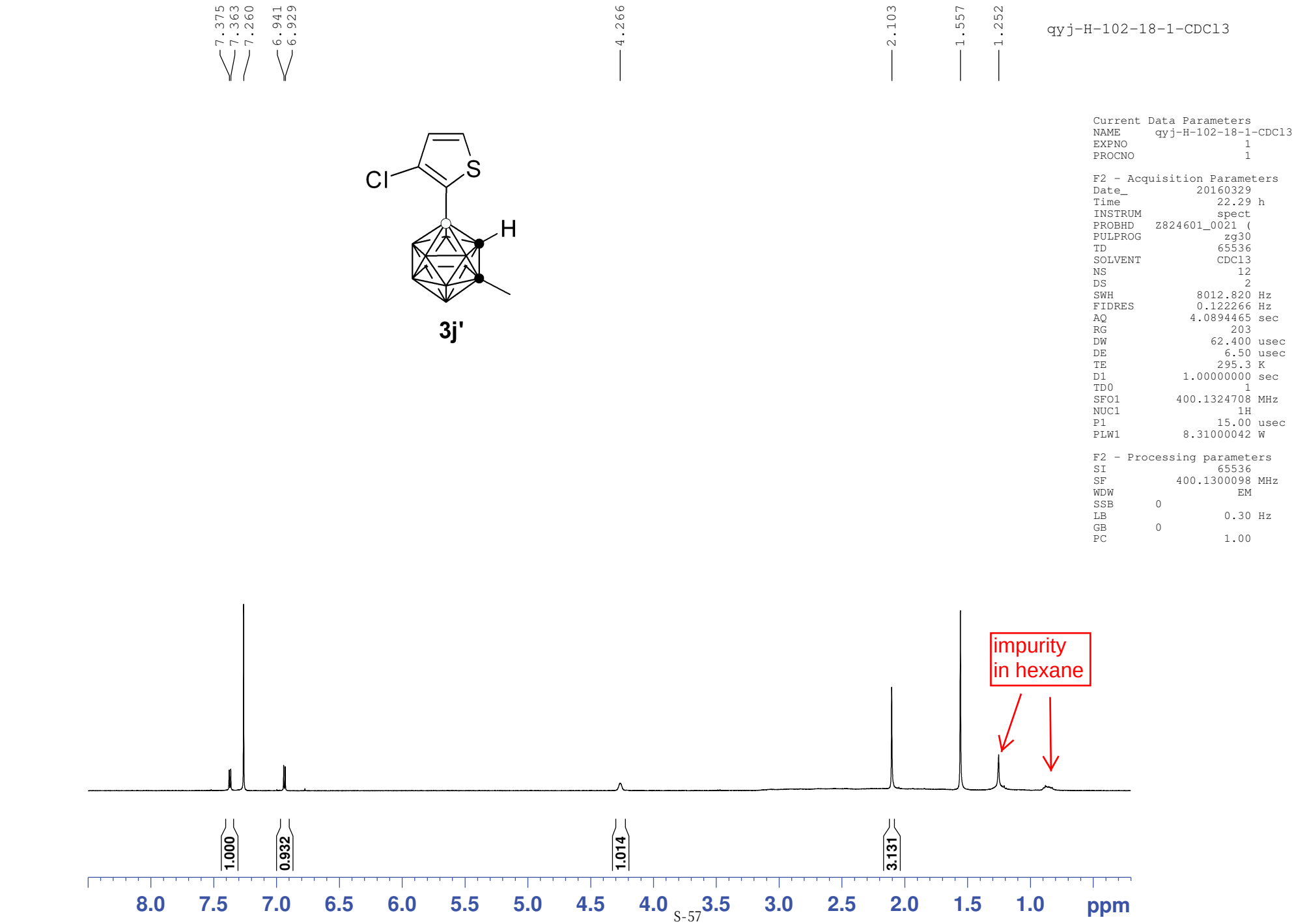
```
Current Data Parameters
NAME      qyj-H-102-18-2-CDCl3
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160329
Time                 22.14 h
INSTRUM              spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                   65536
SOLVENT              CDCl3
NS                      18
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                  295.3 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             400.1300098 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```



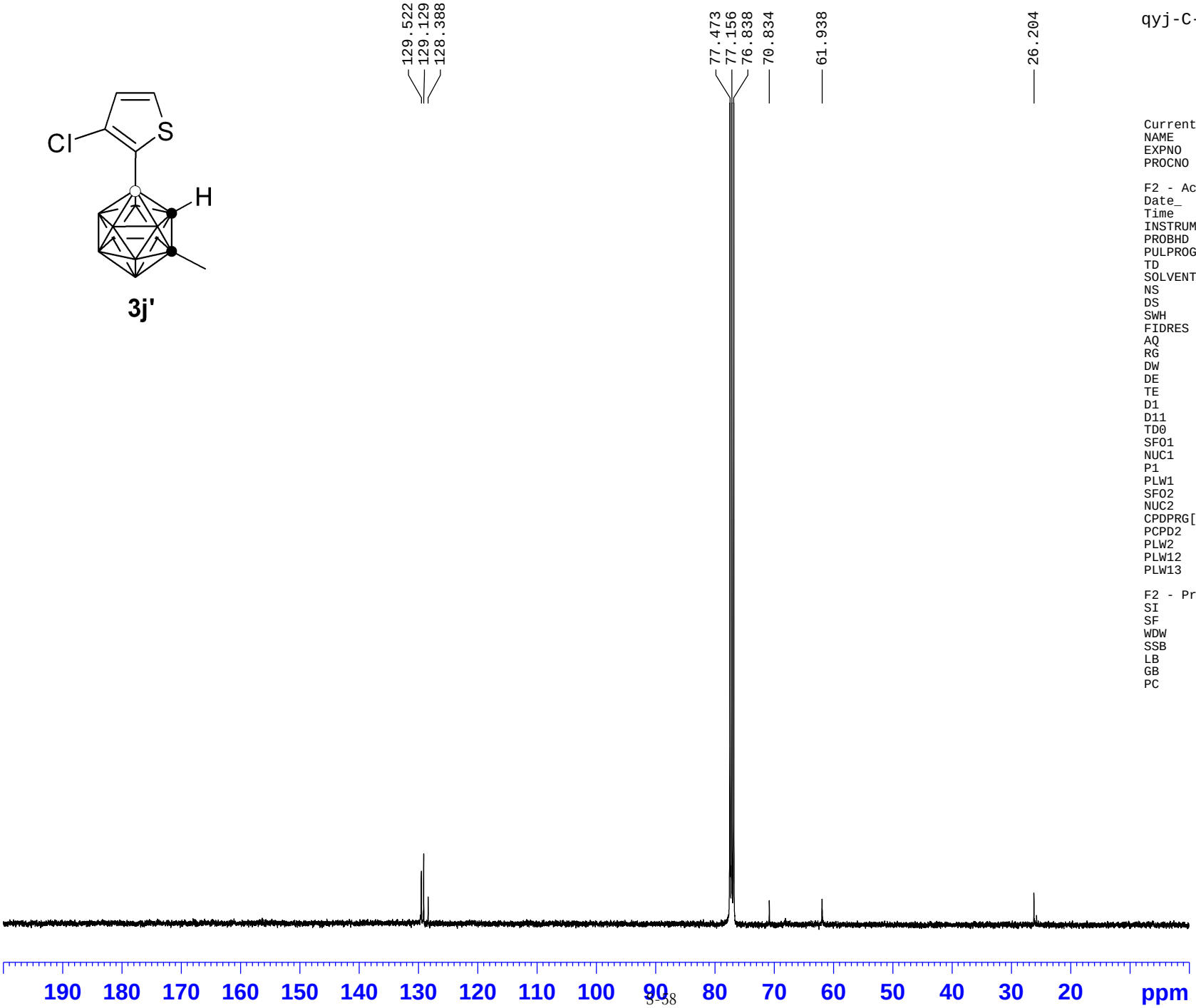

133.694
126.186
123.901
77.475
77.157
76.840
71.570
62.841
26.049
qyj-C-r102-3j-cdcl3
Cl
S
H
3j
Current Data Parameters
NAME qyj-C-r102-3j-cdcl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170318
Time 20.35 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 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 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 100.6127564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


-1.60
-5.96
-8.85
-9.80
-11.28
-12.10
-13.27
qyj-B-0102-18-2-CDCl3
Cl
S
H
3j
Current Data Parameters
NAME qyj-B-0102-18-2-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160330
Time 14.29 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 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 128.4097615 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1.04
2.02
1.13
1.15
4.00
1.12
15
10
5
0
-5
-10
-15
-20
-25
ppm


-0.85
-2.04
-5.21
-5.78
-6.24
-8.12
-9.14
-10.43
-11.76
-12.43
-13.75
qyj-B-0102-18-2-CDCl3(c)
Cl
S
H
3j
Current Data Parameters
NAME qyj-B-0102-18-2-CDCl3(c)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160330
Time 14.30 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 20
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 294.3 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
15
10
5
0
-5
-10
-15
-20
-25
ppm

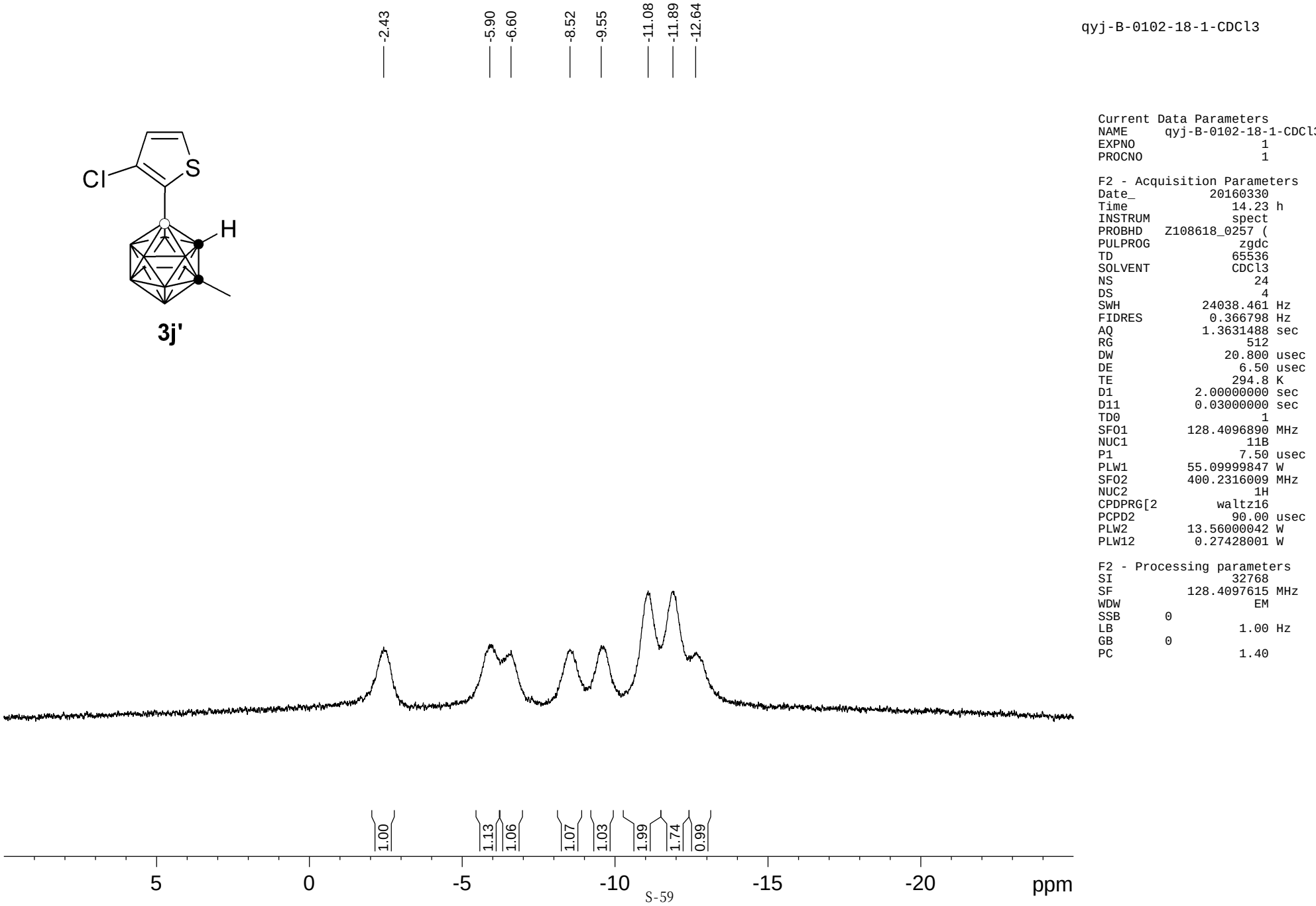

7.375
7.363
7.260
6.941
6.929
4.266
2.103
1.557
1.252
qyj-H-102-18-1-CDCl3
Cl
S
H
3j'
Current Data Parameters
NAME qyj-H-102-18-1-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160329
Time 22.29 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 295.3 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 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
impurity
in hexane
1.000
0.932
1.014
3.131
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

3j'

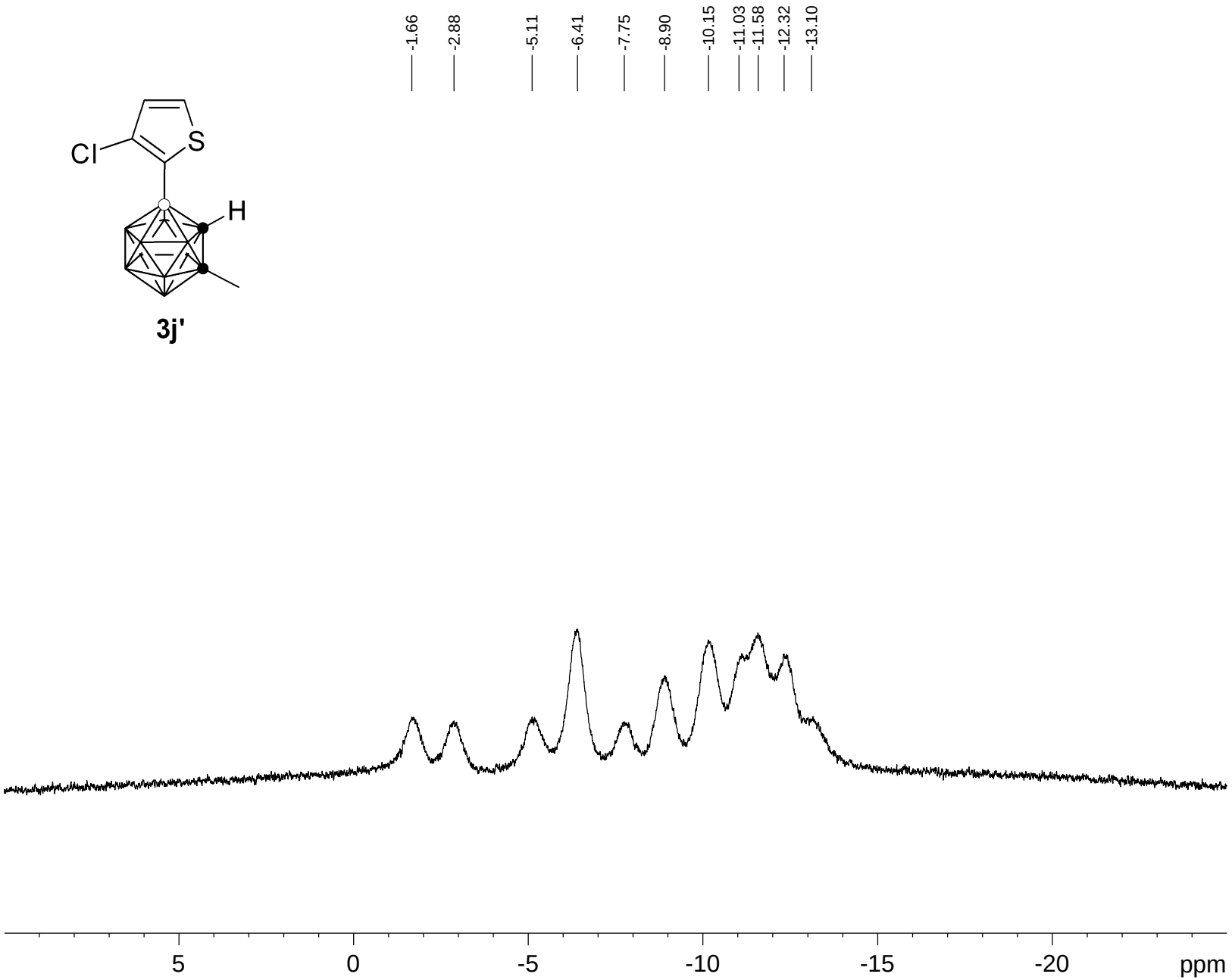


qyj-C-r102-3j'-cdcl3

```
Current Data Parameters
NAME     qyj-C-r102-3j'-cdcl3
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_           20170318
Time              21.26 h
INSTRUM             spect
PROBHD   Z824601_0021 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                 10240
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        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           100.6127557 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

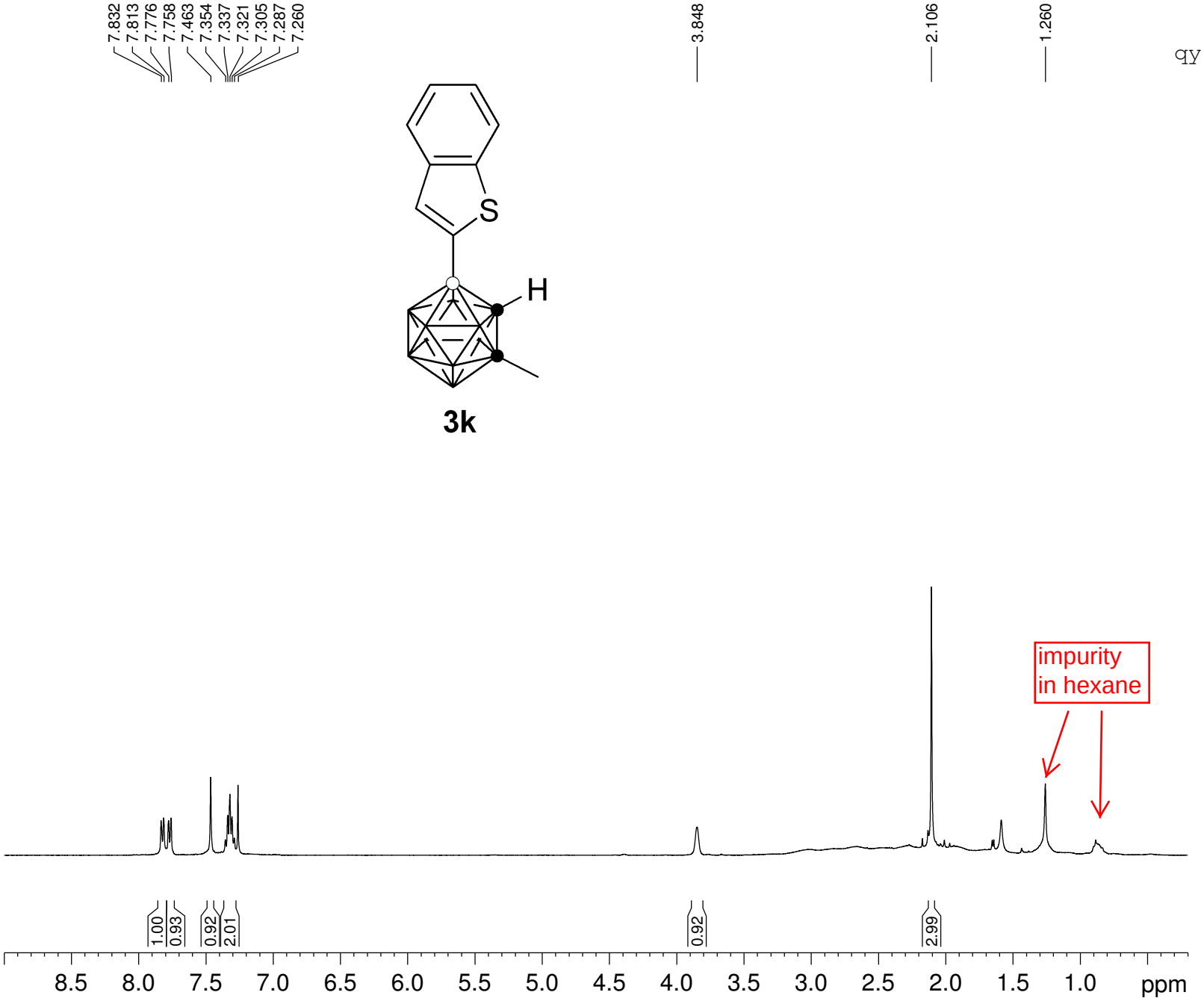

-2.43
-5.90
-6.60
-8.52
-9.55
-11.08
-11.89
-12.64
qyj-B-0102-18-1-CDCl3
Current Data Parameters
NAME qyj-B-0102-18-1-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160330
Time 14.23 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 24
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 512
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
Cl
S
H
3j'
1.00
1.13
1.06
1.07
1.03
1.99
1.74
0.99
5
0
-5
-10
-15
-20
ppm

3j'



qyj-B-0102-18-1-CDCl3(c)

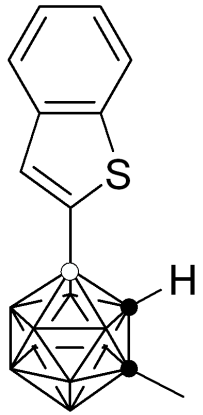
```
Current Data Parameters
NAME     qyj-B-0102-18-1-CDCl3(c)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20160330
Time              14.26 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                   36
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  512
DW                20.800 usec
DE                 6.50 usec
TE                294.2 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
```



Current Data Parameters
NAME qyj-H-102-19-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160403
Time 21.51 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 101
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 12.80 usec
PLW1 13.56000042 W

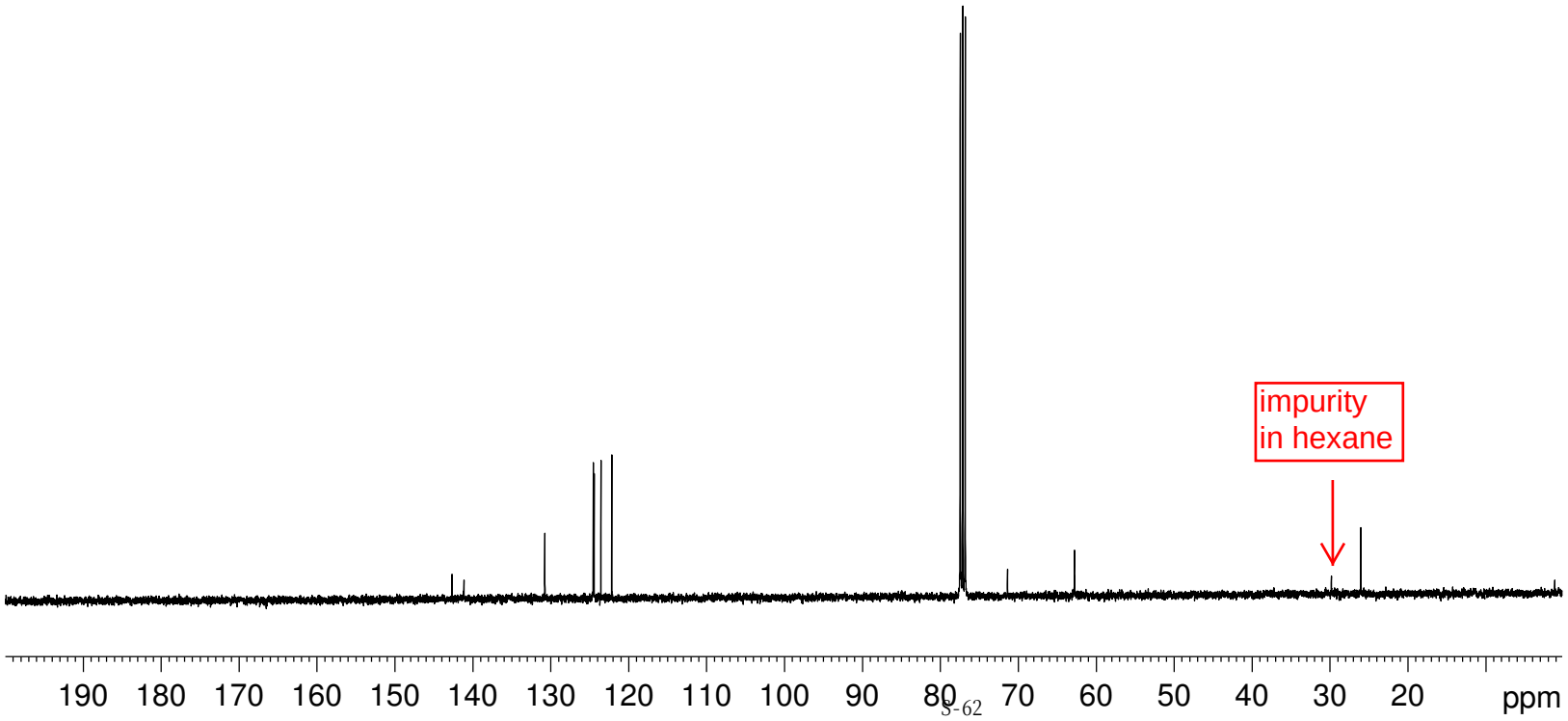
F2 - Processing parameters
SI 65536
SF 400.2300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



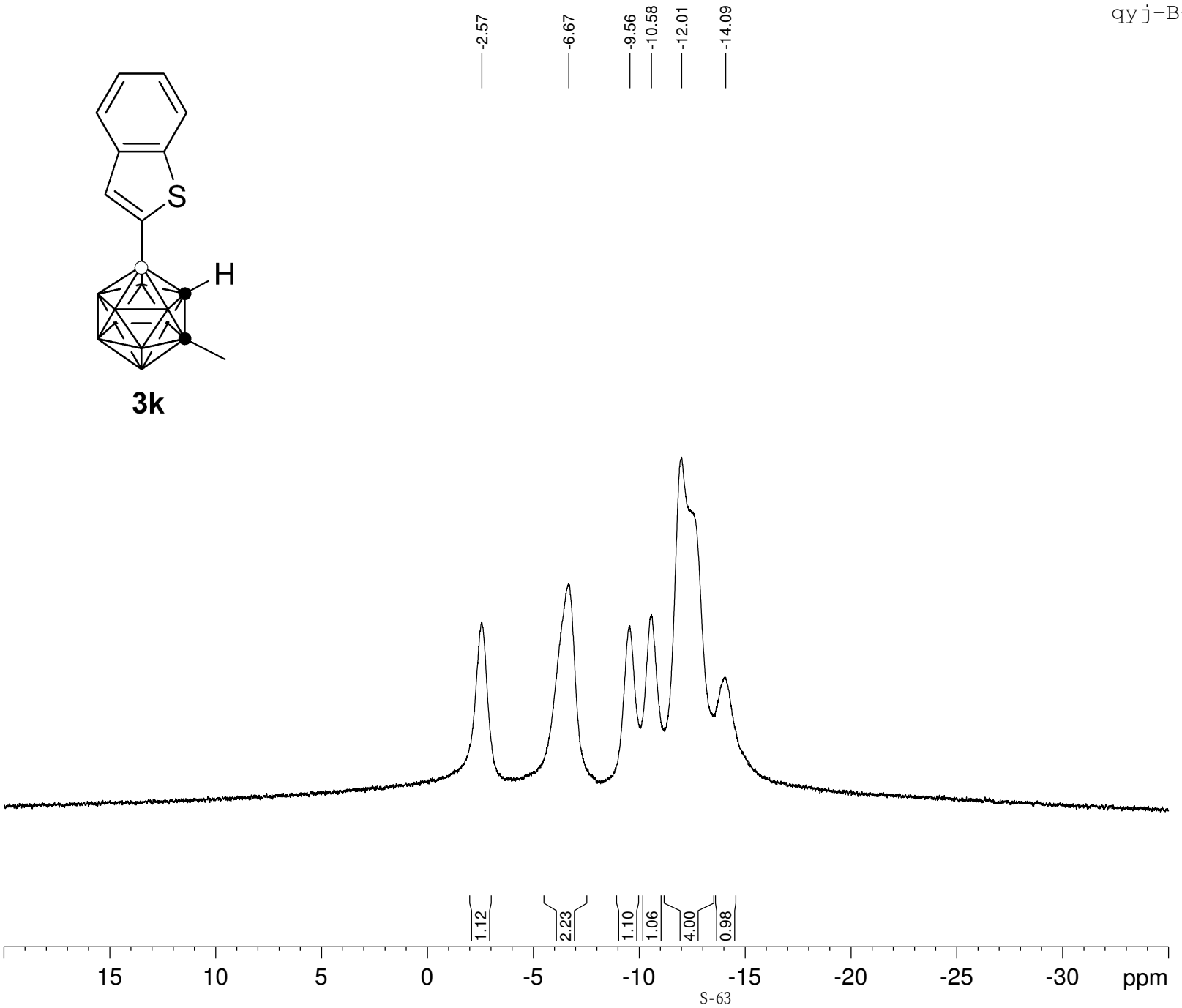
3k

142.66
141.12
130.75
124.54
124.42
123.55
122.16
77.47
77.16
76.84
71.40
62.81
29.84
26.08

qyj-C-r102-19-CDCl3



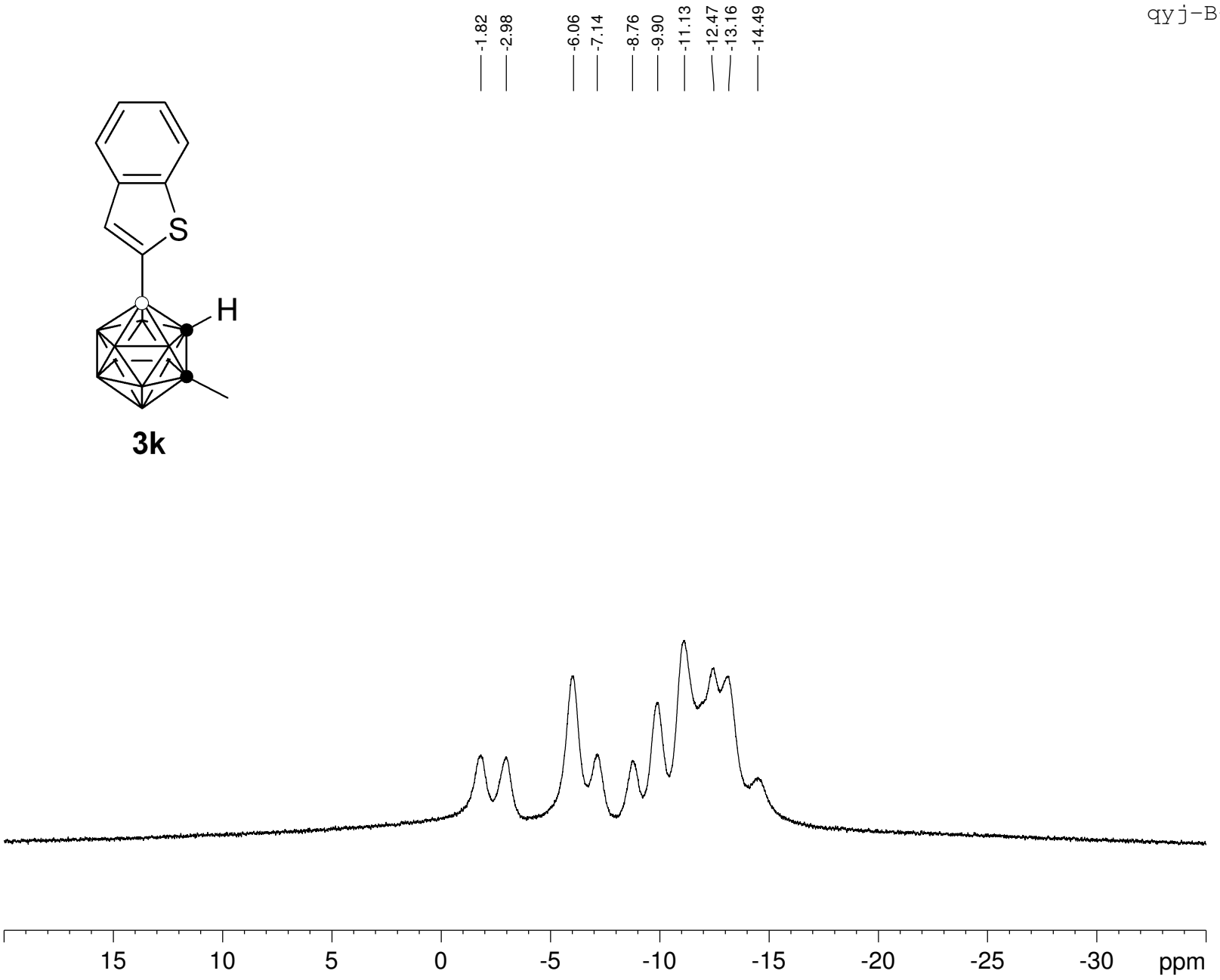

```
Current Data Parameters
NAME      qyj-C-r102-19-CDCl3
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20170317
Time                 17.45 h
INSTRUM              spect
PROBHD    Z108618_0257 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     286
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                     203
DW                  16.800 usec
DE                   6.50 usec
TE                  295.2 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             100.6379024 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



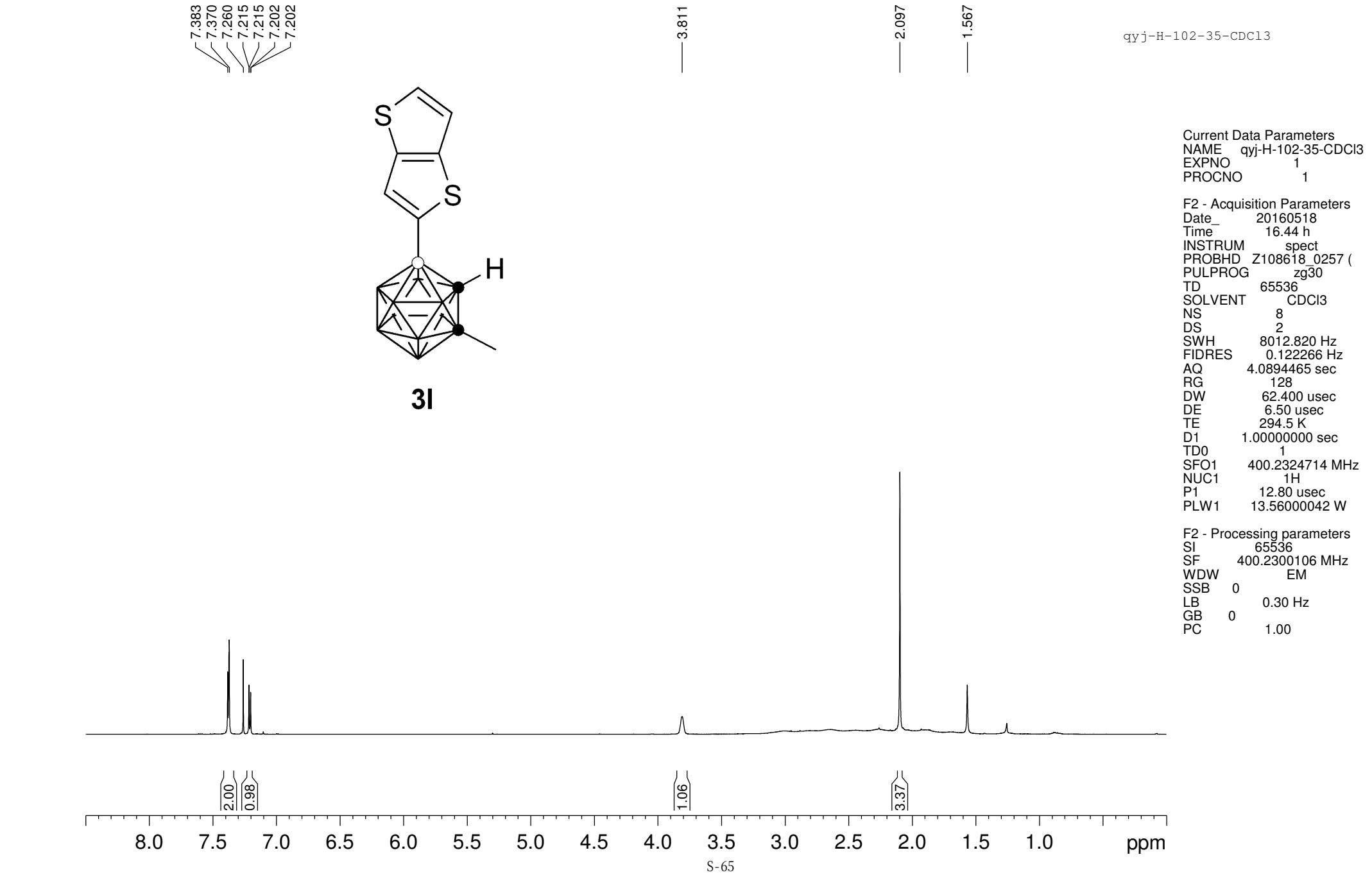

```
Current Data Parameters
NAME      qyj-B-102-19-CDCl3
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20160403
Time                21.44 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     21
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                 295.2 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
```

qyj-B-102-19-CDCl3(c)

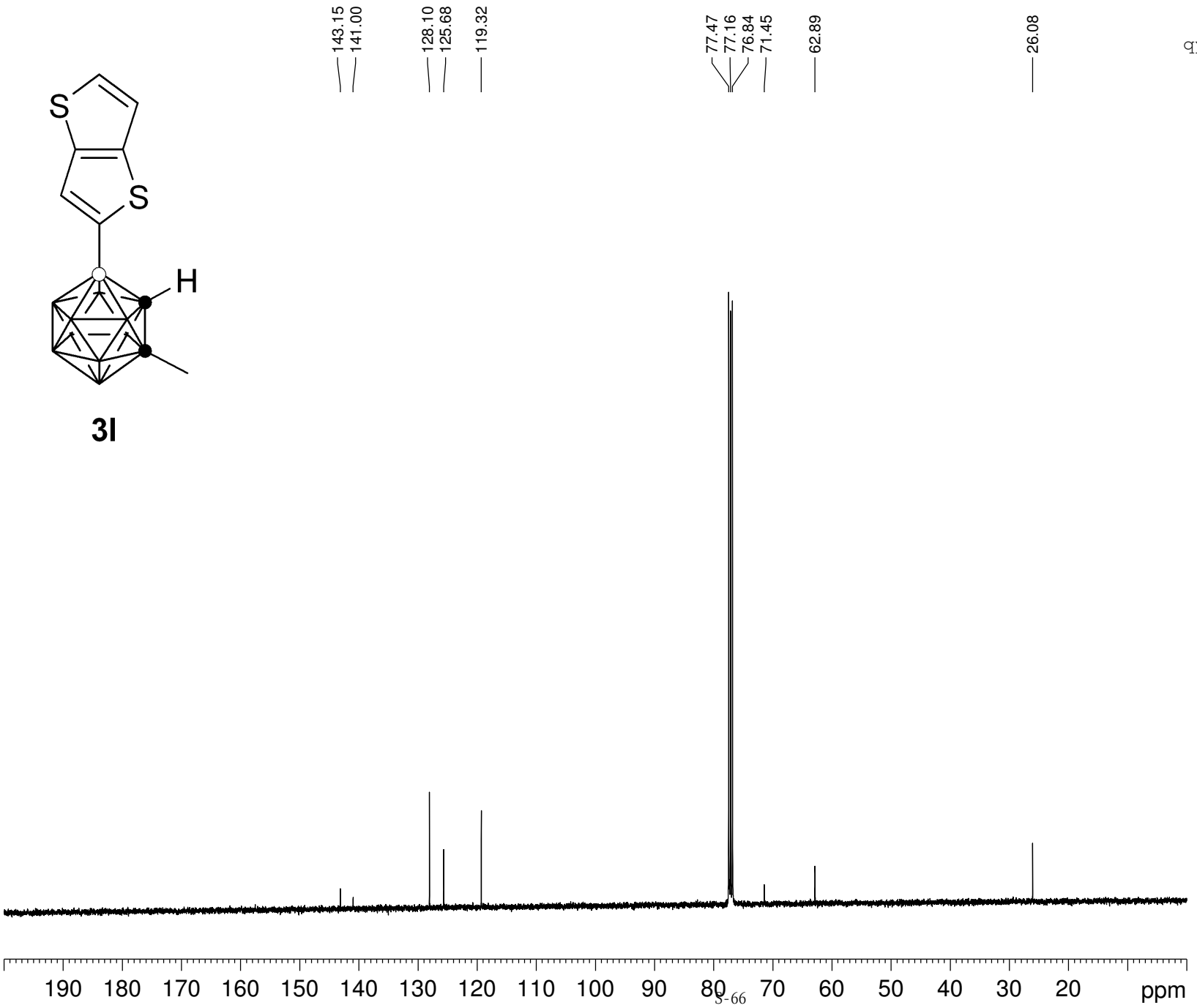
3k




```
Current Data Parameters
NAME      qyj-B-102-19-CDCl3(c)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160403
Time                 21.46 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT                CDCl3
NS                        16
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                    294.8 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
```


7.383
7.370
7.260
7.215
7.215
7.202
7.202
3.811
2.097
1.567
qyj-H-102-35-CDCl3
S
S
H
3I
Current Data Parameters
NAME qyj-H-102-35-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160518
Time 16.44 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 128
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 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
2.00
0.98
1.06
3.37
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

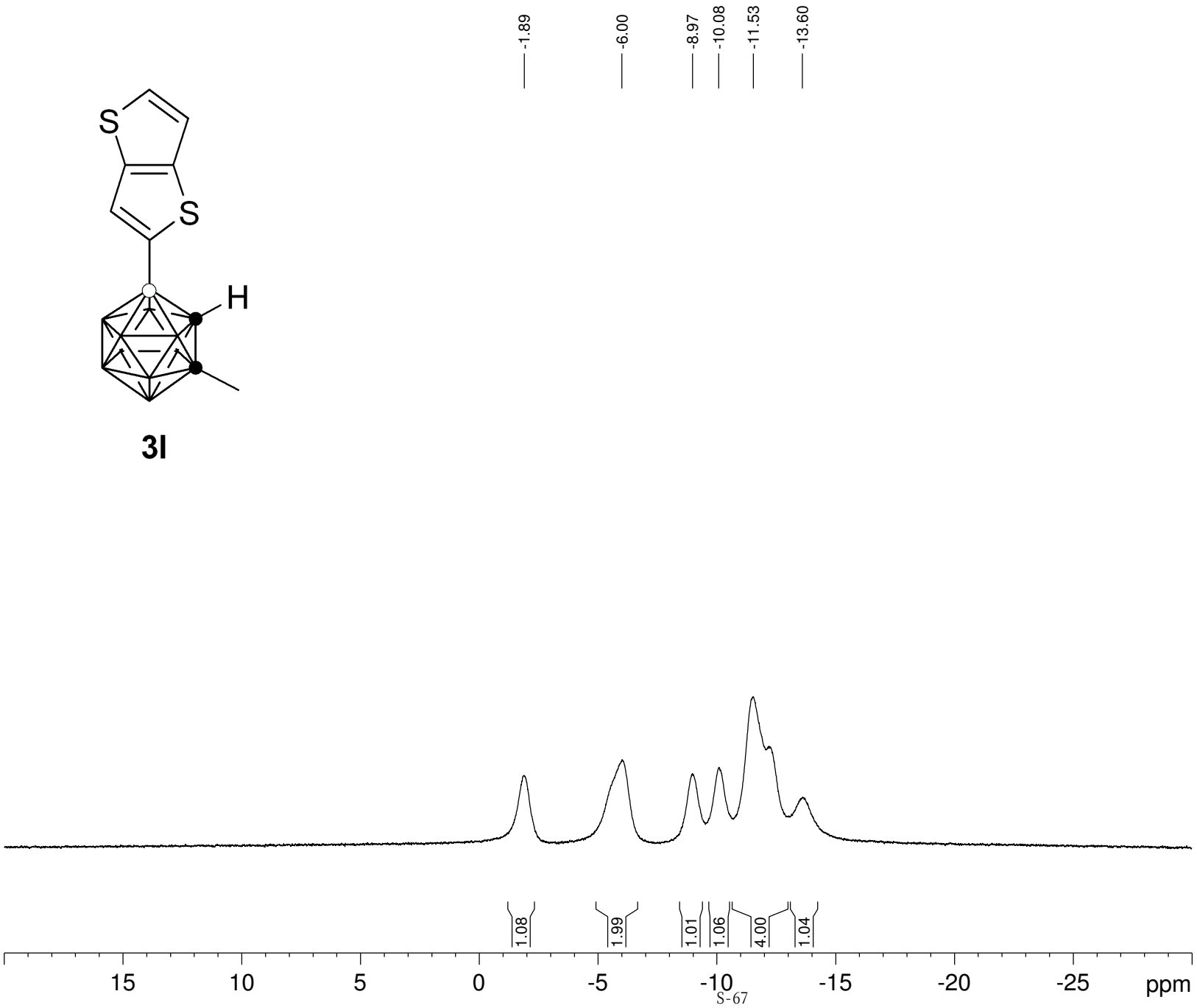
3l



qyj-C-102-35-CDCl3

