

# Electronic Supplementary Information

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

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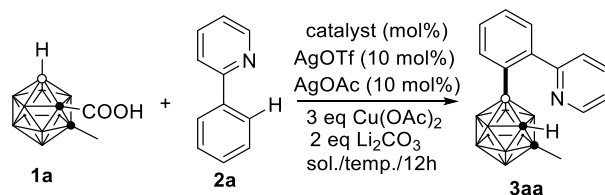
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**General Methods.** All reactions were carried out in flame-dried glassware under an atmosphere of dry argon with the exclusion of air and moisture using standard Schlenk techniques or in drybox. All organic solvents were dried and distilled by standard methods prior to use.  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{11}\text{B}$  and  $^{19}\text{F}$  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  $\delta$  units with references to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, to external  $\text{BF}_3\cdot\text{OEt}_2$  (0.00 ppm) for boron chemical shifts, and to external  $\text{CFCl}_3$  (0.00) for fluorine chemical shifts. High Resolution Mass Spectra (HRMS) were obtained on a Thermo Q Exactive<sup>TM</sup> Focus Hybrid Quadrupole-Orbitrap<sup>TM</sup> 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.<sup>1</sup> 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<sup>a</sup>



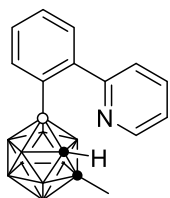
entry	catalyst (mol%)	sol.	temp. (°C)	yield (%) <sup>b</sup>
1	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	tol	100	91
2	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	tol	110	92
3	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	tol	120	95
4	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	tol	130	99 (90 <sup>c</sup> )
5	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	tol	140	89
6 <sup>d</sup>	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	tol	130	93
7 <sup>e</sup>	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	tol	130	63
8	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	OX	130	84
9	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	DCE	130	68
10 <sup>f</sup>	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (2.5)	tol	130	75
11	-	tol	130	0
12	[Cp*RhCl <sub>2</sub> ] <sub>2</sub> (5)	tol	130	0
13	Pd(OAc) <sub>2</sub> (10)	tol	130	0
14	[RuCl <sub>2</sub> ( <i>p</i> -cymene)] <sub>2</sub> (5)	tol	130	0
15 <sup>g</sup>	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	tol	130	0
16 <sup>h</sup>	[Cp*IrCl <sub>2</sub> ] <sub>2</sub> (5)	tol	130	22

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

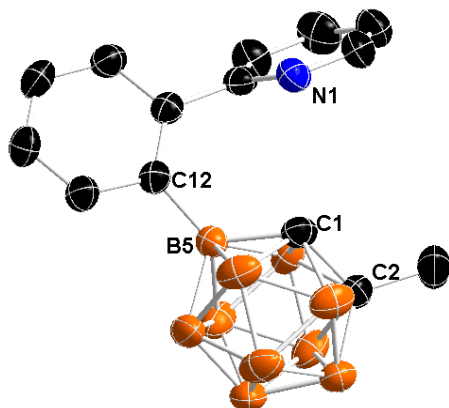
## General Procedures

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

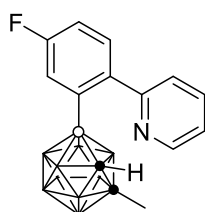
**A representative procedure.** 1-COOH-2-CH<sub>3</sub>-*o*-carborane (**1a**; 20.2 mg, 0.10 mmol), 2-phenylpyridine (**2a**; 15.5 mg, 0.10 mmol), [Cp\*IrCl<sub>2</sub>]<sub>2</sub> (4.0 mg, 0.005 mmol), AgOTf (2.6 mg, 0.01 mmol), AgOAc (1.7 mg, 0.01 mmol), Li<sub>2</sub>CO<sub>3</sub> (14.8 mg, 0.20 mmol) and Cu(OAc)<sub>2</sub> (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 (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%).



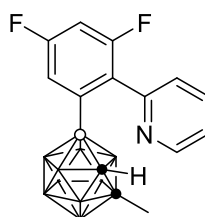
**3aa:** Yield 90%. Colorless crystals. Mp: 141–142 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.57 (d, *J* = 4.4 Hz, 1H), 7.83 (dd, *J* = 6.4, 2.4 Hz, 1H), 7.76 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.37 (m, 4H), 7.19 (dd, *J* = 4.9, 2.4 Hz, 1H) (aryl CH), 3.96 (s, 1H) (Cage CH), 1.88 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 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 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): 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<sub>14</sub>H<sub>21</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N [M+H]<sup>+</sup>: 312.2750. Found: 312.2747.



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

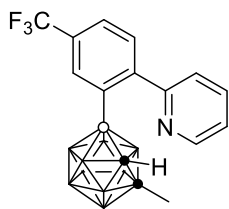


**3ab**: Yield 87%. Pale yellow solid. Mp: 132–133 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.57 (d,  $J = 4.8$  Hz, 1H), 7.77 (ddd,  $J = 7.7, 7.7, 1.8$  Hz, 1H), 7.53 (dd,  $J = 10.4, 2.4$  Hz, 1H), 7.40 (d,  $J = 7.8$  Hz, 1H), 7.33 (dd,  $J = 7.5, 4.9$  Hz, 1H), 7.16 (dd,  $J = 8.4, 5.7$  Hz, 1H), 7.03 (ddd,  $J = 8.2, 8.2, 2.7$  Hz, 1H) (aryl CH), 4.00 (s, 1H) (Cage CH), 1.88 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.1 (d,  $^1J_{\text{C-F}} = 245.9$  Hz), 161.6, 147.9, 141.2 (d,  $^4J_{\text{C-F}} = 3.1$  Hz), 136.8, 131.6 (d,  $^3J_{\text{C-F}} = 7.7$  Hz), 125.4, 123.6 (d,  $^2J_{\text{C-F}} = 21.0$  Hz), 122.8, 114.8 (d,  $^2J_{\text{C-F}} = 21.0$  Hz) (aryl C), 70.4, 63.5 (Cage C), 26.0 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.85 (1B), -4.12 (1B), -6.01 (1B), -8.38 (1B), -10.03 (1B), -11.87 (5B).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  -115.61 (s, 1F). HRMS (ESI):  $m/z$  calcd for  $\text{C}_{14}\text{H}_{20}^{10}\text{B}_2^{11}\text{B}_8\text{NF}$   $[\text{M}+\text{Na}]^+$ : 352.2475. Found: 352.2473.

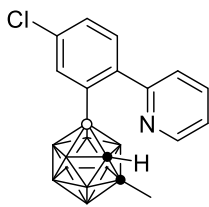


**3ac**: Yield 87%. Pale yellow solid. Mp: 128–129 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.64 (d,  $J = 4.9$  Hz, 1H), 7.79 (ddd,  $J = 7.7, 7.7, 1.8$  Hz, 1H), 7.38 (m, 3H), 6.85 (ddd,  $J = 8.8, 8.8, 2.5$  Hz, 1H) (aryl CH), 3.58 (s, 1H) (Cage CH), 1.85 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.0 (dd,  $^{1,3}J_{\text{C-F}} = 248.2, 12.0$  Hz), 160.2 (dd,  $^{1,3}J_{\text{C-F}} = 245.5, 11.6$  Hz), 155.1, 148.8, 136.5, 128.4 (dd,  $^{2,4}J_{\text{C-F}} = 15.7, 3.7$  Hz), 127.0, 123.5, 119.4 (dd,  $^{2,4}J_{\text{C-F}} = 20.5, 3.4$  Hz), 103.7 (dd,

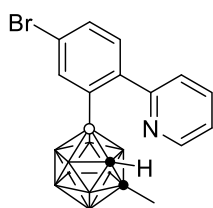
$^{2,2}J_{C-F} = 26.5, 25.3$  Hz) (aryl C), 70.5, 62.9 (Cage C), 26.0 (CH<sub>3</sub>).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz, CDCl<sub>3</sub>):  $\delta$  -2.97 (1B), -4.86 (1B), -6.28 (1B), -8.65 (1B), -10.11 (1B), -12.15 (5B).  $^{19}\text{F}$  NMR (376 MHz, CD<sub>2</sub>Cl<sub>2</sub>):  $\delta$  -110.48 (s, 1F), -111.26 (s, 1F). HRMS (ESI):  $m/z$  calcd for C<sub>14</sub>H<sub>19</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>NF<sub>2</sub> [M+Na]<sup>+</sup>: 370.2381. Found: 329.2379.



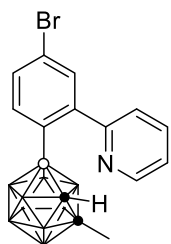
**3ad**: Yield 91%. White solid. Mp: 144–145 °C.  $^1\text{H}$  NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  8.60 (d,  $J = 4.4$  Hz, 1H), 8.08 (s, 1H), 7.80 (ddd,  $J = 7.7, 7.7, 1.8$  Hz, 1H), 7.61 (d,  $J = 8.0$  Hz, 1H), 7.37 (m, 3H) (aryl CH), 3.95 (s, 1H) (Cage CH), 1.89 (s, 3H) (CH<sub>3</sub>).  $^{13}\text{C}$  NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  161.2, 148.5, 148.2, 137.0, 133.8 (q,  $^3J_{C-F} = 4.0$  Hz), 130.1, 129.8 (q,  $^2J_{C-F} = 30.7$  Hz), 125.0, 124.8 (q,  $^3J_{C-F} = 3.7$  Hz) (aryl C), 124.4 (q,  $^1J_{C-F} = 270.7$  Hz) (CF<sub>3</sub>), 123.2 (aryl C), 70.6, 63.5 (Cage C), 26.1 (CH<sub>3</sub>).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz, CDCl<sub>3</sub>):  $\delta$  -2.71 (1B), -4.12 (1B), -5.95 (1B), -8.34 (1B), -9.92 (1B), -11.83 (5B).  $^{19}\text{F}$  NMR (376 MHz, CD<sub>2</sub>Cl<sub>2</sub>):  $\delta$  -62.45 (s, 3F). HRMS (ESI):  $m/z$  calcd for C<sub>15</sub>H<sub>20</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>NF<sub>3</sub> [M+Na]<sup>+</sup>: 380.2624. Found: 380.2618.



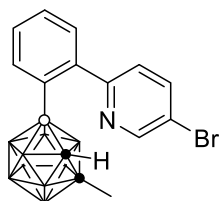
**3ae**: Yield 88%. White solid. Mp: 110–111 °C.  $^1\text{H}$  NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.58 (d,  $J = 4.6$  Hz, 1H), 7.80 (m, 2H), 7.40 (dd,  $J = 7.8$  Hz, 1H), 7.35 (m, 2H), 7.12 (d,  $J = 8.1$  Hz, 1H) (aryl CH), 4.04 (s, 1H) (Cage CH), 1.89 (s, 3H) (CH<sub>3</sub>).  $^{13}\text{C}$  NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  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 (CH<sub>3</sub>).  $^{11}\text{B}\{^1\text{H}\}$  NMR (160 MHz, CDCl<sub>3</sub>):  $\delta$  -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<sub>14</sub>H<sub>20</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>NCl [M]<sup>+</sup>: 346.2276. Found: 346.2274.



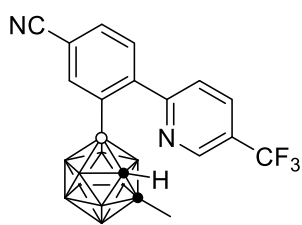
**3af:** Yield 68%. White solid. Mp: 115–116 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.57 (d,  $J = 4.8$  Hz, 1H), 7.94 (d,  $J = 1.8$  Hz, 1H), 7.77 (ddd,  $J = 7.7, 7.7, 1.8$  Hz, 1H), 7.48 (dd,  $J = 8.2, 2.1$  Hz, 1H), 7.35 (m, 2H), 7.06 (d,  $J = 8.2$  Hz, 1H) (aryl CH), 3.99 (s, 1H) (Cage CH), 1.88 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  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 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.86 (1B), -4.36 (1B), -6.08 (1B), -8.46 (1B), -10.05 (1B), -11.98 (5B). HRMS (ESI):  $m/z$  calcd for  $\text{C}_{14}\text{H}_{20}^{10}\text{B}_2^{11}\text{B}_8\text{NBr}$  [ $\text{M}+\text{H}$ ] $^+$ : 391.1836. Found: 391.1837.



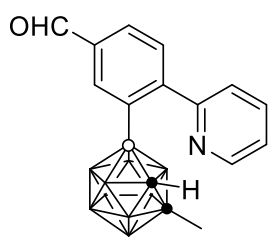
**3ag:** Yield 77%. White solid. Mp: 112–113 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.57 (d,  $J = 4.9$  Hz, 1H), 7.78 (ddd,  $J = 7.7, 7.7, 1.8$  Hz, 1H), 7.68 (d,  $J = 8.3$  Hz, 1H), 7.49 (dd,  $J = 8.3, 2.1$  Hz, 1H), 7.41 (d,  $J = 7.8$  Hz, 1H), 7.34 (m, 2H) (aryl CH), 3.93 (s, 1H) (Cage CH), 1.87 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  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 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.06 (1B), -4.05 (1B), -6.22 (1B), -8.60 (1B), -10.18 (1B), -12.14 (5B). HRMS (ESI):  $m/z$  calcd for  $\text{C}_{14}\text{H}_{20}^{10}\text{B}_2^{11}\text{B}_8\text{NBr}$  [ $\text{M}+\text{H}$ ] $^+$ : 391.1836. Found: 391.1831.



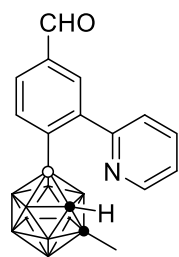
**3ah:** Yield 81%. White solid. Mp: 107–108 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.65 (d,  $J = 2.3$  Hz, 1H), 7.89 (dd,  $J = 8.3, 2.4$  Hz, 1H), 7.83 (dd,  $J = 5.8, 3.0$  Hz, 1H), 7.37 (m, 2H), 7.33 (d,  $J = 8.3$  Hz, 1H), 7.16 (dd,  $J = 7.1, 2.9$  Hz, 1H) (aryl CH), 4.08 (s, 1H) (Cage CH), 1.94 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  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 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.78 (2B), -6.70 (1B), -9.08 (1B), -10.84 (1B), -12.58 (4B), -13.53 (1B). HRMS (ESI):  $m/z$  calcd for  $\text{C}_{14}\text{H}_{20}^{10}\text{B}_2^{11}\text{B}_8\text{NBr}$  [ $\text{M}+\text{H}$ ] $^+$ : 392.1836. Found: 392.1829.



**3ai:** Yield 84%. Pale yellow solid. Mp: 146–147 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  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 CH), 4.13 (s, 1H) (Cage CH), 1.95 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.0, 148.4, 145.3 (q,  $J_{\text{C-F}} = 4.0$  Hz), 140.7, 134.2 (q,  $J_{\text{C-F}} = 3.3$  Hz), 131.5, 130.4, 126.6 (q,  $J_{\text{C-F}} = 33.5$  Hz), 124.8 (aryl C), 123.5 (q,  $J_{\text{C-F}} = 269.7$  Hz) ( $\text{CF}_3$ ), 118.7 (CN), 112.6 (aryl C), 71.1, 63.5 (Cage C), 26.1 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.32 (1B), -5.02 (1B), -6.12 (1B), -8.68 (1B), -9.79 (1B), -12.03 (5B).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  -62.07 (s, 3F). HRMS (ESI):  $m/z$  calcd for  $\text{C}_{16}\text{H}_{19}^{10}\text{B}_2^{11}\text{B}_8\text{N}_2\text{F}_3$   $[\text{M}+\text{Na}]^+$ : 427.2396. Found: 427.2392.



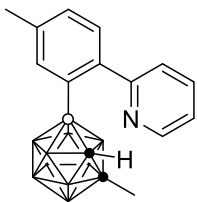
**3aj:** Yield 81%. White solid. Mp: 170–171 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  10.07 (s, 1H), 8.60 (d,  $J = 4.6$  Hz, 1H), 8.30 (s, 1H), 7.87 (dd,  $J = 7.8$ , 1.6 Hz, 1H), 7.81 (ddd,  $J = 7.7$ , 7.7, 1.6 Hz, 1H), 7.39 (m, 3H) (aryl CH), 4.01 (s, 1H) (Cage CH), 1.90 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  192.5 (CHO), 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 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.73 (1B), -5.25 (1B), -7.07 (1B), -9.53 (1B), -11.00 (1B), -12.95 (5B). HRMS (ESI):  $m/z$  calcd for  $\text{C}_{15}\text{H}_{21}^{10}\text{B}_2^{11}\text{B}_8\text{NO}$   $[\text{M}+\text{Na}]^+$ : 362.2519. Found: 362.2513.



**3ak:** Yield 76%. White solid. Mp: 165–166 °C.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  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 CH), 3.95 (s, 1H) (Cage CH), 1.87 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  192.1 (CHO), 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 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (160 MHz,

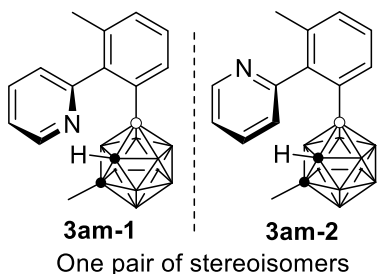


CDCl<sub>3</sub>):  $\delta$  -2.48 (1B), -4.02 (1B), -5.71 (1B), -8.08 (1B), -9.69 (1B), -11.70 (5B). HRMS (APCI):  $m/z$  calcd for C<sub>15</sub>H<sub>21</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>NO [M+H]<sup>+</sup>: 340.2707. Found: 340.2695.



**3al**: Yield 89%. White solid. Mp: 126–127 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  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 CH), 4.00 (s, 1H) (Cage

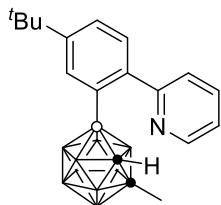
CH), 2.40 (s, 3H) (Aryl CH<sub>3</sub>), 1.88 (s, 3H) (Cage CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  162.7, 147.8, 142.5, 138.0, 137.1, 136.6, 129.7, 128.7, 125.4, 122.4 (aryl C), 70.2, 63.5 (Cage C), 26.1, 21.4 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>):  $\delta$  -3.32 (2B), -6.21 (1B), -8.52 (1B), -10.38 (1B), -12.07 (5B). HRMS (ESI):  $m/z$  calcd for C<sub>15</sub>H<sub>23</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N [M+H]<sup>+</sup>: 326.2907. Found: 326.2900.



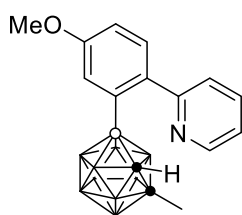
**3am**: Yield 89%. (Yield of one pair of stereoisomers, resulting from the restricted rotation of pyridyl unit).<sup>2</sup>

White solid. Mp: 117–120 °C. For one isomer **3am-1**: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  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 CH), 3.11 (s, 1H) (Cage CH), 1.96 (s, 3H) (Cage CH<sub>3</sub>), 1.84 (s, 3H) (Aryl CH<sub>3</sub>). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  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 (CH<sub>3</sub>). For another isomer **3am-2**: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  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 CH), 2.64 (s, 1H) (Cage CH), 1.96 (s, 3H) (Cage CH<sub>3</sub>), 1.76 (s, 3H) (Aryl CH<sub>3</sub>). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  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 (CH<sub>3</sub>). For **3am**: <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>):  $\delta$  -2.95 (2B), -

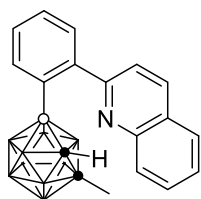
5.93 (1B), -8.11 (1B), -9.81 (1B), -11.25 (5B). HRMS (APCI):  $m/z$  calcd for  $C_{15}H_{23}^{10}B_2^{11}B_8N$   $[M+H]^+$ : 326.2907. Found: 326.2906.



**3an**: Yield 95%. White solid. Mp: 132–133 °C.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  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 CH), 4.01 (s, 1H) (Cage CH), 1.88 (s, 3H) (Cage  $CH_3$ ), 1.37 (s, 9H) ( $^tBu$ ).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  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 ( $^tBu$ ), 26.1 (Cage  $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -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.

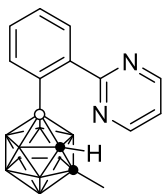


**3ao**: Yield 66%. Pale yellow solid. Mp: 137–138 °C.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.55 (d,  $J = 3.5$  Hz, 1H), 7.75 (t,  $J = 7.7$  Hz, 1H), 7.40 (m, 2H), 7.30 (dd,  $J = 6.1, 6.1$  Hz, 1H), 7.13 (d,  $J = 8.4$  Hz, 1H), 6.89 (d,  $J = 8.4$  Hz, 1H) (aryl CH), 4.12 (s, 1H) (Cage CH), 3.85 (s, 3H) ( $OCH_3$ ), 1.88 (s, 3H) (Cage  $CH_3$ ).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  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 ( $OCH_3$ ), 26.1 (Cage  $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -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.



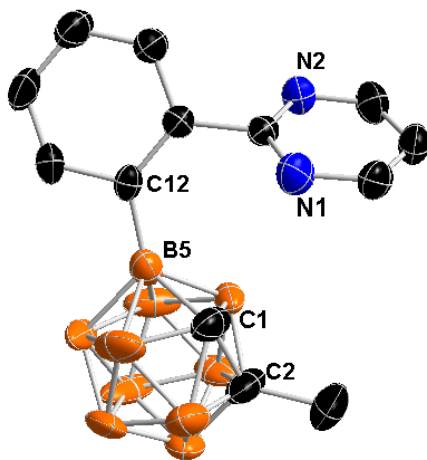
**3ap**: Yield 59%. Pale yellow solid. Mp: 148–149 °C.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.27 (d,  $J = 8.4$  Hz, 1H), 8.03 (d,  $J = 8.4$  Hz, 1H), 7.91 (m, 2H), 7.75 (dd,  $J = 7.7, 7.7$  Hz, 1H), 7.60 (m, 2H), 7.41 (m, 2H), 7.31 (dd,  $J = 5.6, 3.4$  Hz, 1H) (aryl CH), 4.28 (s, 1H) (Cage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

(CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 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 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -4.29 (2B), -7.24 (1B), -9.48 (1B), -11.41 (1B), -12.97 (5B). HRMS (ESI): *m/z* calcd for C<sub>18</sub>H<sub>23</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N [M+Na]<sup>+</sup>: 384.2726. Found: 384.2720.

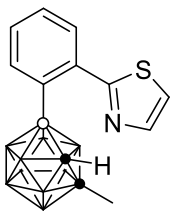


**3aq:** Yield 88%. Colorless crystals. Mp: 155–156 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.80 (d, *J* = 4.9 Hz, 2H), 7.85 (dd, *J* = 3.8, 3.8 Hz, 1H), 7.40 (m, 3H), 7.32 (dd, *J* = 4.9, 4.9 Hz, 1H) (aryl CH), 4.46 (s, 1H) (Cage CH), 1.96 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 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 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): 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<sub>13</sub>H<sub>20</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N<sub>2</sub> [M+Na]<sup>+</sup>: 335.2522. Found: 335.2520.



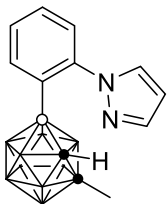
**Figure S2.** Molecular Structure of **3aq**.



**3ar:** Yield 81%. White solid. Mp: 100–102 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 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 CH), 4.59 (s, 1H) (Cage CH), 1.95 (s, 3H) (CH<sub>3</sub>).

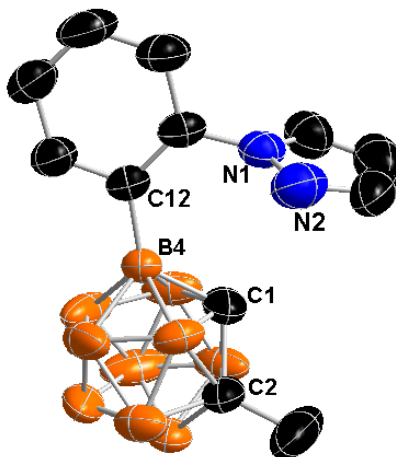
<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ 170.3, 141.6, 137.7, 137.0, 131.1, 129.1, 128.0, 121.5 (aryl C), 70.5, 64.2 (Cage C), 26.1 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>):

$\delta$  -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.

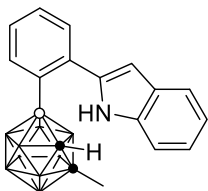


**3as**: Yield 72%. Colorless crystals. Mp: 112–113 °C.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.80 (d,  $J = 7.2$  Hz, 1H), 7.66 (d,  $J = 1.5$  Hz, 1H), 7.59 (d,  $J = 2.1$  Hz, 1H), 7.41 (m, 2H), 7.17 (dd,  $J = 7.6, 1.3$  Hz, 1H), 6.45 (dd,  $J = 2.1, 2.1$  Hz, 1H) (aryl  $CH$ ), 3.08 (s, 1H) (Cage  $CH$ ), 1.88 (s, 3H) ( $CH_3$ ).  $^{13}C$

NMR (100 MHz,  $CDCl_3$ ):  $\delta$  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 ( $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -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.



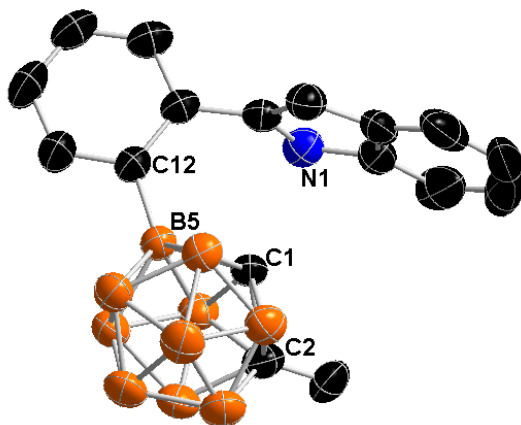
**Figure S3.** Molecular Structure of **3as**.



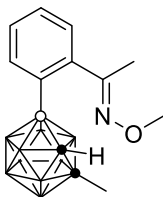
**3at**: Yield 72%. Colorless crystals. Mp: 119–120 °C.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.10 (s, 1H), 7.73 (d,  $J = 7.5$  Hz, 1H), 7.64 (d,  $J = 7.9$  Hz, 1H), 7.39 (m, 4H), 7.24 (ddd,  $J = 7.2, 7.2, 1.2$  Hz, 1H), 7.17 (ddd,  $J = 7.5, 7.5, 1.1$  Hz, 1H), 6.49 (d,  $J = 2.1$  Hz, 1H) (aryl  $CH$ ), 2.25 (s, 1H)

(Cage  $CH$ ), 1.56 (s, 3H) ( $CH_3$ ).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  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),

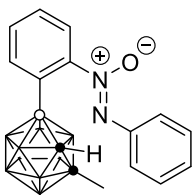
25.8 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -3.68 (2B), -6.30 (1B), -8.42 (1B), -9.96 (1B), -11.57 (5B). HRMS (ESI): *m/z* calcd for C<sub>17</sub>H<sub>23</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N [M+Na]<sup>+</sup>: 372.2726. Found: 372.2728.



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

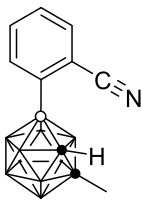


**3au**: Yield 67%. Pale yellow solid. Mp: 104–105 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.72 (d, *J* = 7.0 Hz, 1H), 7.31 (m, 2H), 7.12 (dd, *J* = 7.0, 1.9 Hz, 1H) (aryl *CH*), 4.21 (s, 1H) (Cage *CH*), 3.93 (s, 3H) (OCH<sub>3</sub>), 2.19 (s, 3H), 2.07 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 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<sub>3</sub>), 26.3, 18.2 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): 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<sub>12</sub>H<sub>23</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>NO [M+Na]<sup>+</sup>: 328.2675. Found: 328.2671.



**3av**: Yield 62%. Pale yellow solid. Mp: 123–124 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.17 (d, *J* = 7.5 Hz, 2H), 7.85 (dd, *J* = 3.9, 3.9 Hz, 1H), 7.48 (m, 6H) (aryl *CH*), 4.32 (s, 1H) (Cage *CH*), 1.86 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 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<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>):

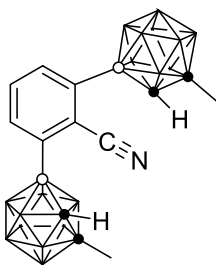
$\delta$  -2.32 (1B), -4.78 (1B), -5.57 (1B), -7.96 (1B), -9.37 (1B), -10.89 (5B). HRMS (ESI):  $m/z$  calcd for  $C_{15}H_{22}^{10}B_2^{11}B_8N_2O$   $[M+Na]^+$ : 377.2628. Found: 377.2623.



**3aw**: Yield 76%. White solid. Mp: 143–144 °C.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):

$\delta$  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 CH), 4.78 (s, 1H) (Cage CH), 2.13 (s, 3H) ( $CH_3$ ).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  136.9, 133.6, 132.3,

128.6 (aryl C), 120.5 (CN), 113.3 (aryl C), 71.0, 60.8 (Cage C), 26.1 ( $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -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.

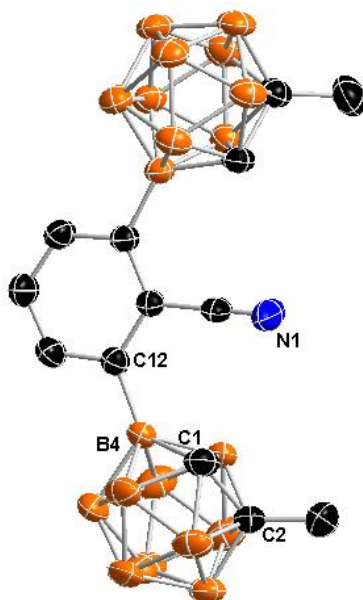


**3ax**: Yield 57%. Colorless crystals. Mp: 179–180 °C.  $^1H$  NMR (400

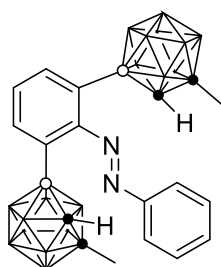
MHz,  $CDCl_3$ ):  $\delta$  7.74 (d,  $J = 7.7$  Hz, 2H), 7.46 (dd,  $J = 7.7, 7.7$  Hz, 1H) (aryl CH), 4.81 (s, 2H) (Cage CH), 2.12 (s, 6H) ( $CH_3$ ).  $^{13}C$  NMR (100

MHz,  $CDCl_3$ ):  $\delta$  136.9, 131.4 (aryl C), 121.9 (CN), 113.7 (aryl C), 70.8, 60.9 (Cage C), 26.2 ( $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -2.50

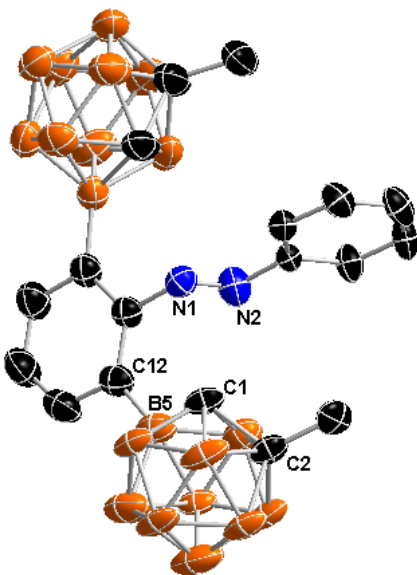
(2B), -4.52 (2B), -5.80 (2B), -8.07 (2B), -9.29 (2B), -10.98 (10B). HRMS (ESI):  $m/z$  calcd for  $C_{13}H_{29}^{10}B_2^{11}B_8N$   $[M+Na]^+$ : 438.4199. Found: 438.4196.



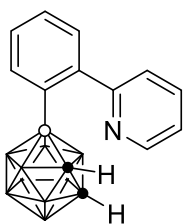
**Figure S5.** Molecular Structure of **3ax**.



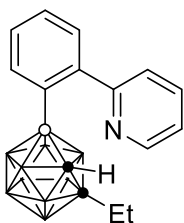
**3ay**: Yield 74%. Orange crystals. Mp: 183–184 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.89 (m, 2H), 7.71 (d,  $J = 7.6$  Hz, 2H), 7.60 (m, 3H), 7.25 (dd,  $J = 7.6, 7.6$  Hz, 1H) (aryl  $\text{CH}$ ), 3.73 (s, 2H) (Cage  $\text{CH}$ ), 1.67 (s, 3H), 1.63 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  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 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.01 (2B), -4.17 (2B), -6.33 (2B), -8.39 (2B), -10.10 (2B), -11.75 (10B). HRMS (ESI):  $m/z$  calcd for  $\text{C}_{18}\text{H}_{34}^{10}\text{B}_2^{11}\text{B}_8\text{N}_2$   $[\text{M}+\text{Na}]^+$ : 517.4631. Found: 517.4624.



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



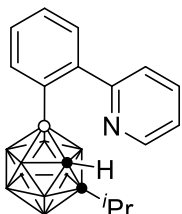
**3ba:** Yield 51%. White solid. Mp: 159–160 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.55 (d,  $J = 4.4$  Hz, 1H), 7.86 (d,  $J = 5.0$  Hz, 1H), 7.75 (ddd,  $J = 7.7, 7.7, 1.7$  Hz, 1H), 7.39 (m, 3H), 7.30 (dd,  $J = 7.4, 5.0$  Hz, 1H), 7.18 (d,  $J = 5.0$  Hz, 1H) (aryl CH), 3.96 (s, 1H), 3.46 (s, 1H) (Cage CH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  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).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -1.72 (1B), -3.81 (2B), -8.69 (1B), -10.32 (1B), -13.06 (1B), -14.83 (4B). HRMS (ESI):  $m/z$  calcd for  $\text{C}_{13}\text{H}_{19}^{10}\text{B}_2^{11}\text{B}_8\text{N}$   $[\text{M}+\text{Na}]^+$ : 320.2413. Found: 320.2411.



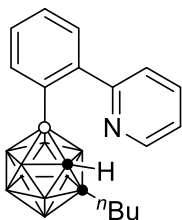
**3ca:** Yield 93%. White solid. Mp: 133–134 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.56 (d,  $J = 4.9$  Hz, 1H), 7.84 (d,  $J = 4.4$  Hz, 1H), 7.77 (ddd,  $J = 7.7, 7.7, 1.8$  Hz, 1H), 7.42 (d,  $J = 7.8$  Hz, 1H), 7.35 (m, 3H), 7.17 (d,  $J = 5.0$  Hz, 1H) (aryl CH), 3.85 (s, 1H) (Cage CH), 2.13 (m, 2H), 0.97 (t,  $J = 7.6$  Hz, 3H), (Et).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  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 ( $\text{CH}_2\text{CH}_3$ ) 13.5



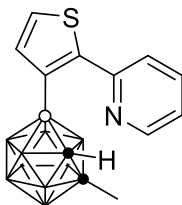
(CH<sub>2</sub>CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -3.87 (2B), -5.31 (1B), -8.65 (1B), -10.43 (1B), -12.59 (5B). HRMS (ESI): *m/z* calcd for C<sub>15</sub>H<sub>23</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N [M+Na]<sup>+</sup>: 348.2726. Found: 348.2721.



**3da:** Yield 41%. White solid. Mp: 121–122 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): 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 CH), 3.92 (s, 1H) (Cage CH), 2.36 (m, 1H), 1.00 (t, *J* = 6.2 Hz, 6H) (*i*Pr). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 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). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -4.44 (3B), -8.68 (1B), -10.37 (1B), -12.91 (5B). HRMS (ESI): *m/z* calcd for C<sub>16</sub>H<sub>25</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N [M+Na]<sup>+</sup>: 362.2883. Found: 362.2878.

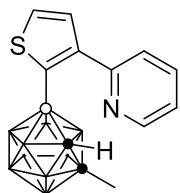


**3ea:** Yield 73%. White solid. Mp: 109–110 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.58 (d, *J* = 4.8 Hz, 1H), 7.84 (dd, *J* = 5.8, 3.1 Hz, 1H), 7.76 (ddd, *J* = 7.7, 7.7, 1.8 Hz, 1H), 7.35 (m, 4H), 7.17 (dd, *J* = 7.1, 2.7 Hz, 1H) (aryl CH), 3.87 (s, 1H) (Cage CH), 2.05 (m, 2H), 1.26 (m, 4H), 0.89 (t, *J* = 7.0 Hz, 3H) (*n*Bu). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): 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). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -3.84 (2B), -5.13 (1B), -8.62 (1B), -10.35 (1B), -12.46 (5B). HRMS (ESI): *m/z* calcd for C<sub>17</sub>H<sub>27</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N [M+Na]<sup>+</sup>: 376.3039. Found: 376.3036.

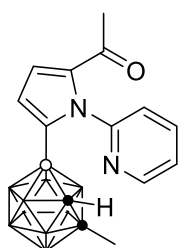


**4aa:** Yield 81%. White solid. Mp: 117–118 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 8.43 (d, *J* = 4.9 Hz, 1H), 7.61 (ddd, *J* = 7.8, 7.8, 1.8 Hz, 1H), 7.46 (d, *J* = 7.9 Hz, 1H), 7.17 (m, 3H) (aryl CH), 4.96 (s, 1H) (Cage CH), 1.88 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): 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<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR

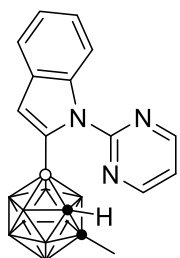
(128 MHz, CDCl<sub>3</sub>):  $\delta$  -4.23 (1B), -7.06 (2B), -9.57 (1B), -11.22 (1B), -13.10 (4B), -14.07 (1B). HRMS (APCI):  $m/z$  calcd for C<sub>12</sub>H<sub>29</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>NS [M-H]<sup>-</sup>: 316.2175. Found: 316.2170.



**4ab:** Yield 69%. White solid. Mp: 135–136 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  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 CH), 5.16 (s, 1H) (Cage CH), 2.05 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  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 (CH<sub>3</sub>). <sup>11</sup>B {<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>):  $\delta$  -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<sub>12</sub>H<sub>29</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>NS [M-H]<sup>-</sup>: 316.2175. Found: 316.2171.



**4ac:** Yield 85%. Pale yellow solid. Mp: 141–142 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  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 CH), 3.81 (s, 1H) (Cage CH), 2.37 (s, 3H) (COCH<sub>3</sub>), 1.94 (s, 3H) (Cage CH<sub>3</sub>). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  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 (CH<sub>3</sub>). <sup>11</sup>B {<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>):  $\delta$  -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<sub>14</sub>H<sub>24</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N<sub>2</sub>O [M+H]<sup>+</sup>: 344.2777. Found: 344.2778.

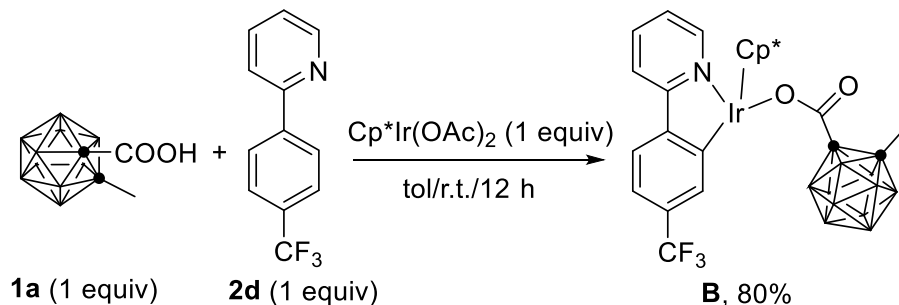


**4ad:** Yield 90%. White solid. Mp: 179–180 °C. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.81 (d,  $J$  = 8.2 Hz, 1H), 8.67 (d,  $J$  = 4.8 Hz, 2H), 8.36 (s, 1H), 7.96 (d,  $J$  = 7.8 Hz, 1H), 7.36 (dd,  $J$  = 5.7, 5.7 Hz, 1H), 7.29 (dd,  $J$  = 7.9, 7.9 Hz, 1H), 7.01 (dd,  $J$  = 4.8, 4.8 Hz, 1H) (aryl CH), 3.79 (s, 1H) (Cage CH), 2.05 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  158.3, 157.5,

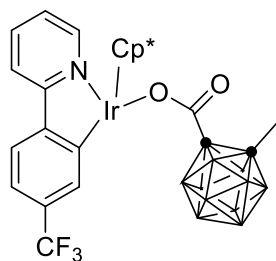
136.4, 134.6, 131.3, 123.8, 122.4, 121.3, 116.5, 116.4 (aryl C), 70.6, 63.4 (Cage C), 26.1 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -2.26 (1B), -5.27 (1B), -6.24 (1B), -9.06 (1B), -10.02 (1B), -11.38 (5B). HRMS (APCI): *m/z* calcd for C<sub>15</sub>H<sub>21</sub><sup>10</sup>B<sub>2</sub><sup>11</sup>B<sub>8</sub>N<sub>3</sub> [M-H]<sup>-</sup>: 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)<sub>2</sub> (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%).

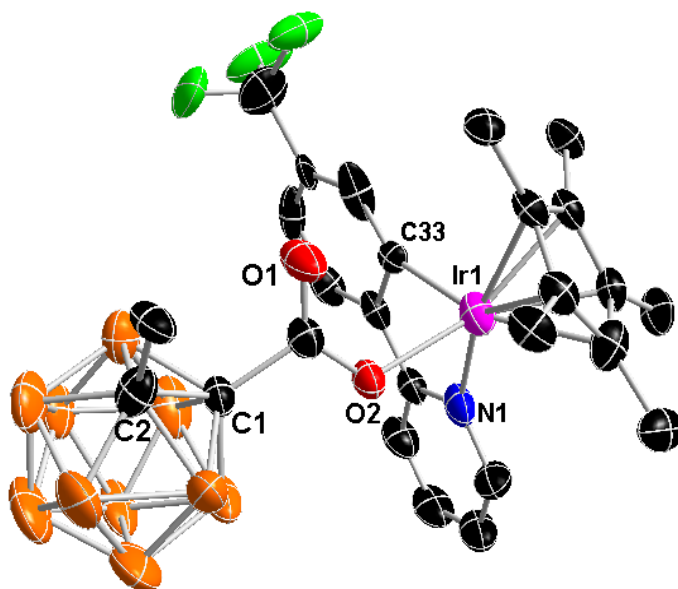


### Scheme S1. Preparation of Intermediate B.



**B:** Yield 80%. Yellow crystals. Mp: > 250 °C. <sup>1</sup>H NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>): 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 CH), 1.67 (s, 15H) (Cp\*), 1.25 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C NMR (125 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 166.0, 163.2, 162.5, 152.5, 138.3, 131.8 (q, <sup>3</sup>*J*<sub>C-F</sub> = 3.8 Hz), 130.8 (q, <sup>2</sup>*J*<sub>C-F</sub> = 30.4 Hz) (aryl C), 124.6 (q, <sup>1</sup>*J*<sub>C-F</sub> = 270.9 Hz) (CF<sub>3</sub>), 123.3, 123.1, 119.5 (q, <sup>3</sup>*J*<sub>C-F</sub> = 3.8 Hz), 119.3 (aryl C), 87.7 (C<sub>5</sub>Me<sub>5</sub>), 77.9, 74.7 (Cage C), 23.6 (Cage CH<sub>3</sub>), 8.9 (C<sub>5</sub>Me<sub>5</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ -3.95 (1B),

-7.09 (1B), -11.18 (8B).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  -62.21 (s, 3F). HRMS (ESI):  $m/z$  calcd for  $\text{C}_{26}\text{H}_{35}^{10}\text{B}_2^{11}\text{B}_8\text{F}_3\text{IrNO}_2$  [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<sub>3</sub>-*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<sub>2</sub>CO<sub>3</sub> (14.8 mg, 0.20 mmol) and Cu(OAc)<sub>2</sub> (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.**

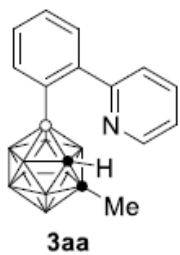
Intermediate **B** (75.1 mg, 0.10 mmol), Li<sub>2</sub>CO<sub>3</sub> (14.8 mg, 0.20 mmol), and/or Cu(OAc)<sub>2</sub> (54.6 mg, 0.30 mmol), LiOTf (46.8 mg, 0.30 mmol), Cu(OTf)<sub>2</sub> (108.5 mg, 0.30 mmol) were mixed in dry toluene (5 mL) in a sealed flask. The reaction mixture was heated at 130 °C for 12 h under Argon. The resulting reaction mixture was cooled to room temperature, 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-K $\alpha$  radiation. An empirical absorption correction was applied using the SADABS program.<sup>3</sup> 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.<sup>4</sup> 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](http://www.ccdc.cam.ac.uk/data_request/cif).

7.785  
7.781  
7.766  
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7.747  
7.742  
7.432  
7.412  
7.390  
7.378  
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7.366  
7.362  
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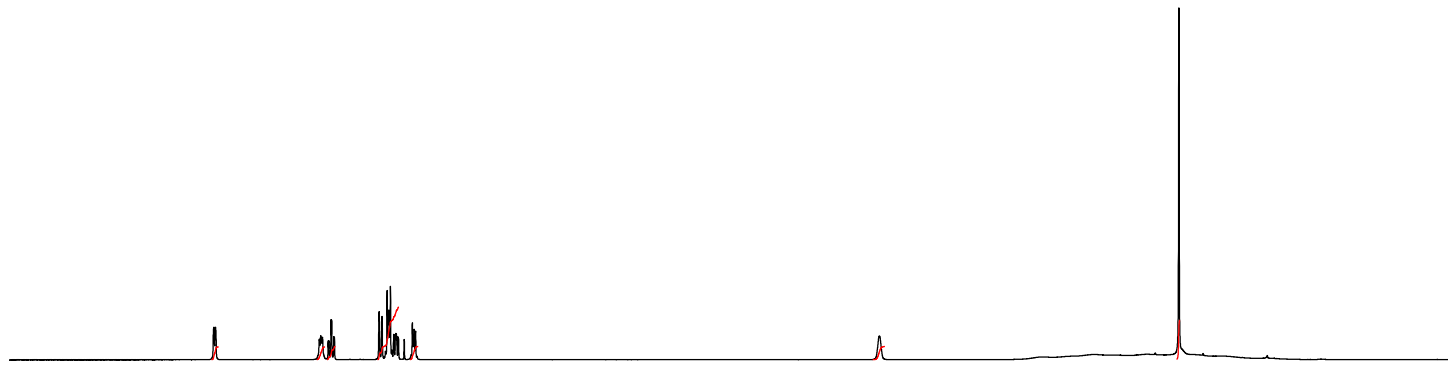
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1.00

1.00

3.06

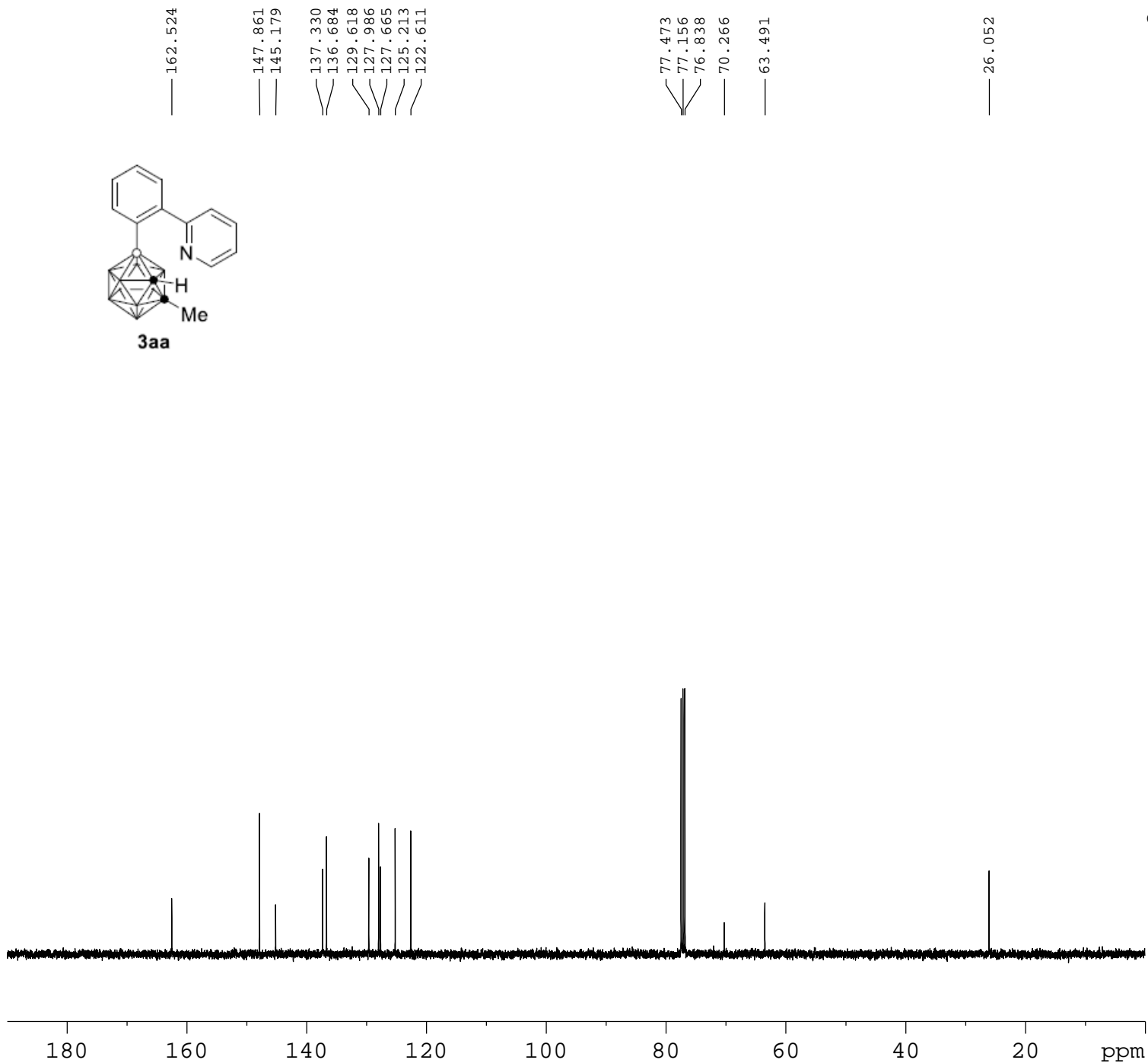
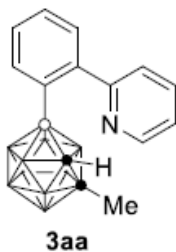
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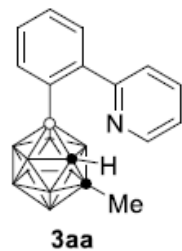
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PROBHD z824601\_0021 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 48  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 294.5 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 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





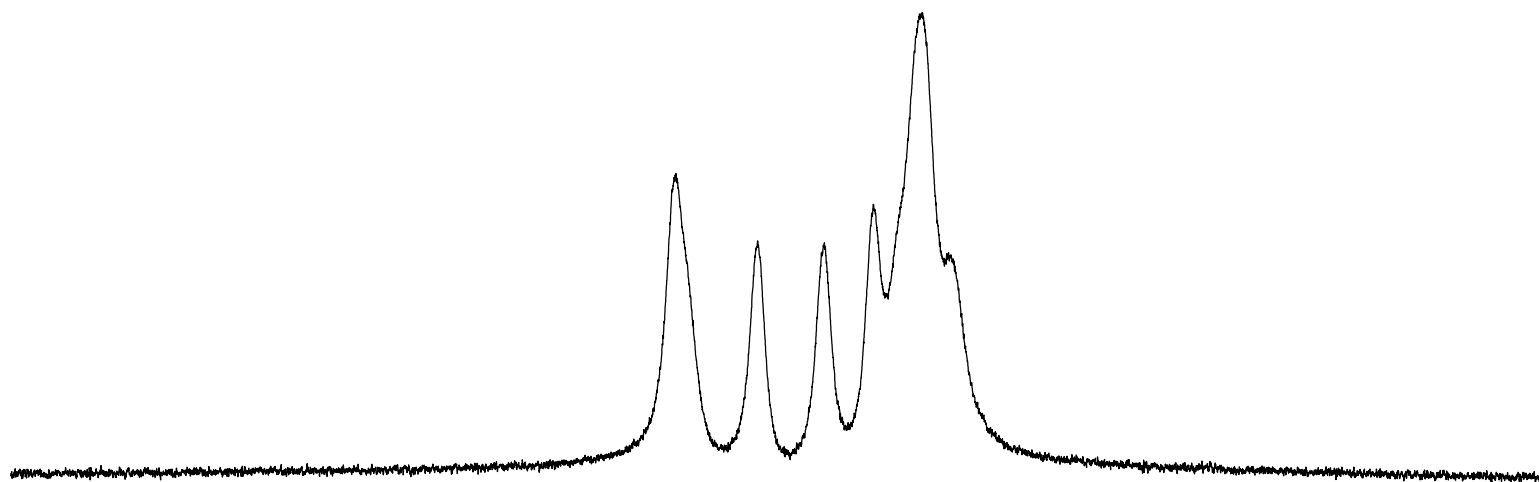
— 3.78  
 — 6.70  
 — 9.08  
 — 10.84  
 — 12.58  
 — 13.53

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 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 11B  
 P1 7.50 usec  
 PLW1 55.09999847 W  
 SFO2 400.2316009 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 13.56000042 W  
 PLW12 0.27428001 W

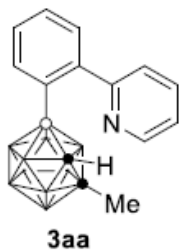
F2 - Processing parameters  
 SI 32768  
 SF 128.4097615 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



2.01  
 1.03  
 1.02  
 1.06  
 4.00  
 1.06

15 10 5 0 -5 -10 -15 -20 -25 -30 ppm





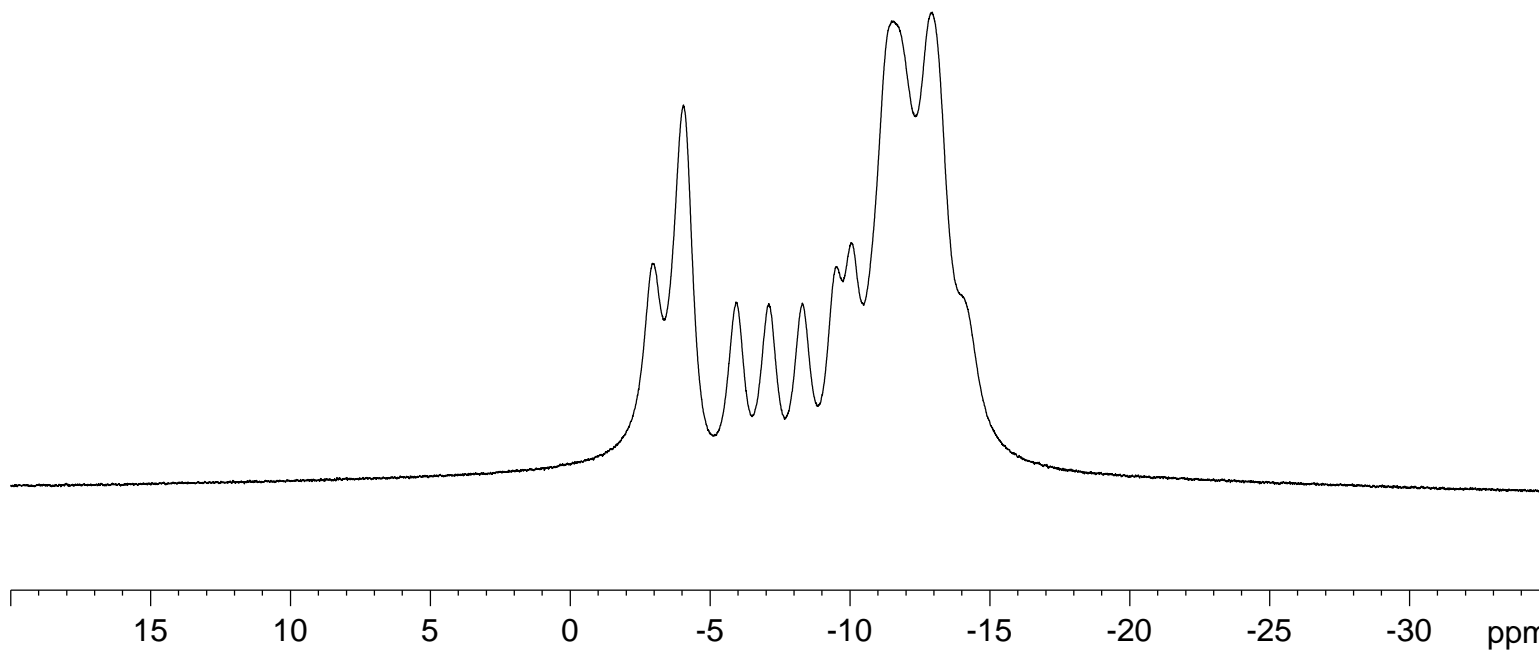
-2.95  
 -4.05  
 -5.93  
 -7.10  
 -8.30  
 -9.51  
 -10.04  
 -11.49  
 -12.94  
 -14.05

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

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

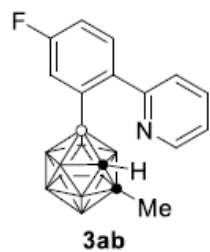
F2 - Acquisition Parameters  
 Date\_ 20160804  
 Time 16.52 h  
 INSTRUM spect  
 PROBHD z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT MeOD  
 NS 33  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 287  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.9 K  
 D1 2.00000000 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



7.770  
7.765  
7.750  
7.746  
7.544  
7.538  
7.518  
7.512  
7.407  
7.387  
7.342  
7.340  
7.330  
7.327  
7.323  
7.321  
7.311  
7.309  
7.260  
7.182  
7.168  
7.161  
7.147  
7.058  
7.052  
7.038  
7.031  
7.017  
7.010  
— 3.996

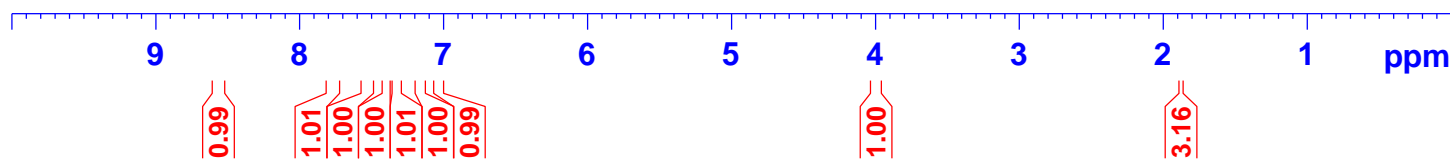
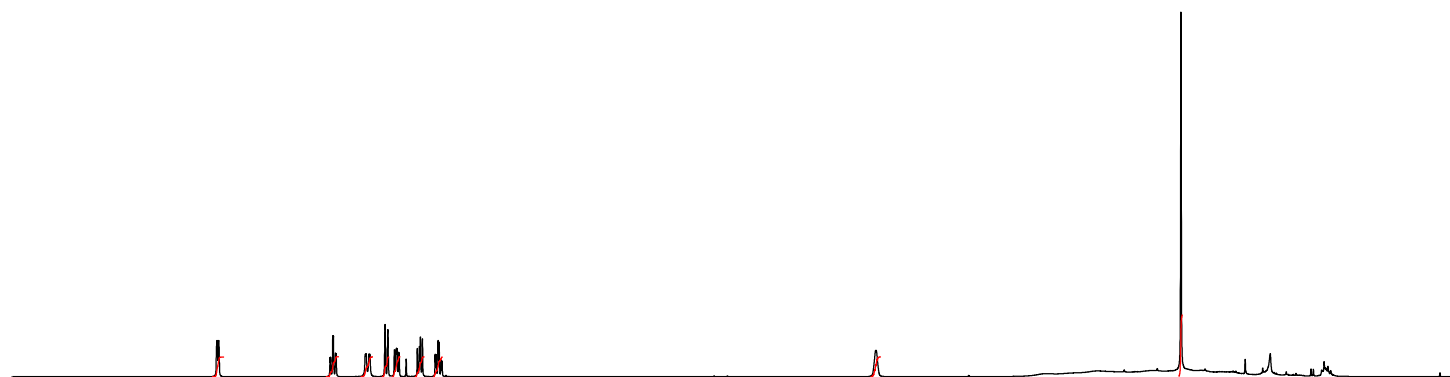
— 1.877



Current Data Parameters  
 NAME CY-H-A-58p-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161111  
 Time 12.23 h  
 INSTRUM spect  
 PROBHD z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 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



163.344  
161.590  
160.885

147.932

141.232  
141.201

136.843

131.591  
131.514

125.377  
123.739  
123.531

122.810

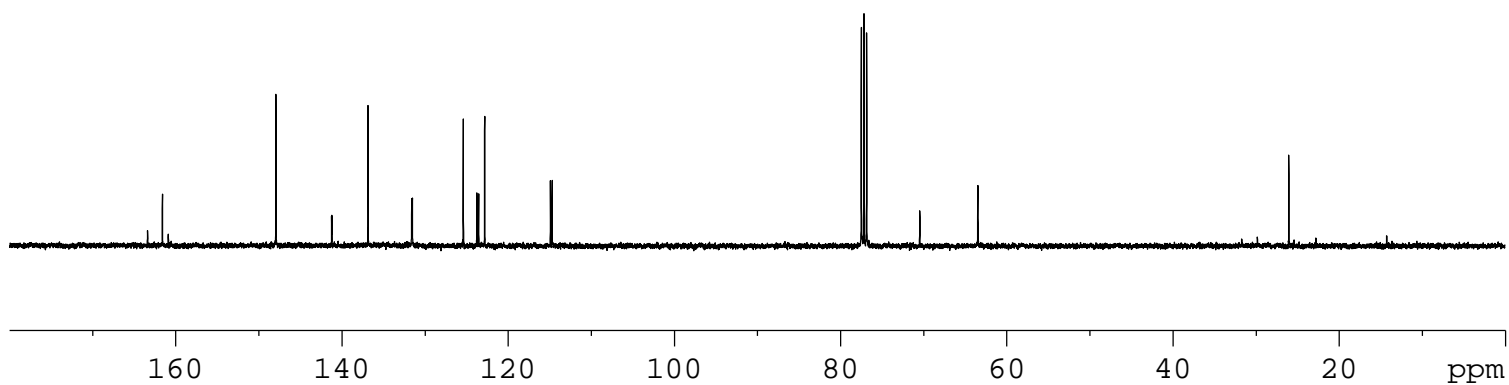
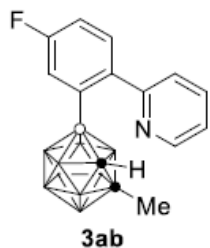
114.894  
114.683

77.475  
77.157  
76.839

70.443

63.450

26.036



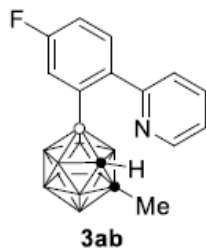
CY-C-A-58P-CDCl3

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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 41.2500000 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



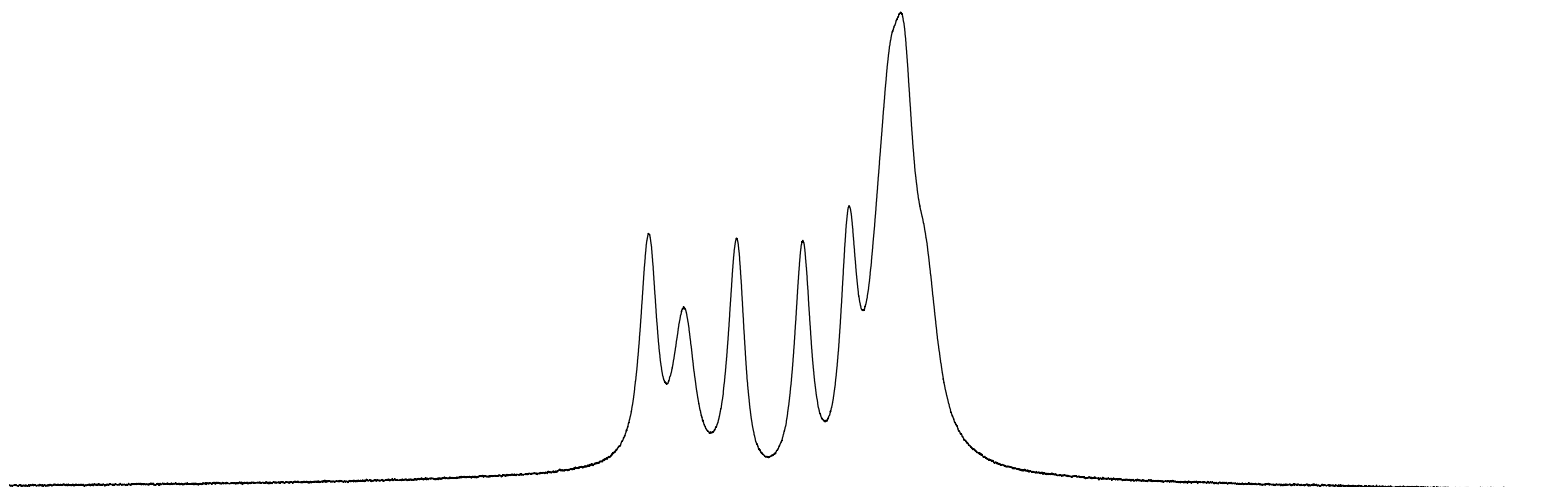
— -2.85  
 — -4.12  
 — -6.01  
 — -8.38  
 — -10.03  
 — -11.87

