

# Supplementary Information

## **Rhodium Catalyzed Cascade Cyclization Featuring B-H and C-H Activation: One-Step Construction of Carborane-Fused N-Polyheterocycles**

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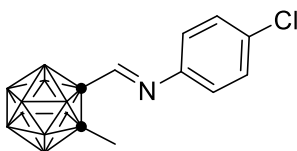
### Table of Contents

General Procedures	S-2
Experimental Section	S-2
Control Experiments	S-25
References	S-29
NMR Spectra	S-30

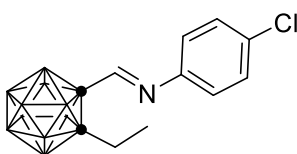
**General Procedures.** All reactions were carried out in flame-dried glassware using standard Schlenk techniques. All organic solvents were dried and distilled by standard methods prior to use.  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{11}\text{B}$  and  $^{19}\text{F}$  NMR spectra were recorded on Bruker DPX 400/500 spectrometers 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  $\text{CFCl}_3$  (0.00 ppm) for fluorine chemical shifts. High resolution mass spectra (HRMS) were obtained on a Thermo Finnigan MAT 95 XL spectrometer. GC-MS analyses were performed on Agilent GC-MS 6890N.  $\text{Cu}(\text{OPiv})_2$  and *o*-carboranyl aldehydes were synthesized according to the reported procedures.<sup>1,2</sup> All other chemicals were purchased from either Aldrich or Acros Chemical Co. and used as received unless otherwise specified.

### **Preparation of Starting Materials.**

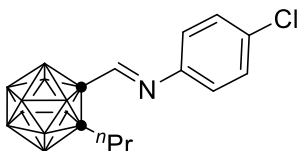
**Preparation of Carboranyl *N*-Arylimines (1). A Representative Procedure.** *o*-Carboranyl aldehyde (1.0 mmol) and aniline (1.5 mmol) were dissolved in toluene (3 ml) in the presence of molecular sieves (3 Å, 100 mg). The resulting solution was stirred at 100 °C for 18 h. After cooling to room temperature, the reaction mixture was filtered through a pad of Celite and concentrated. The residue was subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (100 : 1 in V/V) as eluent to afford carboranyl *N*-arylimines **1**.



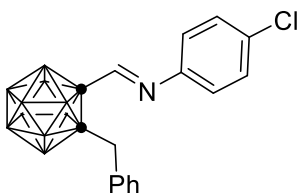
**1a:** Yield 93%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.80 (s, 1H) (imine *CH*), 7.37 (d,  $J = 8.8$  Hz, 2H), 7.06 (d,  $J = 8.8$  Hz, 2H) (aryl *CH*), 2.10 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  152.3 (imine *CH*), 147.0, 134.0, 129.7, 122.3 (aryl C), 75.3 (cage C), 23.7 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.2 (1B), -5.9 (1B), -9.7 (8B). HRMS:  $m/z$  calcd for  $\text{C}_{10}\text{H}_{18}\text{B}_{10}\text{ClN}$   $[\text{M}]^+$ : 295.2125. Found: 295.2125.



**1b:** Yield 82%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.78 (s, 1H) (imine *CH*), 7.36 (d,  $J = 8.8$  Hz, 2H), 7.06 (d,  $J = 8.8$  Hz, 2H) (aryl *CH*), 2.36 (q,  $J = 7.4$  Hz, 2H), 1.15 (t,  $J = 7.4$  Hz, 3H) (Et).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  152.2 (imine *CH*), 147.0, 134.0, 129.7, 122.3 (aryl C), 83.1, 76.6 (cage C), 29.2, 14.3 (Et).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -1.8 (1B), -4.4 (1B), -9.1 (2B), -10.3 (6B). HRMS:  $m/z$  calcd for  $\text{C}_{11}\text{H}_{20}\text{B}_{10}\text{ClN}$   $[\text{M}]^+$ : 309.2282. Found: 309.2283.

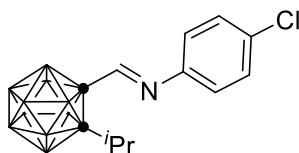


**1c:** Yield 86%. White solid.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.78 (s, 1H) (imine *CH*), 7.37 (d,  $J = 9.0$  Hz, 2H), 7.05 (d,  $J = 9.0$  Hz, 2H) (aryl *CH*), 2.26 (m, 2H), 1.58 (m, 2H), 0.90 (t,  $J = 7.5$  Hz, 3H) ( $^i\text{Pr}$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  152.2 (imine *CH*), 147.1, 134.0, 129.7, 122.3 (aryl C), 82.2, 76.5 (cage C), 37.5, 23.3, 13.9 ( $^i\text{Pr}$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (160 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.2 (1B), -4.7 (1B), -9.4 (2B), -10.6 (6B). HRMS:  $m/z$  calcd for  $\text{C}_{12}\text{H}_{22}\text{B}_{10}\text{ClN}$   $[\text{M}]^+$ : 324.2418. Found: 324.2419.

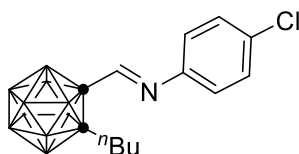


**1d:** Yield 89%. White solid.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.87 (s, 1H) (imine *CH*), 7.42 (d,  $J = 9.0$  Hz, 2H), 7.32 (m, 3H), 7.15 (m, 4H) (aryl *CH*), 3.63 (s, 2H) ( $\text{CH}_2$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,

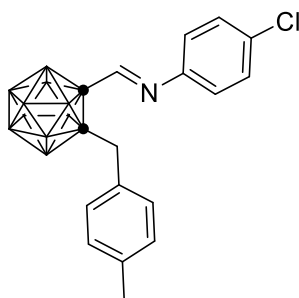
CDCl<sub>3</sub>): δ 152.4 (imine CH), 146.8, 135.3, 134.3, 130.4, 129.8, 128.7, 128.2, 122.5 (aryl C), 82.2, 76.8 (cage C), 41.0 (CH<sub>2</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -2.0 (1B), -4.3 (1B), -9.0 (2B), -10.4 (6B). HRMS: *m/z* calcd for C<sub>16</sub>H<sub>22</sub>B<sub>10</sub>CIN [M]<sup>+</sup>: 371.2438. Found: 371.2436.



**1e:** Yield 78%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.77 (s, 1H) (imine CH), 7.37 (d, *J* = 9.0 Hz, 2H), 7.06 (d, *J* = 9.0 Hz, 2H) (aryl CH), 2.45 (m, 1H), 1.22 (d, *J* = 7.0 Hz, 6H) (<sup>i</sup>Pr). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 152.0 (imine CH), 147.1, 134.0, 129.7, 122.3 (aryl C), 88.6, 78.3 (cage C), 32.3, 24.3 (<sup>i</sup>Pr). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -2.6 (1B), -3.9 (1B), -9.2 (2B), -11.4 (6B). HRMS: *m/z* calcd for C<sub>12</sub>H<sub>22</sub>B<sub>10</sub>CIN [M]<sup>+</sup>: 324.2418. Found: 324.2418.



**1f:** Yield 87%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.78 (s, 1H) (imine CH), 7.37 (d, *J* = 8.5 Hz, 2H), 7.05 (d, *J* = 9.0 Hz, 2H) (aryl CH), 2.29 (m, 2H), 1.53 (m, 2H), 1.27 (m, 2H), 0.88 (t, *J* = 7.5 Hz, 3H) (<sup>n</sup>Bu). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 152.3 (imine CH), 147.1, 134.0, 129.7, 122.2 (aryl C), 82.4, 76.5 (cage C), 35.3, 31.9, 22.4, 13.8 (<sup>n</sup>Bu). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -2.2 (1B), -4.7 (1B), -9.4 (2B), -10.5 (6B). HRMS: *m/z* calcd for C<sub>13</sub>H<sub>24</sub>B<sub>10</sub>CIN [M]<sup>+</sup>: 338.2576. Found: 338.2577.

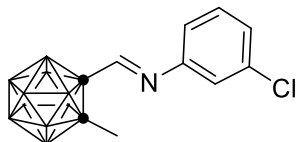


**1g:** Yield 86%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.87 (s, 1H) (imine CH), 7.43 (d, *J* = 9.0 Hz, 2H), 7.16 (m, 4H), 7.04 (d, *J* = 8.0 Hz, 2H) (aryl CH), 3.60 (s, 2H) (CH<sub>2</sub>), 2.37 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 152.4 (imine CH), 146.8, 138.0, 134.2, 132.2, 130.2, 129.8, 129.3, 122.5 (aryl C), 82.4, 76.8 (cage C), 40.7 (CH<sub>2</sub>), 21.3



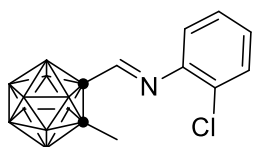
(CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -2.0 (1B), -4.4 (1B), -9.0 (2B), -10.4 (6B).

HRMS: *m/z* calcd for C<sub>17</sub>H<sub>24</sub>B<sub>10</sub>ClN [M]<sup>+</sup>: 386.2578. Found: 386.2578.



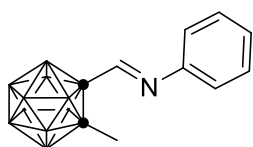
**1j**: Yield 77%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.81 (s, 1H) (imine CH), 7.30 (m, 2H), 7.10 (s, 1H), 7.00 (d, *J* = 8.0 Hz, 1H) (aryl CH), 2.12 (s, 3H) (CH<sub>3</sub>).

<sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 153.3 (imine CH), 149.8, 135.2, 130.6, 128.0, 121.1, 119.2 (aryl C), 75.1 (cage C), 23.7 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -1.6 (1B), -5.5 (1B), -9.3 (8B). HRMS: *m/z* calcd for C<sub>10</sub>H<sub>18</sub>B<sub>10</sub>ClN [M]<sup>+</sup>: 295.2134. Found: 295.2133.



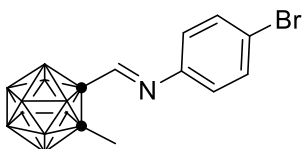
**1k**: Yield 70%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.80 (s, 1H) (imine CH), 7.44 (d, *J* = 8.0 Hz, 1H), 7.28 (m, 1H), 7.22 (m, 1H), 6.90 (d, *J* = 8.0 Hz, 1H) (aryl CH), 2.22 (s, 3H) (CH<sub>3</sub>).

<sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 153.3 (imine CH), 149.8, 135.2, 130.6, 128.0, 121.1, 119.2 (aryl C), 75.1 (cage C), 23.7 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -1.6 (1B), -5.5 (1B), -9.3 (8B). HRMS: *m/z* calcd for C<sub>10</sub>H<sub>18</sub>B<sub>10</sub>ClN [M]<sup>+</sup>: 295.2134. Found: 295.2133.

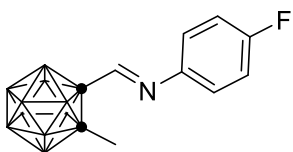


**1l**: Yield 90%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.82 (s, 1H) (imine CH), 7.41 (t, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.12

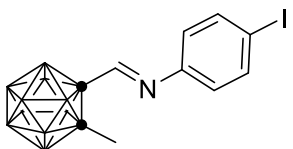
(d, *J* = 7.5 Hz, 2H) (phenyl CH), 2.12 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 151.9 (imine CH), 148.7, 129.6, 128.2, 120.9 (phenyl C), 75.5 (cage C), 23.7 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -1.9 (1B), -5.5 (1B), -9.4 (8B). HRMS: *m/z* calcd for C<sub>10</sub>H<sub>19</sub>B<sub>10</sub>N [M]<sup>+</sup>: 261.2520. Found: 261.2521.



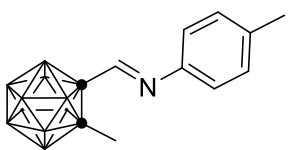
**1m:** Yield 91%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.81 (s, 1H) (imine CH), 7.52 (d,  $J = 8.4$  Hz, 2H), 7.00 (d,  $J = 8.4$  Hz, 2H) (aryl CH), 2.11 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  152.4 (imine CH), 147.5, 132.7, 122.6, 121.9 (aryl C), 76.9, 75.3 (cage C), 23.7 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.2 (1B), -6.0 (1B), -9.8 (8B). HRMS:  $m/z$  calcd for  $\text{C}_{10}\text{H}_{18}\text{B}_{10}\text{BrN}$   $[\text{M}]^+$ : 340.1611. Found: 340.1612.



**1n:** Yield 83%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.82 (s, 1H) (imine CH), 7.13 (m, 4H) (aryl CH), 2.12 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.6 (d,  $^1J_{\text{C-F}} = 247$  Hz) (aryl C), 151.4 (imine CH), 144.6 (d,  $^4J_{\text{C-F}} = 3$  Hz), 122.8 (d,  $^3J_{\text{C-F}} = 8$  Hz), 116.4 (d,  $^2J_{\text{C-F}} = 22$  Hz) (aryl C), 77.0, 75.5 (cage C), 23.6 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.4 (1B), -6.1 (1B), -9.9 (5B), -10.9 (3B).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ):  $\delta$  -105.5 (m, 1F). HRMS:  $m/z$  calcd for  $\text{C}_{10}\text{H}_{18}\text{B}_{10}\text{FN}$   $[\text{M}]^+$ : 279.2426. Found: 279.2426.

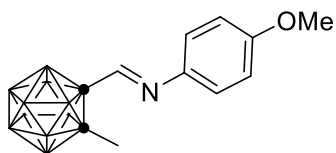


**1o:** Yield 80%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.80 (s, 1H) (imine CH), 7.71 (d,  $J = 8.4$  Hz, 2H), 6.87 (d,  $J = 8.8$  Hz, 2H) (aryl CH), 2.11 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  152.4 (imine CH), 148.2, 138.6, 122.8, 93.1 (aryl C), 76.9, 75.2 (cage C), 23.7 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.2 (1B), -6.0 (1B), -9.9 (8B). HRMS:  $m/z$  calcd for  $\text{C}_{10}\text{H}_{18}\text{B}_{10}\text{IN}$   $[\text{M}]^+$ : 387.1487. Found: 387.1486.



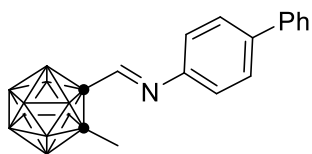
**1p:** Yield 86%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.85 (s, 1H) (imine CH), 7.23 (d,  $J = 8.0$  Hz, 2H), 7.08 (d,  $J = 8.4$  Hz, 2H)

(aryl CH), 2.40 (s, 3H), 2.12 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): δ 150.6 (imine CH), 146.0, 138.5, 130.1, 121.0 (aryl C), 77.0, 75.8 (cage C), 23.6, 21.2 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -2.5 (1B), -6.1 (1B), -10.0 (8B). HRMS: *m/z* calcd for C<sub>11</sub>H<sub>21</sub>B<sub>10</sub>N [M]<sup>+</sup>: 275.2677. Found: 275.2678.



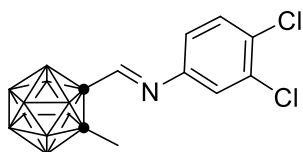
**1q:** Yield 85%. White solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.82 (s, 1H) (imine CH), 7.17 (d, *J* = 8.8 Hz, 2H), 6.92 (d, *J* = 8.8 Hz,

2H) (aryl CH), 3.83 (s, 3H) (OCH<sub>3</sub>), 2.09 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): δ 160.1 (aryl C), 148.8 (imine CH), 141.3, 122.8, 114.7 (aryl C), 77.0, 76.1 (cage C), 55.7 (OCH<sub>3</sub>), 23.6 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -2.2 (1B), -5.6 (1B), -9.6 (8B). HRMS: *m/z* calcd for C<sub>11</sub>H<sub>21</sub>B<sub>10</sub>NO [M]<sup>+</sup>: 291.2626. Found: 291.2626.



**1r:** Yield 82%. White solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.90 (s, 1H) (imine CH), 7.62 (m, 4H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.39

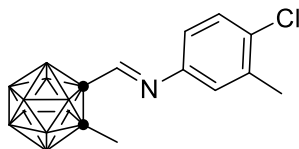
(m, 1H), 7.23 (dd, *J* = 1.6, 6.4 Hz, 2H) (aryl CH), 2.15 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): δ 151.5 (imine CH), 147.6, 141.3, 140.1, 129.1, 128.2, 127.9, 127.1, 121.5 (aryl C), 77.0, 75.6 (cage C), 23.7 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -2.2 (1B), -5.6 (1B), -9.6 (8B). HRMS: *m/z* calcd for C<sub>20</sub>H<sub>25</sub>B<sub>10</sub>N [M]<sup>+</sup>: 387.2998. Found: 387.3005.



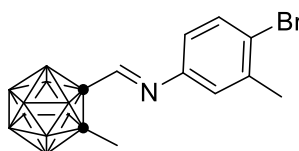
**1s:** Yield 77%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.81 (s, 1H) (imine CH), 7.47 (d, *J* = 8.5 Hz, 1H), 7.22 (d, *J* = 2.5 Hz, 1H),

6.98 (dd, *J* = 2.5, 8.5 Hz, 1H) (aryl CH), 2.11 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 153.6 (imine CH), 147.8, 133.6, 132.1, 131.2, 122.9, 120.4 (aryl C), 74.9 (cage C),

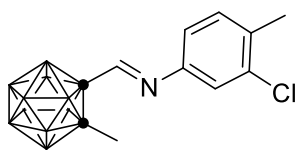
23.7 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -1.7 (1B), -5.6 (1B), -9.4 (8B). HRMS: *m/z* calcd for C<sub>10</sub>H<sub>10</sub>B<sub>17</sub>Cl<sub>2</sub>N [M-H]<sup>+</sup>: 329.1641. Found: 329.1641.



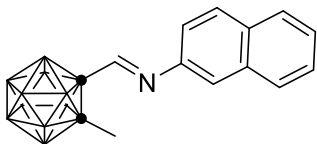
**1t:** Yield 76%. White solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.81 (s, 1H) (imine CH), 7.35 (d, *J* = 8.4 Hz, 1H), 7.01 (s, 1H), 6.91 (d, *J* = 8.4 Hz, 1H) (aryl CH), 2.40, 2.11 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): δ 151.9 (imine CH), 147.0, 137.5, 134.1, 130.0, 123.5, 119.4 (aryl C), 76.9, 75.4 (cage C), 23.7, 20.2 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -2.4 (1B), -6.1 (1B), -10.0 (8B). HRMS: *m/z* calcd for C<sub>11</sub>H<sub>20</sub>B<sub>10</sub>ClN [M]<sup>+</sup>: 309.2282. Found: 309.2288.



**1u:** Yield 79%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.81 (s, 1H) (imine CH), 7.53 (d, *J* = 8.5 Hz, 1H), 7.00 (s, 1H), 6.82 (d, *J* = 8.0 Hz, 1H) (aryl CH), 2.42, 2.11 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 152.0 (imine CH), 147.7, 139.4, 133.3, 124.3, 123.4, 119.6 (aryl C), 75.4 (cage C), 23.7, 23.1 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -2.4 (1B), -6.1 (1B), -10.0 (8B). HRMS: *m/z* calcd for C<sub>11</sub>H<sub>20</sub>B<sub>10</sub>BrN [M]<sup>+</sup>: 354.1768. Found: 354.1766.

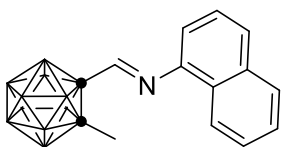


**1v:** Yield 75%. White solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.82 (s, 1H) (imine CH), 7.26 (d, *J* = 8.0 Hz, 1H), 7.15 (s, 1H), 6.96 (d, *J* = 8.0 Hz, 1H) (aryl CH), 2.40, 2.11 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (100 MHz, CDCl<sub>3</sub>): δ 152.0 (imine CH), 147.7, 139.4, 133.3, 124.3, 123.4, 119.6 (aryl C), 75.4 (cage C), 23.7, 23.1 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (128 MHz, CDCl<sub>3</sub>): δ -2.3 (1B), -6.1 (1B), -9.9 (8B). HRMS: *m/z* calcd for C<sub>11</sub>H<sub>20</sub>B<sub>10</sub>ClN [M]<sup>+</sup>: 309.2282. Found: 309.2284.



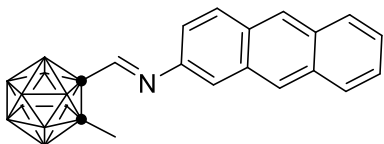
**1w:** Yield 82%. White solid.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.97 (s, 1H) (imine *CH*), 7.87 (m, 3H), 7.53 (m, 3H), 7.32 (d,  $J = 8.5$

Hz, 1H) (aryl *H*), 2.17 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  151.7 (imine *CH*), 146.0, 133.7, 133.0, 129.6, 128.3, 127.9, 127.1, 126.6, 119.7, 119.4 (aryl *C*), 77.0, 75.7 (cage *C*), 23.7 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (160 MHz,  $\text{CDCl}_3$ ):  $\delta$  -1.8 (1B), -5.4 (1B), -9.3 (8B). HRMS:  $m/z$  calcd for  $\text{C}_{14}\text{H}_{21}\text{B}_{10}\text{N}$   $[\text{M}]^+$ : 311.2679. Found: 311.2677.



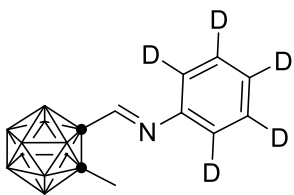
**1x:** Yield 72%. Yellow solid.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.12 (t,  $J = 7.5$  Hz, 1H) (aryl *CH*), 7.95 (s, 1H) (imine *CH*), 7.86 (t,  $J = 6.0$

Hz, 1H), 7.81 (d,  $J = 10.0$  Hz, 1H), 7.56 (m, 2H), 7.44 (t,  $J = 10.0$  Hz, 1H), 6.94 (d,  $J = 9.0$  Hz, 1H) (aryl *CH*), 2.20 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  152.0 (imine *CH*), 145.8, 134.1, 128.5, 128.3, 128.0, 127.1, 126.8, 125.7, 123.4, 112.7 (aryl *C*), 76.8, 75.8 (cage *C*), 23.9 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.3 (1B), -5.9 (1B), -9.8 (8B). HRMS:  $m/z$  calcd for  $\text{C}_{14}\text{H}_{21}\text{B}_{10}\text{N}$   $[\text{M}]^+$ : 311.2672. Found: 311.2672.



**1y:** Yield 70%. Yellow solid.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.44 (s, 1H), 8.43 (s, 1H), 8.01 (m, 4H), 7.70 (s, 1H), 7.51

(m, 2H), 7.33 (dd,  $J = 2.0, 9.0$  Hz, 1H) (aryl *CH* and imine *CH*), 2.18 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  151.3 (imine *CH*), 145.3, 132.4, 132.2, 131.6, 130.9, 130.1, 128.4, 128.2, 127.1, 126.6, 126.2, 126.1, 119.9, 119.7 (aryl *C*), 77.1, 75.8 (cage *C*), 23.8 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (160 MHz,  $\text{CDCl}_3$ ):  $\delta$  -1.7 (1B), -5.5 (1B), -9.3 (8B). HRMS:  $m/z$  calcd for  $\text{C}_{18}\text{H}_{23}\text{B}_{10}\text{N}$   $[\text{M}]^+$ : 361.2837. Found: 361.2836.



**11-d<sub>5</sub>**: Yield 91%. White solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.82

(s, 1H) (imine CH), 2.12 (s, 3H) (CH<sub>3</sub>). <sup>2</sup>H NMR (61 MHz, CDCl<sub>3</sub>):

δ 7.47, 7.19 (aryl CD). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 151.9

(imine CH), 148.6, 129.1 (t, *J*<sub>C-D</sub> = 11.3 Hz), 127.7 (t, *J*<sub>C-D</sub> = 11.3 Hz), 120.5 (t, *J*<sub>C-D</sub> = 11.3

Hz) (aryl C), 75.5 (cage C), 23.7 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -1.9 (1B), -5.6

(1B), -9.4 (8B). HRMS: *m/z* calcd for C<sub>10</sub>H<sub>14</sub>B<sub>10</sub>ND<sub>5</sub> [M-H]<sup>-</sup>: 265.2764. Found: 265.2762.

### Synthesis of C,B-Substituted *o*-Carborane-Fused *N*-Polyheterocycles (3). A

**Representative Procedure.** Carboranyl *N*-arylimine **1** (0.10 mmol), vinyl ketone (0.50 mmol,

5.0 equiv), [Cp\**Rh*Cl<sub>2</sub>]<sub>2</sub> (3.1 mg, 0.005 mmol, 5 mol%), AgSbF<sub>6</sub> (34.4 or 17.2 mg, 0.10 or

0.05 mmol, 1.0 or 0.5 equiv), Cu(OPiv)<sub>2</sub> (66.0 mg, 0.25 mmol, 2.5 equiv) and

2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane

(2 mL). The resulting mixture was stirred at 90 °C for 6 h or 10 h under argon. After cooling

to room temperature and the addition of pyridine (0.1 mL), the reaction mixture was filtered

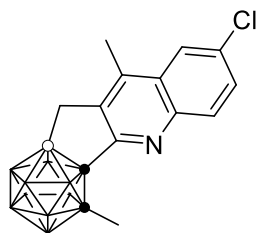
through a pad of Celite and washed with dichloromethane. The filtrate was concentrated to

dryness in vacuo, and subjected to flash column chromatography on silica gel (230-400

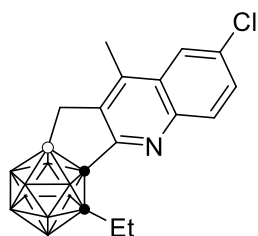
mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **3**. It

is noted that cage B(4)-H and B(5)-H are identical according to the symmetry of the cluster,

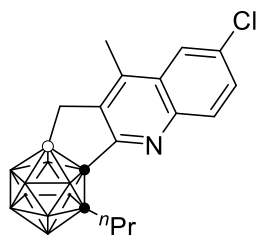
which will generate a pair of enantiomers in the reactions.<sup>3</sup>



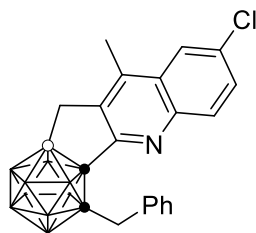
**3a:** Yield 70%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.96 (m, 2H), 7.61 (dd,  $J = 2.0, 8.8$  Hz, 1H) (aryl CH), 2.62 (s, 3H) ( $\text{CH}_3$ ), 2.53 (m, 2H) ( $\text{CH}_2$ ), 2.42 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  156.9, 144.2, 142.1, 140.7, 133.1, 131.9, 129.9, 128.3, 122.9 (aryl C), 83.0, 75.4 (cage C), 22.3, 15.1 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.3 (1B) (B-C), -5.3 (1B), -6.5 (1B), -8.2 (2B), -9.8 (4B), -13.1 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{14}\text{H}_{20}\text{B}_{10}\text{ClN}$  [ $\text{M}$ ] $^+$ : 346.2263. Found: 346.2264.



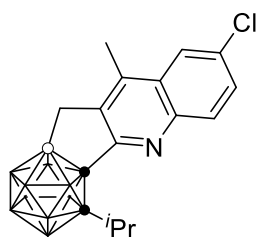
**3b:** Yield 72%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.96 (m, 2H), 7.61 (dd,  $J = 2.0, 8.8$  Hz, 1H) (aryl CH), 2.91 (m, 1H), 2.72 (m, 1H) ( $\text{CH}_2$ ), 2.61 (s, 3H) ( $\text{CH}_3$ ), 2.51 (m, 2H) ( $\text{CH}_2$ ), 1.22 (t,  $J = 7.2$  Hz, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  156.9, 144.1, 142.1, 140.8, 133.1, 131.9, 129.9, 128.3, 122.9 (aryl C), 84.1, 81.7 (cage C), 27.9, 15.1, 14.4 ( $\text{CH}_3$  and Et).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.4 (1B) (B-C), -5.7 (2B), -8.4 (2B), -10.5 (3B), -12.0 (1B), -14.5 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{15}\text{H}_{22}\text{B}_{10}\text{ClN}$  [ $\text{M}$ ] $^+$ : 360.2420. Found: 360.2427.



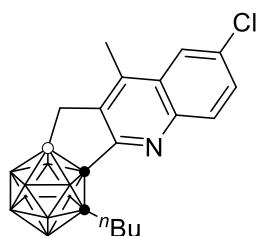
**3c:** Yield 74%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.95 (m, 2H), 7.62 (dd,  $J = 2.4, 8.8$  Hz, 1H) (aryl CH), 2.79 (m, 1H), 2.62 (m, 4H), 2.51 (m, 2H), 1.79 (m, 1H), 1.52 (m, 1H), 0.92 (t,  $J = 7.2$  Hz, 3H) ( $\text{CH}_2$ ,  $\text{CH}_3$  and  $^n\text{Pr}$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  156.9, 144.1, 142.1, 140.8, 133.1, 131.9, 129.9, 128.3, 122.9 (aryl C), 83.9, 80.8 (cage C), 36.2, 23.5, 15.1, 13.9 ( $\text{CH}_3$  and  $^n\text{Pr}$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.5 (1B) (B-C), -5.7 (2B), -10.0 (6B), -14.4 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{24}\text{B}_{10}\text{ClN}$  [ $\text{M}$ ] $^+$ : 374.2577. Found: 374.2579.



**3d:** Yield 69%. White solid.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.05 (d,  $J = 9.0$  Hz, 1H), 8.01 (d,  $J = 2.5$  Hz, 1H), 7.66 (dd,  $J = 2.0, 9.0$  Hz, 1H), 7.30 (m, 5H) (aryl CH), 4.27 (d,  $J = 15.0$  Hz, 1H), 3.96 (d,  $J = 15.0$  Hz, 1H) ( $\text{CH}_2$ ), 2.64 (s, 3H) ( $\text{CH}_3$ ), 2.53 (m, 2H) ( $\text{CH}_2$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  157.0, 144.1, 142.4, 140.9, 136.3, 133.3, 131.8, 130.8, 130.1, 128.5, 128.4, 127.9, 123.0 (aryl C), 84.3, 80.2 (cage C), 39.4, 15.2 ( $\text{CH}_2$  and  $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.6 (1B) (B-C), -5.5 (2B), -10.1 (5B), -12.4 (1B), -14.1 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{20}\text{H}_{24}\text{B}_{10}\text{ClN}$   $[\text{M}]^+$ : 421.2596. Found: 421.2593.



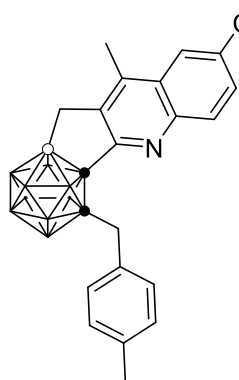
**3e:** Yield 64%. White solid.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.95 (m, 2H), 7.61 (dd,  $J = 2.5, 9.0$  Hz, 1H) (aryl CH), 3.39 (m, 1H) (CH), 2.61 (s, 3H) ( $\text{CH}_3$ ), 2.50 (m, 2H) ( $\text{CH}_2$ ), 1.45 (d,  $J = 6.5$  Hz, 3H), 1.08 (d,  $J = 7.0$  Hz, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  157.0, 144.1, 142.1, 140.8, 133.1, 132.0, 129.9, 128.3, 122.9 (aryl C), 87.1, 85.5 (cage C), 30.9, 24.6, 24.5, 15.1 ( $\text{CH}_3$  and  $^i\text{Pr}$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.5 (1B) (B-C), -5.0 (1B), -5.9 (1B), -9.6 (3B), -10.6 (3B), -15.4 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{24}\text{B}_{10}\text{ClN}$   $[\text{M}]^+$ : 373.2595. Found: 373.2593.



**3f:** Yield 74%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.95 (m, 2H), 7.61 (dd,  $J = 2.0, 8.8$  Hz, 1H) (aryl CH), 2.83 (m, 1H), 2.65 (m, 4H), 2.51 (m, 2H), 1.75 (m, 1H), 1.46 (m, 1H), 1.50 (m, 2H), 0.94 (t,  $J = 7.2$  Hz, 3H), ( $\text{CH}_2$ ,  $\text{CH}_3$  and  $^n\text{Bu}$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  156.9, 144.1, 142.1, 140.8, 133.1, 131.8, 129.9, 128.3, 122.9 (aryl C), 84.0, 80.9 (cage C), 33.8, 32.1, 22.5, 15.1, 13.8 ( $\text{CH}_3$  and  $^n\text{Bu}$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -1.9 (1B) (B-C), -4.0 (2B), -8.3

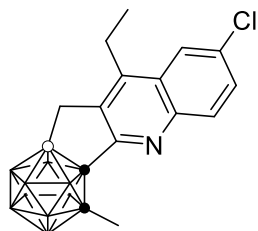


(5B), -10.3 (1B), -12.7 (1B). HRMS:  $m/z$  calcd for  $C_{17}H_{26}B_{10}ClN$   $[M]^+$ : 387.2751. Found: 387.2752.



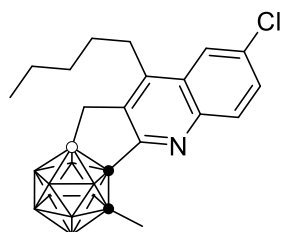
**3g**: Yield 71%. White solid.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.04 (d,  $J$  = 8.8 Hz, 1H), 8.00 (d,  $J$  = 2.0 Hz, 1H), 7.66 (dd,  $J$  = 2.4, 8.8 Hz, 1H), 7.17 (d,  $J$  = 8.0 Hz, 2H), 7.11 (d,  $J$  = 8.0 Hz, 2H) (aryl CH), 4.21 (d,  $J$  = 15.2 Hz, 1H), 3.92 (d,  $J$  = 15.2 Hz, 1H) ( $CH_2$ ), 2.64 (s, 3H) ( $CH_3$ ), 2.52 (m, 2H) ( $CH_2$ ), 2.33 (s, 3H) ( $CH_3$ ).  $^{13}C\{^1H\}$  NMR (100 MHz,

$CDCl_3$ ):  $\delta$  157.0, 144.1, 142.3, 140.9, 137.5, 133.3, 133.3, 131.8, 130.7, 130.1, 129.2, 128.4, 123.0 (aryl C), 84.2, 80.5 (cage C), 39.0, 12.3, 15.2 ( $CH_2$  and  $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -4.1 (1B) (B-C), -6.1 (2B), -10.7 (5B), -13.0 (1B), -14.6 (1B). HRMS:  $m/z$  calcd for  $C_{21}H_{26}B_{10}ClN$   $[M]^+$ : 435.2751. Found: 435.2739.



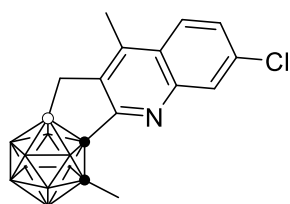
**3h**: Yield 63%. White solid.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.97 (m, 2H), 7.62 (dd,  $J$  = 2.0, 8.8 Hz, 1H) (aryl CH), 3.06 (q,  $J$  = 7.6 Hz, 2H), 2.53 (m, 2H) ( $CH_2$ ), 2.42 (s, 3H), 1.30 (t,  $J$  = 7.6 Hz, 3H) ( $CH_3$ ).

