Electronic Supplementary Information

Ir-Catalyzed Selective Dehydrogenative Cross-Coupling of Aryls with *o*-Carboranes via Mixed Directing-Group Strategy

Yu Chen, Yangjian Quan,* and Zuowei Xie*

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

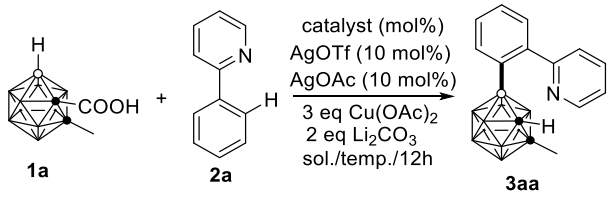
E-mail: yjquan@cuhk.edu.hk, zxie@cuhk.edu.hk

Table of Contents

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

Optimization of Reaction Conditions

Table S1. Screening of the optimal reaction conditions[a]



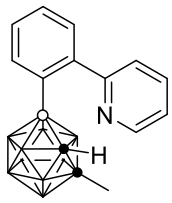
entry	catalyst (mol%)	sol.	temp. (°C)	yield (%)[b]
1	$[Cp^*IrCl_2]_2$ (5)	tol	100	91
2	$[Cp^*IrCl_2]_2$ (5)	tol	110	92
3	$[Cp^*IrCl_2]_2$ (5)	tol	120	95
4	$[Cp^*IrCl_2]_2$ (5)	tol	130	99 (90[c])
5	$[Cp^*IrCl_2]_2$ (5)	tol	140	89
6[d]	$[Cp^*IrCl_2]_2$ (5)	tol	130	93
7[e]	$[Cp^*IrCl_2]_2$ (5)	tol	130	63
8	$[Cp^*IrCl_2]_2$ (5)	OX	130	84
9	$[Cp^*IrCl_2]_2$ (5)	DCE	130	68
10[f]	$[Cp^*IrCl_2]_2$ (2.5)	tol	130	75
11	-	tol	130	0
12	$[Cp^*RhCl_2]_2$ (5)	tol	130	0
13	$Pd(OAc)_2$ (10)	tol	130	0
14	$[RuCl_2(p\text{-cymene})]_2$ (5)	tol	130	0
15[g]	$[Cp^*IrCl_2]_2$ (5)	tol	130	0
16[h]	$[Cp^*IrCl_2]_2$ (5)	tol	130	22

[a]Reactions were conducted on 0.05 mmol scale in toluene (3 mL) in a closed flask; tol = tolunene, OX = *o*-xylene, DCE = 1,2-dichloroethane. [b]GC yield. [c]Isolated yield. [d]20 mol% AgOTf was used as the sole silver salt. [e]20 mol% AgOAc was used as the sole silver salt. [f]5 mol% AgOTf and 5 mol% AgOAc were added. [g]1-Methyl-*o*-carborane was used as the feedstock. [h]The reaction was carried out in air.

General Procedures

Preparation of B(4)-arylated carborane derivatives (**3** and **4**)

A representative procedure. 1-COOH-2-CH_3-*o*-carborane (**1a**; 20.2 mg, 0.10 mmol), 2-phenylpyridine (**2a**; 15.5 mg, 0.10 mmol), $[Cp^*IrCl_2]_2$ (4.0 mg, 0.005 mmol), AgOTf (2.6 mg, 0.01 mmol), AgOAc (1.7 mg, 0.01 mmol), Li_2CO_3 (14.8 mg, 0.20 mmol) and $Cu(OAc)_2$ (54.6 mg, 0.30 mmol) were mixed in dry toluene (5 mL) in a sealed flask. The reaction mixture was heated at 130 ºC (bath temperature) for 12 h under Argon. The resulting reaction mixture was cooled to room temperature. After filtration, the solid was washed with dichloromethane (5 mL x 3). The organic portions were combined and concentrated under reduced pressure. The residue was then subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (50/1 to 10/1 in V/V) as eluent to give **3aa** (27.9 mg, 90%).



3aa: Yield 90%. Colorless crystals. Mp: 141–142 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, *J* = 4.4 Hz, 1H), 7.83 (dd, *J* = 6.4, 2.4 Hz, 1H), 7.76 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.37 (m, 4H), 7.19 (dd, *J* = 4.9, 2.4 Hz, 1H) (aryl C*H*), 3.96 (s, 1H) (Cage C*H*), 1.88 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.5, 147.9, 145.2, 137.3, 136.7, 129.6, 128.0, 127.7, 125.2, 122.6 (aryl *C*), 70.3, 63.5 (Cage *C*), 26.1 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.78 (2B), -6.70 (1B), -9.08 (1B), -10.84 (1B), -12.58 (4B), -13.53 (1B). HRMS (ESI): *m/z* calcd for $C_{14}H_{21}{}^{10}B_2{}^{11}B_8N$ $[M+H]^+$: 312.2750. Found: 312.2747.

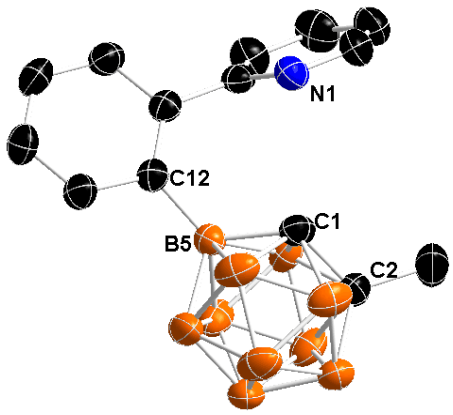
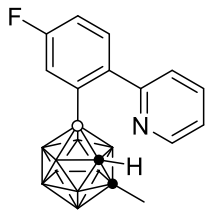
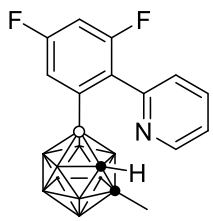


Figure S1. Molecular Structure of **3aa**.

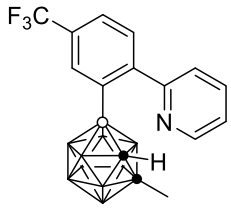


3ab: Yield 87%. Pale yellow solid. Mp: 132–133 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, J = 4.8 Hz, 1H), 7.77 (ddd, J = 7.7, 7.7, 1.8 Hz, 1H), 7.53 (dd, J = 10.4, 2.4 Hz, 1H), 7.40 (d, J = 7.8 Hz, 1H), 7.33 (dd, J = 7.5, 4.9 Hz, 1H), 7.16 (dd, J = 8.4, 5.7 Hz, 1H), 7.03 (ddd, J = 8.2, 8.2, 2.7 Hz, 1H) (aryl C*H*), 4.00 (s, 1H) (Cage C*H*), 1.88 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.1 (d, $^{1}J_{C\text{-}F}$ = 245.9 Hz), 161.6, 147.9, 141.2 (d, $^{4}J_{C\text{-}F}$ = 3.1 Hz), 136.8, 131.6 (d, $^{3}J_{C\text{-}F}$ = 7.7 Hz), 125.4, 123.6 (d, $^{2}J_{C\text{-}F}$ = 21.0 Hz), 122.8, 114.8 (d, $^{2}J_{C\text{-}F}$ = 21.0 Hz) (aryl *C*), 70.4, 63.5 (Cage *C*), 26.0 (CH_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.85 (1B), -4.12 (1B), -6.01 (1B), -8.38 (1B), -10.03 (1B), -11.87 (5B). ^{19}F NMR (376 MHz, CD_2Cl_2): δ -115.61 (s, 1F). HRMS (ESI): *m/z* calcd for $C_{14}H_{20}{}^{10}B_2{}^{11}B_8NF$ $[M+Na]^+$: 352.2475. Found: 352.2473.

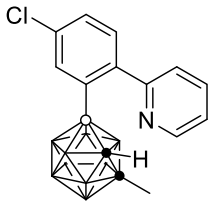


3ac: Yield 87%. Pale yellow solid. Mp: 128–129 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.64 (d, J = 4.9 Hz, 1H), 7.79 (ddd, J = 7.7, 7.7, 1.8 Hz, 1H), 7.38 (m, 3H), 6.85 (ddd, J = 8.8, 8.8, 2.5 Hz, 1H) (aryl C*H*), 3.58 (s, 1H) (Cage C*H*), 1.85 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.0 (dd, $^{1,3}J_{C\text{-}F}$ = 248.2, 12.0 Hz), 160.2 (dd, $^{1,3}J_{C\text{-}F}$ = 245.5, 11.6 Hz), 155.1, 148.8, 136.5, 128.4 (dd, $^{2,4}J_{C\text{-}F}$ = 15.7, 3.7 Hz), 127.0, 123.5, 119.4 (dd, $^{2,4}J_{C\text{-}F}$ = 20.5, 3.4 Hz), 103.7 (dd,

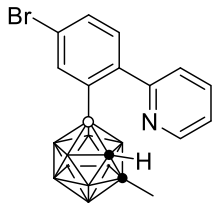
$^{2,2}J_{C\text{-}F}$ = 26.5, 25.3 Hz) (aryl *C*), 70.5, 62.9 (Cage *C*), 26.0 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, CDCl$_3$): δ -2.97 (1B), -4.86 (1B), -6.28 (1B), -8.65 (1B), -10.11 (1B), -12.15 (5B). ^{19}F NMR (376 MHz, CD$_2$Cl$_2$): δ -110.48 (s, 1F), -111.26 (s, 1F). HRMS (ESI): *m/z* calcd for $C_{14}H_{19}{}^{10}B_2{}^{11}B_8NF_2$ [M+Na]$^+$: 370.2381. Found: 329.2379.



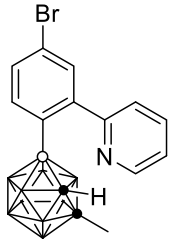
3ad: Yield 91%. White solid. Mp: 144–145 °C. ^{1}H NMR (400 MHz, CDCl$_3$): δ 8.60 (d, *J* = 4.4 Hz, 1H), 8.08 (s, 1H), 7.80 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.37 (m, 3H) (aryl C*H*), 3.95 (s, 1H) (Cage C*H*), 1.89 (s, 3H) (C*H*$_3$). ^{13}C NMR (100 MHz, CDCl$_3$): δ 161.2, 148.5, 148.2, 137.0, 133.8 (q, $^3J_{C\text{-}F}$ = 4.0 Hz), 130.1, 129.8 (q, $^2J_{C\text{-}F}$ = 30.7 Hz), 125.0, 124.8 (q, $^3J_{C\text{-}F}$ = 3.7 Hz) (aryl *C*), 124.4 (q, $^1J_{C\text{-}F}$ = 270.7 Hz) (*C*F$_3$), 123.2 (aryl *C*), 70.6, 63.5 (Cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, CDCl$_3$): δ -2.71 (1B), -4.12 (1B), -5.95 (1B), -8.34 (1B), -9.92 (1B), -11.83 (5B). ^{19}F NMR (376 MHz, CD$_2$Cl$_2$): δ -62.45 (s, 3F). HRMS (ESI): *m/z* calcd for $C_{15}H_{20}{}^{10}B_2{}^{11}B_8NF_3$ [M+Na]$^+$: 380.2624. Found: 380.2618.



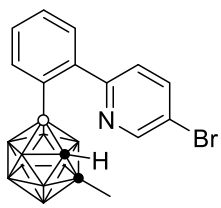
3ae: Yield 88%. White solid. Mp: 110–111 °C. ^{1}H NMR (500 MHz, CDCl$_3$): δ 8.58 (d, *J* = 4.6 Hz, 1H), 7.80 (m, 2H), 7.40 (dd, *J* = 7.8 Hz, 1H), 7.35 (m, 2H), 7.12 (d, *J* = 8.1 Hz, 1H) (aryl C*H*), 4.04 (s, 1H) (Cage C*H*), 1.89 (s, 3H) (C*H*$_3$). ^{13}C NMR (125 MHz, CDCl$_3$): δ 161.2, 147.7, 143.2, 137.2, 136.9, 134.2, 131.1, 128.1, 125.5, 123.0 (aryl *C*), 70.6, 63.5 (Cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (160 MHz, CDCl$_3$): δ -2.57 (1B), -4.07 (1B), -5.82 (1B), -8.22 (1B), -9.78 (1B), -11.79 (5B). HRMS (APCI): *m/z* calcd for $C_{14}H_{20}{}^{10}B_2{}^{11}B_8NCl$ [M]$^-$: 346.2276. Found: 346.2274.



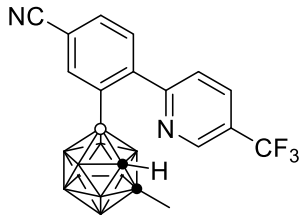
3af: Yield 68%. White solid. Mp: 115−116 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, *J* = 4.8 Hz, 1H), 7.94 (d, *J* = 1.8 Hz, 1H), 7.77 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.48 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.35 (m, 2H), 7.06 (d, *J* = 8.2 Hz, 1H) (aryl C*H*), 3.99 (s, 1H) (Cage C*H*), 1.88 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.4, 148.0, 144.0, 139.7, 136.9, 131.4, 131.0, 125.2, 122.9, 122.5 (aryl *C*), 70.5, 63.5 (Cage *C*), 26.1 (*C*H$_3$).^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.86 (1B), -4.36 (1B), -6.08 (1B), -8.46 (1B), -10.05 (1B), -11.98 (5B). HRMS (ESI): *m/z* calcd for $C_{14}H_{20}{}^{10}B_2{}^{11}B_8NBr$ $[M+H]^+$: 391.1836. Found: 391.1837.



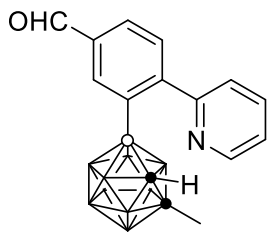
3ag: Yield 77%. White solid. Mp: 112−113 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, *J* = 4.9 Hz, 1H), 7.78 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.68 (d, *J* = 8.3 Hz, 1H), 7.49 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.34 (m, 2H) (aryl C*H*), 3.93 (s, 1H) (Cage C*H*), 1.87 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.0, 148.1, 146.8, 139.0, 136.9, 132.4, 130.7, 125.1, 123.1, 122.5 (aryl *C*), 70.4, 63.4 (Cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.06 (1B), -4.05 (1B), -6.22 (1B), -8.60 (1B), -10.18 (1B), -12.14 (5B). HRMS (ESI): *m/z* calcd for $C_{14}H_{20}{}^{10}B_2{}^{11}B_8NBr$ $[M+H]^+$: 391.1836. Found: 391.1831.



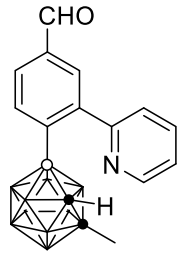
3ah: Yield 81%. White solid. Mp: 107−108 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.65 (d, *J* = 2.3 Hz, 1H), 7.89 (dd, *J* = 8.3, 2.4 Hz, 1H), 7.83 (dd, *J* = 5.8, 3.0 Hz, 1H), 7.37 (m, 2H), 7.33 (d, *J* = 8.3 Hz, 1H), 7.16 (dd, *J* = 7.1, 2.9 Hz, 1H) (aryl C*H*), 4.08 (s, 1H) (Cage C*H*), 1.94 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.9, 148.9, 144.3, 139.3, 137.3, 129.7, 128.2, 128.0, 126.6, 119.8 (aryl *C*), 70.6, 63.6 (Cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.78 (2B), -6.70 (1B), -9.08 (1B), -10.84 (1B), -12.58 (4B), -13.53 (1B). HRMS (ESI): *m/z* calcd for $C_{14}H_{20}{}^{10}B_2{}^{11}B_8NBr$ $[M+H]^+$: 392.1836. Found: 392.1829.



3ai: Yield 84%. Pale yellow solid. Mp: 146–147 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.88 (s, 1H), 8.11 (s, 1H), 8.06 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.56 (d, *J* = 8.2 Hz, 1H), 7.29 (d, *J* = 7.9 Hz, 1H) (aryl C*H*), 4.13 (s, 1H) (Cage C*H*), 1.95 (s, 3H) (C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0, 148.4, 145.3 (q, J_{C-F} = 4.0 Hz), 140.7, 134.2 (q, J_{C-F} = 3.3 Hz), 131.5, 130.4, 126.6 (q, J_{C-F} = 33.5 Hz), 124.8 (aryl *C*), 123.5 (q, J_{C-F} = 269.7 Hz) (*C*F$_3$), 118.7 (*C*N), 112.6 (aryl *C*), 71.1, 63.5 (Cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.32 (1B), -5.02 (1B), -6.12 (1B), -8.68 (1B), -9.79 (1B), -12.03 (5B). ^{19}F NMR (376 MHz, CD_2Cl_2): δ -62.07 (s, 3F). HRMS (ESI): *m/z* calcd for $C_{16}H_{19}{}^{10}B_2{}^{11}B_8N_2F_3$ $[M+Na]^+$: 427.2396. Found: 427.2392.

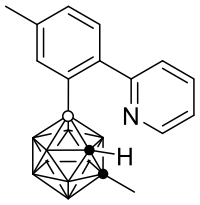


3aj: Yield 81%. White solid. Mp: 170–171 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.07 (s, 1H), 8.60 (d, *J* = 4.6 Hz, 1H), 8.30 (s, 1H), 7.87 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.81 (ddd, *J* = 7.7, 7.7, 1.6 Hz, 1H), 7.39 (m, 3H) (aryl C*H*), 4.01 (s, 1H) (Cage C*H*), 1.90 (s, 3H) (C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.5 (*C*HO), 161.1, 150.8, 148.1, 139.6, 137.0, 135.3, 130.6, 128.4, 125.0, 123.3 (aryl *C*), 70.7, 63.5 (Cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.73 (1B), -5.25 (1B), -7.07 (1B), -9.53 (1B), -11.00 (1B), -12.95 (5B). HRMS (ESI): *m/z* calcd for $C_{15}H_{21}{}^{10}B_2{}^{11}B_8NO$ $[M+Na]^+$: 362.2519. Found: 362.2513.

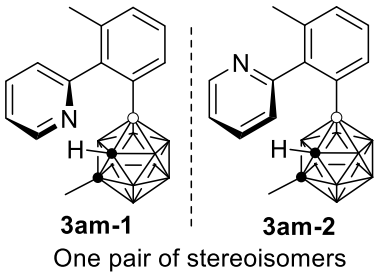


3ak: Yield 76%. White solid. Mp: 165–166 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.01 (s, 1H), 8.59 (d, *J* = 4.5 Hz, 1H), 8.00 (dd, *J* = 7.9 Hz, 1H), 7.82 (m, 2H), 7.69 (s, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.36 (dd, *J* = 7.3, 5.1 Hz, 1H) (aryl C*H*), 3.95 (s, 1H) (Cage C*H*), 1.87 (s, 3H) (C*H*$_3$). ^{13}C NMR (125 MHz, $CDCl_3$): δ 192.1 (*C*HO), 161.1, 148.0, 145.8, 138.1, 137.1, 135.5, 130.4, 128.3, 125.2, 123.2 (aryl *C*), 70.6, 63.4 (Cage *C*), 26.0 (*C*H$_3$). ^{11}B{^{1}H} NMR (160 MHz,

$CDCl_3$): δ -2.48 (1B), -4.02 (1B), -5.71 (1B), -8.08 (1B), -9.69 (1B), -11.70 (5B). HRMS (APCI): *m/z* calcd for $C_{15}H_{21}{}^{10}B_2{}^{11}B_8NO$ $[M+H]^+$: 340.2707. Found: 340.2695.

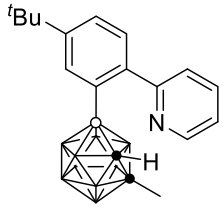


3al: Yield 89%. White solid. Mp: 126–127 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (d, *J* = 4.2 Hz, 1H), 7.74 (ddd, *J* = 7.7, 7.7, 1.7 Hz, 1H), 7.63 (s, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.29 (dd, *J* = 7.3, 4.9 Hz, 1H), 7.17 (d, *J* = 7.7 Hz, 1H), 7.08 (d, *J* = 7.7 Hz, 1H) (aryl C*H*), 4.00 (s, 1H) (Cage C*H*), 2.40 (s, 3H) (Aryl CH_3), 1.88 (s, 3H) (Cage CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.7, 147.8, 142.5, 138.0, 137.1, 136.6, 129.7, 128.7, 125.4, 122.4 (aryl *C*), 70.2, 63.5 (Cage *C*), 26.1, 21.4 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.32 (2B), -6.21 (1B), -8.52 (1B), -10.38 (1B), -12.07 (5B). HRMS (ESI): *m/z* calcd for $C_{15}H_{23}{}^{10}B_2{}^{11}B_8N$ $[M+H]^+$: 326.2907. Found: 326.2900.

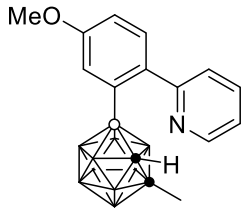


3am: Yield 89%. (Yield of one pair of stereoisomers, resulting from the restricted rotation of pyridyl unit).[2] White solid. Mp: 117–120 °C. For one isomer **3am-1**: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67 (d, *J* = 4.3 Hz, 1H), 7.75 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.62 (d, *J* = 7.4 Hz, 1H), 7.35 (m, 2H), 7.24 (m, 2H) (aryl C*H*), 3.11 (s, 1H) (Cage C*H*), 1.96 (s, 3H) (Cage CH_3), 1.84 (s, 3H) (Aryl CH_3). ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.3, 149, 144.1, 136.7, 135.4, 134.8, 130.2, 127.7, 126.3, 122.6 (aryl *C*), 70.3, 62.6 (Cage *C*), 26.0, 20.6 (*C*H_3). For another isomer **3am-2**: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67 (d, *J* = 4.3 Hz, 1H), 7.75 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.57 (d, *J* = 7.4 Hz, 1H), 7.35 (m, 2H), 7.24 (m, 2H) (aryl C*H*), 2.64 (s, 1H) (Cage C*H*), 1.96 (s, 3H) (Cage CH_3), 1.76 (s, 3H) (Aryl CH_3). ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.2, 148.9, 143.7, 136.5, 135.4, 134.7, 130.1, 127.7, 126.1, 122.6 (aryl *C*), 69.7, 61.8 (Cage *C*), 26.0, 20.5 (*C*H_3). For **3am**: ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -2.95 (2B), -

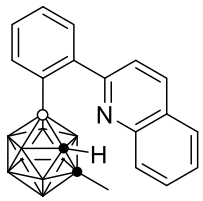
5.93 (1B), -8.11 (1B), -9.81 (1B), -11.25 (5B). HRMS (APCI): *m/z* calcd for $C_{15}H_{23}{}^{10}B_2{}^{11}B_8N$ $[M+H]^+$: 326.2907. Found: 326.2906.



3an: Yield 95%. White solid. Mp: 132–133 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (d, *J* = 4.9 Hz, 1H), 7.90 (s, 1H), 7.75 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.39 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.30 (dd, *J* = 7.5, 4.9 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 1H) (aryl C*H*), 4.01 (s, 1H) (Cage C*H*), 1.88 (s, 3H) (Cage CH_3), 1.37 (s, 9H) (^{t}Bu). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.7, 150.1, 147.8, 142.3, 136.7, 134.8, 129.4, 125.2, 125.0, 122.4 (aryl *C*), 70.2, 63.5 (Cage *C*), 34.8, 31.4 (^{t}Bu), 26.1 (Cage *C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.26 (2B), -6.11 (1B), -8.43 (1B), -10.35 (1B), -11.99 (5B). HRMS (ESI): *m/z* calcd for $C_{18}H_{29}{}^{10}B_2{}^{11}B_8N$ $[M+Na]^+$: 390.3196. Found: 390.3193.

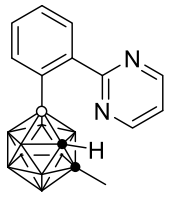


3ao: Yield 66%. Pale yellow solid. Mp: 137–138 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, *J* = 3.5 Hz, 1H), 7.75 (t, *J* = 7.7 Hz, 1H), 7.40 (m, 2H), 7.30 (dd, *J* = 6.1, 6.1 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H) (aryl C*H*), 4.12 (s, 1H) (Cage C*H*), 3.85 (s, 3H) (OCH_3), 1.88 (s, 3H) (Cage CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4, 158.7, 147.8, 138.0, 136.7, 131.2, 125.5, 122.9, 122.4, 113.2 (aryl *C*), 70.2, 63.6 (Cage *C*), 55.4 (O*C*H_3), 26.1 (Cage *C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -4.04 (2B), -7.01 (1B), -9.34 (1B), -11.24 (1B), -12.84 (5B). HRMS (ESI): *m/z* calcd for $C_{15}H_{23}{}^{10}B_2{}^{11}B_8NO$ $[M+H]^+$: 342.2856. Found: 342.2849.



3ap: Yield 59%. Pale yellow solid. Mp: 148–149 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (d, *J* = 8.4 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.91 (m, 2H), 7.75 (dd, *J* = 7.7, 7.7 Hz, 1H), 7.60 (m, 2H), 7.41 (m, 2H), 7.31 (dd, *J* = 5.6, 3.4 Hz, 1H) (aryl C*H*), 4.28 (s, 1H) (Cage C*H*), 1.57 (s, 3H)

(C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6, 146.4, 145.3, 137.7, 136.9, 130.4, 129.5, 128.6, 128.2, 128.1, 127.9, 127.1, 127.0, 123.3 (aryl *C*), 70.2, 63.9 (Cage *C*), 25.7 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -4.29 (2B), -7.24 (1B), -9.48 (1B), -11.41 (1B), -12.97 (5B). HRMS (ESI): *m/z* calcd for $C_{18}H_{23}{}^{10}B_2{}^{11}B_8N$ [M+Na]$^+$: 384.2726. Found: 384.2720.



3aq: Yield 88%. Colorless crystals. Mp: 155–156 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80 (d, *J* = 4.9 Hz, 2H), 7.85 (dd, *J* = 3.8, 3.8 Hz, 1H), 7.40 (m, 3H), 7.32 (dd, *J* = 4.9, 4.9 Hz, 1H) (aryl C*H*), 4.46 (s, 1H) (Cage C*H*), 1.96 (s, 3H) (C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.9, 156.6, 144.2, 137.1, 130.0, 128.3, 128.2, 119.7 (aryl *C*), 70.6, 64.0 (Cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.90 (1B), -3.72 (1B), -5.94 (1B), -8.58 (1B), -10.24 (1B), -12.11 (5B). HRMS (ESI): *m/z* calcd for $C_{13}H_{20}{}^{10}B_2{}^{11}B_8N_2$ [M+Na]$^+$: 335.2522. Found: 335.2520.

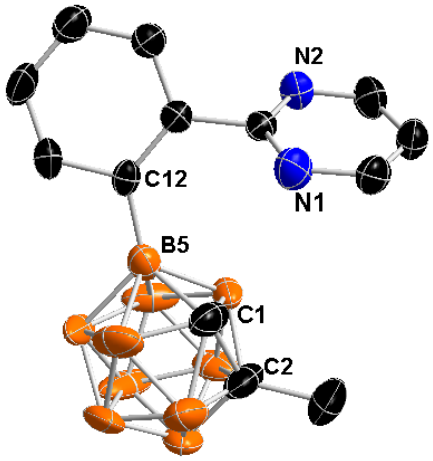
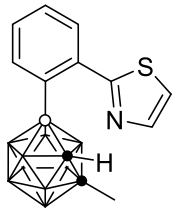
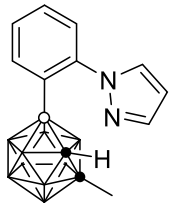


Figure S2. Molecular Structure of **3aq**.



3ar: Yield 81%. White solid. Mp: 100–102 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, *J* = 7.4 Hz, 1H), 7.80 (d, *J* = 3.3 Hz, 1H), 7.47 (d, *J* = 3.4 Hz, 1H), 7.39 (m, 3H) (aryl C*H*), 4.59 (s, 1H) (Cage C*H*), 1.95 (s, 3H) (C*H*$_3$). ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.3, 141.6, 137.7, 137.0, 131.1, 129.1, 128.0, 121.5 (aryl *C*), 70.5, 64.2 (Cage *C*), 26.1 (*C*H$_3$). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$):

δ -3.24 (1B), -4.00 (1B), -6.14 (1B), -8.42 (1B), -10.29 (1B), -11.94 (5B). HRMS (ESI): *m/z* calcd for $C_{12}H_{19}{}^{10}B_2{}^{11}B_8NS$ $[M+Na]^+$: 340.2134. Found: 340.2130.



3as: Yield 72%. Colorless crystals. Mp: 112–113 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 7.2 Hz, 1H), 7.66 (d, *J* = 1.5 Hz, 1H), 7.59 (d, *J* = 2.1 Hz, 1H), 7.41 (m, 2H), 7.17 (dd, *J* = 7.6, 1.3 Hz, 1H), 6.45 (dd, *J* = 2.1, 2.1 Hz, 1H) (aryl C*H*), 3.08 (s, 1H) (Cage C*H*), 1.88 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.5, 139.4, 137.9, 132.4, 129.1, 129.0, 127.9, 106.6 (aryl *C*), 70.1, 62.1 (Cage *C*), 25.9 (CH_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.48 (1B), -4.13 (1B), -5.51 (1B), -7.70 (1B), -9.23 (1B), -10.71 (5B). HRMS (ESI): *m/z* calcd for $C_{12}H_{20}{}^{10}B_2{}^{11}B_8N_2$ $[M+Na]^+$: 323.2522. Found: 323.2519.

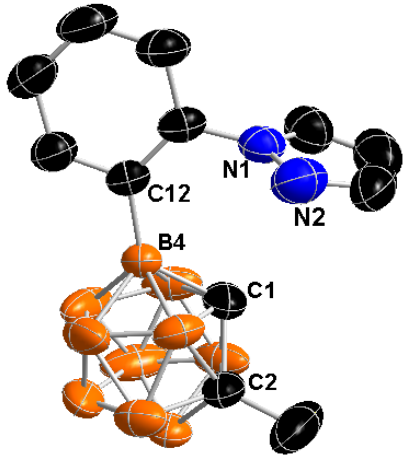
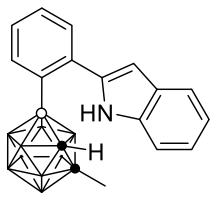


Figure S3. Molecular Structure of **3as**.



3at: Yield 72%. Colorless crystals. Mp: 119–120 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (s, 1H), 7.73 (d, *J* = 7.5 Hz, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.39 (m, 4H), 7.24 (ddd, *J* = 7.2, 7.2, 1.2 Hz, 1H), 7.17 (ddd, *J* = 7.5, 7.5, 1.1 Hz, 1H), 6.49 (d, *J* = 2.1 Hz, 1H) (aryl C*H*), 2.25 (s, 1H) (Cage C*H*), 1.56 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.8, 136.8, 135.5, 134.9, 130.8, 128.5, 127.9, 127.6, 122.7, 120.8, 120.7, 111.0, 102.9 (aryl *C*), 69.6, 61.0 (Cage *C*),

25.8 (CH_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -3.68 (2B), -6.30 (1B), -8.42 (1B), -9.96 (1B), -11.57 (5B). HRMS (ESI): *m/z* calcd for $C_{17}H_{23}{}^{10}B_2{}^{11}B_8N$ $[M+Na]^+$: 372.2726. Found: 372.2728.

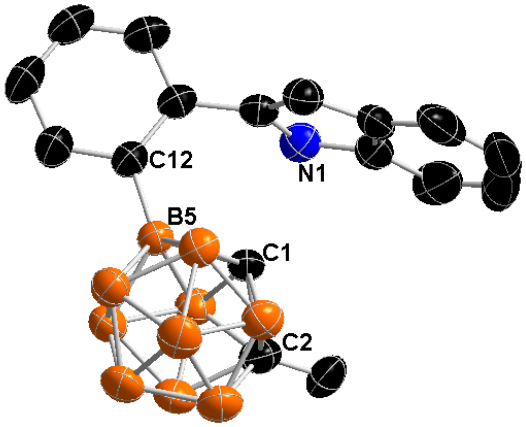
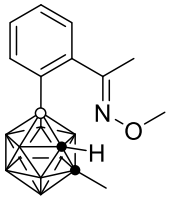
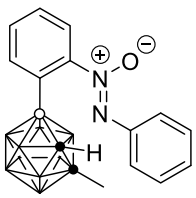


Figure S4. Molecular Structure of **3at**.

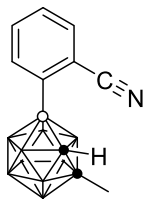


3au: Yield 67%. Pale yellow solid. Mp: 104–105 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 7.0 Hz, 1H), 7.31 (m, 2H), 7.12 (dd, *J* = 7.0, 1.9 Hz, 1H) (aryl C*H*), 4.21 (s, 1H) (Cage C*H*), 3.93 (s, 3H) (OCH_3), 2.19 (s, 3H), 2.07 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.3 (*C*=N), 141.6, 137.3, 128.3, 128.1, 127.9 (aryl *C*), 70.7, 63.6 (Cage *C*), 61.8 (OCH_3), 26.3, 18.2 (CH_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.85 (1B), -3.60 (1B), -5.98 (1B), -8.47 (1B), -9.94 (1B), -11.83 (5B). HRMS (ESI): *m/z* calcd for $C_{12}H_{23}{}^{10}B_2{}^{11}B_8NO$ $[M+Na]^+$: 328.2675. Found: 328.2671.

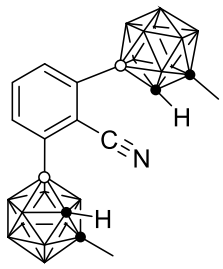


3av: Yield 62%. Pale yellow solid. Mp: 123–124 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 7.5 Hz, 2H), 7.85 (dd, *J* = 3.9, 3.9 Hz, 1H), 7.48 (m, 6H) (aryl C*H*), 4.32 (s, 1H) (Cage C*H*), 1.86 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0, 143.7, 138.2, 130.6, 129.4, 129.3, 129.1, 125.6, 123.3 (aryl *C*), 70.4, 62.5 (Cage *C*), 25.9 (CH_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$):

δ -2.32 (1B), -4.78 (1B), -5.57 (1B), -7.96 (1B), -9.37 (1B), -10.89 (5B). HRMS (ESI): *m/z* calcd for $C_{15}H_{22}{}^{10}B_2{}^{11}B_8N_2O$ $[M+Na]^+$: 377.2628. Found: 377.2623.



3aw: Yield 76%. White solid. Mp: 143−144 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 7.6 Hz, 1H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.54 (ddd, *J* = 7.6, 7.6, 1.3 Hz, 1H), 7.40 (ddd, *J* = 7.6, 7.6, 1.2 Hz, 1H) (aryl C*H*), 4.78 (s, 1H) (Cage C*H*), 2.13 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.9, 133.6, 132.3, 128.6 (aryl *C*), 120.5 (*C*N), 113.3 (aryl *C*), 71.0, 60.8 (Cage *C*), 26.1 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.66 (1B), -4.91 (1B), -6.18 (1B), -8.46 (1B), -9.41 (1B), -11.06 (5B). HRMS (ESI): *m/z* calcd for $C_{10}H_{17}{}^{10}B_2{}^{11}B_8N$ $[M+Na]^+$: 282.2256. Found: 282.2253.



3ax: Yield 57%. Colorless crystals. Mp: 179−180 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 7.7 Hz, 2H), 7.46 (dd, *J* = 7.7, 7.7 Hz, 1H) (aryl C*H*), 4.81 (s, 2H) (Cage C*H*), 2.12 (s, 6H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.9, 131.4 (aryl *C*), 121.9 (*C*N), 113.7 (aryl *C*), 70.8, 60.9 (Cage *C*), 26.2 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.50 (2B), -4.52 (2B), -5.80 (2B), -8.07 (2B), -9.29 (2B), -10.98 (10B). HRMS (ESI): *m/z* calcd for $C_{13}H_{29}{}^{10}B_2{}^{11}B_8N$ $[M+Na]^+$: 438.4199. Found: 438.4196.

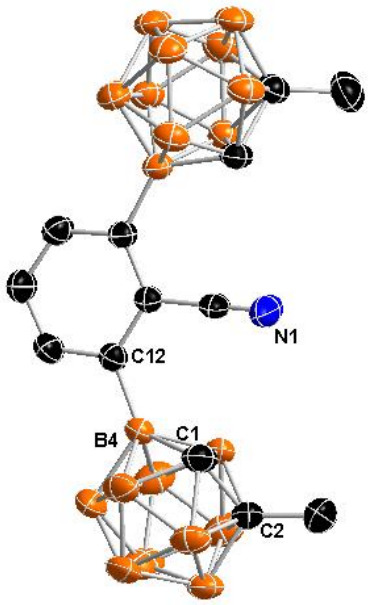
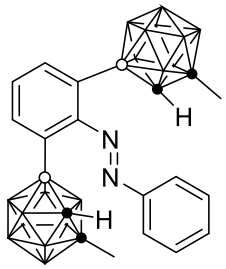


Figure S5. Molecular Structure of **3ax**.



3ay: Yield 74%. Orange crystals. Mp: 183–184 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (m, 2H), 7.71 (d, *J* = 7.6 Hz, 2H), 7.60 (m, 3H), 7.25 (dd, *J* = 7.6, 7.6 Hz, 1H) (aryl C*H*), 3.73 (s, 2H) (Cage C*H*), 1.67 (s, 3H), 1.63 (s, 3H) (CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.9, 150.5, 150.4, 137.5, 132.7, 130.0, 126.6, 123.1 (aryl *C*), 70.6, 70.5, 62.9, 62.8 (Cage *C*), 25.7, 25.6 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.01 (2B), -4.17 (2B), -6.33 (2B), -8.39 (2B), -10.10 (2B), -11.75 (10B). HRMS (ESI): *m/z* calcd for $C_{18}H_{34}{}^{10}B_2{}^{11}B_8N_2$ $[M+Na]^+$: 517.4631. Found: 517.4624.

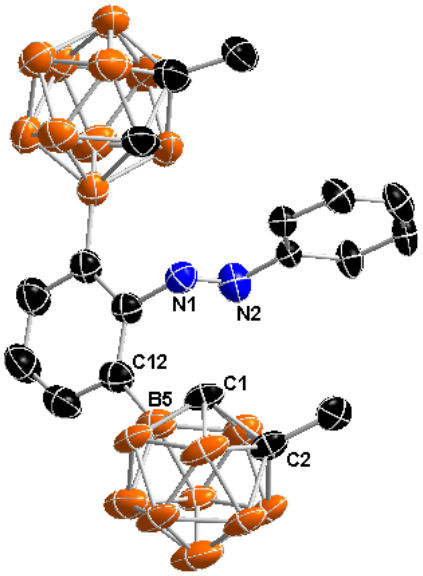
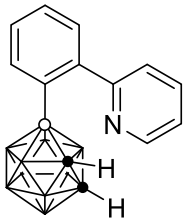
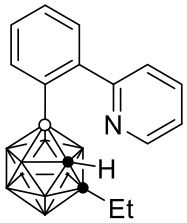


Figure S6. Molecular Structure of **3ay**.

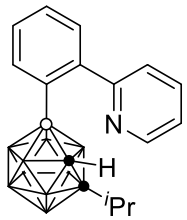


3ba: Yield 51%. White solid. Mp: 159–160 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, *J* = 4.4 Hz, 1H), 7.86 (d, *J* = 5.0 Hz, 1H), 7.75 (ddd, *J* = 7.7, 7.7, 1.7 Hz, 1H), 7.39 (m, 3H), 7.30 (dd, *J* = 7.4, 5.0 Hz, 1H), 7.18 (d, *J* = 5.0 Hz, 1H) (aryl C*H*), 3.96 (s, 1H), 3.46 (s, 1H) (Cage C*H*). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4, 148.1, 145.3, 137.4, 136.7, 129.8, 128.1, 127.7, 125.2, 122.6 (aryl *C*), 56.0, 54.7 (Cage *C*). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.72 (1B), -3.81 (2B), -8.69 (1B), -10.32 (1B), -13.06 (1B), -14.83 (4B). HRMS (ESI): *m/z* calcd for $C_{13}H_{19}{}^{10}B_2{}^{11}B_8N$ $[M+Na]^+$: 320.2413. Found: 320.2411.

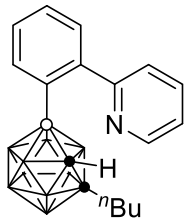


3ca: Yield 93%. White solid. Mp: 133–134 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (d, *J* = 4.9 Hz, 1H), 7.84 (d, *J* = 4.4 Hz, 1H), 7.77 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.35 (m, 3H), 7.17 (d, *J* = 5.0 Hz, 1H) (aryl C*H*), 3.85 (s, 1H) (Cage C*H*), 2.13 (m, 2H), 0.97 (t, *J* = 7.6 Hz, 3H), (Et). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6, 148.0, 145.1, 137.4, 136.7, 129.6, 127.9, 127.7, 125.2, 122.6 (aryl *C*), 76.1, 62.2 (Cage *C*), 31.7 (CH_2CH_3) 13.5

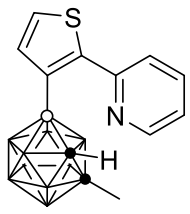
(CH_2CH_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -3.87 (2B), -5.31 (1B), -8.65 (1B), -10.43 (1B), -12.59 (5B). HRMS (ESI): *m/z* calcd for $C_{15}H_{23}{}^{10}B_2{}^{11}B_8N$ $[M+Na]^+$: 348.2726. Found: 348.2721.



3da: Yield 41%. White solid. Mp: 121–122 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 8.58 (d, *J* = 4.7 Hz, 1H), 7.85 (d, *J* = 6.6 Hz, 1H), 7.76 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.34 (m, 4H), 7.15 (d, *J* = 5.9 Hz, 1H) (aryl C*H*), 3.92 (s, 1H) (Cage C*H*), 2.36 (m, 1H), 1.00 (t, *J* = 6.2 Hz, 6H) (^{i}Pr). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6, 148.2, 145.0, 137.4, 136.7, 129.7, 127.9, 127.7, 125.2, 122.5 (aryl *C*), 81.3, 61.2 (Cage *C*), 34.9, 22.9 (^{i}Pr). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -4.44 (3B), -8.68 (1B), -10.37 (1B), -12.91 (5B). HRMS (ESI): *m/z* calcd for $C_{16}H_{25}{}^{10}B_2{}^{11}B_8N$ $[M+Na]^+$: 362.2883. Found: 362.2878.

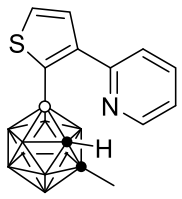


3ea: Yield 73%. White solid. Mp: 109–110 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 8.58 (d, *J* = 4.8 Hz, 1H), 7.84 (dd, *J* = 5.8, 3.1 Hz, 1H), 7.76 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.35 (m, 4H), 7.17 (dd, *J* = 7.1, 2.7 Hz, 1H) (aryl C*H*), 3.87 (s, 1H) (Cage C*H*), 2.05 (m, 2H), 1.26 (m, 4H), 0.89 (t, *J* = 7.0 Hz, 3H) (^{n}Bu). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6, 148.0, 145.1, 137.3, 136.7, 129.6, 127.9, 127.6, 125.2, 122.5 (aryl *C*), 75.4, 62.3 (Cage *C*), 37.9, 31.1, 22.2, 13.8 (^{n}Bu). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -3.84 (2B), -5.13 (1B), -8.62 (1B), -10.35 (1B), -12.46 (5B). HRMS (ESI): *m/z* calcd for $C_{17}H_{27}{}^{10}B_2{}^{11}B_8N$ $[M+Na]^+$: 376.3039. Found: 376.3036.

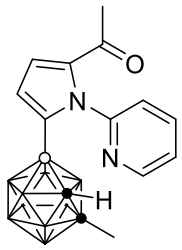


4aa: Yield 81%. White solid. Mp: 117–118 °C. ^1H NMR (500 MHz, $CDCl_3$): δ 8.43 (d, *J* = 4.9 Hz, 1H), 7.61 (ddd, *J* = 7.8, 7.8, 1.8 Hz, 1H), 7.46 (d, *J* = 7.9 Hz, 1H), 7.17 (m, 3H) (aryl C*H*), 4.96 (s, 1H) (Cage C*H*), 1.88 (s, 3H) (CH_3). ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.5, 148.3, 145.2, 136.8, 136.7, 125.4, 125.1, 122.8 (aryl *C*), 70.4, 64.6 (Cage *C*), 26.1 (CH_3). $^{11}B\{^1H\}$ NMR

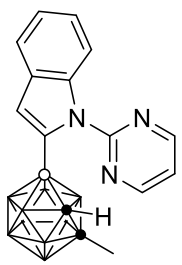
(128 MHz, $CDCl_3$): δ -4.23 (1B), -7.06 (2B), -9.57 (1B), -11.22 (1B), -13.10 (4B), -14.07 (1B). HRMS (APCI): *m/z* calcd for $C_{12}H_{29}{}^{10}B_2{}^{11}B_8NS$ $[M-H]^-$: 316.2175. Found: 316.2170.



4ab: Yield 69%. White solid. Mp: 135–136 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, *J* = 4.4 Hz, 1H), 7.77 (ddd, *J* = 7.8, 7.8, 1.4 Hz, 1H), 7.50 (m, 2H), 7.29 (dd, *J* = 5.7, 5.7 Hz, 1H), 7.20 (d, *J* = 4.9 Hz, 1H) (aryl C*H*), 5.16 (s, 1H) (Cage C*H*), 2.05 (s, 3H) (CH_3). ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.7, 148.0, 145.1, 136.6, 130.6, 129.0, 124.4, 122.3 (aryl *C*), 70.5, 64.5 (Cage *C*), 26.0 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -3.18 (1B), -5.91 (2B), -8.54 (1B), -10.26 (1B), -12.01 (4B), -13.07 (1B). HRMS (APCI): *m/z* calcd for $C_{12}H_{29}{}^{10}B_2{}^{11}B_8NS$ $[M-H]^-$: 316.2175. Found: 316.2171.



4ac: Yield 85%. Pale yellow solid. Mp: 141–142 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 8.52 (d, *J* = 4.9 Hz, 1H), 7.80 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.42 (dd, *J* = 7.4, 4.9 Hz, 1H), 7.31 (d, *J* = 7.9 Hz, 1H), 7.02 (d, *J* = 3.9 Hz, 1H), 6.59 (d, *J* = 3.8 Hz, 1H) (aryl C*H*), 3.81 (s, 1H) (Cage C*H*), 2.37 (s, 3H) (COCH_3), 1.94 (s, 3H) (Cage CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 187.3 (*C*=O), 153.9, 148.2, 138.0, 135.2, 124.6, 124.2, 120.1, 119.6 (aryl *C*), 70.9, 62.8 (Cage *C*), 27.2, 26.0 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -1.97 (1B), -5.77 (1B), -7.00 (1B), -8.54 (1B), -9.57 (1B), -11.05 (5B). HRMS (APCI): *m/z* calcd for $C_{14}H_{24}{}^{10}B_2{}^{11}B_8N_2O$ $[M+H]^+$: 344.2777. Found: 344.2778.

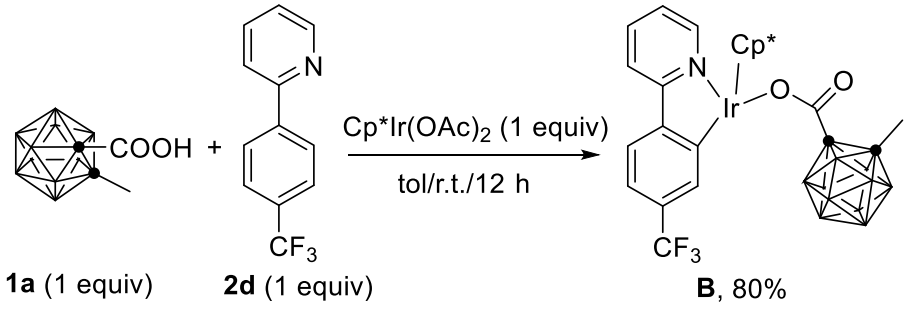


4ad: Yield 90%. White solid. Mp: 179–180 °C. ^1H NMR (500 MHz, $CDCl_3$): δ 8.81 (d, *J* = 8.2 Hz, 1H), 8.67 (d, *J* = 4.8 Hz, 2H), 8.36 (s, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.36 (dd, *J* = 5.7, 5.7 Hz, 1H), 7.29 (dd, *J* = 7.9, 7.9 Hz, 1H), 7.01 (dd, *J* = 4.8, 4.8 Hz, 1H) (aryl C*H*), 3.79 (s, 1H) (Cage C*H*), 2.05 (s, 3H) (CH_3). ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.3, 157.5,

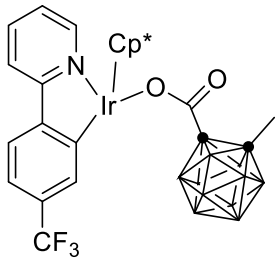
136.4, 134.6, 131.3, 123.8, 122.4, 121.3, 116.5, 116.4 (aryl *C*), 70.6, 63.4 (Cage *C*), 26.1 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.26 (1B), -5.27 (1B), -6.24 (1B), -9.06 (1B), -10.02 (1B), -11.38 (5B). HRMS (APCI): *m/z* calcd for $C_{15}H_{21}{}^{10}B_2{}^{11}B_8N_3$ $[M-H]^-$: 350.2673. Found: 350.2667.

Preliminary mechanistic study

Preparation of Intermediate B. Compound 1a (20.2 mg, 0.10 mmol), 2d (22.3 mg, 0.10 mmol) and Cp*Ir(OAc)2 (44.5 mg, 0.10 mmol) were mixed in dry toluene (5 mL) in a closed flask. The resultant mixture was stirred at room temperature for 12 h. Complex B was isolated as bright yellow crystals via slow evaporation of toluene (59.7 mg, 80%).



Scheme S1. Preparation of Intermediate **B**.



B: Yield 80%. Yellow crystals. Mp: > 250 °C. ^1H NMR (400 MHz, CD_2Cl_2): δ 8.99 (d, *J* = 5.3 Hz, 1H), 8.21 (s, 1H), 7.86 (m, 2H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 7.27 (dd, *J* = 6.5, 6.5 Hz, 1H) (aryl C*H*), 1.67 (s, 15H) (Cp*), 1.25 (s, 3H) (CH_3). ^{13}C NMR (125 MHz, CD_2Cl_2): δ 166.0, 163.2, 162.5, 152.5, 138.3, 131.8 (q, $^3J_{C\text{-}F}$ = 3.8 Hz), 130.8 (q, $^2J_{C\text{-}F}$ = 30.4 Hz) (aryl *C*), 124.6 (q, $^1J_{C\text{-}F}$ = 270.9 Hz) (*C*F_3), 123.3, 123.1, 119.5 (q, $^3J_{C\text{-}F}$ = 3.8 Hz), 119.3 (aryl *C*), 87.7 (*C*$_5$Me$_5$), 77.9, 74.7 (Cage *C*), 23.6 (Cage *C*H_3), 8.9 (C$_5$*Me*$_5$). $^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2): δ -3.95 (1B),

-7.09 (1B), -11.18 (8B). ^{19}F NMR (376 MHz, CD_2Cl_2): δ -62.21 (s, 3F). HRMS (ESI): *m/z* calcd for $C_{26}H_{35}{}^{10}B_2{}^{11}B_8F_3IrNO_2$ $[M-H]^-$: 750.3174. Found: 750.3178.

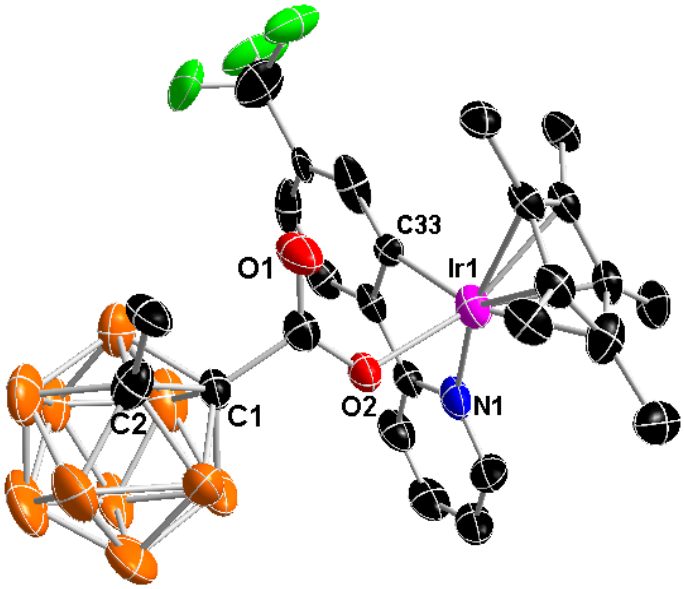


Figure S7. Molecular Structure of Intermediate **B**.

Control experiments using intermediate B as the catalyst. 1-COOH-2-CH_3-*o*-carborane **1a** (20.2 mg, 0.10 mmol), 2-[4-(trifluoromethyl)phenyl]-pyridine **2d** (22.3 mg, 0.10 mmol), **B** (7.5 mg, 0.01 mmol), AgOTf (2.6 mg, 0.01 mmol), AgOAc (1.7 mg, 0.01 mmol), Li_2CO_3 (14.8 mg, 0.20 mmol) and $Cu(OAc)_2$ (54.6 mg, 0.30 mmol) were mixed in dry toluene (5 mL) in a sealed flask. The reaction mixture was heated at 130 °C for 12 h under Argon. The resulting reaction mixture was cooled to room temperature. After filtration, the solid was washed with dichloromethane (5 mL x 3). The organic portions were combined and concentrated under reduced pressure. The residue was then subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (50/1 to 10/1 in V/V) as eluent to give **3ad** (29.3 mg, 77%).

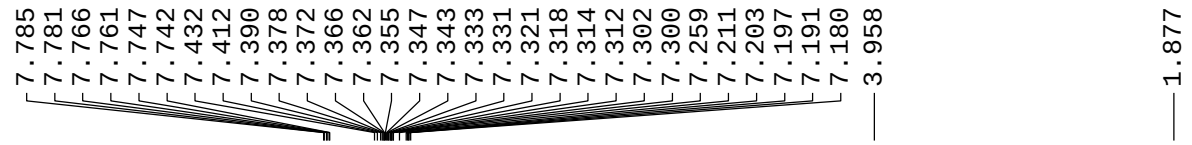
Transformation of intermediate B in toluene with different additives.

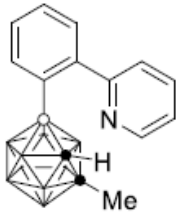
Intermediate **B** (75.1 mg, 0.10 mmol), Li_2CO_3 (14.8 mg, 0.20 mmol), and/or $Cu(OAc)_2$ (54.6 mg. 0.30 mmol), LiOTf (46.8 mg. 0.30 mmol), $Cu(OTf)_2$ (108.5 mg. 0.30 mmol) were mixed in dry toluene (5 mL) in a sealed flask. The reaction mixture was heated at 130 ^oC for 12 h under Argon. The resulting reaction mixture was cooled to room temperature, filtered and washed with dichloromethane (5 mL x 3). The organic portions were combined and concentrated under reduced pressure. The residue was then subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (50/1 to 10/1 in V/V) as eluent to give the product **3ad**.

X-ray Structure Determination. X-ray data of **3aa**, **3aq**, **3as**, **3at**, **3ax**, **3ay** and **B** 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.[3] 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.[4] All hydrogen atoms were geometrically fixed using the riding model.

CCDC 1987436-1987442 for **3aa**, **3aq**, **3as**, **3at**, **3ax**, **3ay** and **B** contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

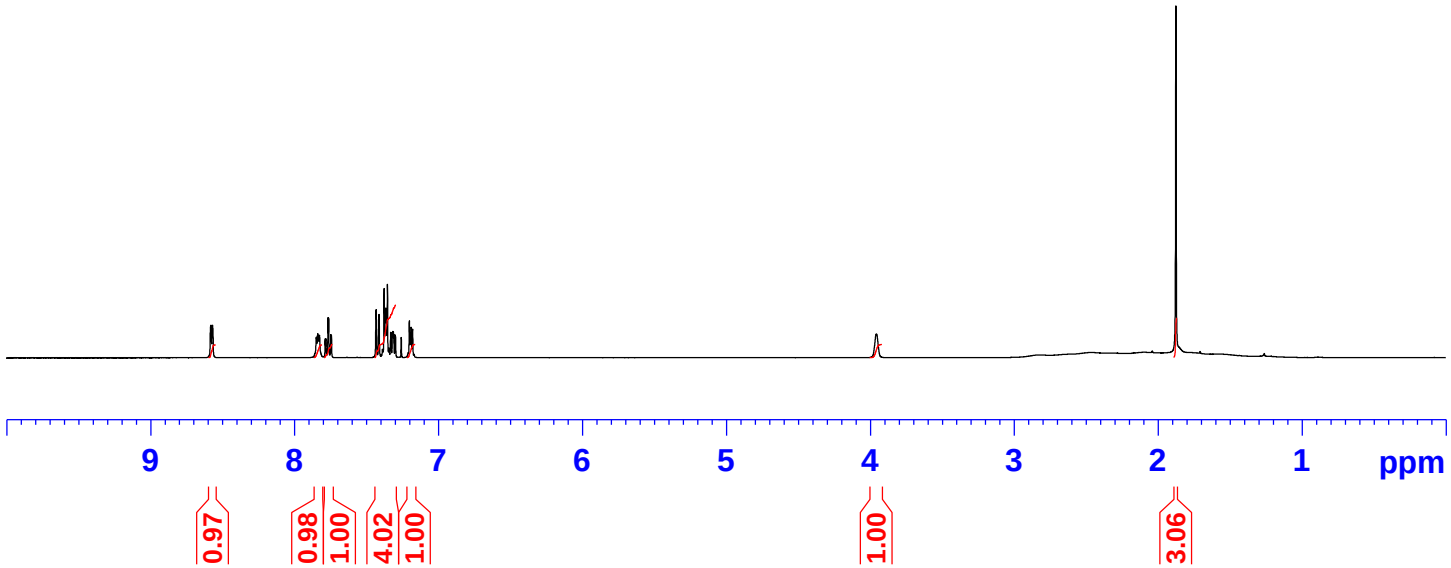
CY-H-A-01p-CDCl3-re

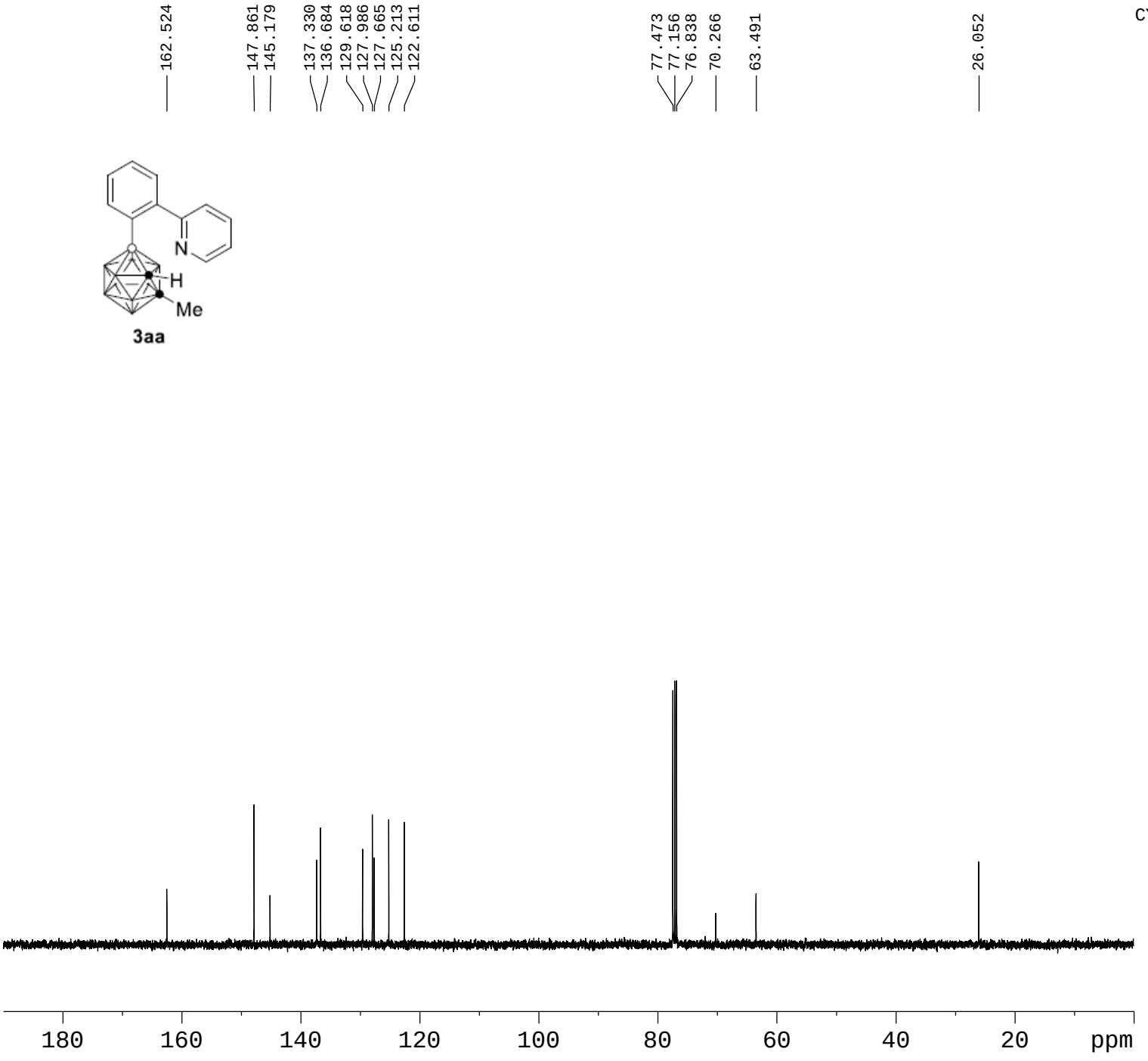




3aa

```
Current Data Parameters
NAME      CY-H-A-01p-CDCl3-re
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20161128
Time                13.45 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                 294.3 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            400.1300101 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```





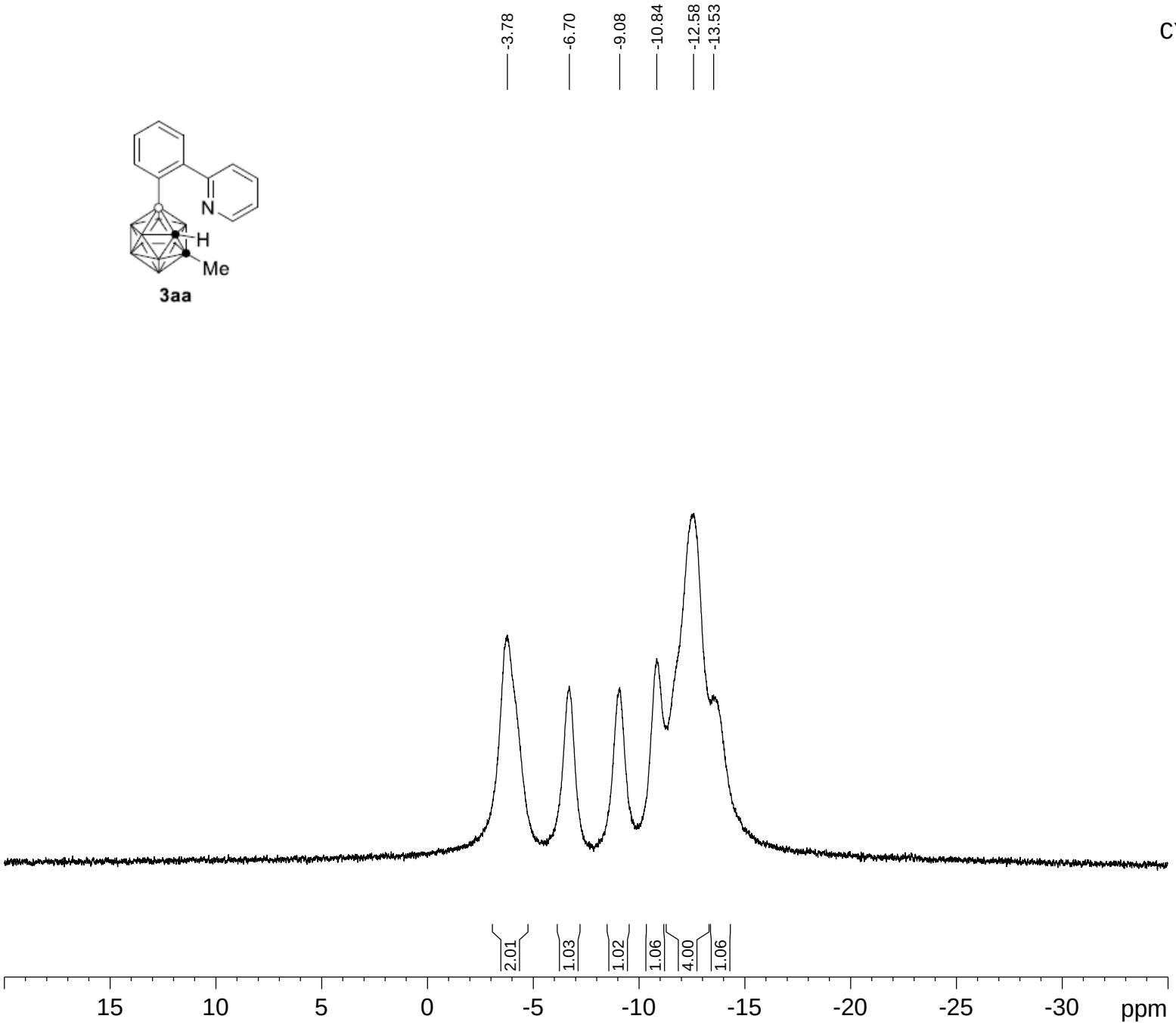
CY-C-A-01P-CDCl3-re

Bruker Advance III 400

Current Data Parameters
NAME CY-C-A-01P-CDCl3-re
EXPNO 1
PROCNO 1

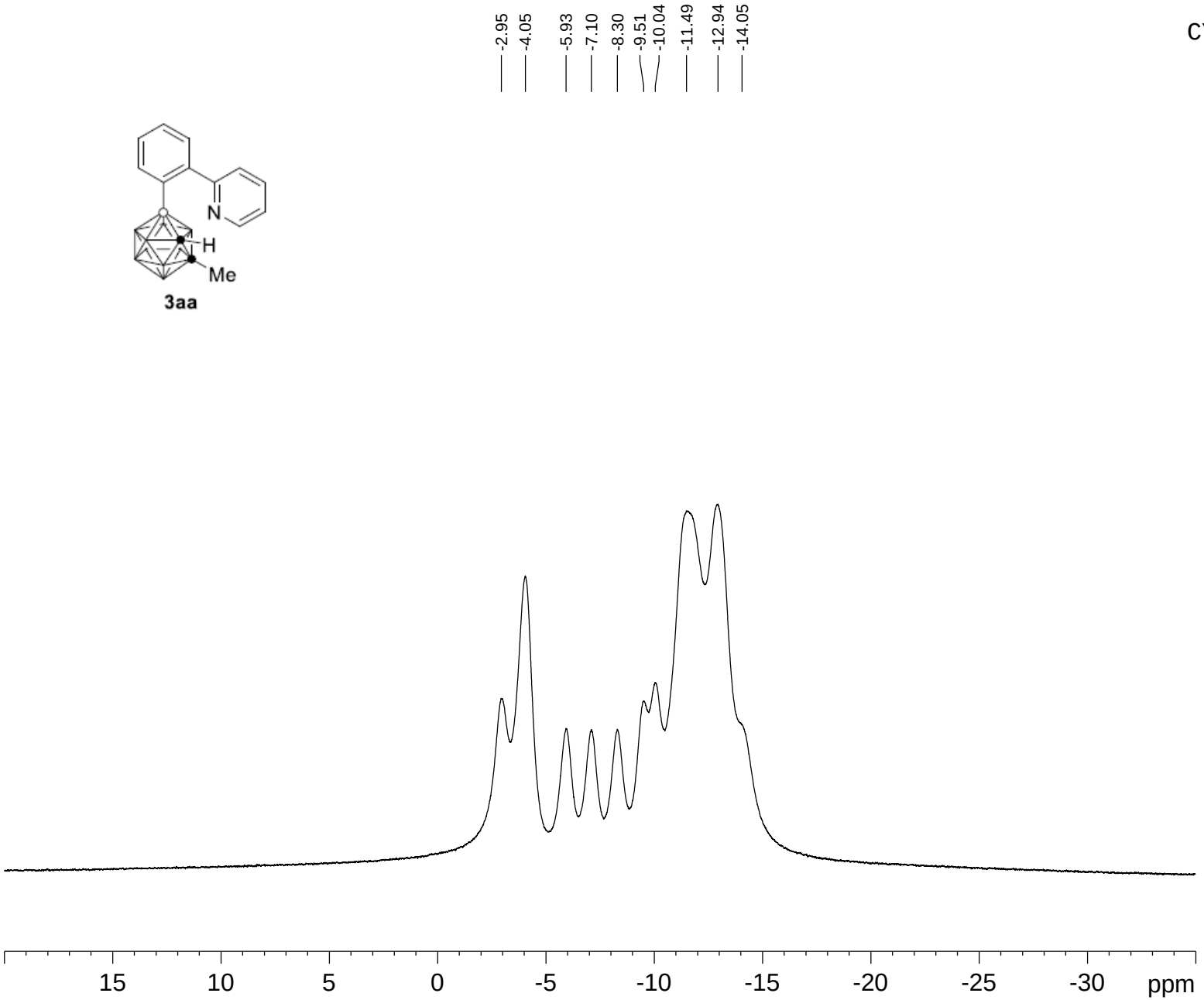
F2 - Acquisition Parameters
Date_ 20161128
Time 13.49 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
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 100.6127614 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



CY-B-A-1p

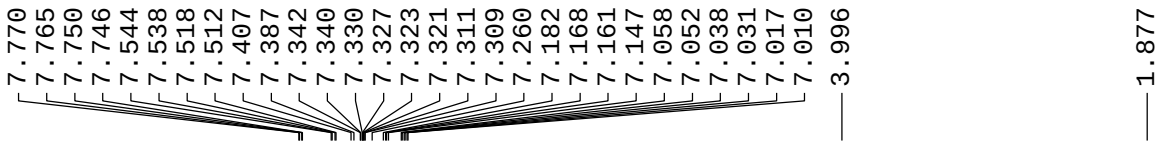
```
Current Data Parameters
NAME                  CY-B-A-1P
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20160804
Time                      16.49 h
INSTRUM                   spect
PROBHD   Z108618_0257 (
PULPROG                    zgdc
TD                        65536
SOLVENT                    MeOD
NS                           32
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.366798 Hz
AQ                    1.3631488 sec
RG                            1
DW                       20.800 usec
DE                        6.50 usec
TE                       295.3 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1
SFO1                128.4096890 MHz
NUC1                        11B
P1                        7.50 usec
PLW1                55.09999847 W
SFO2                400.2316009 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                13.56000042 W
PLW12                0.27428001 W

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

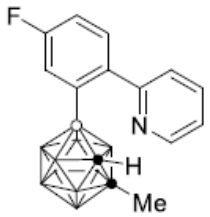


CY-B-A-1P-(C)

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

F2 - Acquisition Parameters
Date_           20160804
Time              16.52 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG               zg
TD                 65536
SOLVENT             MeOD
NS                    33
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   287
DW                20.800 usec
DE                 6.50 usec
TE                294.9 K
D1           2.00000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W