CY-B-A-58p

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

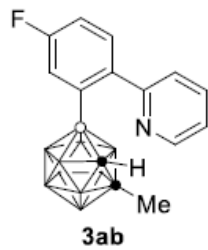
F2 - Acquisition Parameters  
 Date\_ 20161111  
 Time 12.41 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 12  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 181  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.8 K  
 D1 2.00000000 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

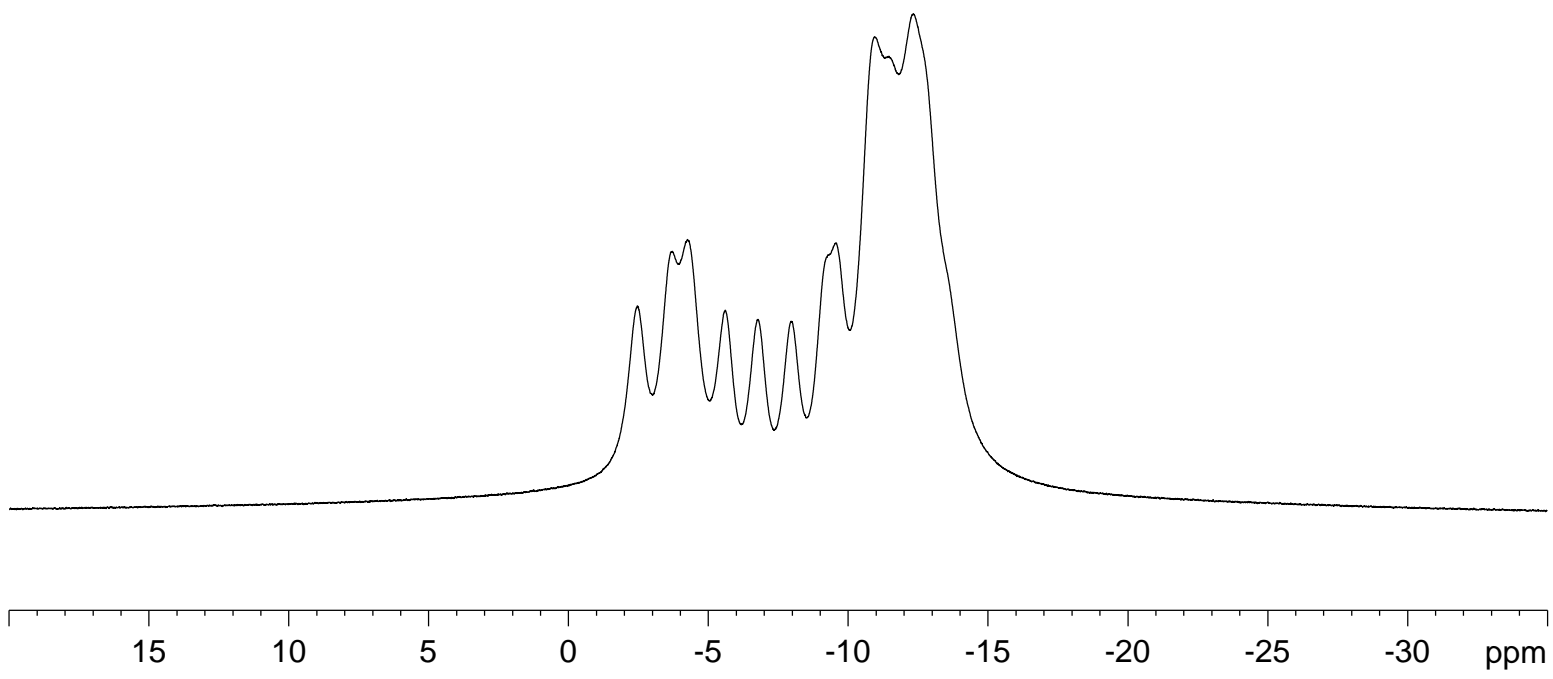


1.10  
 1.05  
 1.07  
 1.09  
 1.09  
 5.00

15 10 5 0 -5 -10 -15 -20 -25 -30 ppm



| -2.46  
 | -3.71  
 | -4.25  
 | -5.61  
 | -6.78  
 | -7.98  
 | -9.58  
 | -10.96  
 | -12.33



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

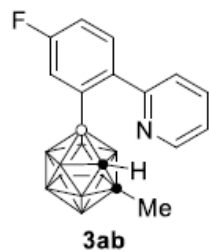
Current Data Parameters  
 NAME CY-B-A-58p-(C)  
 EXPNO 1  
 PROCNO 1

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

-115.61

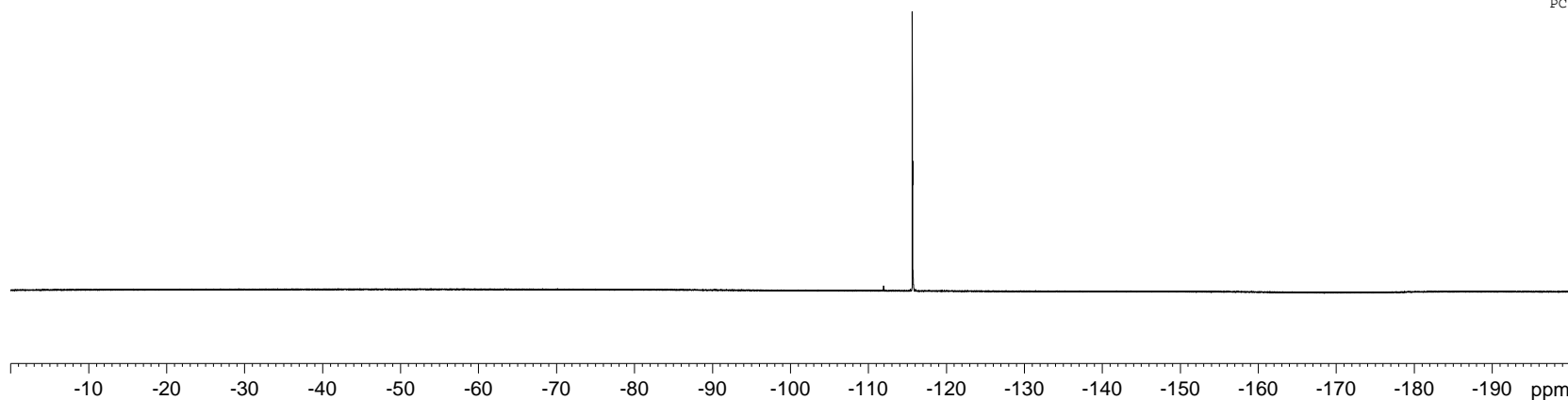
CY-F-A-58P-re



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 zgfhigpn.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 1.0000000 sec  
D11 0.0300000 sec  
D12 0.0000200 sec  
TD0 1  
SFO1 376.5548010 MHz  
NUC1 19F  
P1 14.70 usec  
PLW1 18.3600061 W  
SFO2 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.5600042 W  
PLW12 0.27428001 W

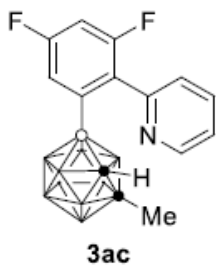
F2 - Processing parameters  
SI 65536  
SF 376.5924602 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



8.637  
7.801  
7.796  
7.781  
7.777  
7.762  
7.758  
7.428  
7.409  
7.377  
7.365  
7.361  
7.358  
7.346  
7.324  
7.260  
6.876  
6.870  
6.853  
6.849  
6.847  
6.832  
6.826

3.578

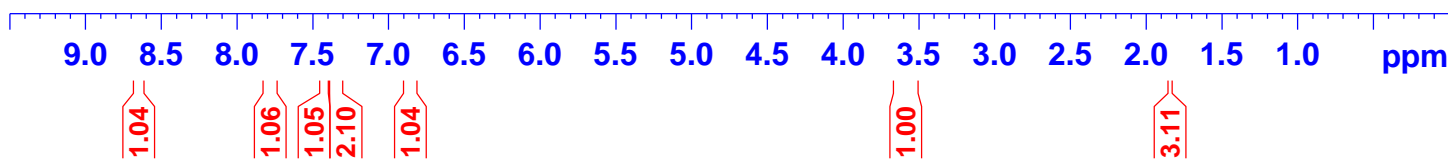
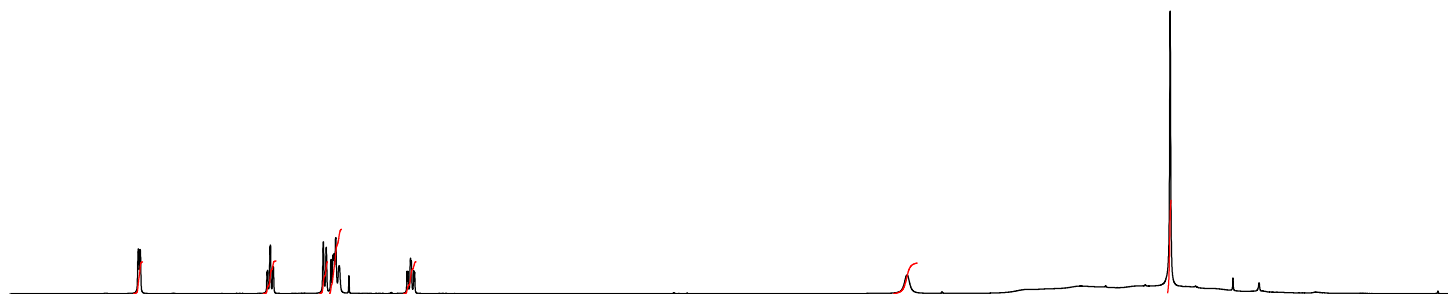
1.841



Current Data Parameters  
 NAME CY-H-A-66p-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161120  
 Time 11.36 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 400.1324708 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 8.31000042 W

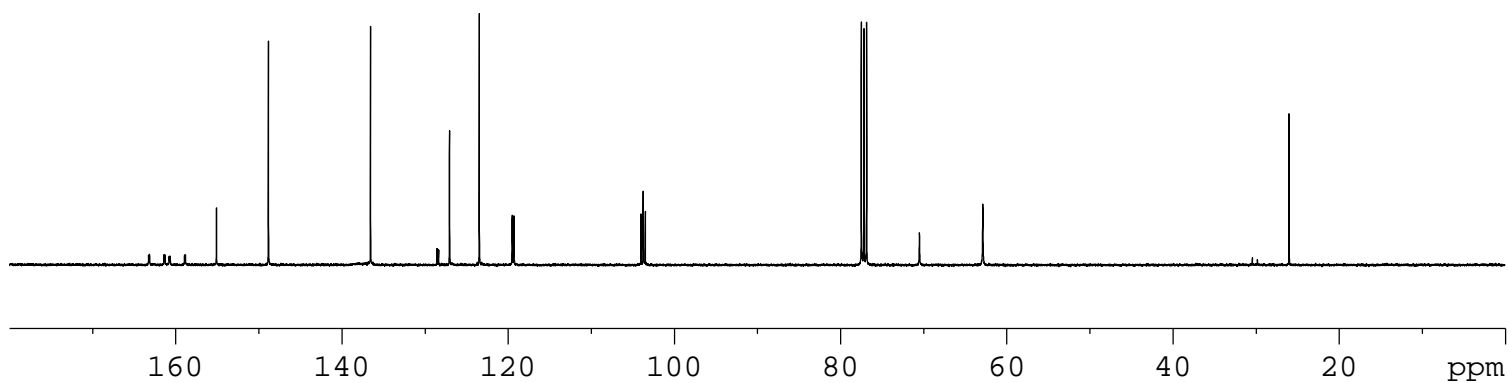
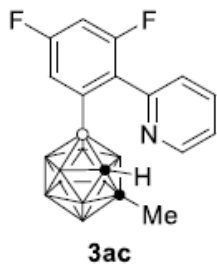
F2 - Processing parameters  
 SI 65536  
 SF 400.1300101 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



163.260  
163.140  
161.390  
161.274  
160.778  
160.658  
158.935  
158.820  
155.088  
148.834  
136.545  
128.539  
128.502  
128.382  
128.345  
127.038  
123.455  
119.515  
119.481  
119.310  
119.277  
103.991  
103.738  
103.726  
103.474

77.476  
77.159  
76.841  
70.481  
62.854

25.990



CY-C-A-66P-CDCl3

Bruker Advance III 400

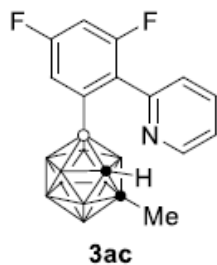
Current Data Parameters  
NAME CY-C-A-66P-CDCl3  
EXPNO 1  
PROCNO 1

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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 41.2500000 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

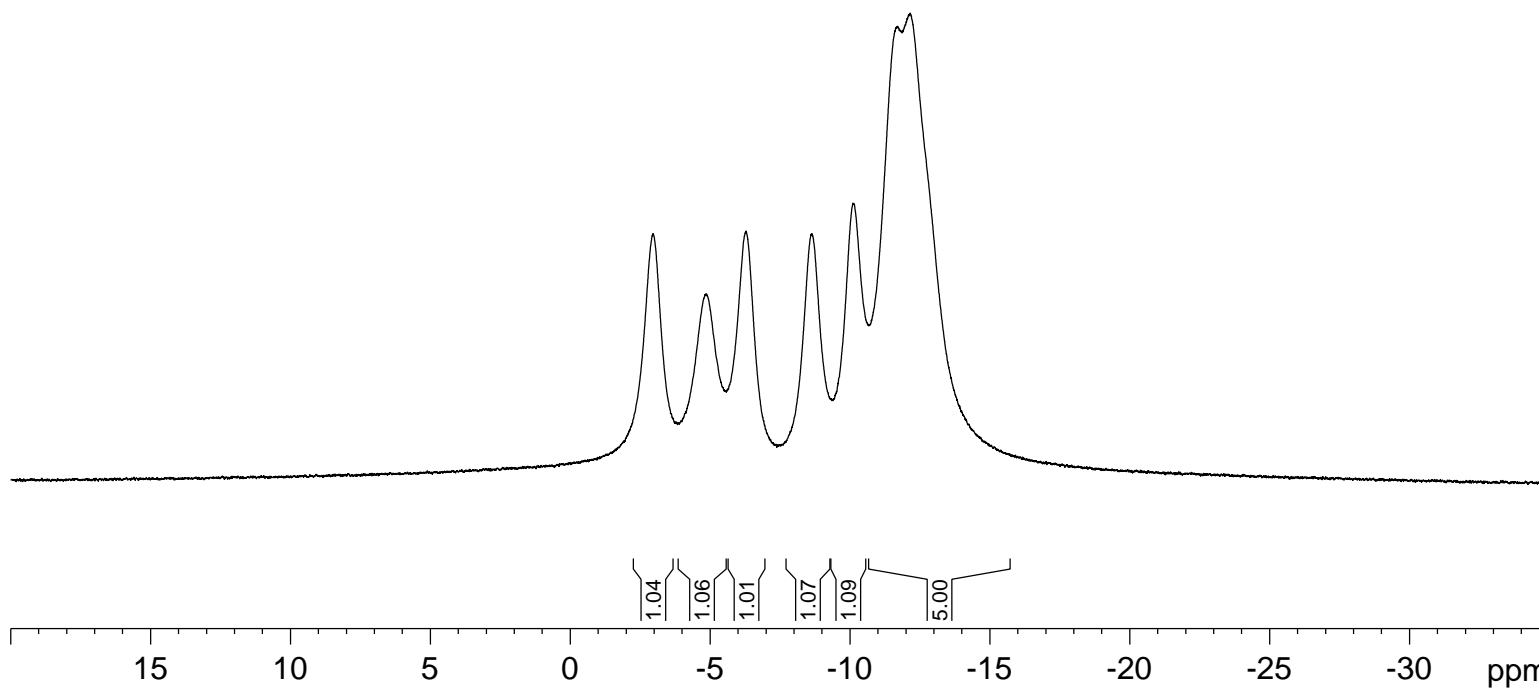


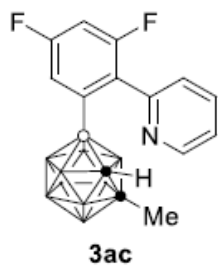
— -2.97  
— -4.86  
— -6.28  
— -8.65  
— -10.11  
— -12.15

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 CDC13  
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





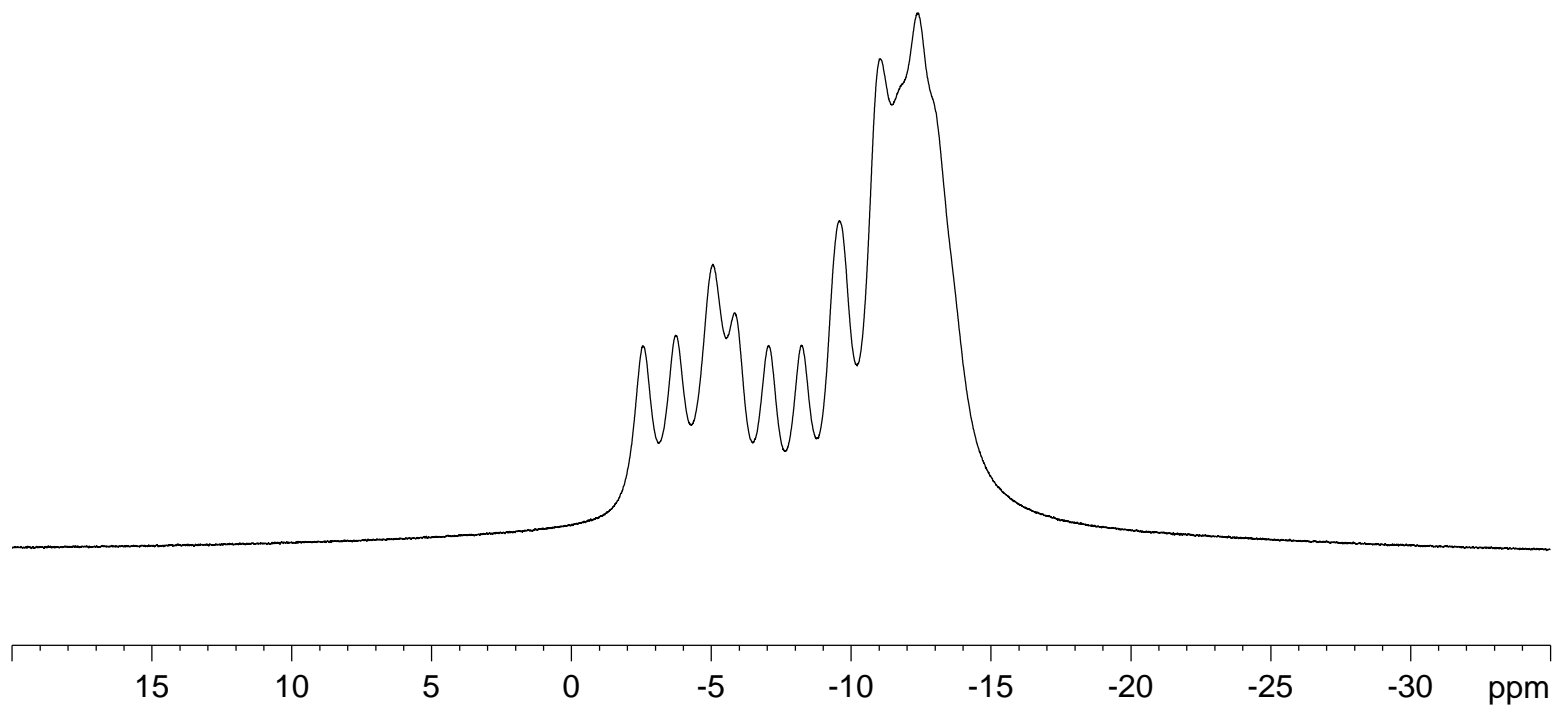
| -2.54  
 | -3.72  
 | -5.05  
 | -5.82  
 | -7.05  
 | -8.22  
 | -9.58  
 | -11.05  
 | -12.35

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

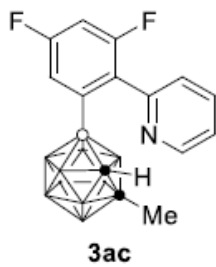


CY-F-A-66P

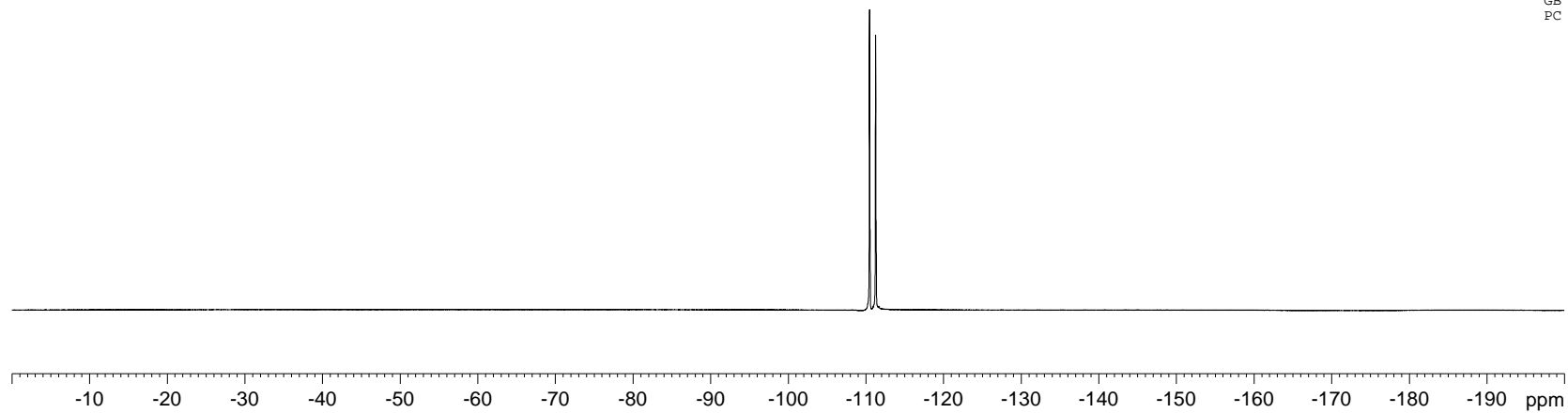
Current Data Parameters  
NAME CY-F-A-66P  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161120  
Time 19.47 h  
INSTRUM spect  
PROBHD Z108618\_0257 ( )  
PULPROG zgfhggn.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  
CPDPRGf2 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



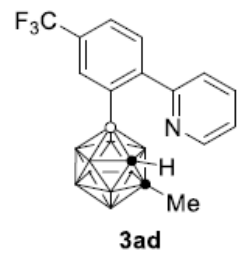
-110.48  
-111.26



8.072  
7.843  
7.839  
7.824  
7.820  
7.805  
7.801  
7.626  
7.623  
7.606  
7.603  
7.436  
7.417  
7.401  
7.388  
7.386  
7.382  
7.369  
7.323  
7.303  
7.260

3.985

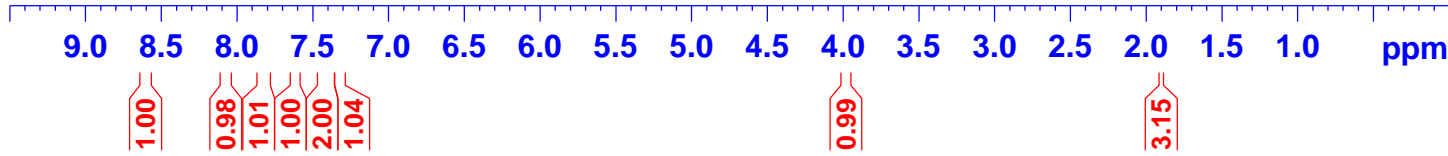
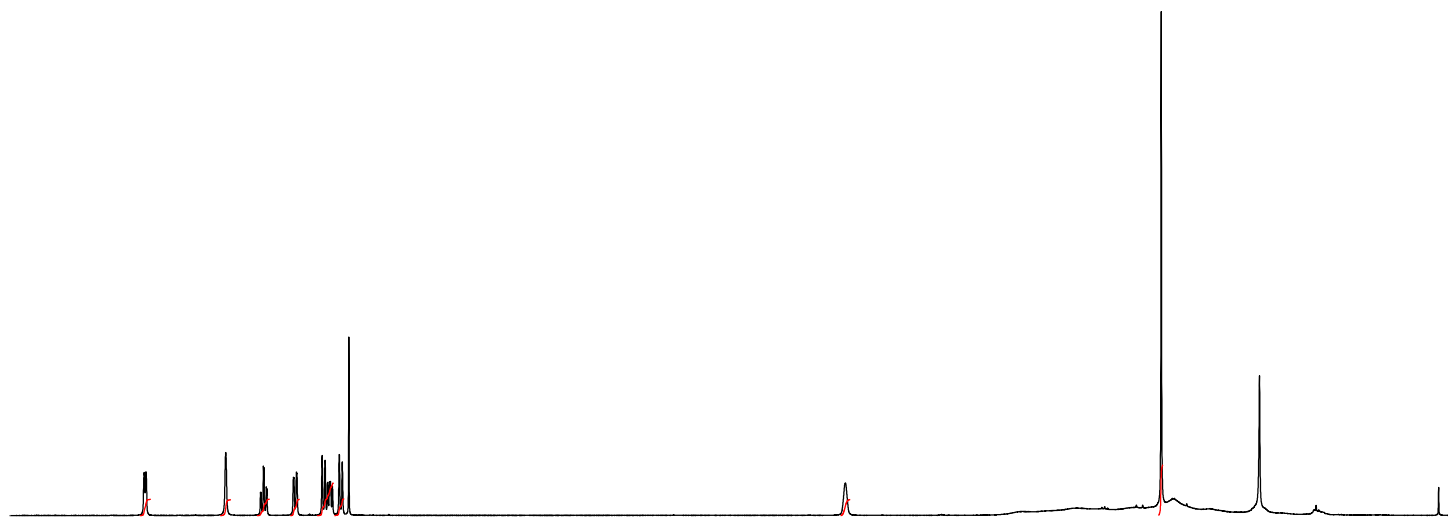
1.900

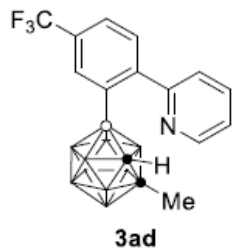


Current Data Parameters  
 NAME CY-H-A-34p-p  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160913  
 Time 21.32 h  
 INSTRUM spect  
 PROBHD z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 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





161.20  
148.49  
148.15  
136.98  
133.88  
133.83  
133.79  
133.76  
130.30  
130.09  
129.98  
129.66  
129.38  
128.41  
125.70  
125.03  
124.82  
124.79  
124.75  
124.71  
123.21  
122.99  
120.29

77.48  
77.16  
76.84  
70.64  
63.48

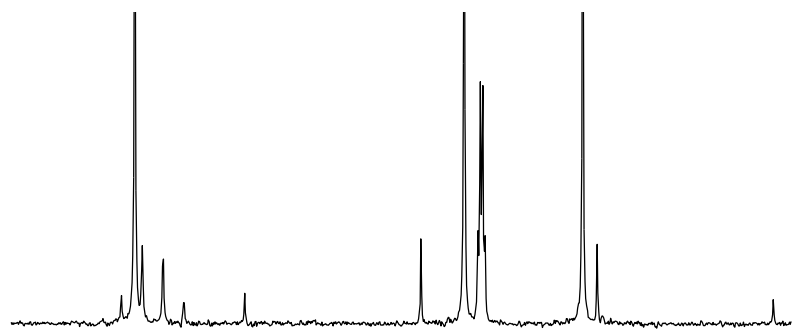
26.05

CY-C-A-34p-re

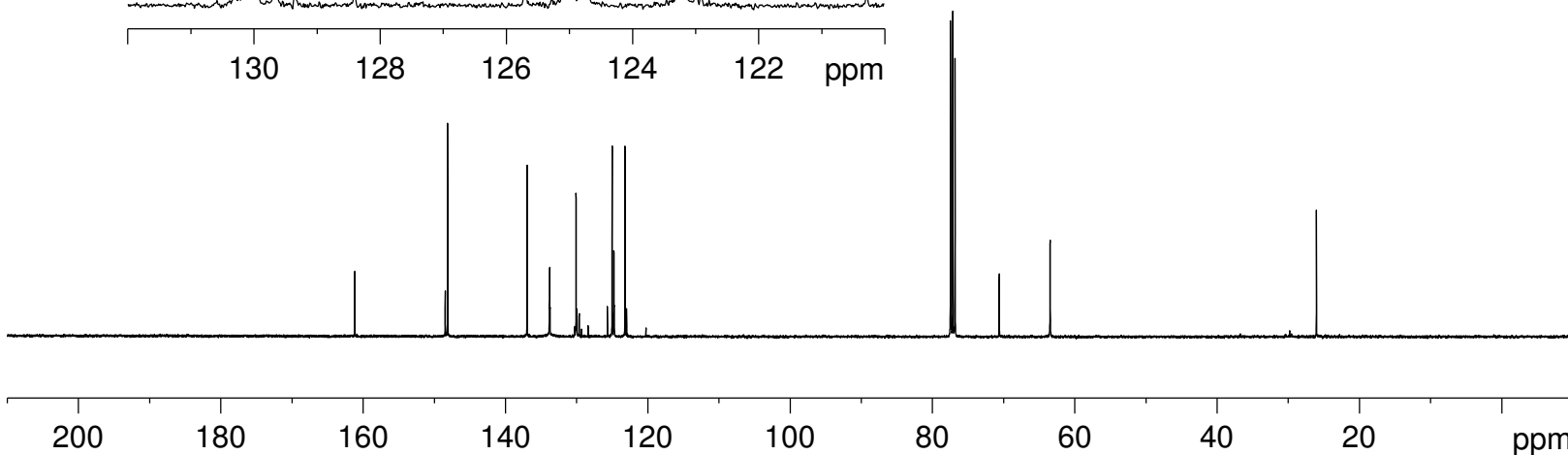
Current Data Parameters  
NAME CY-C-A-34p-re2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161123  
Time 19.45 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
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 2.0000000 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

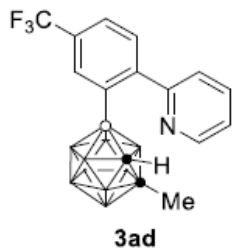
130.30  
130.09  
129.98  
129.66  
129.38  
128.41  
125.70  
125.03  
124.82  
124.79  
124.75  
124.71  
123.21  
122.99  
120.29



130 128 126 124 122 ppm



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



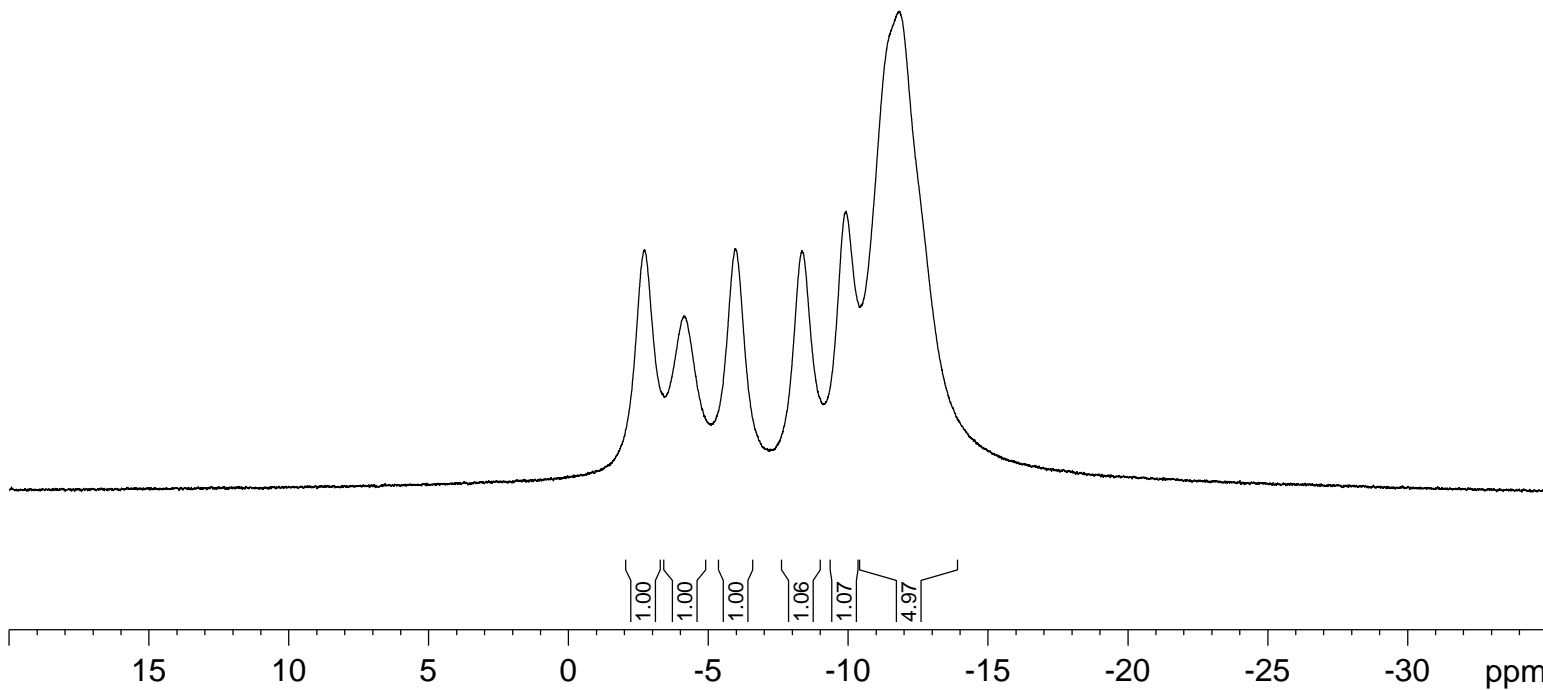
— 2.71  
 — 4.12  
 — 5.95  
 — 8.34  
 — 9.92  
 — 11.83

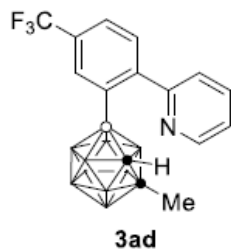
CY-B-A-34p

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





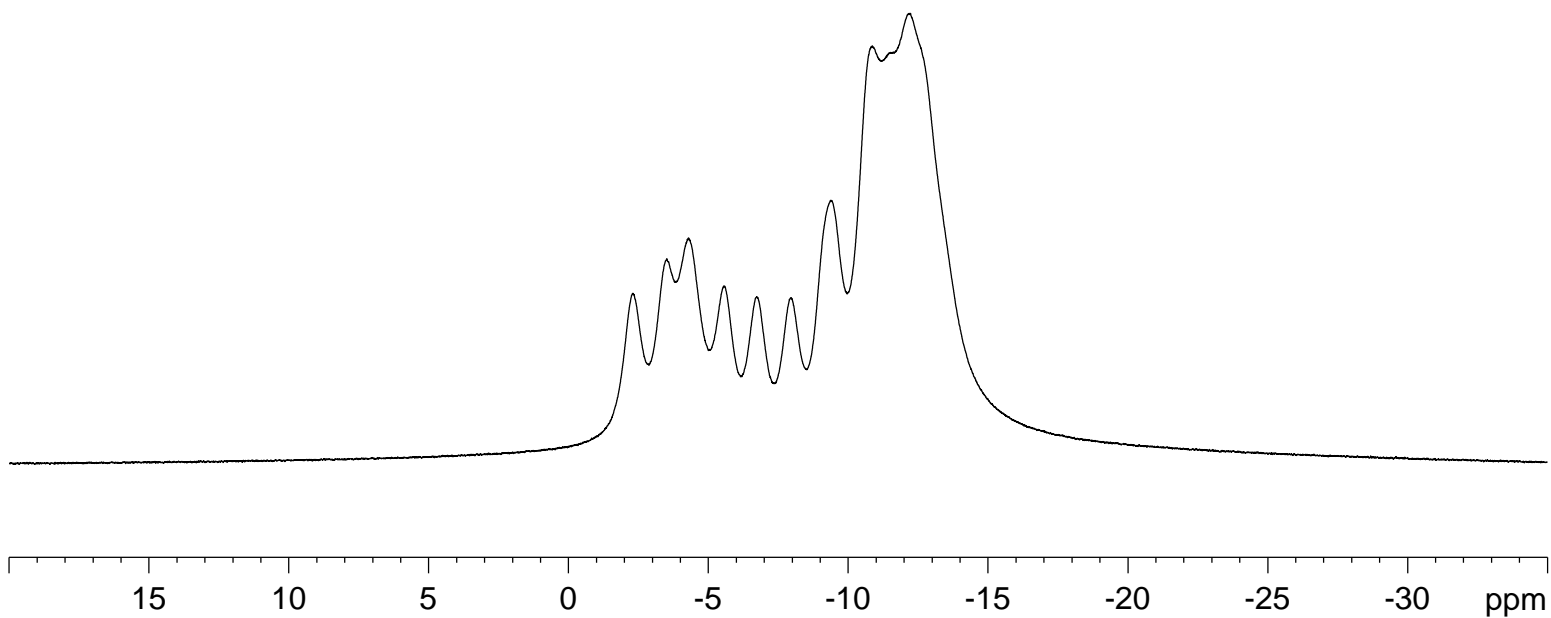
-2.30  
 -3.51  
 -4.29  
 -5.56  
 -6.74  
 -7.96  
 -9.38  
 -10.86  
 -11.44  
 -12.23

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

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

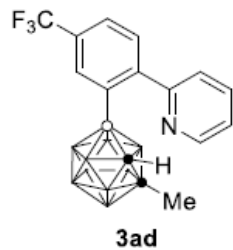
F2 - Acquisition Parameters  
 Date\_ 20161124  
 Time 16.55 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 32  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 181  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.5 K  
 D1 2.00000000 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

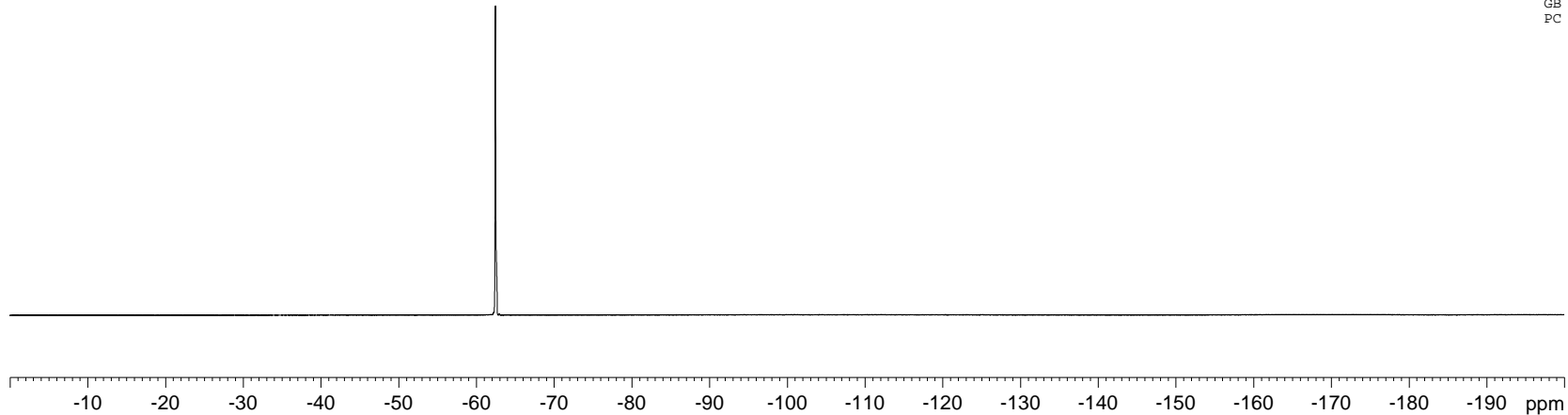
CY-F-A-34P



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

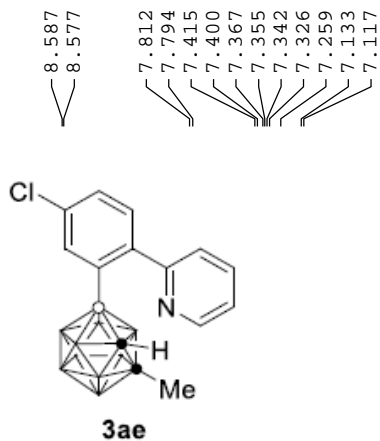
F2 - Acquisition Parameters  
Date\_ 20161124  
Time 16.38 h  
INSTRUM spect  
PROBHD Z108618\_0257 ( )  
PULPROG zgfhggn.2  
TD 131072  
SOLVENT CDCl3  
NS 20  
DS 4  
SWH 89285.711 Hz  
FIDRES 0.681196 Hz  
AQ 0.7340032 sec  
RG 645  
DW 5.600 usec  
DE 6.50 usec  
TE 296.0 K  
D1 1.00000000 sec  
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  
CPDPRGf2 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



8.587  
8.577  
7.812  
7.794  
7.415  
7.400  
7.367  
7.355  
7.342  
7.326  
7.259  
7.133  
7.117

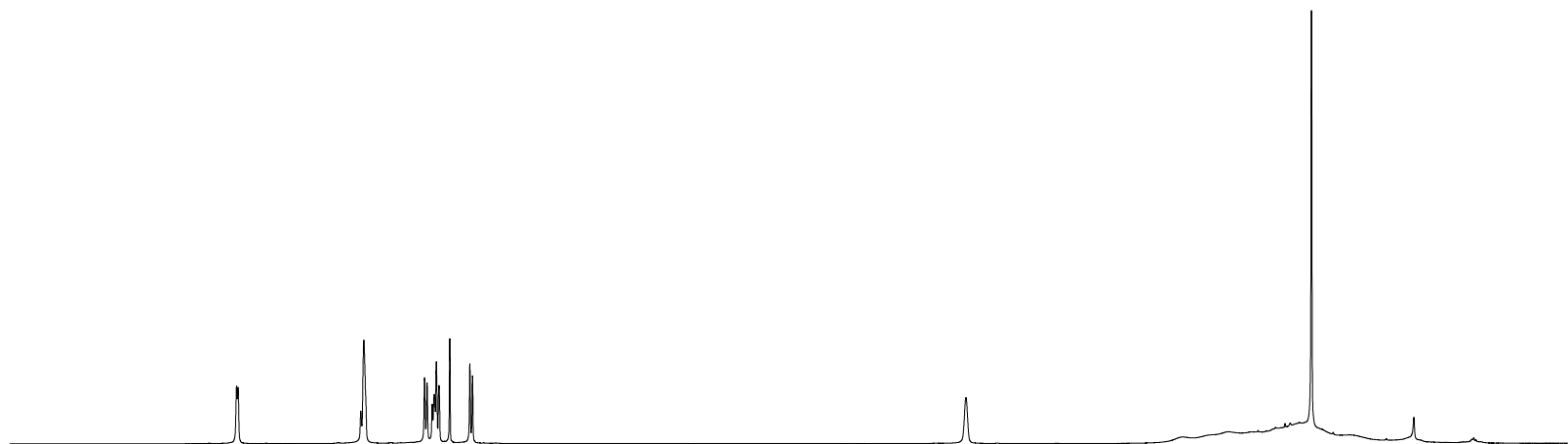
4.043

1.891

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  
SF01 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



9 8 7 6 5 4 3 2 1 ppm

1.000

1.966

1.003

1.981

1.004

1.031

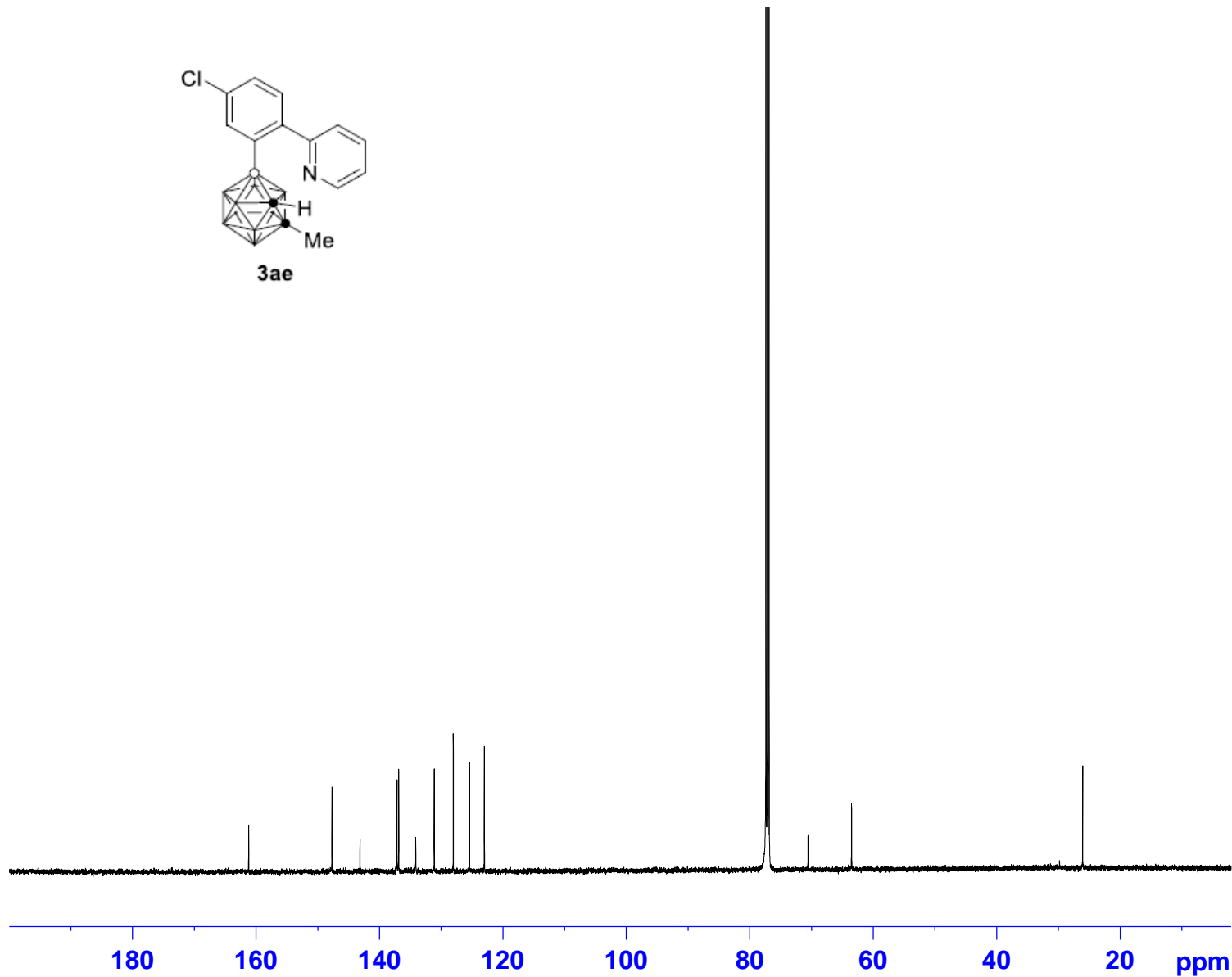
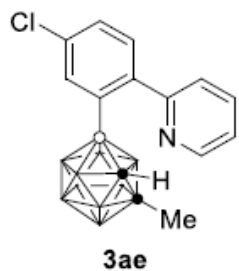
3.099

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

161.23  
147.73  
143.18  
137.19  
136.91  
134.15  
131.14  
128.07  
125.45  
123.03

77.40  
77.15  
76.89  
70.57  
63.52

26.08

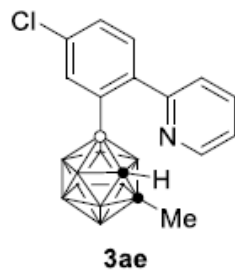


Current Data Parameters  
NAME CY-C-B-199P-4-Cl  
EXPNO 1  
PROCNO 1

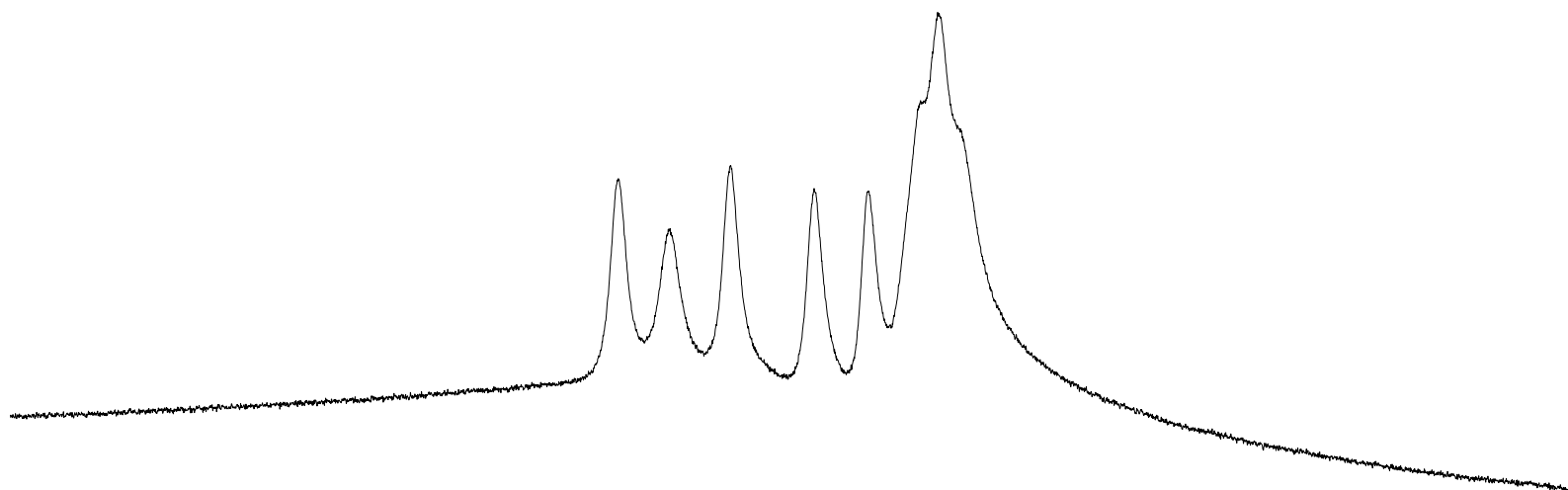
F2 - Acquisition Parameters  
Date\_ 20190228  
Time 14.28 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 640  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
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



— -2.57  
— -4.07  
— -5.82  
— -8.22  
— -9.78  
— -11.79



0.97 1.09 0.97 0.99 0.94 5.00

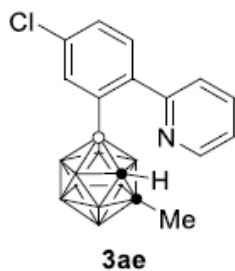
Current Data Parameters  
NAME CY-B-B-199P-4-Cl  
EXPNO 1  
PROCNO 1

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)

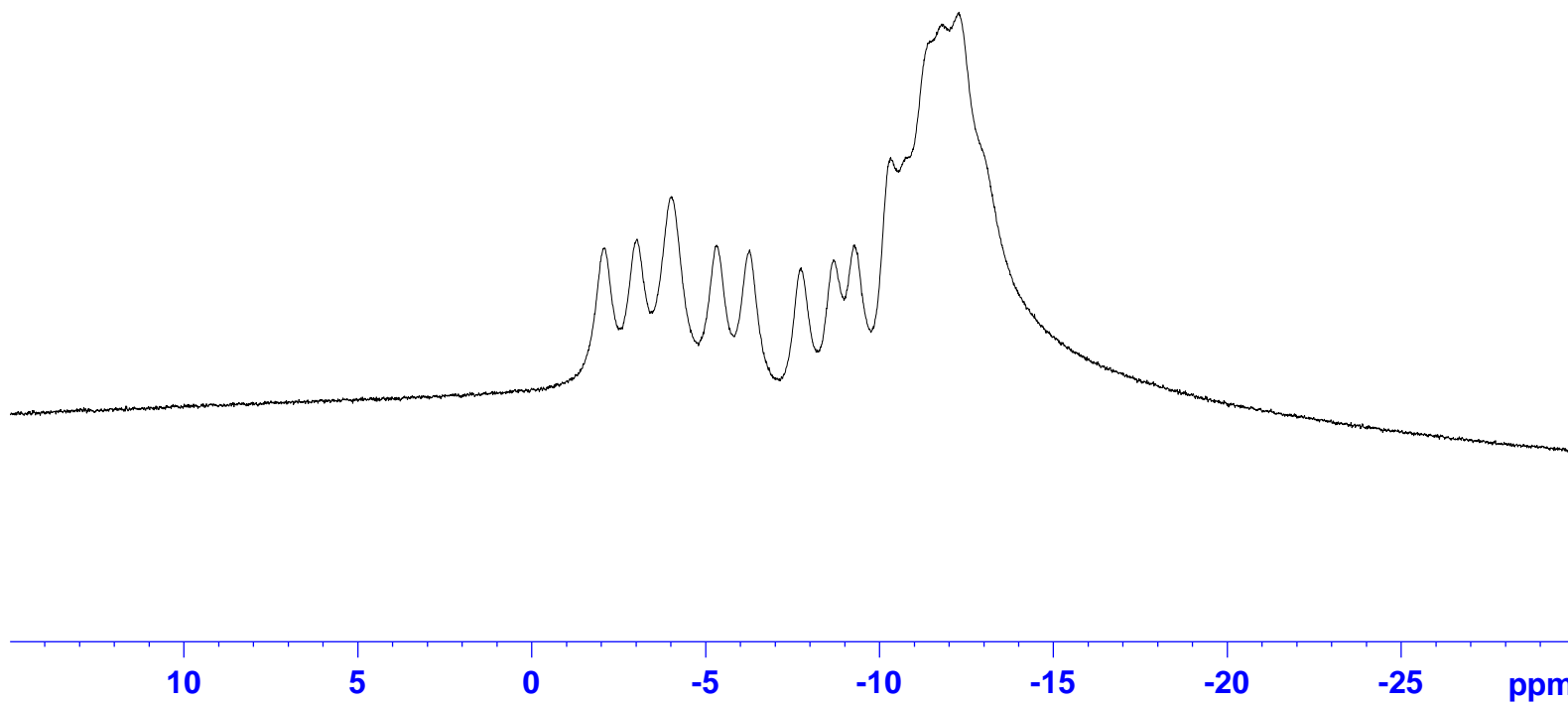
— 2.09  
— 3.03  
— 4.02  
— 5.32  
— 6.27  
— 7.75  
— 8.68  
— 9.29  
— 10.29  
— 10.70  
— 11.37  
— 11.78  
— 12.28



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  
SF01 160.4615792 MHz  
NUC1 11B  
P1 15.00 usec  
PLW1 50.00000000 W

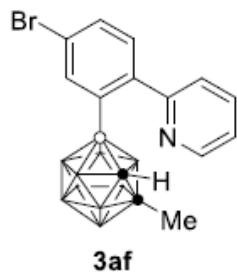
F2 - Processing parameters  
SI 16384  
SF 160.4615997 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



8.563  
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

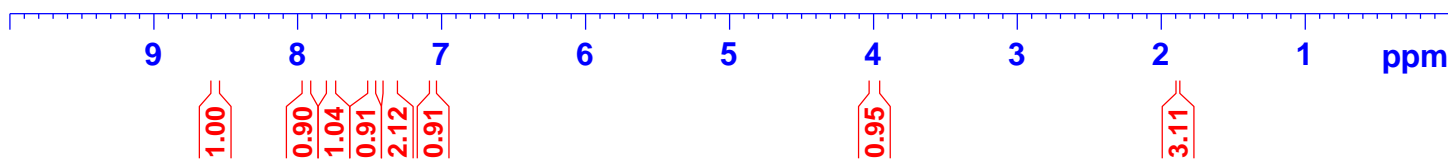
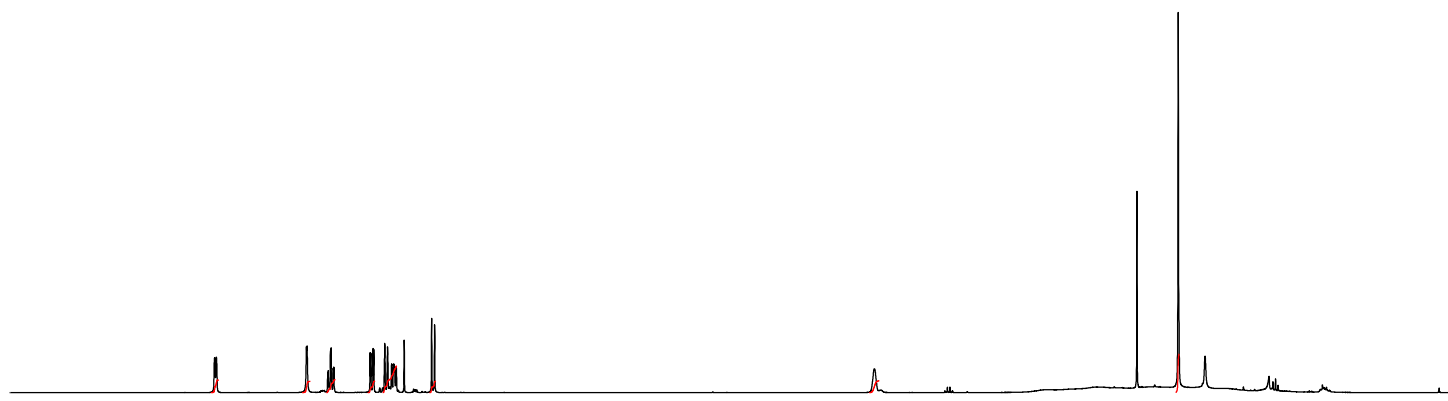
1.882

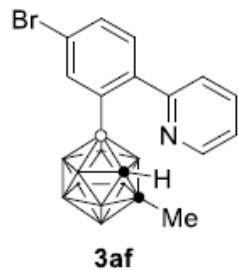


Current Data Parameters  
 NAME CY-H-A-57p-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161104  
 Time 18.25 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 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





161.438  
 148.034  
 144.024  
 139.665  
 136.869  
 131.388  
 130.985  
 125.198  
 122.924  
 122.500

77.474  
 77.156  
 76.838  
 70.488  
 63.481

26.072

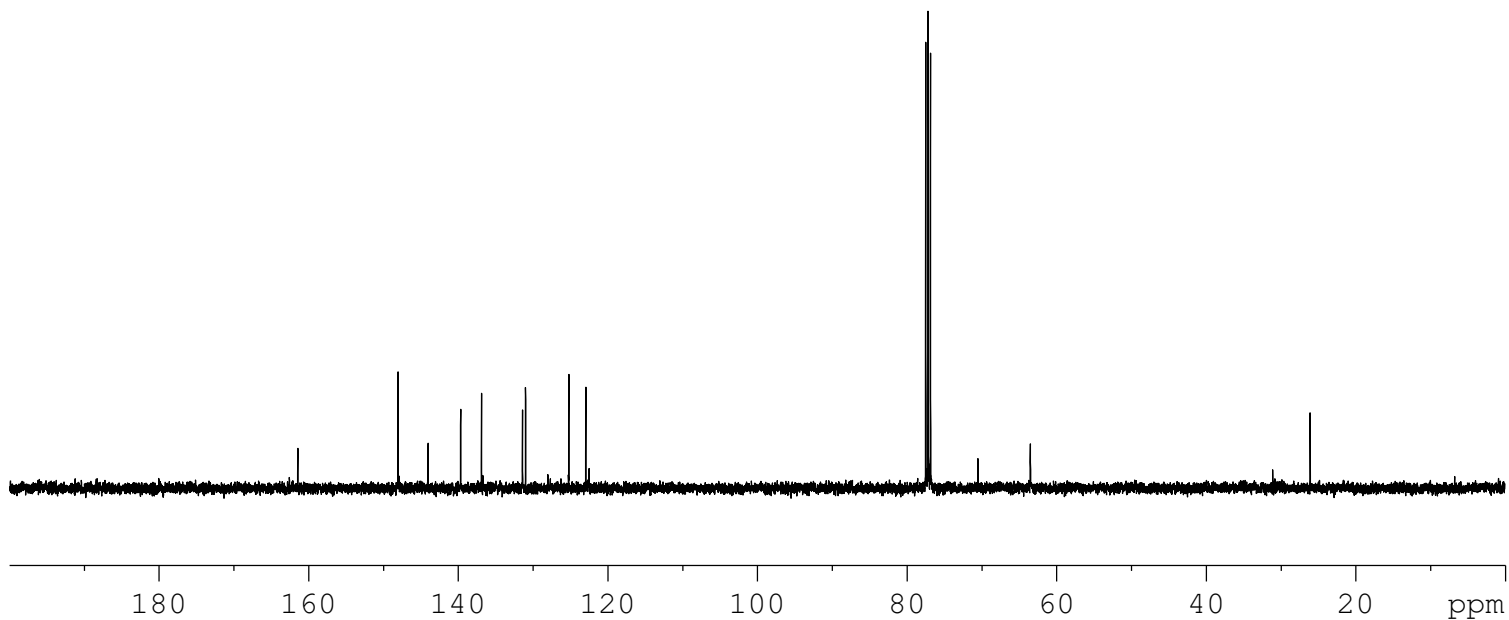
CY-C-A-57P-CDCl3

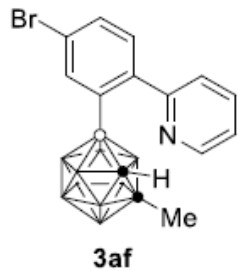
Bruker Advance III 400

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 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 41.2500000 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 FCPD2 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





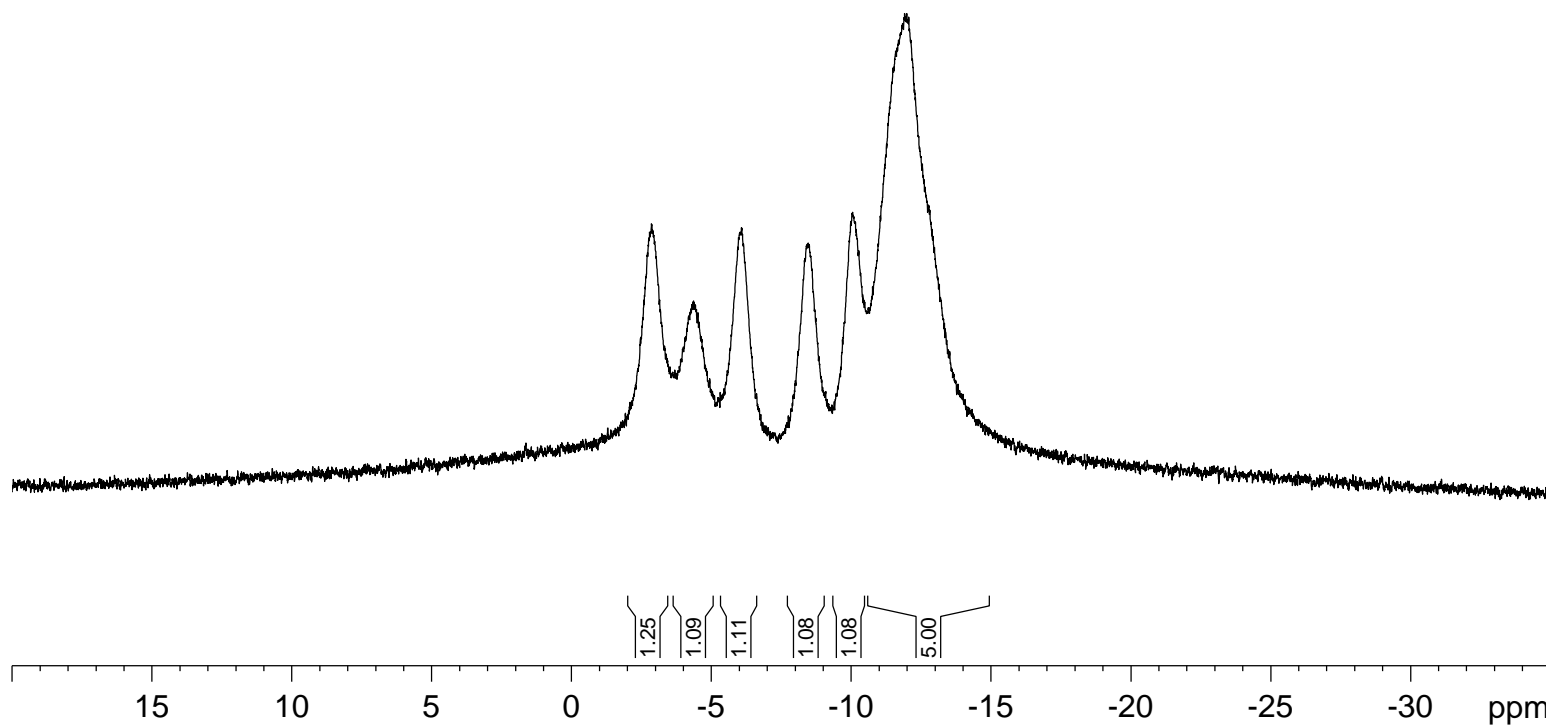
— -2.86  
 — -4.36  
 — -6.08  
 — -8.46  
 — -10.05  
 — -11.98