$^{13}C\{^1H\}$  NMR (125 MHz,  $CDCl_3$ ):  $\delta$  157.1, 147.9, 144.7, 139.9, 133.2, 132.1, 129.9, 127.3, 122.7 (aryl C), 83.0, 75.4 (cage C), 22.5, 22.3, 13.9 ( $CH_2$  and  $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -3.5 (1B) (B-C), -5.5 (1B), -6.7 (3B), -9.9 (2B), -10.7 (2B), -13.2 (1B). HRMS:  $m/z$  calcd for  $C_{15}H_{22}B_{10}ClN$   $[M]^+$ : 360.2420. Found: 360.2424.



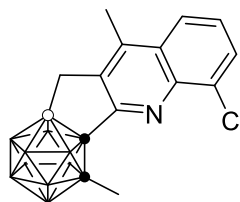
**3i**: Yield 35%. White solid.  $^1H$  NMR (500 MHz,  $CDCl_3$ ):  $\delta$  7.96 (m, 2H), 7.61 (dd,  $J$  = 2.5, 9.0 Hz, 1H) (aryl CH), 3.01 (t,  $J$  = 8.0 Hz, 2H), 2.53 (m, 2H) ( $CH_2$ ), 2.42 (s, 3H) ( $CH_3$ ), 1.64 (m, 2H), 1.48 (m,

2H), 1.42 (m, 2H) ( $CH_2$ ), 0.94 (t,  $J = 7.5$  Hz, 3H) ( $CH_3$ ).  $^{13}C\{^1H\}$  NMR (125 MHz,  $CDCl_3$ ):  $\delta$  157.0, 146.8, 144.6, 140.2, 133.1, 132.1, 129.9, 127.6, 122.8 (aryl C), 83.0, 75.4 (cage C), 32.4, 29.5, 29.3, 22.6, 22.3, 14.2 ( $CH_2$  and  $CH_3$ ).  $^{11}B\{^1H\}$  NMR (160 MHz,  $CDCl_3$ ):  $\delta$  -2.9 (1B) (B-C), -4.8 (1B), -5.9 (1B), -7.6 (2B), -9.9 (4B), -12.5 (1B). HRMS:  $m/z$  calcd for  $C_{18}H_{28}B_{10}ClN$  [M] $^+$ : 402.2892. Found: 402.2893.



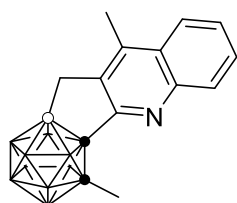
**3j**: Yield 68%. White solid.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.04 (d,  $J = 2.0$  Hz, 1H), 7.94 (d,  $J = 8.8$  Hz, 1H), 7.53 (dd,  $J = 2.0, 9.2$  Hz, 1H) (aryl CH), 2.64 (s, 3H) ( $CH_3$ ), 2.51 (m, 2H) ( $CH_2$ ), 2.41 (s, 3H)

( $CH_3$ ).  $^{13}C\{^1H\}$  NMR (125 MHz,  $CDCl_3$ ):  $\delta$  157.7, 146.3, 143.1, 140.1, 135.1, 129.2, 128.1, 126.0, 125.1 (aryl C), 82.9, 75.4 (cage C), 22.3, 15.1 ( $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -3.2 (1B) (B-C), -5.3 (1B), -6.4 (1B), -8.2 (2B), -9.7 (2B), -10.4 (2B), -12.9 (1B). HRMS:  $m/z$  calcd for  $C_{14}H_{20}B_{10}ClN$  [M] $^+$ : 345.2282. Found: 345.2287.



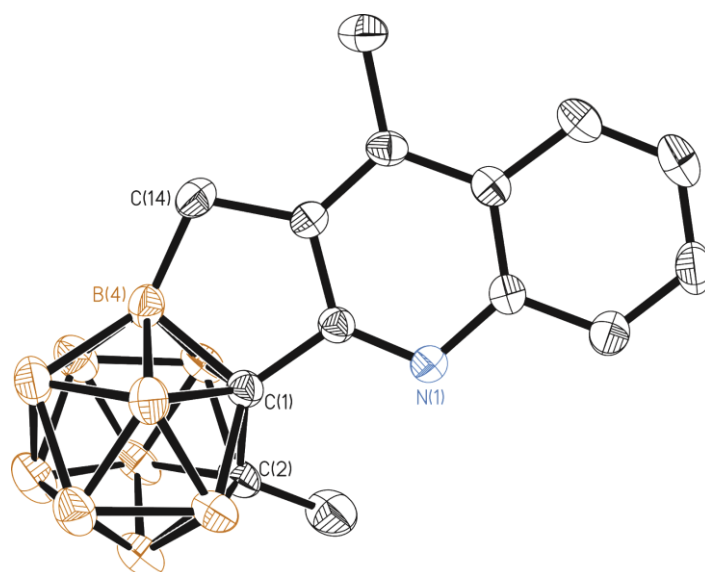
**3k**: Yield 39%. White solid.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  7.94 (dd,  $J = 1.2, 8.4$  Hz, 1H), 7.80 (dd,  $J = 1.2, 7.6$  Hz, 1H), 7.49 (dd,  $J = 7.6, 8.4$  Hz, 1H) (aryl CH), 2.67 (s, 3H) ( $CH_3$ ), 2.54 (m, 2H) ( $CH_2$ ), 2.49 (s, 3H)

( $CH_3$ ).  $^{13}C\{^1H\}$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  157.0, 143.5, 142.2, 140.6, 134.8, 129.4, 128.9, 127.0, 122.8 (aryl C), 82.8, 75.4 (cage C), 22.2, 15.4 ( $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -3.5 (1B) (B-C), -5.3 (1B), -6.5 (1B), -8.2 (2B), -9.8 (2B), -10.5 (2B), -12.9 (1B). HRMS:  $m/z$  calcd for  $C_{14}H_{20}B_{10}ClN$  [M] $^+$ : 346.2263. Found: 346.2264.

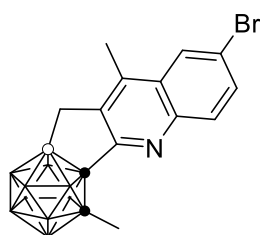


**3l**: Yield 62%. Colorless crystals.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.03 (m, 2H), 7.69 (t,  $J = 7.2$  Hz, 1H), 7.59 (t,  $J = 6.8$  Hz, 1H) (aryl CH), 2.67

(s, 3H) ( $CH_3$ ), 2.54 (m, 2H) ( $CH_2$ ), 2.45 (s, 3H) ( $CH_3$ ).  $^{13}C\{^1H\}$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  156.5, 145.7, 143.0, 139.8, 130.3, 129.1, 127.5, 127.3, 123.7 (aryl C), 83.3, 75.4 (cage C), 22.3, 15.1 ( $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -3.6 (1B) (B-C), -5.9 (1B), -6.9 (1B), -8.5 (2B), -10.8 (4B), -13.4 (1B). HRMS:  $m/z$  calcd for  $C_{14}H_{21}B_{10}N [M]^+$ : 311.2672. Found: 311.2675.

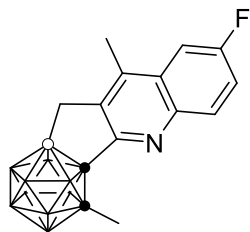


**Supplementary Figure 1.** Molecular structure of **3l** drawn with 30% probability ellipsoids.

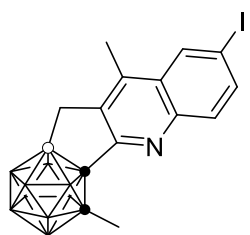


**3m:** Yield 67%. White solid.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.15 (d,  $J$  = 2.0 Hz, 1H), 7.89 (d,  $J$  = 8.8 Hz, 1H), 7.74 (dd,  $J$  = 2.0, 8.8 Hz, 1H) (aryl CH), 2.62 (s, 3H) ( $CH_3$ ), 2.54 (m, 2H) ( $CH_2$ ), 2.41 (s, 3H) ( $CH_3$ ).

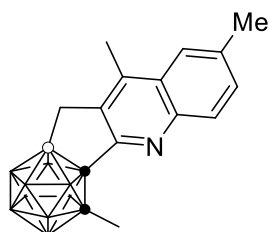
$^{13}C\{^1H\}$  NMR (125 MHz,  $CDCl_3$ ):  $\delta$  157.0, 144.4, 142.1, 140.7, 132.5, 132.0, 128.8, 126.3, 121.4 (aryl C), 83.0, 75.4 (cage C), 22.3, 15.1 ( $CH_3$ ).  $^{11}B\{^1H\}$  NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -3.3 (1B) (B-C), -5.3 (1B), -6.4 (1B), -8.3 (2B), -9.7 (2B), -10.4 (2B), -13.1 (1B). HRMS:  $m/z$  calcd for  $C_{14}H_{20}B_{10}BrN [M-H]^+$ : 390.1696. Found: 390.1691.



**3n**: Yield 58%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.02 (dd,  $J$  = 6.0, 9.2 Hz, 1H), 7.59 (dd,  $J$  = 2.4, 10.0 Hz, 1H), 7.45 (t,  $J$  = 9.2 Hz, 1H) (aryl CH), 2.61 (s, 3H) ( $\text{CH}_3$ ), 2.53 (m, 2H) ( $\text{CH}_2$ ), 2.42 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  161.1 (d,  $^1J_{\text{C-F}}$  = 247 Hz), 156.0, 142.8, 142.3 (d,  $^4J_{\text{C-F}}$  = 6 Hz), 140.5, 132.8 (d,  $^3J_{\text{C-F}}$  = 10 Hz), 128.6 (d,  $^3J_{\text{C-F}}$  = 10 Hz), 119.1 (d,  $^2J_{\text{C-F}}$  = 25 Hz), 107.5 (d,  $^2J_{\text{C-F}}$  = 22 Hz) (aryl C), 83.1, 75.4 (cage C), 22.3, 15.2 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.3 (1B) (B-C), -5.4 (1B), -6.5 (1B), -8.1 (2B), -9.8 (2B), -10.5 (1B), -11.3 (1B), -13.0 (1B).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ ):  $\delta$  -111.4 (m, 1F). HRMS:  $m/z$  calcd for  $\text{C}_{14}\text{H}_{20}\text{B}_{10}\text{FN} [\text{M}]^+$ : 329.2584. Found: 329.2585.



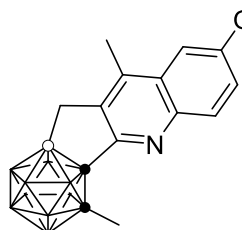
**3o**: Yield 42%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.37 (d,  $J$  = 1.6 Hz, 1H), 7.91 (dd,  $J$  = 1.6, 8.8 Hz, 1H), 7.74 (d,  $J$  = 8.8 Hz, 1H) (aryl CH), 2.61 (s, 3H) ( $\text{CH}_3$ ), 2.52 (m, 2H) ( $\text{CH}_2$ ), 2.41 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  157.1, 144.8, 141.8, 140.6, 137.9, 133.0, 131.9, 129.3, 93.2 (aryl C), 83.0, 75.4 (cage C), 22.3, 15.1 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.2 (1B) (B-C), -5.2 (1B), -6.4 (1B), -8.1 (2B), -9.7 (2B), -10.3 (2B), -13.0 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{14}\text{H}_{20}\text{B}_{10}\text{IN} [\text{M}]^+$ : 437.1638. Found: 437.1639.



**3p**: Yield 53%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.92 (d,  $J$  = 8.8 Hz, 1H), 7.76 (s, 1H), 7.51 (dd,  $J$  = 1.2, 8.8 Hz, 1H) (aryl CH), 2.63 (s, 3H), 2.57 (s, 3H) ( $\text{CH}_3$ ), 2.51 (m, 2H) ( $\text{CH}_2$ ), 2.43 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  155.7, 144.3, 142.2, 139.7, 137.2, 131.3, 130.0, 127.5, 122.8 (aryl C), 83.4, 75.3 (cage C), 22.3, 22.1, 15.0 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,

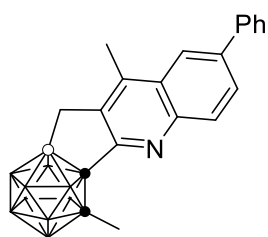
$\text{CDCl}_3$ ):  $\delta$  -3.1 (1B) (B-C), -5.6 (1B), -6.6 (1B), -8.1 (2B), -9.9 (2B), -10.5 (2B), -13.1 (1B).

HRMS:  $m/z$  calcd for  $\text{C}_{15}\text{H}_{23}\text{B}_{10}\text{N}$   $[\text{M}]^+$ : 325.2836. Found: 325.2837.



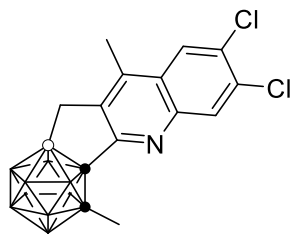
**3q**: Yield 32%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.92 (d,  $J = 9.2$  Hz, 1H), 7.34 (dd,  $J = 2.8, 9.2$  Hz, 1H), 7.19 (d,  $J = 1.2$  Hz, 1H) (aryl CH), 3.96 (s, 3H) ( $\text{OCH}_3$ ), 2.60 (s, 3H) ( $\text{CH}_3$ ), 2.51 (m,

2H) ( $\text{CH}_2$ ), 2.42 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  158.5, 154.2, 141.6, 141.4, 140.1, 131.8, 128.6, 121.2, 102.1 (aryl C), 83.5, 75.2 (cage C), 55.7 ( $\text{OCH}_3$ ), 22.3, 15.2 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.2 (1B) (B-C), -5.7 (1B), -6.6 (3B), -10.0 (4B), -13.0 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{15}\text{H}_{23}\text{B}_{10}\text{NO}$   $[\text{M}]^-$ : 341.2790. Found: 341.2796.



**3r**: Yield 56%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.16 (d,  $J = 1.6$  Hz, 1H), 8.10 (d,  $J = 8.8$  Hz, 1H), 7.94 (dd,  $J = 1.2, 8.8$  Hz, 1H), 7.72 (d,  $J = 7.6$  Hz, 2H), 7.52 (t,  $J = 7.6$  Hz, 2H), 7.43 (t,  $J = 7.2$  Hz,

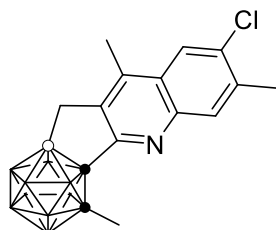
1H) (aryl CH), 2.71 (s, 3H) ( $\text{CH}_3$ ), 2.55 (m, 2H) ( $\text{CH}_2$ ), 2.45 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  156.5, 145.1, 143.0, 140.8, 140.2, 140.1, 130.8, 129.2, 128.9, 128.0, 127.7, 127.7, 121.7 (aryl C), 83.3, 75.4 (cage C), 22.3, 15.2 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.1 (1B) (B-C), -6.5 (4B), -9.8 (2B), -10.4 (2B), -12.9 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{20}\text{H}_{25}\text{B}_{10}\text{N}$   $[\text{M}]^-$ : 387.2998. Found: 387.3005.



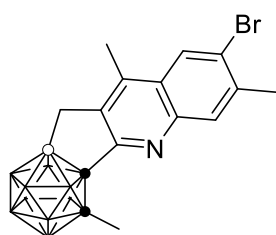
**3s**: Yield 63%. White solid.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.16 (s, 1H), 8.09 (s, 1H) (aryl CH), 2.62 (s, 3H) ( $\text{CH}_3$ ), 2.51 (m, 2H) ( $\text{CH}_2$ ), 2.40 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  158.0,

144.6, 142.2, 140.9, 133.6, 131.8, 131.2, 126.9, 124.8 (aryl C), 82.7, 75.5 (cage C), 22.3, 15.2

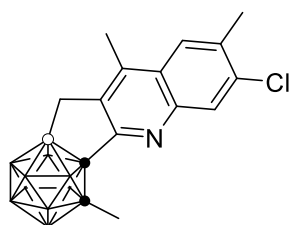
(CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -2.8 (1B) (B-C), -4.6 (1B), -5.9 (1B), -7.7 (2B), -9.9 (4B), -12.5 (1B). HRMS: *m/z* calcd for C<sub>14</sub>H<sub>19</sub>B<sub>10</sub>Cl<sub>2</sub>N [M]<sup>+</sup>: 379.1804. Found: 379.1811.



**3t:** Yield 70%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.98 (s, 1H), 7.89 (s, 1H) (aryl CH), 2.60 (s, 3H), 2.55 (s, 3H) (CH<sub>3</sub>), 2.50 (m, 2H) (CH<sub>2</sub>), 2.41 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 156.8, 144.5, 141.9, 139.8, 137.8, 134.5, 131.4, 126.8, 123.2 (aryl C), 83.1, 75.3 (cage C), 22.3, 20.6, 15.1 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -2.8 (1B) (B-C), -4.9 (1B), -6.0 (1B), -7.1 (2B), -9.9 (3B), -10.9 (1B), -12.5 (1B). HRMS: *m/z* calcd for C<sub>15</sub>H<sub>22</sub>B<sub>10</sub>ClN [M]<sup>+</sup>: 360.2420. Found: 360.2423.



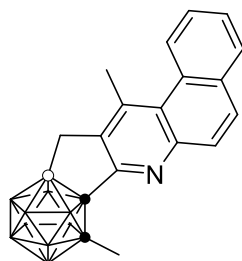
**3u:** Yield 66%. White solid. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 8.19 (s, 1H), 7.89 (s, 1H) (aryl CH), 2.60 (s, 3H), 2.58 (s, 3H) (CH<sub>3</sub>), 2.51 (m, 2H) (CH<sub>2</sub>), 2.41 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 157.0, 144.9, 141.8, 139.8, 139.2, 131.1, 127.1, 126.9, 125.1 (aryl C), 83.1, 75.3 (cage C), 22.3, 20.6, 15.1 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -2.6 (1B) (B-C), -4.8 (1B), -5.9 (1B), -7.6 (2B), -9.9 (4B), -12.5 (1B). HRMS: *m/z* calcd for C<sub>15</sub>H<sub>22</sub>B<sub>10</sub>BrN [M-H]<sup>+</sup>: 404.1849. Found: 404.1849.



**3v:** Yield 64%. White solid. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 8.05 (s, 1H), 7.82 (s, 1H) (aryl CH), 2.62 (s, 3H), 2.58 (s, 3H) (CH<sub>3</sub>), 2.50 (m, 2H) (CH<sub>2</sub>), 2.41 (s, 3H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 156.8, 145.0, 142.3, 140.0, 136.4, 135.7, 129.4, 126.3, 124.6 (aryl C), 83.1, 75.4 (cage C), 22.3, 21.0, 15.1 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -2.9 (1B) (B-C), -5.0

(1B), -6.2 (1B), -7.8 (2B), -10.1 (4B), -12.7 (1B). HRMS:  $m/z$  calcd for  $C_{15}H_{22}B_{10}ClN [M]^+$ :

360.2420. Found: 360.2420.



**3w**: Yield 50%. Colorless crystals.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  8.78

(d,  $J = 9.2$  Hz, 1H), 7.94 (m, 3H), 7.67 (m, 2H) (aryl CH), 3.06 (s, 3H)

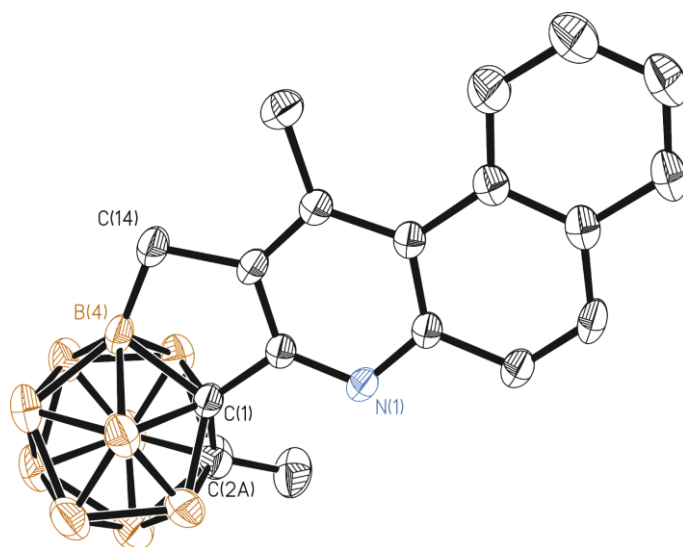
( $CH_3$ ), 2.61 (m, 2H) ( $CH_2$ ), 2.46 (s, 3H) ( $CH_3$ ).  $^{13}C\{^1H\}$  NMR (100

MHz,  $CDCl_3$ ):  $\delta$  154.8, 147.3, 144.2, 142.5, 133.5, 131.0, 130.5, 129.1,

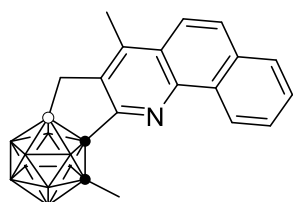
129.0, 128.1, 127.0, 126.3, 125.7 (aryl C), 83.5, 75.1 (cage C), 22.3, 22.0 ( $CH_3$ ).  $^{11}B\{^1H\}$

NMR (128 MHz,  $CDCl_3$ ):  $\delta$  -3.3 (1B) (B-C), -6.5 (4B), -10.3 (4B), -12.9 (1B). HRMS:  $m/z$

calcd for  $C_{18}H_{23}B_{10}N [M-H]^+$ : 360.2769. Found: 360.2770.



**Supplementary Figure 2.** Molecular structure of **3w** drawn with 30% probability ellipsoids.



**3x**: Yield 37%. White solid.  $^1H$  NMR (500 MHz,  $CDCl_3$ ):  $\delta$  9.17 (d,

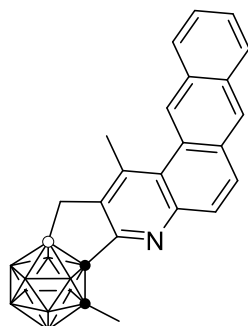
$J = 7.5$  Hz, 1H), 7.90 (m, 3H), 7.70 (m, 2H) (aryl CH), 2.72 (s, 3H)

( $CH_3$ ), 2.58 (m, 2H) ( $CH_2$ ), 2.55 (s, 3H) ( $CH_3$ ).  $^{13}C\{^1H\}$  NMR (125

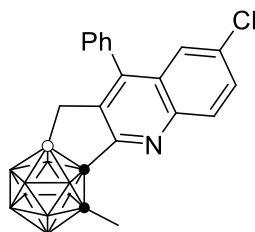
MHz,  $CDCl_3$ ):  $\delta$  154.8, 143.7, 143.3, 141.2, 133.3, 131.9, 128.3, 128.3, 127.9, 127.3, 125.3,

124.6, 121.3 (aryl C), 83.8, 74.8 (cage C), 22.4, 15.4 ( $CH_3$ ).  $^{11}B\{^1H\}$  NMR (160 MHz,

$\text{CDCl}_3$ ):  $\delta$  -2.6 (1B) (B-C), -5.1 (1B), -6.0 (3B), -9.9 (4B), -12.5 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{18}\text{H}_{23}\text{B}_{10}\text{N}$  [M]<sup>-</sup>: 361.2835. Found: 361.2850.



**3y**: Yield 29%. White solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  9.26 (s, 1H), 8.45 (s, 1H), 8.16 (m, 1H), 8.09 (m, 1H), 8.00 (d,  $J = 9.2$  Hz, 1H), 7.73 (d,  $J = 9.2$  Hz, 1H), 7.63 (t,  $J = 8.8$  Hz, 2H) (aryl CH), 3.16 (s, 3H) ( $\text{CH}_3$ ), 2.65 (m, 2H) ( $\text{CH}_2$ ), 2.47 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  154.6, 148.3, 145.0, 143.4, 132.0, 131.9, 131.8, 131.8, 129.2, 129.0, 128.8, 128.7, 127.8, 127.4, 127.2, 126.6, 126.3 (aryl C), 84.1, 75.6 (cage C), 22.4, 22.0 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  -3.1 (1B) (B-C), -6.6 (4B), -10.4 (4B), -13.0 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{22}\text{H}_{25}\text{B}_{10}\text{N}$  [M-H]<sup>-</sup>: 410.2921. Found: 410.2928.



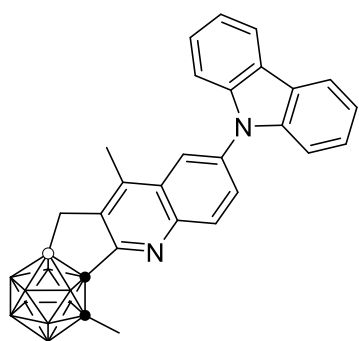
**3z**: Yield 38%. Colorless oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.03 (d,  $J = 8.8$  Hz, 1H), 7.60 (d,  $J = 8.8$  Hz, 1H), 7.54 (m, 4H), 7.30 (m, 2H), (aryl CH), 2.47 (s, 3H) ( $\text{CH}_3$ ), 2.34 (m, 2H) ( $\text{CH}_2$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  157.1, 146.8, 144.6, 140.5, 135.4, 133.4, 131.4, 130.3, 129.1, 129.1, 128.8, 128.9, 124.9 (aryl C), 82.8, 75.4 (cage C), 22.3 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.0 (1B) (B-C), -6.3 (4B), -9.5 (4B), -12.9 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{19}\text{H}_{22}\text{B}_{10}\text{ClN}$  [M+H]<sup>+</sup>: 408.2529. Found: 408.2520.

### Transformations of 3m.

**Reaction of 3m with Carbazole.** Compound **3m** (39.0 mg, 0.10 mmol), carbazole (20.0 mg, 0.12 mmol, 1.2 equiv),  $\text{Pd}_2(\text{dba})_3$  (4.6 mg, 0.005 mmol, 5 mol%), lithium tert-butoxide (36.0



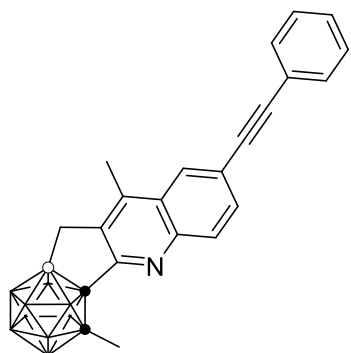
mg, 0.45 mmol, 4.5 equiv) and tri-tert-butylphosphine (1M in toluene, 8.0  $\mu$ L, 8 mol%) were mixed in *o*-xylene (2 mL). The resultant mixture was stirred at 140 °C for 24 h under argon, and then cooled down to room temperature. After filtration through a Celite pad, the filtrate was concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **4m** as a white solid (45.0 mg, 95%).



**4m.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.27 (d,  $J = 8.5$  Hz, 1H), 8.23 (s, 1H), 8.20 (d,  $J = 8.0$  Hz, 2H), 7.90 (d,  $J = 9.0$  Hz, 1H), 7.45 (m, 4H), 7.34 (t,  $J = 7.0$  Hz, 2H) (aryl CH), 2.66 (s, 3H) ( $\text{CH}_3$ ), 2.59 (m, 2H) ( $\text{CH}_2$ ), 2.49 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  157.1, 144.6, 142.8, 140.9, 140.7, 136.4, 132.3, 128.5, 128.4, 126.3, 123.7, 121.5, 120.7, 120.5, 109.6 (aryl C), 83.1, 75.4 (cage C), 22.3, 15.3 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (160 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.6 (1B) (B-C), -5.9 (4B), -9.8 (4B), -12.4 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{26}\text{H}_{28}\text{B}_{10}\text{N}_2$  [ $\text{M}-\text{H}$ ] $^-$ : 475.3179. Found: 475.3195.

**Reaction of 3m with Phenylacetylene.** Compound **3m** (39.0 mg, 0.10 mmol),  $\text{PdCl}_2(\text{PPh}_3)_2$  (3.5 mg, 0.005 mmol, 5 mol%),  $\text{CuI}$  (1.9 mg, 0.01 mmol, 10 mol%), phenylacetylene (13.2  $\mu$ L, 0.12 mmol, 1.2 equiv), and triethylamine (70.0  $\mu$ L, 0.50 mmol, 5.0 equiv) were dissolved in DMF (2 mL). The resultant mixture was stirred at 60 °C for 16 h under argon. The reaction was quenched with water, and extracted with diethyl ether (5 mL x 3). The organic portions were combined, washed with water (5 mL x 3), dried with  $\text{MgSO}_4$ , and concentrated to dryness in vacuo. Then, the obtained residue was subjected to flash column chromatography

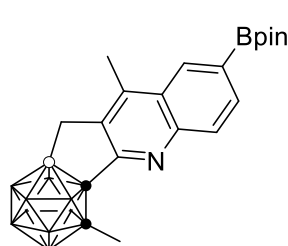
on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **5m** as a white solid (39.5 mg, 96%).



**5m.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.19 (d,  $J = 1.2$  Hz, 1H), 7.99 (d,  $J = 8.4$  Hz, 1H), 7.78 (dd,  $J = 1.6, 8.8$  Hz, 1H), 7.60 (m, 2H), 7.39 (m, 3H) (aryl CH), 2.67 (s, 3H) ( $\text{CH}_3$ ), 2.53 (m, 2H) ( $\text{CH}_2$ ), 2.44 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  157.1, 145.2, 142.7, 140.5, 131.9, 131.8, 130.5, 128.8, 128.6,

127.4, 127.3, 123.0, 122.2 (aryl C), 91.0, 89.4 (alkynyl C), 83.1, 75.4 (cage C), 22.3, 15.1 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (160 MHz,  $\text{CDCl}_3$ ):  $\delta$  -2.6 (1B) (B-C), -4.7 (1B), -5.9 (3B), -9.2 (2B), -9.9 (2B), -12.5 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{22}\text{H}_{25}\text{B}_{10}\text{N}$  [ $\text{M}-\text{H}$ ] $^-$ : 410.2927. Found: 410.2928.

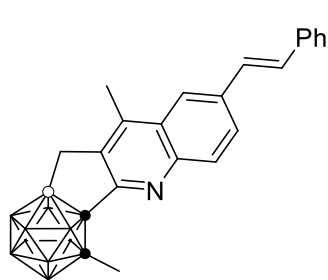
**Reaction of 3m with  $\text{B}_2\text{pin}_2$ .** Compound **3m** (39.0 mg, 0.10 mmol), bis(pinacolato)diboron (28.0 mg, 0.11 mmol, 1.1 equiv),  $\text{Pd}(\text{dppf})\text{Cl}_2$  (dppf = 1,1'-bis(diphenylphosphino)ferrocene) (7.3 mg, 0.01 mmol, 10 mol%), and potassium acetate (29.4 mg, 0.30 mmol, 3.0 equiv) were mixed in toluene (2 mL). The resultant mixture was stirred at 90 °C under Ar for 18 h. The reaction mixture was allowed to cool to room temperature before filtered through a pad of Celite and washed with diethyl ether. The filtrate was concentrated to dryness in vacuo and subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (10 : 1 in V/V) as eluent to give the product **6m** as a white solid (39.0 mg, 89%).



**6m.**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.50 (s, 1H), 8.04 (d,  $J = 8.5$  Hz, 1H), 7.99 (d,  $J = 8.5$  Hz, 1H) (aryl CH), 2.71 (s, 3H) ( $\text{CH}_3$ ), 2.52 (m, 2H) ( $\text{CH}_2$ ), 2.44 (s, 3H) ( $\text{CH}_3$ ), 1.40 (s, 12H) (pinacolato  $\text{CH}_3$ ).

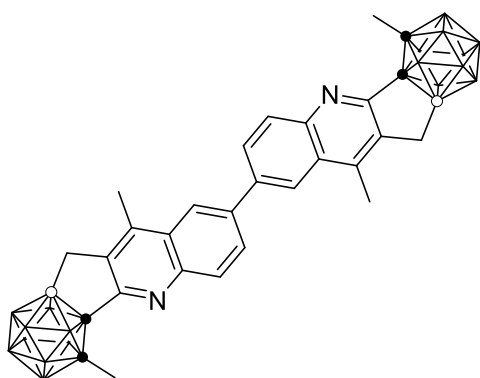
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  157.4, 147.4, 143.8, 139.8, 134.0, 131.8, 129.4, 126.8 (aryl C), 84.4 (pinacolato C), 83.3, 75.4 (cage C), 25.1 (pinacolato  $\text{CH}_3$ ), 22.3, 15.2 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (160 MHz,  $\text{CDCl}_3$ ):  $\delta$  -31.6 (1B) (Bpin), -2.7 (1B) (B-C), -4.9 (1B), -6.0 (3B), -10.0 (4B), -12.6 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{20}\text{H}_{32}\text{B}_{11}\text{NO}_2$   $[\text{M}+\text{H}]^+$ : 438.3608. Found: 438.3613.

**Reaction of 3m with Styrene.** Compound **3m** (39.0 mg, 0.10 mmol), styrene (12.5 mg, 0.12 mmol, 1.2 equiv),  $\text{PdCl}_2(\text{PPh}_3)_2$  (7.0 mg, 0.01 mmol, 10 mol%), and potassium carbonate (55.0 mg, 0.40 mmol, 4.0 equiv) were mixed in toluene (2 mL). The resultant mixture was stirred at 130 °C under Ar for 12 h. The reaction mixture was allowed to cool to room temperature and filtered through a pad of Celite. The filtrate was then concentrated in vacuo, and purified by column chromatography on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **7m** as a white solid (29.0 mg, 70%).



**7m.**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.98 (m, 3H), 7.58 (d,  $J = 7.6$  Hz, 2H), 7.40 (t,  $J = 7.6$  Hz, 2H), 7.30 (m, 3H) (aryl CH and alkenyl CH), 2.68 (s, 3H) ( $\text{CH}_3$ ), 2.53 (m, 2H) ( $\text{CH}_2$ ), 2.44 (s, 3H) ( $\text{CH}_3$ ).  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  156.2, 145.6, 142.7, 140.3, 137.1, 136.2, 130.7, 130.5, 129.0, 128.3, 128.2, 127.8, 126.8, 126.6, 122.3 (aryl C and alkenyl C), 83.4, 75.3 (cage C), 22.3, 15.1 ( $\text{CH}_3$ ).  $^{11}\text{B}\{^1\text{H}\}$  NMR (128 MHz,  $\text{CDCl}_3$ ):  $\delta$  -3.1 (1B) (B-C), -6.5 (4B), -10.4 (4B), -13.0 (1B). HRMS:  $m/z$  calcd for  $\text{C}_{22}\text{H}_{27}\text{B}_{10}\text{N}$   $[\text{M}-\text{H}]^-$ : 412.3083. Found: 412.3085.

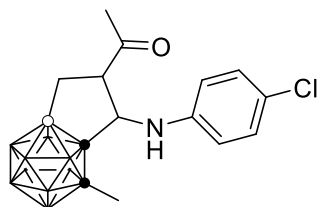
**Homo-coupling Reaction of 3m.** A solution of NiCl<sub>2</sub> (13.0 mg, 0.10 mmol, 1.0 equiv) and PPh<sub>3</sub> (105.0 mg, 0.40 mmol, 4.0 equiv) in DMF (3 mL) was stirred at 50 °C under Ar for 0.5 h. The resulting blue suspension was treated with Zn dust (6.5 mg, 0.10 mmol, 1.0 equiv) to produce a red-brown suspension, which was stirred for another 0.5 h. To which was added a solution of **3a** (39.0 mg, 0.10 mmol) in DMF (2 mL), and the resulting mixture was stirred at 50 °C under Ar overnight. The reaction was quenched by aqueous ammonia solution (2 M, 5 mL) and extracted with diethyl ether (5 mL x 3). The organic portions were combined, washed with water (5 mL x 3), dried with MgSO<sub>4</sub> and evaporated to dryness. The residue was purified by column chromatography on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **8m** as a white solid (25.5 mg, 83%).