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

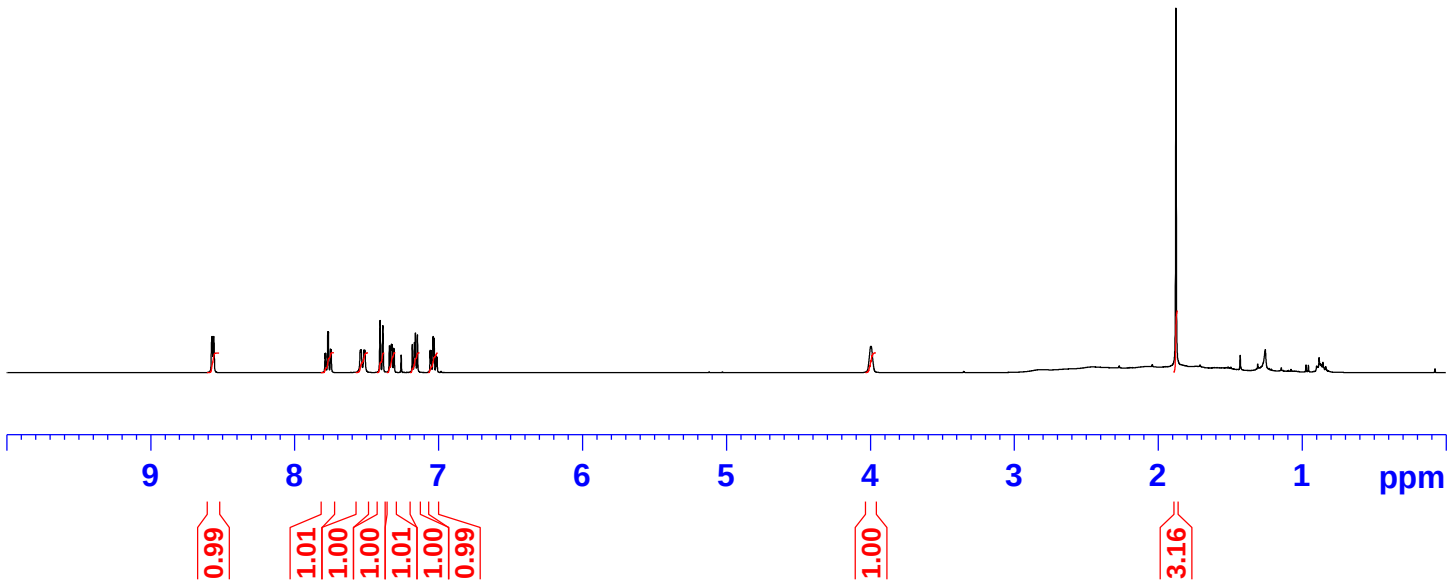
CY-H-A-58p-CDCl3

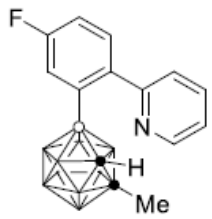




3ab

```
Current Data Parameters
NAME      CY-H-A-58p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20161111
Time                12.23 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                    71.8
DW                  62.400 usec
DE                   6.50 usec
TE                  294.5 K
D1             1.00000000 sec
TD0                     1
SFO1         400.1324708 MHz
NUC1                   1H
P1                  15.00 usec
PLW1          8.31000042 W

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



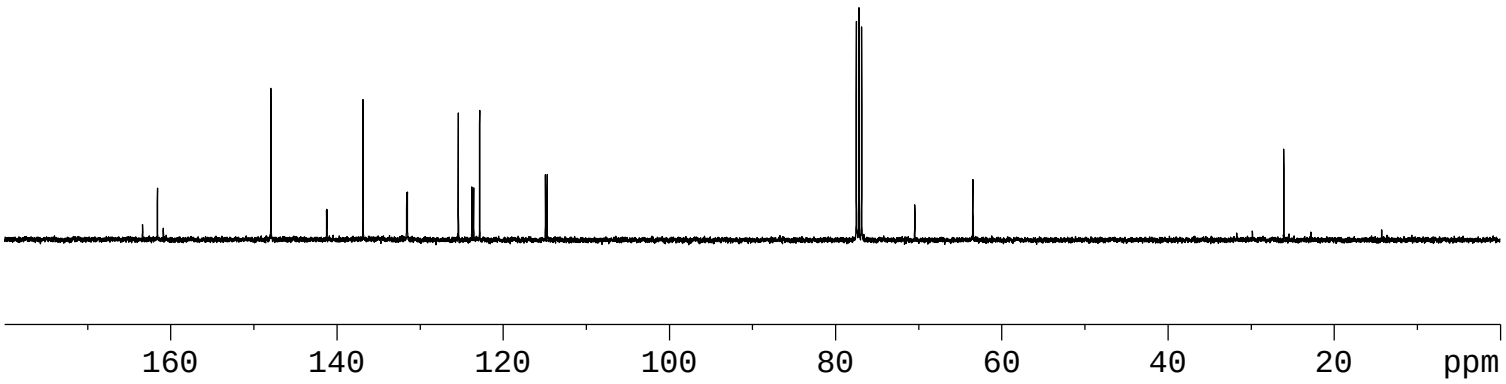


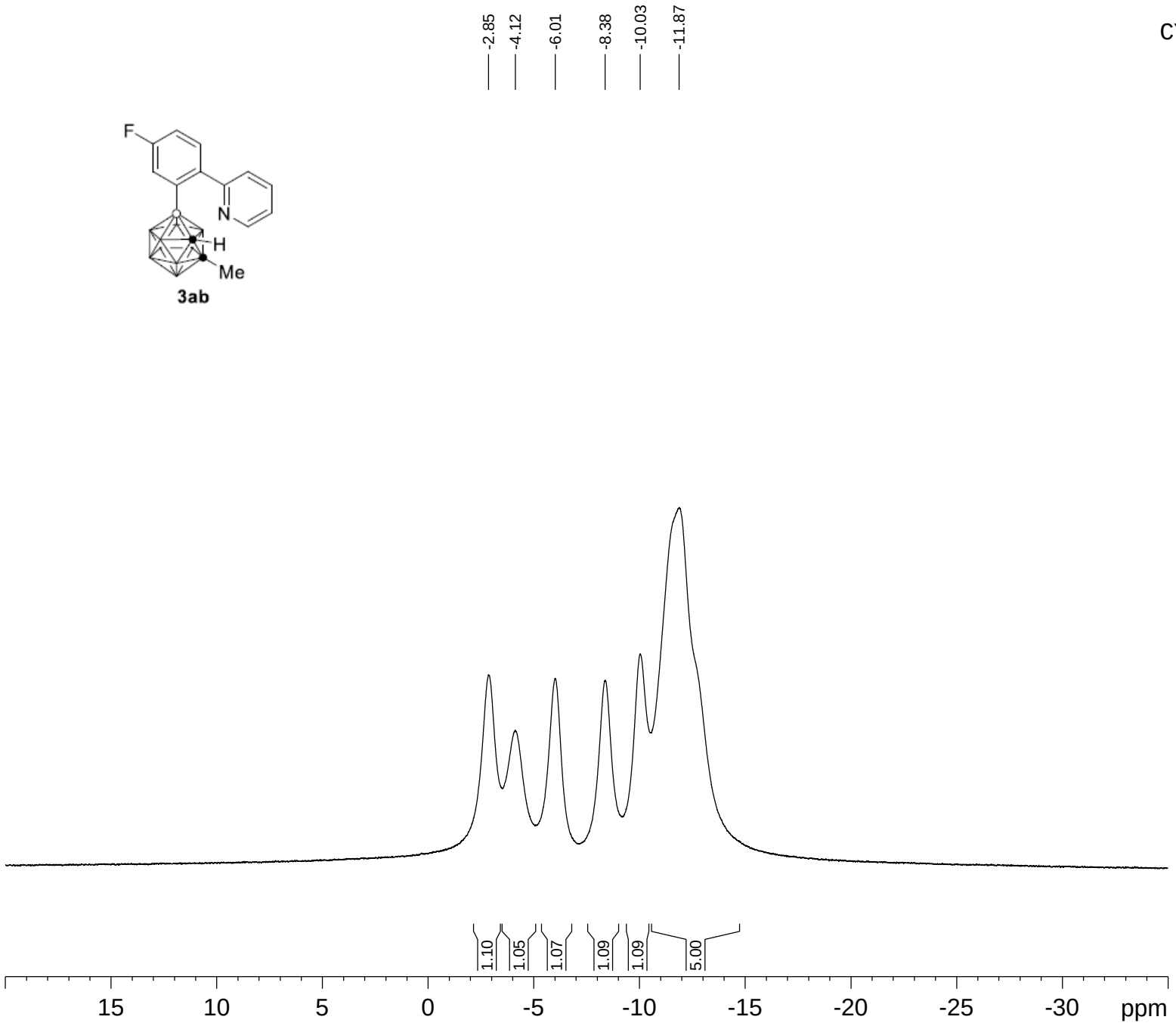
3ab

CY-C-A-58P-CDCl3

Bruker Advance III 400

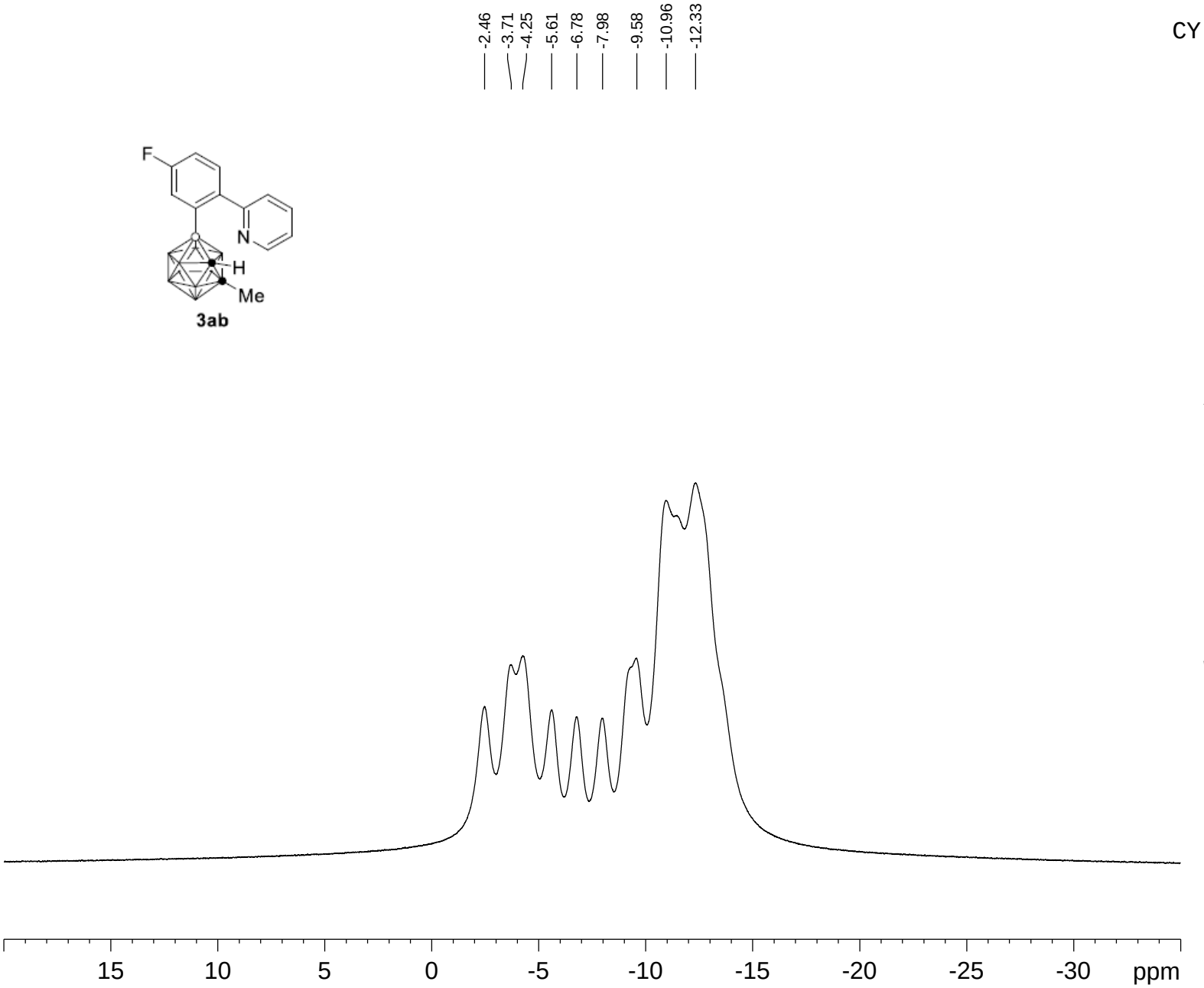
```
Current Data Parameters
NAME      CY-C-A-58P-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20161111
Time               12.29 h
INSTRUM             spect
PROBHD   Z824601_0021 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    160
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          100.6127601 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





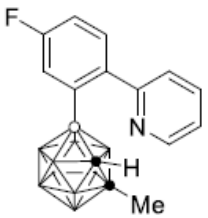
CY-B-A-58p

```
Current Data Parameters
NAME          CY-B-A-58P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161111
Time               12.41 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                   181
DW                20.800 usec
DE                 6.50 usec
TE                295.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-58p-(C)

```
Current Data Parameters
NAME      CY-B-A-58p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161111
Time                12.45 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      47
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     181
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            128.4097881 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

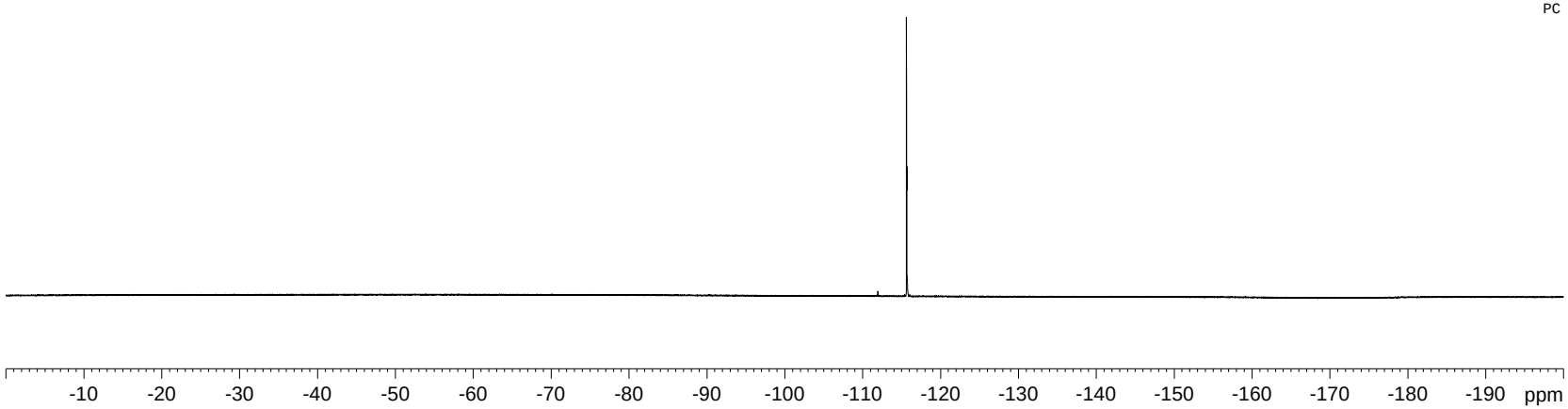


3ab

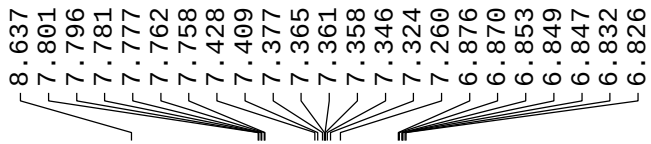
-115.61

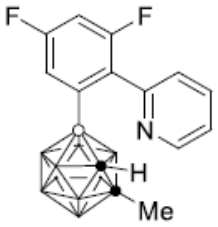
CY-F-A-58P-re

```
Current Data Parameters
NAME      CY-F-A-58P-re
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20161127
Time             16.17 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG      zgfhigqn.2
TD               131072
SOLVENT          Acetone
NS                   32
DS                    4
SWH           89285.711 Hz
FIDRES         0.681196 Hz
AQ            0.7340032 sec
RG                 645
DW                5.600 usec
DE                 6.50 usec
TE                296.2 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                  1
SFO1        376.5548010 MHz
NUC1               19F
P1                14.70 usec
PLW1        18.36000061 W
SFO2        400.2316009 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W

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



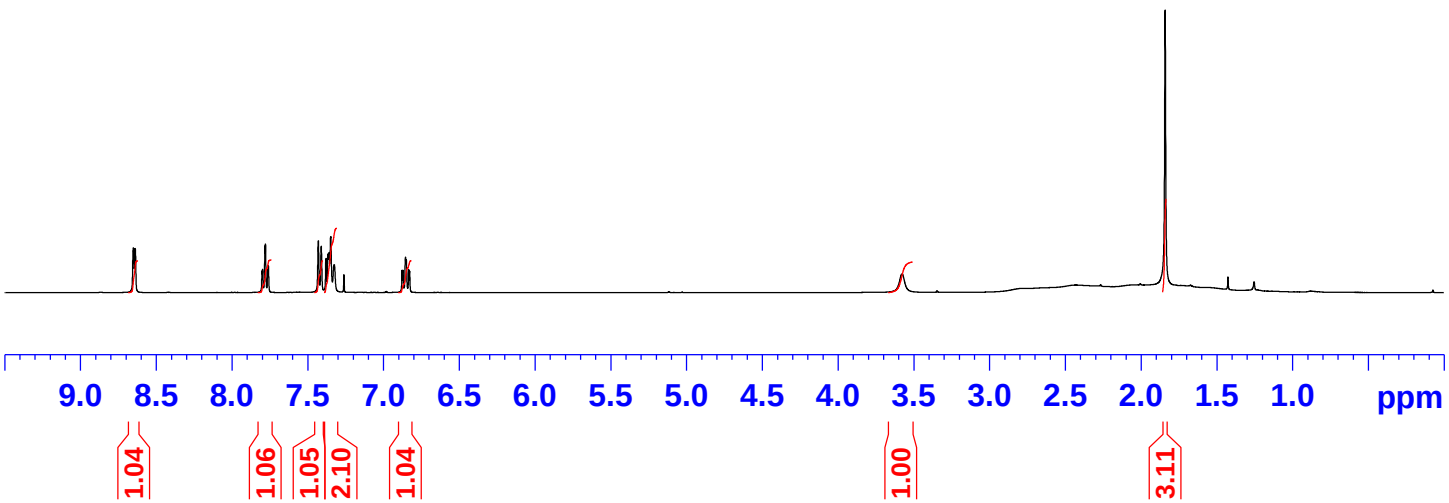
CY-H-A-66p-CDCl3

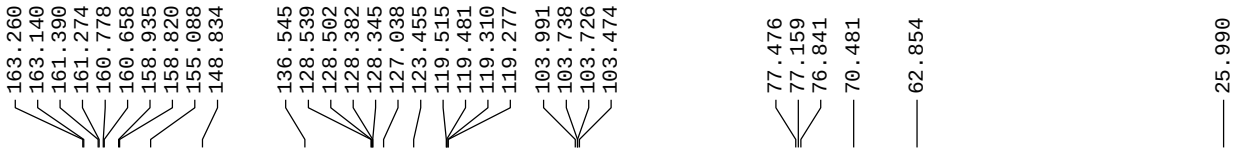


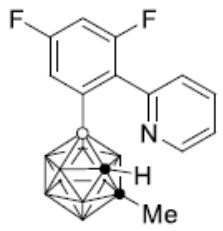


3ac

```
Current Data Parameters
NAME      CY-H-A-66p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20161120
Time                11.36 h
INSTRUM              spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                    80.6
DW                  62.400 usec
DE                   6.50 usec
TE                  294.8 K
D1             1.00000000 sec
TD0                     1
SFO1          400.1324708 MHz
NUC1                   1H
P1                  15.00 usec
PLW1           8.31000042 W

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





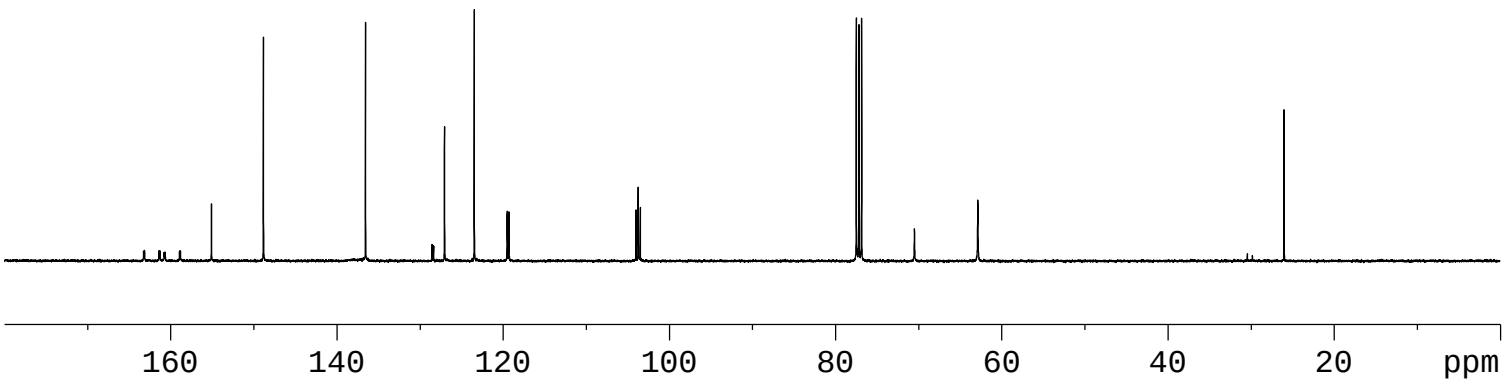


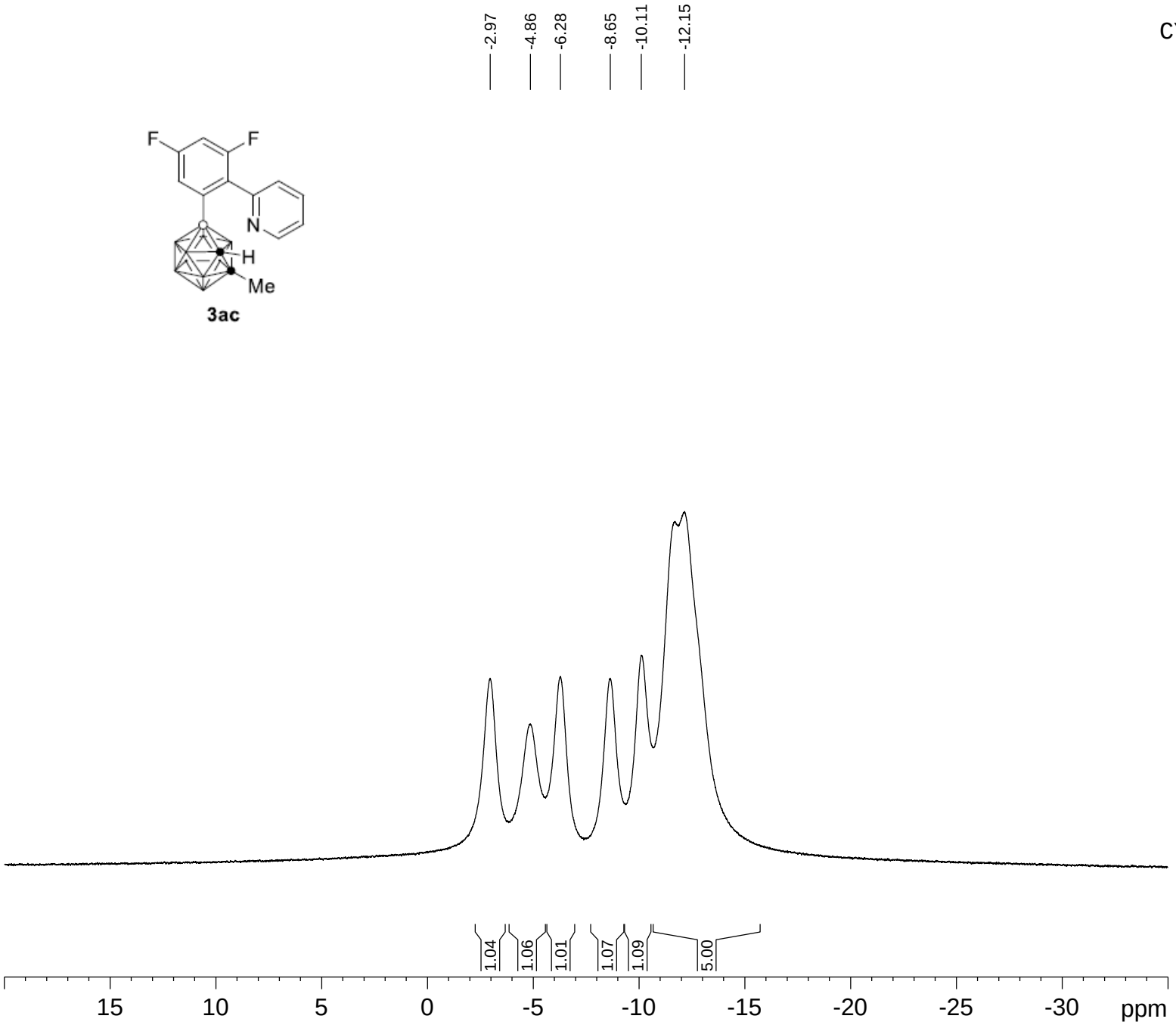
3ac

CY-C-A-66P-CDCl3

Bruker Advance III 400

```
Current Data Parameters
NAME      CY-C-A-66P-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20161120
Time               11.42 h
INSTRUM             spect
PROBHD   Z824601_0021 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2447
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           100.6127594 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

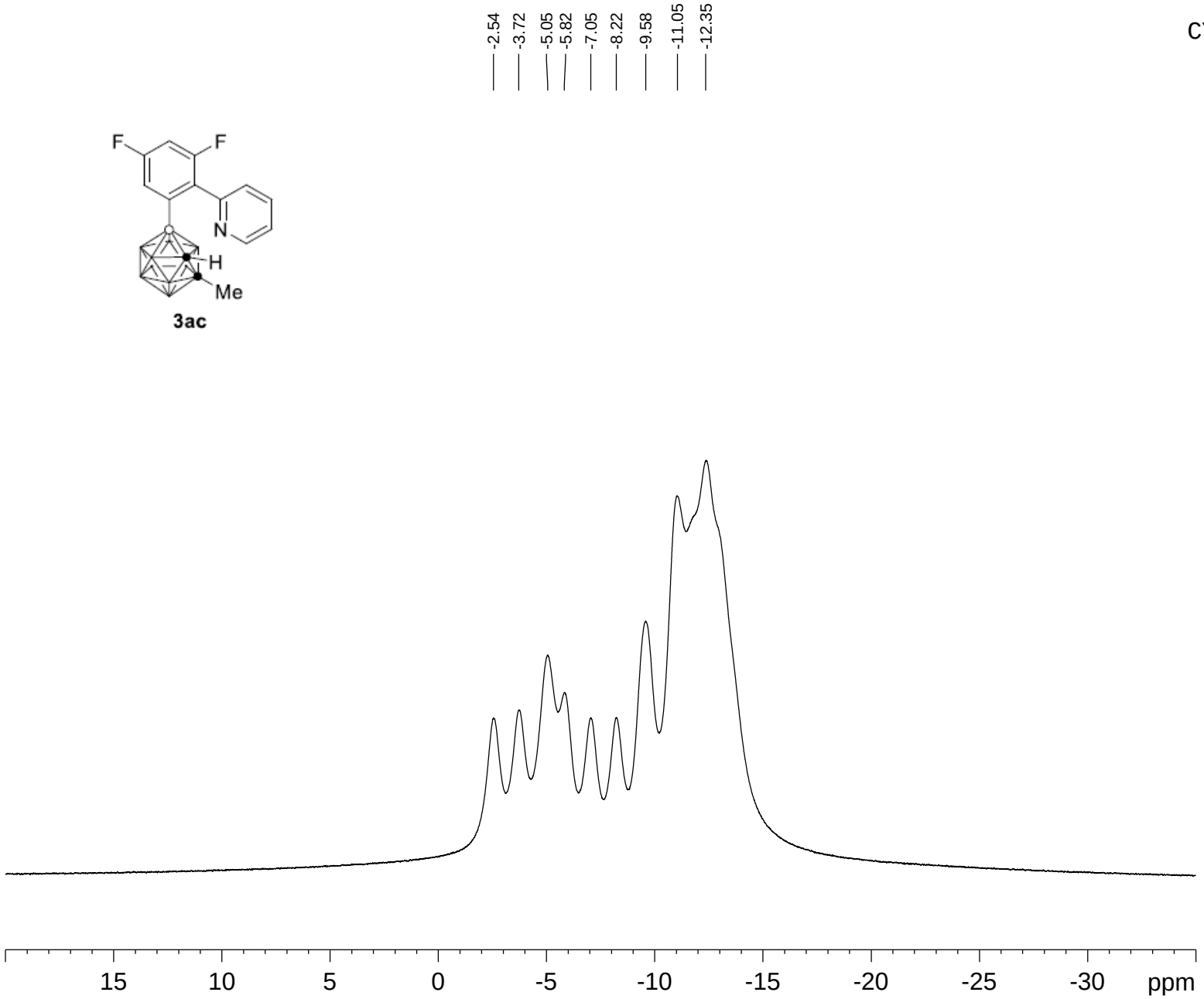




CY-B-A-66p

```
Current Data Parameters
NAME          CY-B-A-66p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161120
Time               19.38 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                   203
DW                20.800 usec
DE                 6.50 usec
TE                296.4 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
```

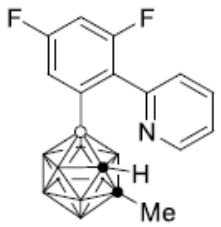
3ac



CY-B-A-66p-(C)

```
Current Data Parameters
NAME      CY-B-A-66p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161120
Time                19.42 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                  65536
SOLVENT             CDCl3
NS                     56
DS                      2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                    203
DW                 20.800 usec
DE                  6.50 usec
TE                 296.0 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            128.4097881 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

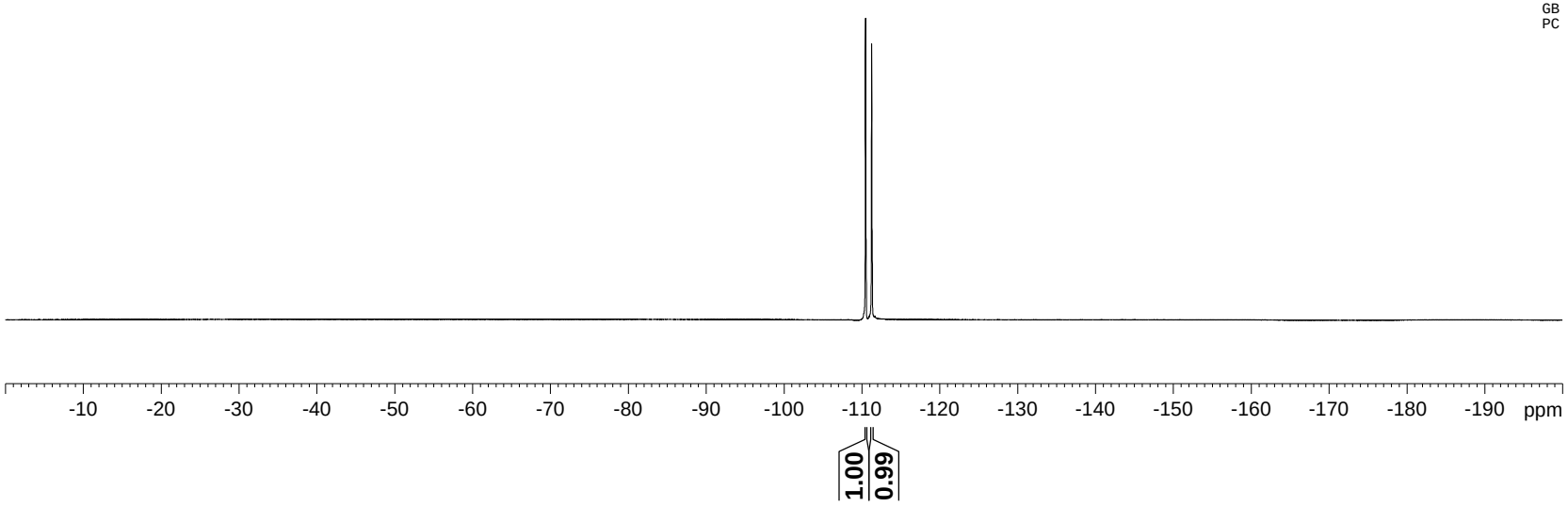
CY-F-A-66P



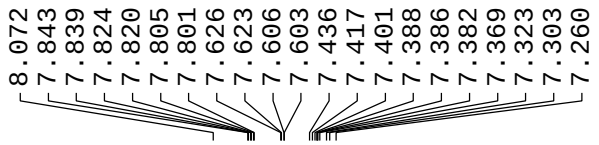
3ac

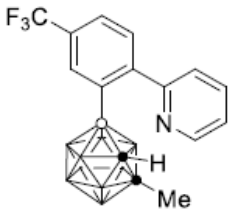
-110.48
-111.26

```
Current Data Parameters
NAME          CY-F-A-66P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161120
Time              19.47 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                    104
DS                      4
SWH            89285.711 Hz
FIDRES          0.681196 Hz
AQ             0.7340032 sec
RG                    645
DW                5.600 usec
DE                6.50 usec
TE                296.1 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1
SFO1         376.5548010 MHz
NUC1                 19F
P1                14.70 usec
PLW1         18.36000061 W
SFO2         400.2316009 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



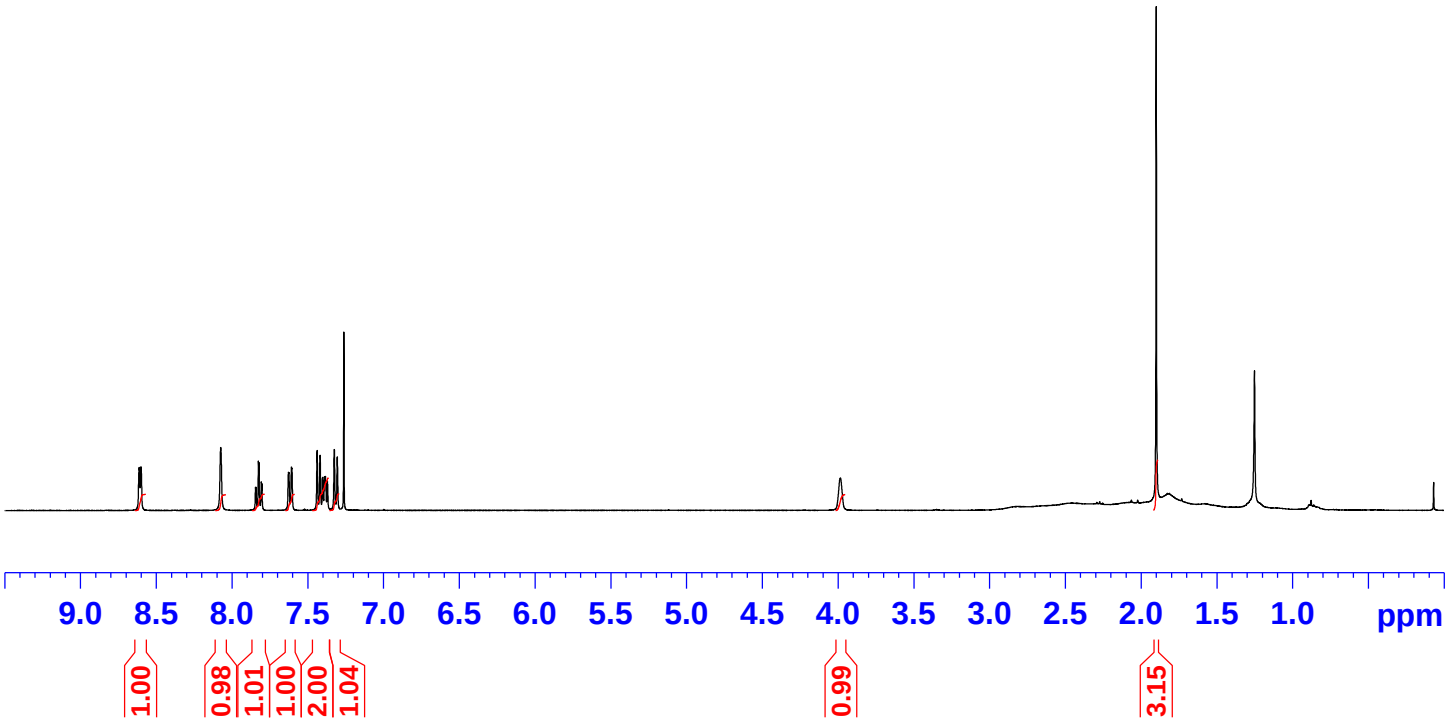
CY-H-A-34p-p

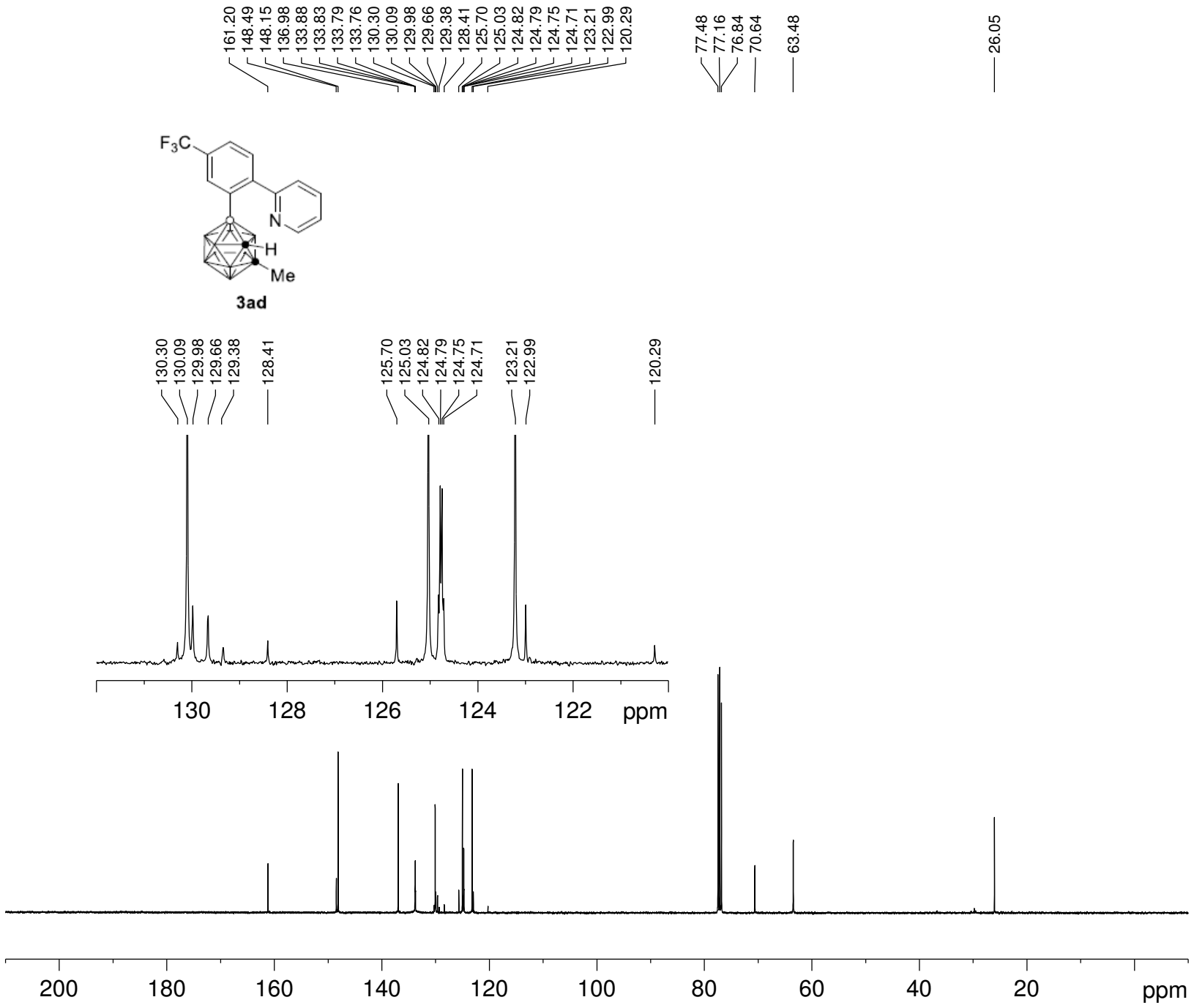




3ad

```
Current Data Parameters
NAME       CY-H-A-34p-p
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20160913
Time              21.32 h
INSTRUM           spect
PROBHD   Z824601_0021 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  11
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               295.1 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          400.1300097 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
```

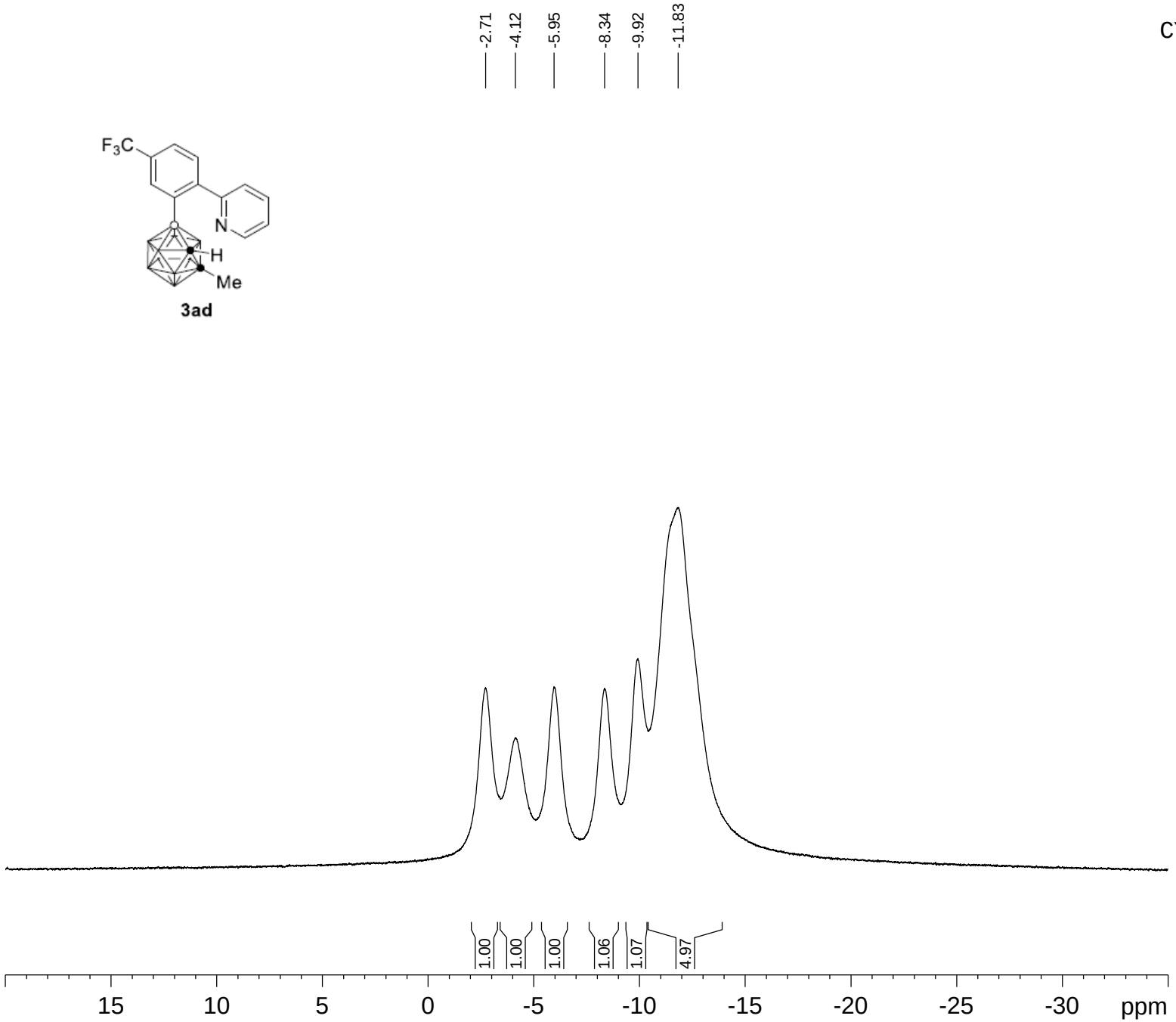




CY-C-A-34p-re

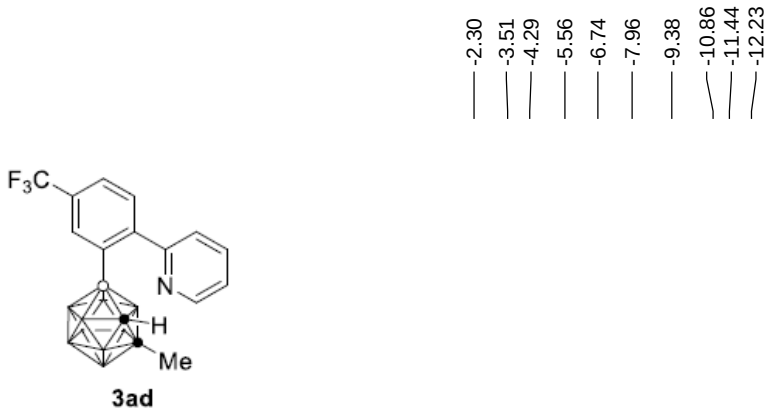
```
Current Data Parameters
NAME      CY-C-A-34p-re2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161123
Time              19.45 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1627
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ            0.8039083 sec
RG                  203
DW               12.267 usec
DE                6.50 usec
TE               296.9 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          100.6379028 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

3ad



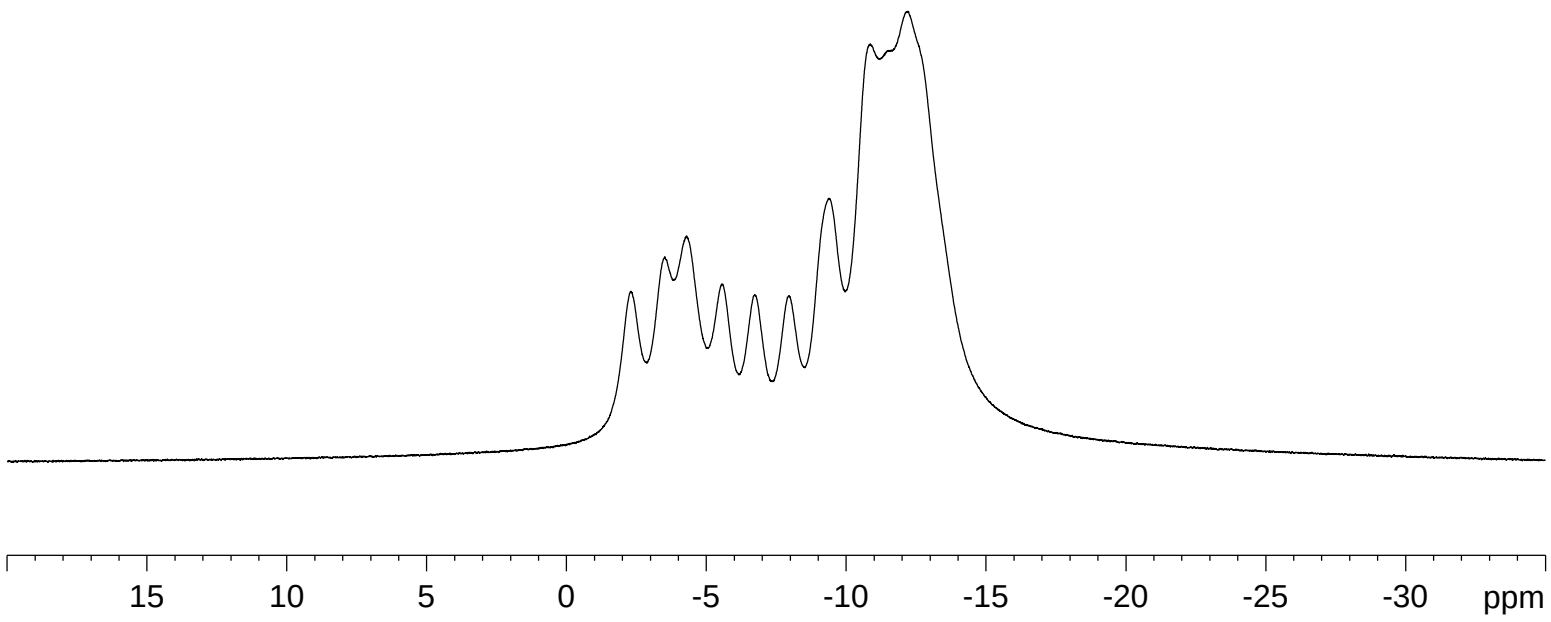
CY-B-A-34p

```
Current Data Parameters
NAME          CY-B-A-34p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161124
Time               16.53 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                   181
DW                20.800 usec
DE                 6.50 usec
TE                295.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



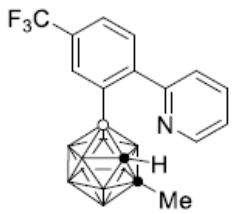
CY-B-A-34p-(C)

```
Current Data Parameters
NAME      CY-B-A-34p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161124
Time                16.55 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                    181
DW                 20.800 usec
DE                  6.50 usec
TE                 295.5 K
D1            2.00000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                  11B
P1                  7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                  32768
SF            128.4097881 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



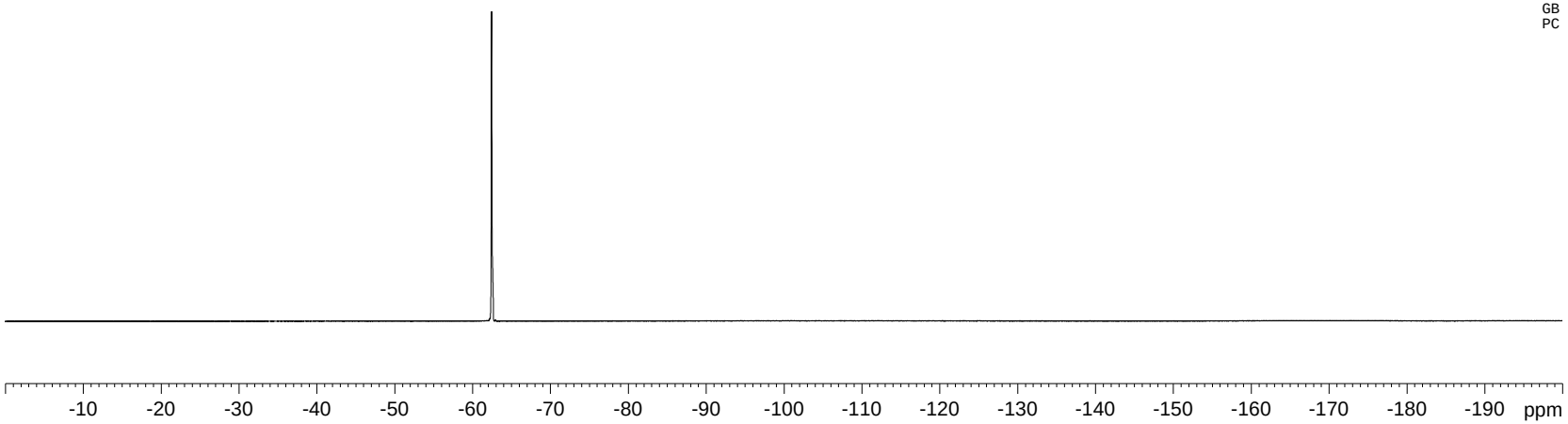
-62.45

CY-F-A-34P

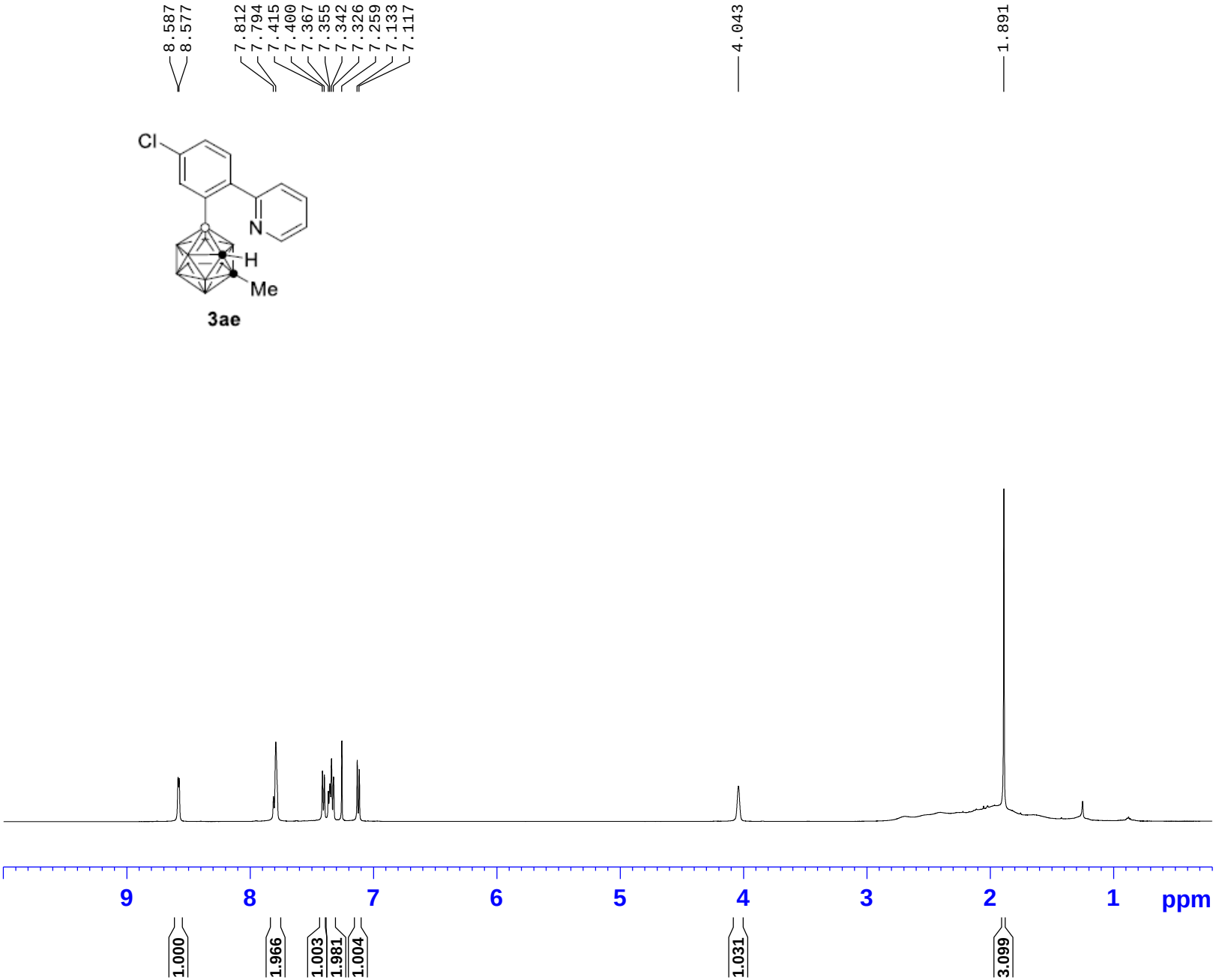


3ad

```
Current Data Parameters
NAME          CY-F-A-34P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161124
Time               16.38 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     20
DS                      4
SWH             89285.711 Hz
FIDRES          0.681196 Hz
AQ              0.7340032 sec
RG                    645
DW                5.600 usec
DE                6.50 usec
TE                296.0 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1
SFO1         376.5548010 MHz
NUC1                  19F
P1                14.70 usec
PLW1         18.36000061 W
SFO2         400.2316009 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

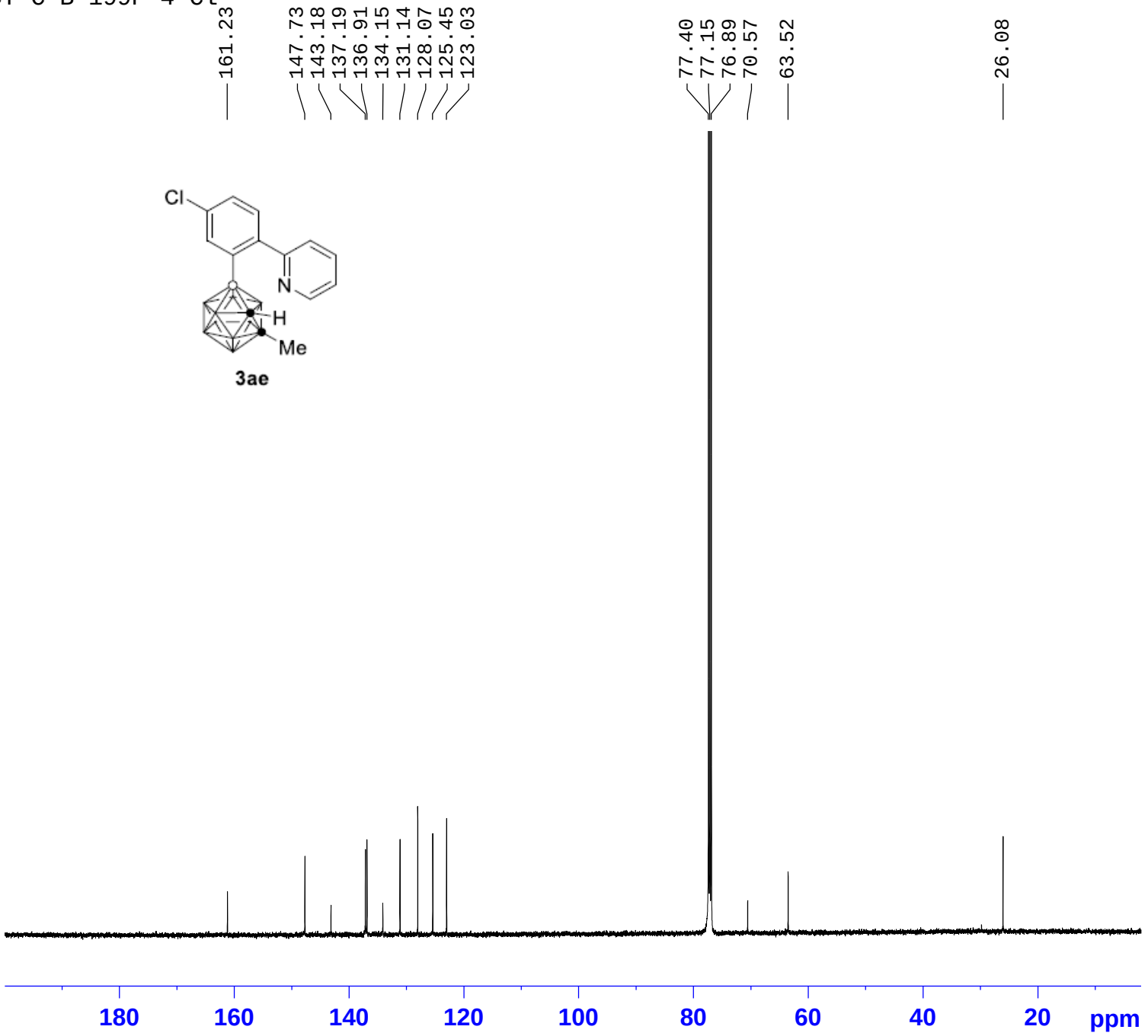


CY-H-B-199P-4-Cl



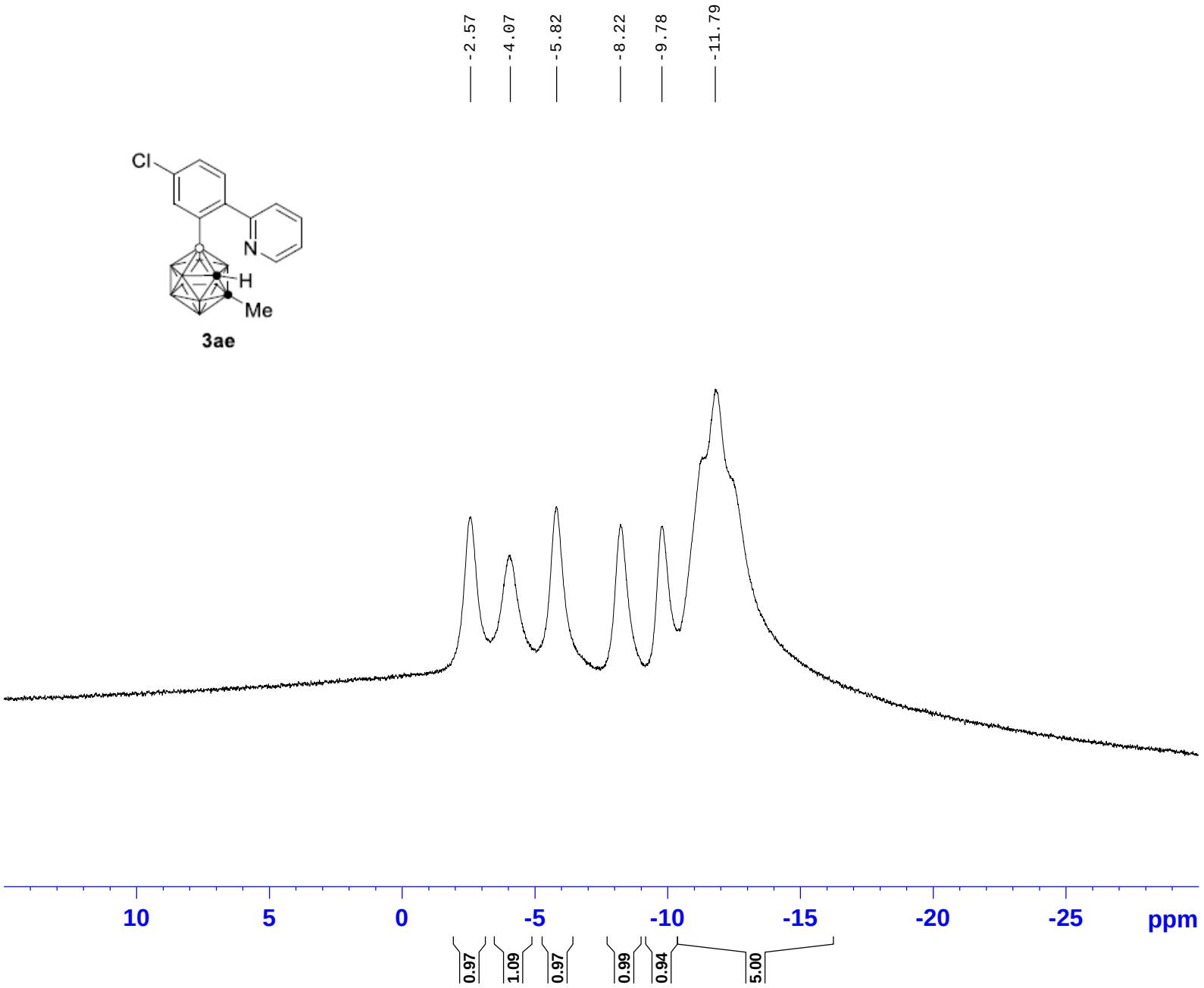

```
Current Data Parameters
NAME      CY-H-B-199P-4-Cl
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190228
Time               13.53 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.305176 Hz
AQ              3.2767999 sec
RG                  50.6
DW                 50.000 usec
DE                 10.00 usec
TE                 298.0 K
D1              1.00000000 sec
TD0                    1
SFO1           500.1330883 MHz
NUC1                  1H
P1                 11.25 usec
PLW1           15.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300140 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

CY-C-B-199P-4-Cl



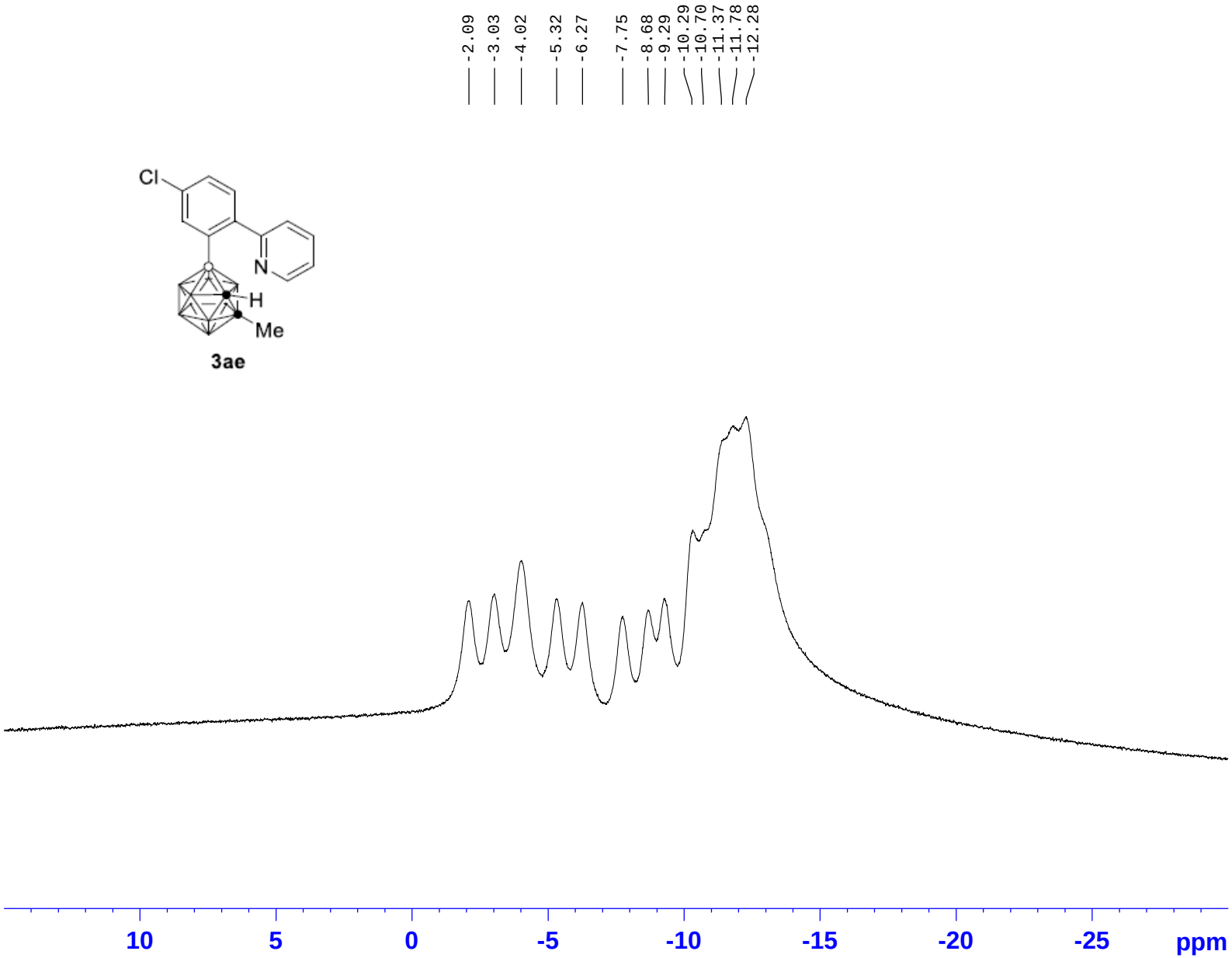

```
Current Data Parameters
NAME      CY-C-B-199P-4-Cl
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190228
Time              14.28 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  640
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

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

CY-B-B-199P-4-Cl




```
Current Data Parameters
NAME      CY-B-B-199P-4-Cl
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190228
Time               14.32 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 32768
SOLVENT             None
NS                    32
DS                     4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                206.72
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         160.4615790 MHz
NUC1                11B
P1                15.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

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

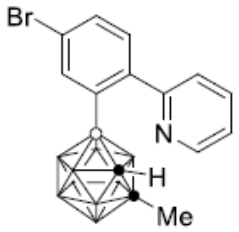
CY-B-B-199P-4-Cl-(C)




```
Current Data Parameters
NAME      CY-B-B-199P-4-Cl-(C)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190228
Time              14.33 h
INSTRUM           spect
PROBHD    Z149001_0010 (
PULPROG              zg
TD                32768
SOLVENT            None
NS                   32
DS                    4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG                142.5
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1           1.00000000 sec
TD0                  1
SFO1        160.4615792 MHz
NUC1               11B
P1               15.00 usec
PLW1        50.00000000 W

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

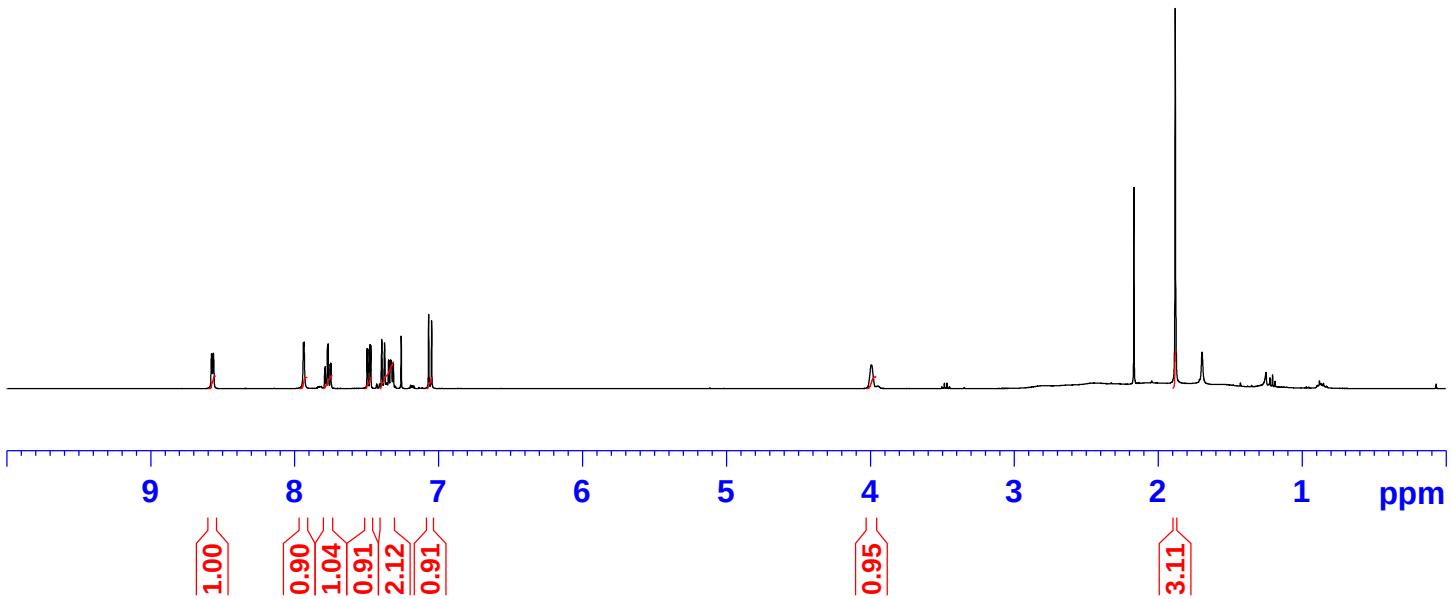
CY-H-A-57p-CDCl3

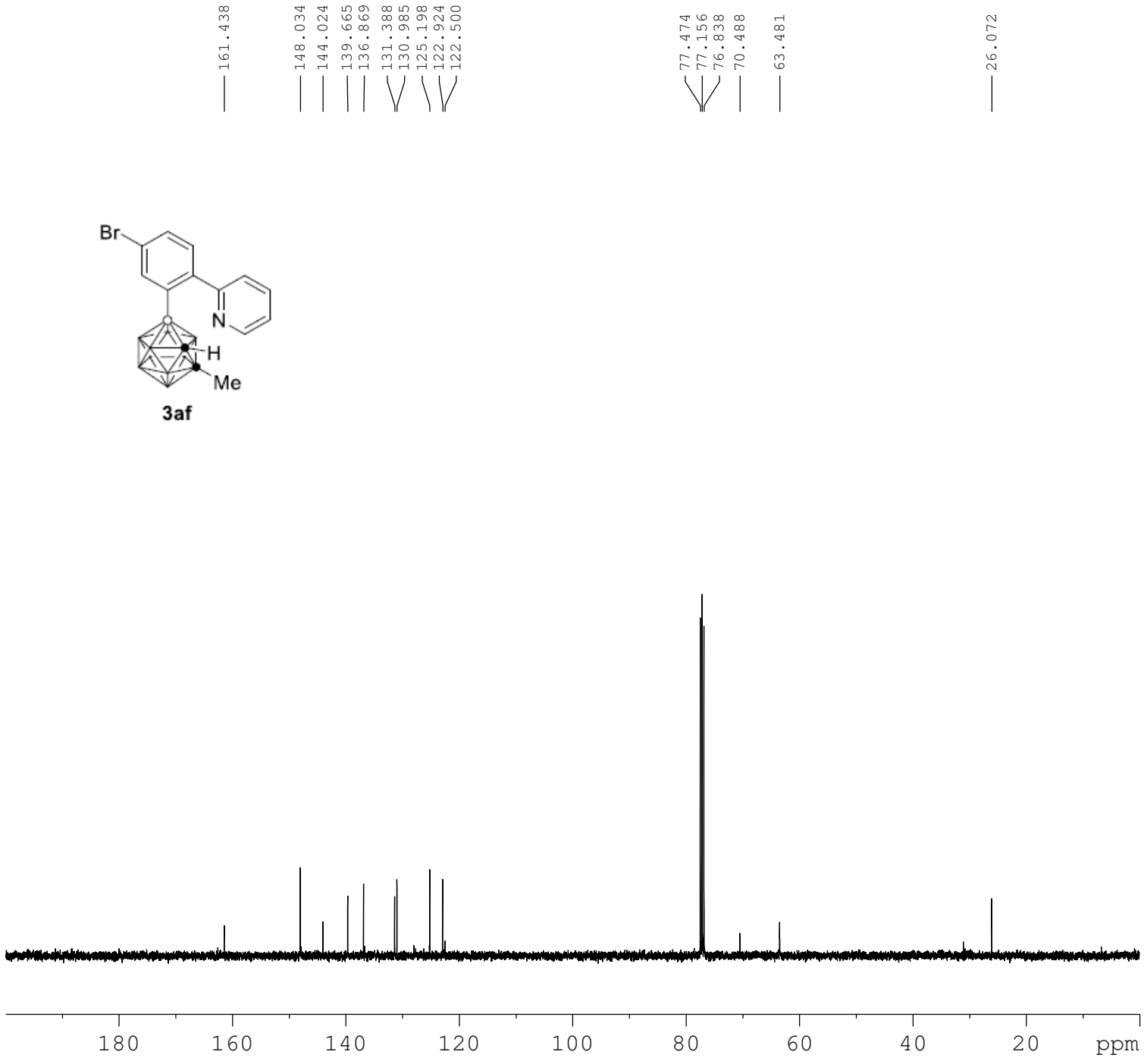
8.563 7.939 7.934 7.791 7.787 7.772 7.768 7.753 7.748 7.497 7.491 7.476 7.471 7.395 7.375 7.347 7.345 7.335 7.332 7.328 7.326 7.316 7.314 7.260 7.069 7.048 3.993 1.882



3af

```
Current Data Parameters
NAME      CY-H-A-57p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20161104
Time                18.25 h
INSTRUM              spect
PROBHD    Z824601_0021 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        7
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                  294.4 K
D1              1.00000000 sec
TD0                       1
SFO1           400.1324708 MHz
NUC1                     1H
P1                  15.00 usec
PLW1            8.31000042 W