```
Current Data Parameters
NAME      qyj-C-102-35-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160519
Time              10.34 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  562
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG                  114
DW                16.800 usec
DE                 6.50 usec
TE                295.0 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          100.6379020 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

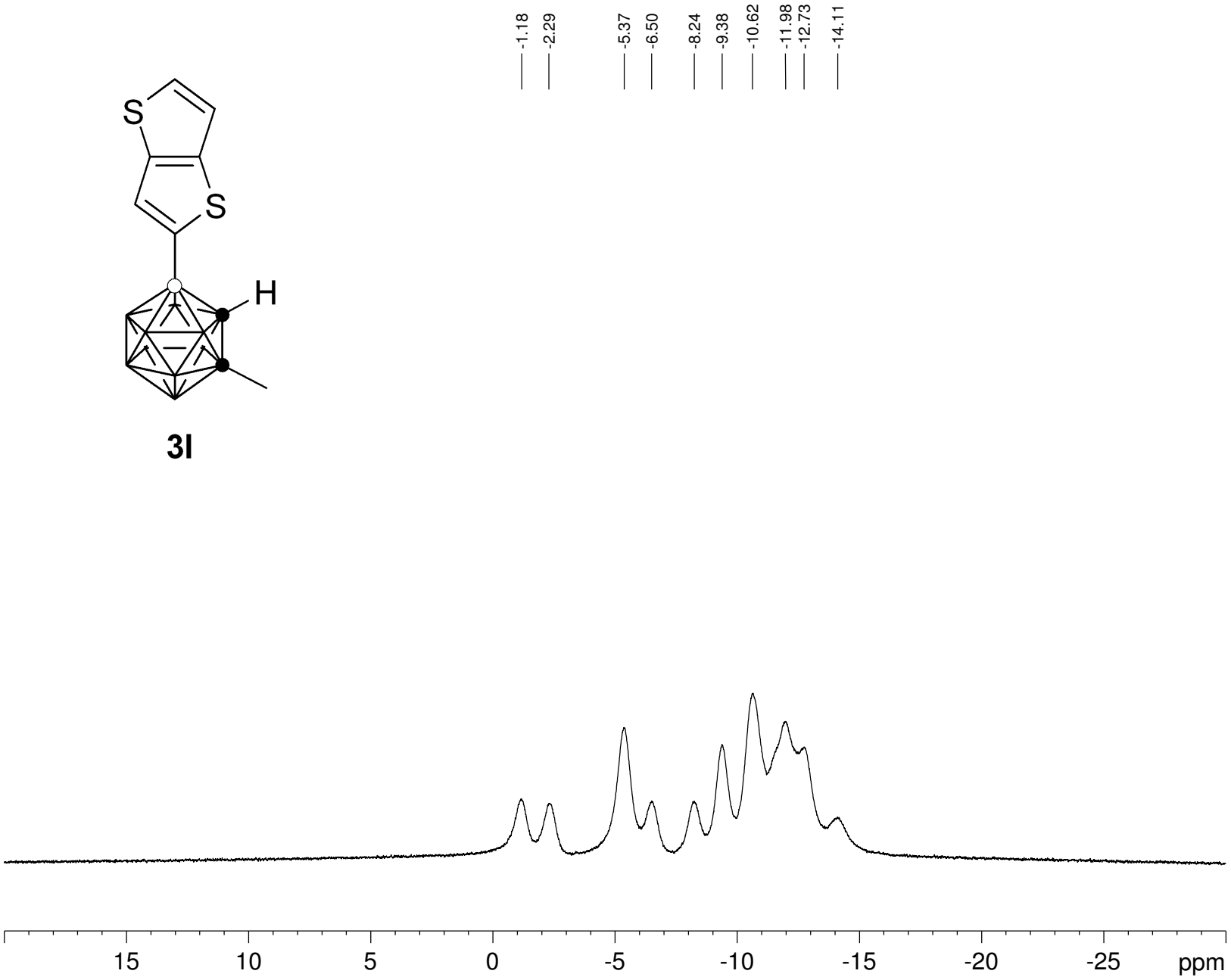
3l



qyj-B-102-35-CDCl3

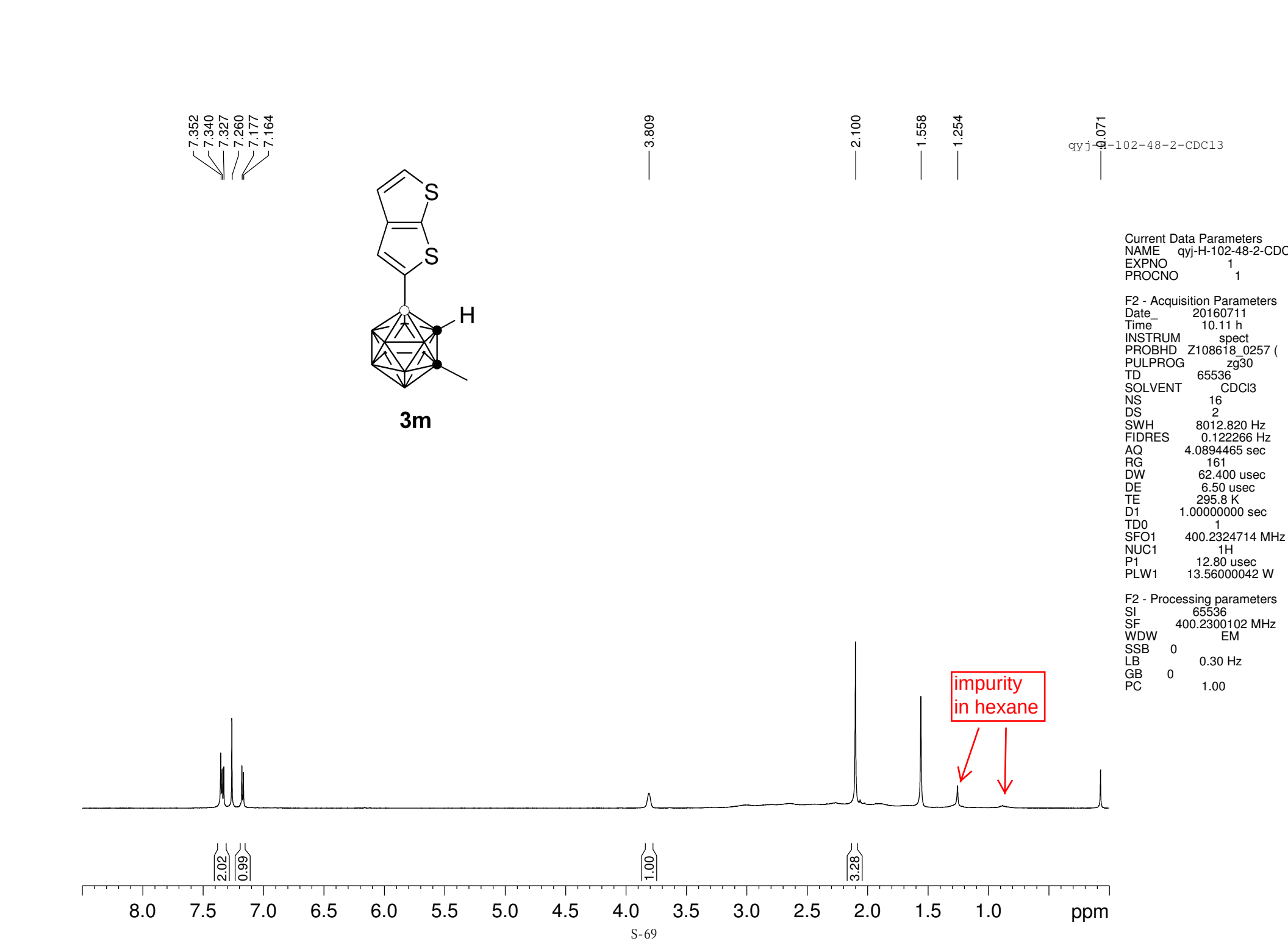
```
Current Data Parameters
NAME      qyj-B-102-35-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20160518
Time                16.46 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                      8
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                 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            128.4097615 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

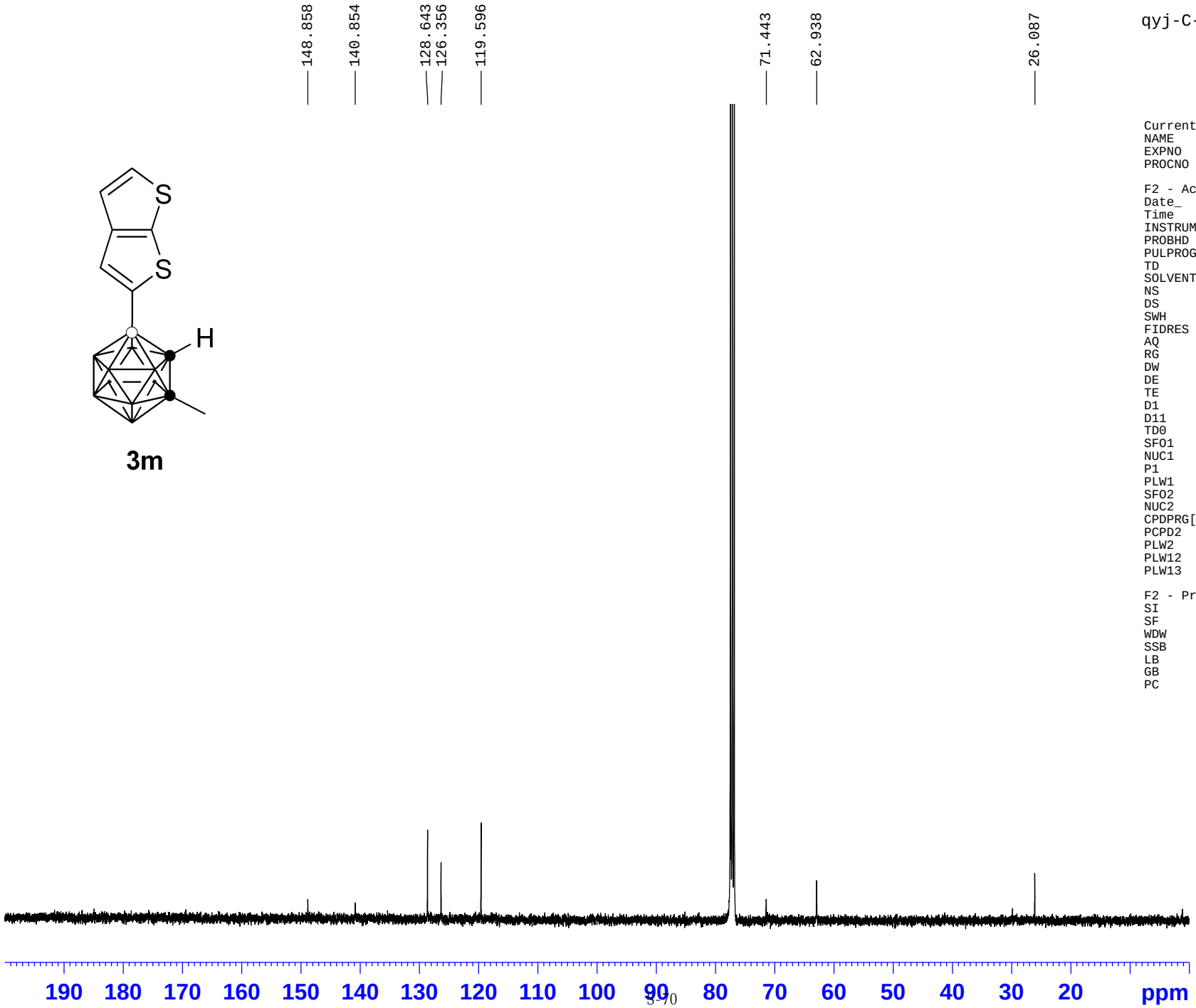
3l



qyj-B-102-35-CDCl3(C)

```
Current Data Parameters
NAME      qyj-B-102-35-CDCl3(C)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160518
Time              16.47 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     12
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                 294.5 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
```


7.352
7.340
7.327
7.260
7.177
7.164
3.809
2.100
1.558
1.254
0.071
qyj-H-102-48-2-CDCl3
S
S
H
3m
Current Data Parameters
NAME qyj-H-102-48-2-CDC
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160711
Time 10.11 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 295.8 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 400.2300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
impurity
in hexane
2.02
0.99
1.00
3.28
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

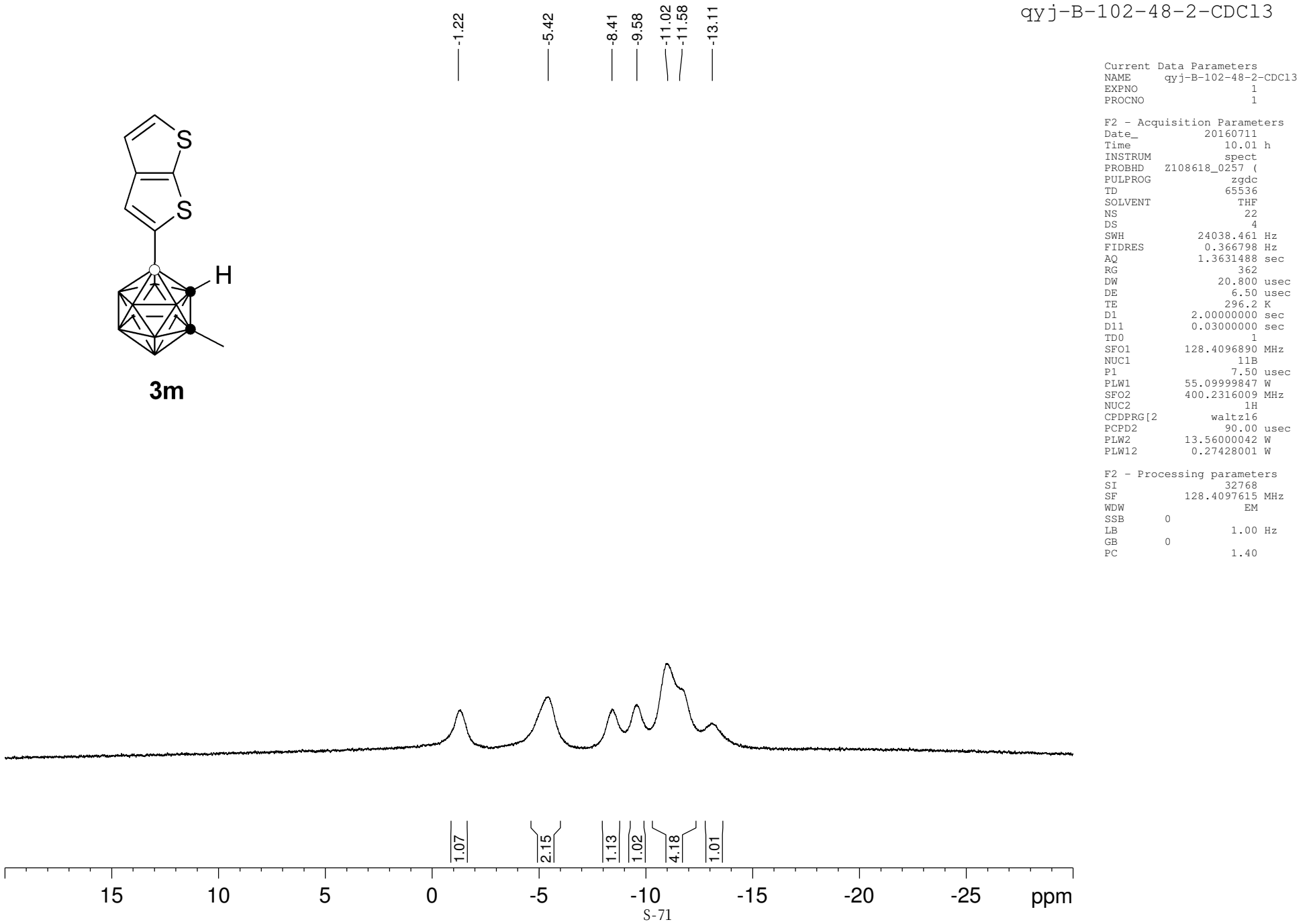


qyj-C-102-48-2-CDCl3

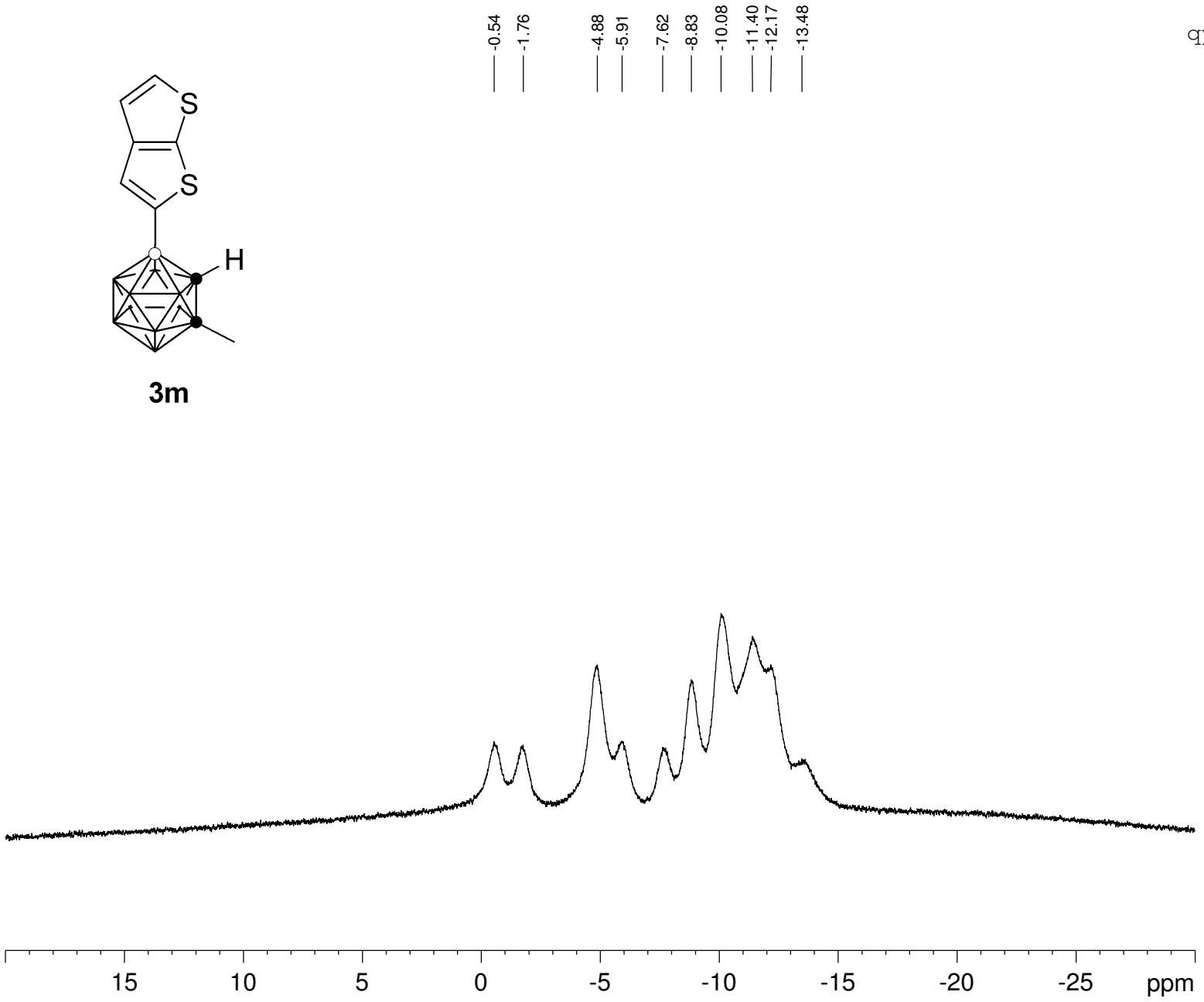
Current Data Parameters
NAME qyj-C-102-48-2-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160714
Time 17.04 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3027
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 294.9 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 100.6127561 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

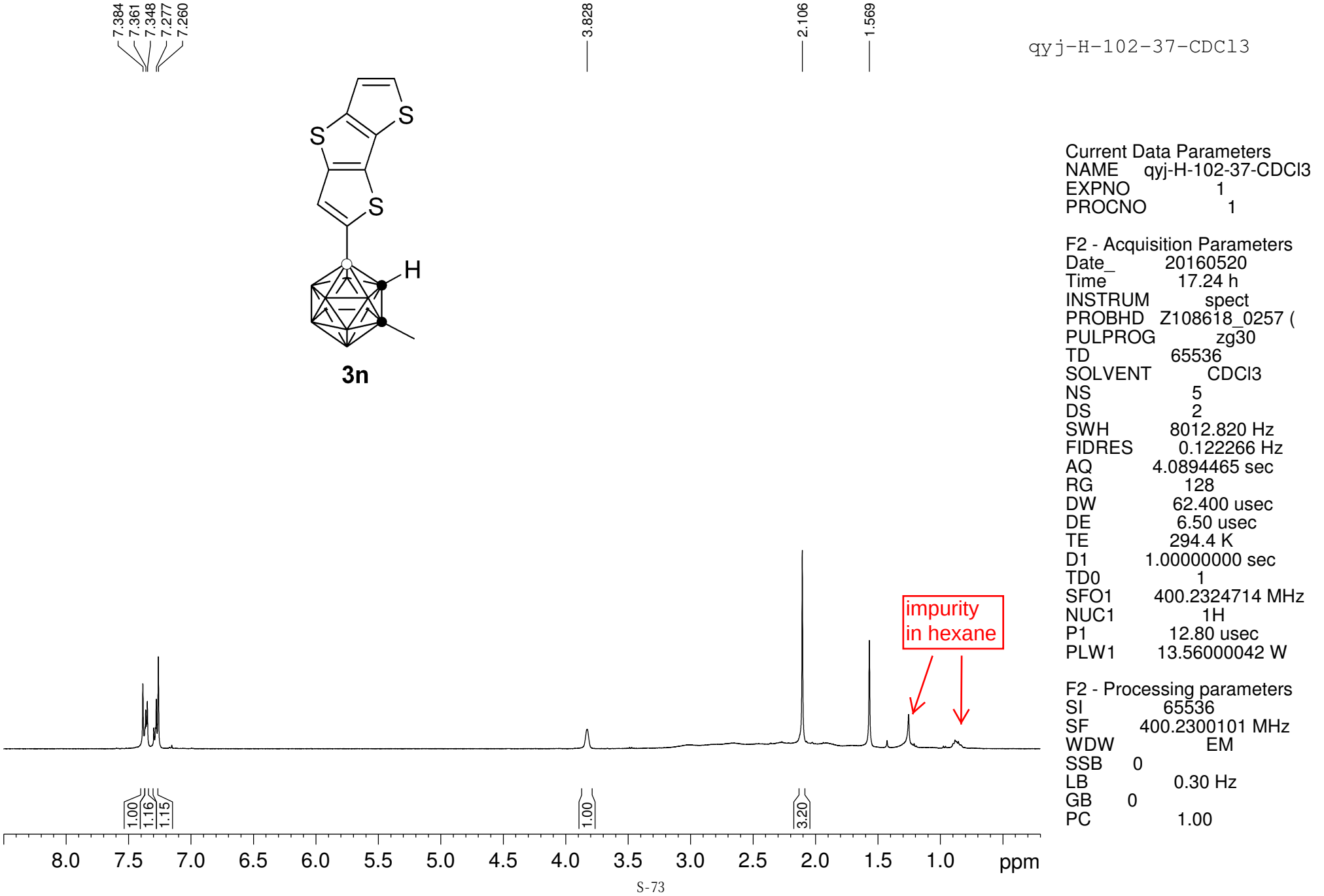

-1.22
-5.42
-8.41
-9.58
-11.02
-11.58
-13.11
qyj-B-102-48-2-CDCl3
Current Data Parameters
NAME qyj-B-102-48-2-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160711
Time 10.01 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgdc
TD 65536
SOLVENT THF
NS 22
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.50 usec
TE 296.2 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
S
S
H
3m
1.07
2.15
1.13
1.02
4.18
1.01
15
10
5
0
-5
-10
-15
-20
-25
ppm

3m



qyj-B-102-48-2-CDCl3(c)

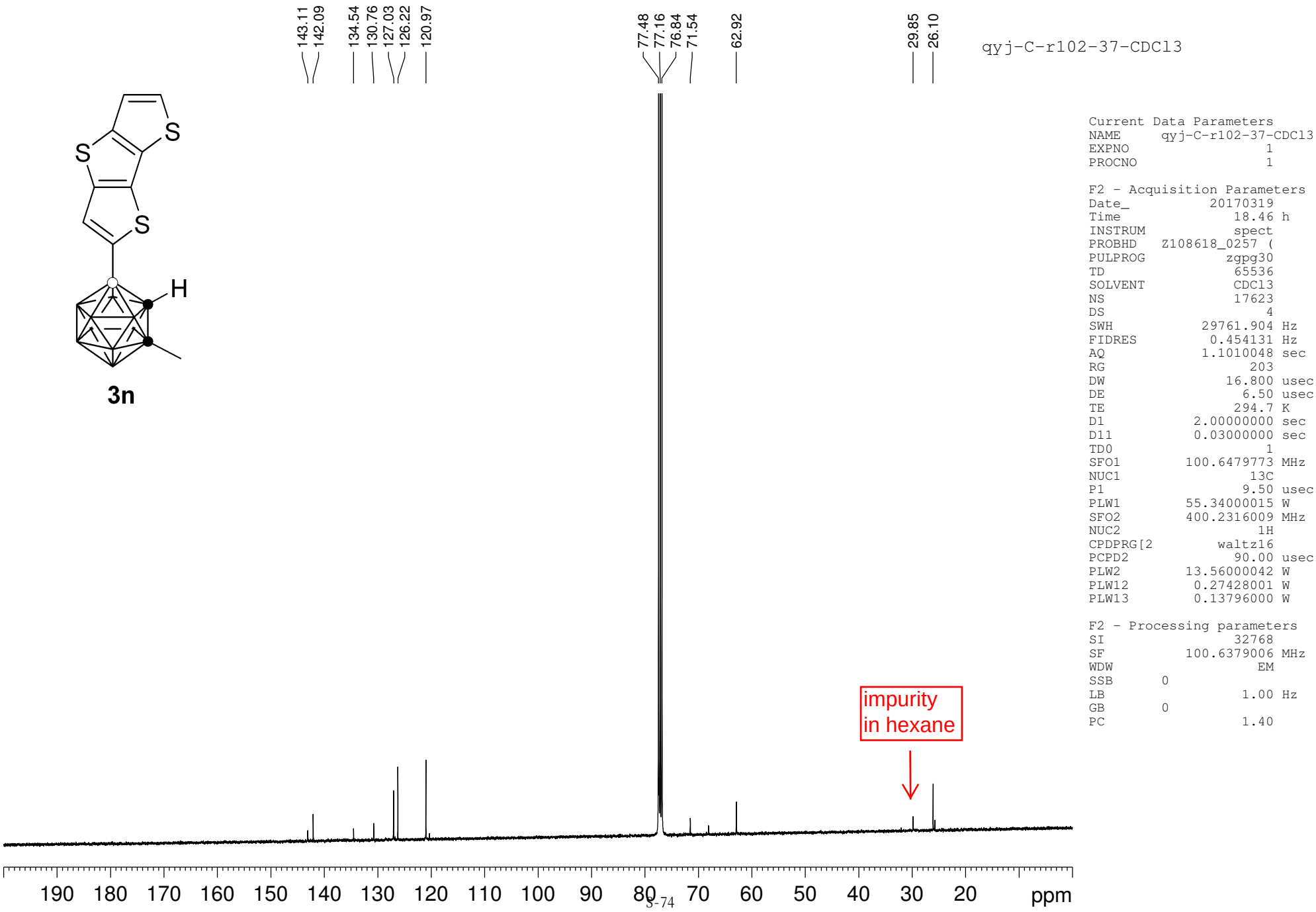
```
Current Data Parameters
NAME      qyj-B-102-48-2-CDCl3(c)
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20160711
Time                   10.04 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT                  THF
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                     295.6 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
```



Current Data Parameters
NAME qyj-H-102-37-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160520
Time 17.24 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
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 294.4 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

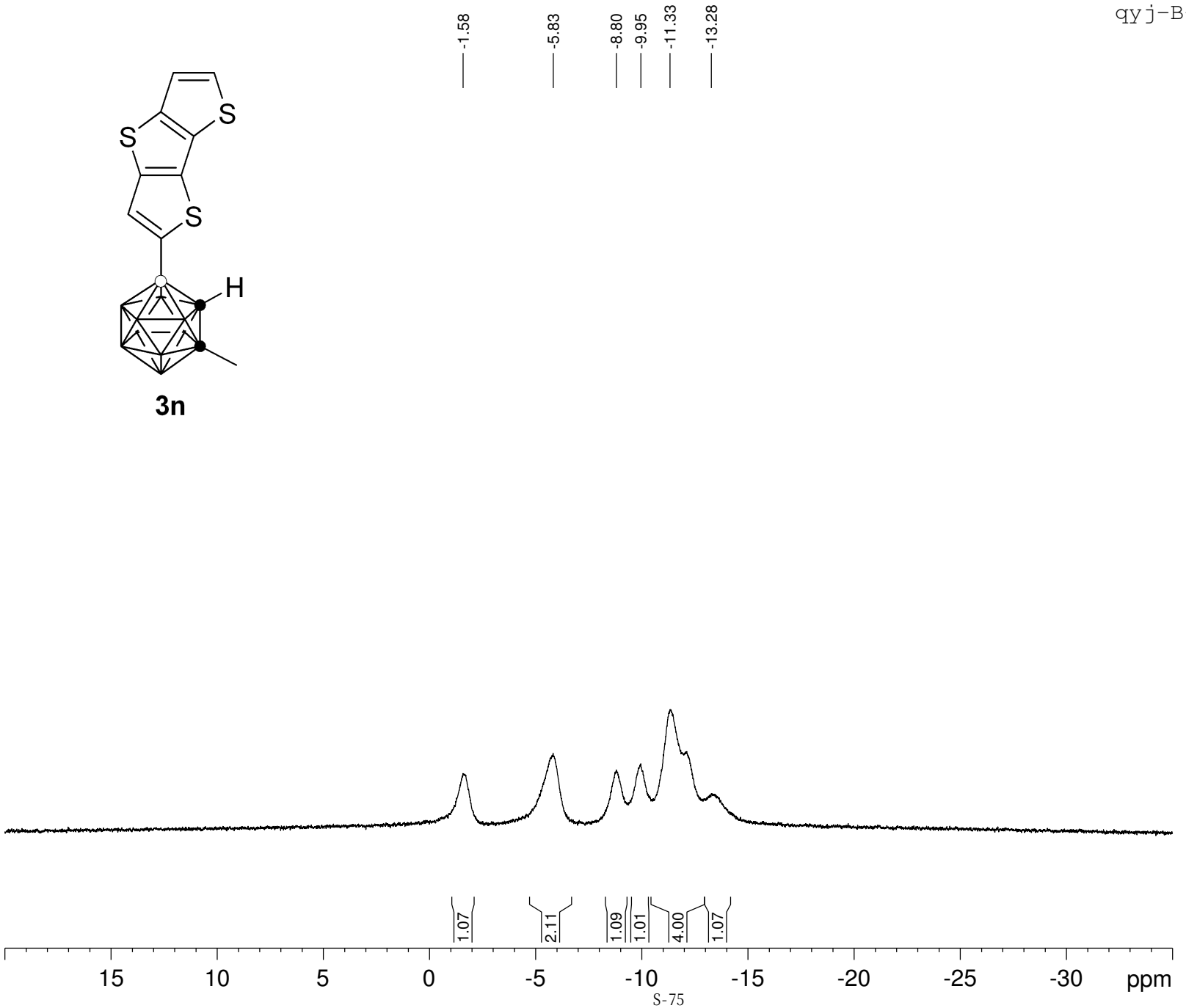


Current Data Parameters
NAME qyj-C-r102-37-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170319
Time 18.46 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 17623
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 294.7 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 100.6379006 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

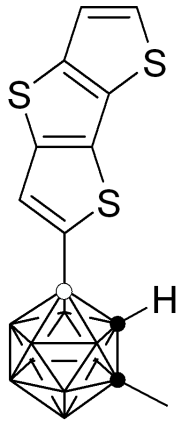
3n



qyj-B-102-37-CDCl3

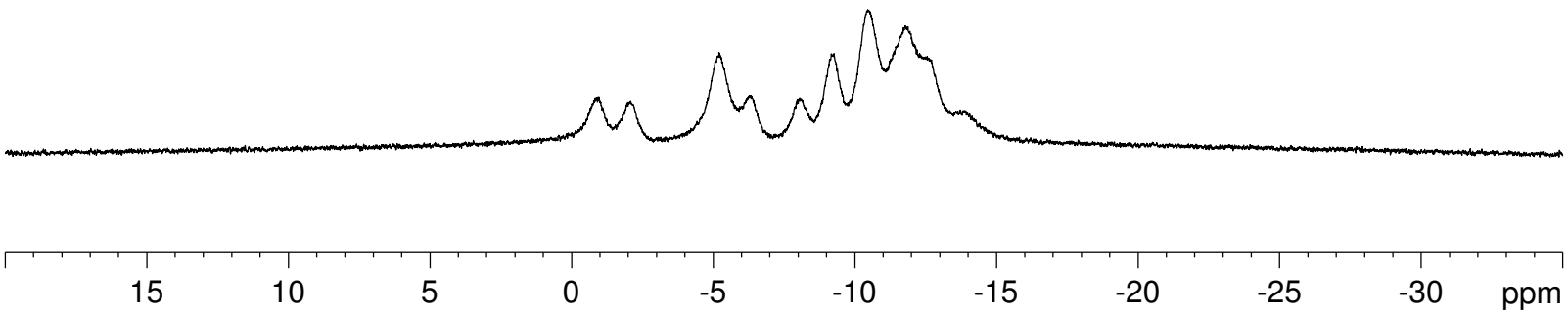
```
Current Data Parameters
NAME      qyj-B-102-37-CDCl3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160520
Time              16.40 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                     8
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                294.5 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
```

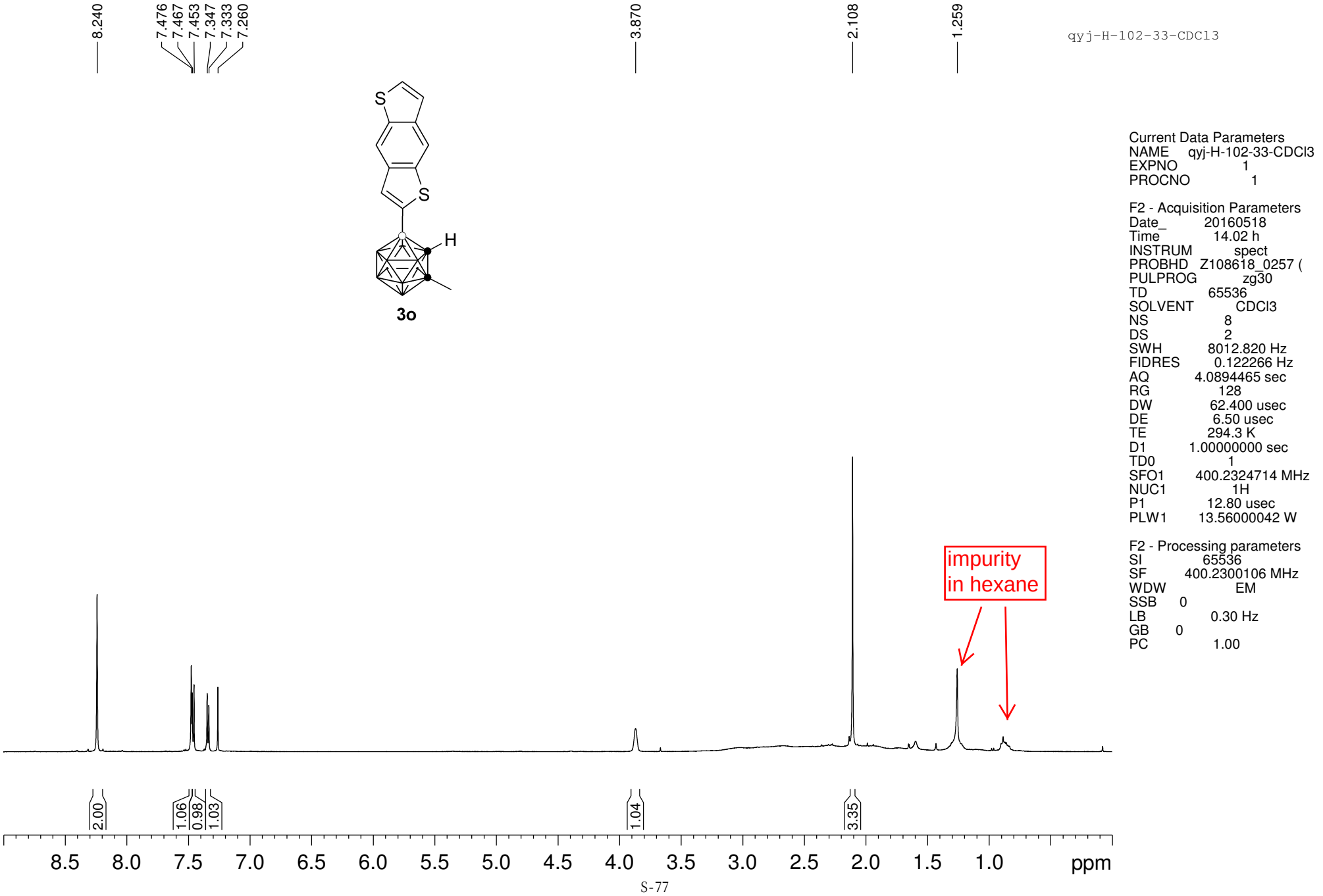
qyj-B-102-37-CDCl3(C)



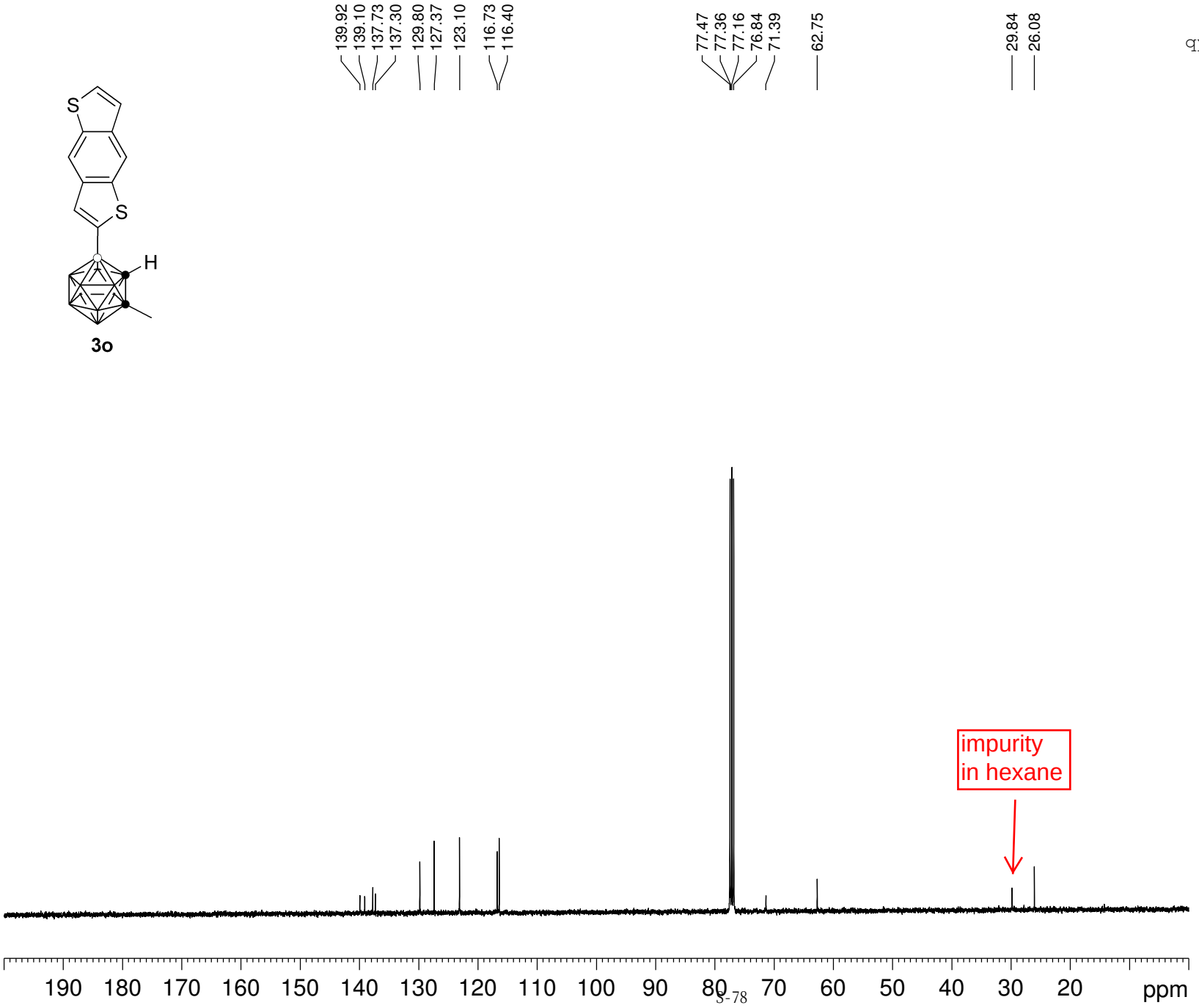
3n