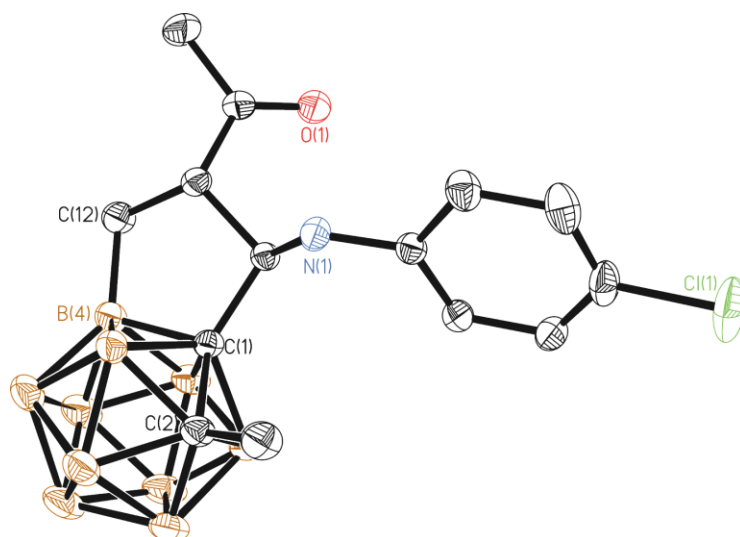
**8m.** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 8.26 (s, 2H), 8.16 (d, *J* = 8.5 Hz, 2H), 8.05 (d, *J* = 8.5 Hz, 2H) (aryl CH), 2.75 (s, 6H) (CH<sub>3</sub>), 2.57 (m, 4H) (CH<sub>2</sub>), 2.46 (s, 6H) (CH<sub>3</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>): δ 156.9, 145.3, 143.1, 140.5, 139.6, 131.1, 128.9, 127.8, 122.3 (aryl C), 83.2, 75.4 (cage C), 22.3, 15.2 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>): δ -2.7 (2B) (*B-C*), -5.9 (8B), -9.9 (8B), -12.2 (2B). HRMS: *m/z* calcd for C<sub>28</sub>H<sub>40</sub>B<sub>20</sub>N<sub>2</sub> [M-H]<sup>-</sup>: 619.5142. Found: 619.5142.

## Supplementary Discussion

**Control Experiments. Isolation of the Reaction Intermediate D.** Carboranyl *N*-4-chlorophenylimine **1a** (29.5 mg, 0.10 mmol), 2-butenone (42.0  $\mu$ L, 0.50 mmol, 5.0 equiv), [Cp\**RhCl*<sub>2</sub>]<sub>2</sub> (3.1 mg, 0.005 mmol, 5 mol%), AgSbF<sub>6</sub> (34.4 mg, 0.10 mmol, 1.0 equiv) and Cu(OPiv)<sub>2</sub> (66.0 mg, 0.25 mmol, 2.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 °C for 30 min under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite and washed with dichloromethane. The obtained filtrate was concentrated to dryness in vacuo and subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ether acetate (100 : 1 to 5 : 1 in V/V) as eluent to give intermediate **D** (10.5 mg, 28%) and **3a** (5.2 mg, 15%).



**D.** Colorless crystals. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.14 (d, *J* = 8.5 Hz, 2H), 6.58 (d, *J* = 8.0 Hz, 2H) (aryl CH), 5.21 (t, *J* = 9.0 Hz, 1H) (CH), 3.48 (d, *J* = 8.5 Hz, 1H) (NH), 3.23 (m, 1H) (CH), 2.19 (s, 3H), 1.95 (s, 3H) (CH<sub>3</sub>), 1.73 (dd, *J* = 10.0, 14.0 Hz, 1H), 1.23 (t, *J* = 13.5 Hz, 1H) (CH<sub>2</sub>). <sup>13</sup>C{<sup>1</sup>H} NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  205.5 (carbonyl C), 143.9, 129.8, 124.0, 114.0 (aryl C), 82.8, 77.8 (cage C), 67.4, 61.0 (CH), 28.6, 23.5 (CH<sub>3</sub>). <sup>11</sup>B{<sup>1</sup>H} NMR (160 MHz, CDCl<sub>3</sub>):  $\delta$  -1.2 (1B) (B-C), -5.3 (2B), -7.5 (2B), -11.5 (3B), -12.5 (1B), -13.5 (1B). HRMS: *m/z* calcd for C<sub>14</sub>H<sub>24</sub>B<sub>10</sub>ClNO [M+H]<sup>+</sup>: 366.2626. Found: 366.2633.



**Supplementary Figure 3.** Molecular structure of **D** drawn with 30% probability ellipsoids.

**Further Transformation of Intermediate D.** Compound **D** (36.5 mg, 0.10 mmol),  $[\text{Cp}^*\text{RhCl}_2]_2$  (3.1 mg, 0.005 mmol, 5 mol%),  $\text{AgSbF}_6$  (34.4 mg, 0.10 mmol, 1.0 equiv),  $\text{Cu}(\text{OPiv})_2$  (66.0 mg, 0.25 mmol, 2.5 equiv) and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 °C for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was concentrated to dryness in vacuo and analyzed by  $^1\text{H}$  NMR spectroscopy. Product **3a** was detected in 95% yield using dibromomethane as an internal standard.

Compound **D** (36.5 mg, 0.10 mmol),  $\text{AgSbF}_6$  (34.4 mg, 0.10 mmol, 1.0 equiv),  $\text{Cu}(\text{OPiv})_2$  (66.0 mg, 0.25 mmol, 2.5 equiv) and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 °C for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was diluted

with ethyl acetate and subjected to GC-MS analysis. Only trace amount of product **3a** was detected.

Compound **D** (36.5 mg, 0.10 mmol), [Cp\* $\text{RhCl}_2$ ]<sub>2</sub> (3.1 mg, 0.005 mmol, 5 mol%), Cu(OPiv)<sub>2</sub> (66.0 mg, 0.25 mmol, 2.5 equiv) and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 °C for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was diluted with ethyl acetate and subjected to GC-MS analysis. Only trace amount of product **3a** was detected.

Compound **D** (36.5 mg, 0.10 mmol), [Cp\* $\text{RhCl}_2$ ]<sub>2</sub> (3.1 mg, 0.005 mmol, 5 mol%), AgSbF<sub>6</sub> (34.4 mg, 0.10 mmol, 1.0 equiv), and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 °C for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was concentrated to dryness in vacuo and analyzed by <sup>1</sup>H NMR spectroscopy. Product **3a** was detected in 43% yield using dibromomethane as an internal standard.

Compound **D** (36.5 mg, 0.10 mmol), [Cp\* $\text{RhCl}_2$ ]<sub>2</sub> (3.1 mg, 0.005 mmol, 5 mol%), AgSbF<sub>6</sub> (68.8 mg, 0.20 mmol, 2.0 equiv), and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 °C for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was

concentrated to dryness in vacuo and analyzed by  $^1\text{H}$  NMR spectroscopy. Product **3a** was detected in 84% yield using dibromomethane as an internal standard.

**Kinetic Isotope Experiment.** Compounds **1l** (26.1 mg, 0.10 mmol, 1.0 equiv), **1l-d<sub>5</sub>** (26.6 mg, 0.10 mmol, 1.0 equiv), 2-butenone (42.0  $\mu\text{L}$ , 0.50 mmol, 5.0 equiv),  $[\text{Cp}^*\text{RhCl}_2]_2$  (3.1 mg, 0.005 mmol, 5 mol%),  $\text{AgSbF}_6$  (17.2 mg, 0.05 mmol, 0.5 equiv),  $\text{Cu}(\text{OPiv})_2$  (66.0 mg, 0.25 mmol, 2.5 equiv) and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 °C for 1 h under argon. After cooling to room temperature and the addition of pyridine (0.1 mL), the reaction mixture was filtered through a pad of Celite and washed with dichloromethane. The filtrate was concentrated to dryness in vacuo and subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give **3l** / **3l-d<sub>4</sub>** as a white solid (6.0 mg, 19%). The KIE value  $k_{\text{H}}/k_{\text{D}} = 1.7$  was measured according to  $^1\text{H}$  NMR spectroscopy.

**Radical Scavenger Experiment.** Compounds **1a** (29.5 mg, 0.10 mmol), 2-butenone (42.0  $\mu\text{L}$ , 0.50 mmol, 5.0 equiv),  $[\text{Cp}^*\text{RhCl}_2]_2$  (3.1 mg, 0.005 mmol, 5 mol%),  $\text{AgSbF}_6$  (34.4 mg, 0.10 mmol, 1.0 equiv),  $\text{Cu}(\text{OPiv})_2$  (66.0 mg, 0.25 mmol, 2.5 equiv), 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) and 1,1-diphenylethene (18.0 mg, 0.10 mmol, 1.0 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 °C for 6 h under argon. After cooling to room temperature and the addition of pyridine (0.1 mL), the reaction mixture was filtered through a pad of Celite and washed with dichloromethane. The filtrate



was concentrated to dryness in vacuo and analyzed by  $^1\text{H}$  NMR spectroscopy. Product **3a** was detected in 73% yield using dibromomethane as an internal standard.

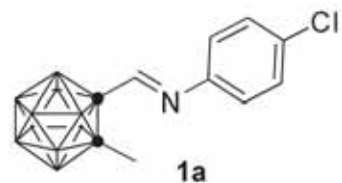
**X-ray Structure Determination.** X-ray data of **3l**, **3w**, and **D** were collected at 293 K on a Bruker SMART 1000 CCD diffractometer using Cu-K $\alpha$  radiation. An empirical absorption correction was applied using the SADABS program.<sup>4</sup> All structures were solved by direct methods 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>5</sup> All hydrogen atoms were geometrically fixed using the riding model.

CCDC 1823584-1823586 (**3l**, **3w**, and **D**) 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).

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7.804  
7.377  
7.355  
7.260  
7.075  
7.053



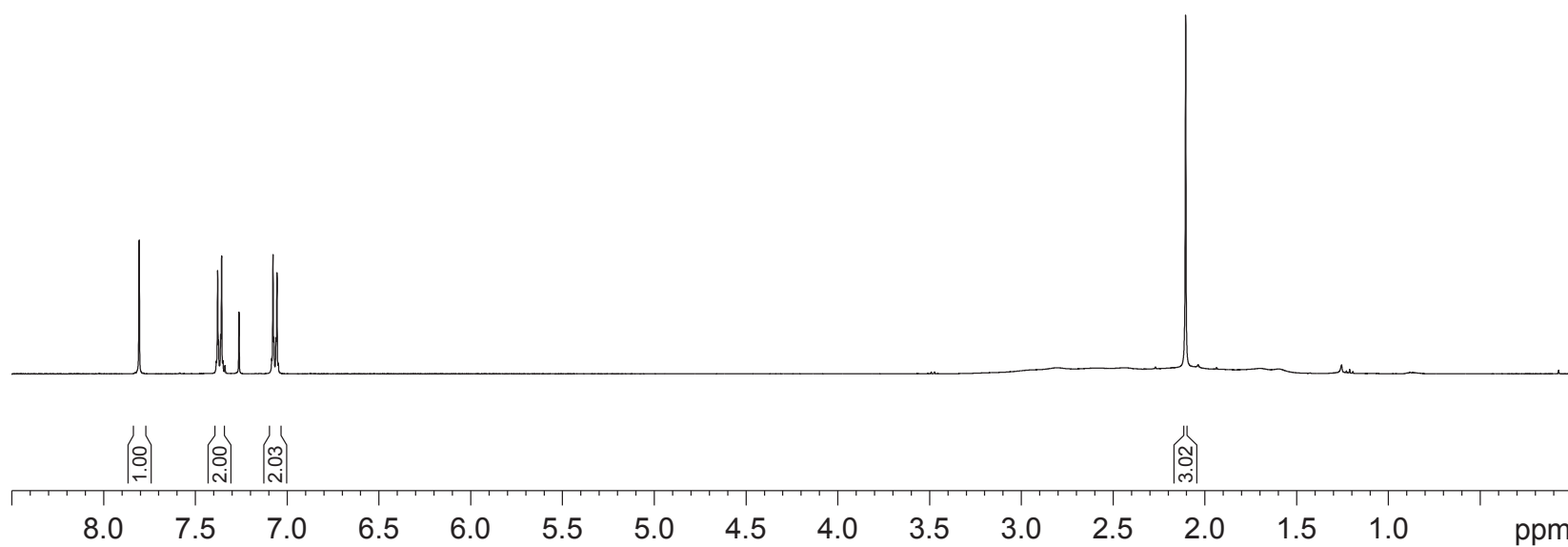
2.103

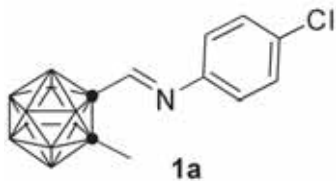
1hr-H-cassm-0409-CDCl3

Current Data Parameters  
NAME 1hr-H-cassm-0409-CDI  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160622  
Time 20.20 h  
INSTRUM spect  
PROBHD Z108618\_0257 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 128  
DW 62.400 usec  
DE 6.50 usec  
TE 294.4 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

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





— 152.348  
 — 147.035  
 — 134.023  
 — 129.709  
 — 122.324

77.477  
 77.160  
 76.842  
 75.292

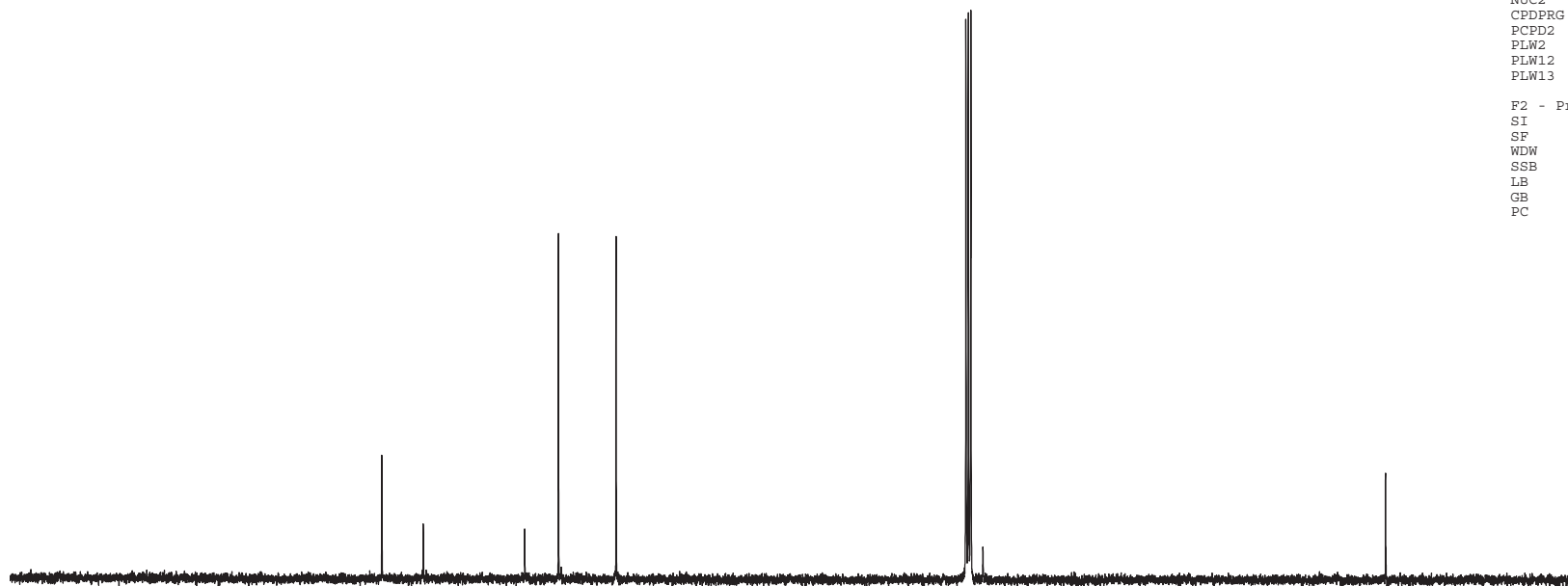
— 23.690

lhr-C-cassmCl-409-CDCl3

Current Data Parameters  
 NAME lhr-C-cassmCl-409-CDCl3  
 EXPNO 1  
 PROCNO 1

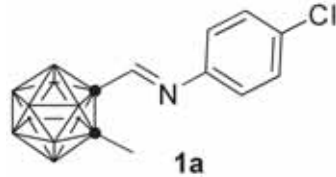
F2 - Acquisition Parameters  
 Date\_ 20160628  
 Time 9.30 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 3409  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 41.25000000 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 8.31000042 W  
 PLW12 0.23083000 W  
 PLW13 0.11611000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127559 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



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

1hr-B-cassm-0409-CDCl3

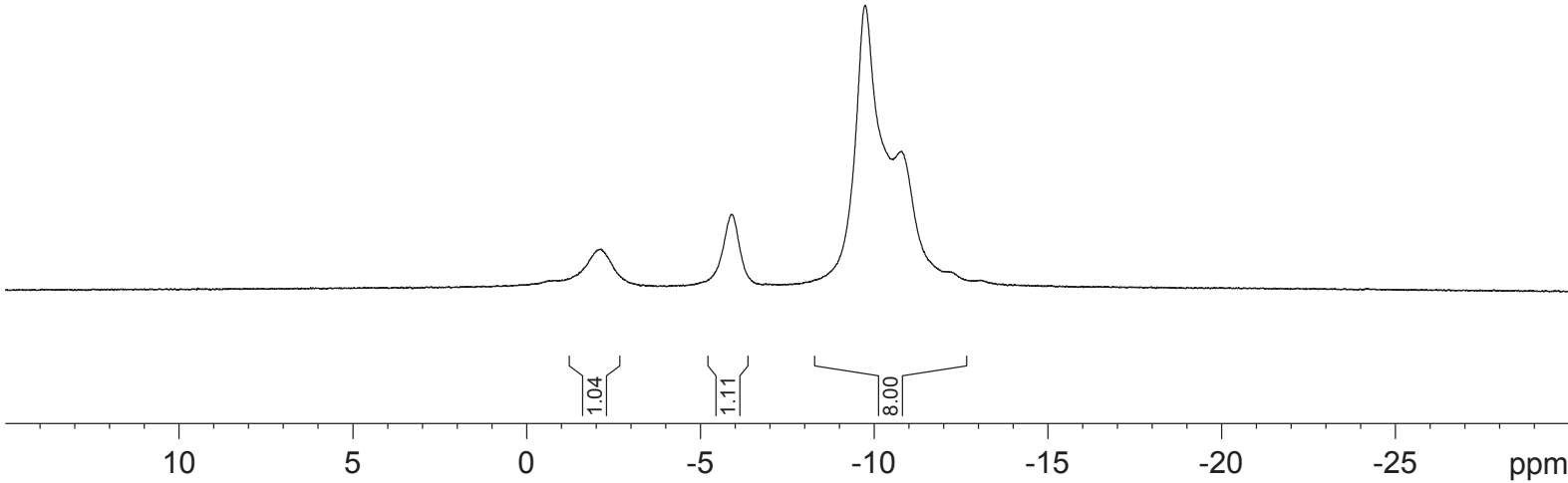


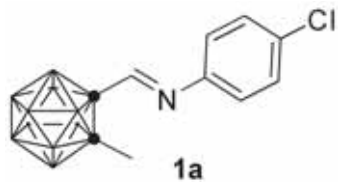
— -2.16  
— -5.89  
— -9.74  
— -10.79

Current Data Parameters  
NAME 1hr-B-cassm-0409-CDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160622  
Time\_ 20.14 h  
INSTRUM spect  
PROBHD Z108618\_0257 (   
PULPROG zgdc  
TD 65536  
SOLVENT CD2Cl2  
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 295.3 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 128.4096890 MHz  
NUC1 1H  
P1 7.50 usec  
PLW1 55.09999847 W  
SFO2 400.2316009 MHz  
NUC2 1H  
PCPD2 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





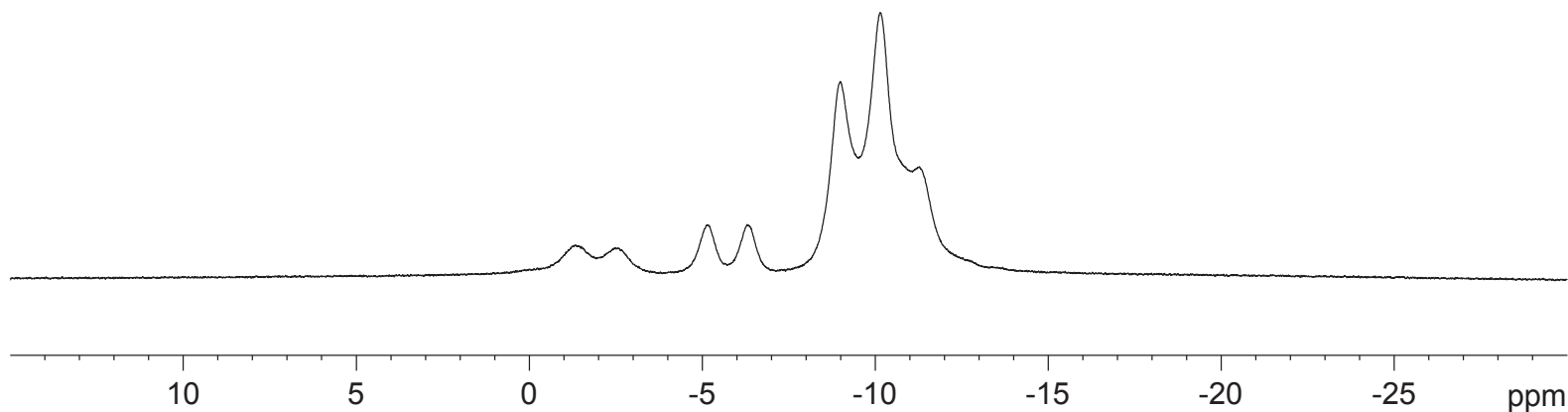
— -1.35  
 — -2.49  
 — -5.15  
 — -6.30  
 — -8.99  
 — -10.14  
 — -11.27

lhr-B-cassm-0409-CDCl3 (C)

Current Data Parameters  
 NAME lhr-B-cassm-0409-CDCl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160622  
 Time\_ 20.15 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zgpg  
 TD 65536  
 SOLVENT CDCl2  
 NS 12  
 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 294.9 K  
 D1 2.0000000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 13B  
 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

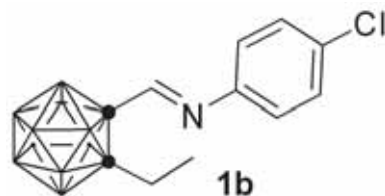


7.776  
7.375  
7.353  
7.260  
7.068  
7.046

2.388  
2.369  
2.351  
2.332

1.165  
1.146  
1.127

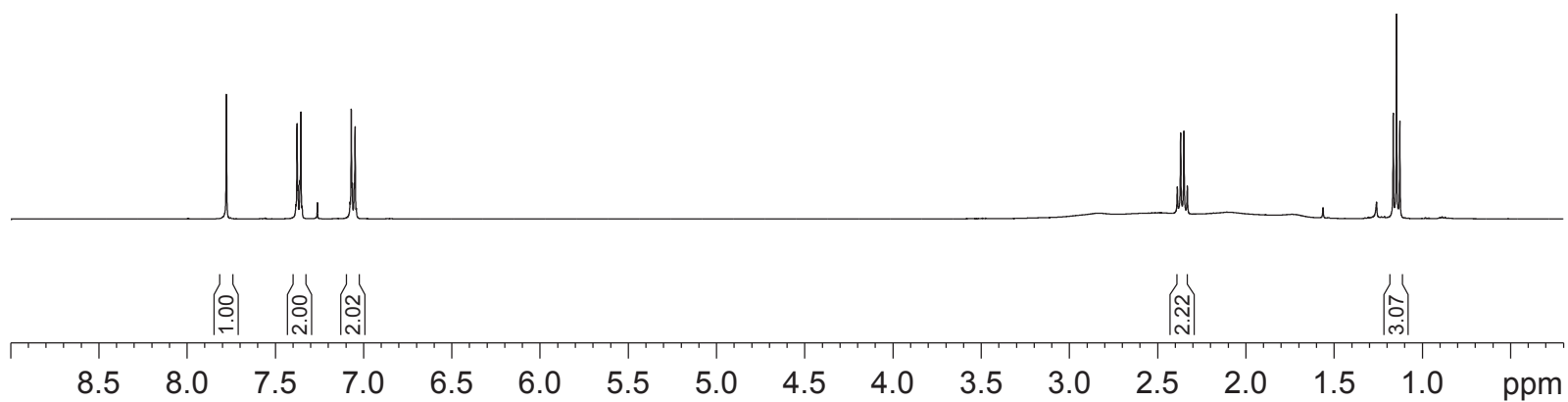
1hr-H-cassm716-CDCl3

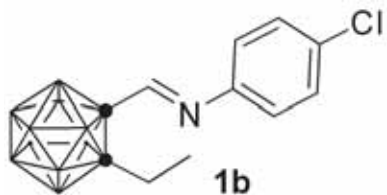


Current Data Parameters  
NAME 1hr-H-cassm716-CDCl3et  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170814  
Time 10.36 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 40.3  
DW 62.400 usec  
DE 6.50 usec  
TE 294.7 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

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





152.20  
147.04  
134.00  
129.70  
122.31

83.09

83.09  
77.48  
77.16  
76.84  
76.62  
77.48  
77.16  
76.84  
76.62

29.19

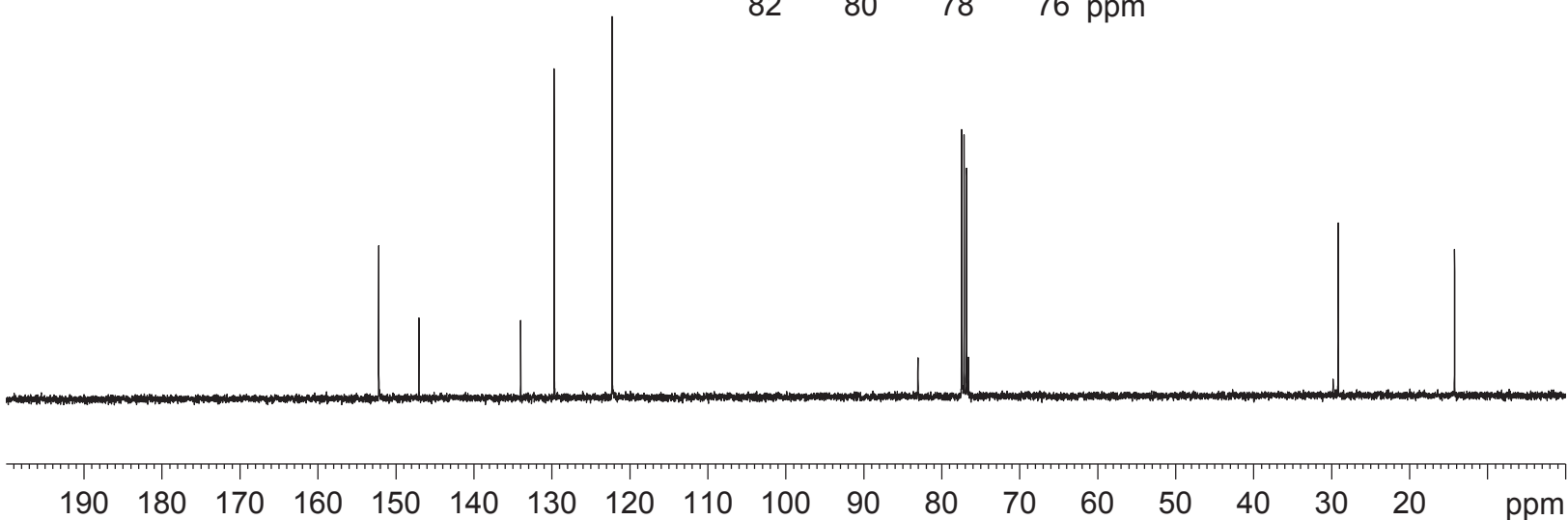
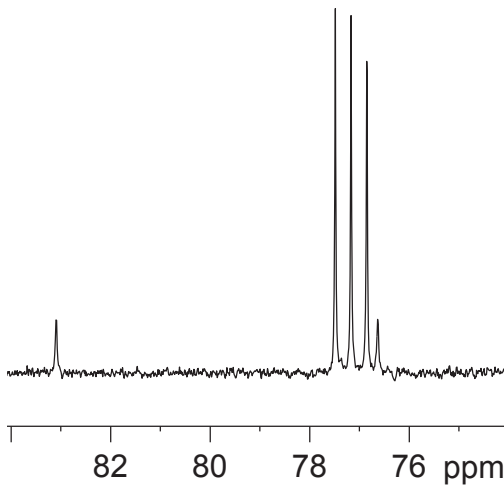
14.26

1hr-C-cassm716-CDC'

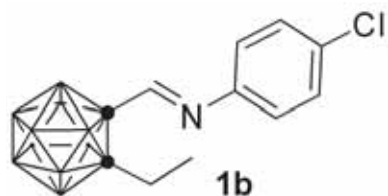
Current Data Parameters  
NAME 1hr-C-cassm716-CDC13et  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170814  
Time 10.39 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgpgg30  
TD 65536  
SOLVENT CDCl3  
NS 80  
DS 4  
SWH 40760.871 Hz  
FIDRES 0.621962 Hz  
AQ 0.8039083 sec  
RG 161  
DW 12.267 usec  
DE 6.50 usec  
TE 295.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6479773 MHz  
NUC1 13C  
P1 9.50 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 100.6379029 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



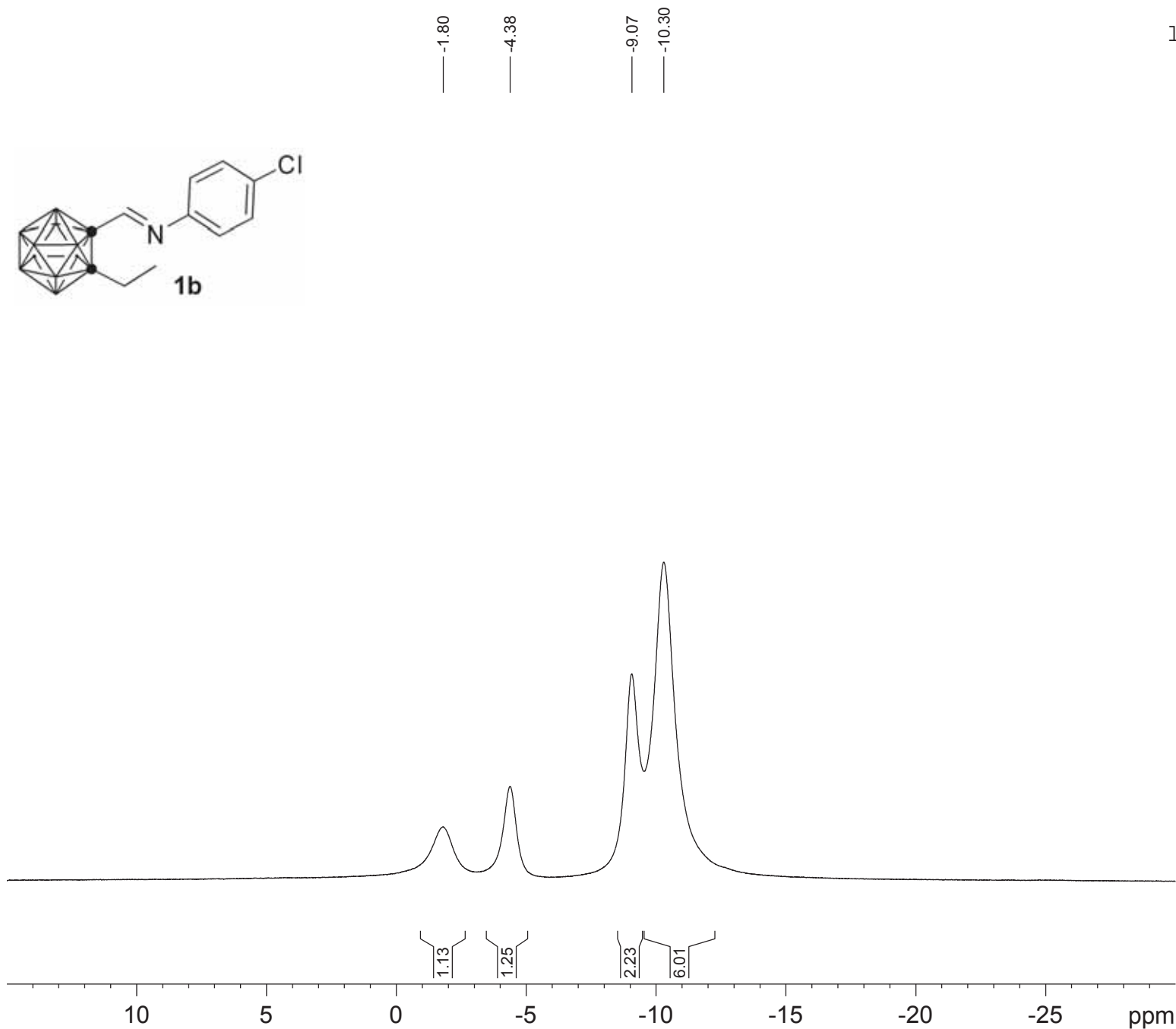
1hr-B-cassm716-CDCl3et



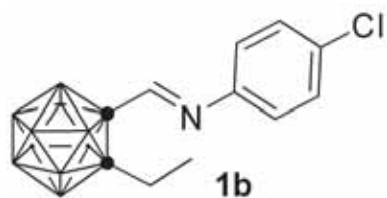
Current Data Parameters  
NAME 1hr-B-cassm716-CDCl3et  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170814  
Time 10.29 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT C6D6  
NS 15  
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 2.0000000 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