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





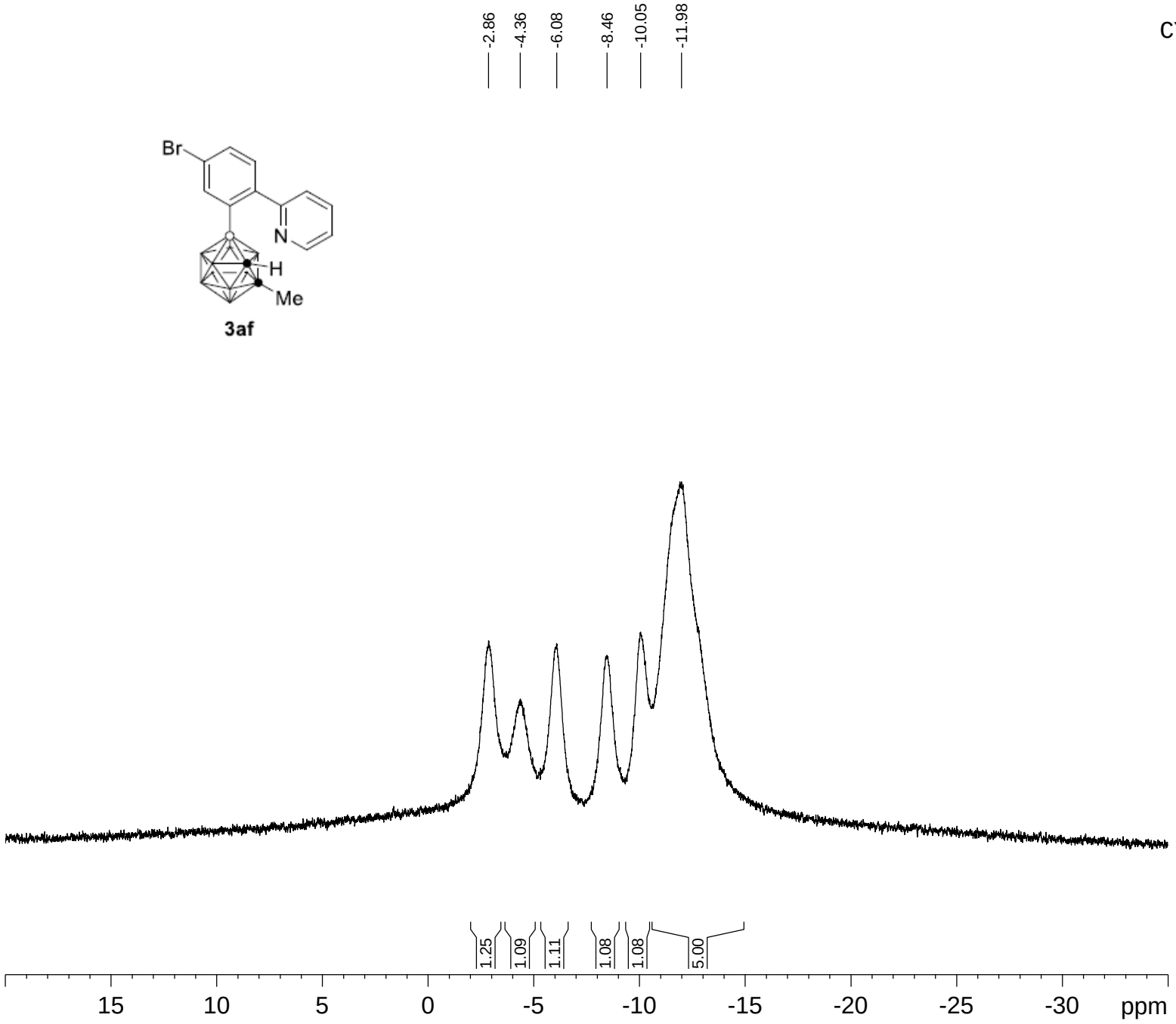
CY-C-A-57P-CDCl3

Bruker Advance III 400

Current Data Parameters
NAME CY-C-A-57P-CDCl3
EXPNO 1
PROCNO 1

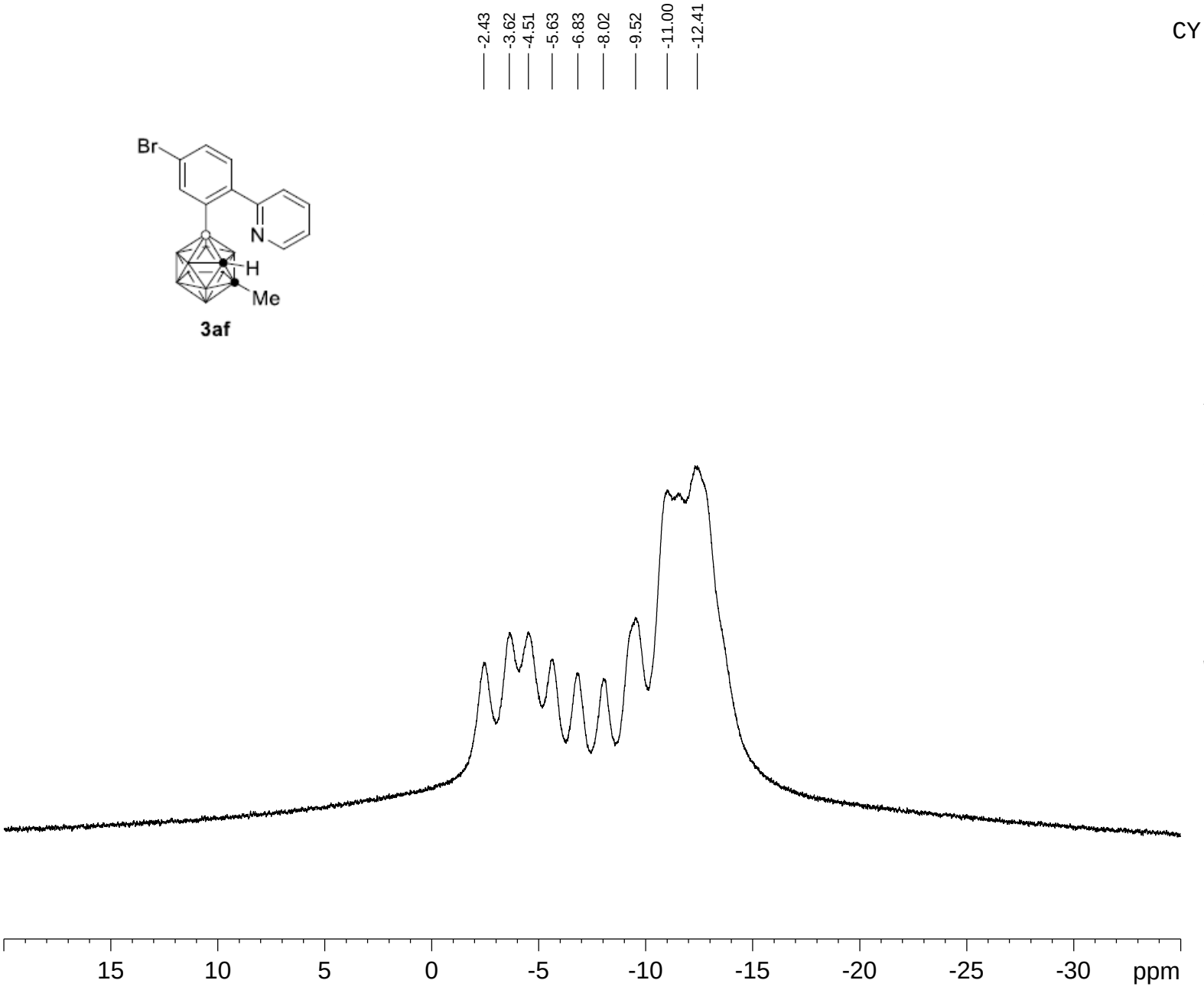
F2 - Acquisition Parameters
Date_ 20161104
Time 18.30 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 133
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 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 100.6127580 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



CY-B-A-57P

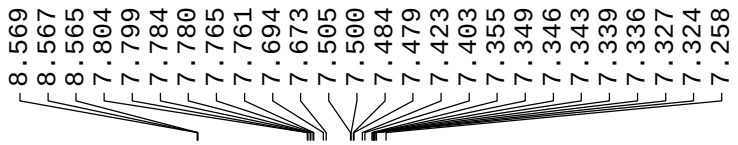
```
Current Data Parameters
NAME          CY-B-A-57P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161104
Time               18.42 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                296.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

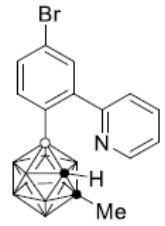


CY-B-A-57P-(C)

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

F2 - Acquisition Parameters
Date_            20161104
Time                18.45 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      57
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                  296.1 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            128.4097881 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

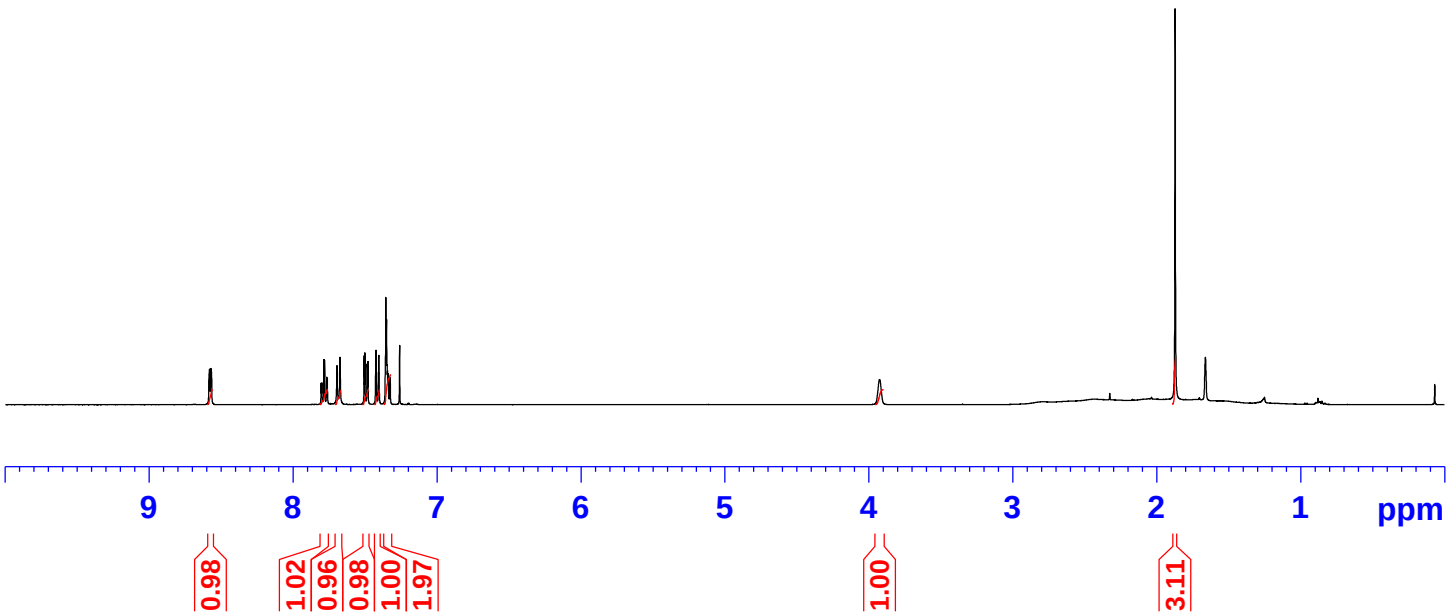
CY-H-A-56p-CDCl3

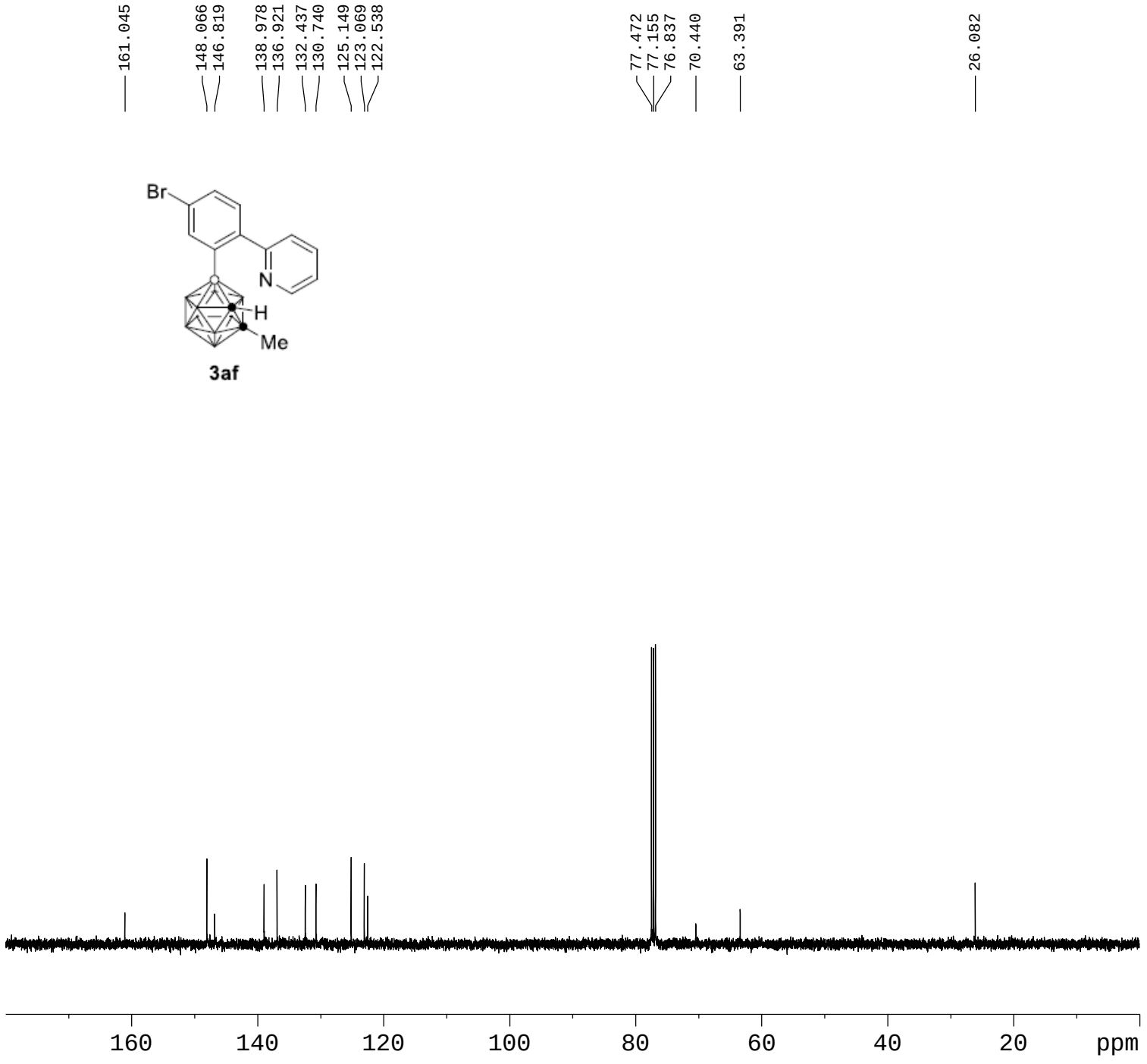




3ag

```
Current Data Parameters
NAME      CY-H-A-56p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20161104
Time                14.40 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      9
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                 294.3 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            400.1300105 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

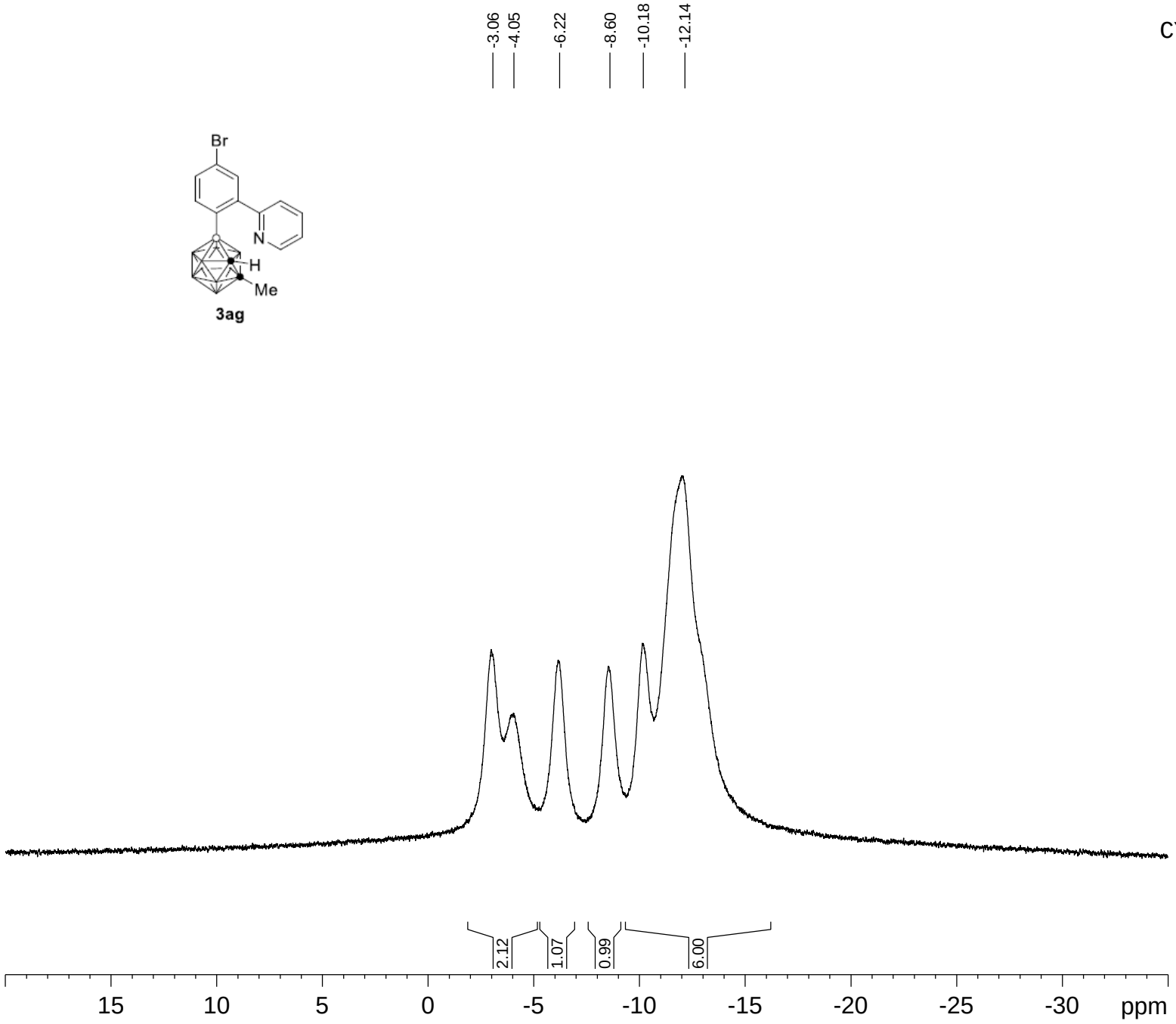




CY-C-A-56P-CDCl3

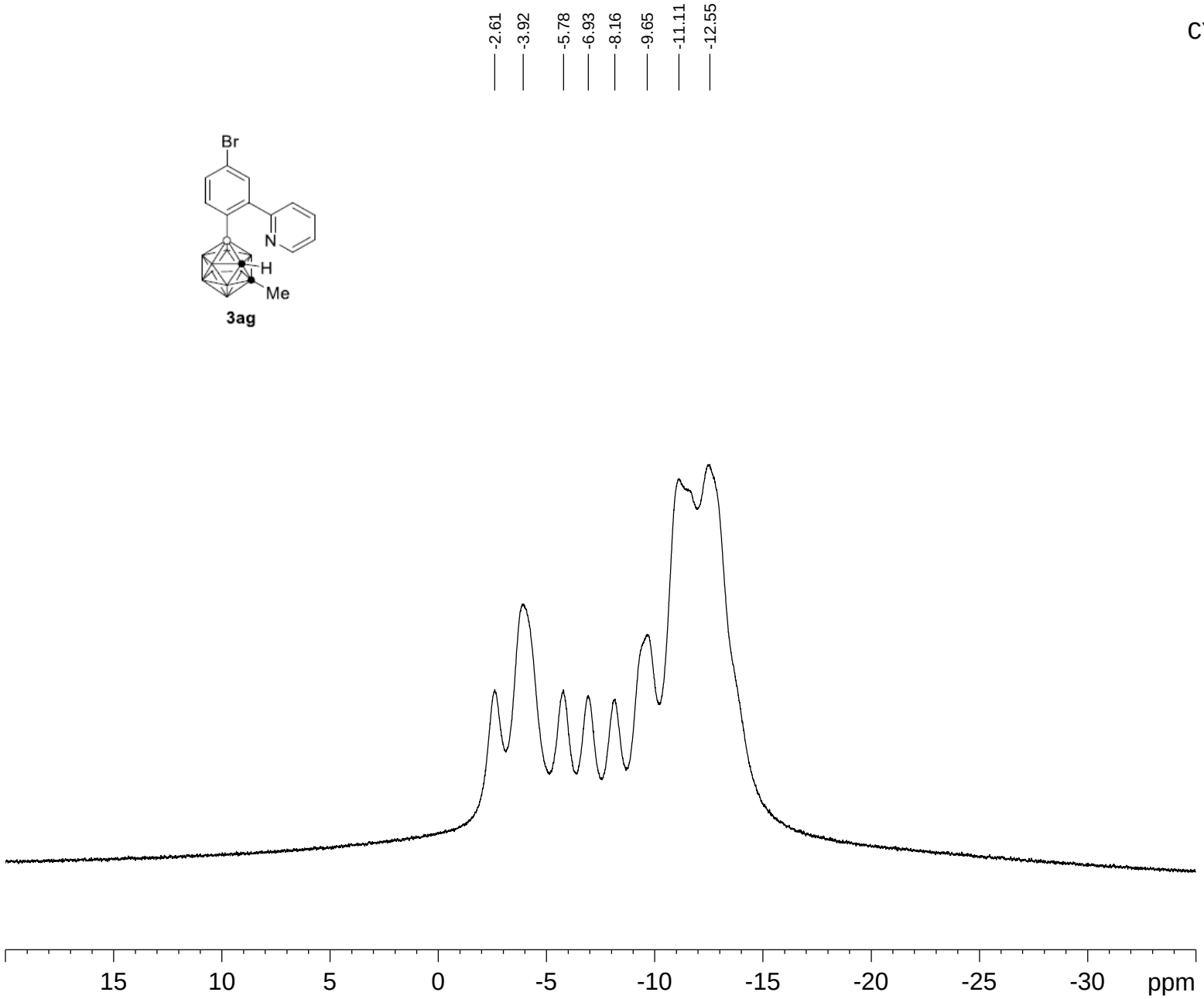
Bruker Advance III 400

```
Current Data Parameters
NAME      CY-C-A-56P-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20161104
Time               14.44 h
INSTRUM             spect
PROBHD   Z824601_0021 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     88
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                 294.6 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           100.6127578 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



CY-B-A-56P

```
Current Data Parameters
NAME          CY-B-A-56P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161104
Time               15.27 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                     7
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   256
DW                20.800 usec
DE                 6.50 usec
TE                295.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

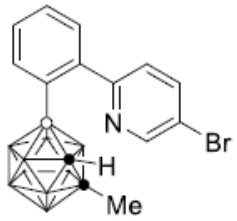


CY-B-A-56P-(C)

```
Current Data Parameters
NAME      CY-B-A-56P-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161104
Time                15.30 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      38
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     256
DW                20.800 usec
DE                 6.50 usec
TE                 295.8 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            128.4097881 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

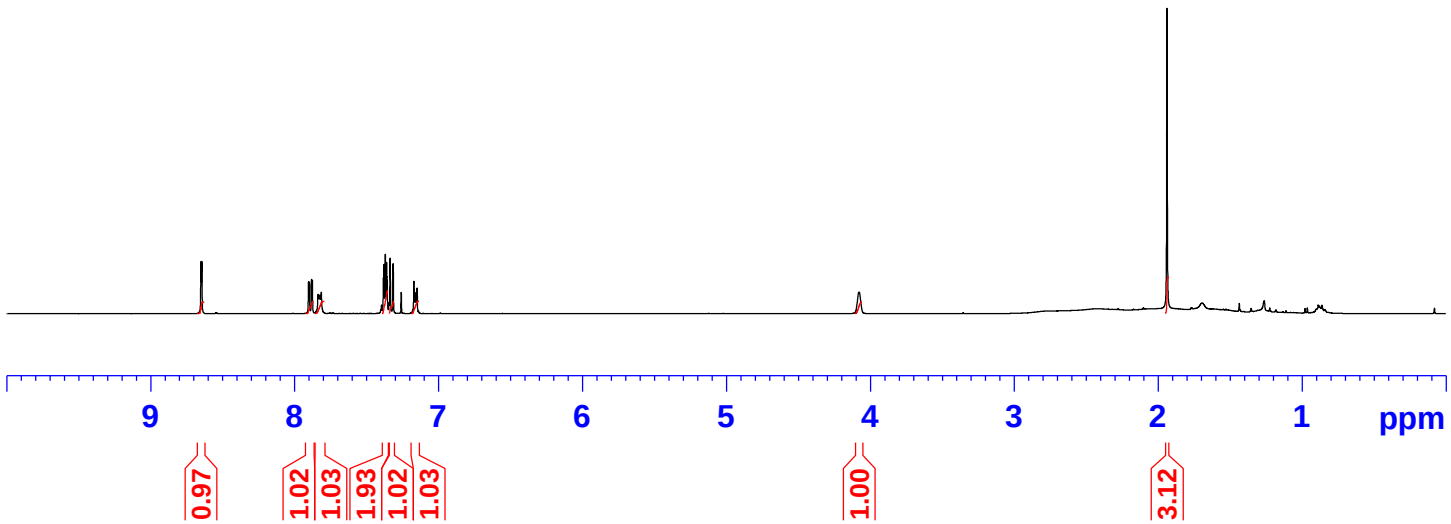
CY-H-A-64p-CDCl3

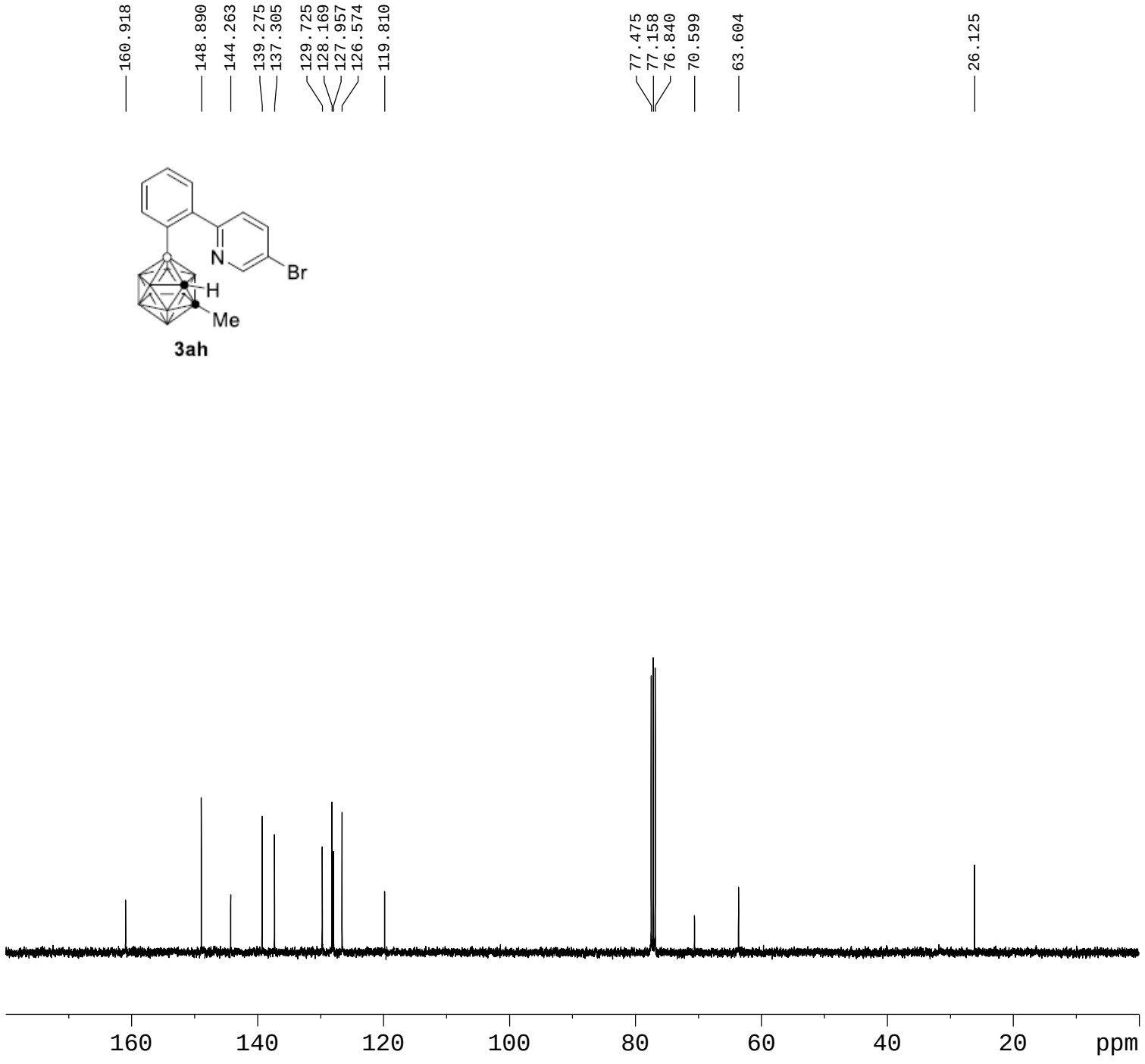
8.650
8.645
7.903
7.897
7.883
7.877
7.837
7.830
7.815
7.396
7.383
7.379
7.370
7.361
7.357
7.344
7.336
7.316
7.259
7.171
7.167
7.161
7.156
7.149
4.079
1.939



3ah

```
Current Data Parameters
NAME      CY-H-A-64p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20161115
Time                19.28 h
INSTRUM              spect
PROBHD    Z824601_0021 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
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                    295.1 K
D1              1.00000000 sec
TD0                       1
SFO1           400.1324708 MHz
NUC1                     1H
P1                    15.00 usec
PLW1           8.31000042 W

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





CY-C-A-64P-CDCl3

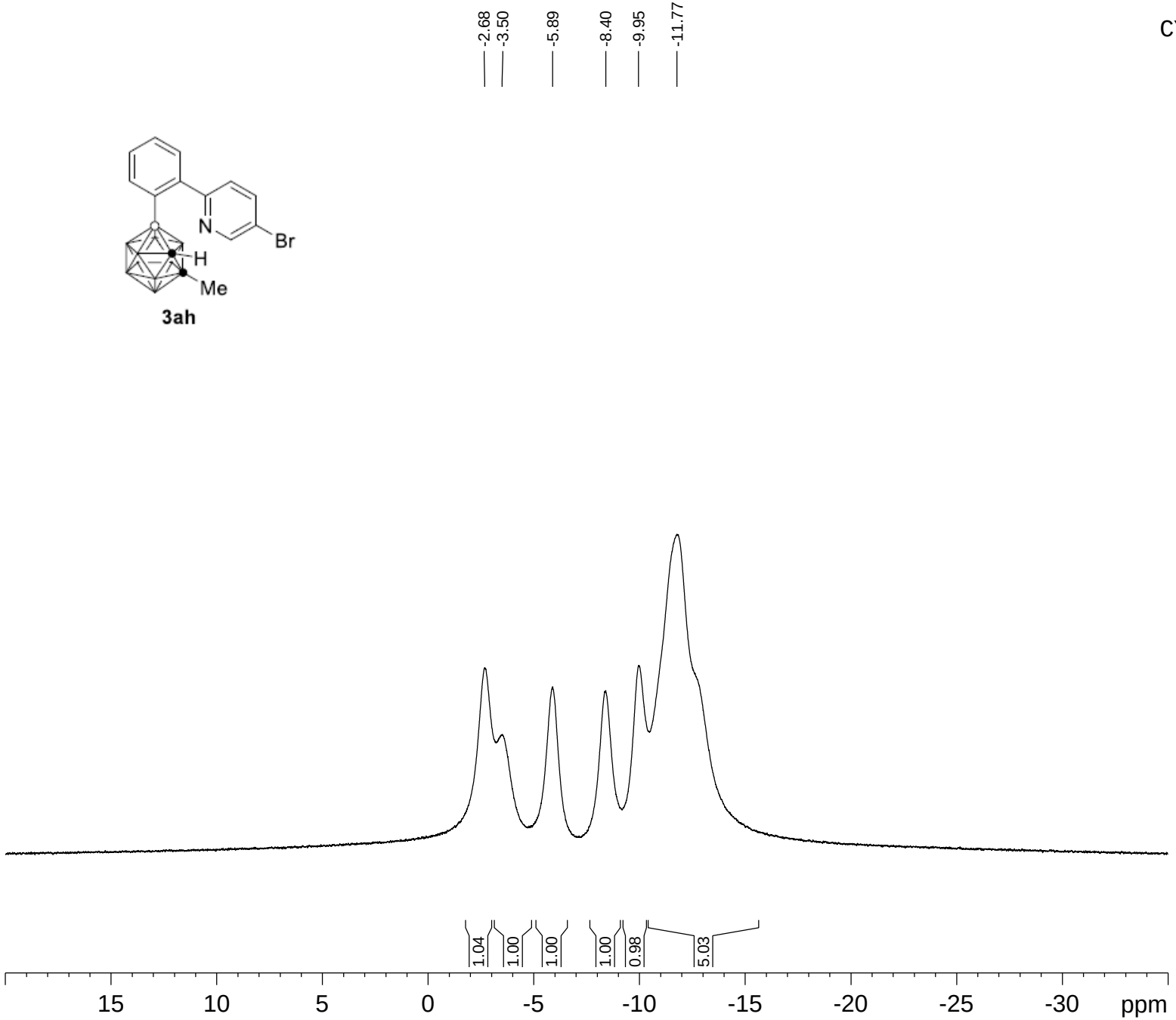
Bruker Advance III 400

Current Data Parameters
NAME CY-C-A-64P-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161115
Time 19.24 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 108
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 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W

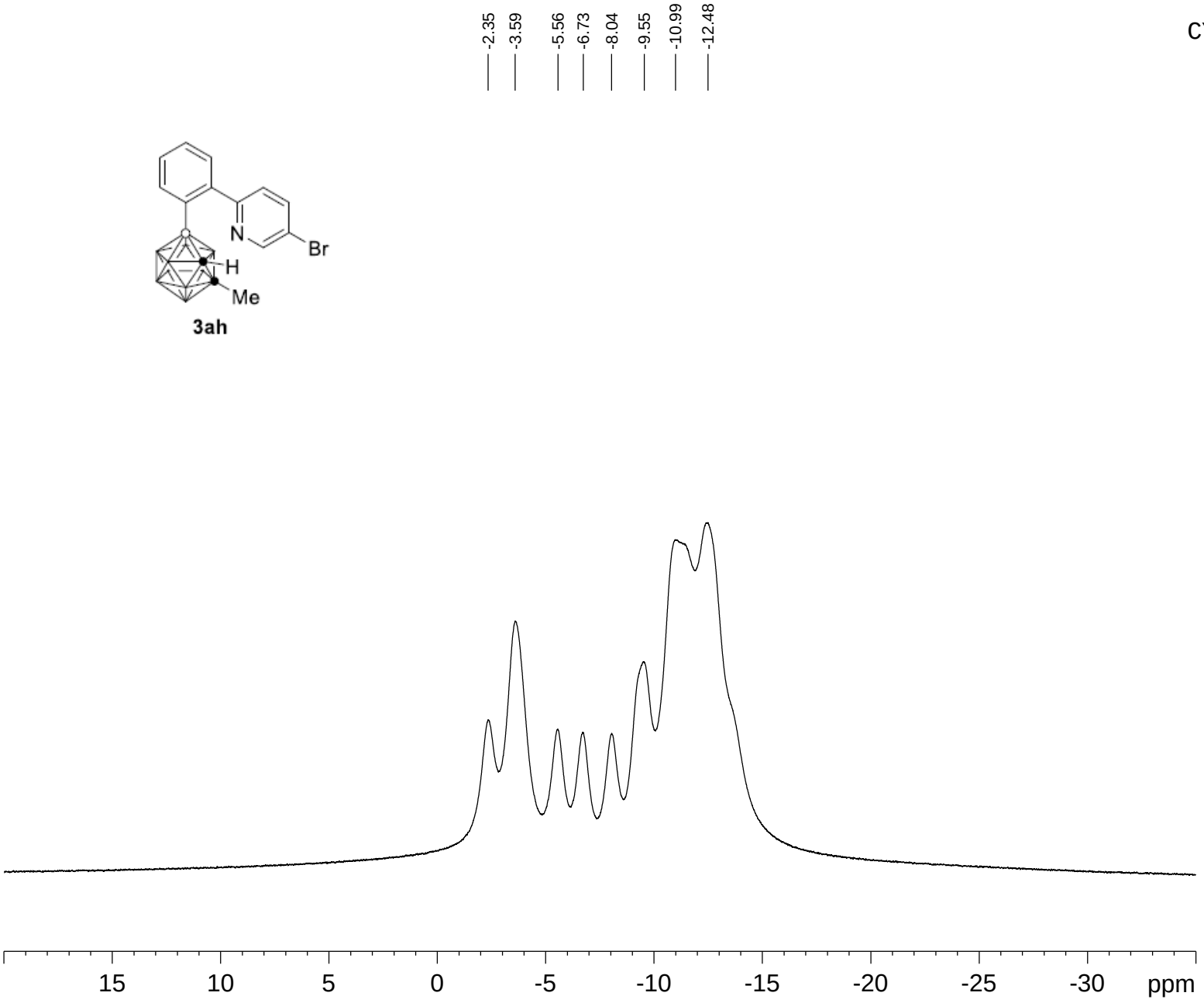
F2 - Processing parameters
SI 32768
SF 100.6127598 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3ah



CY-B-A-64p

```
Current Data Parameters
NAME          CY-B-A-64p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161115
Time               19.13 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                   256
DW                20.800 usec
DE                 6.50 usec
TE                296.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-64p-(C)

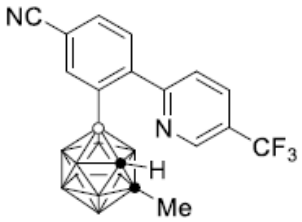
```
Current Data Parameters
NAME      CY-B-A-64p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161115
Time                19.11 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      48
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     256
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           128.4097881 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

CY-H-A-43p-CDCl3-re

8.882
8.111
8.075
8.071
8.055
8.050
7.678
7.675
7.659
7.656
7.568
7.548
7.304
7.284
7.259

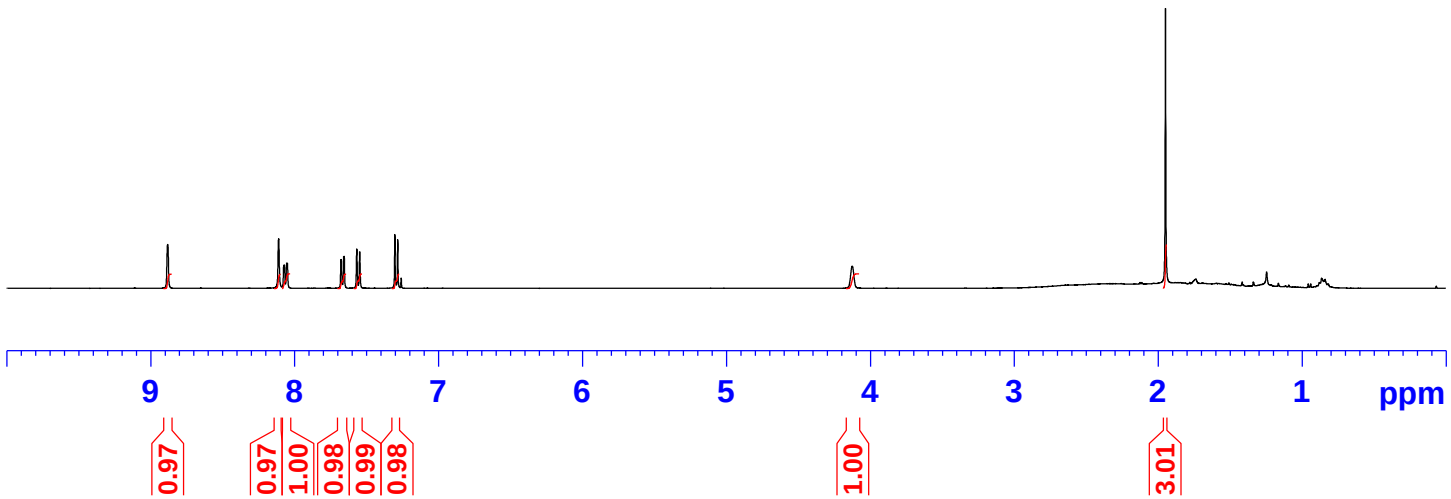
4.125

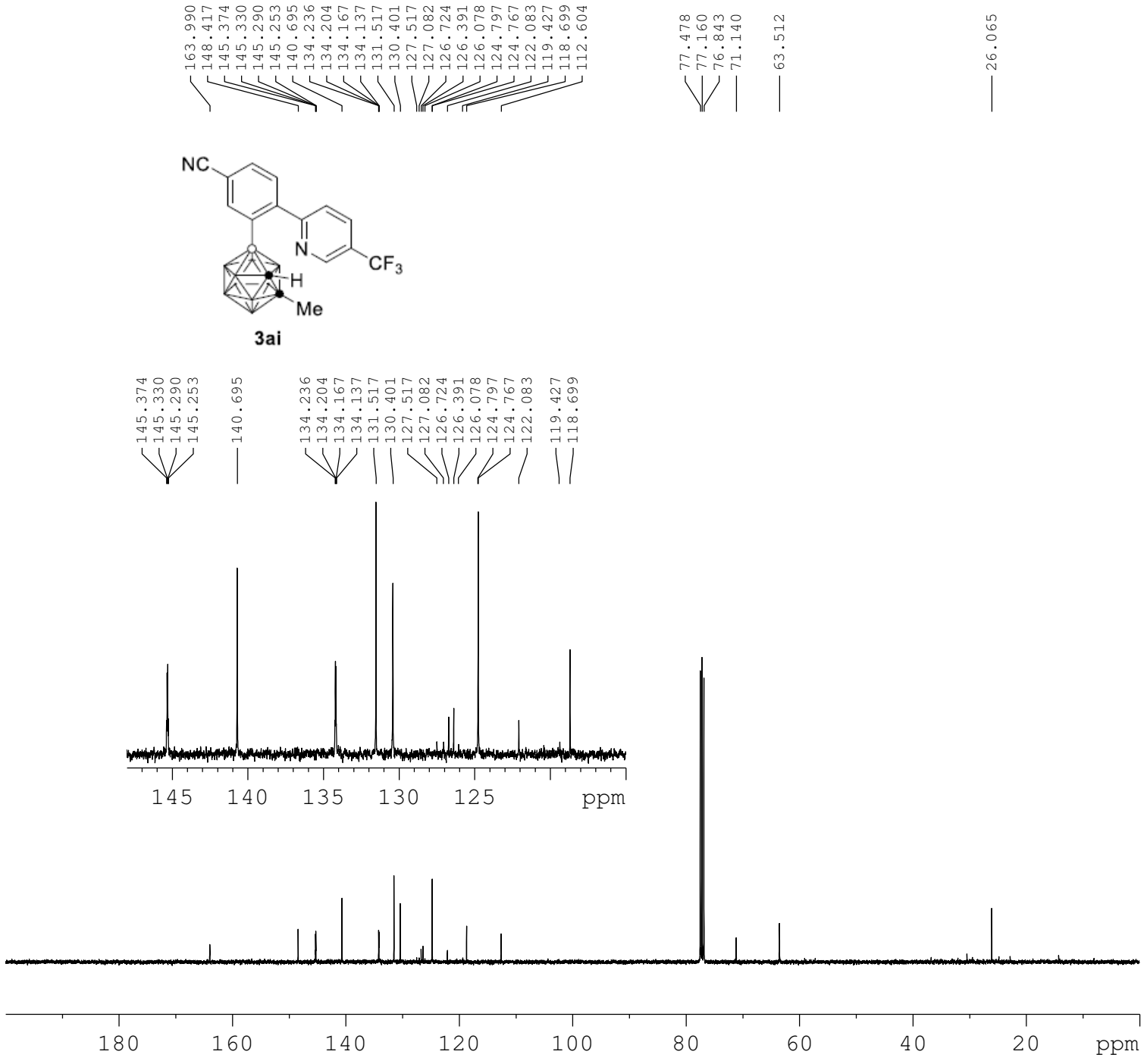
1.950



3ai

```
Current Data Parameters
NAME      CY-H-A-43p-CDCl3-re
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20161124
Time                17.16 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                      1
DW                 62.400 usec
DE                  6.50 usec
TE                 294.2 K
D1              1.00000000 sec
TD0                     1
SFO1          400.1324708 MHz
NUC1                   1H
P1                 15.00 usec
PLW1           8.31000042 W

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

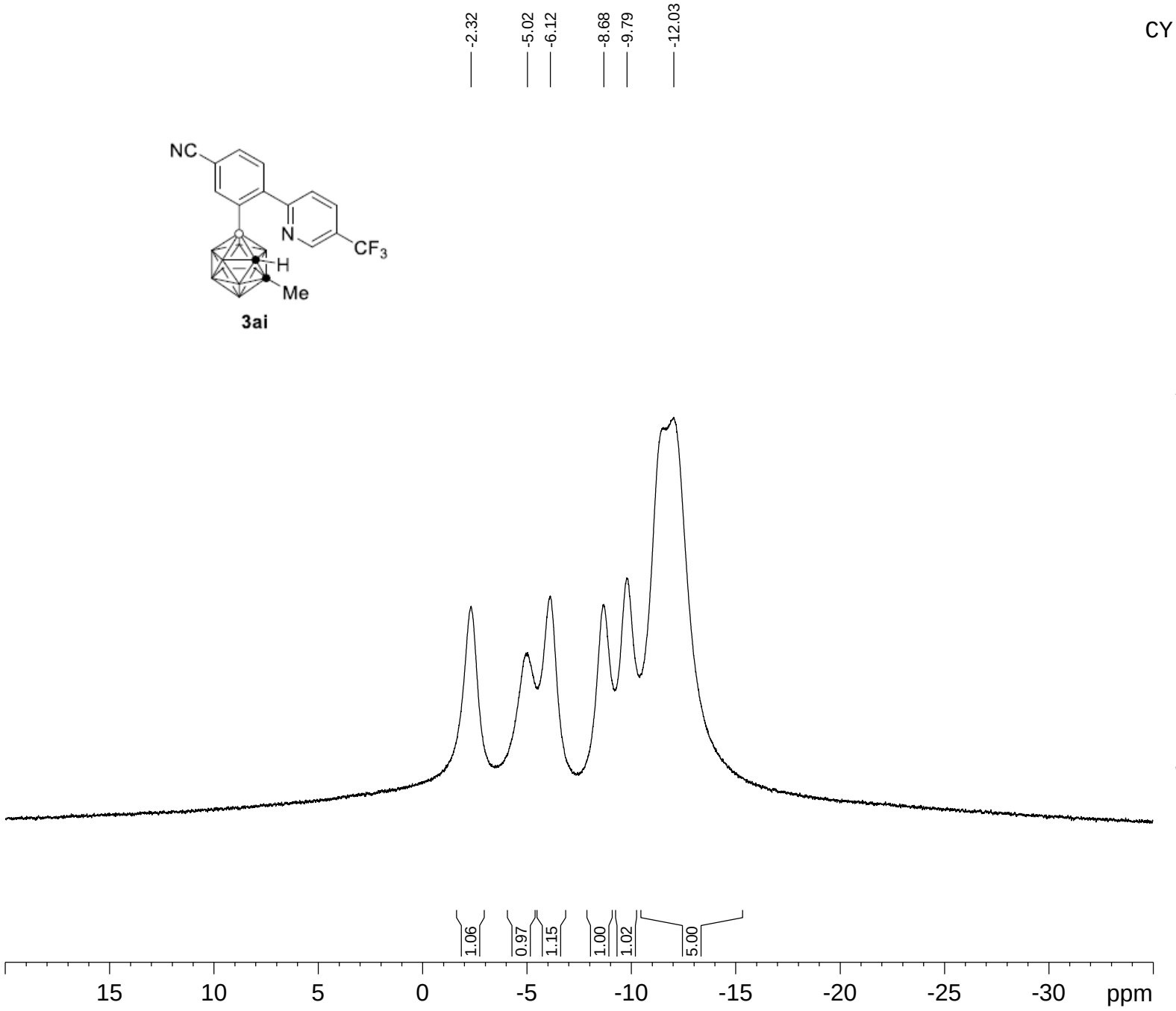




CY-C-A-43P-CDCl3

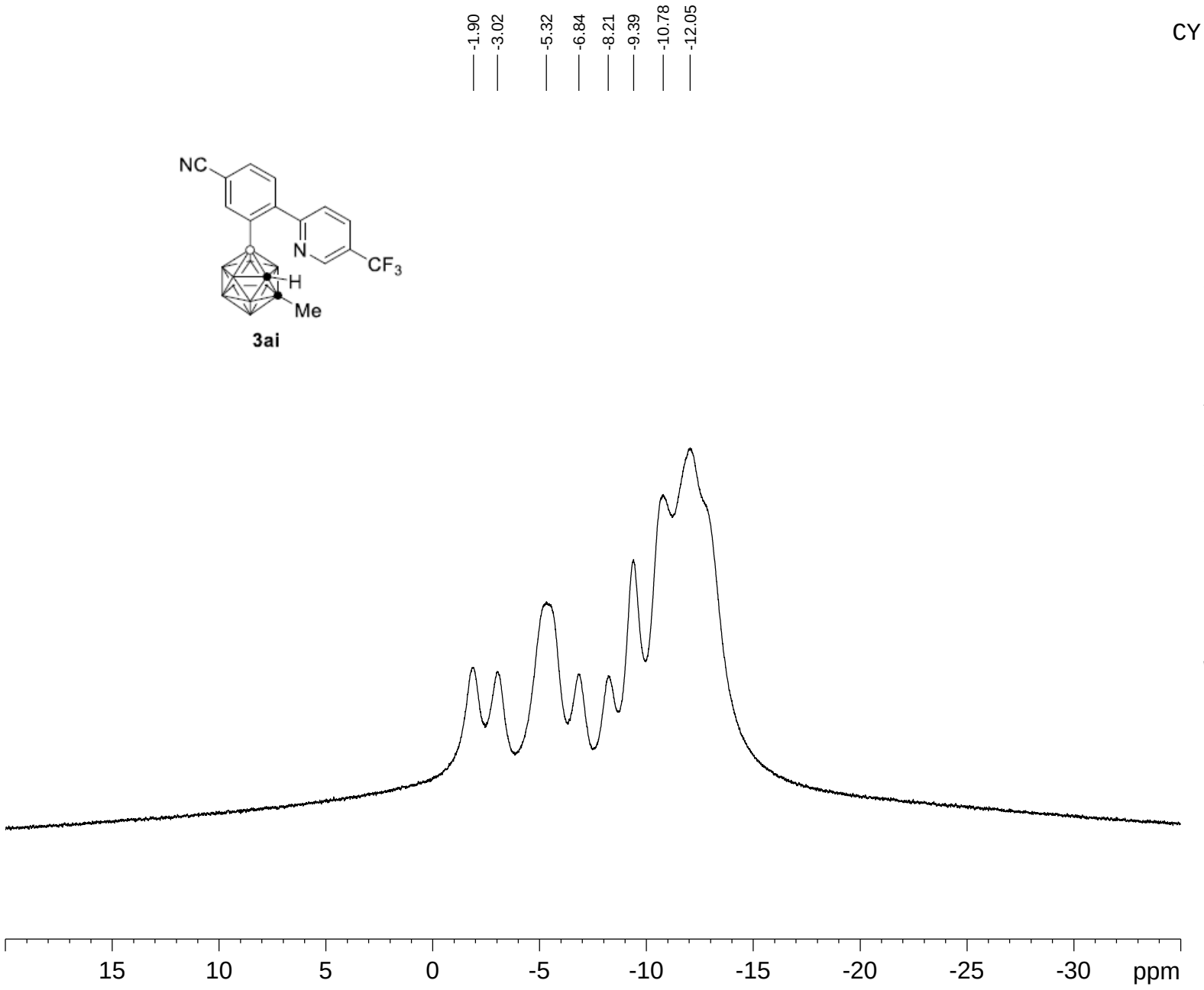
Bruker Advance III 400

Current Data Parameters	
NAME	CY-C-A-43P-CDCl3
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Date_	20161114
Time	20.33 h
INSTRUM	spect
PROBHD	Z824601_0021 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	568
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	100.6127568 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



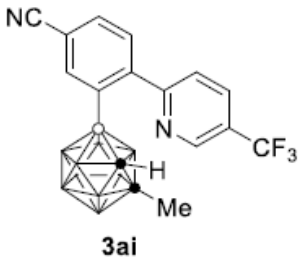
CY-B-A-43p

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

F2 - Acquisition Parameters
Date_           20161114
Time               21.17 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    52
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   456
DW                20.800 usec
DE                 6.50 usec
TE                296.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



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

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

F2 - Acquisition Parameters
Date_            20161114
Time                21.24 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                     456
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            128.4097881 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

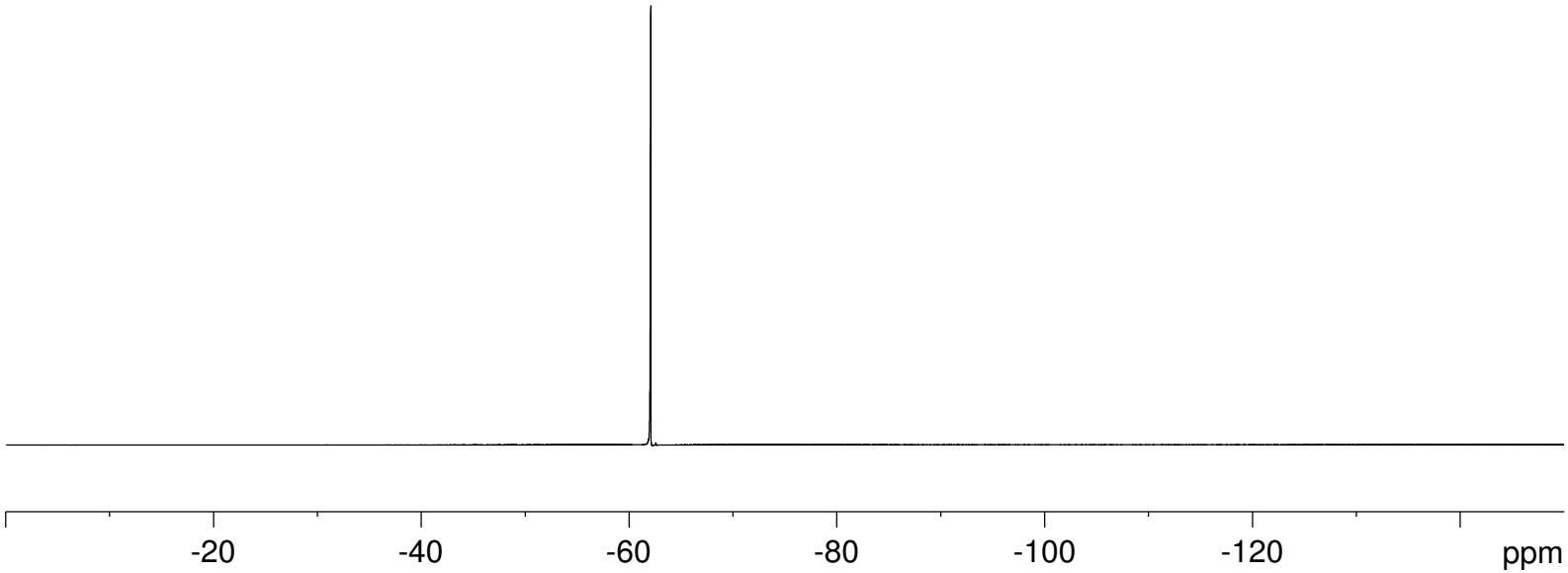


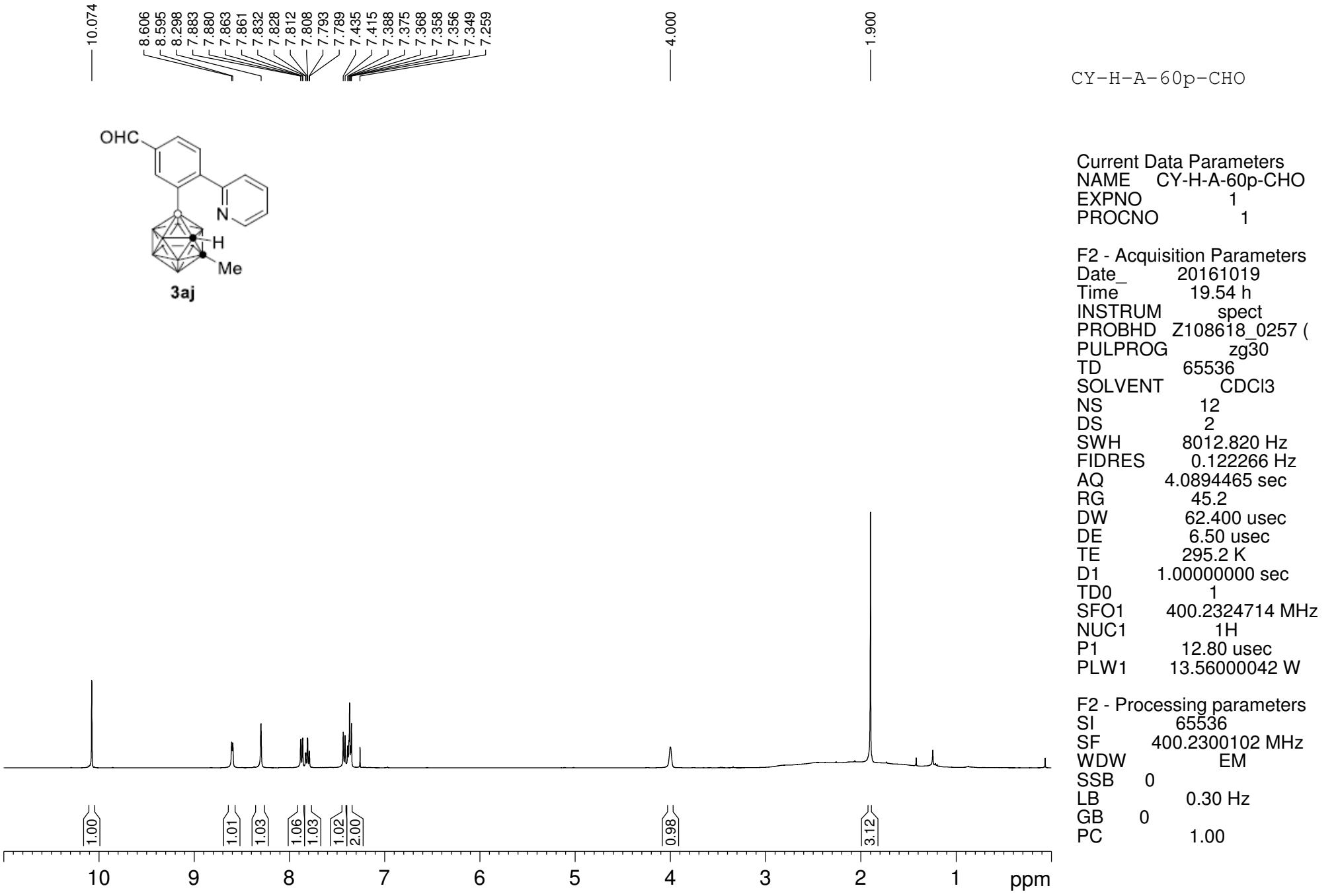
3ai

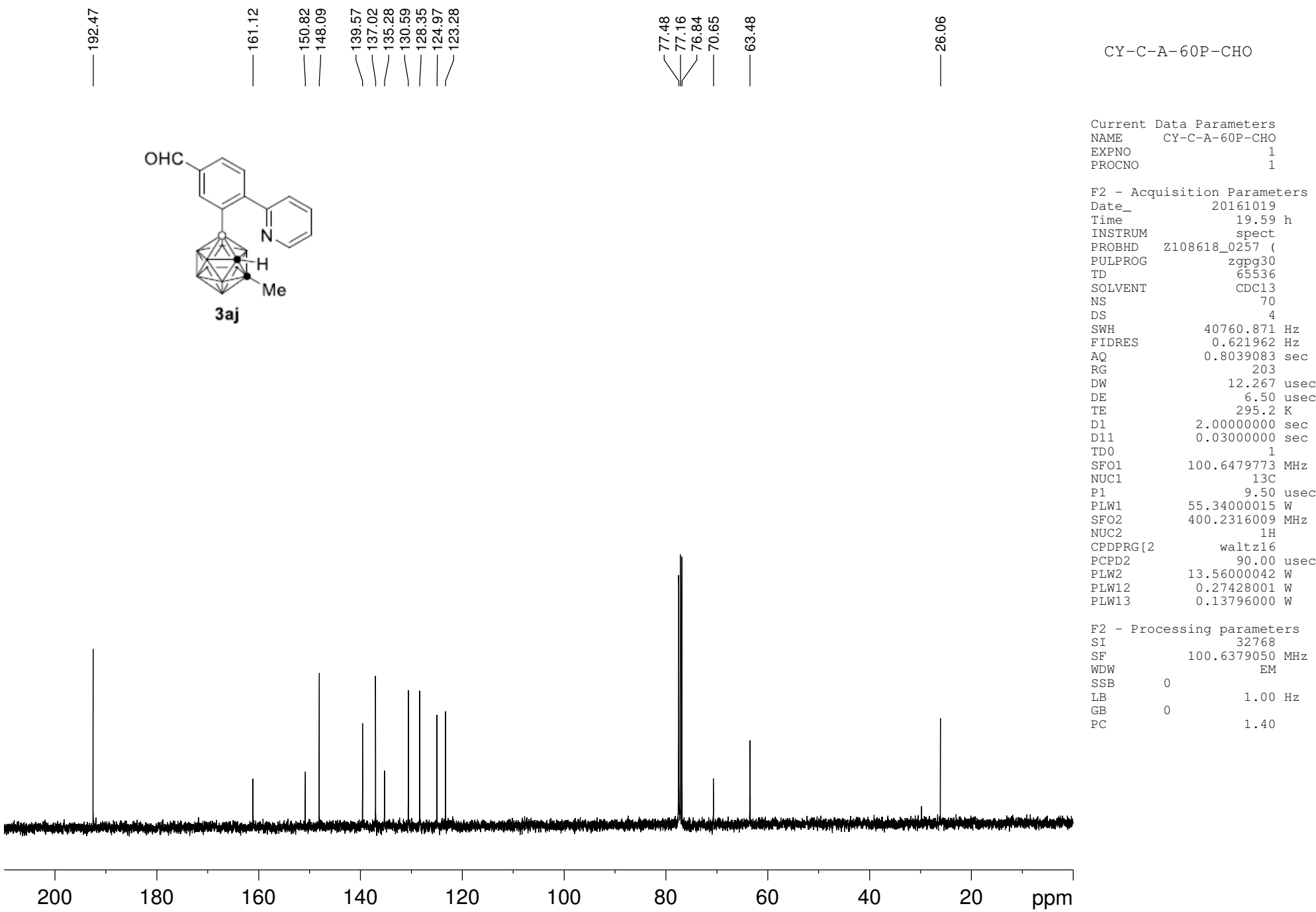
-62.07

CY-F-A-43P

```
Current Data Parameters
NAME          CY-F-A-43P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161124
Time              16.42 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG       zgfhigqn.2
TD               131072
SOLVENT             CDCl3
NS                     36
DS                      4
SWH            89285.711 Hz
FIDRES         0.681196 Hz
AQ             0.7340032 sec
RG                   645
DW                 5.600 usec
DE                 6.50 usec
TE                 296.1 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1
SFO1         376.5548010 MHz
NUC1                  19F
P1                14.70 usec
PLW1         18.36000061 W
SFO2         400.2316009 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

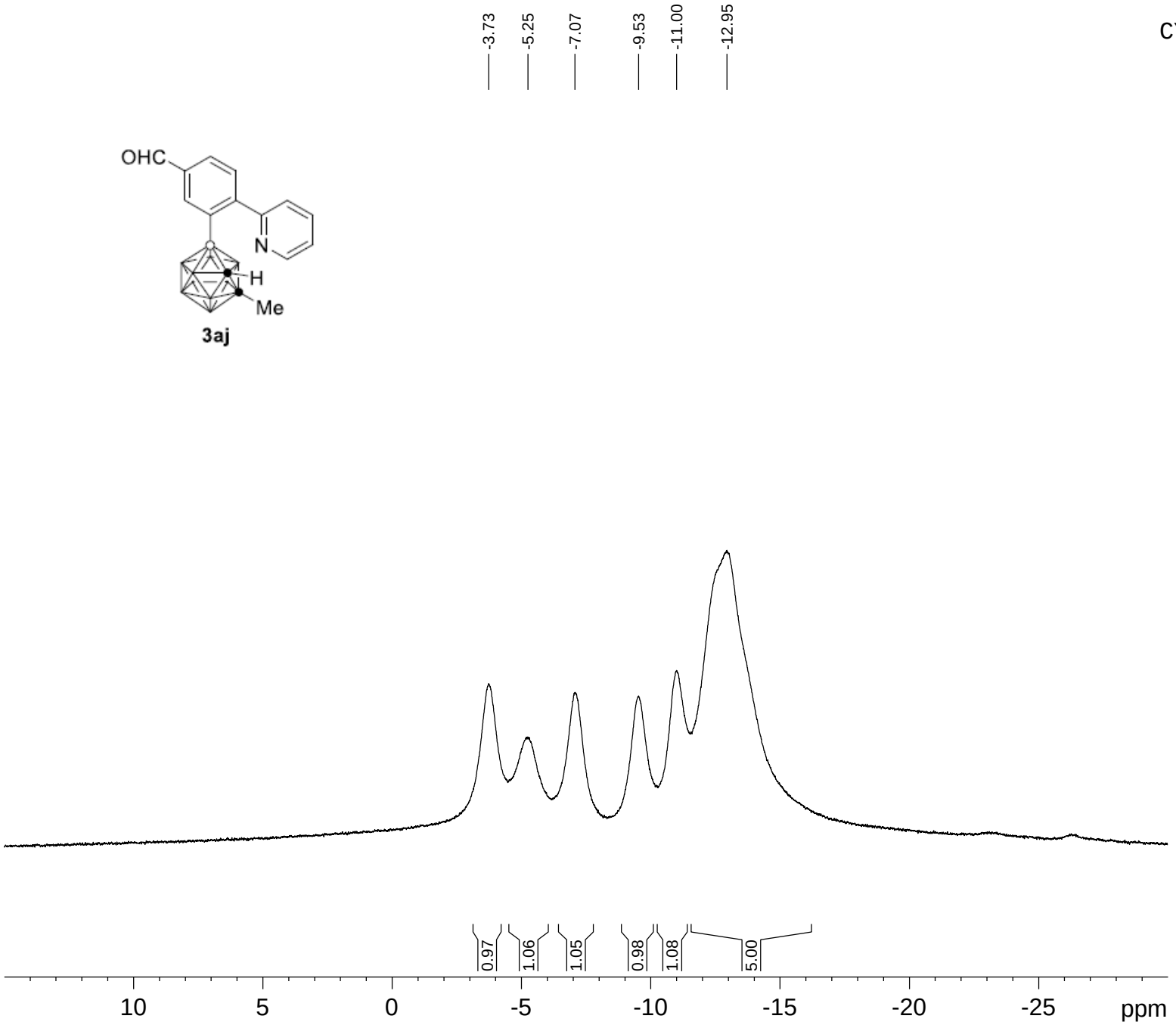



10.074
8.606
8.595
8.298
7.883
7.880
7.863
7.861
7.832
7.828
7.812
7.808
7.793
7.789
7.435
7.415
7.388
7.375
7.368
7.358
7.356
7.349
7.259
4.000
1.900
CY-H-A-60p-CHO
OHC
N
H
Me
3aj
Current Data Parameters
NAME CY-H-A-60p-CHO
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161019
Time 19.54 h
INSTRUM 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 45.2
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.00
1.01
1.03
1.06
1.03
1.02
2.00
0.98
3.12
10
9
8
7
6
5
4
3
2
1
ppm



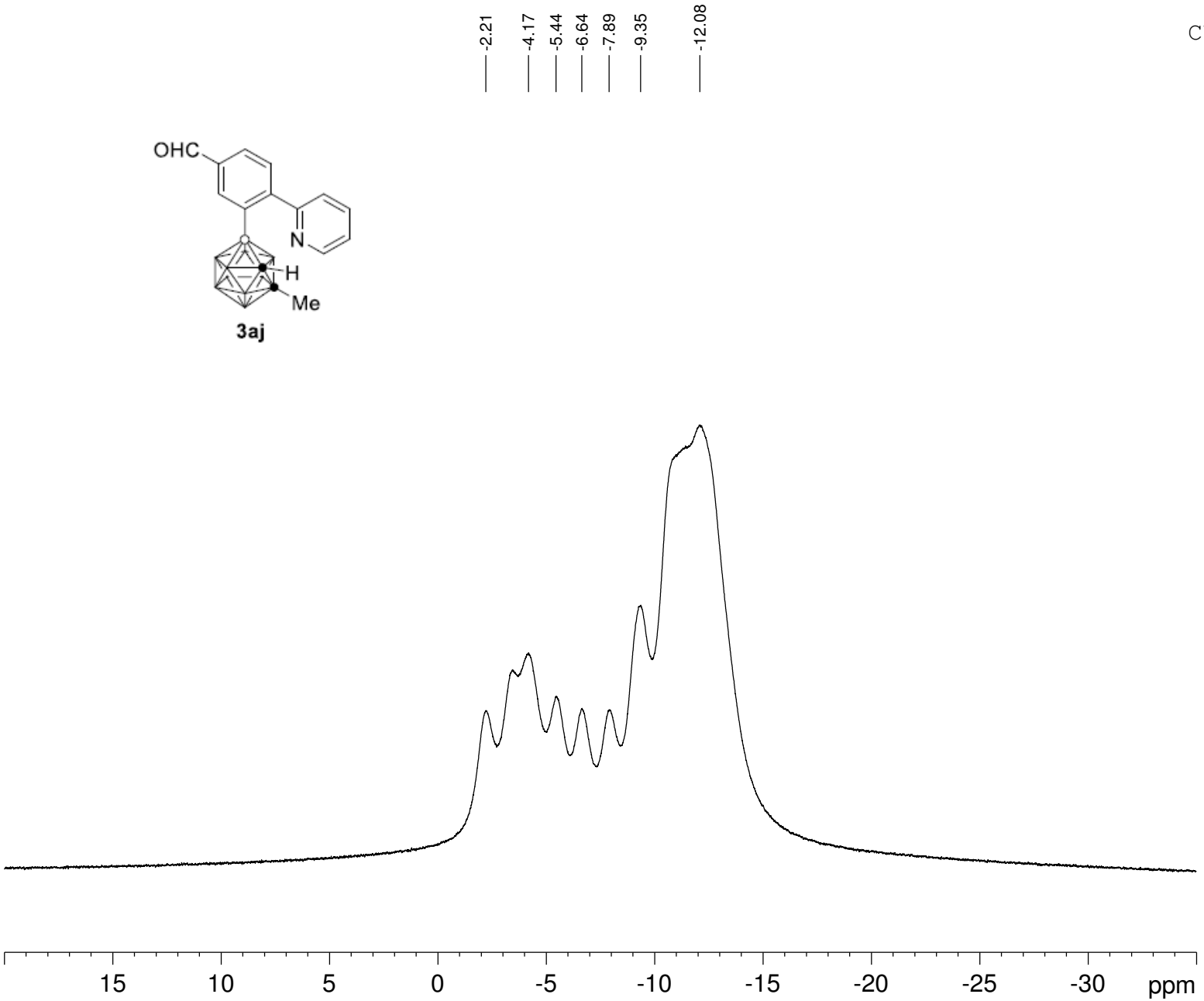
CY-C-A-60P-CHO

```
Current Data Parameters
NAME      CY-C-A-60P-CHO
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20161019
Time              19.59 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   70
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ            0.8039083 sec
RG                  203
DW               12.267 usec
DE                6.50 usec
TE                295.2 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          100.6379050 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



CY-B-A-55p-re3

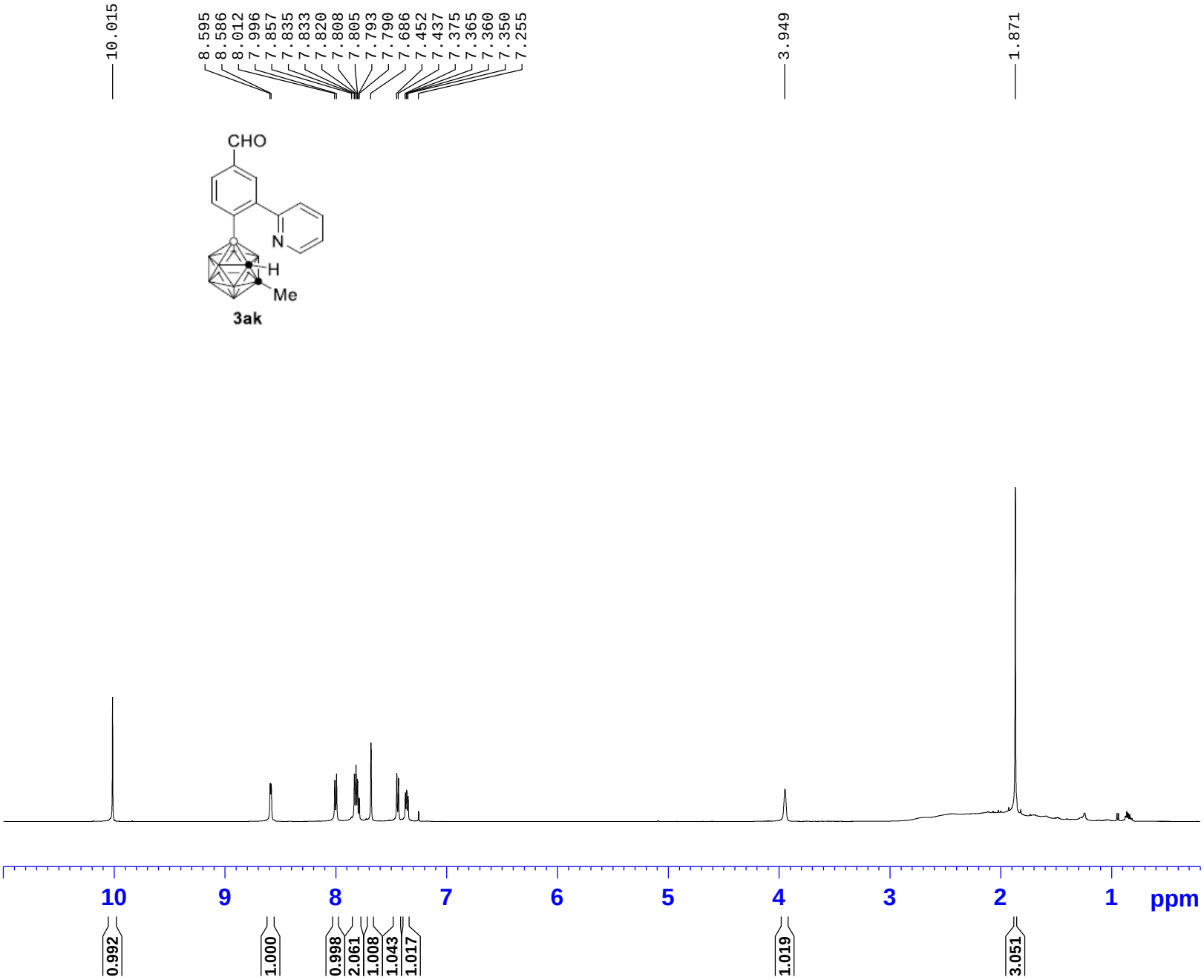
```
Current Data Parameters
NAME      CY-B-A-55p-re3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161127
Time              16.09 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT          Acetone
NS                    36
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   256
DW                20.800 usec
DE                 6.50 usec
TE                296.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-55P-(C)

```
Current Data Parameters
NAME      CY-B-A-55P-(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161015
Time               20.48 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                  203
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097881 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

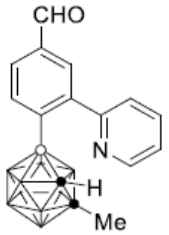
CY-H-B-200P-Ir-CDC-CHO




```
Current Data Parameters
NAME      CY-H-B-200P-Ir-CDC-CHO
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20190129
Time                   16.47 h
INSTRUM                spect
PROBHD    Z149001_0010 (
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                     30.85
DW                    50.000 usec
DE                    10.00 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                        1
SFO1              500.1330883 MHz
NUC1                       1H
P1                    11.25 usec
PLW1              15.00000000 W

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

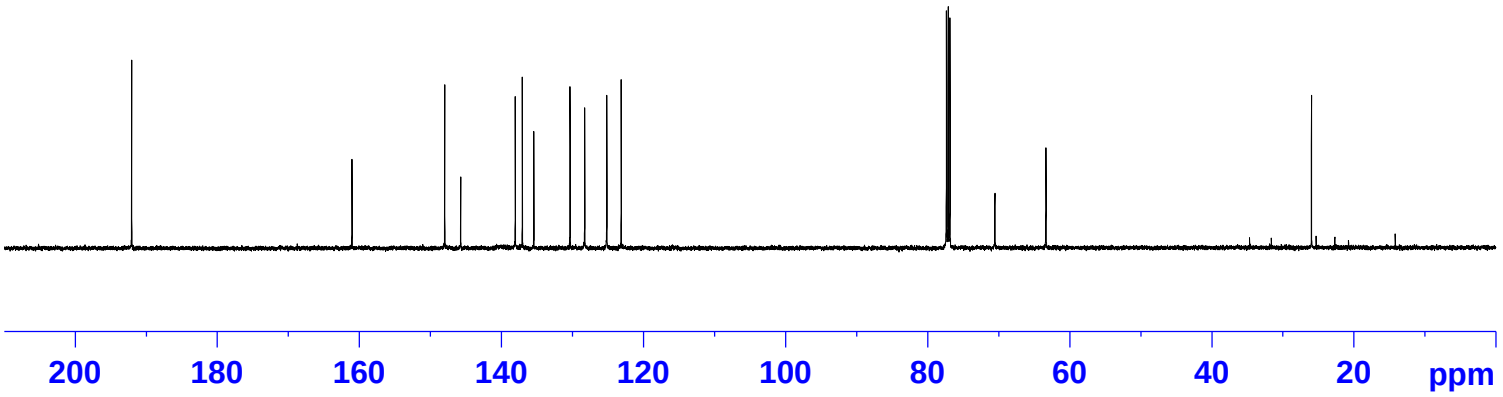
CY-C-B-200P-Ir-CDC-CHO-re

192.09 161.08 148.01 145.77 138.10 137.10 135.48 130.37 128.31 125.20 123.18 77.40 77.14 76.89 70.56 63.38 26.00