```
Current Data Parameters
NAME      qyj-B-102-37-CDCl3(C)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160520
Time                 16.41 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      11
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     456
DW                  20.800 usec
DE                   6.50 usec
TE                  294.3 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
```




8.240
7.476
7.467
7.453
7.347
7.333
7.260
3.870
2.108
1.259
qyj-H-102-33-CDCl3
S
S
H
3o
Current Data Parameters
NAME qyj-H-102-33-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160518
Time 14.02 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 128
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 400.2300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
impurity
in hexane
2.00
1.06
0.98
1.03
1.04
3.35
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
ppm

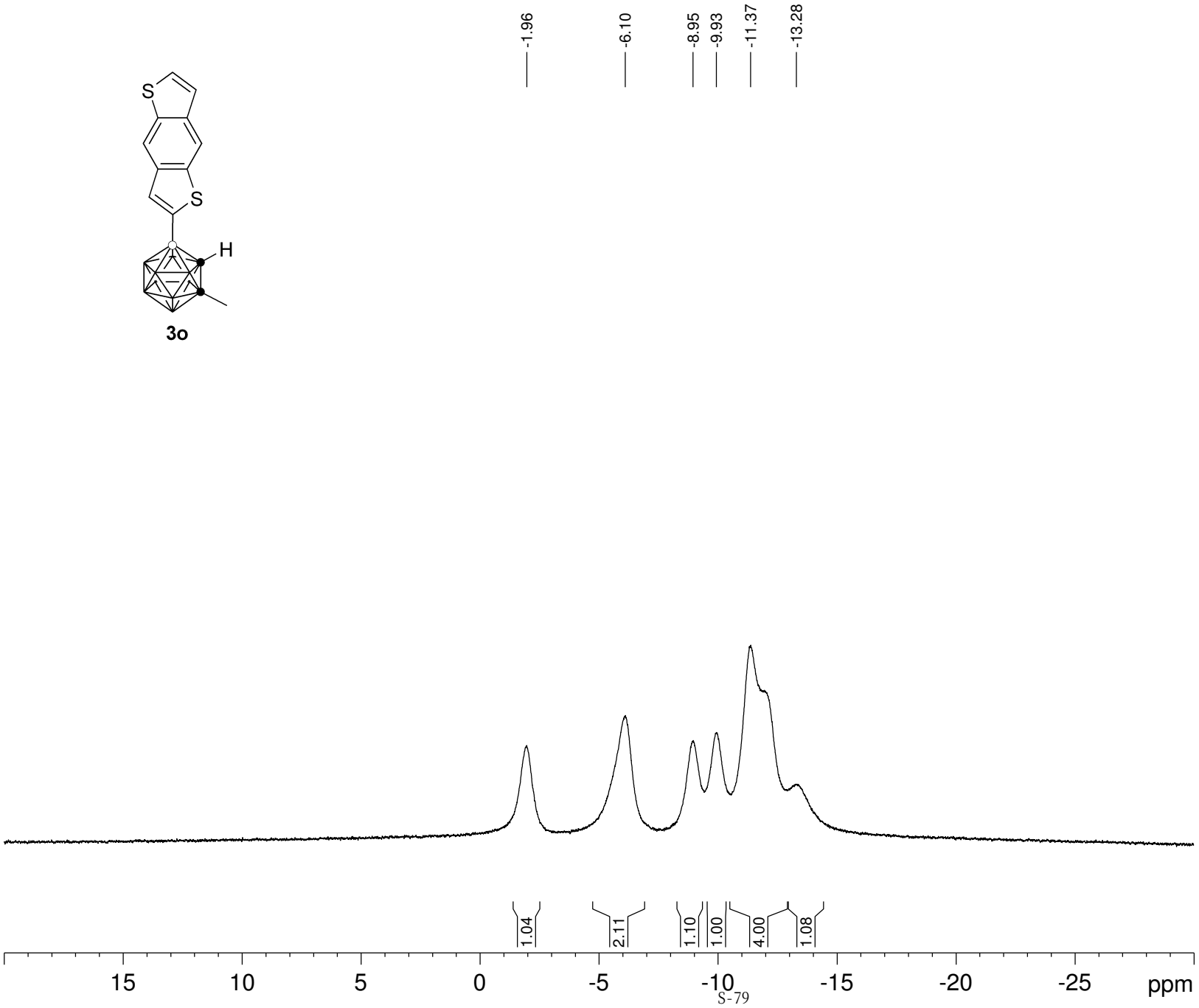
3o



qyj-C-102-33-CDCl3

```
Current Data Parameters
NAME      qyj-C-102-33-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160520
Time              17.35 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  522
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  114
DW                16.800 usec
DE                 6.50 usec
TE                294.4 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           100.6379024 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

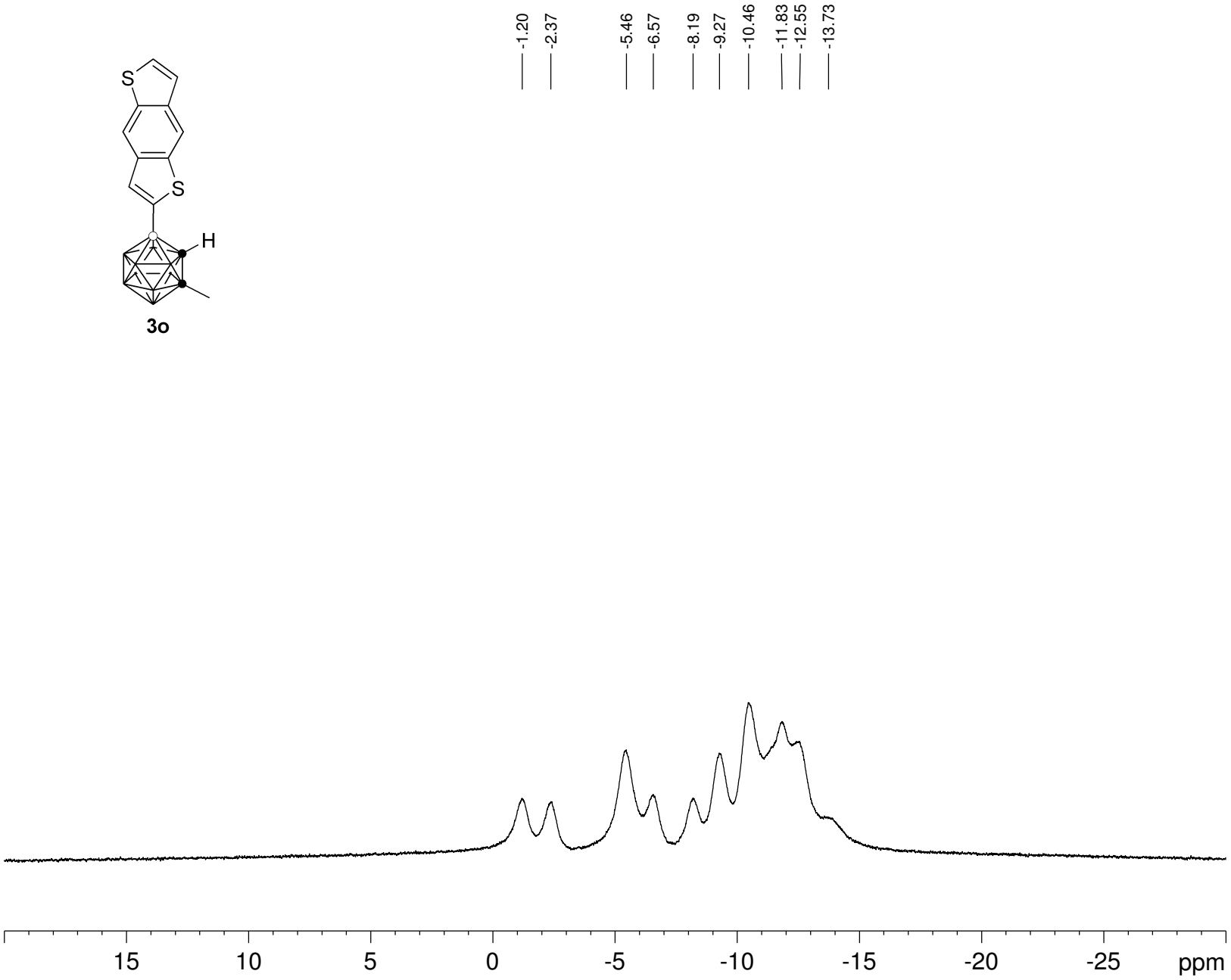
3o



qyj-B-102-33-CDCl3

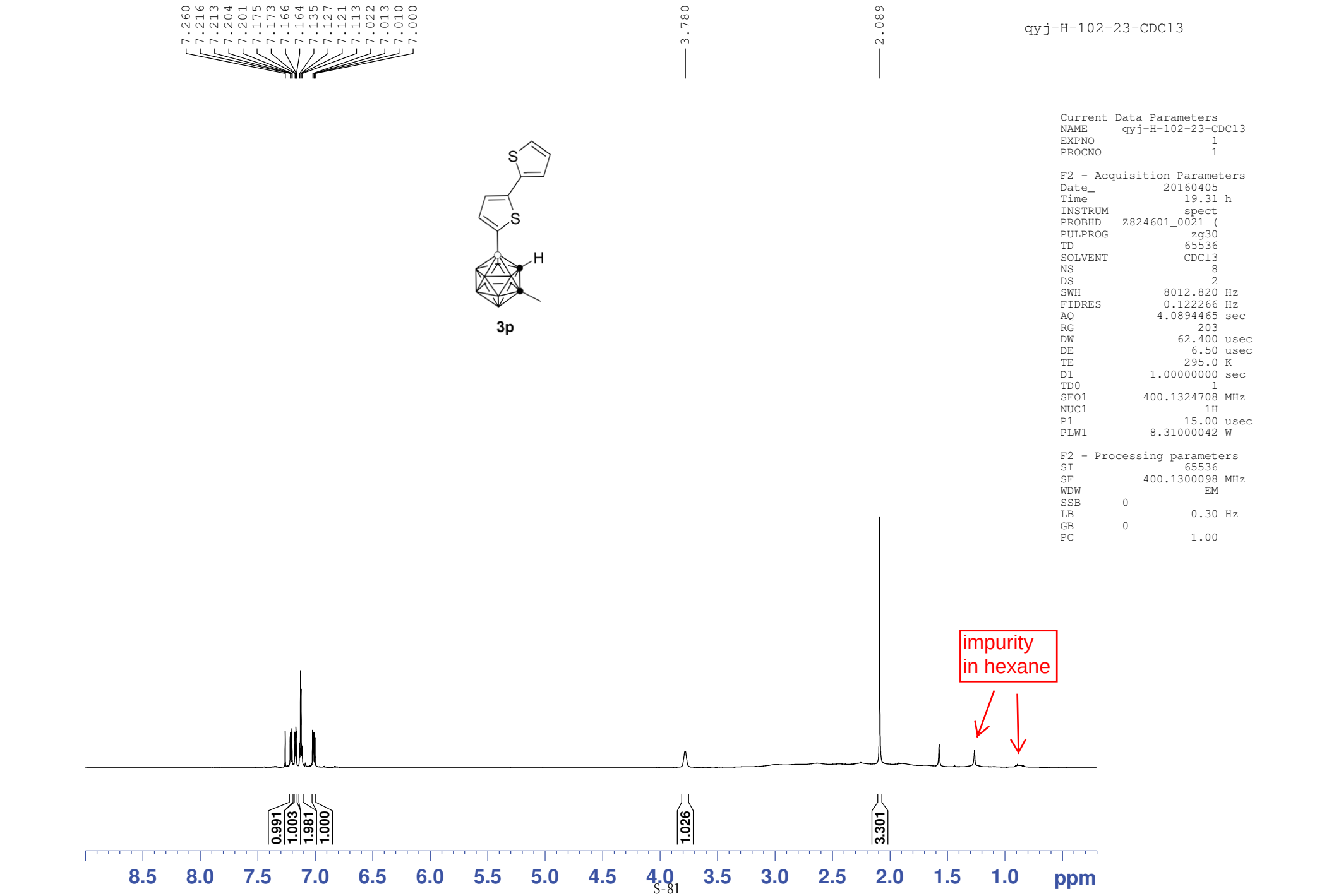
```
Current Data Parameters
NAME      qyj-B-102-33-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20160518
Time                14.04 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     12
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                 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            128.4097615 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

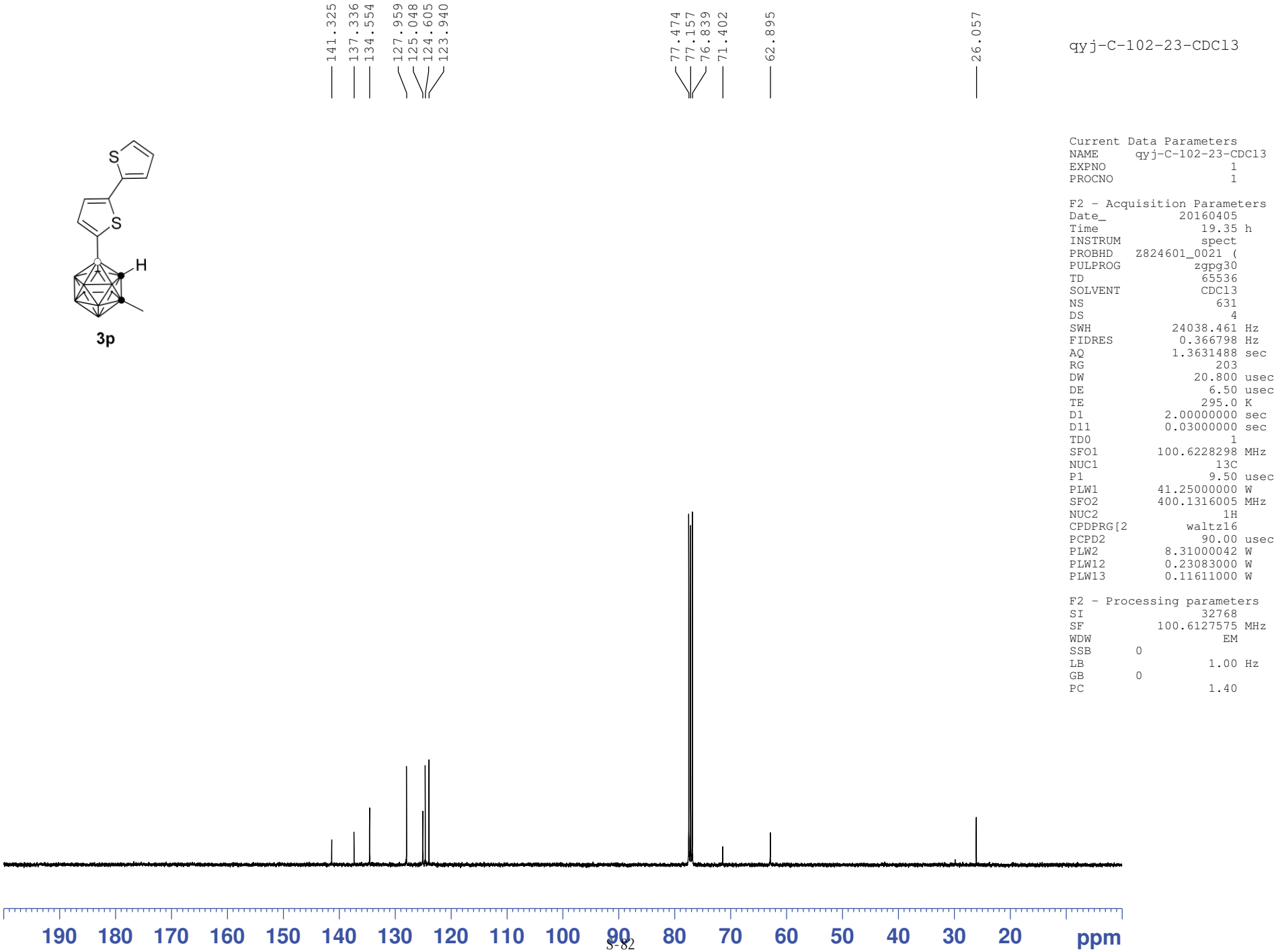
3o



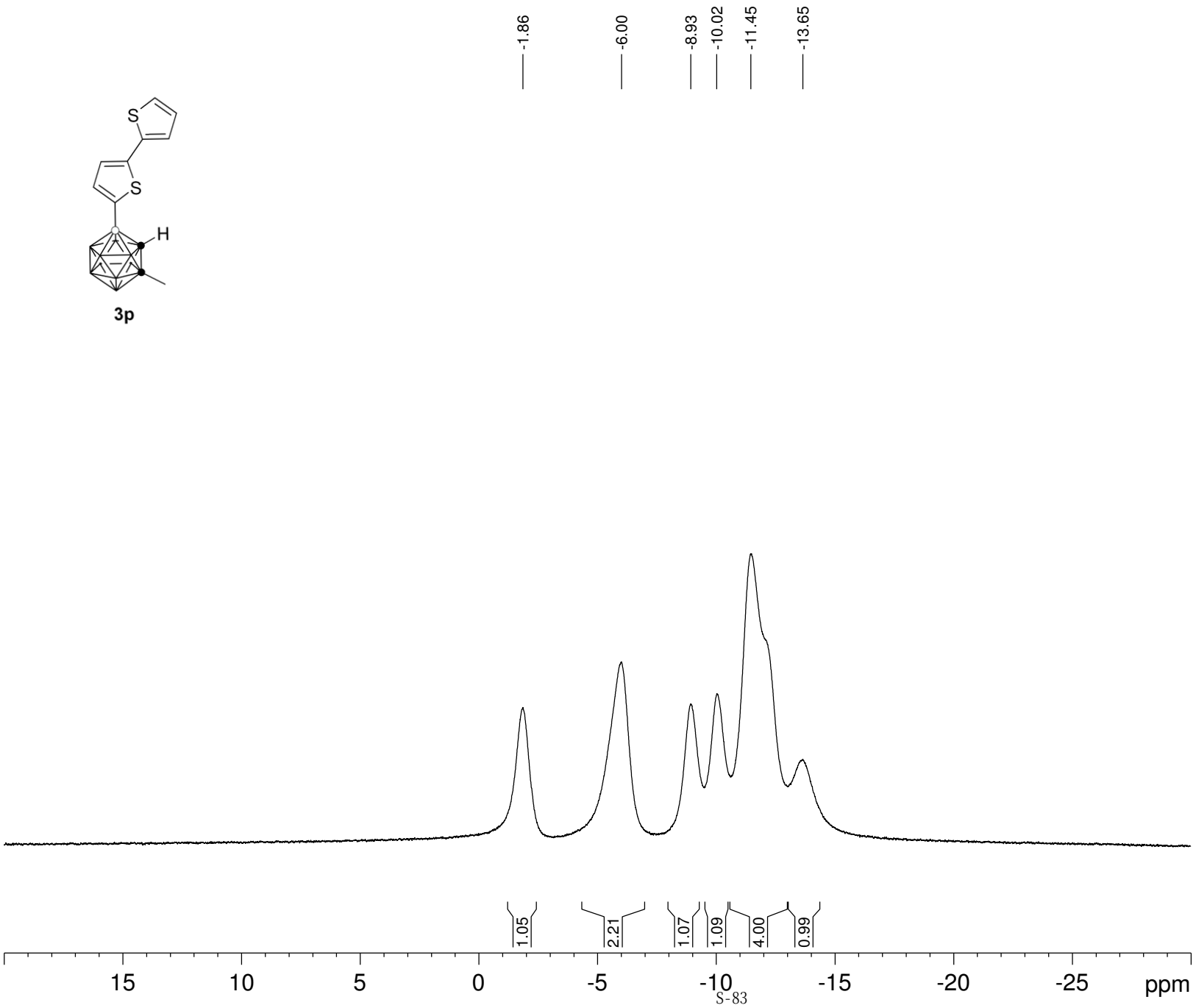
qyj-B-102-33-CDCl3(C)

```
Current Data Parameters
NAME      qyj-B-102-33-CDCl3(C)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160518
Time                  14.06 h
INSTRUM               spect
PROBHD    Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT                CDCl3
NS                        13
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                    294.5 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
```


7.260
7.216
7.213
7.204
7.201
7.175
7.173
7.166
7.164
7.135
7.127
7.121
7.113
7.022
7.013
7.010
7.000
3.780
2.089
qyj-H-102-23-CDCl3
Current Data Parameters
NAME qyj-H-102-23-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160405
Time 19.31 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
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 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 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
S
S
H
3p
impurity
in hexane
0.991
1.003
1.981
1.000
1.026
3.301
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
ppm

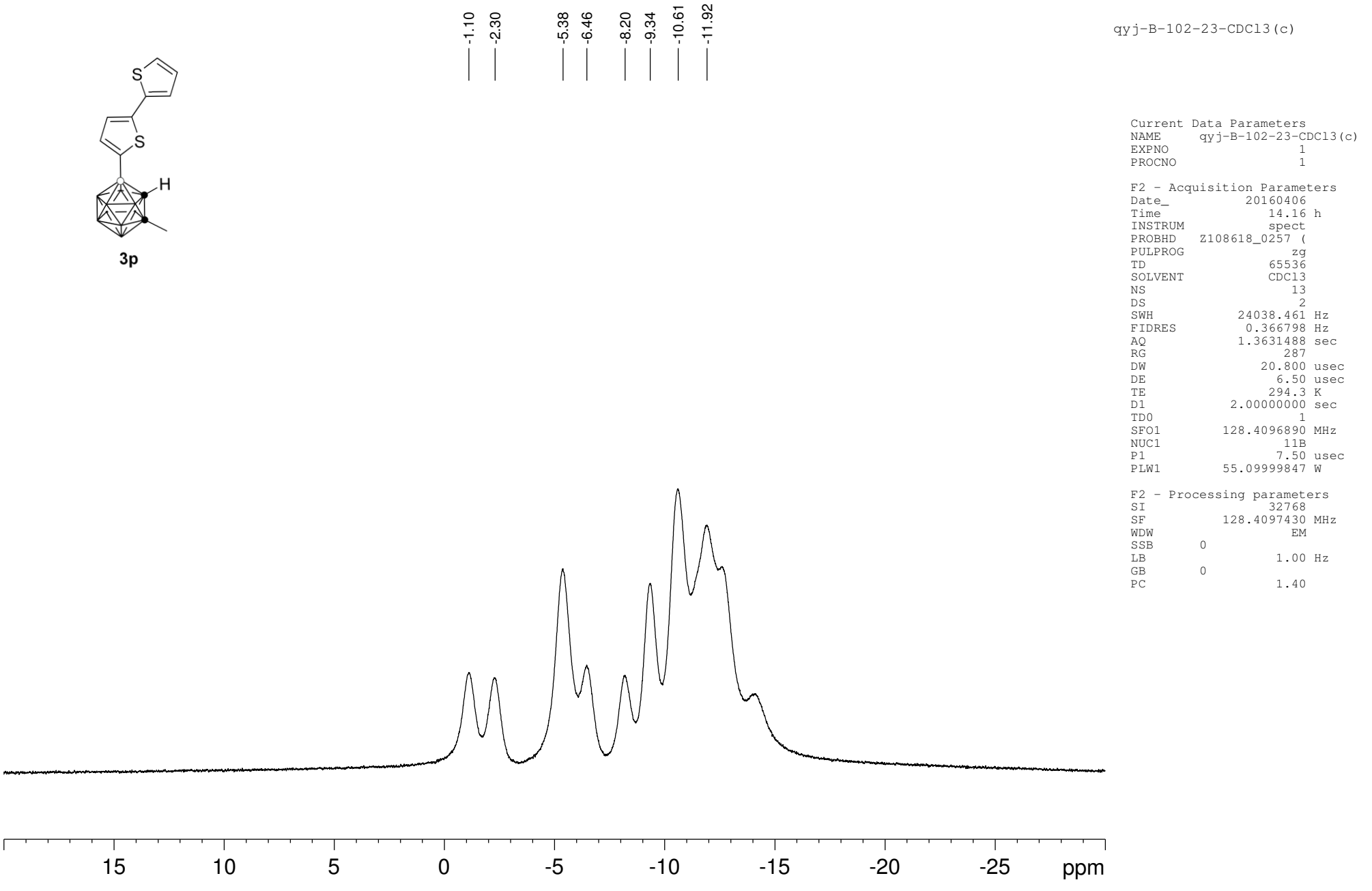

141.325
137.336
134.554
127.959
125.048
124.605
123.940
77.474
77.157
76.839
71.402
62.895
26.057
qyj-C-102-23-CDCl3
Current Data Parameters
NAME qyj-C-102-23-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160405
Time 19.35 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 631
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 295.0 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 100.6127575 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
S
S
H
3p
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

3p



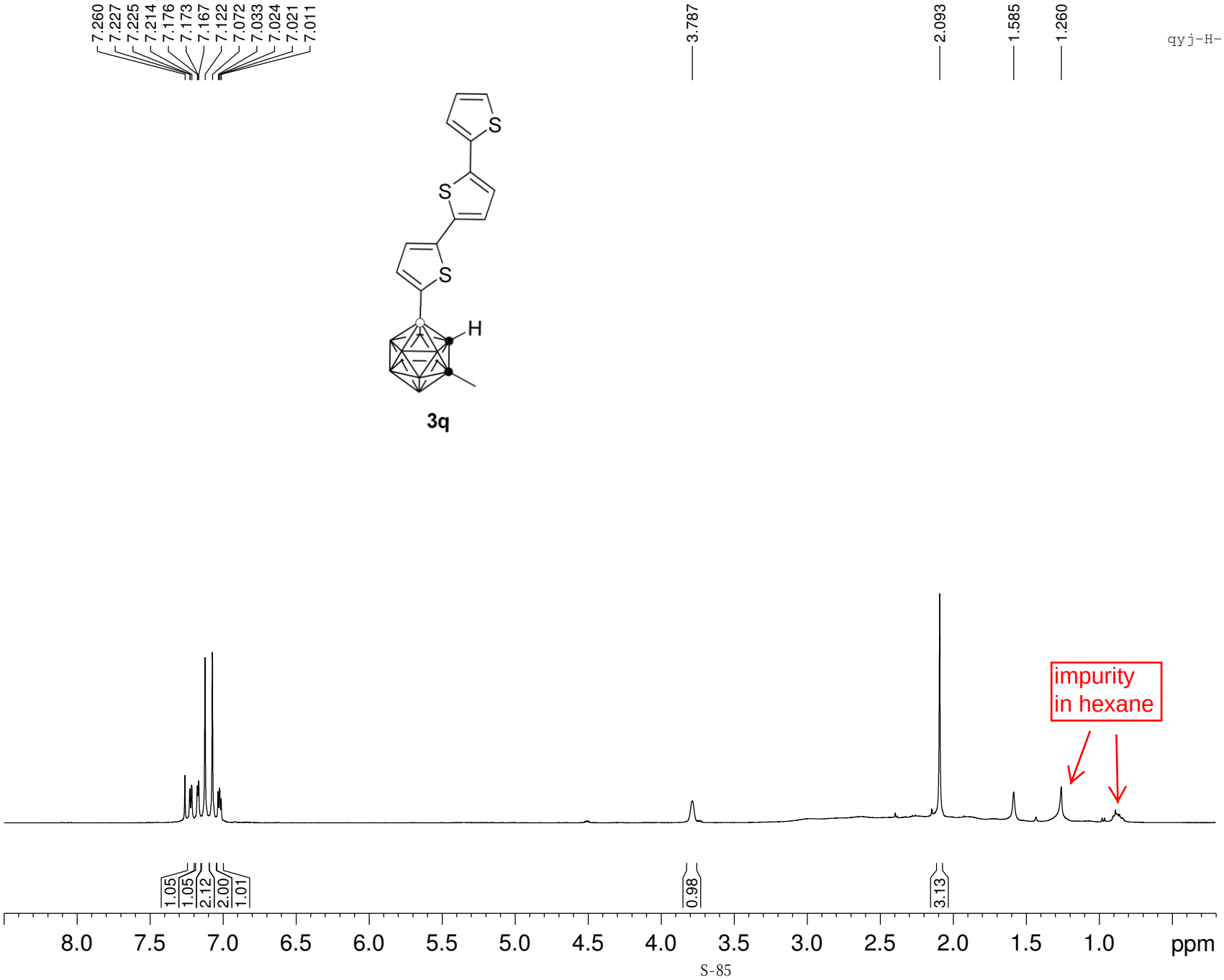
qyj-B-102-23-CDCl3

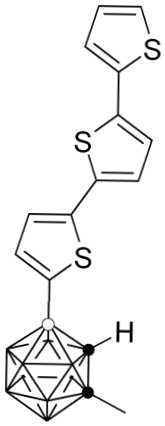
```
Current Data Parameters
NAME      qyj-B-102-23-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160406
Time              14.14 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    12
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                294.5 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
```



qyj-B-102-23-CDCl3(c)

```
Current Data Parameters
NAME      qyj-B-102-23-CDCl3(c)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160406
Time                  14.16 h
INSTRUM               spect
PROBHD    Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT                CDCl3
NS                        13
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                    294.3 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
```

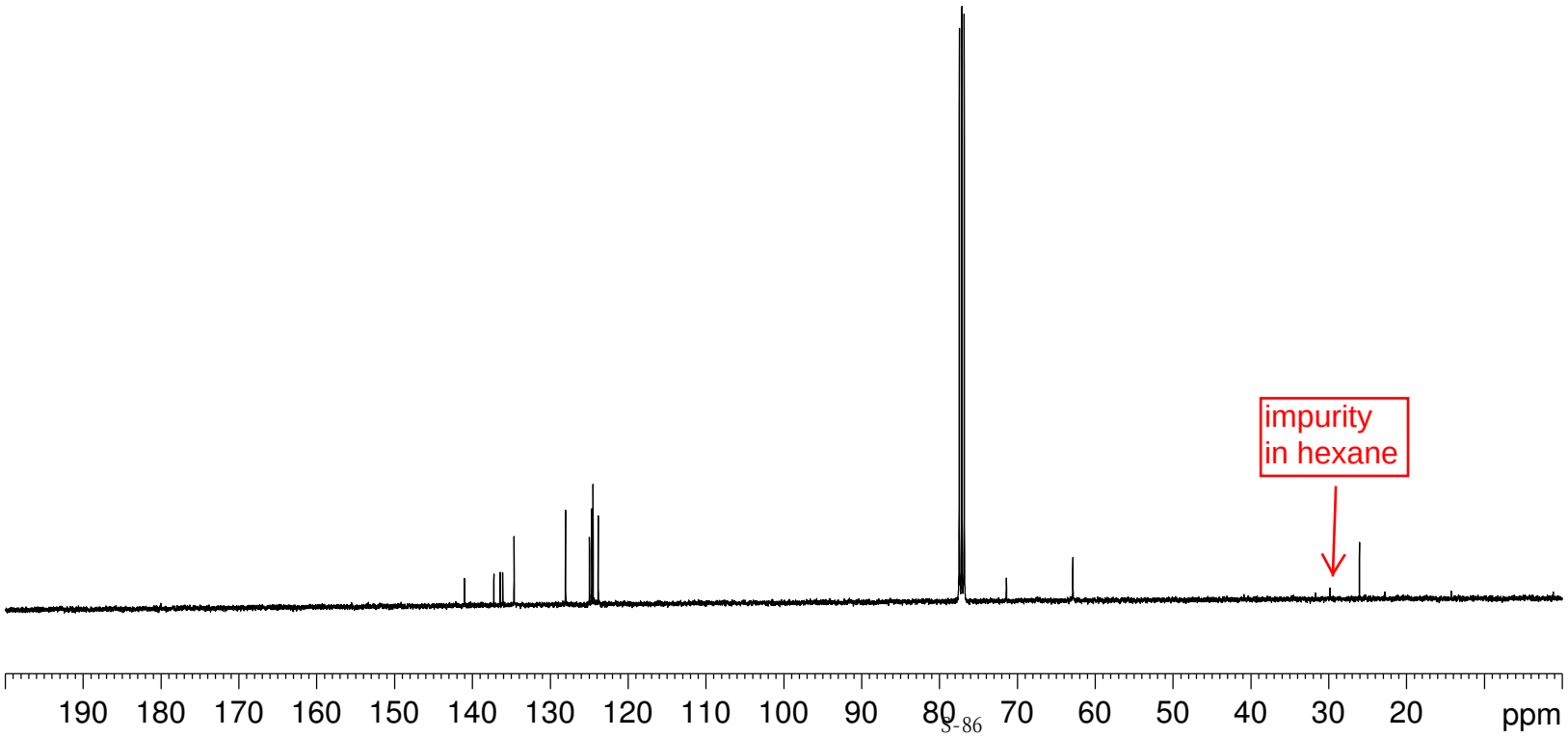

7.260
7.227
7.225
7.214
7.176
7.173
7.167
7.122
7.072
7.033
7.024
7.021
7.011
3.787
2.093
1.585
1.260
qyj-H-102-28-CDCl3
S
S
S
H
3q
Current Data Parameters
NAME qyj-H-102-28-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160504
Time 20.23 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 71.8
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 400.2300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
impurity
in hexane
1.05
1.05
2.12
2.00
1.01
0.98
3.13
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



3q

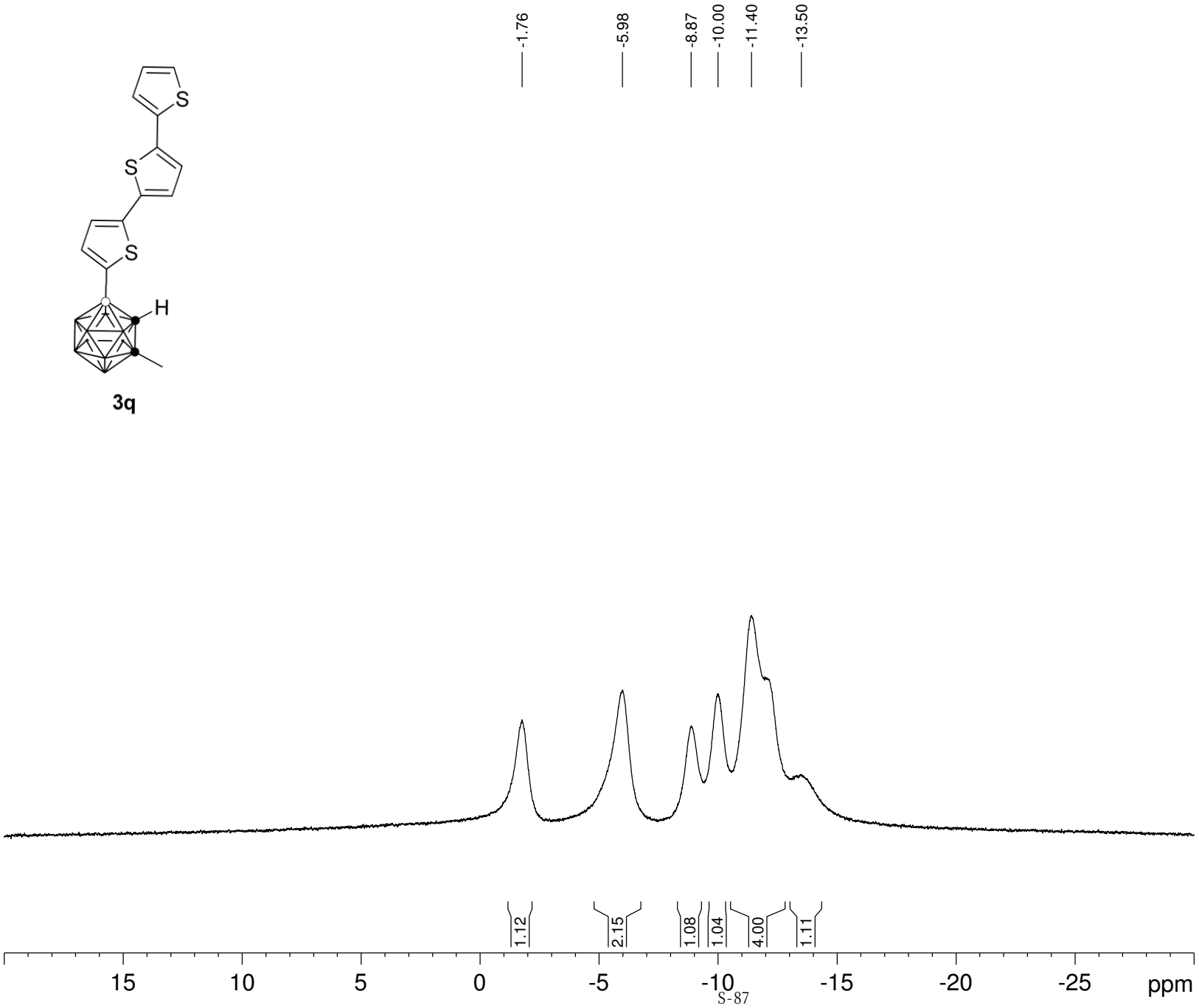
141.00
137.23
136.42
136.10
134.64
128.03
124.95
124.64
124.51
124.48
123.83
77.47
77.16
76.84
71.42
62.88
26.07

qyj-C-102-28-CDCl3




```
Current Data Parameters
NAME      qyj-C-102-28-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160504
Time              20.26 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  809
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  128
DW               16.800 usec
DE                6.50 usec
TE                294.9 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           100.6379024 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

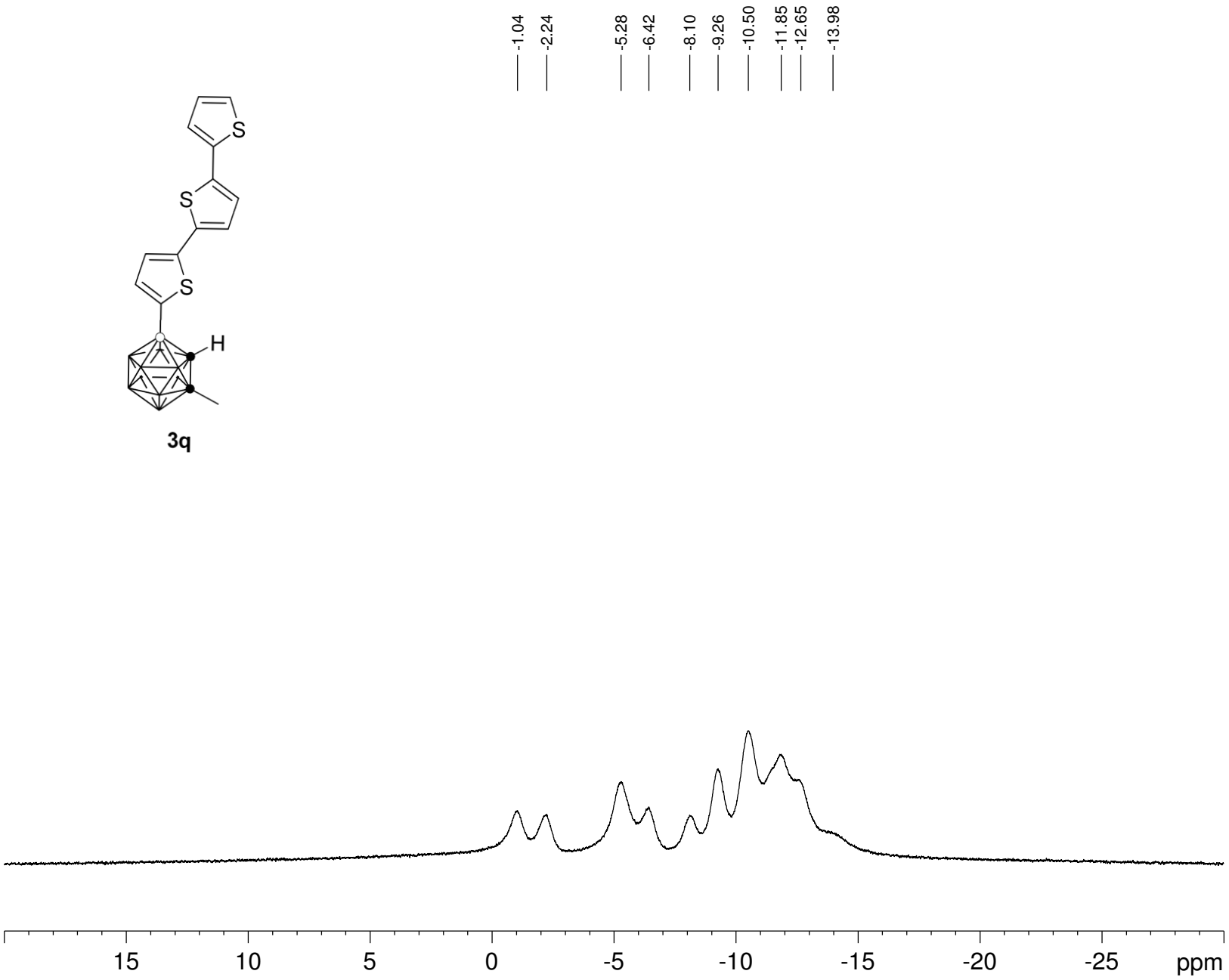
3q



qyj-B-102-28-CDCl3

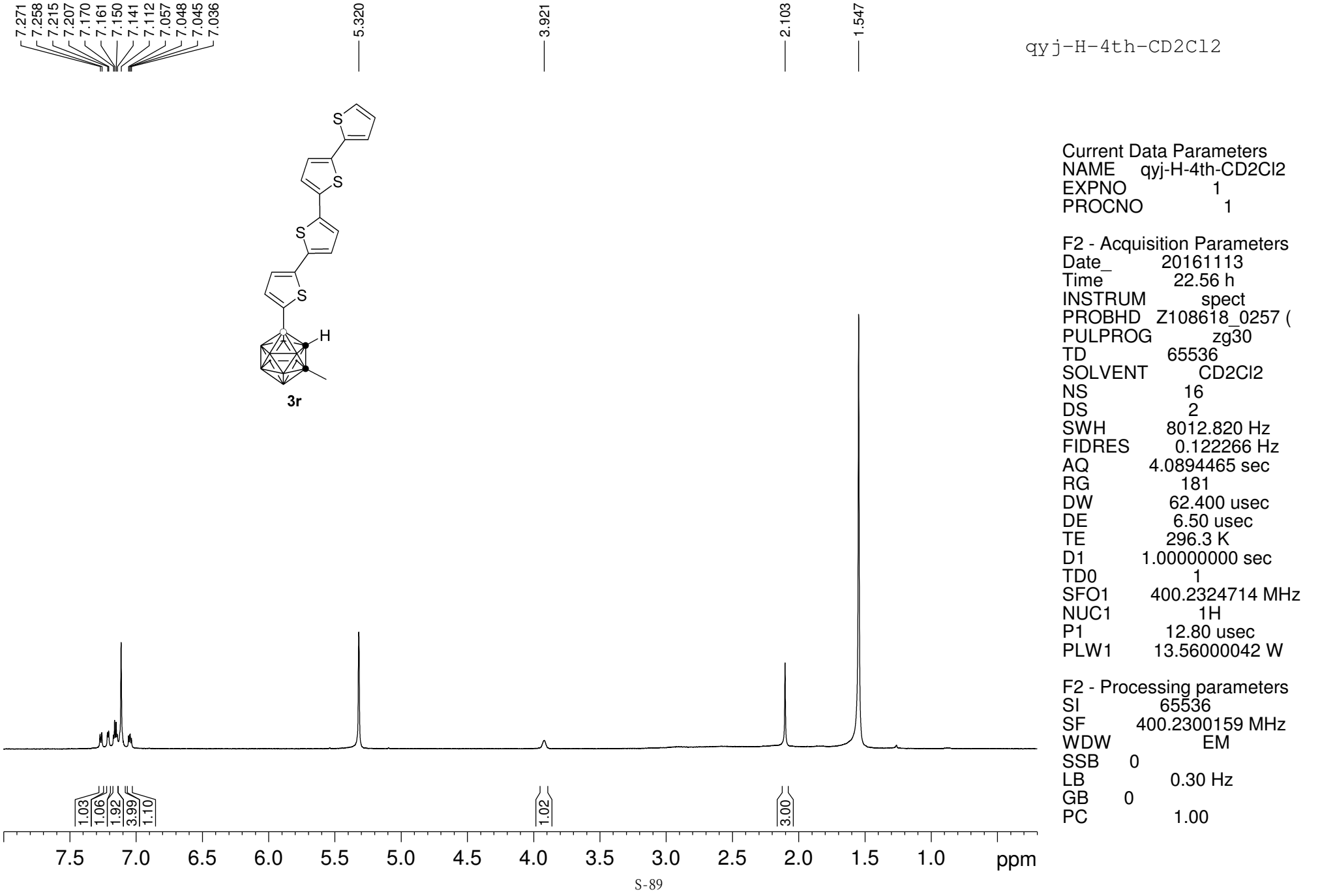
```
Current Data Parameters
NAME      qyj-B-102-28-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160504
Time                20.16 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     12
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                 295.1 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
```