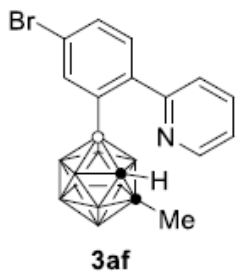
CY-B-A-57P

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





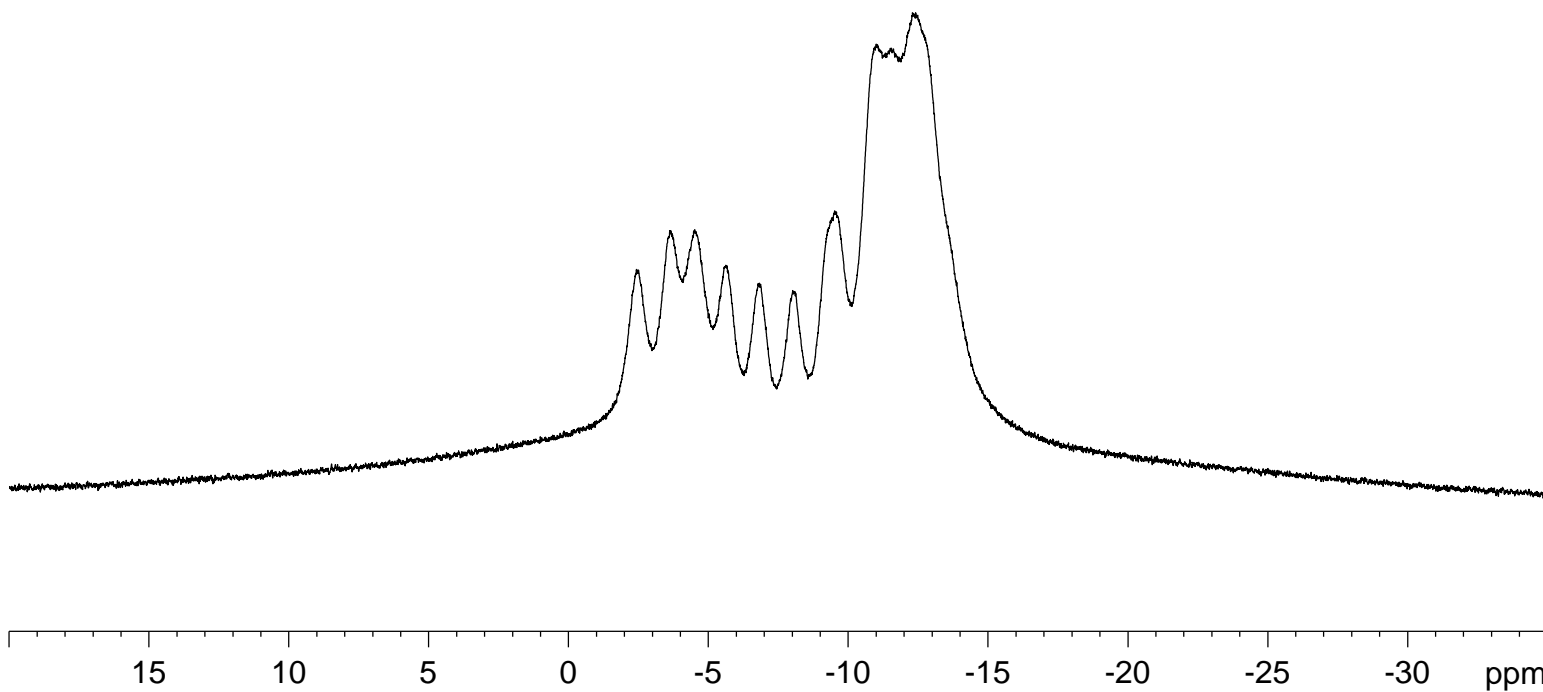
| -2.43  
 | -3.62  
 | -4.51  
 | -5.63  
 | -6.83  
 | -8.02  
 | -9.52  
 | -11.00  
 | -12.41

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

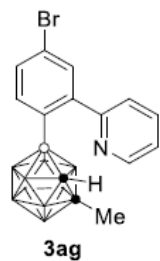
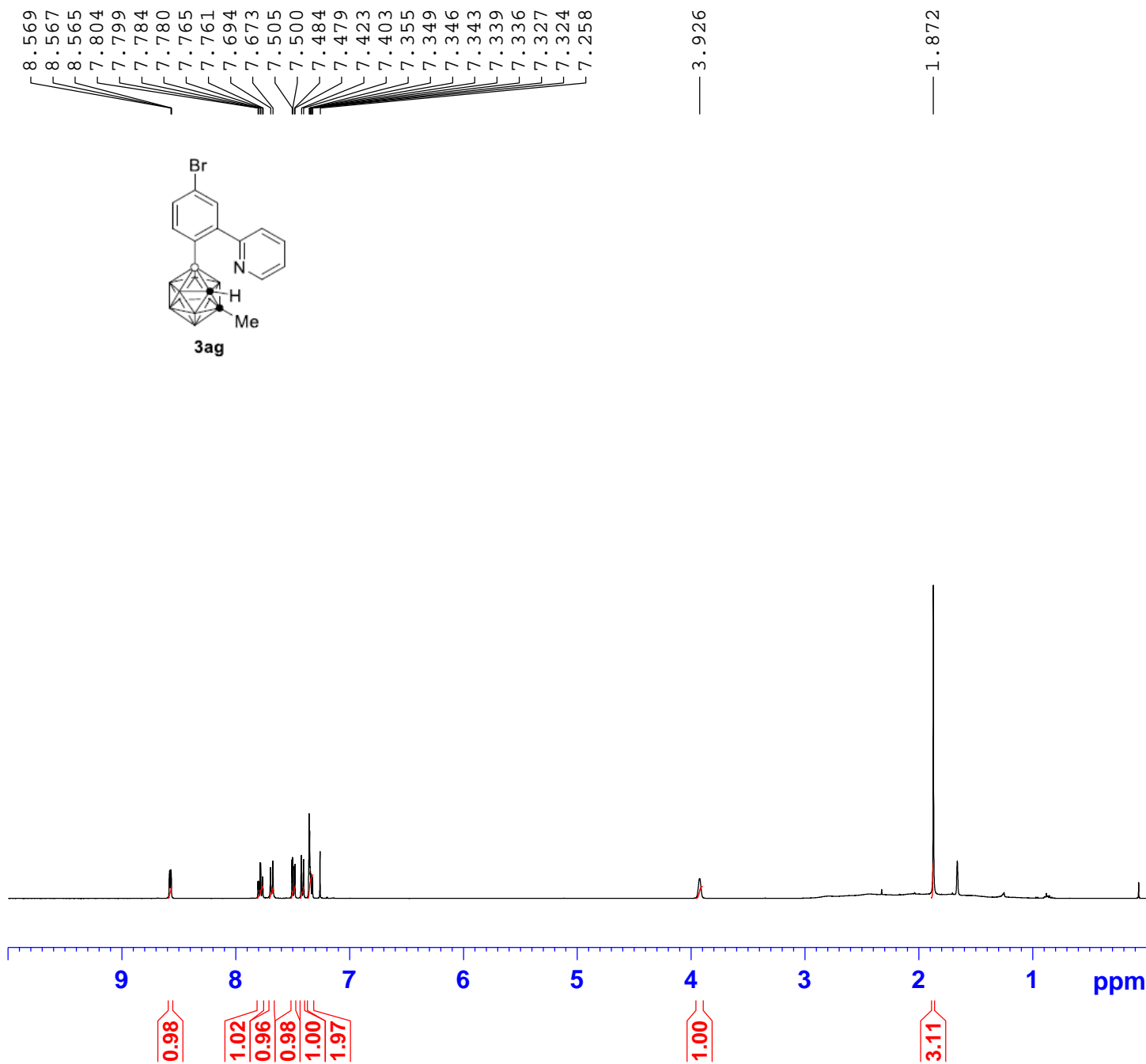
Current Data Parameters  
 NAME CY-B-A-57P-(C)  
 EXPNO 1  
 PROCNO 1

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







Current Data Parameters  
 NAME CY-H-A-56p-CDC13  
 EXPNO 1  
 PROCNO 1

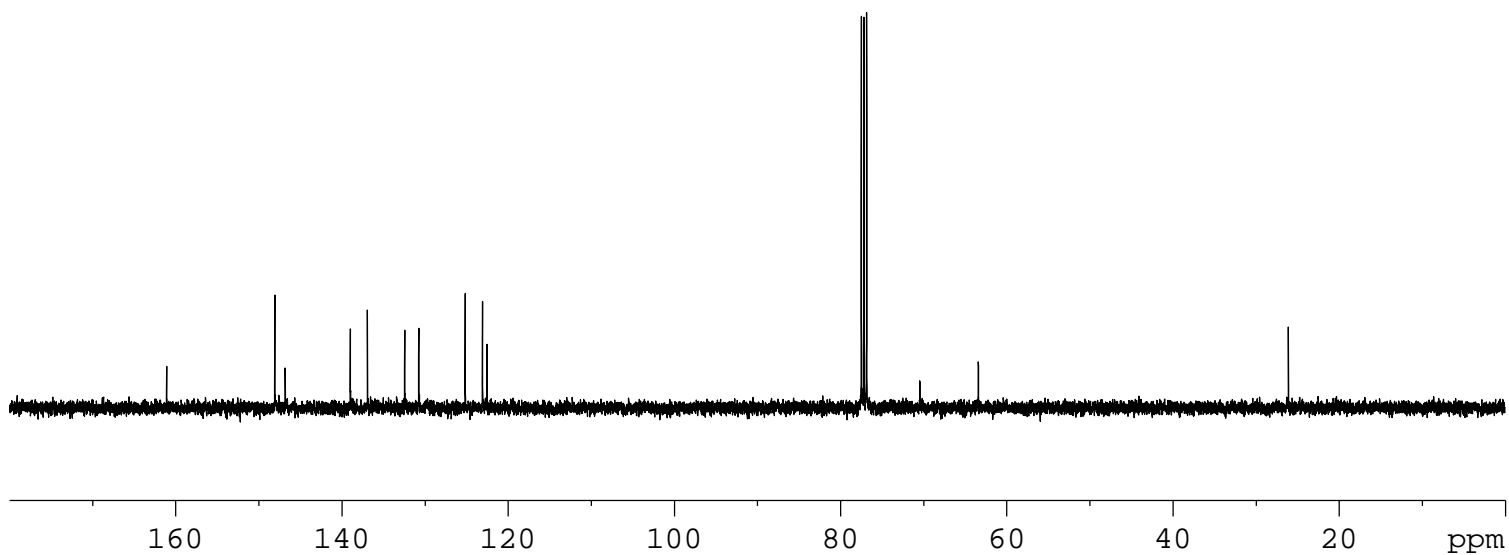
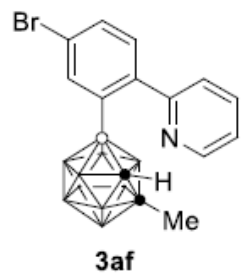
F2 - Acquisition Parameters  
 Date\_ 20161104  
 Time 14.40 h  
 INSTRUM spect  
 PROBHD z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 9  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.3 K  
 D1 1.00000000 sec  
 TD0 1  
 SF01 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

— 161.045  
 — 148.066  
 — 146.819  
 — 138.978  
 — 136.921  
 — 132.437  
 — 130.740  
 — 125.149  
 — 123.069  
 — 122.538

— 77.472  
 — 77.155  
 — 76.837  
 — 70.440  
 — 63.391

— 26.082



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 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 41.2500000 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 FCPD2 90.00 usec  
 PLW2 8.31000042 W  
 PLW12 0.23083000 W  
 PLW13 0.11611000 W

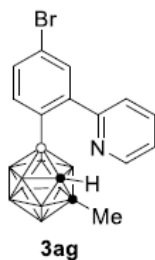
F2 - Processing parameters  
 SI 32768  
 SF 100.6127578 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

CY-B-A-56P

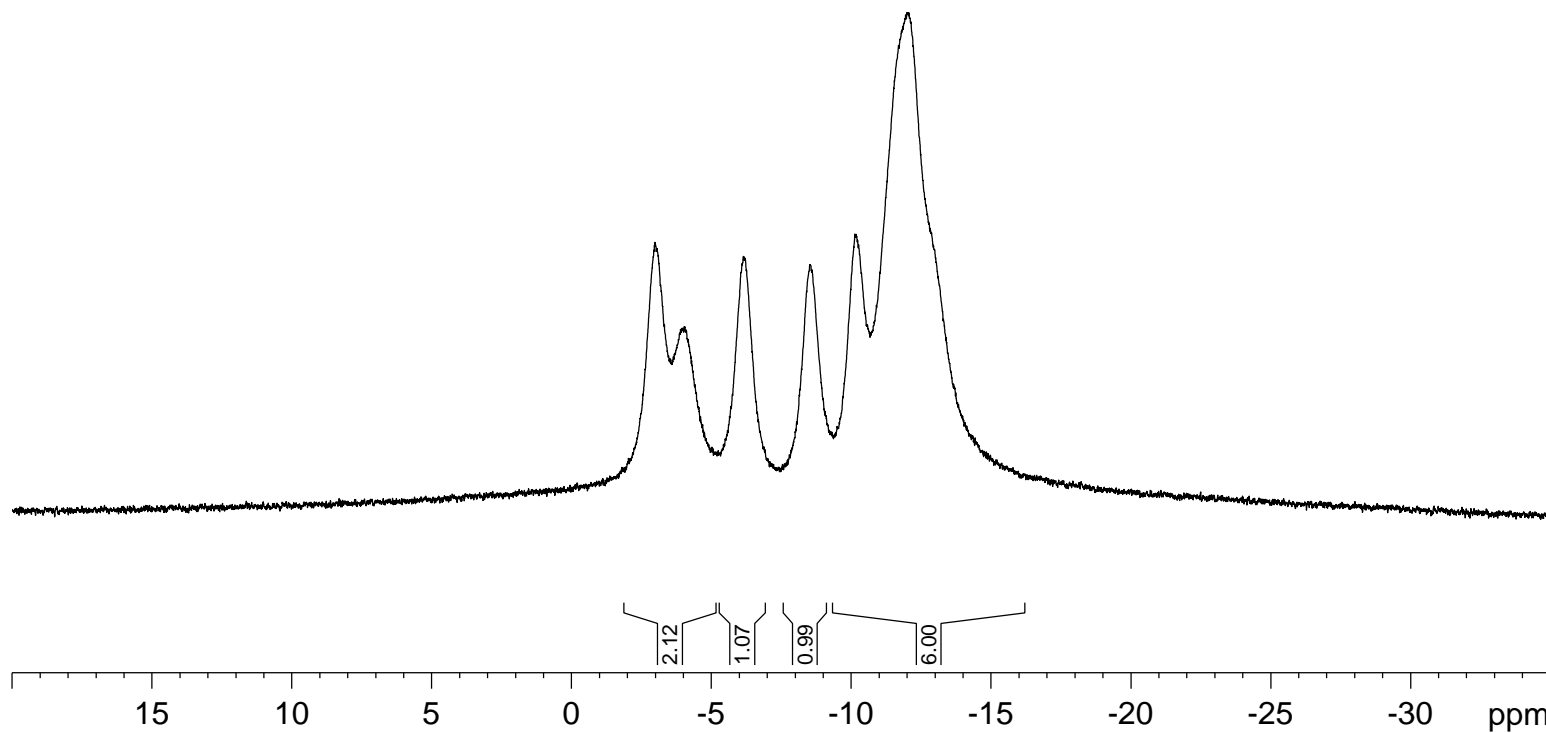
Current Data Parameters  
NAME CY-B-A-56P  
EXPNO 1  
PROCNO 1

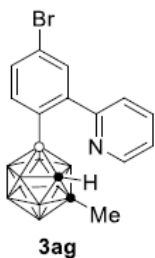
F2 - Acquisition Parameters  
Date\_ 20161104  
Time 15.27 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 7  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 256  
DW 20.800 usec  
DE 6.50 usec  
TE 295.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W  
SF02 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



— 3.06  
— 4.05  
— 6.22  
— 8.60  
— 10.18  
— 12.14





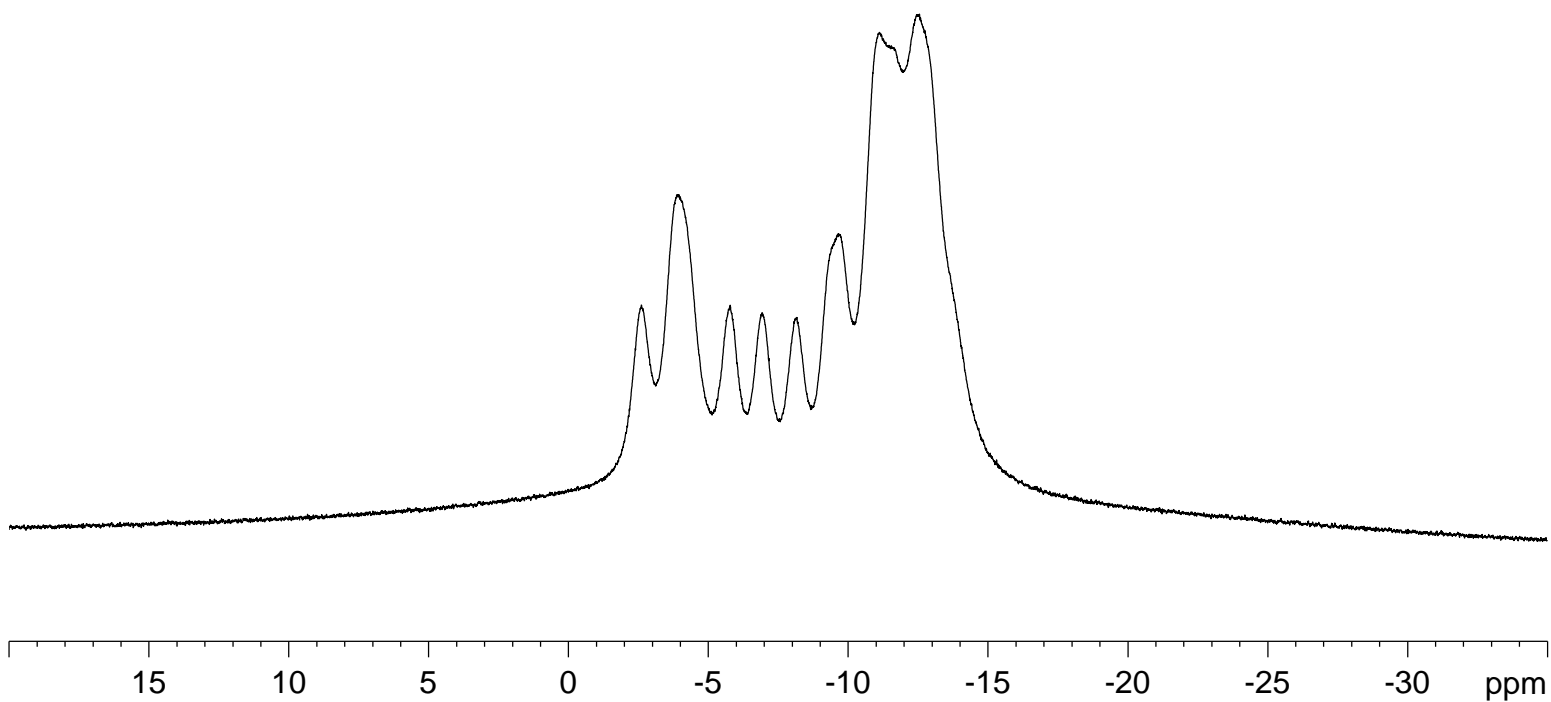
| -2.61  
 | -3.92  
 | -5.78  
 | -6.93  
 | -8.16  
 | -9.65  
 | -11.11  
 | -12.55

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

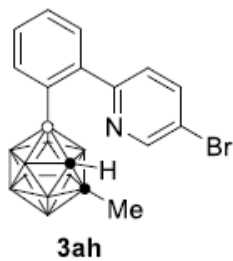
F2 - Processing parameters  
 SI 32768  
 SF 128.4097881 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



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

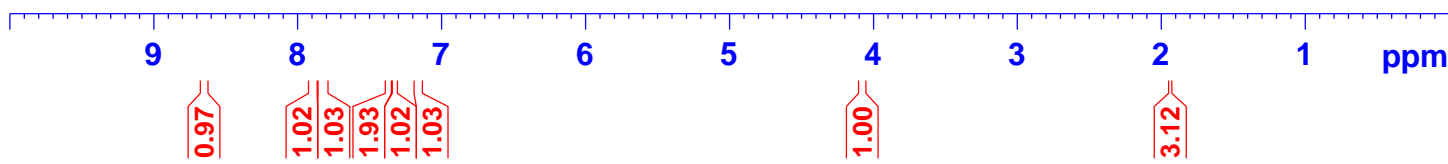
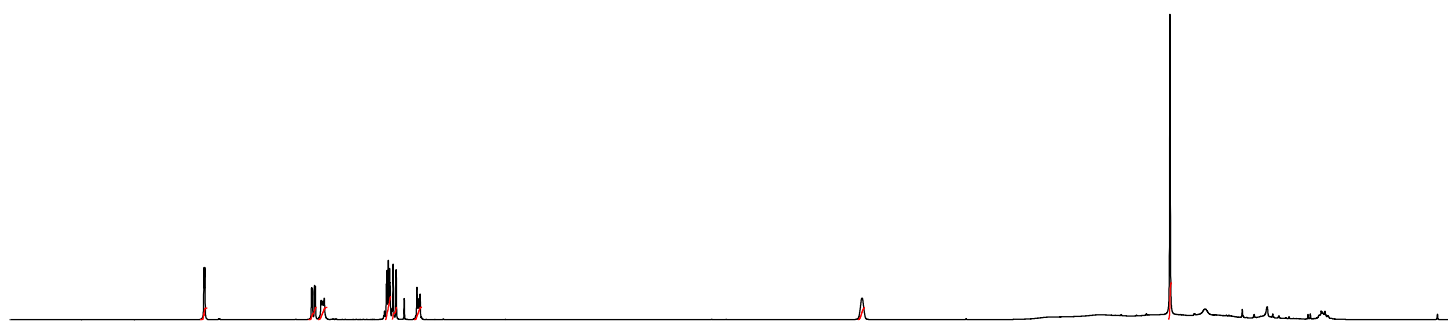
— 1.939



Current Data Parameters  
 NAME CY-H-A-64p-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161115  
 Time 19.28 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 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



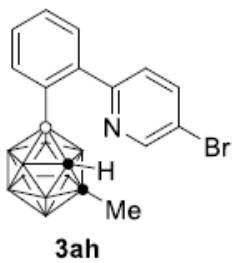
160.918  
148.890  
144.263  
139.275  
137.305  
129.725  
128.169  
127.957  
126.574  
119.810

77.475  
77.158  
76.840  
70.599  
63.604

26.125

CY-C-A-64P-CDCl3

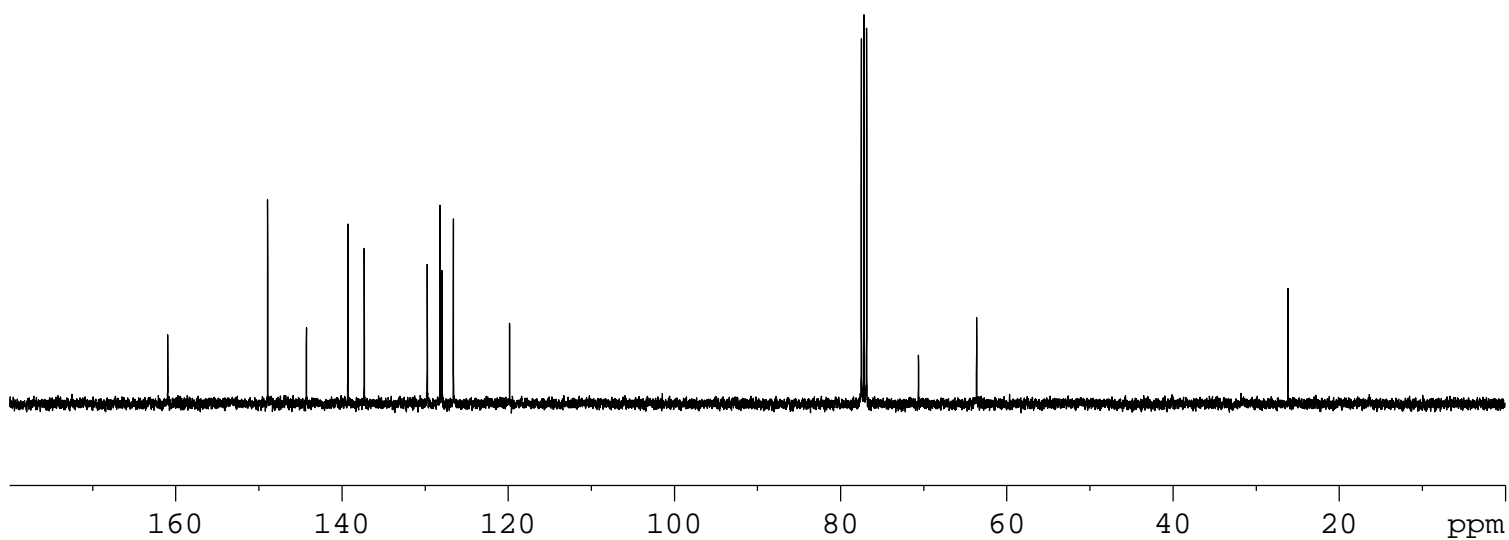
Bruker Advance III 400



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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 41.2500000 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

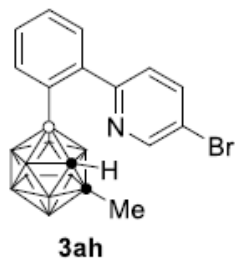


CY-B-A-64p

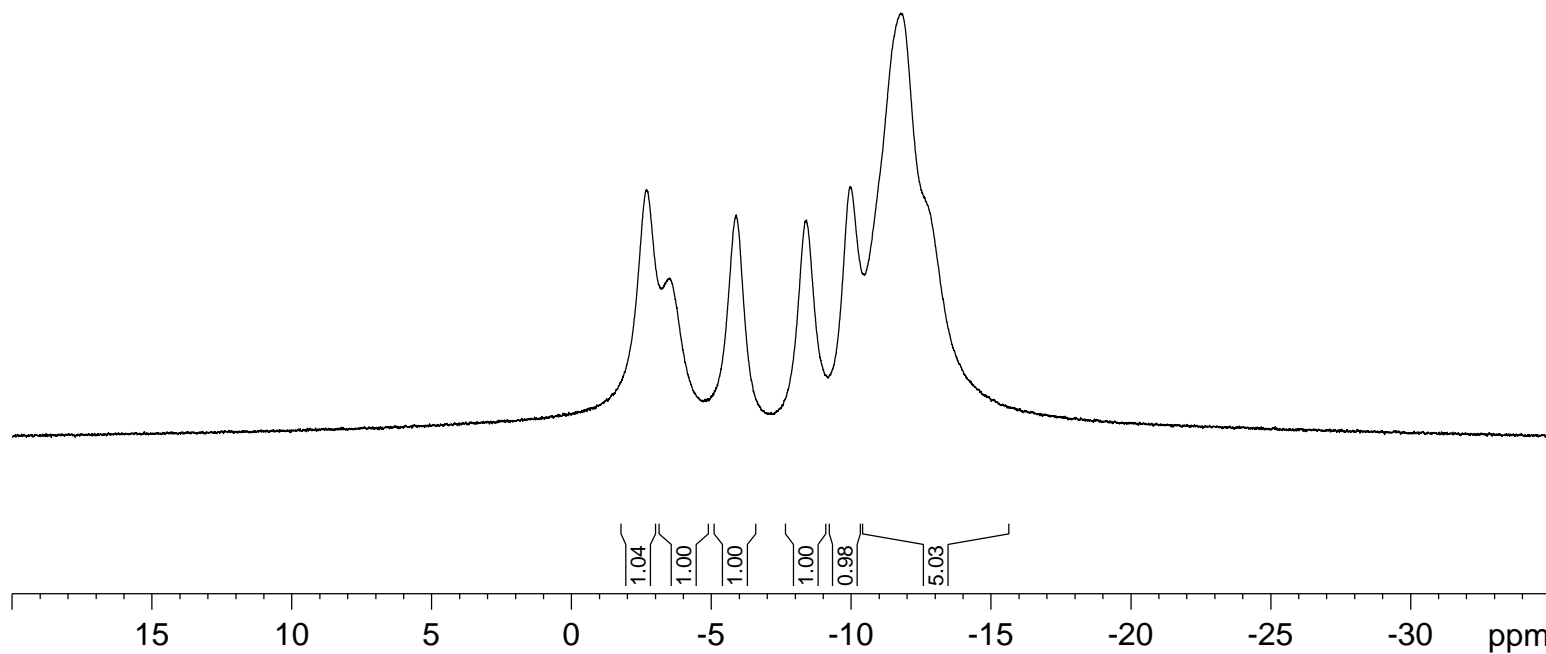
Current Data Parameters  
NAME CY-B-A-64p  
EXPNO 1  
PROCNO 1

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

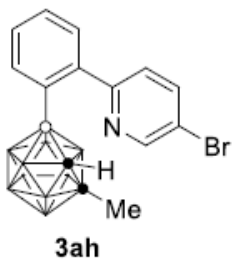
F2 - Processing parameters  
SI 32768  
SF 128.4097615 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



— 2.68  
— 3.50  
— 5.89  
— 8.40  
— 9.95  
— 11.77



| -2.35  
 | -3.59  
 | -5.56  
 | -6.73  
 | -8.04  
 | -9.55  
 | -10.99  
 | -12.48



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

Current Data Parameters

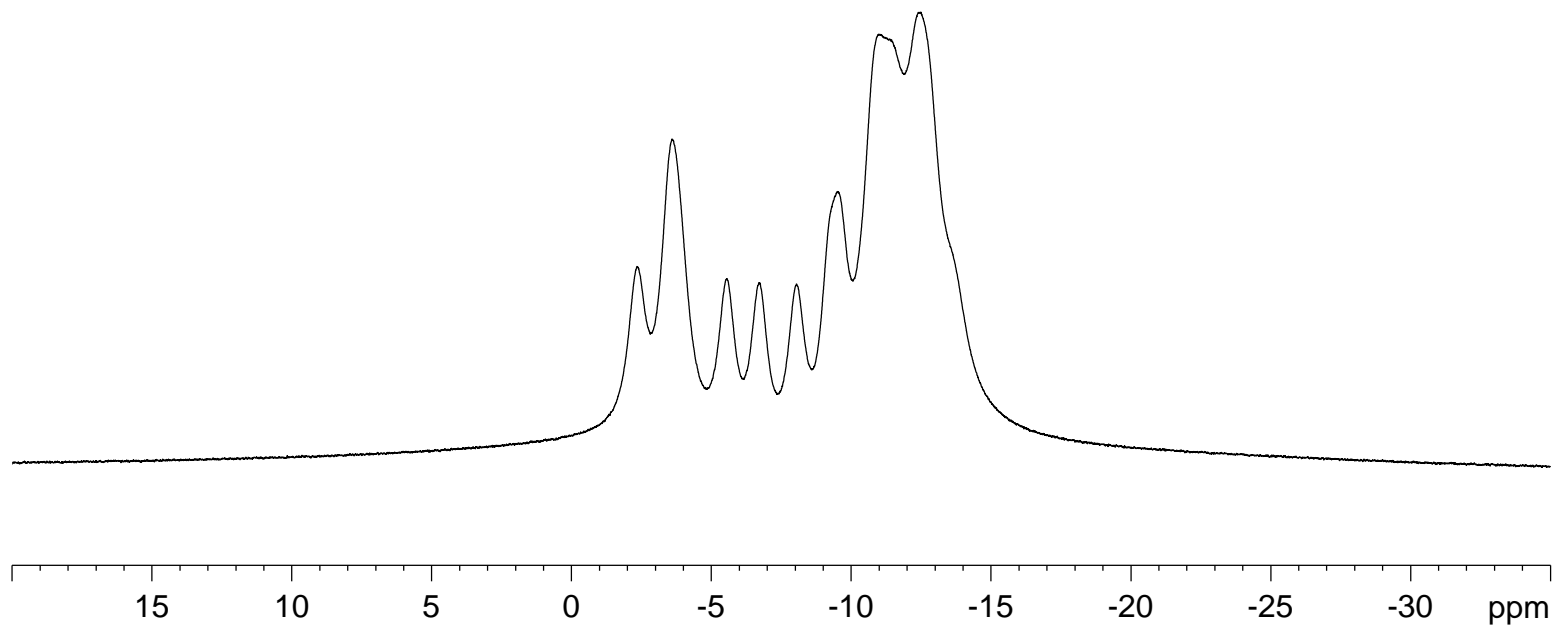
NAME CY-B-A-64p-(C)  
 EXPNO 1  
 PROCNO 1

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

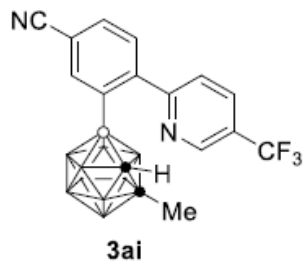




8.882  
8.111  
8.075  
8.071  
8.055  
8.050  
7.678  
7.675  
7.659  
7.656  
7.568  
7.548  
7.304  
7.284  
7.259

4.125

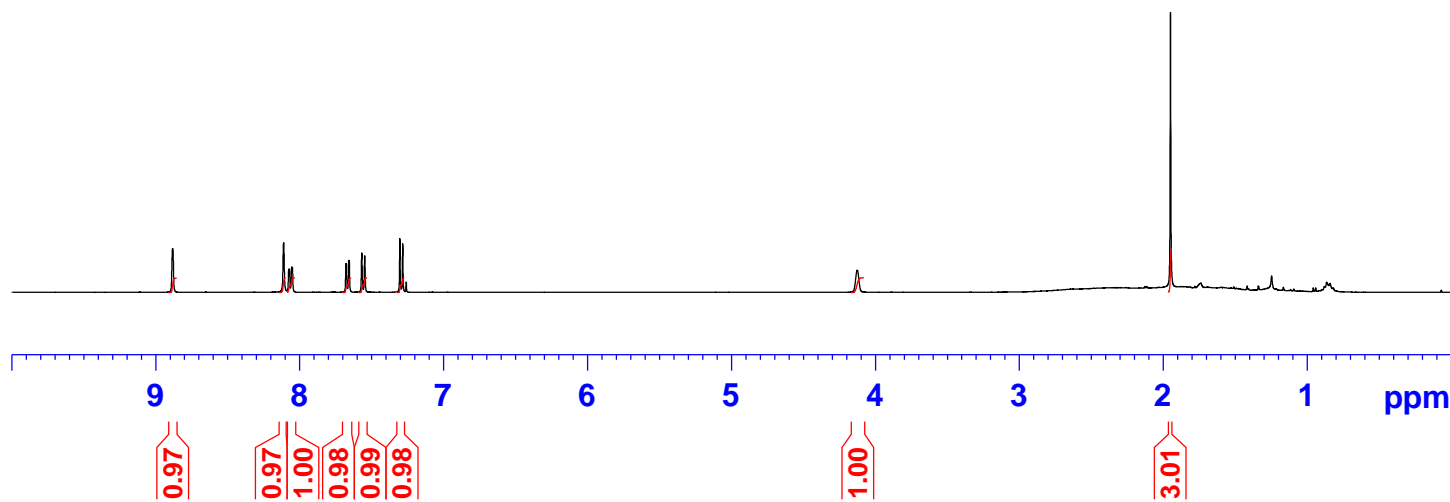
1.950



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  
SF01 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

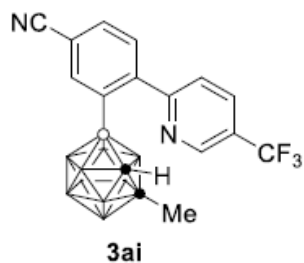
Current Data Parameters  
NAME CY-C-A-43P-CDCl3  
EXPNO 1  
PROCNO 1

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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 41.2500000 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

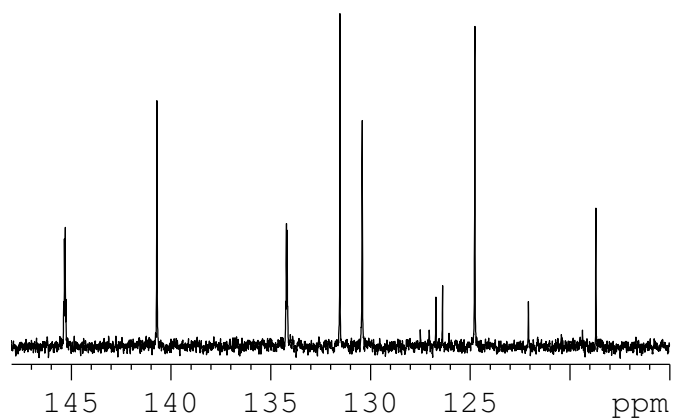
F2 - Processing parameters  
SI 32768  
SF 100.6127568 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

163.990  
148.417  
145.374  
145.330  
145.290  
145.253  
140.695  
134.236  
134.204  
134.167  
134.137  
131.517  
130.401  
127.517  
127.082  
126.724  
126.391  
126.078  
124.797  
124.767  
122.083  
119.427  
118.699  
112.604

77.478  
77.160  
76.843  
71.140  
63.512  
26.065



145.374  
145.330  
145.290  
145.253  
140.695  
134.236  
134.204  
134.167  
134.137  
131.517  
130.401  
127.517  
127.082  
126.724  
126.391  
126.078  
124.797  
124.767  
122.083  
119.427  
118.699



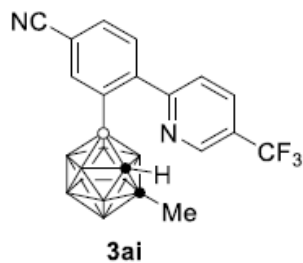
180 160 140 120 100 80 60 40 20 ppm

CY-B-A-43p

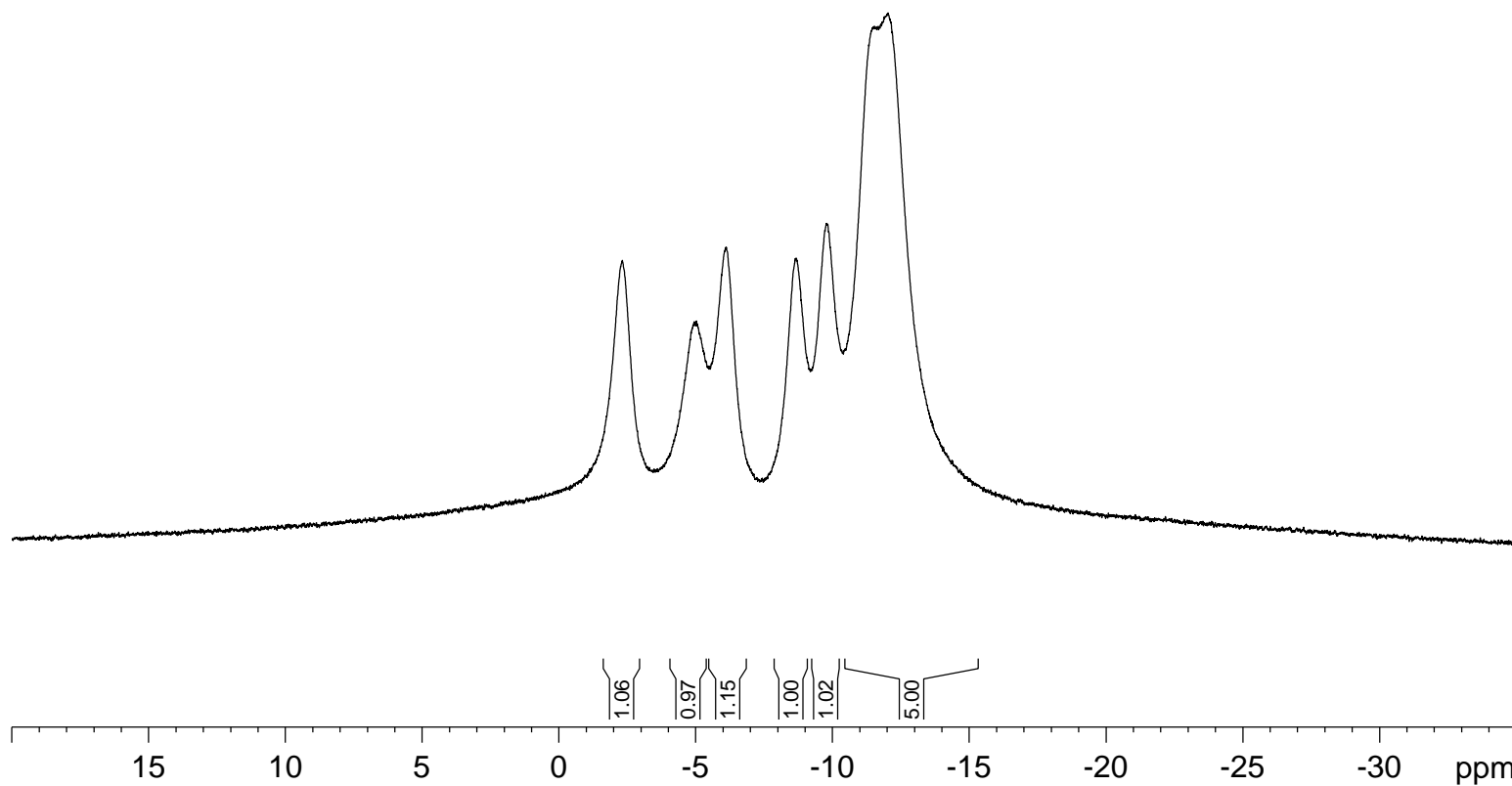
Current Data Parameters  
NAME CY-B-A-43p  
EXPNO 1  
PROCNO 1

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  
SF01 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W  
SF02 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.56000042 W  
PLW12 0.27428001 W

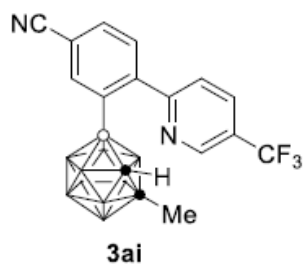
F2 - Processing parameters  
SI 32768  
SF 128.4097615 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



— -2.32  
— -5.02  
— -6.12  
— -8.68  
— -9.79  
— -12.03



| 1.90  
 | 3.02  
 | 5.32  
 | 6.84  
 | 8.21  
 | 9.39  
 | 10.78  
 | 12.05

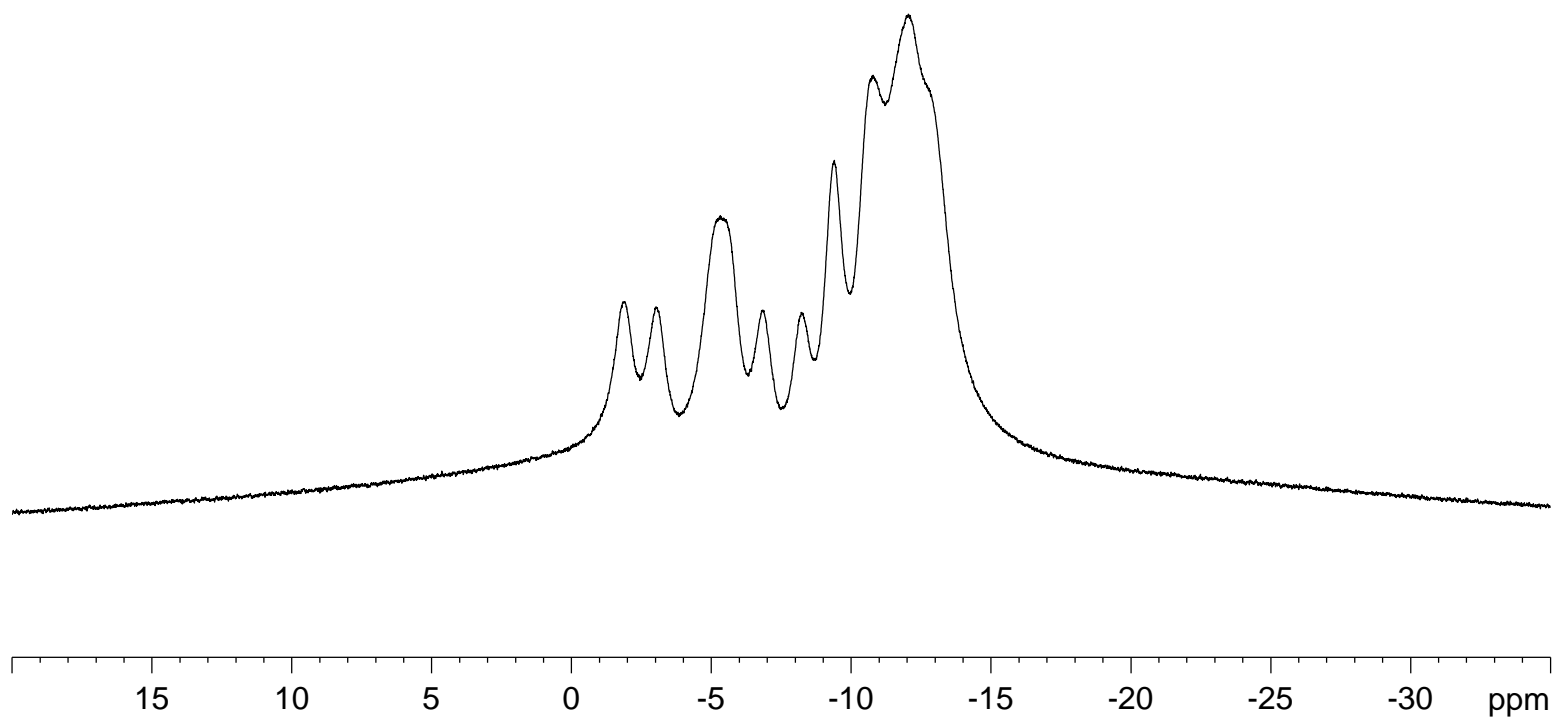


CY-B-A-43p-(C)

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

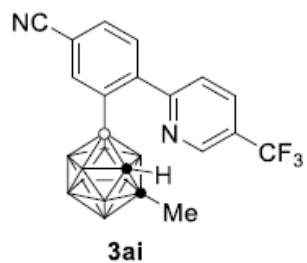
F2 - Acquisition Parameters  
 Date\_ 20161114  
 Time 21.24 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (   
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 80  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 456  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 2.00000000 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



-62.07

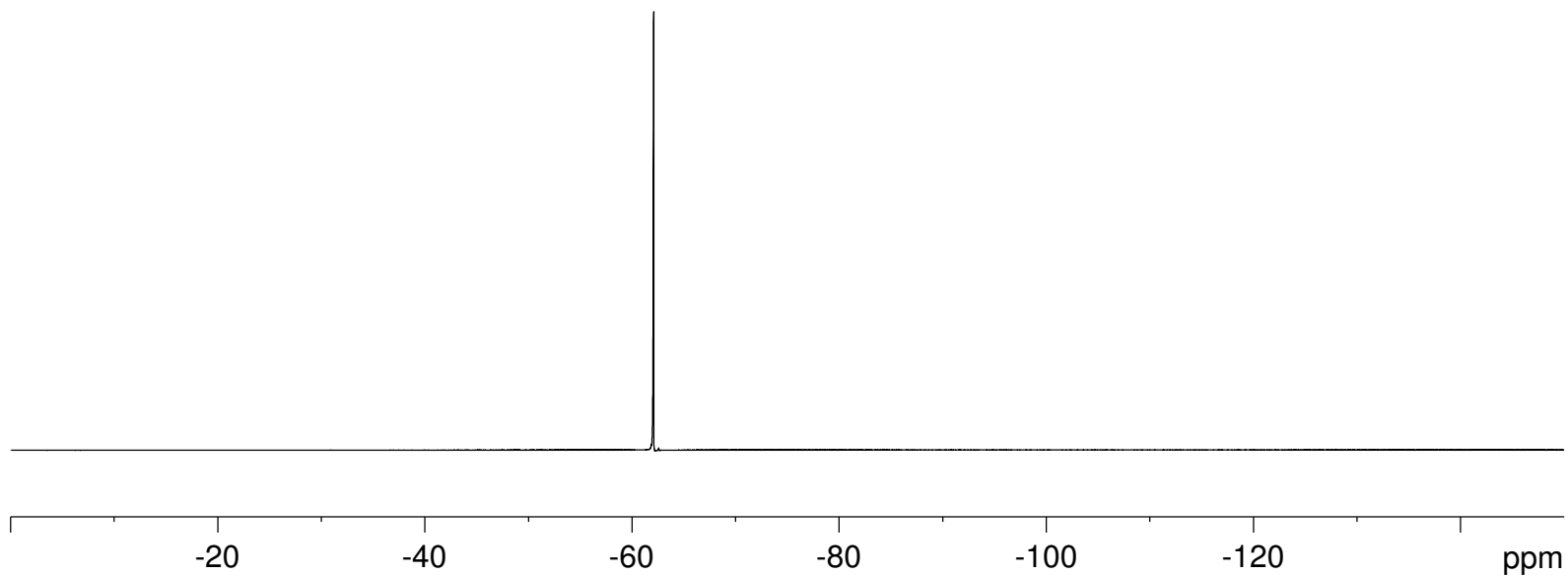
CY-F-A-43P

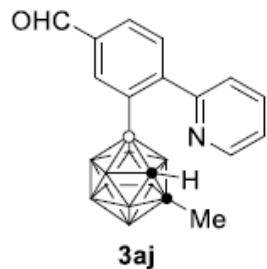
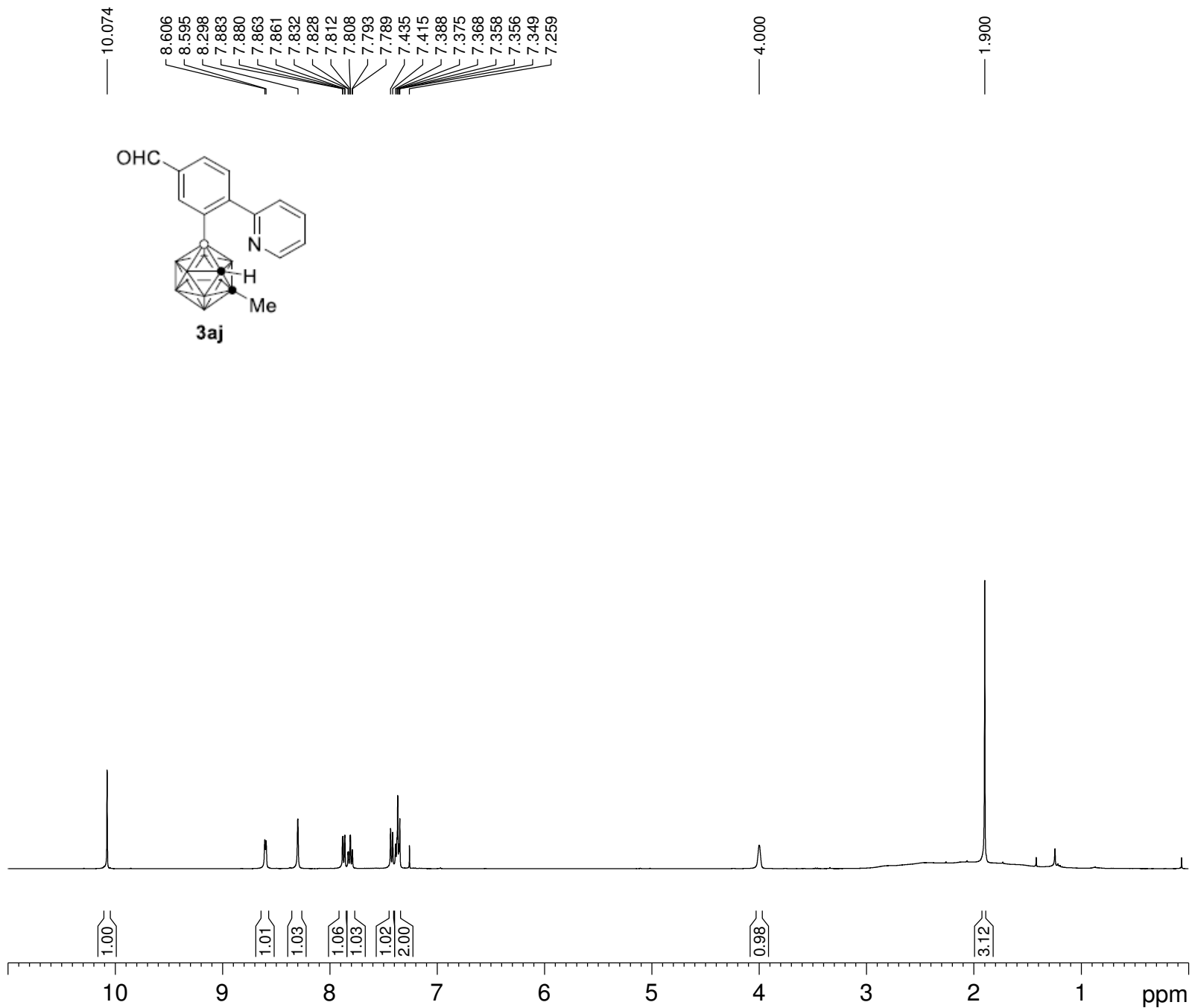


```
Current Data Parameters
NAME      CY-F-A-43P
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20161124
Time      16.42 h
INSTRUM   spect
PROBHD    Z108618_0257 (
PULPROG   zgfhigqn.2
TD        131072
SOLVENT   CDC13
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
```





CY-H-A-60p-CHO

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

192.47

161.12

150.82

148.09

139.57

137.02

135.28

130.59

128.35

124.97

123.28

77.48

77.16

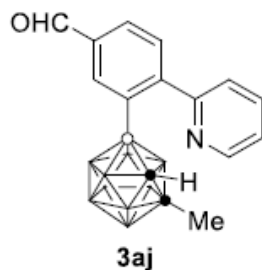
76.84

70.65

63.48

26.06

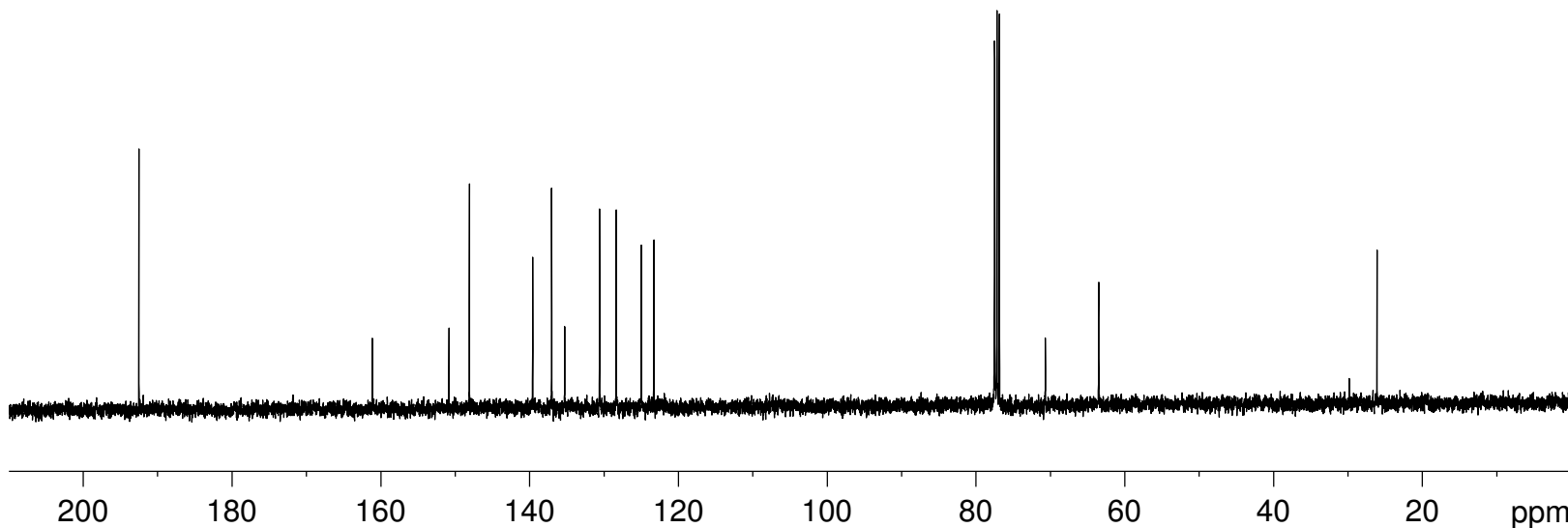
CY-C-A-60P-CHO



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

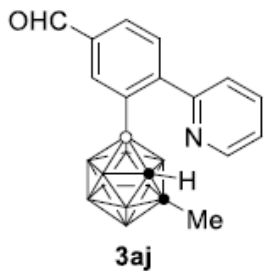


CY-B-A-55p-re3

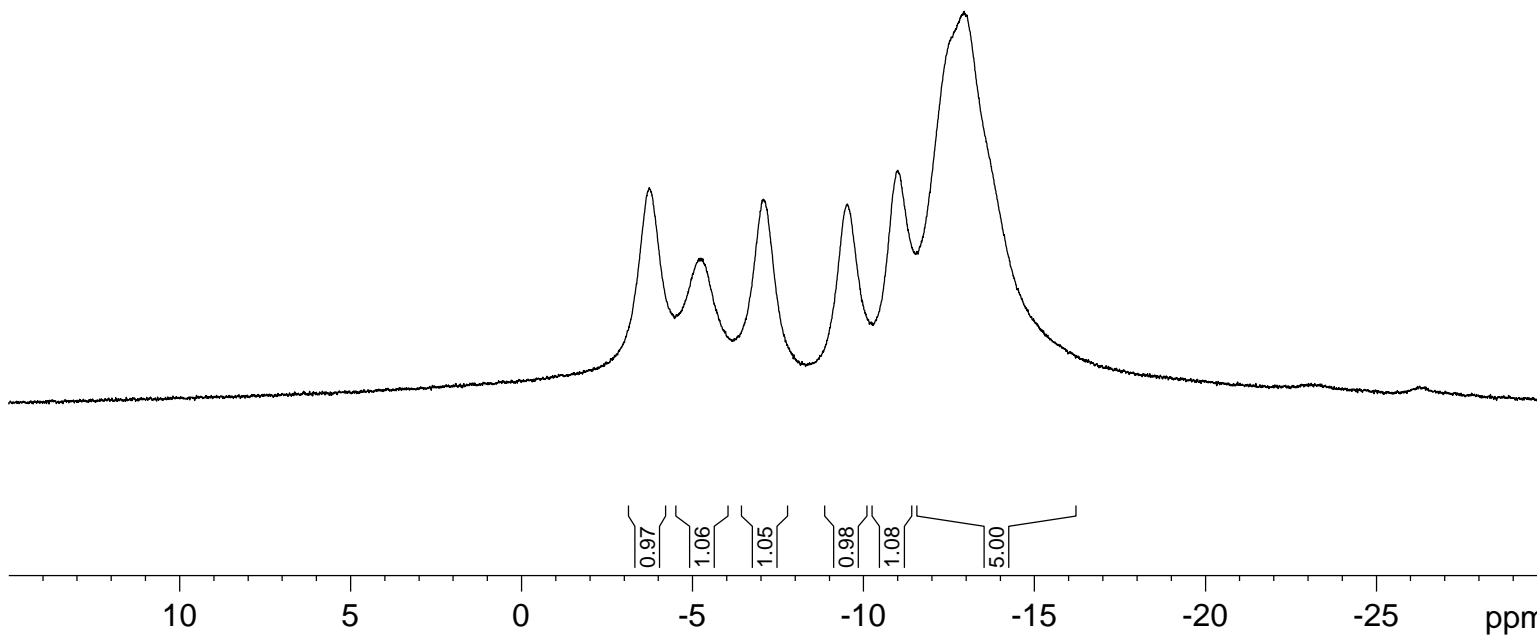
Current Data Parameters  
NAME CY-B-A-55p-re3  
EXPNO 1  
PROCNO 1

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 2.0000000 sec  
D11 0.0300000 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



— 3.73  
— 5.25  
— 7.07  
— 9.53  
— 11.00  
— 12.95





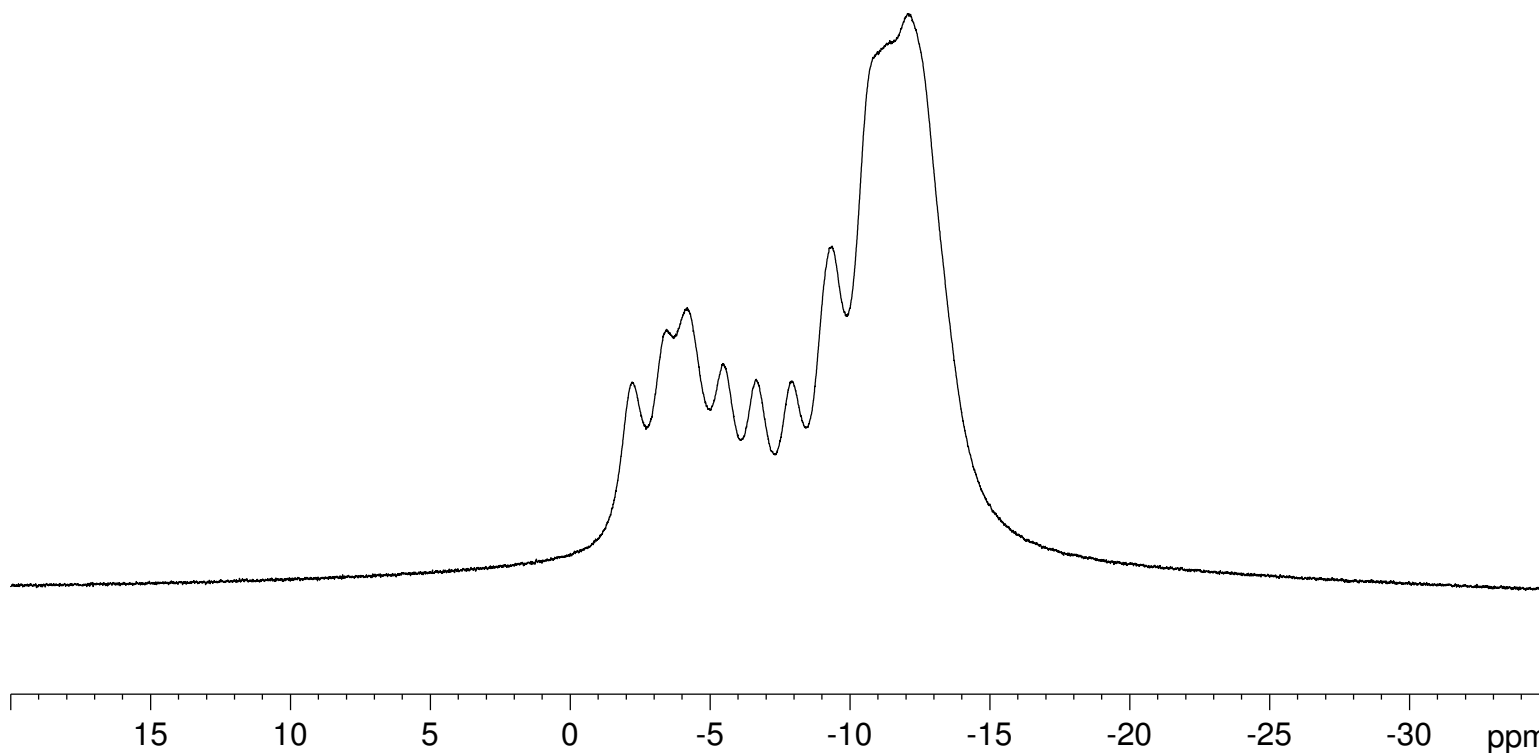
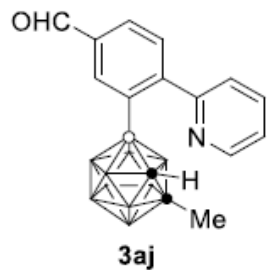
CY-B-A-55P- (C)

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 CDC13  
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

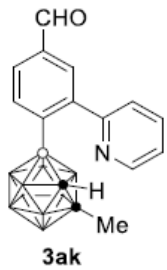
F2 - Processing parameters  
SI 32768  
SF 128.4097881 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