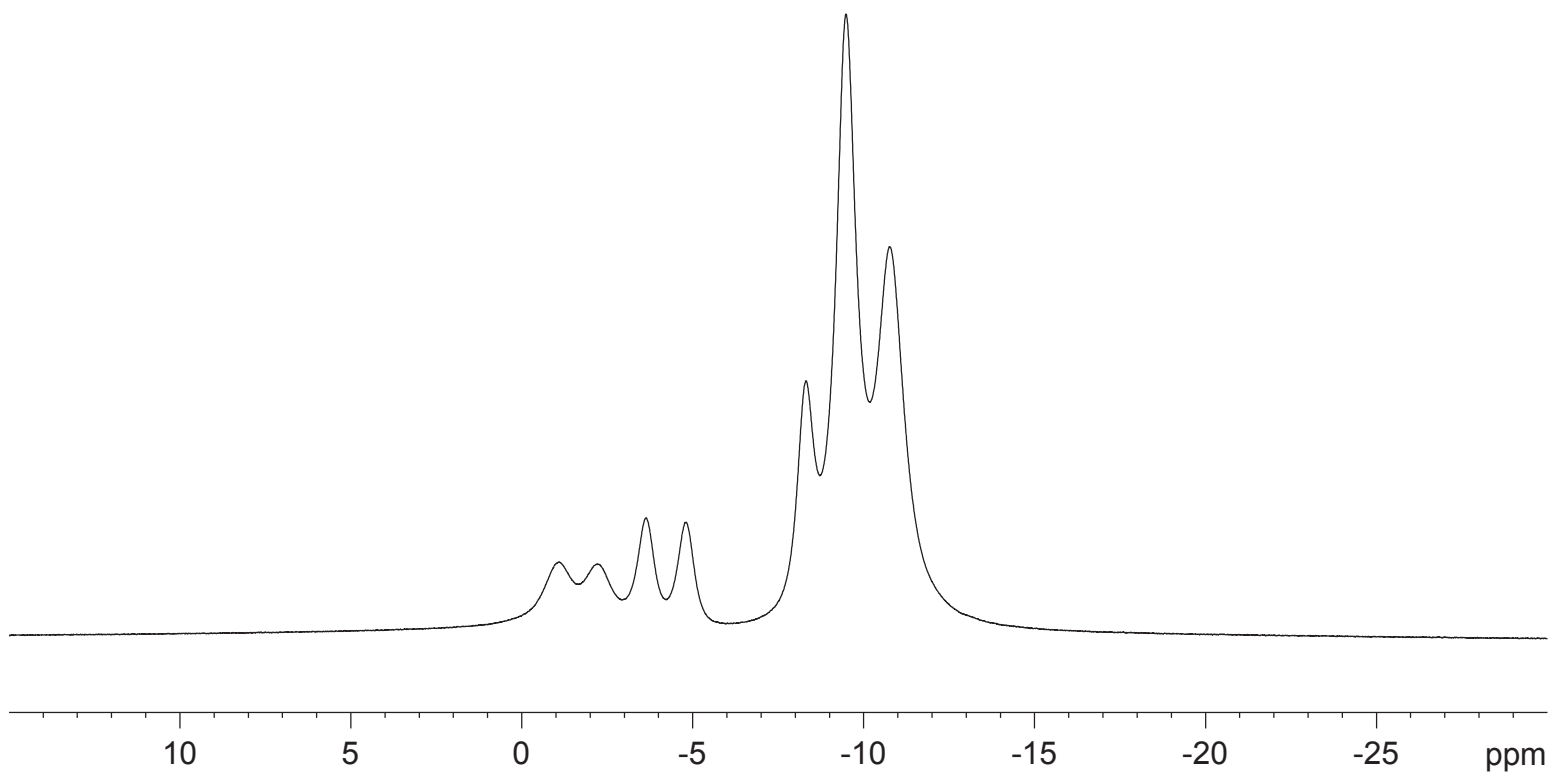
| -1.08  
 | -2.23  
 | -3.63  
 | -4.80  
  
 | -8.32  
 | -9.49  
 | -10.76

1hr-B-cassm716-CDCl3et (C)

Current Data Parameters  
 NAME 1hr-B-cassm716-CDCl3et (C)  
 EXPNO 1  
 PROCNO 1

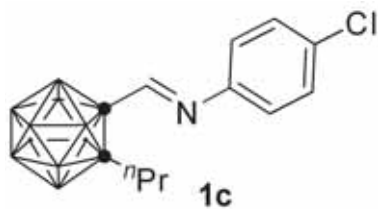
F2 - Acquisition Parameters  
 Date\_ 20170814  
 Time 10.31 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zg  
 TD 65536  
 SOLVENT C6D6  
 NS 28  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.9 K  
 D1 2.00000000 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



7.780  
7.379  
7.362  
7.260  
7.063  
7.046

2.272  
2.264  
2.261  
2.255  
2.249  
2.245  
2.238  
1.614  
1.599  
1.591  
1.584  
1.577  
1.573  
1.565  
1.558  
1.550  
1.536  
0.914  
0.899  
0.885

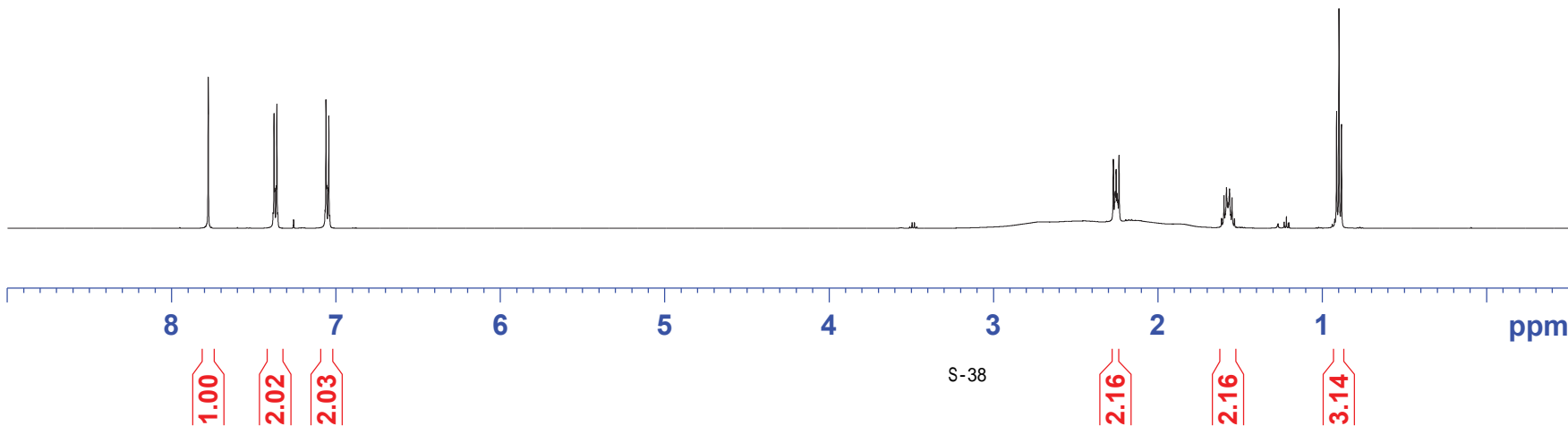


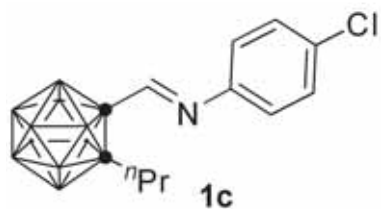
l hr-H-cassm-728NPR

Current Data Parameters  
NAME l hr-H-cassm-728  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170814  
Time 19.04  
INSTRUM spect  
PROBHD Z149001\_0010 (C  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 14.97  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300127  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00





— 152.21  
— 147.07

— 133.96  
— 129.71  
— 122.25

82.24  
77.41  
77.16  
76.91  
76.49

— 37.54

— 23.32

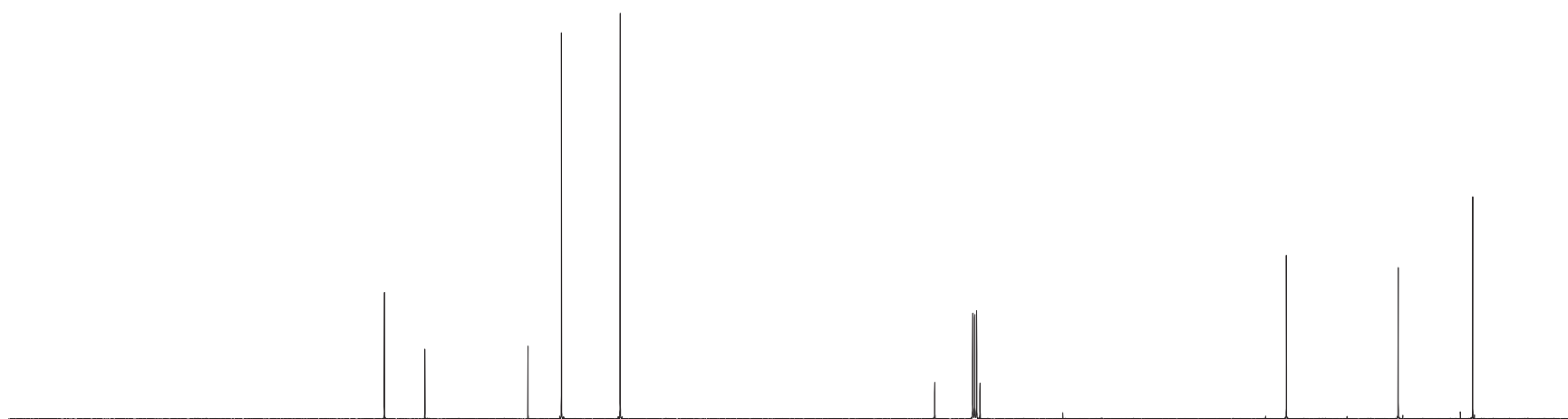
— 13.85

1 hr-C-cassm-728NPR

Current Data Parameters  
NAME 1 hr-C-cassm-728NPR  
EXPNO 1  
PROCNO 1

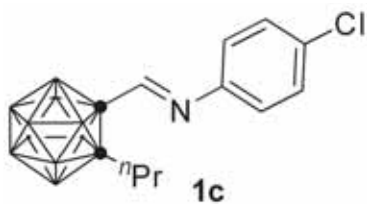
F2 - Acquisition Parameters  
Date\_ 20170814  
Time 19.10 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 60  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters  
SI 32768  
SF 125.7577789 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

I hr-B-cassm-728NPR

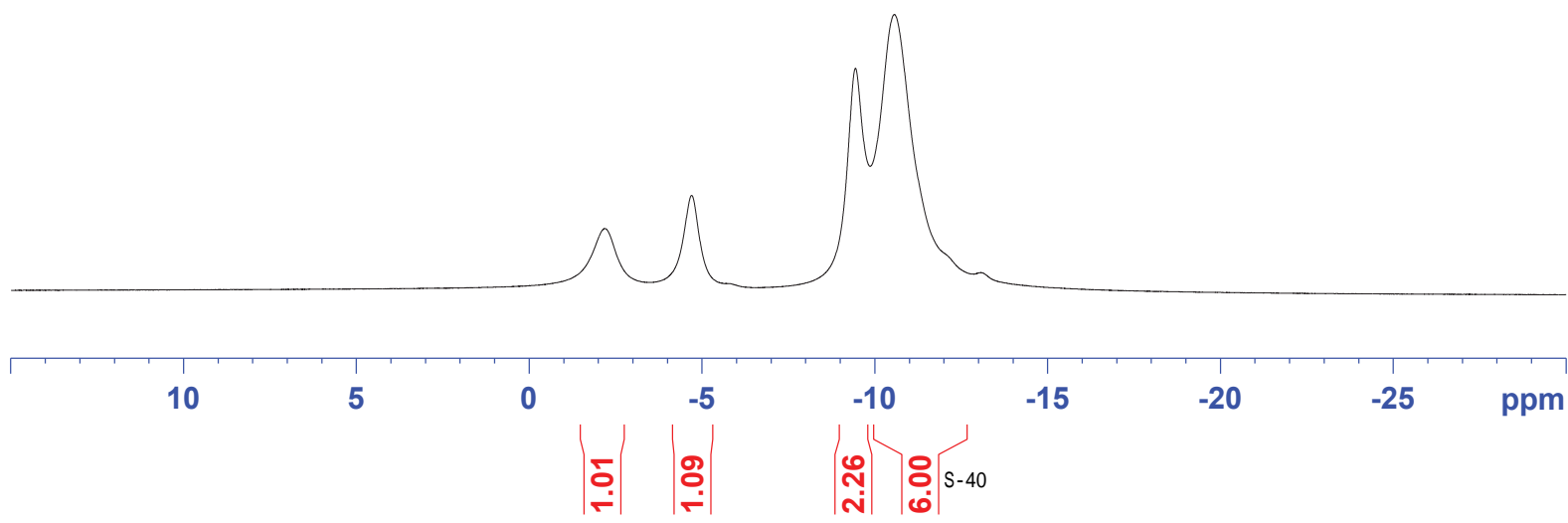


Chemical shift markers (ppm):  
-2.18  
-4.69  
-9.43  
-10.56

Current Data Parameters  
NAME I hr-B-cassm-728NPR  
EXPNO 2  
PROCNO 1

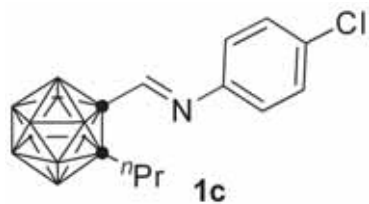
F2 - Acquisition Parameters  
Date\_ 20170814  
Time 19.13 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 12  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 50.6  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.00000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.00000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



I hr-B-cassm-728NPR(c)

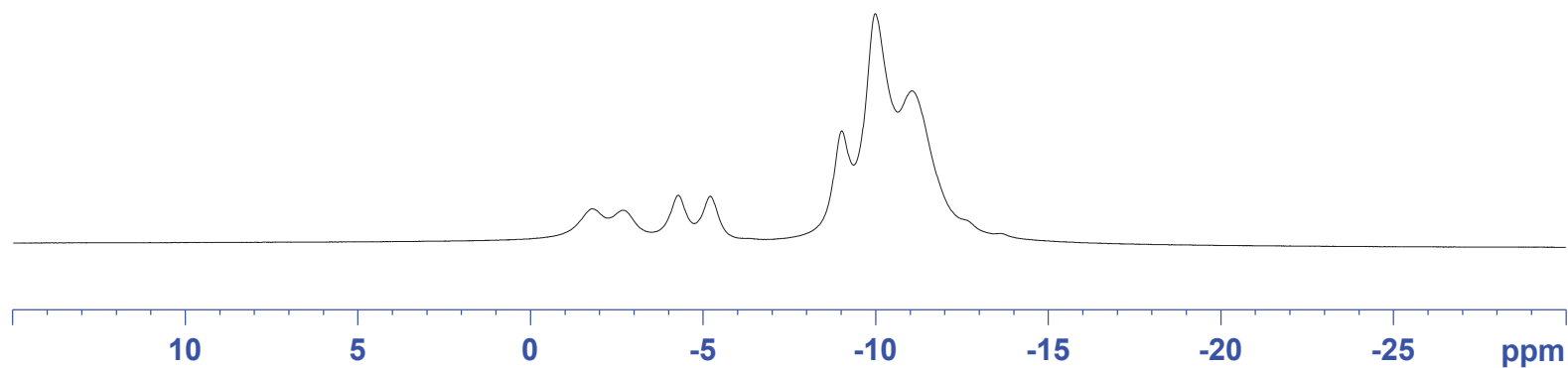
-1.78  
-2.68  
-4.28  
-5.20  
-9.01  
-9.99  
-11.05



Current Data Parameters  
NAME I hr-B-cassm-728NPR(c)  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170814  
Time 19.14 h  
INSTRUM spect  
PROBHD Z149001\_0010 (zg)  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 12  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 56.83  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

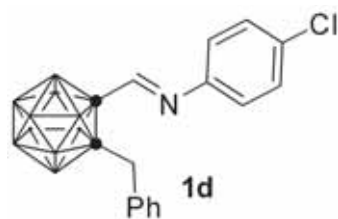
F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1 hr-H-cassm718-bn

7.870  
7.427  
7.410  
7.329  
7.322  
7.317  
7.260  
7.171  
7.154  
7.142  
7.137

3.629



Current Data Parameters  
NAME 1 hr-H-cassm718-bn  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170816  
Time 9.49 h  
INSTRUM spect  
PROBHD Z149001\_0010 (CP  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.2767999 sec  
RG 17.56  
DW 50.000 usec  
DE 10.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 500.1330883 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 15.0000000 W

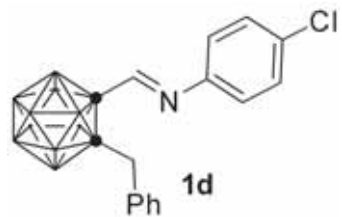
F2 - Processing parameters  
SI 65536  
SF 500.1300127 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



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

1.00  
2.04  
3.00  
4.09

2.08 S-42



152.42  
146.81  
135.27  
134.27  
130.42  
129.80  
128.68  
128.21  
122.52

82.18  
77.41  
77.16  
76.91  
76.80

41.03

1 hr-C-cassm718-bn

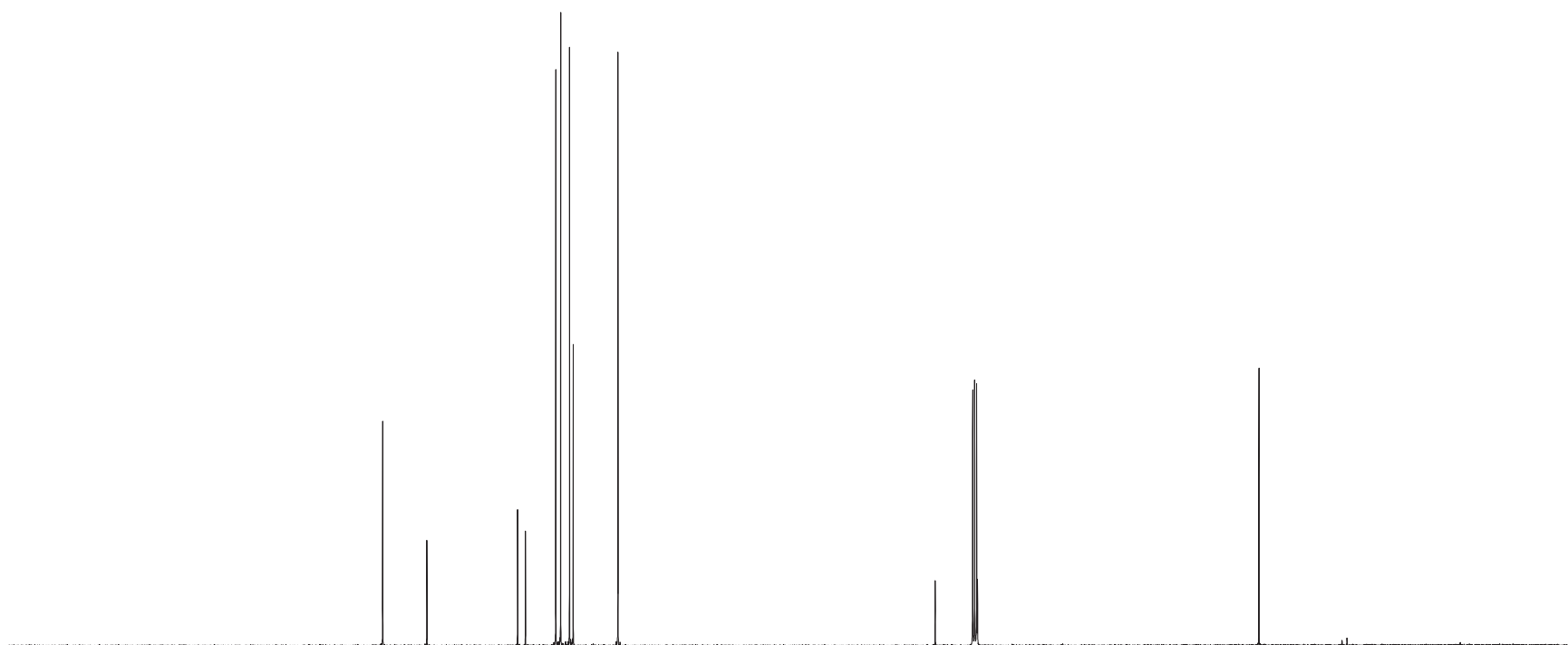
Current Data Parameters  
NAME 1 hr-C-cassm718-bn  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170816  
Time 9.57 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 120  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

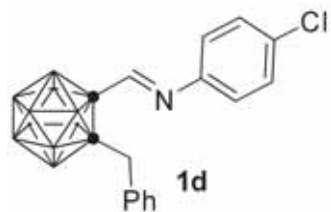
F2 - Processing parameters

SI 32768  
SF 125.7577794 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

l hr-B-cassm718-bn

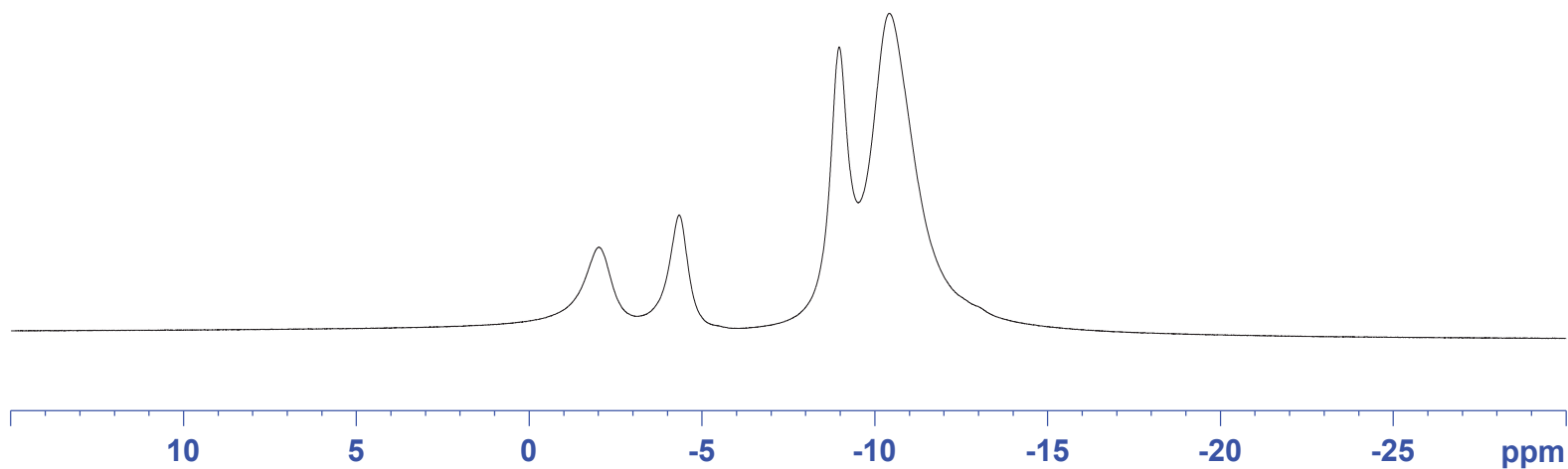


— -2.00  
— -4.33  
— -8.96  
— -10.41

Current Data Parameters  
NAME l hr-B-cassm718-bn  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170816  
Time 10.00 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 12  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 102.6  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

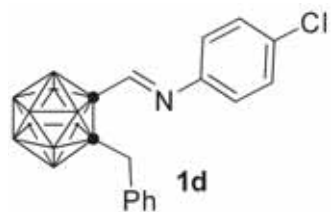


1.06  
1.13  
2.14  
6.00 S-44



I hr-B-cassm718-bn(C)

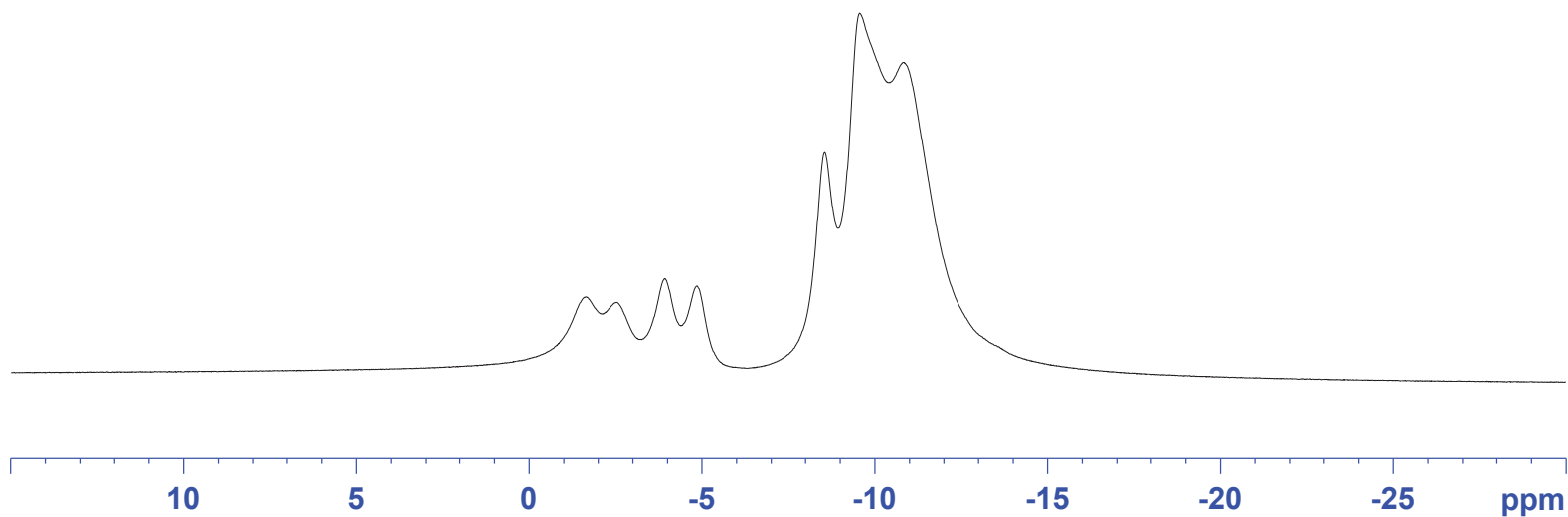
-1.65  
-2.52  
-3.92  
-4.86  
-8.54  
-9.56  
-10.03  
-10.81



Current Data Parameters  
NAME I hr-B-cassm718-bn(C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170816  
Time 10.01 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 12  
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 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

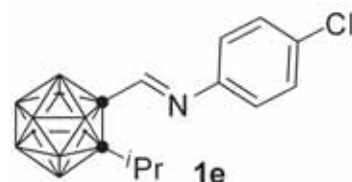


7.772  
7.375  
7.358  
7.260  
7.070  
7.053

2.473  
2.460  
2.446  
2.432  
2.418

1.225  
1.211

1 hr-H-cassm734-i pr



Current Data Parameters  
NAME 1 hr-H-cassm734-i pr  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170816  
Time 10.06 h  
INSTRUM spect  
PROBHD Z149001\_0010 (H  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.305176 Hz  
AQ 3.2767999 sec  
RG 14.97  
DW 50.000 usec  
DE 10.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SFO1 500.1330883 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 15.0000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300125 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

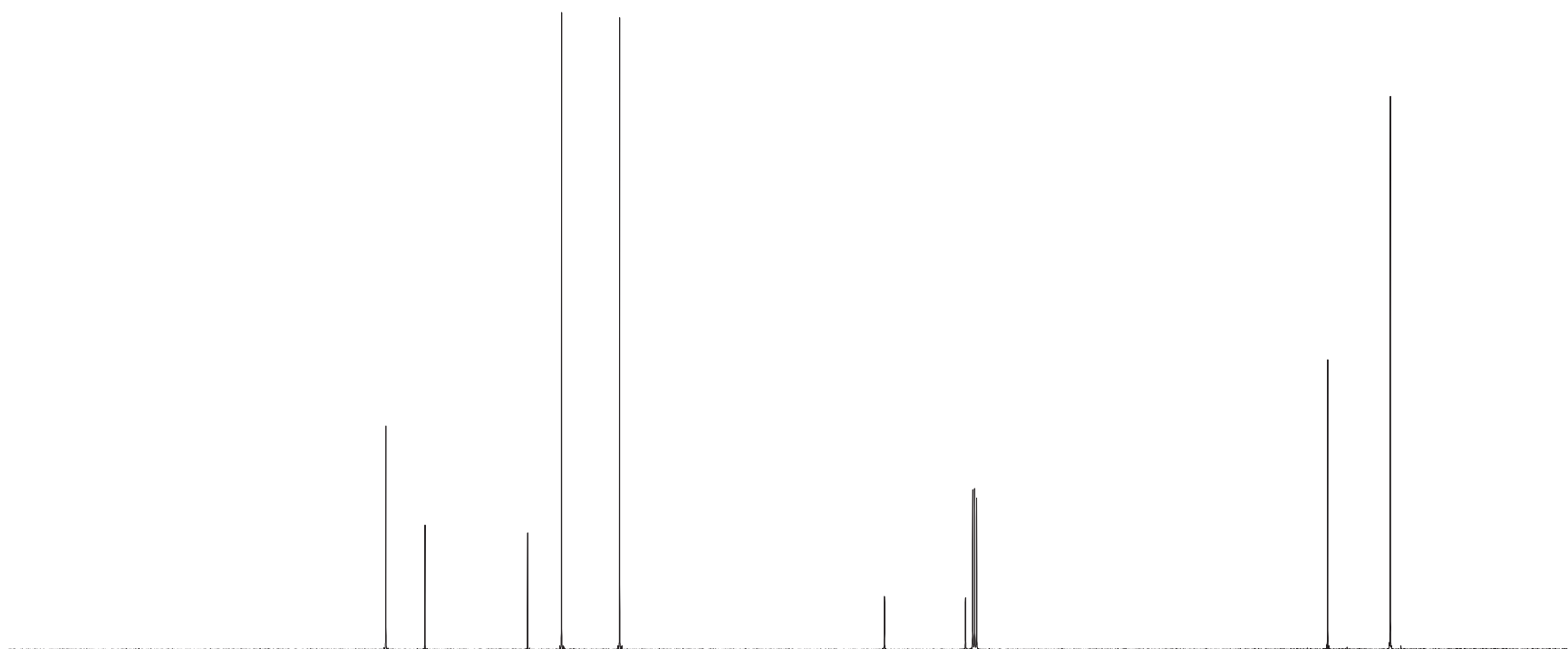
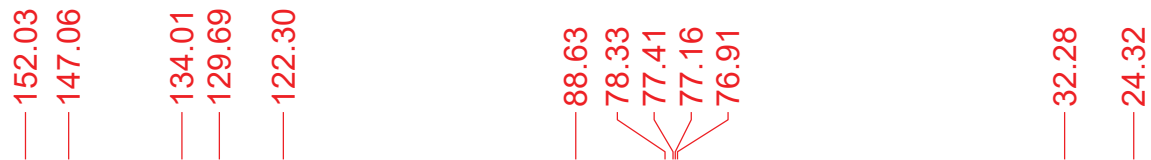
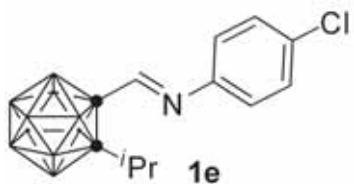


1.00  
2.02  
2.04

S-46

1.22  
6.25

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



1 hr-C-cassm734-i pr

Current Data Parameters  
 NAME 1 hr-C-cassm734-i pr  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

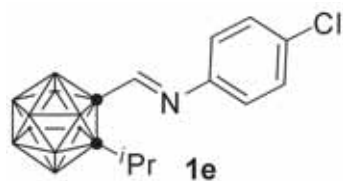
Date\_ 20170816  
 Time 10.14 h  
 INSTRUM spect  
 PROBHD Z149001\_0010 ( )  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 120  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 1.1010048 sec  
 RG 206.72  
 DW 16.800 usec  
 DE 18.00 usec  
 TE 298.0 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1  
 SF01 125.7703643 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 61.0000000 W  
 SF02 500.1320005 MHz  
 NUC2 1H  
 CPDPRG[2] wal tz16  
 PCPD2 80.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.33750001 W  
 PLW13 0.16976000 W

F2 - Processing parameters

SI 32768  
 SF 125.7577792 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

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

l hr-B-cassm734-i pr



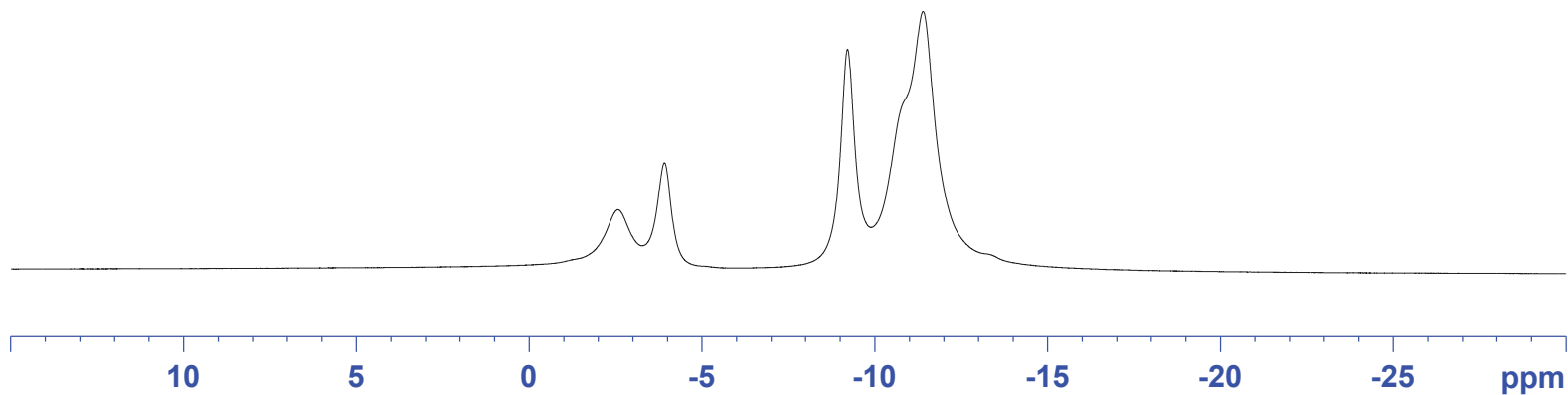
-2.56  
-3.90

-9.21  
-10.75  
-11.39

Current Data Parameters  
NAME l hr-B-cassm734-i pr  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170816  
Time 10.17 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 12  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 50.6  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

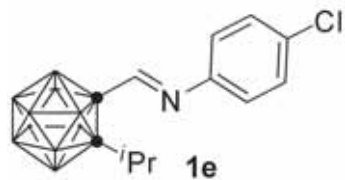


0.96  
0.96  
2.00  
6.02

6.48

I hr-B-cassm734-i pr(C)

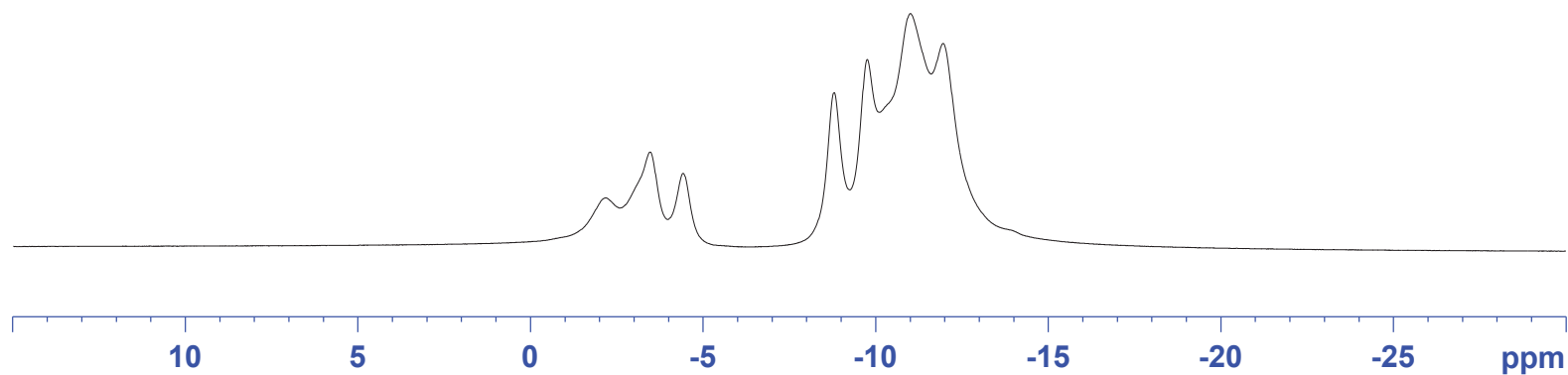
-2.17  
-3.03  
-3.46  
-4.42  
-8.79  
-9.75  
-10.32  
-11.00  
-11.95