3q



qyj-B-102-28-CDCl3(c)

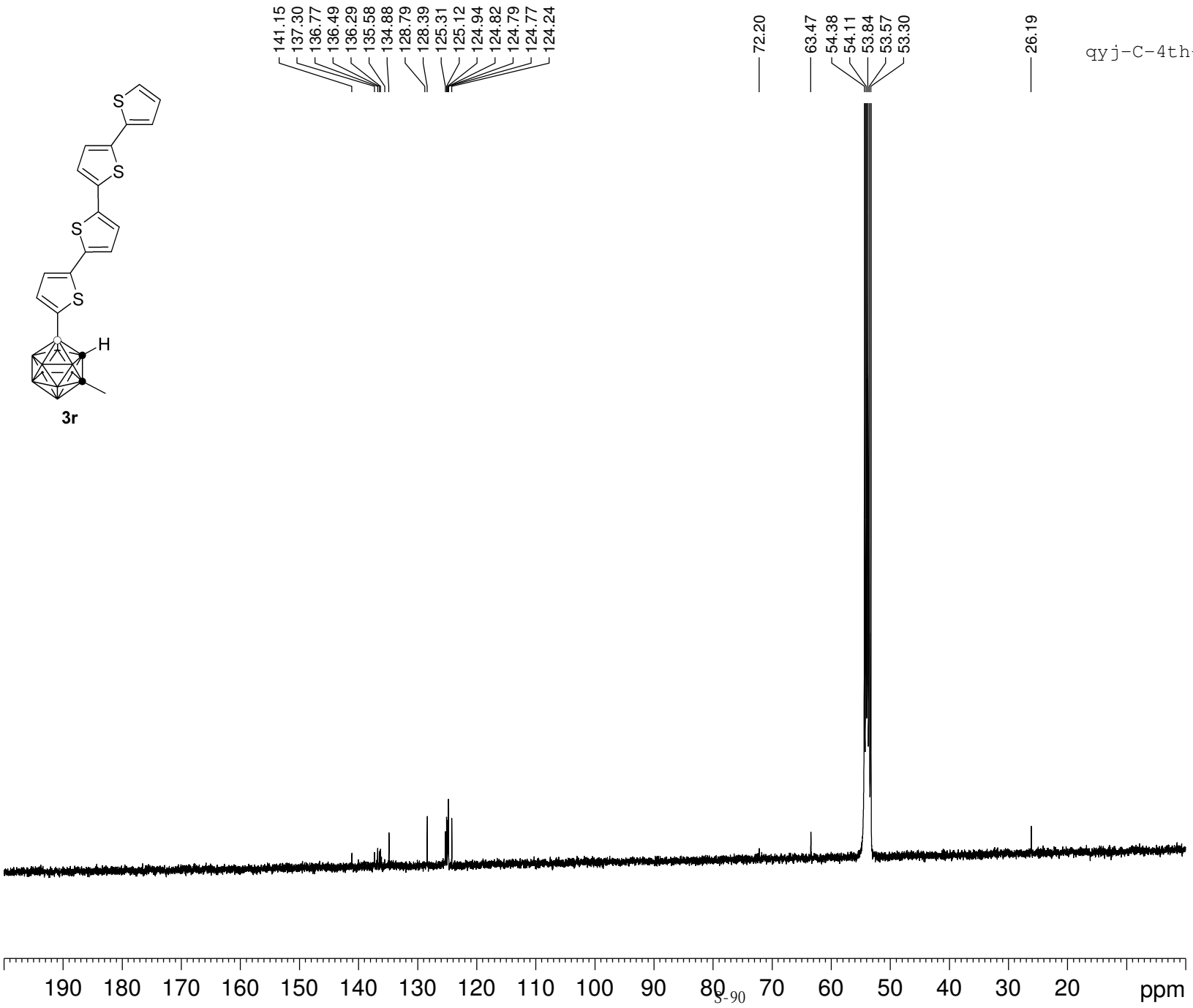
```
Current Data Parameters
NAME      qyj-B-102-28-CDCl3(c)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160504
Time                  20.18 h
INSTRUM               spect
PROBHD    Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT                CDCl3
NS                         9
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 qyj-H-4th-CD2Cl2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161113
Time 22.56 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 181
DW 62.400 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

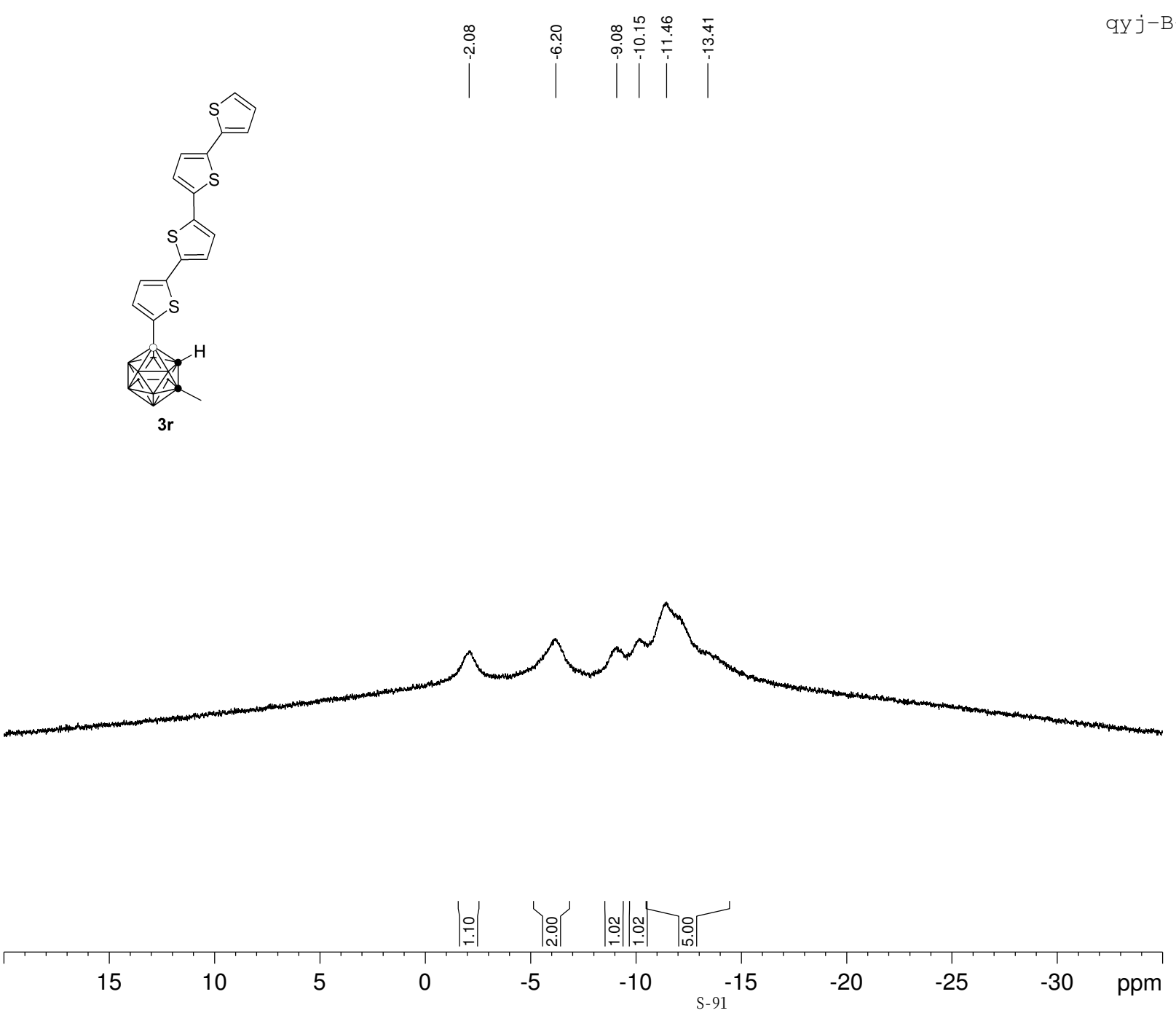
F2 - Processing parameters
SI 65536
SF 400.2300159 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

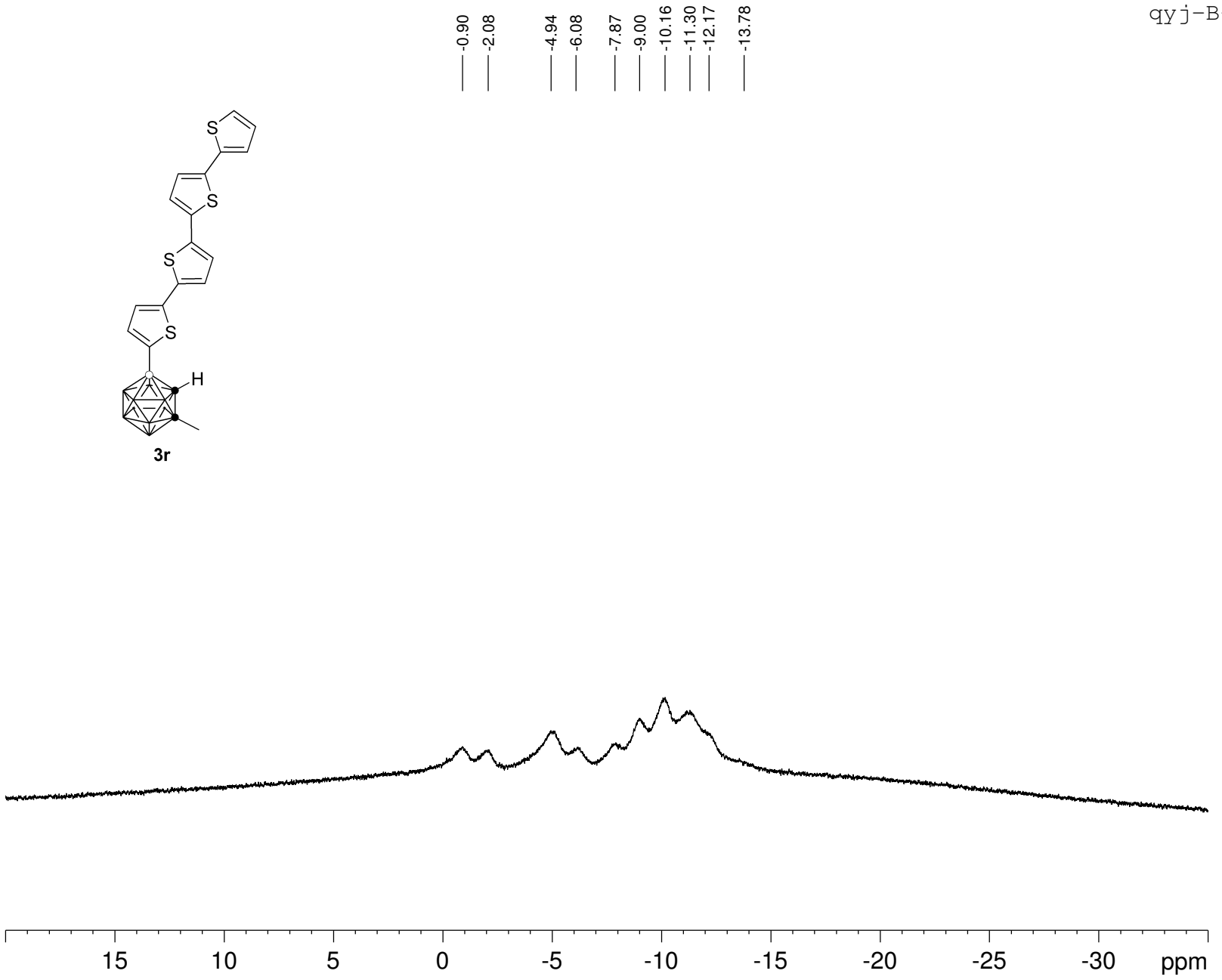


Current Data Parameters
NAME qyj-C-4th-CD2Cl2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161113
Time 23.02 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 13151
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.7 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 100.6378728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


qyj-B-4th-CD2Cl2
-2.08
-6.20
-9.08
-10.15
-11.46
-13.41
S
S
S
S
H
3r
Current Data Parameters
NAME qyj-B-4th-CD2Cl2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161107
Time 14.49 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 200
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 296.6 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
1.10
2.00
1.02
1.02
5.00
15
10
5
0
-5
-10
-15
-20
-25
-30
ppm

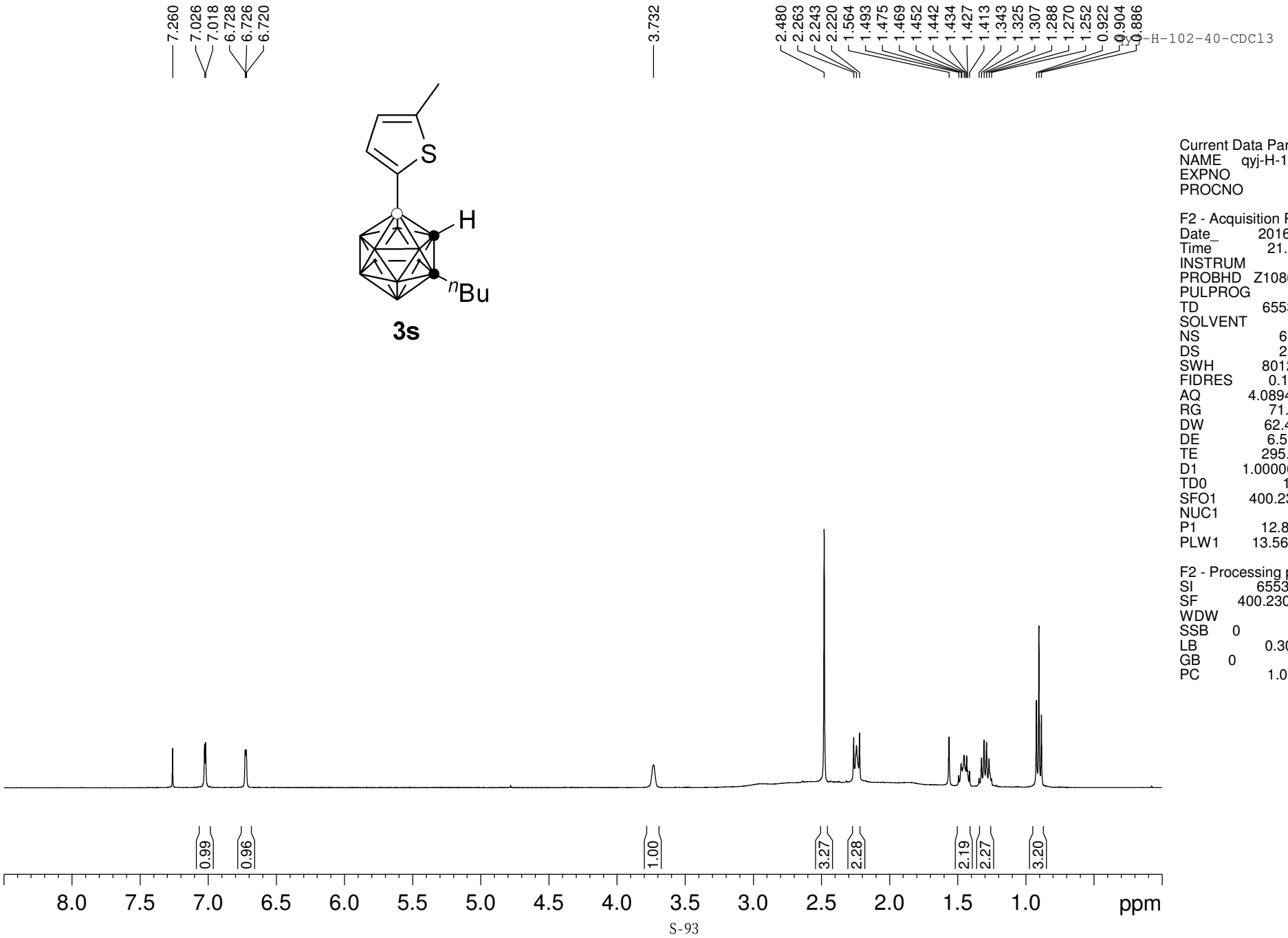


qyj-B-4th-CD2Cl2(C)

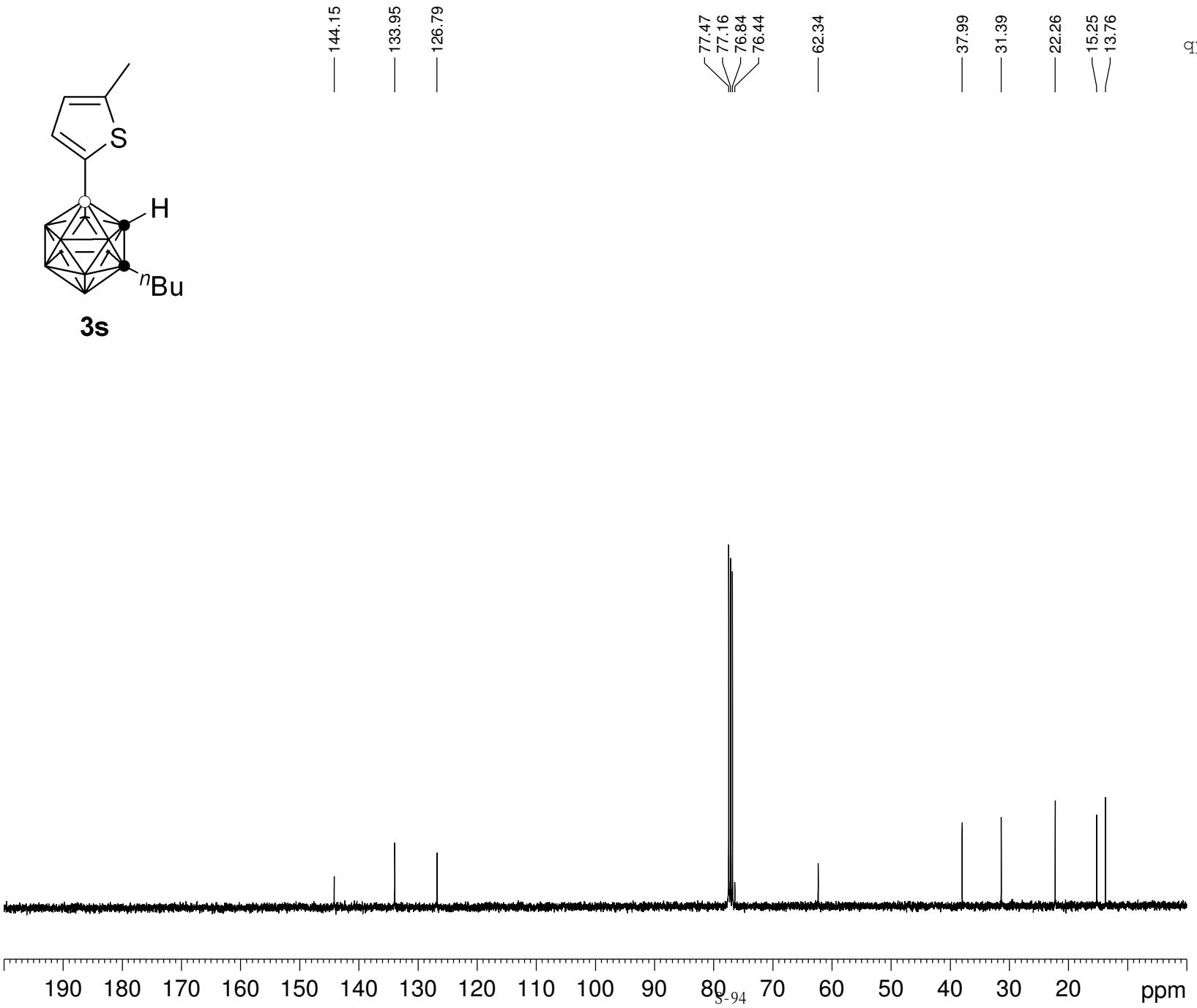
Current Data Parameters
NAME qyj-B-4th-CD2Cl2(C)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161116
Time 16.18 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 100
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 295.9 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 128.4097504 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


7.260
7.026
7.018
6.728
6.726
6.720
3.732
2.480
2.263
2.243
2.220
1.564
1.493
1.475
1.469
1.452
1.442
1.434
1.427
1.413
1.343
1.325
1.307
1.288
1.270
1.252
0.922
0.904
0.886
qyj-H-102-40-CDCl3
S
H
nBu
3s
Current Data Parameters
NAME qyj-H-102-40-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160529
Time 21.52 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
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 295.1 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
0.99
0.96
1.00
3.27
2.28
2.19
2.27
3.20
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

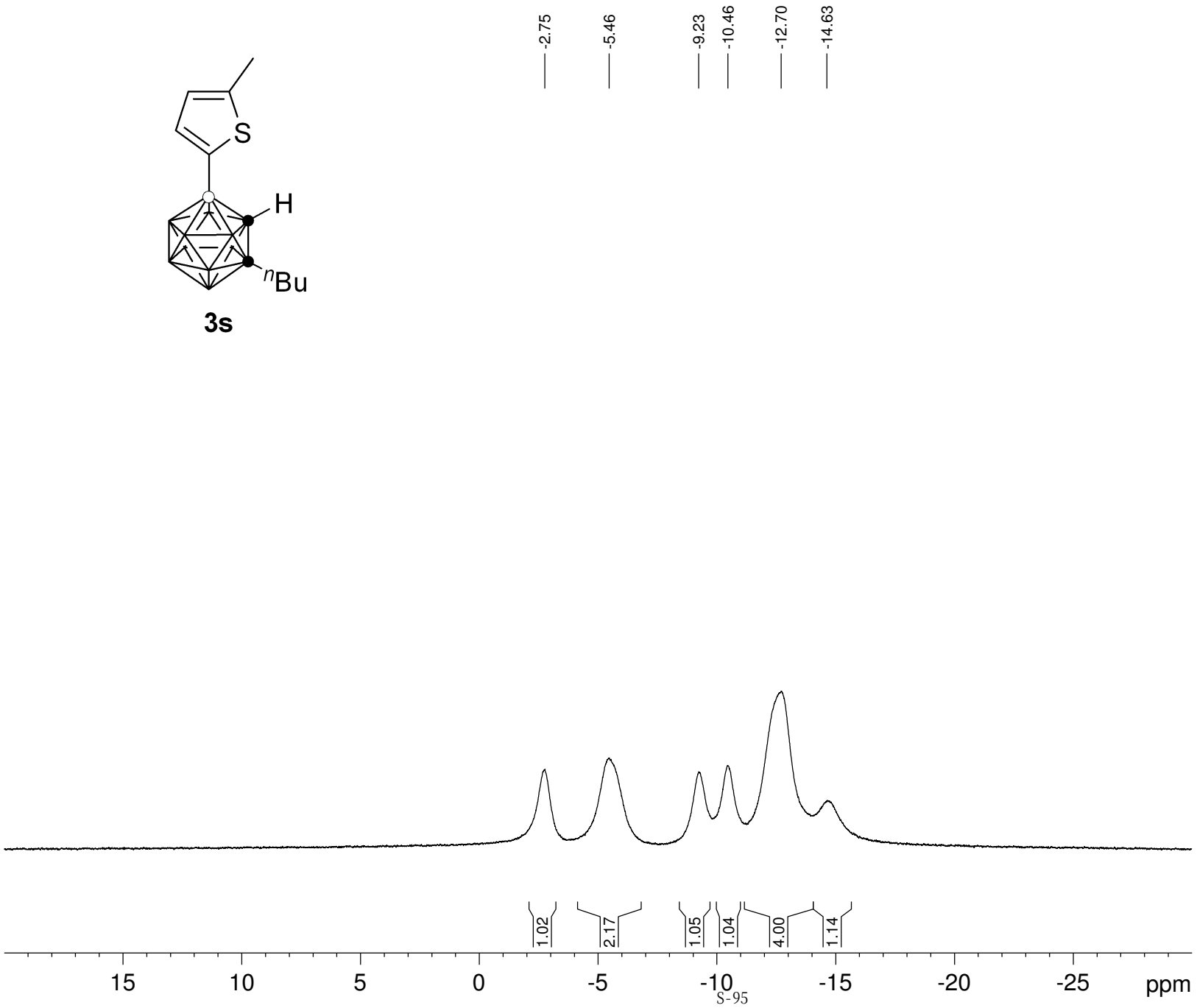
3s



qyj-C-102-40-CDCl3

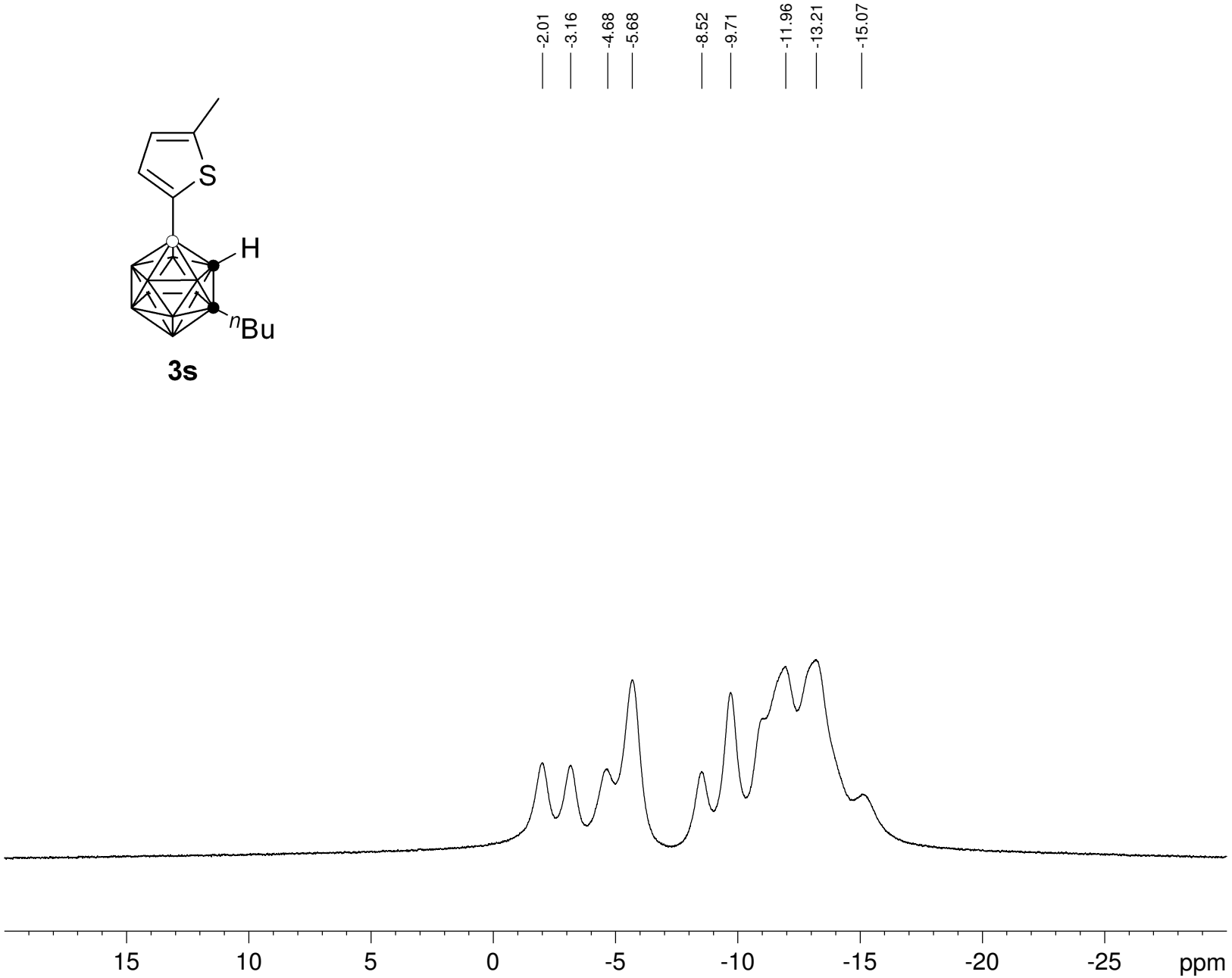
```
Current Data Parameters
NAME      qyj-C-102-40-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160529
Time              21.55 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   120
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                   114
DW                16.800 usec
DE                 6.50 usec
TE                295.4 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           100.6379020 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

3s



qyj-B-102-40-CDCl3

```
Current Data Parameters
NAME      qyj-B-102-40-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20160529
Time                22.02 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                      6
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
```



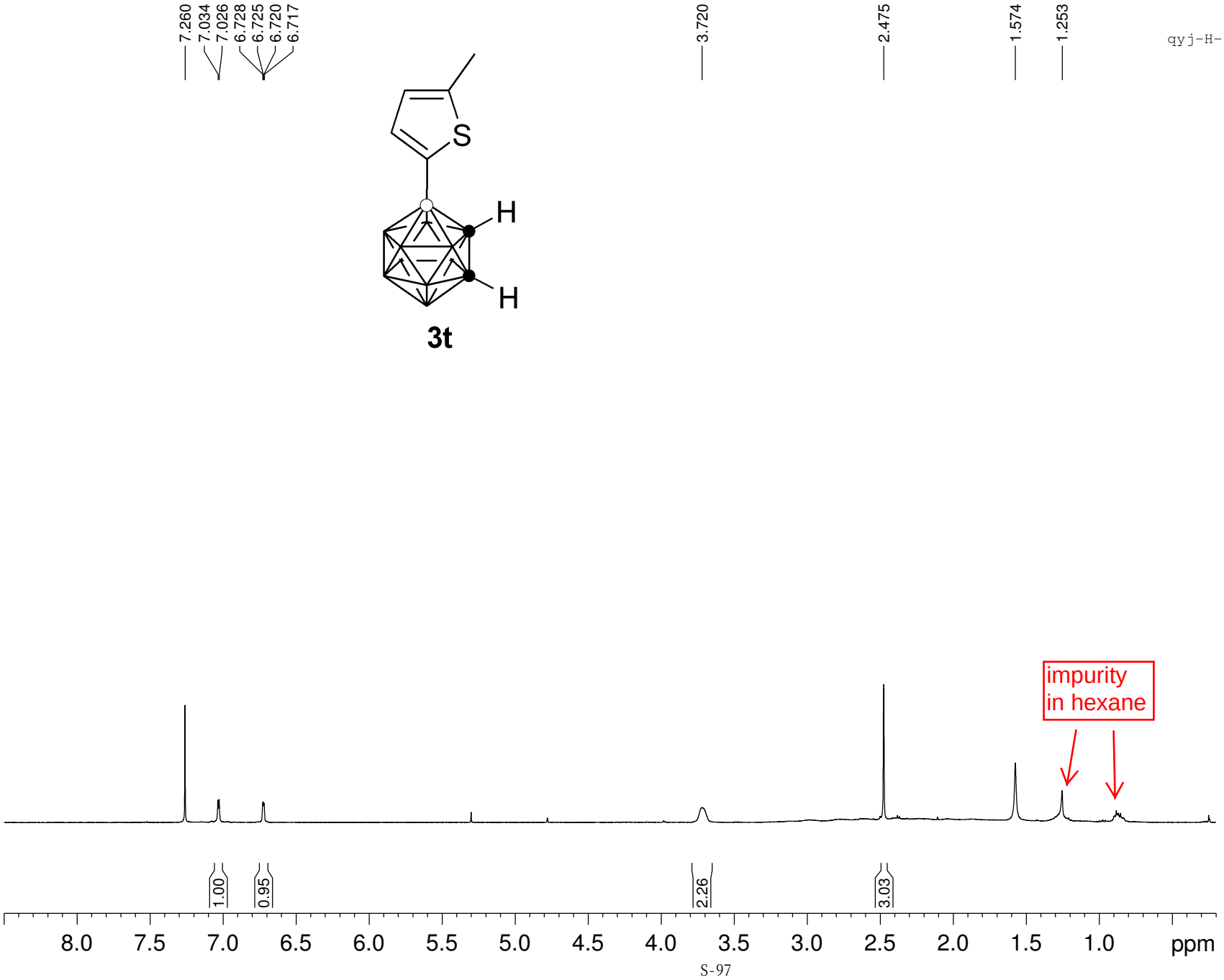
3s

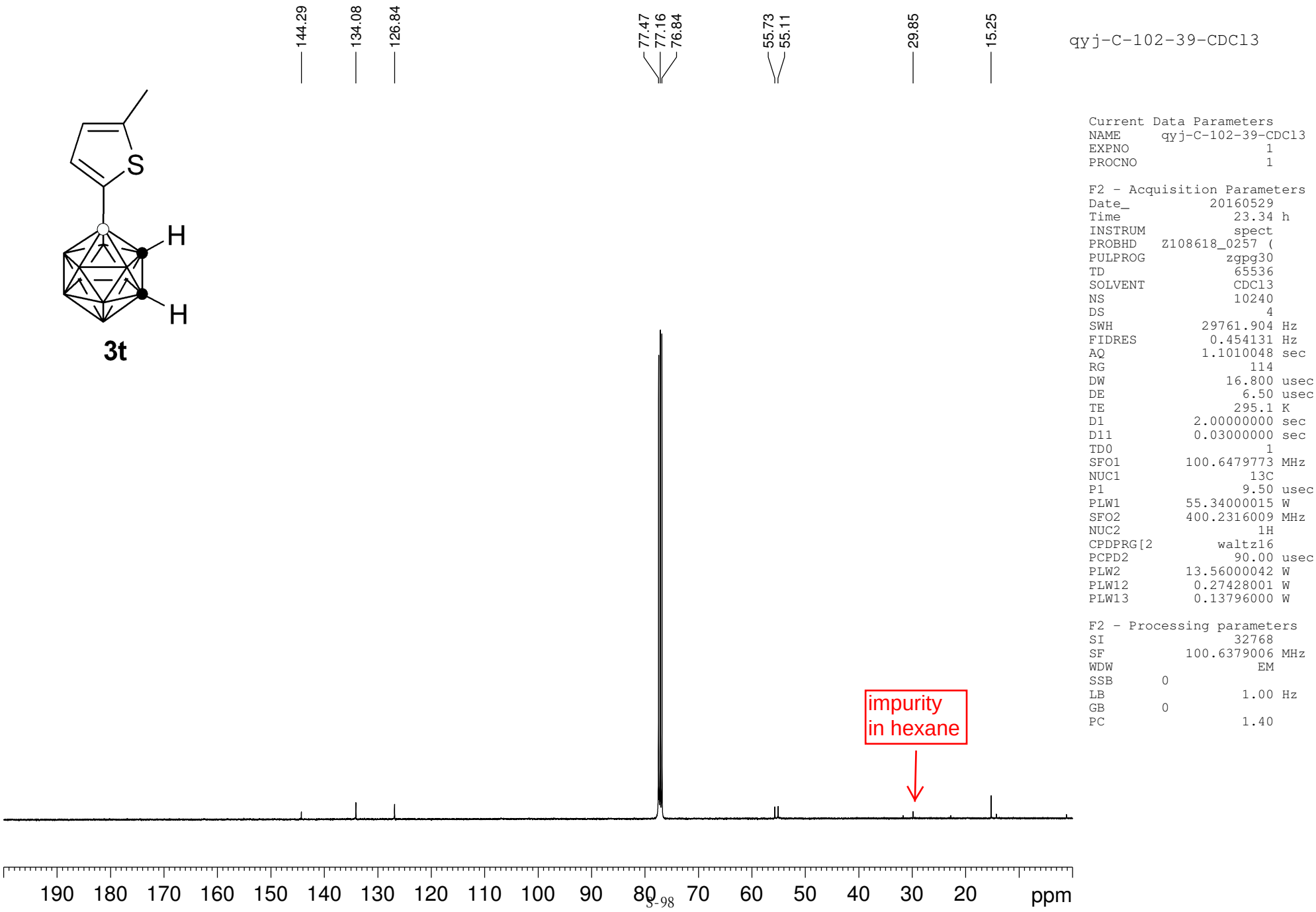
qyj-B-102-40-CDCl3(c)

Current Data Parameters
NAME qyj-B-102-40-CDCl3(c)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160529
Time 22.04 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 25
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

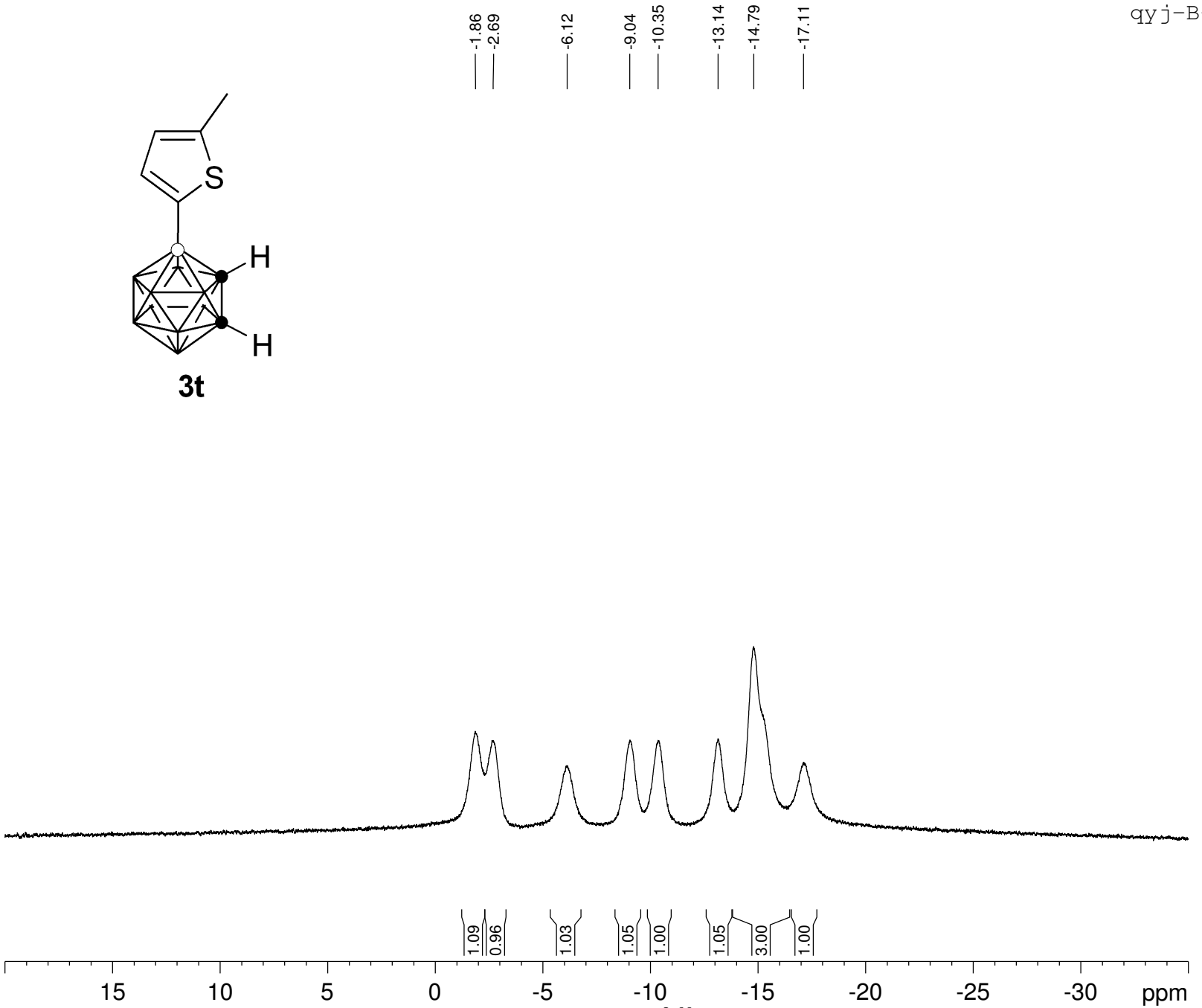
F2 - Processing parameters
SI 32768
SF 128.4097430 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


7.260
7.034
7.026
6.728
6.725
6.720
6.717
3.720
2.475
1.574
1.253
qyj-H-102-39-CDCl3
S
H
H
3t
Current Data Parameters
NAME qyj-H-102-39-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160527
Time 16.26 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
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 294.9 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 400.2300107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
impurity
in hexane
1.00
0.95
2.26
3.03
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