— -2.21  
— -4.17  
— -5.44  
— -6.64  
— -7.89  
— -9.35  
— -12.08



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

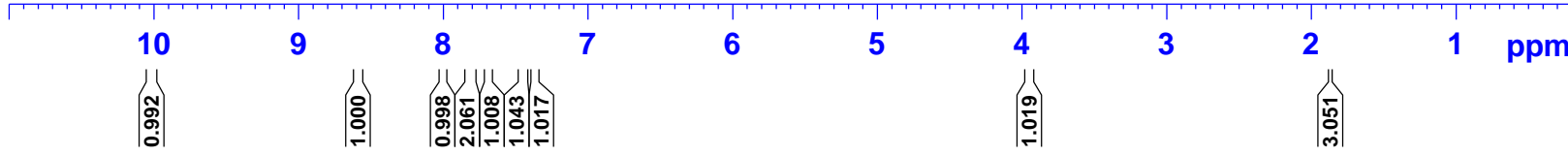
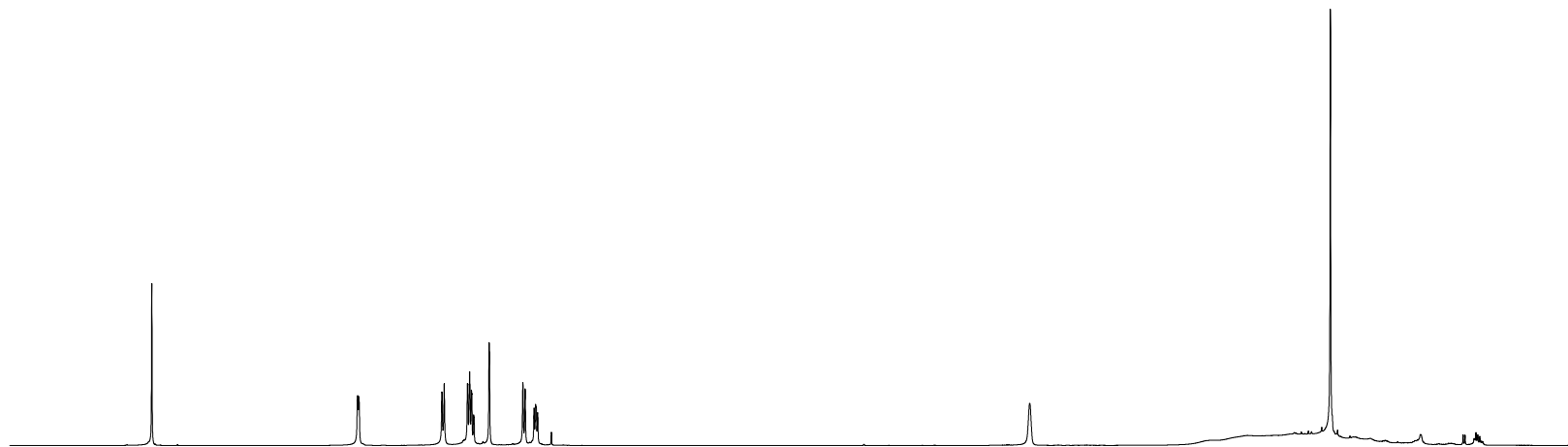
10.015  
 8.595  
 8.586  
 8.012  
 7.996  
 7.857  
 7.835  
 7.833  
 7.820  
 7.808  
 7.805  
 7.793  
 7.790  
 7.686  
 7.452  
 7.437  
 7.375  
 7.365  
 7.360  
 7.350  
 7.255  
 3.949  
 1.871



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 CDC13  
 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

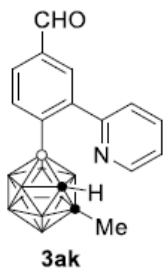


CY-C-B-200P-Ir-CDC-CHO-K

— 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

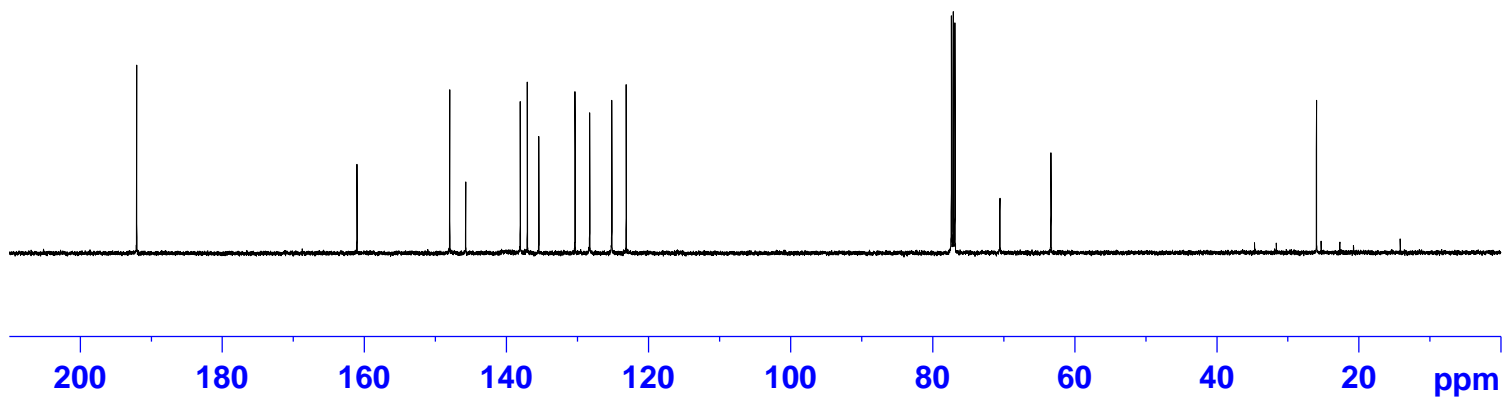
— 26.00



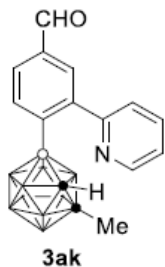
Current Data Parameters  
 NAME CY-C-B-200P-Ir-CDC-CHO-re  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190129  
 Time\_ 17.29 h  
 INSTRUM spect  
 PROBHD Z149001\_0010 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 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 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 125.7703643 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 61.0000000 W  
 SFO2 500.1320005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.29663000 W  
 PLW13 0.14920001 W

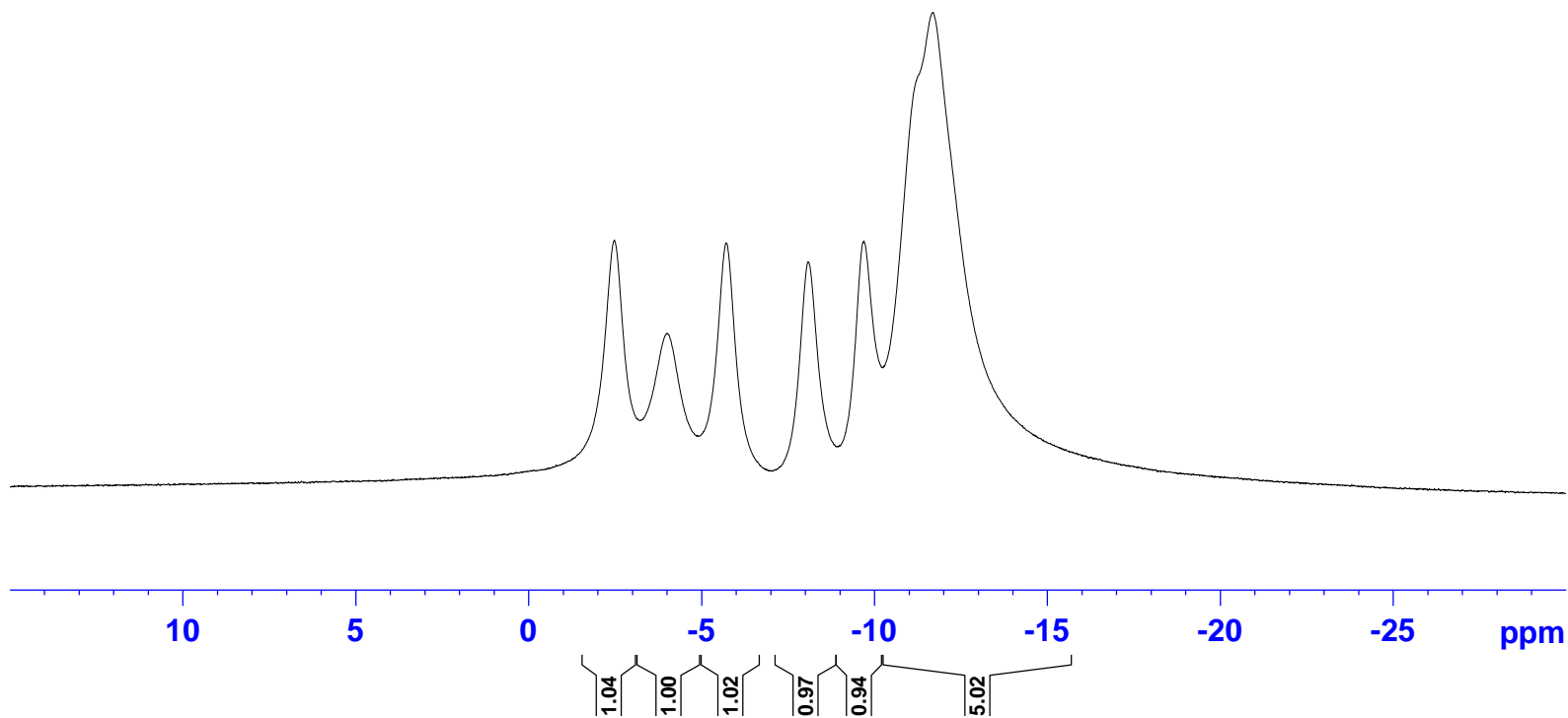
F2 - Processing parameters  
 SI 32768  
 SF 125.7577824 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



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



— 2.48  
 — 4.02  
 — 5.71  
 — 8.08  
 — 9.69  
 — 11.70



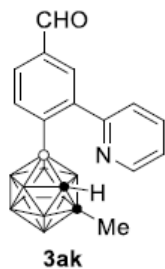
Current Data Parameters  
 NAME CY-B-B-200P-Ir-CDC-CHO  
 EXPNO 1  
 PROCNO 1

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)

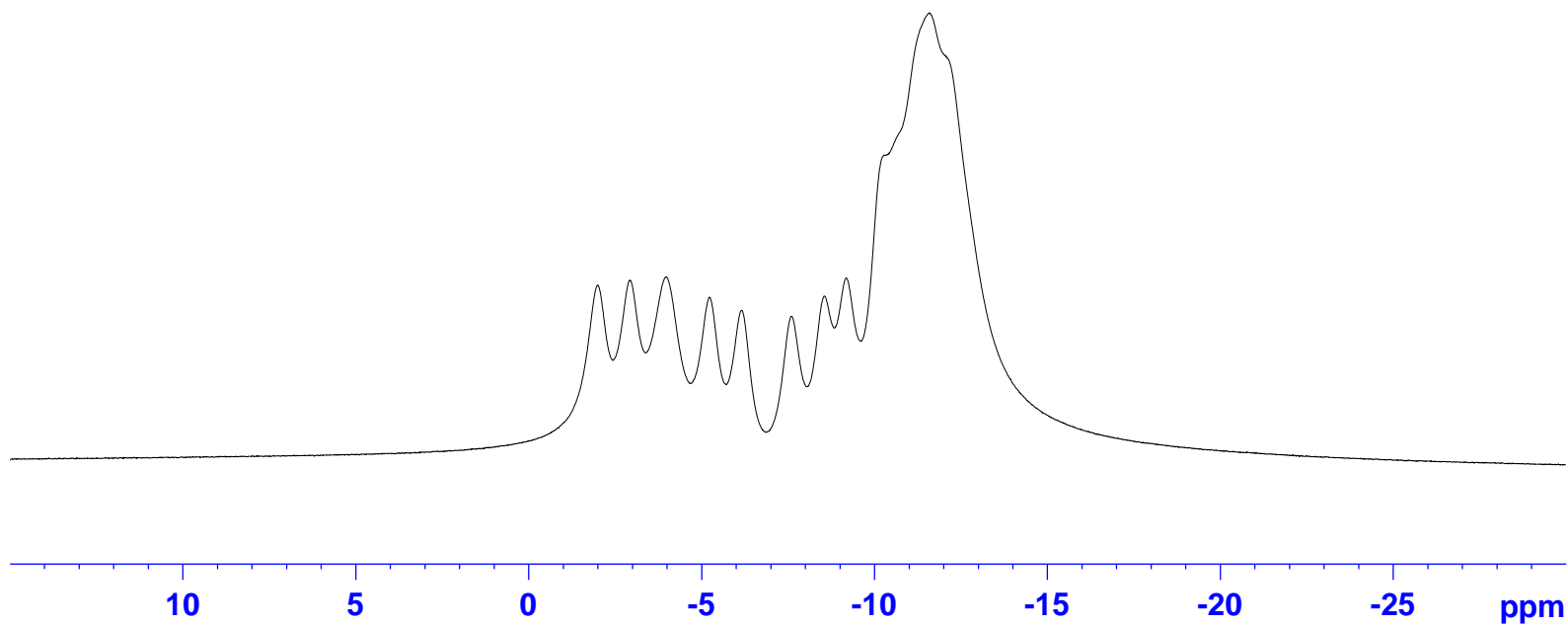
-2.00  
 -2.91  
 -3.99  
 -5.23  
 -6.16  
 -7.61  
 -8.56  
 -9.18  
 -10.29  
 -11.59  
 -12.08



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  
 SF01 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



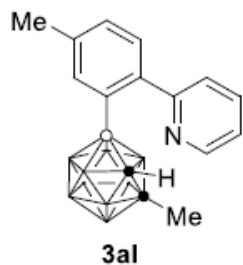
8.561  
8.550  
7.766  
7.762  
7.747  
7.743  
7.728  
7.723  
7.634  
7.412  
7.392  
7.309  
7.307  
7.297  
7.295  
7.291  
7.278  
7.276  
7.258  
7.181  
7.162  
7.092  
7.072

4.007

2.398

1.875

CY-H-A-42P



Current Data Parameters

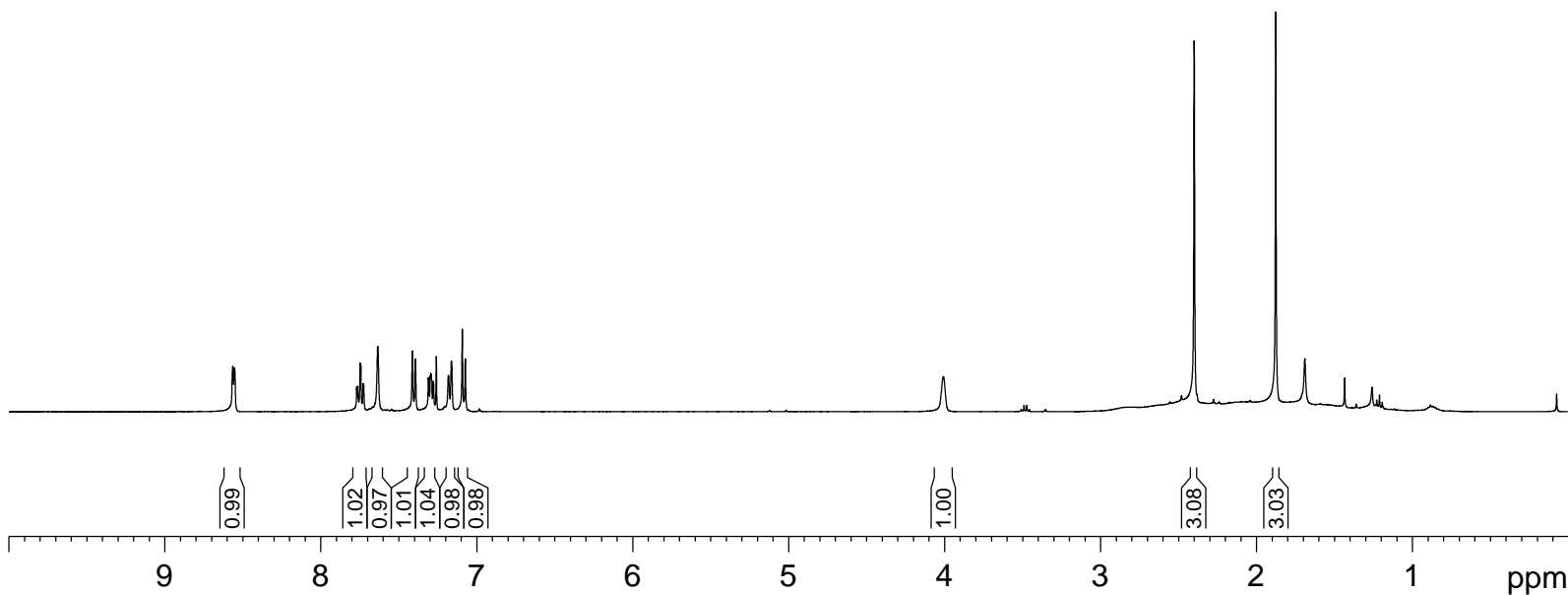
NAME CY-H-A-42P  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20161103  
Time 19.39 h  
INSTRUM spect  
PROBHD Z108618\_0257 (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 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters

SI 65536  
SF 400.2300103 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



162.684

147.814

142.470

138.028

137.142

136.623

129.704

128.727

125.353

122.438

77.462

77.145

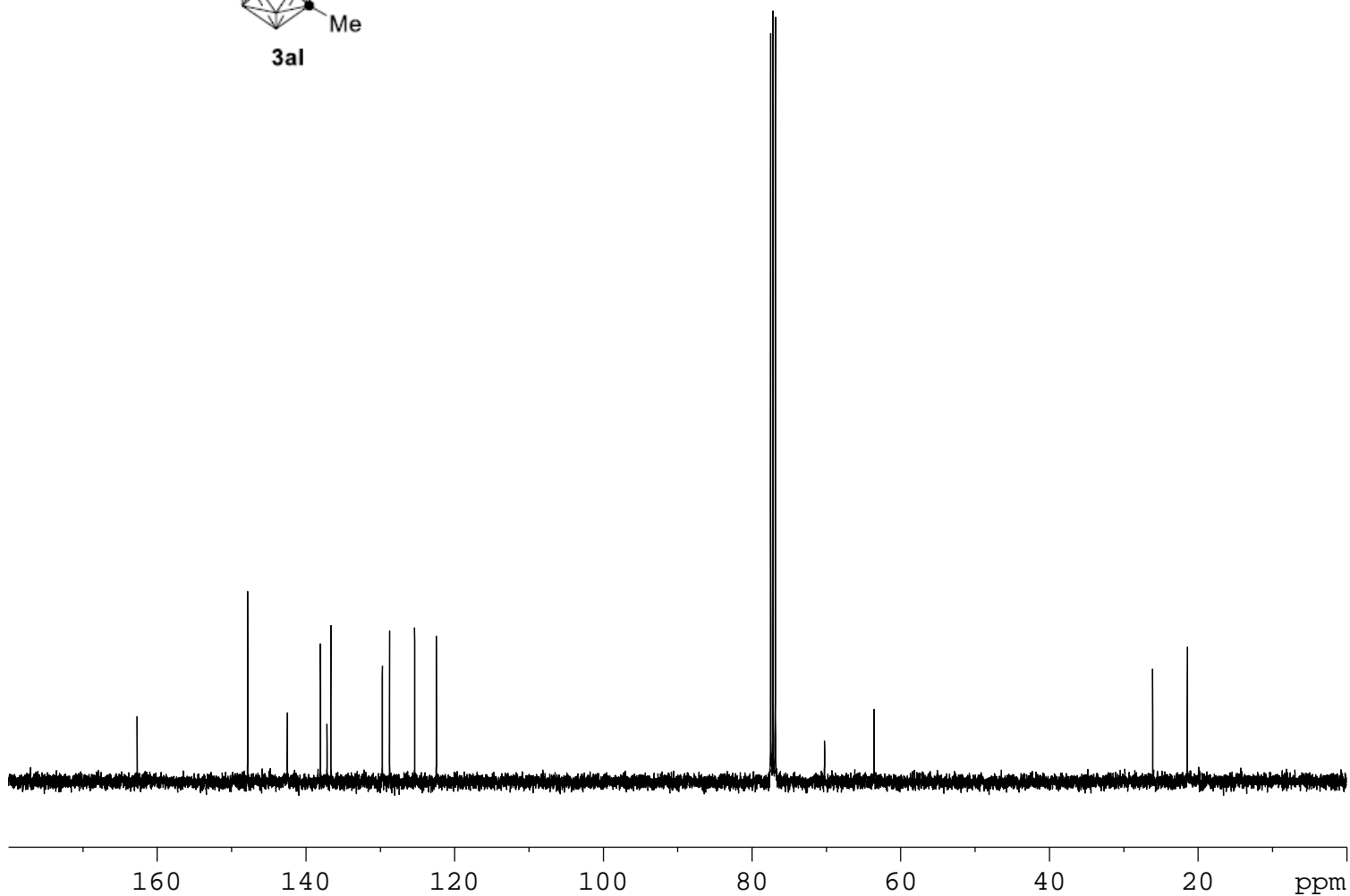
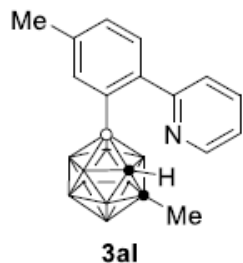
76.826

70.206

63.547

26.071

21.404



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

CY-B-A-42P-RE2

Current Data Parameters

NAME CY-B-A-42P-RE2  
EXPNO 1  
PROCNO 1

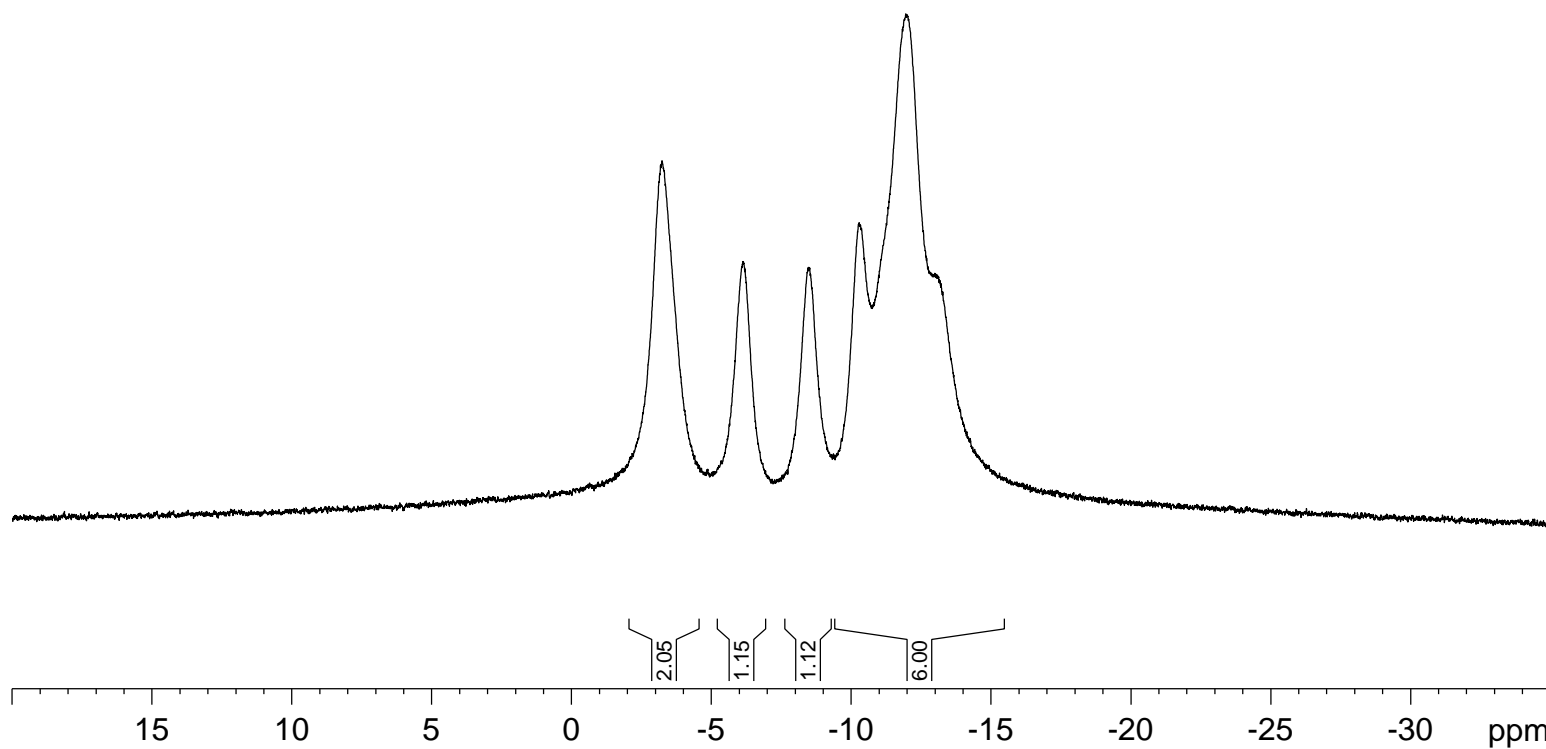
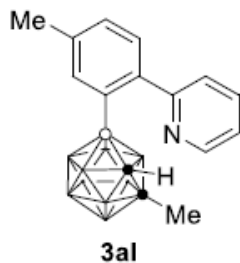
F2 - Acquisition Parameters

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

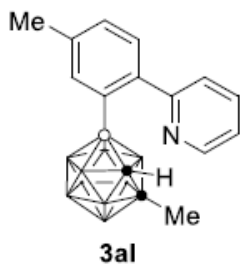
F2 - Processing parameters

SI 32768  
SF 128.4097615 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

— -3.32  
— -6.21  
— -8.52  
— -10.38  
— -12.07







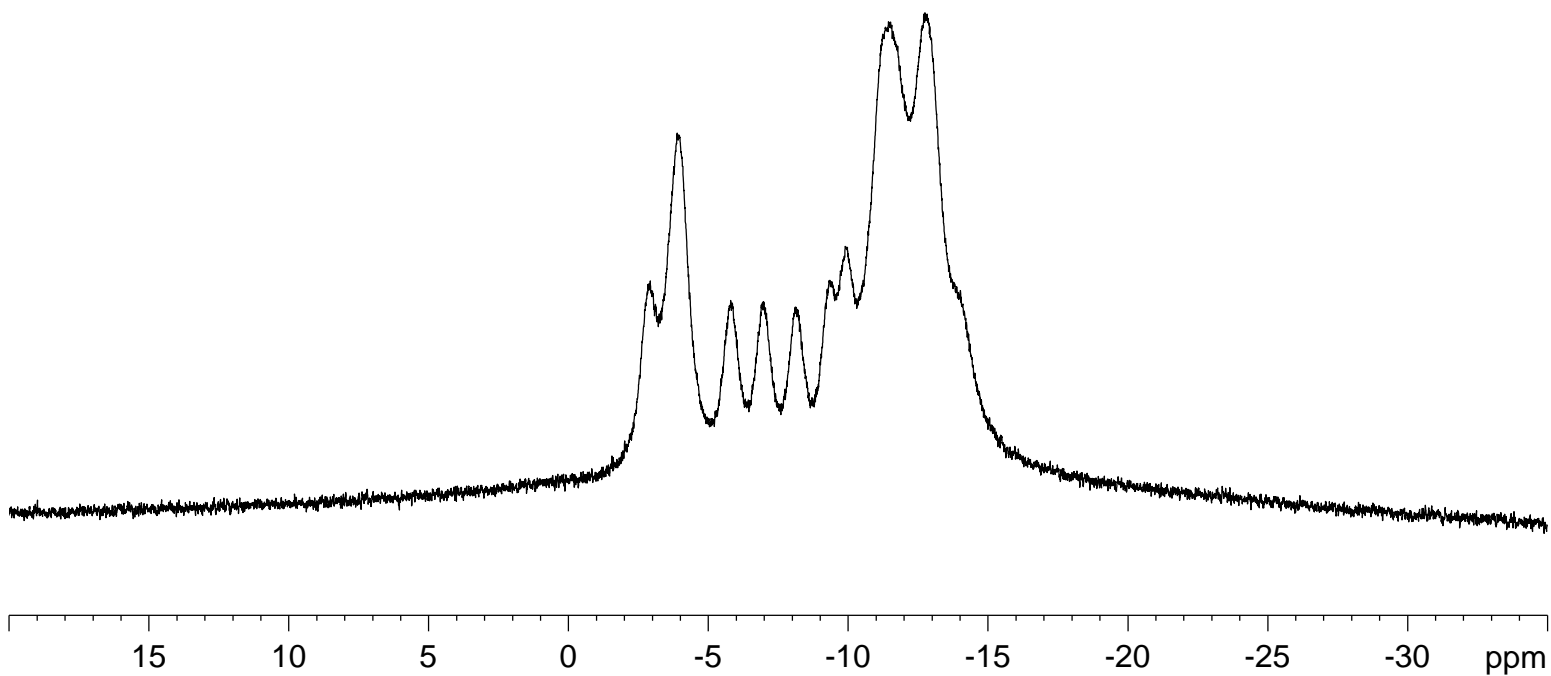
| -2.92  
 | -3.98  
 | -5.89  
 | -6.99  
 | -8.21  
 | -9.97  
 | -11.56  
 | -12.92

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

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

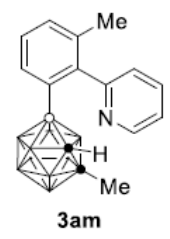
F2 - Acquisition Parameters  
 Date\_ 20161103  
 Time 19.53 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 4  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 256  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.4 K  
 D1 2.00000000 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

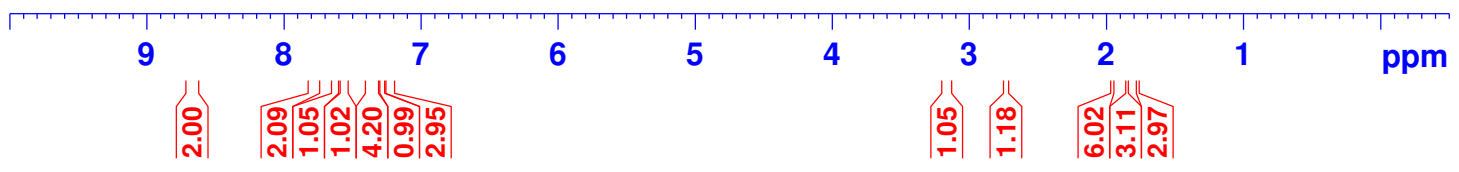
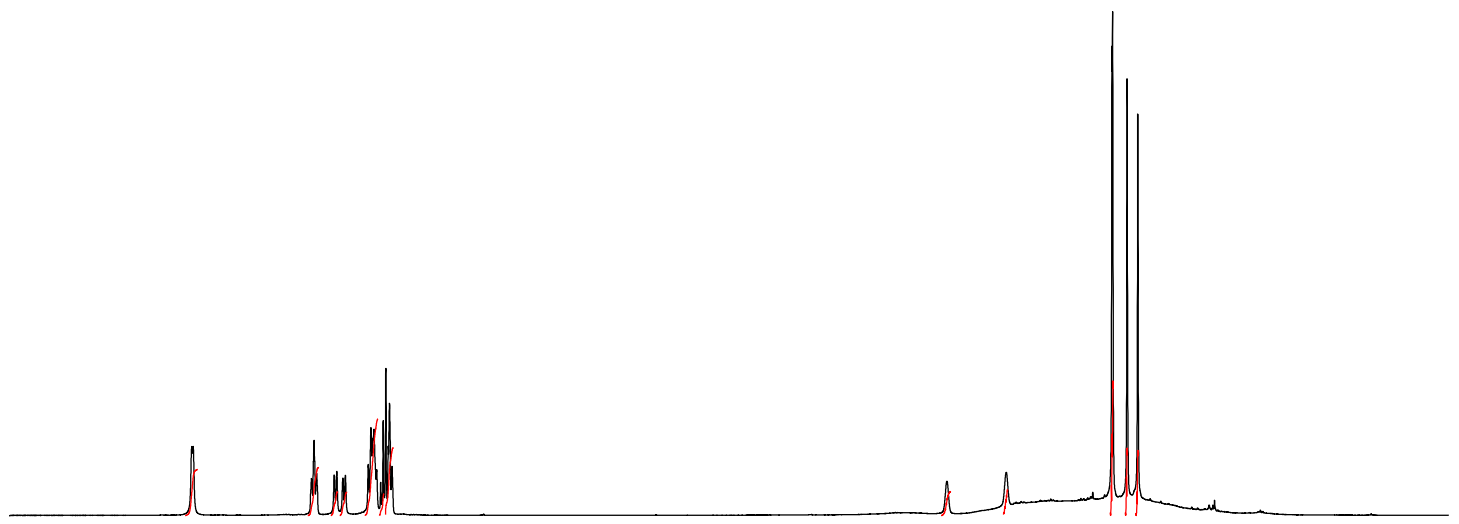
3.163  
2.731  
1.959  
1.955  
1.849  
1.771



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 CDC13  
 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



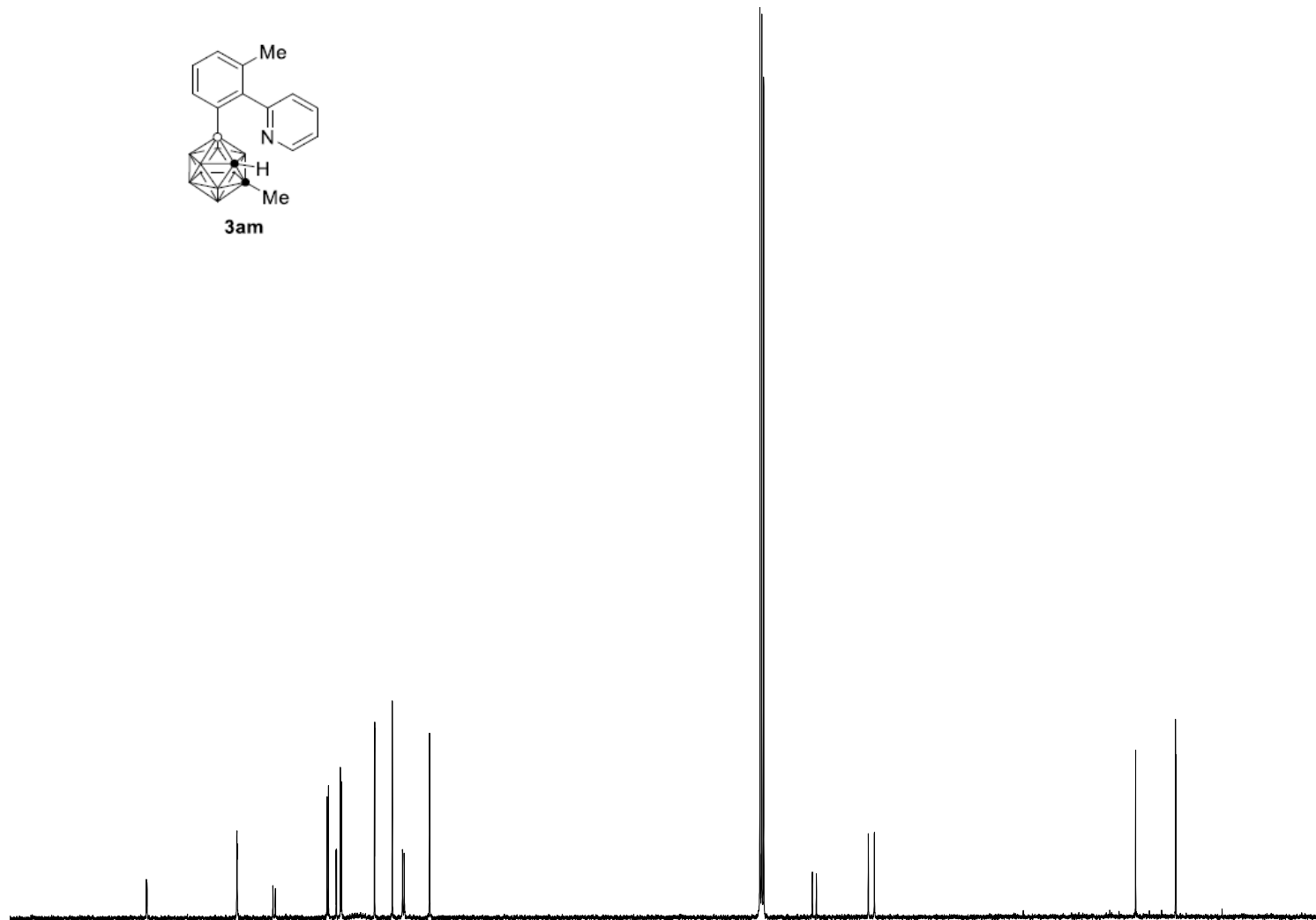
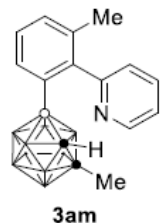
2.00  
2.09  
1.05  
1.02  
4.20  
0.99  
2.95  
1.05  
1.18  
6.02  
3.11  
2.97

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



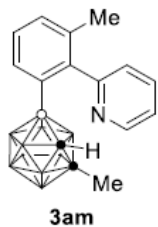
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

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

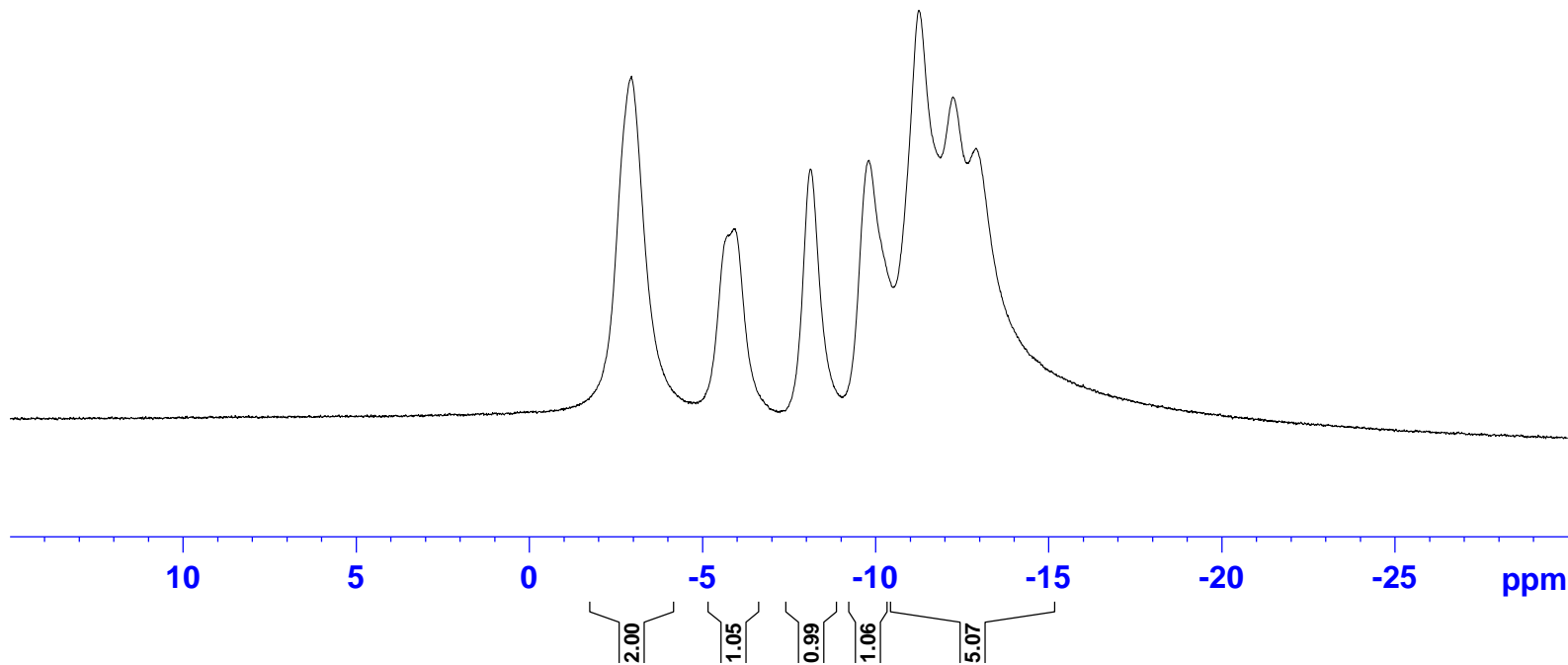
F2 - Acquisition Parameters  
Date\_ 20190129  
Time 16.38 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 208  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 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



— -2.95  
 — -5.93  
 — -8.11  
 — -9.81  
 — -11.25  
 — -12.24

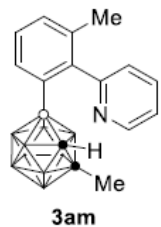


Current Data Parameters  
 NAME CY-B-B-124P-IrCDC-Me  
 EXPNO 1  
 PROCNO 1

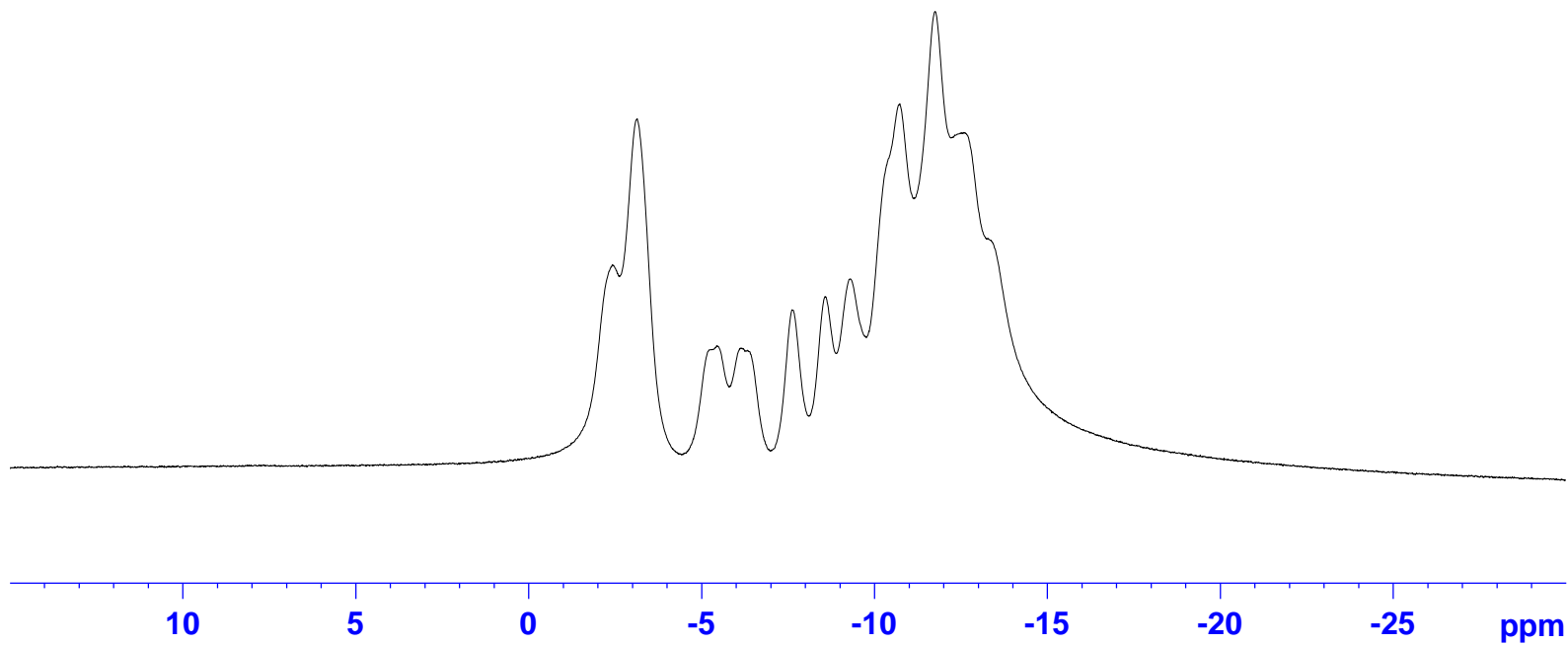
F2 - Acquisition Parameters  
 Date\_ 20190129  
 Time 16.42 h  
 INSTRUM spect  
 PROBHD Z149001\_0010 (  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT None  
 NS 16  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 1.467191 Hz  
 AQ 0.6815744 sec  
 RG 206.72  
 DW 20.800 usec  
 DE 18.00 usec  
 TE 298.0 K  
 D1 1.00000000 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)



-2.36  
 -3.13  
 -5.19  
 -5.44  
 -6.15  
 -6.38  
 -7.62  
 -8.58  
 -9.30  
 -10.73  
 -11.75  
 -12.58  
 -13.36



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

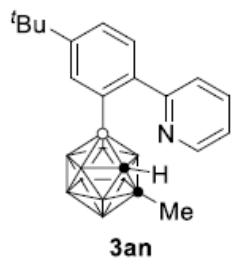
8.564  
8.562  
8.551  
8.549  
7.902  
7.898  
7.775  
7.770  
7.756  
7.751  
7.737  
7.732  
7.448  
7.428  
7.398  
7.393  
7.378  
7.373  
7.313  
7.310  
7.300  
7.297  
7.294  
7.291  
7.281  
7.279  
7.259  
7.141  
7.121

4.011

1.879

1.374

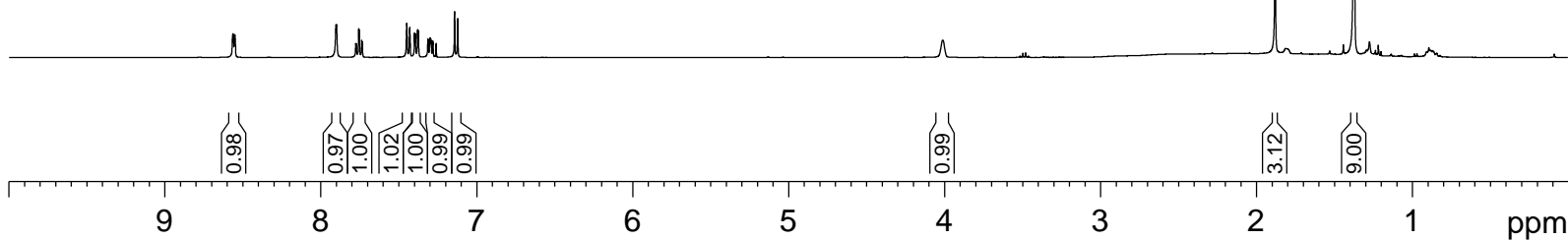
CY-H-A-59p



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 (Z  
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 MHz  
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

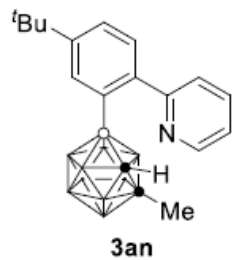


162.71  
150.08  
147.79  
142.31  
136.66  
134.81  
129.40  
125.16  
124.98  
122.42

77.47  
77.16  
76.84  
70.21  
63.54

34.79  
31.43  
26.06

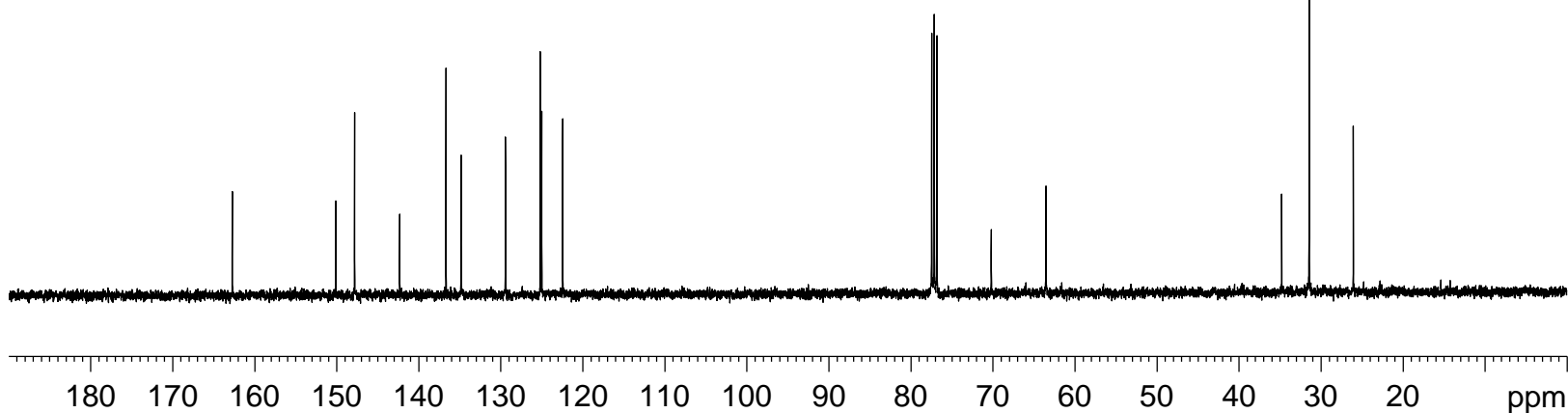
CY-C-A-59p



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

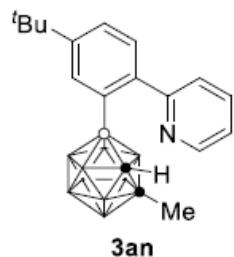
NAME CY-B-A-59p  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

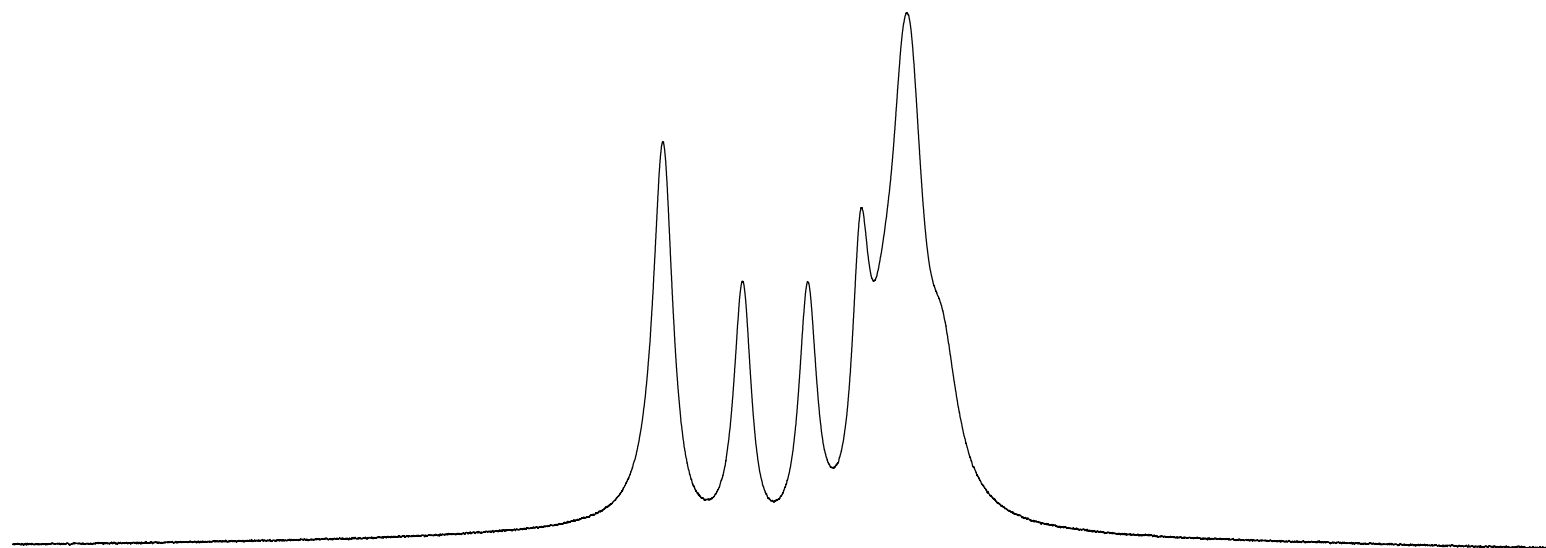
Date\_ 20161111  
Time 16.26 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 24  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 296.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 128.4096890 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



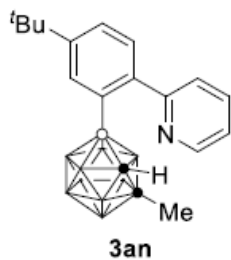
— -3.26  
— -6.11  
— -8.43  
— -10.35  
— -11.99



2.00  
1.06  
1.07  
1.09  
5.00

15 10 5 0 -5 -10 -15 -20 -25 -30 ppm





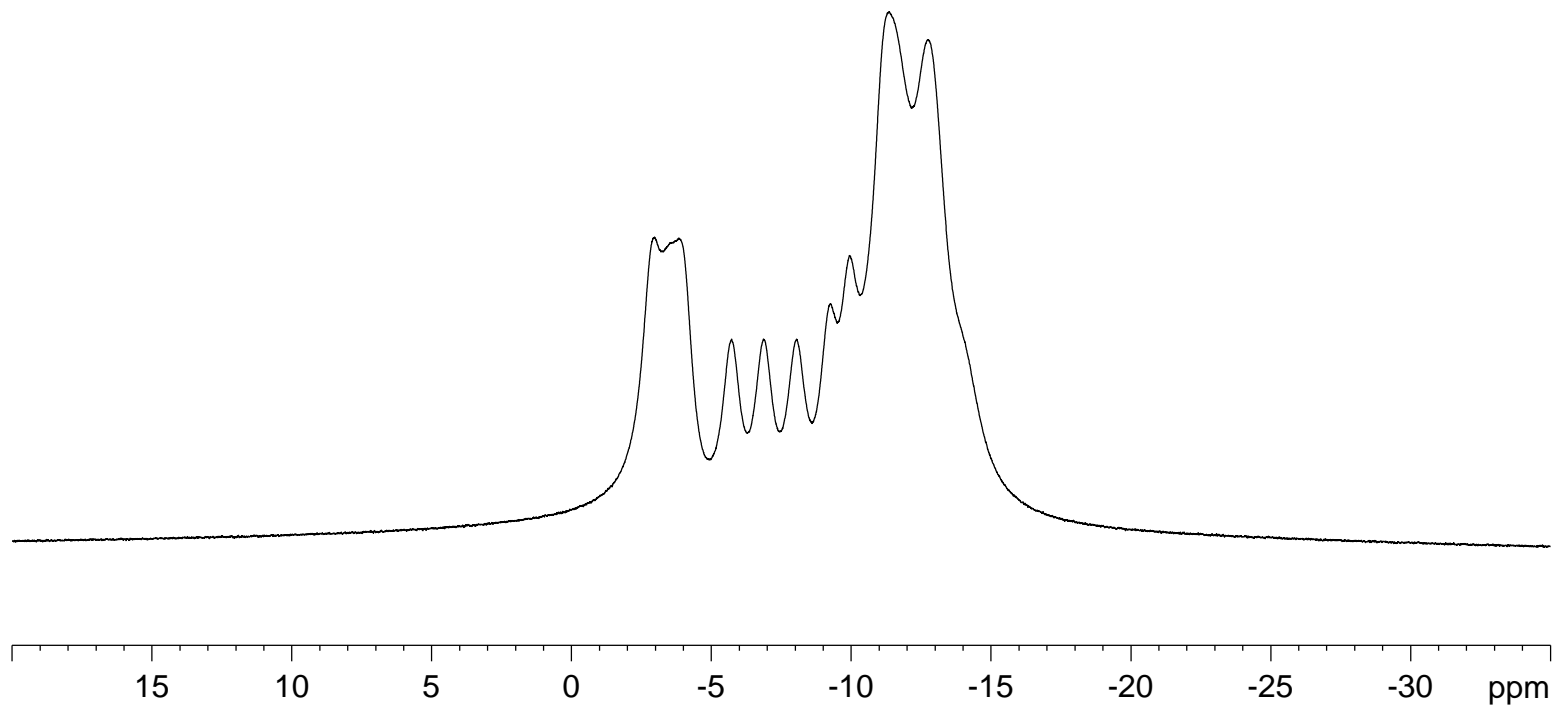
— 2.97  
 — 5.73  
 — 6.87  
 — 8.05  
 — 9.25  
 — 9.94  
 — 11.36  
 — 12.74

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

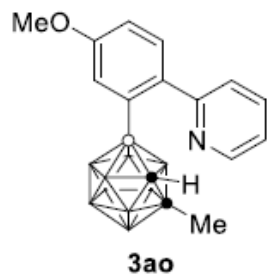
F2 - Processing parameters  
 SI 32768  
 SF 128.4097881 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



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

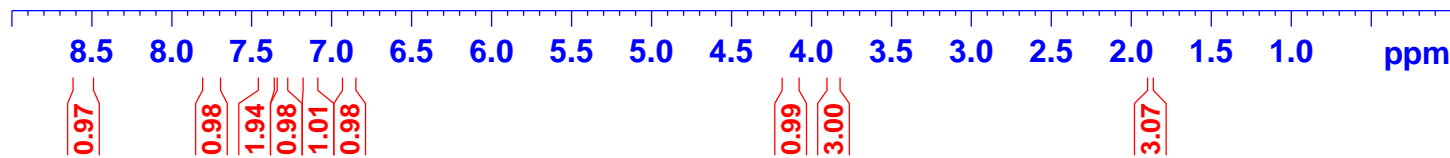
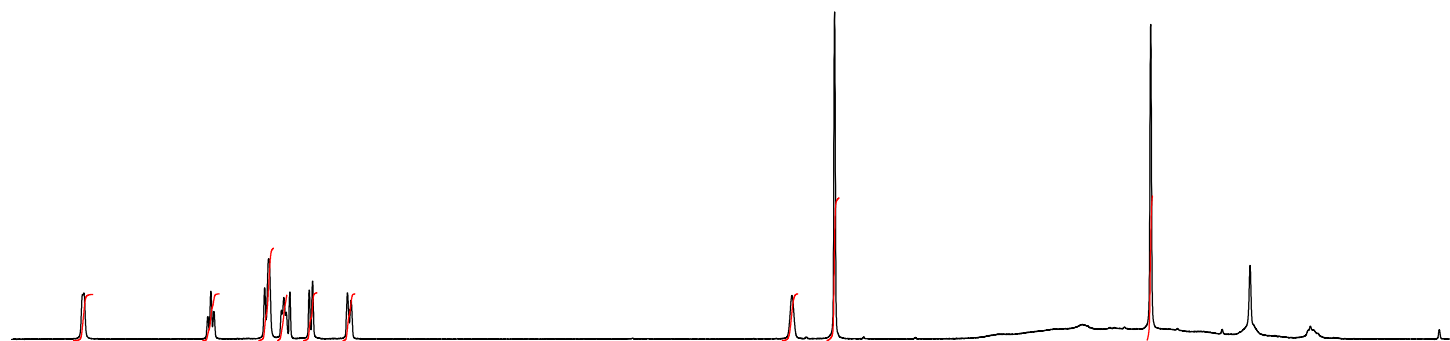
1.878



Current Data Parameters  
 NAME CY-H-A-26p-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160829  
 Time 13.21 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 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

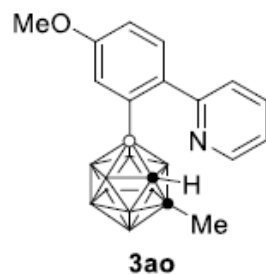


162.42  
158.71  
147.76  
137.96  
136.70  
131.18  
125.51  
122.85  
122.40  
113.24

77.47  
77.15  
76.84  
70.24  
63.60  
55.38

26.07

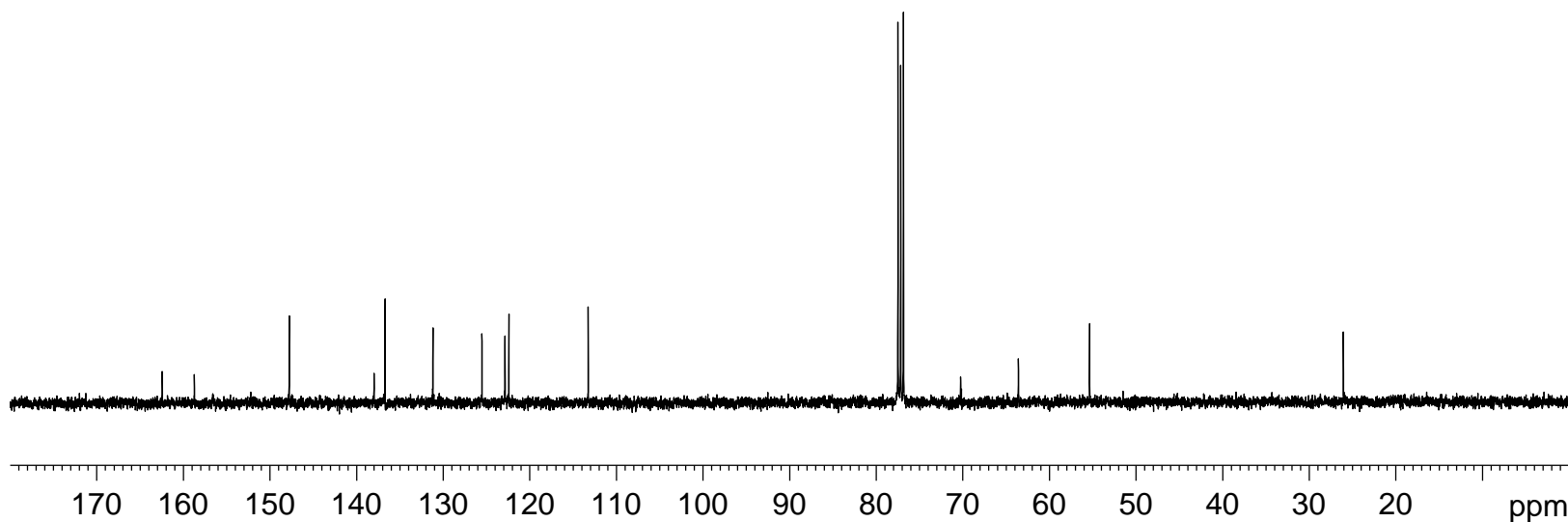
CY-C-A-26P-re



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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6479773 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 55.3400015 W  
SFO2 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.5600042 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

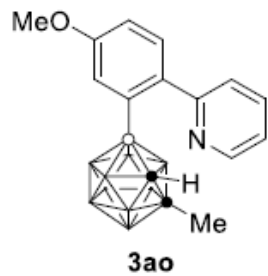


CY-B-A-26P

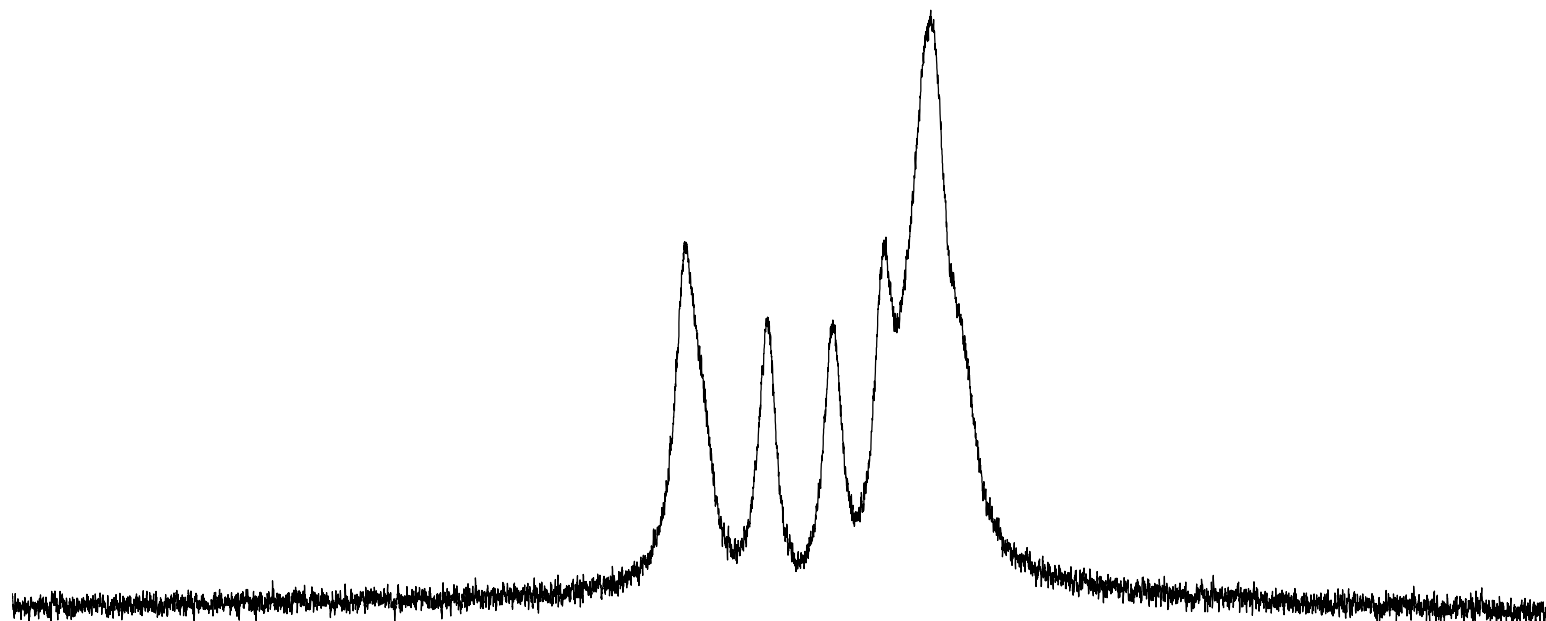
Current Data Parameters  
NAME CY-B-A-26P  
EXPNO 1  
PROCNO 1