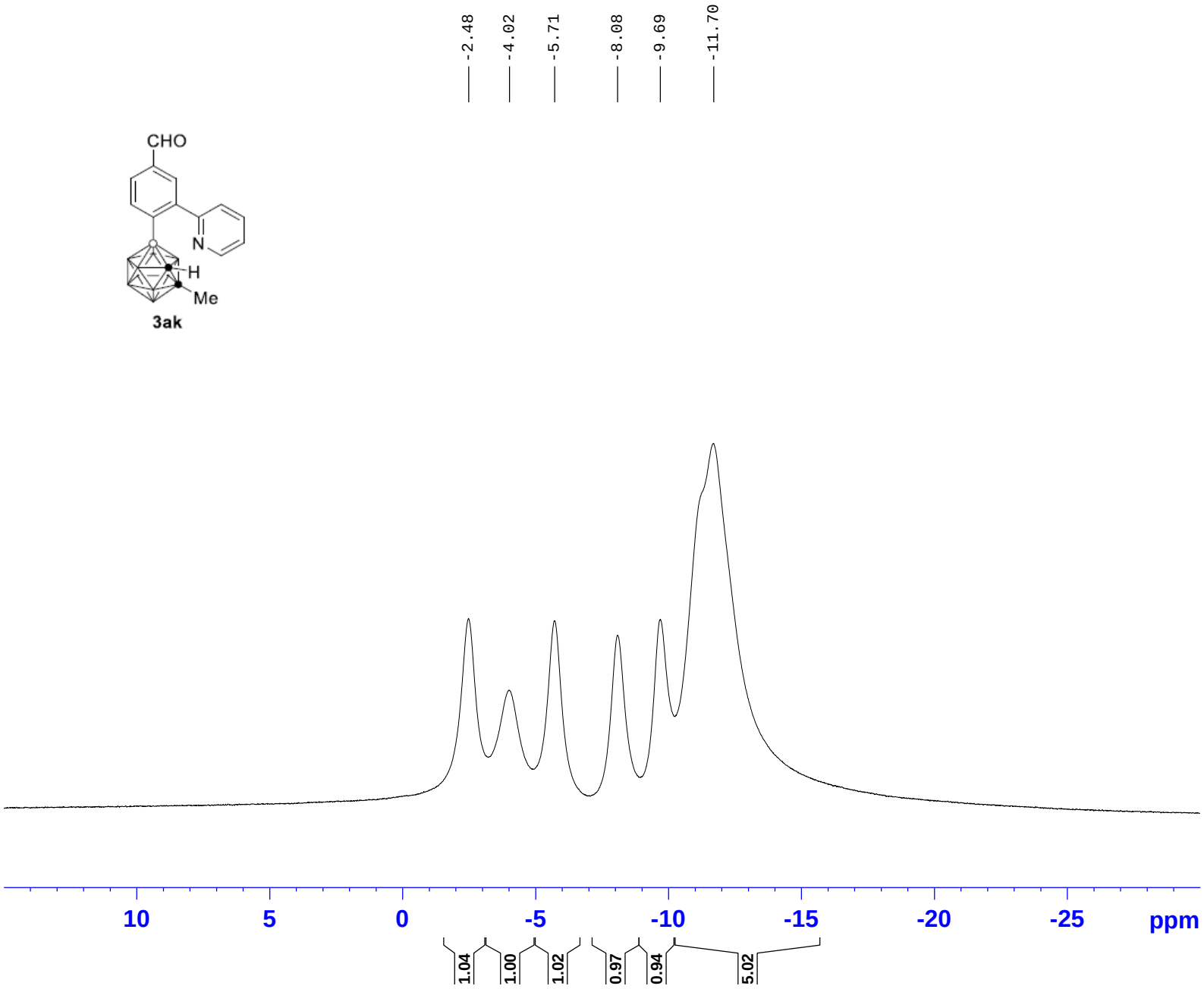


3ak

```
Current Data Parameters
NAME     CY-C-B-200P-Ir-CDC-CHO-re
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20190129
Time              17.29 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                32768
SF          125.7577824 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

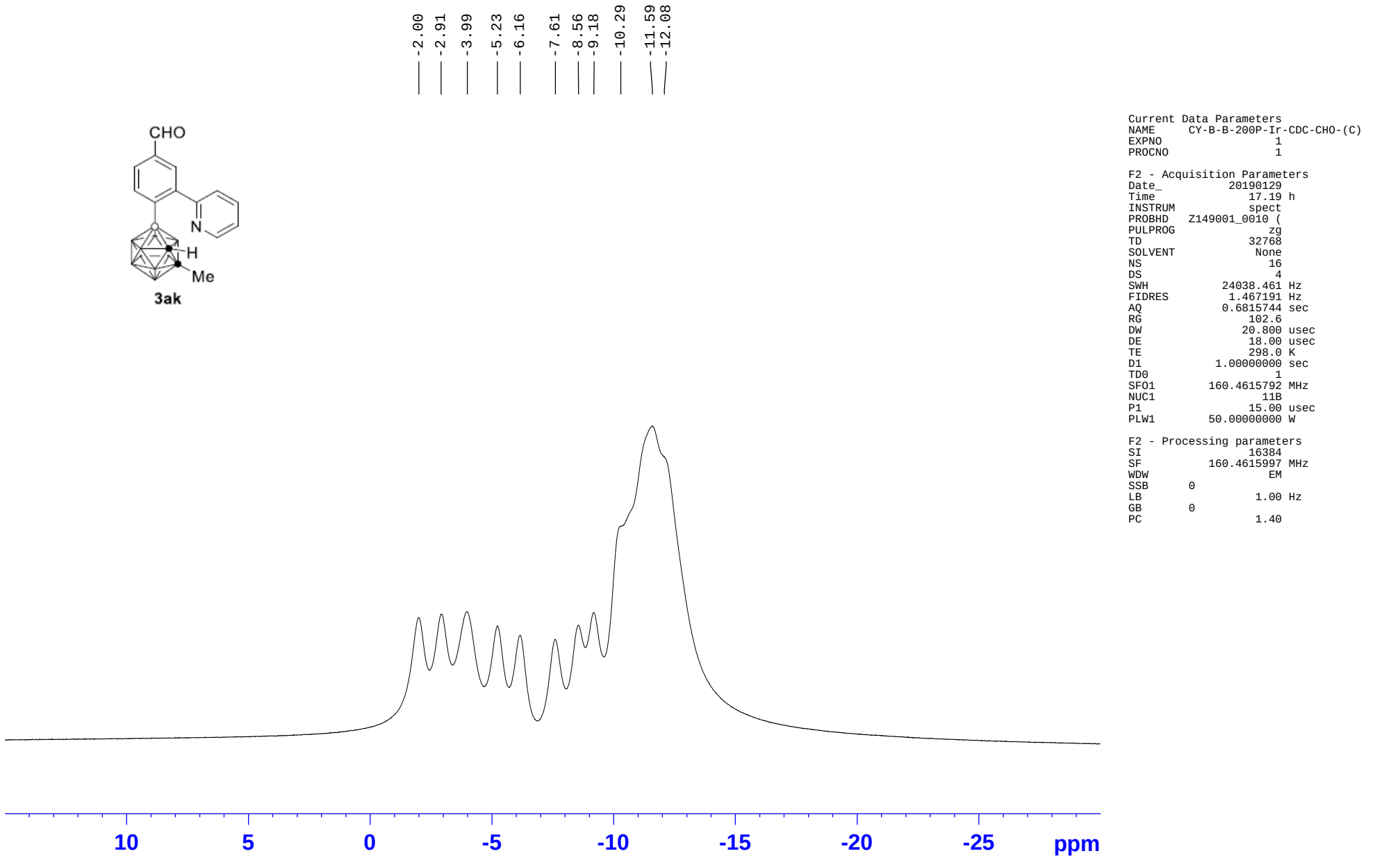


CY-B-B-200P-Ir-CDC-CHO

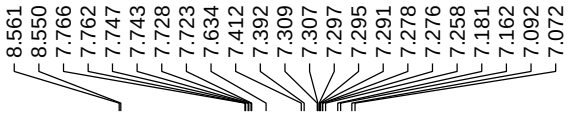



```
Current Data Parameters
NAME      CY-B-B-200P-Ir-CDC-CHO
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_           20190129
Time              17.18 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 32768
SOLVENT             None
NS                    16
DS                     4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               206.72
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         160.4615790 MHz
NUC1                11B
P1                15.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

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

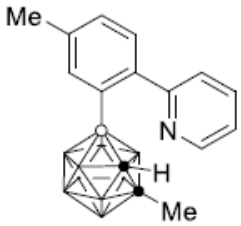
CY-B-B-200P-Ir-CDC-CHO-(C)



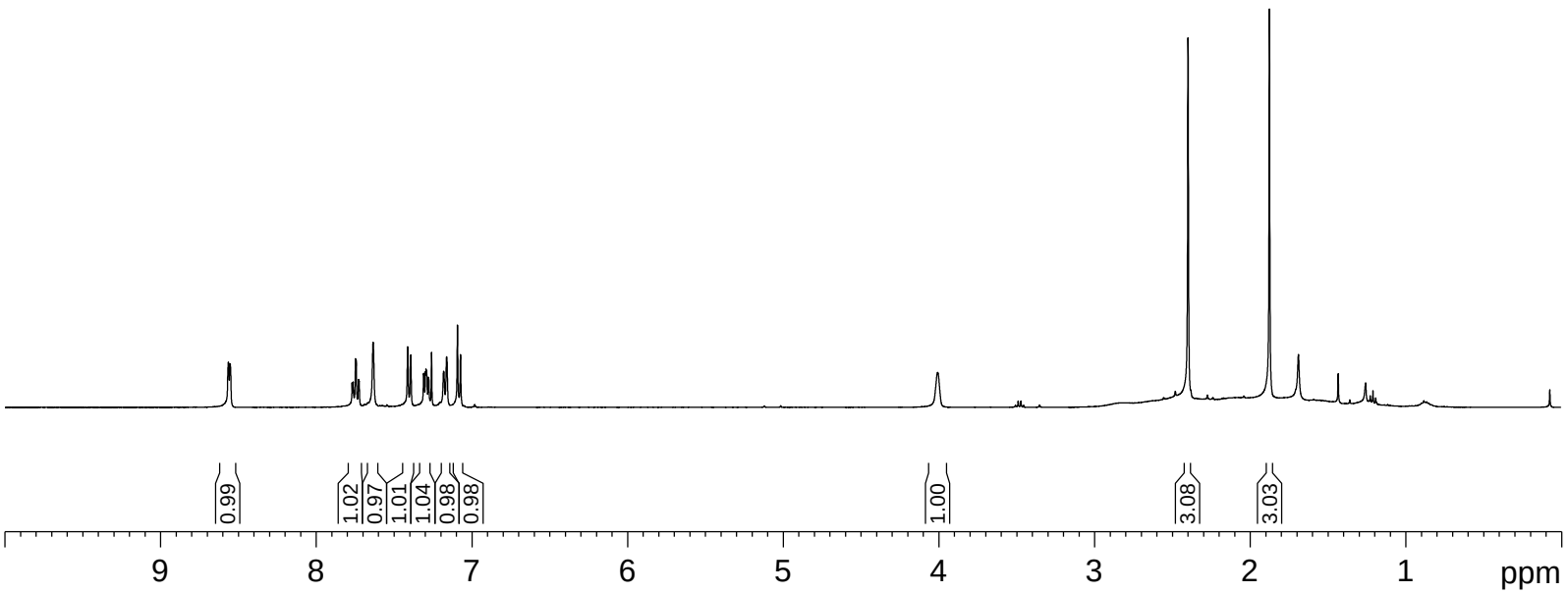

```
Current Data Parameters
NAME     CY-B-B-200P-Ir-CDC-CHO-(C)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20190129
Time              17.19 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG               zg
TD                32768
SOLVENT            None
NS                   16
DS                    4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG                102.6
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1          1.00000000 sec
TD0                   1
SFO1        160.4615792 MHz
NUC1                11B
P1                15.00 usec
PLW1        50.00000000 W

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



CY-H-A-42P



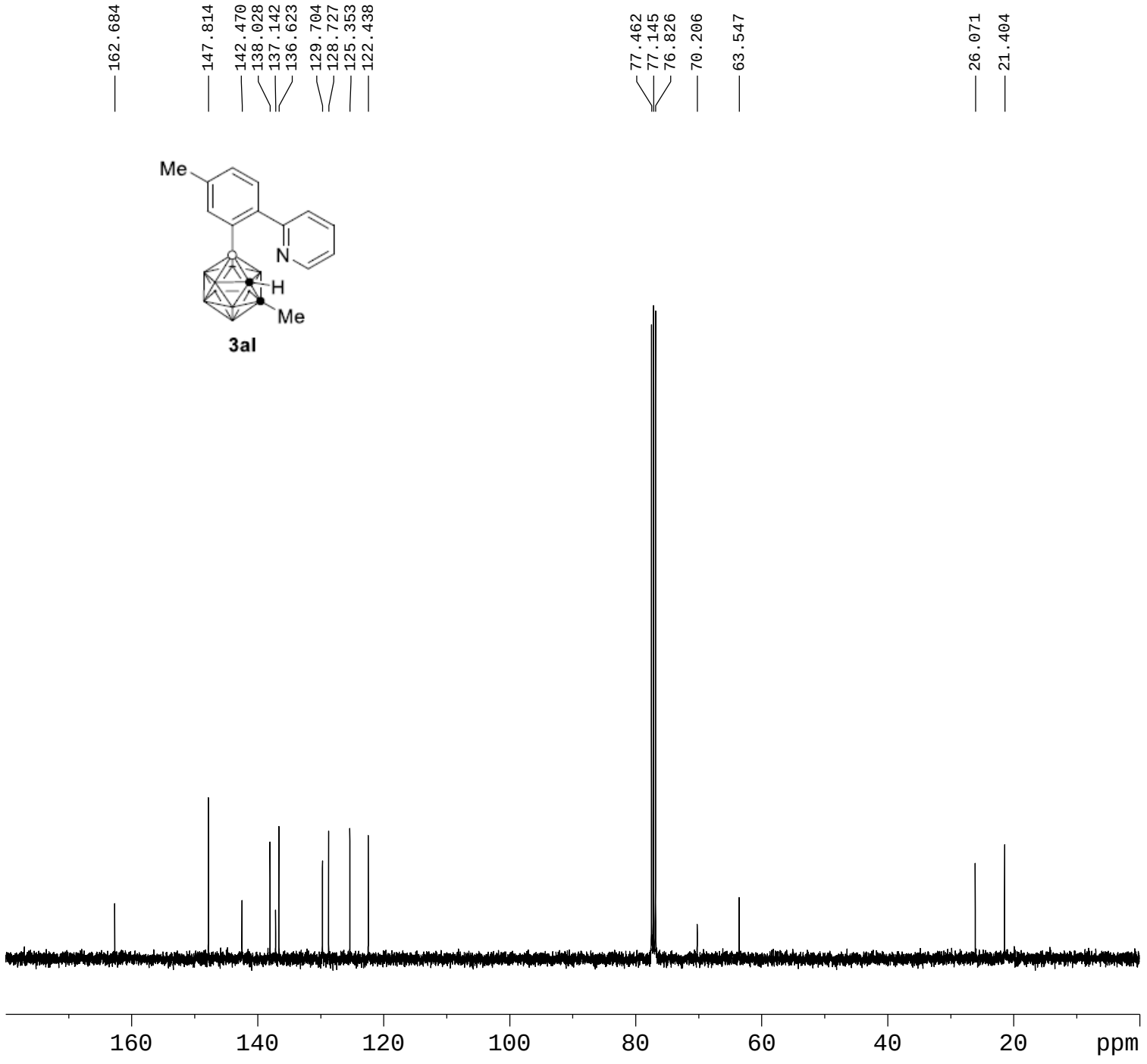
3al



Current Data Parameters
NAME CY-H-A-42P
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161103
Time 19.39 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 80.6
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MH
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

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



CY-C-A-42P-CDCl3

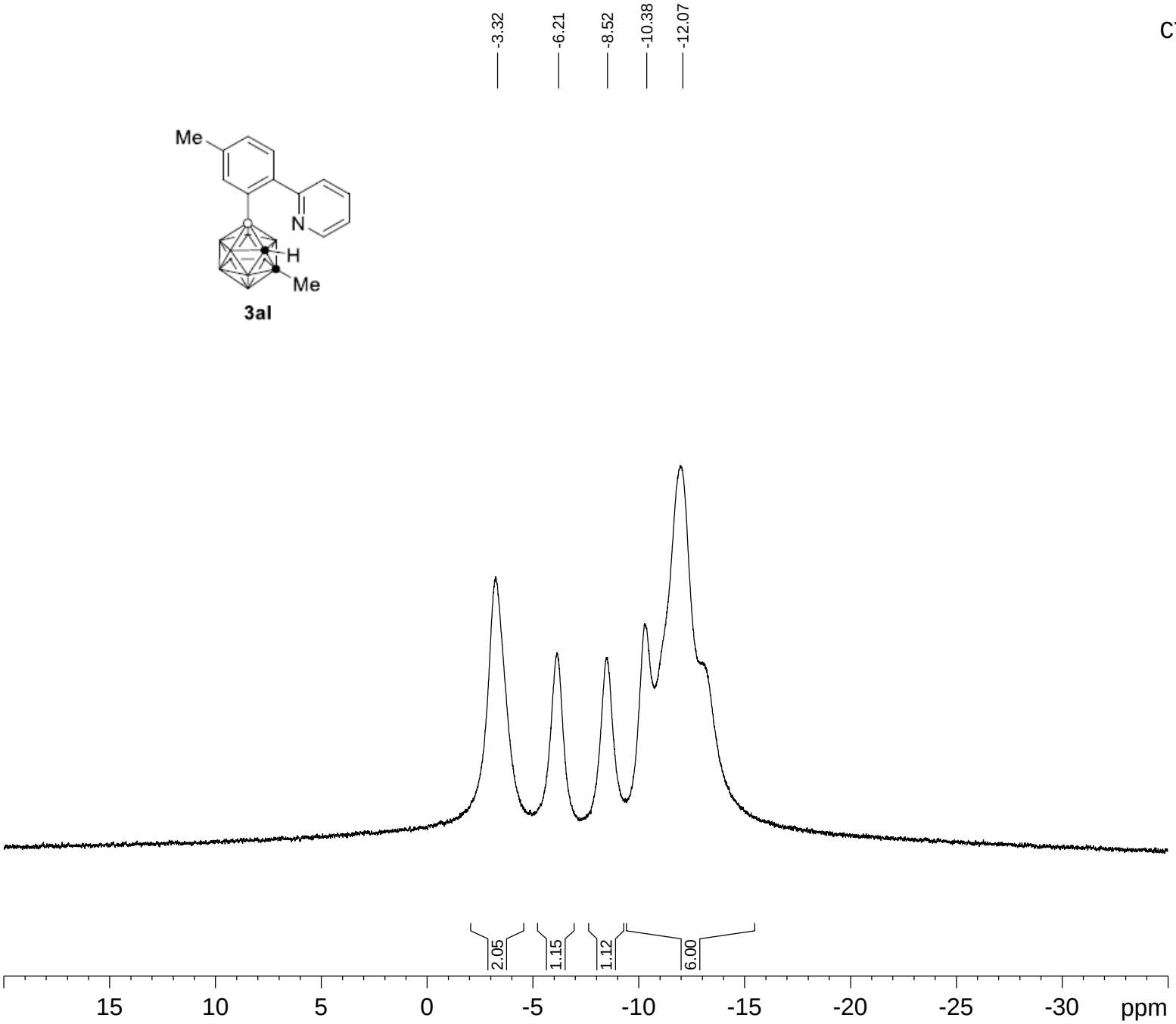
Bruker Advance III 400

Current Data Parameters
NAME CY-C-A-42P-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161103
Time 21.18 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 176
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 294.5 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

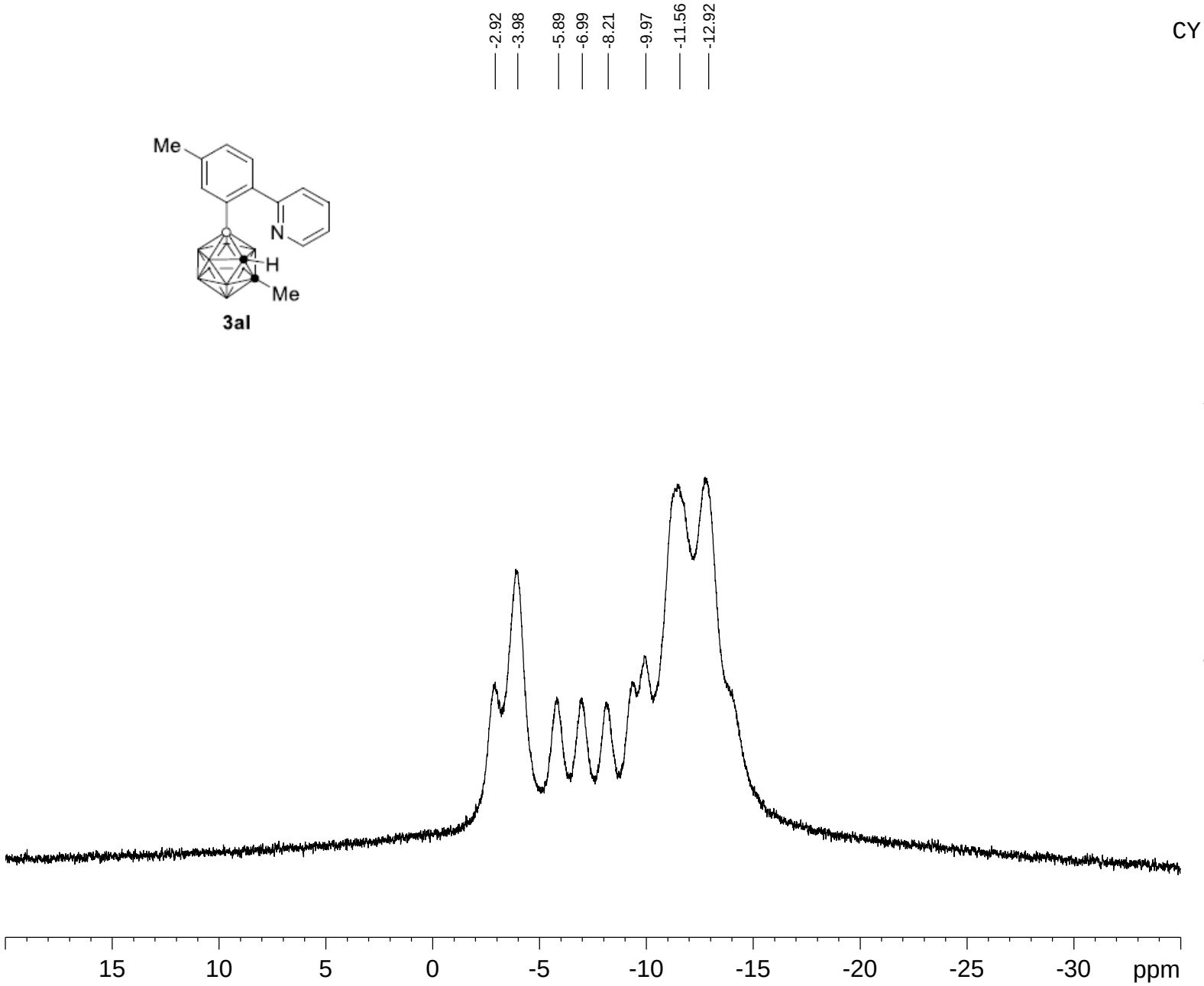
F2 - Processing parameters
SI 32768
SF 100.6127589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3al



CY-B-A-42P-RE2

```
Current Data Parameters
NAME      CY-B-A-42P-RE2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161103
Time               21.59 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    10
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   256
DW                20.800 usec
DE                 6.50 usec
TE                296.3 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
```



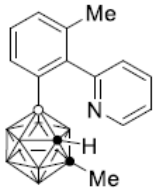
3al

CY-B-A-42P-(C)

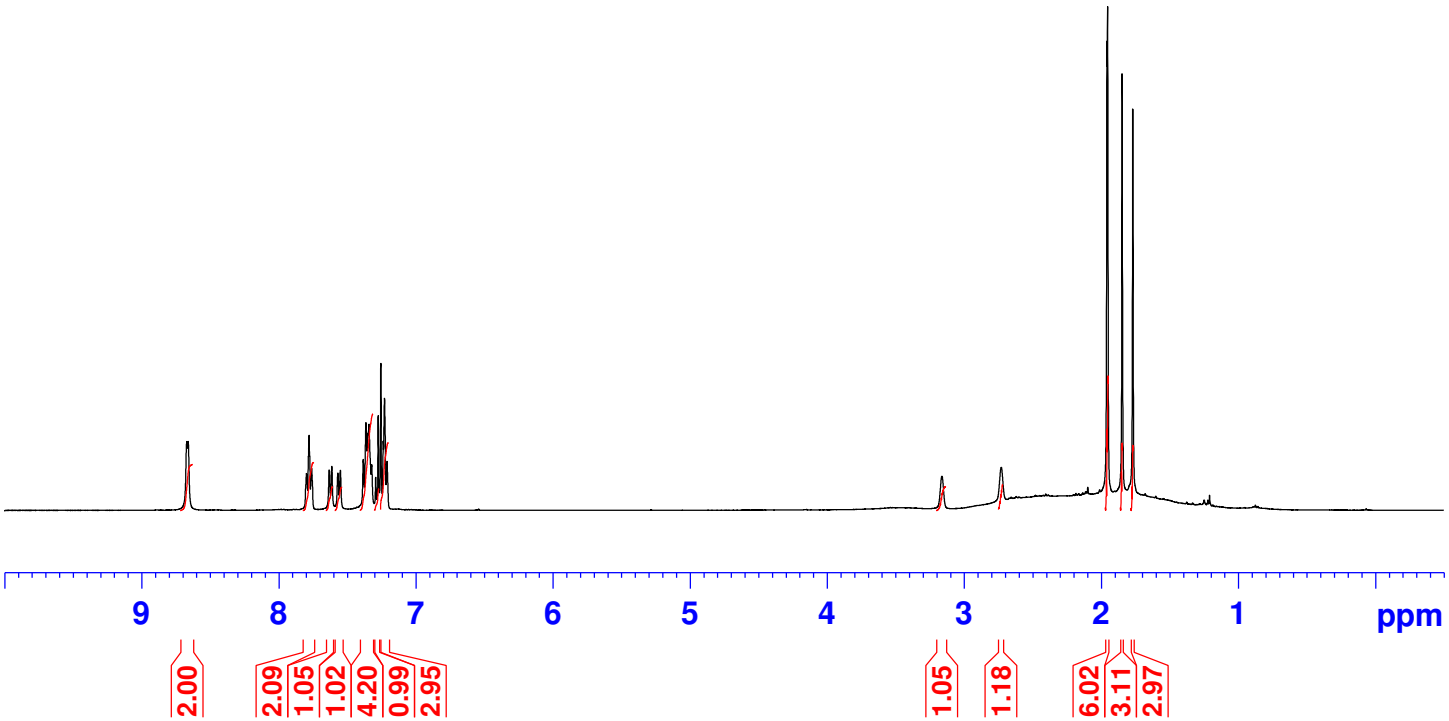
```
Current Data Parameters
NAME      CY-B-A-42P-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161103
Time                19.53 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                      4
DS                      2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                    256
DW                 20.800 usec
DE                  6.50 usec
TE                 296.4 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            128.4097881 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

8.672 8.662 7.799 7.794 7.780 7.766 7.761 7.633 7.614 7.570 7.552 7.385 7.365 7.350 7.343 7.323 7.294 7.276 7.257 7.239 7.230 7.211

3.163 2.731 1.959 1.955 1.849 1.771



3am




```
Current Data Parameters
NAME      CY-H-B-124p-o-CH3
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20190320
Time               16.24 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     14
DS                      2
SWH              8012.820 Hz
FIDRES           0.244532 Hz
AQ              4.0894465 sec
RG                    114
DW                 62.400 usec
DE                  6.50 usec
TE                 294.9 K
D1            1.00000000 sec
TD0                     1
SFO1         400.1324708 MHz
NUC1                   1H
P1                 15.00 usec
PLW1          8.31000042 W

F2 - Processing parameters
SI                  65536
SF           400.1300116 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

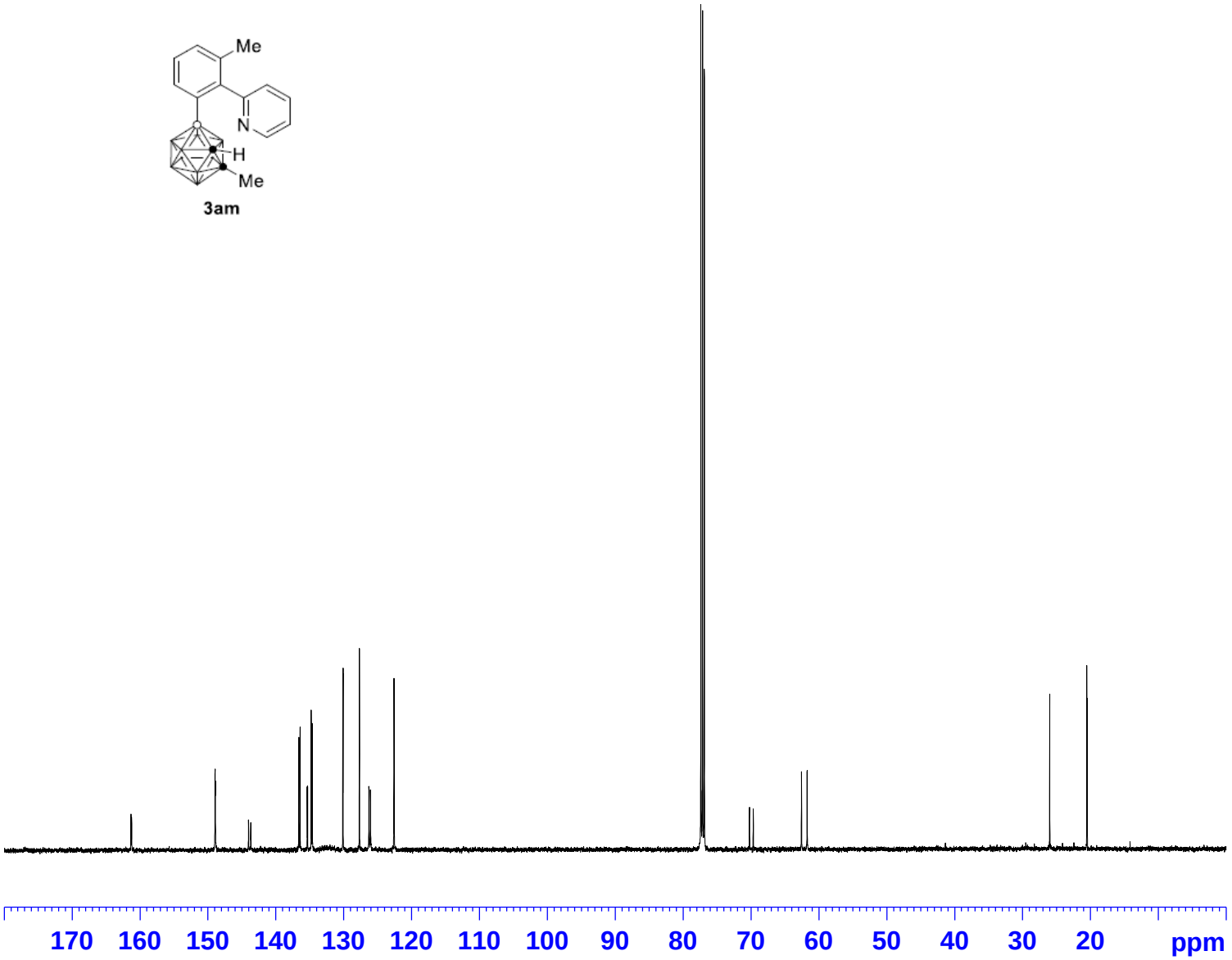
CY-C-B-124P-IrCDC-Me

161.34
161.24
148.95
148.90
144.05
143.72
136.65
136.47
135.41
135.35
134.81
134.66
130.16
130.13
127.72
126.32
126.08
122.62

77.42
77.16
76.91
70.25
69.70
62.59
61.76

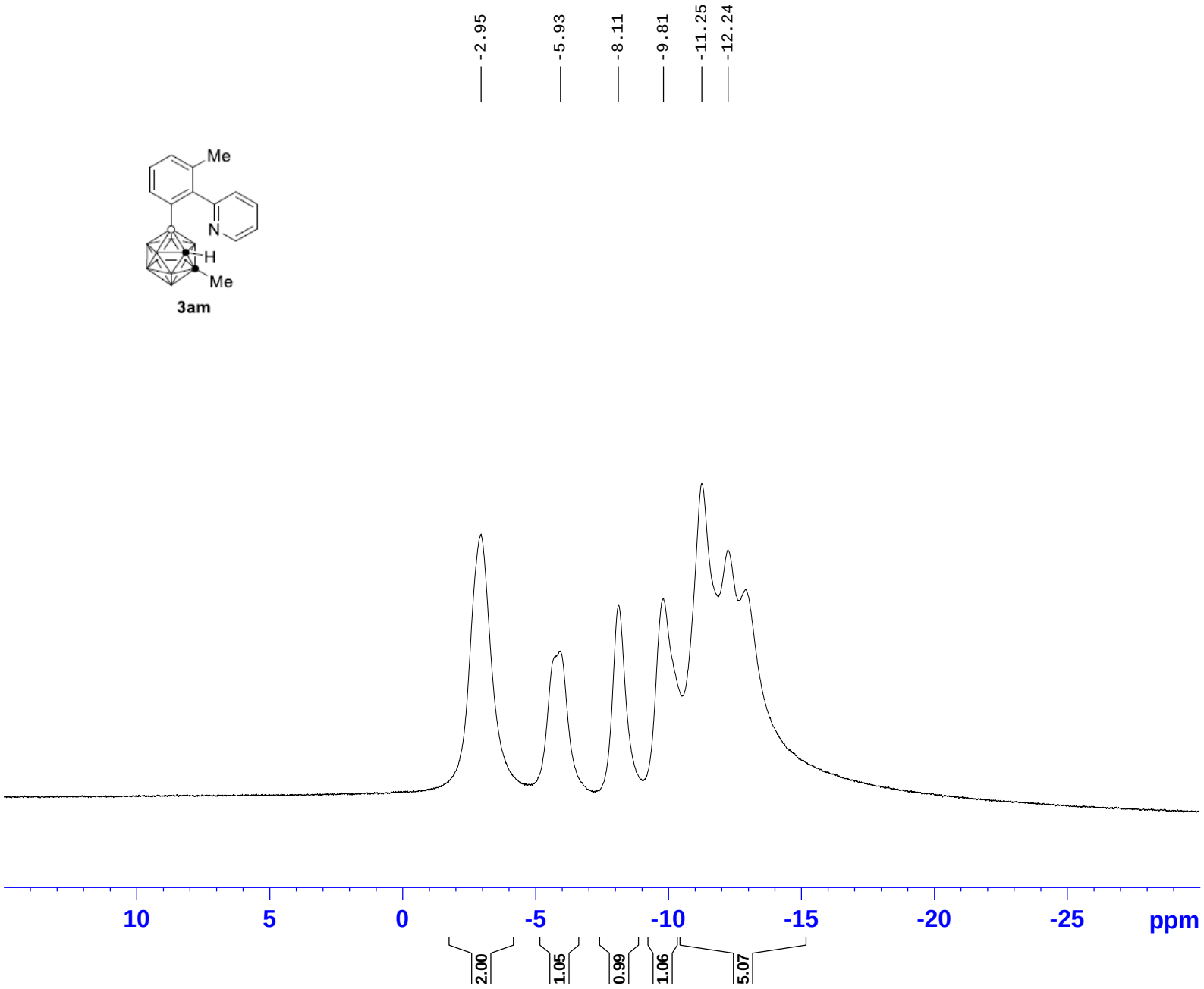
26.02
20.56
20.49

3am



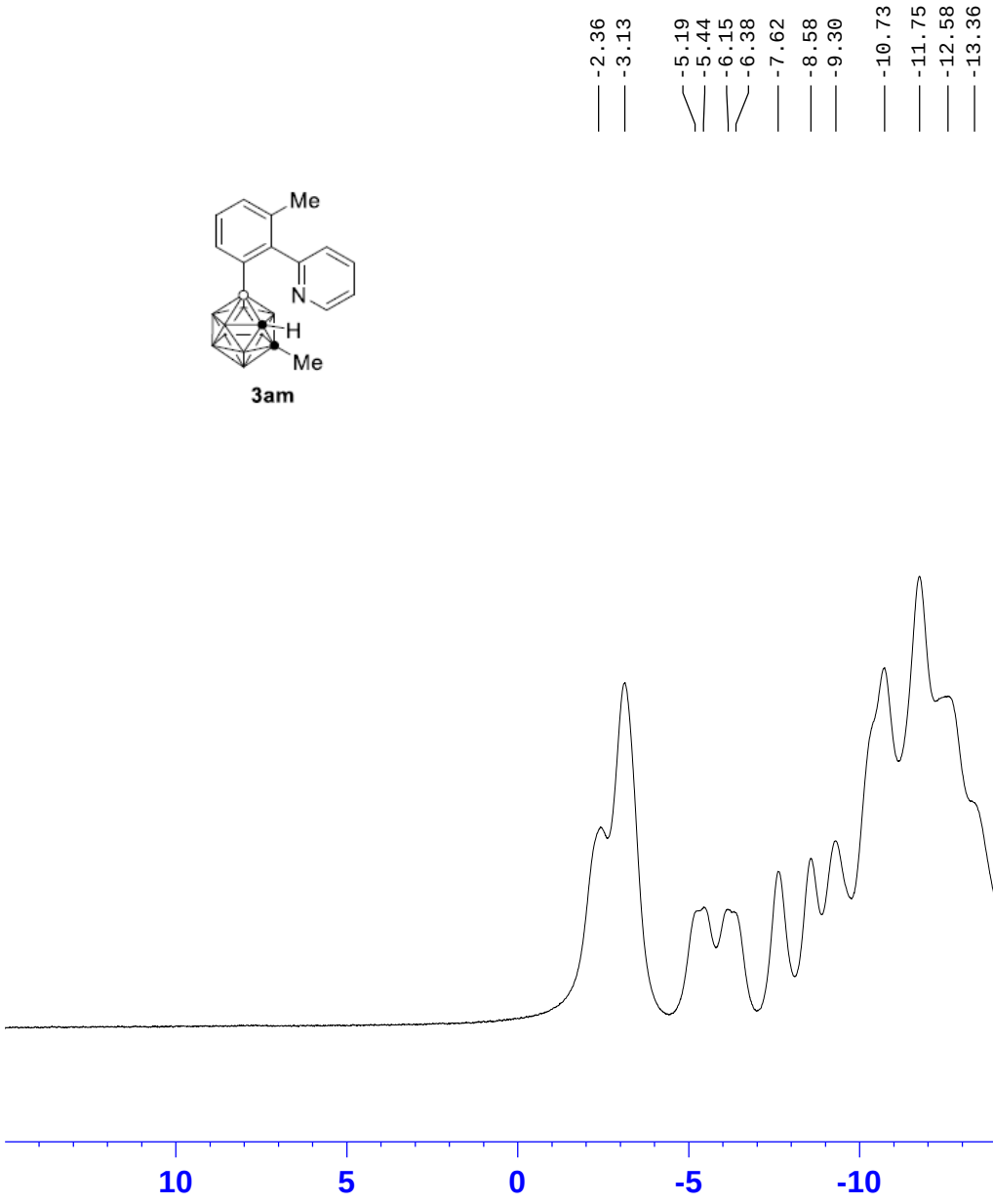

```
Current Data Parameters
NAME      CY-C-B-124P-IrCDC-Me
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190129
Time               16.38 h
INSTRUM             spect
PROBHD    Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   208
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.29663000 W
PLW13         0.14920001 W

F2 - Processing parameters
SI                 32768
SF           125.7577763 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

CY-B-B-124P-IrCDC-Me

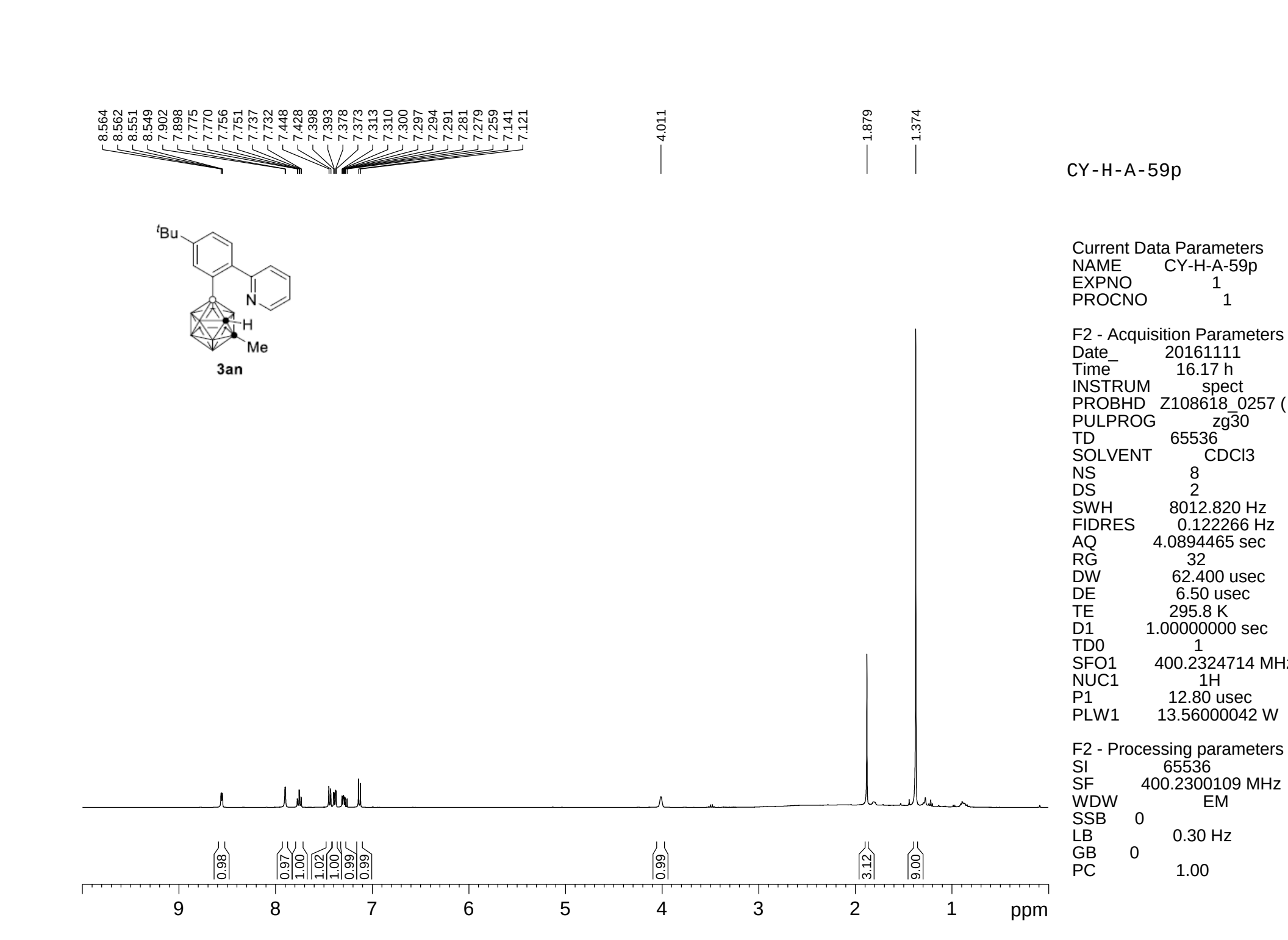


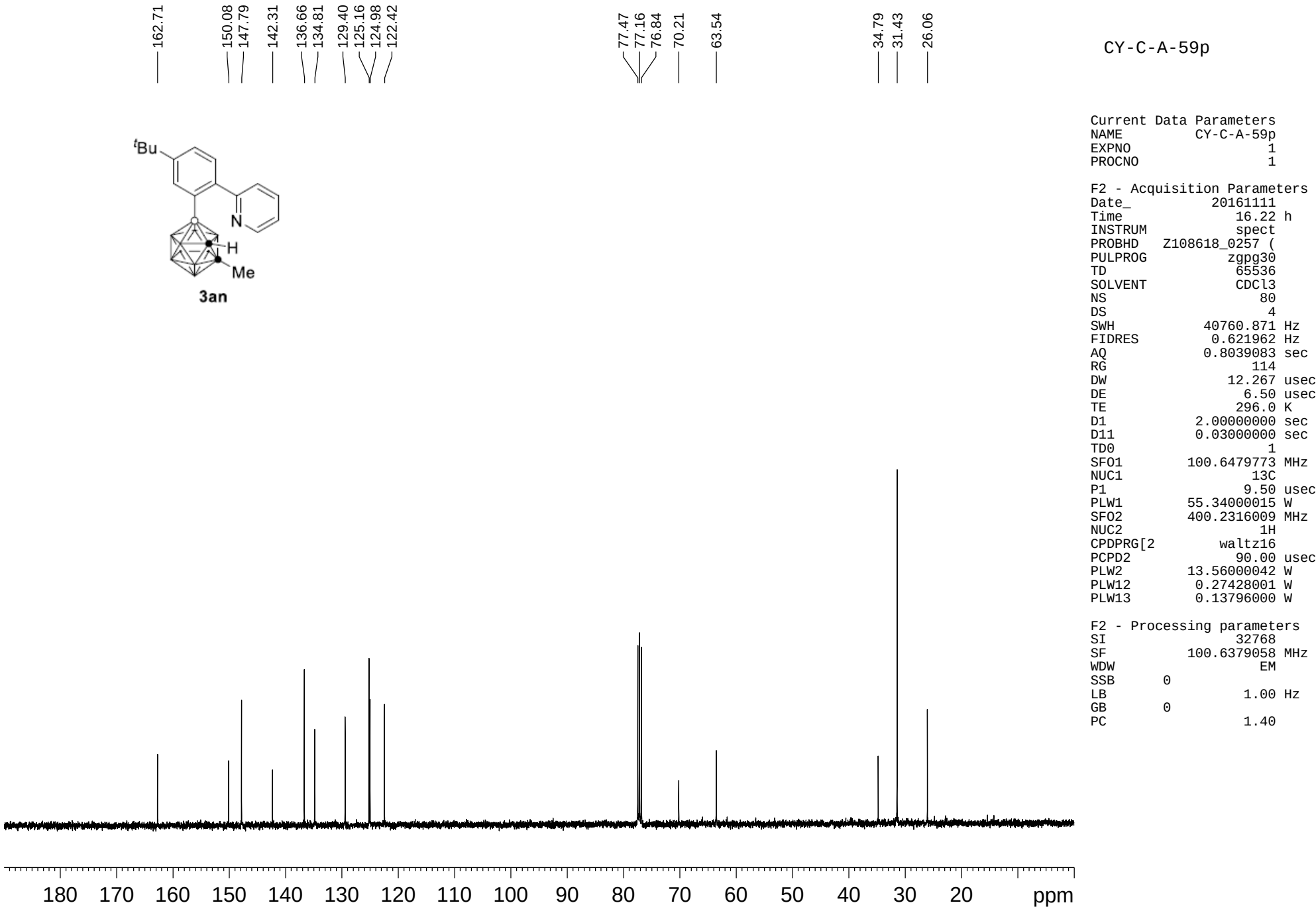

```
Current Data Parameters
NAME      CY-B-B-124P-IrCDC-Me
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190129
Time              16.42 h
INSTRUM             spect
PROBHD    Z149001_0010 (
PULPROG           zgpg30
TD                32768
SOLVENT            None
NS                   16
DS                    4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               206.72
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        160.4615790 MHz
NUC1                11B
P1                15.00 usec
PLW1        50.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

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

CY-B-B-124P-IrCDC-Me-(C)



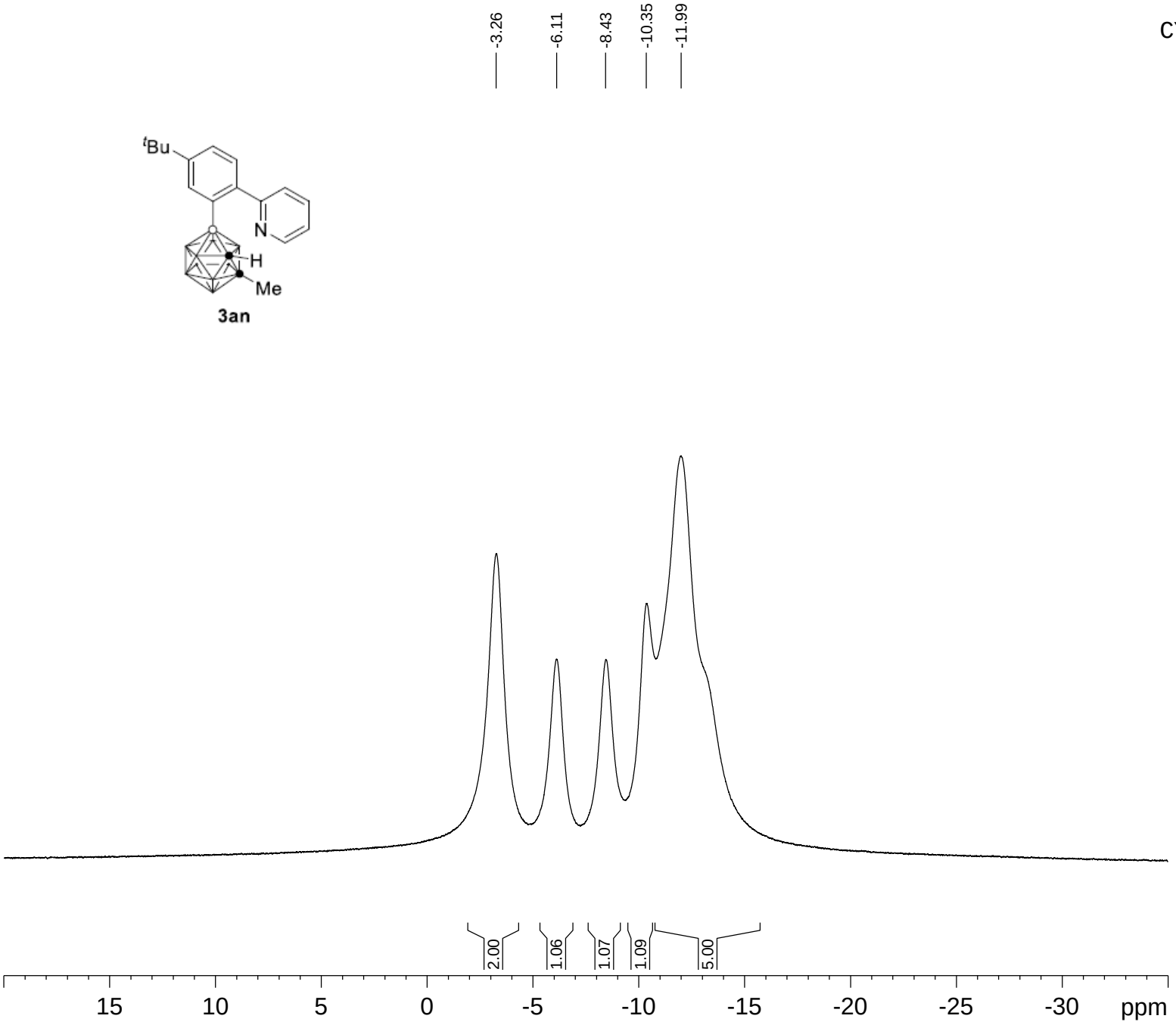

```
Current Data Parameters
NAME      CY-B-B-124P-IrCDC-Me-(C)
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_              20190129
Time                  16.43 h
INSTRUM                spect
PROBHD    Z149001_0010 (
PULPROG                   zg
TD                     32768
SOLVENT                None
NS                       16
DS                        4
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                 0.6815744 sec
RG                     142.5
DW                    20.800 usec
DE                    18.00 usec
TE                    298.0 K
D1              1.00000000 sec
TD0                       1
SFO1            160.4615792 MHz
NUC1                    11B
P1                    15.00 usec
PLW1            50.00000000 W

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


8.564
8.562
8.551
8.549
7.902
7.898
7.775
7.770
7.756
7.751
7.737
7.732
7.448
7.428
7.398
7.393
7.378
7.373
7.313
7.310
7.300
7.297
7.294
7.291
7.281
7.279
7.259
7.141
7.121
4.011
1.879
1.374
CY-H-A-59p
tBu
N
H
Me
3an
Current Data Parameters
NAME CY-H-A-59p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161111
Time 16.17 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 32
DW 62.400 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MH
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0.98
0.97
1.00
1.02
1.00
0.99
0.99
0.99
3.12
9.00
9
8
7
6
5
4
3
2
1
ppm



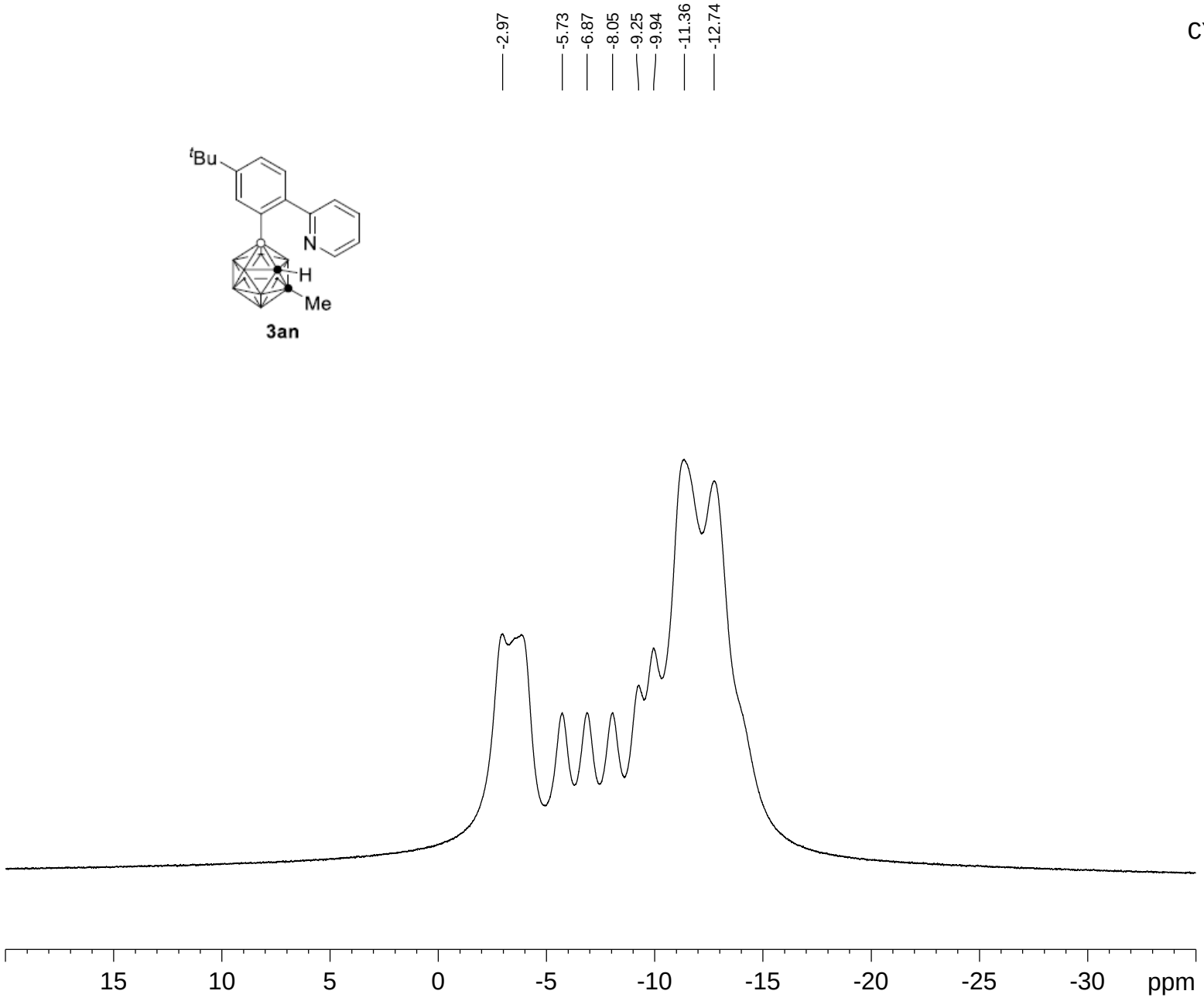
CY-C-A-59p

```
Current Data Parameters
NAME                  CY-C-A-59p
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20161111
Time                      16.22 h
INSTRUM                    spect
PROBHD    Z108618_0257 (
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                           80
DS                            4
SWH                   40760.871 Hz
FIDRES                 0.621962 Hz
AQ                     0.8039083 sec
RG                           114
DW                        12.267 usec
DE                          6.50 usec
TE                         296.0 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                  100.6379058 MHz
WDW                           EM
SSB       0
LB                          1.00 Hz
GB        0
PC                          1.40
```



CY-B-A-59p

```
Current Data Parameters
NAME          CY-B-A-59p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161111
Time              16.26 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                   203
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-59p-(C)

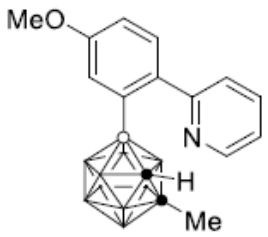
```
Current Data Parameters
NAME      CY-B-A-59p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161111
Time                16.29 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     40
DS                      2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    203
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            128.4097881 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

CY-H-A-26p-CDCl3

8.556
8.547
7.773
7.753
7.734
7.416
7.391
7.312
7.297
7.282
7.259
7.138
7.117
6.899
6.878

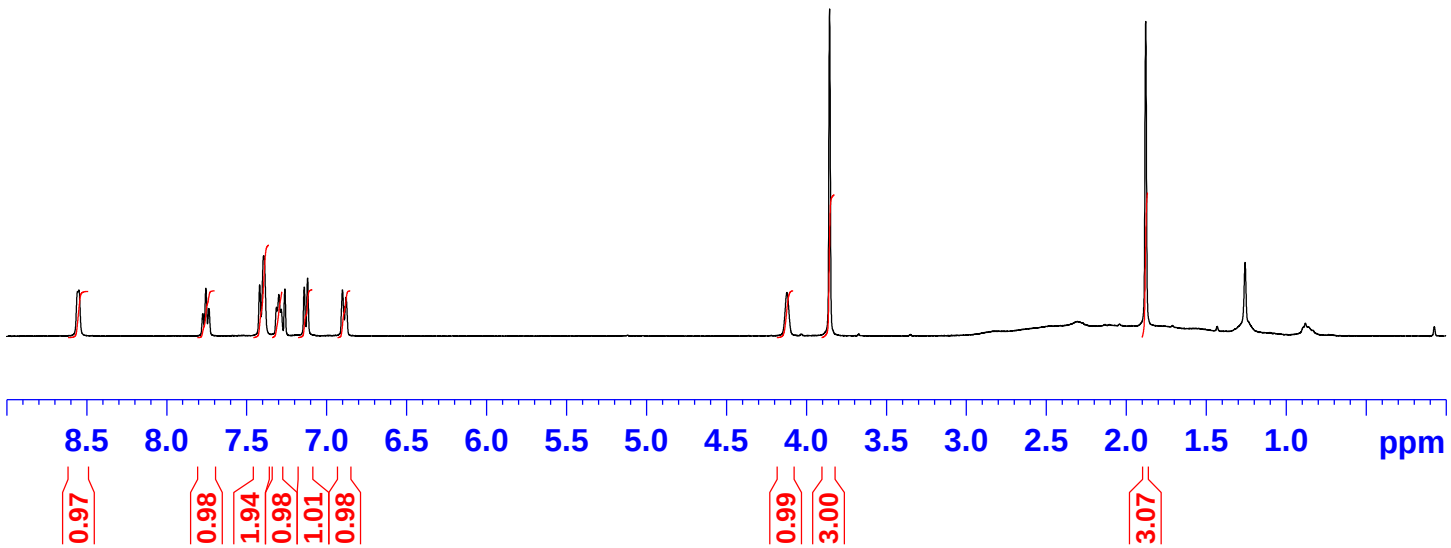
4.121
3.855

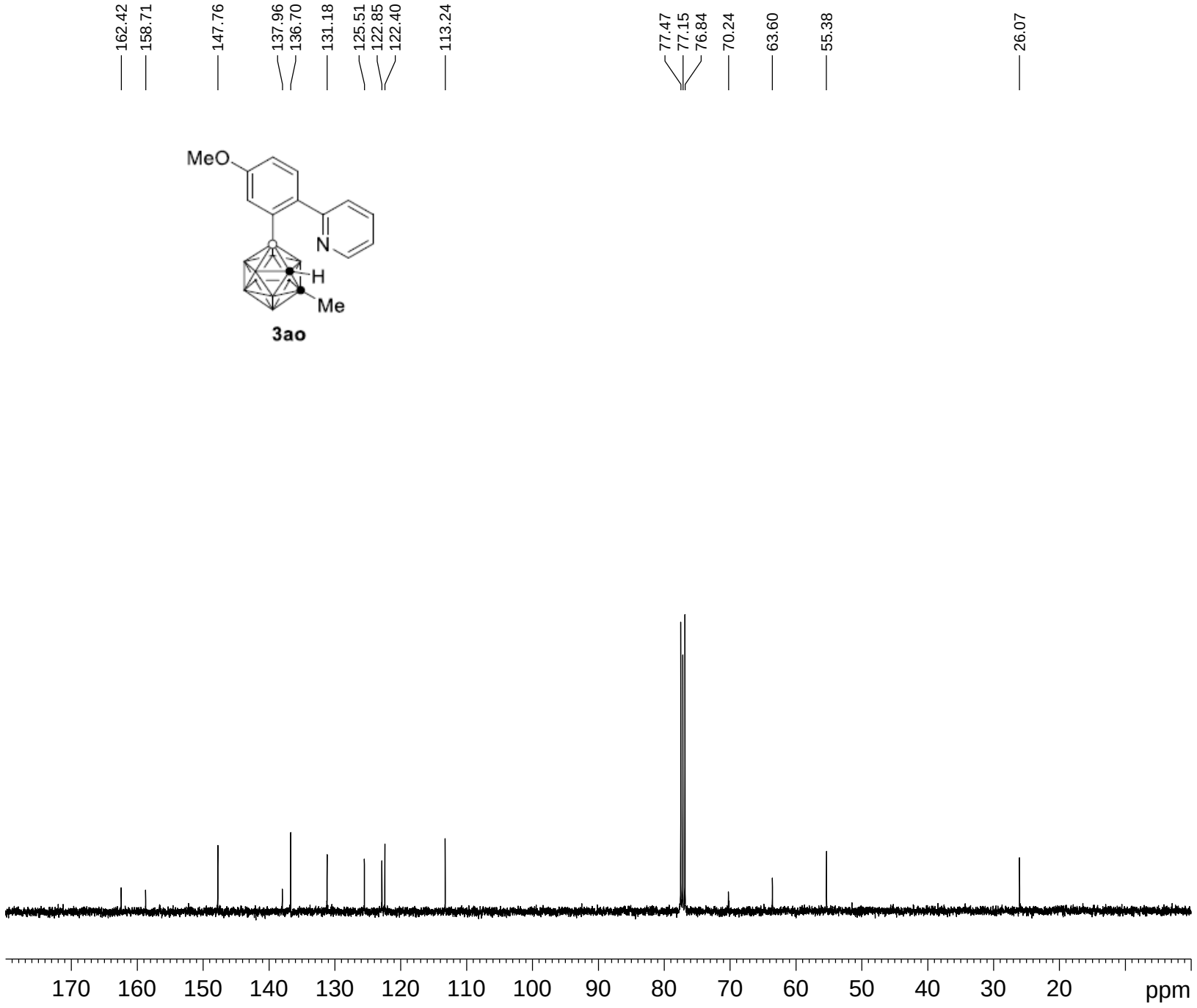
1.878



3ao

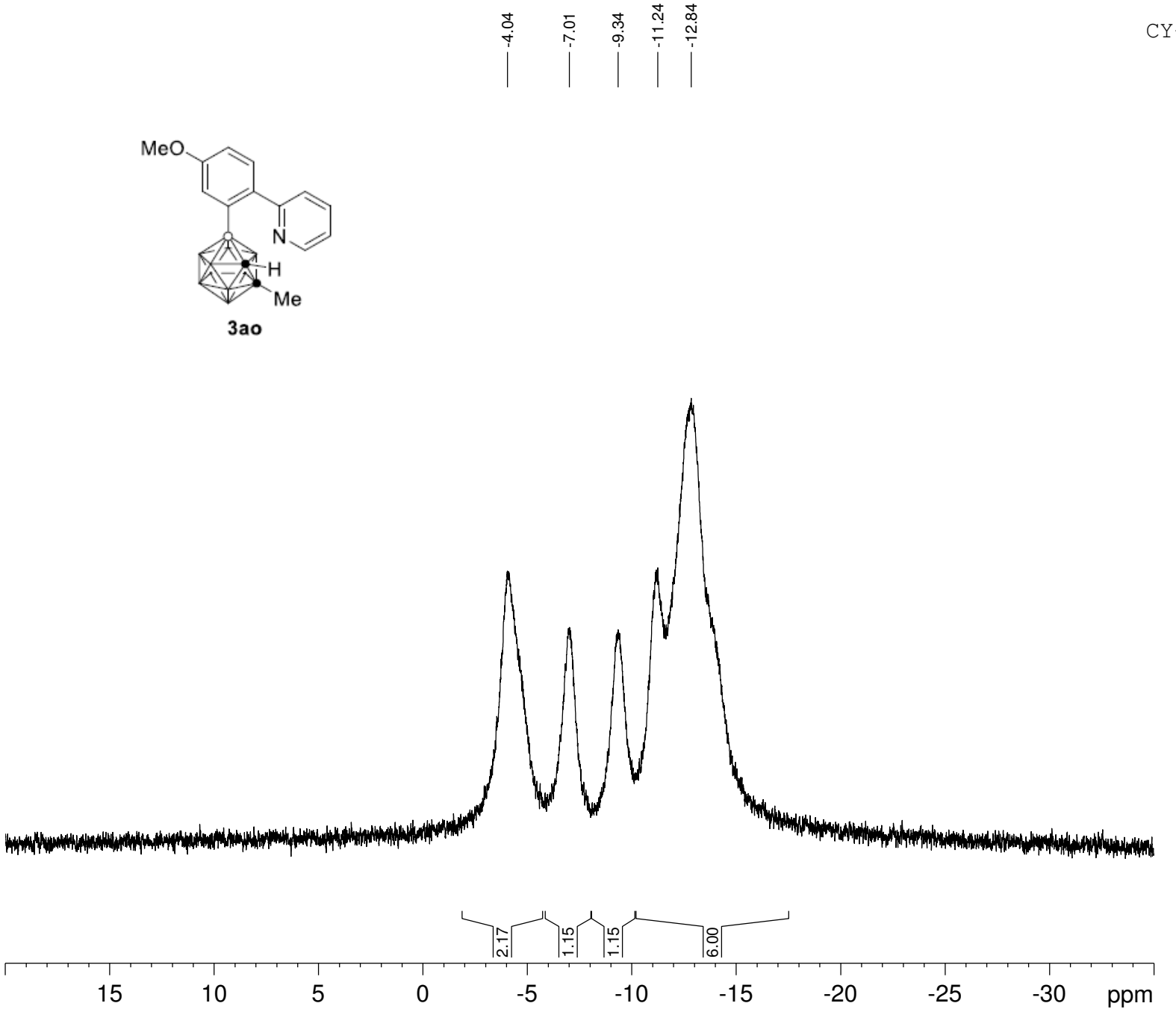
```
Current Data Parameters
NAME      CY-H-A-26p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20160829
Time                13.21 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                      1
DW                 62.400 usec
DE                  6.50 usec
TE                 295.6 K
D1              1.00000000 sec
TD0                     1
SFO1          400.1324708 MHz
NUC1                   1H
P1                 15.00 usec
PLW1            8.31000042 W

F2 - Processing parameters
SI                  65536
SF            400.1300107 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```





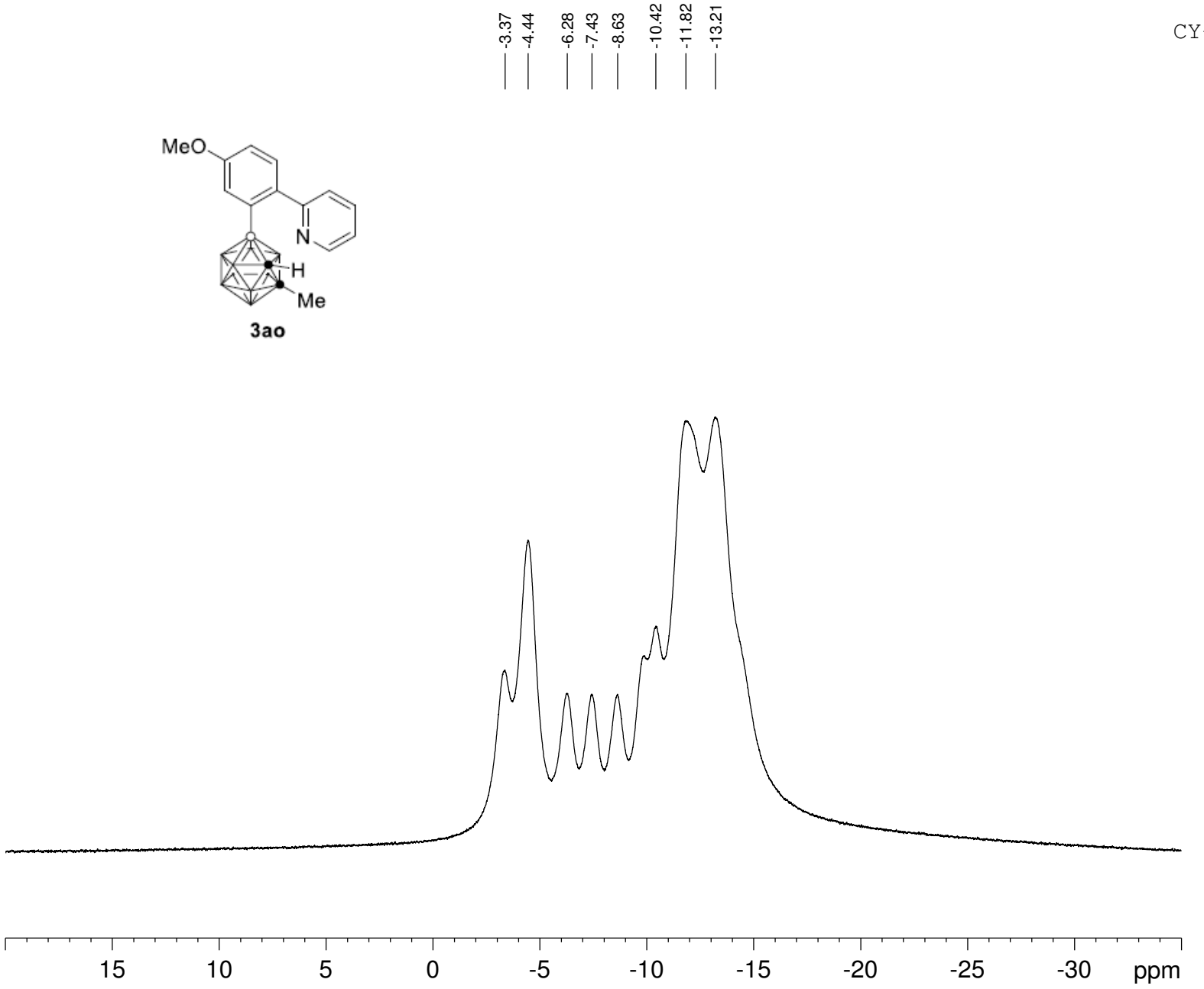
CY-C-A-26P-re

```
Current Data Parameters
NAME      CY-C-A-26P-re
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20161130
Time               9.54 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   80
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ            0.8039083 sec
RG                  203
DW               12.267 usec
DE                6.50 usec
TE                296.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6479773 MHz
NUC1               13C
P1                9.50 usec
PLW1        55.34000015 W
SFO2        400.2316009 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W
PLW13        0.13796000 W