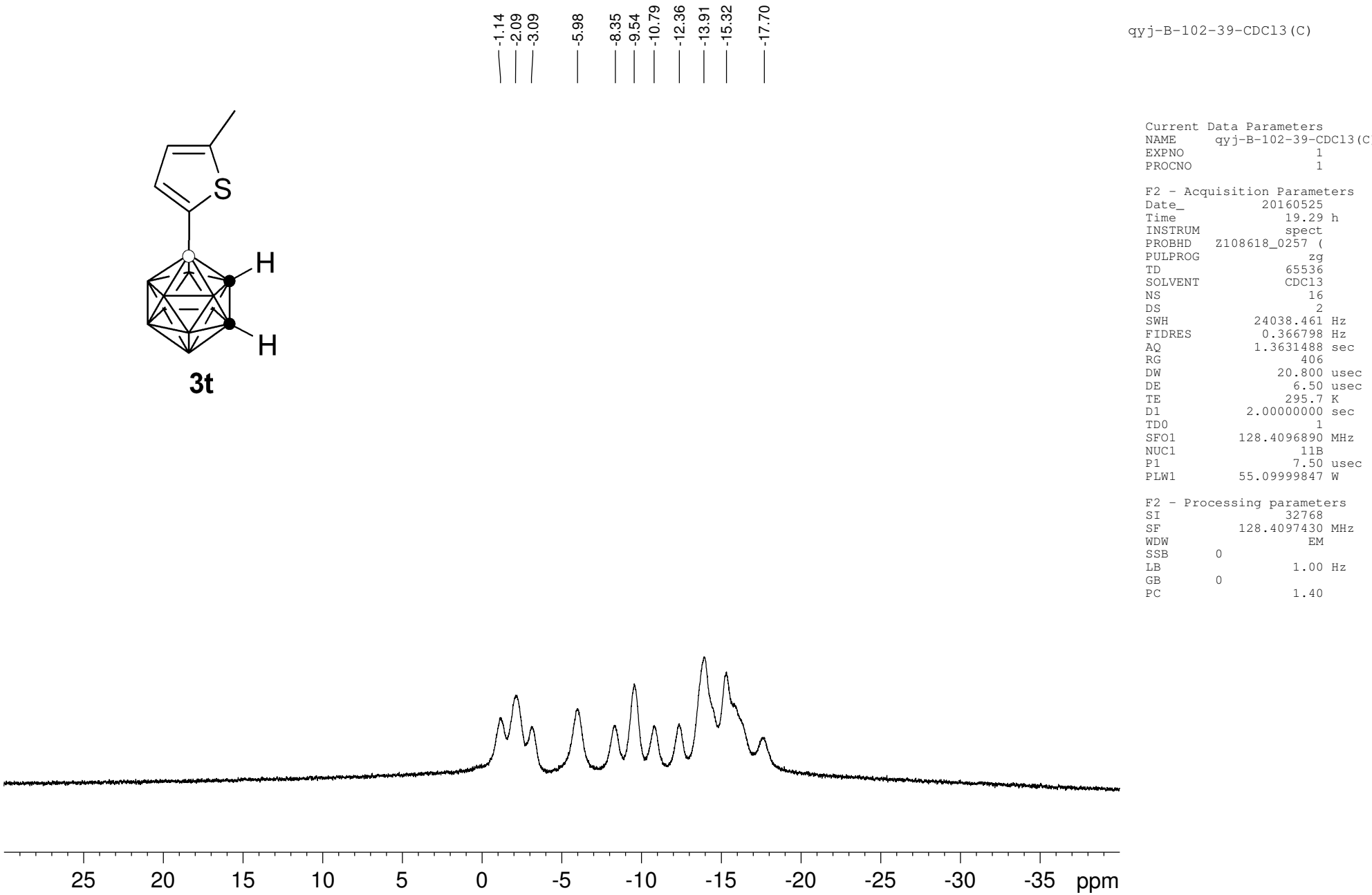

```
Current Data Parameters
NAME      qyj-C-102-39-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160529
Time              23.34 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                10240
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  114
DW               16.800 usec
DE                6.50 usec
TE                295.1 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           100.6379006 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

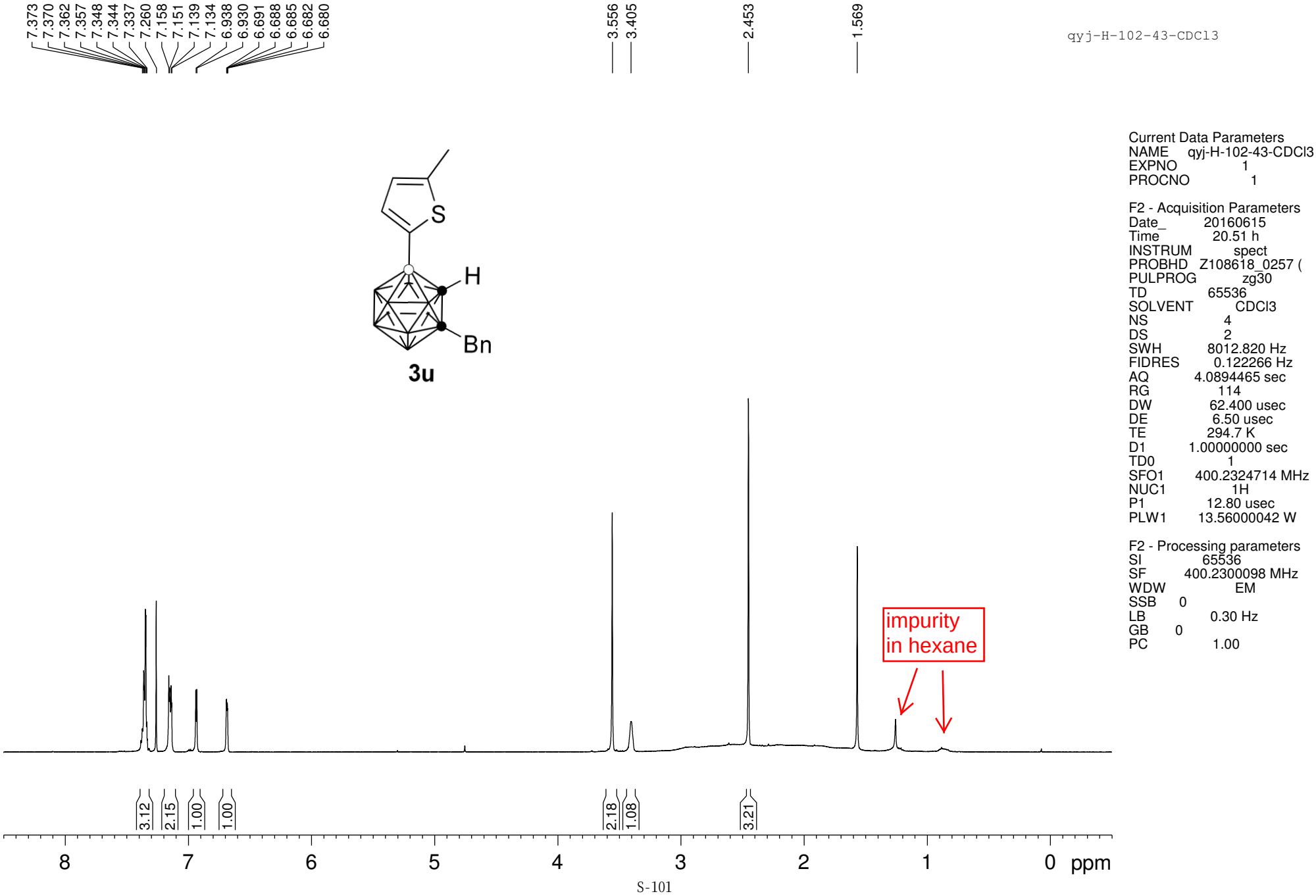
3t



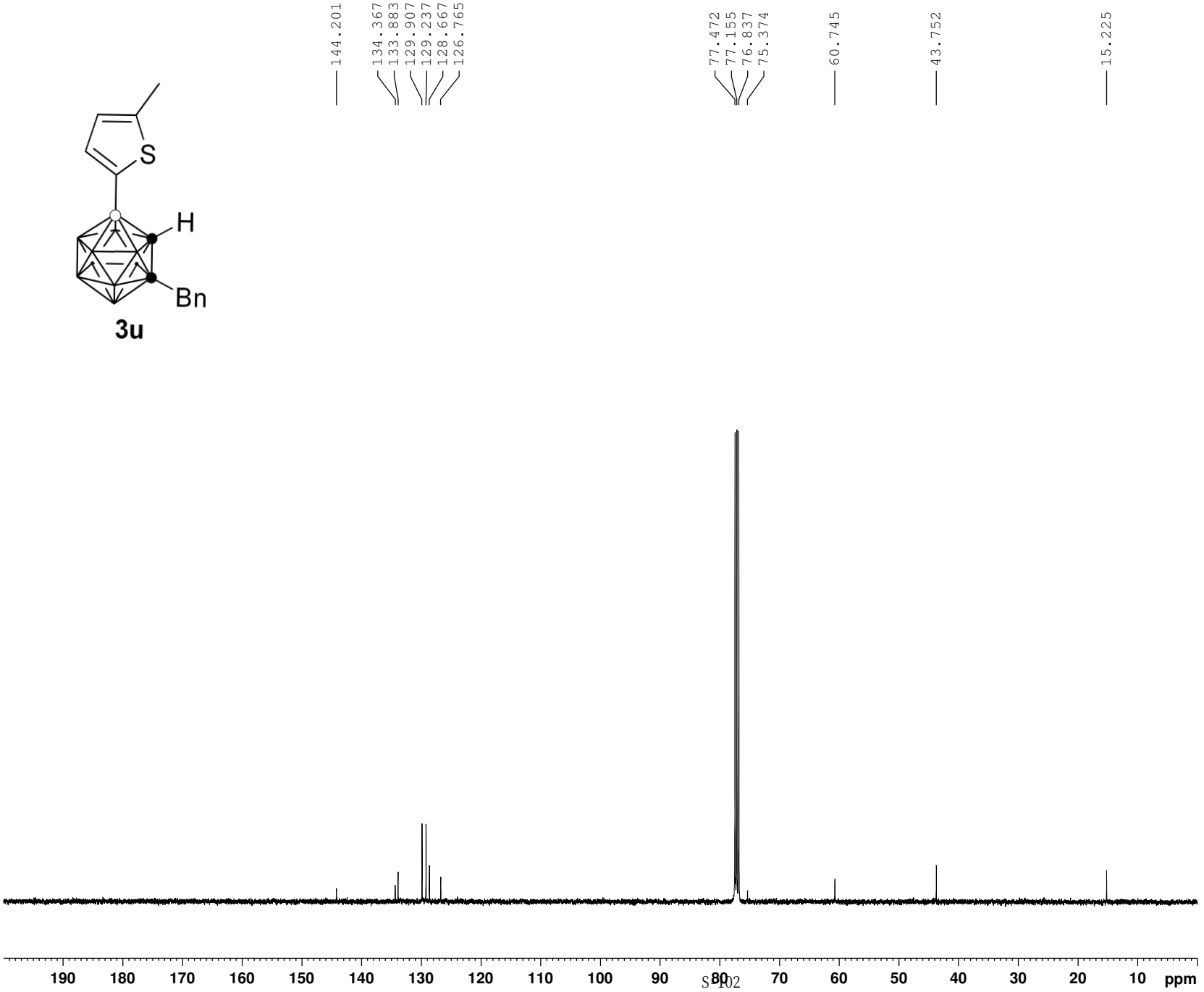
qyj-B-102-39-CDCl3

```
Current Data Parameters
NAME      qyj-B-102-39-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160525
Time              19.27 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG            zgdc
TD                65536
SOLVENT           CDCl3
NS                   16
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                295.7 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           128.4097615 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


-1.14
-2.09
-3.09
-5.98
-8.35
-9.54
-10.79
-12.36
-13.91
-15.32
-17.70
qyj-B-102-39-CDCl3(C)
S
H
H
3t
Current Data Parameters
NAME qyj-B-102-39-CDCl3(C)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160525
Time 19.29 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 16
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 295.7 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
25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 ppm


7.373
7.370
7.362
7.357
7.348
7.344
7.337
7.260
7.158
7.151
7.139
7.134
6.938
6.930
6.691
6.688
6.685
6.682
6.680
3.556
3.405
2.453
1.569
qyj-H-102-43-CDCl3
S
H
Bn
3u
Current Data Parameters
NAME qyj-H-102-43-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160615
Time 20.51 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
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 294.7 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
impurity
in hexane
3.12
2.15
1.00
1.00
2.18
1.08
3.21
8
7
6
5
4
3
2
1
0
ppm

3u

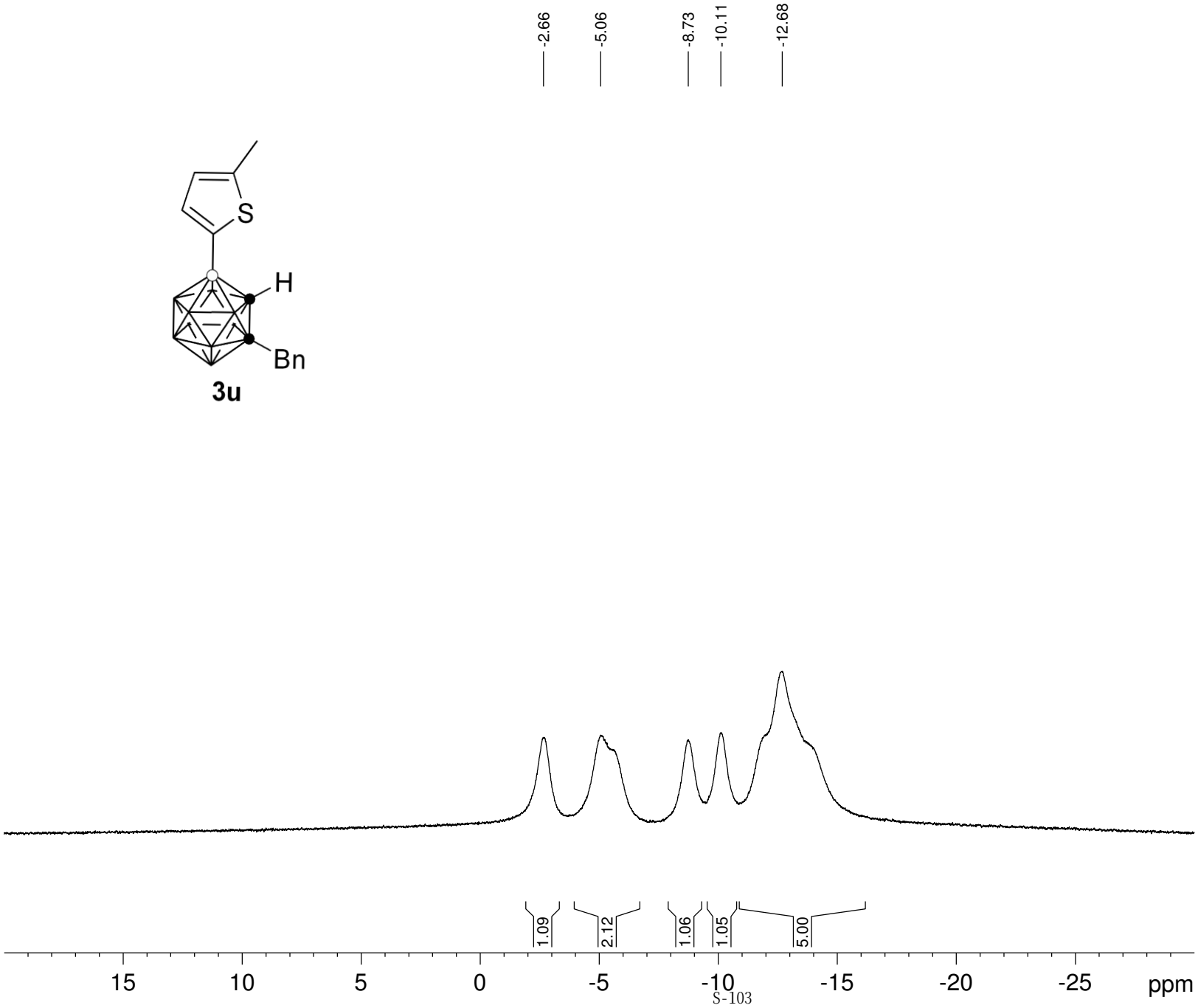


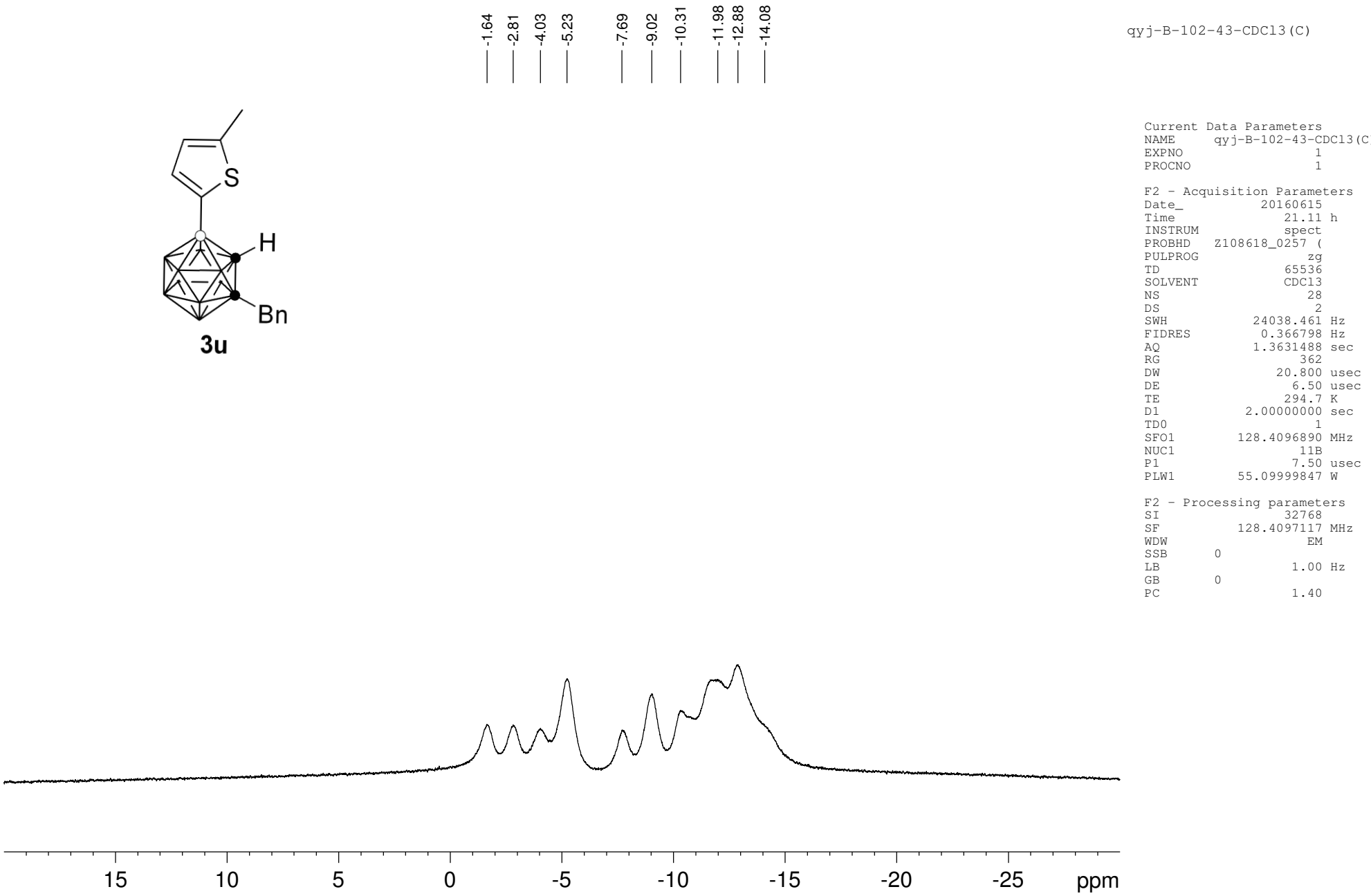
qyj-C-102-43-CDCl3

Current Data Parameters
NAME qyj-C-102-43-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160616
Time 17.48 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 921
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 295.2 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 100.6127564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


-2.66
-5.06
-8.73
-10.11
-12.68
S
H
Bn
3u
qyj-B-102-43-CDCl3
Current Data Parameters
NAME qyj-B-102-43-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160615
Time 21.08 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 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
1.09
2.12
1.06
1.05
5.00
15
10
5
0
-5
-10
-15
-20
-25
ppm

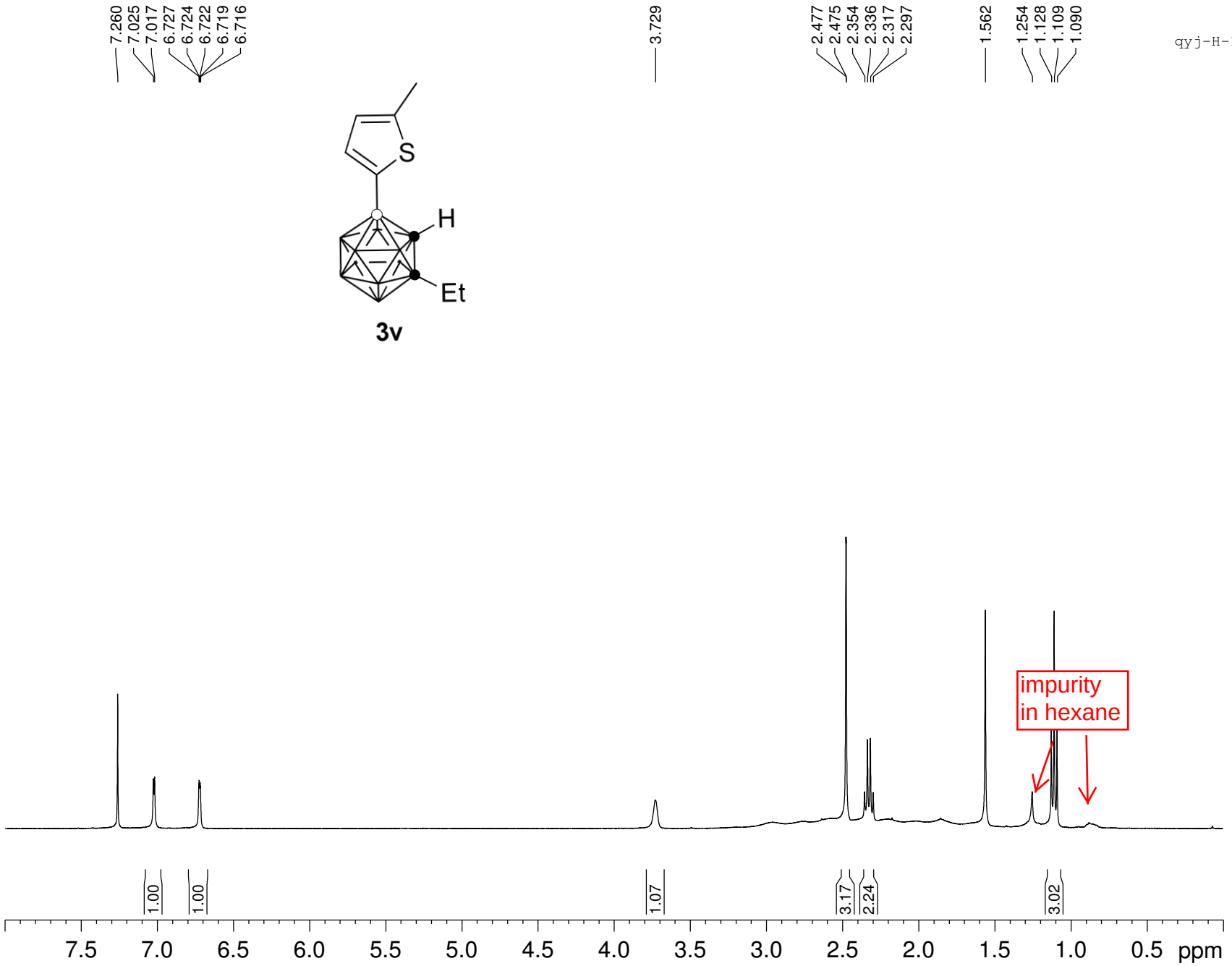


qyj-B-102-43-CDCl3(C)

Current Data Parameters
NAME qyj-B-102-43-CDCl3(C)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160615
Time 21.11 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 28
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 294.7 K
D1 2.00000000 sec
TD0 1
SFO1 128.4096890 MHz
NUC1 11B
P1 7.50 usec
PLW1 55.09999847 W

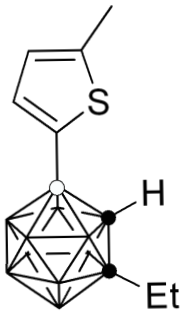
F2 - Processing parameters
SI 32768
SF 128.4097117 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME qyj-H-102-48-CDCl
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160623
Time 20.37 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 128
DW 62.400 usec
DE 6.50 usec
TE 294.4 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



3v

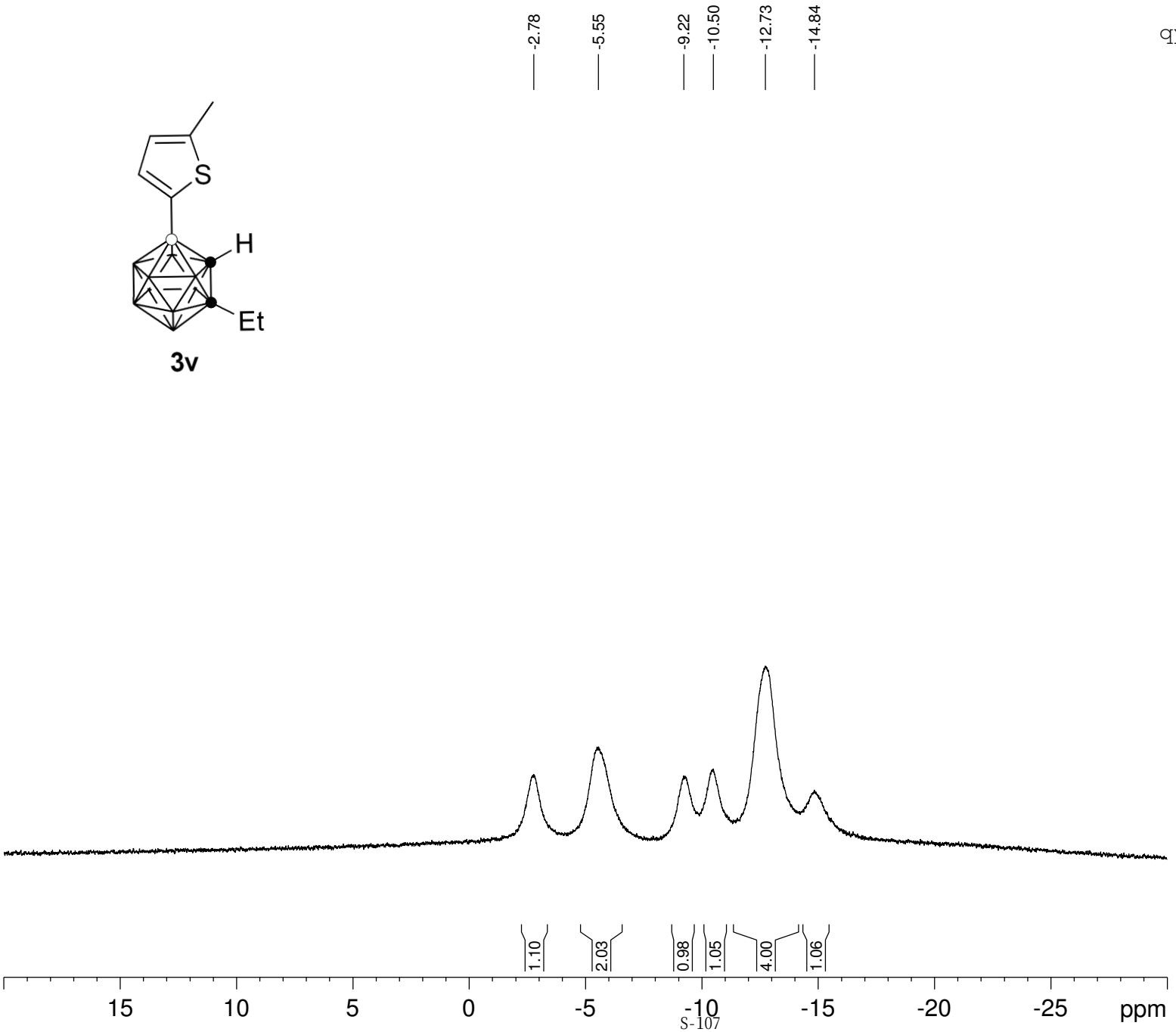
144.180
133.973
126.806
77.475
77.157
76.840
62.190
31.784
15.248
13.659

qyj-C-102-48-CDCl3

```
Current Data Parameters
NAME      qyj-C-102-48-CDCl3
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20160624
Time                9.03 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2298
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               295.5 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           100.6127557 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

impurity
in hexane

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

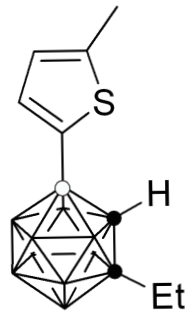


qyj-B-102-48-CDCl3

Current Data Parameters
NAME qyj-B-102-48-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160623
Time 20.31 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 16
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 295.0 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

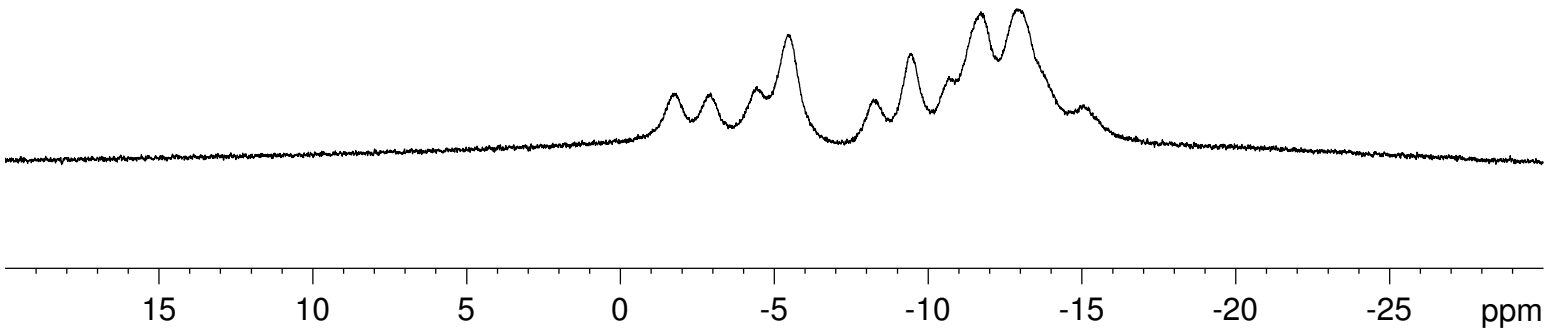


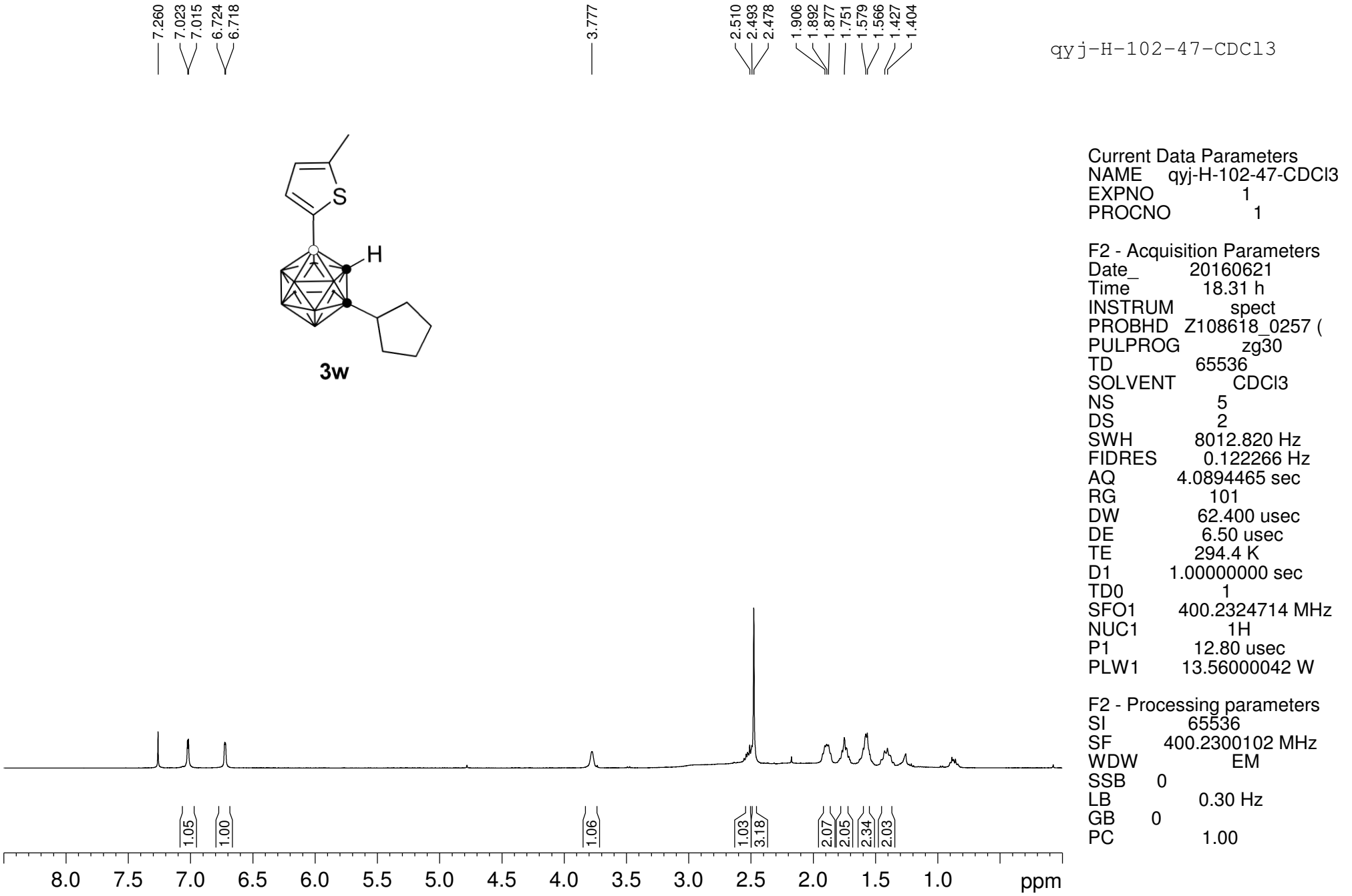
3v

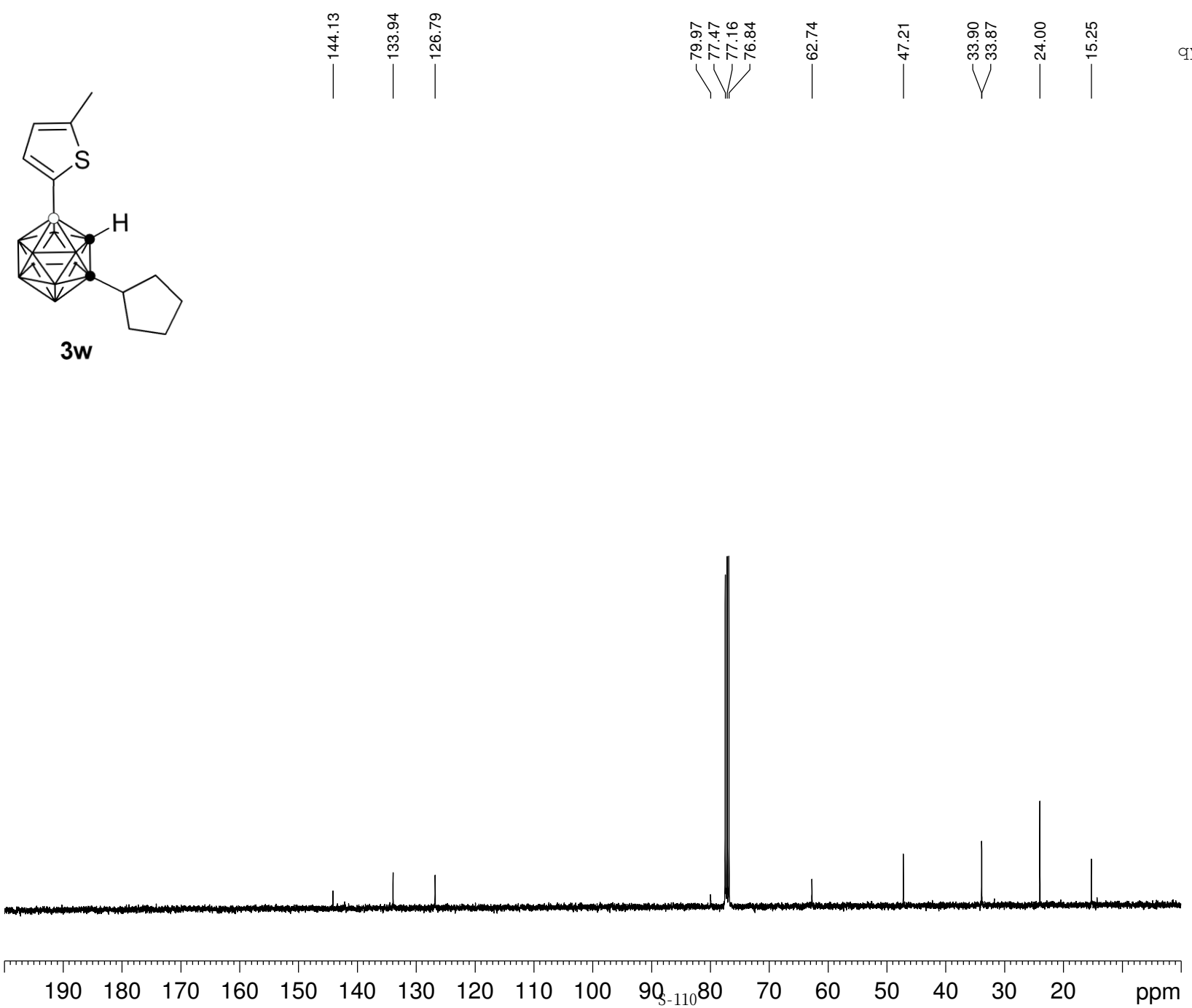
-1.75 -2.93 -4.44 -5.47 -8.22 -9.46 -10.64 -11.72 -12.89 -14.98

qyj-B-102-48-CDCl3(C)

```
Current Data Parameters
NAME      qyj-B-102-48-CDCl3(C)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160623
Time                  20.33 h
INSTRUM               spect
PROBHD   Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT                CDCl3
NS                        21
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                    294.5 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             128.4097117 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```




7.260
7.023
7.015
6.724
6.718
3.777
2.510
2.493
2.478
1.906
1.892
1.877
1.751
1.579
1.566
1.427
1.404
qyj-H-102-47-CDCl3
S
H
3w
Current Data Parameters
NAME qyj-H-102-47-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160621
Time 18.31 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 101
DW 62.400 usec
DE 6.50 usec
TE 294.4 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 400.2300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.05
1.00
1.06
1.03
3.18
2.07
2.05
2.34
2.03
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



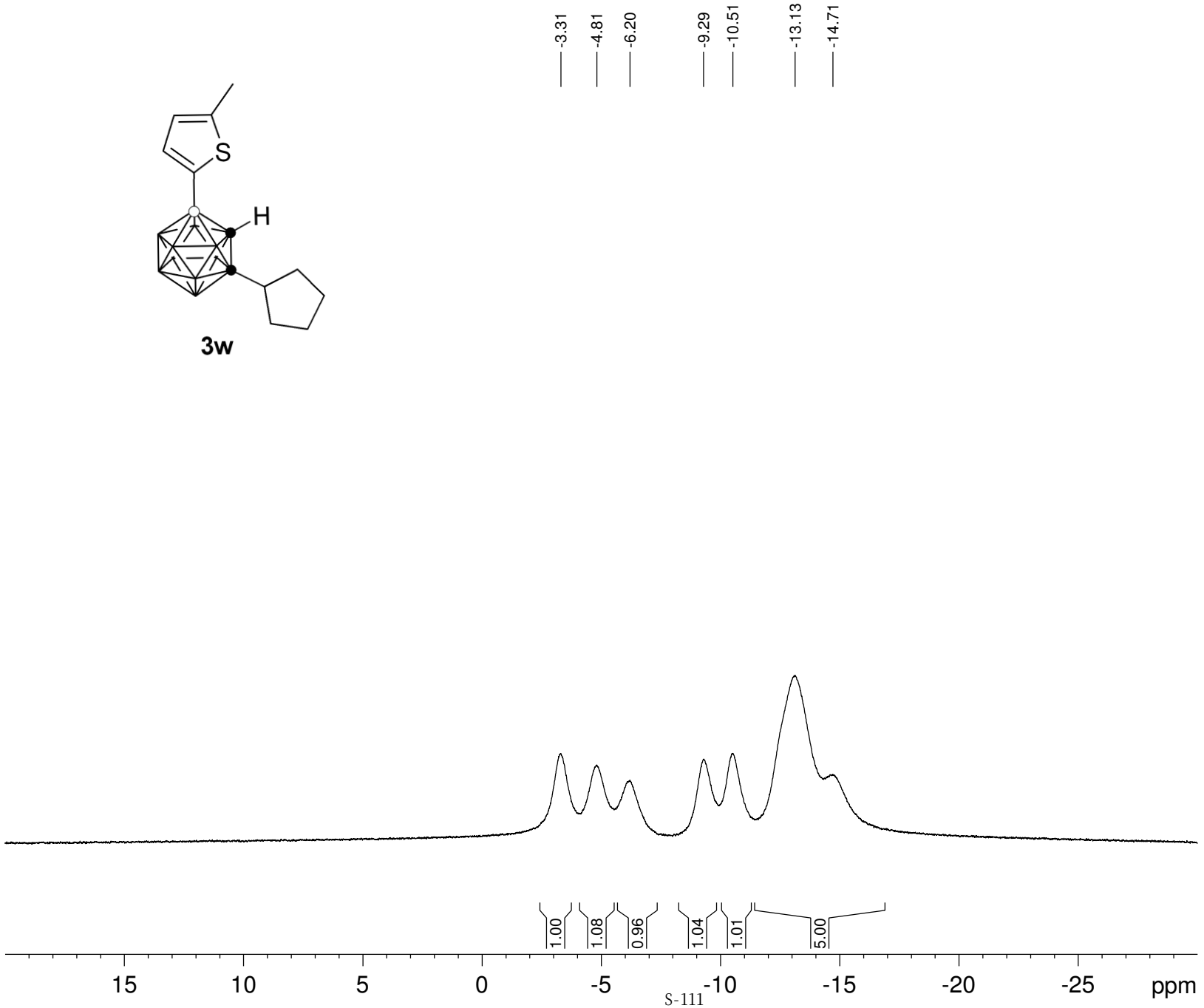
qyj-C-102-47-CDCl3

Current Data Parameters
NAME qyj-C-102-47-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160621
Time 18.33 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 71.8
DW 16.800 usec
DE 6.50 usec
TE 294.5 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

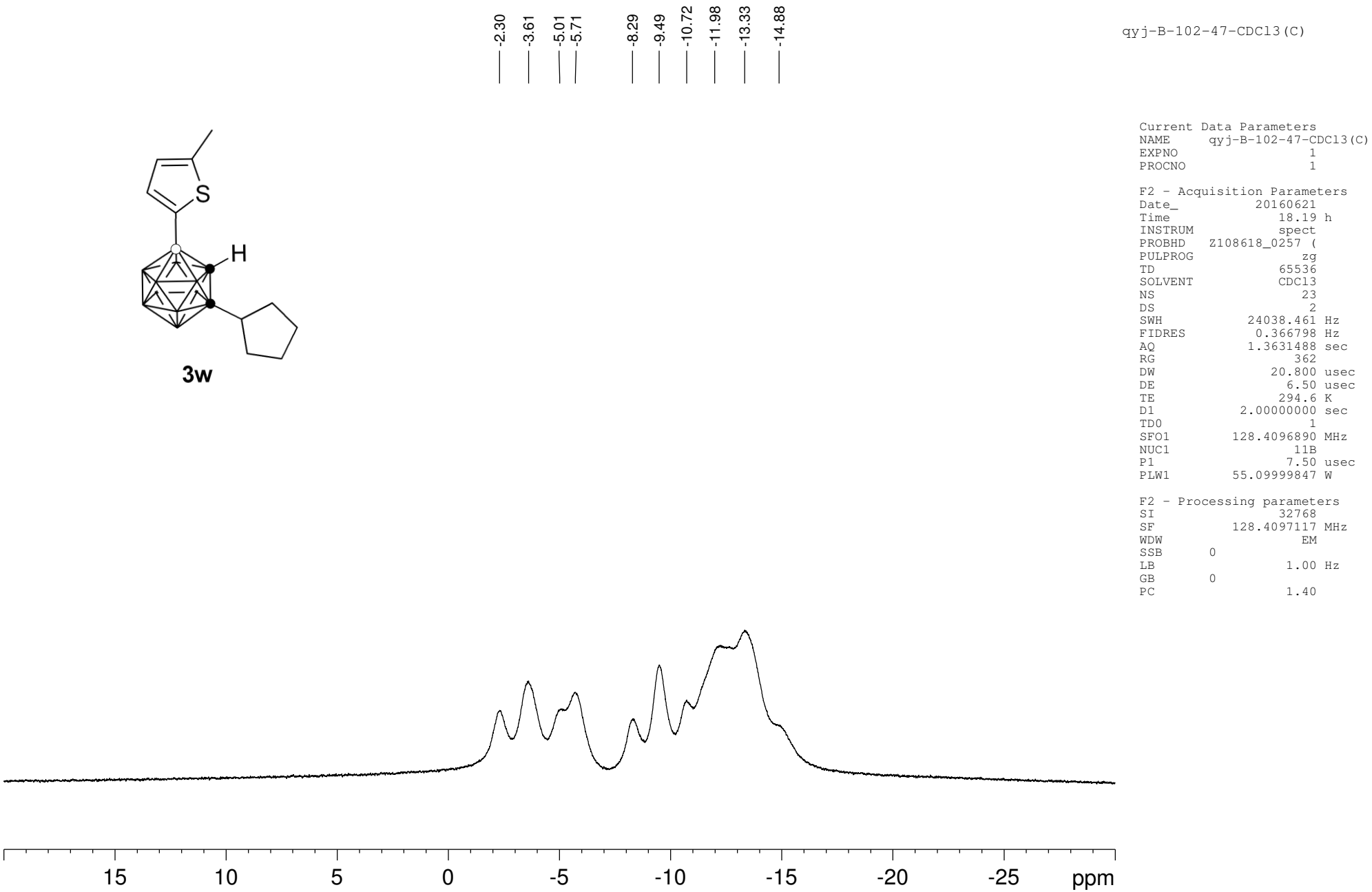
F2 - Processing parameters
SI 32768
SF 100.6379015 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