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

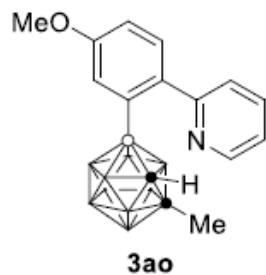


— -4.04  
— -7.01  
— -9.34  
— -11.24  
— -12.84



2.17  
1.15  
1.15  
6.00

15 10 5 0 -5 -10 -15 -20 -25 -30 ppm



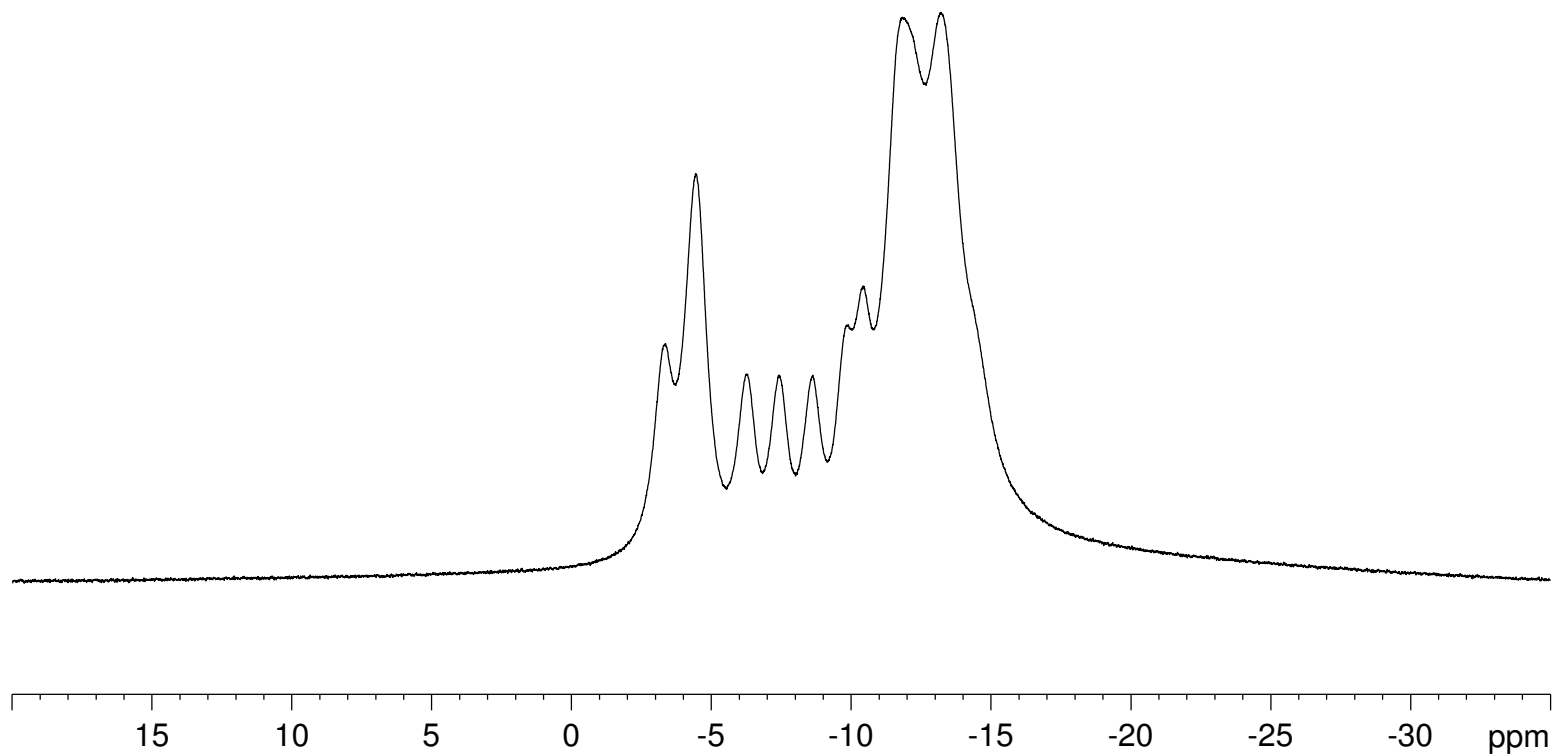
| -3.37  
 | -4.44  
 | -6.28  
 | -7.43  
 | -8.63  
 | -10.42  
 | -11.82  
 | -13.21

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

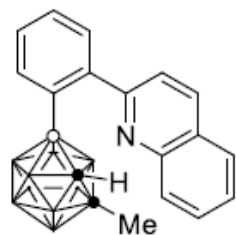
F2 - Processing parameters  
 SI 32768  
 SF 128.4097430 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



7.739  
7.736  
7.619  
7.617  
7.599  
7.596  
7.582  
7.579  
7.574  
7.433  
7.422  
7.413  
7.408  
7.399  
7.388  
7.328  
7.318  
7.310  
7.306  
7.303  
7.296  
7.260

4.277

1.566

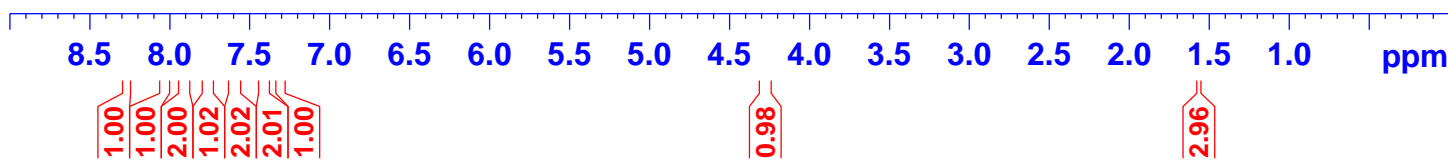
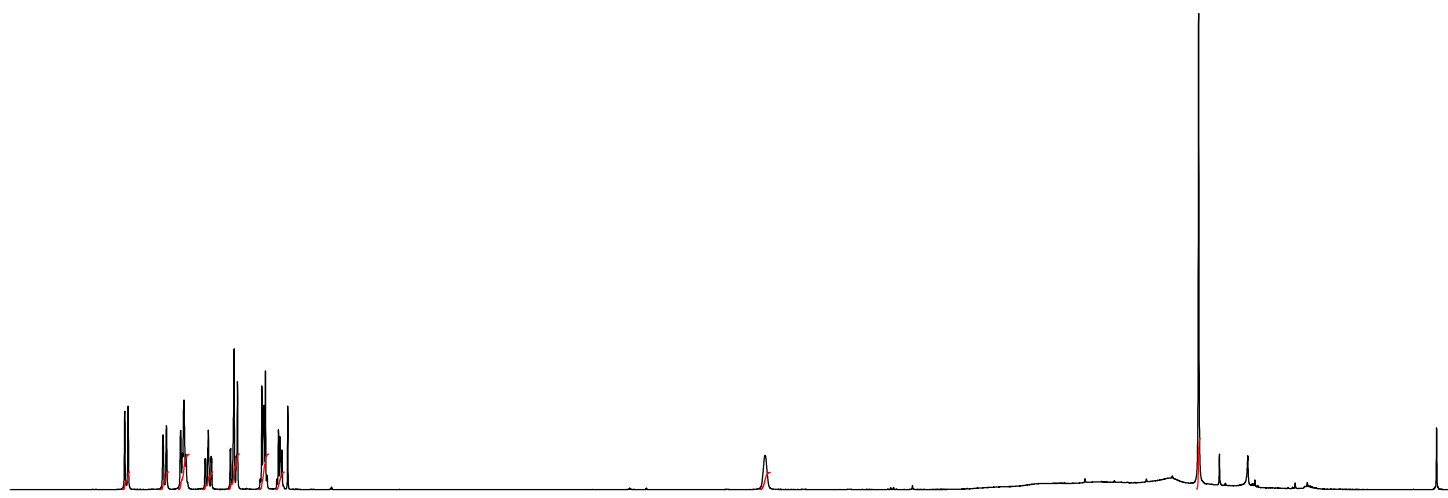


3ap

Current Data Parameters  
 NAME CY-H-A-52p-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161014  
 Time 19.52 h  
 INSTRUM spect  
 PROBHD z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 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

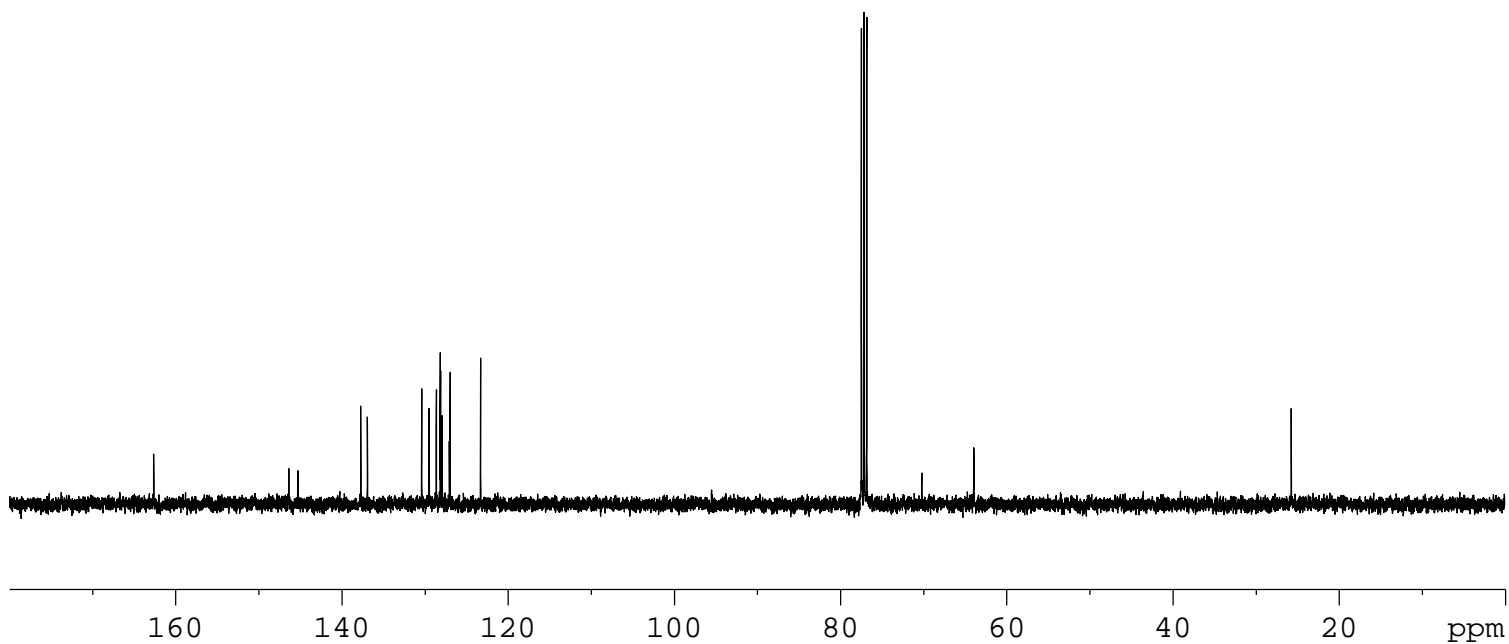
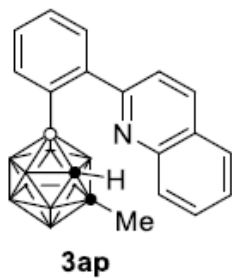


162.607

146.386  
145.289  
137.728  
136.919  
130.387  
129.501  
128.628  
128.160  
128.110  
127.919  
127.062  
126.973  
123.298

77.467  
77.150  
76.832  
70.195  
63.936

25.740



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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 41.2500000 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

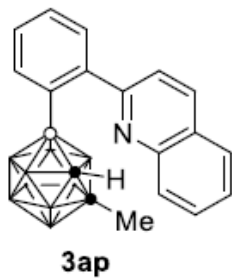
F2 - Processing parameters  
SI 32768  
SF 100.6127584 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

CY-B-A-52p-re3

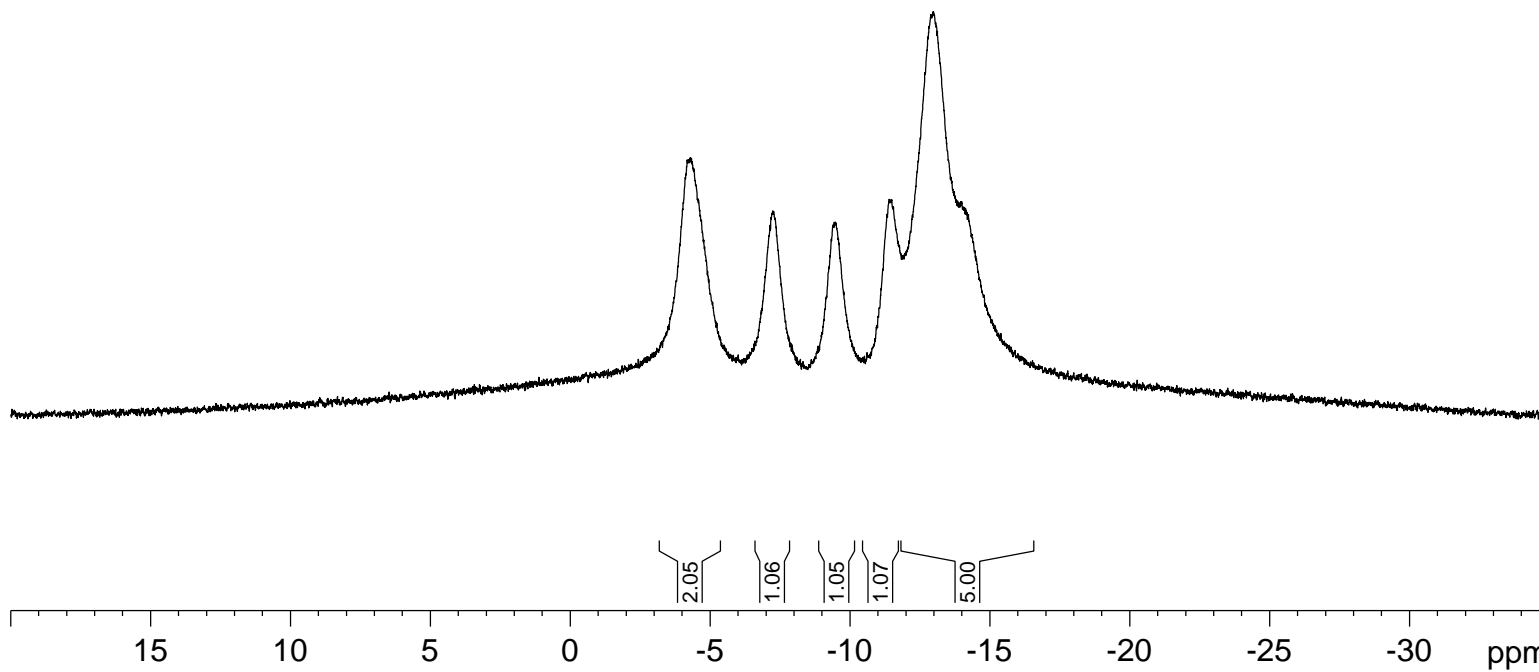
Current Data Parameters  
NAME CY-B-A-52p-re3  
EXPNO 1  
PROCNO 1

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 2.0000000 sec  
D11 0.0300000 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



— 4.29  
— 7.24  
— 9.48  
— 11.41  
— 12.97





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

Current Data Parameters

NAME CY-B-A-52P- (C)  
EXPNO 1  
PROCNO 1

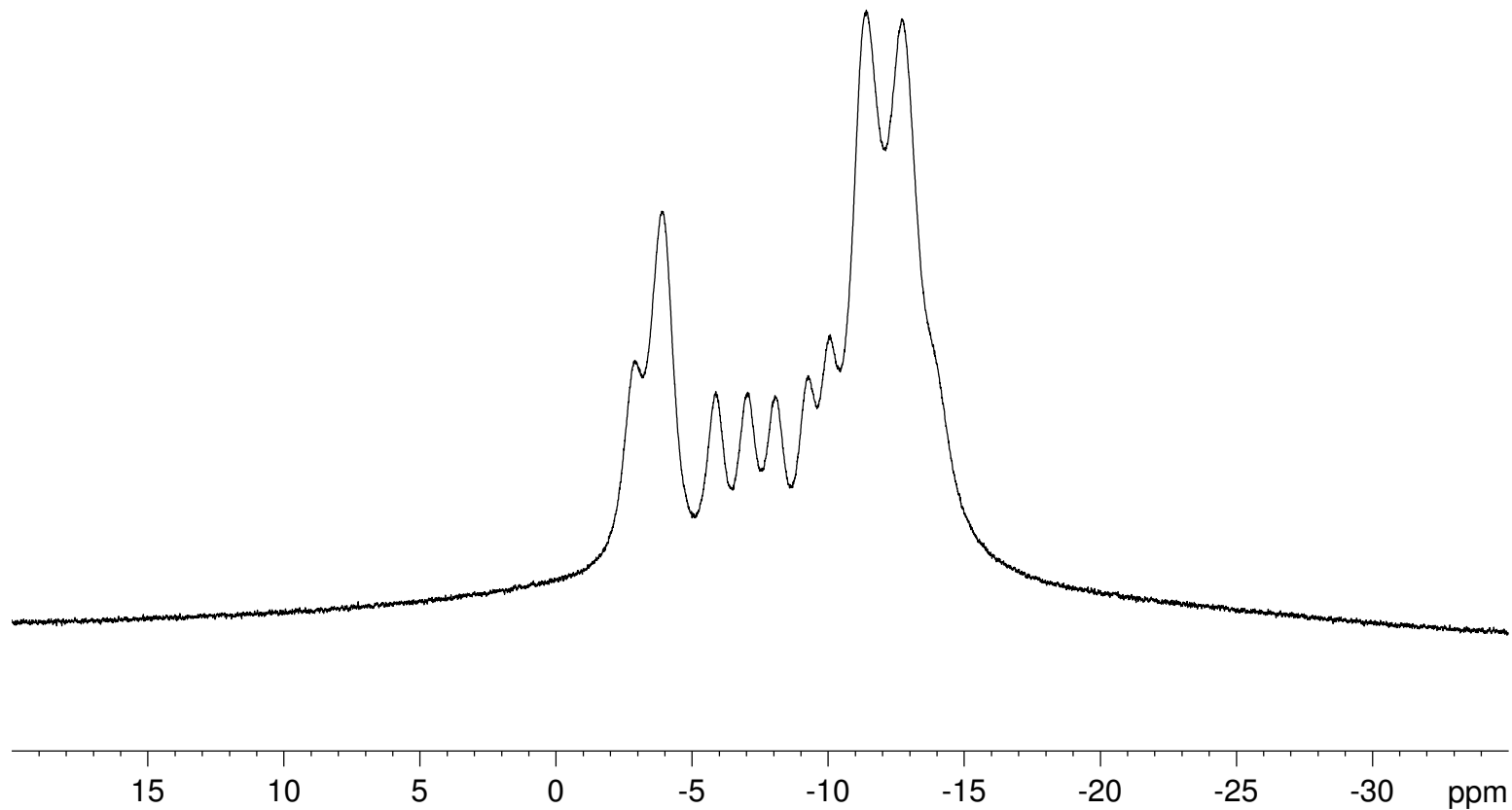
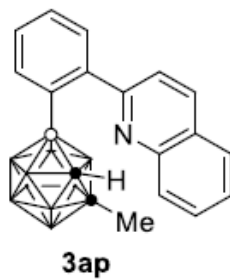
F2 - Acquisition Parameters

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

— -3.88  
— -5.87  
— -7.04  
— -8.04  
— -9.25  
— -10.08  
— -11.40  
— -12.71

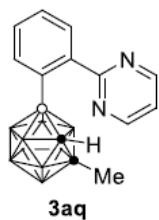


8.806  
8.794  
7.859  
7.849  
7.843  
7.415  
7.403  
7.395  
7.392  
7.382  
7.329  
7.317  
7.304  
7.259

4.461

1.961

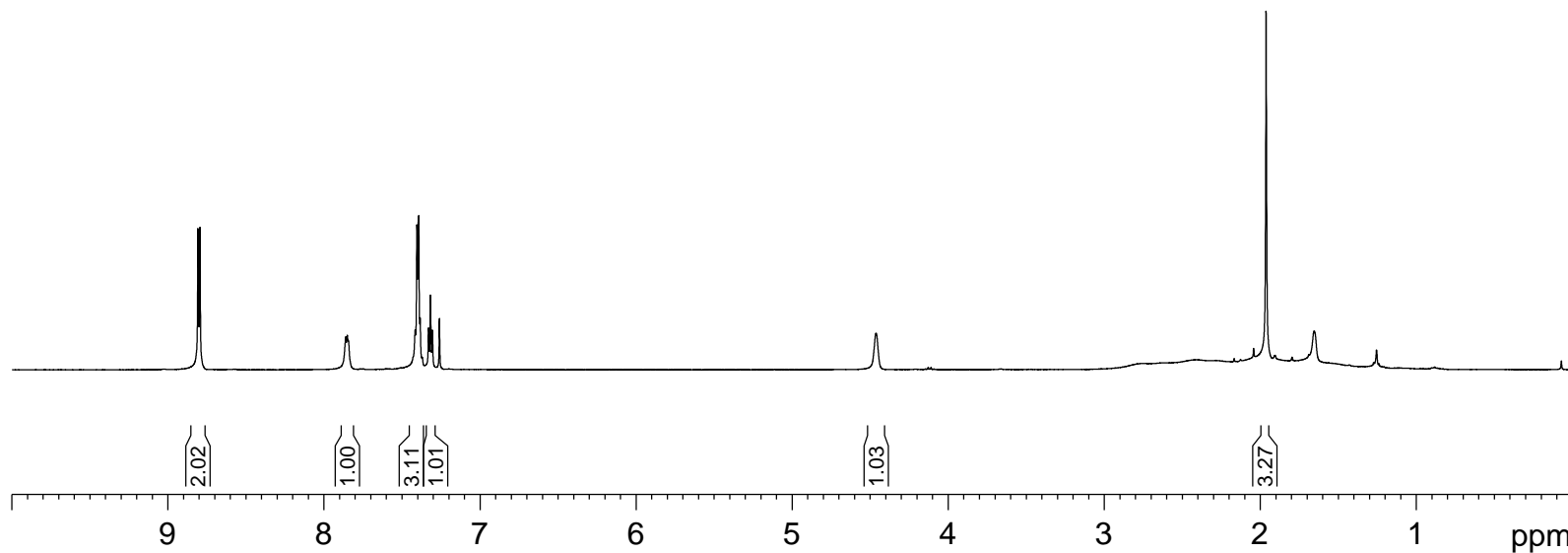
CY-H-A-53P-1



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 (zg30)  
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 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

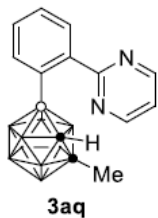


169.87  
156.64  
144.17  
137.09  
129.98  
128.30  
119.66

77.46  
77.14  
76.83  
70.60  
63.96

26.12

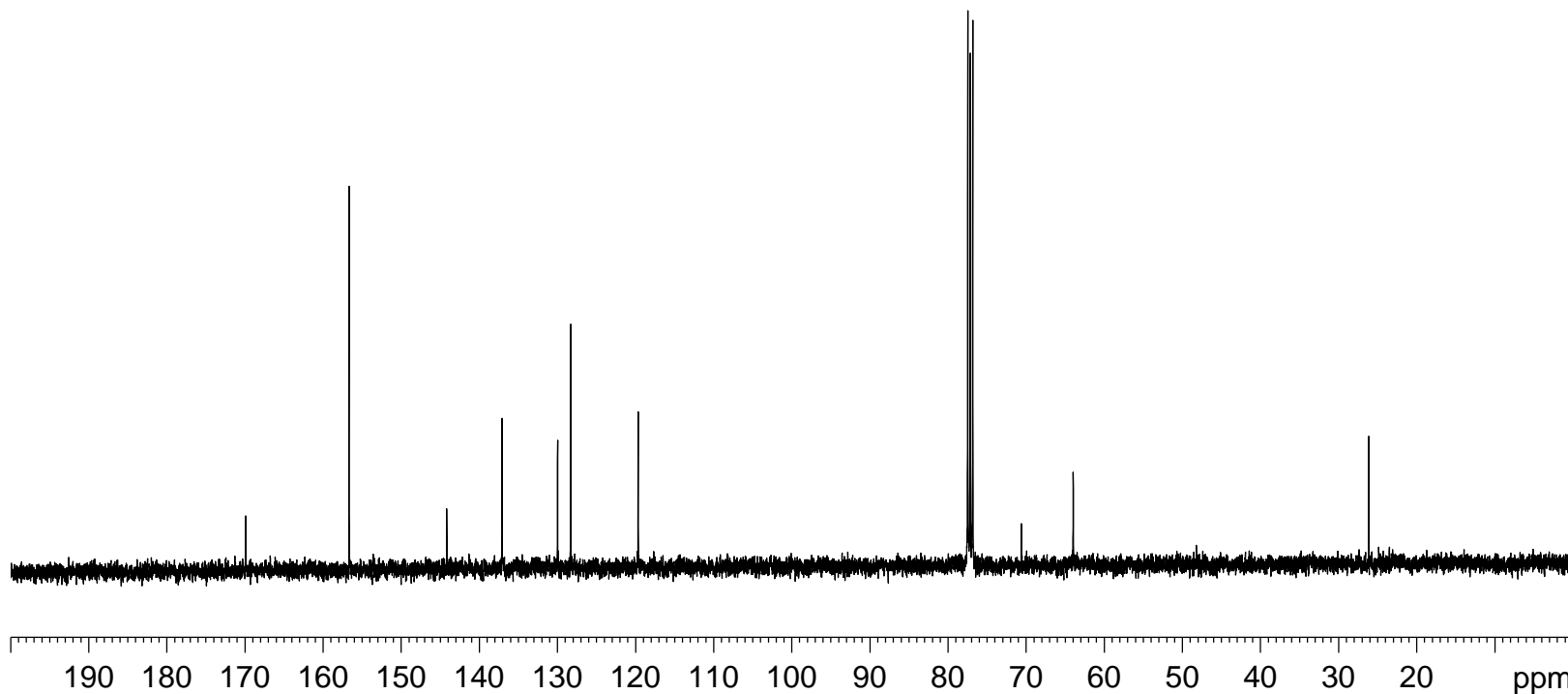
CY-C-A-53P



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

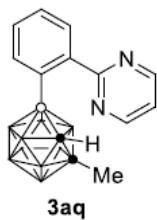
NAME CY-B-A-53P-1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

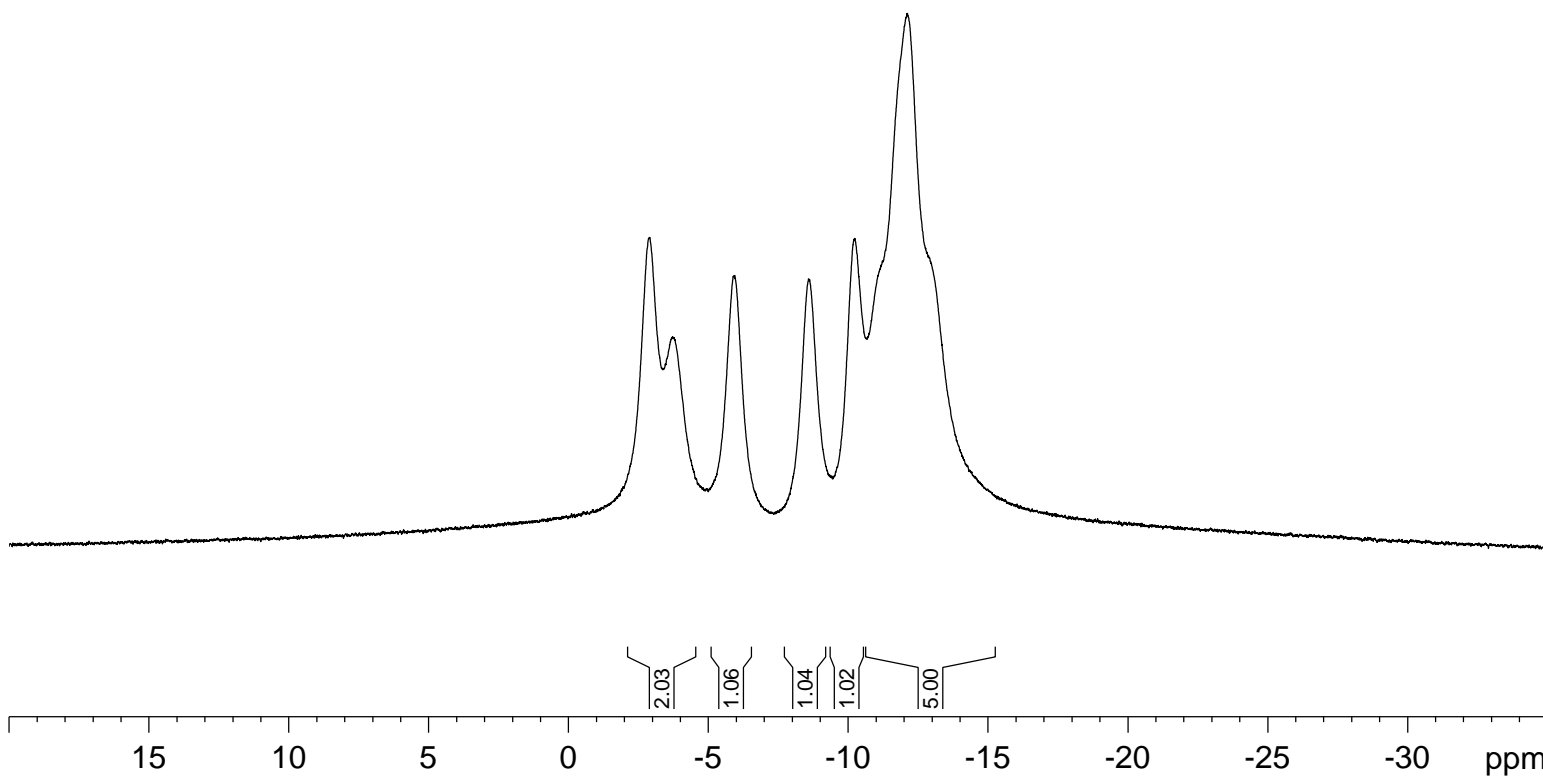
Date\_ 20161104  
Time 22.40 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 40  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 322  
DW 20.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 128.4096890 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



-2.90  
-3.72  
-5.94  
-8.58  
-10.24  
-12.11



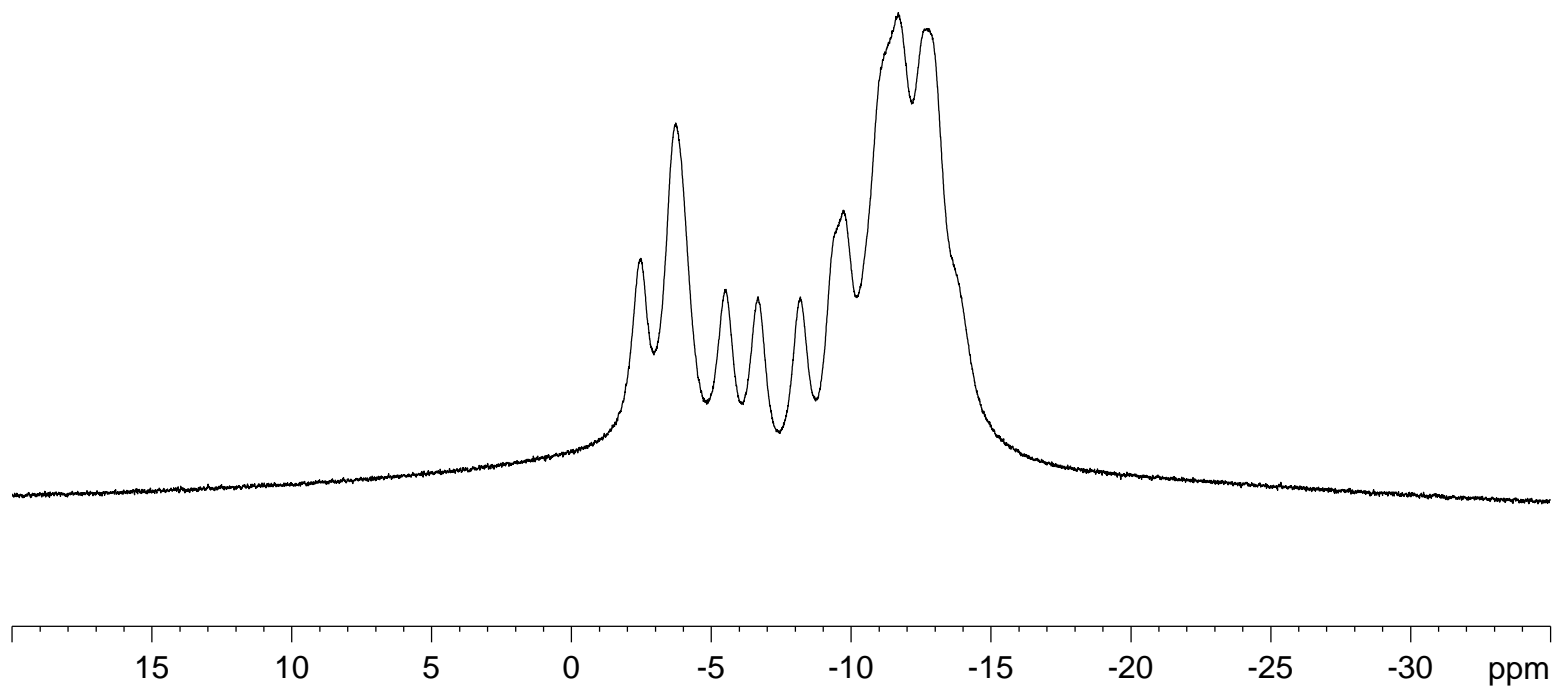
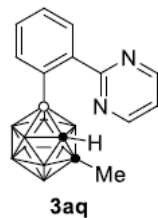
CY-B-A-53P-1-(C)

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

— 2.48  
— 3.73  
— 5.52  
— 6.67  
— 8.18  
— 9.72  
— 11.68  
— 12.74

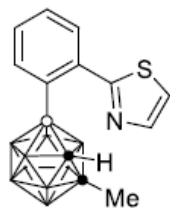


7.902  
7.802  
7.793  
7.473  
7.465  
7.438  
7.430  
7.426  
7.423  
7.418  
7.412  
7.404  
7.395  
7.391  
7.376  
7.372  
7.367  
7.361  
7.358  
7.349  
7.260

4.587

1.946

CY-H-A-62p



3ar

Current Data Parameters

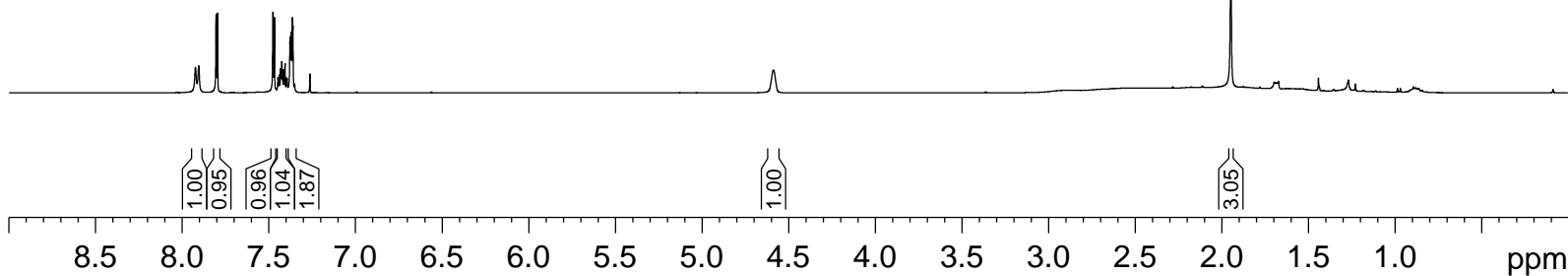
NAME CY-H-A-62p  
EXPNO 1  
PROCNO 1

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 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters

SI 65536  
SF 400.2300100 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



— 170.32

— 141.59

— 137.70

— 136.98

— 131.11

— 129.06

— 127.98

— 121.51

— 77.47

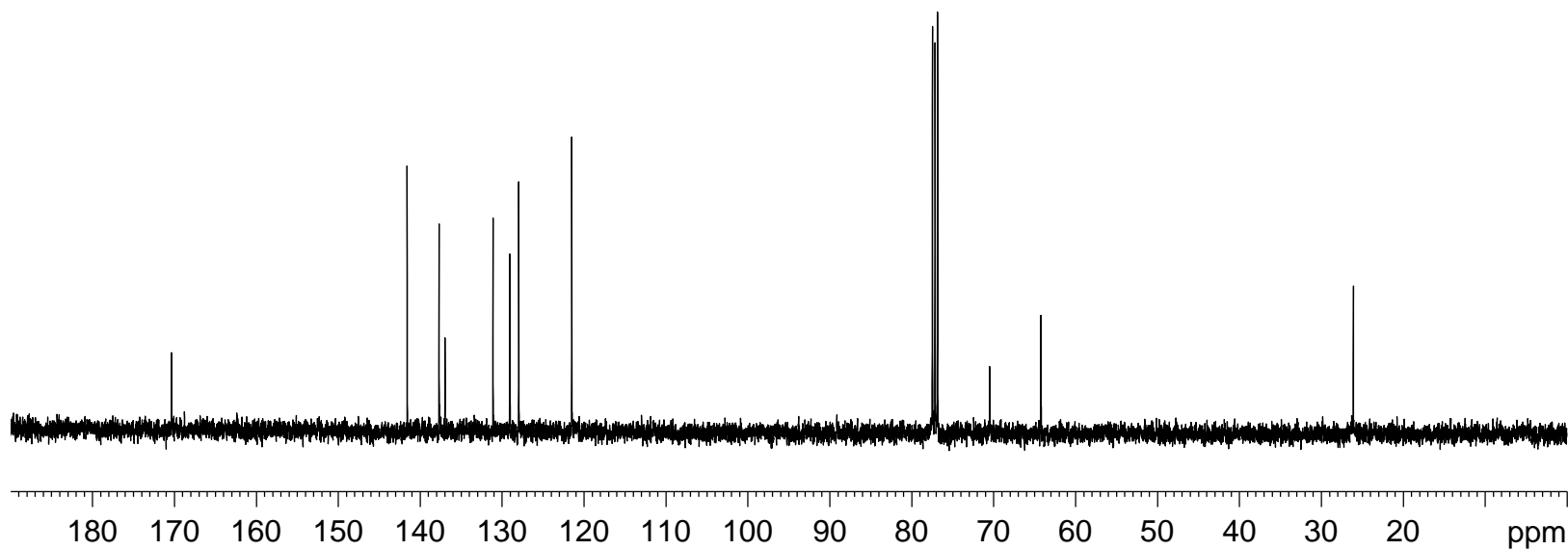
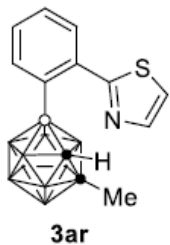
— 77.15

— 76.84

— 70.48

— 64.23

— 26.08



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

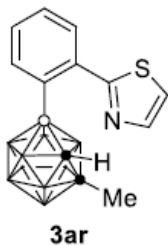
F2 - Processing parameters  
SI 32768  
SF 100.6379054 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

CY-B-A-62p

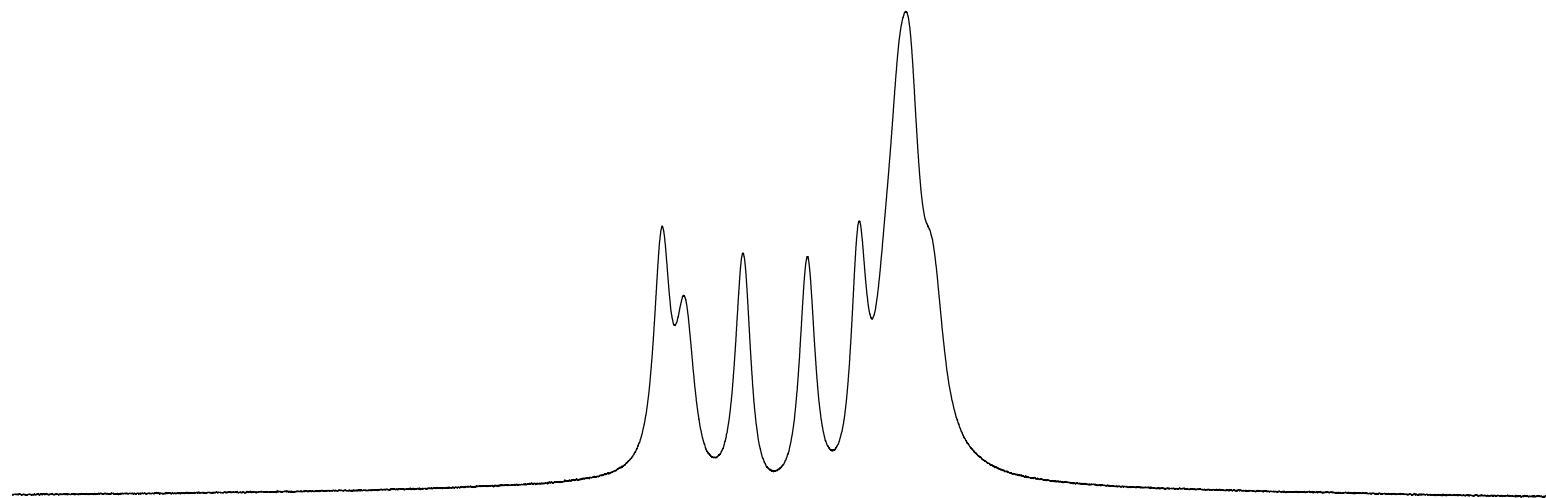
Current Data Parameters  
NAME CY-B-A-62p  
EXPNO 1  
PROCNO 1

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



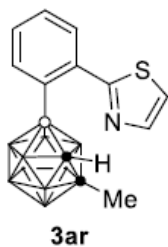
-3.24  
-4.00  
-6.14  
-8.42  
-10.29  
-11.94



1.07  
0.94  
1.05  
0.99  
1.10  
5.00

15 10 5 0 -5 -10 -15 -20 -25 -30 ppm





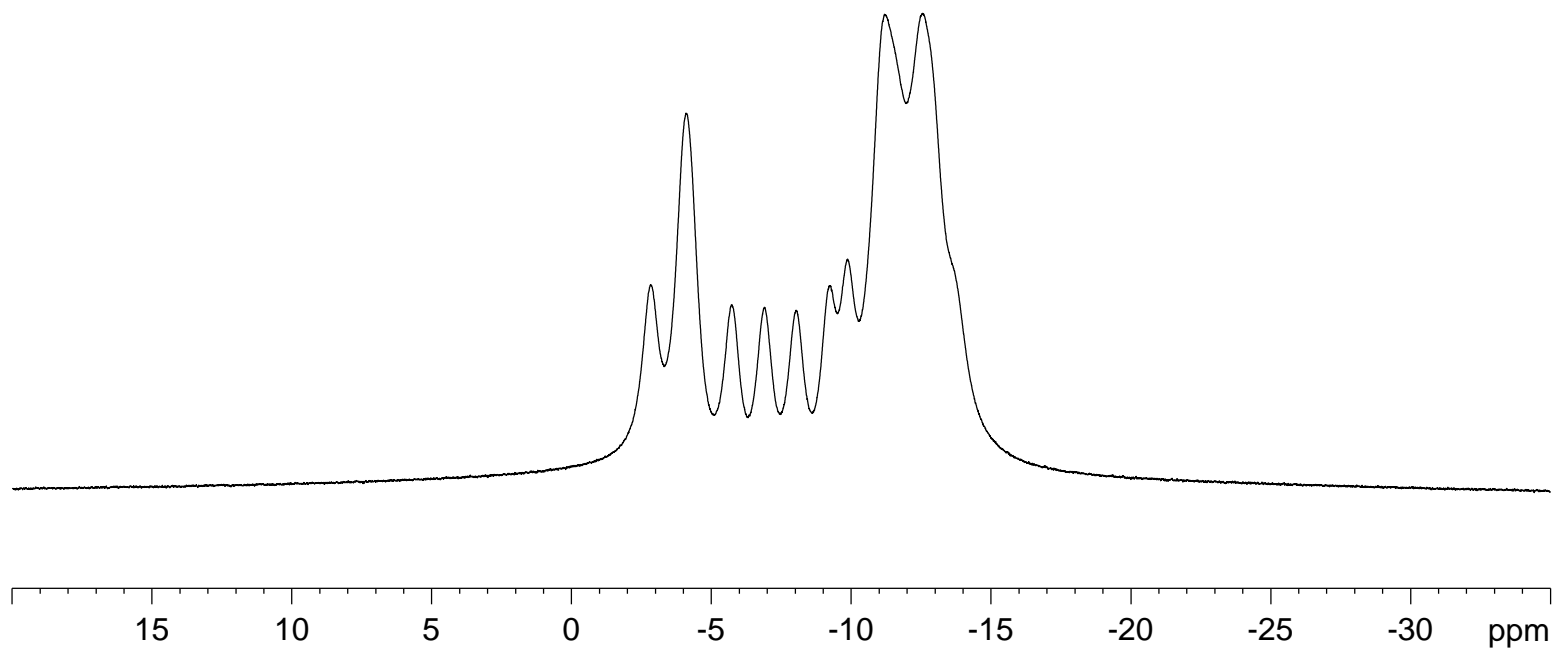
-2.84  
 -4.09  
 -5.72  
 -6.91  
 -8.03  
 -9.24  
 -9.88  
 -11.19  
 -12.55

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

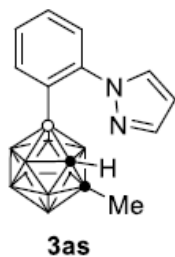
F2 - Processing parameters  
 SI 32768  
 SF 128.4097881 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



7.597  
7.592  
7.456  
7.453  
7.438  
7.434  
7.419  
7.415  
7.408  
7.403  
7.389  
7.385  
7.370  
7.366  
7.259  
7.180  
7.177  
7.161  
7.157  
6.459  
6.454  
6.449

3.084

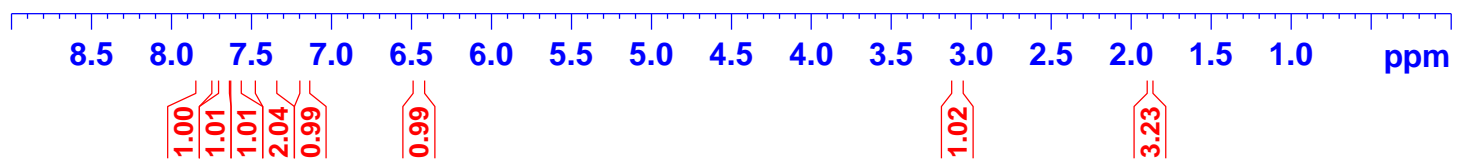
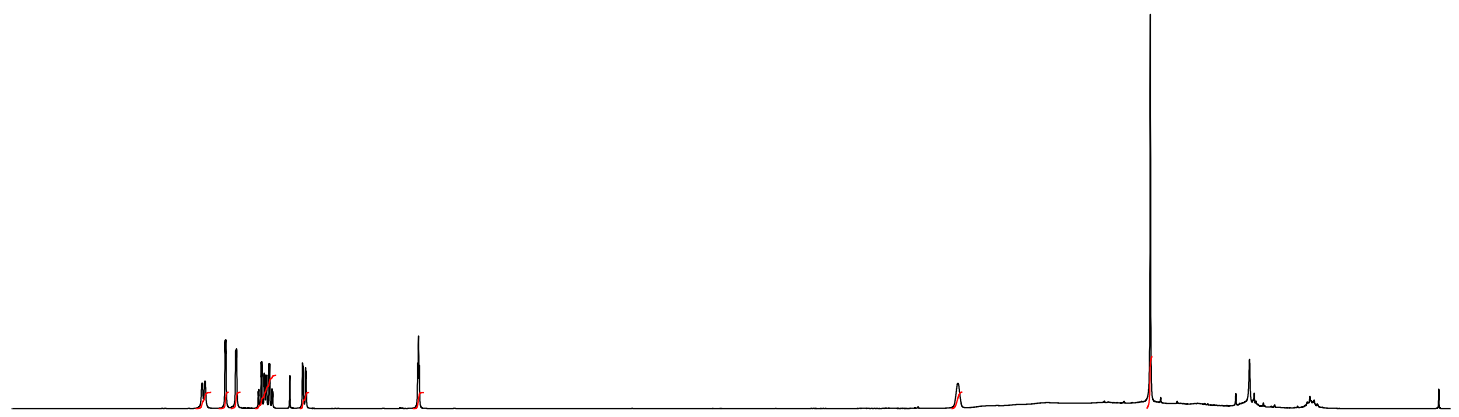
1.880



Current Data Parameters  
 NAME CY-H-A-25P-2-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160827  
 Time 10.31 h  
 INSTRUM spect  
 PROBHD z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 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-CDC13

Bruker Advance III 400

Current Data Parameters  
NAME CY-C-A-25P-2-CDC13  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160827  
Time 10.47 h  
INSTRUM spect  
PROBHD Z824601\_0021 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
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

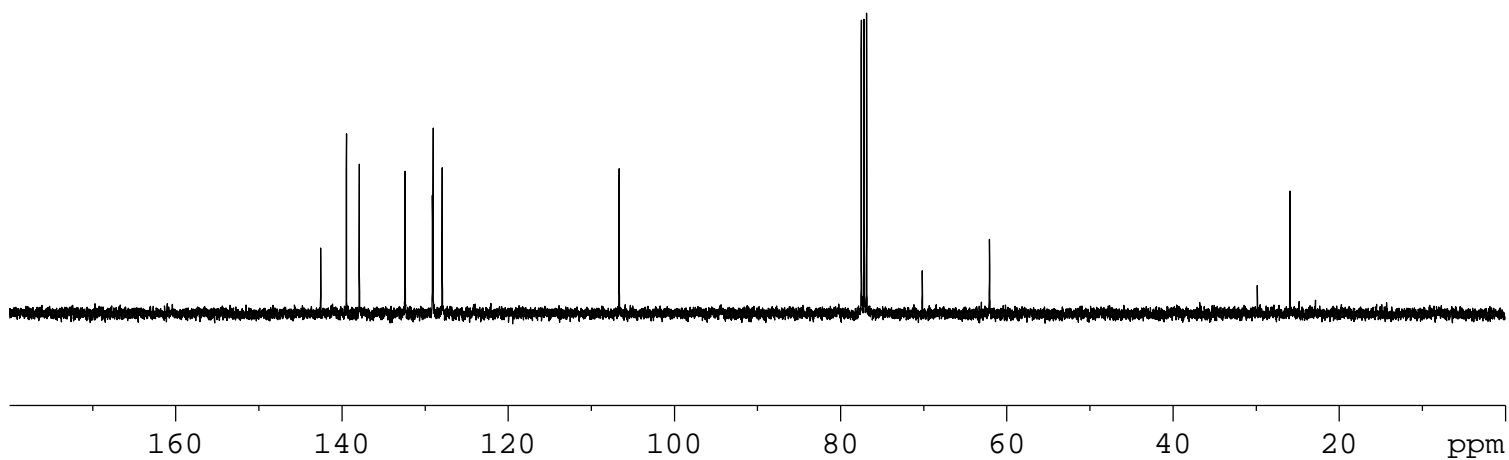
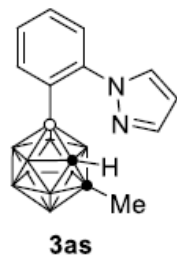
F2 - Processing parameters  
SI 32768  
SF 100.6127590 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

142.548  
139.444  
137.894  
132.382  
129.089  
129.005  
127.912

106.632

77.476  
77.159  
76.840  
70.139  
62.050

25.889



CY-B-A-25P-2

Current Data Parameters

NAME CY-B-A-25P-2  
EXPNO 1  
PROCNO 1

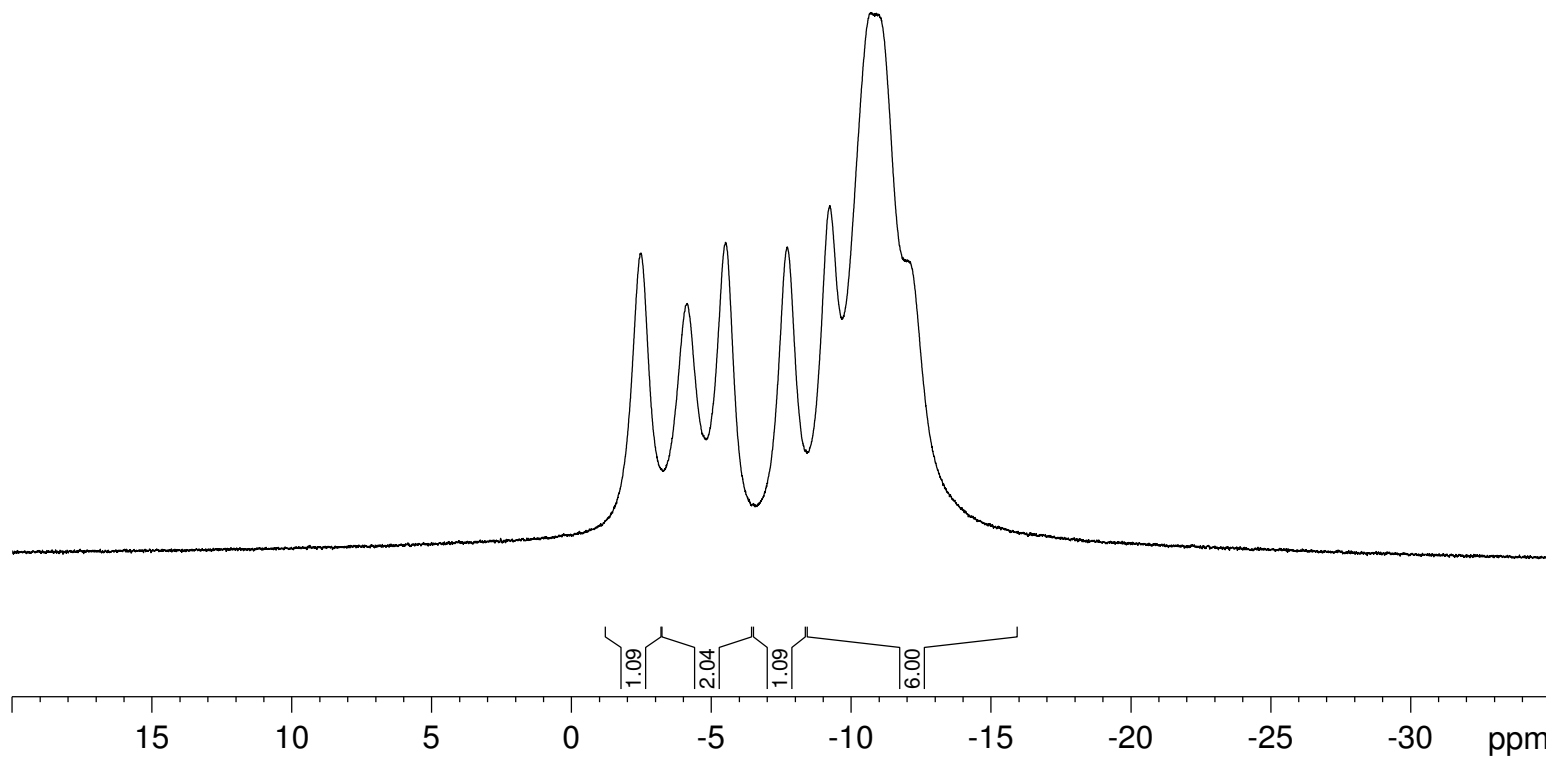
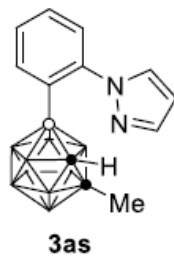
F2 - Acquisition Parameters

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

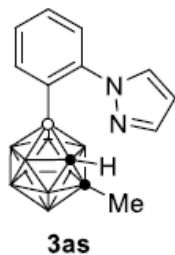
F2 - Processing parameters

SI 32768  
SF 128.4097615 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

— 2.48  
— 4.13  
— 5.51  
— 7.70  
— 9.23  
— 10.71



| -1.75  
 | -2.90  
 | -3.97  
 | -4.70  
 | -5.94  
 | -6.96  
 | -8.33  
 | -9.74  
 | -11.20

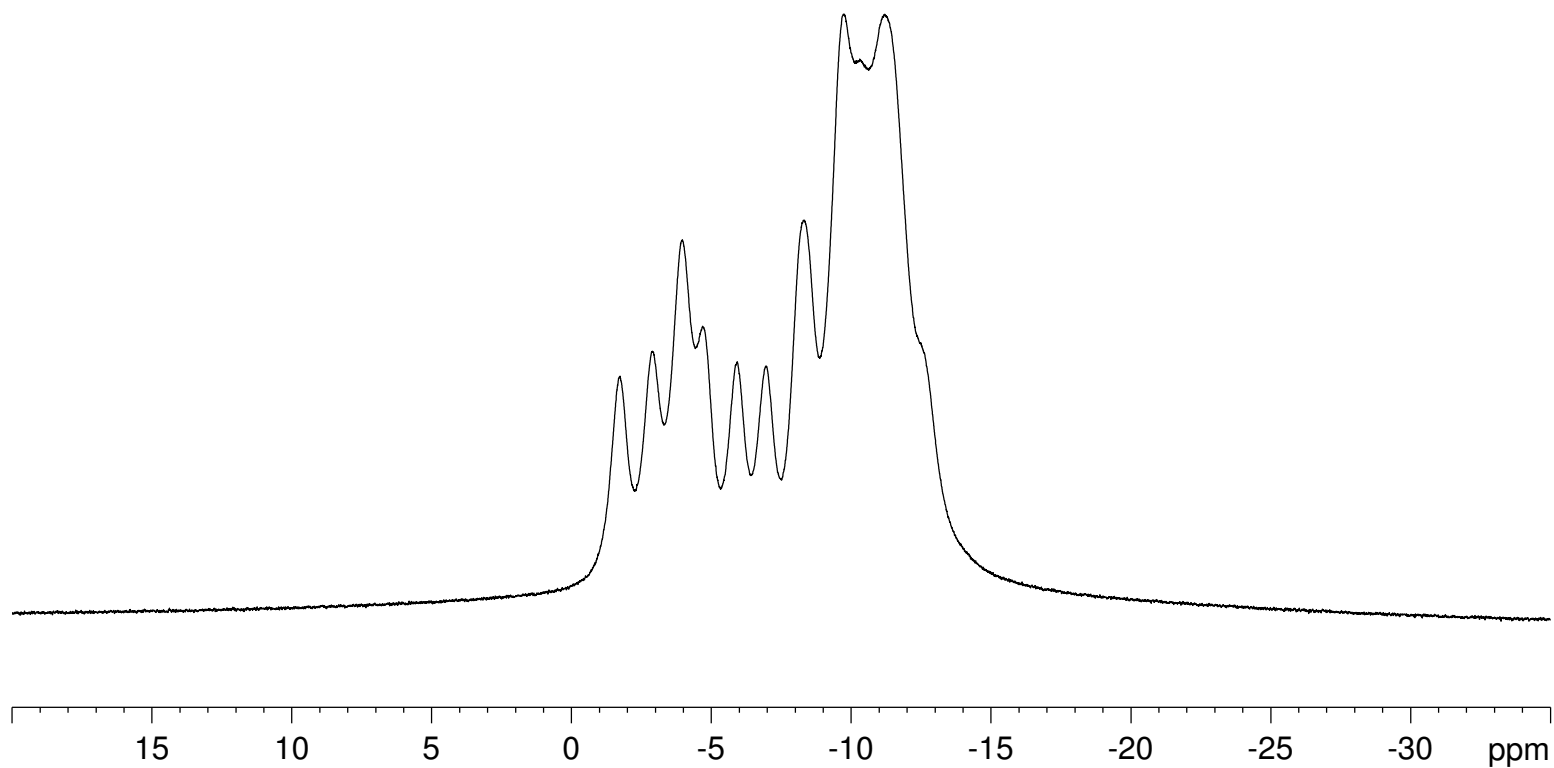


CY-B-A-25P-2- (C)

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

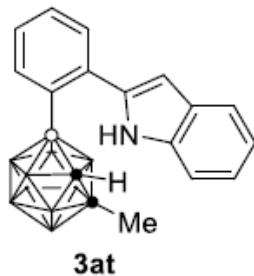
F2 - Acquisition Parameters  
 Date\_ 20160827  
 Time 11.01 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (zg)  
 PULPROG zg  
 TD 65536  
 SOLVENT C6D6  
 NS 22  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 181  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.5 K  
 D1 2.00000000 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



7.411  
7.409  
7.407  
7.391  
7.389  
7.372  
7.369  
7.361  
7.356  
7.354  
7.344  
7.260  
7.256  
7.253  
7.239  
7.236  
7.218  
7.215  
7.193  
7.190  
7.173  
7.171  
7.156  
7.153  
6.495  
6.493  
6.490  
6.488

— 2.245  
— 1.558



Current Data Parameters  
NAME CY-H-A-23p-CDC13-re2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161129  
Time 19.57 h  
INSTRUM spect  
PROBHD Z824601\_0021 (  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
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



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm

0.98  
1.03  
1.04  
4.06  
1.05  
1.03  
1.00

1.08  
3.21

CY-C-A-24P-CDCl3

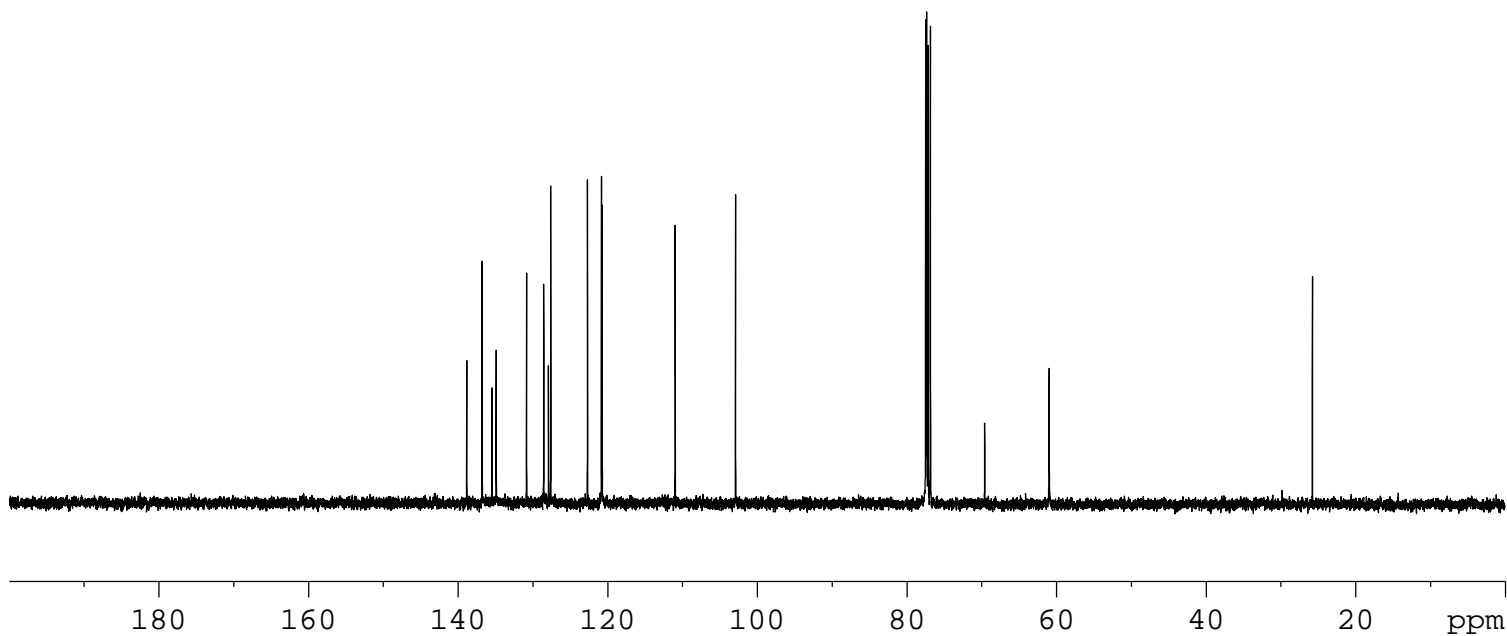
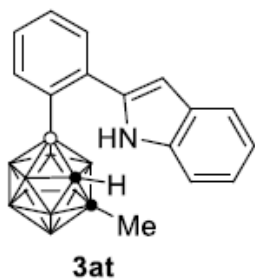
Bruker Advance III 400

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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 41.2500000 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

138.843  
136.803  
135.472  
134.900  
130.841  
128.549  
127.917  
127.615  
122.702  
120.834  
120.737  
110.975  
102.897  
77.473  
77.156  
76.838  
69.589  
60.965  
25.756