Current Data Parameters  
NAME I hr-B-cassm734-i pr(C)  
EXPNO 1  
PROCNO 1

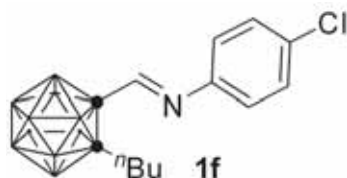
F2 - Acquisition Parameters  
Date\_ 20170816  
Time 10.18 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 12  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 56.83  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



7.777  
7.378  
7.361  
7.260  
7.059  
7.041

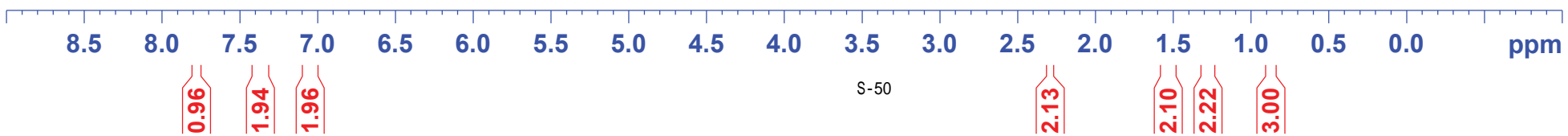
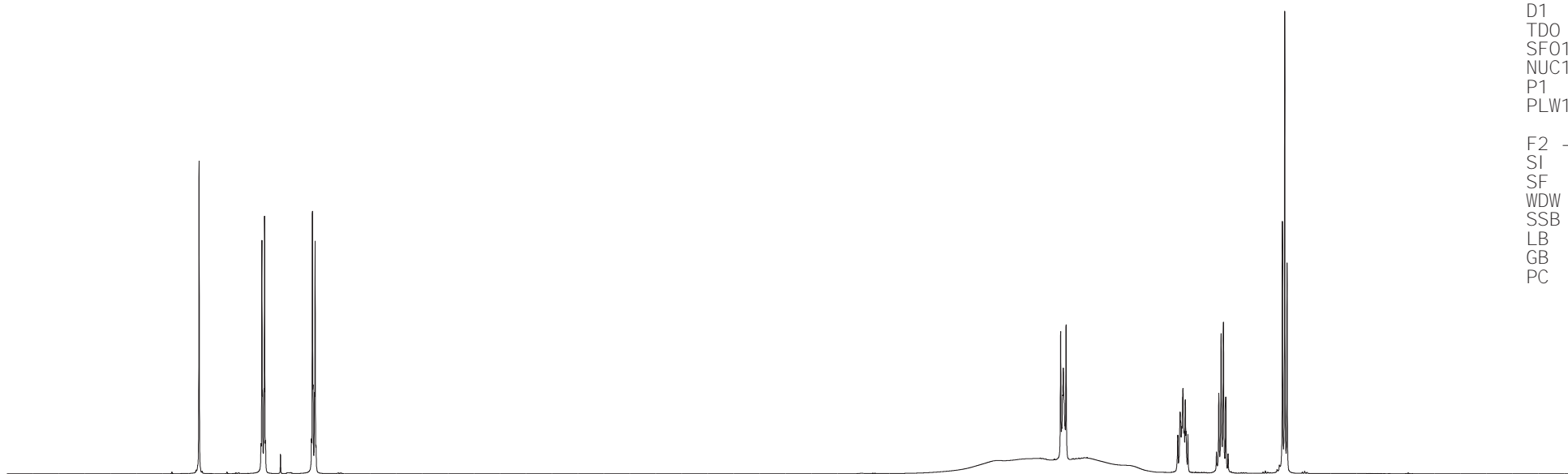
2.302  
2.296  
2.285  
2.275  
2.268  
1.558  
1.543  
1.539  
1.532  
1.525  
1.517  
1.510  
1.505  
1.493  
1.312  
1.297  
1.282  
1.268  
1.253  
1.238  
0.893  
0.878  
0.863

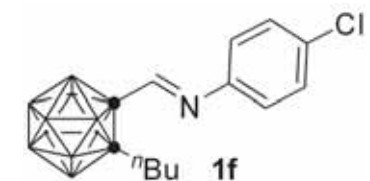


Current Data Parameters  
NAME 1 hr-H-cassm-731  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170814  
Time 19.17  
INSTRUM spect  
PROBHD Z149001\_0010 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 14.97  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300128  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00





152.26  
147.08

133.96  
129.72  
122.23

82.42  
77.41  
77.16  
76.91  
76.54

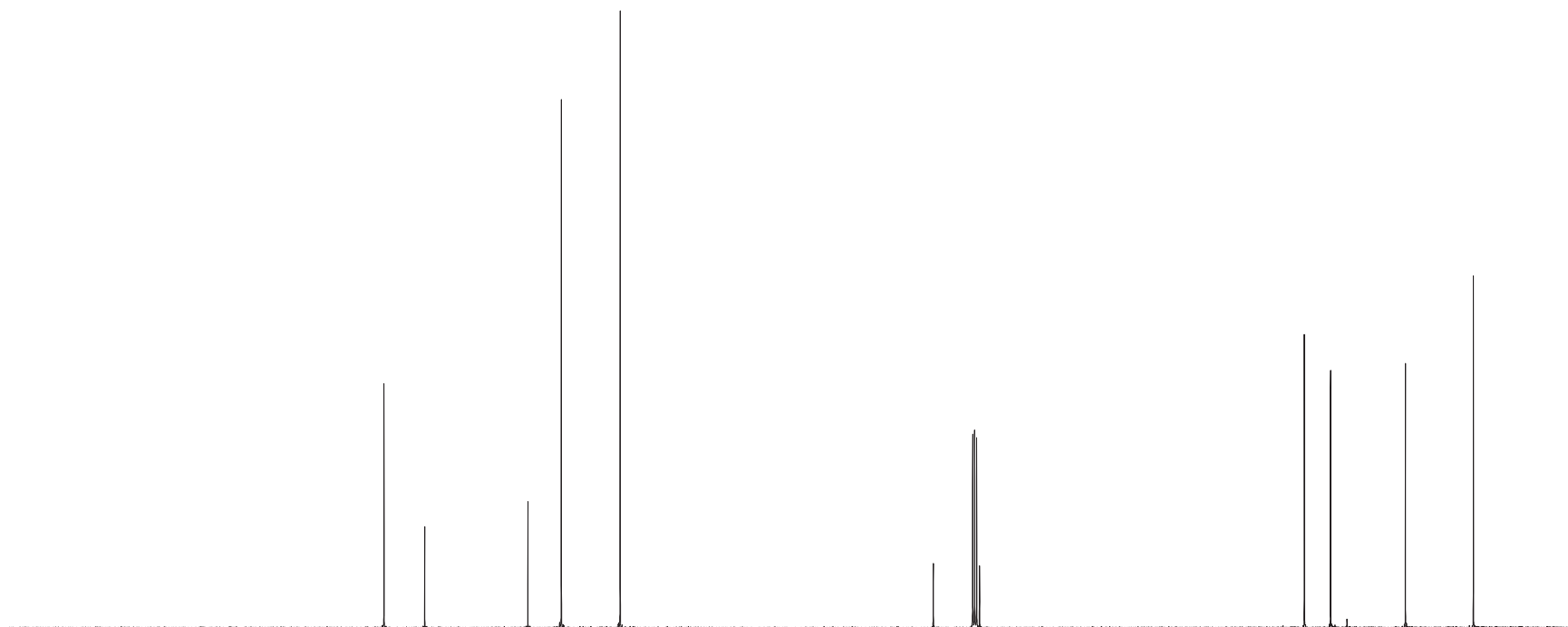
35.25  
31.92  
22.41  
13.76

1 hr-C-cassm-731NBU

Current Data Parameters  
NAME 1 hr-C-cassm-731NBU  
EXPNO 1  
PROCNO 1

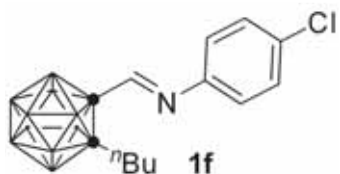
F2 - Acquisition Parameters  
Date\_ 20170814  
Time 19.25 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters  
SI 32768  
SF 125.7577775 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

I hr-B-cassm-731NBU

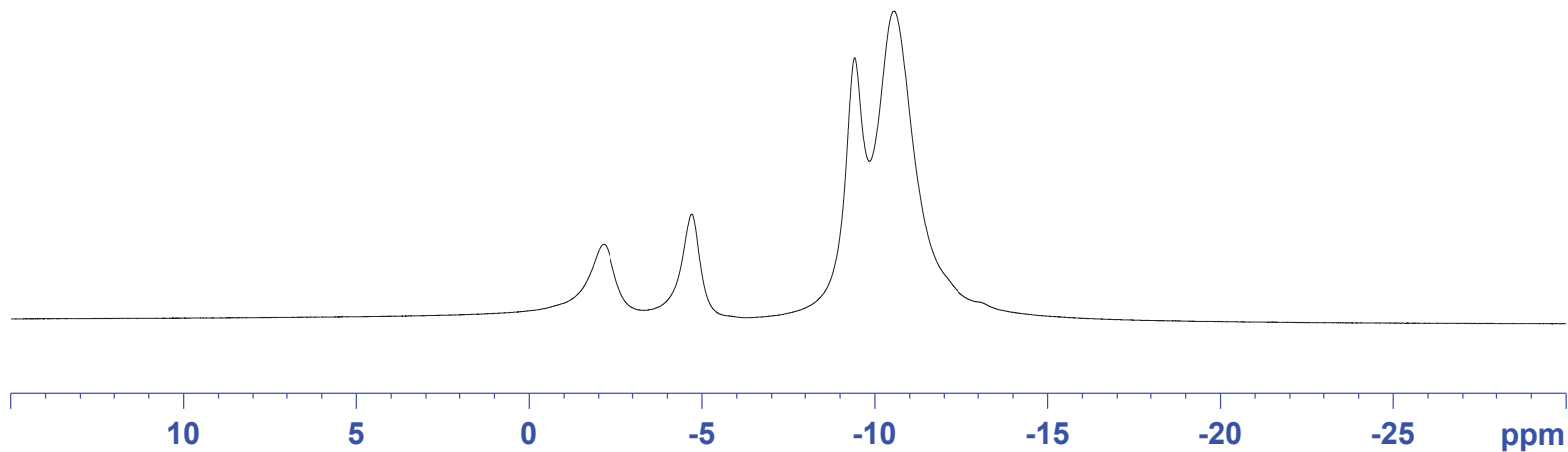


Chemical shift markers (ppm):  
-2.15  
-4.69  
-9.41  
-10.54

Current Data Parameters  
NAME I hr-B-cassm-731NBU  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170814  
Time 19.28 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 12  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 83.35  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

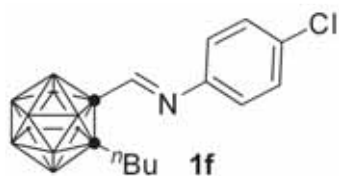


Integration values:  
1.05  
1.08  
2.20  
6.00



I hr-B-cassm-731NBU(c)

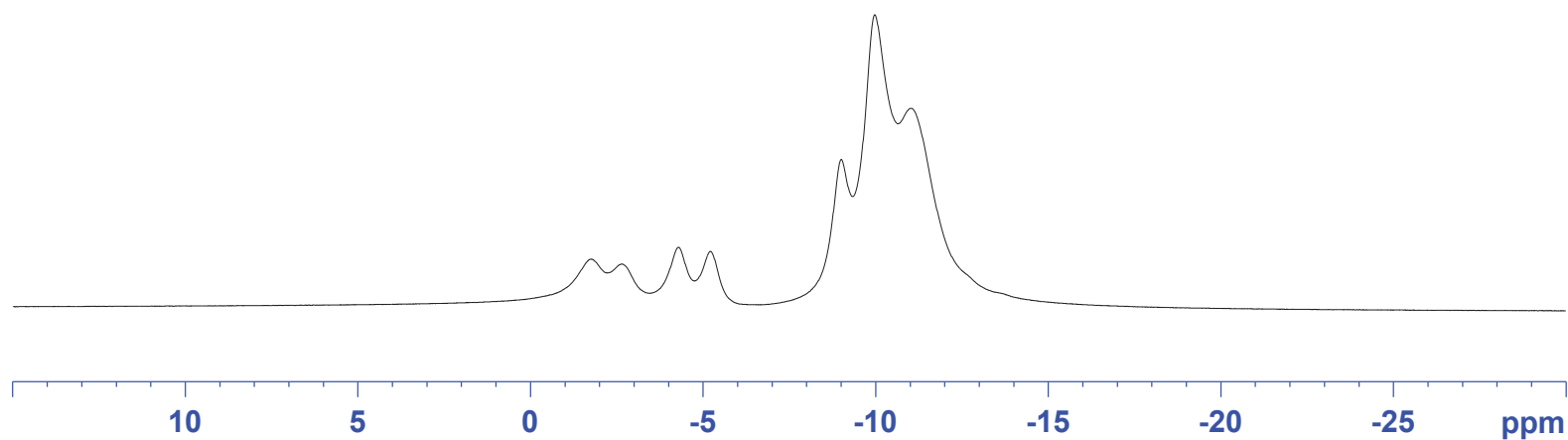
-1.75  
-2.65  
-4.28  
-5.21  
-9.00  
-9.97  
-11.02



Current Data Parameters  
NAME I hr-B-cassm-731NBU(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170814  
Time 19.29 h  
INSTRUM spect  
PROBHD Z149001\_0010 (zg)  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 12  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 56.83  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

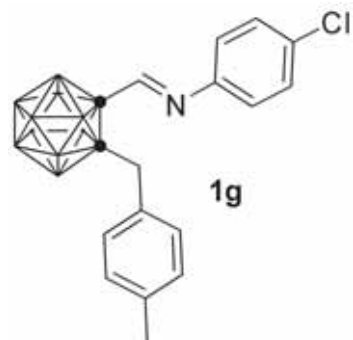


1 hr-H-cassm-740-bnme

Current Data Parameters  
NAME 1 hr-H-cassm-740-bnme  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170815  
Time 15.07 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 13.21  
DW 50.000 usec  
DE 10.00 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1  
SF01 500.1330883 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 15.00000000 W

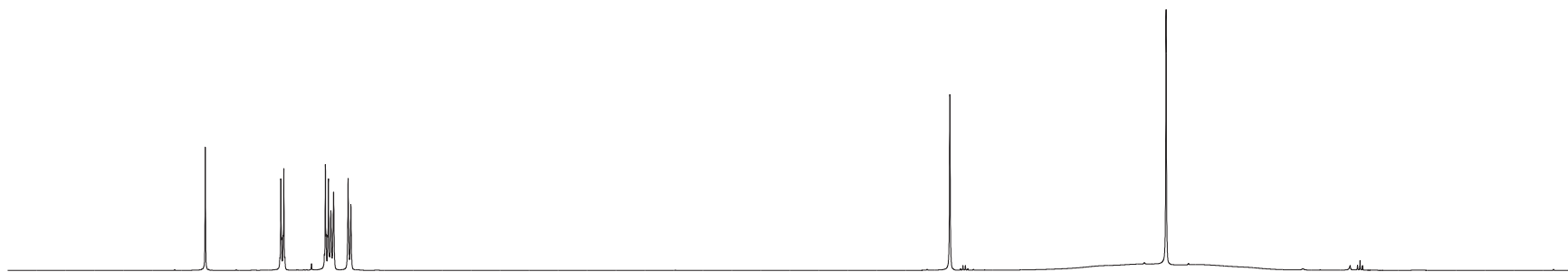
F2 - Processing parameters  
SI 65536  
SF 500.1300124 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



7.869  
7.436  
7.418  
7.260  
7.181  
7.163  
7.149  
7.133  
7.050  
7.034

3.603

2.365

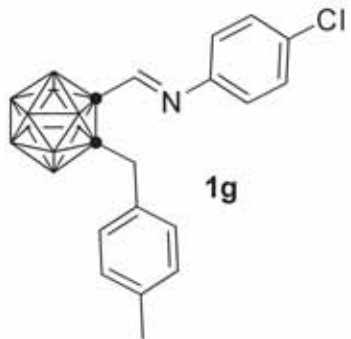


8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

1.00  
2.02  
4.11  
2.03

2.05 S-54

3.16



152.39  
146.82  
137.96  
134.19  
132.24  
130.23  
129.75  
129.34  
122.50

82.43  
77.41  
77.16  
76.91  
76.78

40.71

21.25

1 hr-C-cassm-740-bnme

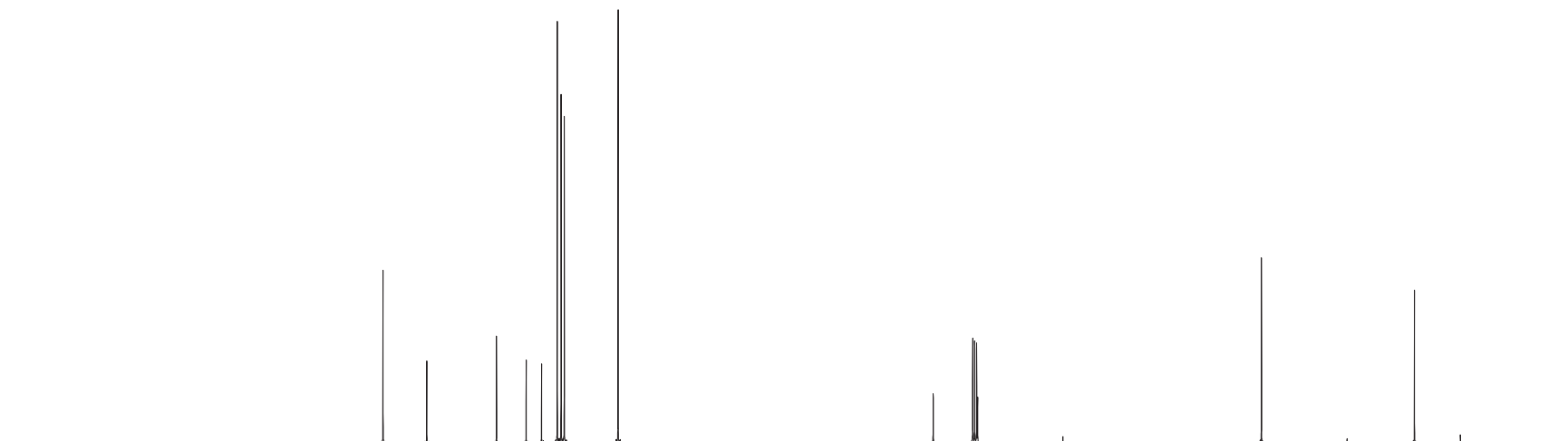
Current Data Parameters  
NAME 1 hr-C-cassm-740-bnme  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170815  
Time 15.14 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 120  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

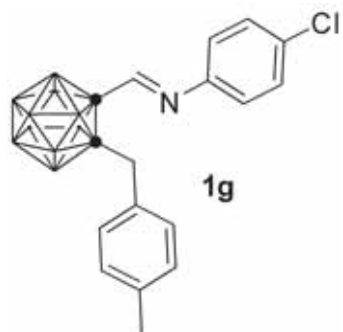
F2 - Processing parameters

SI 32768  
SF 125.7577854 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

I hr-B-cassm-740-bnme

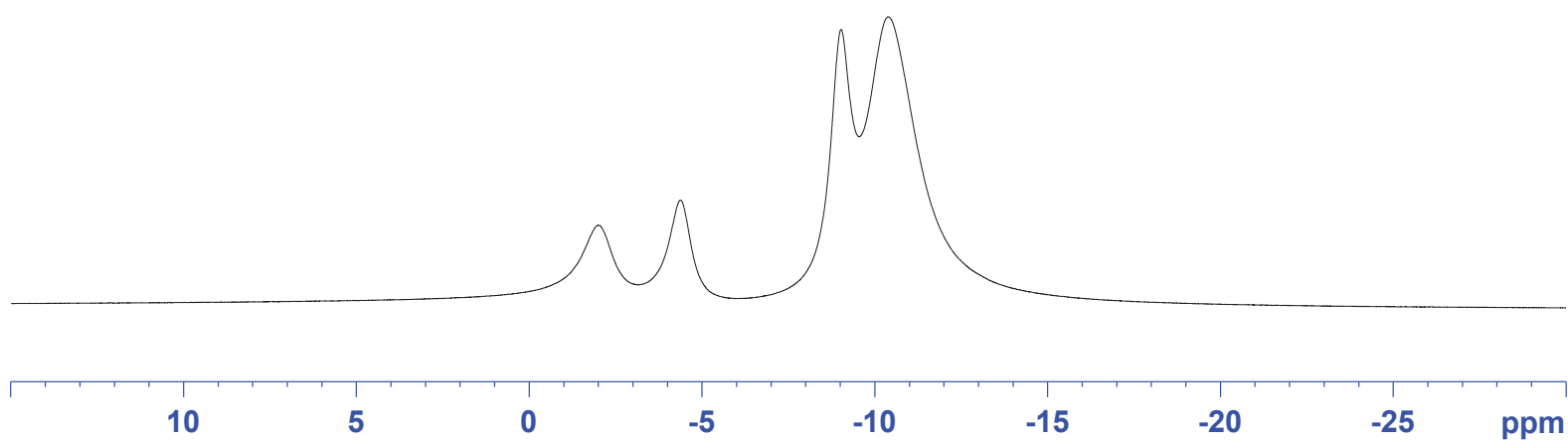


— -2.00  
— -4.38  
— -9.02  
— -10.38

Current Data Parameters  
NAME I hr-B-cassm-740-bnme  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170815  
Time 15.18 h  
INSTRUM spect  
PROBHD Z149001\_0010 (   
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 12  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 50.6  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

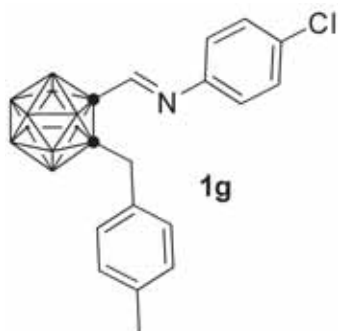
F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.16  
1.01  
2.19  
6.00 S-56

I hr-B-cassm-740-bnme(C)

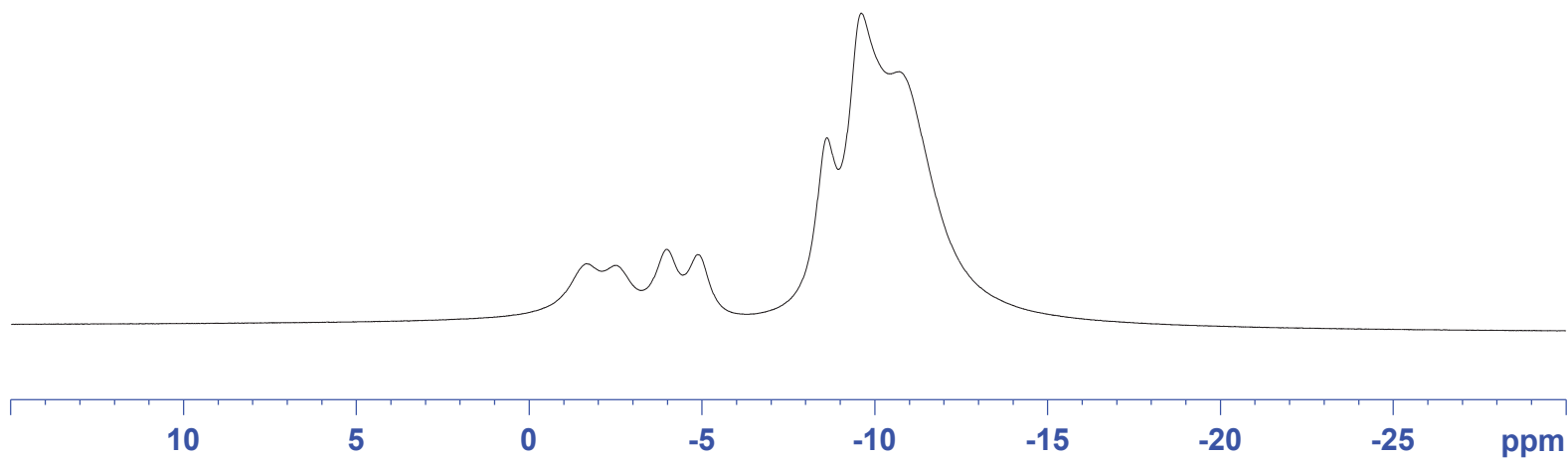
-1.64  
-2.49  
-3.99  
-4.88  
-8.61  
-9.60  
-10.73



Current Data Parameters  
NAME I hr-B-cassm-740-bnme(C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170815  
Time 15.19 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 12  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 56.83  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



7.809  
7.353  
7.337  
7.322  
7.302  
7.300  
7.296  
7.286  
7.283  
7.280  
7.260  
7.107  
7.103  
7.100  
7.009  
7.006  
7.005  
7.003  
6.994  
6.991  
6.990  
6.987

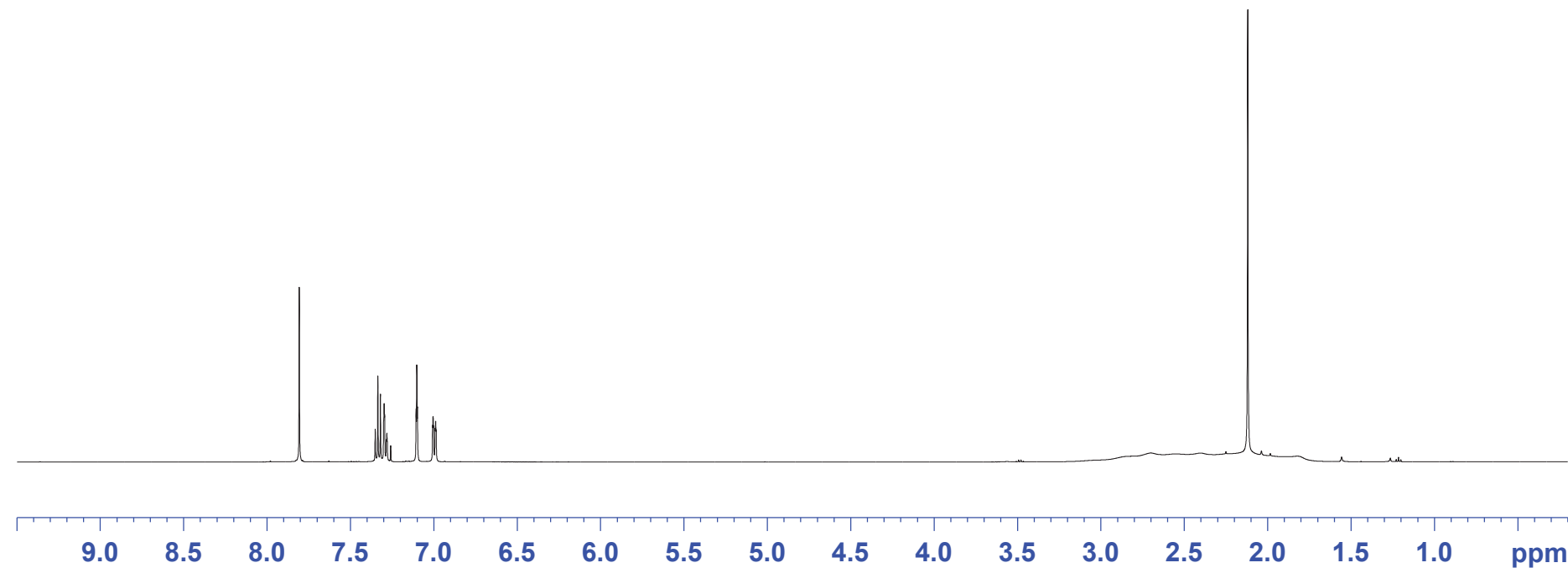
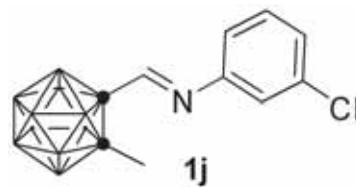
2.120

1 hr-H-cassm-m-cl - 71

Current Data Parameters  
NAME 1 hr-H-cassm-m-cl  
EXPNO 1  
PROCNO 1

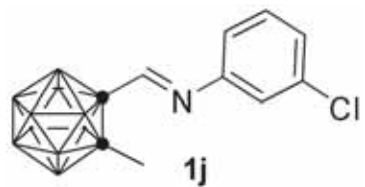
F2 - Acquisition Parameters  
Date\_ 20170815  
Time 15.23 H  
INSTRUM spect  
PROBHD Z149001\_0010 (zg30)  
PULPROG 65536  
TD 16  
SOLVENT CDCl 3  
NS 2  
DS 10000.000 H  
SWH 0.305176 H  
FIDRES 3.2767999 s  
RG 17.56  
DW 50.000 U  
DE 10.00 U  
TE 298.0 K  
D1 1.0000000 s  
TDO 1  
SF01 500.1330883 M  
NUC1 1H  
P1 12.00 U  
PLW1 15.0000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300126 M  
WDW EM  
SSB 0  
LB 0.30 H  
GB 0  
PC 1.00



1.00  
2.04  
0.99  
1.02

3.15



153.25  
149.80

135.24  
130.61  
128.01  
121.06  
119.20

77.41  
77.16  
76.91  
75.09

23.69

1 hr-C-cassm-m-cl -712

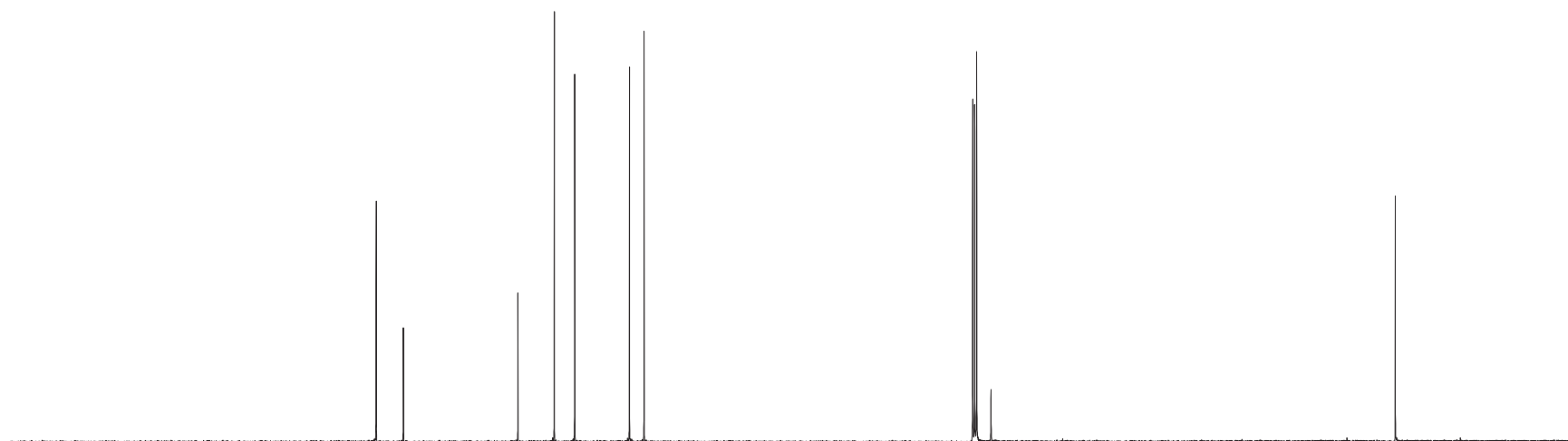
Current Data Parameters  
 NAME 1 hr-C-cassm-m-cl -712  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170815  
 Time 15.32 h  
 INSTRUM spect  
 PROBHD Z149001\_0010 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 120  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 1.1010048 sec  
 RG 206.72  
 DW 16.800 usec  
 DE 18.00 usec  
 TE 298.0 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SF01 125.7703643 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 61.0000000 W  
 SF02 500.1320005 MHz  
 NUC2 1H  
 CPDPRG[2] wal tz16  
 PCPD2 80.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.33750001 W  
 PLW13 0.16976000 W

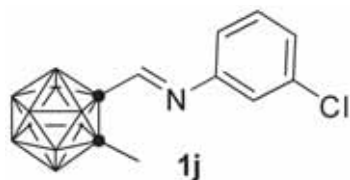
F2 - Processing parameters

SI 32768  
 SF 125.7577763 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



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

I hr-B-cassm-m-cl -712

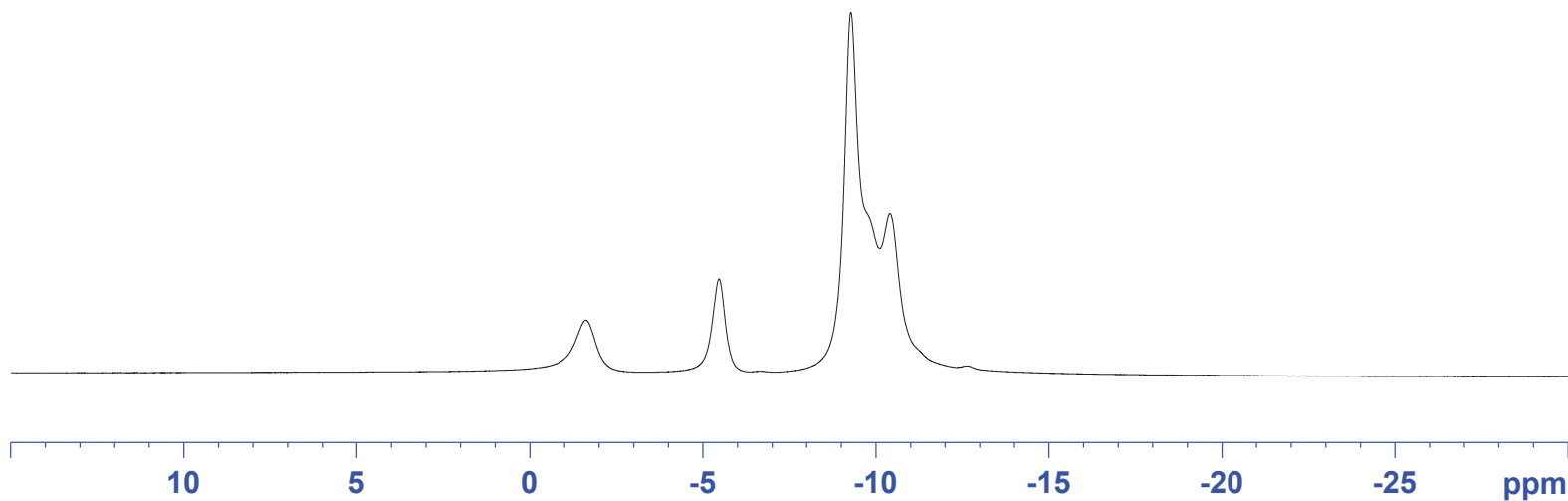


-1.61  
-5.46  
-9.27  
-9.82  
-10.40

Current Data Parameters  
NAME I hr-B-cassm-m-cl -712  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170815  
Time 15.35 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 93.28  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SFO2 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



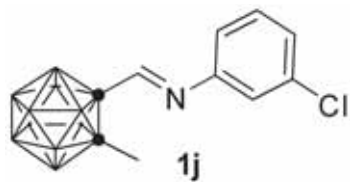
1.02  
1.01  
8.00

S-60



I hr-B-cassm-m-cl -712(c)