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



CY-B-A-26P

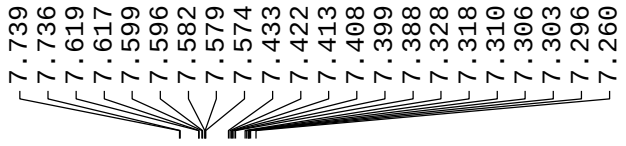
```
Current Data Parameters
NAME          CY-B-A-26P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160829
Time              17.07 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT          Acetone
NS                    10
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                     1
DW                20.800 usec
DE                 6.50 usec
TE                295.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

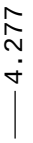


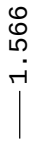
CY-B-A-26P-(C)

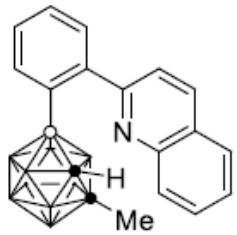
```
Current Data Parameters
NAME      CY-B-A-26P-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160829
Time                17.10 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT           Acetone
NS                      40
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
```

CY-H-A-52p-CDCl3



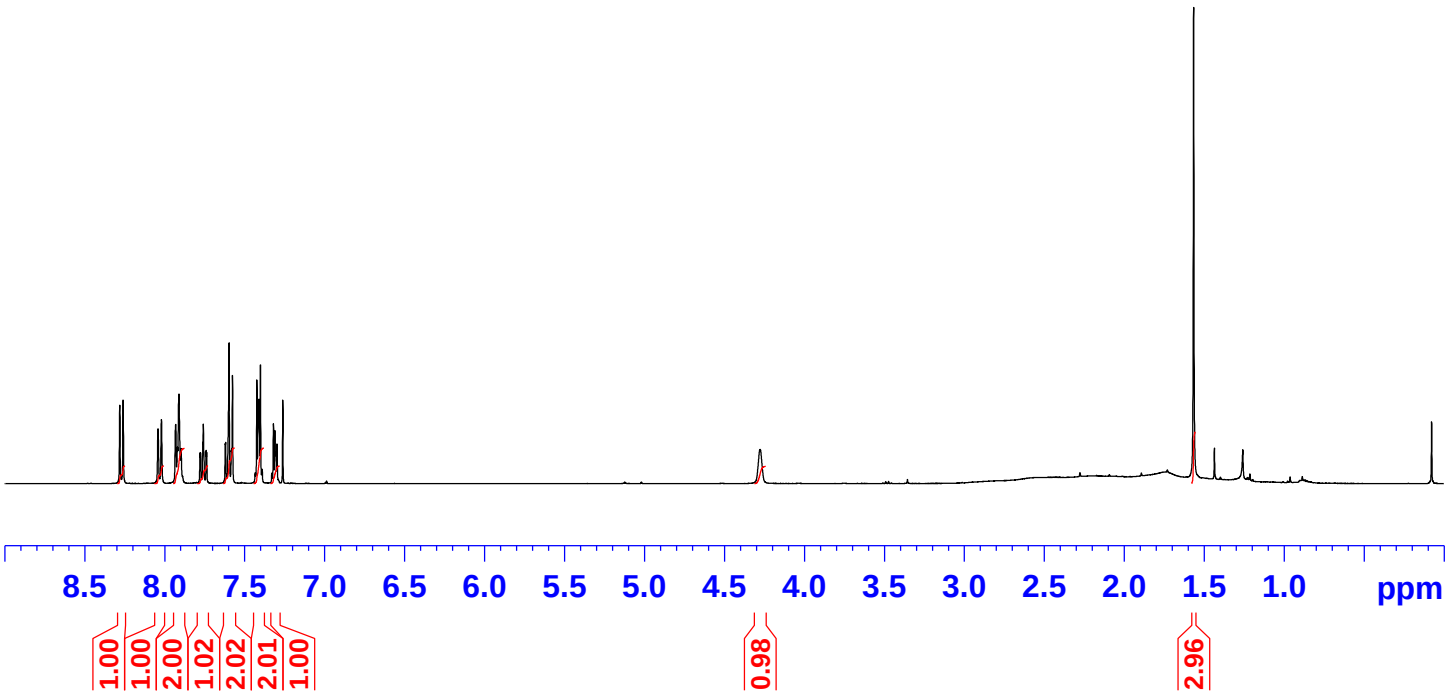


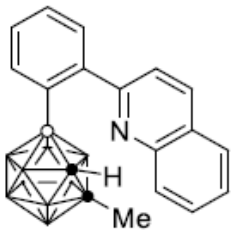




3ap

```
Current Data Parameters
NAME      CY-H-A-52p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20161014
Time               19.52 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     11
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                 294.9 K
D1            1.00000000 sec
TD0                     1
SFO1         400.1324708 MHz
NUC1                   1H
P1                 15.00 usec
PLW1          8.31000042 W

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



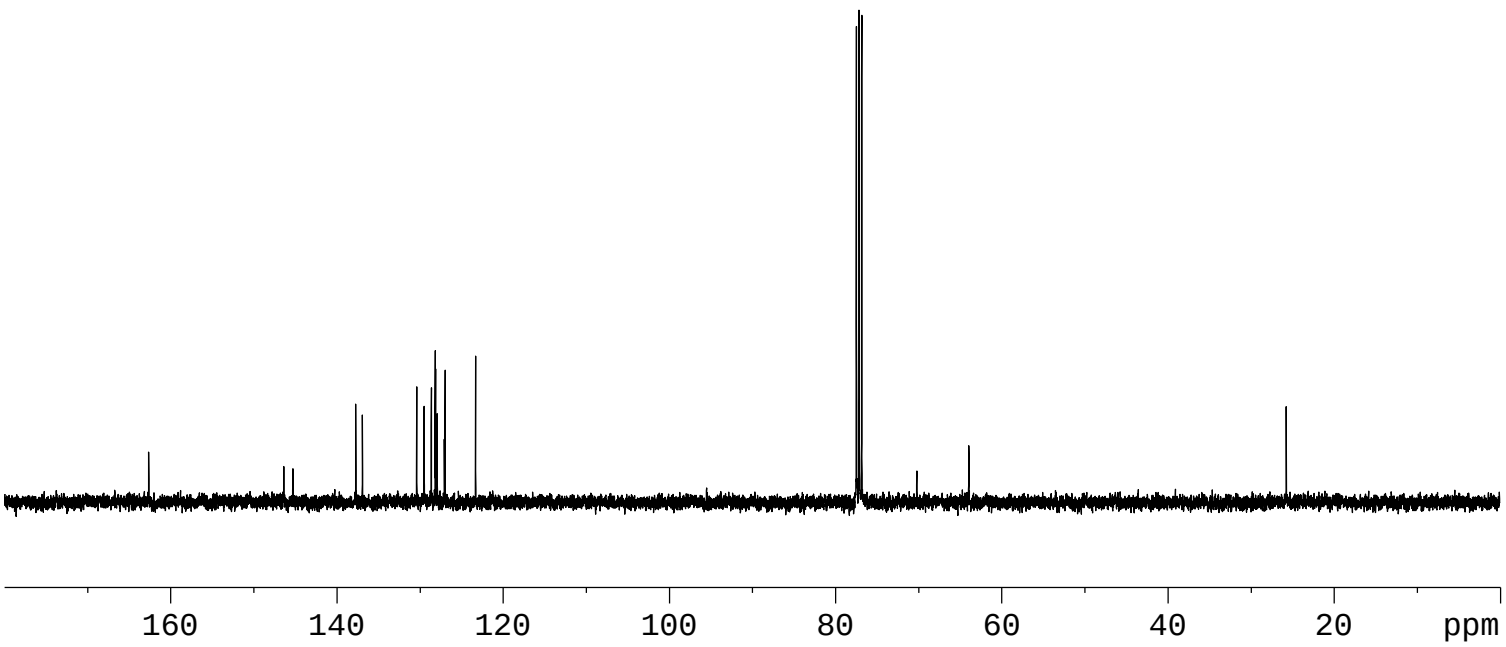


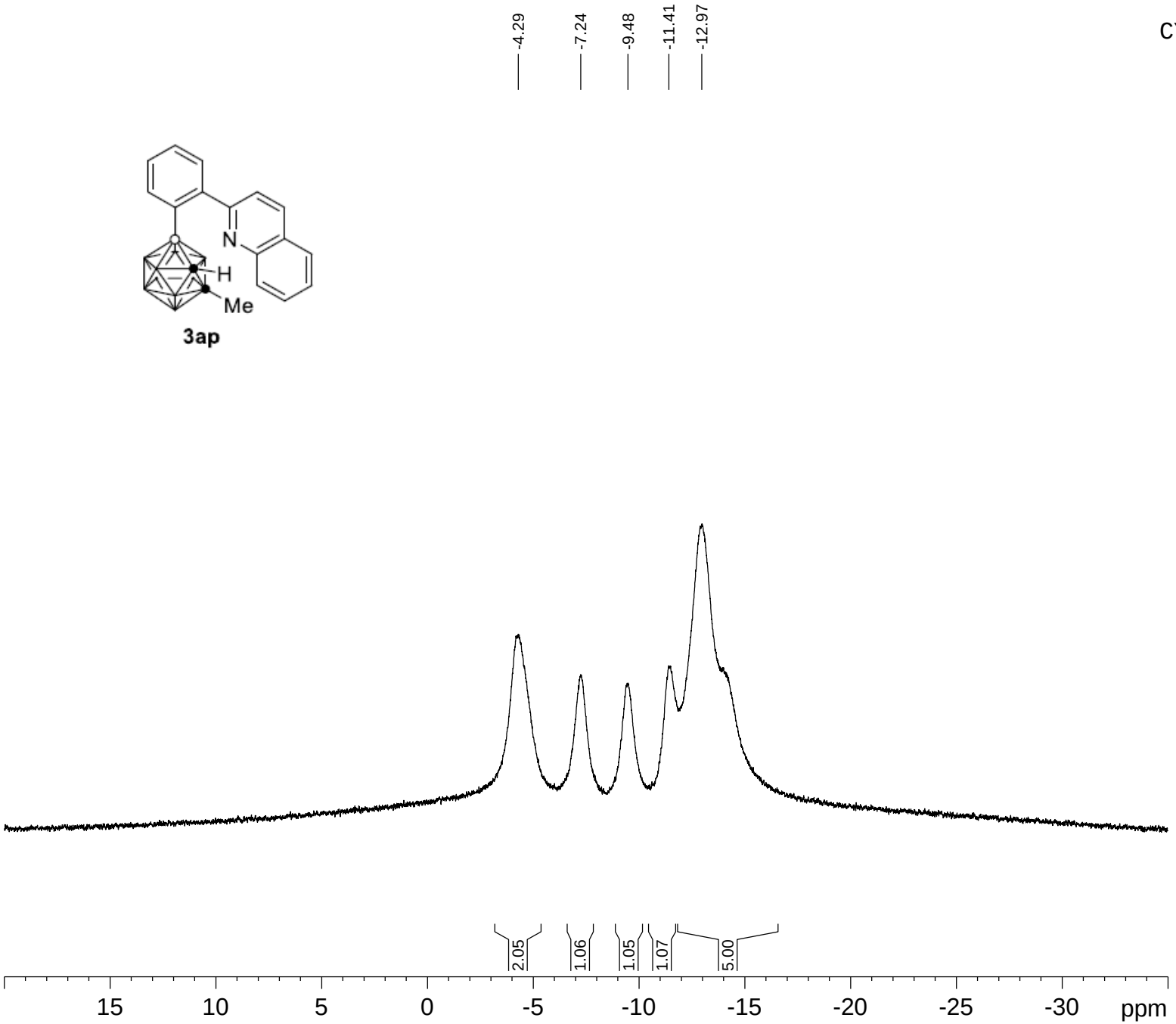
3ap

CY-C-A-52P-CDCl3

Bruker Advance III 400

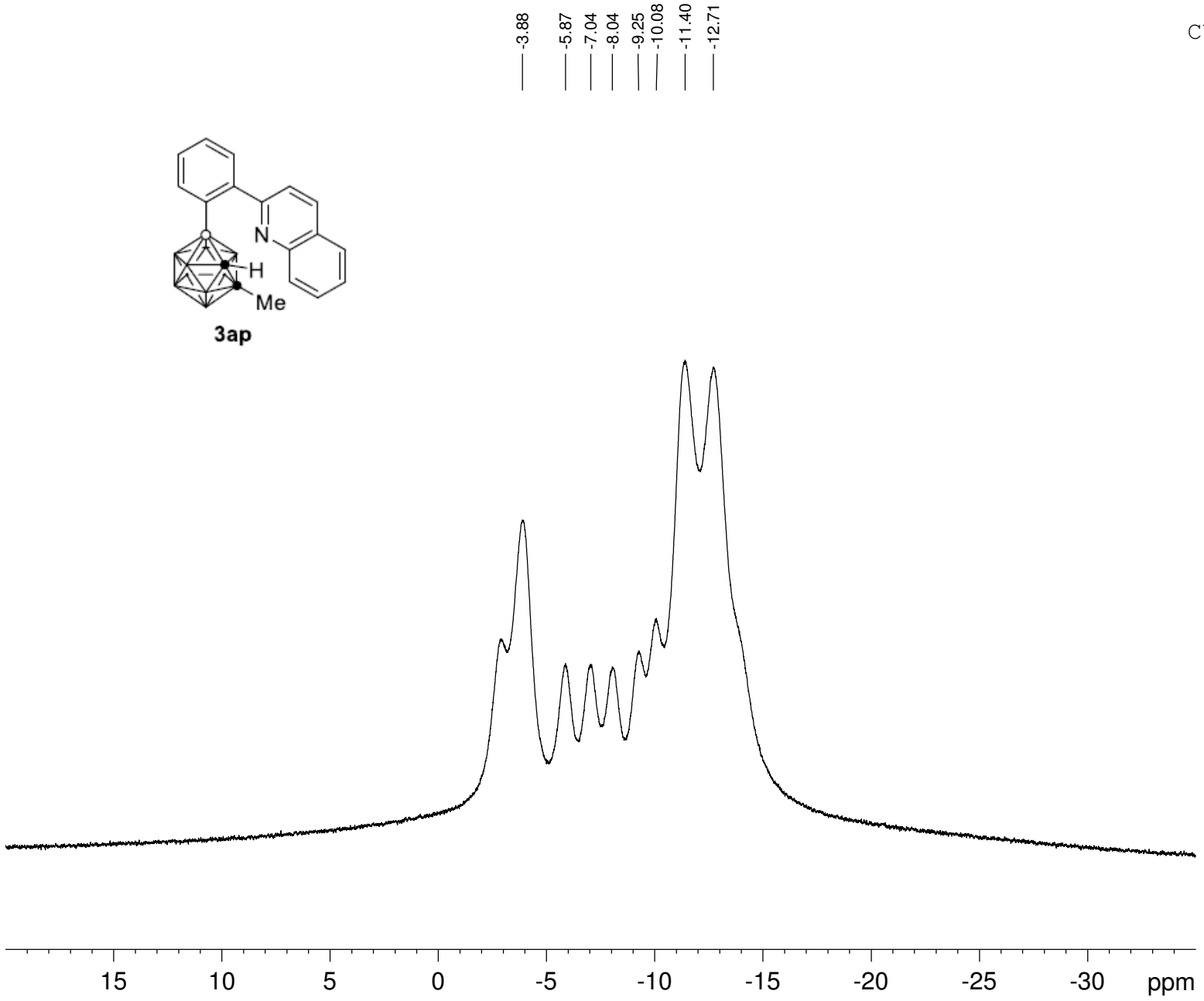
```
Current Data Parameters
NAME      CY-C-A-52P-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20161014
Time               19.58 h
INSTRUM             spect
PROBHD   Z824601_0021 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    121
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           100.6127584 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```





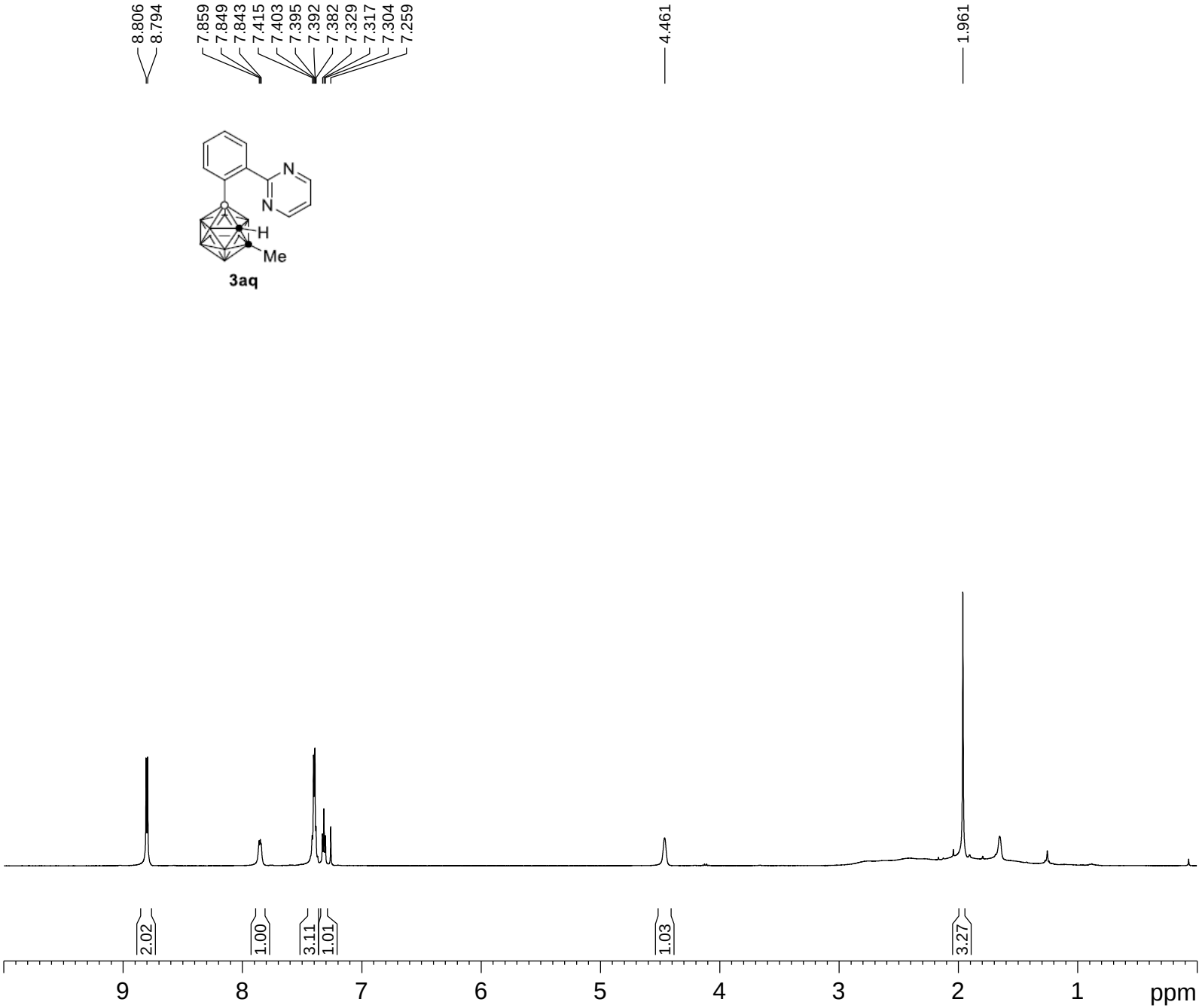
CY-B-A-52p-re3

```
Current Data Parameters
NAME      CY-B-A-52p-re3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161127
Time               16.05 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT          Acetone
NS                    20
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   256
DW                20.800 usec
DE                 6.50 usec
TE                296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-52P-(C)

```
Current Data Parameters
NAME      CY-B-A-52P-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161014
Time               21.37 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                    228
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097881 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

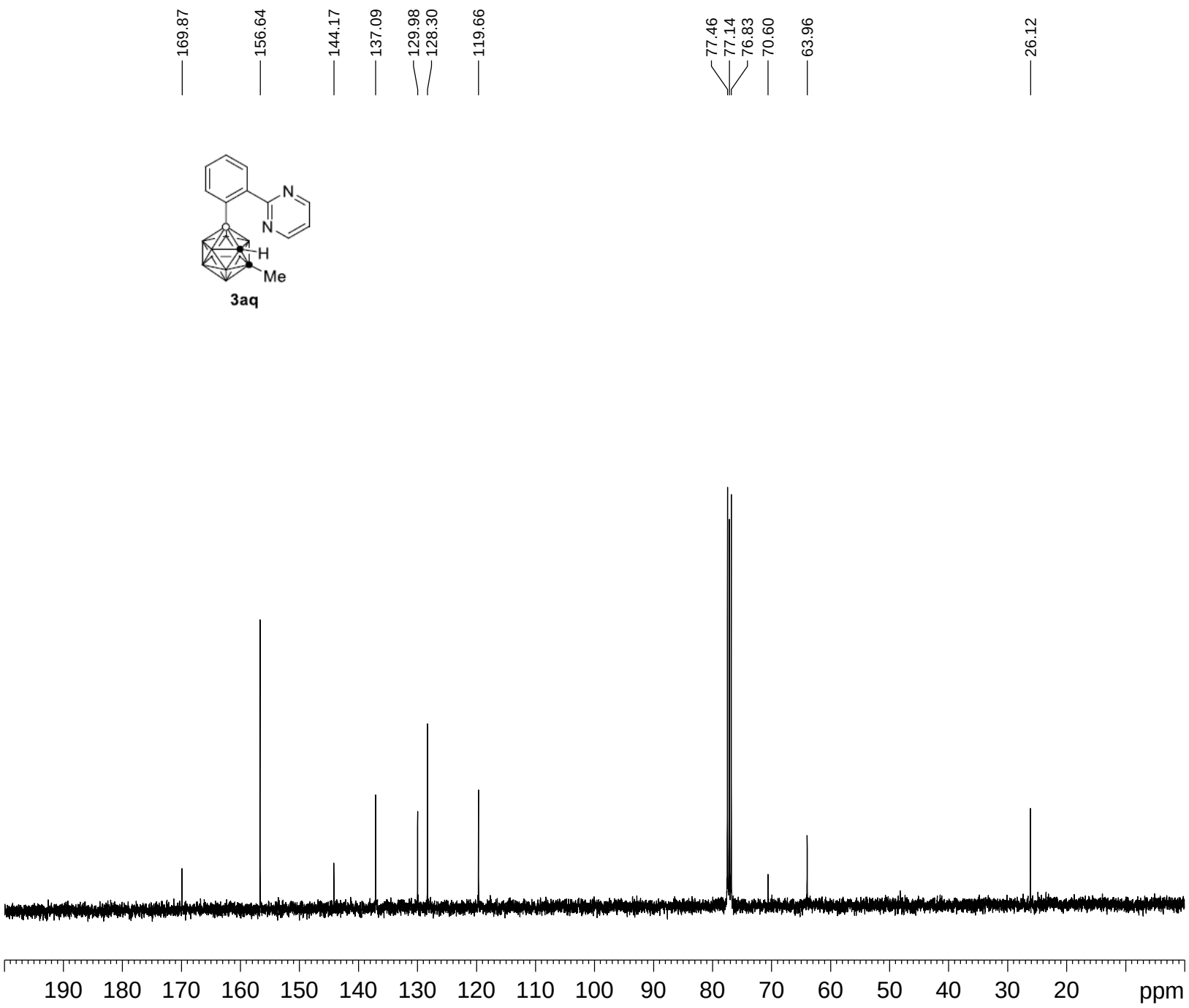


CY-H-A-53P-1

Current Data Parameters
NAME CY-H-A-53P-1
EXPNO 1
PROCNO 1

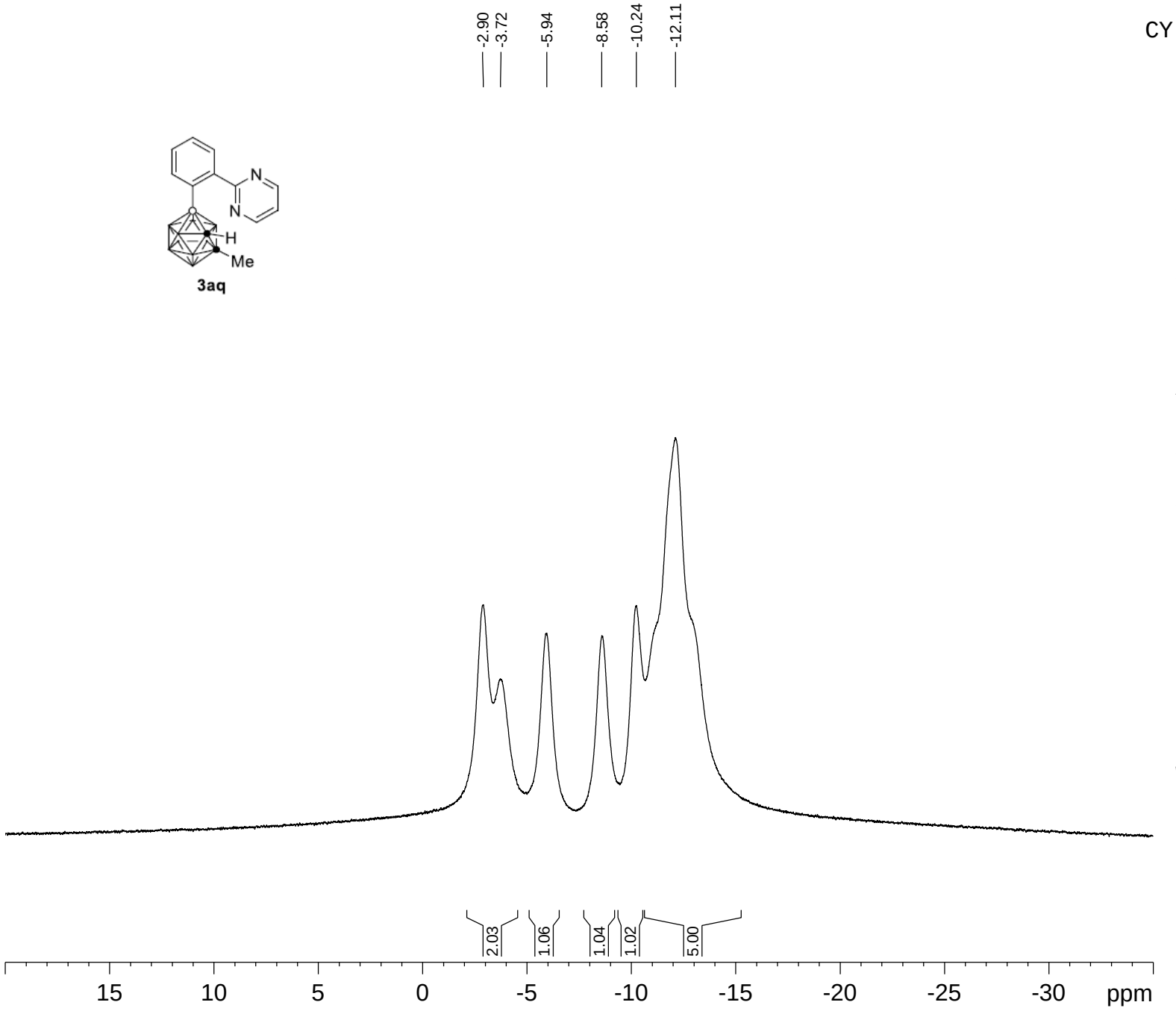
F2 - Acquisition Parameters
Date_ 20161104
Time 22.22 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 80.6
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MH
NUC1 1H
P1 12.80 usec
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



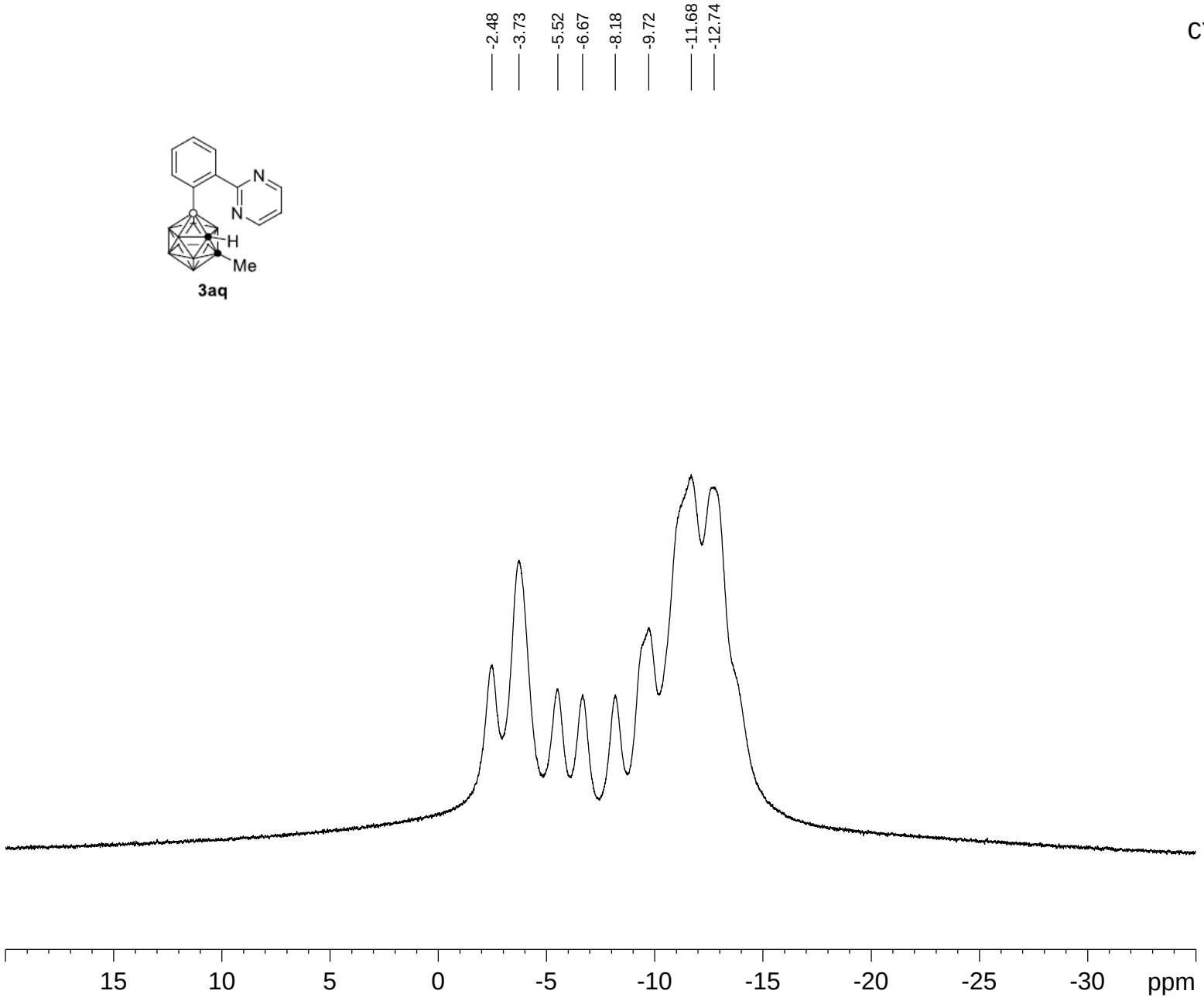
CY-C-A-53P

```
Current Data Parameters
NAME          CY-C-A-53P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161104
Time               22.25 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   135
DS                     4
SWH            40760.871 Hz
FIDRES          0.621962 Hz
AQ              0.8039083 sec
RG                   181
DW                12.267 usec
DE                 6.50 usec
TE                296.4 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           100.6379036 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



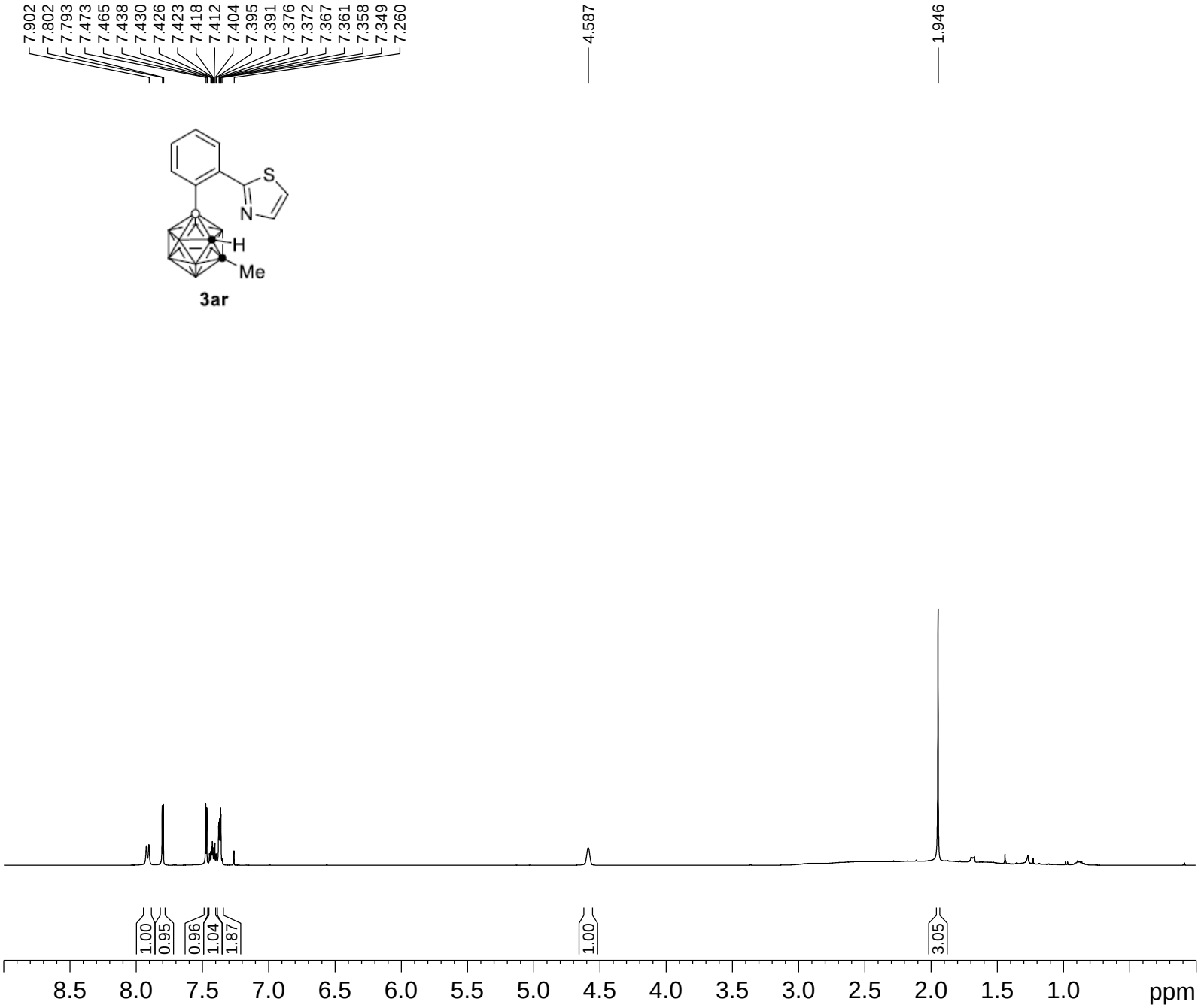
CY-B-A-53P-1

```
Current Data Parameters
NAME        CY-B-A-53P-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161104
Time               22.40 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    40
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                296.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-53P-1-(C)

```
Current Data Parameters
NAME      CY-B-A-53P-1-(C)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20161104
Time                22.43 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                     322
DW                20.800 usec
DE                 6.50 usec
TE                 296.4 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            128.4097881 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

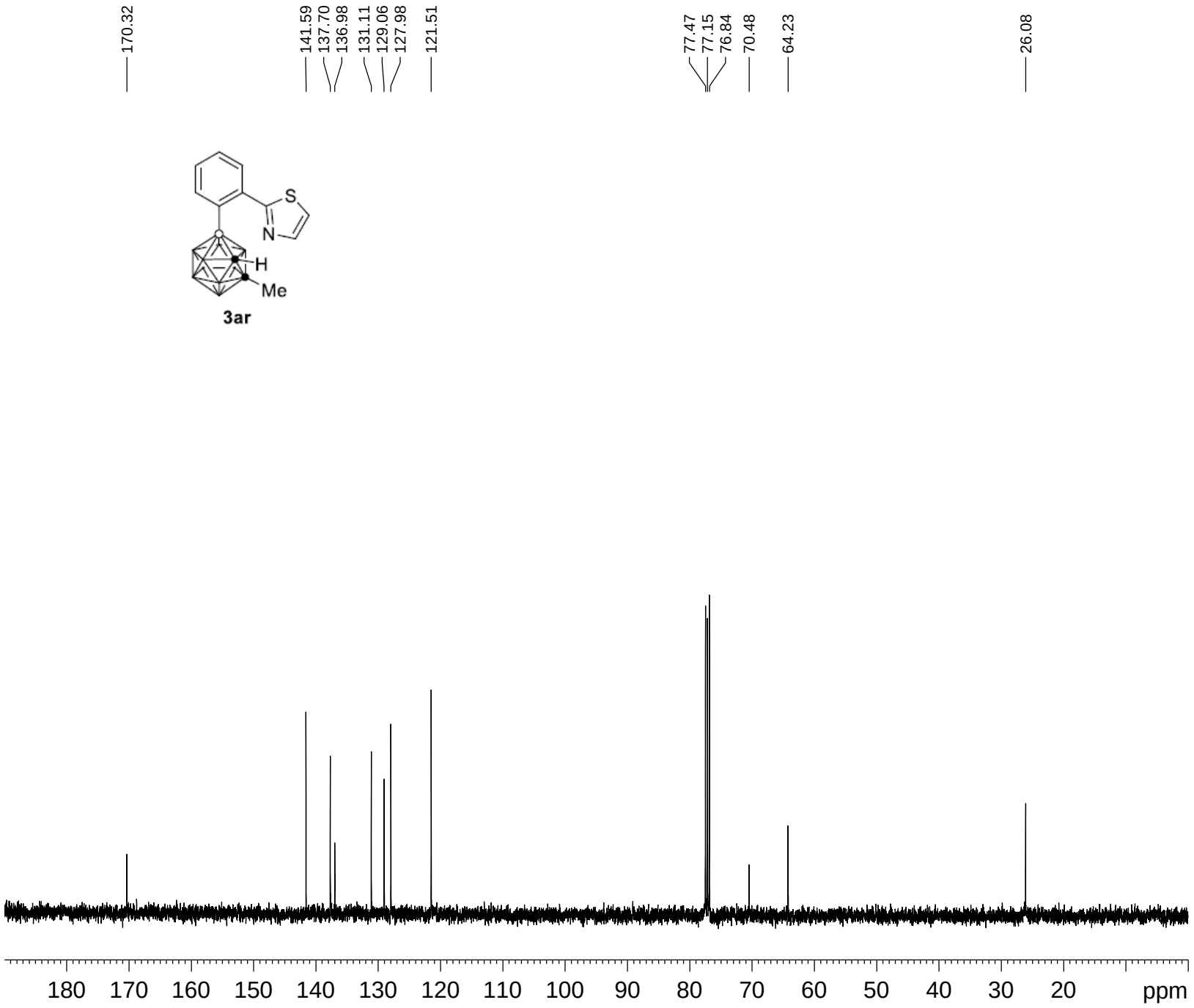


CY-H-A-62p

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

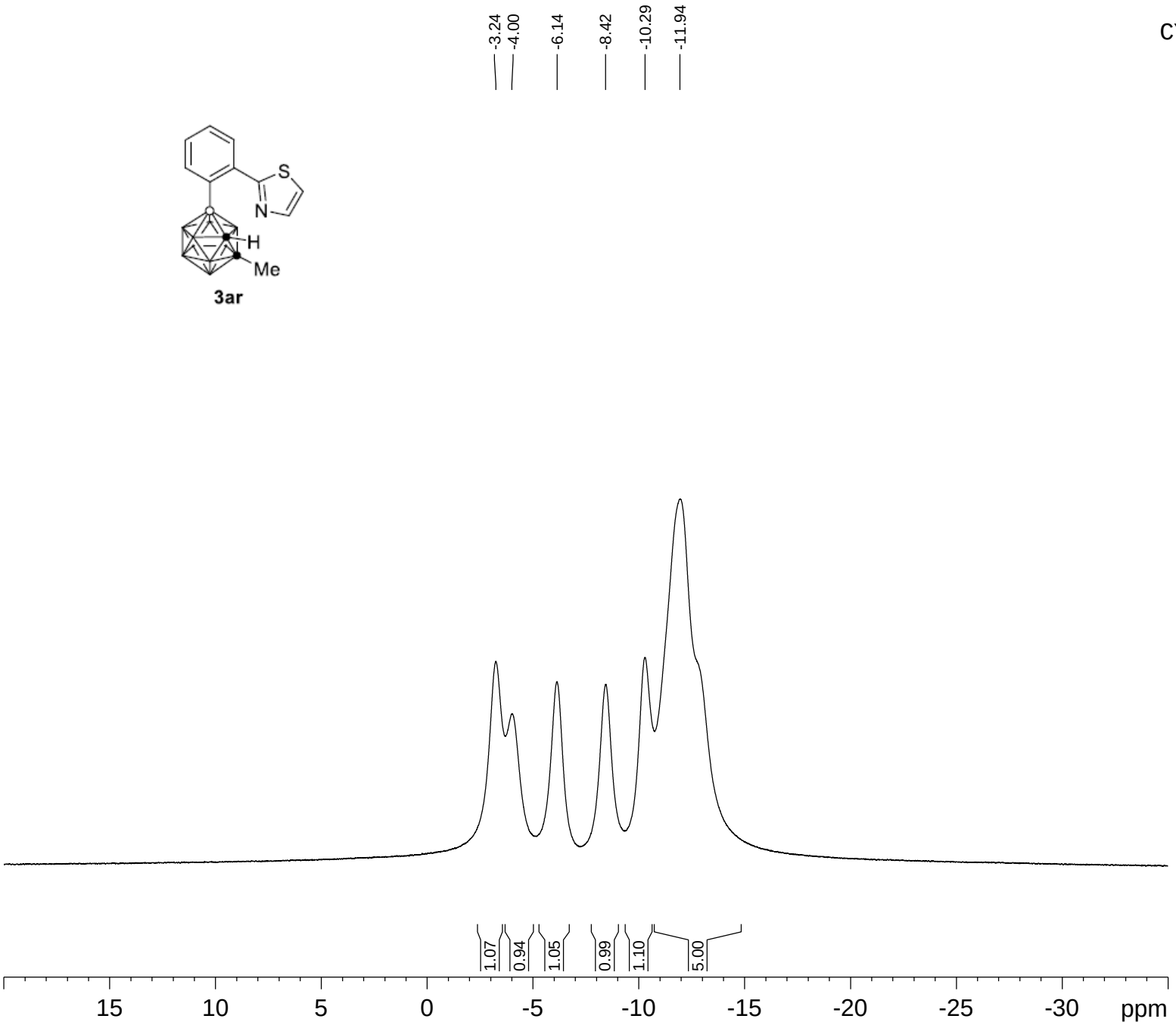
F2 - Acquisition Parameters
Date_ 20161112
Time 12.19 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 32
DW 62.400 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MH
NUC1 1H
P1 12.80 usec
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



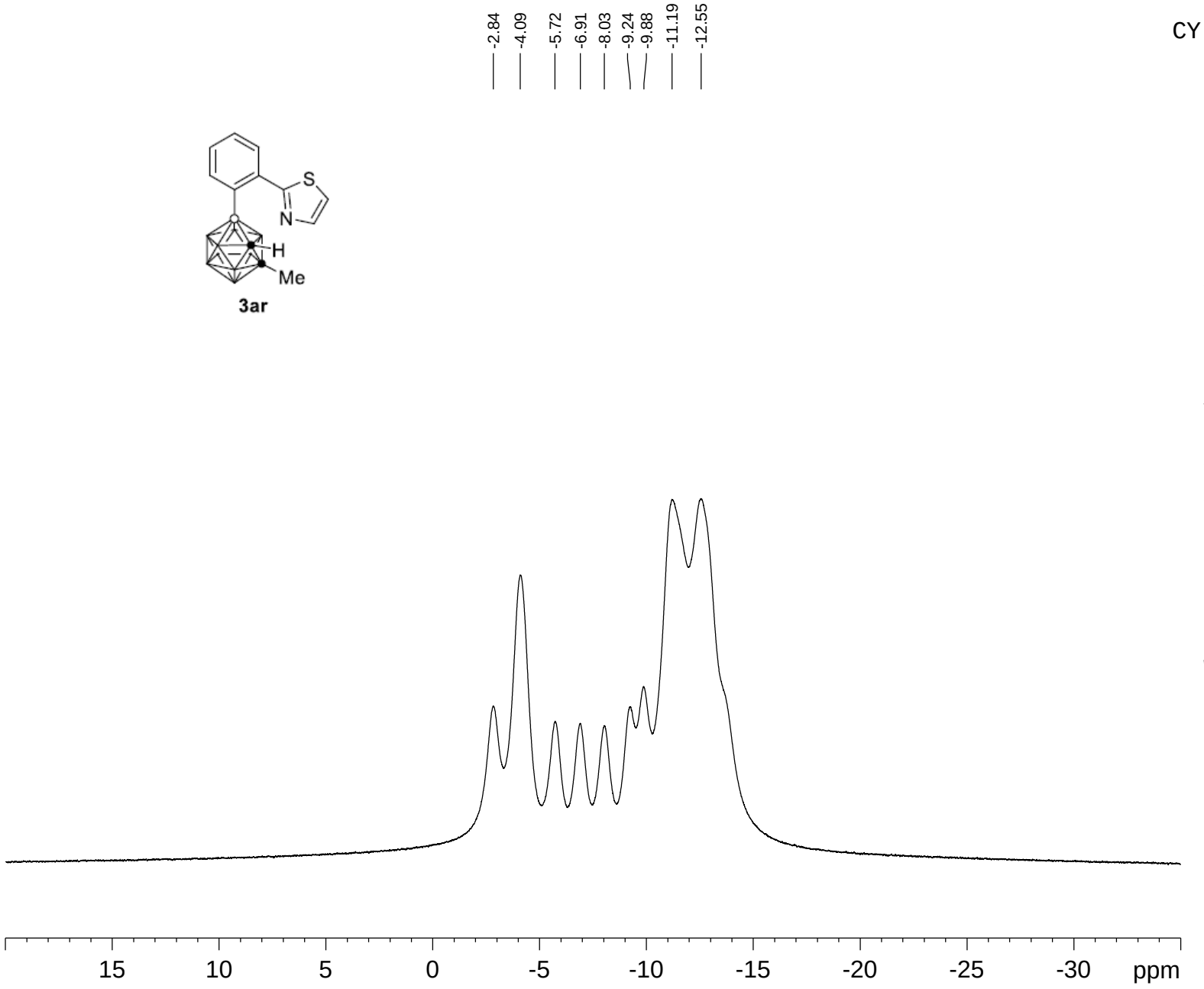
CY-C-A-62p

```
Current Data Parameters
NAME                  CY-C-A-62p
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20161112
Time                       12.21 h
INSTRUM                    spect
PROBHD    Z108618_0257 (
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                            32
DS                             4
SWH                    40760.871 Hz
FIDRES                 0.621962 Hz
AQ                     0.8039083 sec
RG                           203
DW                        12.267 usec
DE                          6.50 usec
TE                         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                  100.6379054 MHz
WDW                           EM
SSB       0
LB                          1.00 Hz
GB        0
PC                          1.40
```



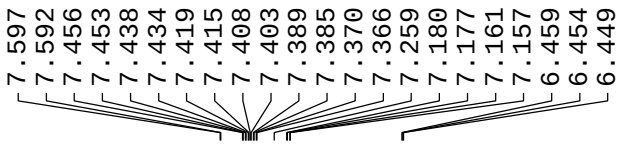
CY-B-A-62p

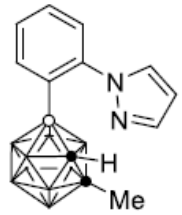
```
Current Data Parameters
NAME          CY-B-A-62p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161112
Time               12.25 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                   203
DW                20.800 usec
DE                 6.50 usec
TE                296.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-62p-(C)

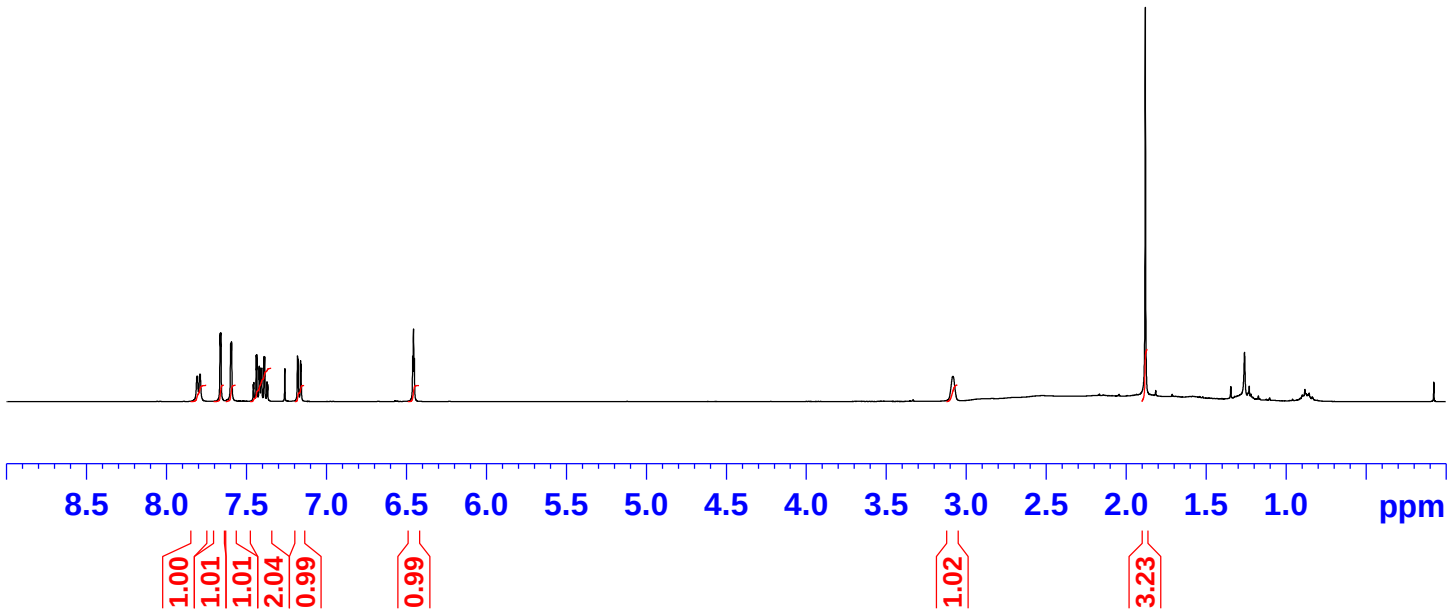
```
Current Data Parameters
NAME      CY-B-A-62p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161112
Time                12.26 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                     203
DW                  20.800 usec
DE                   6.50 usec
TE                  295.8 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            128.4097881 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

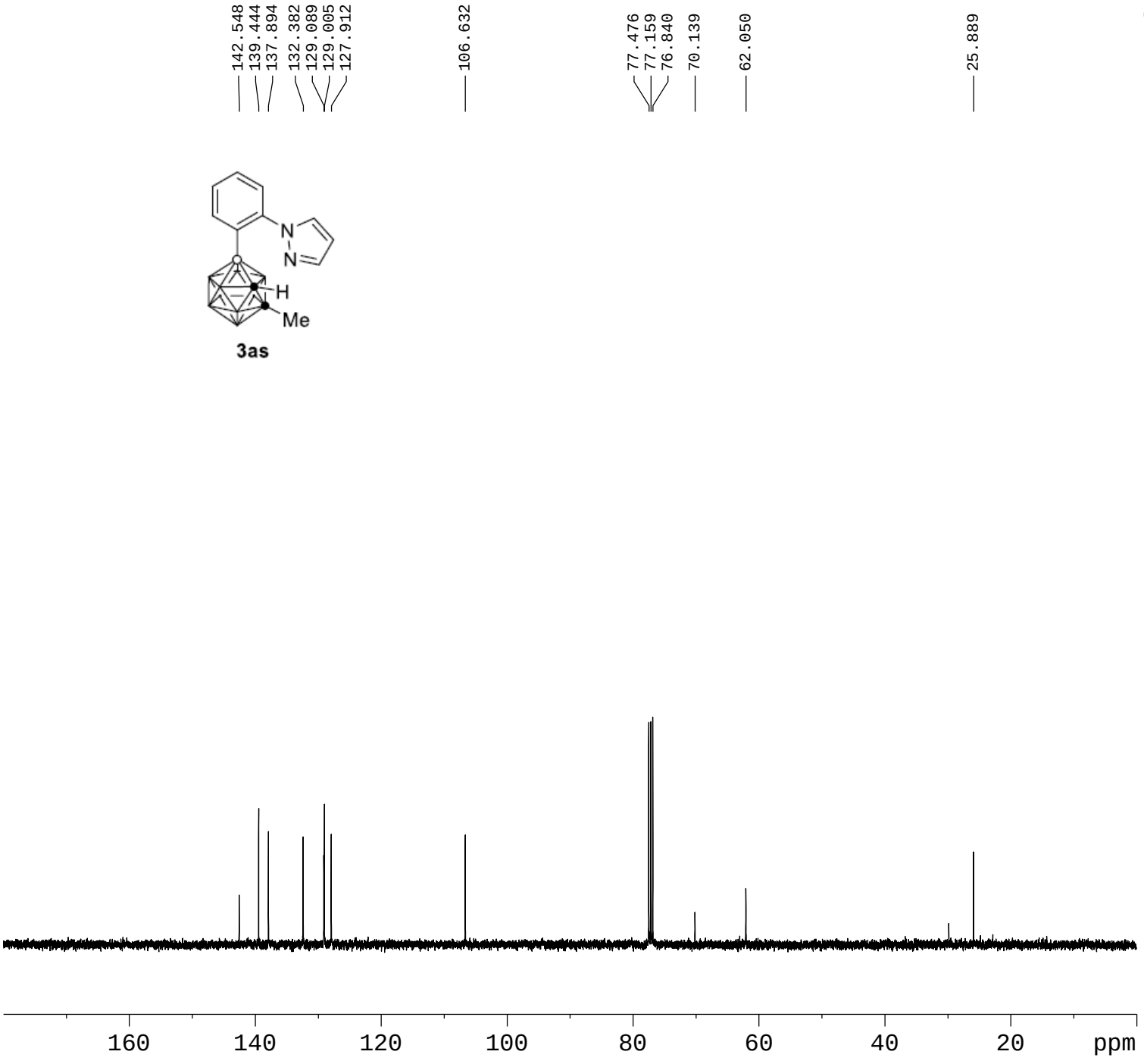




3as

```
Current Data Parameters
NAME      CY-H-A-25P-2-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160827
Time              10.31 h
INSTRUM            spect
PROBHD    Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                   114
DW                62.400 usec
DE                 6.50 usec
TE                295.7 K
D1           1.00000000 sec
TD0                    1
SFO1        400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1          8.31000042 W

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





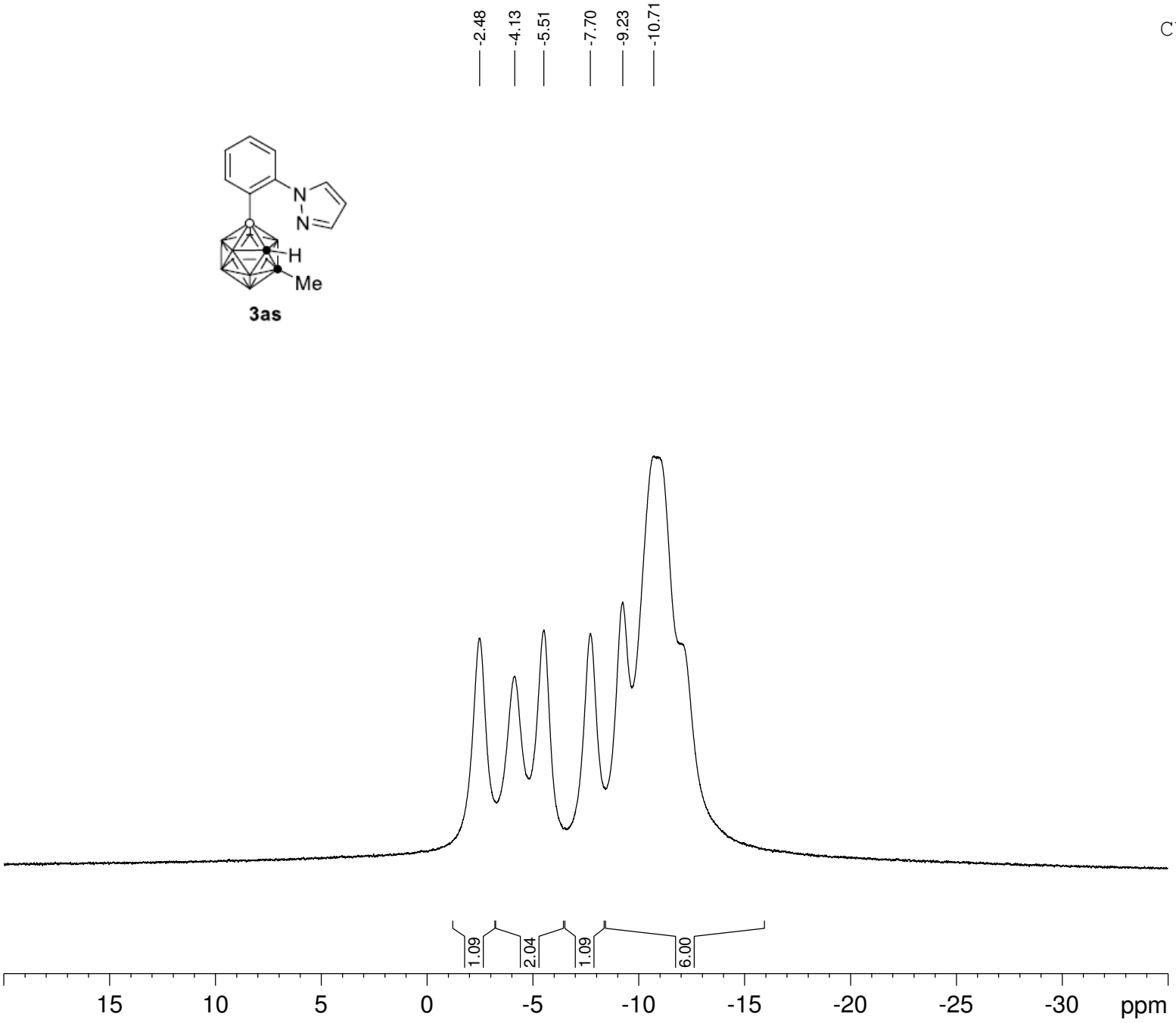
CY-C-A-25P-2-CDCl3

Bruker Advance III 400

Current Data Parameters
NAME CY-C-A-25P-2-CDCl3
EXPNO 1
PROCNO 1

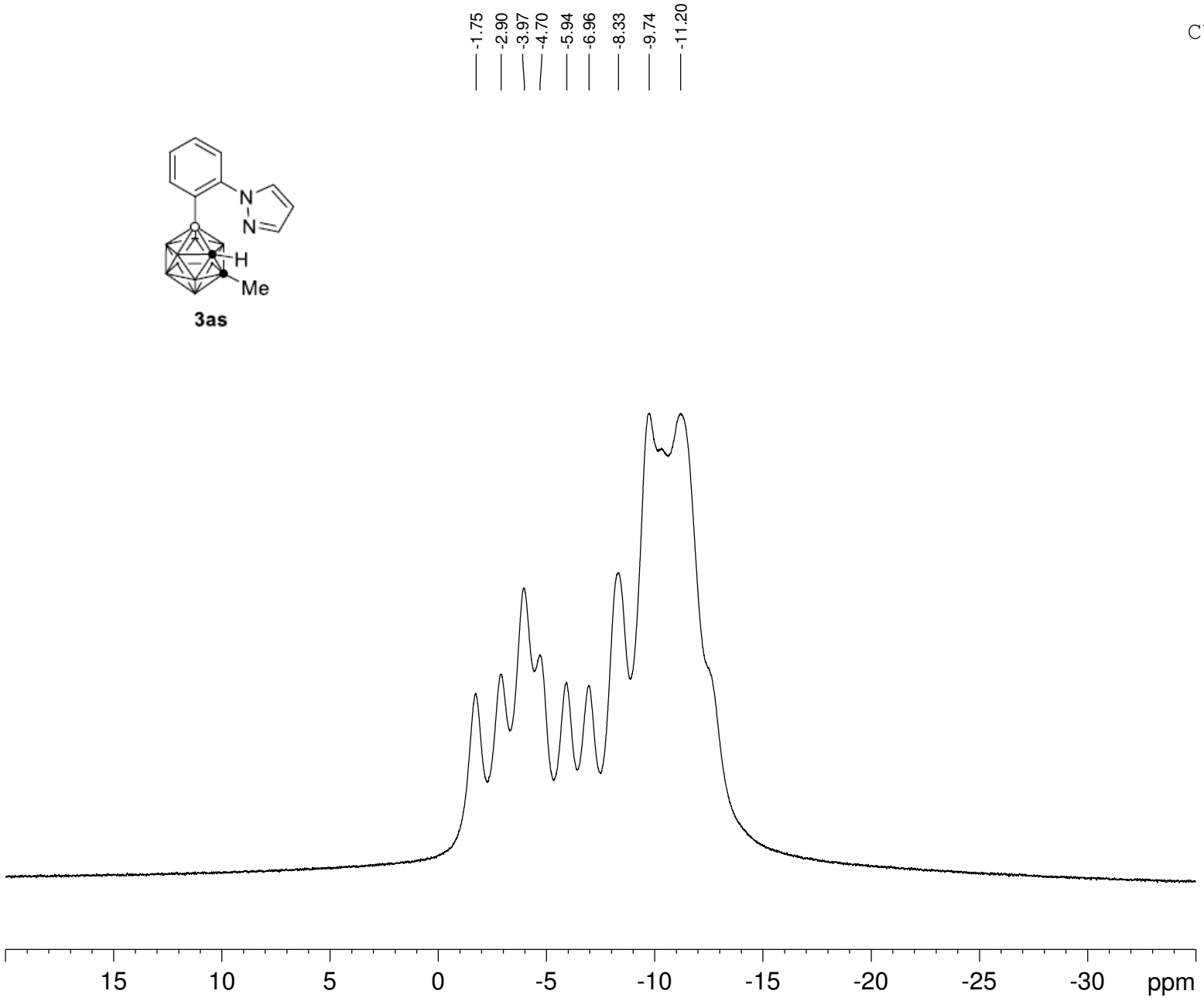
F2 - Acquisition Parameters
Date_ 20160827
Time 10.47 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 82
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
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 100.6127590 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



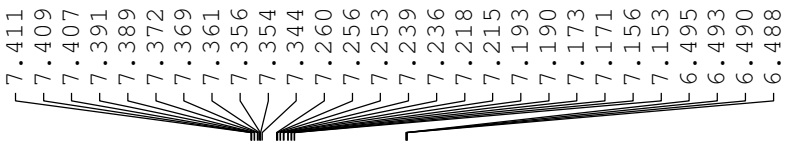
CY-B-A-25P-2

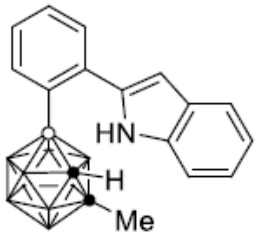
```
Current Data Parameters
NAME        CY-B-A-25P-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160827
Time              10.59 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT             C6D6
NS                    11
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   181
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
```



CY-B-A-25P-2-(C)

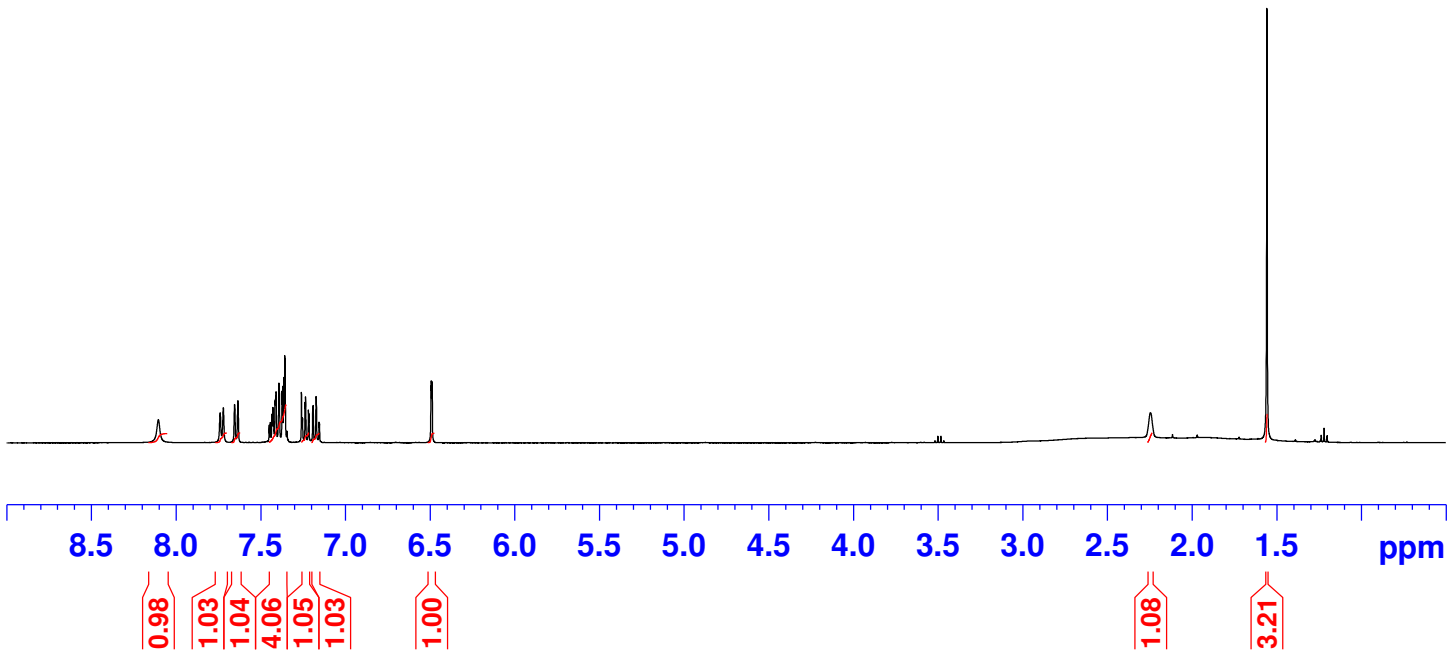
```
Current Data Parameters
NAME      CY-B-A-25P-2-(C)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160827
Time               11.01 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT              C6D6
NS                     22
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    181
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
```

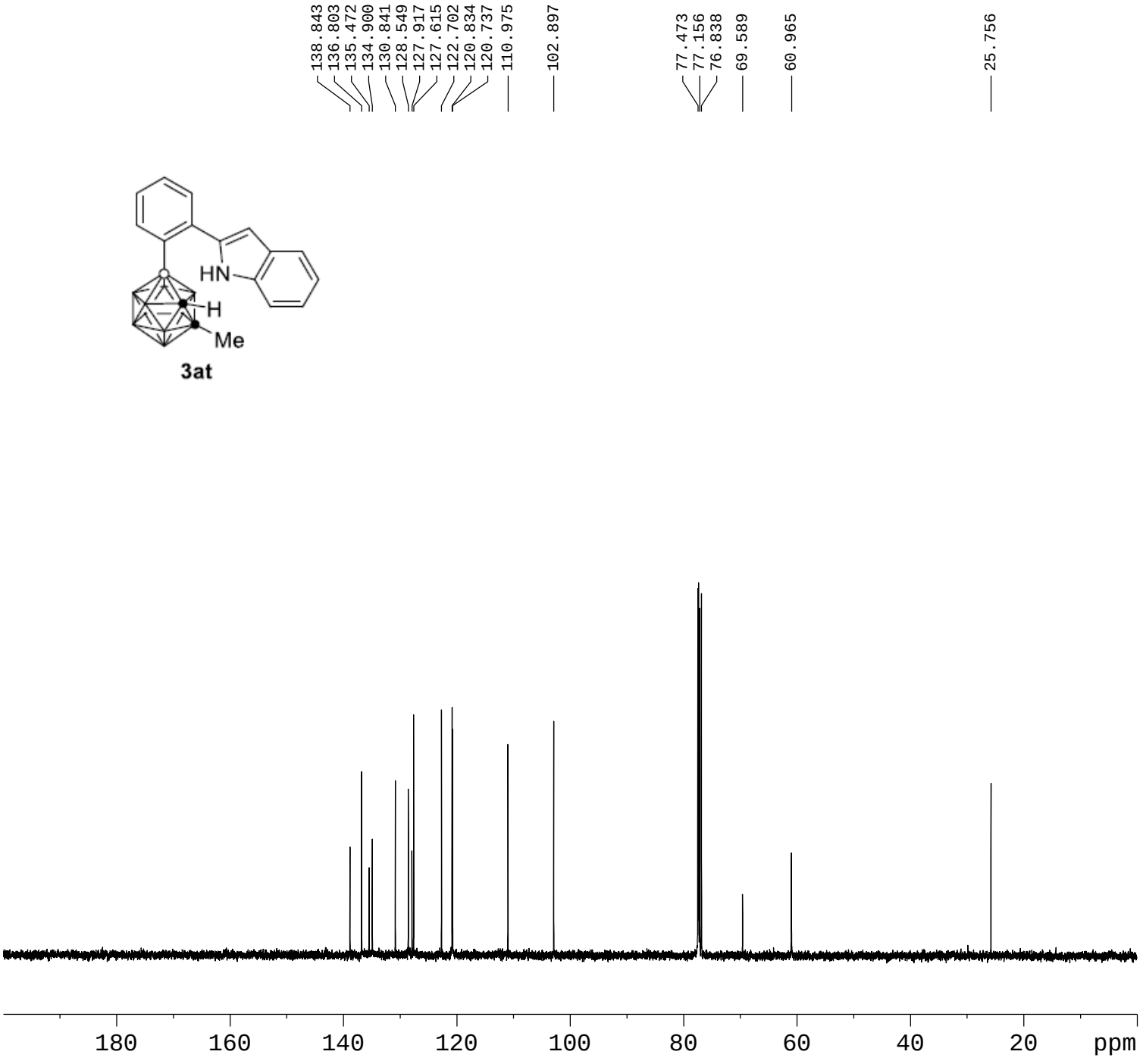




3at

```
Current Data Parameters
NAME      CY-H-A-23p-CDCl3-re2
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20161129
Time                  19.57 h
INSTRUM               spect
PROBHD    Z824601_0021 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
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                    294.4 K
D1              1.00000000 sec
TD0                          1
SFO1           400.1324708 MHz
NUC1                      1H
P1                    15.00 usec
PLW1            8.31000042 W

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





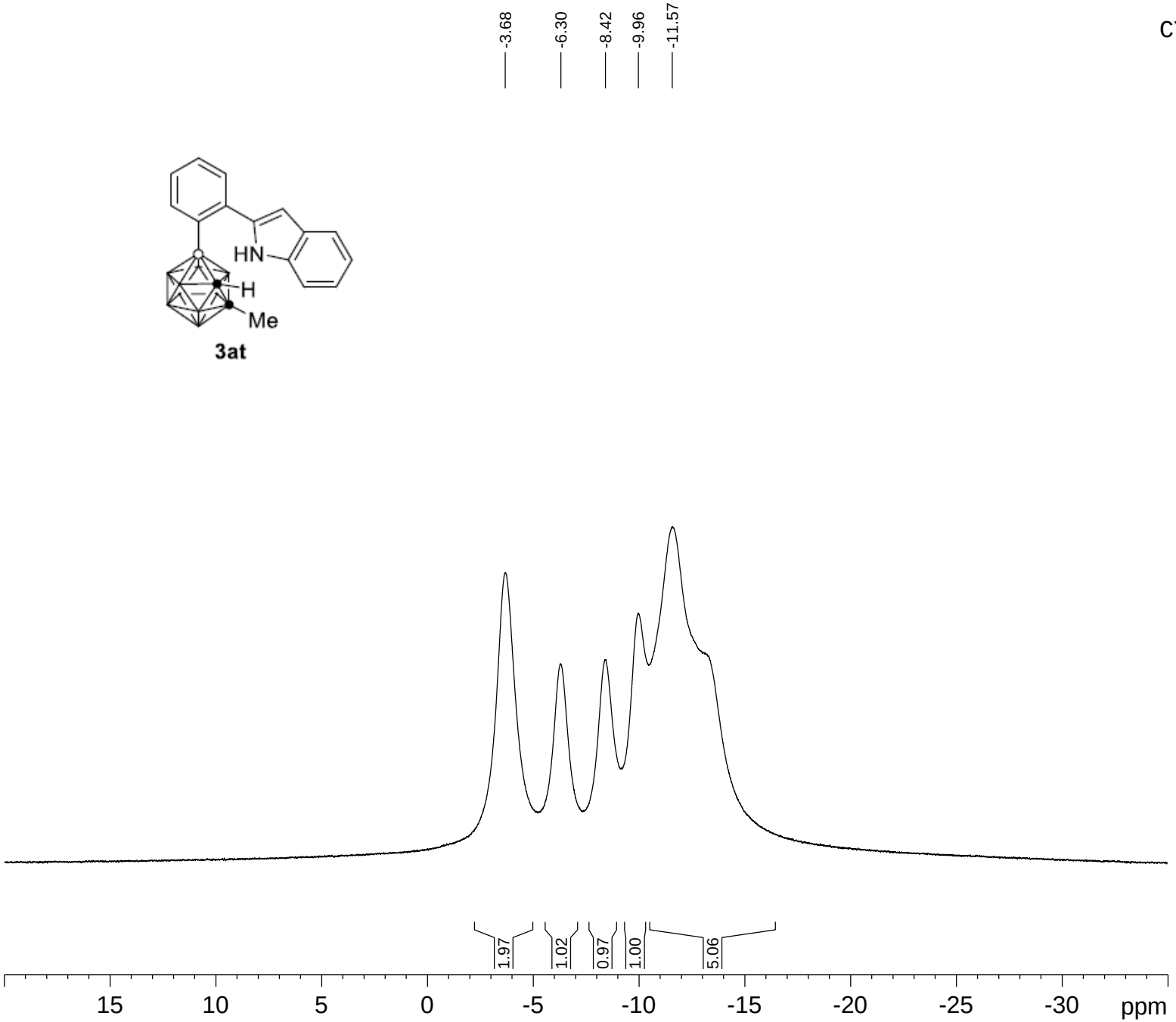
CY-C-A-24P-CDCl3

Bruker Advance III 400

Current Data Parameters
NAME CY-C-A-24P-CDCl3
EXPNO 1
PROCNO 1

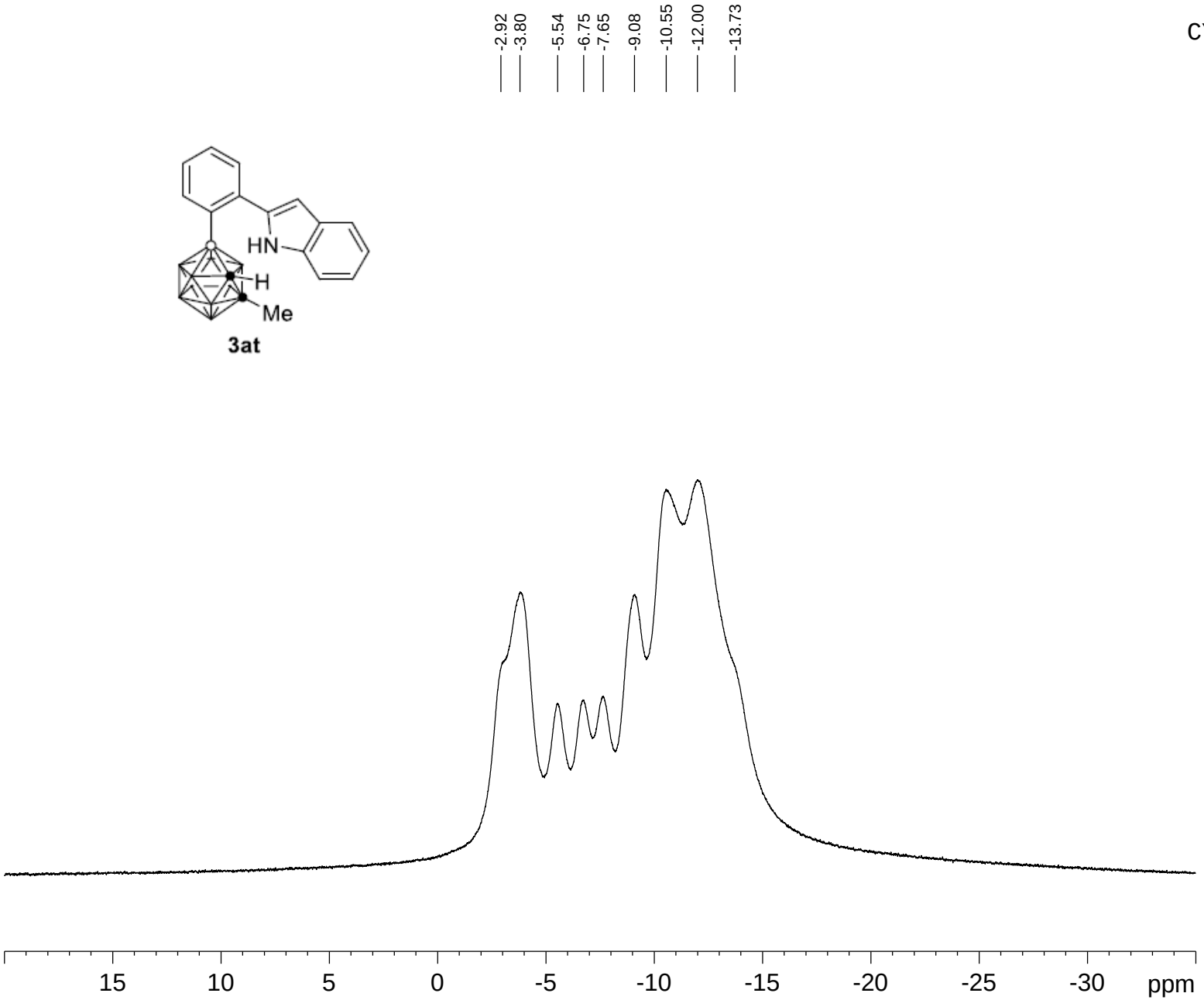
F2 - Acquisition Parameters
Date_ 20160826
Time 19.36 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 312
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 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 100.6127598 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