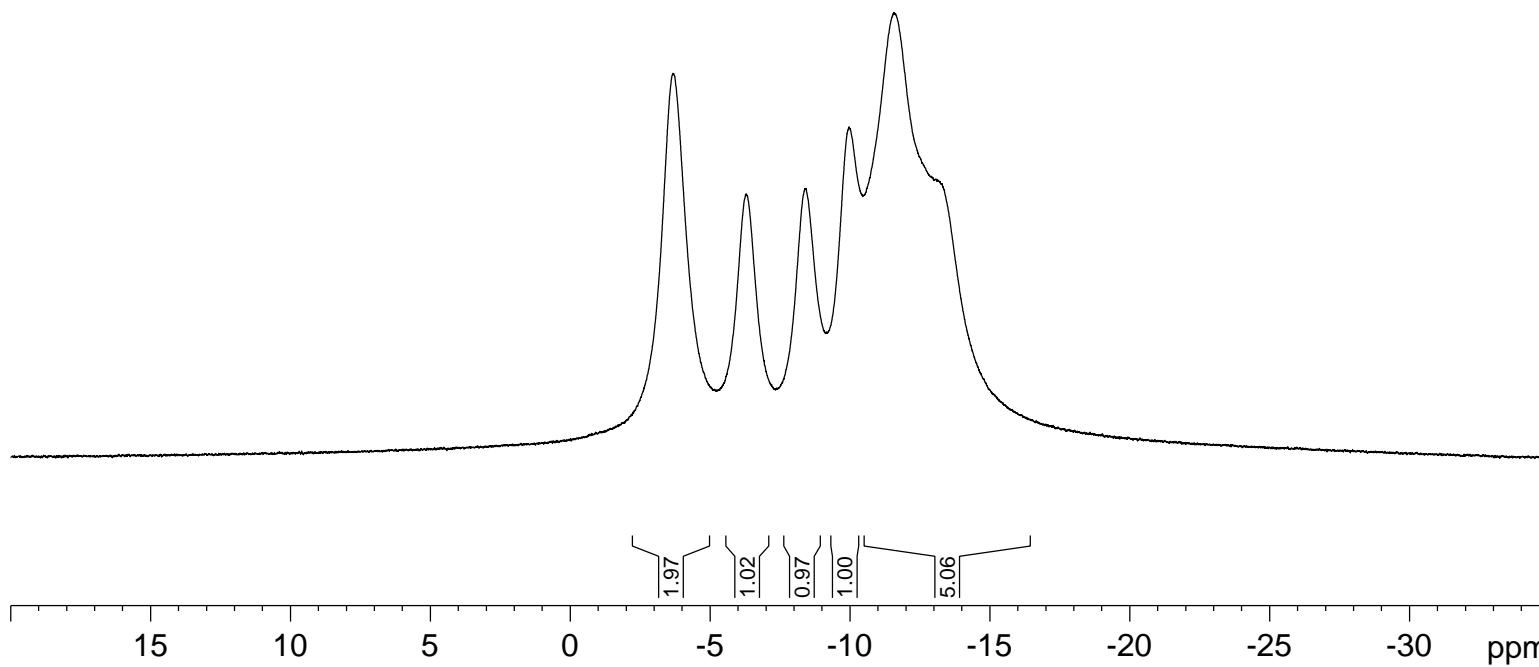
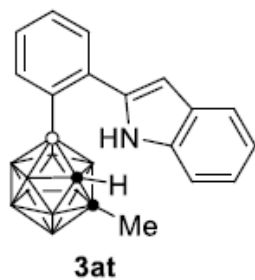
CY-B-A-23P

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 2.0000000 sec  
D11 0.0300000 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

— 3.68  
— 6.30  
— 8.42  
— 9.96  
— 11.57





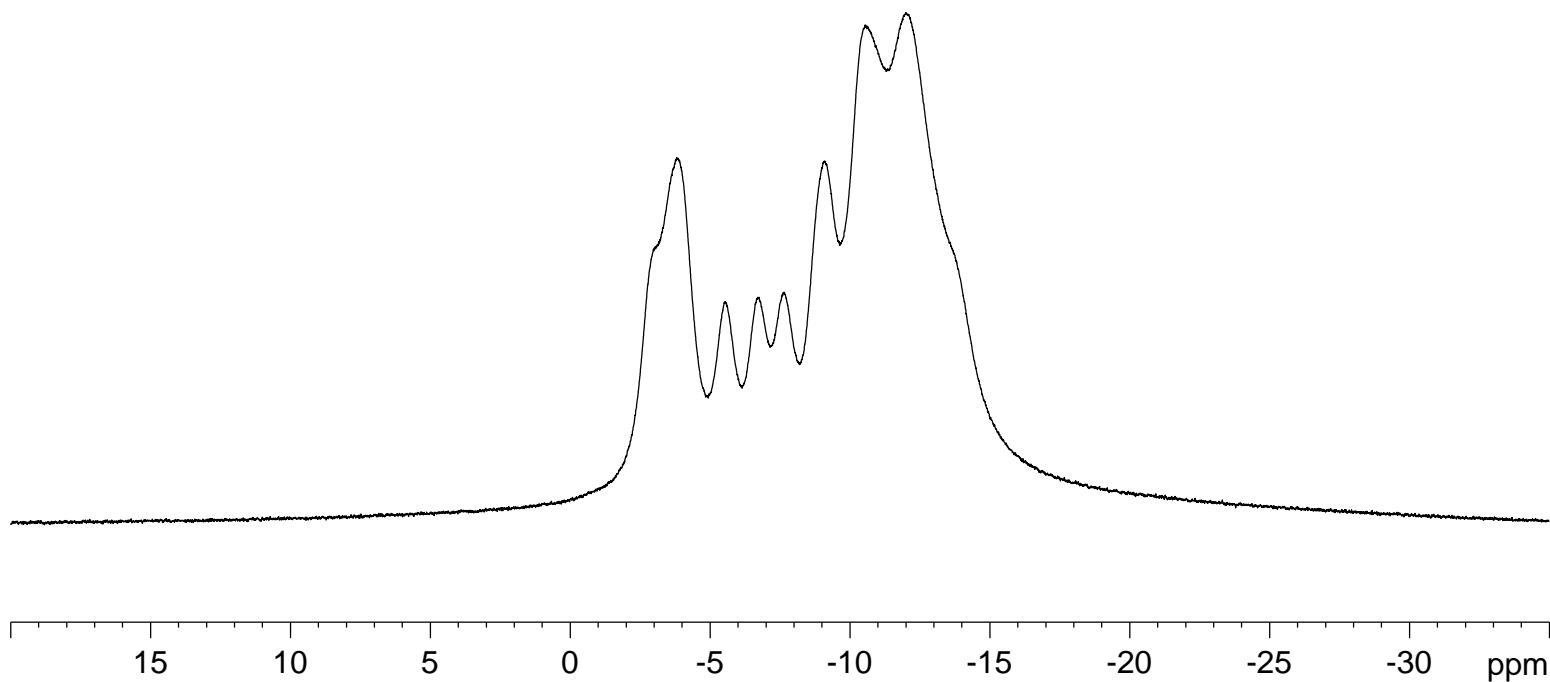
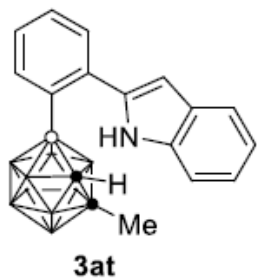
CY-B-A-23P-(C)

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

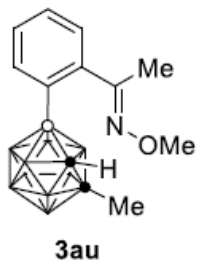
—2.92  
 —3.80  
 —5.54  
 —6.75  
 —7.65  
 —9.08  
 —10.55  
 —12.00  
 —13.73



7.729  
7.712  
7.708  
7.350  
7.345  
7.331  
7.327  
7.314  
7.309  
7.297  
7.293  
7.278  
7.274  
7.259  
7.134  
7.130  
7.118  
7.115  
7.112

— 4.209  
— 3.933

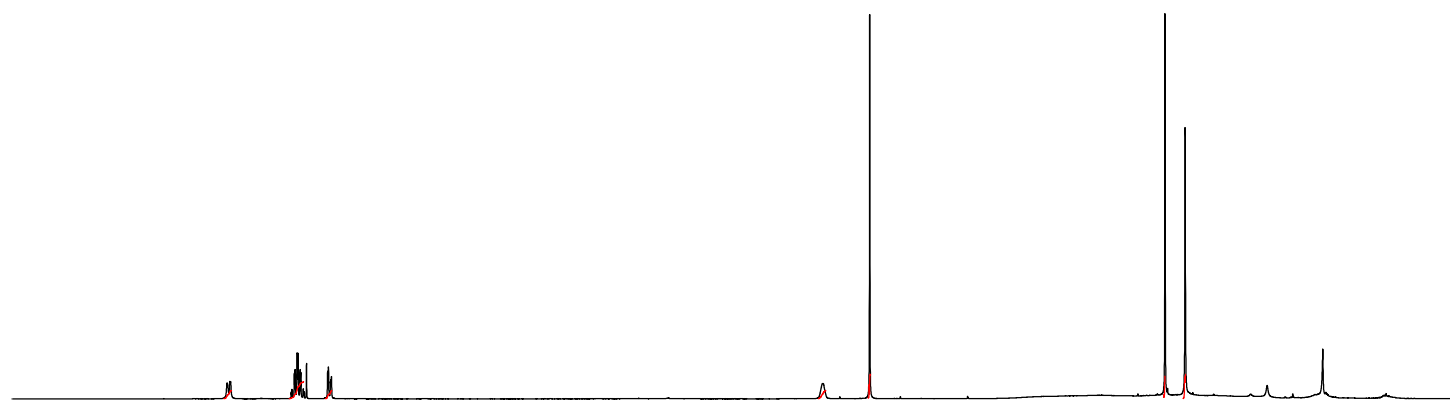
— 2.189  
— 2.070



Current Data Parameters  
NAME CY-H-A-16p-CDC13-re  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161129  
Time 19.42 h  
INSTRUM spect  
PROBHD z824601\_0021 (  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
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  
SF01 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



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm

1.00  
2.08  
1.00

1.00  
2.98

3.02  
3.06

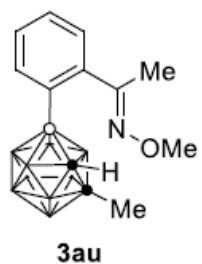
— 159.283  
 — 141.588  
 — 137.266  
 128.344  
 128.099  
 127.919

77.475  
 77.157  
 76.840  
 — 70.748  
 63.564  
 61.838

— 26.271  
 — 18.192

CY-C-A-16P-CDCl3

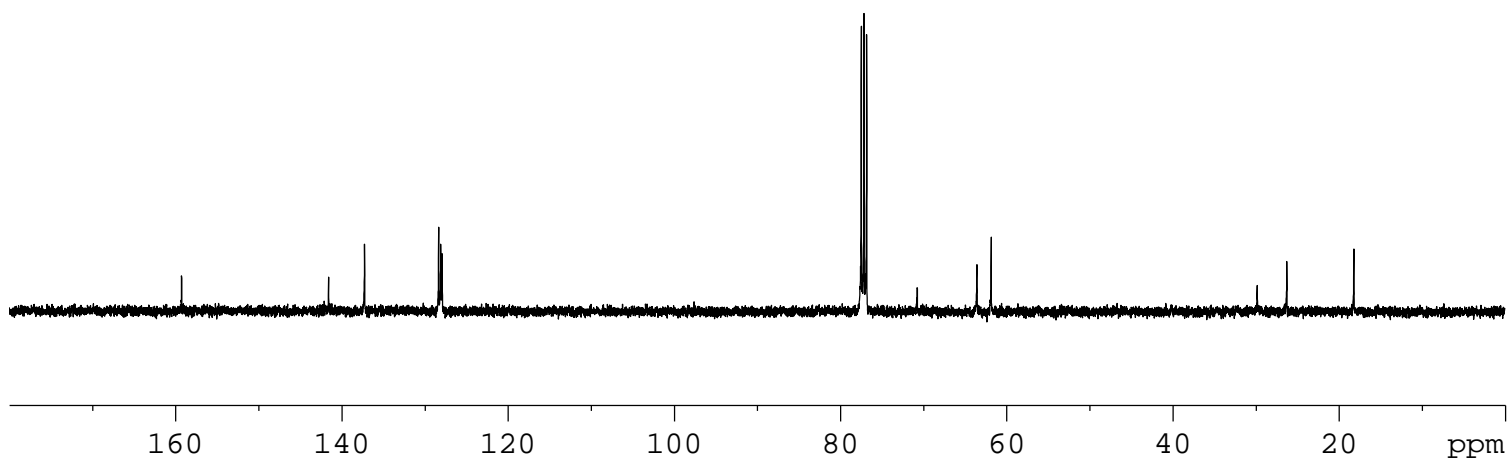
Bruker Advance III 400



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 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 41.2500000 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 FCPD2 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



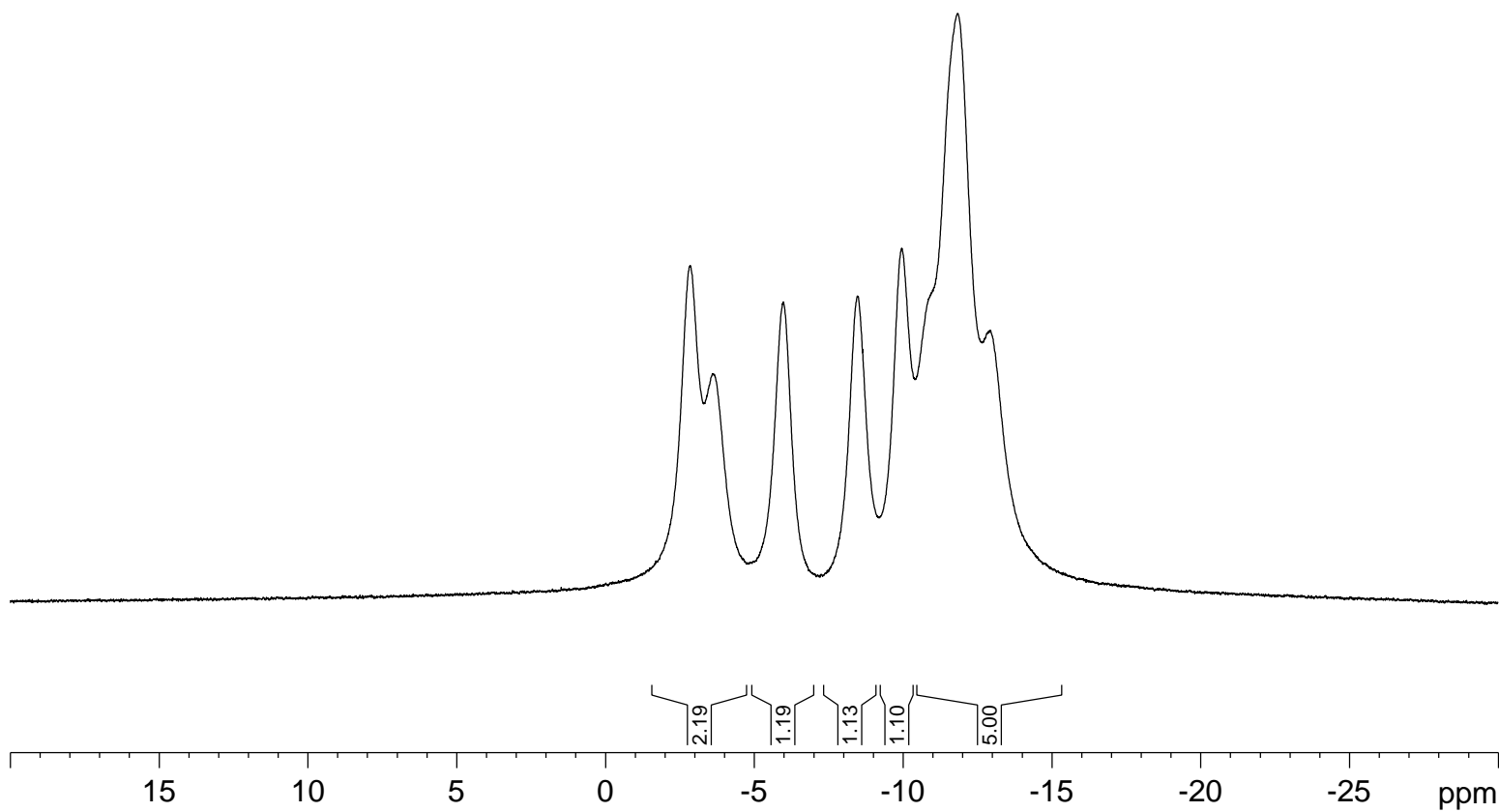
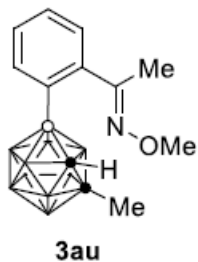
CY-B-A-16P

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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W  
SFO2 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.56000042 W  
PLW12 0.27428001 W

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

— -2.85  
— -3.60  
— -5.98  
— -8.47  
— -9.94  
— -11.83  
— -12.92



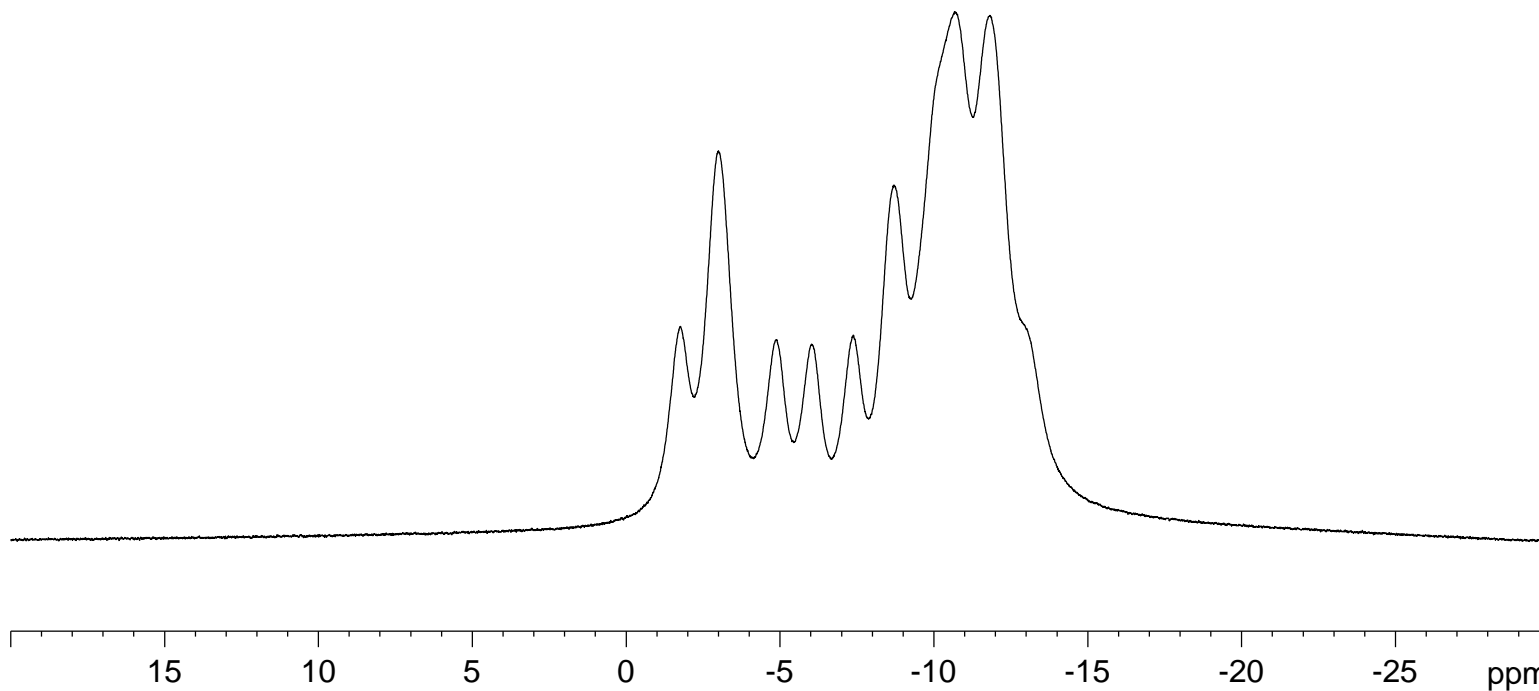
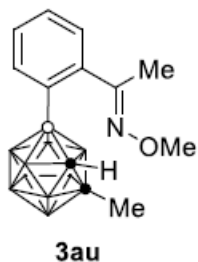
CY-B(C)-A-16P

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

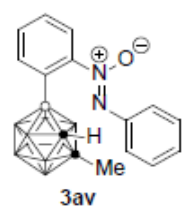
1.77  
3.00  
4.87  
6.03  
7.38  
8.71  
10.68  
11.82



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

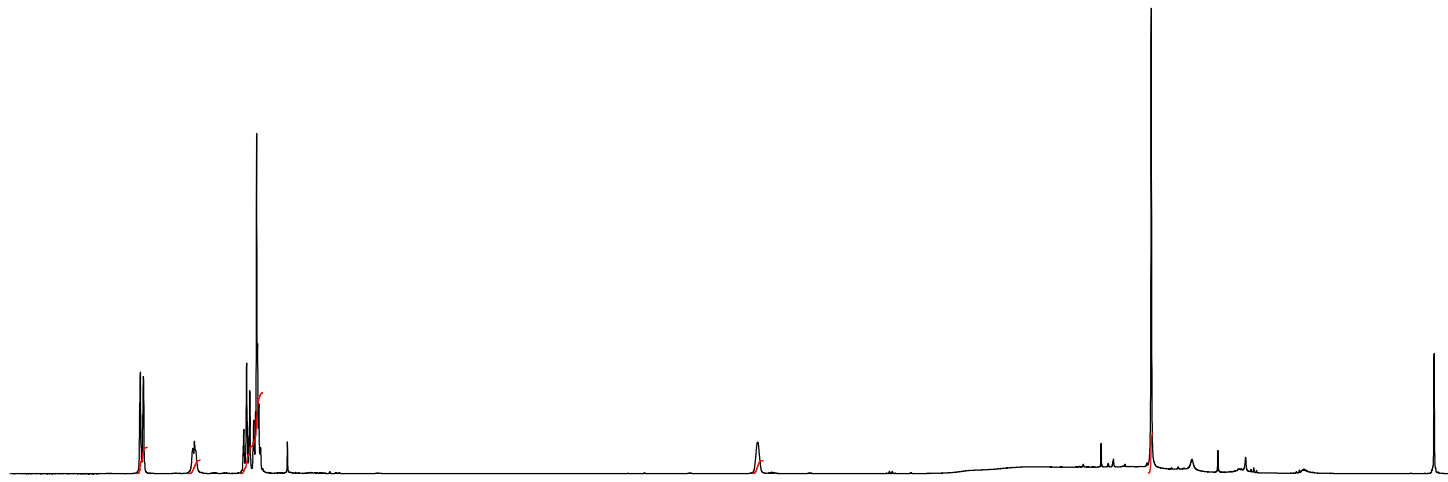
1.862



Current Data Parameters  
 NAME CY-H-A-38p-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161014  
 Time 20.07 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 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



8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

2.00

1.04

6.19

1.00

3.11

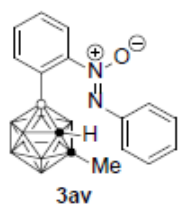
152.971  
 143.724  
 138.202  
 130.608  
 129.443  
 129.315  
 129.077  
 125.603  
 123.303

77.476  
 77.158  
 76.841  
 70.432  
 62.511

25.866

CY-C-A-38P-CDCl3

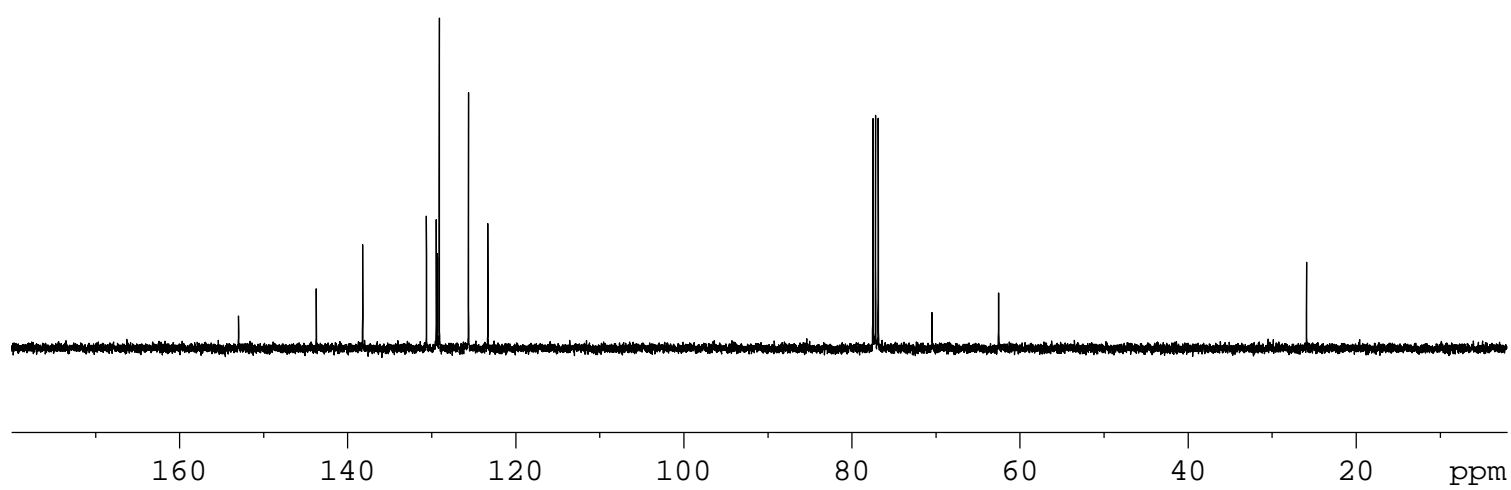
Bruker Advance III 400

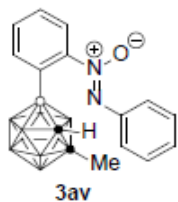


Current Data Parameters  
 NAME CY-C-A-38P-CDCl3  
 EXPNO 1  
 PROCNO 1

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 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 41.2500000 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 FCPD2 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





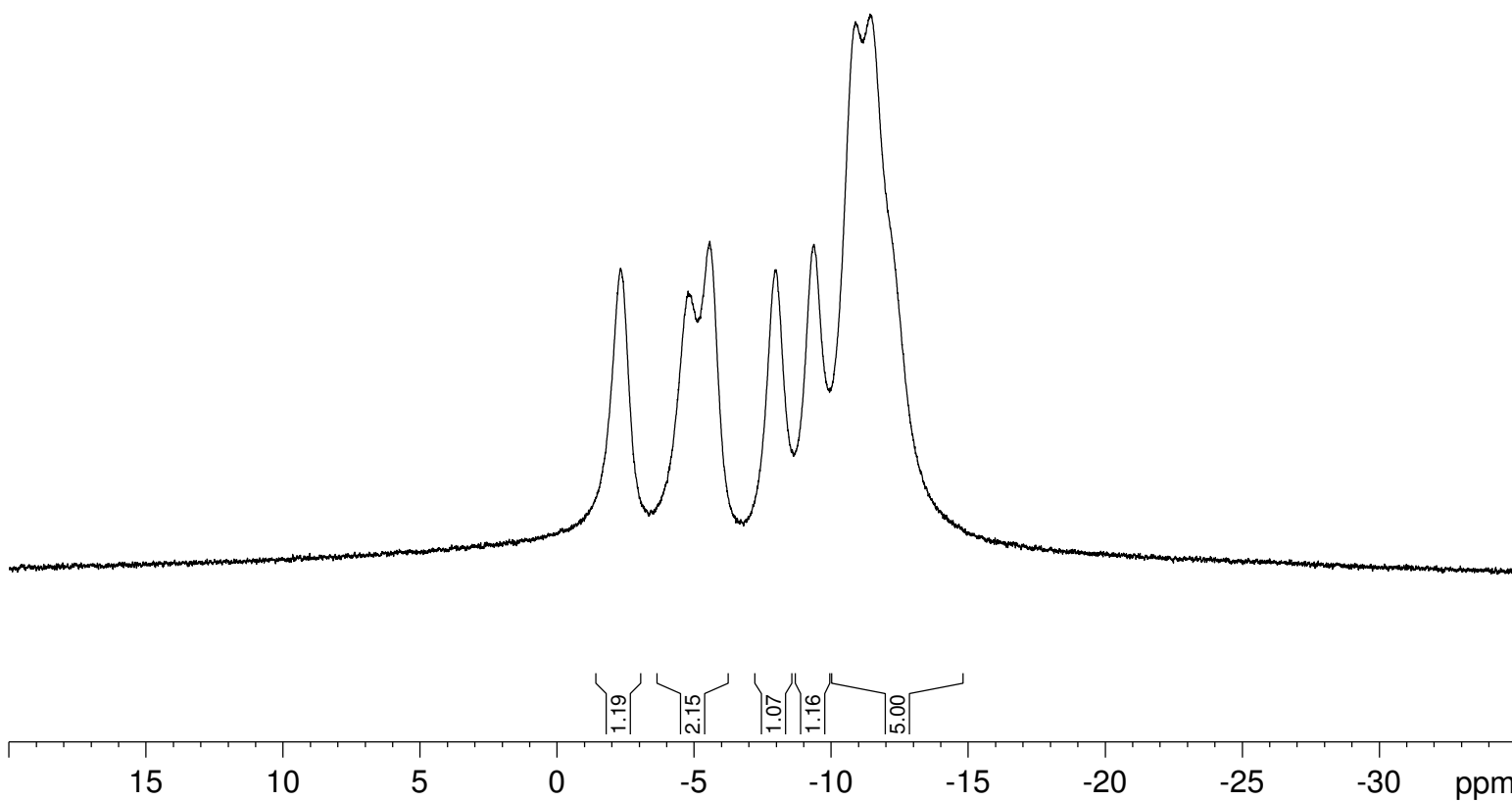
— 2.32  
 — 4.78  
 — 5.57  
 — 7.96  
 — 9.37  
 — 10.89  
 — 11.42

CY-B-38P-p

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

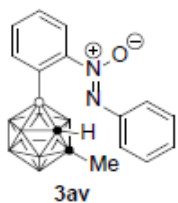
F2 - Acquisition Parameters  
 Date\_ 20160914  
 Time 14.07 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 12  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 287  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.2 K  
 D1 2.00000000 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





| -1.59  
 | -2.74  
 | -4.71  
 | -5.98  
 | -7.19  
 | -8.50  
 | -9.92  
 | -11.32



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

Current Data Parameters

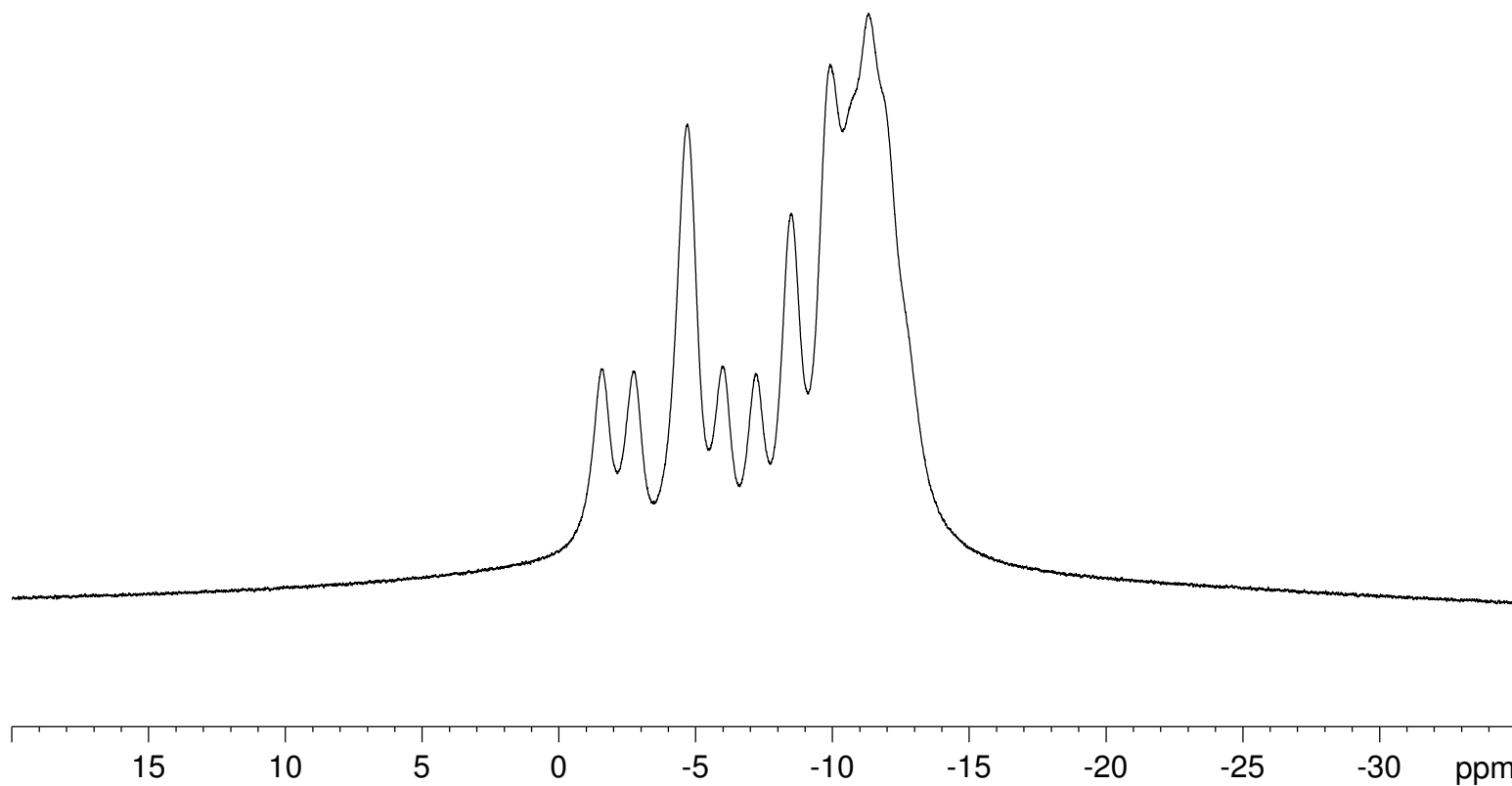
NAME CY-B-38P-p- (C)  
 EXPNO 1  
 PROCNO 1

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

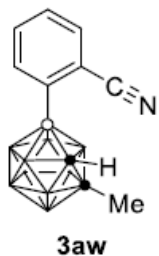


7.768  
7.749  
7.622  
7.620  
7.602  
7.600  
7.556  
7.553  
7.537  
7.534  
7.518  
7.515  
7.422  
7.419  
7.403  
7.400  
7.384  
7.381  
7.259

4.780

2.132

CY-H-A-50p



Current Data Parameters

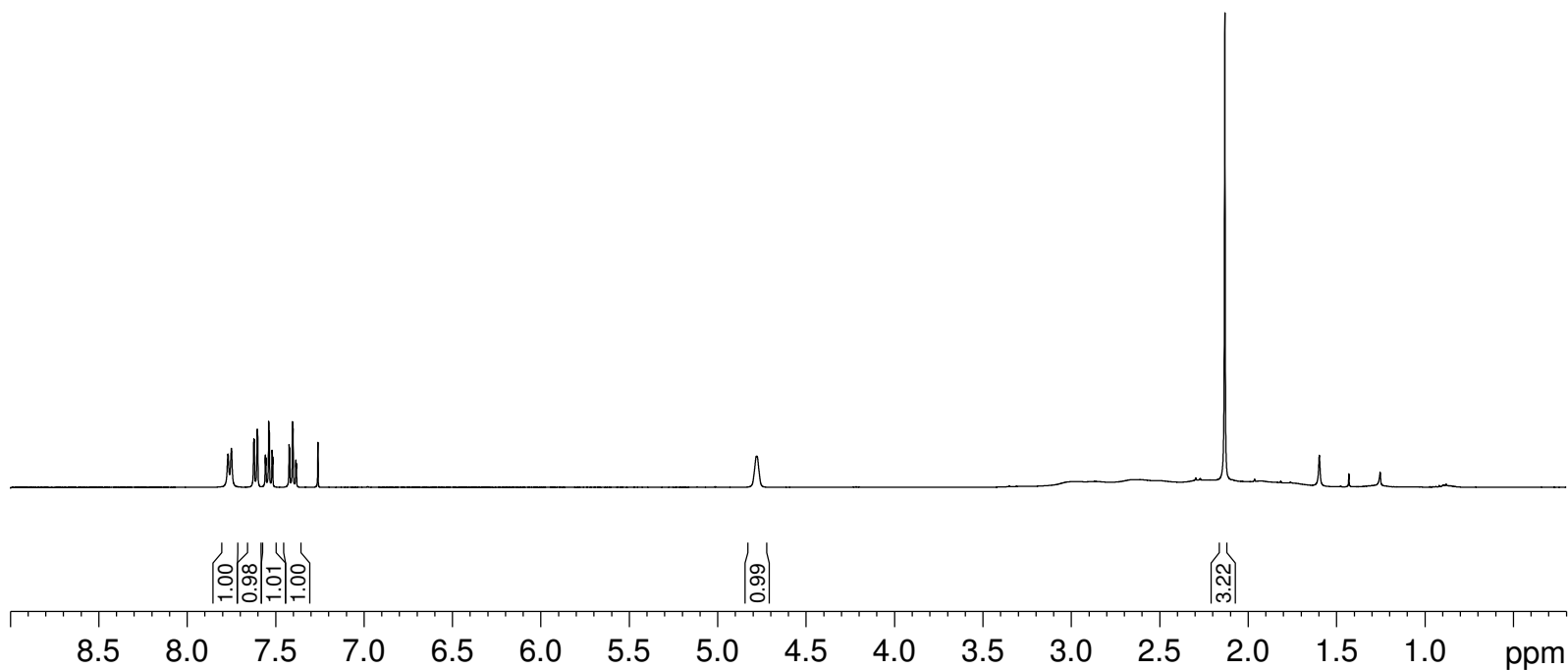
NAME CY-H-A-50p  
EXPNO 1  
PROCNO 1

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 1.0000000 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

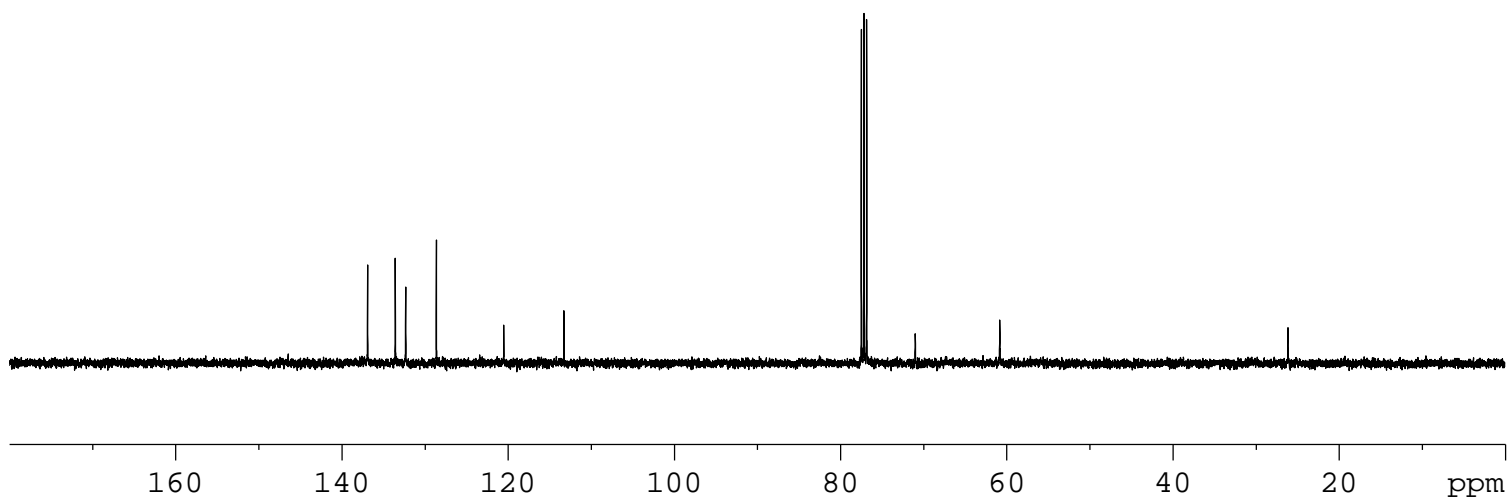
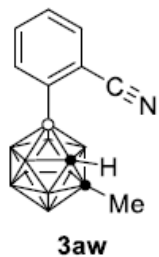
F2 - Acquisition Parameters  
Date\_ 20161012  
Time 10.39 h  
INSTRUM spect  
PROBHD z824601\_0021 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 121  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 41.2500000 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

136.893  
133.569  
132.313  
128.621  
120.519  
113.263

77.472  
77.155  
76.837  
70.992  
60.820

26.128



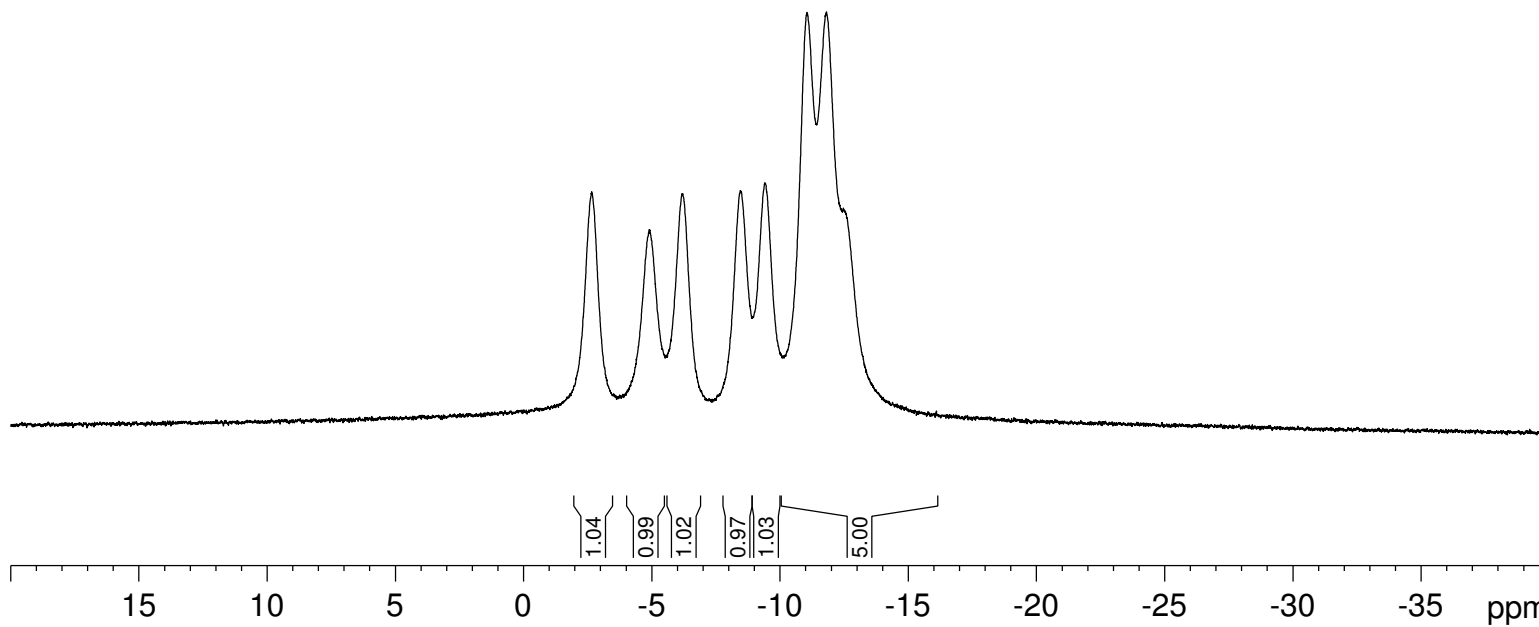
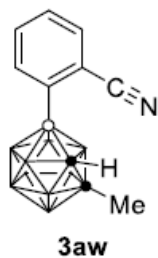
CY-B-A-50P

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 CDC13  
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

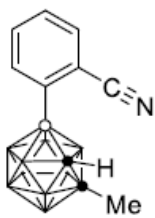
F2 - Processing parameters  
SI 32768  
SF 128.4097793 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

— -2.66  
— -4.91  
— -6.18  
— -8.46  
— -9.41  
— -11.06  
— -11.81

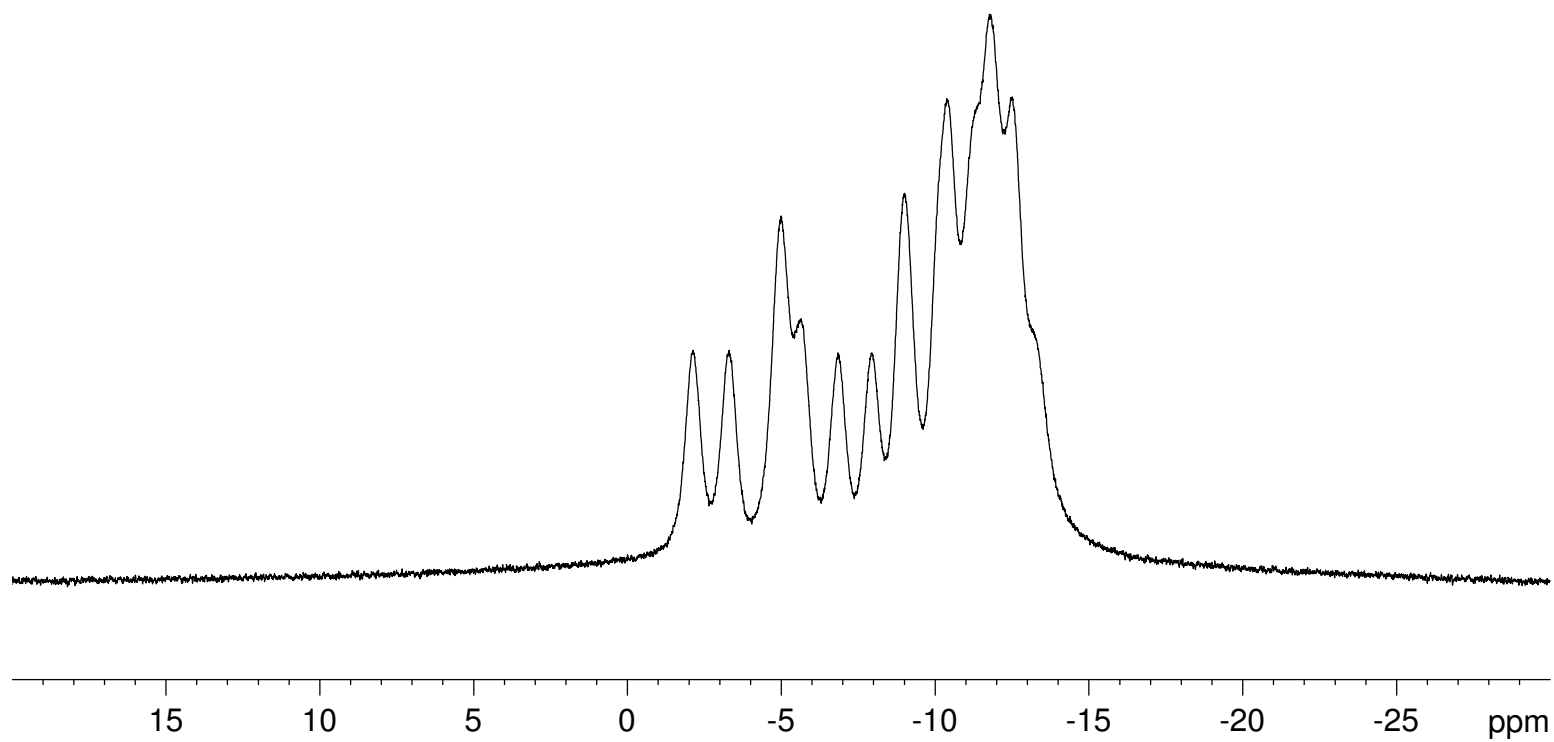


CY-B-A-50P-(C)

— 2.13  
— 3.30  
— 4.99  
— 5.64  
— 6.85  
— 7.93  
— 9.01  
— 10.38  
— 11.77  
— 12.51



3aw



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

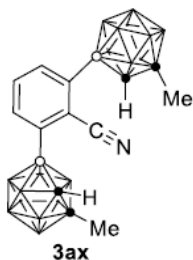
F2 - Processing parameters  
SI 32768  
SF 128.4097881 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

7.748  
7.729  
7.483  
7.464  
7.445  
7.257

4.813

2.122

CY-H-A-14p



Current Data Parameters

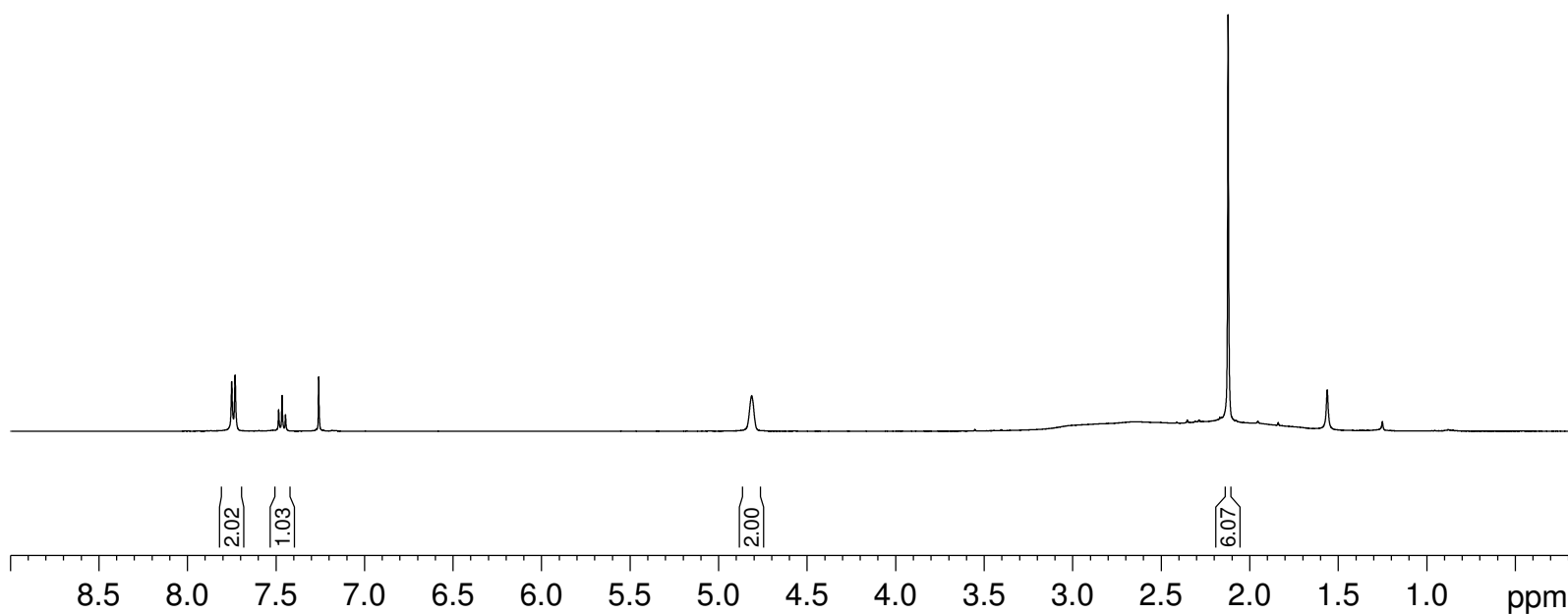
NAME CY-H-A-14p  
EXPNO 1  
PROCNO 1

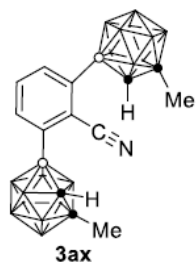
F2 - Acquisition Parameters

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





— 136.90  
— 131.44  
— 121.90  
— 113.67

77.47  
77.15  
76.84  
— 70.80  
— 60.87

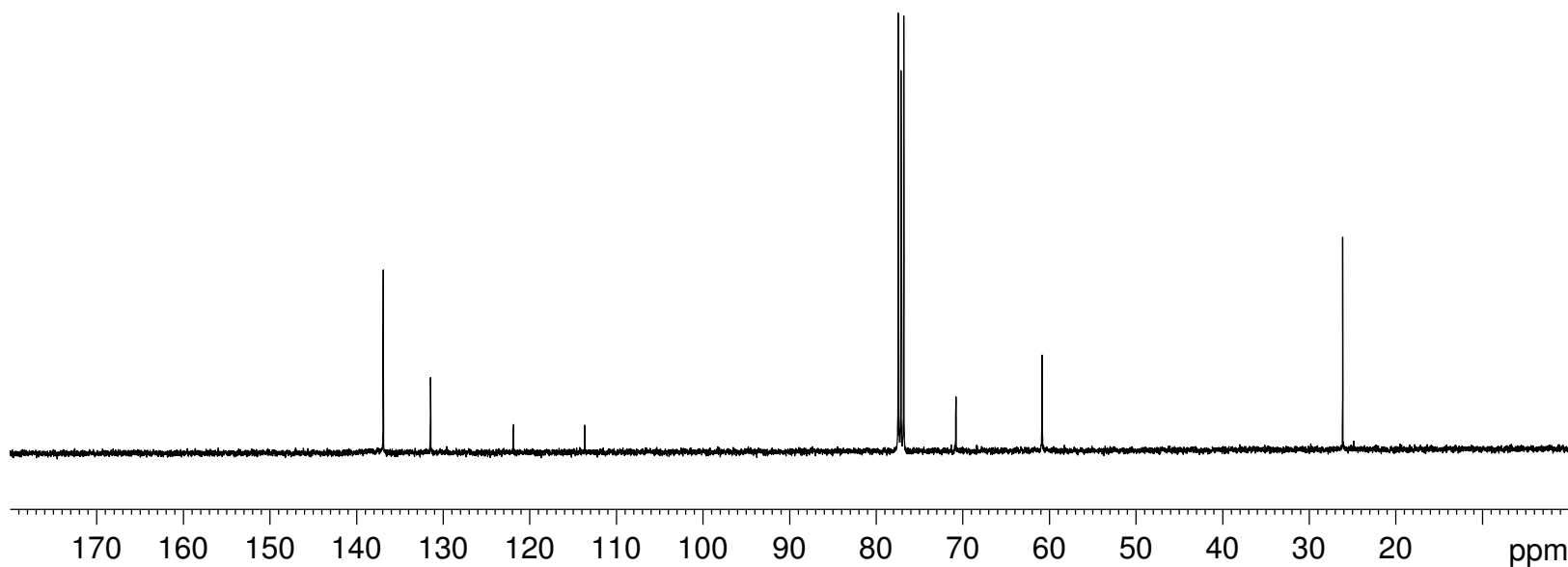
— 26.15

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 CDC13  
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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6479773 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 55.3400015 W  
SFO2 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.5600042 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



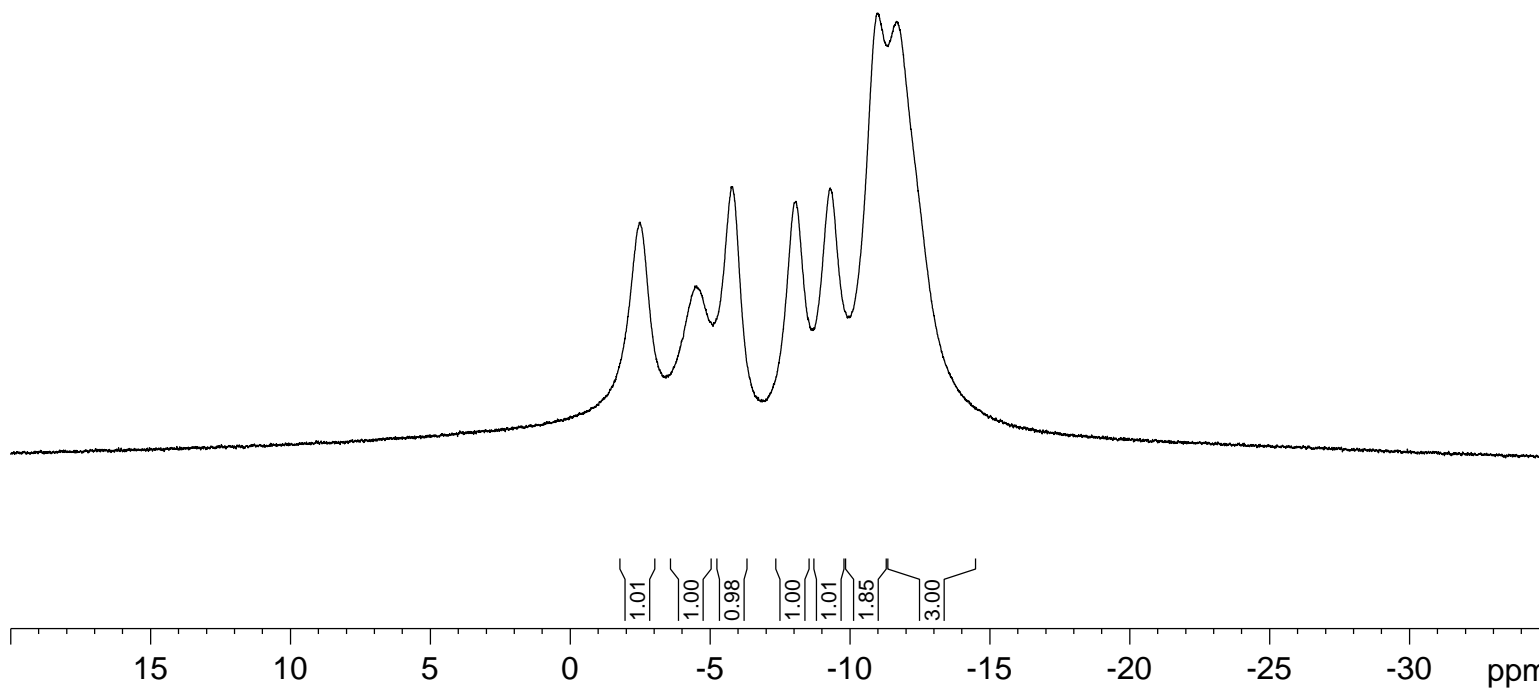
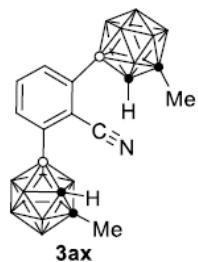
CY-B-A-14p-re2

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

-2.50  
 -4.52  
 -5.80  
 -8.07  
 -9.29  
 -10.98  
 -11.67





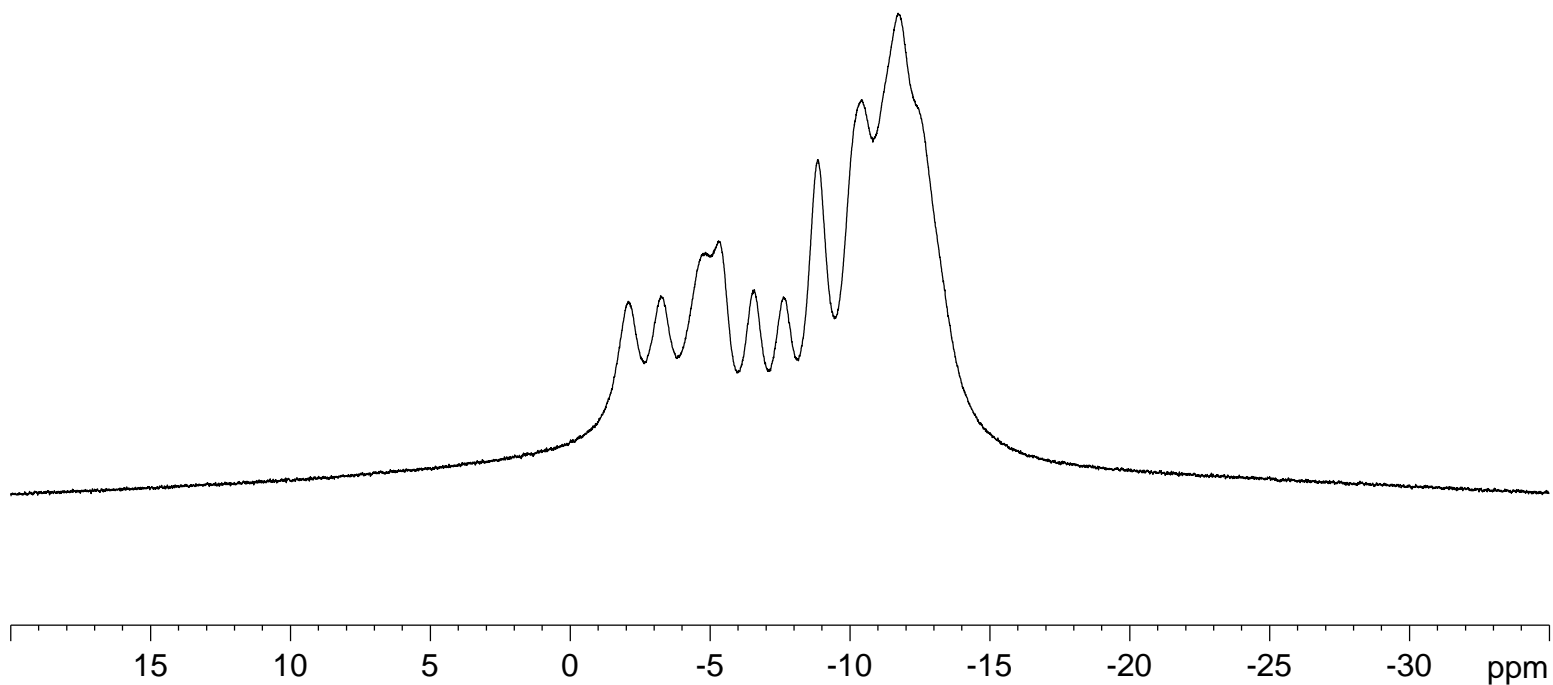
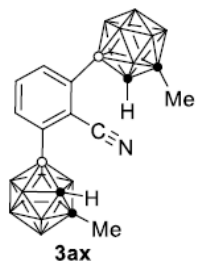
CY-B-A-14p-(C)-re2

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

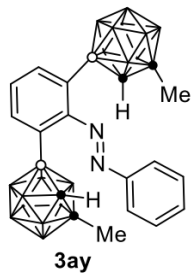
—2.07  
—3.22  
—4.83  
—5.30  
—6.58  
—7.62  
—8.83  
—10.41  
—11.71  
—12.49



7.903  
7.897  
7.883  
7.880  
7.719  
7.700  
7.620  
7.617  
7.608  
7.590  
7.581  
7.269  
7.260  
7.250  
7.231

3.727

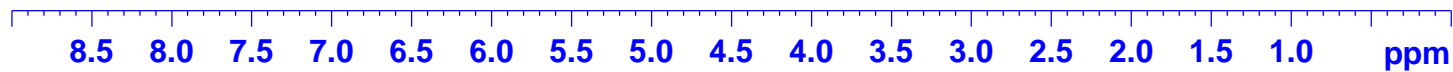
1.666  
1.631



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  
SF01 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



2.05  
2.04  
3.08  
1.07

2.00

3.11  
3.02

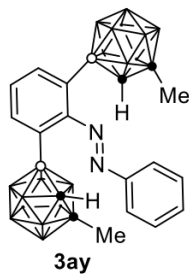
162.878  
 150.448  
 150.379  
 137.543  
 132.690  
 129.965  
 126.604  
 123.073

77.476  
 77.158  
 76.841  
 70.602  
 70.514  
 62.927  
 62.796

25.710  
 25.674

CY-C-A-13p-CDCl3

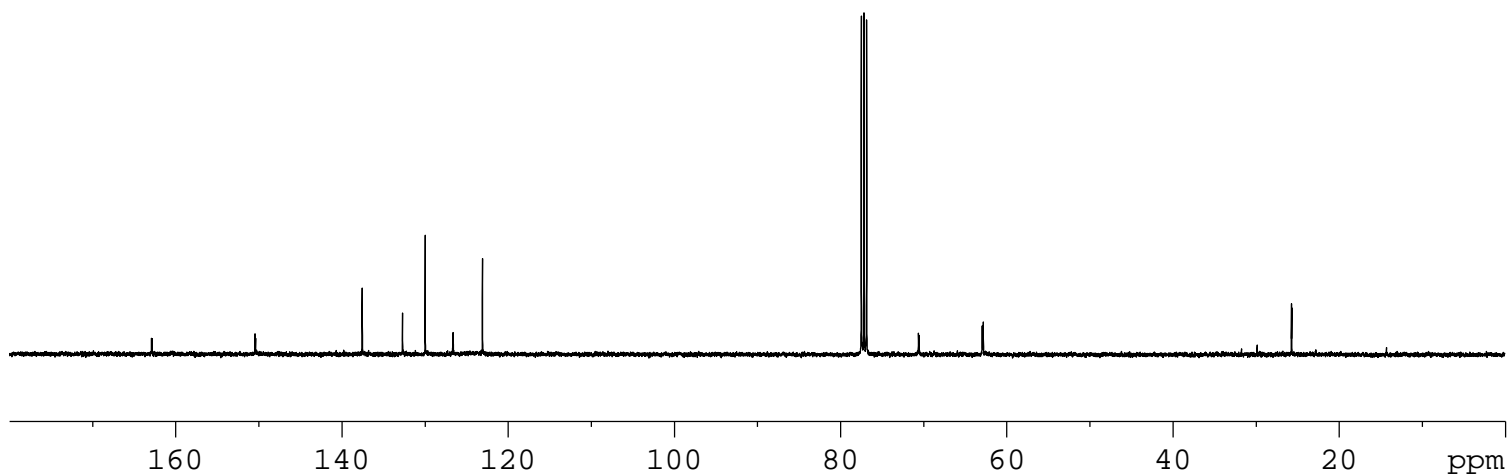
Bruker Advance III 400



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  
 FCPD2 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