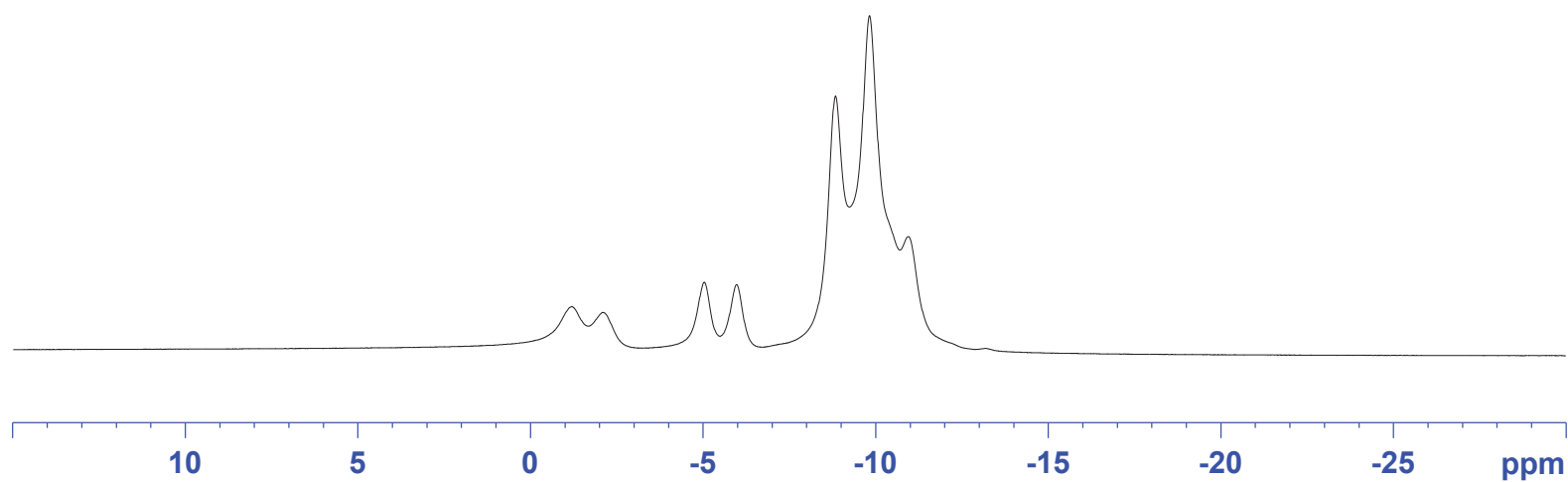
-1.19  
-2.09  
-5.03  
-5.96  
-8.83  
-9.81  
-10.93



Current Data Parameters  
NAME I hr-B-cassm-m-cl -712(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170815  
Time\_ 15.36 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 12  
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 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



7.780  
7.450  
7.447  
7.434  
7.431  
7.298  
7.295  
7.283  
7.280  
7.268  
7.265  
7.260  
7.234  
7.231  
7.218  
7.215  
7.203  
7.200  
6.910  
6.907  
6.895  
6.891

2.220

1.545

I hr-Hcassm-ocl

Current Data Parameters

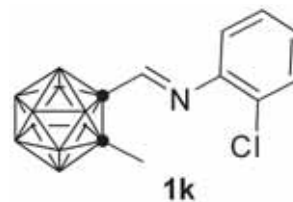
NAME I hr-Hcassm-ocl  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170819  
Time 13.00  
INSTRUM spect  
PROBHD Z149001\_0010 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 30.85  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters

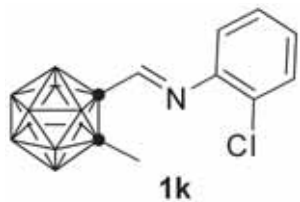
SI 65536  
SF 500.1300126  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00



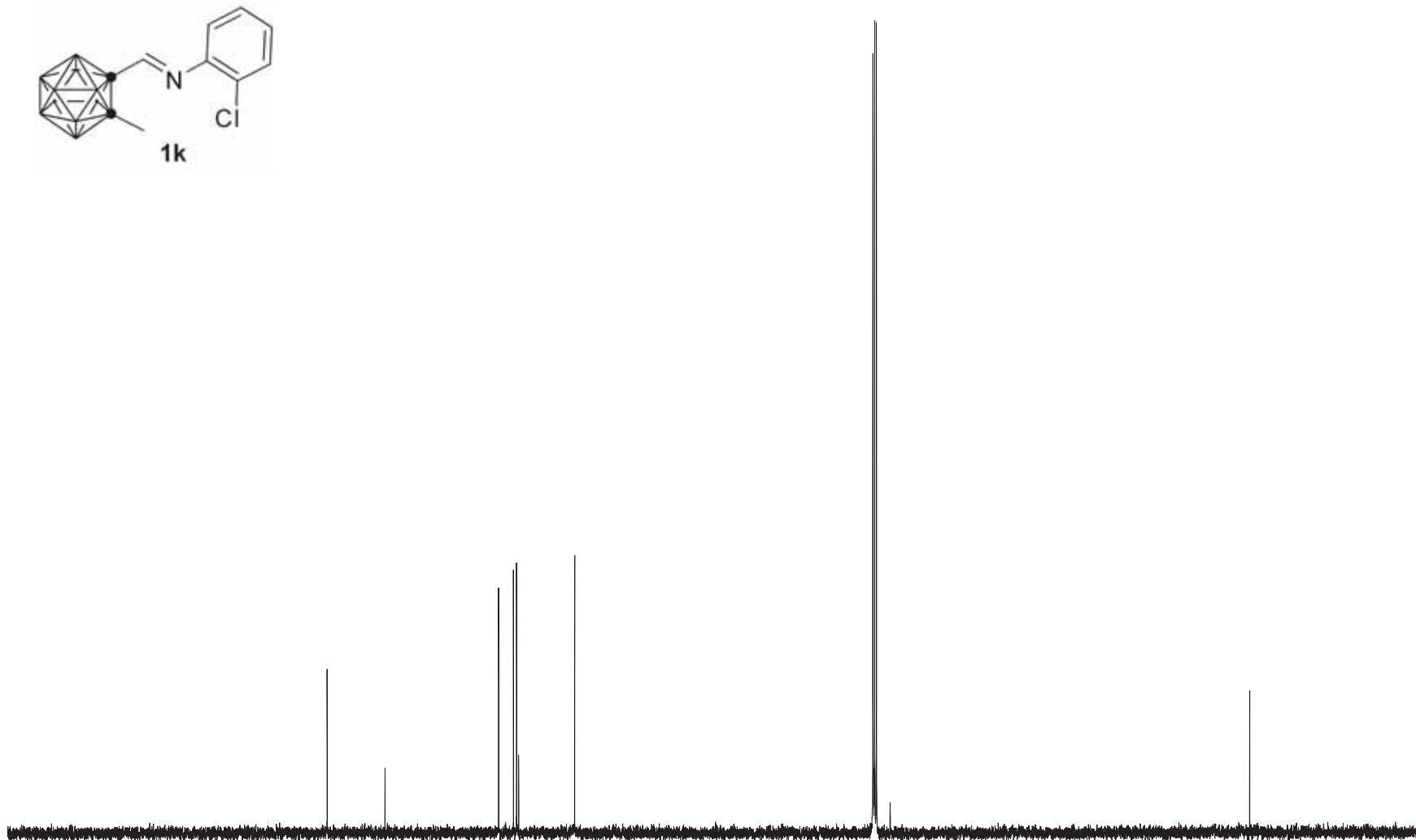
1.01  
1.00  
1.08  
1.03  
1.03

3.06

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm



154.70  
 146.50  
 130.44  
 128.34  
 127.90  
 127.60  
 119.67  
 77.41  
 77.16  
 76.91  
 74.97  
 24.03



1 hr-Ccassm-ocl

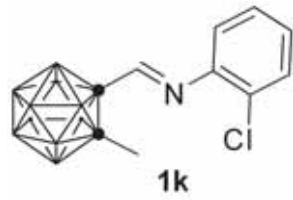
Current Data Parameters  
 NAME 1 hr-Ccassm-ocl  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170819  
 Time 13.21 h  
 INSTRUM spect  
 PROBHD Z149001\_0010 ( )  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 360  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 1.1010048 sec  
 RG 206.72  
 DW 16.800 usec  
 DE 18.00 usec  
 TE 298.0 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1  
 SF01 125.7703643 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 61.0000000 W  
 SF02 500.1320005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.33750001 W  
 PLW13 0.16976000 W

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

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

I hr-Bcassm-ocl

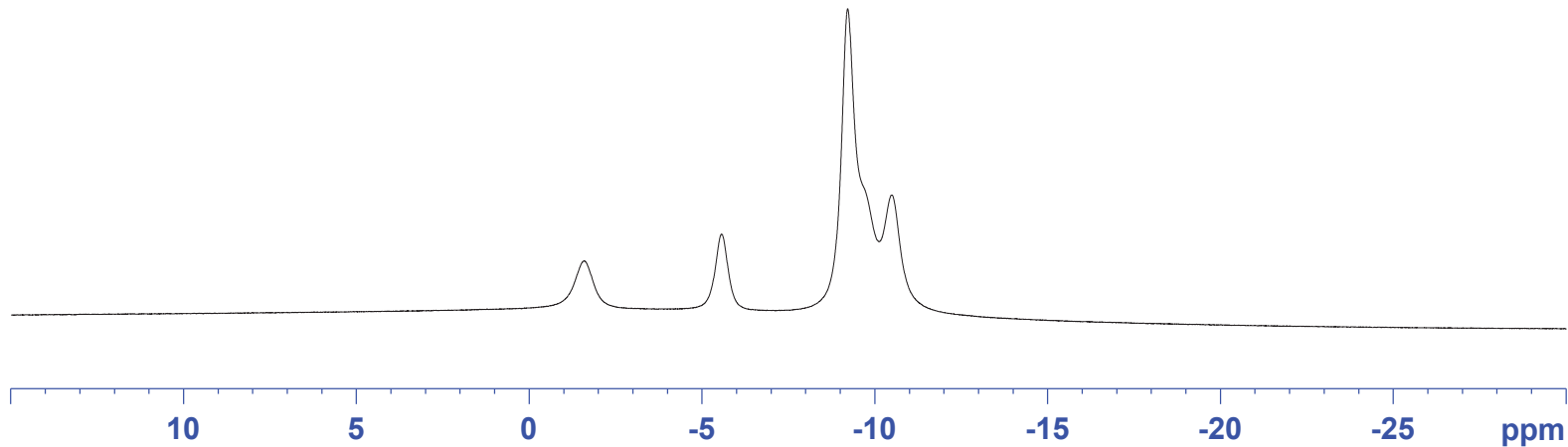


-1.58  
-5.56  
-9.21  
-9.75  
-10.48

Current Data Parameters  
NAME I hr-Bcassm-ocl  
EXPNO 1  
PROCNO 1

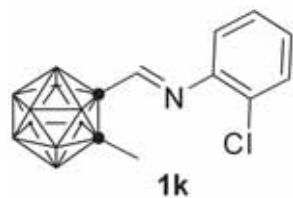
F2 - Acquisition Parameters  
Date\_ 20170819  
Time 13.24 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 12  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 142.5  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.00000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.00000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.02  
1.06  
8.00

I hr-Bcassm-ocl (c)

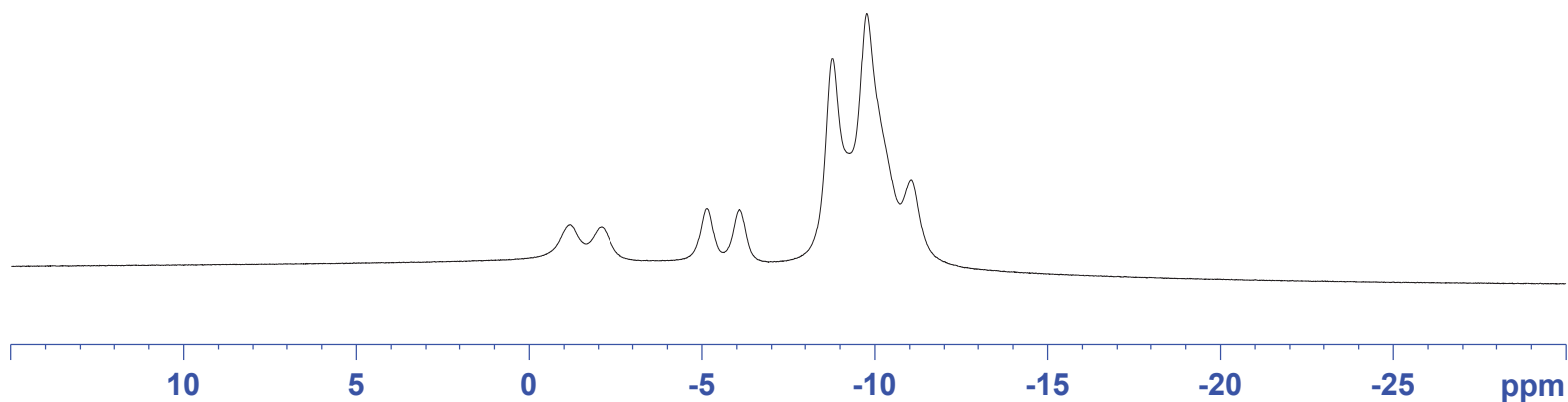


-1.17  
-2.08  
-5.14  
-6.07  
-8.78  
-9.76  
-11.04

Current Data Parameters  
NAME I hr-Bcassm-ocl (c)  
EXPNO 1  
PROCNO 1

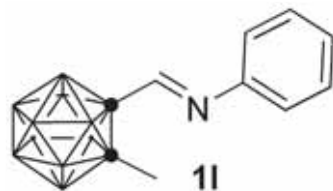
F2 - Acquisition Parameters  
Date\_ 20170819  
Time 13.25 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl 3  
NS 12  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 142.5  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



lhr-H-cassm708

7.822  
7.421  
7.406  
7.390  
7.335  
7.320  
7.305  
7.260  
7.125  
7.110



2.123

Current Data Parameters  
NAME lhr-H-cassm708  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171214  
Time 11.51 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  
TDO 1  
SF01 500.1330883 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300125 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

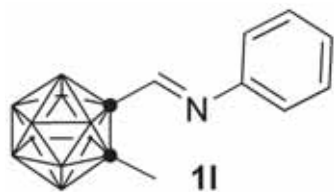


8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

1.005  
2.091  
1.000  
2.059

3.228

lhr-C-cassm708

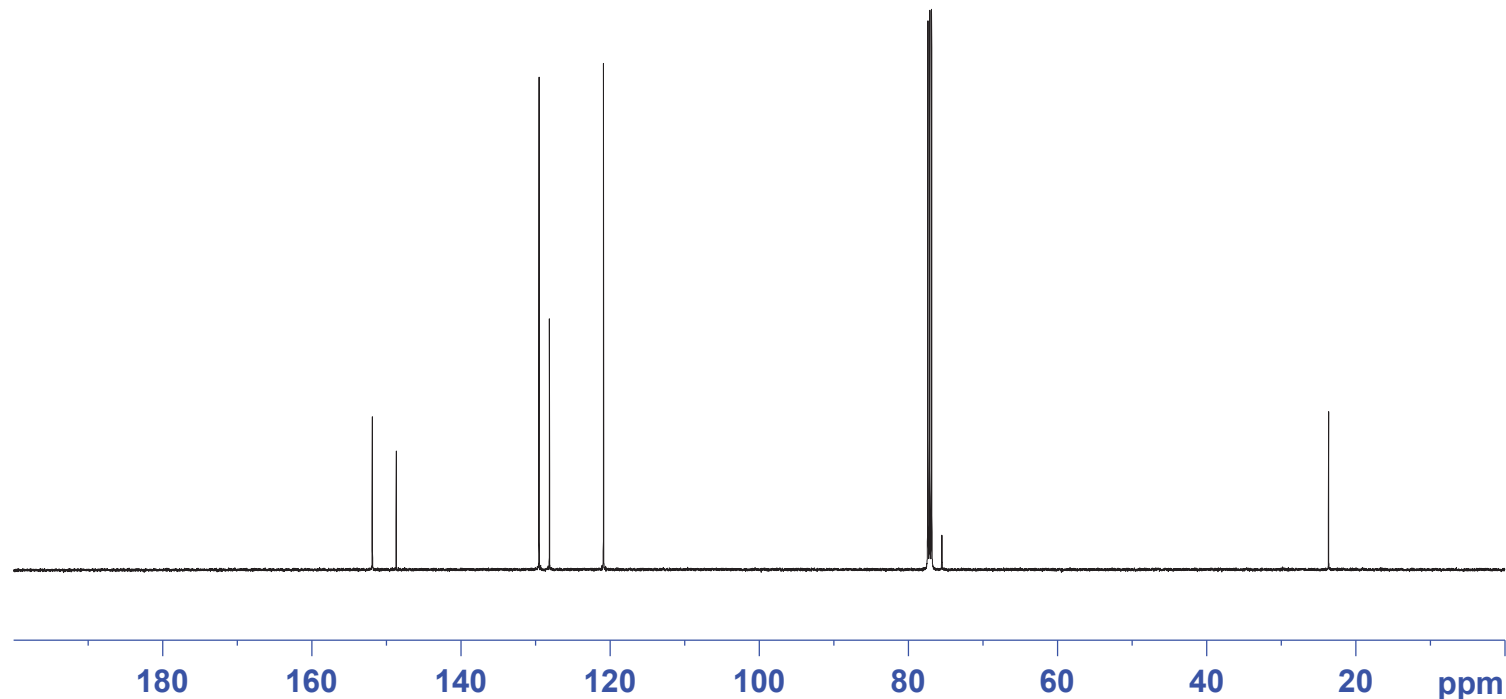


151.91  
148.71

129.56  
128.16  
120.91

77.41  
77.16  
76.91  
75.53

23.68

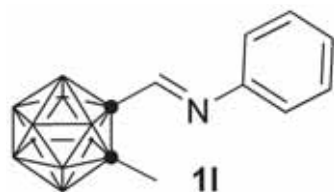


Current Data Parameters  
NAME lhr-C-cassm708  
EXPNO 1  
PROCNO 1

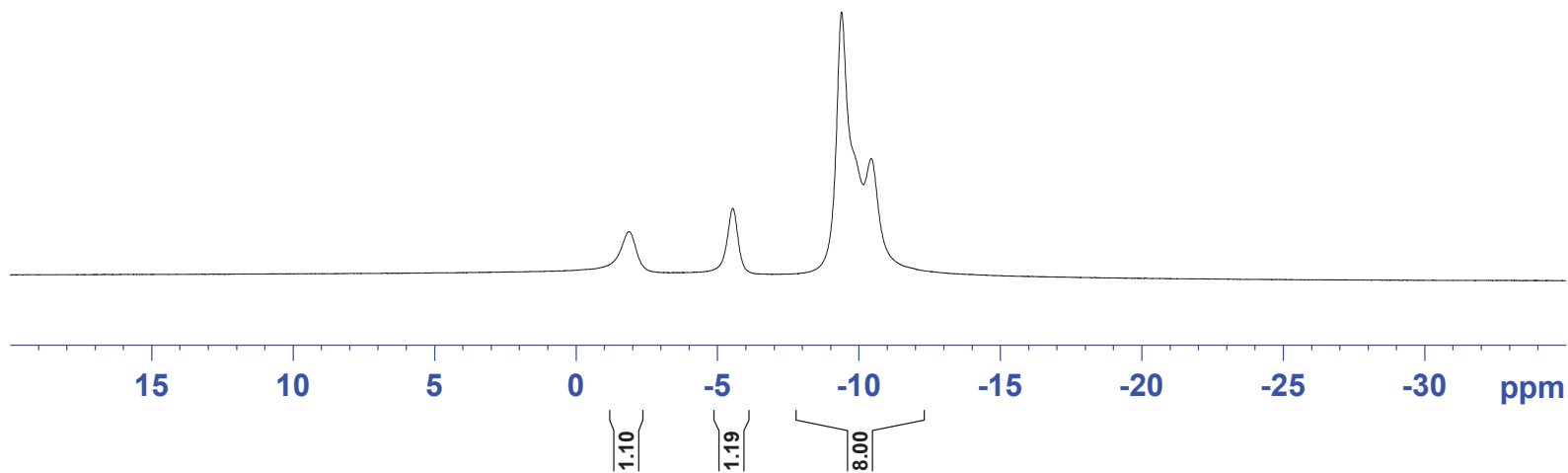
F2 - Acquisition Parameters  
Date\_ 20171214  
Time\_ 12.18 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 500  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.00000000 W  
SFO2 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.00000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

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

lhr-B-cassm708



— -1.87  
— -5.54  
— -9.39  
— -10.44



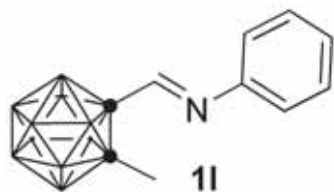
Current Data Parameters  
NAME lhr-B-cassm708  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171214  
Time 12.21 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgig  
TD 32768  
SOLVENT CDCl3  
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  
D11 0.03000000 sec  
TD0 1  
SFO1 160.4615790 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.00000000 W  
SFO2 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.00000000 W  
PLW12 0.33750001 W

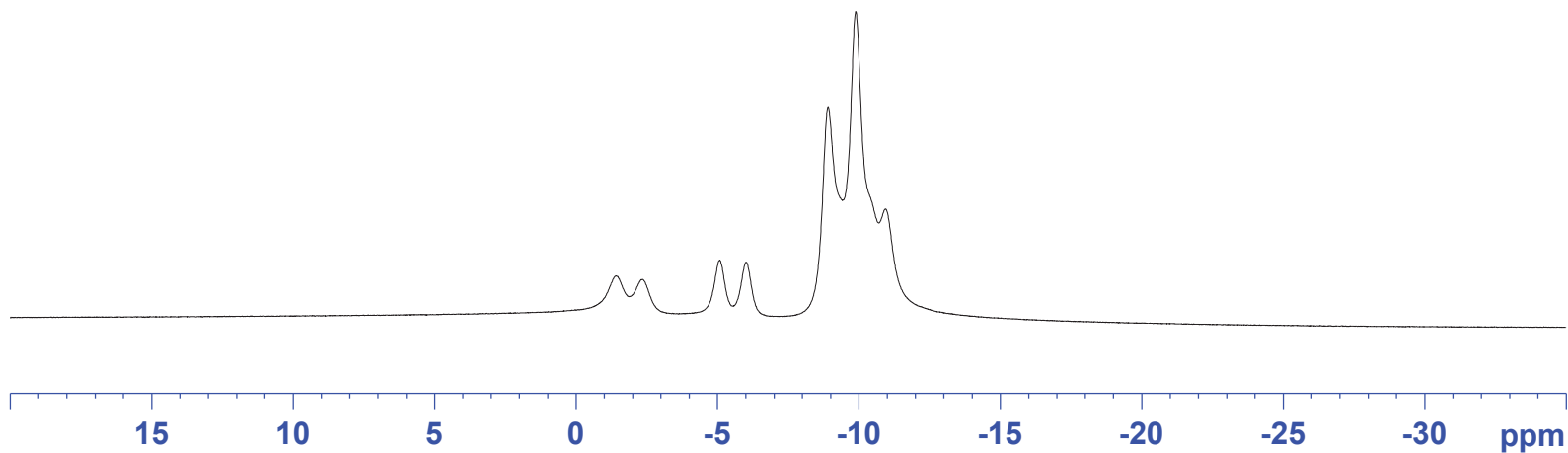
F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1hr-B-cassm708 (C)



— 1.42  
— 2.35  
  
— 5.07  
— 6.01  
  
— 8.91  
— 9.89  
— 10.94



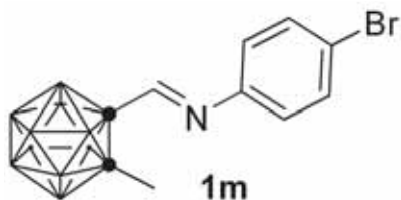
Current Data Parameters  
NAME 1hr-B-cassm708 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171214  
Time 12.22 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
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  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.00000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

7.808  
7.528  
7.507  
7.260  
7.011  
6.990

2.107



1hr-H-cassm715-Br-Cl

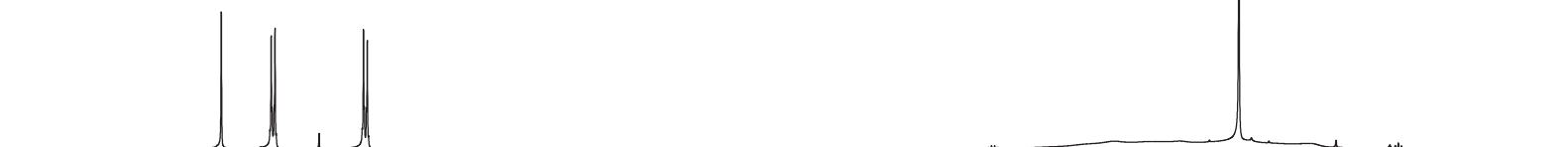
Current Data Parameters  
NAME 1hr-H-cassm715-Br-CDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170812  
Time 18.51 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 40.3  
DW 62.400 usec  
DE 6.50 usec  
TE 294.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters

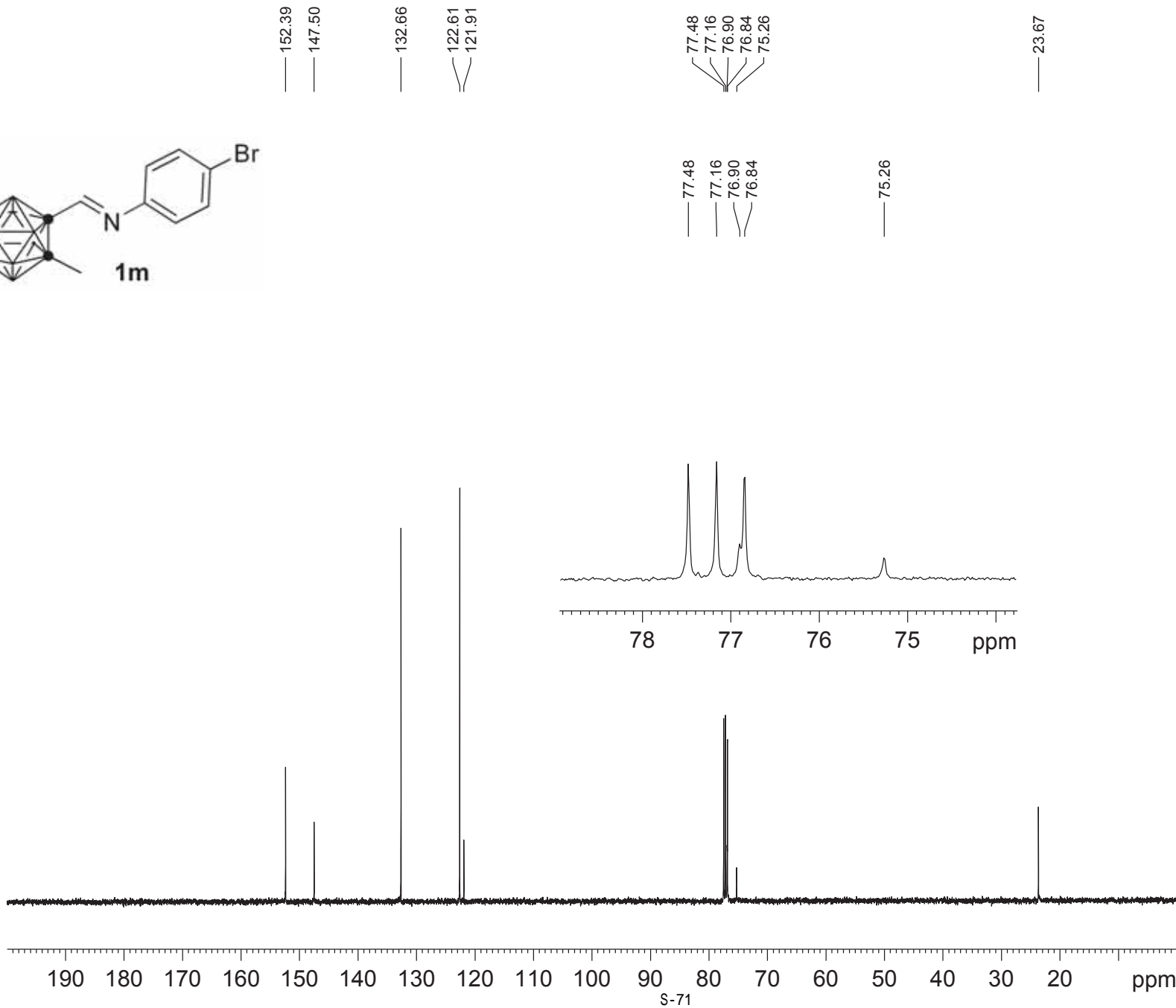
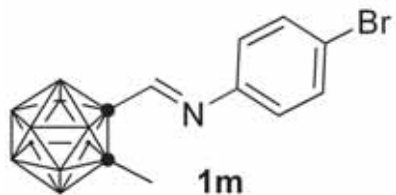
SI 65536  
SF 400.2300105 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



1.00  
2.00  
2.03

3.13

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



1hr-C-cassm715-Br-(

Current Data Parameters  
 NAME 1hr-C-cassm715-Br-CDCl3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170812  
 Time\_ 18.54 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 98  
 DS 4  
 SWH 40760.871 Hz  
 FIDRES 0.621962 Hz  
 AQ 0.8039083 sec  
 RG 161  
 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

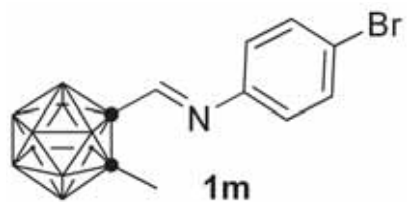
F2 - Processing parameters  
 SI 32768  
 SF 100.6379041 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1hr-B-cassm715-Br-CDCl3

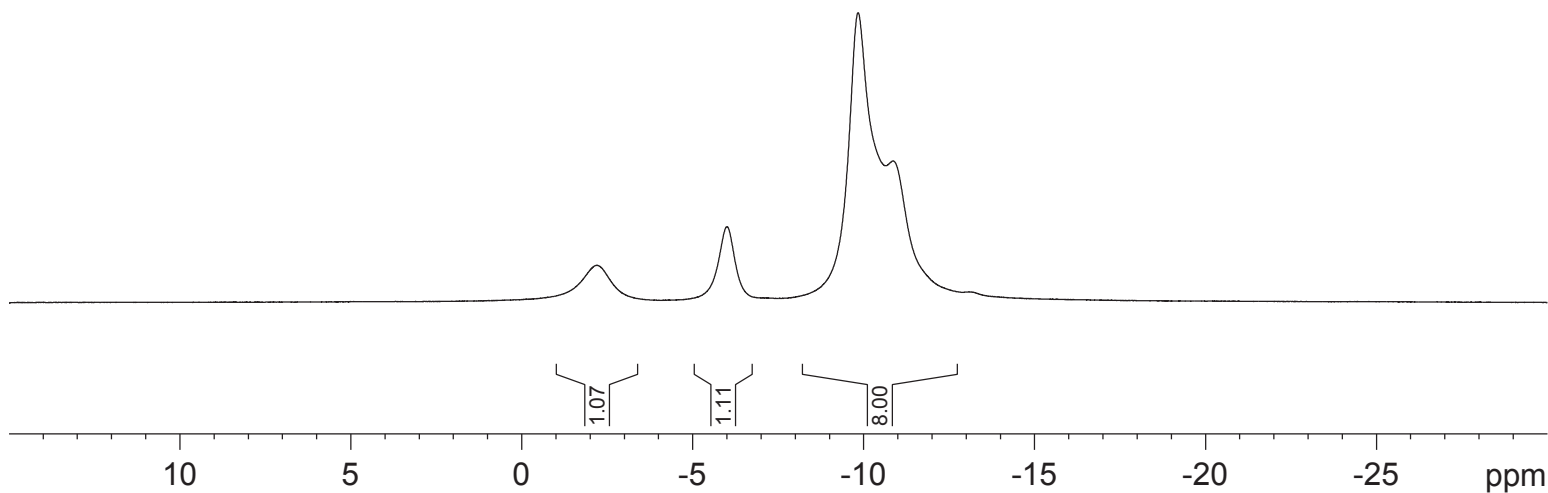
Current Data Parameters  
NAME 1hr-B-cassm715-Br-CDCl3  
EXPNO 1  
PROCNO 1

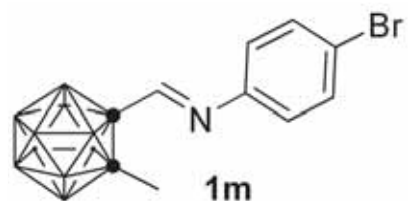
F2 - Acquisition Parameters  
Date\_ 20170812  
Time\_ 19.27 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 17  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 295.4 K  
D1 2.00000000 sec  
D11 0.03000000 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



— -2.20  
— -6.00  
— -9.84  
— -10.87





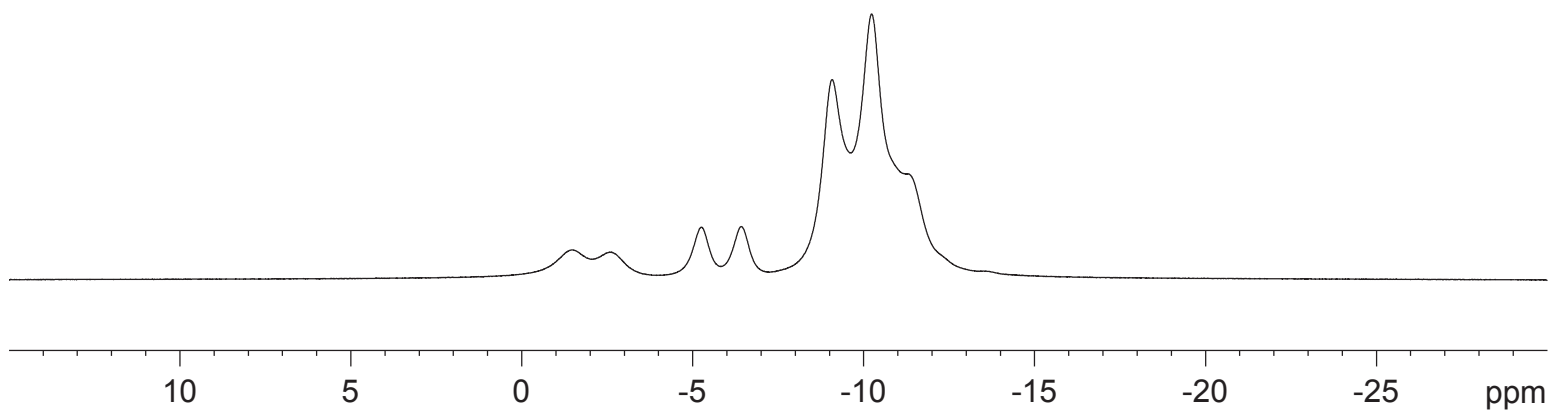
| -1.47  
 | -2.59  
 | -5.25  
 | -6.41  
 | -9.08  
 | -10.24  
 | -11.39

1hr-B-cassm715-Br-CDCl3 (C)

Current Data Parameters  
 NAME 1hr-B-cassm715-Br-CDCl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170812  
 Time 19.29 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 19  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.1 K  
 D1 2.0000000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 11B  
 P1 7.50 usec  
 PLW1 55.09999847 W

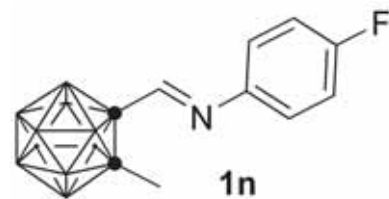
F2 - Processing parameters  
 SI 32768  
 SF 128.4097430 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