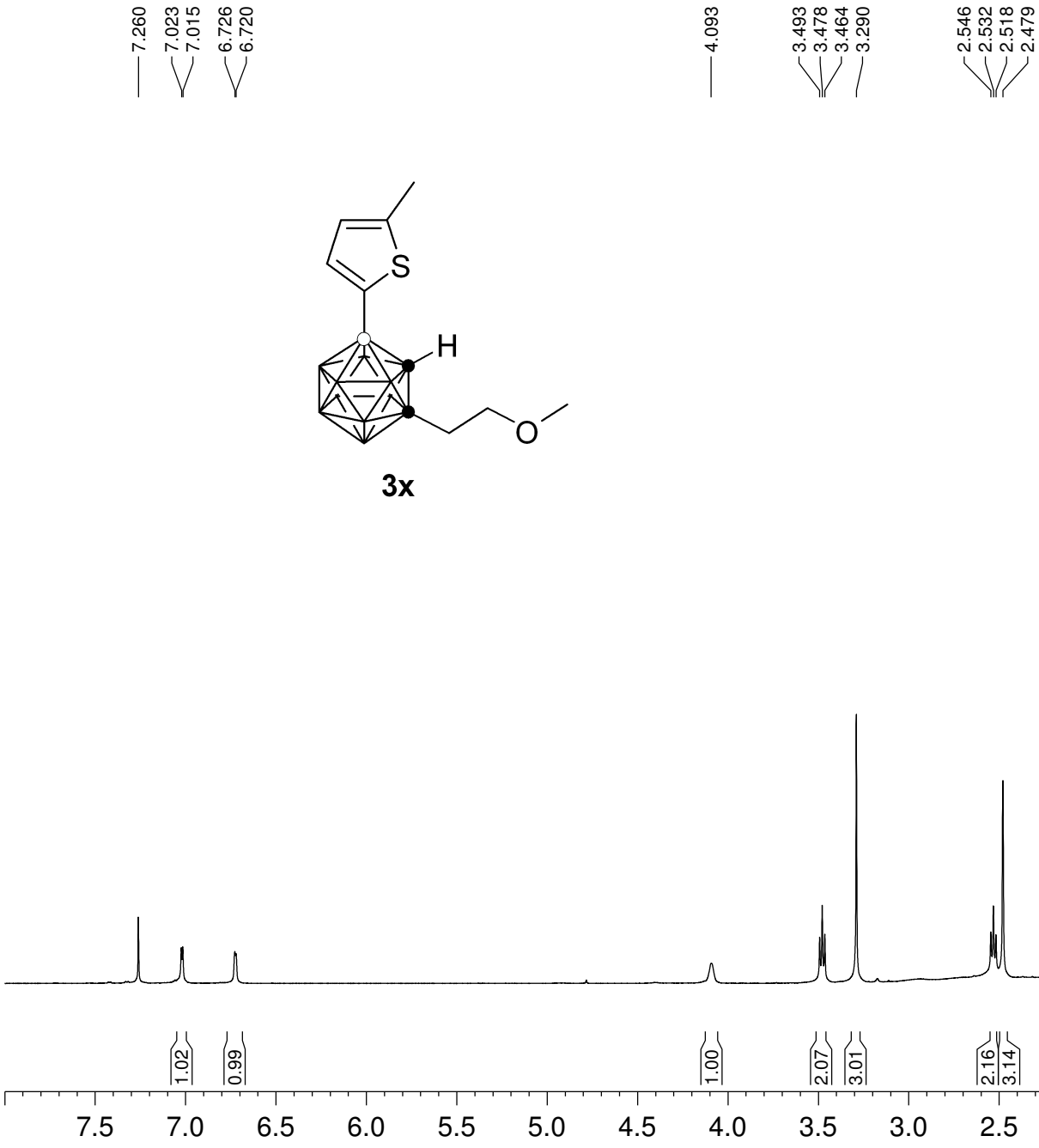
3w



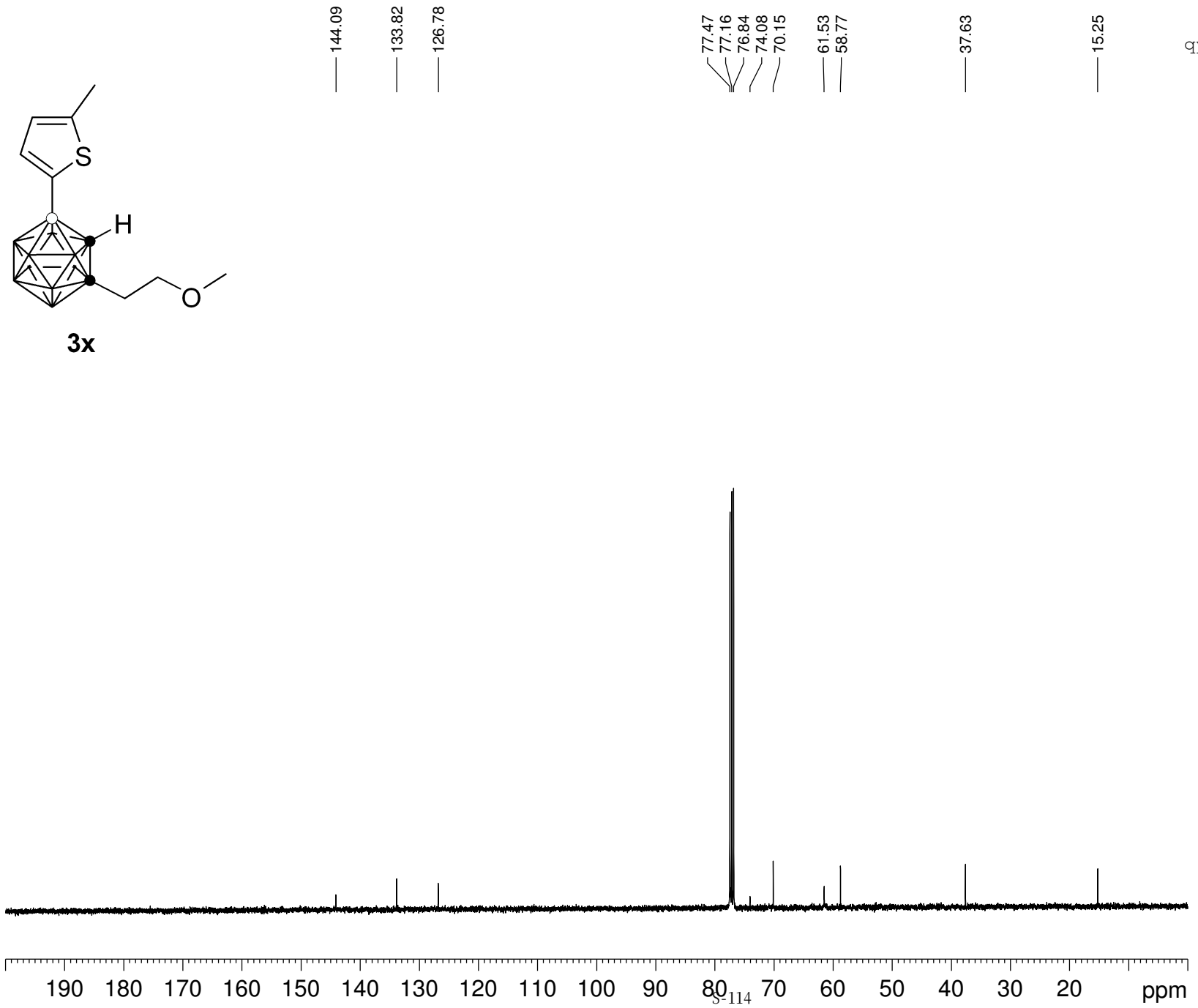
qyj-B-102-47-CDCl3

```
Current Data Parameters
NAME      qyj-B-102-47-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160621
Time              18.17 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    20
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                295.1 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
```


-2.30
-3.61
-5.01
-5.71
-8.29
-9.49
-10.72
-11.98
-13.33
-14.88
qyj-B-102-47-CDCl3(C)
S
H
3w
Current Data Parameters
NAME qyj-B-102-47-CDCl3(C)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160621
Time 18.19 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 23
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 294.6 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 128.4097117 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
15
10
5
0
-5
-10
-15
-20
-25
ppm

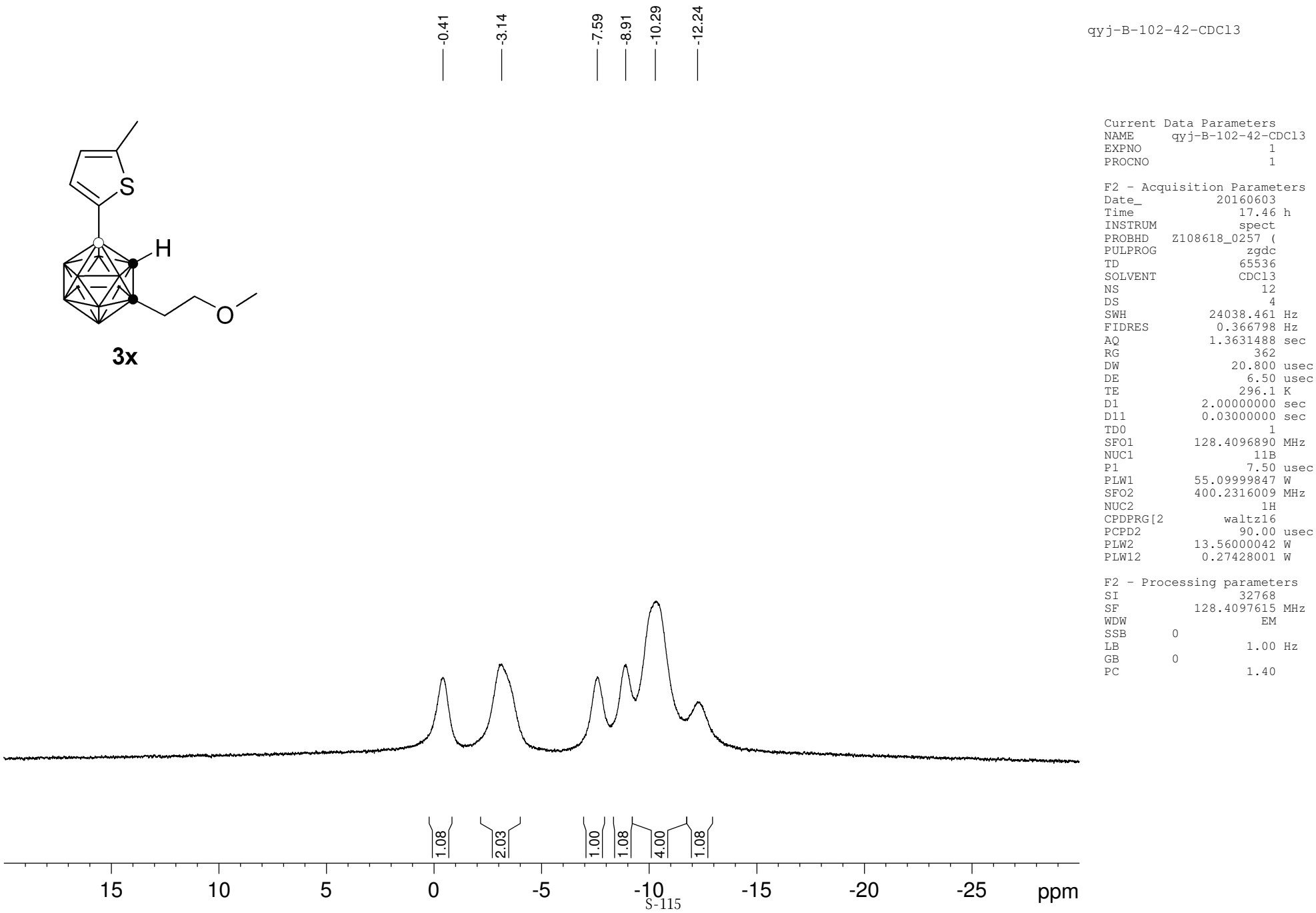

7.260
7.023
7.015
6.726
6.720
4.093
3.493
3.478
3.464
3.290
2.546
2.532
2.518
2.479
qyj-H-120-22-CDCl3
S
H
O
3x
Current Data Parameters
NAME qyj-H-102-42-p-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160603
Time 17.39 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
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 295.9 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 400.2300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.02
0.99
1.00
2.07
3.01
2.16
3.14
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
ppm

3x

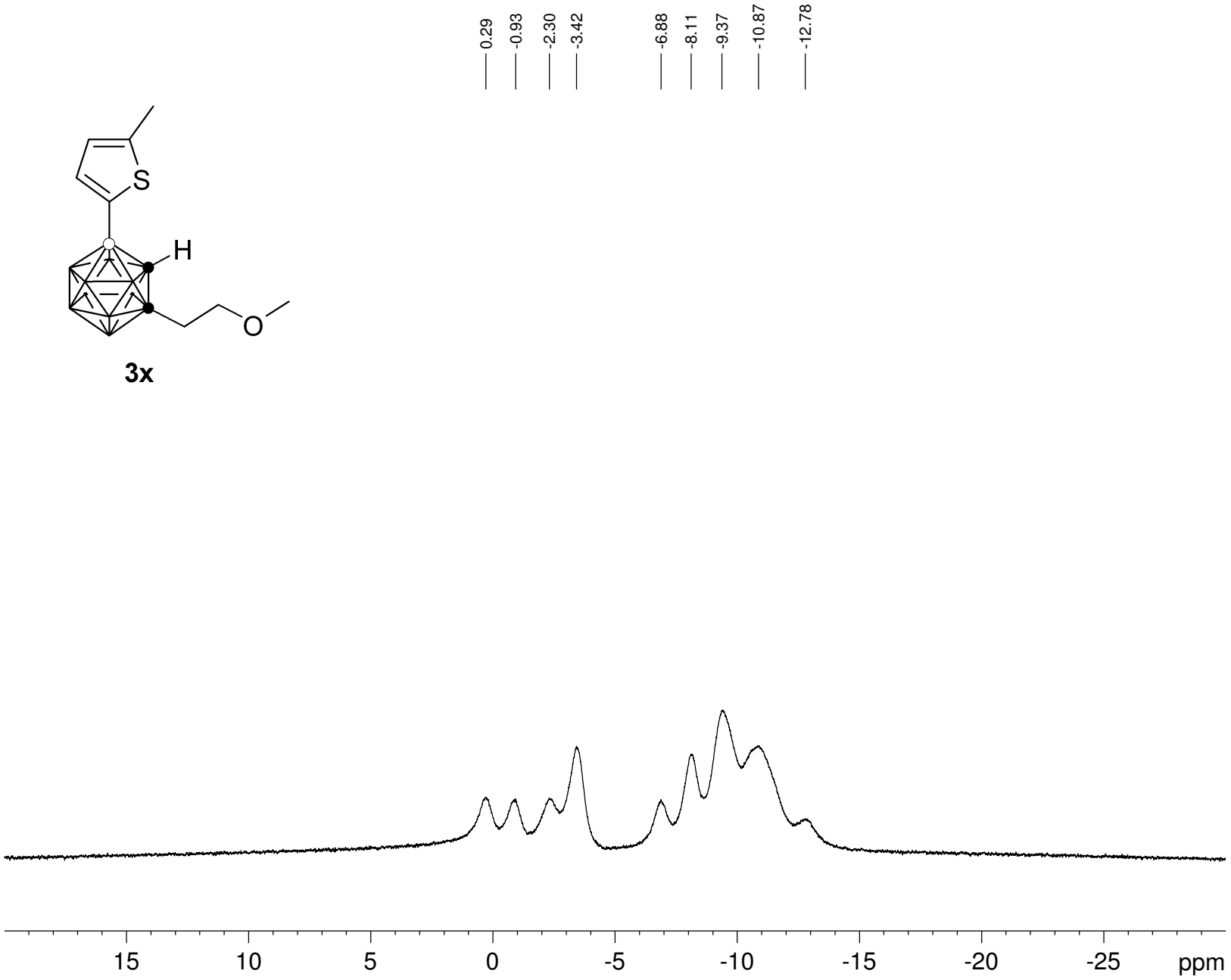


qyj-C-102-42-CDCl3

```
Current Data Parameters
NAME      qyj-C-102-42-CDCl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20160604
Time              16.10 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   350
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                   114
DW                16.800 usec
DE                 6.50 usec
TE                296.2 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           100.6379006 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

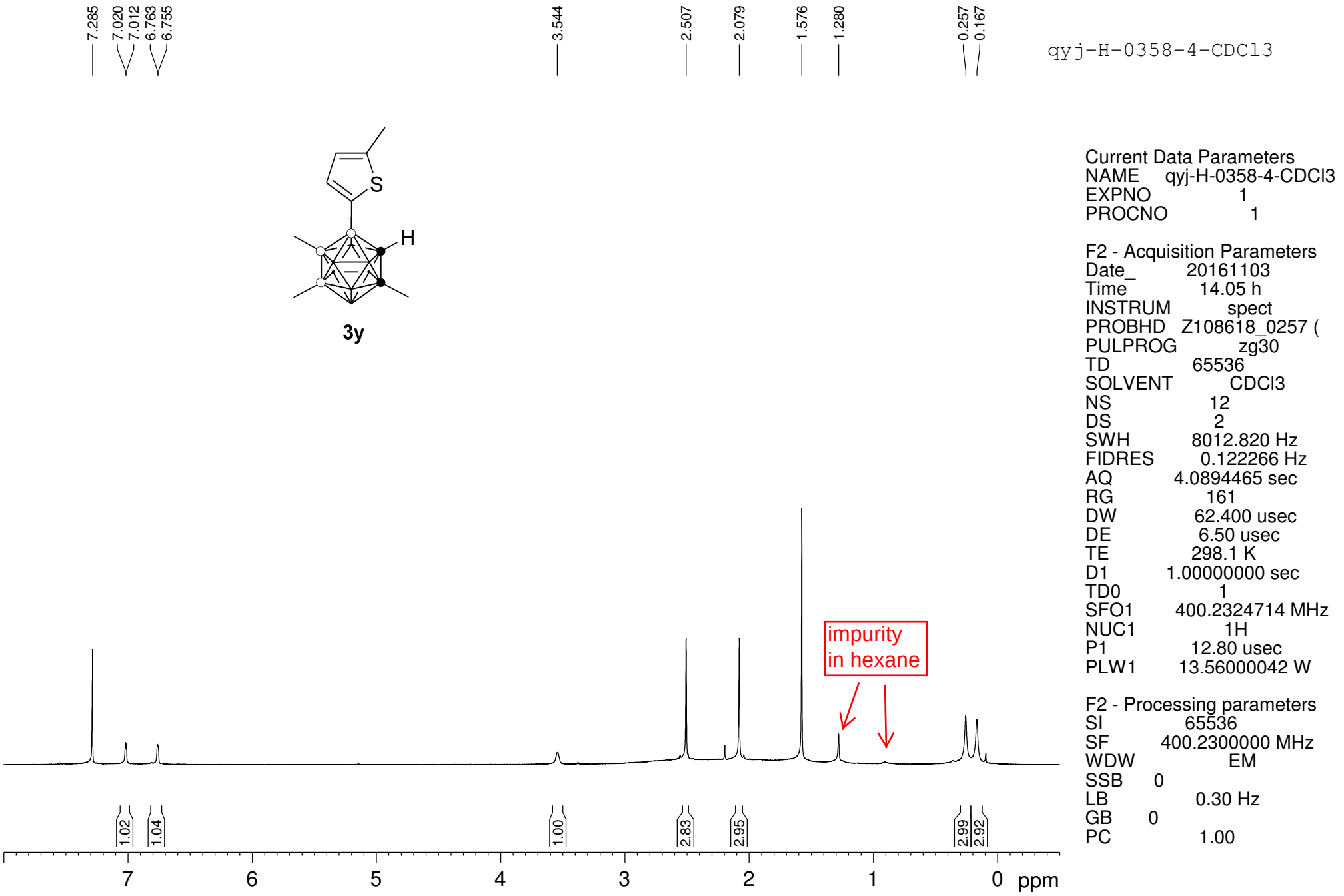

-0.41
-3.14
-7.59
-8.91
-10.29
-12.24
qyj-B-102-42-CDCl3
S
H
O
3x
Current Data Parameters
NAME qyj-B-102-42-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160603
Time 17.46 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 12
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.50 usec
TE 296.1 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
1.08
2.03
1.00
1.08
4.00
1.08
15
10
5
0
-5
-10
-15
-20
-25
ppm

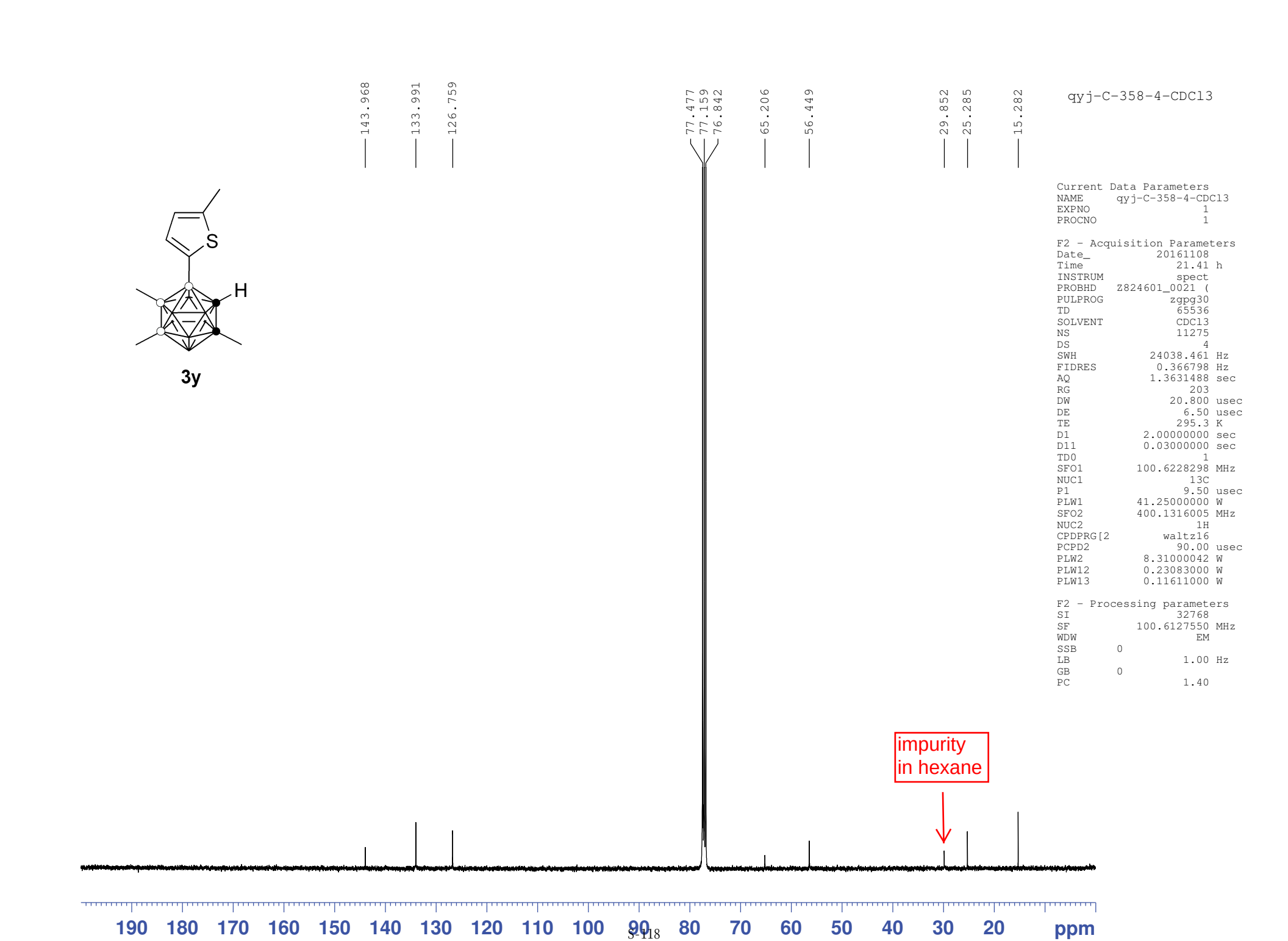
3x



qyj-B-102-42-CDCl3(C)

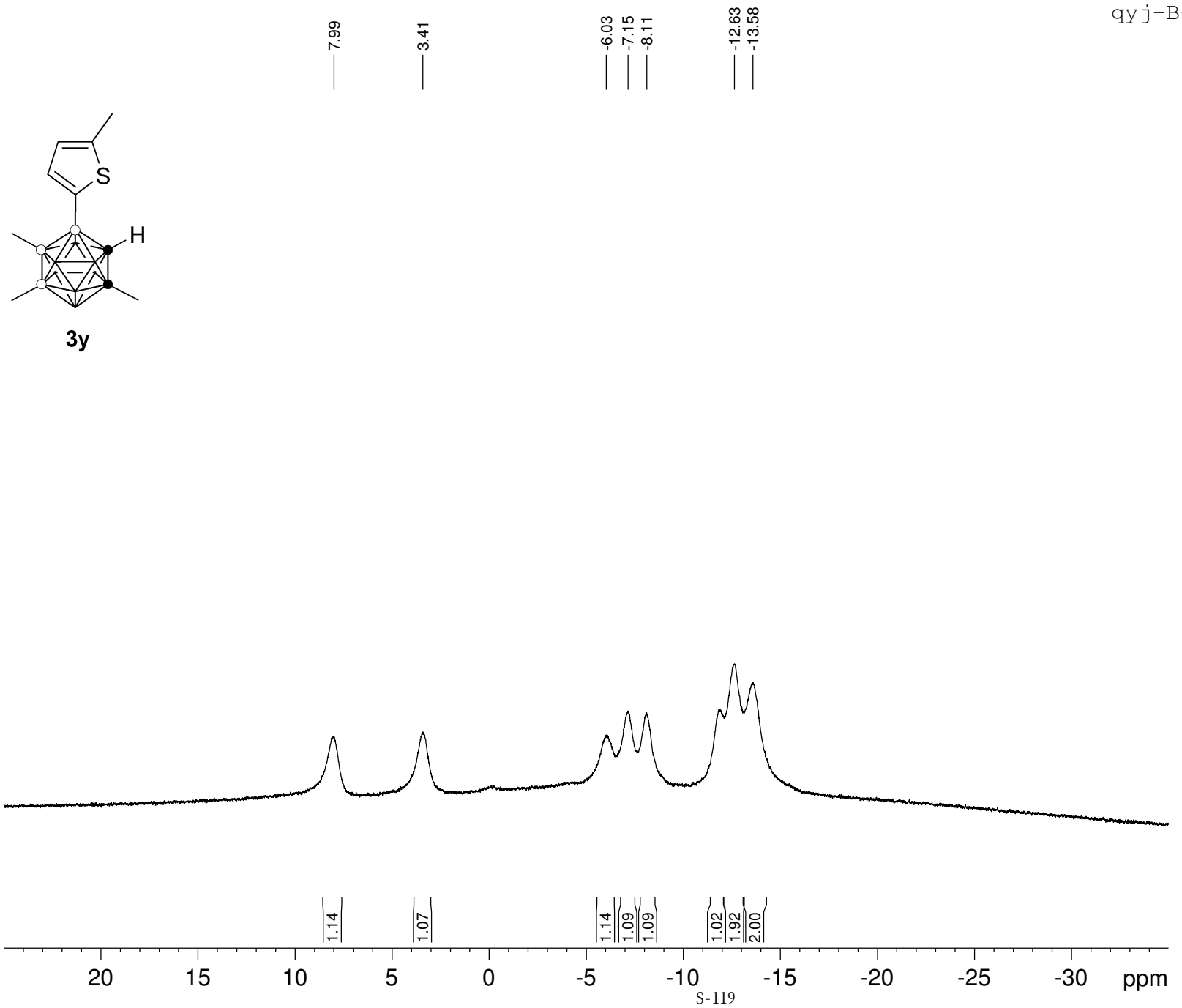
```
Current Data Parameters
NAME      qyj-B-102-42-CDCl3(C)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160603
Time                  17.48 h
INSTRUM               spect
PROBHD    Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT               CDCl3
NS                        14
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                    295.9 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              128.4097504 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```


7.285
7.020
7.012
6.763
6.755
3.544
2.507
2.079
1.576
1.280
0.257
0.167
qyj-H-0358-4-CDCl3
S
H
3y
Current Data Parameters
NAME qyj-H-0358-4-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161103
Time 14.05 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 161
DW 62.400 usec
DE 6.50 usec
TE 298.1 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 400.2300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
impurity
in hexane
1.02
1.04
1.00
2.83
2.95
2.99
2.92
7
6
5
4
3
2
1
0
ppm


143.968
133.991
126.759
77.477
77.159
76.842
65.206
56.449
29.852
25.285
15.282
qyj-C-358-4-CDCl3
S
H
3y
Current Data Parameters
NAME qyj-C-358-4-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161108
Time 21.41 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11275
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 295.3 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 100.6127550 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
impurity
in hexane
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

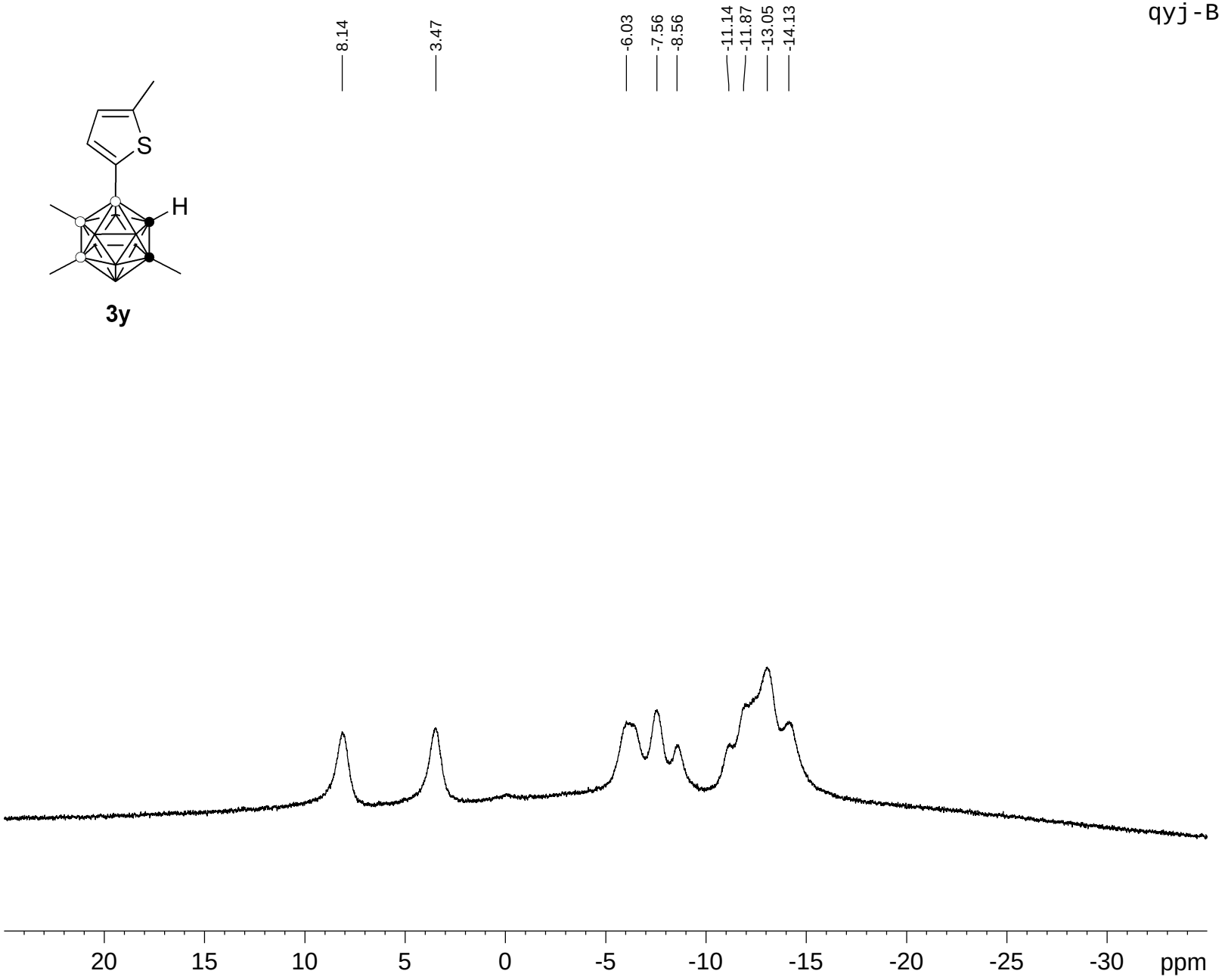
qyj-B-0358-4-CDCl3

3y



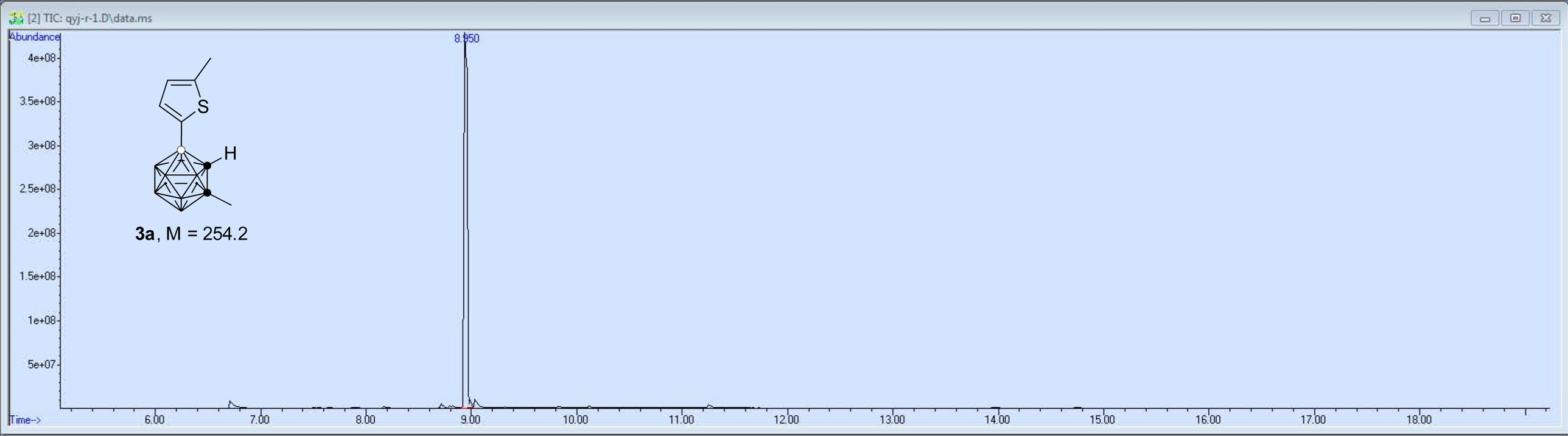

```
Current Data Parameters
NAME      qyj-B-0358-4-CDCl3
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20161103
Time                14.08 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                    100
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                 298.4 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
```

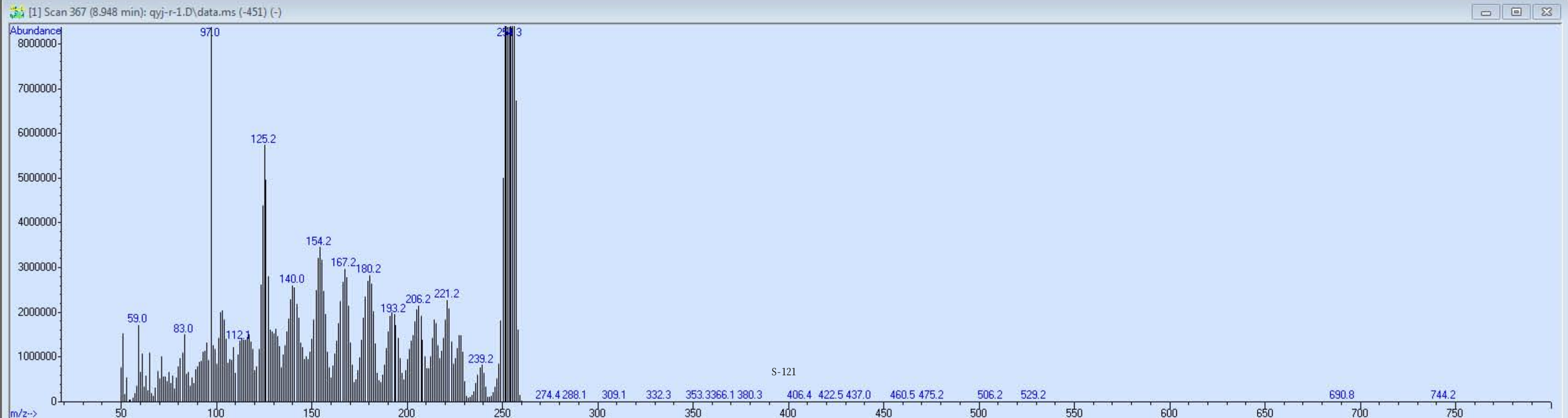
3y

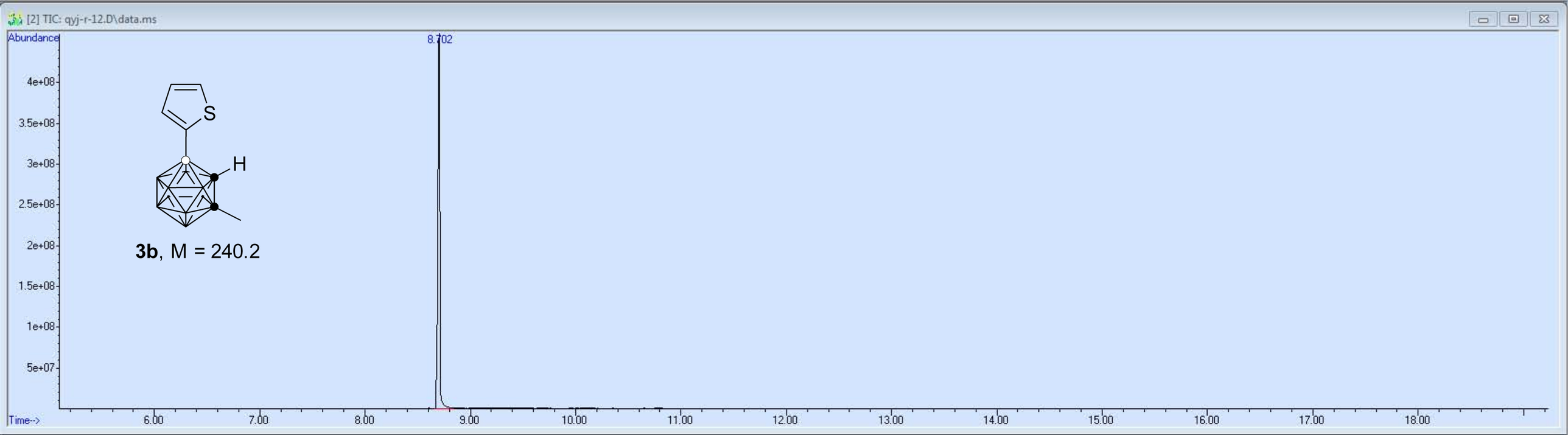


qyj-B-0358-4-CDCl3(c)