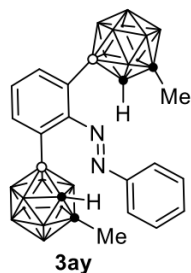


CY-B-A-13p-re2

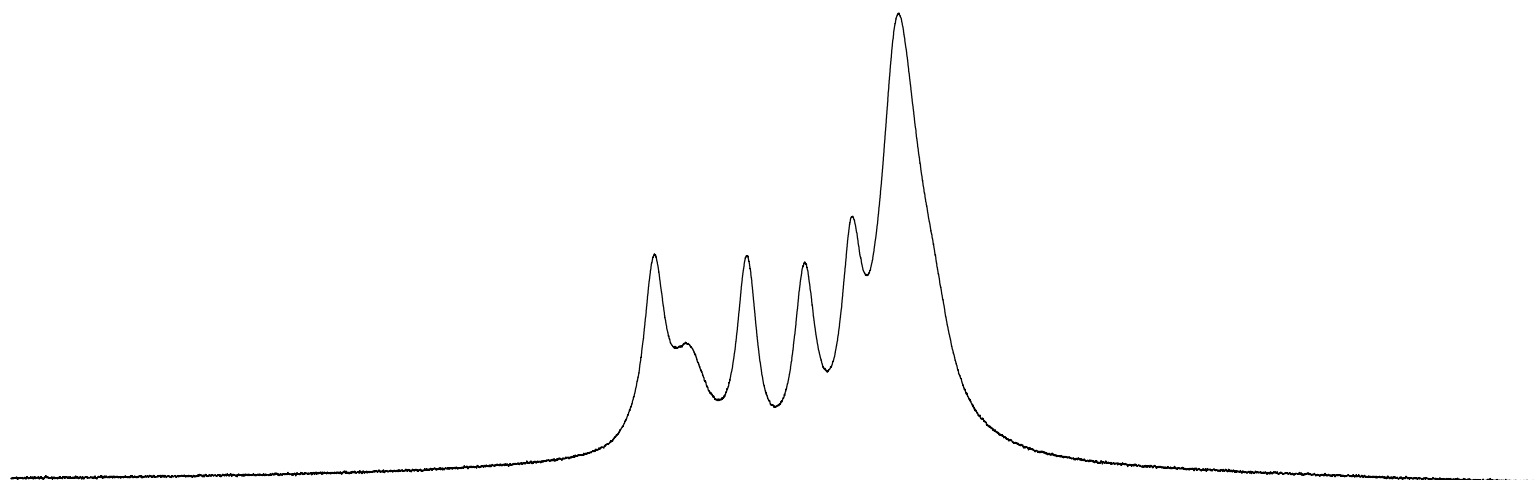
Current Data Parameters  
NAME CY-B-A-13p-re2  
EXPNO 1  
PROCNO 1

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



— 3.01  
— 6.33  
— 8.39  
— 10.10  
— 11.75



1.17 0.92 1.02 1.03 1.07 5.00

15 10 5 0 -5 -10 -15 -20 -25 -30 ppm

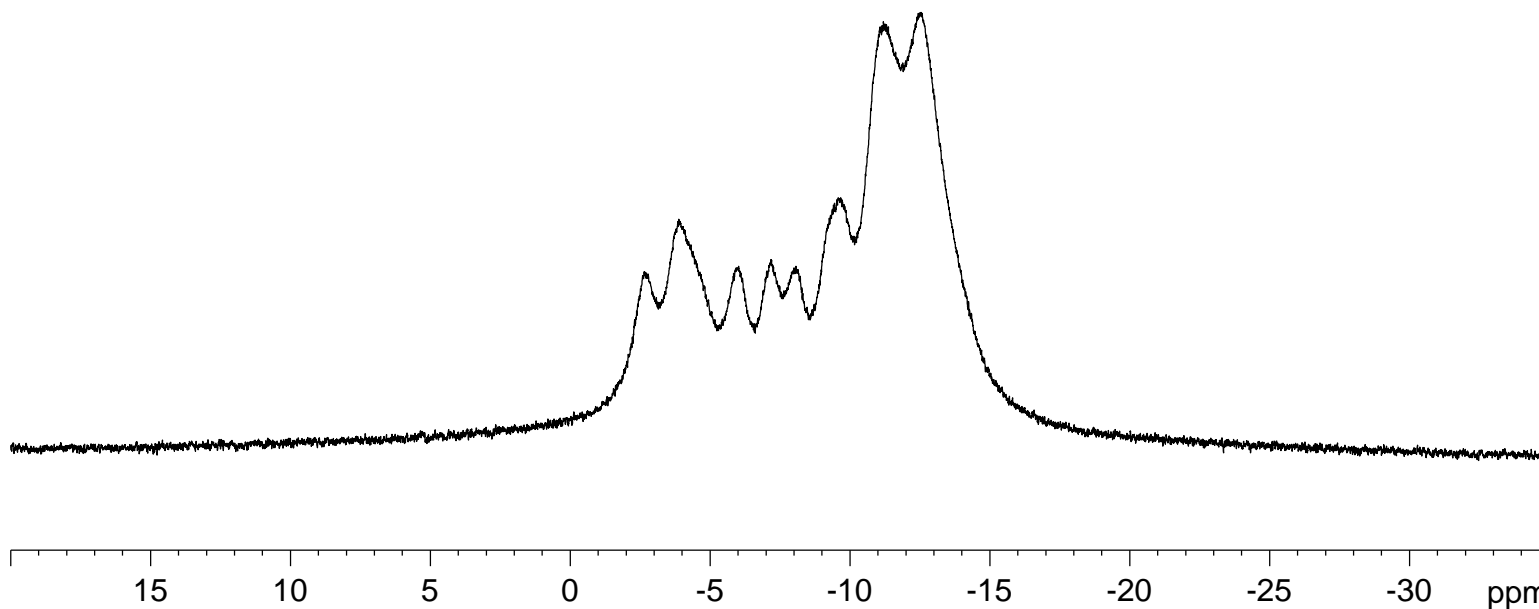
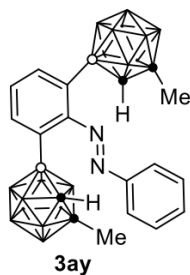
CY-B-A-13p-(C)-re

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

— 2.64  
 — 3.88  
 — 6.01  
 — 7.17  
 — 8.06  
 — 9.66  
 — 11.19  
 — 12.54

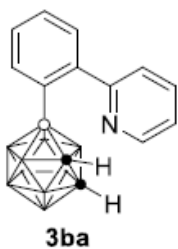


8.556  
8.545  
7.871  
7.862  
7.849  
7.775  
7.771  
7.756  
7.751  
7.737  
7.732  
7.420  
7.400  
7.380  
7.370  
7.362  
7.360  
7.344  
7.317  
7.304  
7.302  
7.298  
7.286  
7.259  
7.188  
7.183  
7.175  
7.166

3.958

3.458

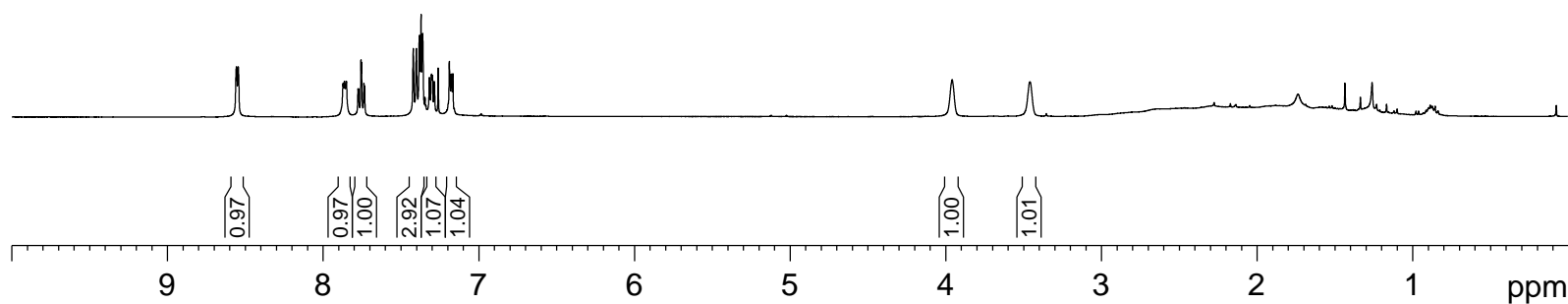
CY-H-A-67p



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 (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 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

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

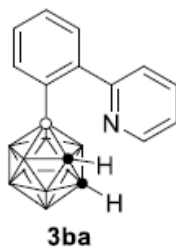


162.37  
 148.07  
 145.28  
 137.43  
 136.69  
 129.76  
 128.08  
 127.70  
 125.18  
 122.64

77.47  
 77.15  
 76.84

55.98  
 54.73

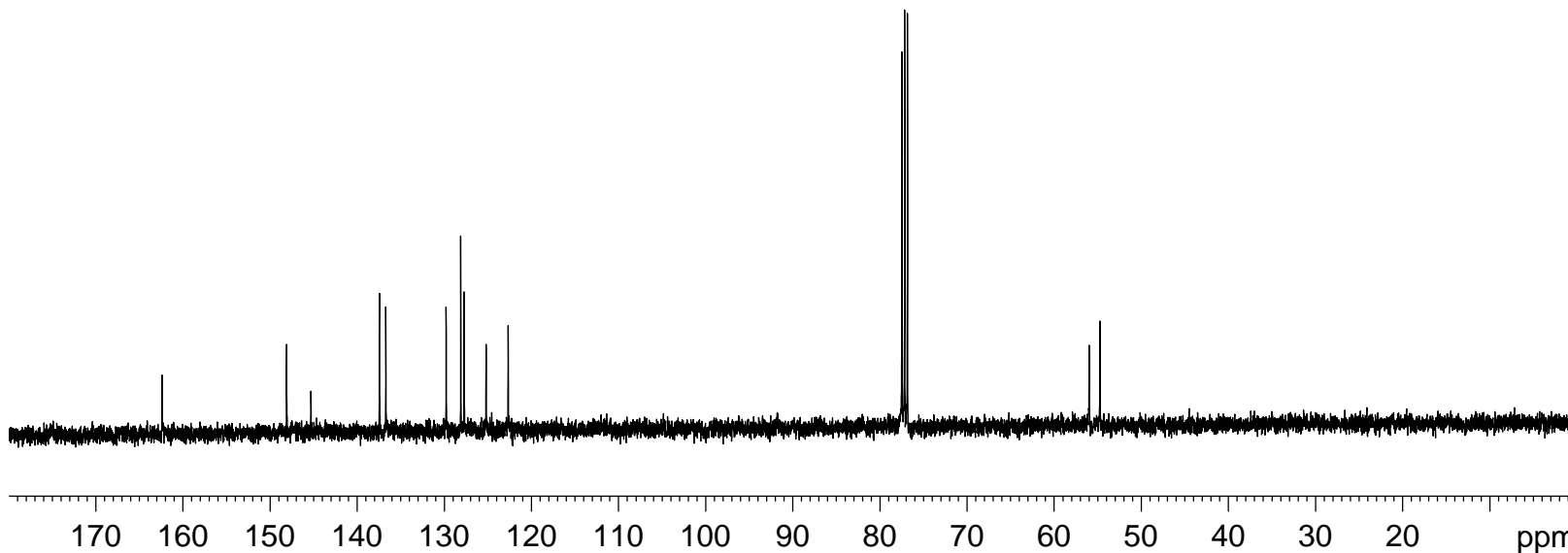
CY-C-A-67P-re



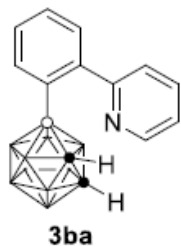
Current Data Parameters  
 NAME CY-C-A-67P-re  
 EXPNO 1  
 PROCNO 1

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

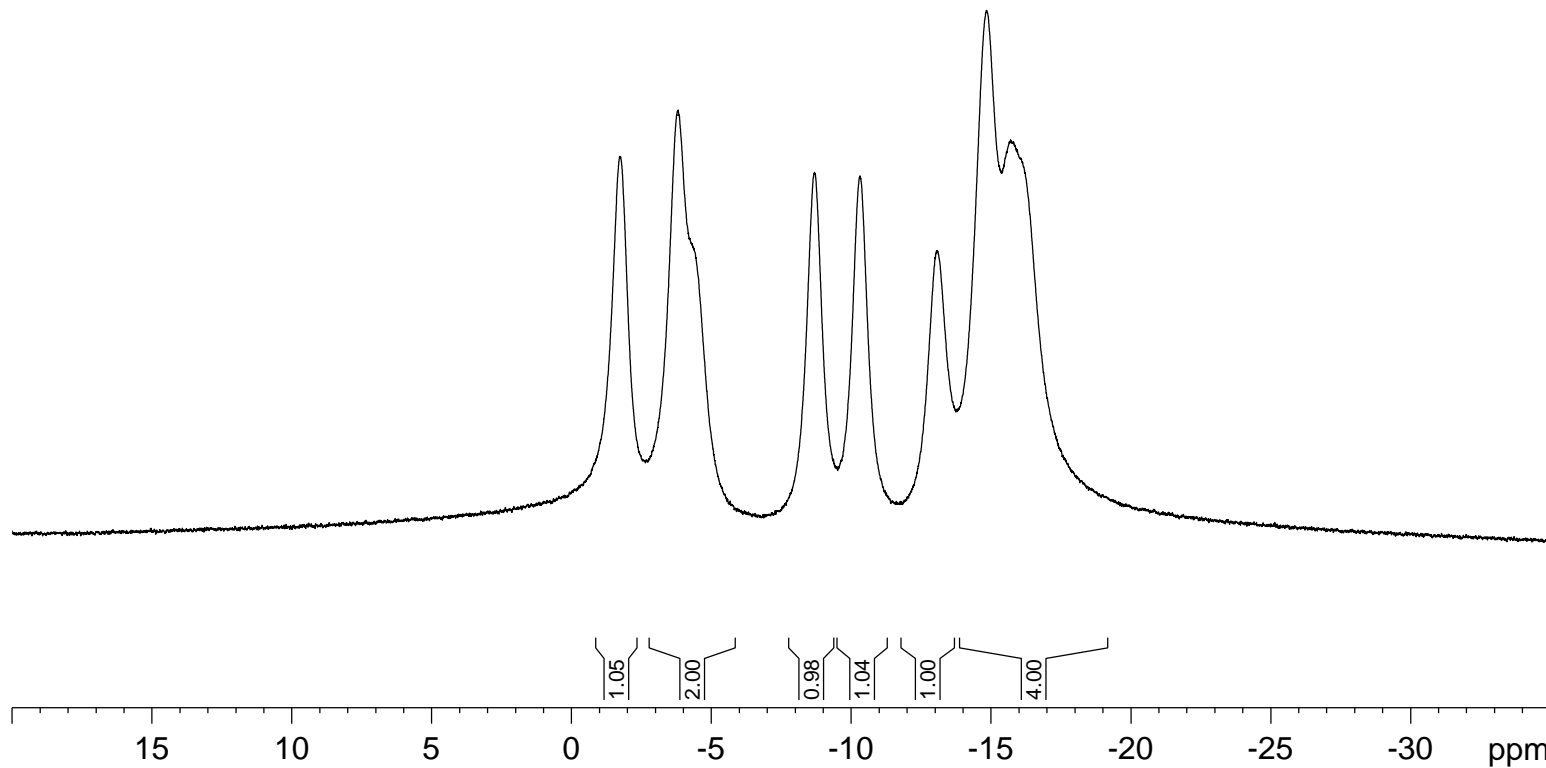
F2 - Processing parameters  
 SI 32768  
 SF 100.6379032 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



CY-B-A-67p



— -1.72  
— -3.81  
— -8.69  
— -10.32  
— -13.06  
— -14.83  
— -15.70

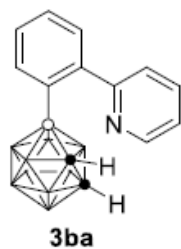


Current Data Parameters  
NAME CY-B-A-67p  
EXPNO 1  
PROCNO 1

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  
SF01 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W  
SF02 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.56000042 W  
PLW12 0.27428001 W

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





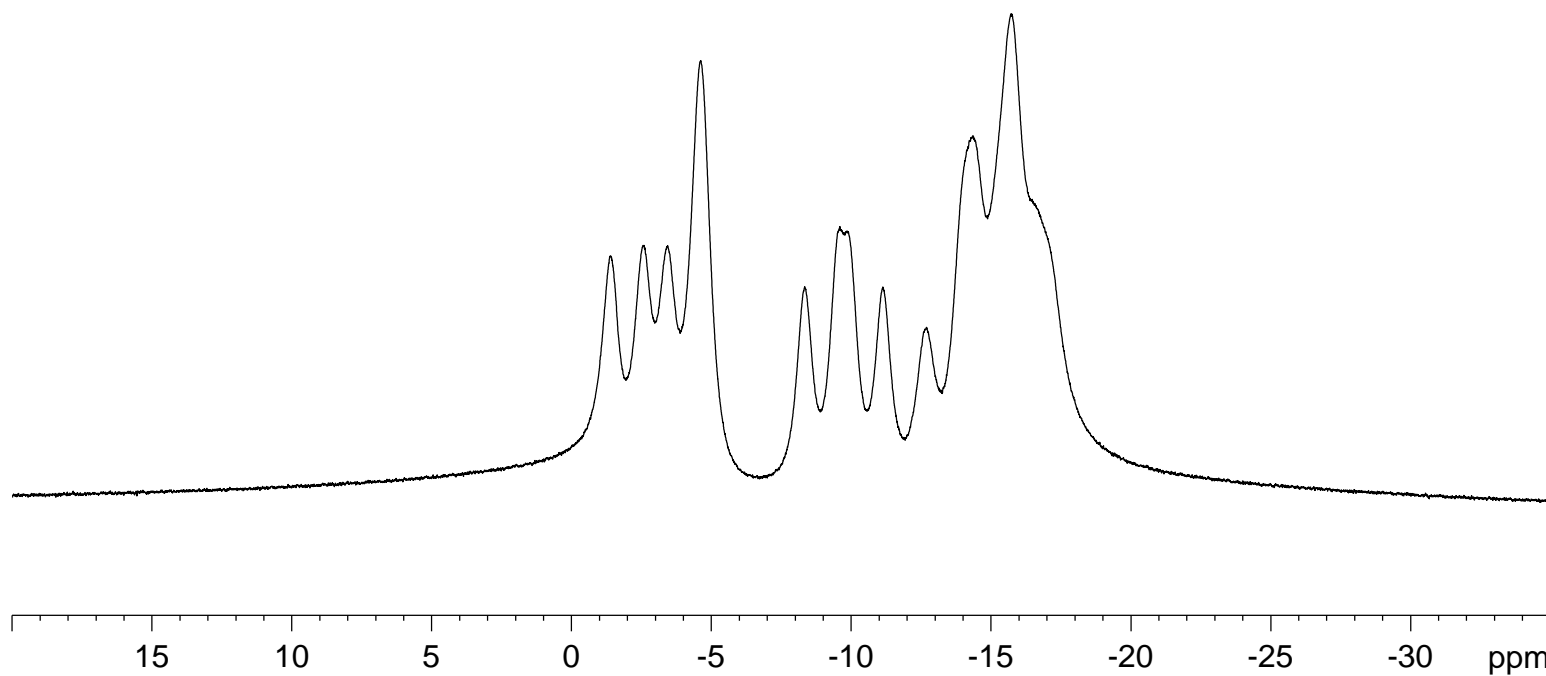
| -1.40  
 | -2.56  
 | -3.44  
 | -4.62  
  
 | -8.34  
 | -9.60  
 | -11.13  
 | -12.69  
 | -14.34  
 | -15.72

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

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

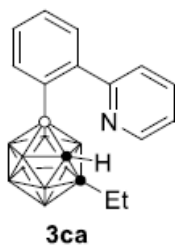
F2 - Acquisition Parameters  
 Date\_ 20161117  
 Time 20.48 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 40  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 256  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.5 K  
 D1 2.00000000 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



7.774  
7.759  
7.755  
7.740  
7.736  
7.425  
7.406  
7.395  
7.389  
7.373  
7.363  
7.354  
7.351  
7.338  
7.323  
7.321  
7.311  
7.308  
7.305  
7.302  
7.292  
7.289  
7.260  
7.187  
7.183  
7.177  
7.174  
7.172  
7.166  
3.872

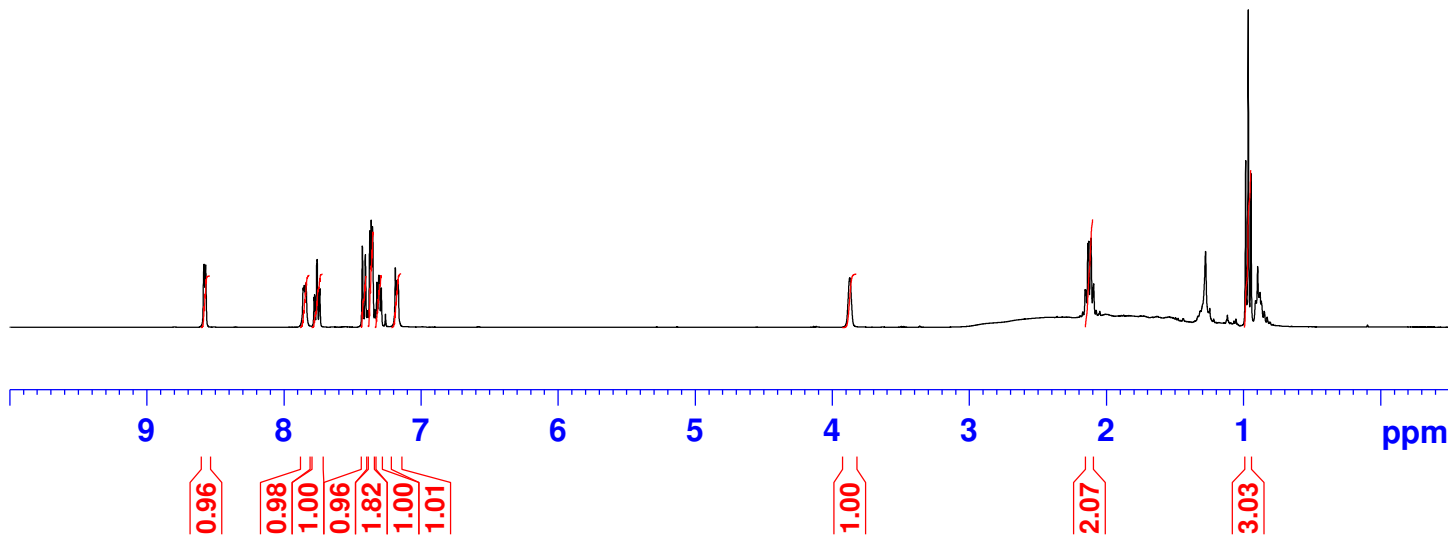
2.155  
2.149  
2.136  
2.130  
2.117  
2.111  
2.098  
2.093  
0.984  
0.965  
0.946



Current Data Parameters  
 NAME CY-H-A-68p-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161119  
 Time 9.40 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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



162.55

148.03  
145.09

137.36  
136.67

129.62  
127.92  
127.65  
125.18  
122.56

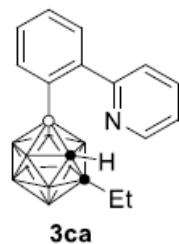
77.47  
77.15  
76.83  
76.09

62.24

31.72

13.45

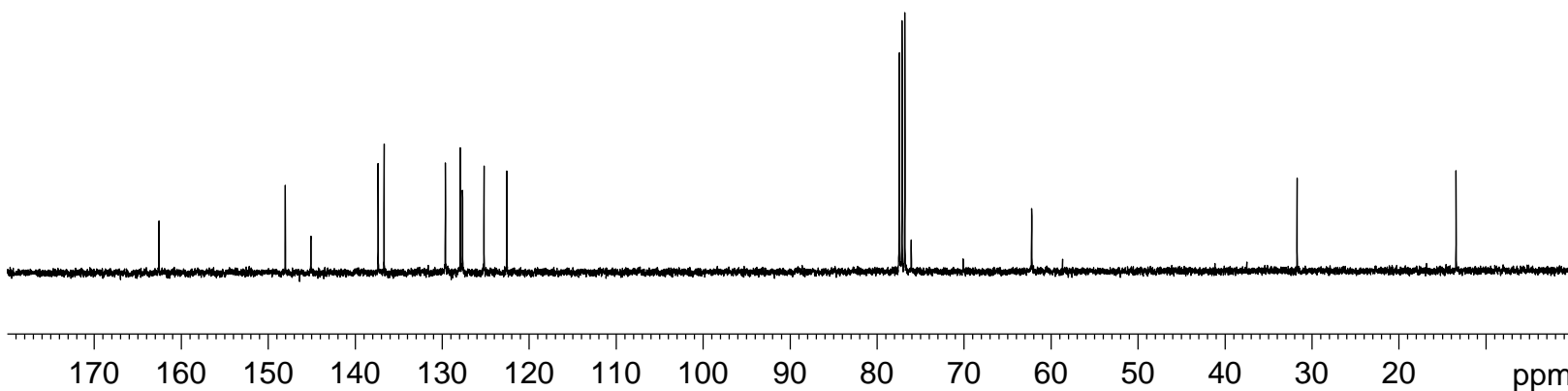
CY-C-A-68P-re

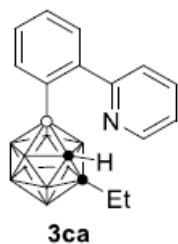


Current Data Parameters  
 NAME CY-C-A-68P-re  
 EXPNO 1  
 PROCNO 1

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 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 100.6479773 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 55.3400015 W  
 SFO2 400.2316009 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 13.5600042 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





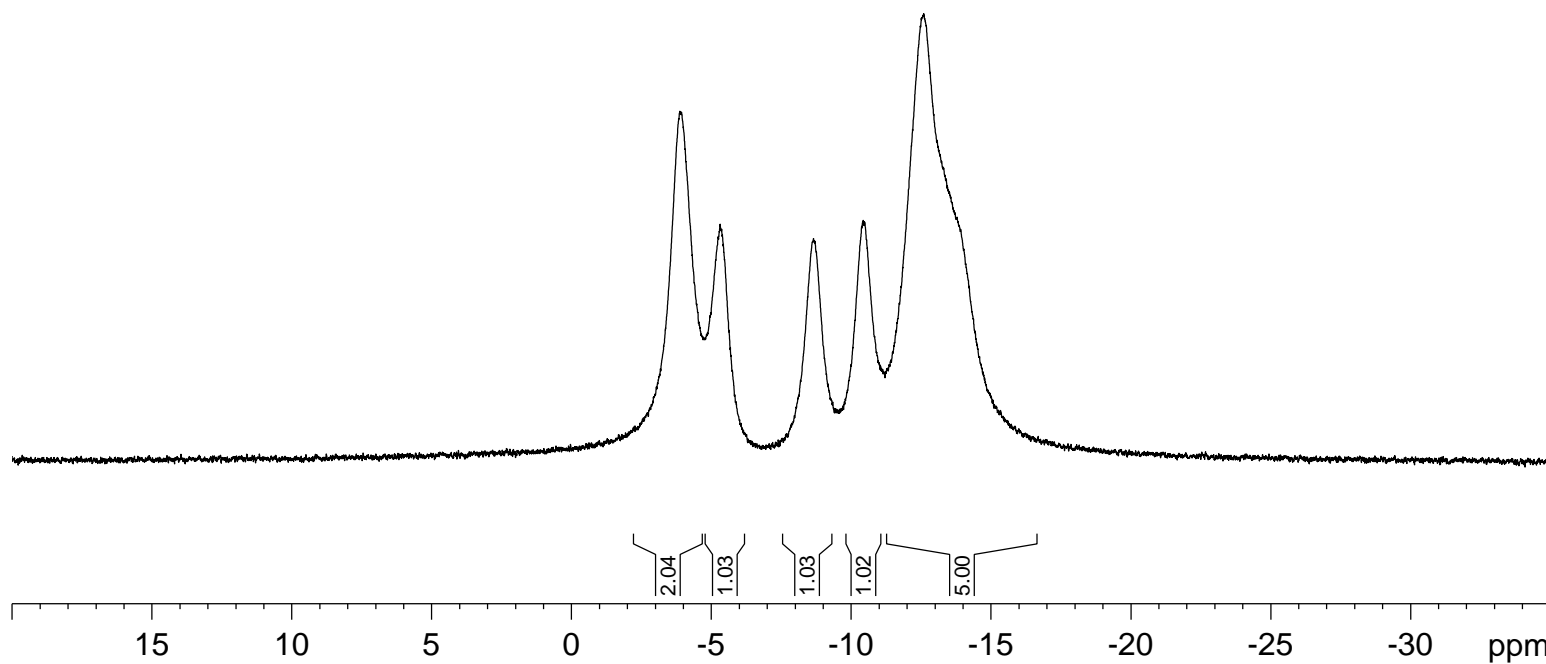
— -3.87  
 — -5.31  
 — -8.65  
 — -10.43  
 — -12.59

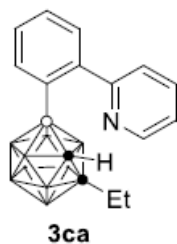
CY-B-A-68p

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





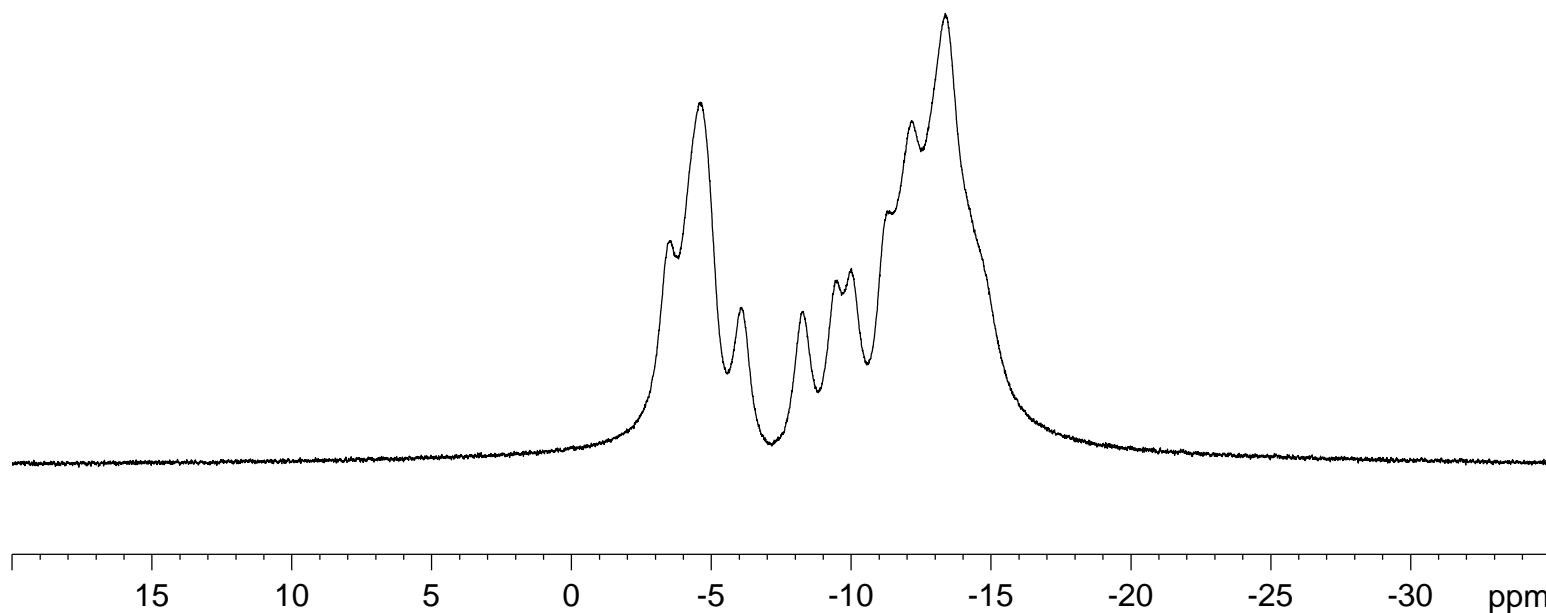
| 3.55  
 | 4.61  
 | 6.07  
 | 8.28  
 | 9.49  
 | 10.01  
 | 12.17  
 | 13.36

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



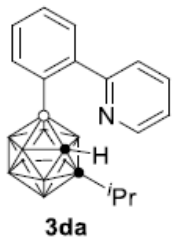
7.853  
7.837  
7.782  
7.777  
7.762  
7.758  
7.743  
7.739  
7.423  
7.404  
7.393  
7.388  
7.374  
7.370  
7.366  
7.359  
7.352  
7.348  
7.344  
7.330  
7.325  
7.316  
7.314  
7.304  
7.302  
7.298  
7.295  
7.285  
7.283  
7.260  
7.158  
7.154  
7.151  
7.142  
7.136

3.917

2.417  
2.399  
2.382  
2.365  
2.348  
2.330  
2.313

1.018  
1.003  
1.001  
0.986

CY-H-A-74p



Current Data Parameters

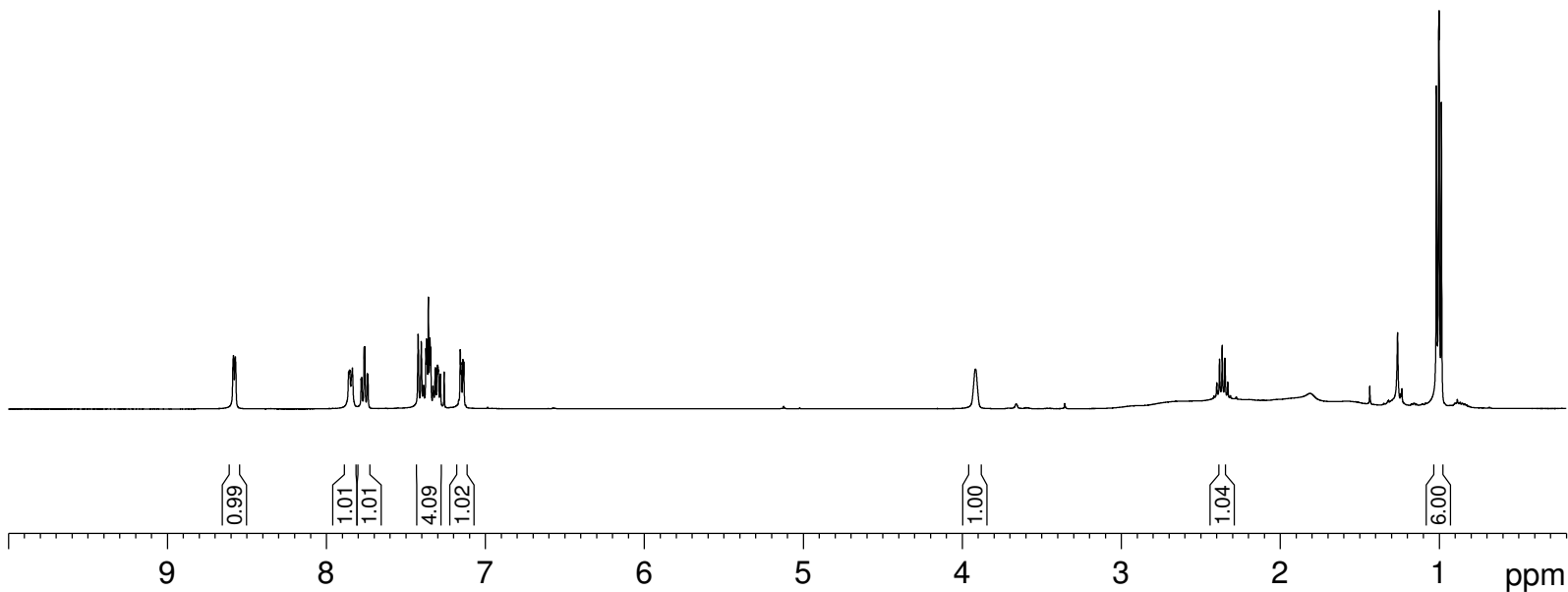
NAME CY-H-A-74p  
EXPNO 1  
PROCNO 1

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 1.0000000 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



162.57  
 148.24  
 144.99  
 137.42  
 136.69  
 129.71  
 127.86  
 127.65  
 125.17  
 122.51

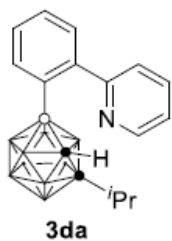
81.27  
 77.47  
 77.15  
 76.83

61.23

34.85

22.88  
 22.85

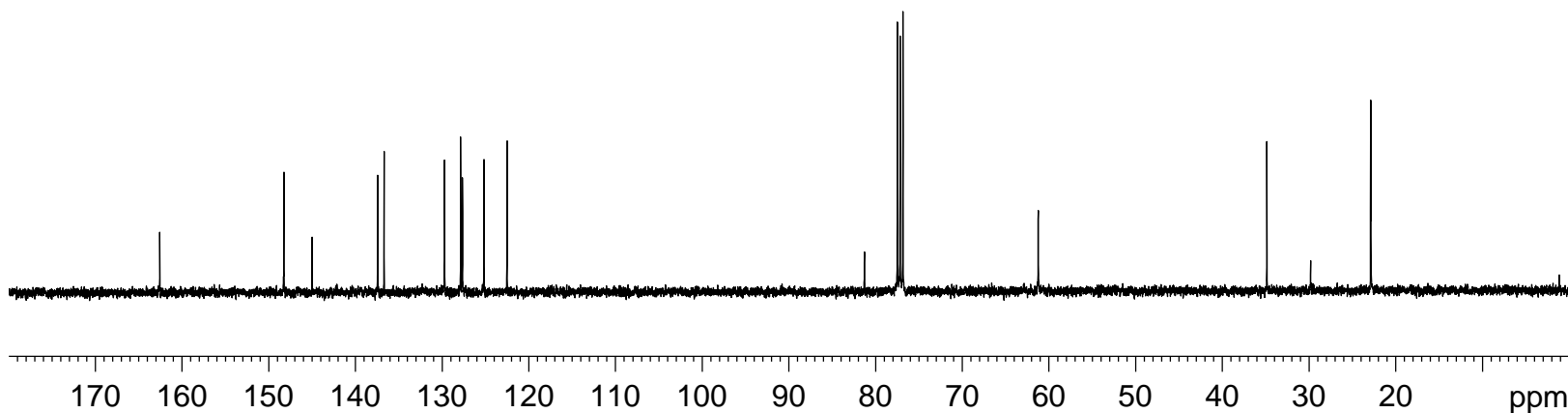
CY-C-A-75p



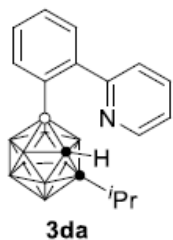
Current Data Parameters  
 NAME CY-C-A-75P  
 EXPNO 1  
 PROCNO 1

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

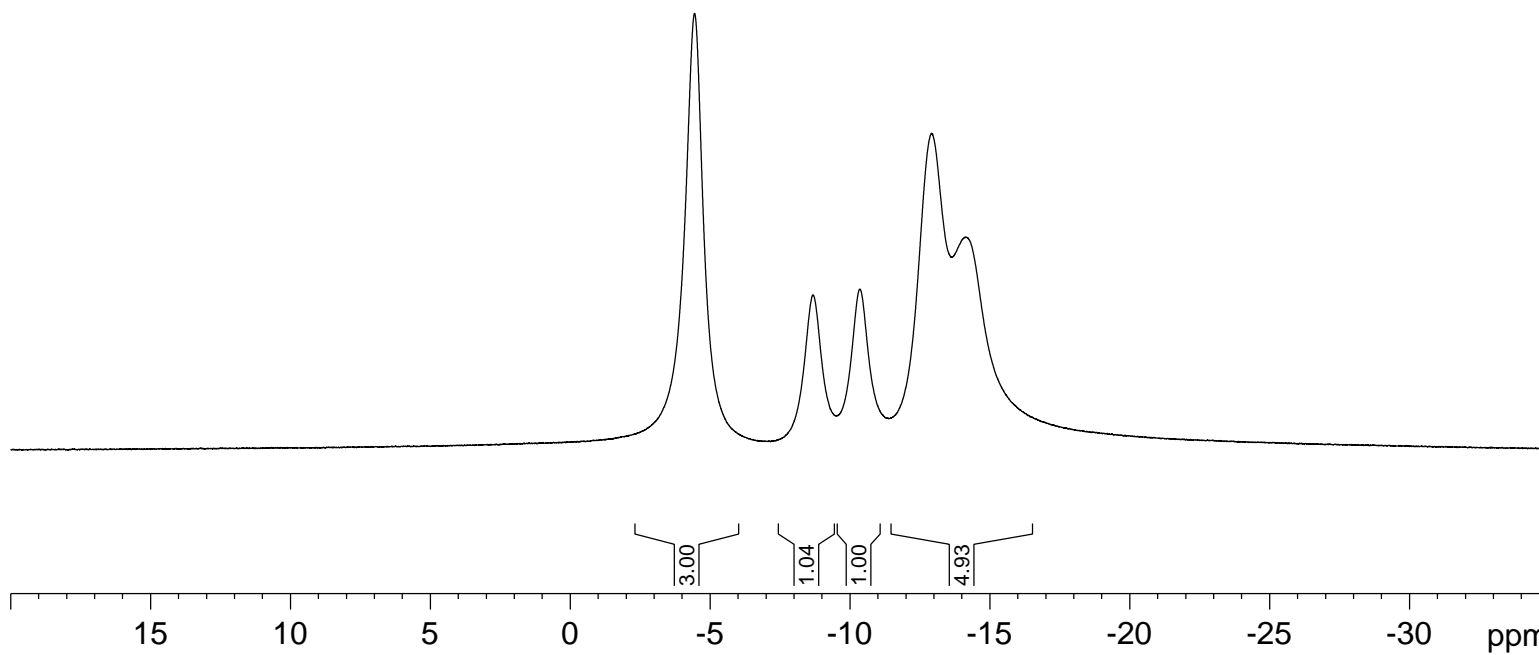


— 4.44  
— 8.68  
— 10.37  
— 12.91  
— 14.16

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





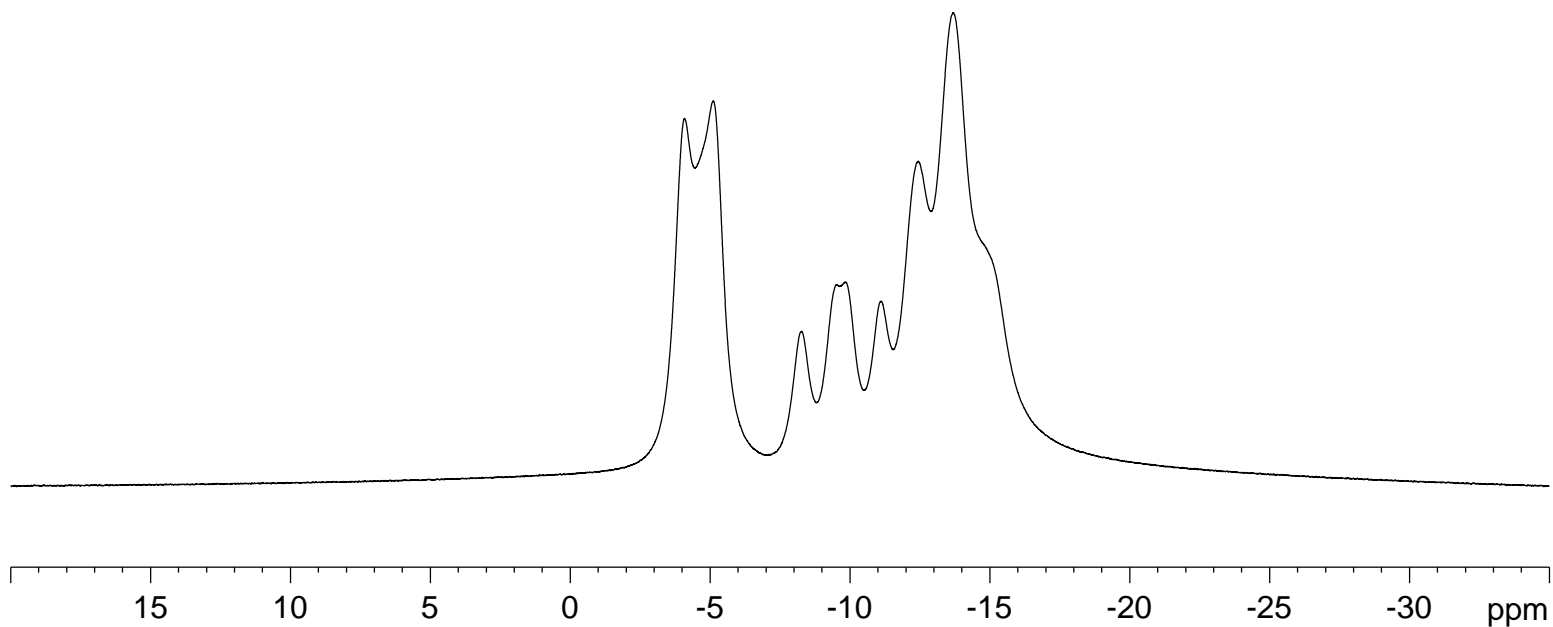
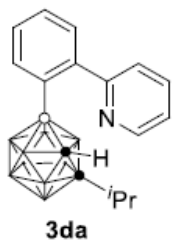
CY-B-A-75p-(C)-re2

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

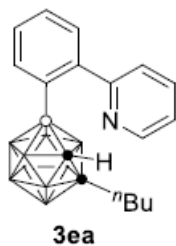
F2 - Acquisition Parameters  
Date\_ 20161121  
Time 20.58 h  
INSTRUM spect  
PROBHD z108618\_0257 (  
PULPROG zg  
TD 65536  
SOLVENT CDC13  
NS 100  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 228  
DW 20.800 usec  
DE 6.50 usec  
TE 296.5 K  
D1 2.00000000 sec  
TD0 1  
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

— 4.07  
— 5.10  
— 8.25  
— 9.43  
— 9.82  
— 11.10  
— 12.44  
— 13.68  
— 15.08



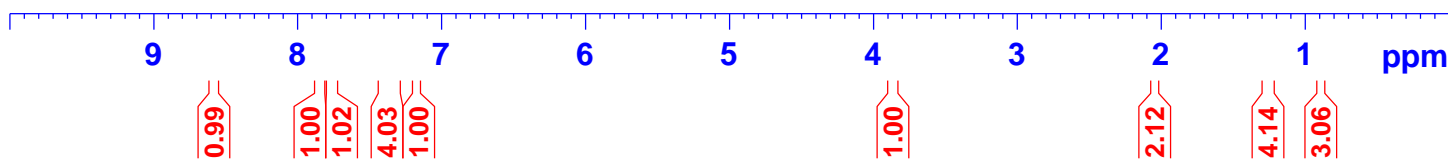
8.582  
8.572  
8.570  
7.851  
7.843  
7.828  
7.783  
7.778  
7.764  
7.759  
7.744  
7.740  
7.427  
7.407  
7.375  
7.370  
7.362  
7.353  
7.349  
7.324  
7.321  
7.311  
7.309  
7.305  
7.302  
7.292  
7.290  
7.260  
7.182  
7.177  
7.172  
7.166  
7.159  
3.866  
2.073  
2.063  
2.057  
2.049  
2.038  
2.031  
2.022  
1.292  
1.284  
1.273  
1.265  
1.257  
1.249  
1.232  
0.911  
0.894  
0.876



Current Data Parameters  
 NAME CY-H-A-74p-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161121  
 Time 20.22 h  
 INSTRUM spect  
 PROBHD z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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  
 SF01 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



0.99  
1.00  
1.02  
4.03  
1.00  
1.00  
2.12  
4.14  
3.06

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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 41.2500000 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

162.561  
148.037  
145.066  
137.333  
136.677  
129.621  
127.892  
127.644  
125.193  
122.540

77.472  
77.154  
76.837  
75.375

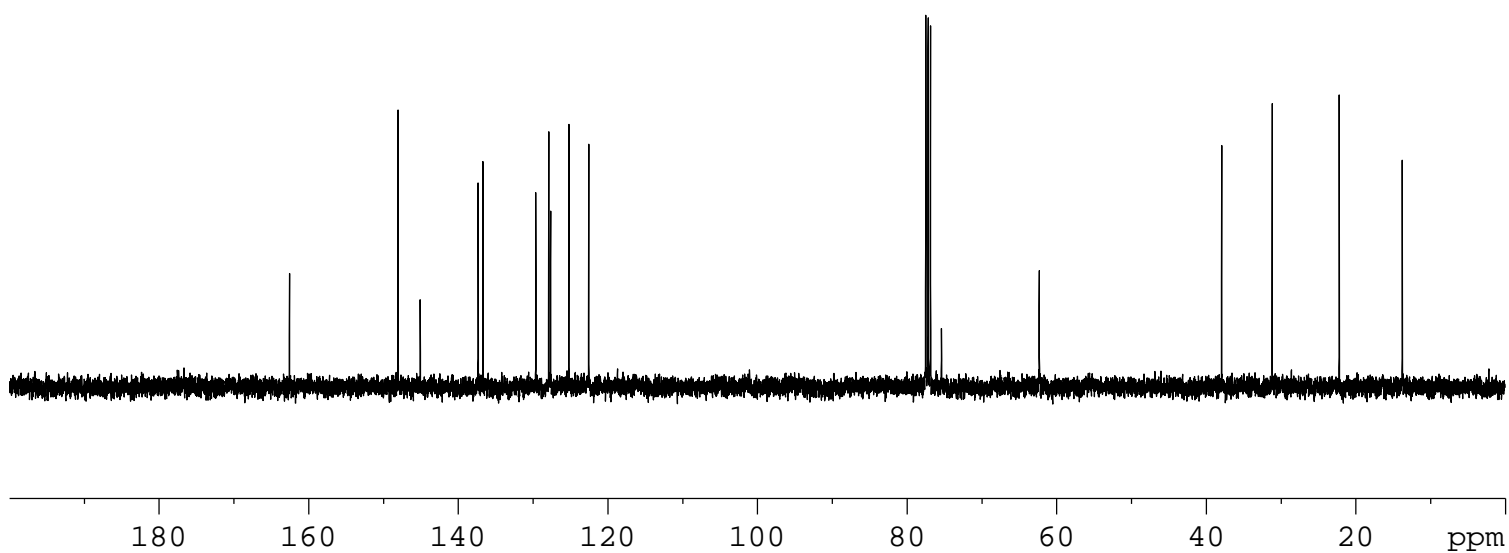
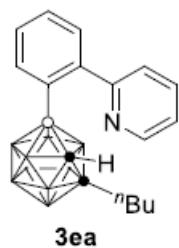
62.294

37.908

31.143

22.182

13.757



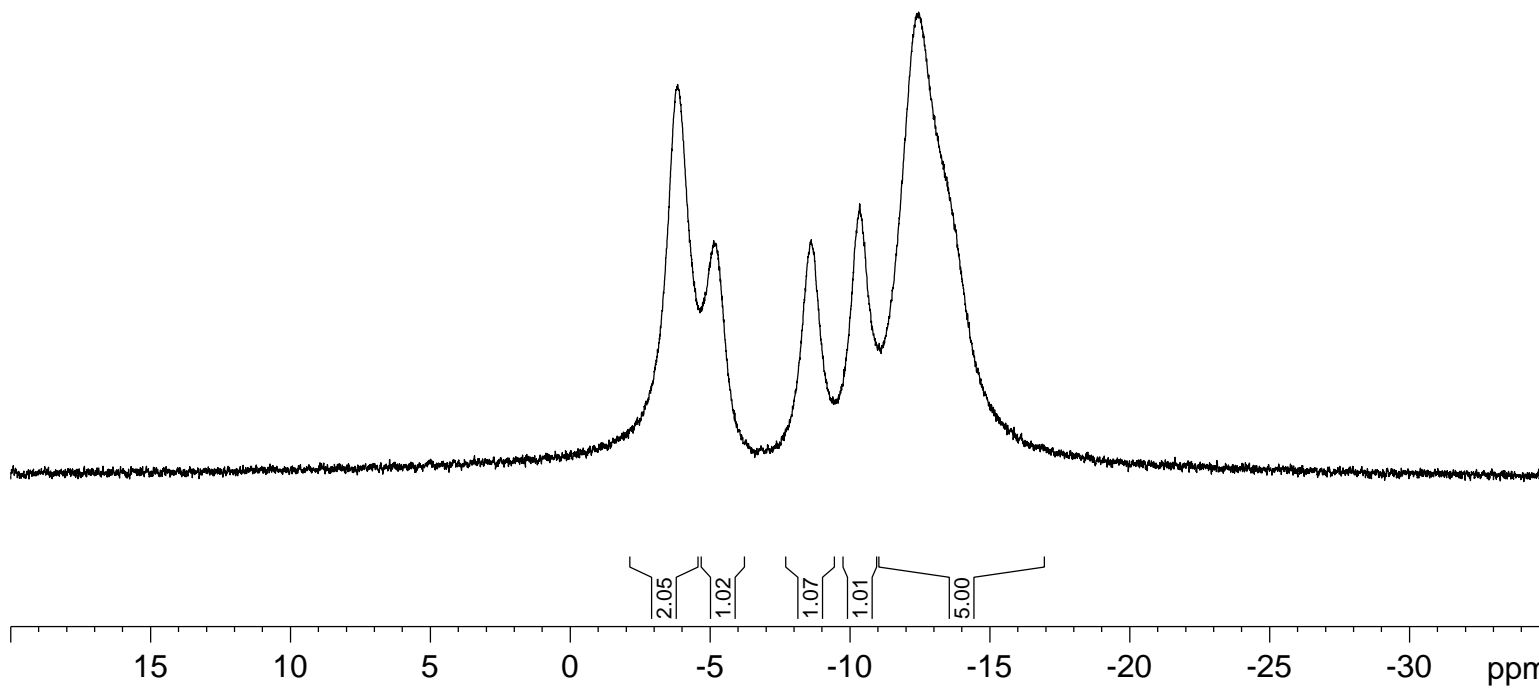
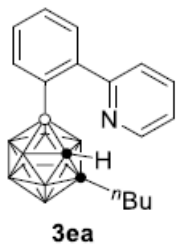
CY-B-A-74p

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 2.0000000 sec  
D11 0.0300000 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

— 3.84  
— 5.13  
— 8.62  
— 10.35  
— 12.46



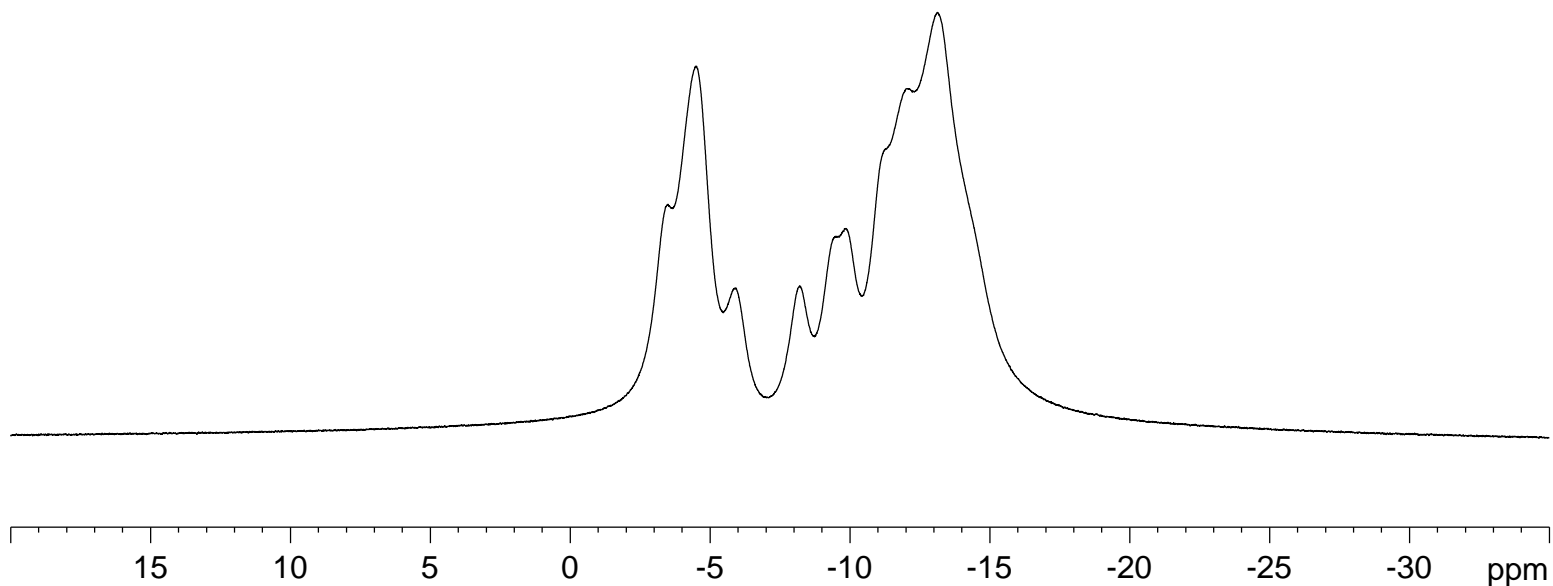
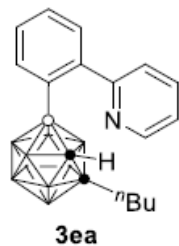
CY-B-A-74p-(C)-re2

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

— 3.38  
— 4.47  
— 5.89  
— 8.19  
— 9.86  
— 11.15  
— 11.91  
— 13.12



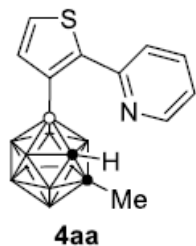
CY-H-A-162P

8.436  
8.434  
8.428  
8.426  
8.425  
7.629  
7.626  
7.614  
7.610  
7.598  
7.595  
7.467  
7.451  
7.217  
7.207  
7.193  
7.183  
7.158  
7.156  
7.148  
7.146  
7.143  
7.140  
7.138  
7.133  
7.131

4.960

1.879

1.559



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  
SF01 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



9 8 7 6 5 4 3 2 1 ppm

1.000

1.043

1.006

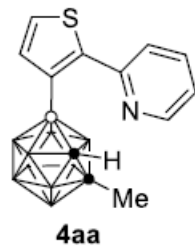
2.026

1.093

1.019

3.121

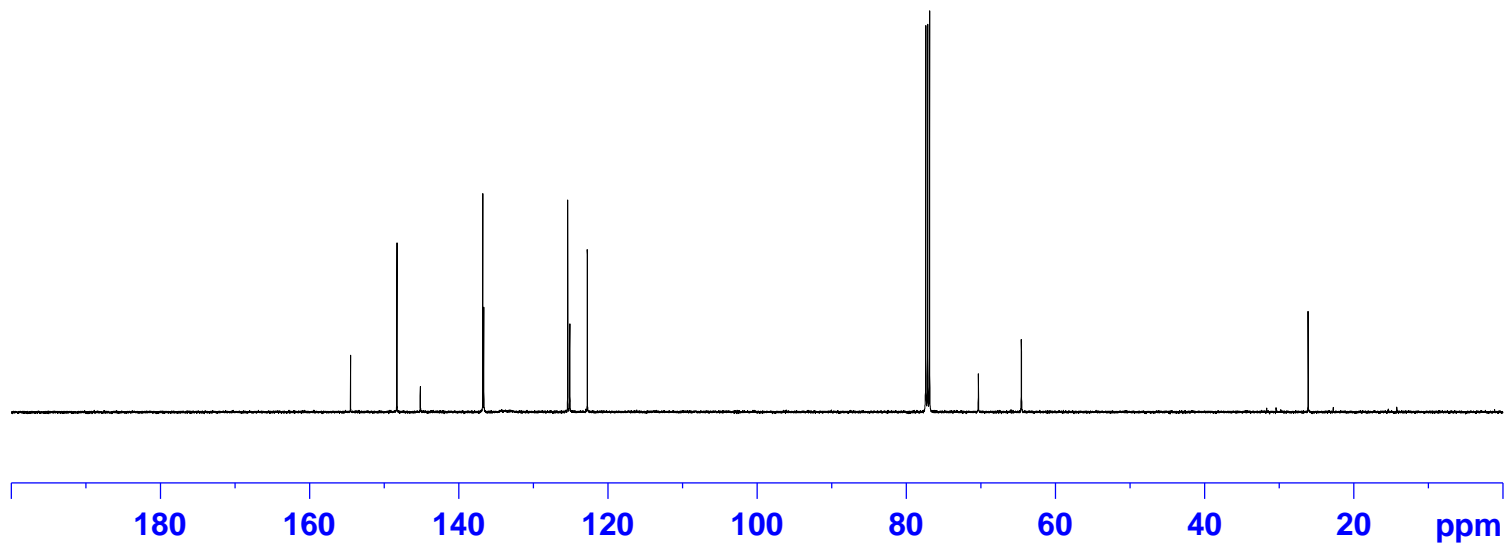
CY-C-A-162P



— 154.54  
 — 148.32  
 — 145.18  
 — 136.82  
 — 136.68  
 — 125.43  
 — 125.14  
 — 122.79

— 77.41  
 — 77.16  
 — 76.90  
 — 70.36  
 — 64.59

— 26.14



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

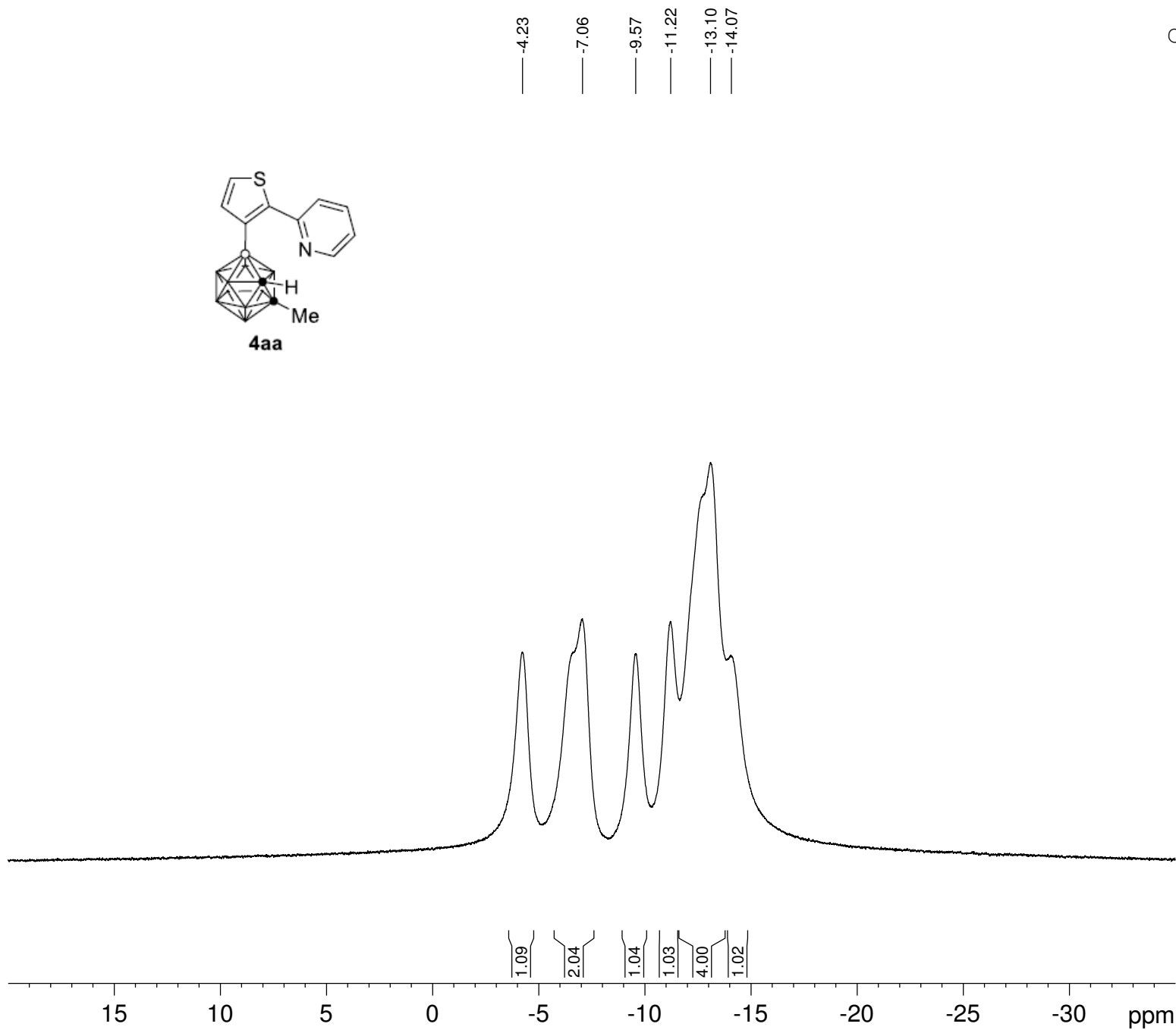
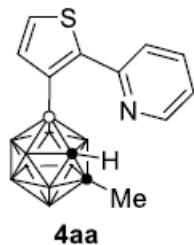
F2 - Processing parameters  
 SI 32768  
 SF 125.7577767 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