7.823  
7.260  
7.166  
7.153  
7.143  
7.131  
7.112  
7.091  
7.069

2.115

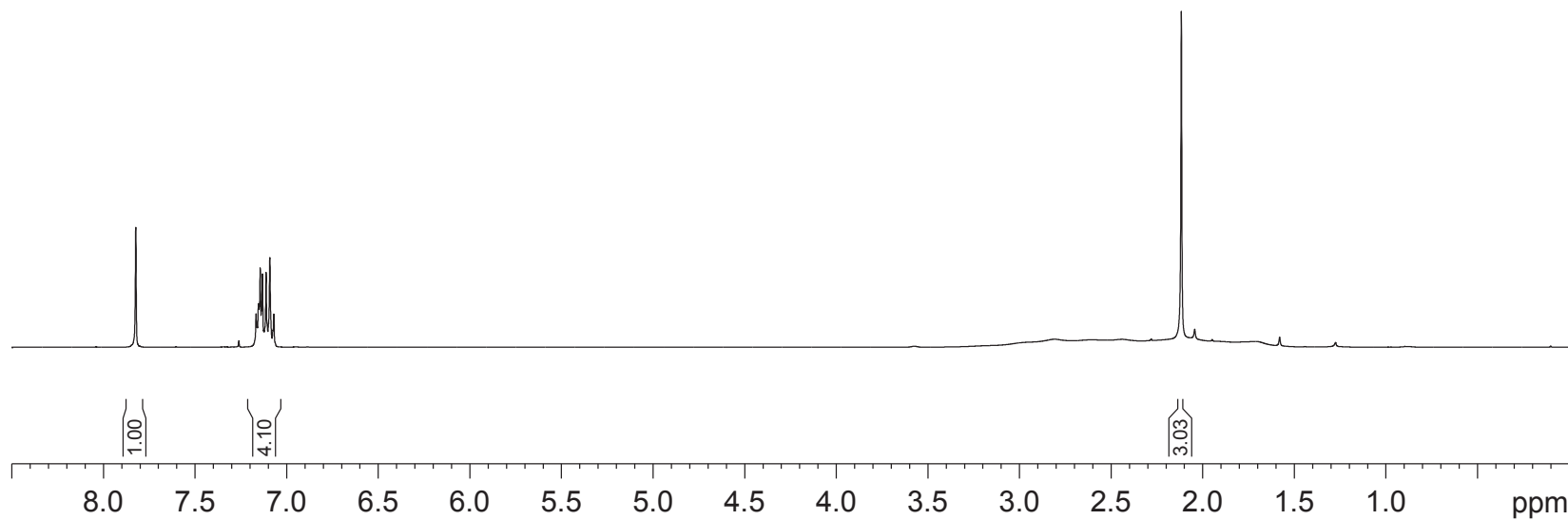
1hr-H-cassm406-F-CDCl3

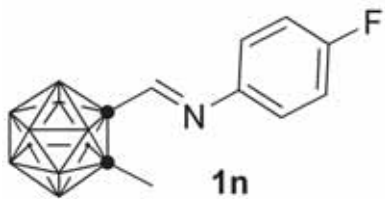


Current Data Parameters  
NAME 1hr-H-cassm406-F-CD  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160701  
Time 15.46 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 22.6  
DW 62.400 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

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





163.79  
161.32

151.40  
144.59  
144.56

122.85  
122.77  
116.51  
116.29

77.48  
77.16  
76.96  
76.84  
75.52

23.64

1hr-C-cassm406-F-CDC13

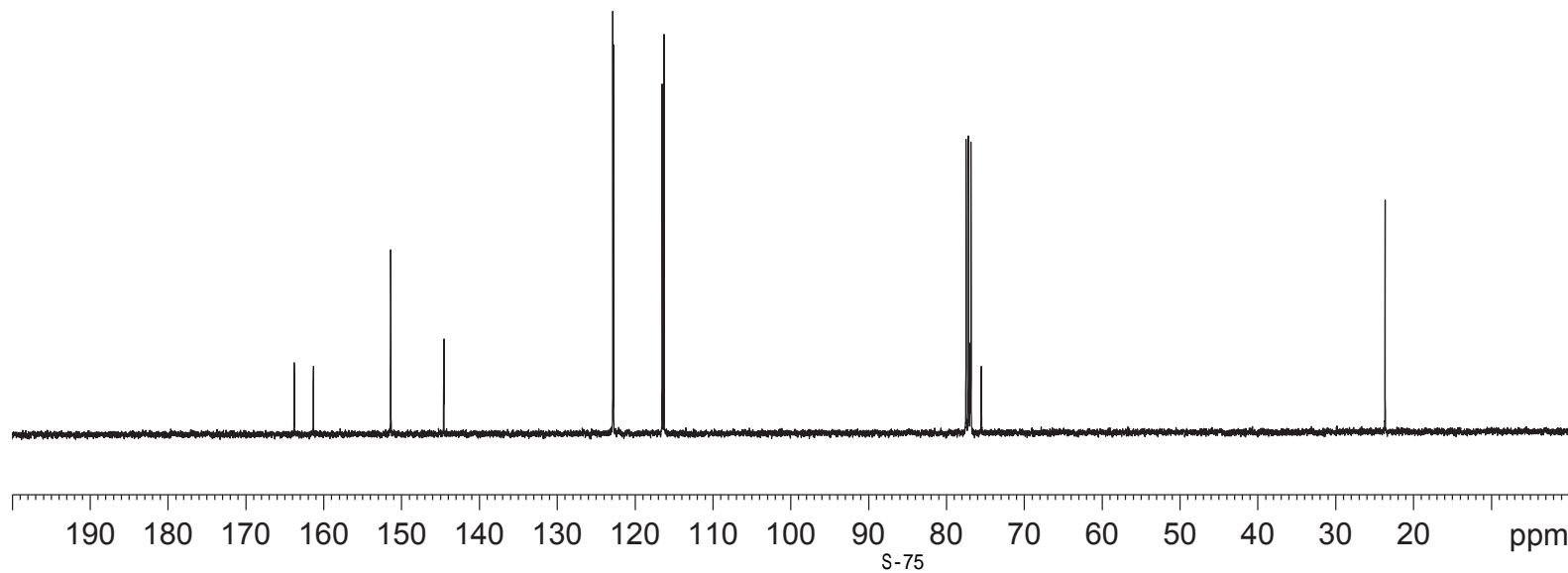
Current Data Parameters  
NAME 1hr-C-cassm406-F-CDC13  
EXPNO 1  
PROCNO 1

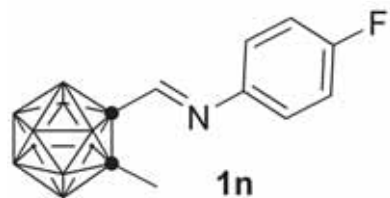
F2 - Acquisition Parameters

Date\_ 20160701  
Time\_ 15.50 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 99  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010048 sec  
RG 128  
DW 16.800 usec  
DE 6.50 usec  
TE 298.4 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 100.6379046 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





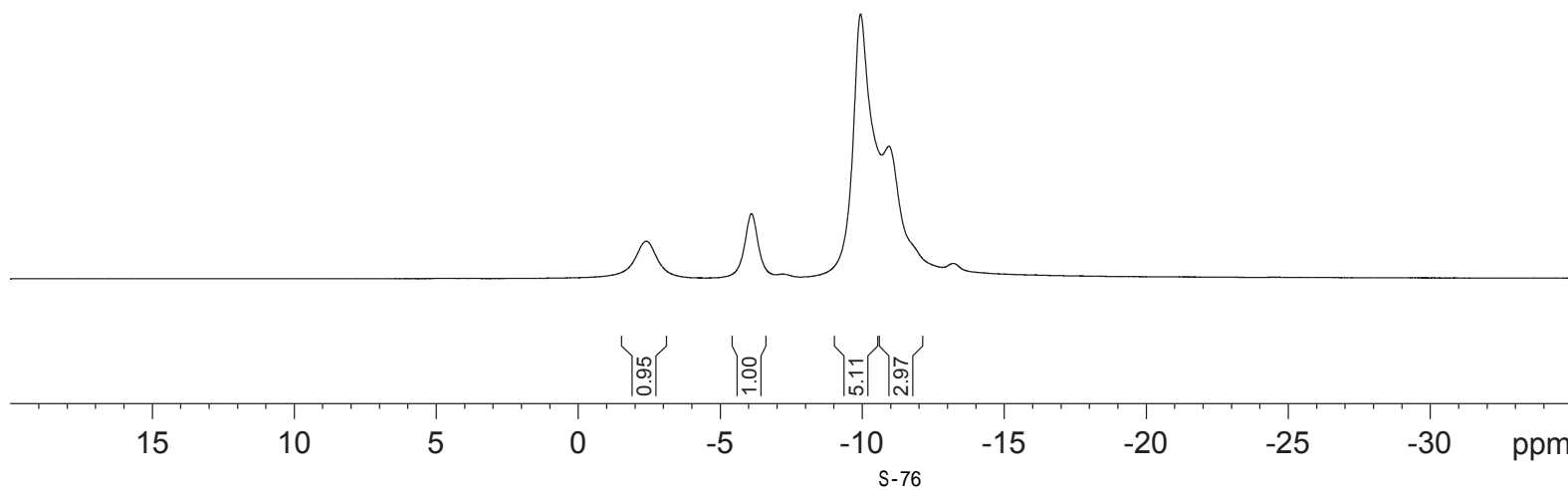
— -2.38  
 — -6.09  
 — -9.94  
 — -10.93

1hr-B-cassm406-F-CDCl3

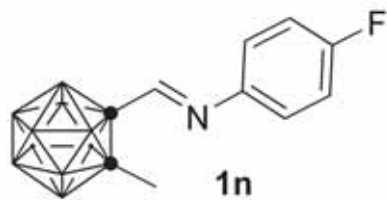
Current Data Parameters  
 NAME 1hr-B-cassm406-F-CDCl3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160701  
 Time\_ 15.58 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (zgdc)  
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 19  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 80.6  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.3 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







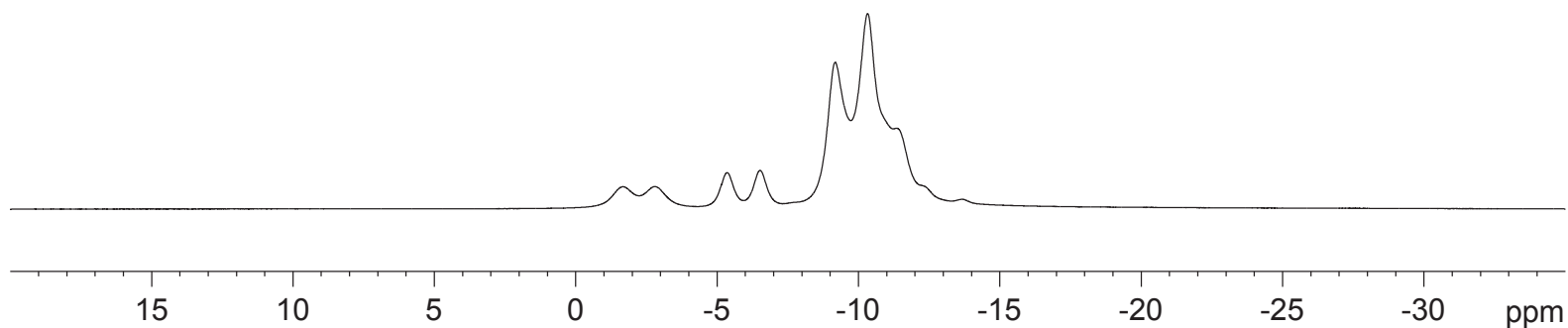
— -1.67  
 — -2.80  
 — -5.35  
 — -6.51  
 — -9.17  
 — -10.32  
 — -11.36

1hr-B-cassm406-F-CDCl3 (C)

Current Data Parameters  
 NAME 1hr-B-cassm406-F-CDCl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160701  
 Time\_ 16.00 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 26  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 80.6  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.8 K  
 D1 2.0000000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 13C  
 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



lhr-F-0704-smcascdcl3

Current Data Parameters  
NAME lhr-F-0704-smcascdcl3  
EXPNO 1  
PROCNO 1

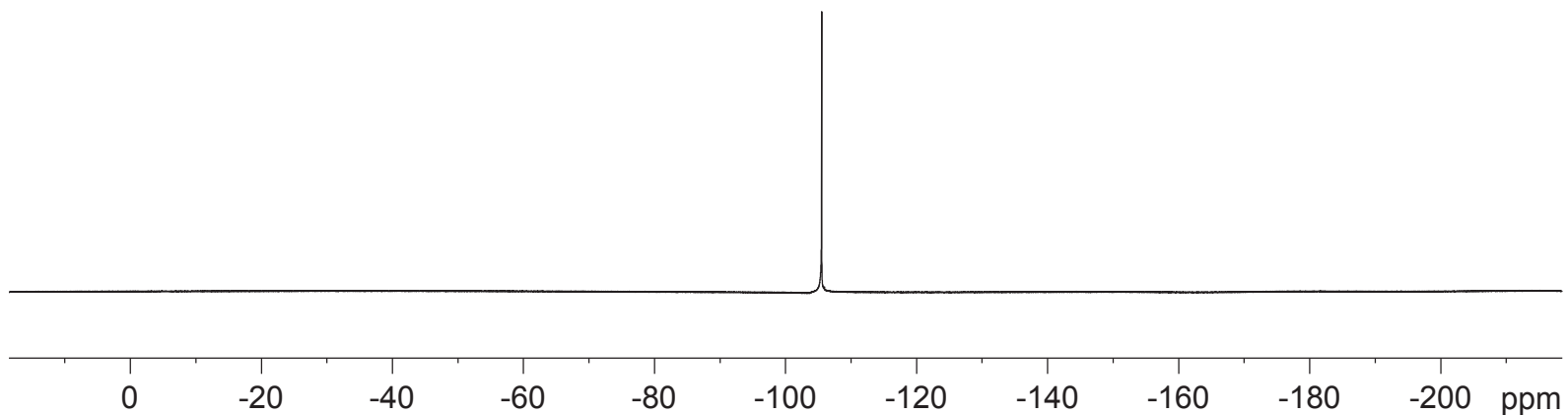
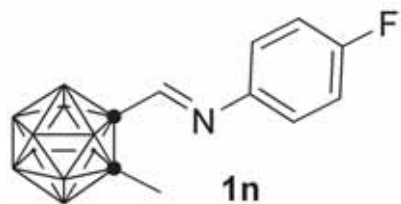
F2 - Acquisition Parameters

Date\_ 20180120  
Time\_ 9.30 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgfhigqn.2  
TD 131072  
SOLVENT D2O  
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 295.3 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

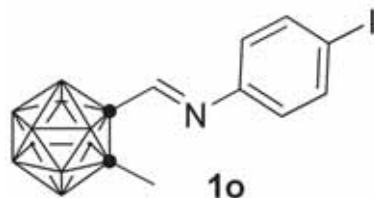
SI 65536  
SF 376.5924602 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

-105.51



7.800  
7.725  
7.704  
7.260  
6.877  
6.855

2.105

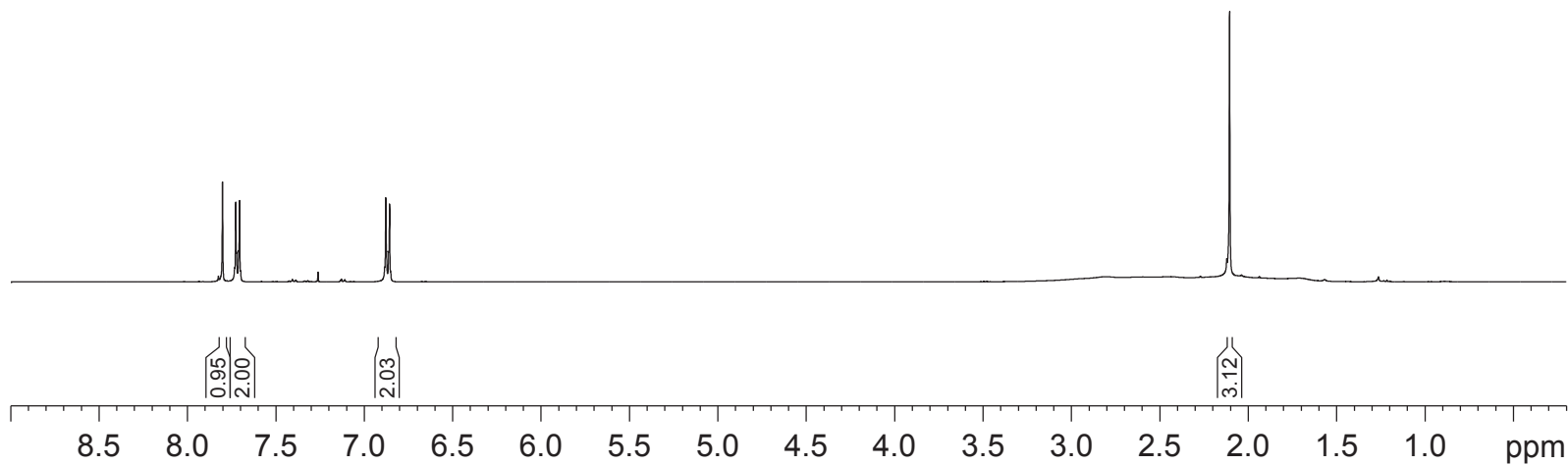


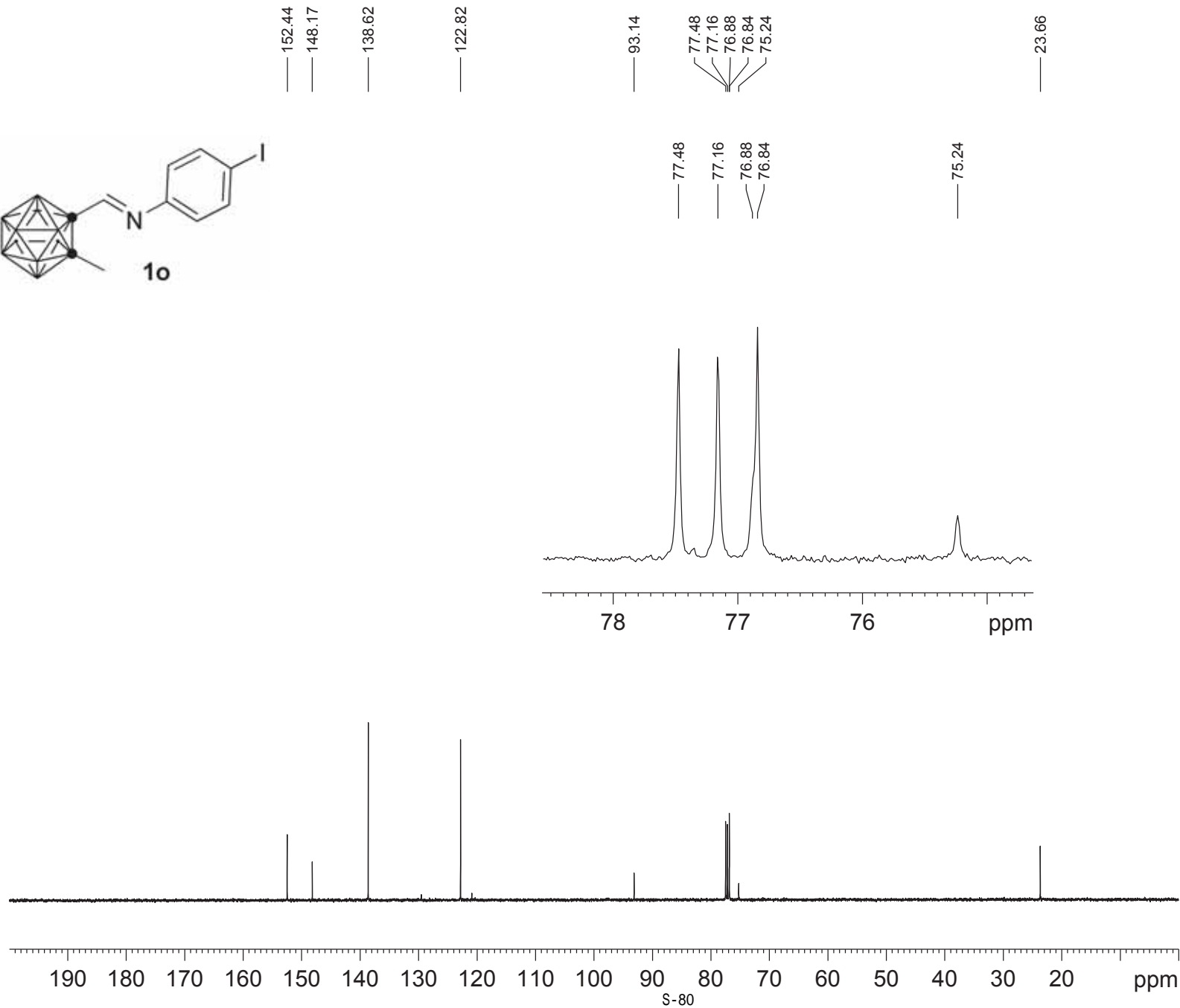
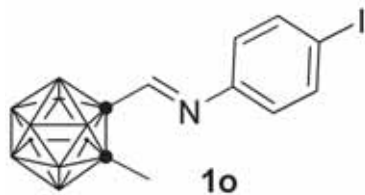
lhr-H-cassm739-I-CDCl<sub>3</sub>

Current Data Parameters  
NAME lhr-H-cassm739-I-CDCl<sub>3</sub>  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170812  
Time 19.38 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 12  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 40.3  
DW 62.400 usec  
DE 6.50 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

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





lhr-C-cassm739-I-Cl

Current Data Parameters  
 NAME lhr-C-cassm739-I-CDC1:  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170812  
 Time\_ 19.41 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 64  
 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

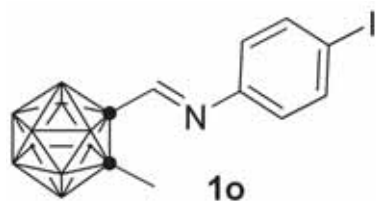
SI 32768  
 SF 100.6379061 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1hr-B-cassm739-I-CDCl3

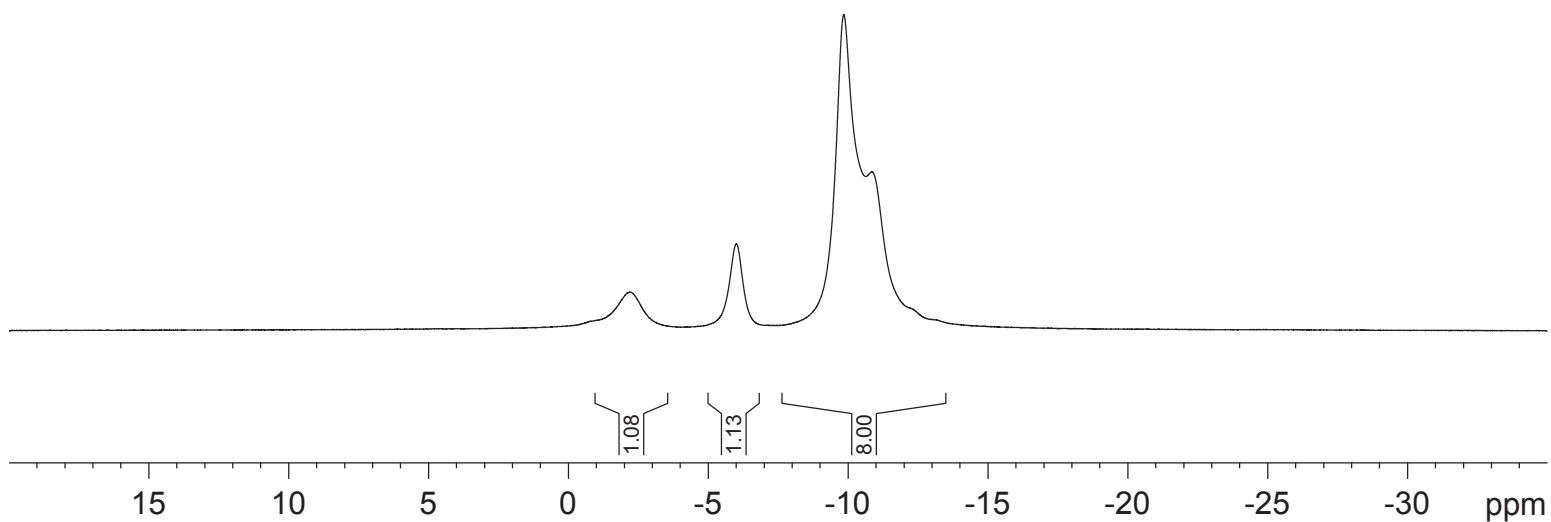
Current Data Parameters  
NAME 1hr-B-cassm739-I-CDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170812  
Time 19.32 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 295.2 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



— -2.20  
— -6.01  
— -9.85  
— -10.85



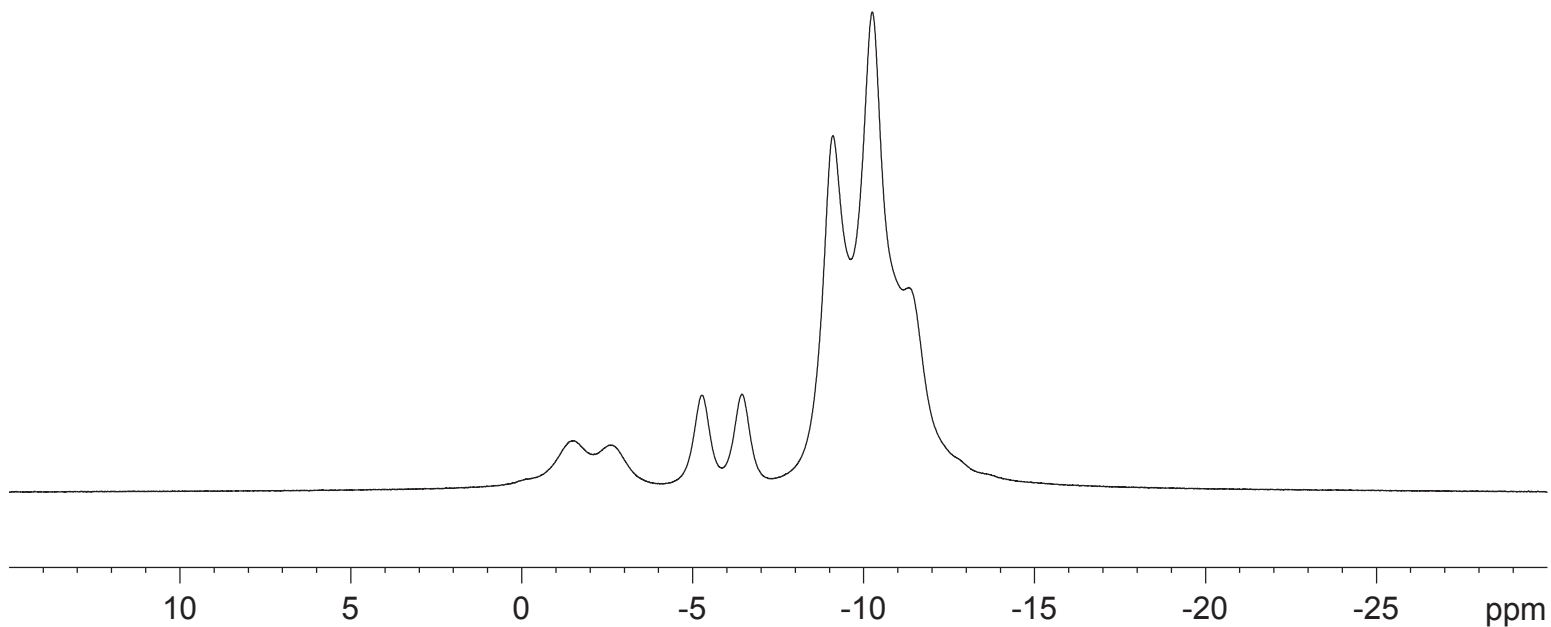
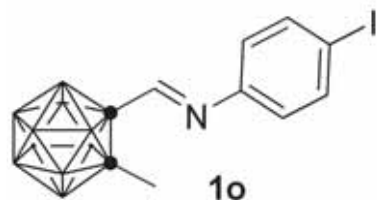
1hr-B-cassm739-I-CDCl3 (C)

Current Data Parameters  
NAME 1hr-B-cassm739-I-CDCl3 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170812  
Time 19.34 h  
INSTRUM spect  
PROBHD Z108618\_0257 ( )  
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 17  
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

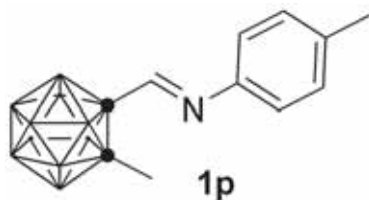
F2 - Processing parameters  
SI 32768  
SF 128.4097430 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

— -1.53  
— -2.64  
— -5.27  
— -6.44  
— -9.10  
— -10.25  
— -11.34



7.848  
7.260  
7.237  
7.217  
7.088  
7.067

2.402  
2.126



1hr-H-0732-cassm-cdc

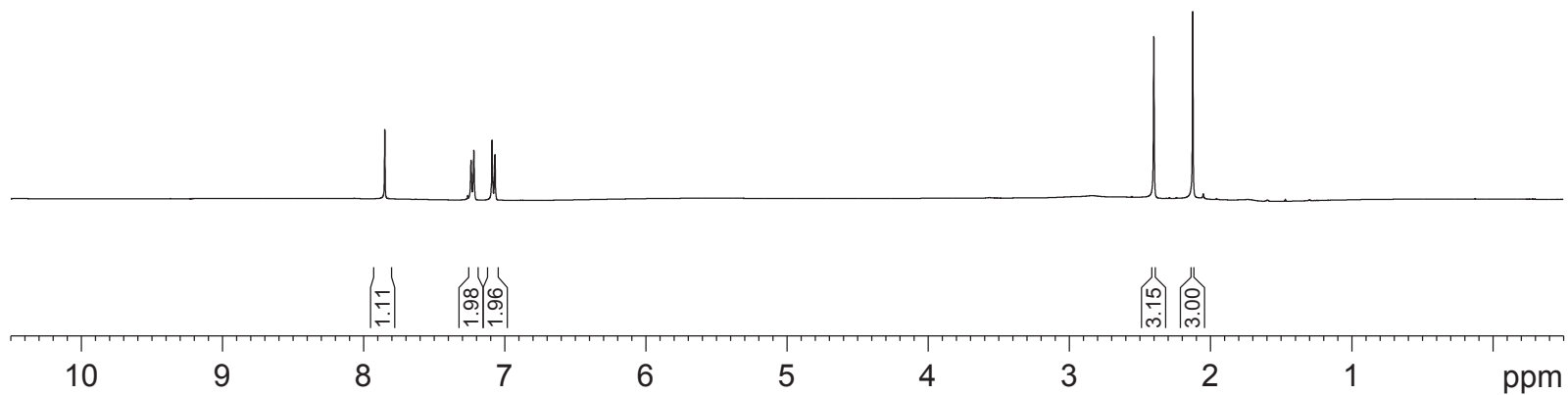
Current Data Parameters  
NAME 1hr-H-0732-cassm-cdcl3  
EXPNO 1  
PROCNO 1

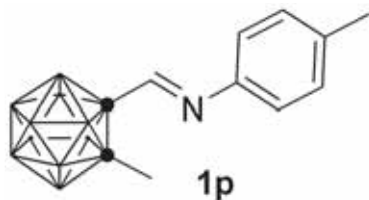
F2 - Acquisition Parameters

Date\_ 20170818  
Time 19.05 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 17  
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 294.8 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 400.2300101 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



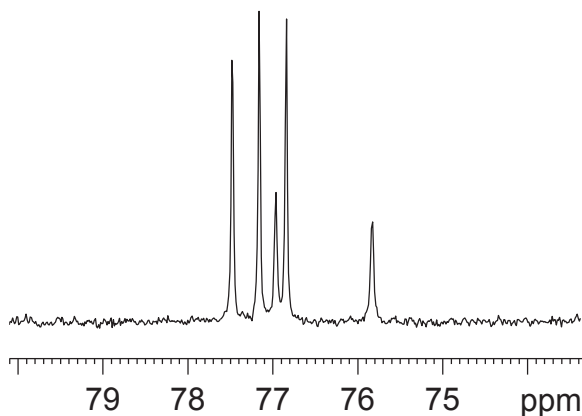


150.57  
146.01  
138.48  
130.10  
120.98

77.48  
77.16  
76.96  
76.84  
75.83

23.59  
21.20

77.48  
77.16  
76.96  
76.84  
75.83



lhr-C-0732-cassm-c

Current Data Parameters  
NAME lhr-C-0732-cassm-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170818  
Time 19.11 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 78  
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 295.3 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 100.6379089 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

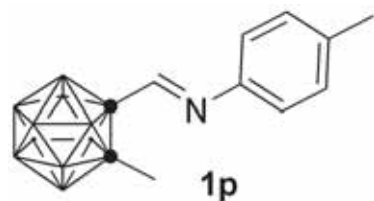


1hr-B-0732-cassm-cdcl3

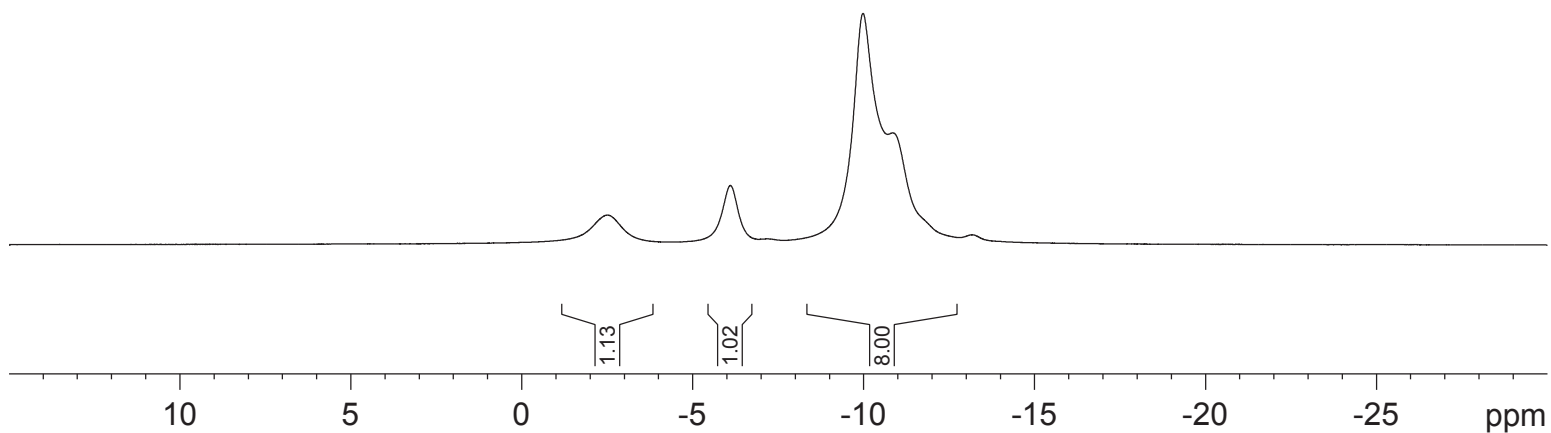
Current Data Parameters  
NAME 1hr-B-0732-cassm-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170818  
Time 19.14 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 50.8  
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