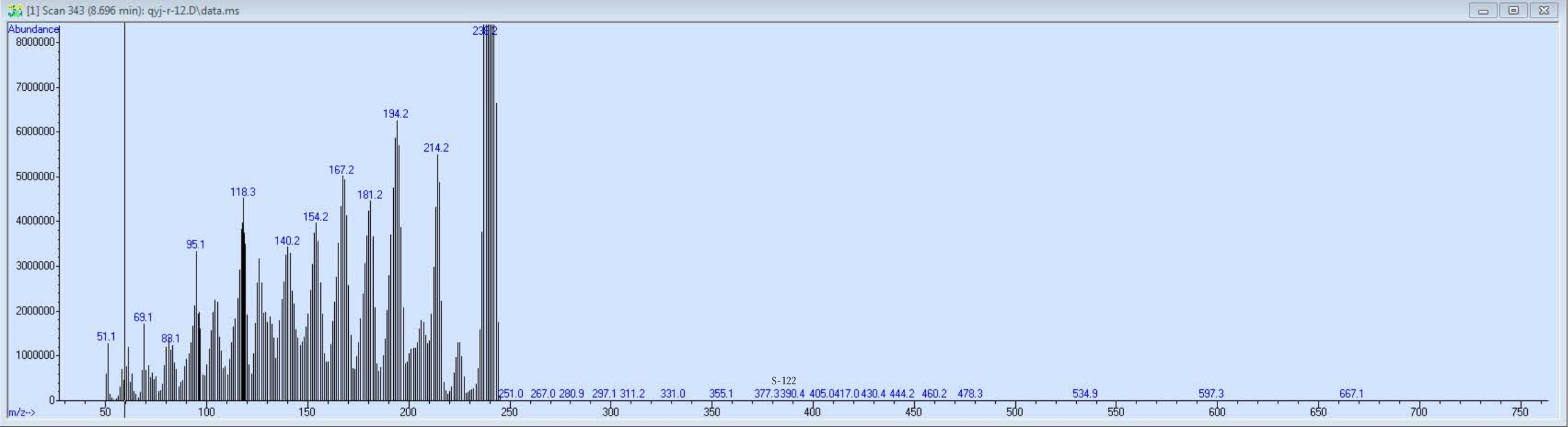
```
Current Data Parameters
NAME     qyj-B-0358-4-CDCl3(c)
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_           20161103
Time              14.17 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG               zg
TD                 65536
SOLVENT            CDCl3
NS                    80
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   512
DW                20.800 usec
DE                 6.50 usec
TE                297.6 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          128.4097504 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

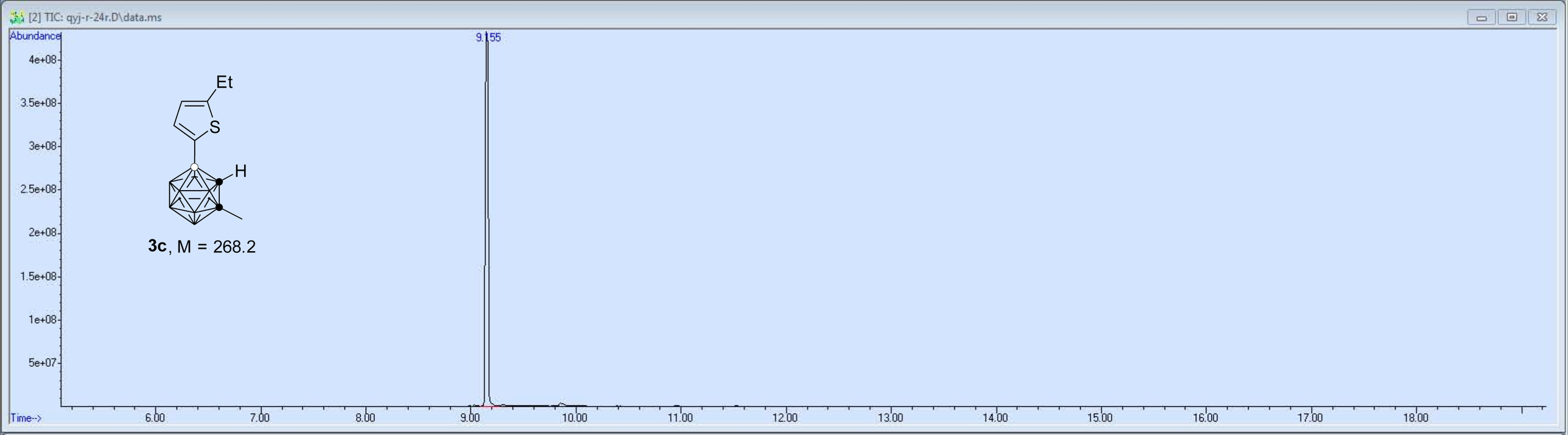

[2] TIC: qyj-r-1.D\data.ms
Abundance
8.950
S
H
3a, M = 254.2
Time-->


[1] Scan 367 (8.948 min): qyj-r-1.D\data.ms (-451) (-)
Abundance
97.0
125.2
154.2
167.2
180.2
140.0
59.0
83.0
112.1
206.2
221.2
193.2
239.2
m/z-->

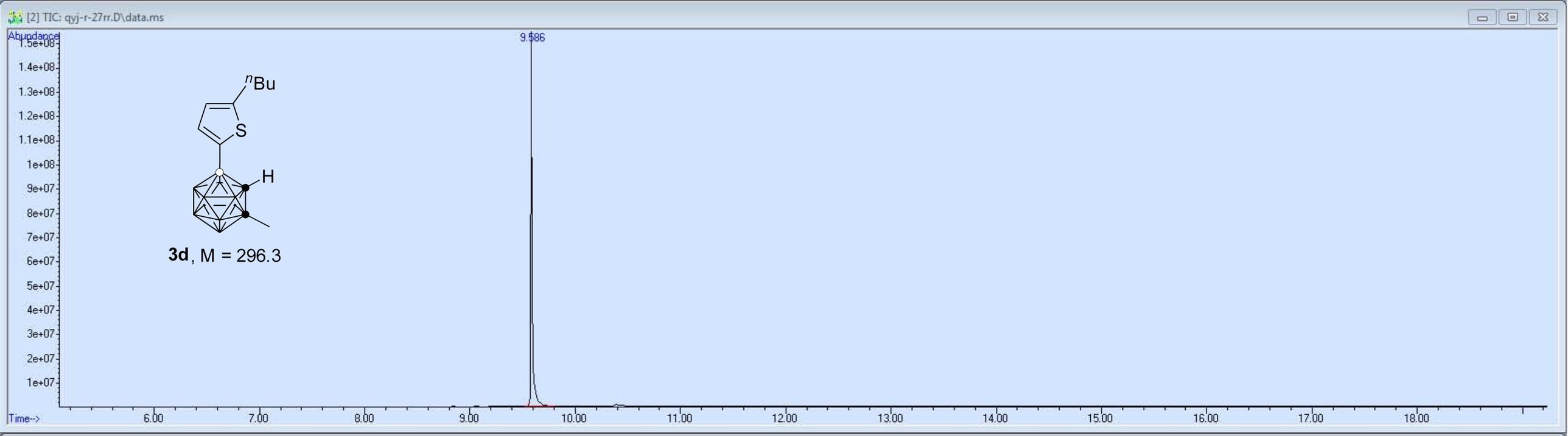

[2] TIC: qyj-r-12.D\data.ms
Abundance
8.702
4e+08
3.5e+08
3e+08
2.5e+08
2e+08
1.5e+08
1e+08
5e+07
Time-->
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00
S
H

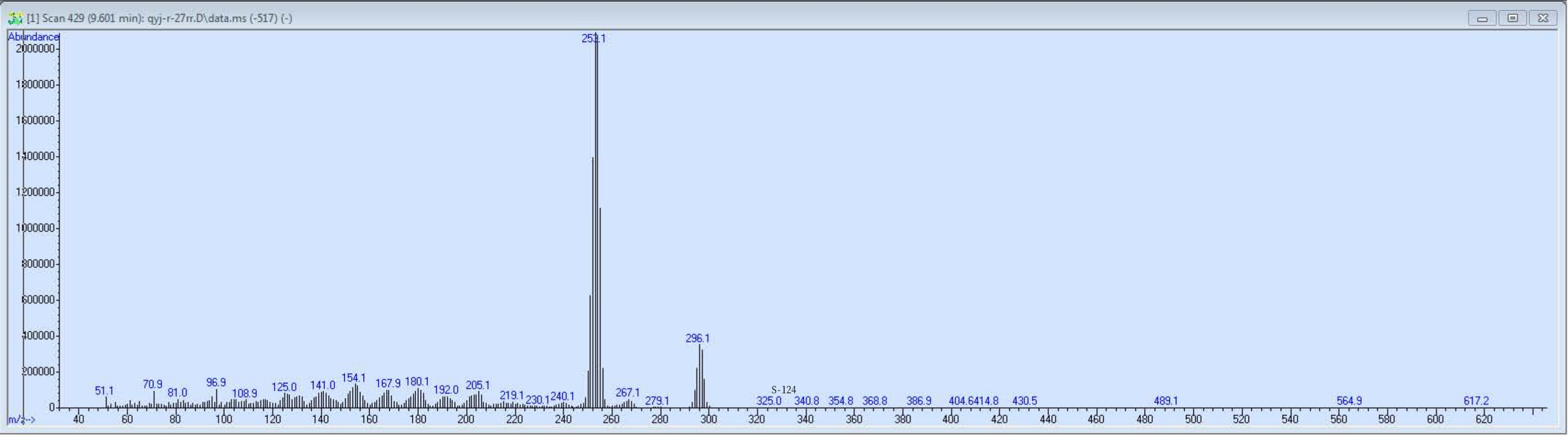
3b, M = 240.2

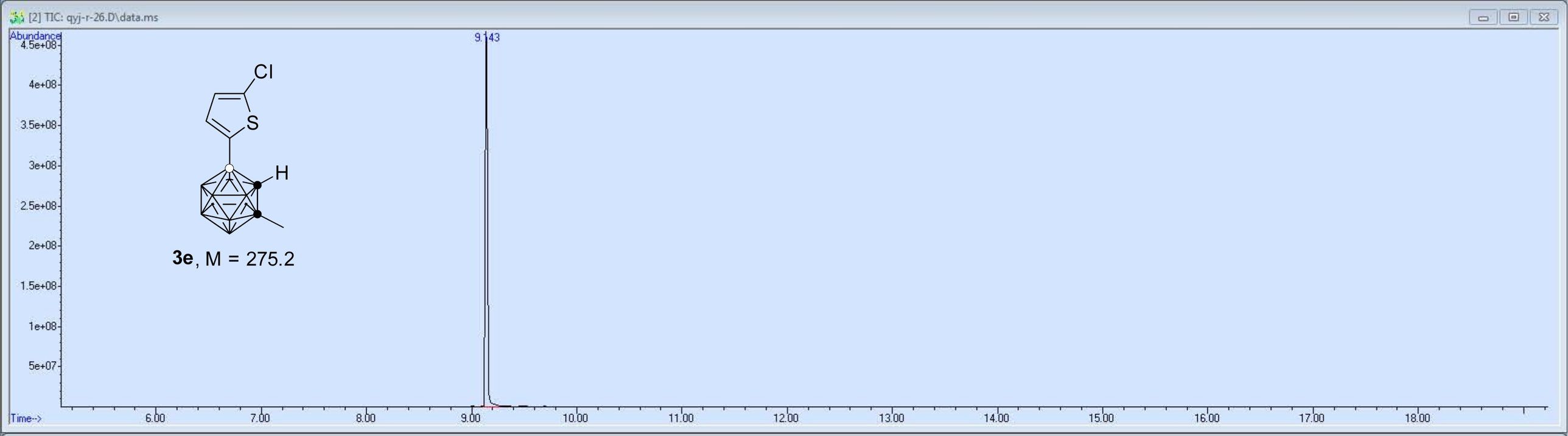

[1] Scan 343 (8.696 min): qyj-r-12.D\data.ms
Abundance
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
m/z-->
51.1
69.1
88.1
95.1
118.3
140.2
154.2
167.2
181.2
194.2
214.2
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750


[2] TIC: qyj-r-24r.D\data.ms
Abundance
9.155
Et
S
H
3c, M = 268.2
Time-->

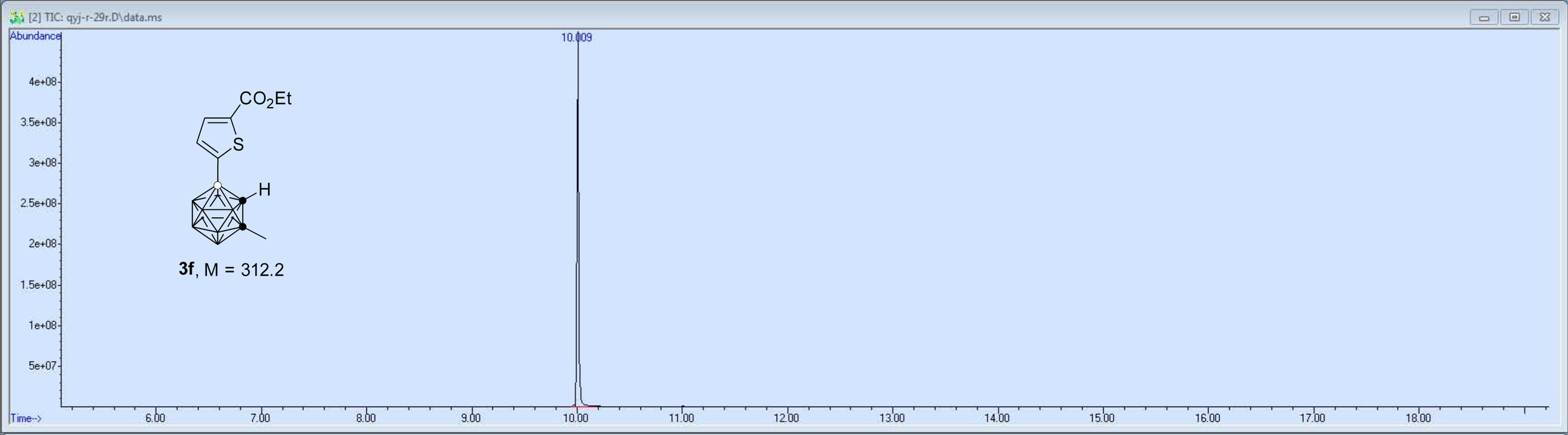

[1] Scan 386 (9.148 min): qyj-r-24r.D\data.ms (-411) (-)
Abundance
132.3
154.2
111.1
167.2
180.2
205.2
51.0
77.0
95.0
219.2
237.2
282.1
m/z-->

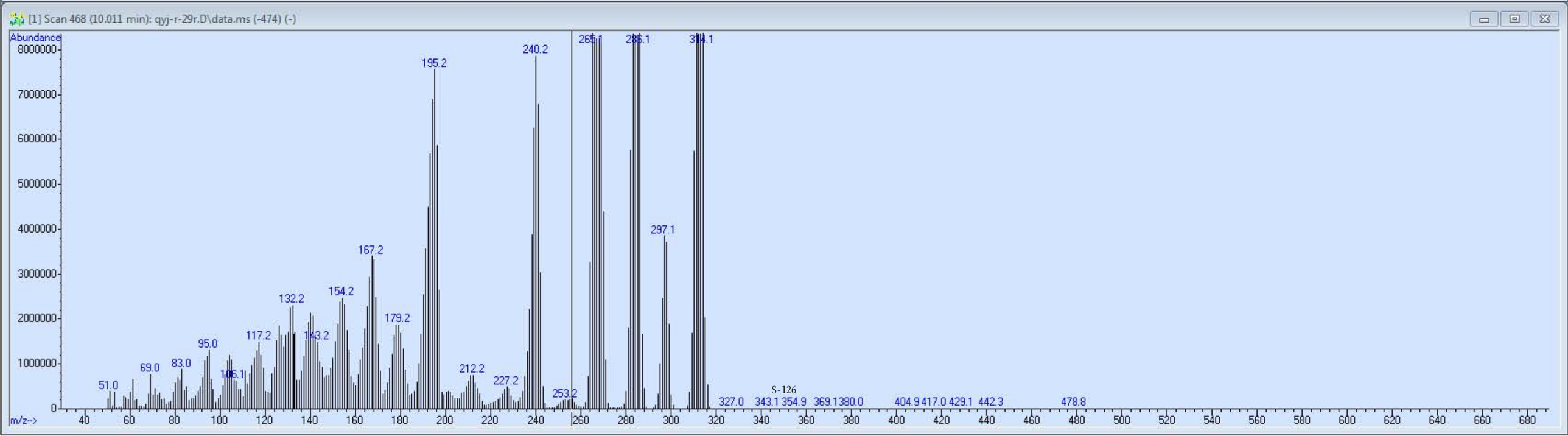

[2] TIC: qyj-r-27rr.D\data.ms
Abundance
9.586
Time-->
nBu
S
H
3d, M = 296.3

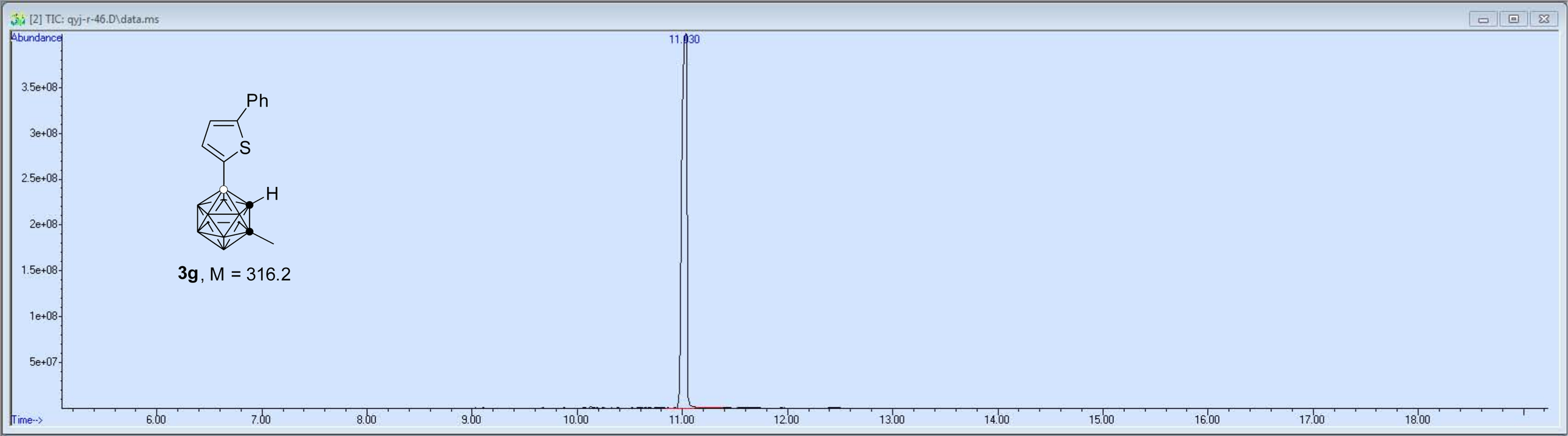

[1] Scan 429 (9.601 min): qyj-r-27rr.D\data.ms (-517) (-)
Abundance
253.1
296.1
m/z-->

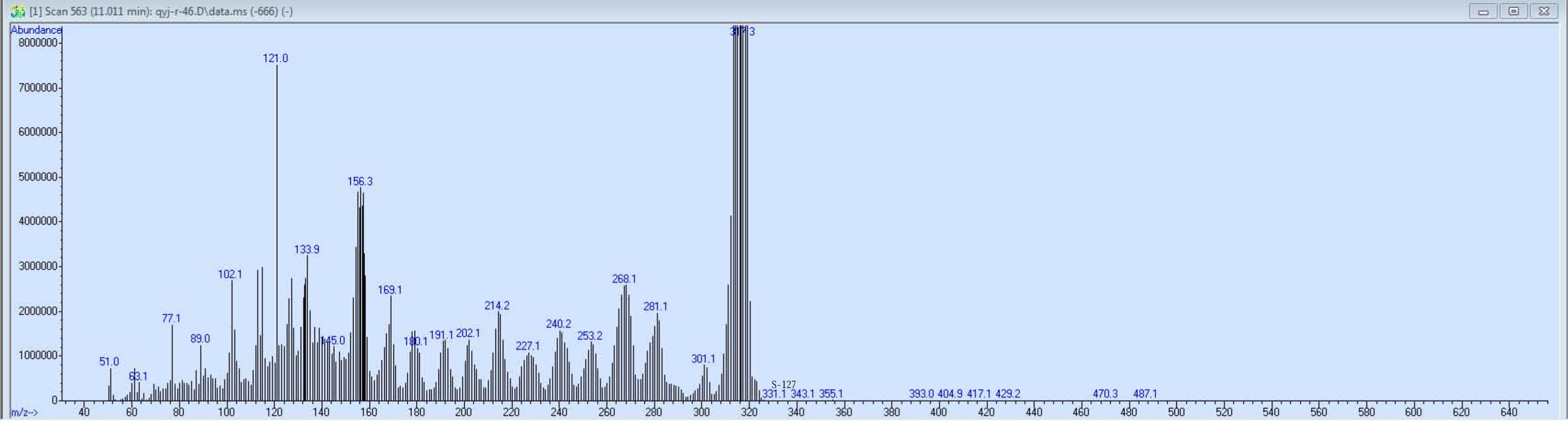

[2] TIC: qyj-r-26.D\data.ms
Abundance
9.143
Cl
S
H
3e, M = 275.2
Time-->

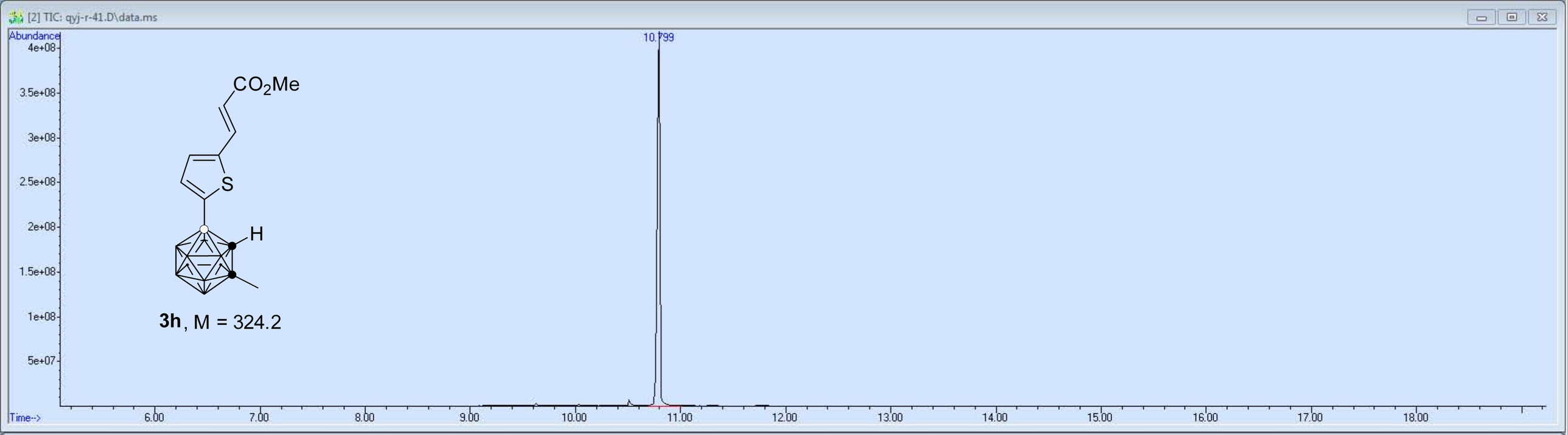

[1] Scan 386 (9.148 min): qyj-r-26.D\data.ms (-466) (-)
Abundance
239.2
194.2
167.2
126.1
140.1
153.2
103.1
213.2
226.2
71.1
51.0
289.1
306.3
320.2
341.1
355.0
370.2
385.0
405.2
421.4
438.2
460.1
474.7
492.0
520.1
547.1
m/z-->

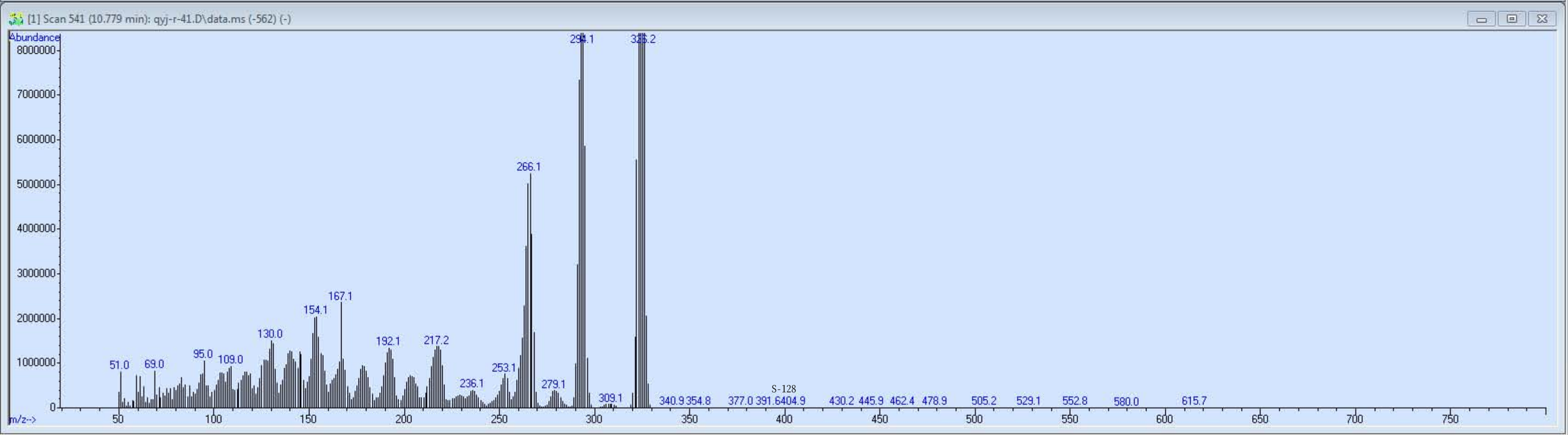

[2] TIC: qyj-r-29r.D\data.ms
Abundance
10.009
4e+08
3.5e+08
3e+08
2.5e+08
2e+08
1.5e+08
1e+08
5e+07
Time-->
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00
CO2Et
S
H
3f, M = 312.2

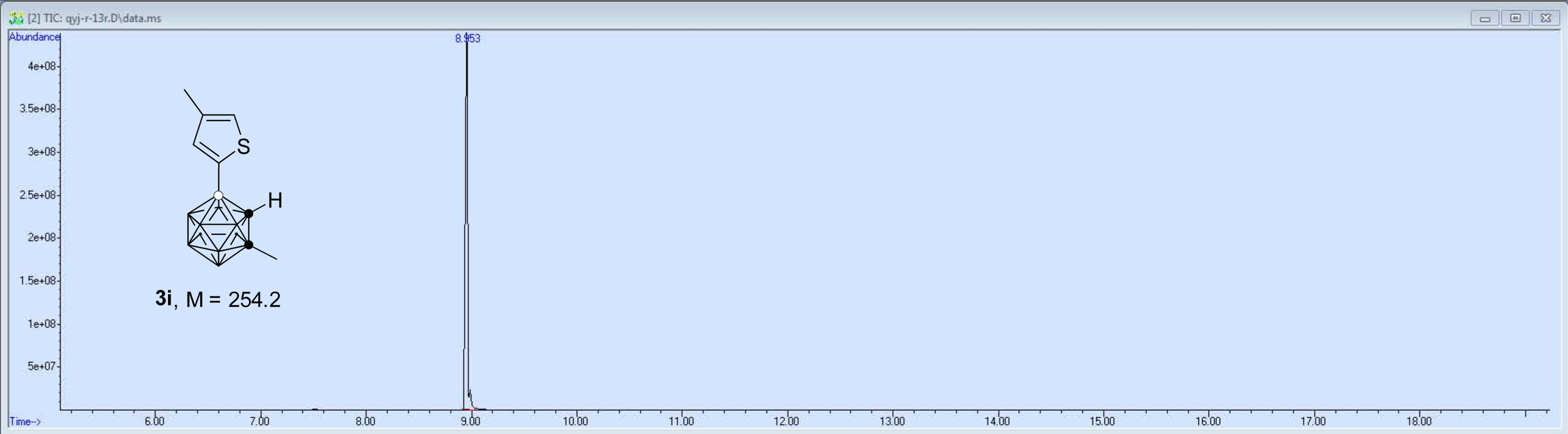

[1] Scan 468 (10.011 min): qyj-r-29r.D\data.ms (-474) (-)
Abundance
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
m/z-->
240.2
195.2
265.1
285.1
314.1
297.1
167.2
154.2
132.2
179.2
117.2
143.2
95.0
69.0
83.0
51.0
106.1
212.2
227.2
253.2
327.0
343.1
354.9
369.1
380.0
404.9
417.0
429.1
442.3
478.8
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
620
640
660
680


[2] TIC: qyj-r-46.D\data.ms
Abundance
11.030
Ph
S
H
3g, M = 316.2
Time-->
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00

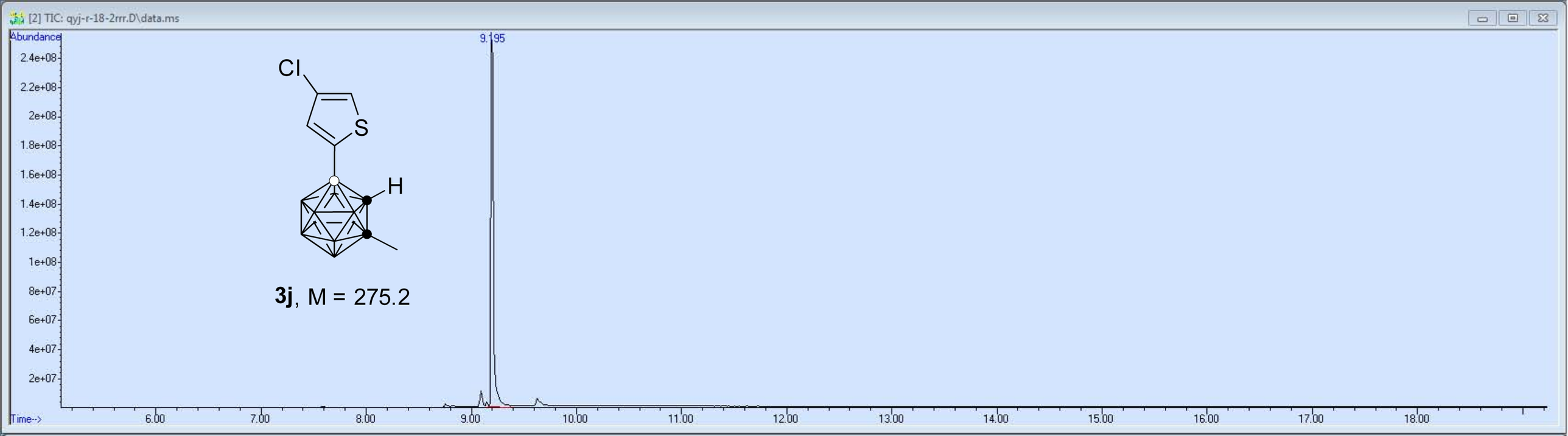

[1] Scan 563 (11.011 min): qyj-r-46.D\data.ms (-666) (-)
Abundance
121.0
156.3
133.9
102.1
169.1
77.1
89.0
145.0
214.2
240.2
253.2
268.1
281.1
227.1
301.1
51.0
63.1
m/z-->
331.1 343.1 355.1
393.0 404.9 417.1 429.2
470.3
487.1

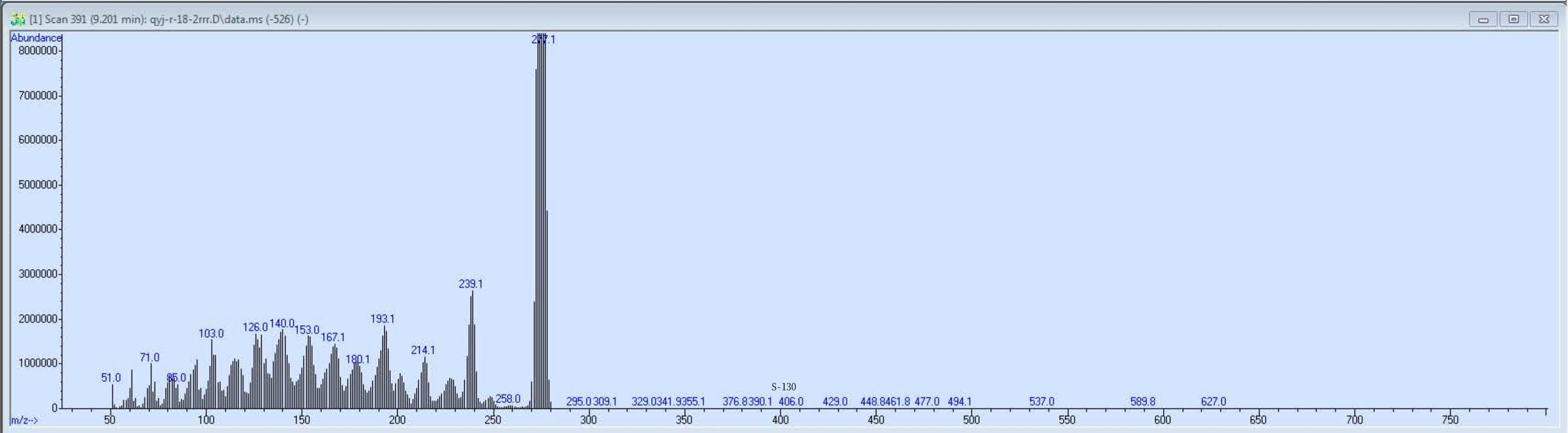

[2] TIC: qyj-r-41.D\data.ms
Abundance
10.799
CO2Me
S
H
3h, M = 324.2
Time-->

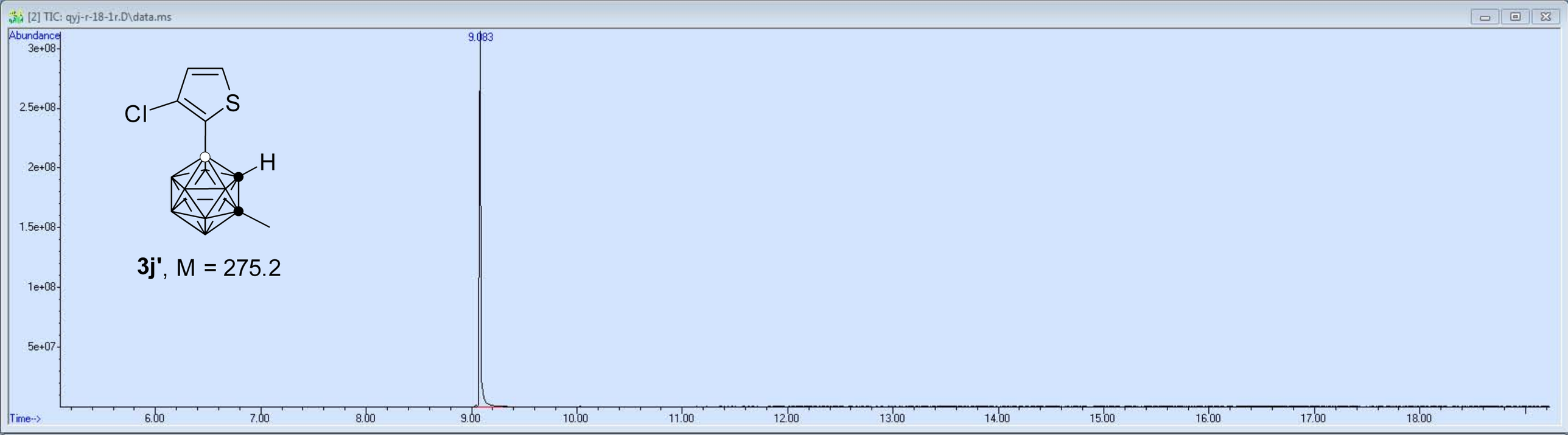

[1] Scan 541 (10.779 min): qyj-r-41.D\data.ms (-562) (-)
Abundance
294.1
324.2
266.1
167.1
154.1
130.0
192.1
217.2
95.0
109.0
51.0
69.0
253.1
236.1
279.1
309.1
m/z-->

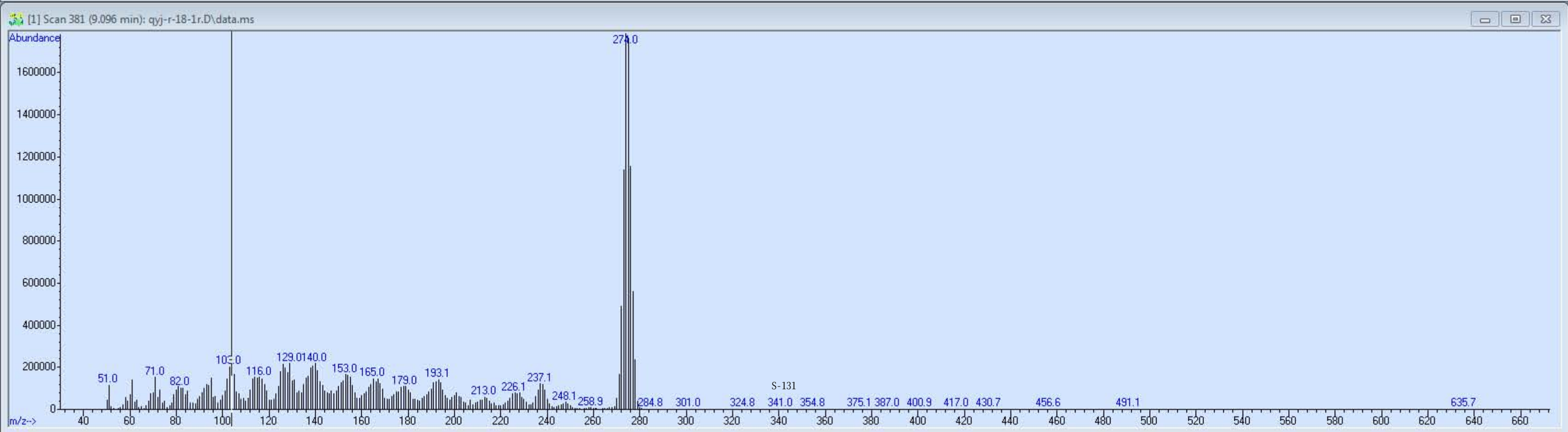

[2] TIC: qyj-r-13r.D\data.ms
Abundance
8.953
S
H
3i, M = 254.2
Time-->

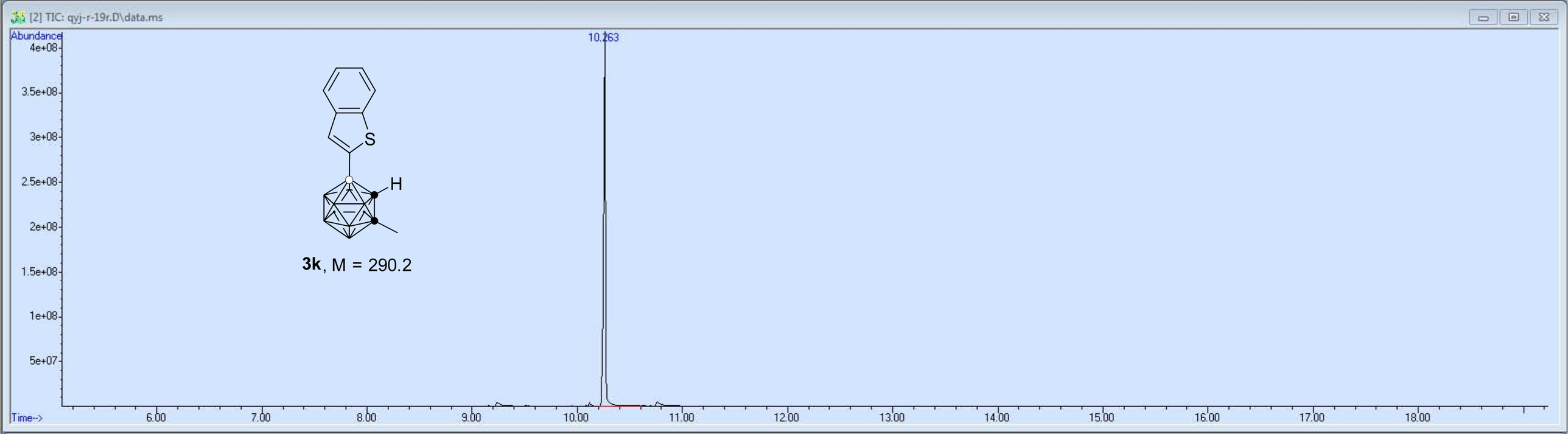

[1] Scan 367 (8.948 min): qyj-r-13r.D\data.ms (-361) (-)
Abundance
97.0
125.2
214.2
154.2
167.2
180.2
140.2
193.2
51.0
83.1
112.2
65.1
227.2
m/z-->

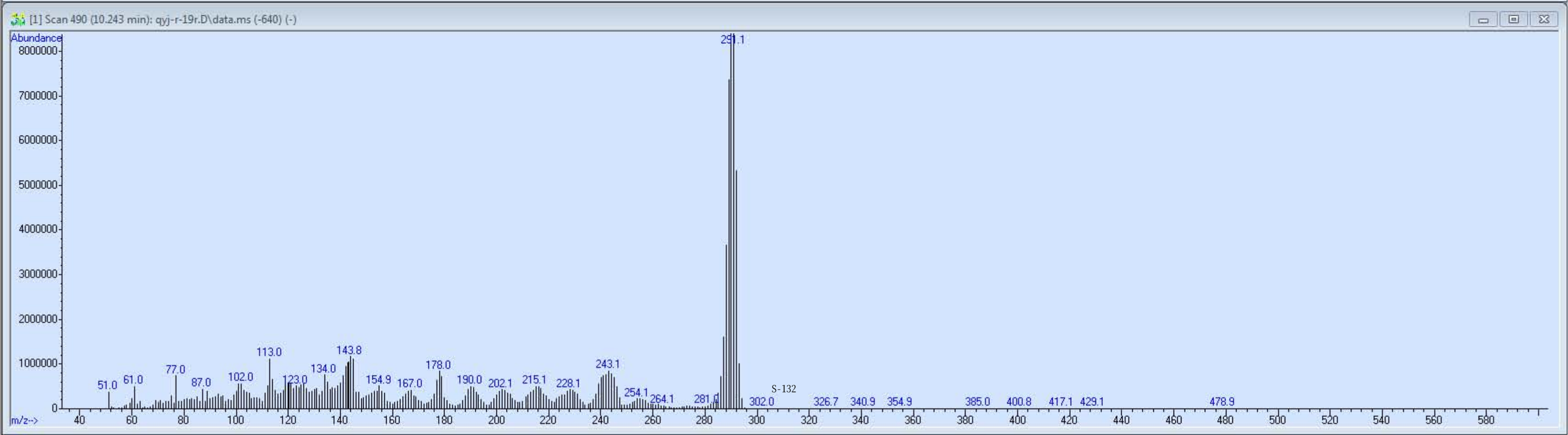

[2] TIC: qyj-r-18-2rrr.D\data.ms
Abundance
9.195
Cl
S
H
3j, M = 275.2
Time-->

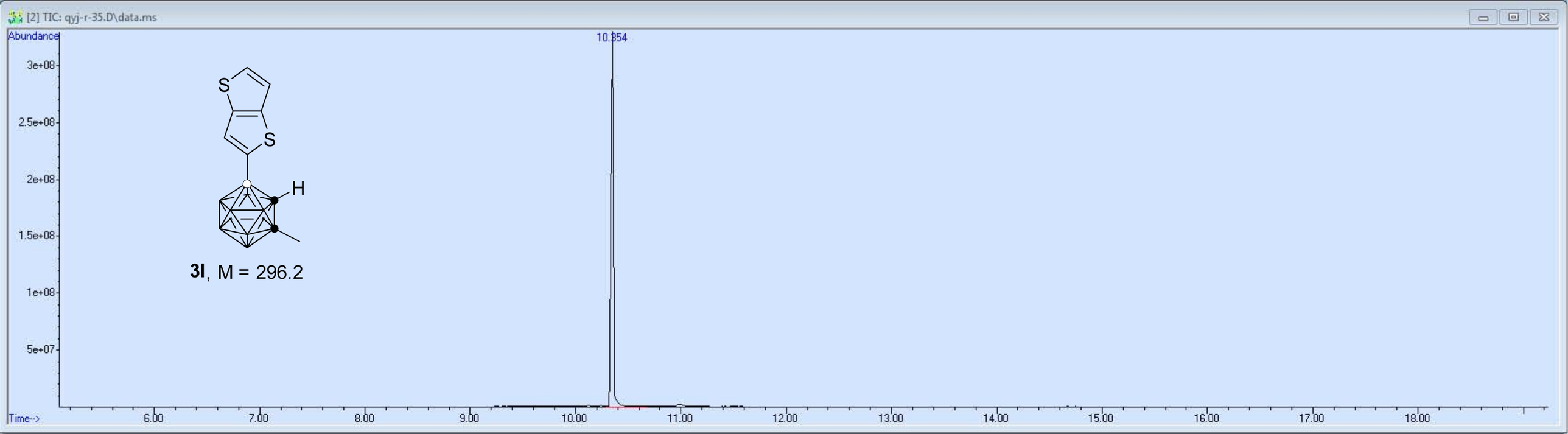

[1] Scan 391 (9.201 min): qyj-r-18-2rrr.D\data.ms (-526) (-)
Abundance
277.1
239.1
193.1
103.0
126.0
140.0
153.0
167.1
214.1
180.1
71.0
51.0
85.0
258.0
m/z-->


[2] TIC: qyj-r-18-1r.D\data.ms
Abundance
9.083
Cl
S
H
3j', M = 275.2
Time-->

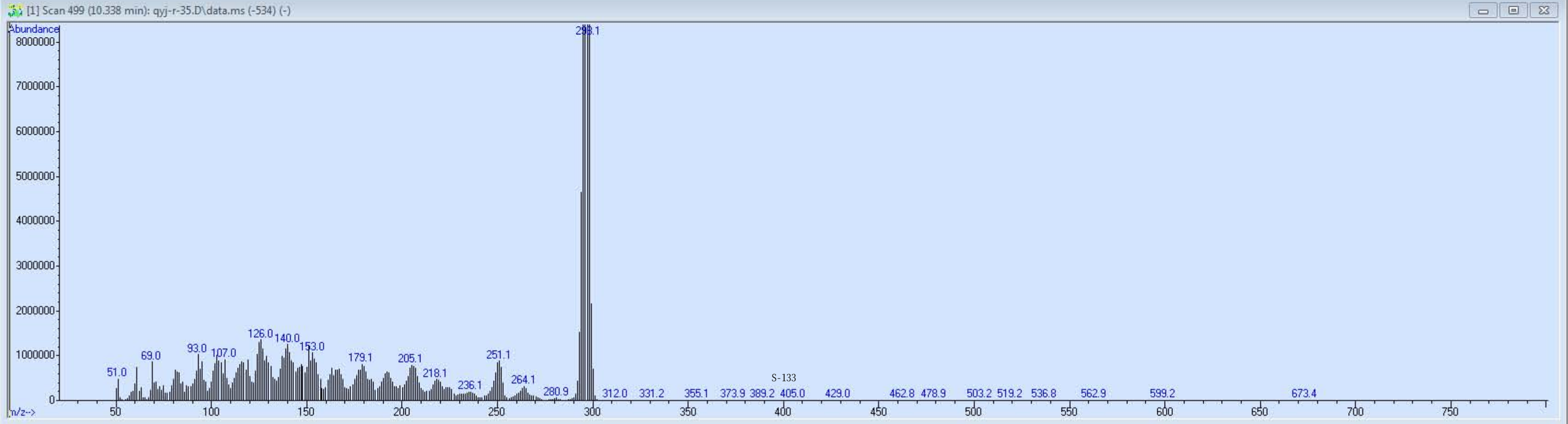

[1] Scan 381 (9.096 min): qyj-r-18-1r.D\data.ms
Abundance
m/z-->

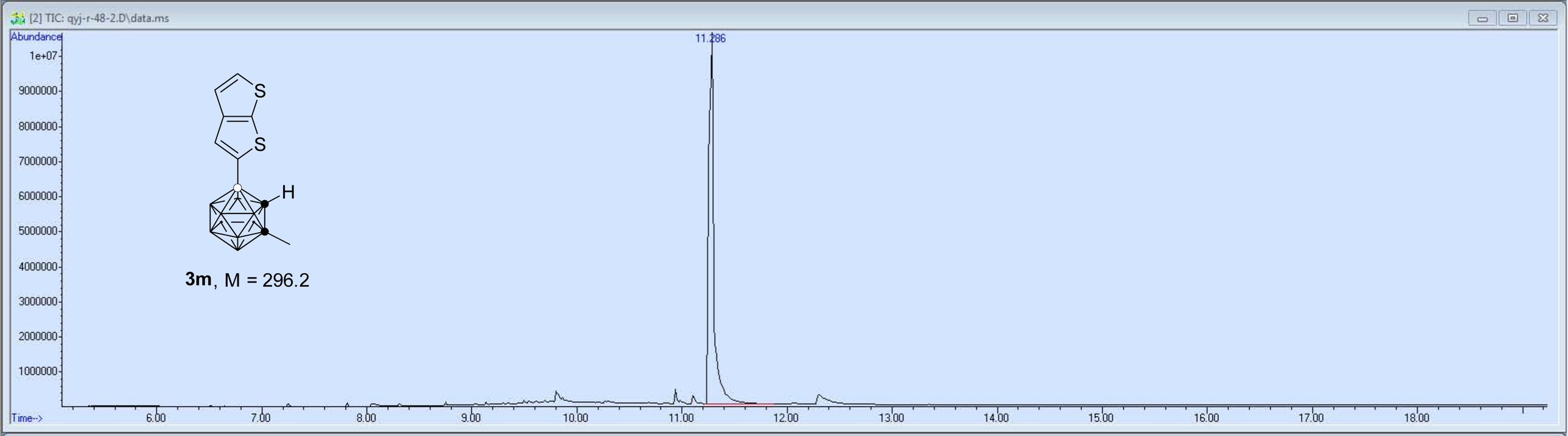

[2] TIC: qyj-r-19r.D\data.ms
Abundance
10.263
S
H