CY-B-A-23P

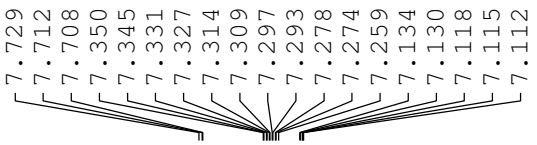
```
Current Data Parameters
NAME          CY-B-A-23P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160826
Time               21.28 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                   181
DW                20.800 usec
DE                 6.50 usec
TE                294.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

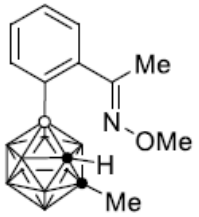


CY-B-A-23P-(C)

```
Current Data Parameters
NAME      CY-B-A-23P-(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160826
Time               21.31 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                  181
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
```

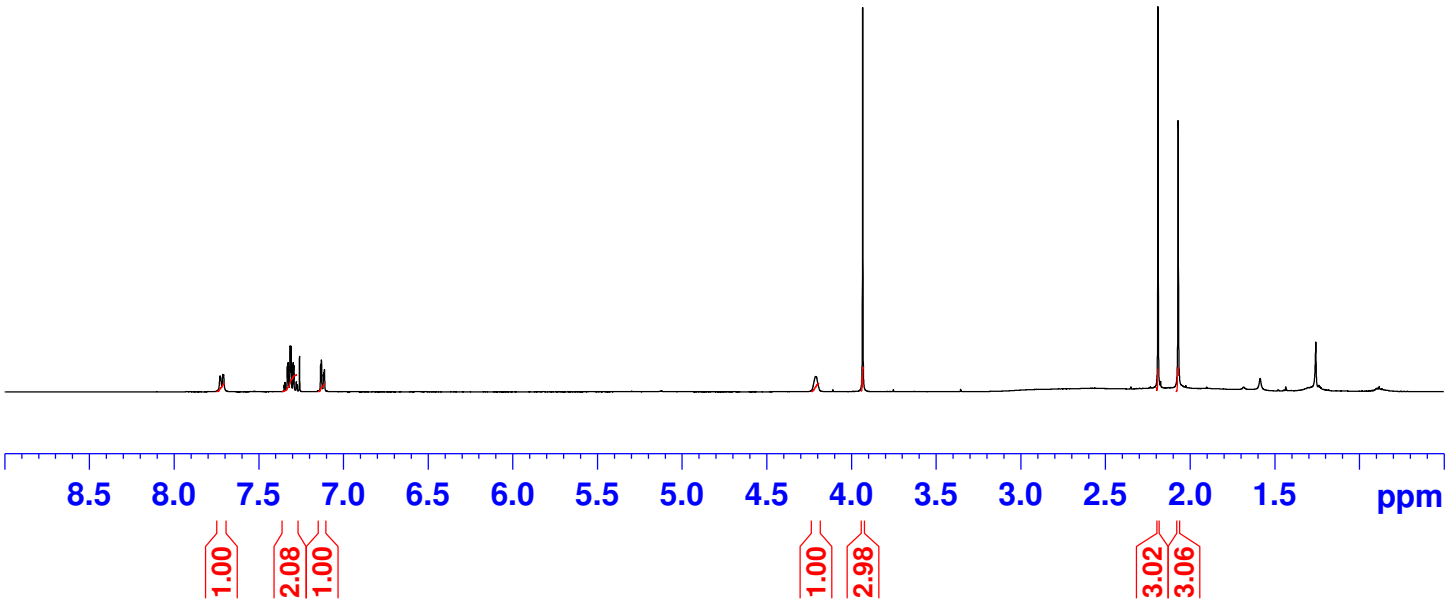
CY-H-A-16p-CDCl3-re

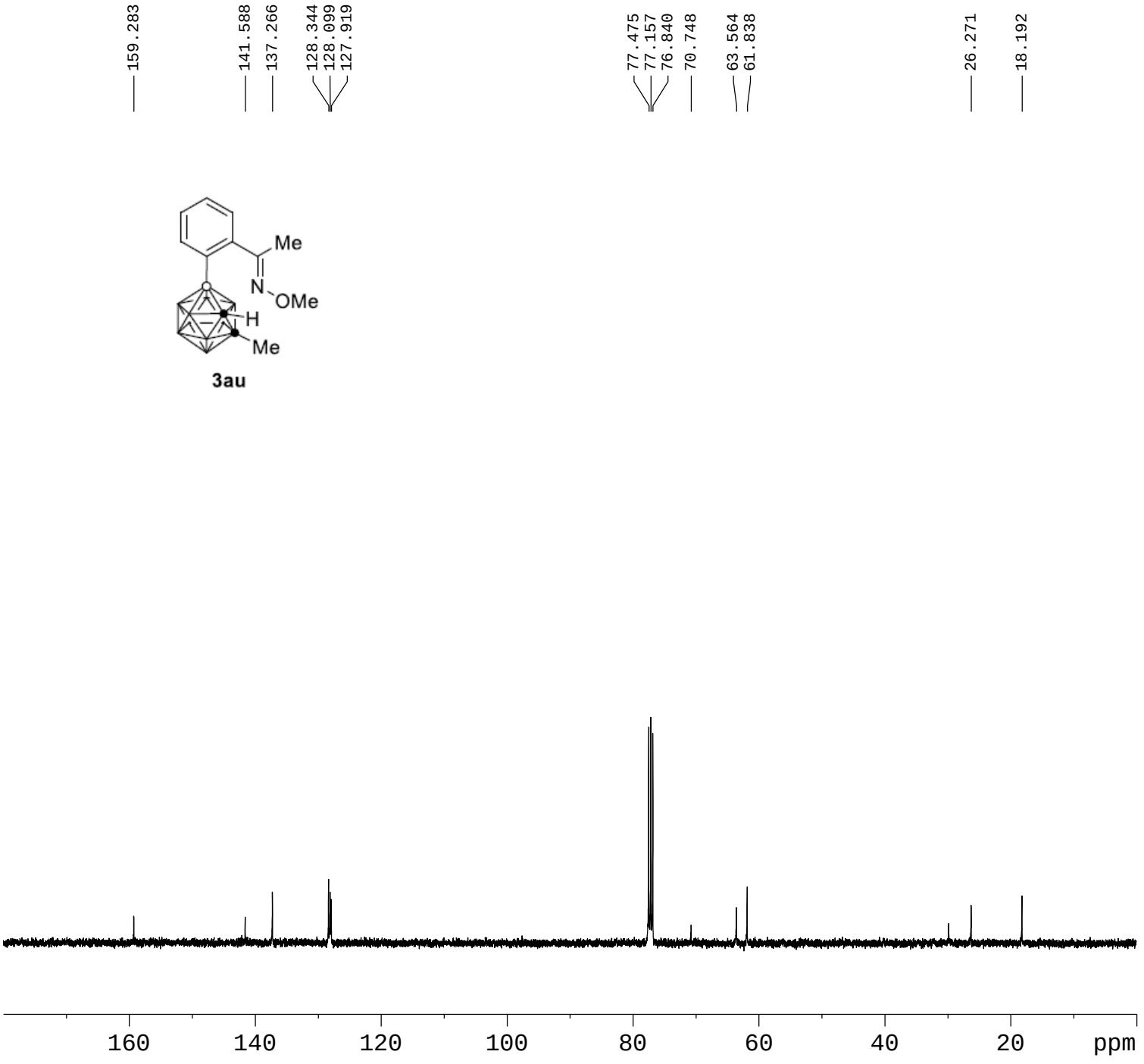




3au

```
Current Data Parameters
NAME      CY-H-A-16p-CDCl3-re
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20161129
Time                19.42 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
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                 294.4 K
D1              1.00000000 sec
TD0                     1
SFO1          400.1324708 MHz
NUC1                   1H
P1                 15.00 usec
PLW1            8.31000042 W

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

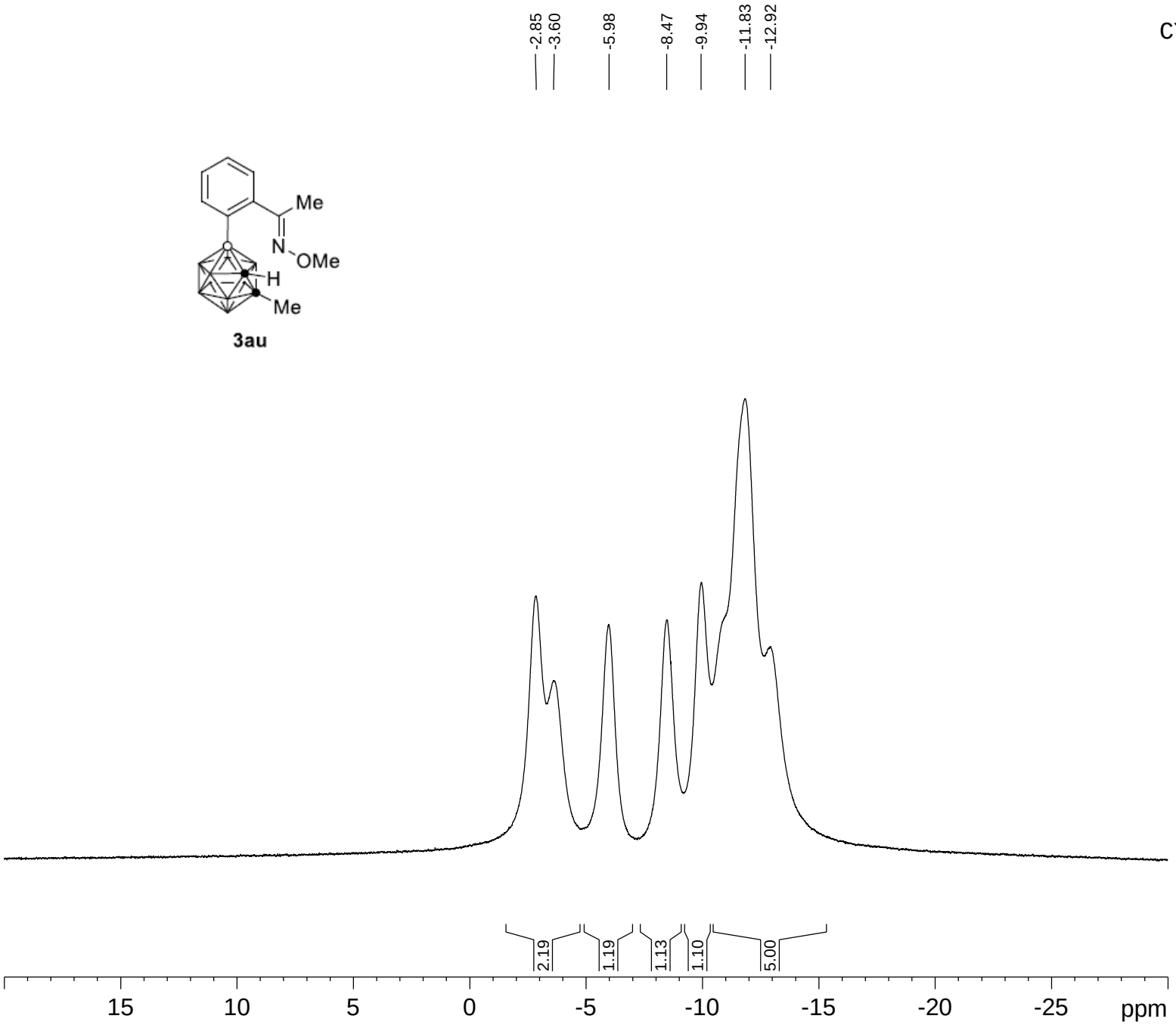




CY-C-A-16P-CDCl3

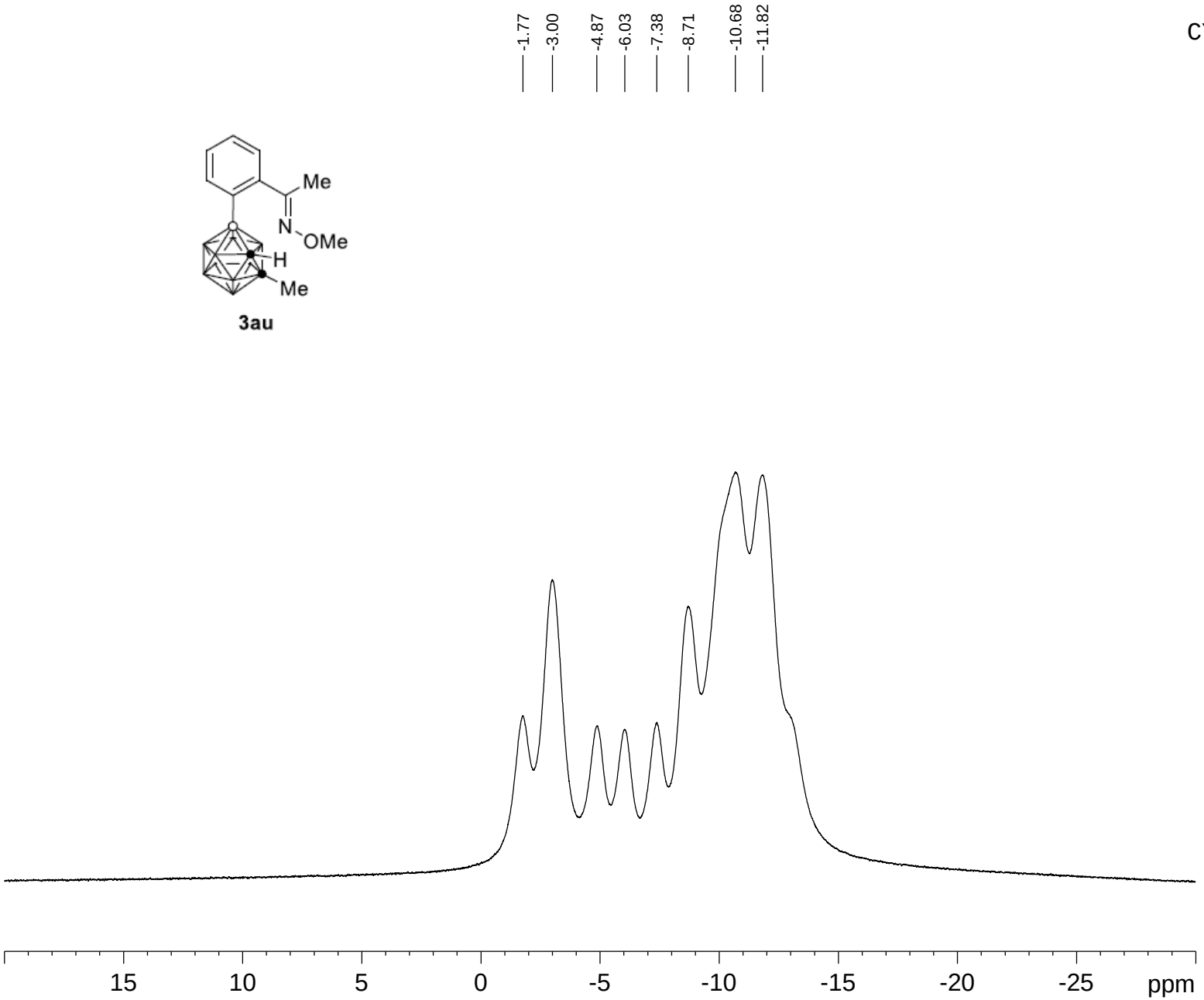
Bruker Advance III 400

```
Current Data Parameters
NAME      CY-C-A-16P-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20160817
Time               13.15 h
INSTRUM             spect
PROBHD   Z824601_0021 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    200
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                 294.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1
SFO1         100.6228298 MHz
NUC1                 13C
P1                  9.50 usec
PLW1         41.25000000 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2               90.00 usec
PLW2          8.31000042 W
PLW12         0.23083000 W
PLW13         0.11611000 W

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



CY-B-A-16P

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

F2 - Acquisition Parameters
Date_           20160817
Time              15.16 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    26
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   256
DW                20.800 usec
DE                 6.50 usec
TE                295.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B(C)-A-16P

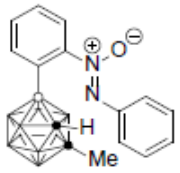
```
Current Data Parameters
NAME       CY-B(C)-A-16P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160817
Time               15.48 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                   44
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  256
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          128.4097504 MHz
WDW                EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

CY-H-A-38p-CDCl3

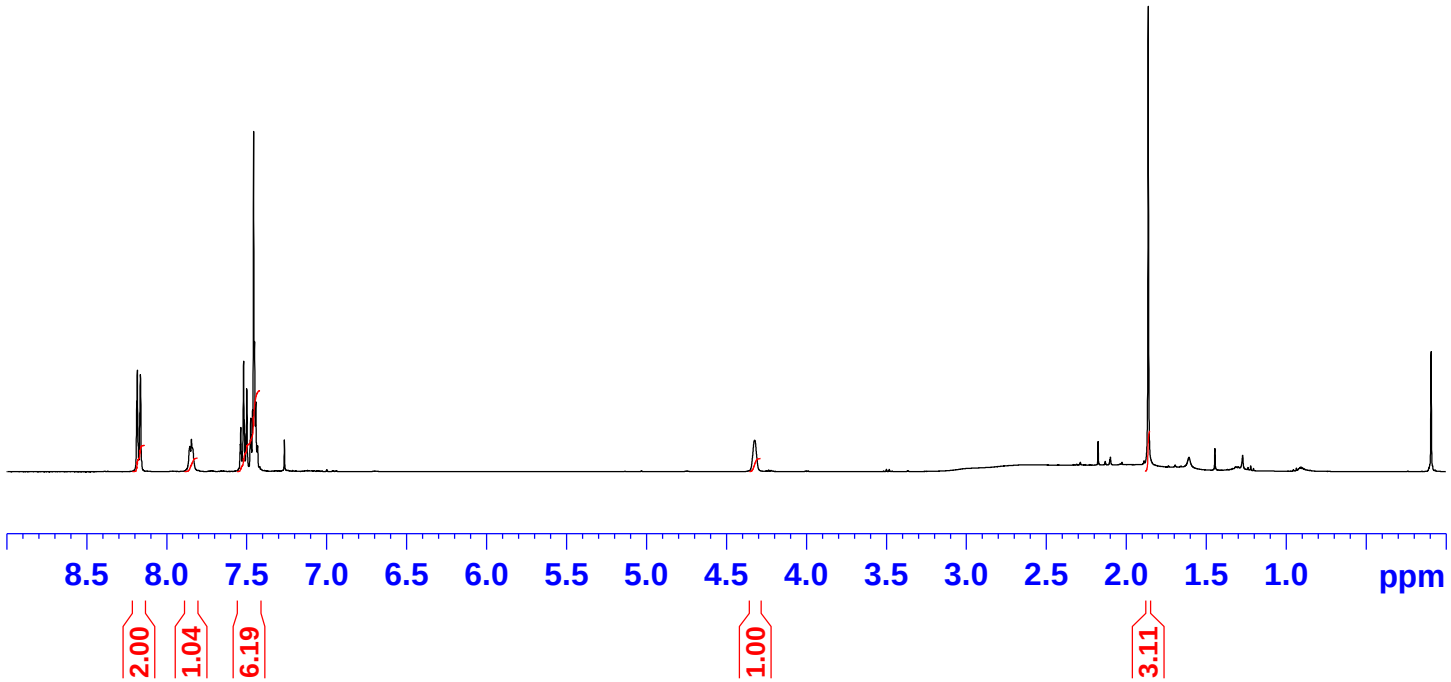
7.853
7.843
7.837
7.538
7.535
7.530
7.517
7.498
7.476
7.473
7.470
7.461
7.455
7.448
7.441
7.429
7.262

4.324

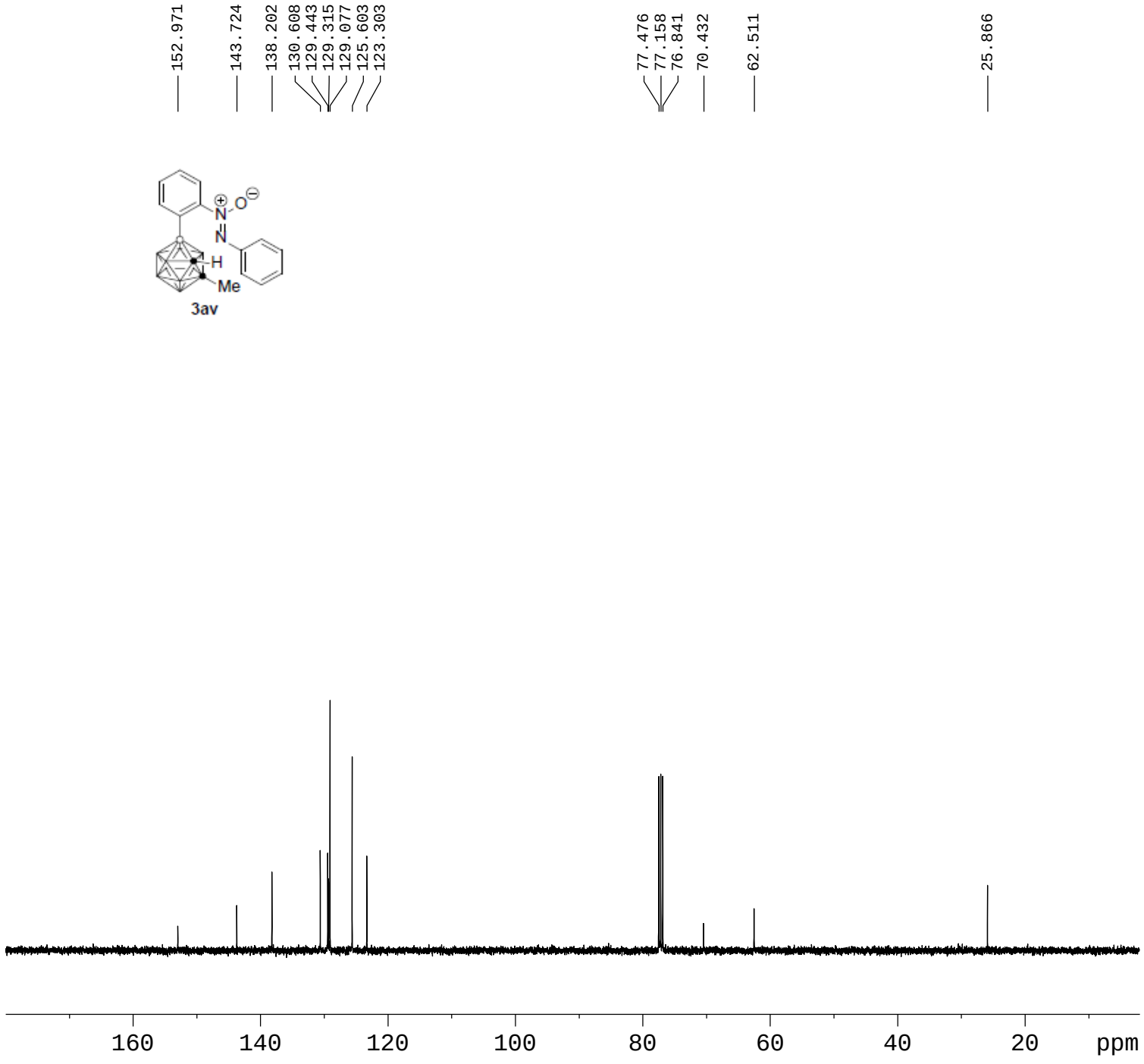
1.862



3av




```
Current Data Parameters
NAME      CY-H-A-38p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20161014
Time               20.07 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      9
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                   80.6
DW                 62.400 usec
DE                  6.50 usec
TE                 294.8 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           400.1300088 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



CY-C-A-38P-CDCl3

Bruker Advance III 400

Current Data Parameters

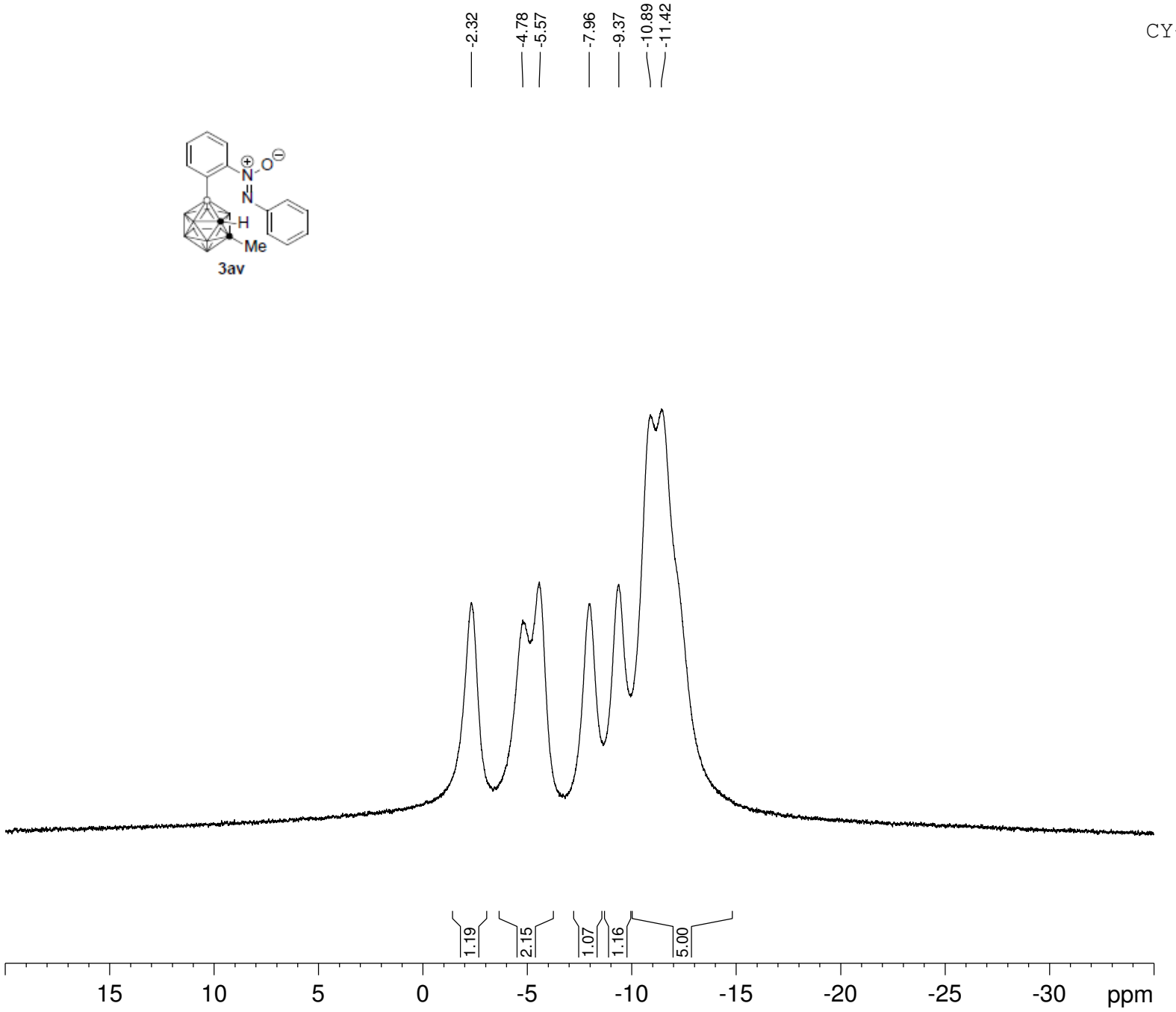
NAME	CY-C-A-38P-CDCl3
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20161014
Time	20.12 h
INSTRUM	spect
PROBHD	Z824601_0021 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	67
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

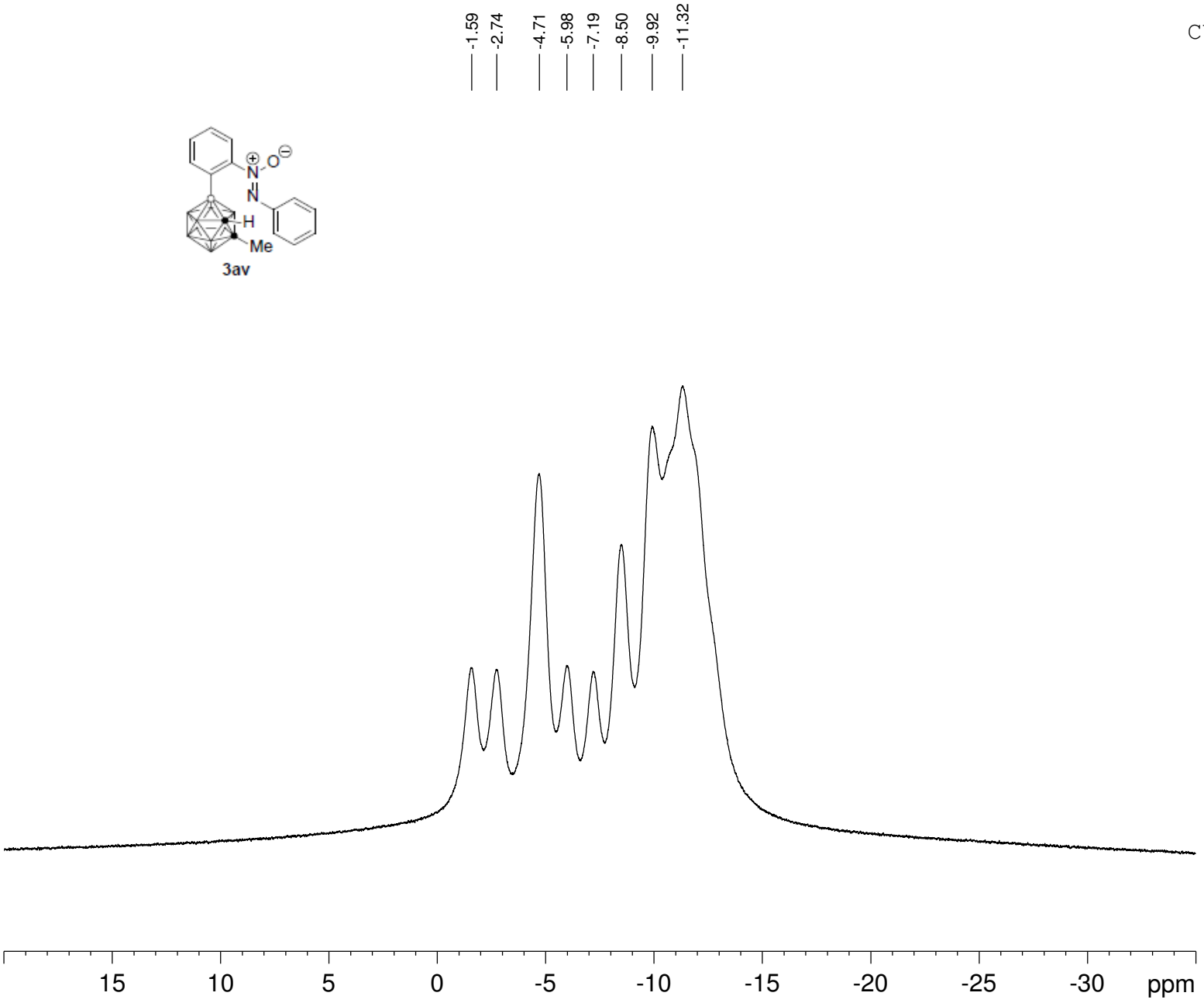
F2 - Processing parameters

SI	32768
SF	100.6127602 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



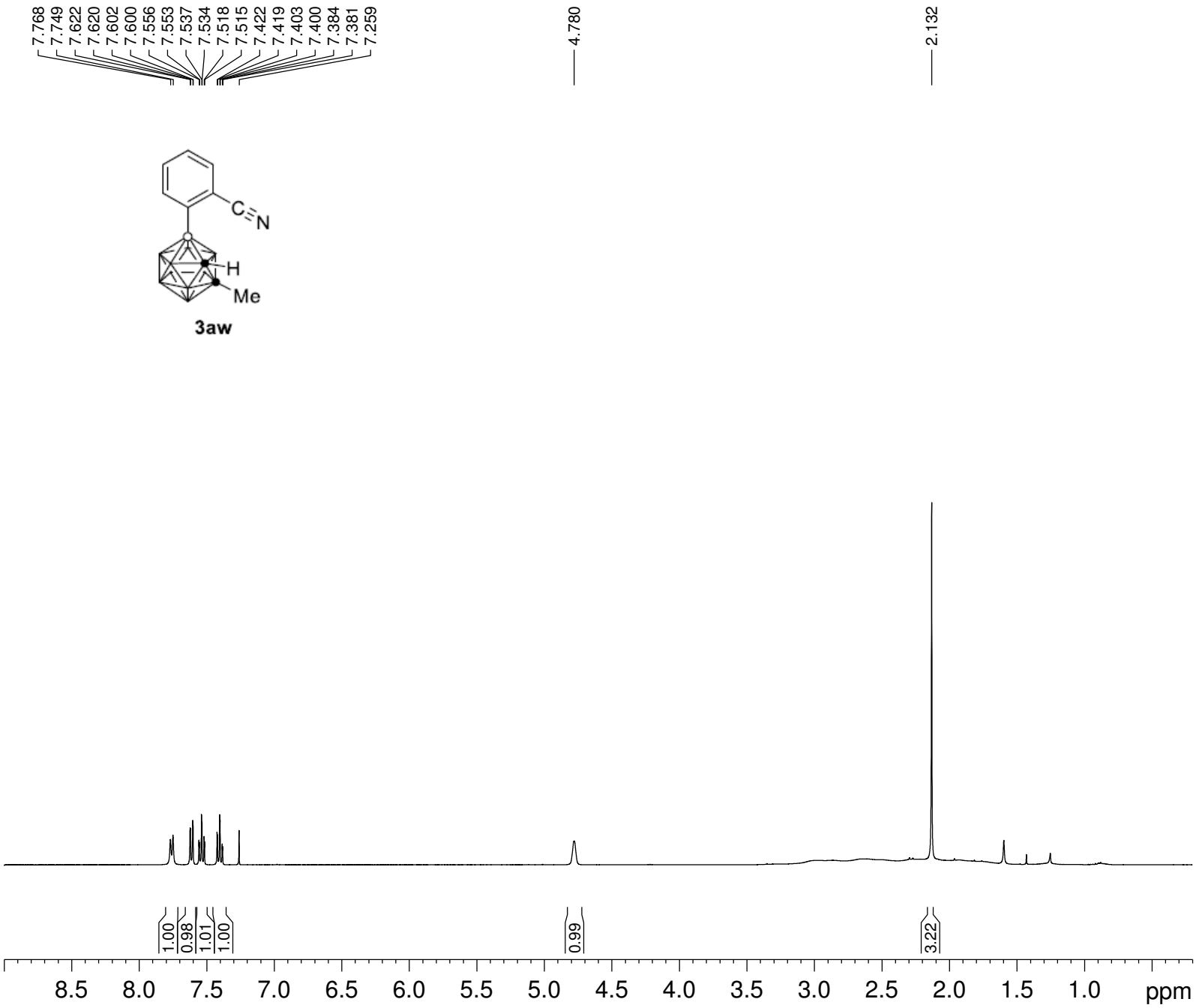
CY-B-38P-p

```
Current Data Parameters
NAME          CY-B-38P-p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160914
Time               14.07 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                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2        400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-38P-p-(C)

```
Current Data Parameters
NAME      CY-B-38P-p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160914
Time               14.10 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     55
DS                      2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   287
DW                20.800 usec
DE                 6.50 usec
TE                294.7 K
D1           2.00000000 sec
TD0                     1
SFO1        128.4096890 MHz
NUC1                  11B
P1                 7.50 usec
PLW1        55.09999847 W

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

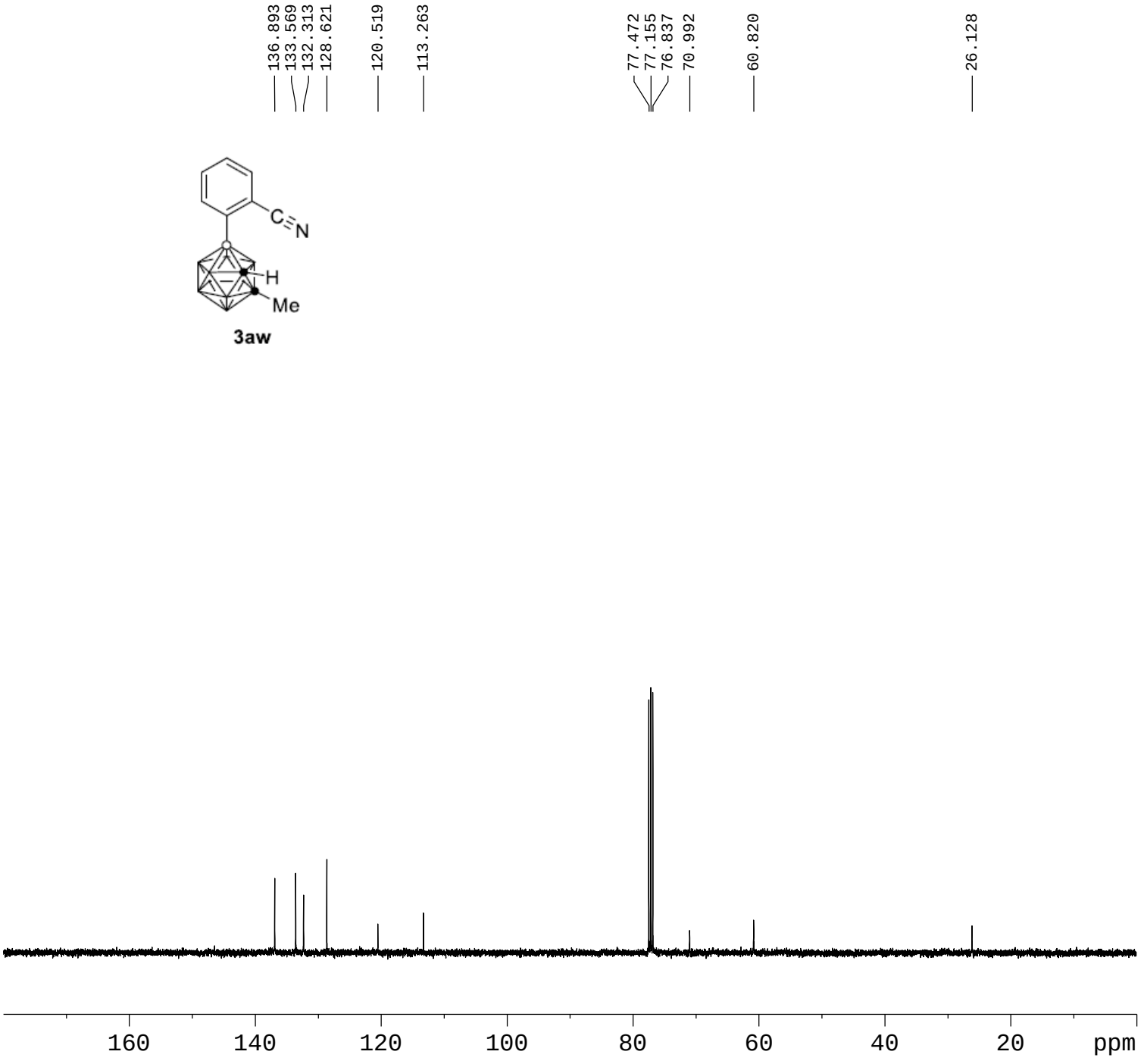


CY-H-A-50p

Current Data Parameters
NAME CY-H-A-50p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161012
Time 10.21 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 15
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 294.9 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



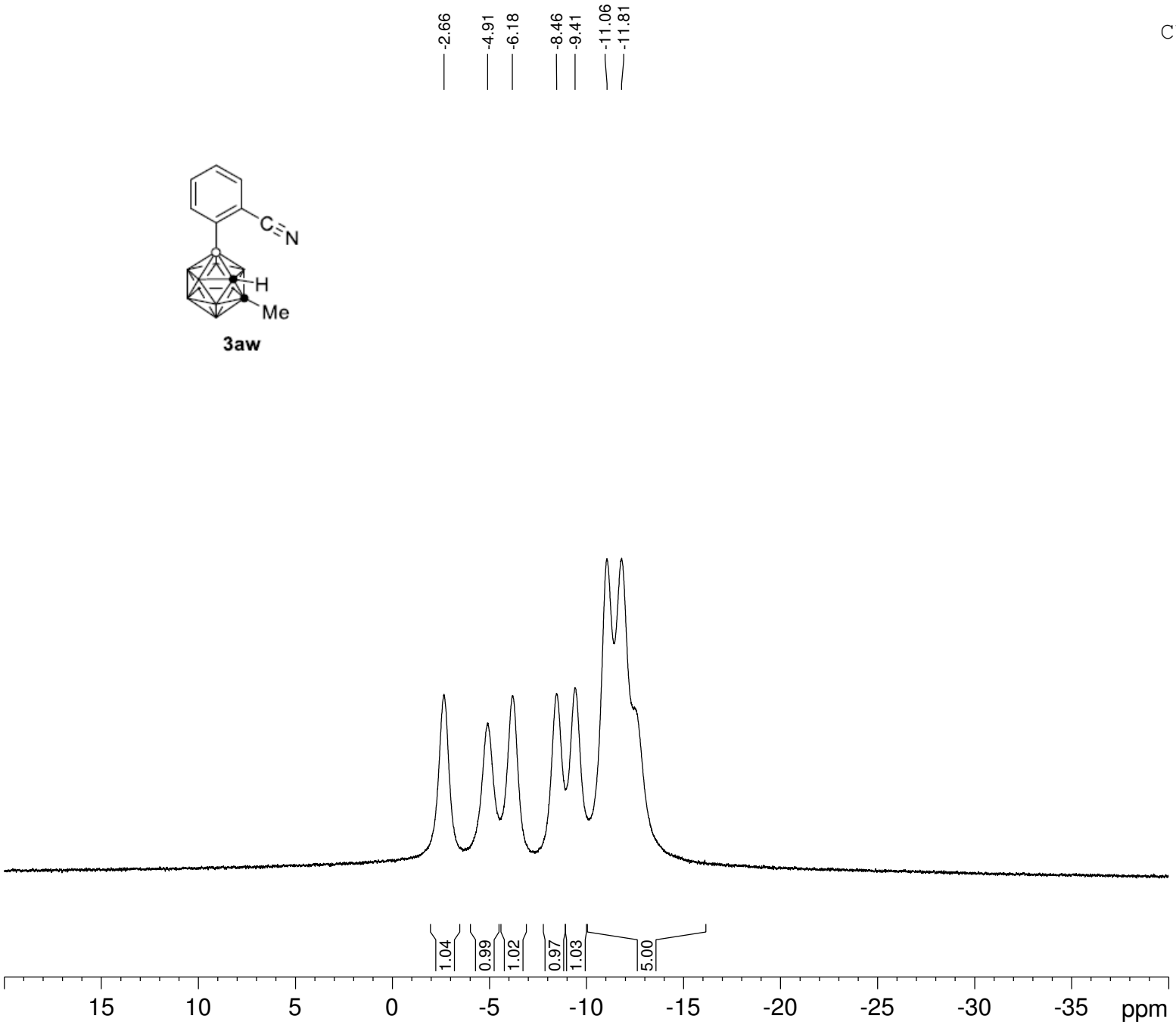
CY-C-A-50P

Bruker Advance III 400

Current Data Parameters
NAME CY-C-A-50P
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161012
Time 10.39 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 121
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

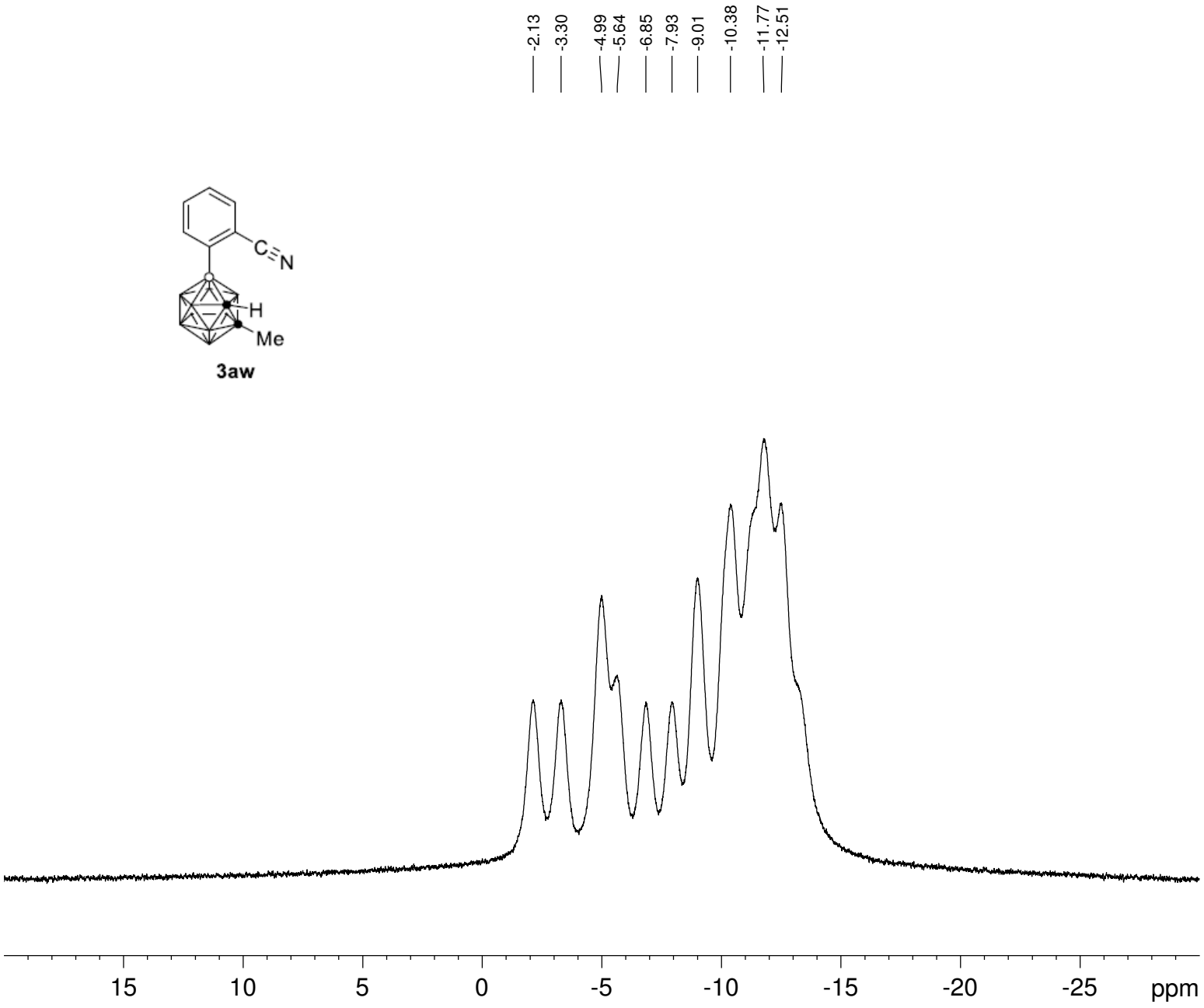
F2 - Processing parameters
SI 32768
SF 100.6127586 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



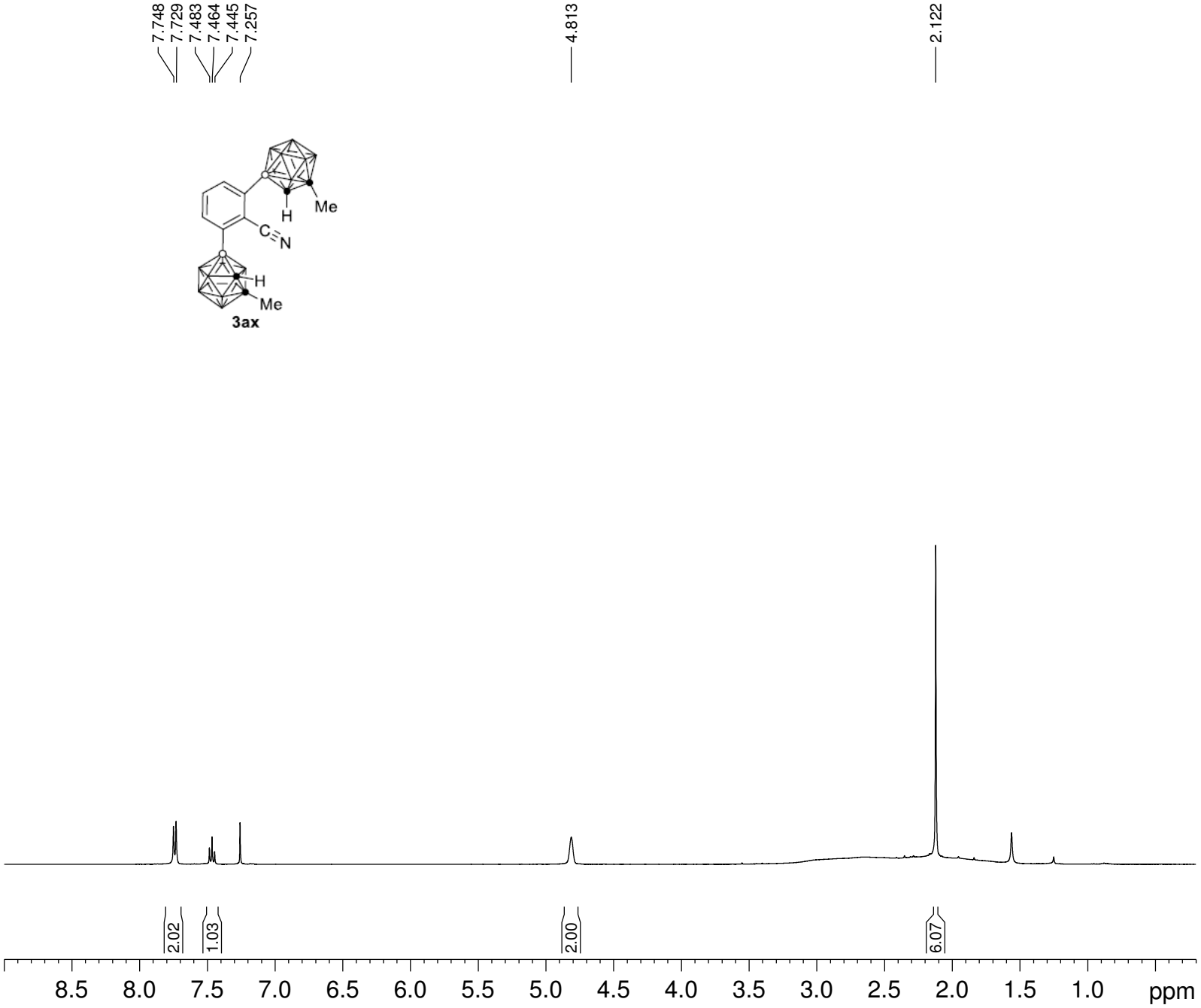
CY-B-A-50P

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

F2 - Acquisition Parameters
Date_           20161012
Time               20.00 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   161
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097793 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

CY-B-A-50P-(C)



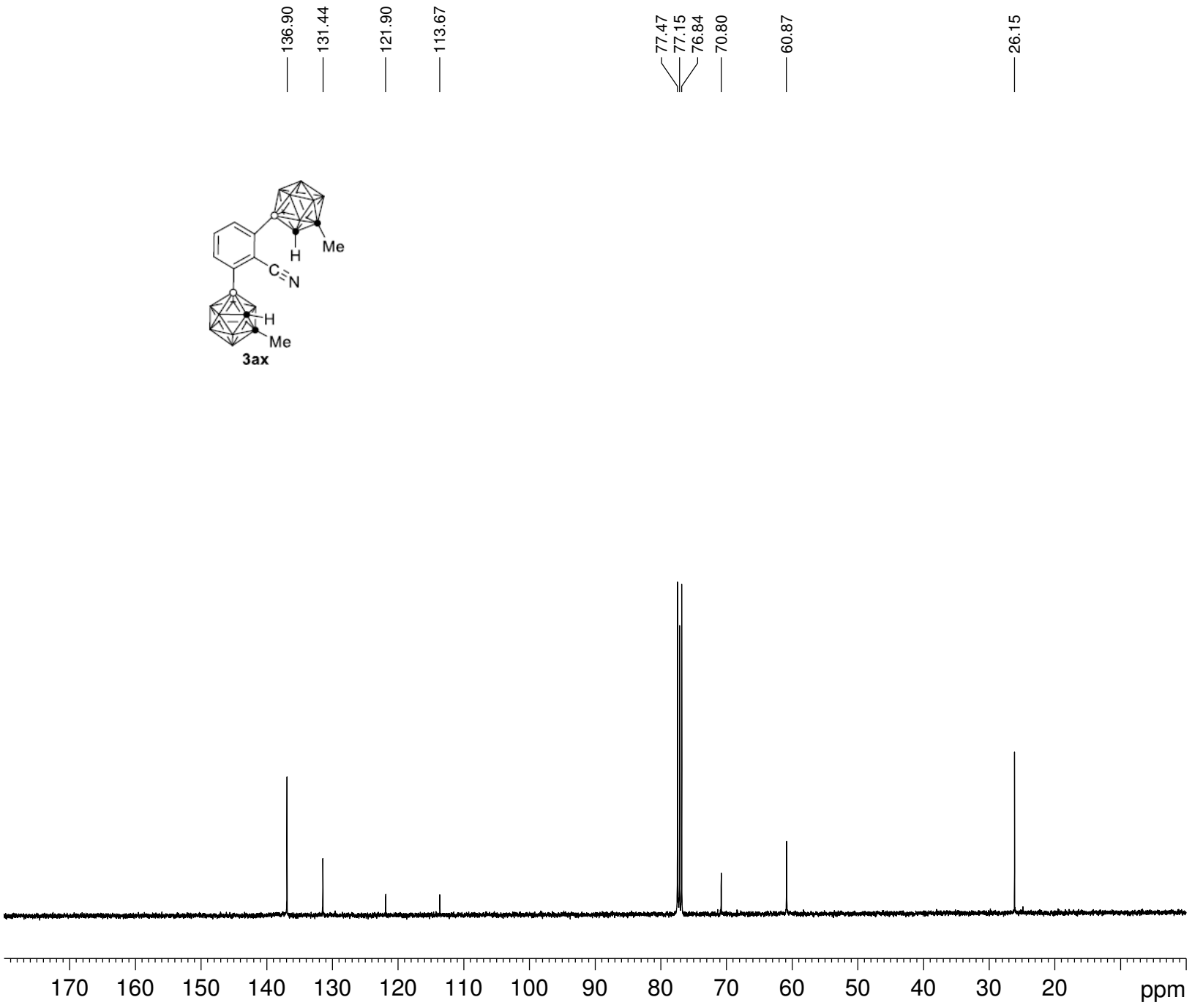

```
Current Data Parameters
NAME      CY-B-A-50P-(C)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20161012
Time              20.01 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  181
DW               20.800 usec
DE                6.50 usec
TE               295.5 K
D1           2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097881 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



Current Data Parameters
NAME CY-H-A-14p
EXPNO 1
PROCNO 1

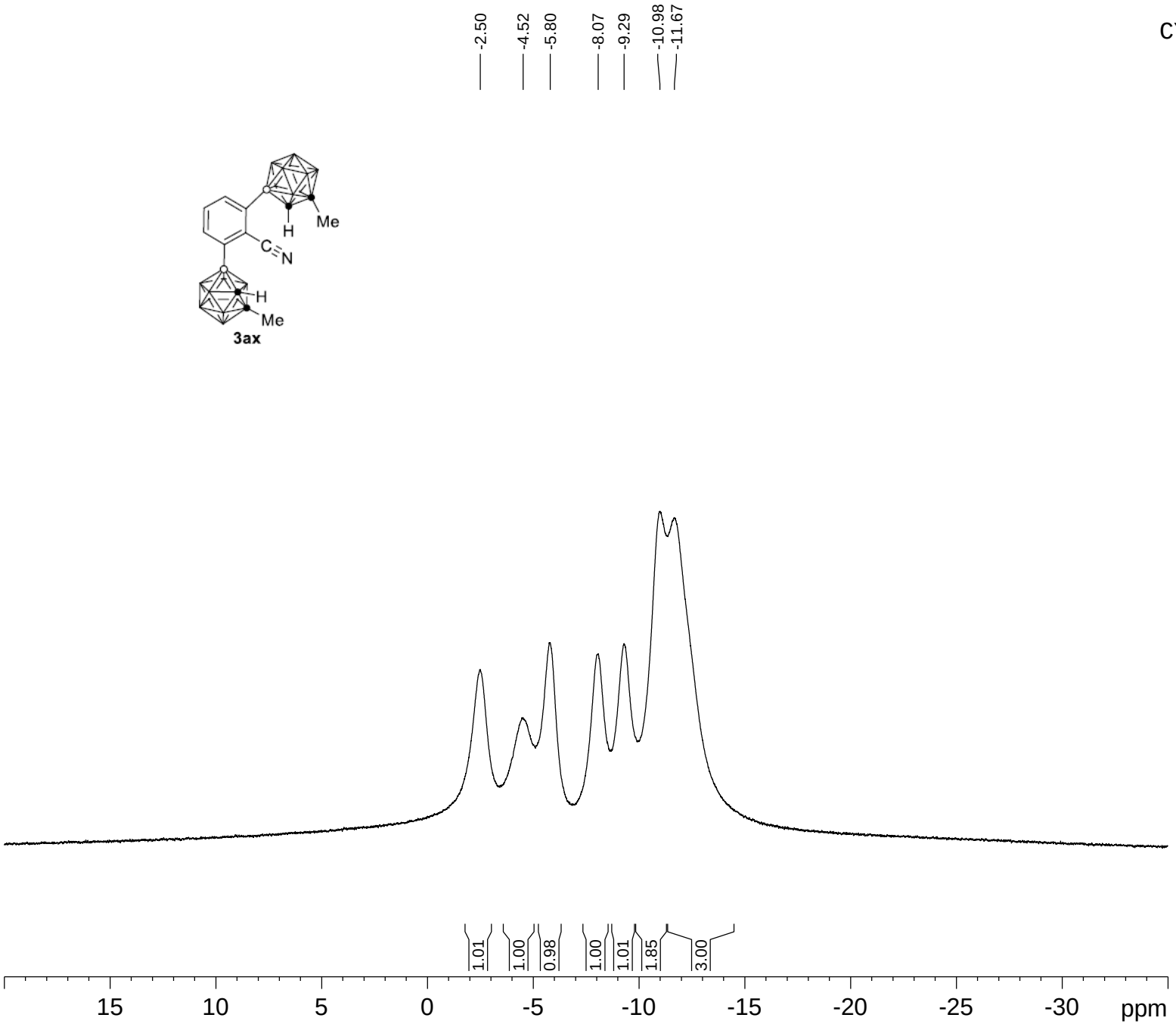
F2 - Acquisition Parameters
Date_ 20161128
Time 13.20 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 101
DW 62.400 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



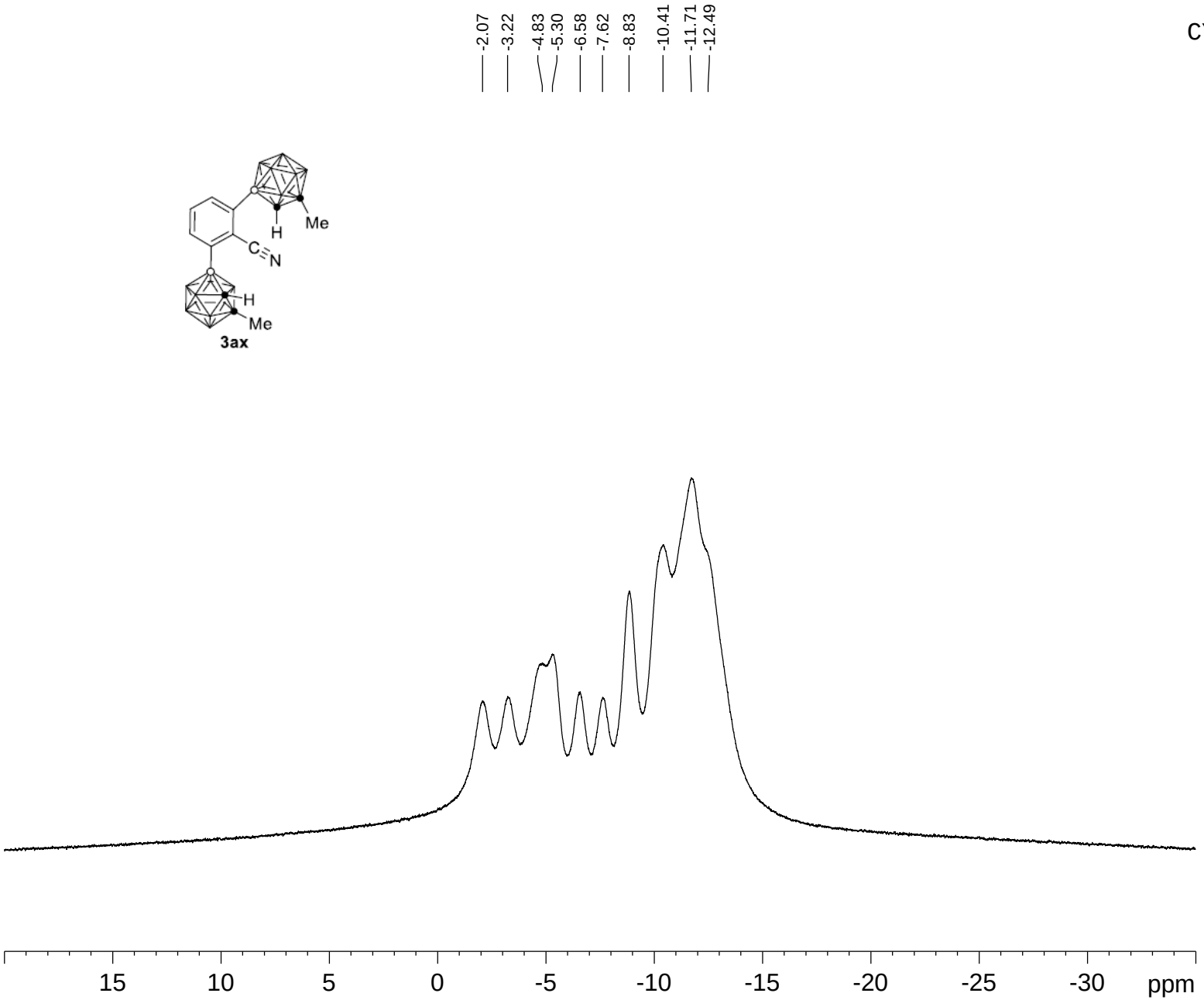
CY-C-A-14ppp

```
Current Data Parameters
NAME        CY-C-A-14ppp
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171021
Time              16.26 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  368
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ            0.8039083 sec
RG                  203
DW               12.267 usec
DE                6.50 usec
TE                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          100.6379027 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



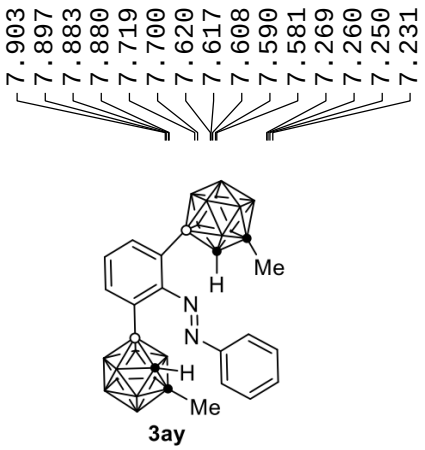
CY-B-A-14p-re2

```
Current Data Parameters
NAME      CY-B-A-14p-re2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161128
Time               13.10 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT             C6D6
NS                    36
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   256
DW                20.800 usec
DE                 6.50 usec
TE                296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

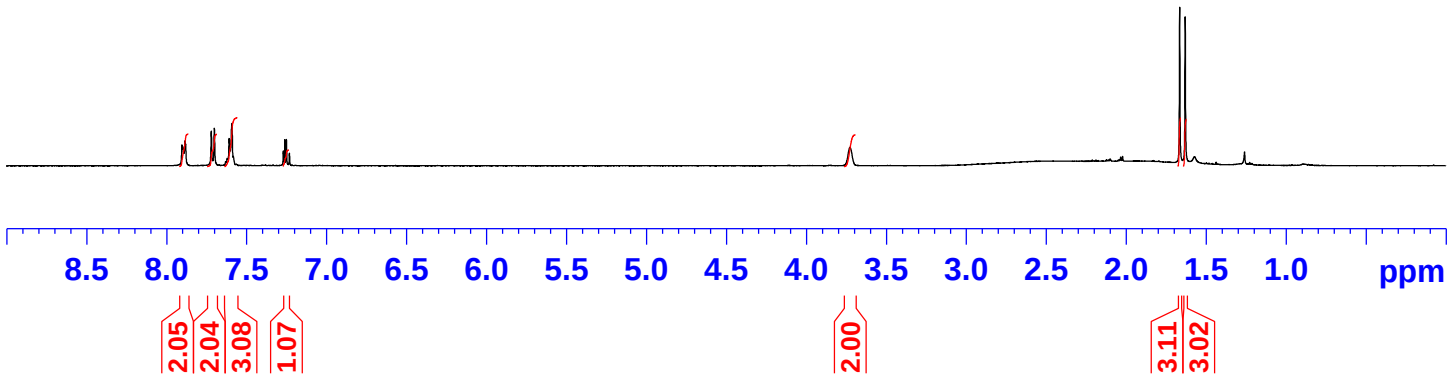


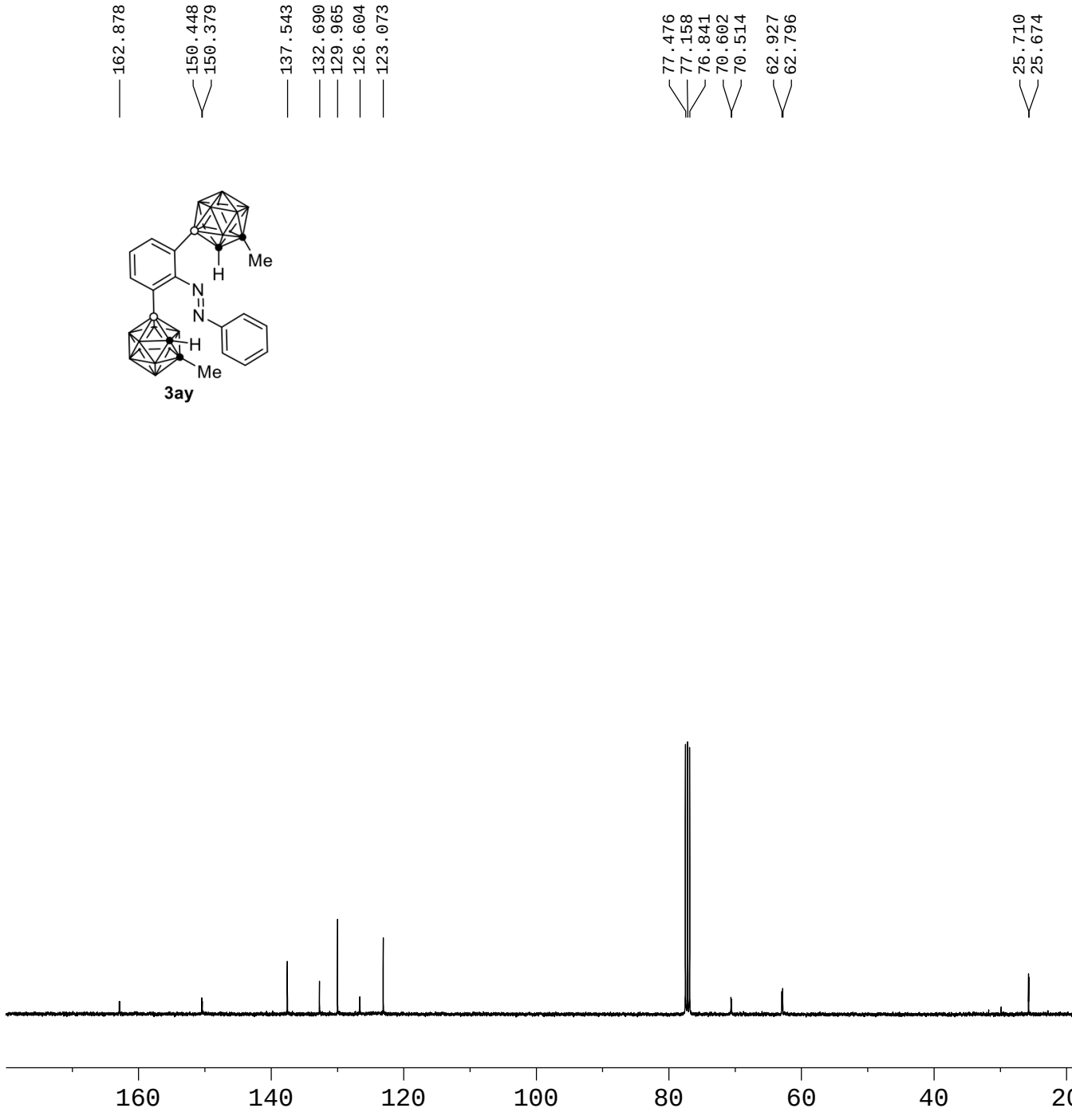
CY-B-A-14p-(C)-re2

```
Current Data Parameters
NAME      CY-B-A-14p-(C)-re2
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20161128
Time                 13.13 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT               C6D6
NS                      56
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                  295.6 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            128.4097881 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```




```
Current Data Parameters
NAME      CY-H-A-13p-CDCl3-re
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20161128
Time                13.41 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                      1
DW                 62.400 usec
DE                  6.50 usec
TE                 294.3 K
D1              1.00000000 sec
TD0                     1
SFO1          400.1324708 MHz
NUC1                   1H
P1                 15.00 usec
PLW1           8.31000042 W

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





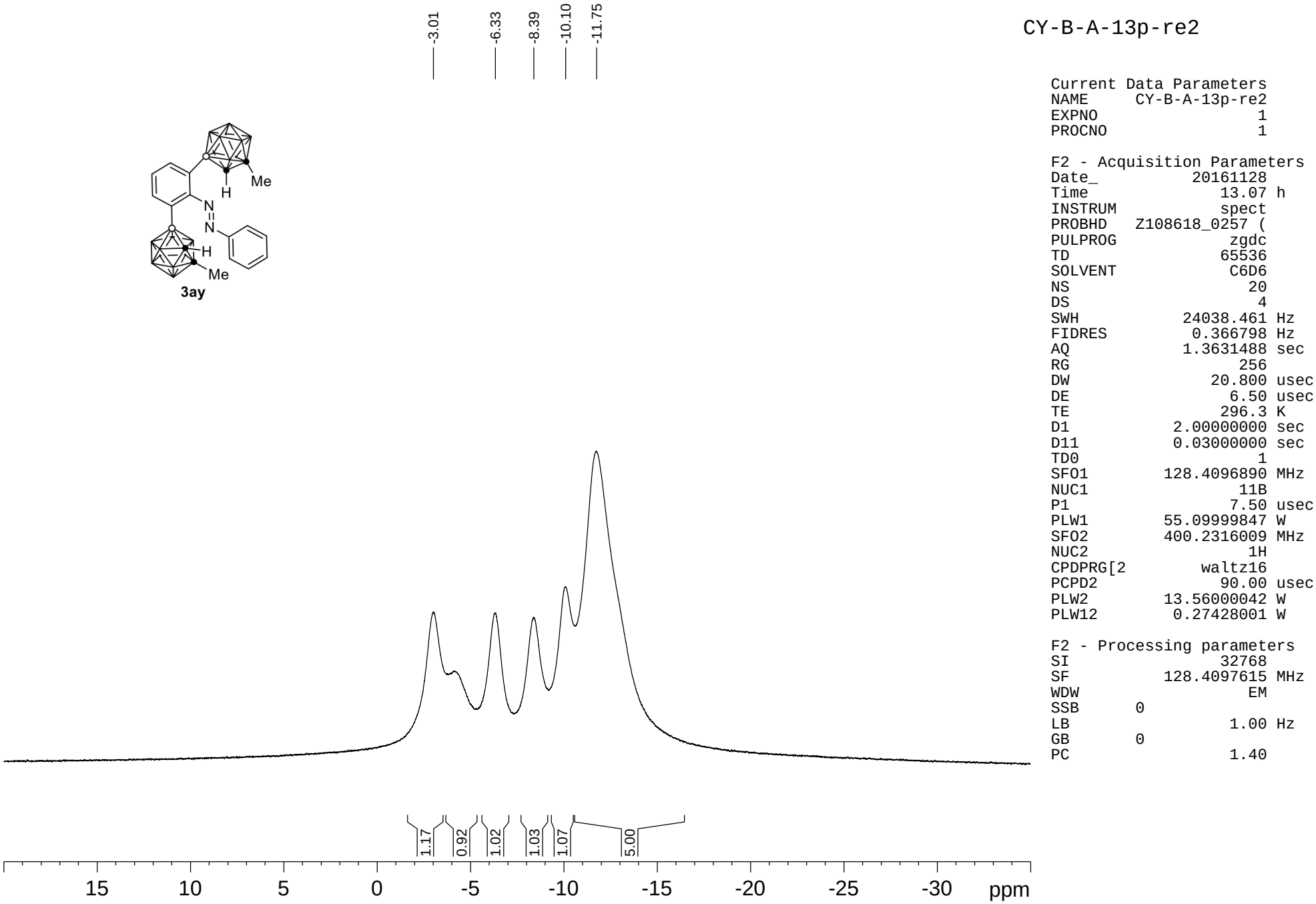
CY-C-A-13p-CDCl3

Bruker Advance III 400

Current Data Parameters
NAME CY-C-A-13p-CDCl3
EXPNO 1
PROCNO 1

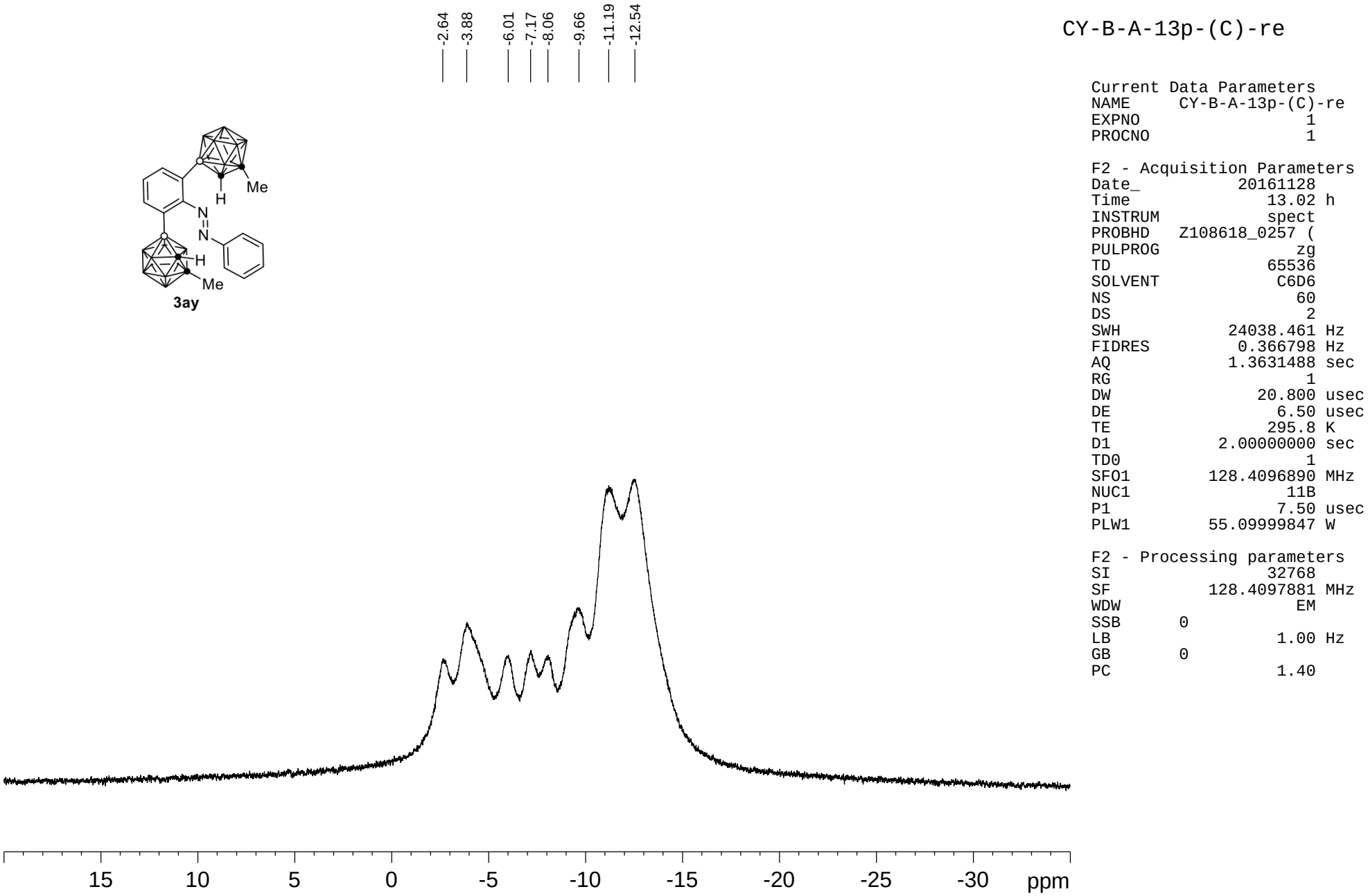
F2 - Acquisition Parameters
Date_ 20160812
Time 19.41 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 448
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 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 100.6127572 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