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 2.0000000 sec  
D11 0.0300000 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

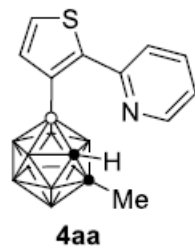
F2 - Processing parameters  
SI 32768  
SF 128.4097615 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





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

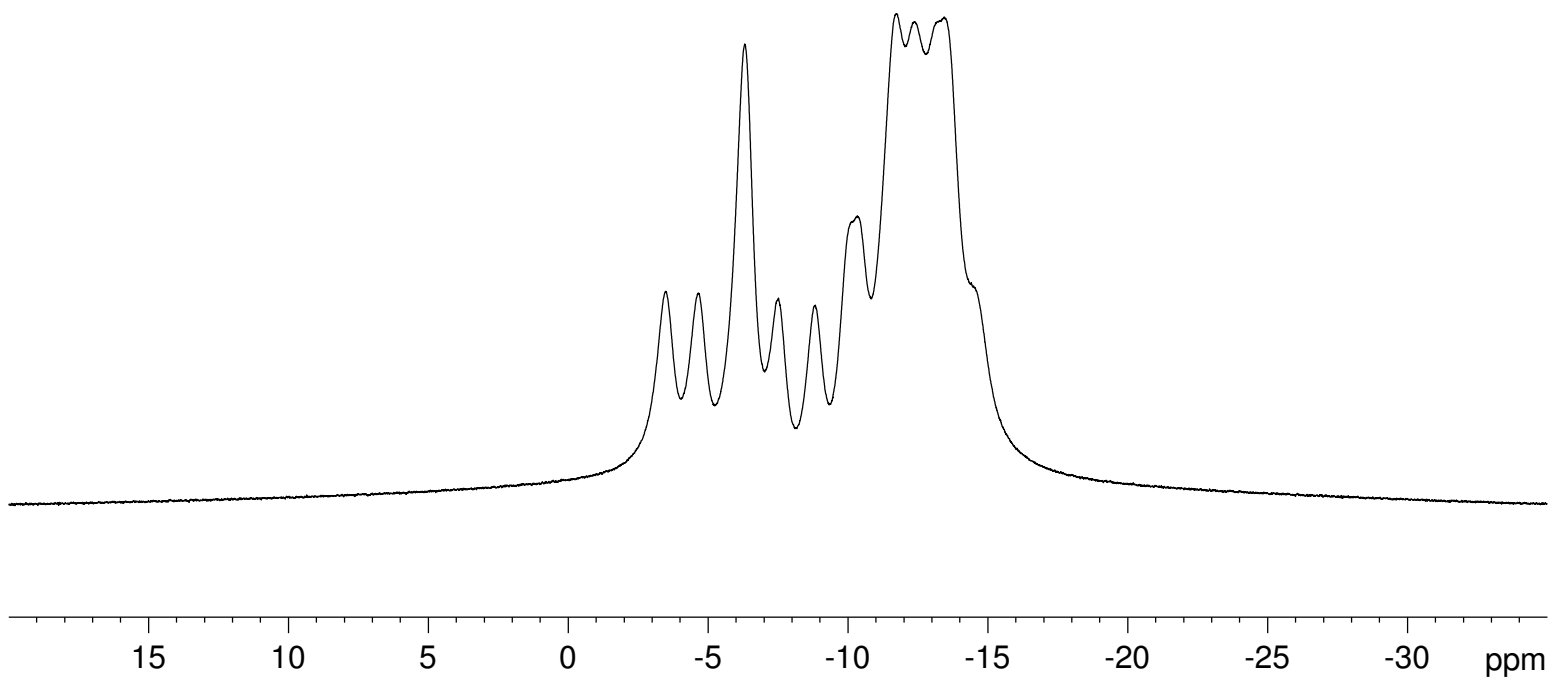
—3.49  
—4.67  
—6.32  
—7.52  
—8.83  
—10.05  
—10.34  
—11.72  
—12.40  
—13.14  
—13.44  
—14.61



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



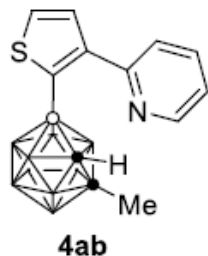
8.579  
8.568  
7.798  
7.795  
7.779  
7.776  
7.760  
7.756  
7.516  
7.492  
7.480  
7.305  
7.291  
7.274  
7.205  
7.192

5.163

2.045

1.675

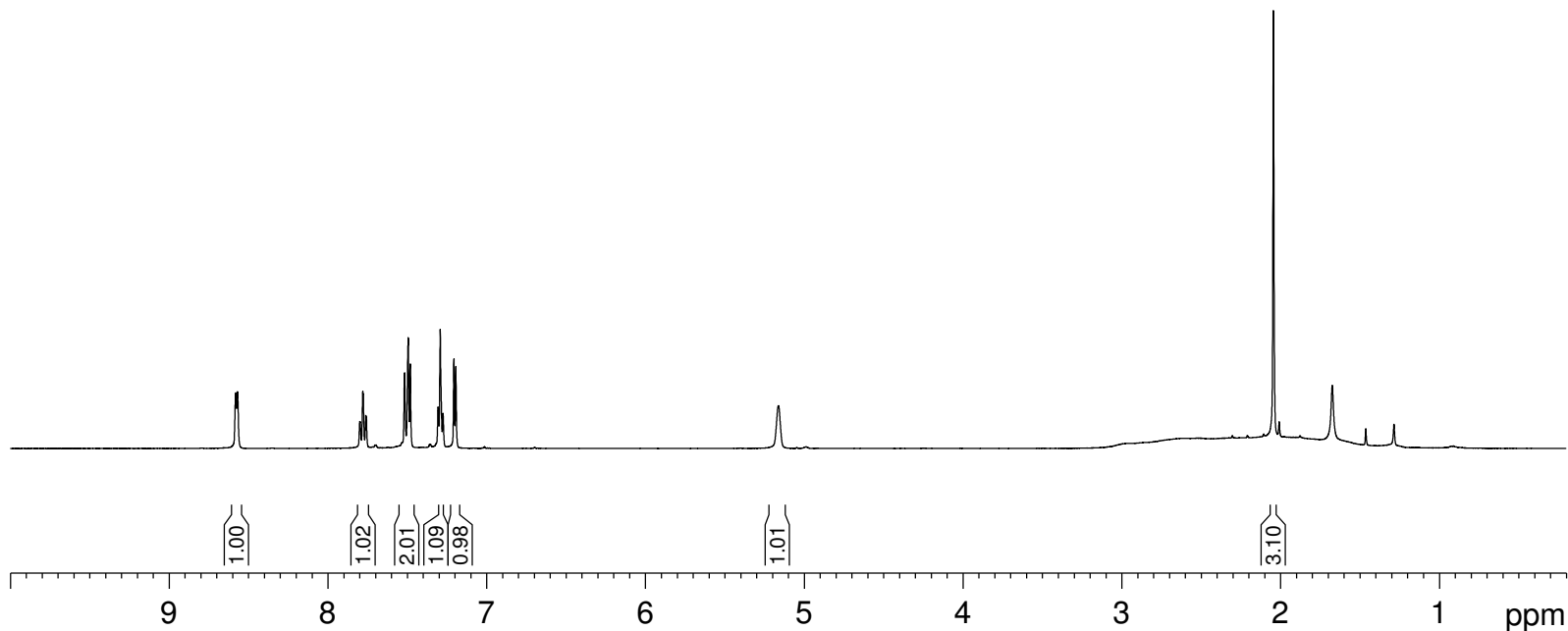
CY-H-A-163p-2



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 (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 1.0000000 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

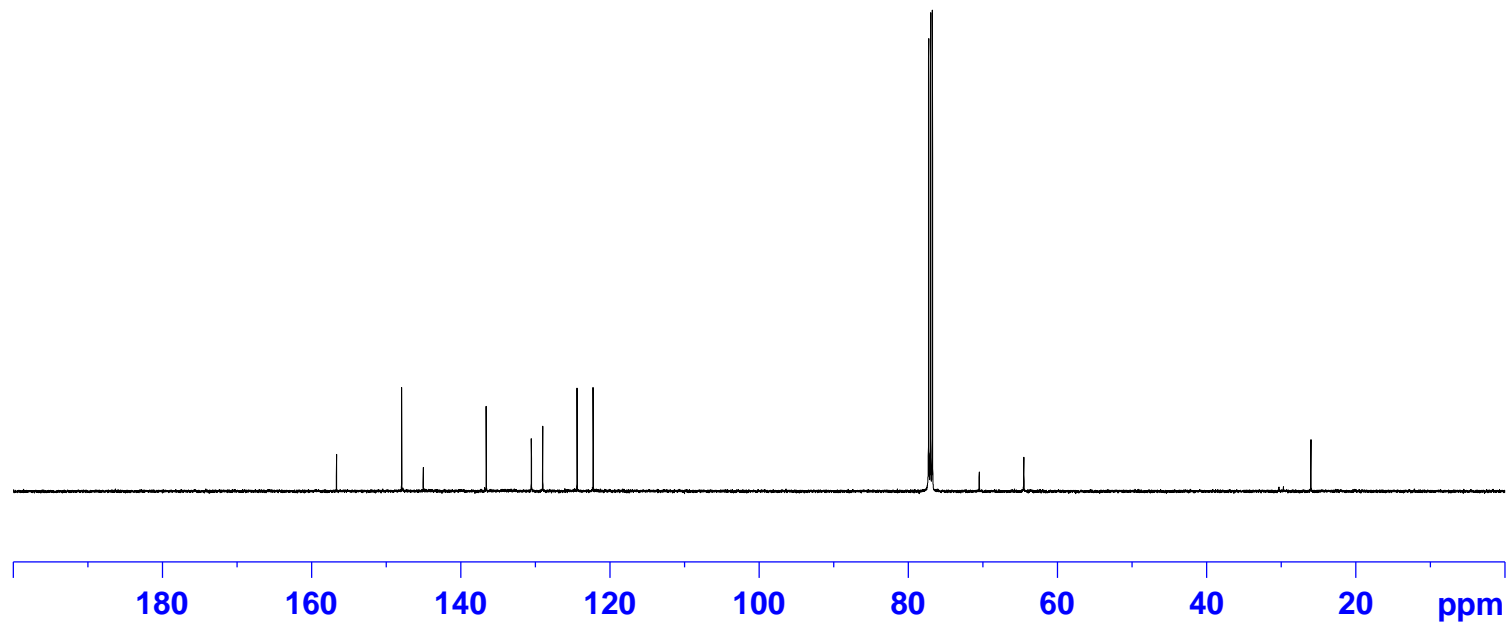
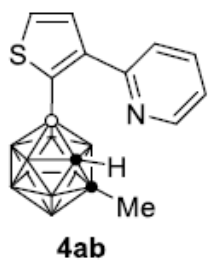


CY-C-A-163P

— 156.69  
— 147.96  
— 145.06  
— 136.62  
— 130.56  
— 129.04  
— 124.44  
— 122.28

— 77.29  
— 77.04  
— 76.78  
— 70.51  
— 64.53

— 26.04



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

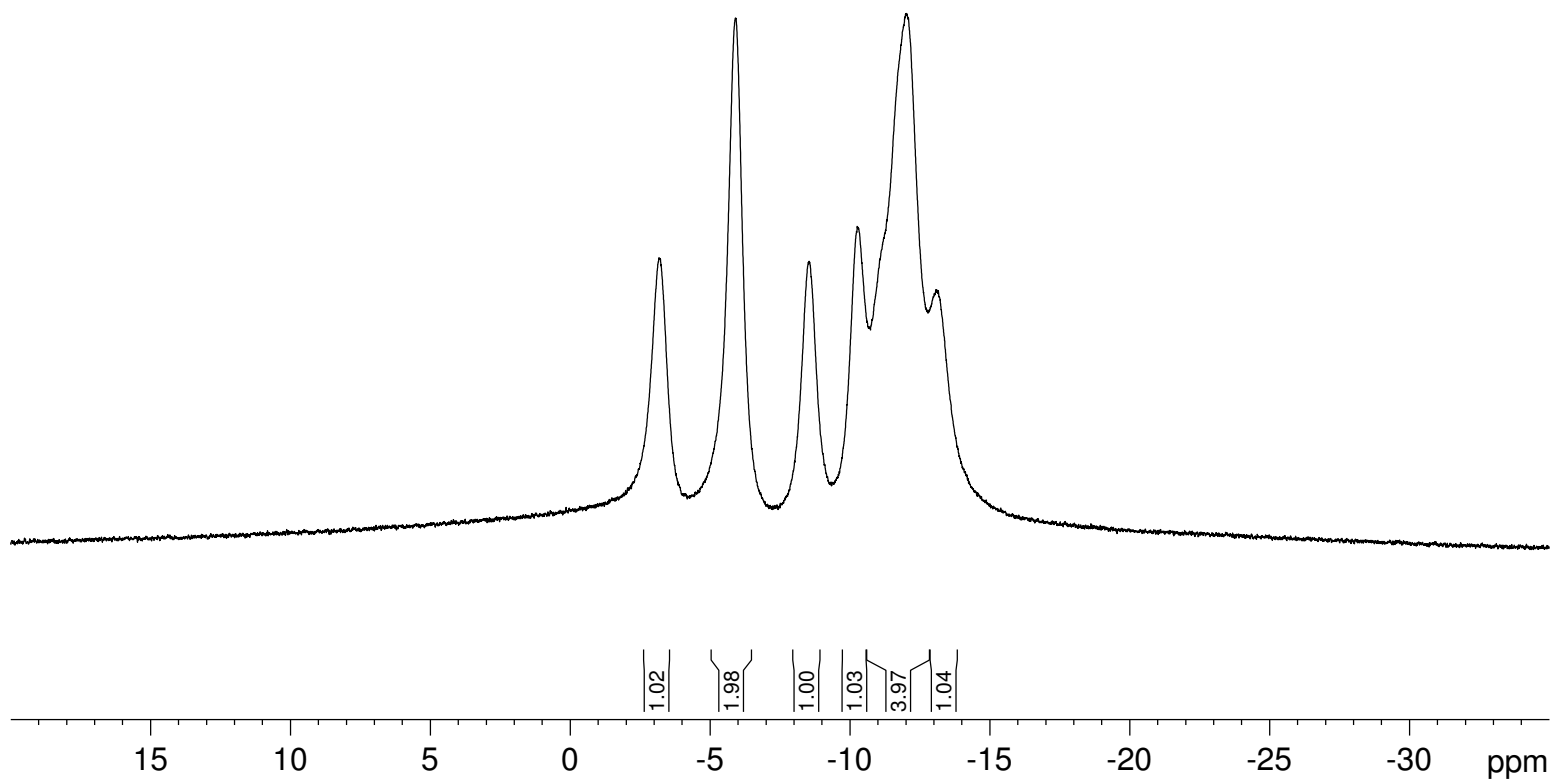
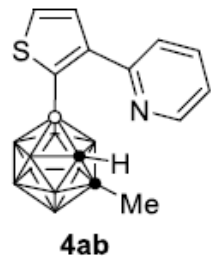
CY-B-A-163p

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 CDC13  
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

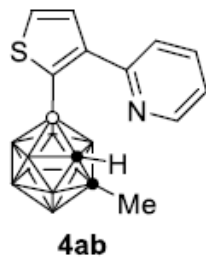
F2 - Processing parameters  
SI 32768  
SF 128.4097615 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

— 3.18  
— 5.91  
— 8.54  
— 10.26  
— 12.01  
— 13.07



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

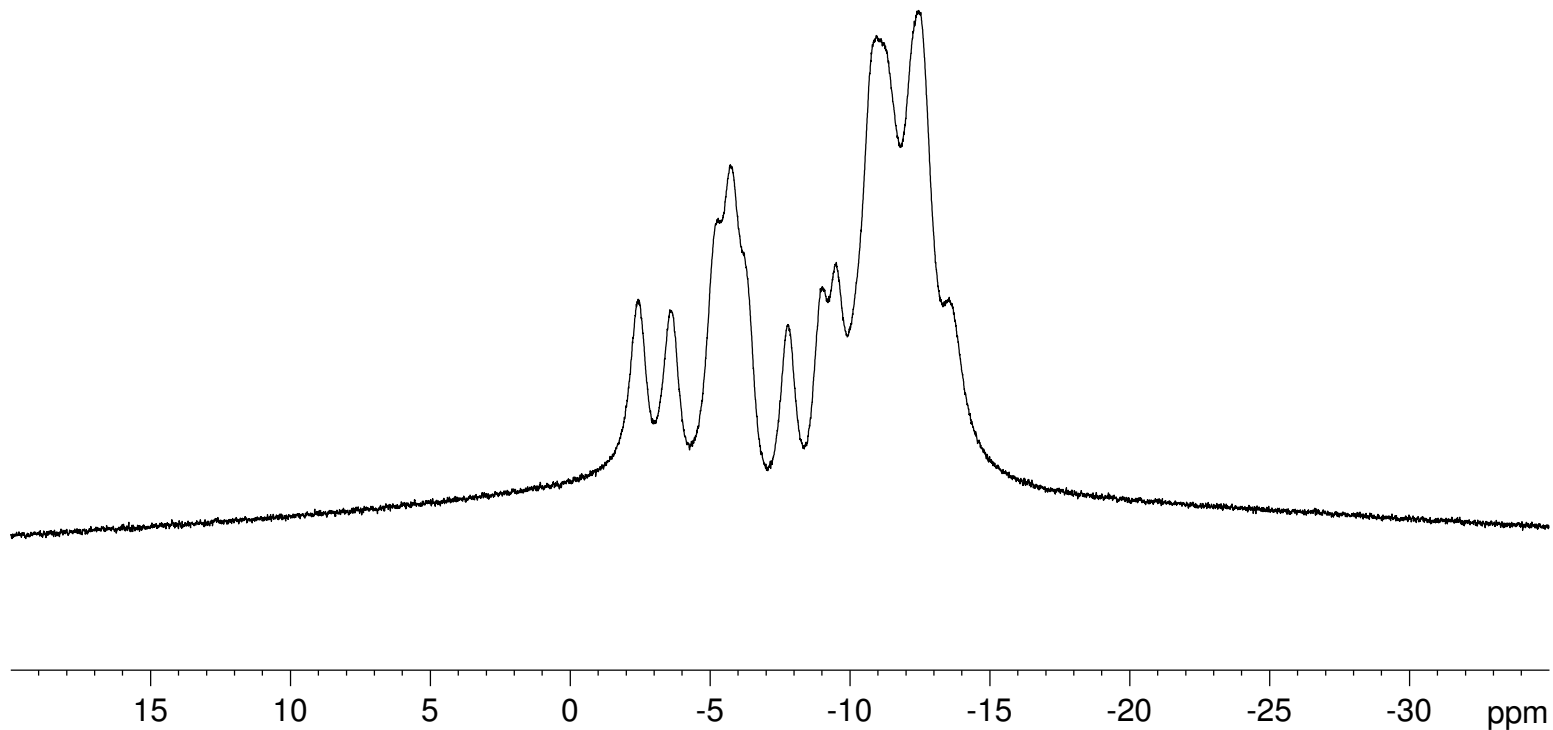
— 2.43  
— 3.56  
— 5.21  
— 5.73  
— 7.77  
— 8.99  
— 9.52  
— 10.95  
— 12.45  
— 13.56



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

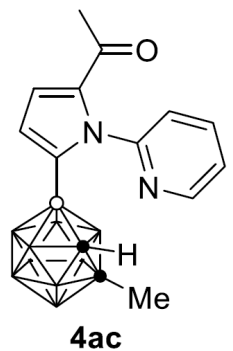
F2 - Acquisition Parameters  
Date\_ 20170920  
Time 17.03 h  
INSTRUM spect  
PROBHD z108618\_0257 (  
PULPROG zg  
TD 65536  
SOLVENT CDC13  
NS 20  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 287  
DW 20.800 usec  
DE 6.50 usec  
TE 295.1 K  
D1 2.00000000 sec  
TD0 1  
SFO1 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



8.521  
8.512  
8.509  
7.823  
7.818  
7.804  
7.799  
7.785  
7.780  
7.433  
7.431  
7.420  
7.418  
7.414  
7.412  
7.402  
7.400  
7.323  
7.303  
7.259  
7.030  
7.020  
6.596  
6.586

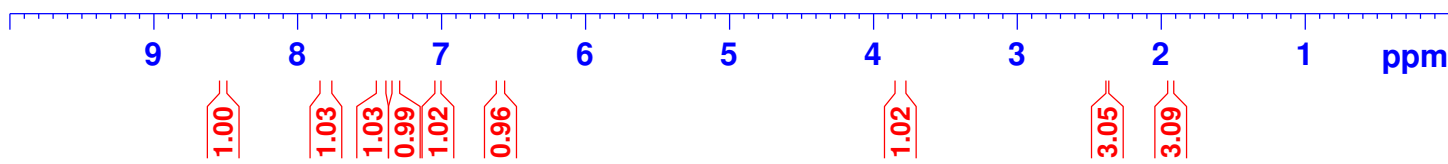
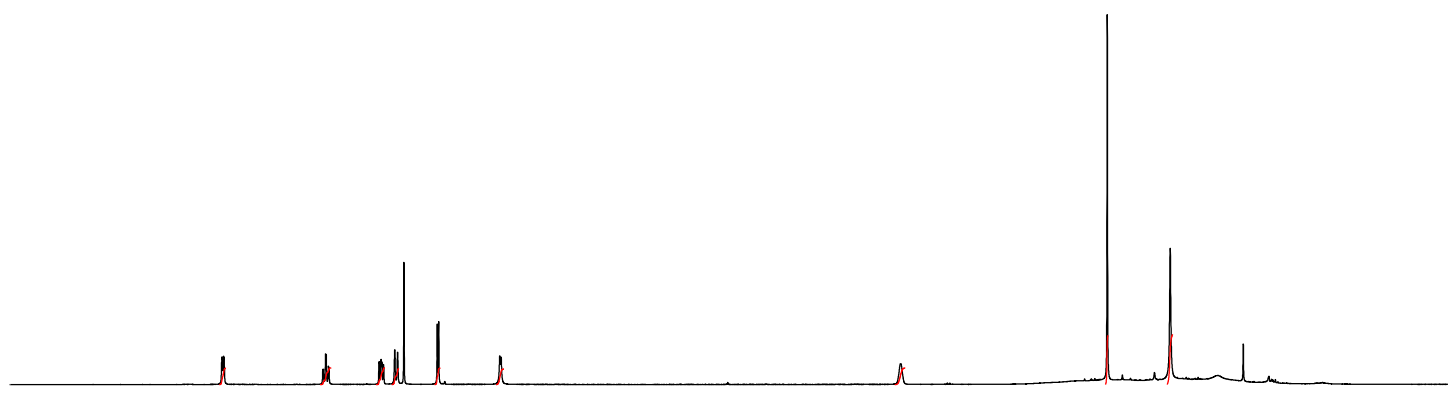
3.811  
2.375  
1.937



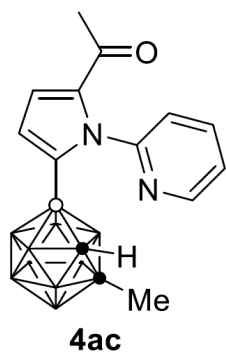
Current Data Parameters  
 NAME CY-H-A-77P-CDC  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190805  
 Time 14.00 h  
 INSTRUM spect  
 PROBHD z820201\_0170 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 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



187.28  
 153.89  
 148.15  
 137.97  
 135.23  
 124.63  
 124.24  
 120.12  
 119.60  
 77.47  
 77.16  
 76.84  
 70.85  
 62.84  
 27.16  
 26.04

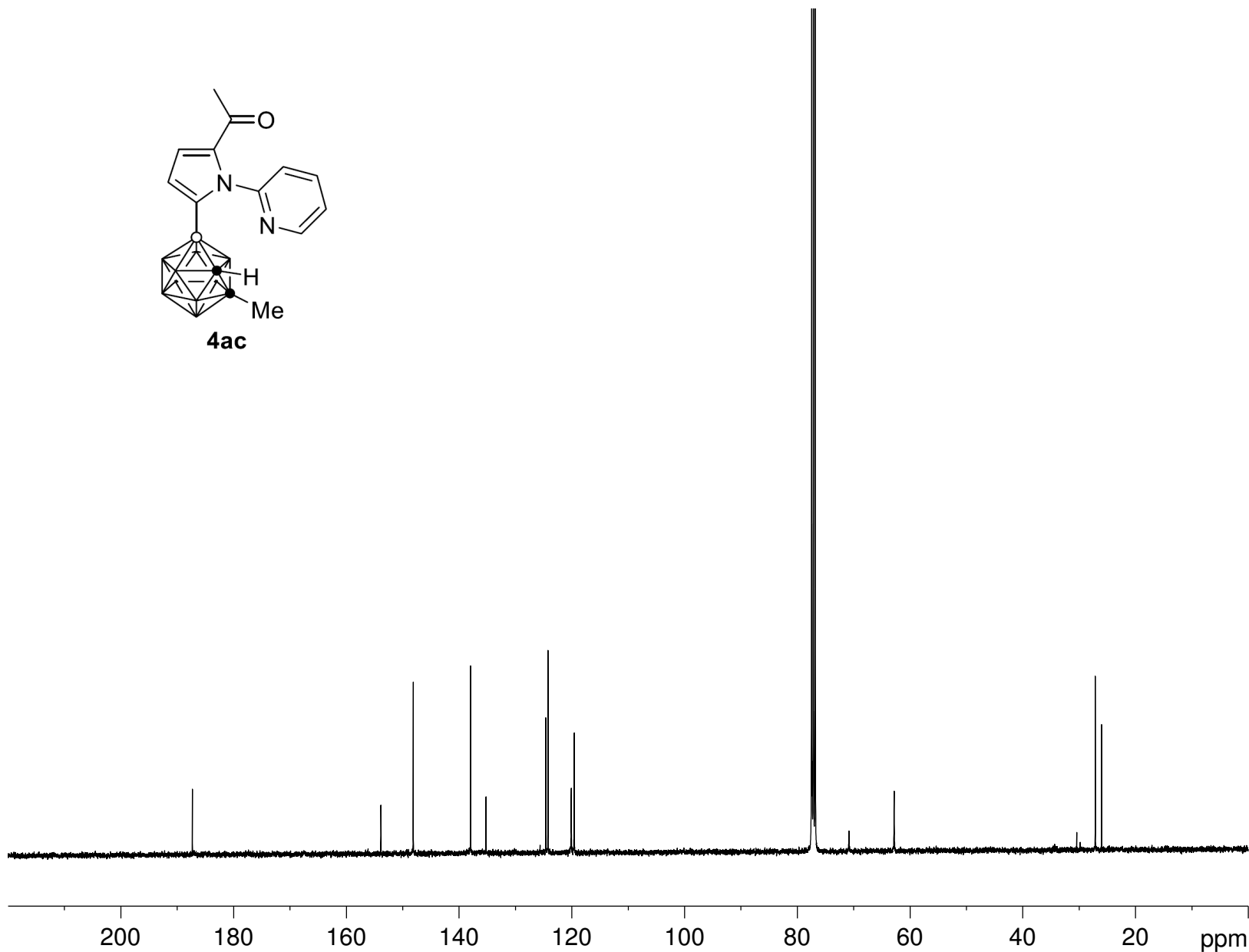


CY-C-A-77P-CDC

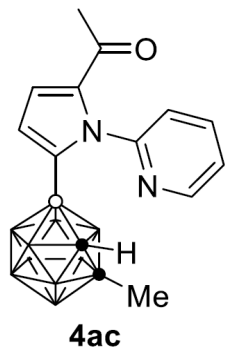
Current Data Parameters  
 NAME CY-C-A-77P-CDC  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190811  
 Time 18.21 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 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 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6479773 MHz  
 NUC1 13C  
 P1 9.36 usec  
 PLW1 40.0000000 W  
 SFO2 400.2316009 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 8.0000000 W  
 PLW12 0.20765001 W  
 PLW13 0.10445000 W

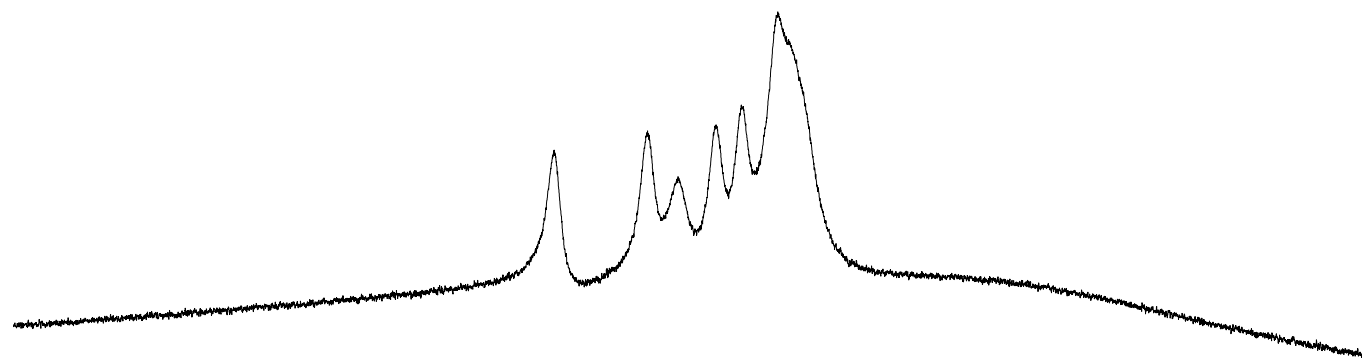
F2 - Processing parameters  
 SI 32768  
 SF 100.6379015 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



CY-B-A-77P



— -1.97  
— -5.77  
— -7.00  
— -8.54  
— -9.57  
— -11.05



15 10 5 0 -5 -10 -15 -20 -25 -30 ppm

1.07 1.06 1.04 1.00 1.07 5.00

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 CDC13  
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

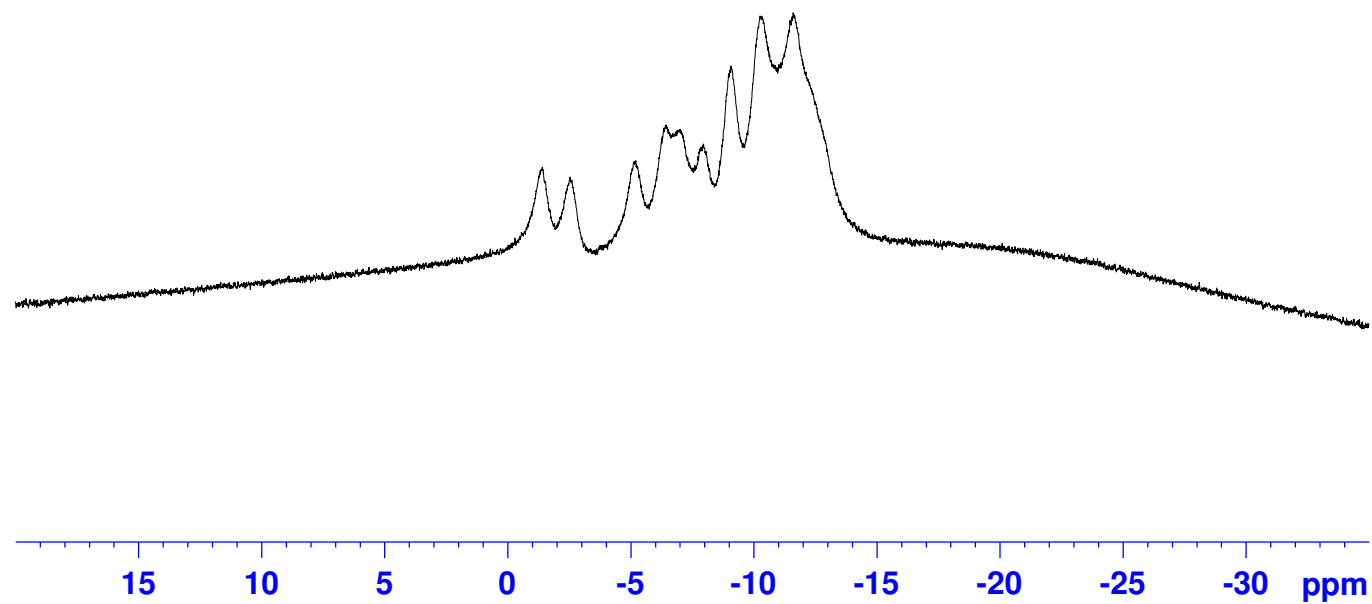
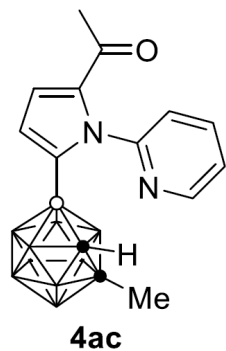
F2 - Processing parameters  
SI 32768  
SF 128.3776052 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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



— 1.42  
— 2.54  
  
— 5.22  
— 6.45  
— 6.94  
— 7.90  
— 9.07  
— 10.25  
— 11.60



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 CDC13  
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

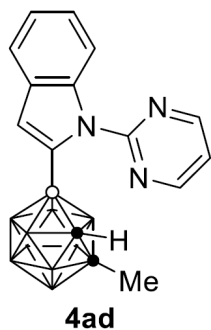
F2 - Processing parameters  
SI 32768  
SF 128.3776052 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

8.787  
8.771  
8.666  
8.657  
8.330  
7.938  
7.922  
7.340  
7.324  
7.309  
7.269  
7.254  
7.239  
7.230  
7.020  
7.011  
7.001

3.799

2.051

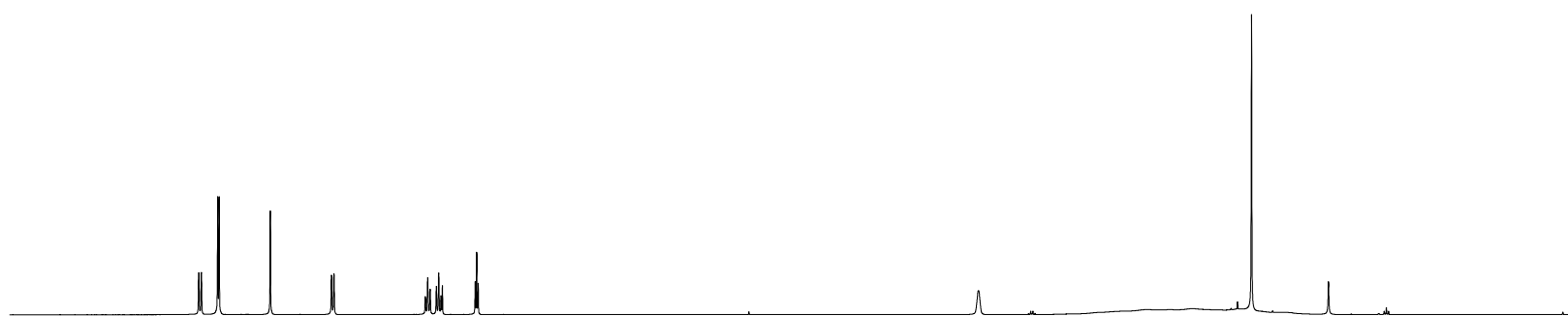
1.559



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

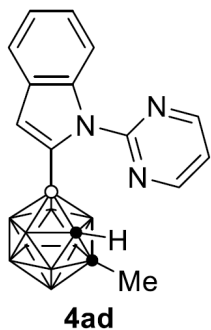
F2 - Acquisition Parameters  
Date\_ 20171012  
Time 10.41 h  
INSTRUM spect  
PROBHD z149001\_0010 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.2767999 sec  
RG 30.85  
DW 50.000 usec  
DE 10.00 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 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



9 8 7 6 5 4 3 2 1 ppm

1.000  
1.978  
0.992  
1.013  
1.046  
0.994  
1.005  
1.019  
2.997

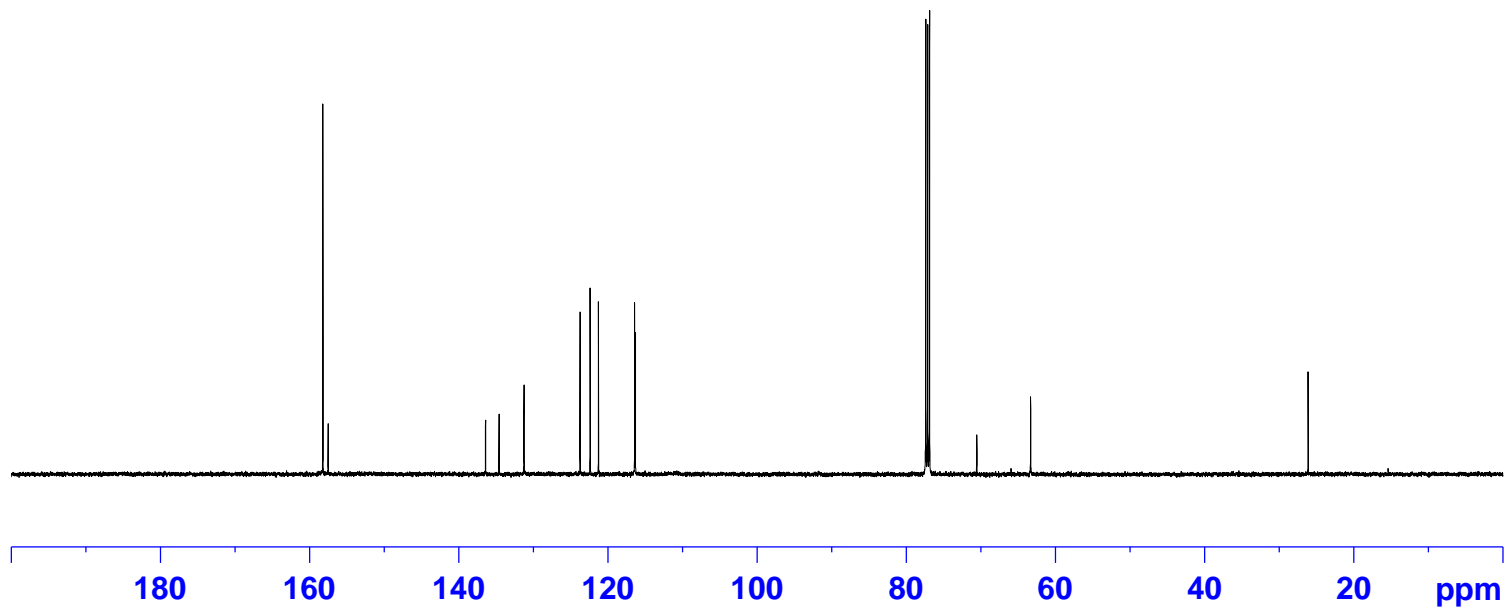


158.25  
157.54

136.44  
134.62  
131.28  
123.76  
122.42  
121.30  
116.45  
116.35

77.41  
77.16  
76.90  
70.57  
63.35

26.14



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

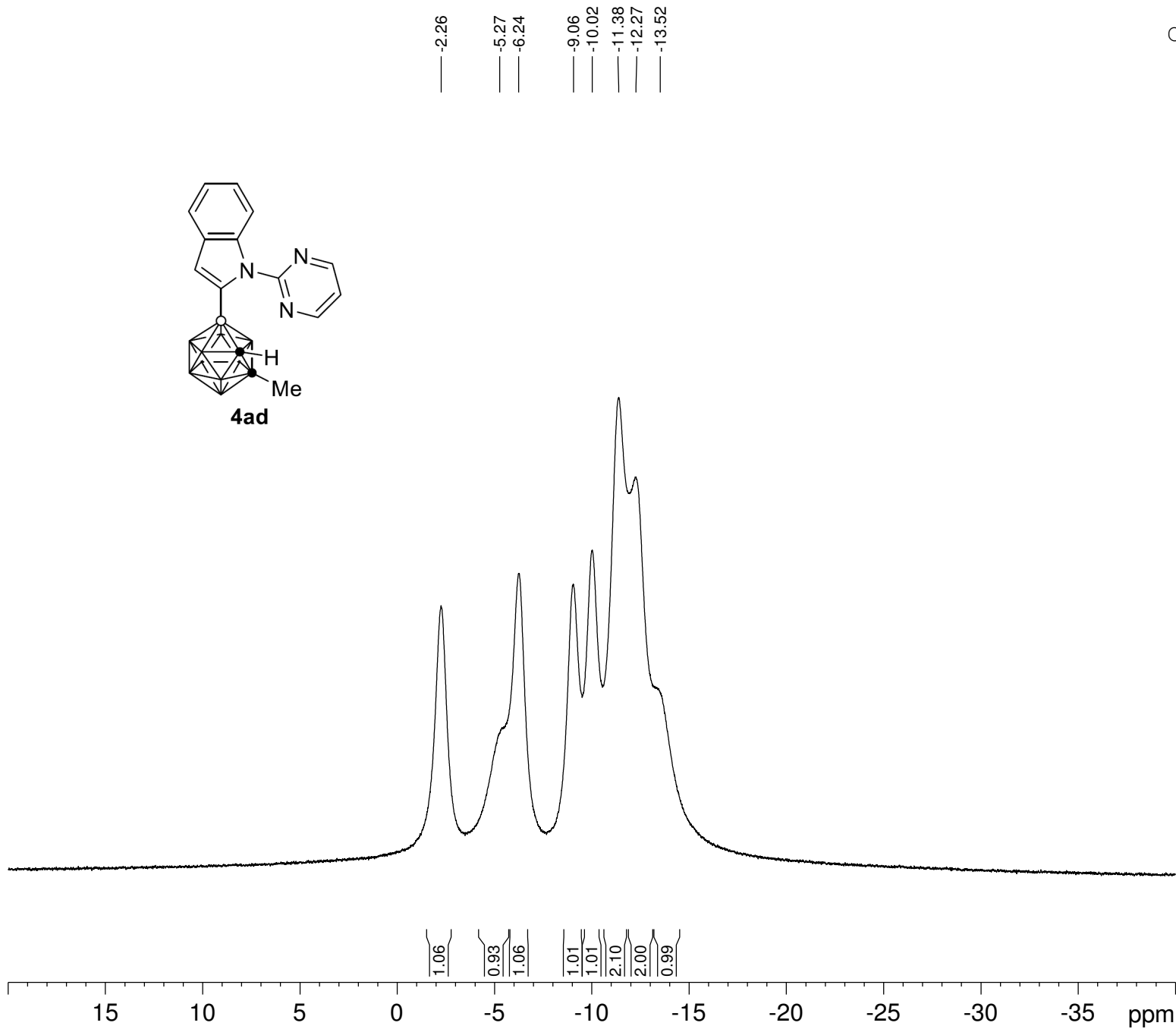
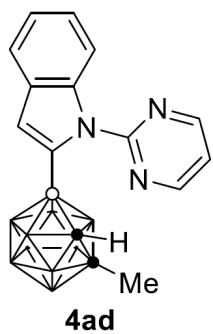
F2 - Processing parameters  
SI 32768  
SF 125.7577754 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

CY-B-A-169p

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

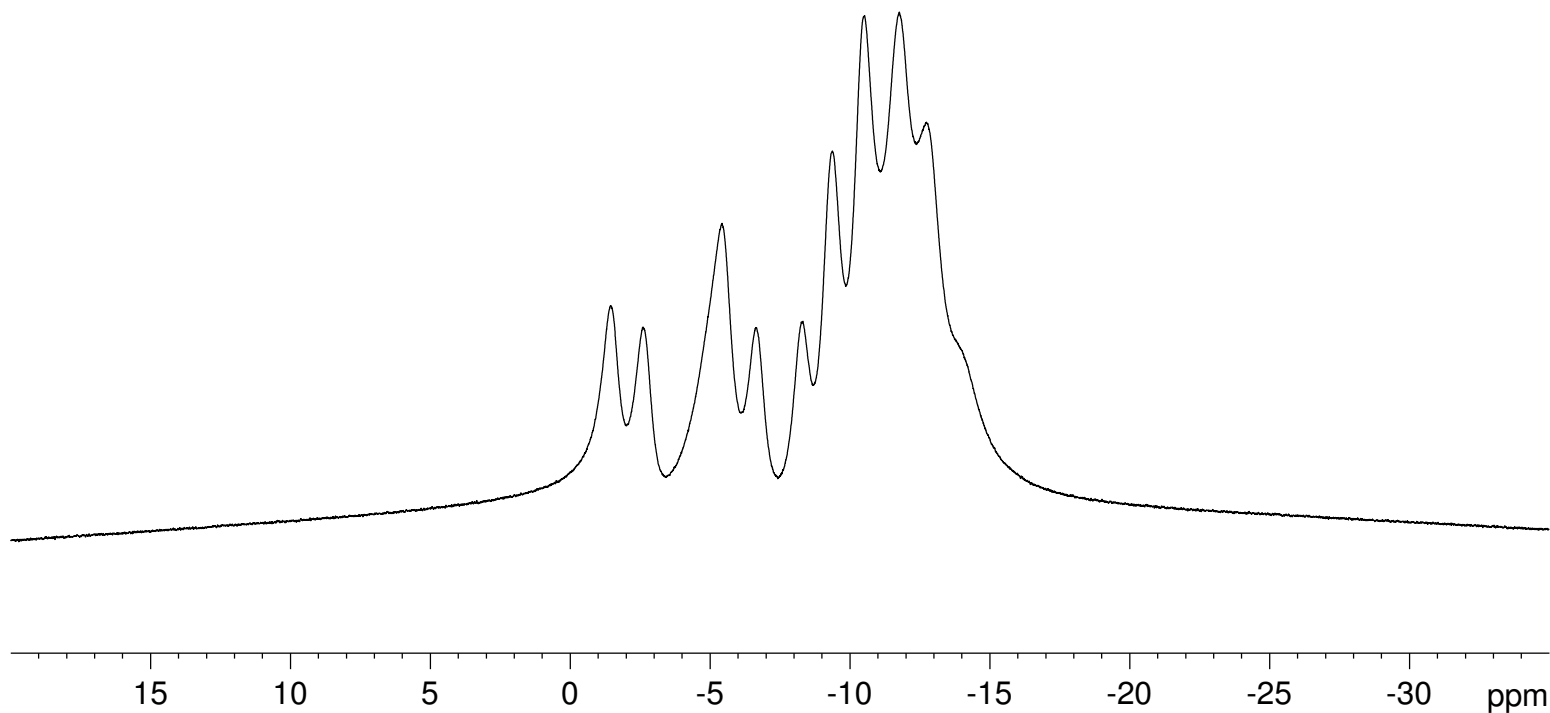
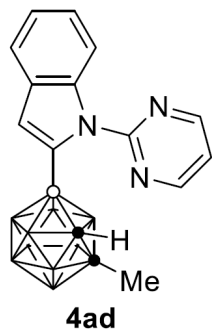
F2 - Acquisition Parameters  
Date\_ 20171009  
Time 15.15 h  
INSTRUM spect  
PROBHD z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDC13  
NS 8  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 406  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.0000000 sec  
D11 0.0300000 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)

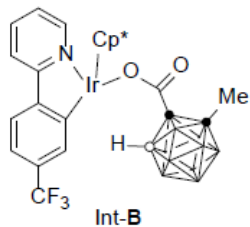
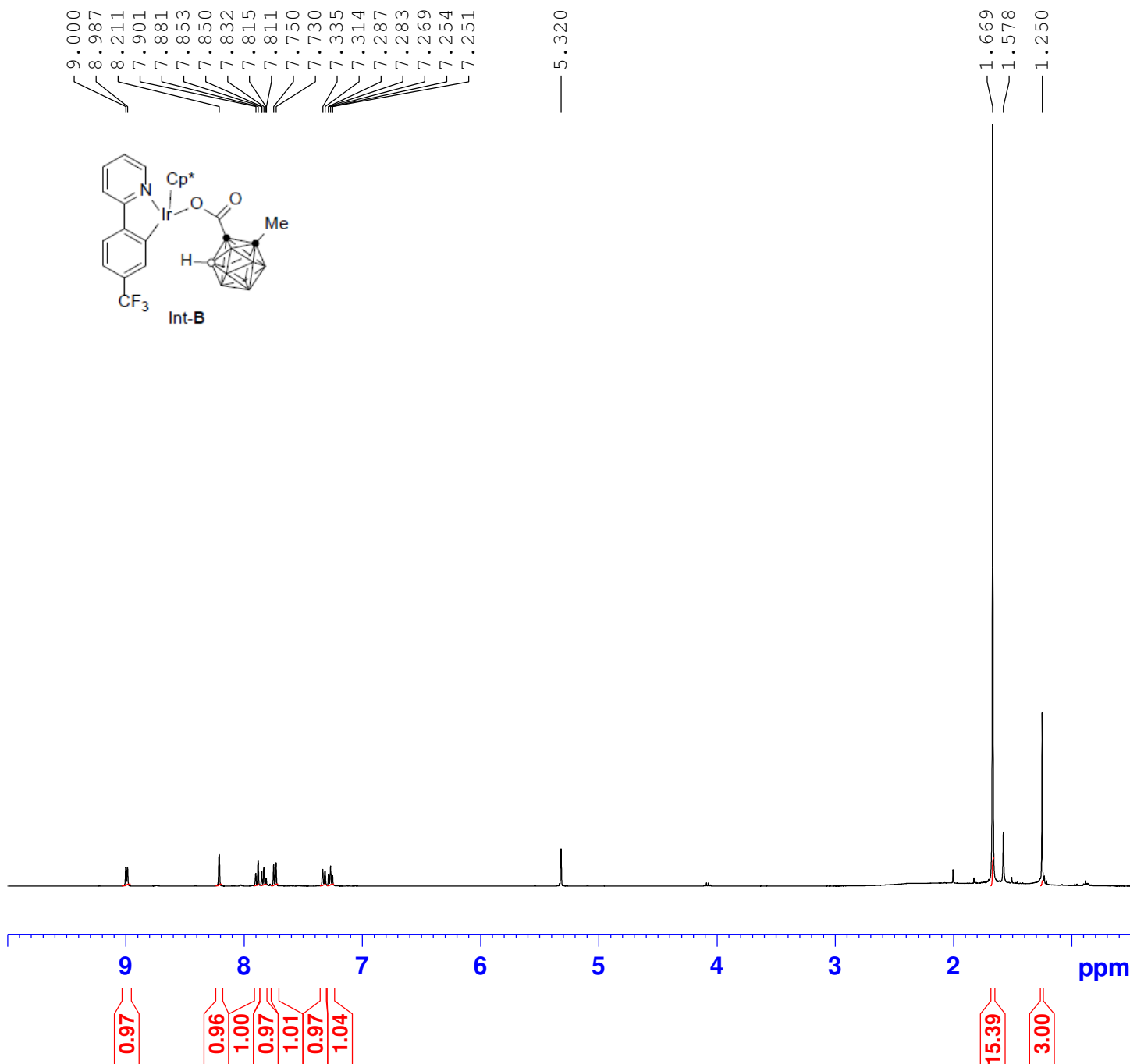
— -1.46  
— -2.61  
  
— -5.43  
— -6.64  
— -8.32  
— -9.37  
— -10.52  
— -11.76  
— -12.73  
— -14.07



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 CDC13  
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

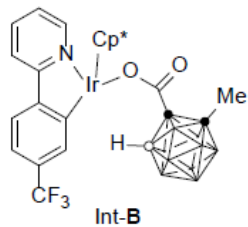
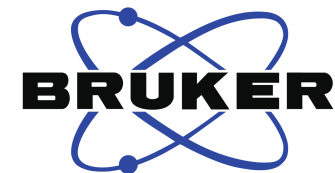


Current Data Parameters  
 NAME CY-H-B-164p  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180604  
 Time 21.43 h  
 INSTRUM spect  
 PROBHD z824601\_0021 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CD2C12  
 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



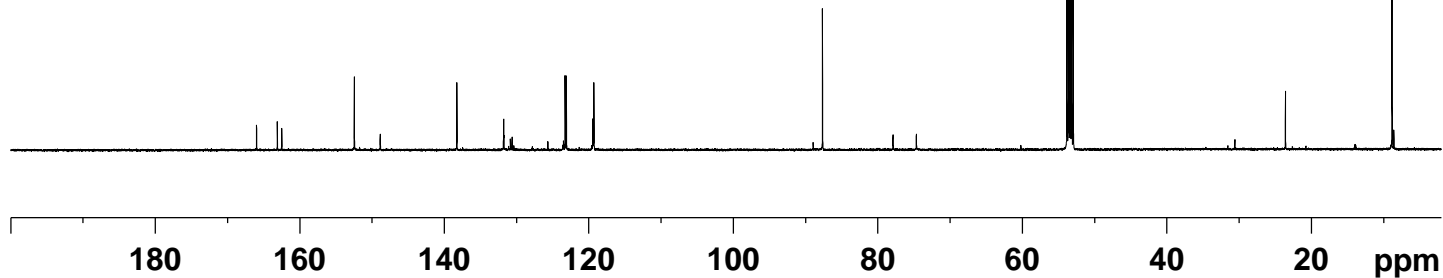
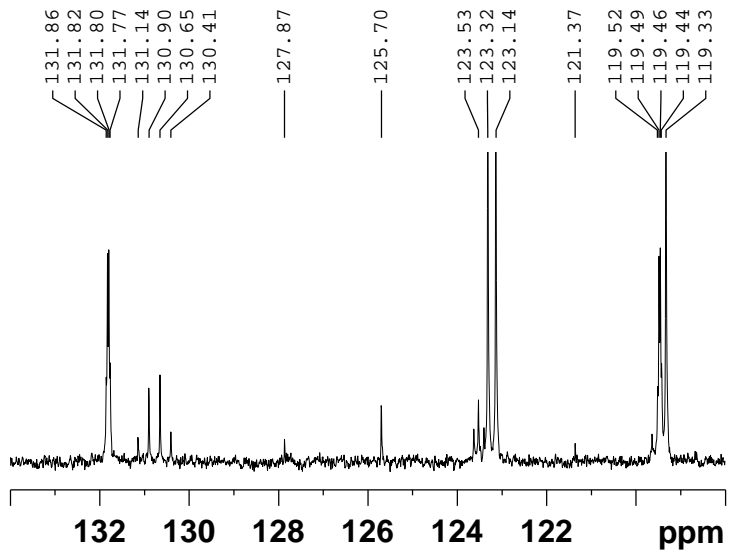
166.02  
163.16  
162.54  
152.49  
148.91  
138.30  
131.86  
131.82  
131.80  
131.77  
131.14  
130.90  
130.65  
130.41  
127.87  
125.70  
123.53  
123.32  
123.14  
121.37  
119.52  
119.49  
119.46  
119.44  
119.33

87.69  
77.93  
74.69

53.86  
53.65  
53.43  
53.21  
53.00

23.61

8.86



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 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SFO2 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.2966300 W  
PLW13 0.14920001 W

F2 - Processing parameters

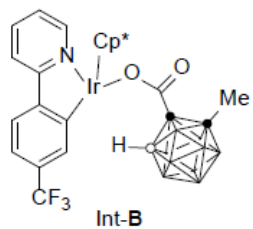
SI 32768  
SF 125.7577885 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

CY-B-A-164p

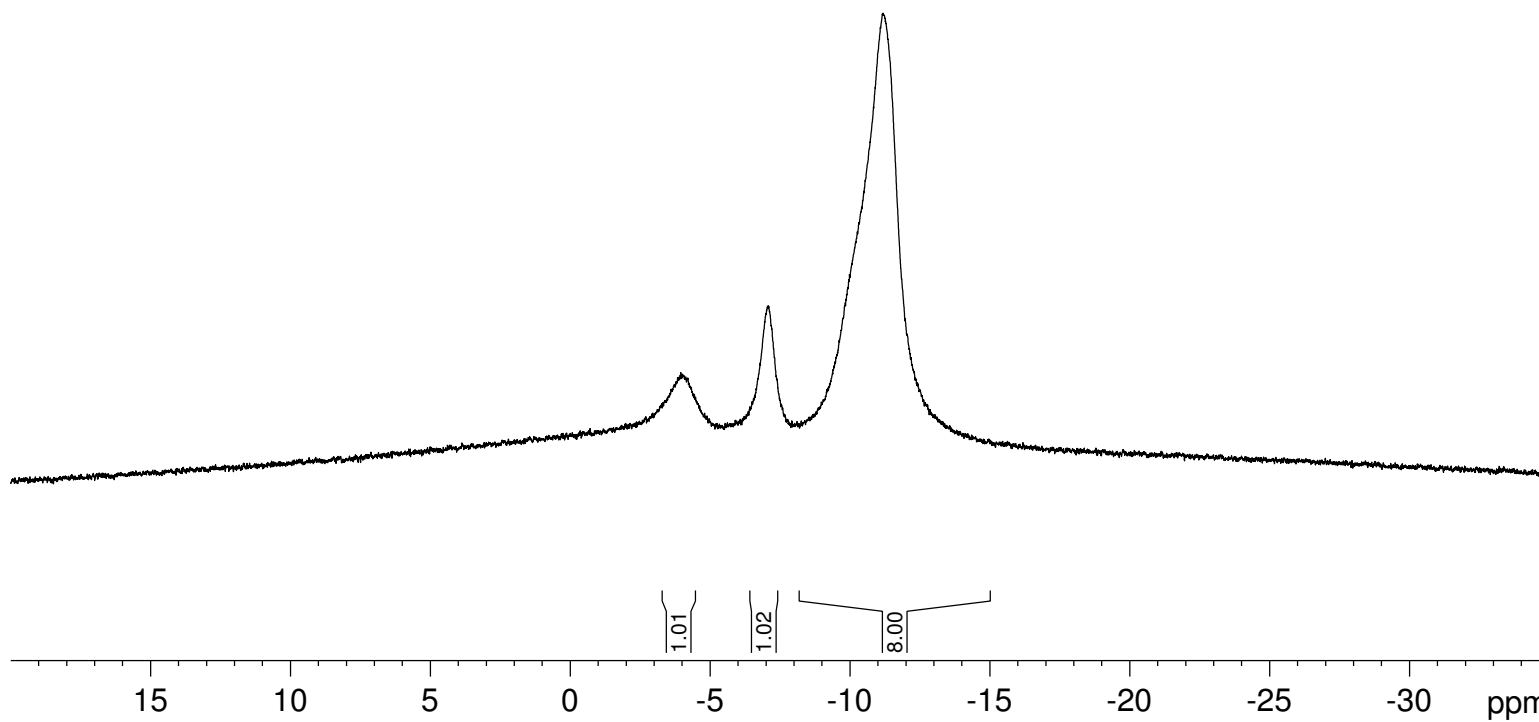
Current Data Parameters  
NAME CY-B-A-164p  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171020  
Time 13.04 h  
INSTRUM spect  
PROBHD z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDC13  
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 2.0000000 sec  
D11 0.0300000 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



— -3.95  
— -7.09  
— -11.18





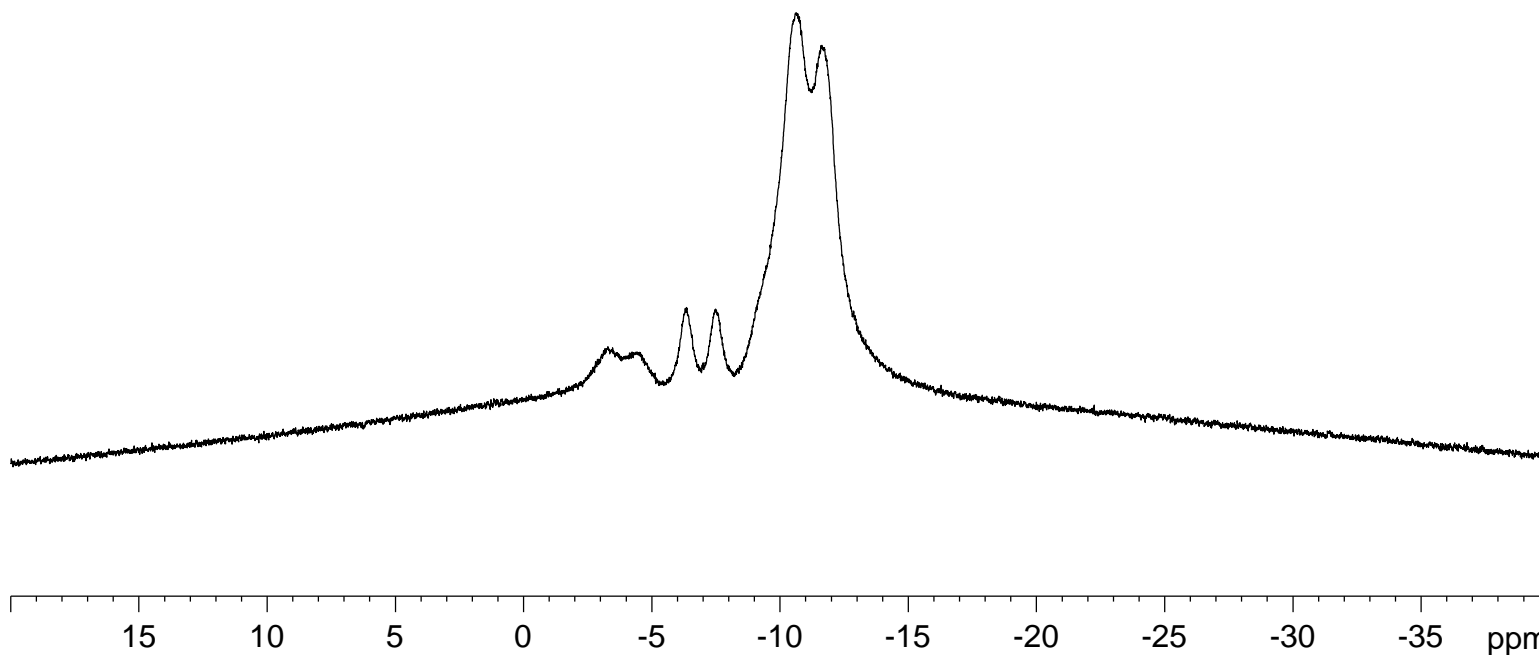
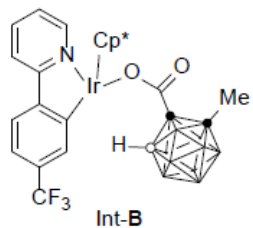
CY-B-A-164p-(C)

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

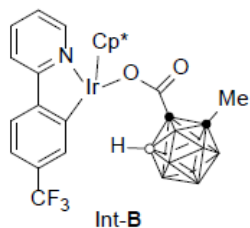
F2 - Processing parameters  
SI 32768  
SF 128.4097430 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

3.30  
4.48  
6.36  
7.50  
-10.61  
-11.62



CY-F-A-164P

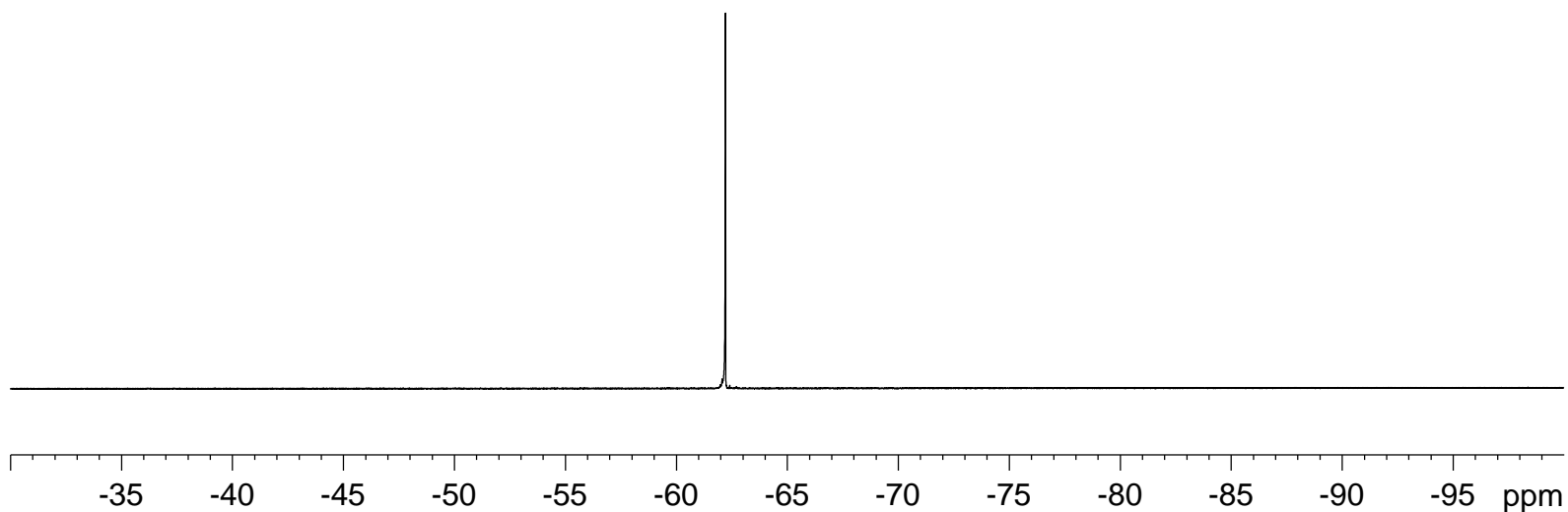
-62.21



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

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2. Y. Quan, J. Zhang and Z. Xie, *J. Am. Chem. Soc.*, 2013, **135**, 18742-18745.
3. G. M. Sheldrick, *SADABS: 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).