3k, M = 290.2
Time-->

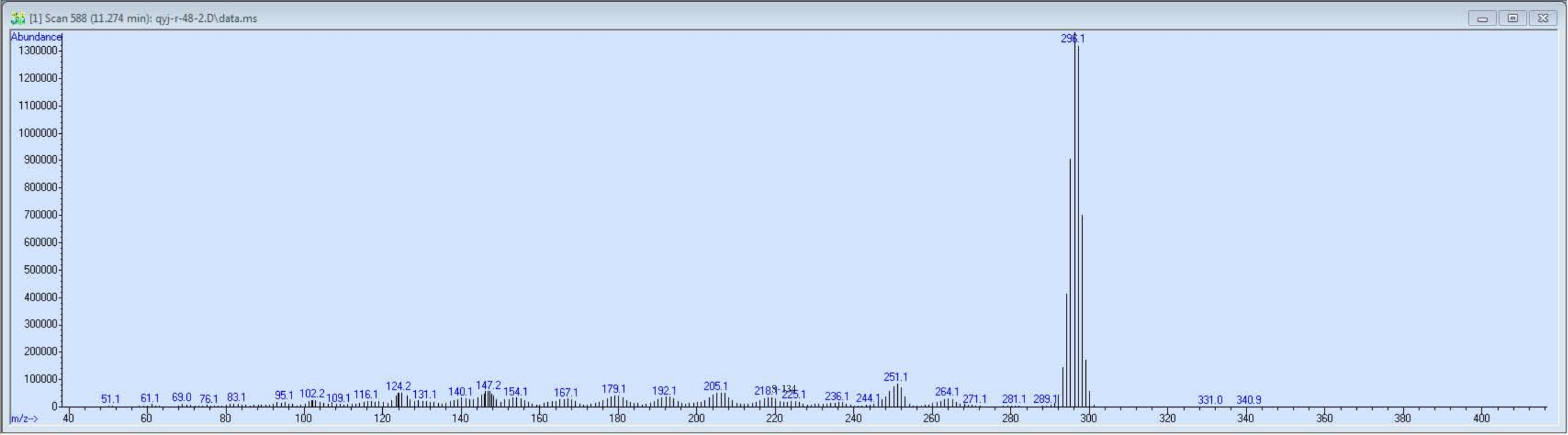

[1] Scan 490 (10.243 min): qyj-r-19r.D\data.ms (-640) (-)
Abundance
291.1
m/z-->

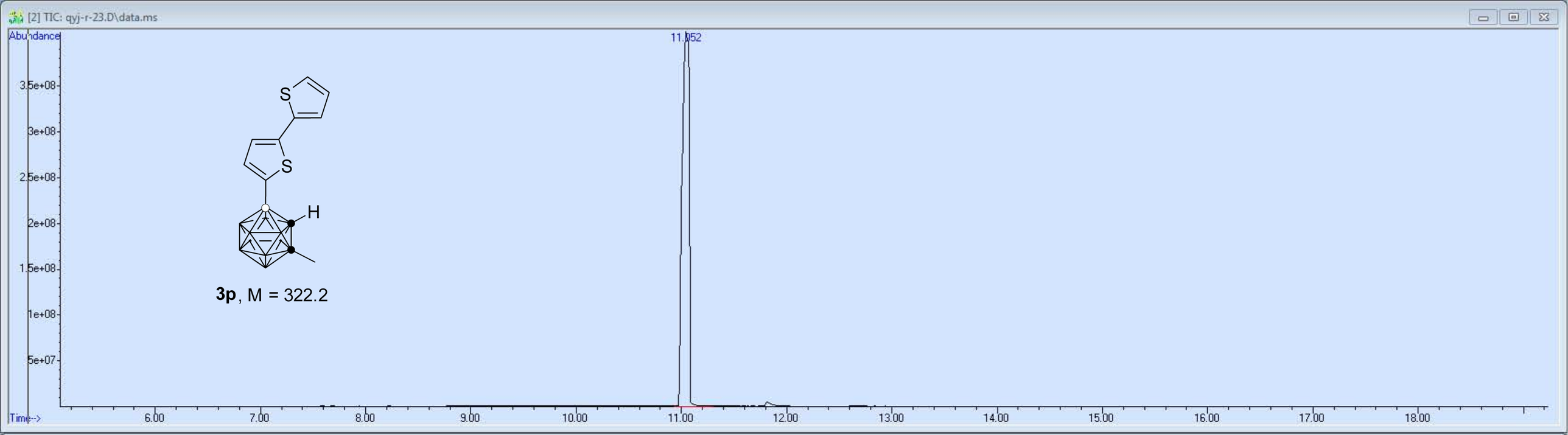

[2] TIC: qyj-r-35.D\data.ms
Abundance
10.354
3e+08
2.5e+08
2e+08
1.5e+08
1e+08
5e+07
Time-->
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00
S
S
H

3l, M = 296.2

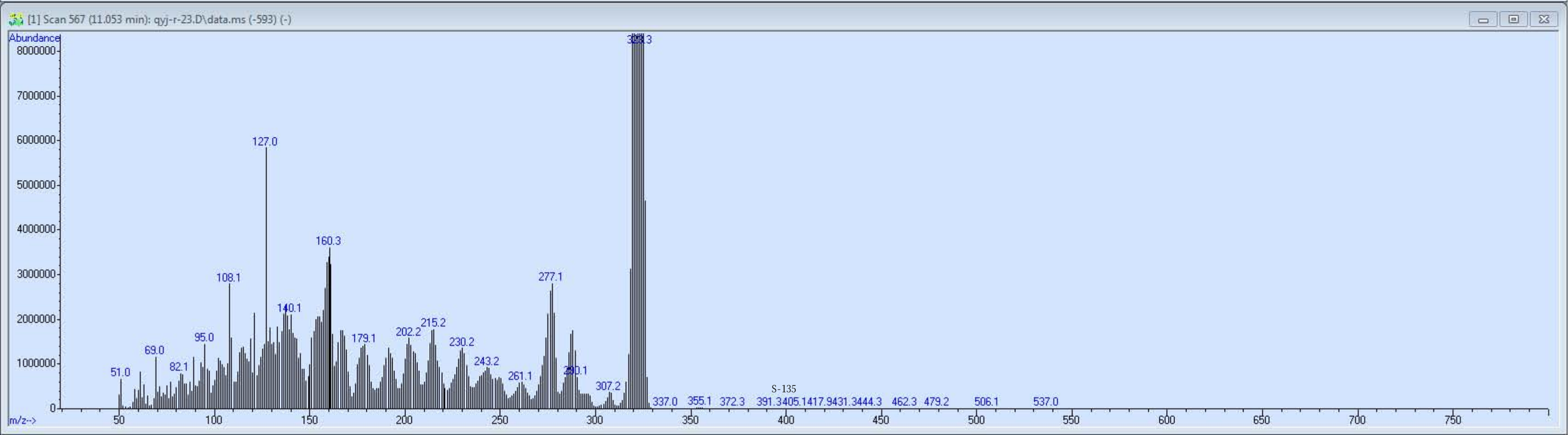

[1] Scan 499 (10.338 min): qyj-r-35.D\data.ms (-534) (-)
Abundance
298.1
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
m/z-->
51.0
69.0
93.0
107.0
126.0
140.0
153.0
179.1
205.1
218.1
236.1
251.1
264.1
280.9
312.0
331.2
355.1
373.9
389.2
405.0
429.0
462.8
478.9
503.2
519.2
536.8
562.9
599.2
673.4
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750

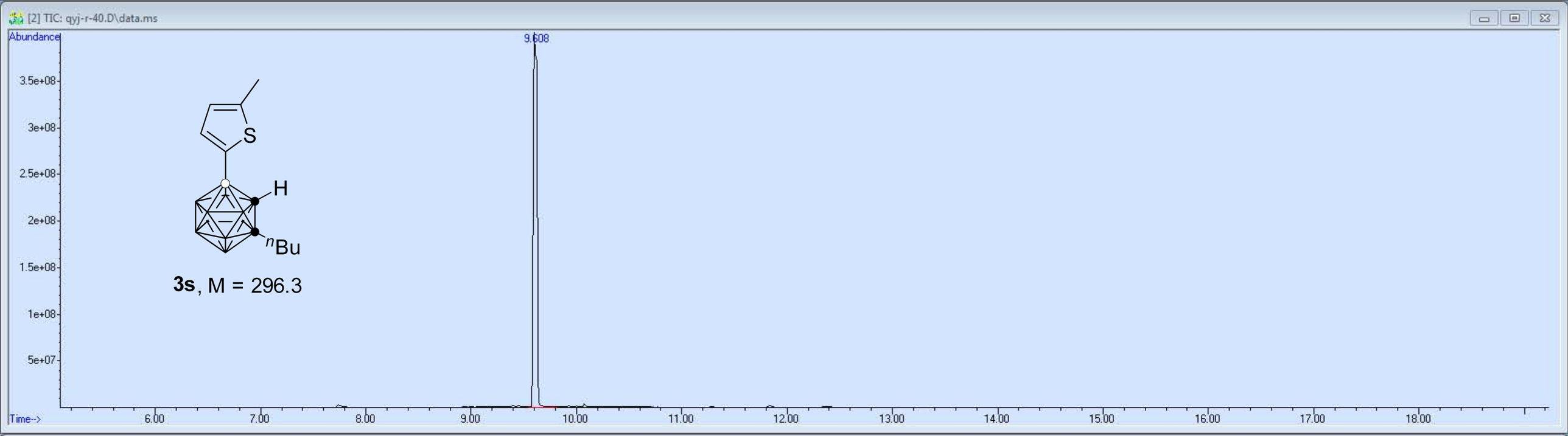

[2] TIC: qyj-r-48-2.D\data.ms
Abundance
11.286
S
S
H
3m, M = 296.2
Time-->

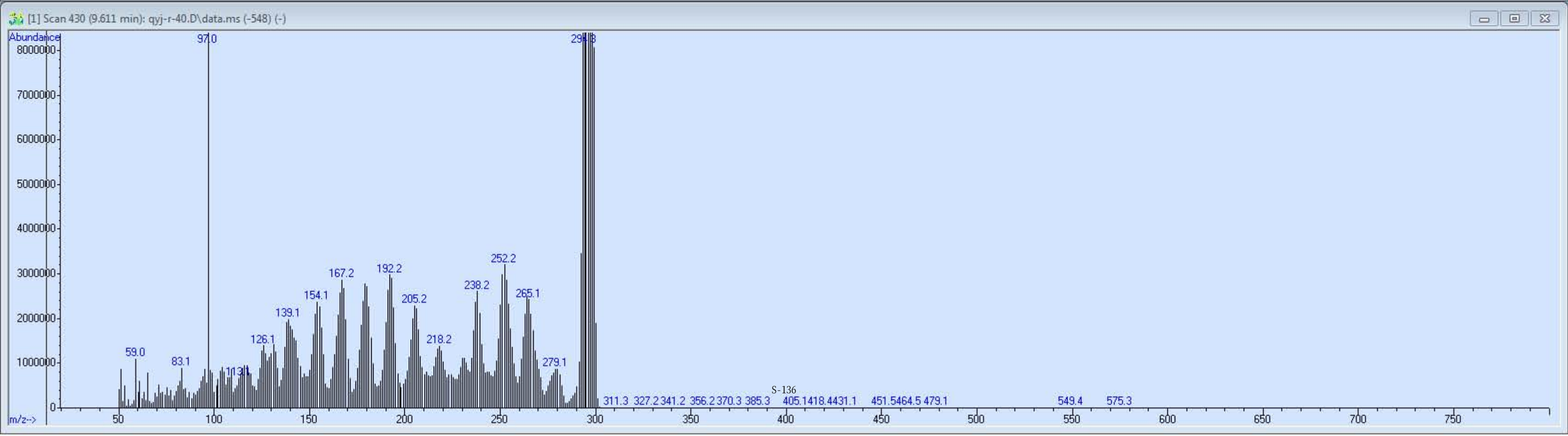

[1] Scan 588 (11.274 min): qyj-r-48-2.D\data.ms
Abundance
296.1
m/z-->

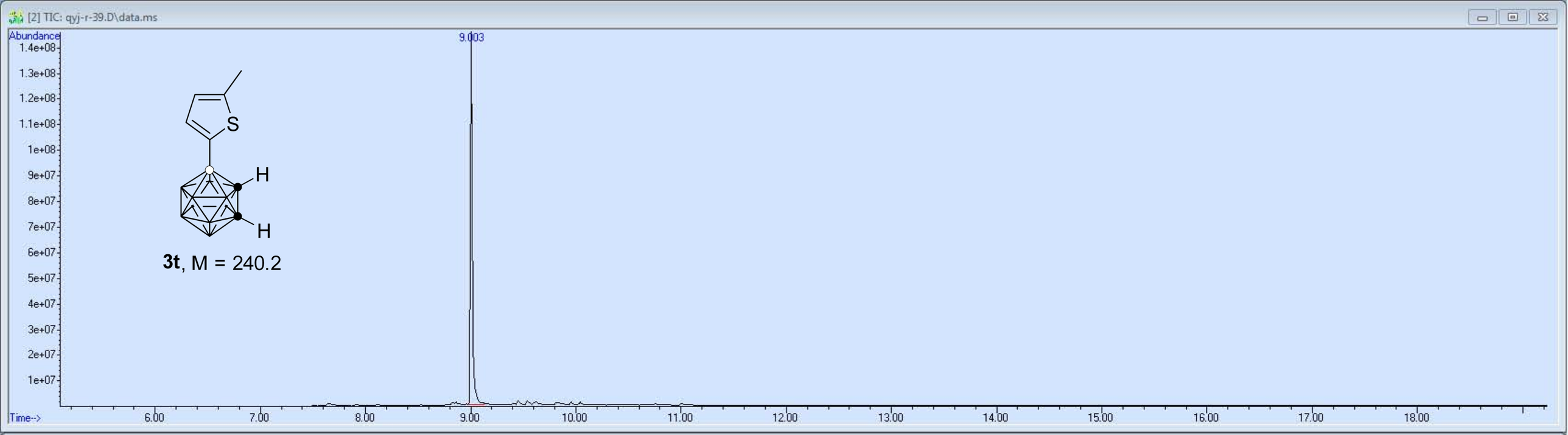

[2] TIC: qyj-r-23.D\data.ms
Abundance
11.052
3.5e+08
3e+08
2.5e+08
2e+08
1.5e+08
1e+08
5e+07
Time-->
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00
S
S
H

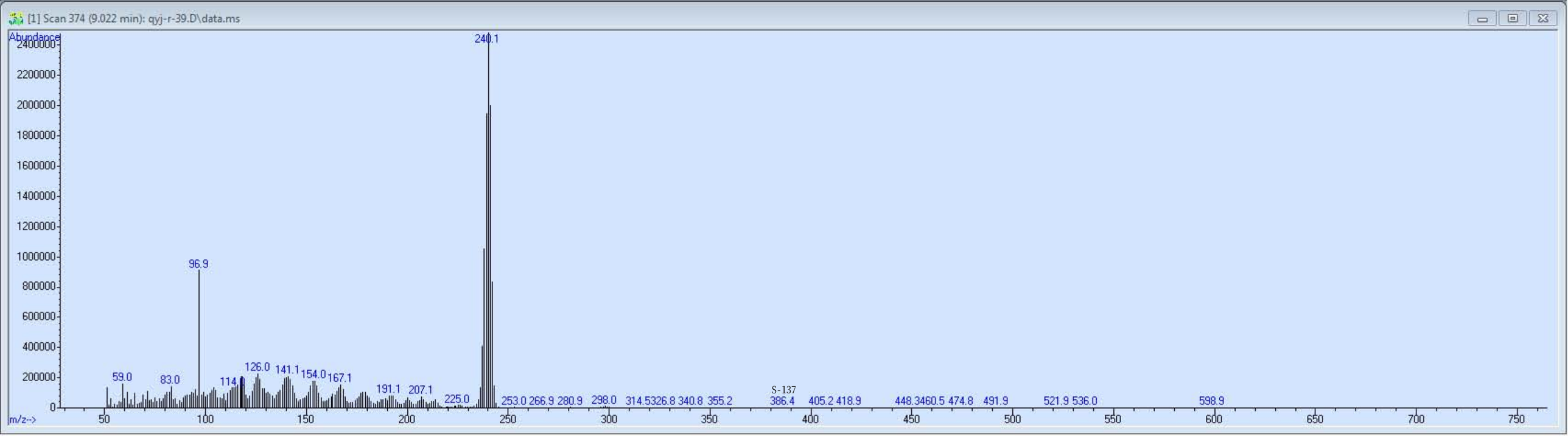
3p, M = 322.2

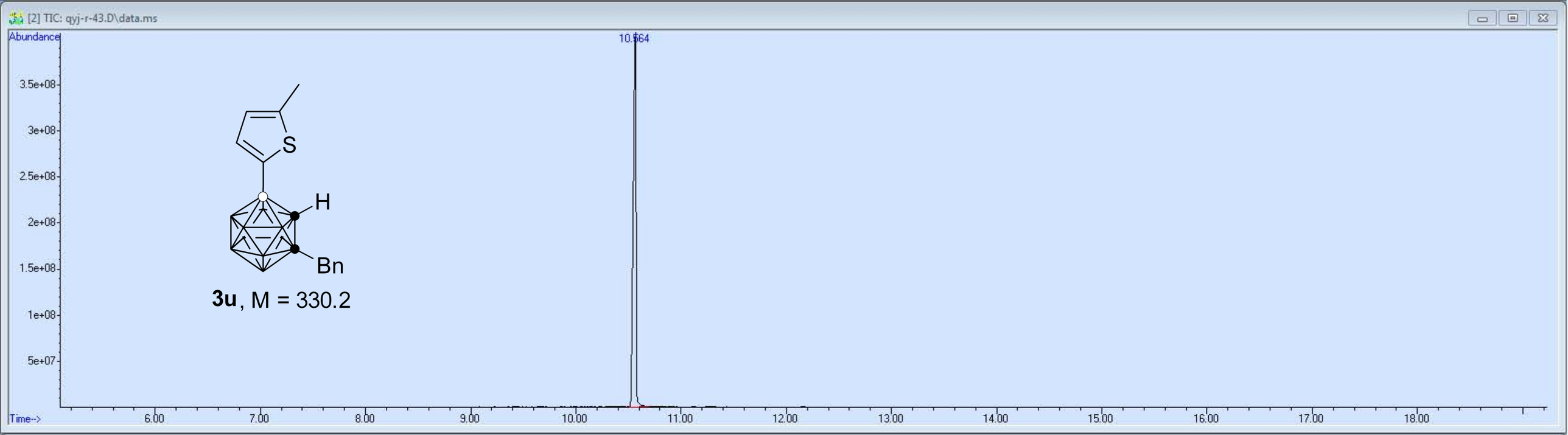

[1] Scan 567 (11.053 min): qyj-r-23.D\data.ms (-593) (-)
Abundance
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
m/z-->
127.0
160.3
108.1
140.1
277.1
179.1
202.2
215.2
230.2
95.0
69.0
82.1
51.0
243.2
261.1
307.2
337.0
355.1
372.3
391.3
405.1
417.9
431.3
444.3
462.3
479.2
506.1
537.0
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750

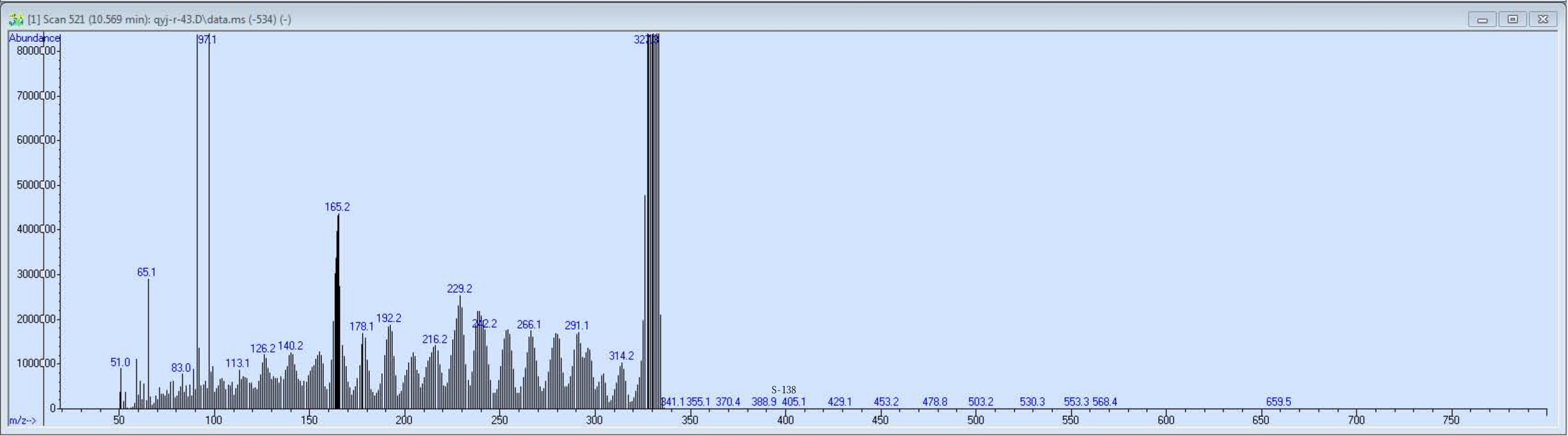

[2] TIC: qyj-r-40.D\data.ms
Abundance
9.608
3.5e+08
3e+08
2.5e+08
2e+08
1.5e+08
1e+08
5e+07
S
H
nBu
3s, M = 296.3
Time-->
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00

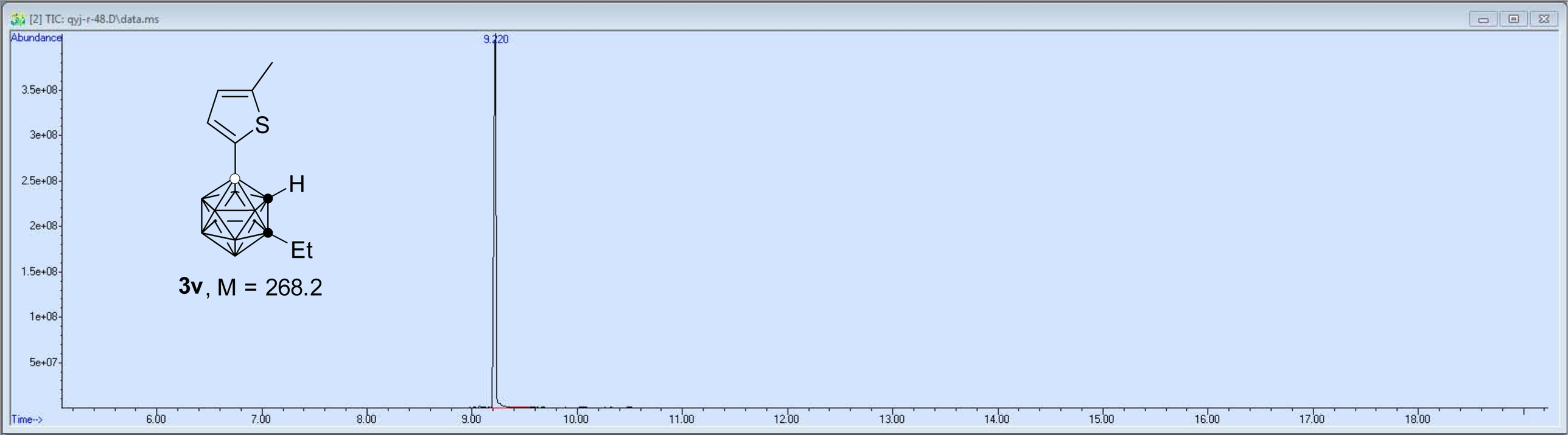

[1] Scan 430 (9.611 min): qyj-r-40.D\data.ms (-548) (-)
Abundance
97.0
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
59.0
83.1
126.1
139.1
154.1
167.2
192.2
205.2
218.2
238.2
252.2
265.1
279.1
311.3 327.2 341.2 356.2 370.3 385.3 405.1 418.4 431.1 451.5 464.5 479.1 549.4 575.3
m/z-->
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750

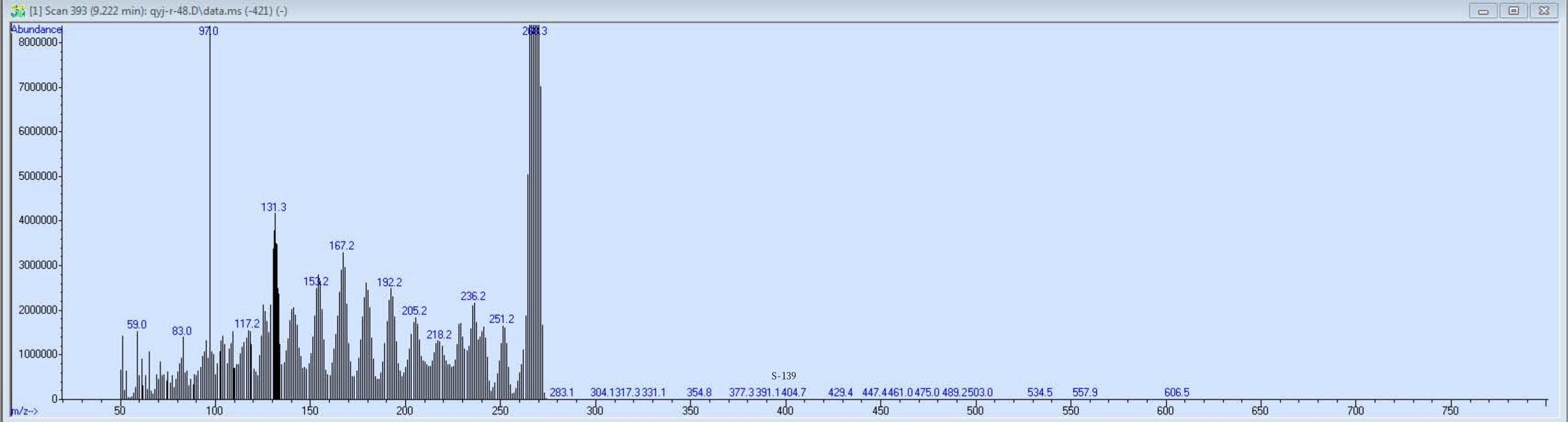

[2] TIC: qyj-r-39.D\data.ms
Abundance
9.003
S
H
H
3t, M = 240.2
Time-->

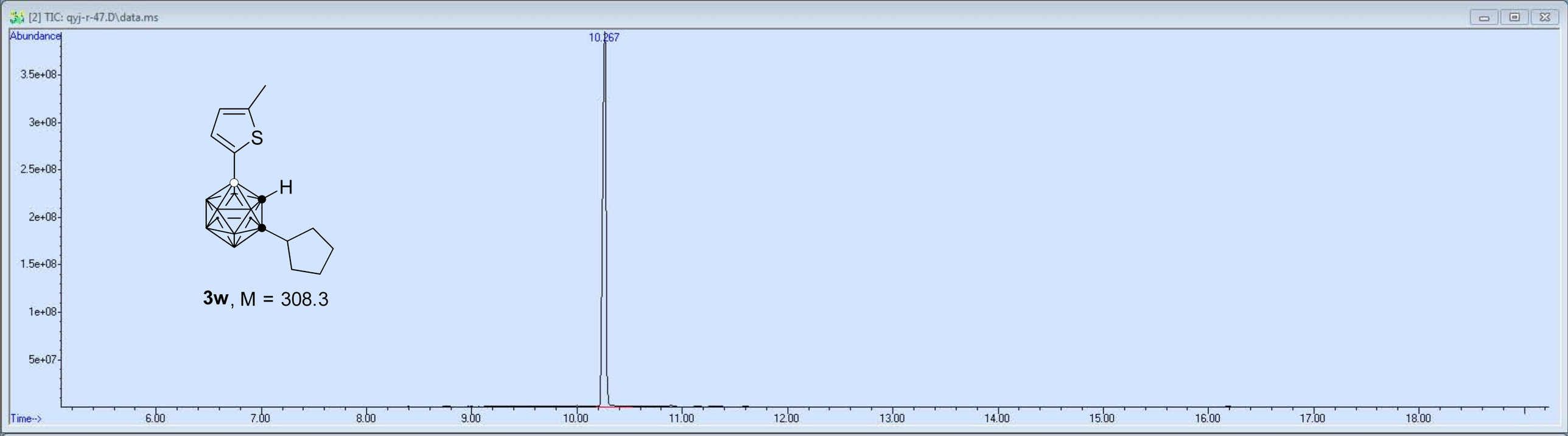

[1] Scan 374 (9.022 min): qyj-r-39.D\data.ms
Abundance
240.1
96.9
59.0
83.0
114.0
126.0
141.1
154.0
167.1
191.1
207.1
225.0
m/z-->


[2] TIC: qyj-r-43.D\data.ms
Abundance
10.564
3.5e+08
3e+08
2.5e+08
2e+08
1.5e+08
1e+08
5e+07
S
H
Bn
3u, M = 330.2
Time-->
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00

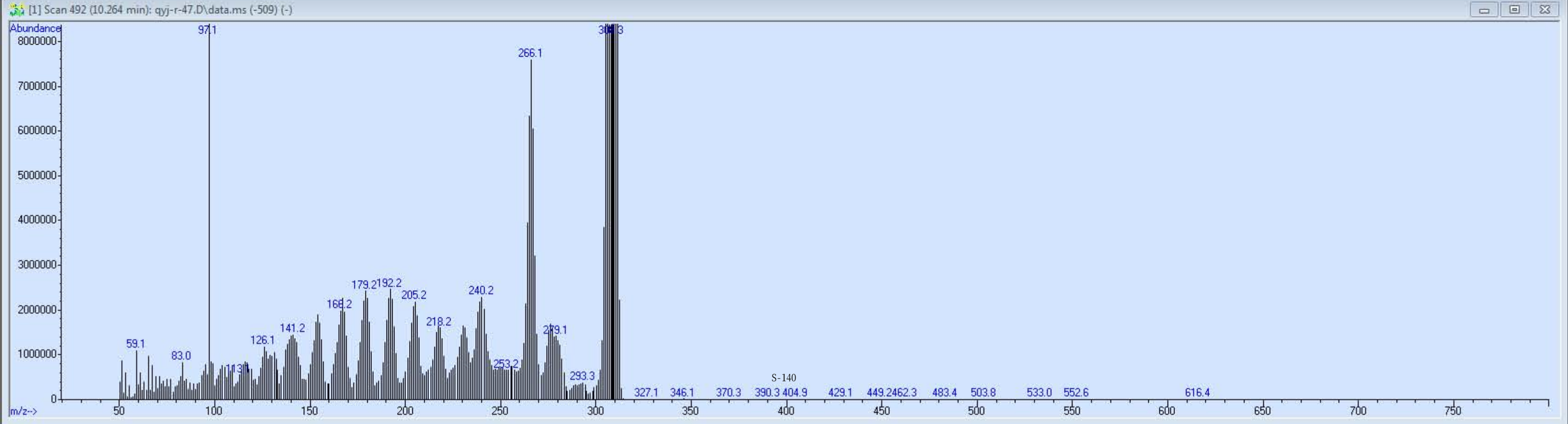

[1] Scan 521 (10.569 min): qyj-r-43.D\data.ms (-534) (-)
Abundance
97.1
321.3
165.2
65.1
229.2
192.2
178.1
216.2
242.2
266.1
291.1
314.2
126.2
140.2
113.1
51.0
83.0
841.1
355.1
370.4
388.9
405.1
429.1
453.2
478.8
503.2
530.3
553.3
568.4
659.5
m/z-->
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750

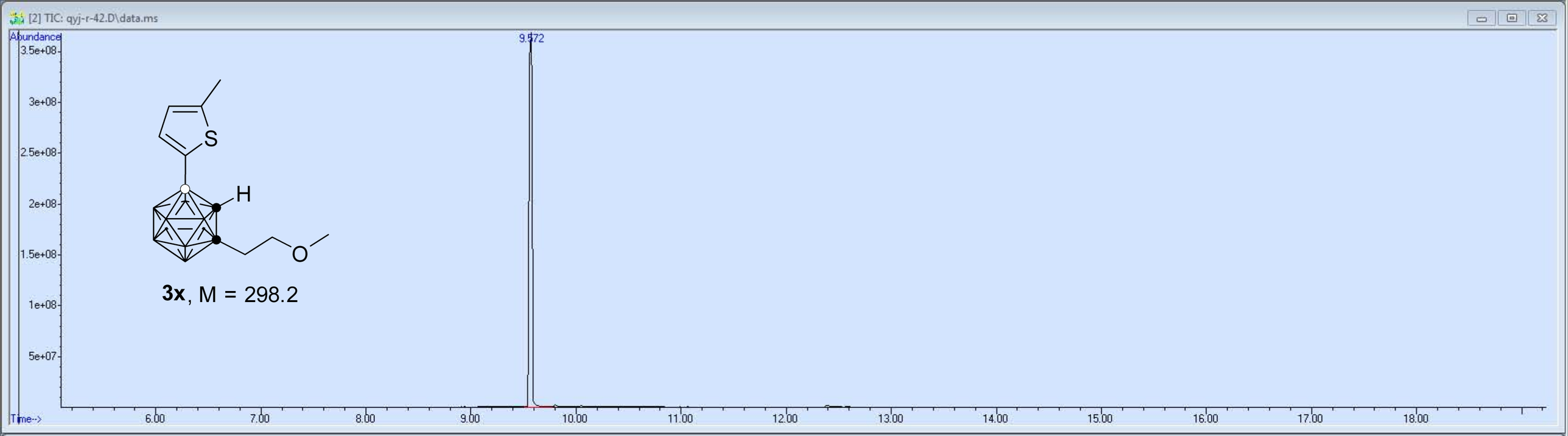

[2] TIC: qyj-r-48.D\data.ms
Abundance
9.220
3.5e+08
3e+08
2.5e+08
2e+08
1.5e+08
1e+08
5e+07
Time-->
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00
S
H
Et
3v, M = 268.2

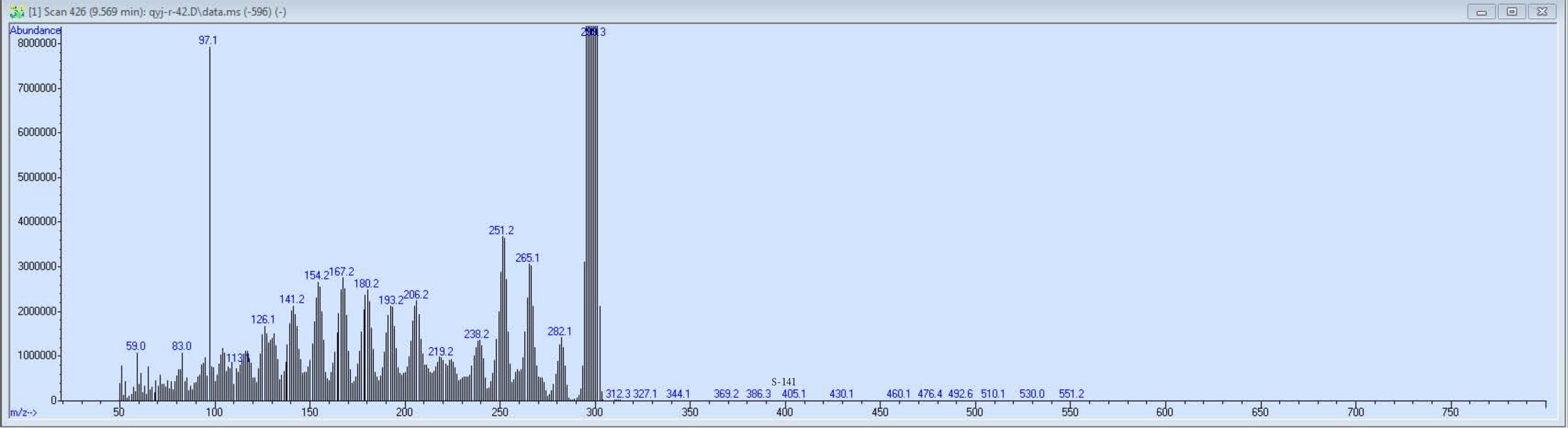

[1] Scan 393 (9.222 min): qyj-r-48.D\data.ms (-421) (-)
Abundance
97.0
131.3
167.2
153.2
192.2
205.2
236.2
251.2
218.2
117.2
59.0
83.0
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
m/z-->
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750

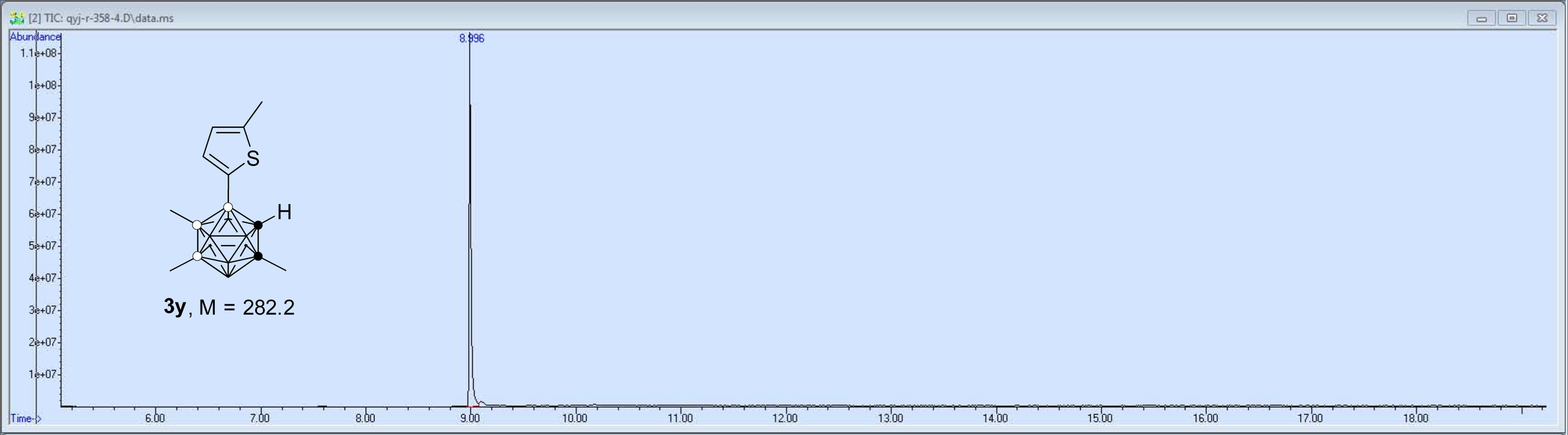

[2] TIC: qyj-r-47.D\data.ms
Abundance
10.267
3.5e+08
3e+08
2.5e+08
2e+08
1.5e+08
1e+08
5e+07
S
H
Time-->
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00

3w, M = 308.3

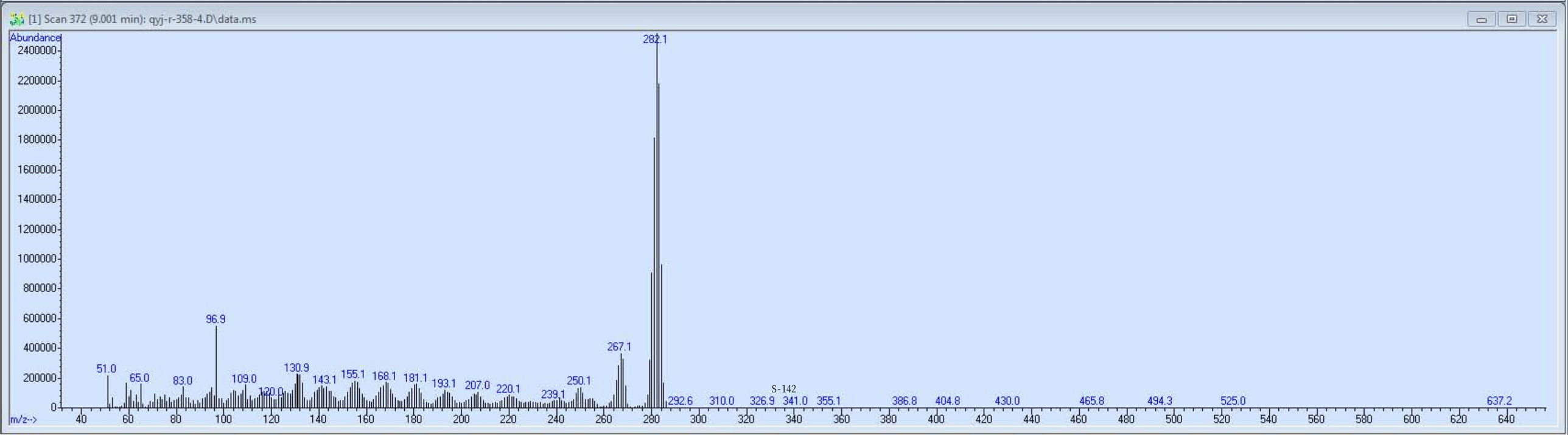

[1] Scan 492 (10.264 min): qyj-r-47.D\data.ms (-509) (-)
Abundance
97.1
308.3
266.1
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
59.1
83.0
126.1
141.2
168.2
179.2
192.2
205.2
218.2
240.2
253.2
279.1
293.3
327.1
346.1
370.3
390.3
404.9
429.1
449.2
462.3
483.4
503.8
533.0
552.6
616.4
m/z-->
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750


[2] TIC: qyj-r-42.D\data.ms
Abundance
9.572
S
H
O
3x, M = 298.2
Time-->


[1] Scan 426 (9.569 min): qyj-r-42.D\data.ms (-596) (-)
Abundance
97.1
251.2
265.1
154.2
167.2
180.2
193.2
206.2
141.2
126.1
59.0
83.0
238.2
219.2
282.1
m/z-->


[2] TIC: qyj-r-358-4.D\data.ms
Abundance
8.996
S
H
Time->

3y, M = 282.2


[1] Scan 372 (9.001 min): qyj-r-358-4.D\data.ms
Abundance
282.1
96.9
267.1
m/z-->