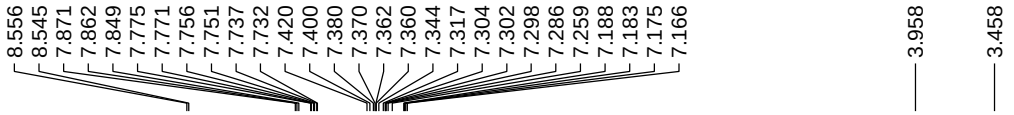
CY-B-A-13p-re2

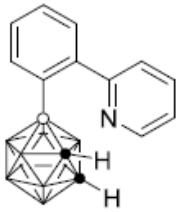
```
Current Data Parameters
NAME      CY-B-A-13p-re2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161128
Time               13.07 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG            zgdc
TD                65536
SOLVENT            C6D6
NS                   20
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  256
DW               20.800 usec
DE                6.50 usec
TE               296.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         128.4096890 MHz
NUC1                11B
P1                7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-13p-(C)-re

```
Current Data Parameters
NAME      CY-B-A-13p-(C)-re
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20161128
Time                 13.02 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT               C6D6
NS                      60
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                       1
DW                  20.800 usec
DE                   6.50 usec
TE                  295.8 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             128.4097881 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```





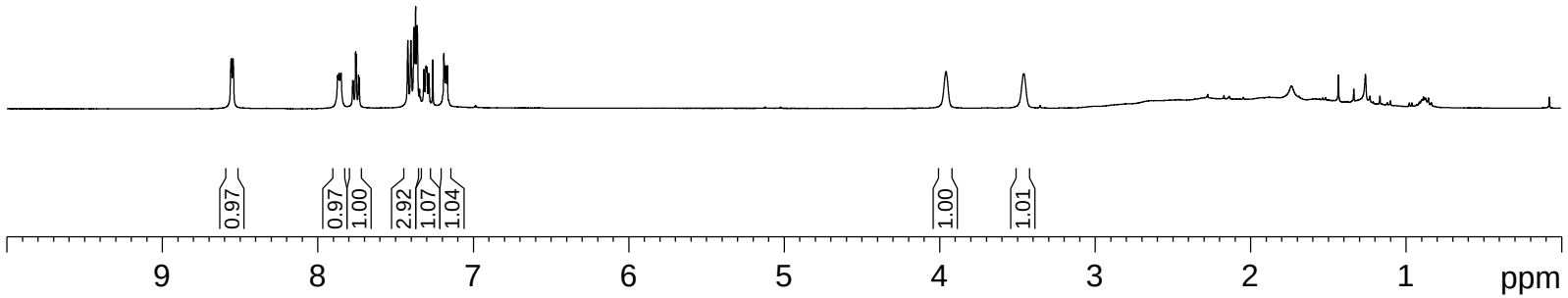
3ba

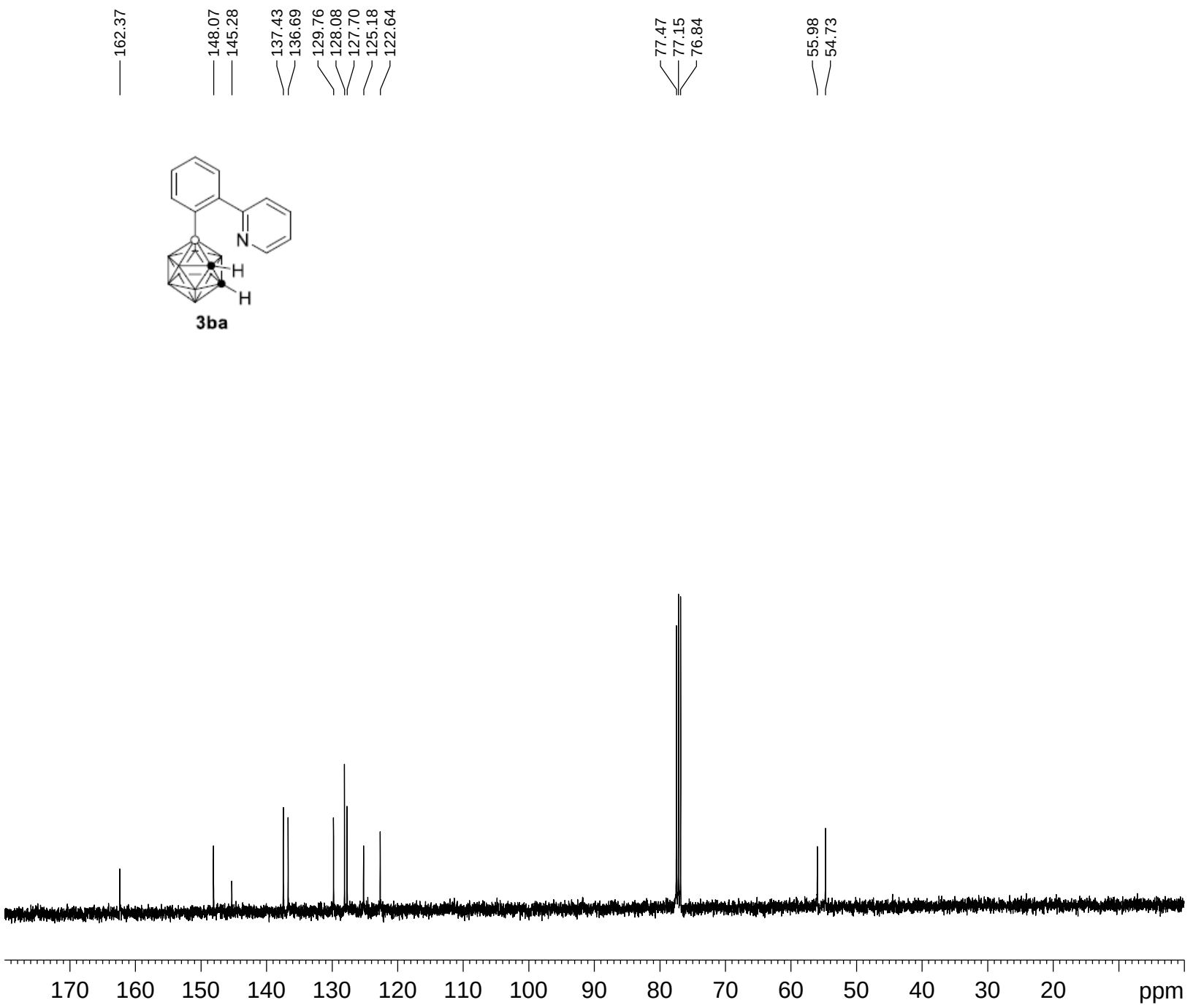
CY-H-A-67p

Current Data Parameters
NAME CY-H-A-67p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161117
Time 19.45 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 45.2
DW 62.400 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MH
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

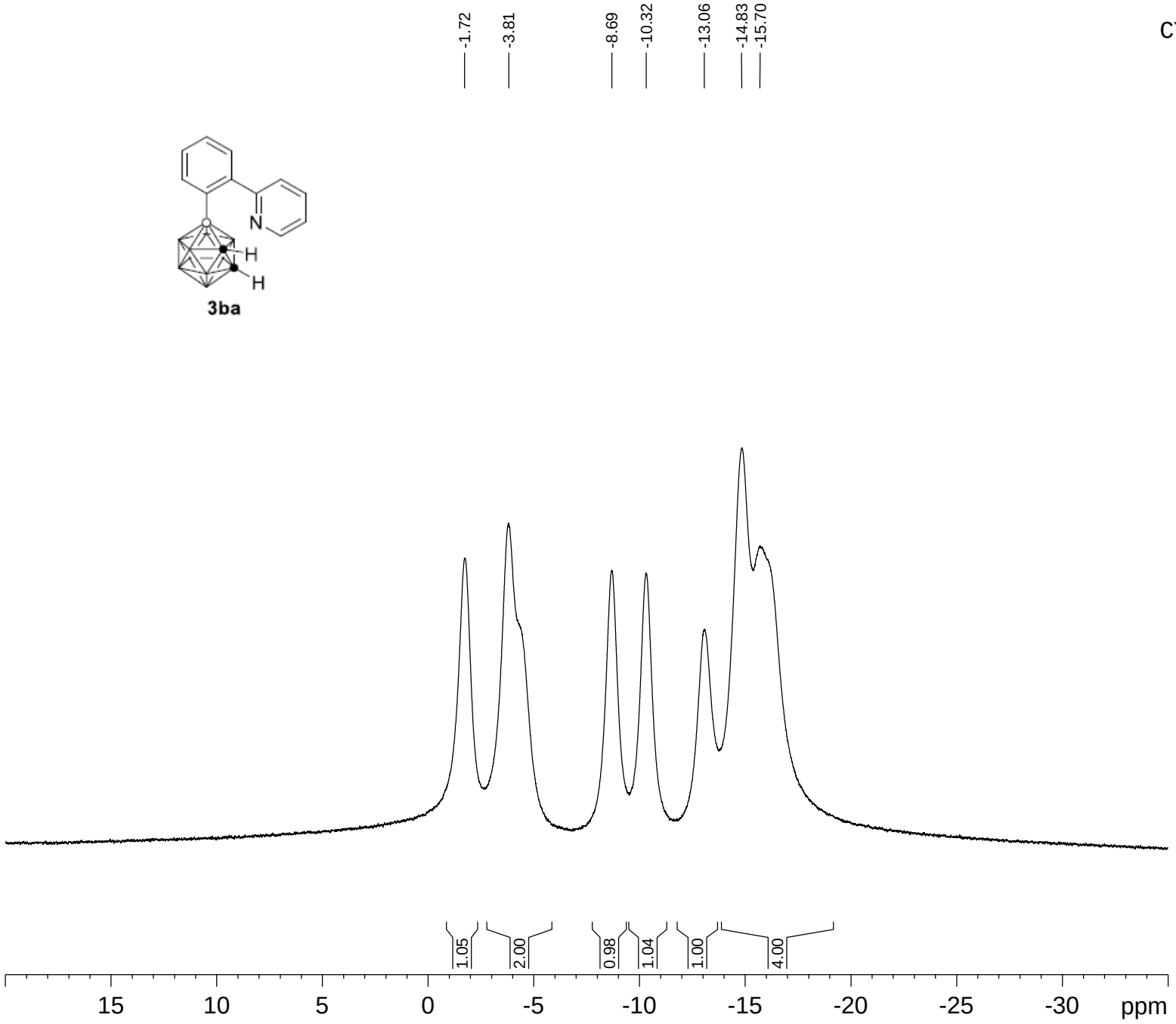
F2 - Processing parameters
SI 65536
SF 400.2300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





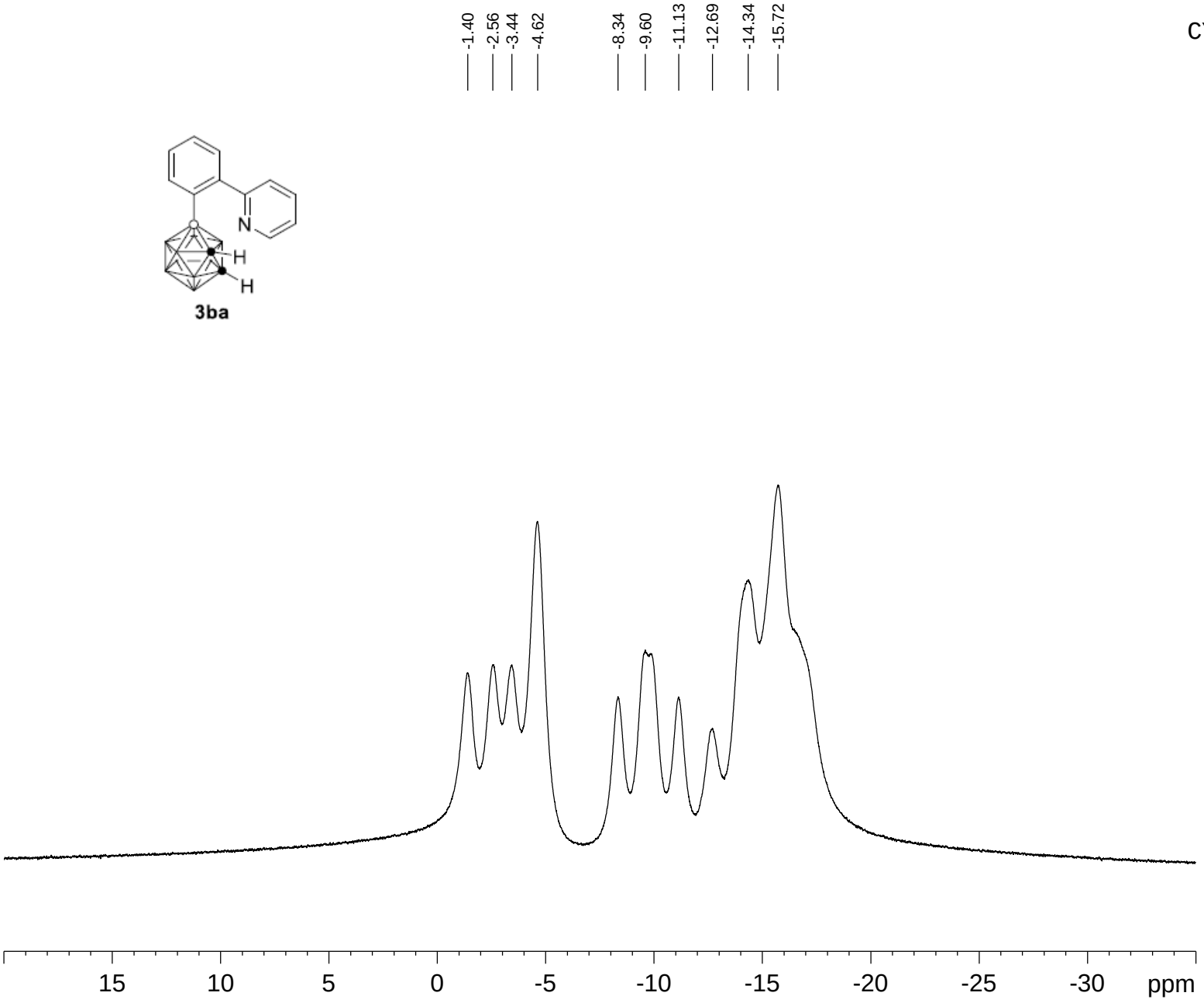
CY-C-A-67P-re

```
Current Data Parameters
NAME       CY-C-A-67P-re
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20161118
Time              13.01 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                   80
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ            0.8039083 sec
RG                  203
DW               12.267 usec
DE                6.50 usec
TE                296.4 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          100.6379032 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



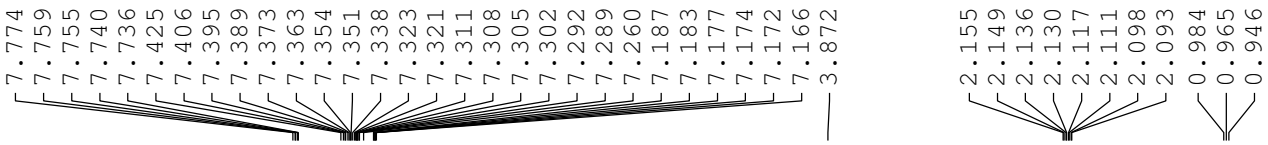
CY-B-A-67p

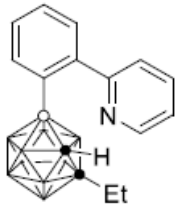
```
Current Data Parameters
NAME          CY-B-A-67p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161117
Time               20.50 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                   256
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



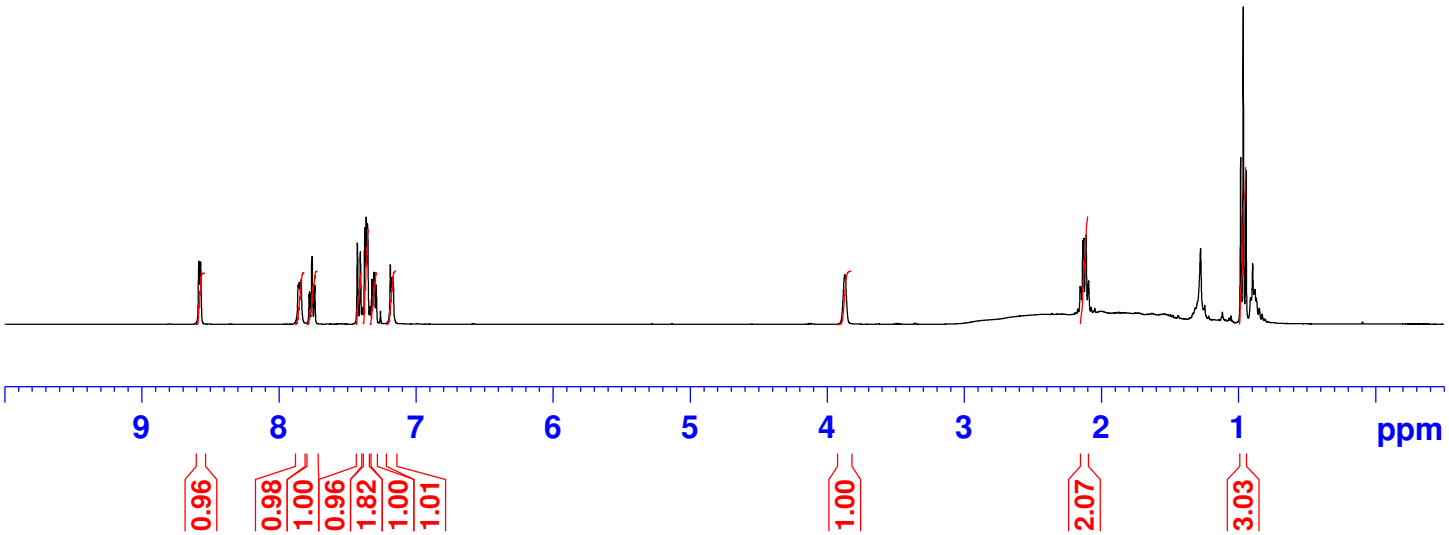
CY-B-A-67p-(C)

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

F2 - Acquisition Parameters
Date_            20161117
Time                20.48 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      40
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     256
DW                  20.800 usec
DE                   6.50 usec
TE                  295.5 K
D1            2.00000000 sec
TD0                      1
SFO1          128.4096890 MHz
NUC1                  11B
P1                   7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                   32768
SF            128.4097881 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

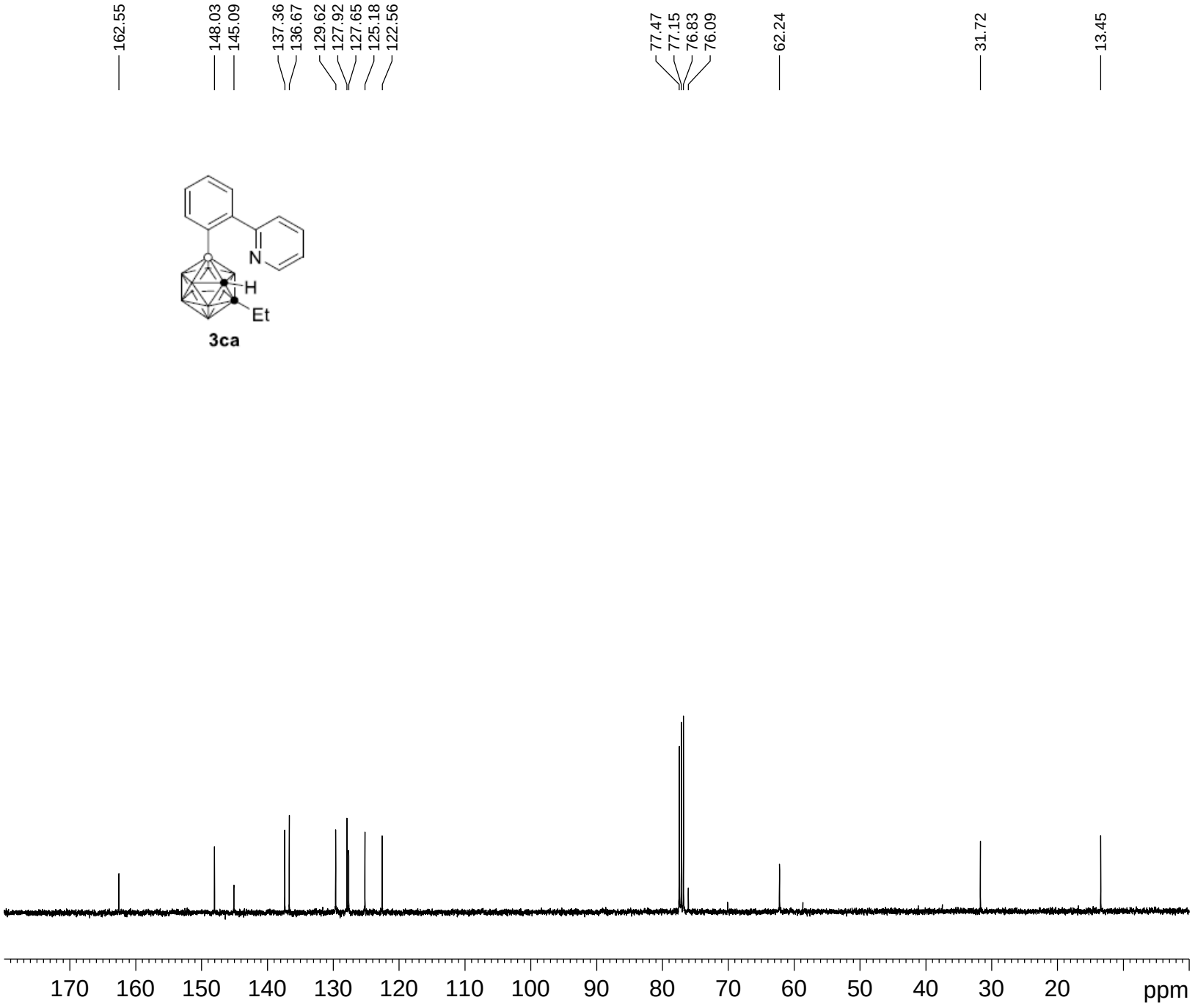




3ca

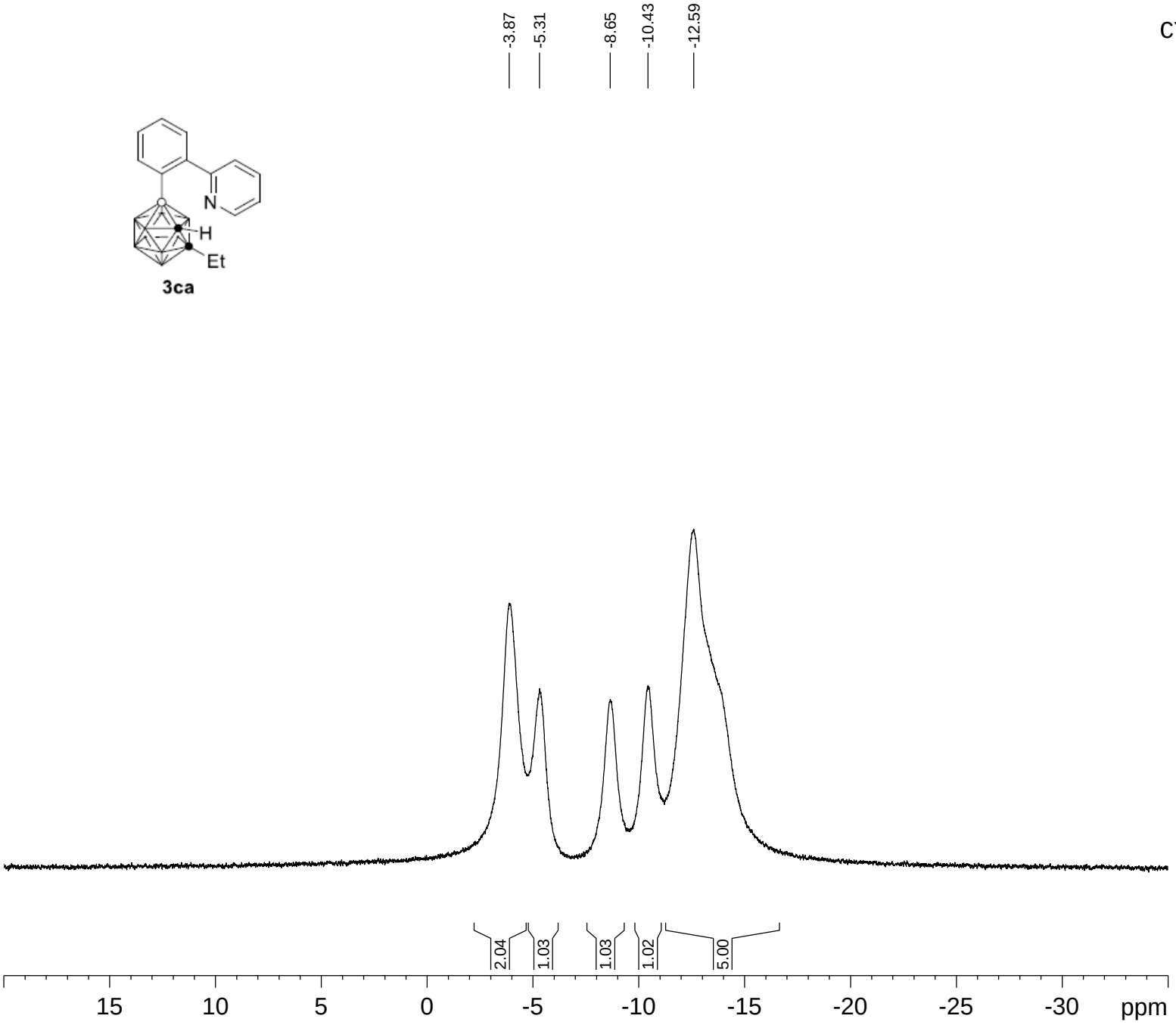



```
Current Data Parameters
NAME      CY-H-A-68p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20161119
Time                9.40 h
INSTRUM            spect
PROBHD   Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                  45.2
DW                62.400 usec
DE                 6.50 usec
TE                294.9 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1          8.31000042 W

F2 - Processing parameters
SI                 65536
SF           400.1300107 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



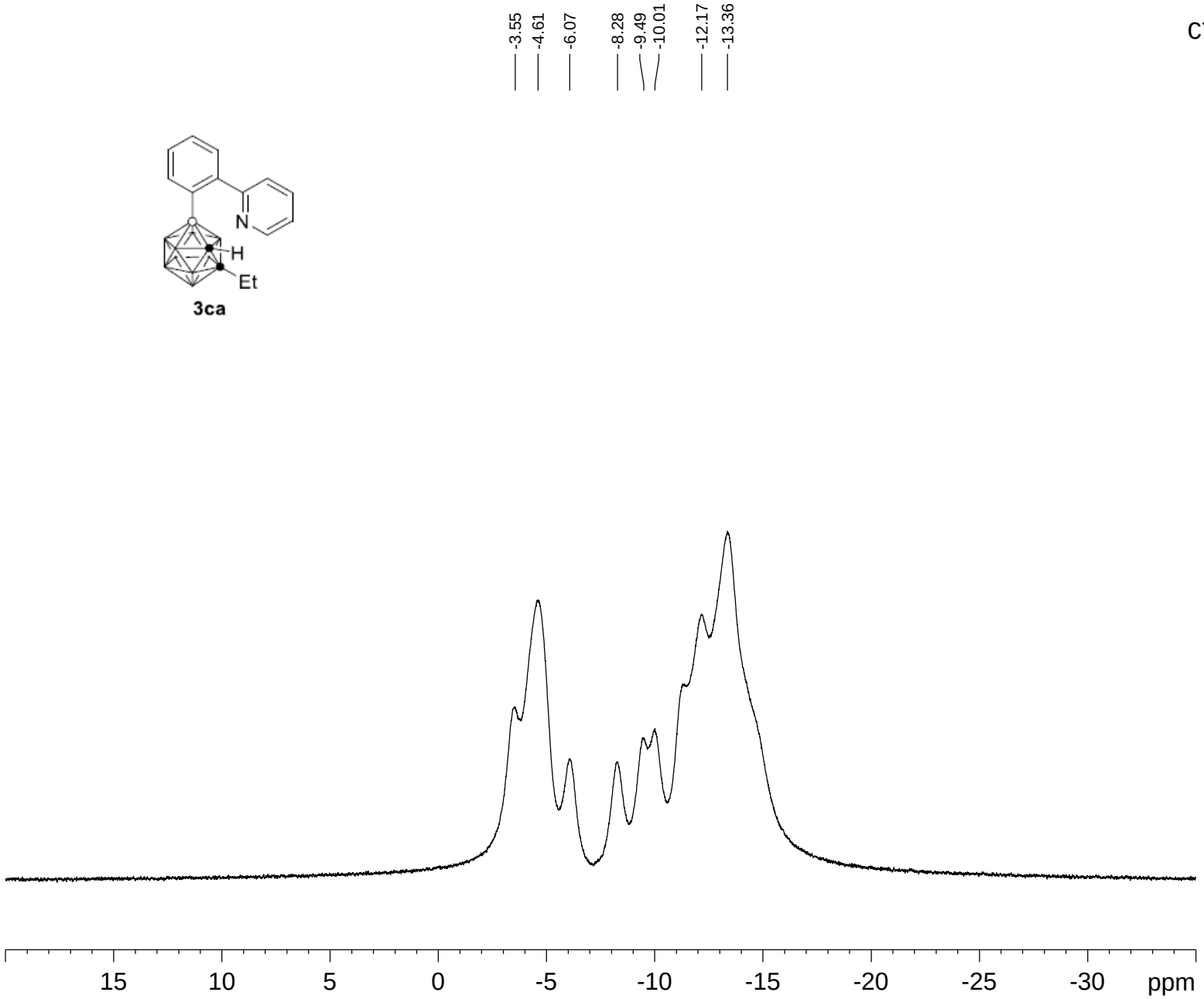
CY-C-A-68P-re

```
Current Data Parameters
NAME      CY-C-A-68P-re
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20161130
Time               9.43 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                  80
DS                   4
SWH          40760.871 Hz
FIDRES        0.621962 Hz
AQ           0.8039083 sec
RG                 203
DW              12.267 usec
DE               6.50 usec
TE               295.9 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          100.6379060 MHz
WDW                EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
```



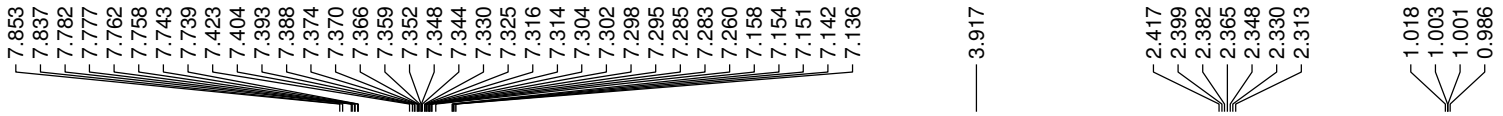
CY-B-A-68p

```
Current Data Parameters
NAME          CY-B-A-68p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161118
Time               22.25 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                     1
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

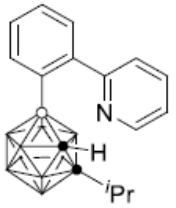


CY-B-A-68p-(C)

```
Current Data Parameters
NAME      CY-B-A-68p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20161118
Time                22.28 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      40
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                       1
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            128.4097881 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



CY-H-A-74p

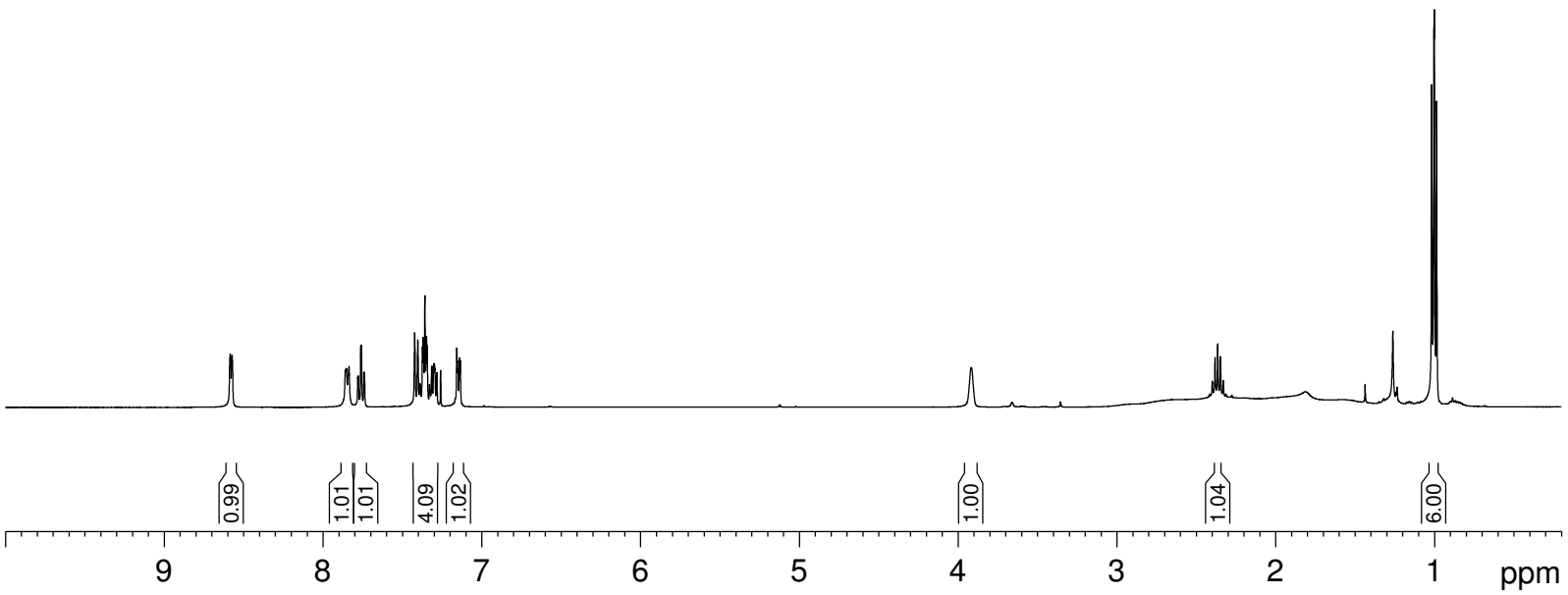


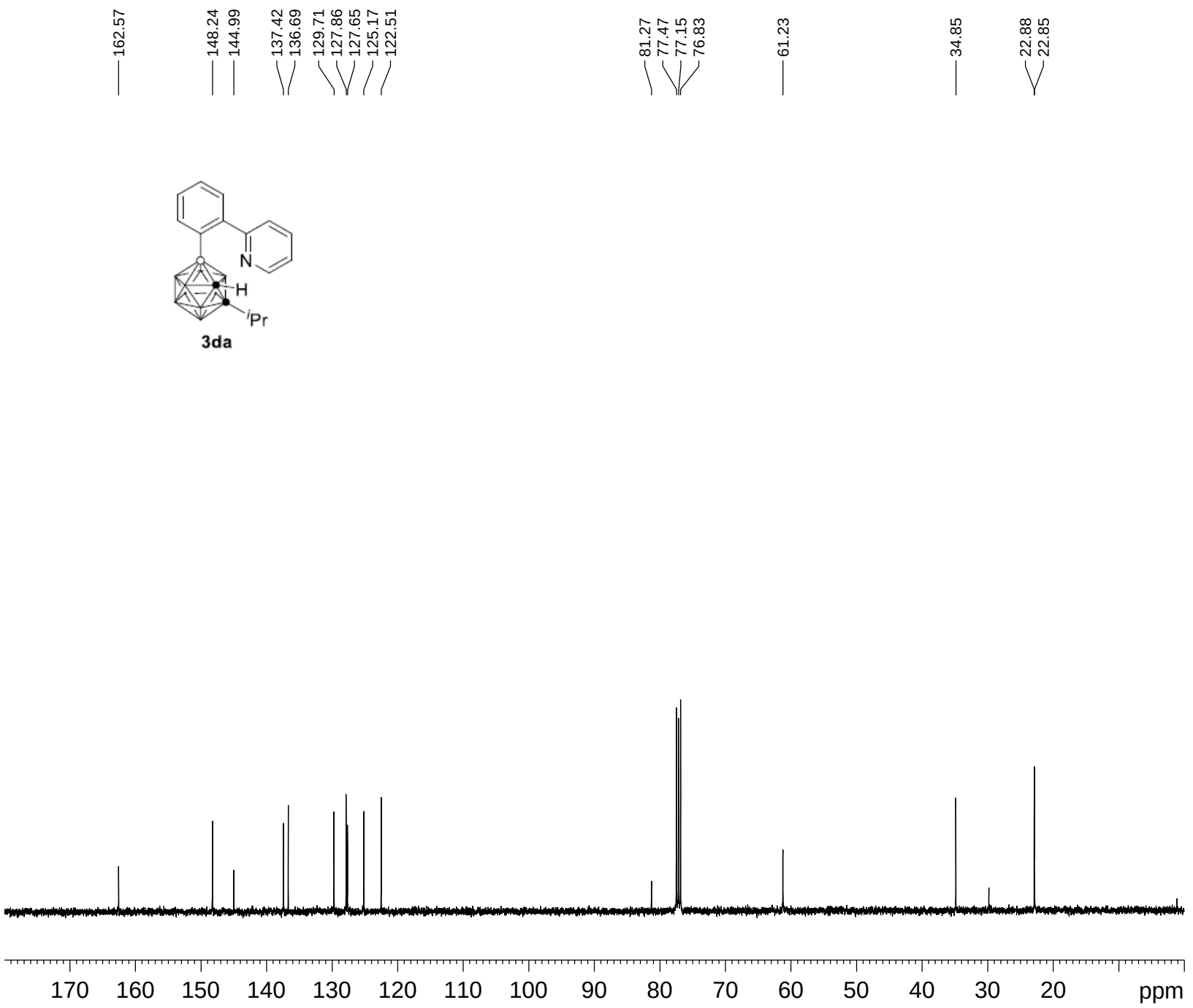
3da

Current Data Parameters
NAME CY-H-A-74p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161121
Time 17.34 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 45.2
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

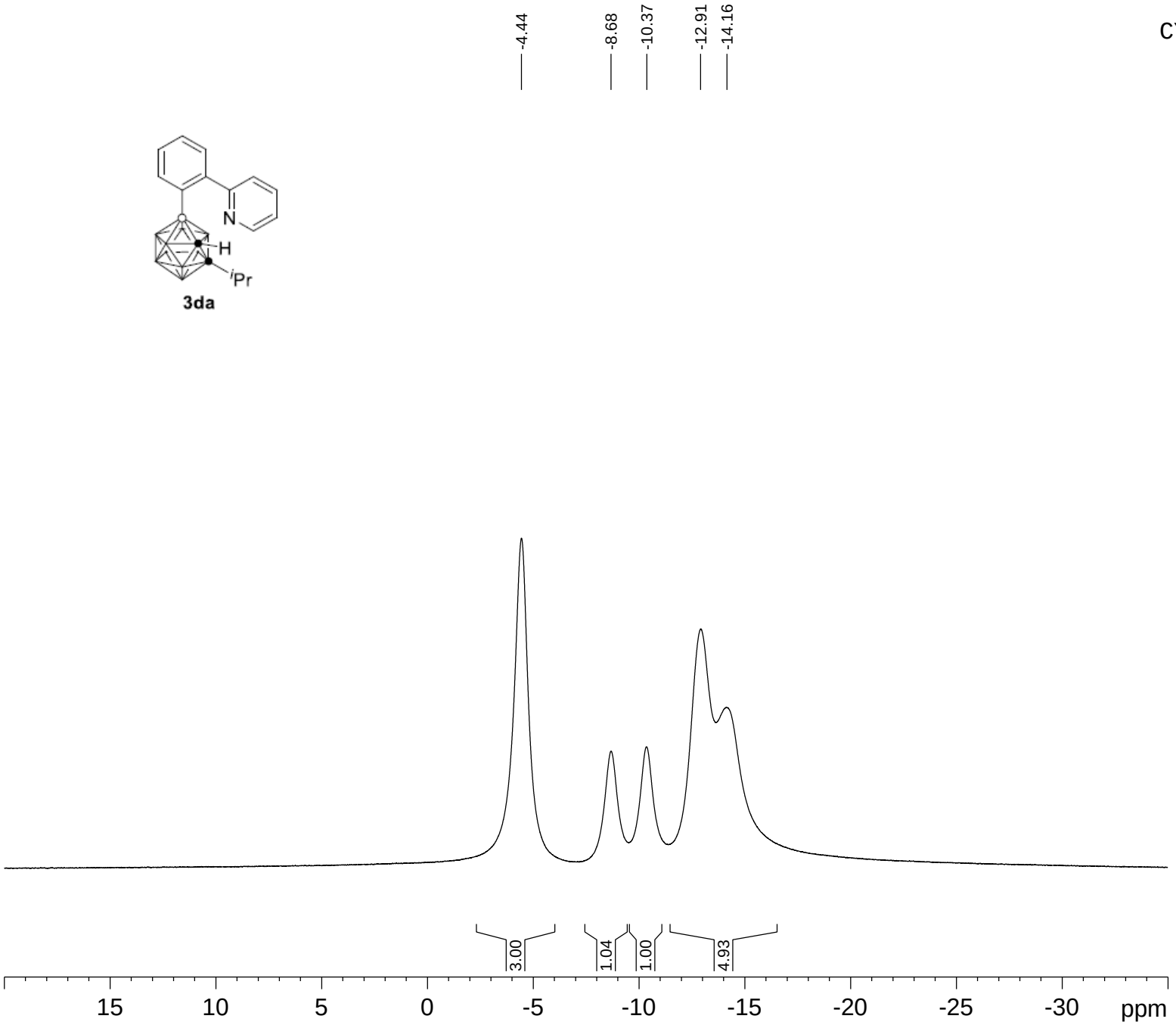
F2 - Processing parameters
SI 65536
SF 400.2300107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





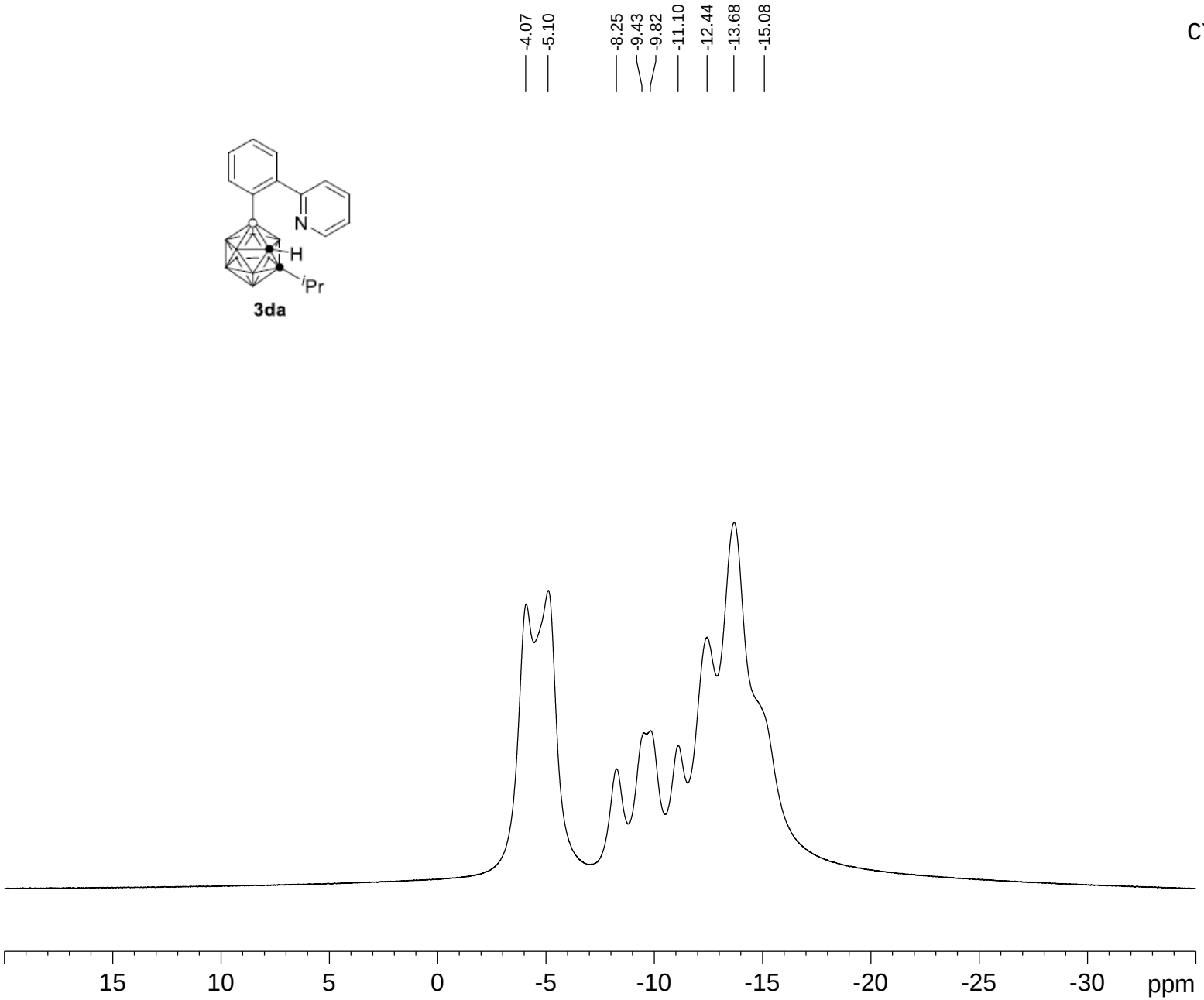
CY-C-A-75p

```
Current Data Parameters
NAME                 CY-C-A-75P
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20161121
Time                     17.38 h
INSTRUM                   spect
PROBHD    Z108618_0257 (
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                          76
DS                           4
SWH                  40760.871 Hz
FIDRES                0.621962 Hz
AQ                    0.8039083 sec
RG                         203
DW                      12.267 usec
DE                        6.50 usec
TE                       296.3 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                  100.6379056 MHz
WDW                         EM
SSB       0
LB                        1.00 Hz
GB        0
PC                        1.40
```



CY-B-A-75p-re2

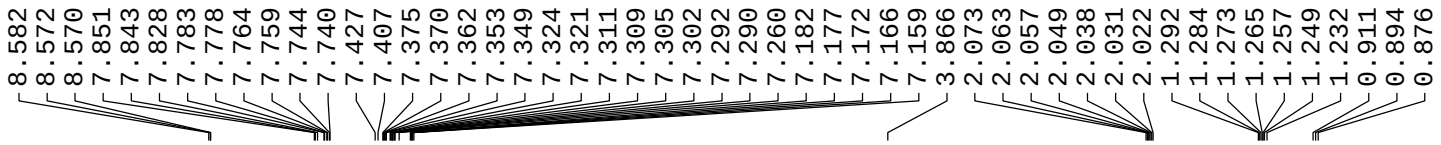
```
Current Data Parameters
NAME      CY-B-A-75p-re2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161121
Time               20.52 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    52
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   228
DW                20.800 usec
DE                 6.50 usec
TE                297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

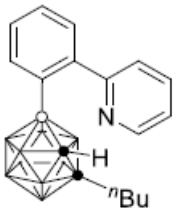


CY-B-A-75p-(C)-re2

```
Current Data Parameters
NAME      CY-B-A-75p-(C)-re2
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20161121
Time                 20.58 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                     228
DW                  20.800 usec
DE                   6.50 usec
TE                  296.5 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             128.4097881 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

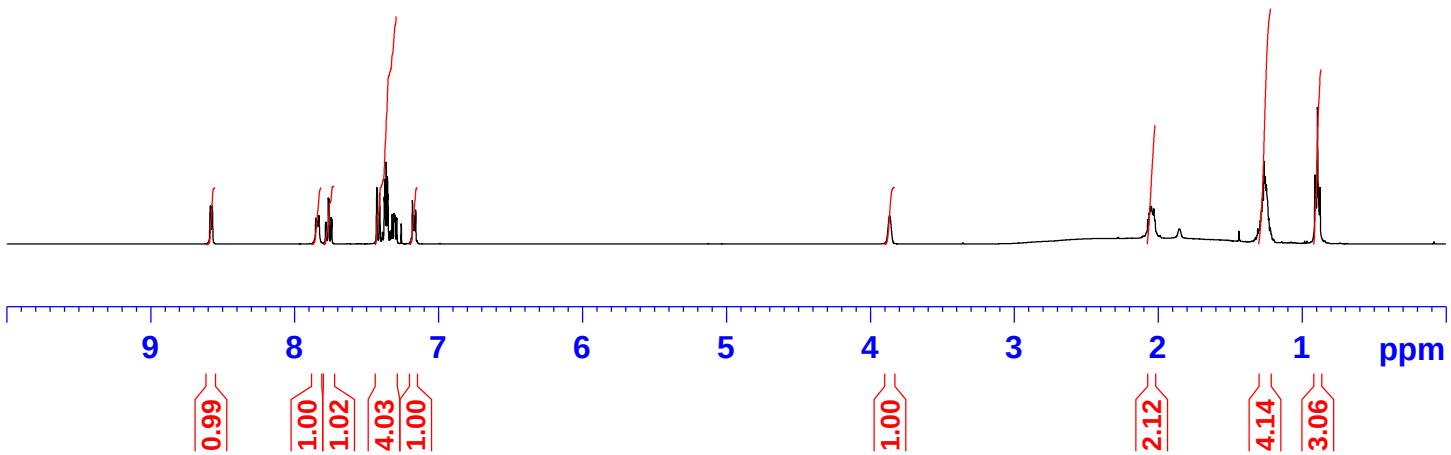
CY-H-A-74p-CDCl3

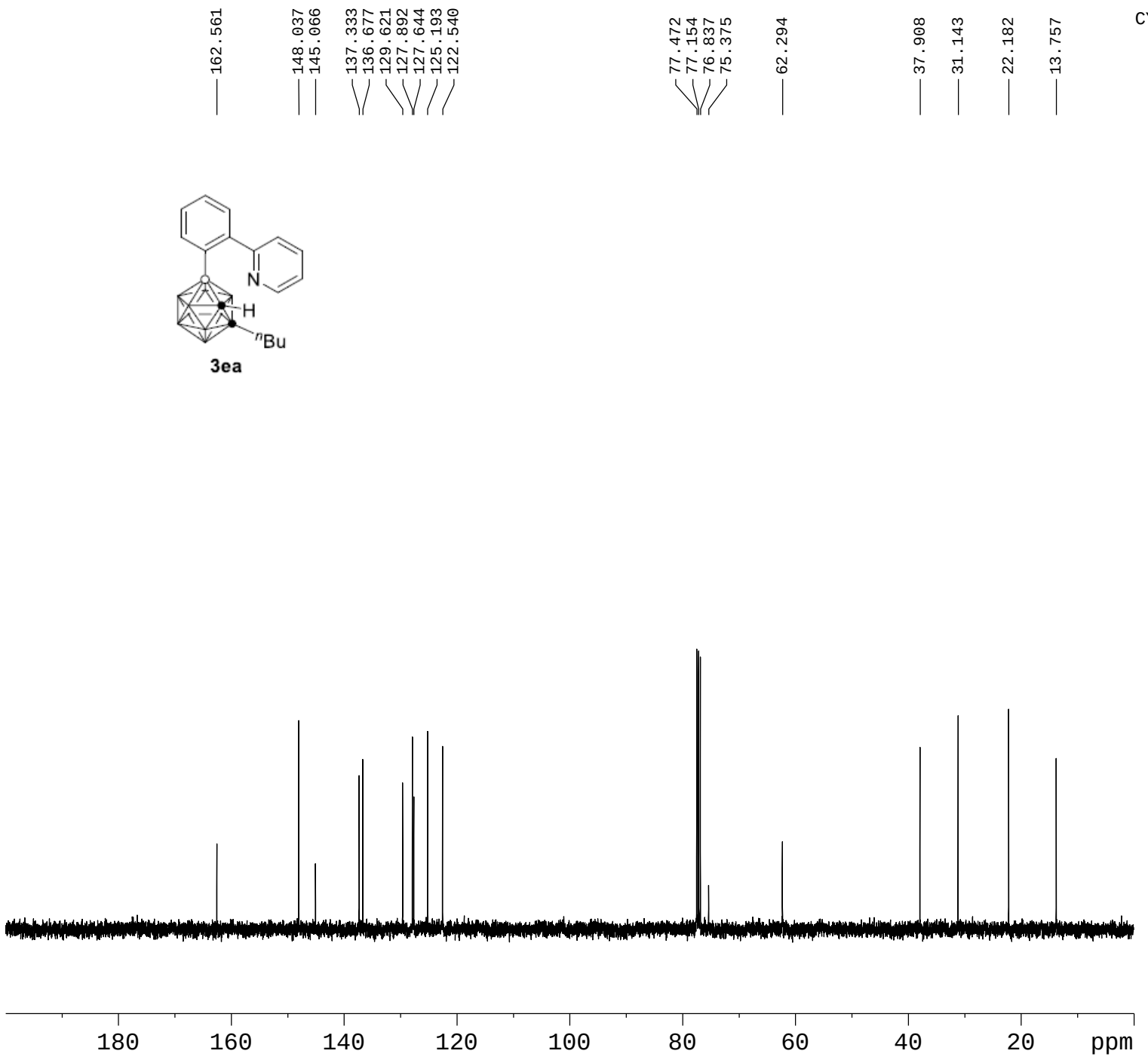




3ea

```
Current Data Parameters
NAME      CY-H-A-74p-CDCl3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20161121
Time              20.22 h
INSTRUM            spect
PROBHD    Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                  80.6
DW                62.400 usec
DE                 6.50 usec
TE                295.0 K
D1           1.00000000 sec
TD0                    1
SFO1        400.1324708 MHz
NUC1                  1H
P1                15.00 usec
PLW1          8.31000042 W

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





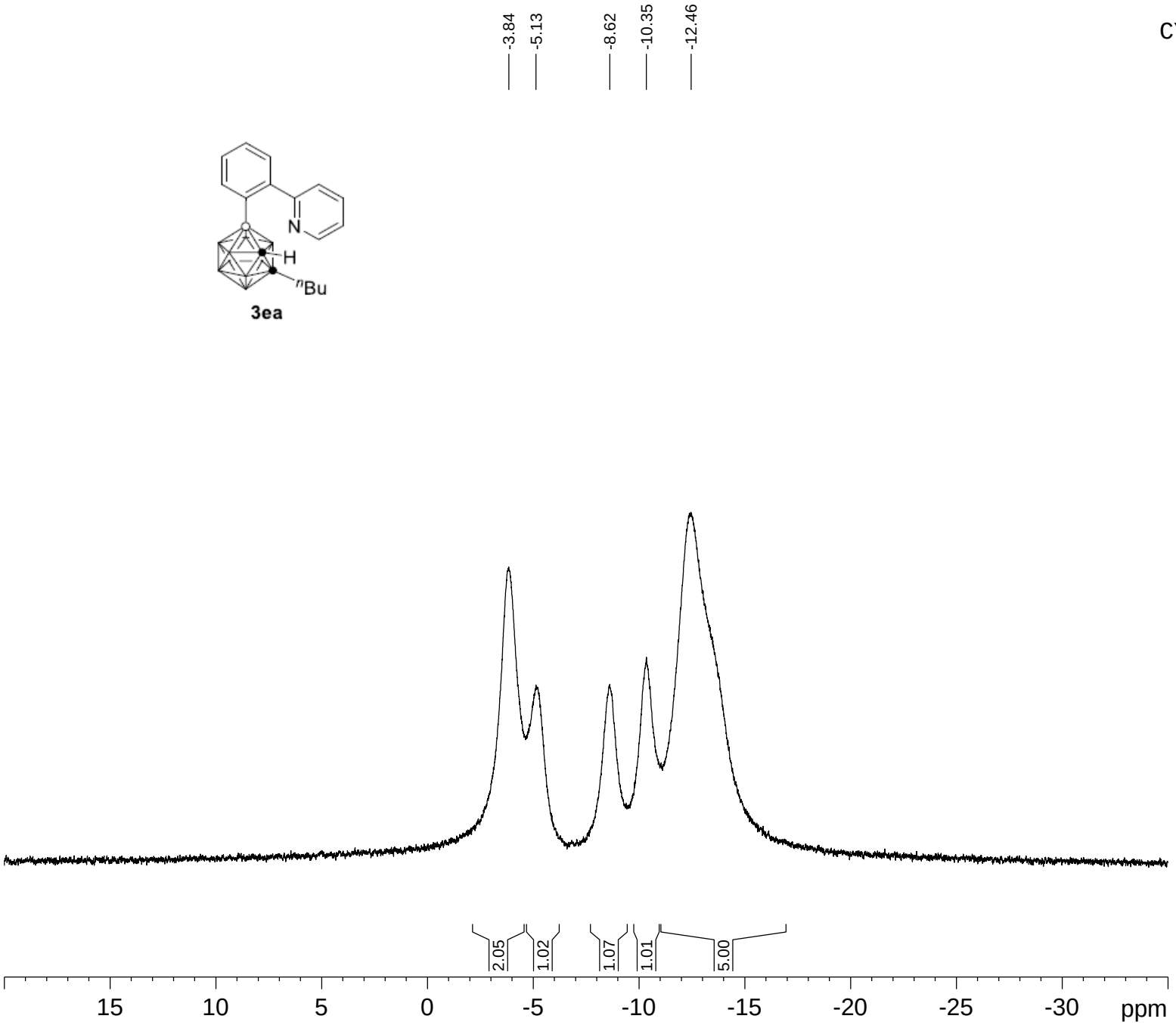
CY-C-A-75P-CDCl3-re

Bruker Advance III 400

Current Data Parameters
NAME CY-C-A-75P-CDCl3-re
EXPNO 1
PROCNO 1

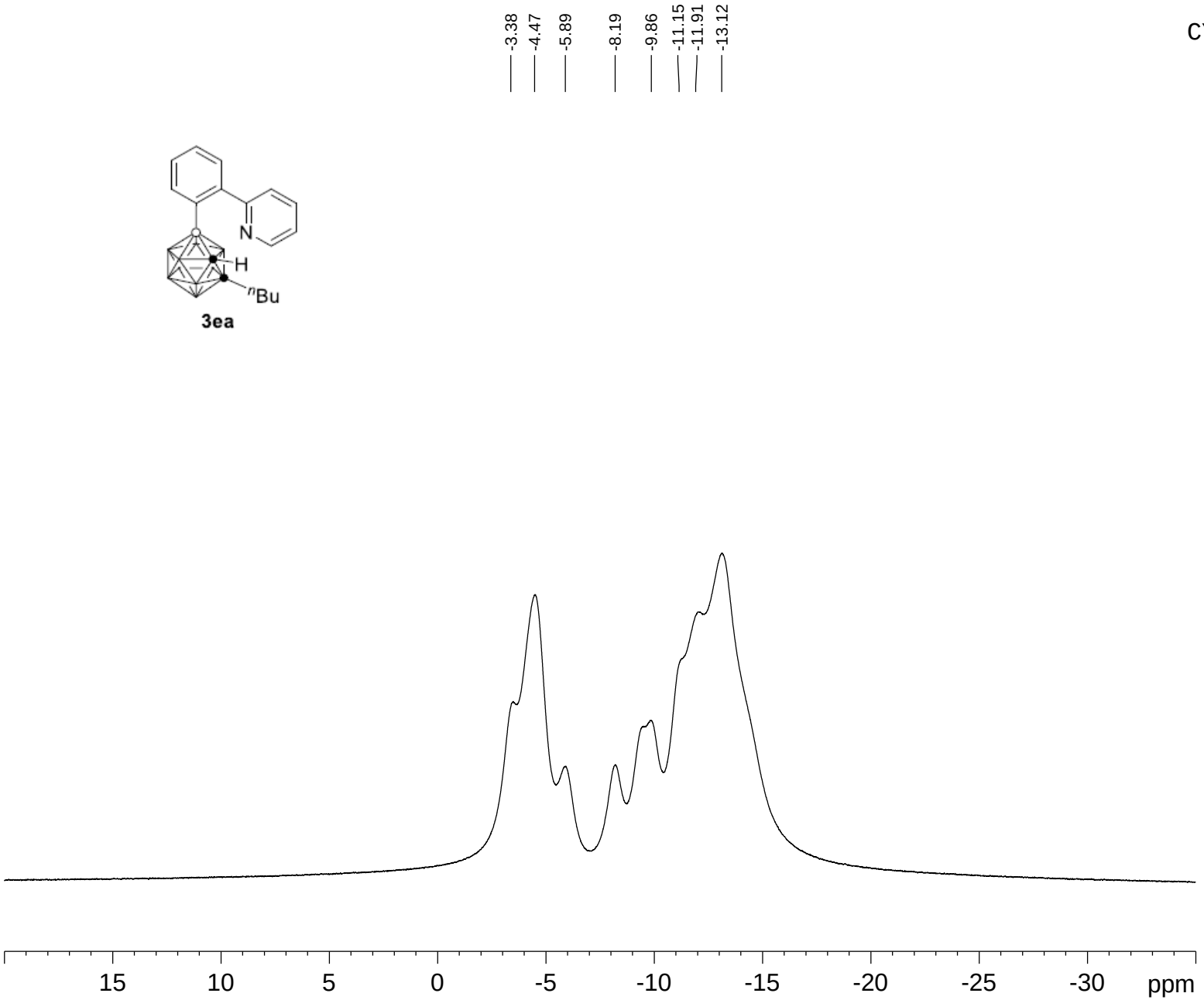
F2 - Acquisition Parameters
Date_ 20161121
Time 21.25 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
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 100.6127620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



CY-B-A-74p

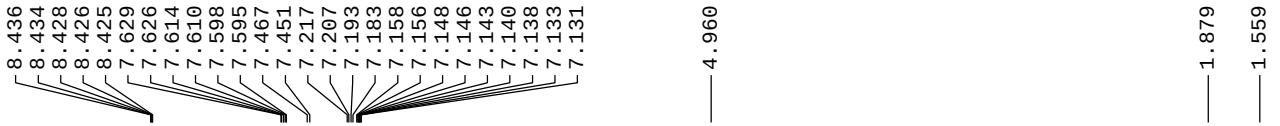
```
Current Data Parameters
NAME          CY-B-A-74p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20161121
Time               20.43 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                     1
DW                20.800 usec
DE                 6.50 usec
TE                296.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

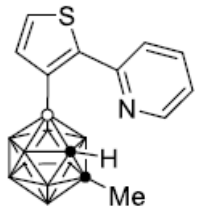


CY-B-A-74p-(C)-re2

```
Current Data Parameters
NAME      CY-B-A-74p-(C)-re2
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20161121
Time                 21.03 h
INSTRUM              spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      40
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     228
DW                  20.800 usec
DE                   6.50 usec
TE                  296.3 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            128.4097881 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

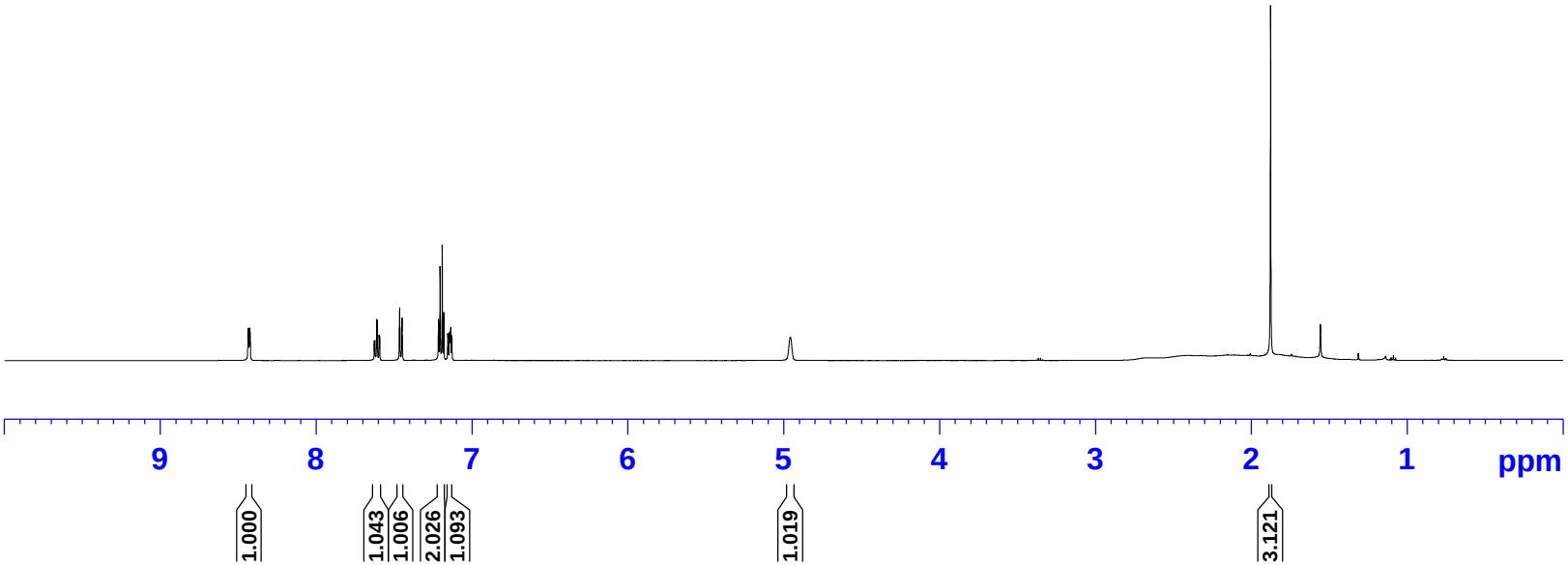
CY-H-A-162P



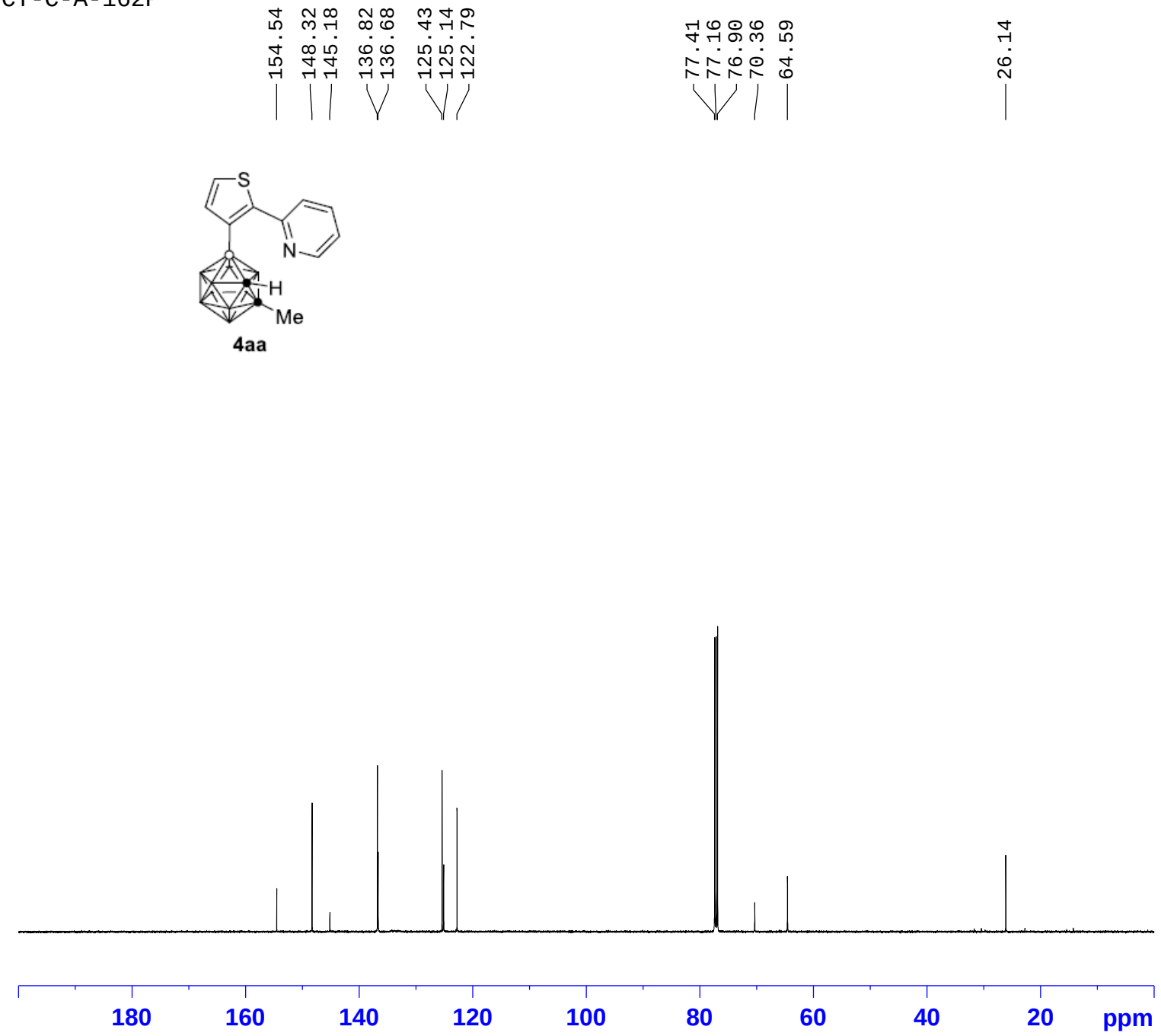


4aa

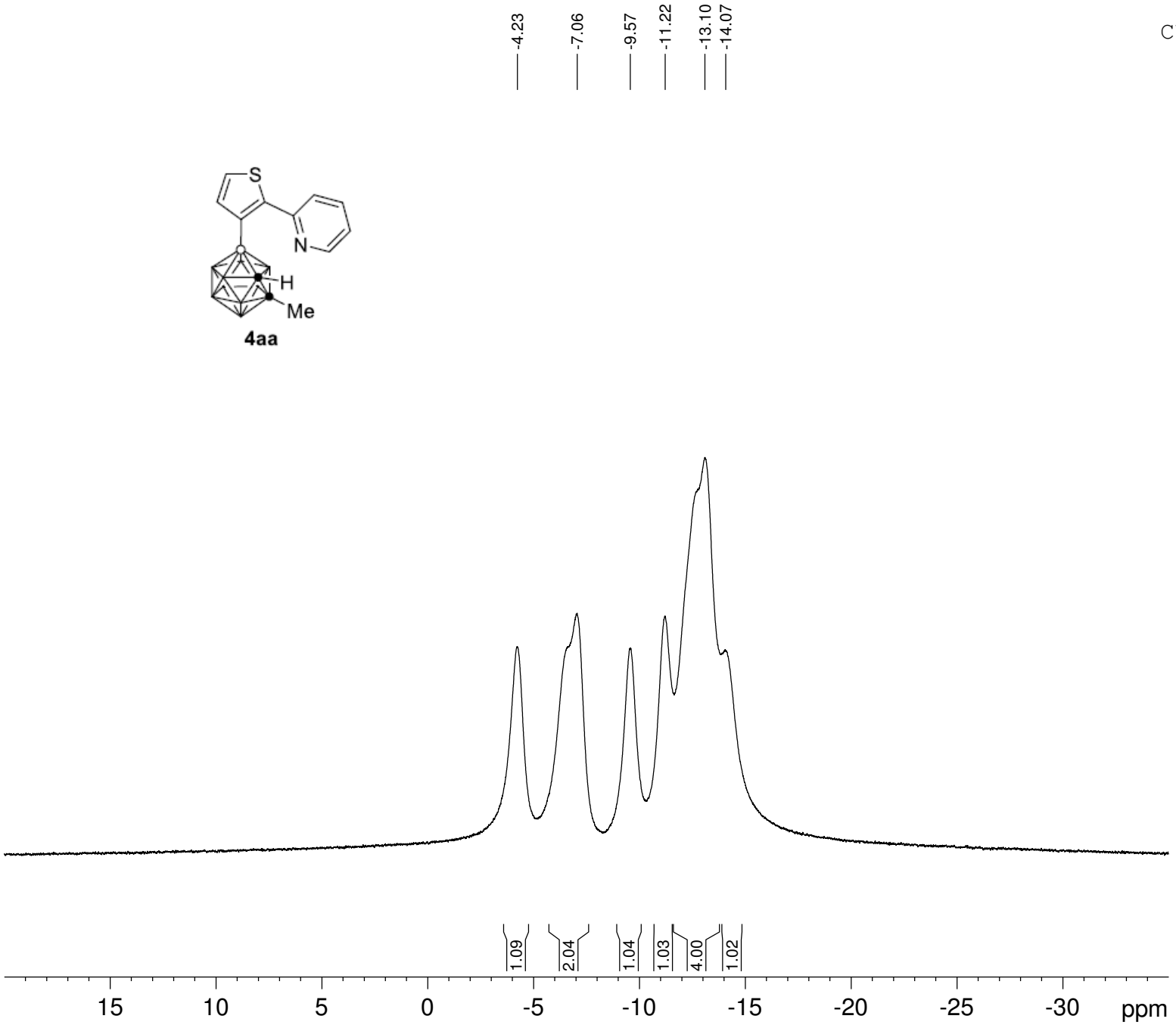
```
Current Data Parameters
NAME         CY-H-A-162P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170918
Time               18.34 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.305176 Hz
AQ             3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                10.00 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                12.00 usec
PLW1          15.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300733 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



CY-C-A-162P

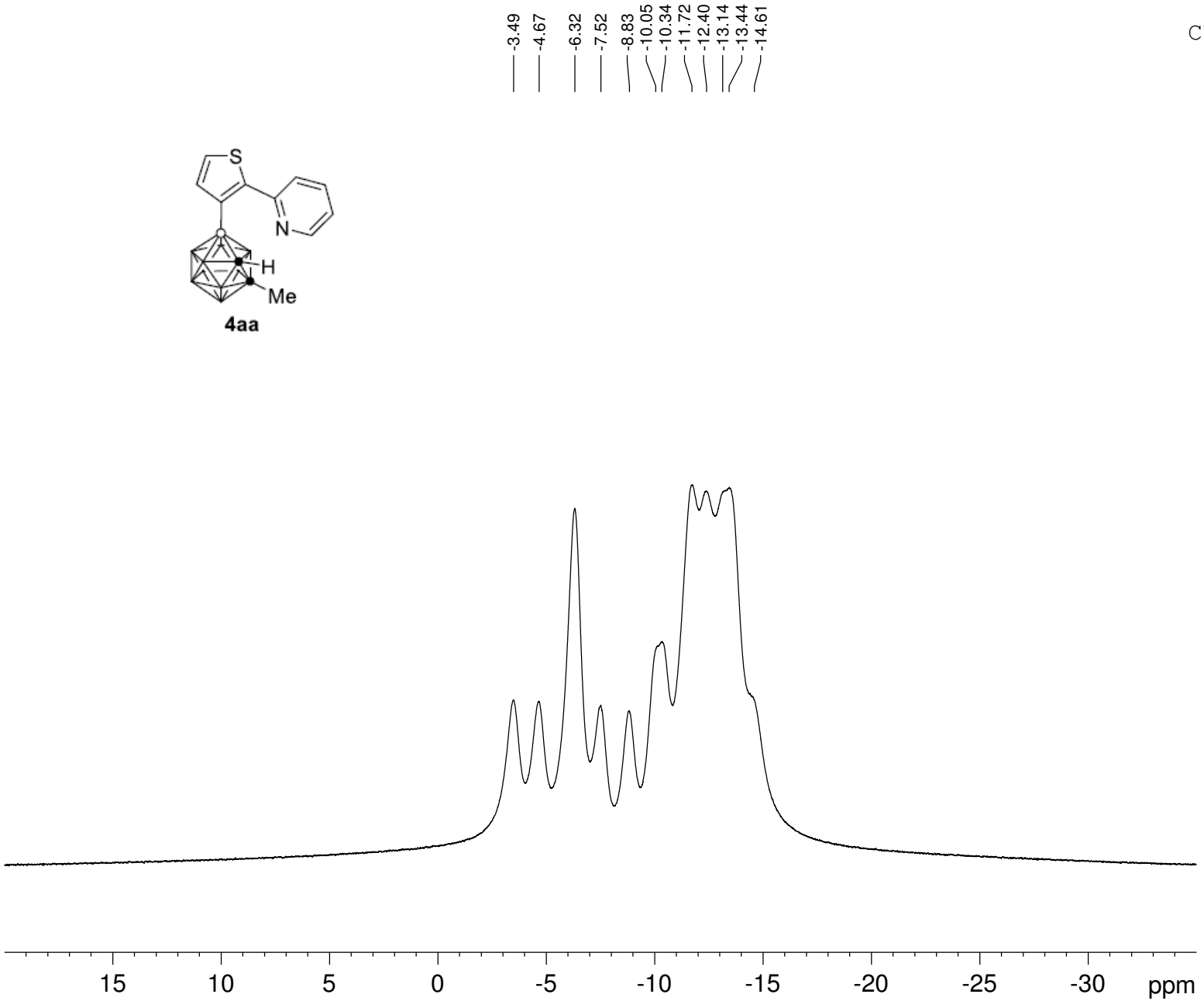



```
Current Data Parameters
NAME         CY-C-A-162P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170918
Time              18.47 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  176
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577767 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



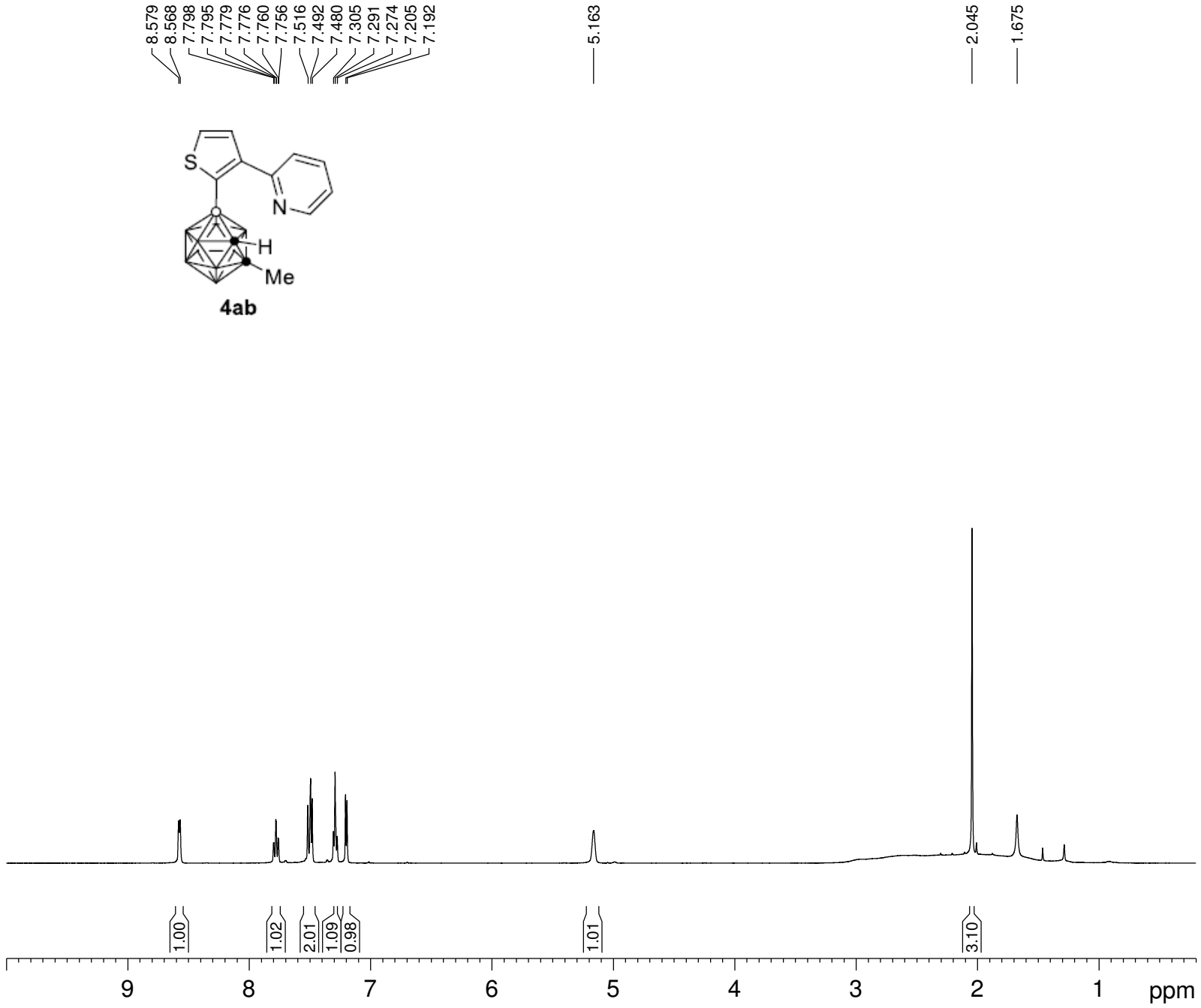
CY-B-A-162p

```
Current Data Parameters
NAME         CY-B-A-162p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170918
Time               18.54 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT          Acetone
NS                    12
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         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-162p-(C)

```
Current Data Parameters
NAME      CY-B-A-162p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170918
Time               18.58 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT          Acetone
NS                     48
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    181
DW                20.800 usec
DE                 6.50 usec
TE                294.6 K
D1           2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                 7.50 usec
PLW1         55.09999847 W

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



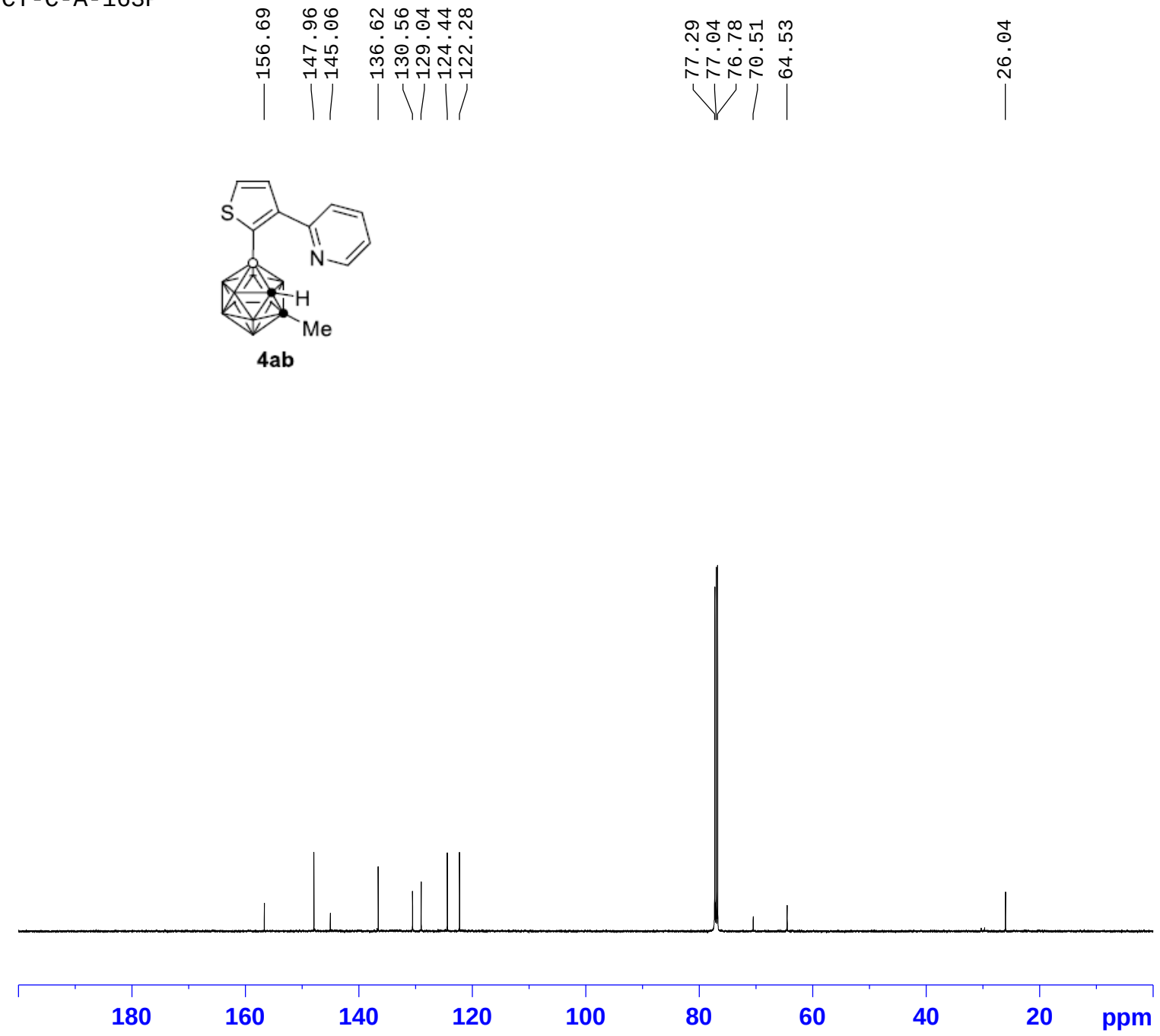
CY-H-A-163p-2

Current Data Parameters
NAME CY-H-A-163p-2
EXPNO 1
PROCNO 1

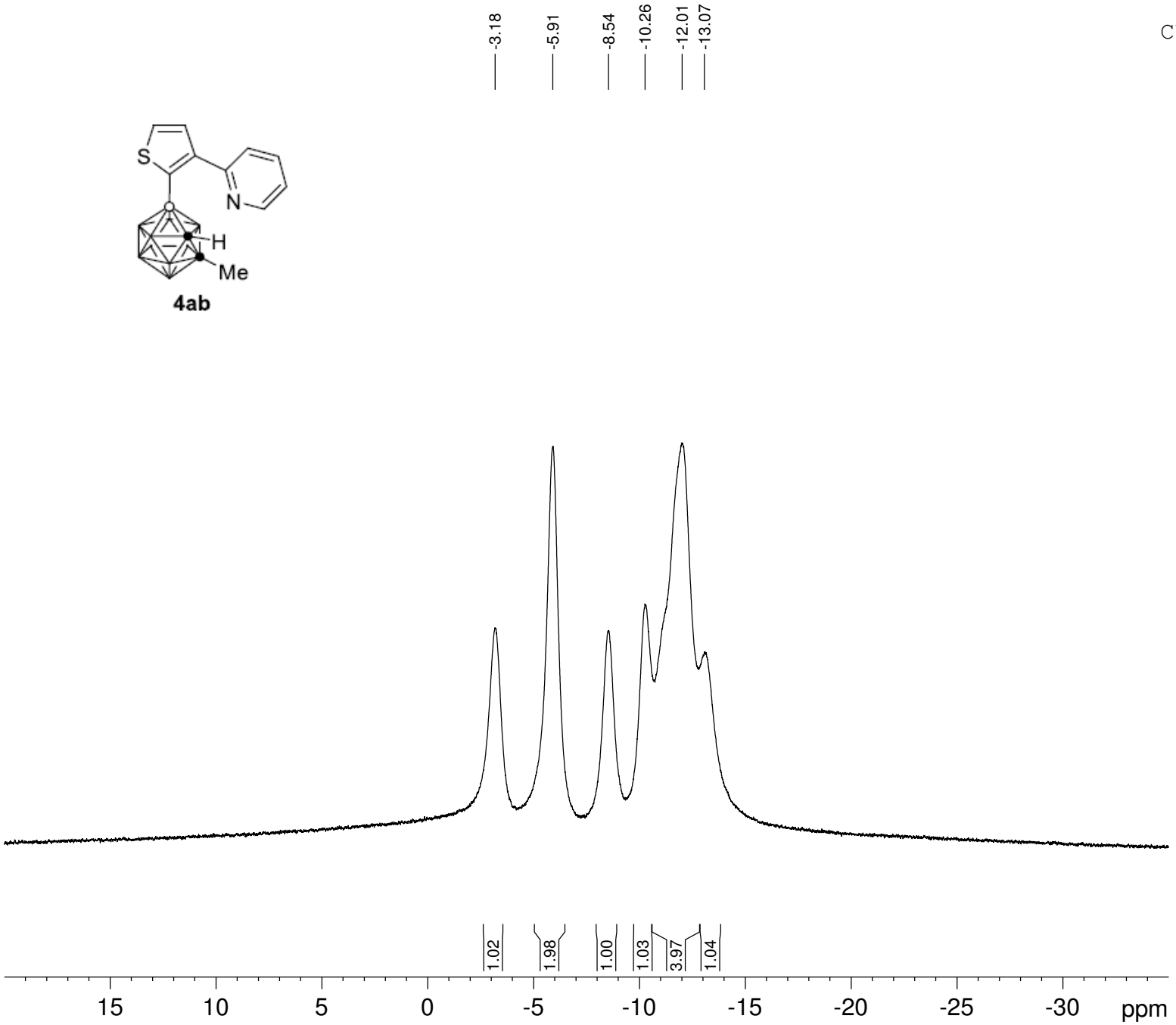
F2 - Acquisition Parameters
Date_ 20170921
Time 21.01 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2299969 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

CY-C-A-163P

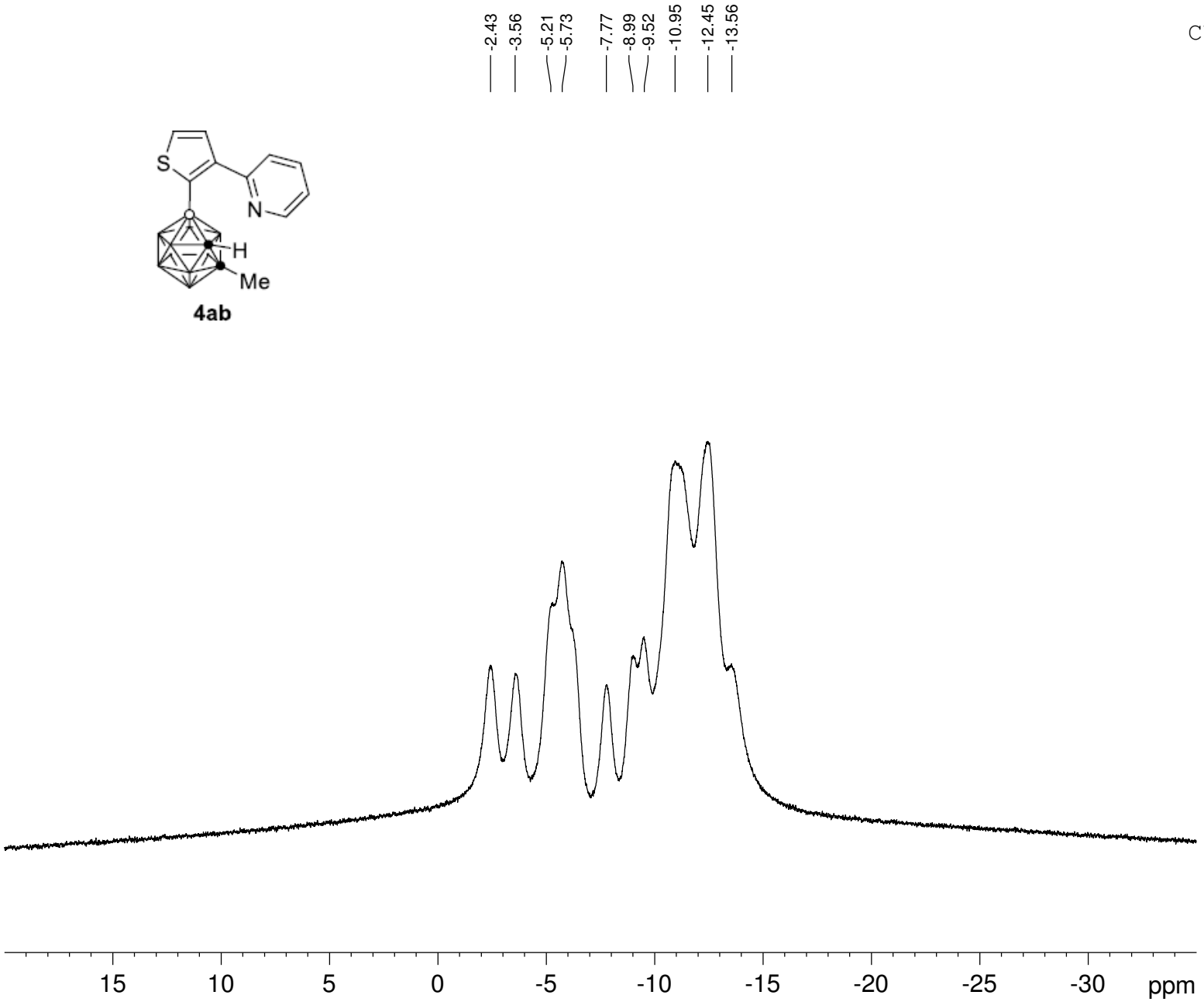



```
Current Data Parameters
NAME         CY-C-A-163P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170922
Time              10.16 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  240
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577885 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



CY-B-A-163p

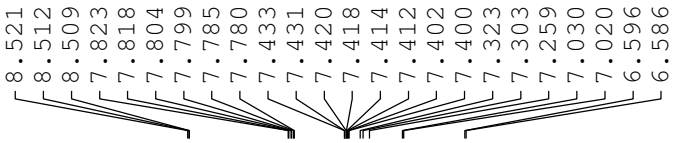
```
Current Data Parameters
NAME         CY-B-A-163p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170920
Time               17.02 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                   203
DW                20.800 usec
DE                 6.50 usec
TE                295.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1          55.09999847 W
SFO2          400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2          13.56000042 W
PLW12          0.27428001 W

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

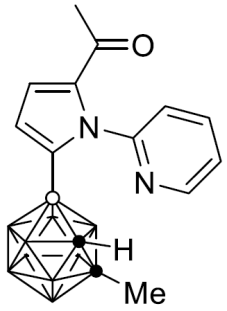


CY-B-A-163p-(C)

```
Current Data Parameters
NAME      CY-B-A-163p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170920
Time               17.03 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                295.1 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                 7.50 usec
PLW1         55.09999847 W

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

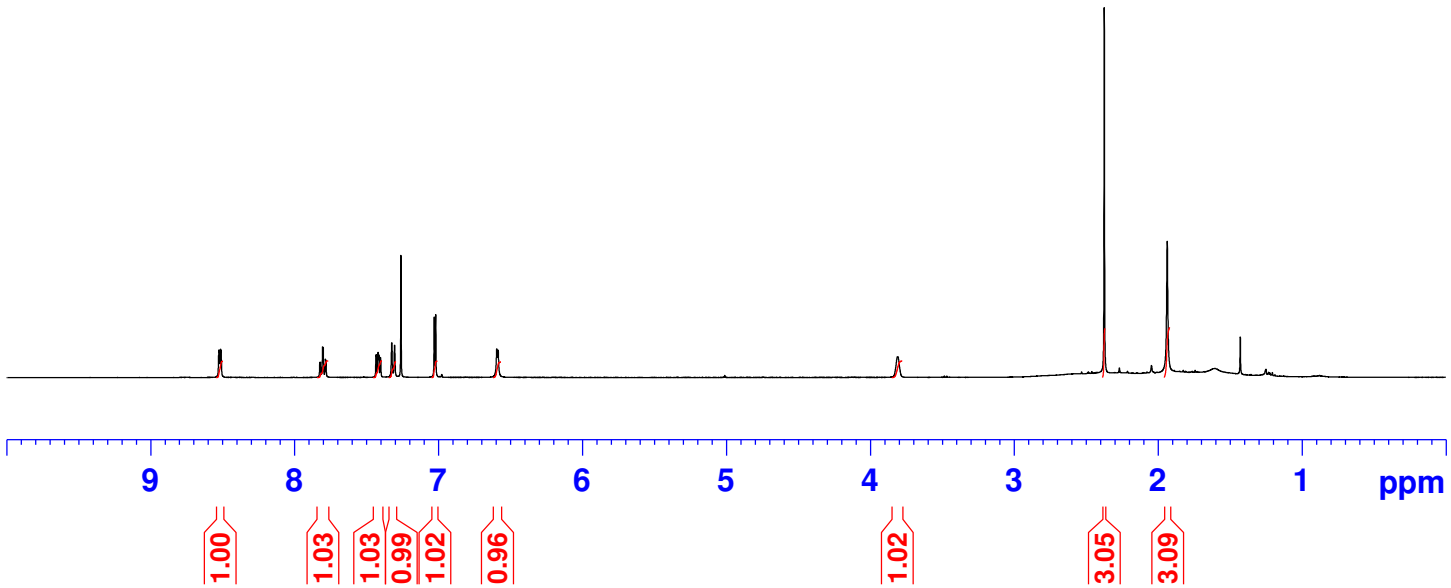
CY-H-A-77P-CDC

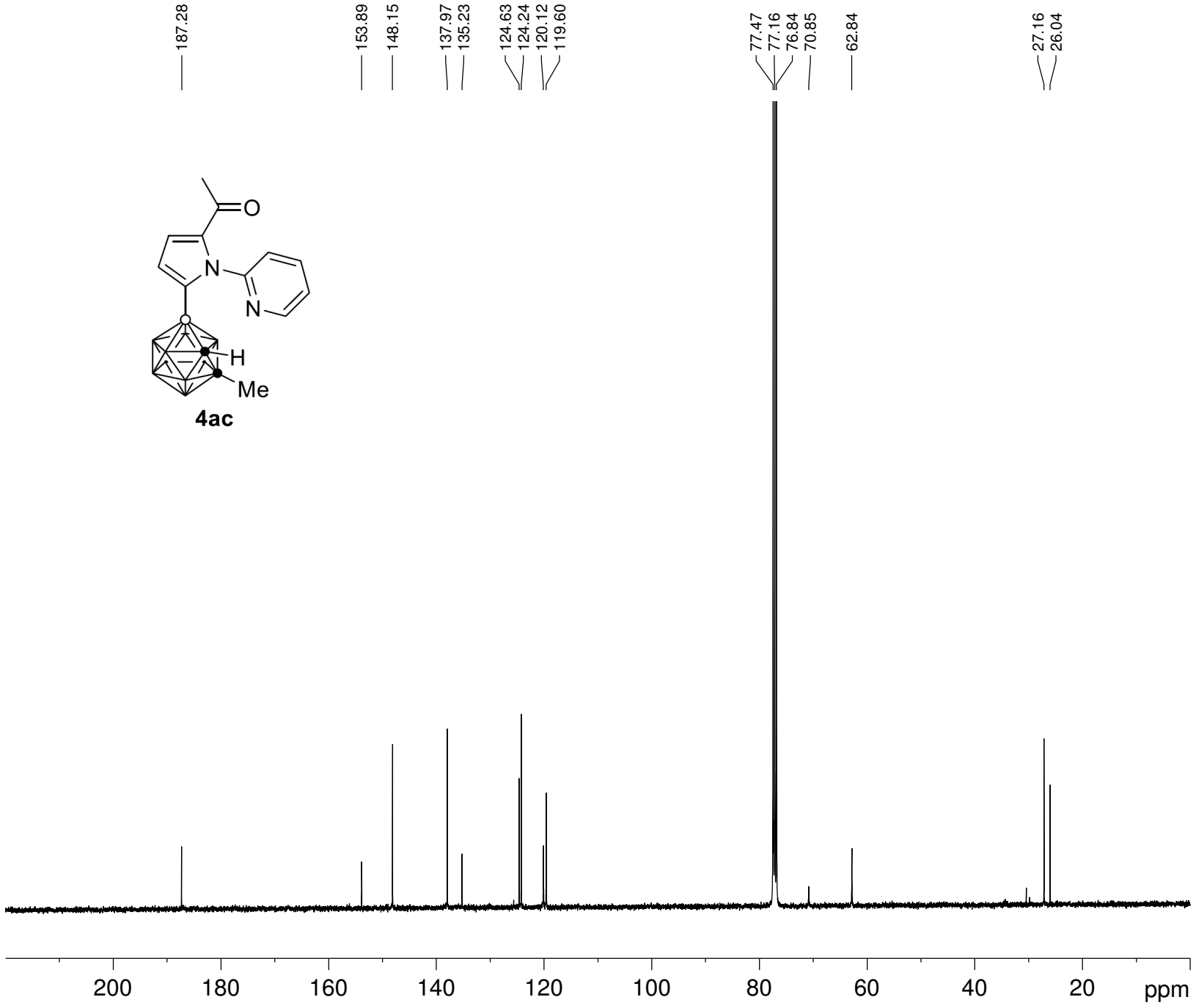




4ac

```
Current Data Parameters
NAME      CY-H-A-77P-CDC
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190805
Time               14.00 h
INSTRUM             spect
PROBHD   Z820201_0170 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                   203
DW                62.400 usec
DE                 6.50 usec
TE                295.9 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                  1H
P1                 6.75 usec
PLW1         13.17700005 W

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





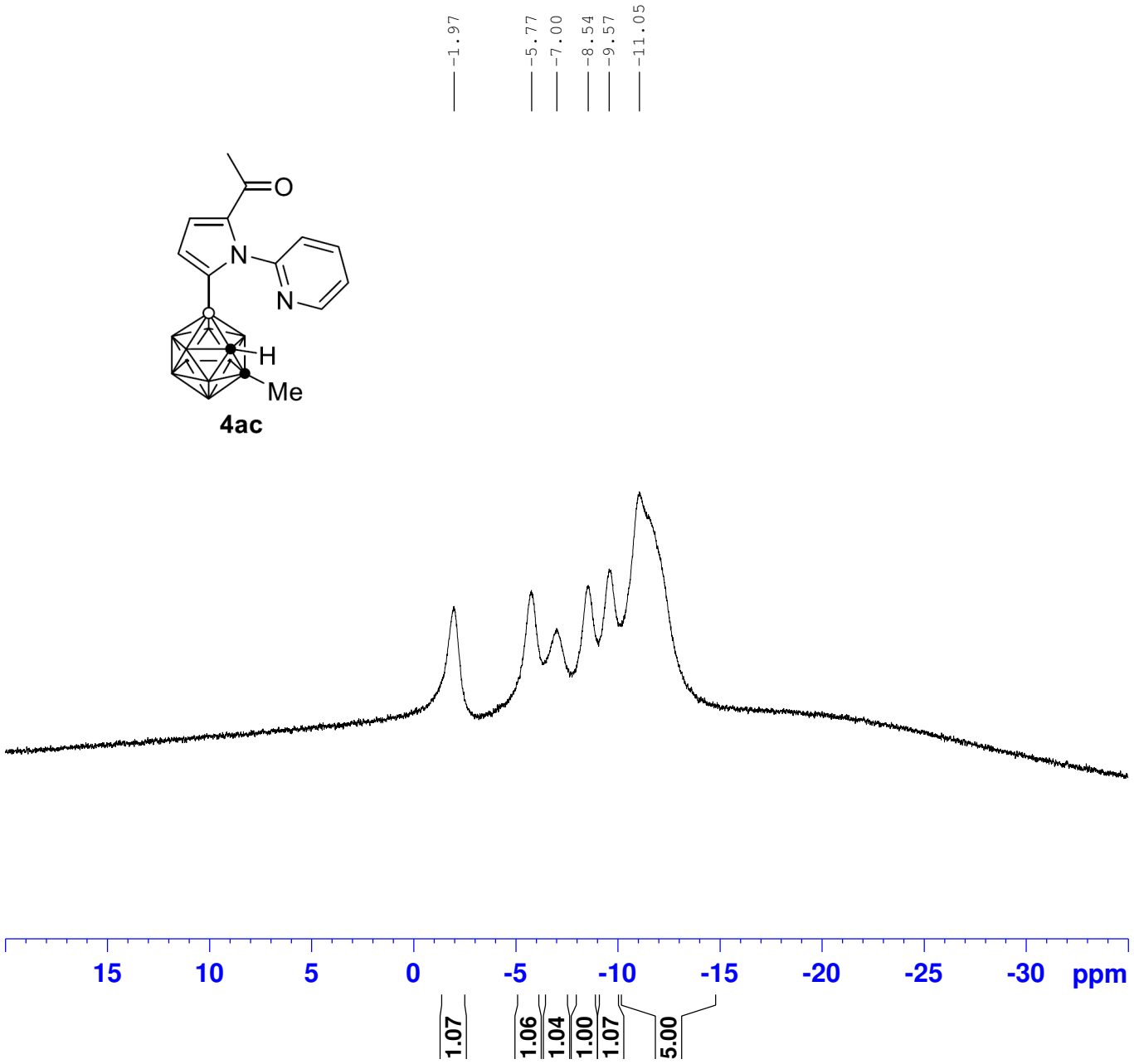
CY-C-A-77P-CDC

Current Data Parameters
NAME CY-C-A-77P-CDC
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190811
Time 18.21 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 12000
DS 4
SWH 40760.871 Hz
FIDRES 0.621962 Hz
AQ 0.8039083 sec
RG 203
DW 12.267 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6479773 MHz
NUC1 13C
P1 9.36 usec
PLW1 40.00000000 W
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.00000000 W
PLW12 0.20765001 W
PLW13 0.10445000 W

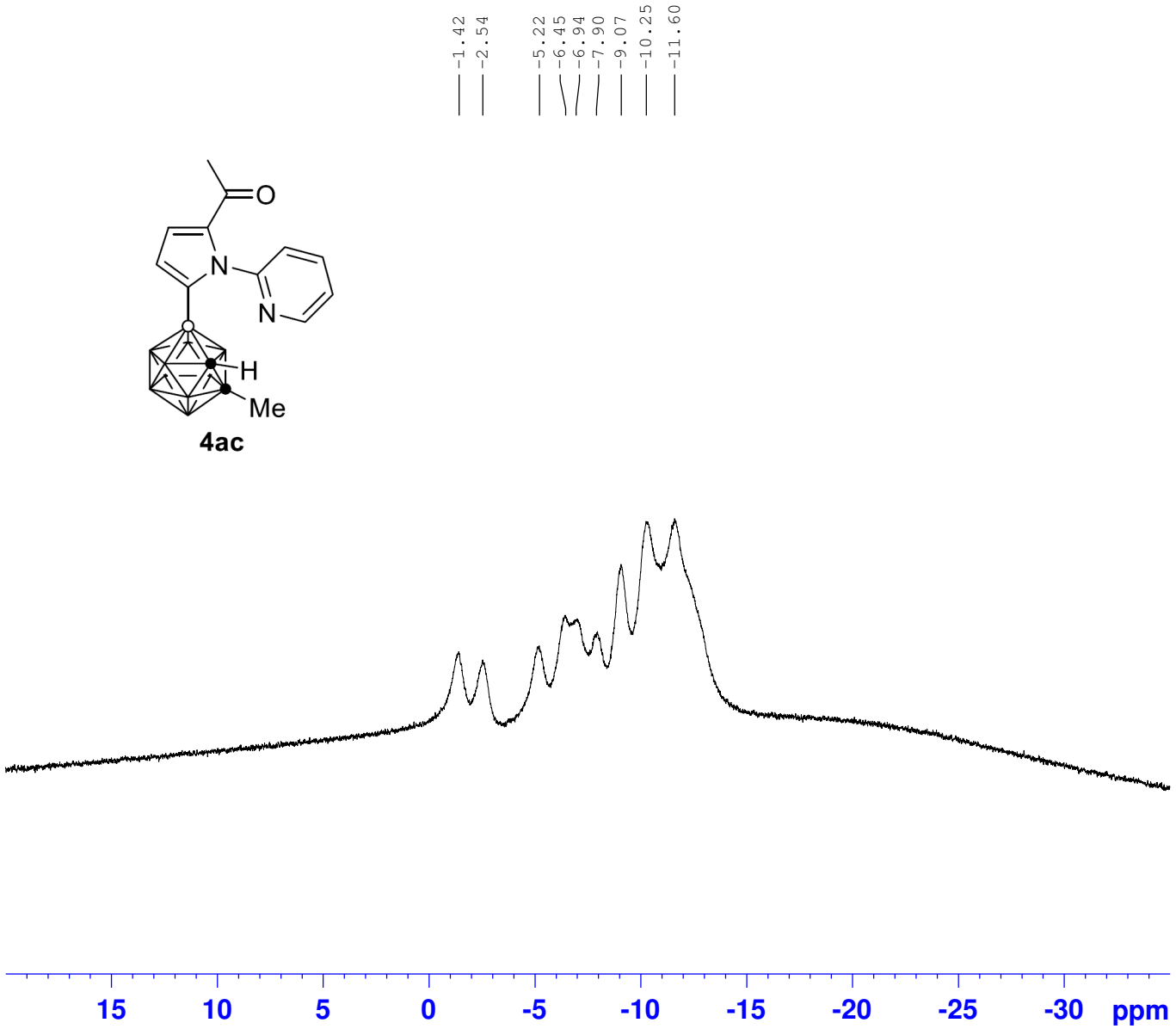
F2 - Processing parameters
SI 32768
SF 100.6379015 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CY-B-A-77P

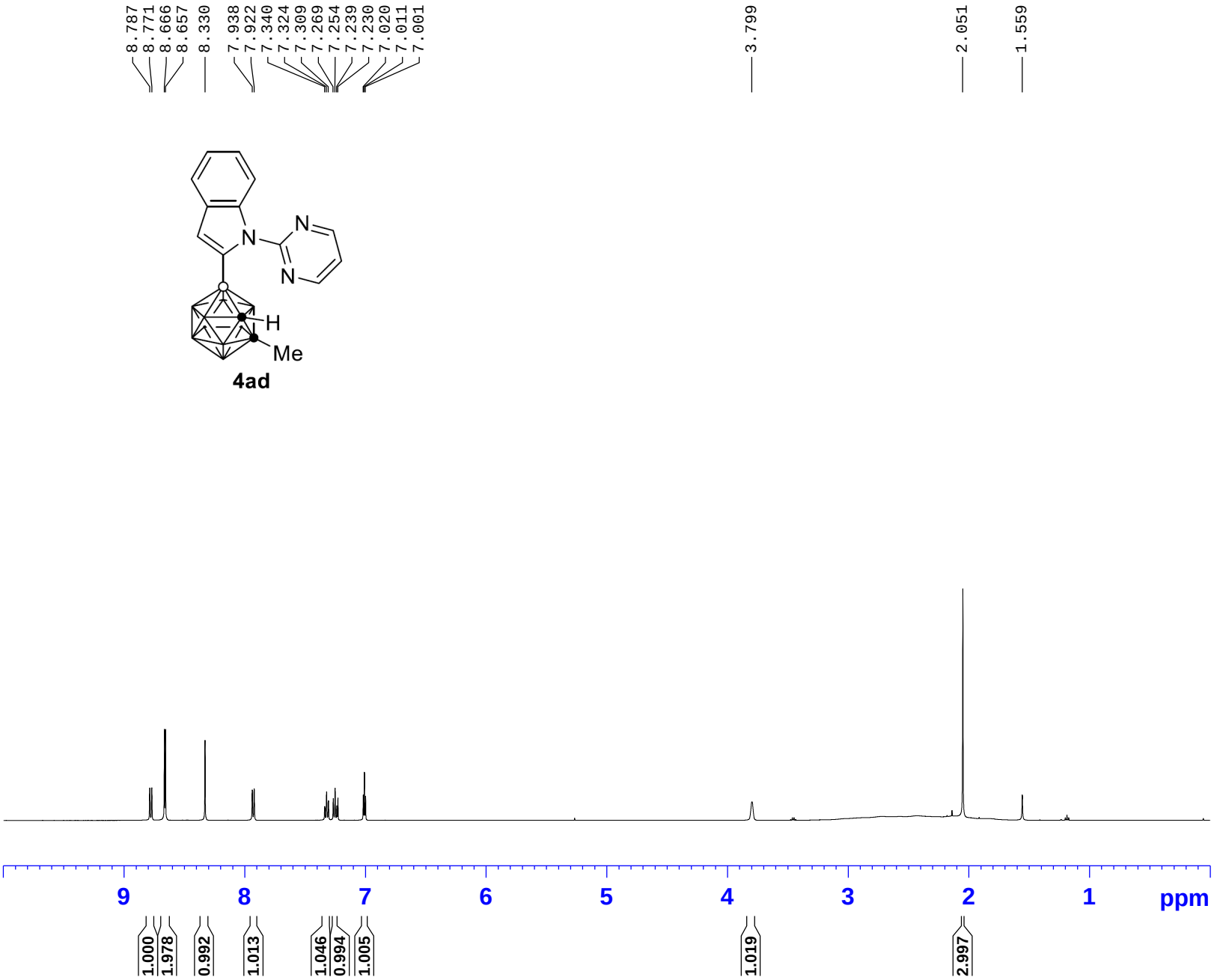



```
Current Data Parameters
NAME          CY-B-A-77P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190805
Time              14.03 h
INSTRUM             spect
PROBHD   Z820201_0170 (
PULPROG             zgig
TD                 65536
SOLVENT            CDCl3
NS                    40
DS                     4
SWH            25510.203 Hz
FIDRES          0.778510 Hz
AQ              1.2845056 sec
RG                   203
DW                19.600 usec
DE                 6.50 usec
TE                296.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.3776050 MHz
NUC1                 11B
P1                28.50 usec
PLW1         14.79100037 W
SFO2         400.1324710 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         13.17000008 W
PLW12         0.07408100 W

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

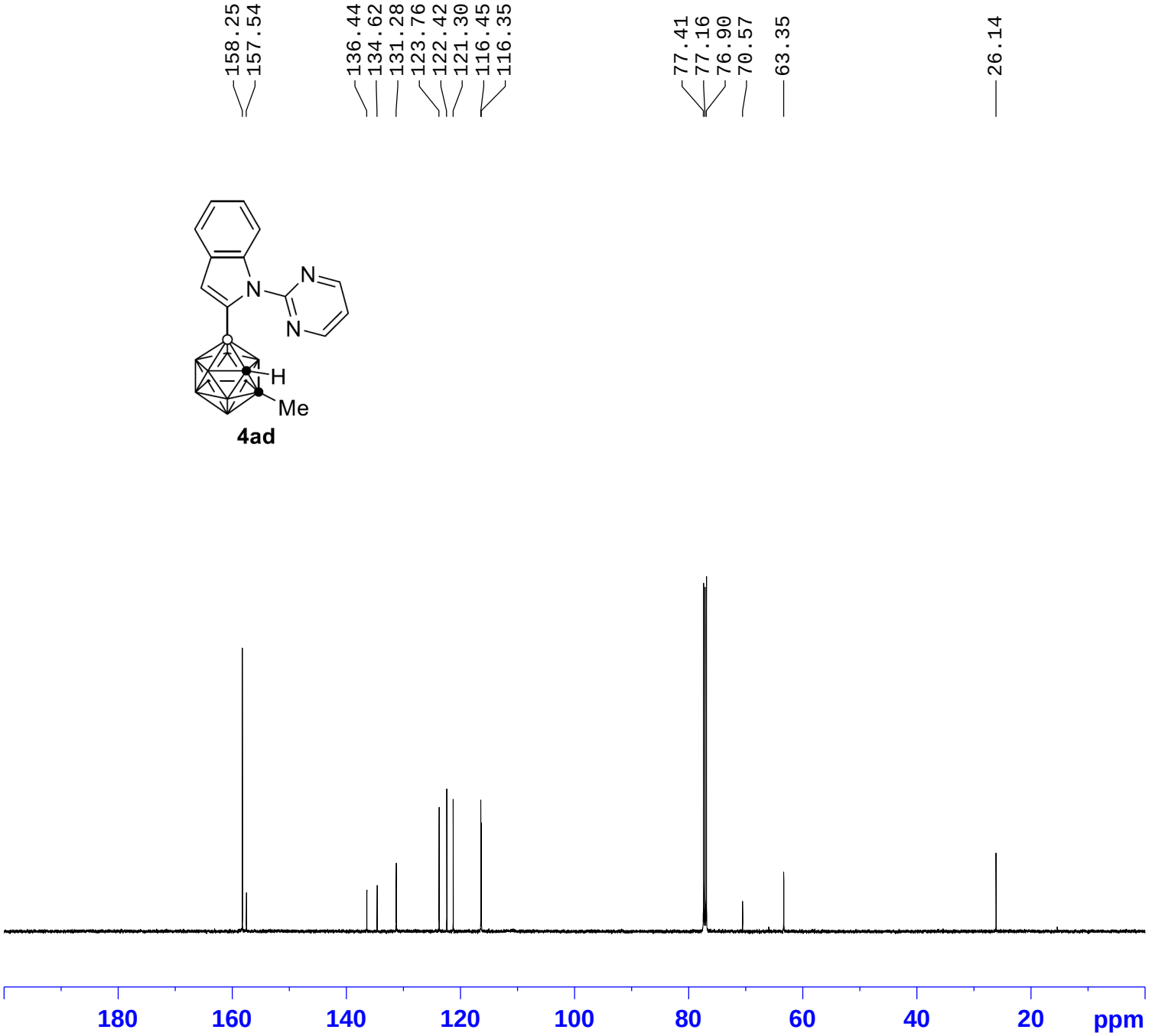
CY-B-A-77P-(C)



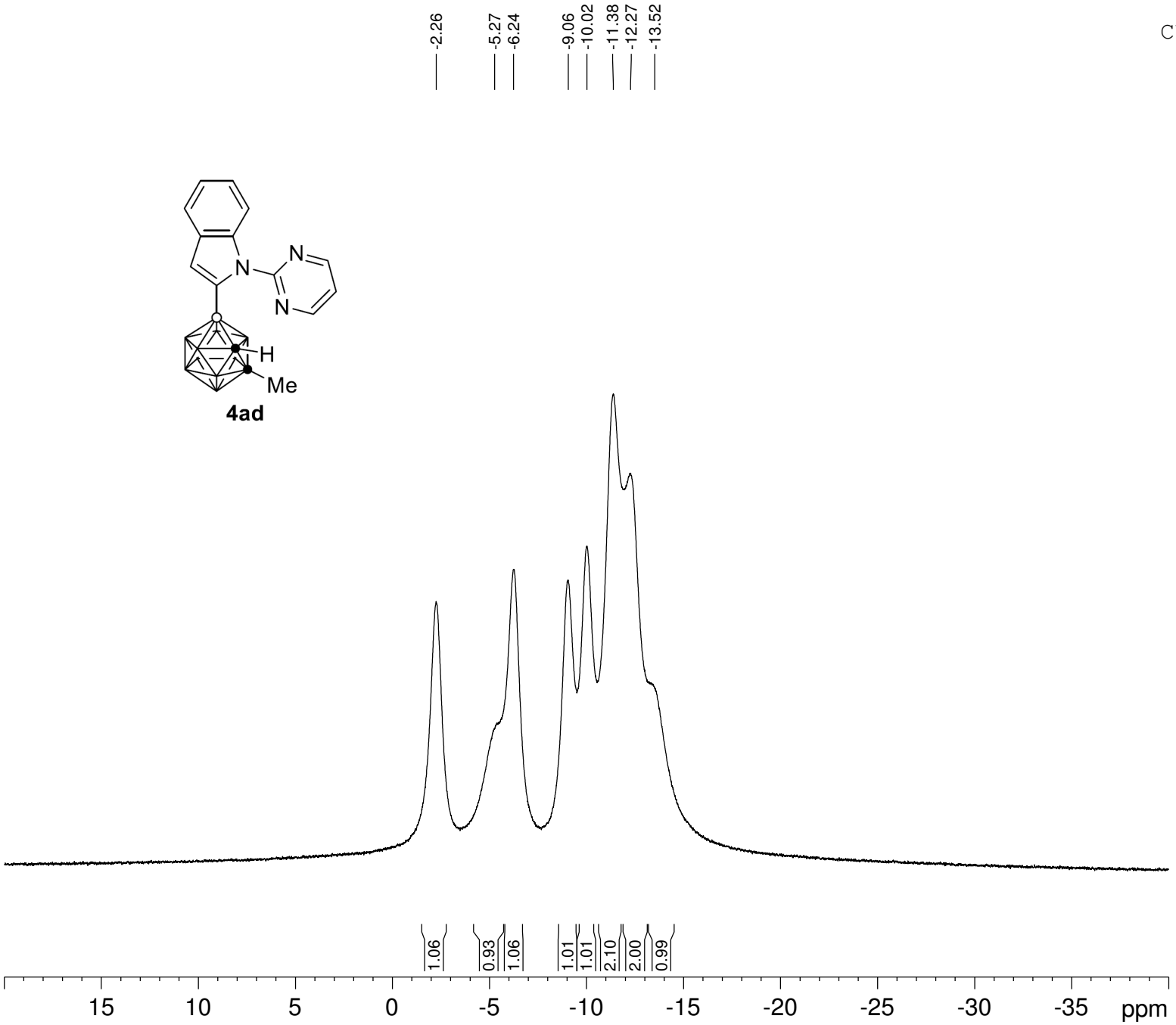

```
Current Data Parameters
NAME      CY-B-A-77P-(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190805
Time              14.06 h
INSTRUM             spect
PROBHD   Z820201_0170 (
PULPROG               zg
TD                 65536
SOLVENT            CDCl3
NS                    50
DS                     4
SWH            25510.203 Hz
FIDRES          0.778510 Hz
AQ              1.2845056 sec
RG                   203
DW                19.600 usec
DE                 6.50 usec
TE                295.9 K
D1           1.00000000 sec
TD0                    1
SFO1         128.3776050 MHz
NUC1                11B
P1                 28.50 usec
PLW1         14.79100037 W

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




```
Current Data Parameters
NAME         CY-H-A-169P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171012
Time               10.41 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.305176 Hz
AQ             3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                10.00 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                12.00 usec
PLW1          15.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300275 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

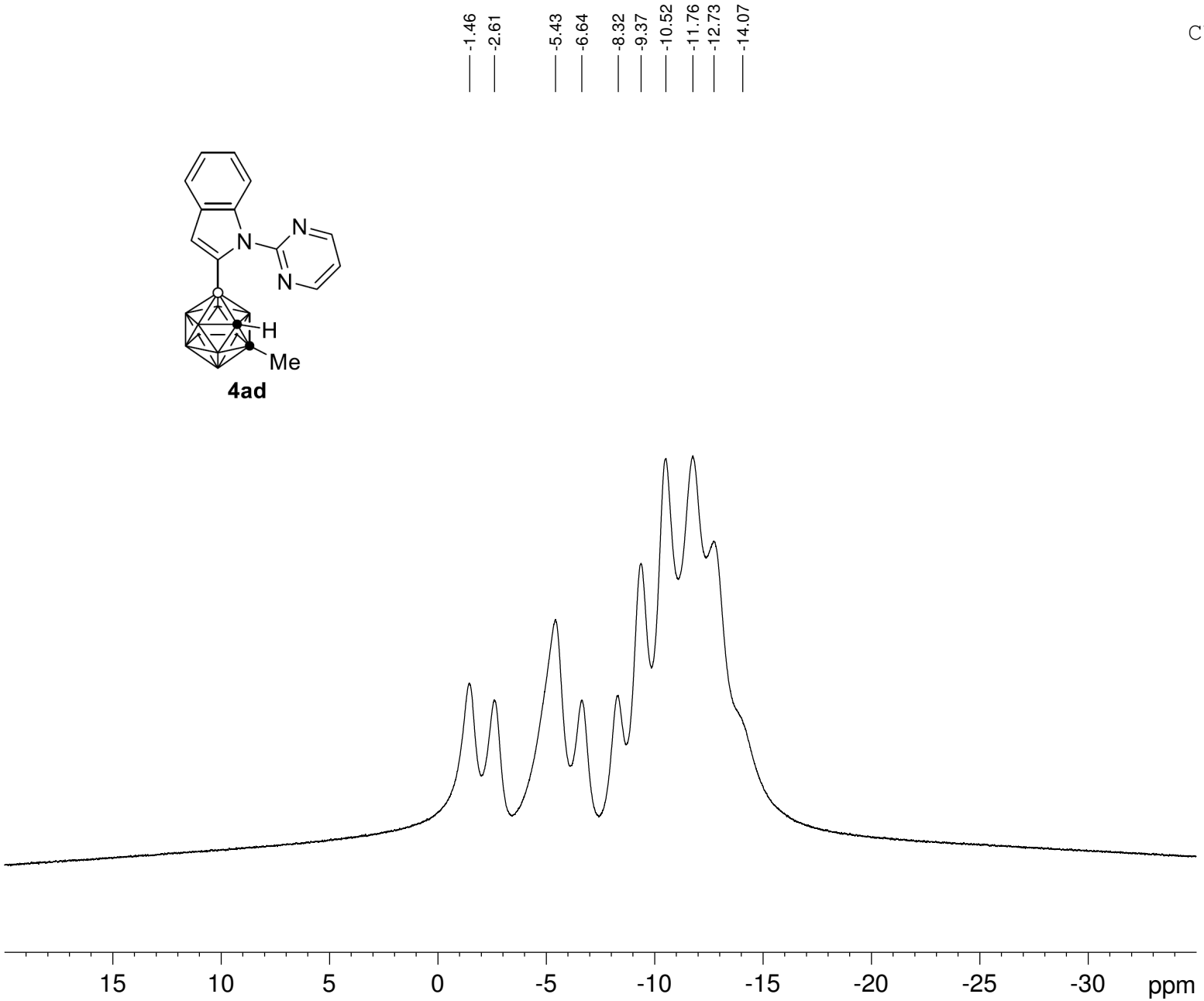



```
Current Data Parameters
NAME         CY-C-A-169P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171012
Time               10.48 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                     96
DS                      4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P1                10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W
PLW13         0.16976000 W

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



CY-B-A-169p

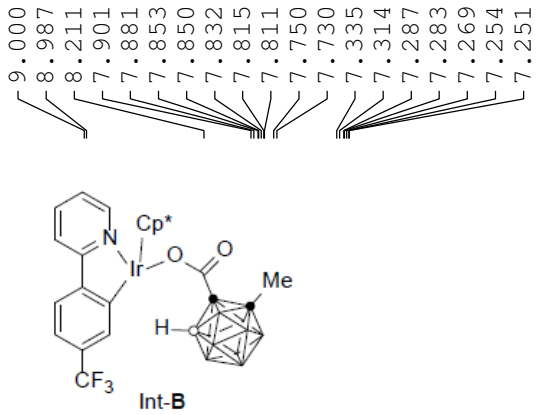
```
Current Data Parameters
NAME         CY-B-A-169p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171009
Time               15.15 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                   406
DW                20.800 usec
DE                 6.50 usec
TE                295.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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

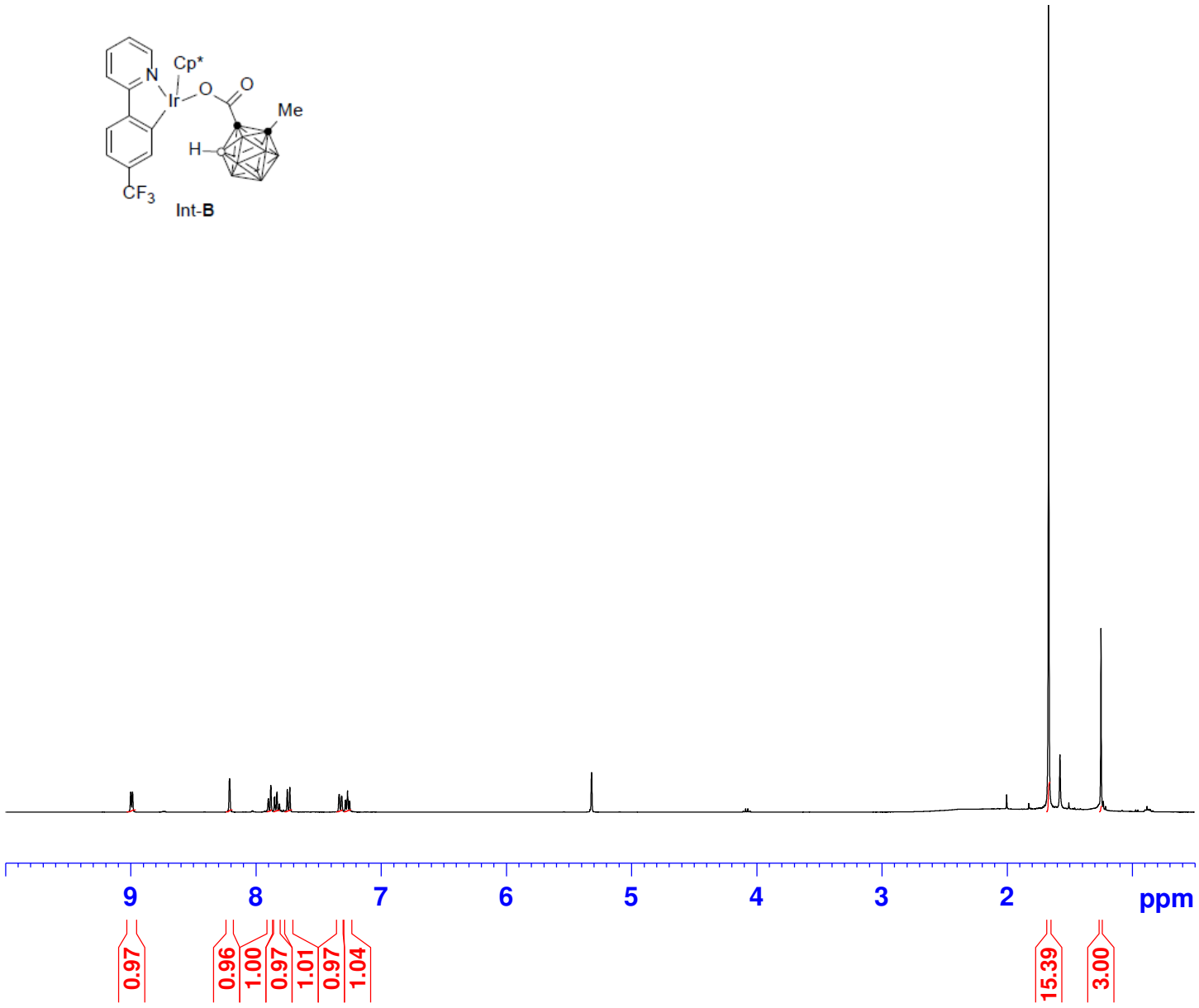


CY-B-A-169p-(C)

```
Current Data Parameters
NAME      CY-B-A-169p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171009
Time               15.17 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                   22
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  406
DW               20.800 usec
DE                6.50 usec
TE               294.6 K
D1            2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

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

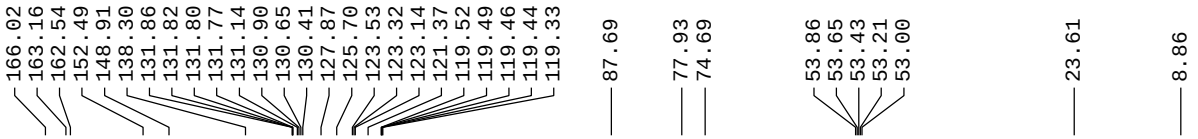
CY-H-B-164p

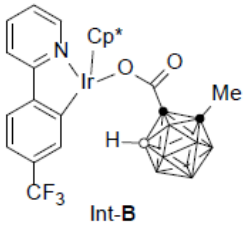




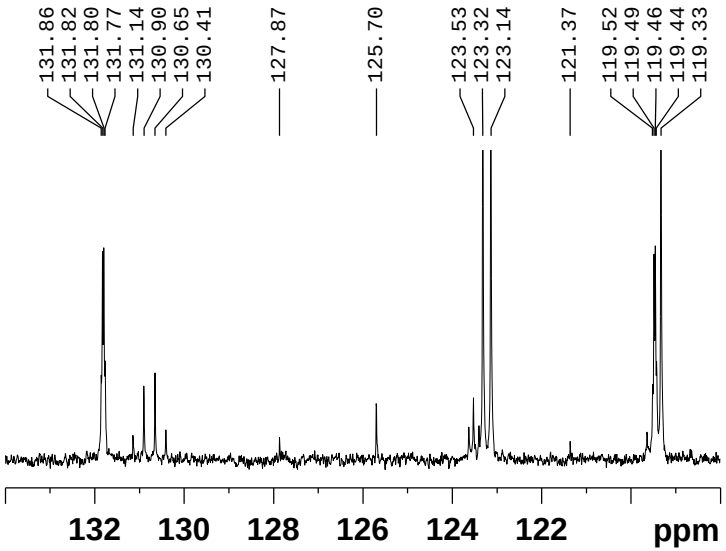

```
Current Data Parameters
NAME         CY-H-B-164p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180604
Time               21.43 h
INSTRUM             spect
PROBHD   Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ             4.0894465 sec
RG                   203
DW                62.400 usec
DE                 6.50 usec
TE                297.1 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          400.1300155 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

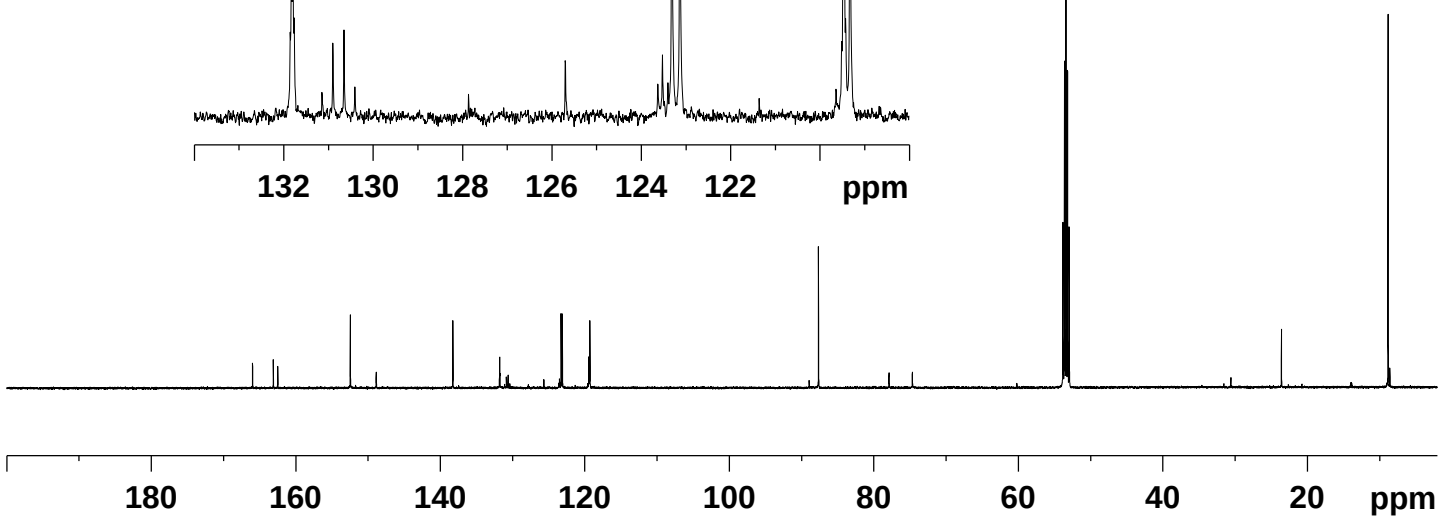
CY-C-B-164P-Ir



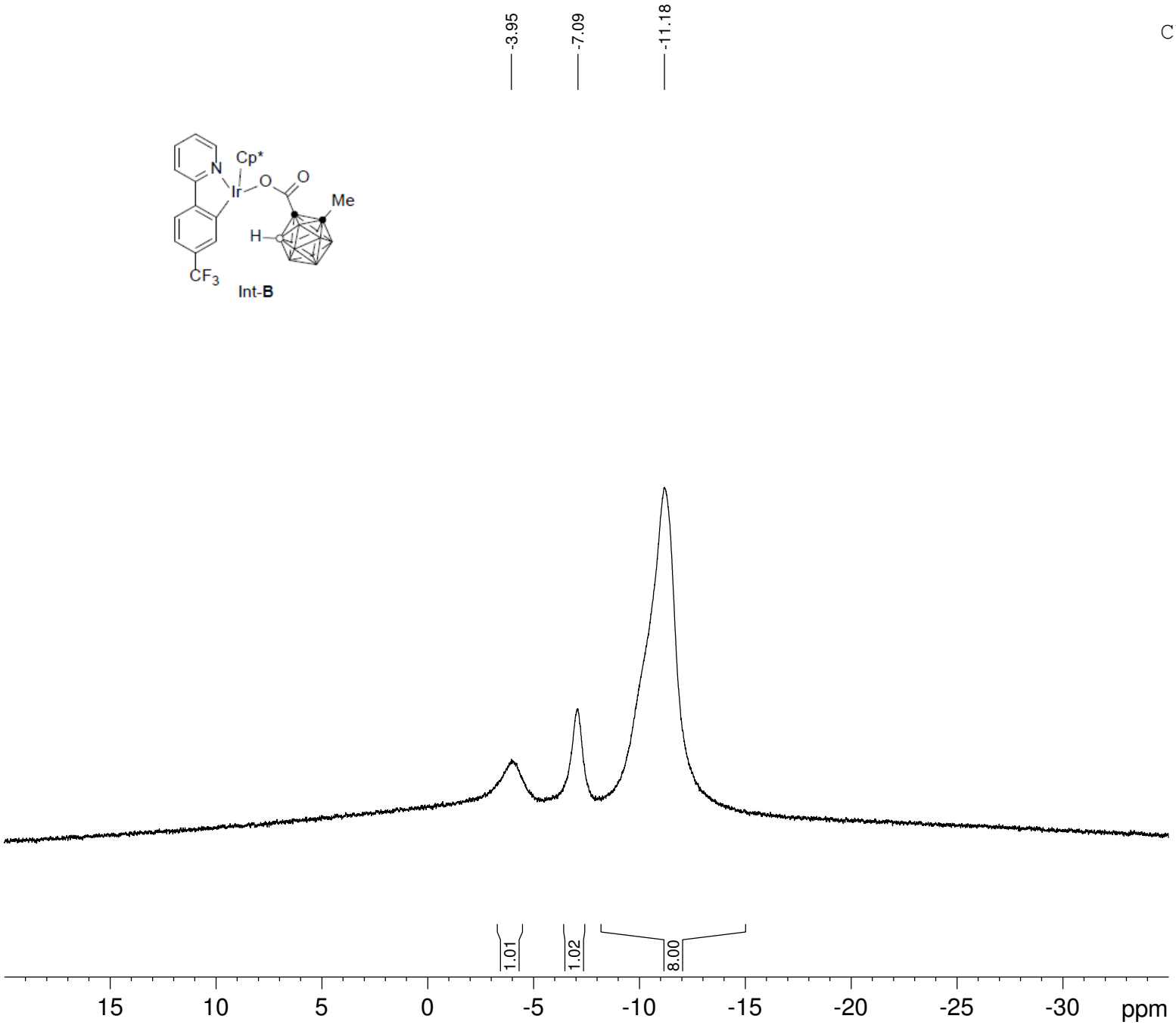


Int-**B**



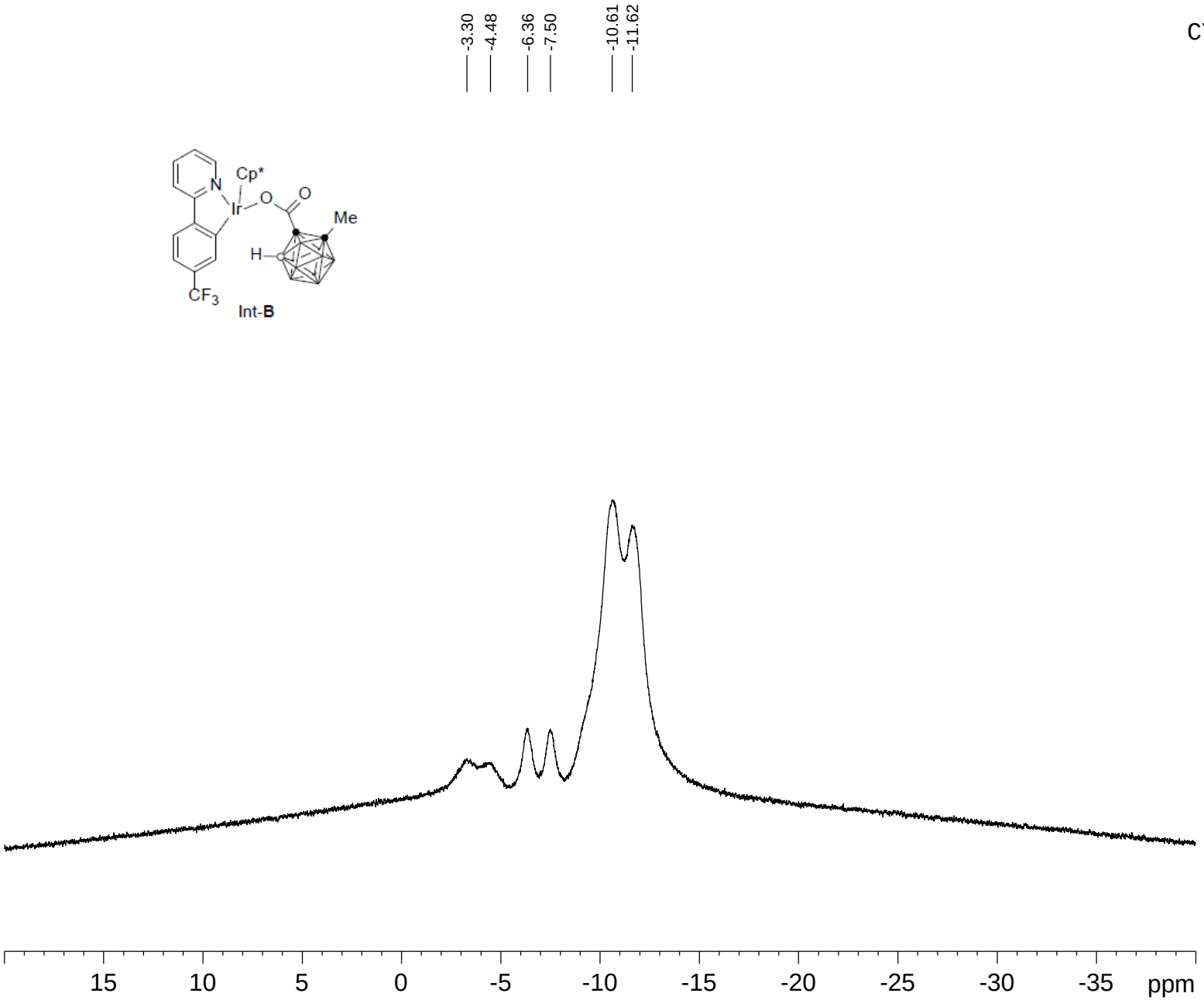



```
Current Data Parameters
NAME      CY-C-B-164P-Ir
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180605
Time               18.56 h
INSTRUM             spect
PROBHD    Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CD2Cl2
NS                   436
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                 13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.29663000 W
PLW13        0.14920001 W

F2 - Processing parameters
SI                 32768
SF          125.7577885 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



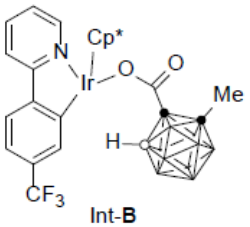
CY-B-A-164p

```
Current Data Parameters
NAME         CY-B-A-164p
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171020
Time               13.04 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                   406
DW                20.800 usec
DE                 6.50 usec
TE                295.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



CY-B-A-164p-(C)

```
Current Data Parameters
NAME      CY-B-A-164p-(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20171020
Time                13.07 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                    406
DW                 20.800 usec
DE                  6.50 usec
TE                 295.0 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

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

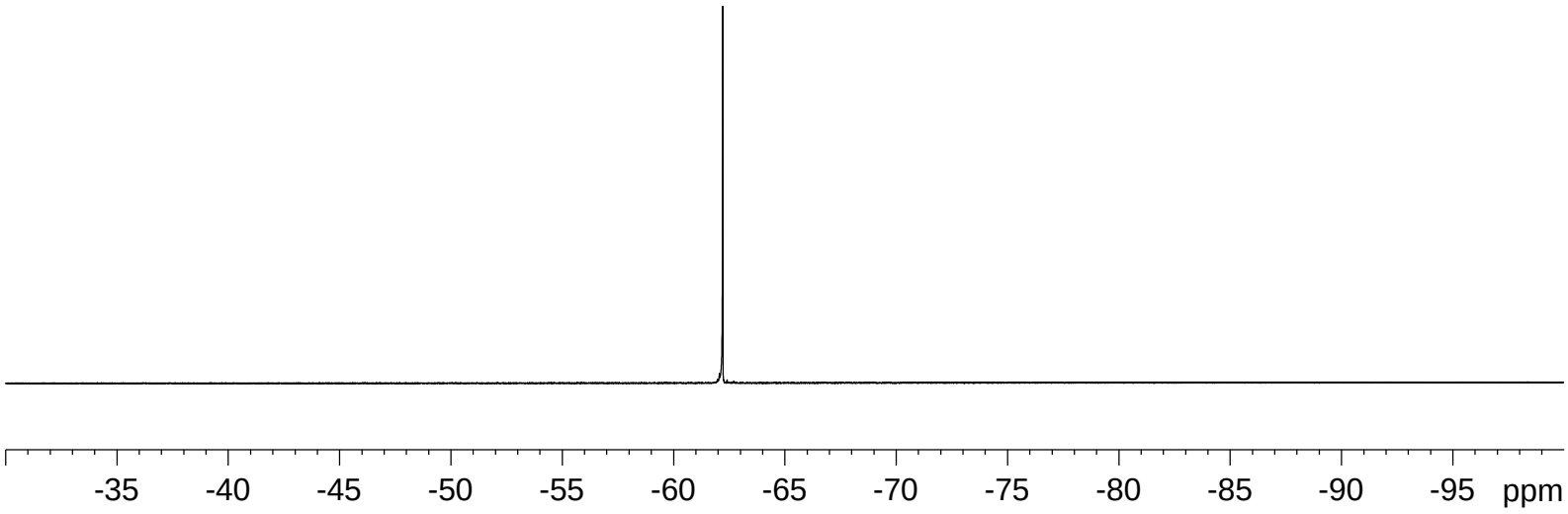


Int-**B**

-62.21

CY-F-A-164P

```
Current Data Parameters
NAME         CY-F-A-164P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171020
Time              13.09 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH            89285.711 Hz
FIDRES         0.681196 Hz
AQ             0.7340032 sec
RG                   645
DW                 5.600 usec
DE                 6.50 usec
TE                 295.0 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1
SFO1         376.5548010 MHz
NUC1                 19F
P1                14.70 usec
PLW1         18.36000061 W
SFO2         400.2316009 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

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



References

1. Y. Quan and Z. Xie, *J. Am. Chem. Soc.*, 2014, **136**, 15513-15516.
2. Y. Quan, J. Zhang and Z. Xie, *J. Am. Chem. Soc.*, 2013, **135**, 18742-18745.
3. G. M. Sheldrick, S*ADABS: Program for Empirical Absorption Correction of Area Detector Data*. (University of Göttingen: Germany, 1996).
4. G. M. Sheldrick, *SHELXTL 5.10 for Windows NT: Structure Determination Software Programs*. (Bruker Analytical X-ray Systems, Inc., Madison, Wisconsin,USA, 1997).