— -2.50  
— -6.10  
— -9.98  
— -10.87



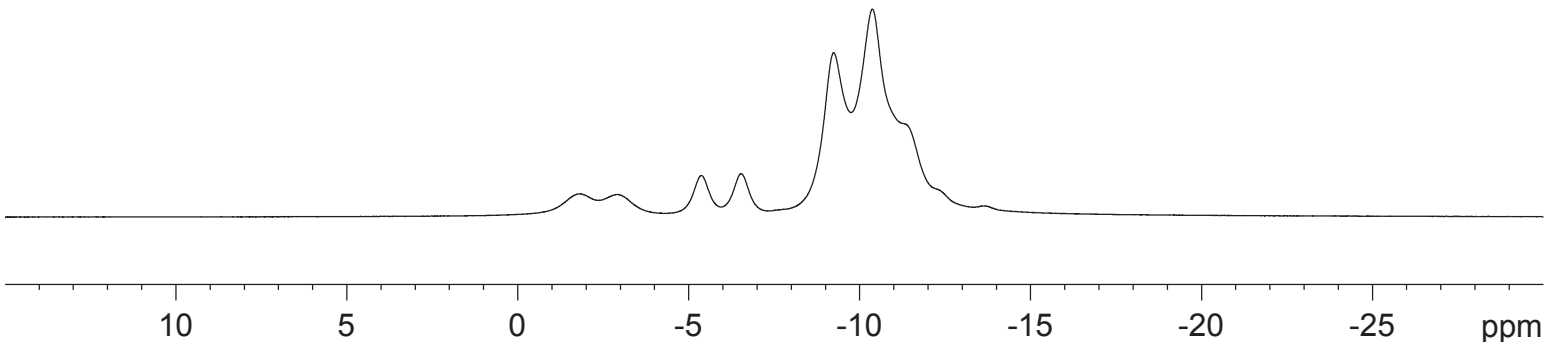
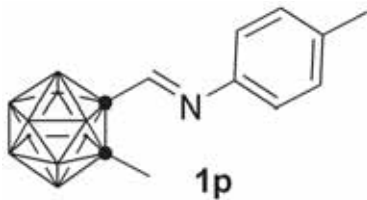
1hr-B-0732-cassm-cdcl3 (C)

Current Data Parameters  
NAME 1hr-B-0732-cassm-cdcl3 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170818  
Time 19.16 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 11  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 57  
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

— -1.81  
— -2.89  
— -5.37  
— -6.53  
— -9.24  
— -10.37  
— -11.35



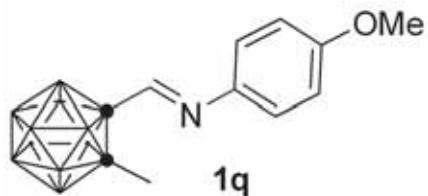
7.824  
7.260  
7.180  
7.158  
6.927  
6.905

3.833

2.090

1.592

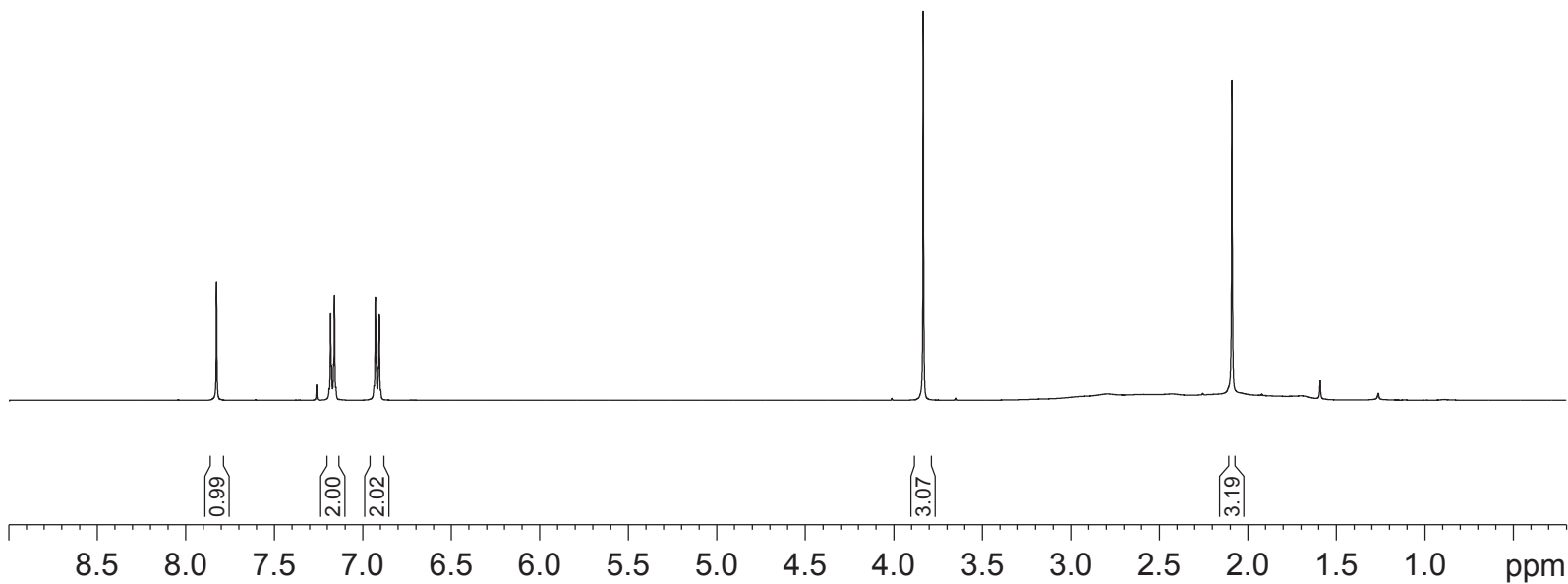
1hr-H-cassm722-omeCI

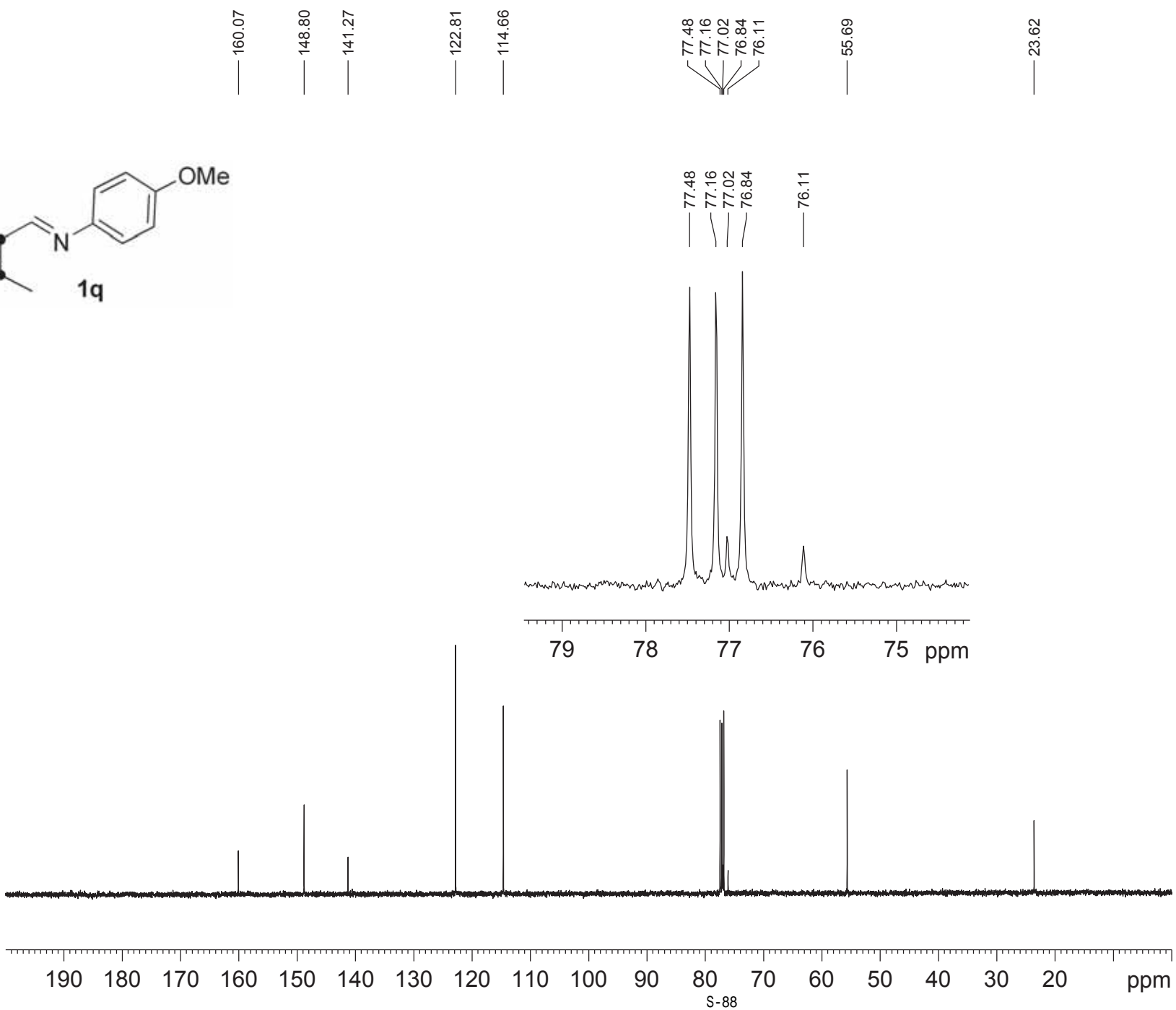
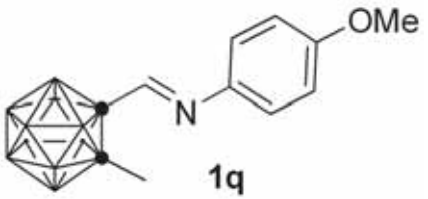


Current Data Parameters  
NAME 1hr-H-cassm722-omeCDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170817  
Time 22.09 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 40.3  
DW 62.400 usec  
DE 6.50 usec  
TE 294.7 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





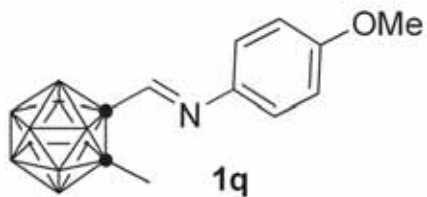
lhr-C-cassm722-omef

```

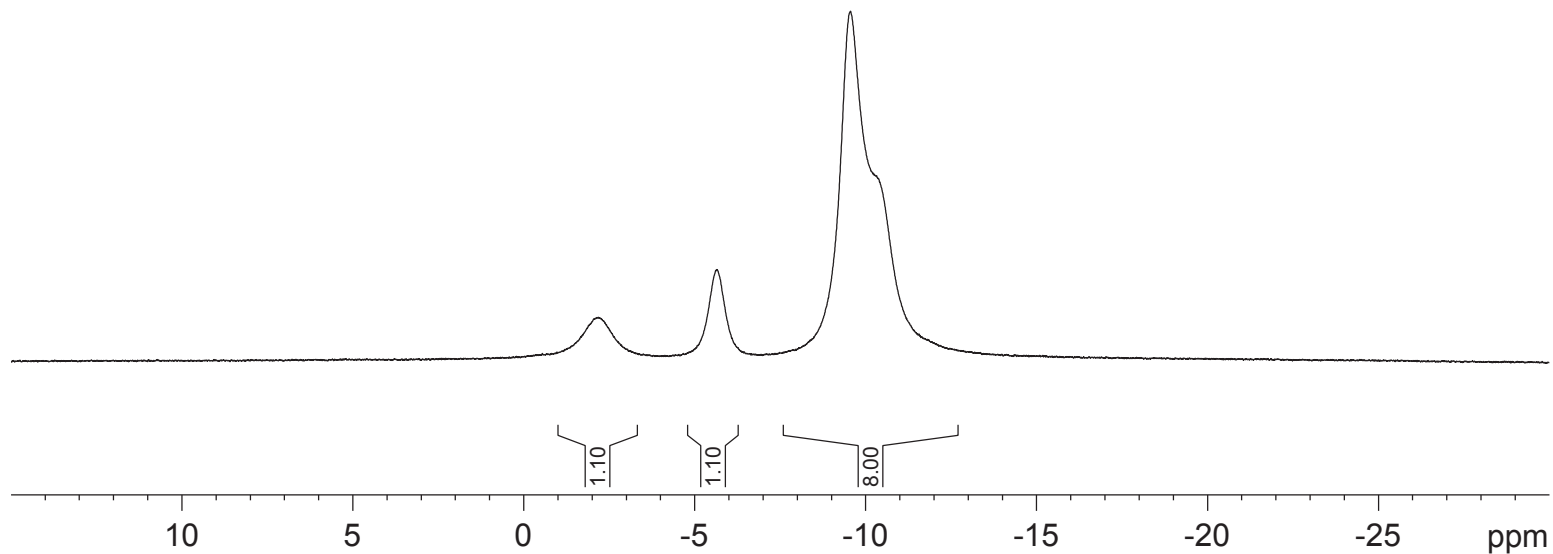
Current Data Parameters
NAME      lhr-C-cassm722-omeCDCl3
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20170817
Time_     22.13 h
INSTRUM   spect
PROBHD    Z108618_0257 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         56
DS         4
SWH       40760.871 Hz
FIDRES    0.621962 Hz
AQ         0.8039083 sec
RG         161
DW         12.267 usec
DE         6.50 usec
TE         294.8 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

F2 - Processing parameters
SI         32768
SF         100.6379037 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



— -2.18  
 — -5.64  
 — -9.56  
 — -10.28



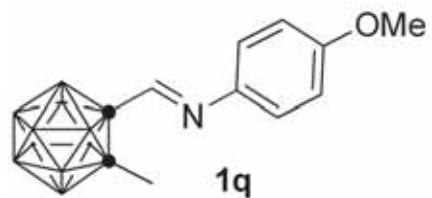
S-89

1hr-B-cassm722-omeCDCl3

Current Data Parameters  
 NAME 1hr-B-cassm722-omeCDCl3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170817  
 Time\_ 22.03 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 11  
 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 295.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 11B  
 P1 7.50 usec  
 PLW1 55.09999847 W  
 SFO2 400.2316009 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 13.56000042 W  
 PLW12 0.27428001 W

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



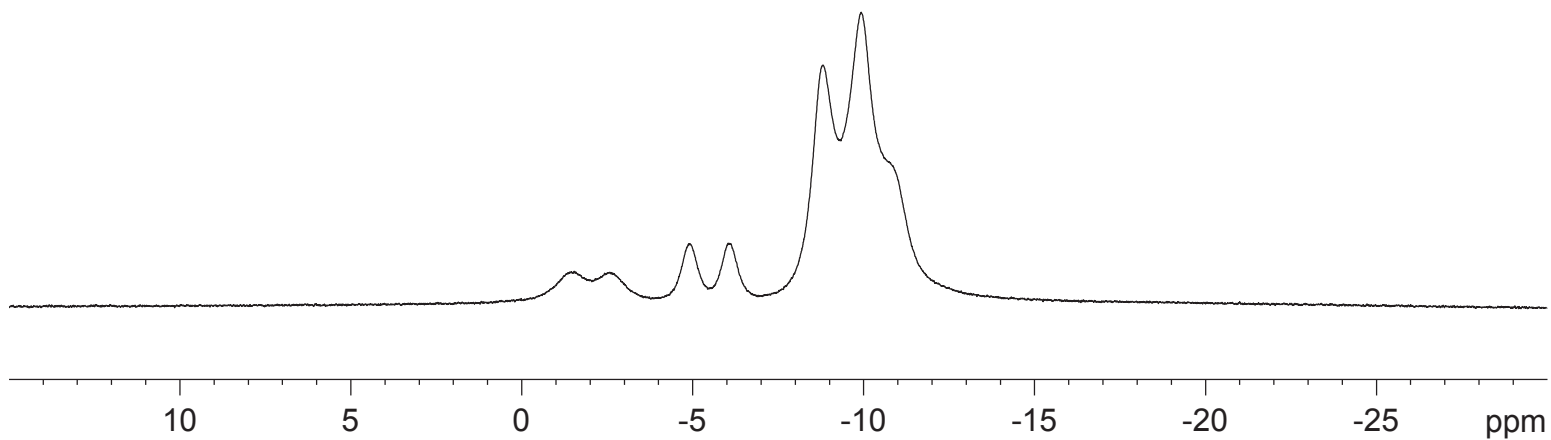
| -1.53  
 | -2.57  
 | -4.90  
 | -6.04  
 | -8.81  
 | -9.93  
 | -10.87

1hr-B-cassm722-omeCDCl3 (C)

Current Data Parameters  
 NAME 1hr-B-cassm722-omeCDCl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170817  
 Time\_ 22.04 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 2.0000000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 11B  
 P1 7.50 usec  
 PLW1 55.09999847 W

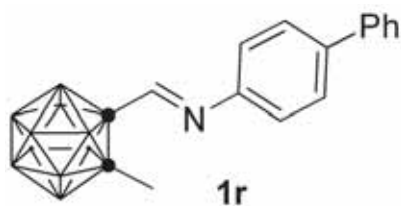
F2 - Processing parameters  
 SI 32768  
 SF 128.4097430 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



7.898  
7.654  
7.632  
7.615  
7.597  
7.494  
7.476  
7.456  
7.410  
7.397  
7.392  
7.374  
7.260  
7.239  
7.235  
7.223  
7.218

2.147

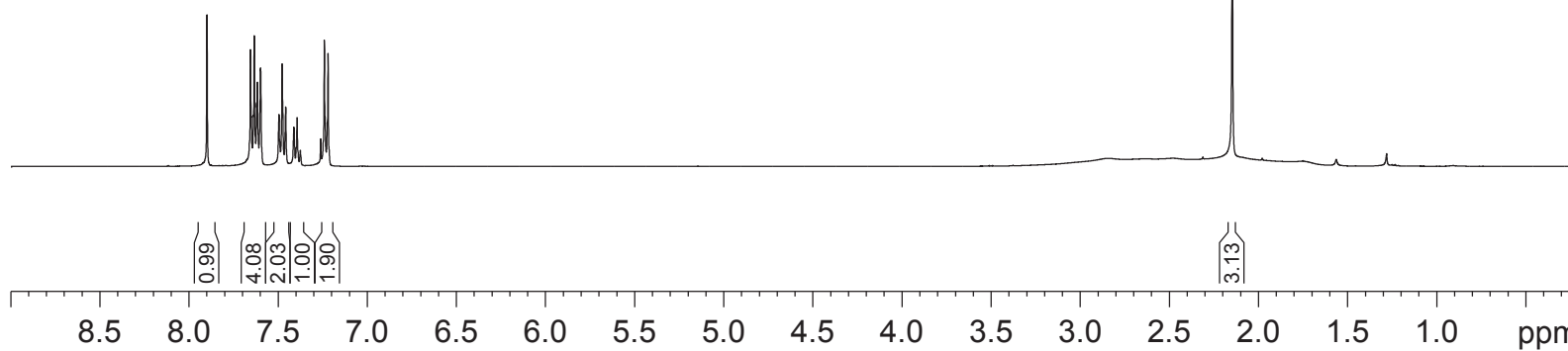
1hr-H-cassm746-ph-Cl

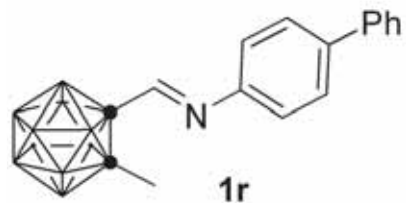


Current Data Parameters  
NAME 1hr-H-cassm746-ph-CDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170812  
Time 19.02 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 203  
DW 62.400 usec  
DE 6.50 usec  
TE 294.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

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

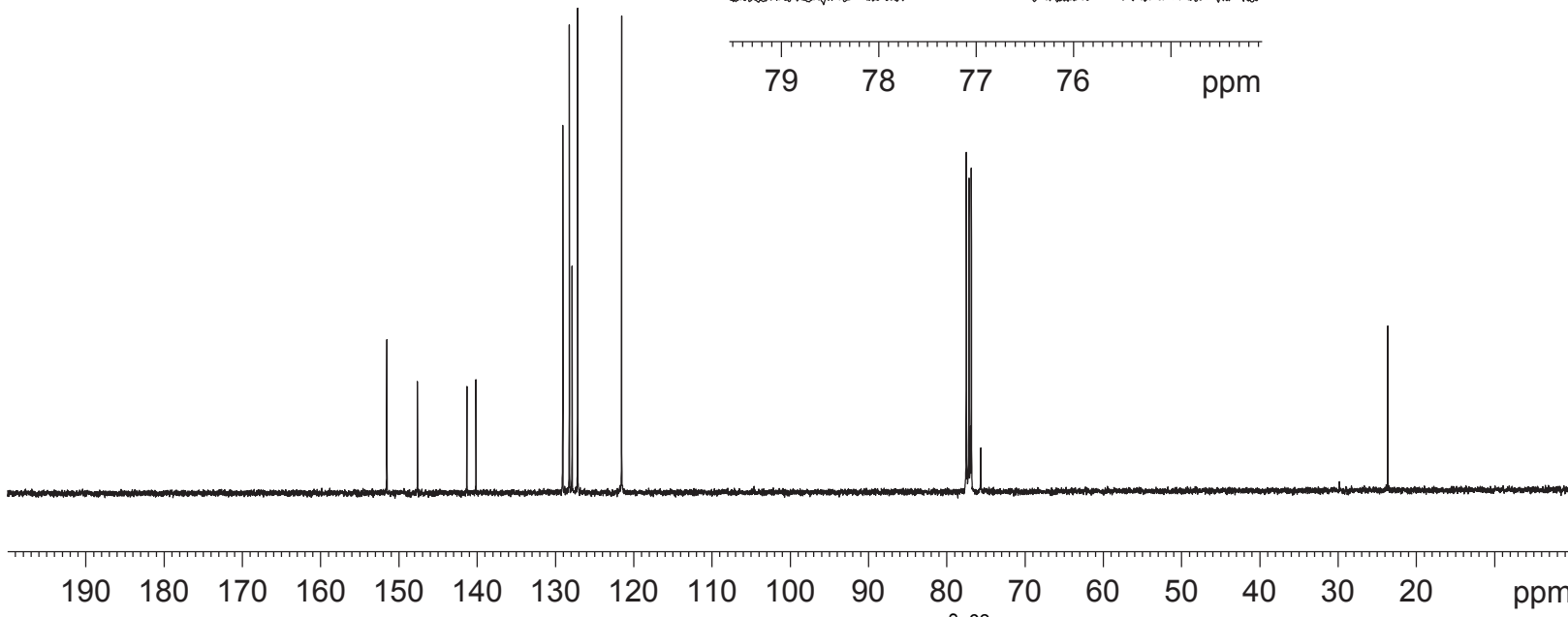
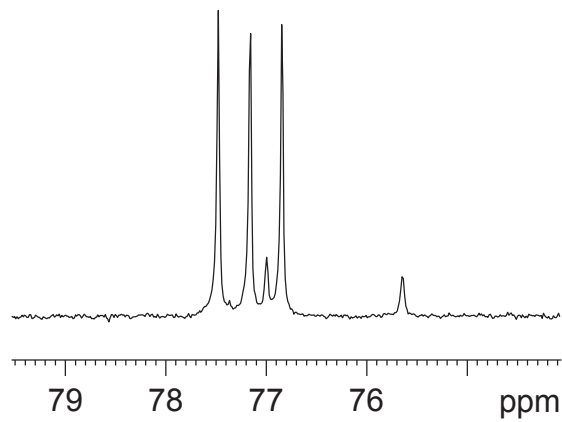




151.54  
147.62  
141.31  
140.13  
129.05  
128.21  
127.86  
127.14  
121.53

77.48  
77.16  
77.00  
76.84  
75.64

23.68



1hr-C-cassm746-Ph-(

Current Data Parameters  
NAME 1hr-C-cassm746-Ph-CDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170812  
Time\_ 19.06 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 349  
DS 4  
SWH 40760.871 Hz  
FIDRES 0.621962 Hz  
AQ 0.8039083 sec  
RG 161  
DW 12.267 usec  
DE 6.50 usec  
TE 295.3 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

F2 - Processing parameters  
SI 32768  
SF 100.6379044 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

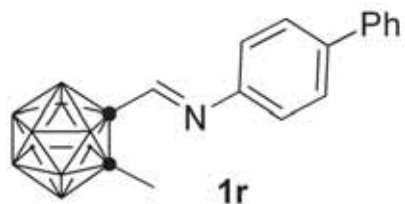


1hr-B-cassm746-ph-CDCl3

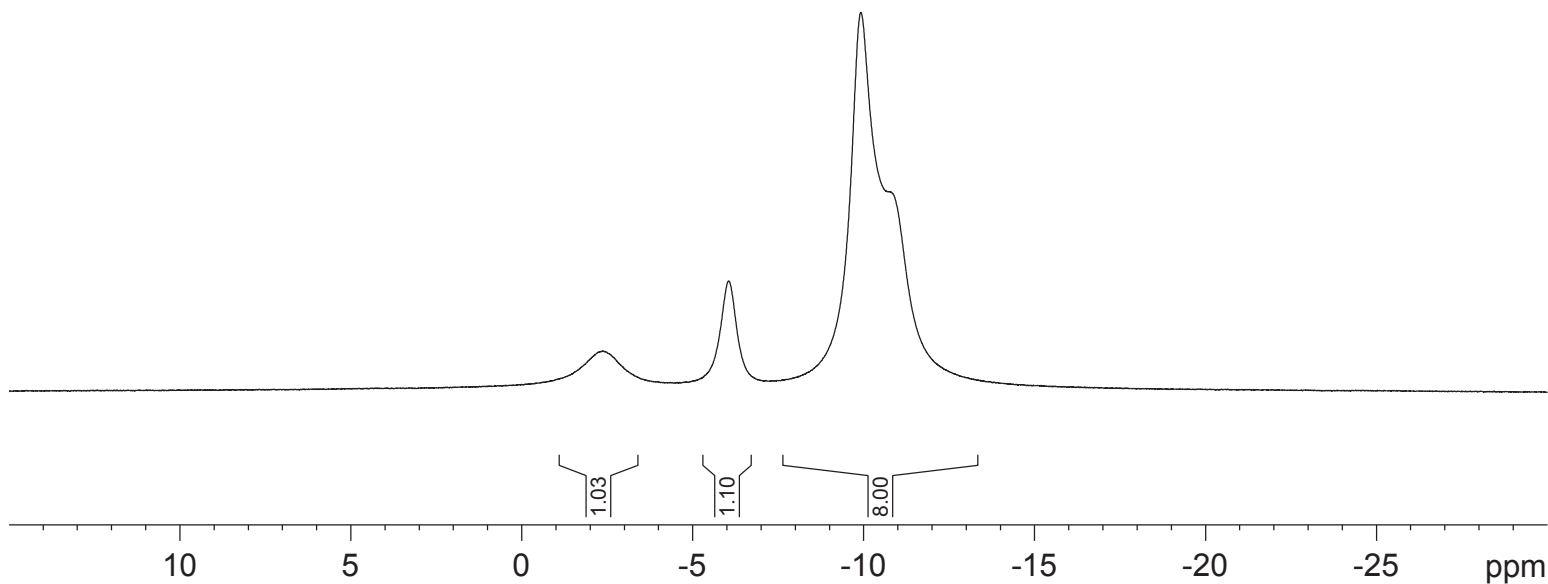
Current Data Parameters  
NAME 1hr-B-cassm746-ph-CDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170812  
Time\_ 19.23 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 15  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 295.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 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



— 2.38  
— 6.06  
— 9.91  
— 10.80



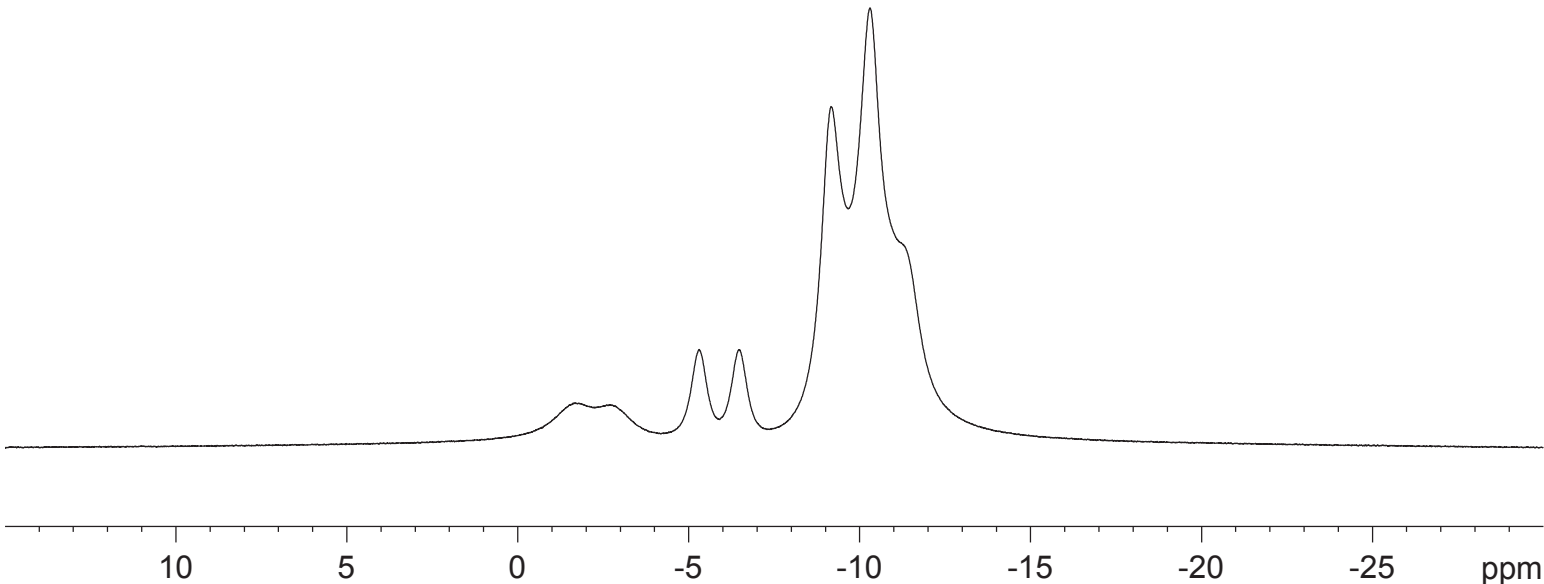
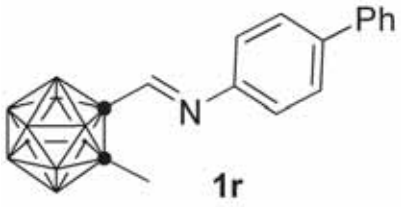
1hr-B-cassm746-ph-CDCl3 (C)

Current Data Parameters  
NAME 1hr-B-cassm746-ph-CDCl3 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170812  
Time 19.25 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 23  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.0000000 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

— -1.66  
— -2.72  
— -5.31  
— -6.49  
— -9.17  
— -10.30  
— -11.29

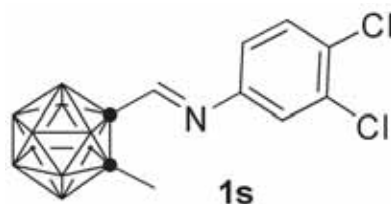


I hr-H-CASSM764

Current Data Parameters  
NAME I hr-H-cassm764  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180124  
Time 9.38  
INSTRUM spect  
PROBHD Z149001\_0010 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 30.85  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300116  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00



7.809  
7.475  
7.458  
7.260  
7.224  
7.219  
6.989  
6.984  
6.972  
6.967

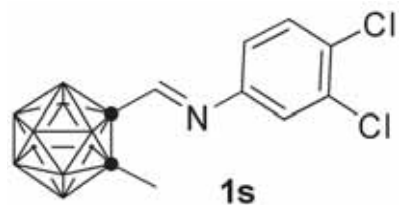
2.108



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

1.00  
1.01  
0.97  
1.03

3.17



153.55  
147.82  
133.57  
132.13  
131.24  
122.89  
120.43

77.41  
77.16  
76.91  
74.93

23.71

1 hr-C-CASSM764

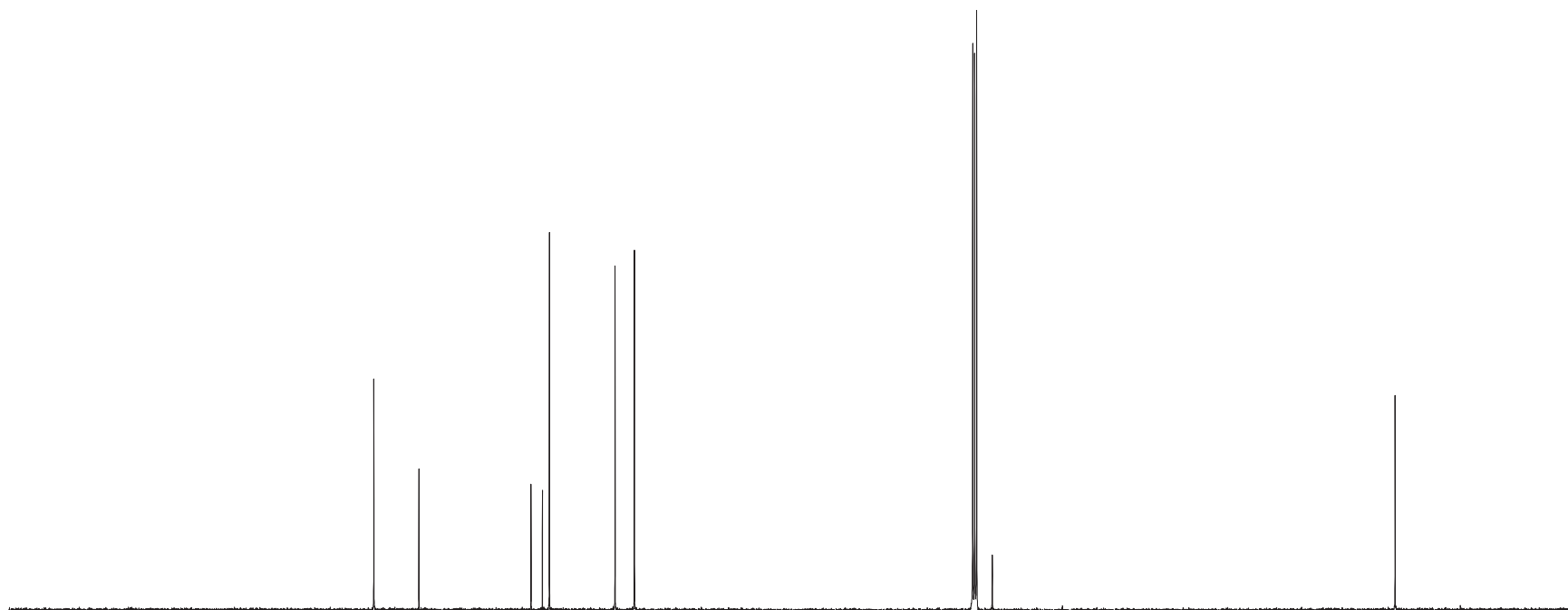
Current Data Parameters  
NAME 1 hr-C-cassm764  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20180124  
Time 9.44 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 102  
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  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

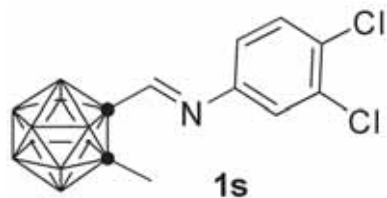
F2 - Processing parameters

SI 32768  
SF 125.7577745 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

I hr-B-CASSM764

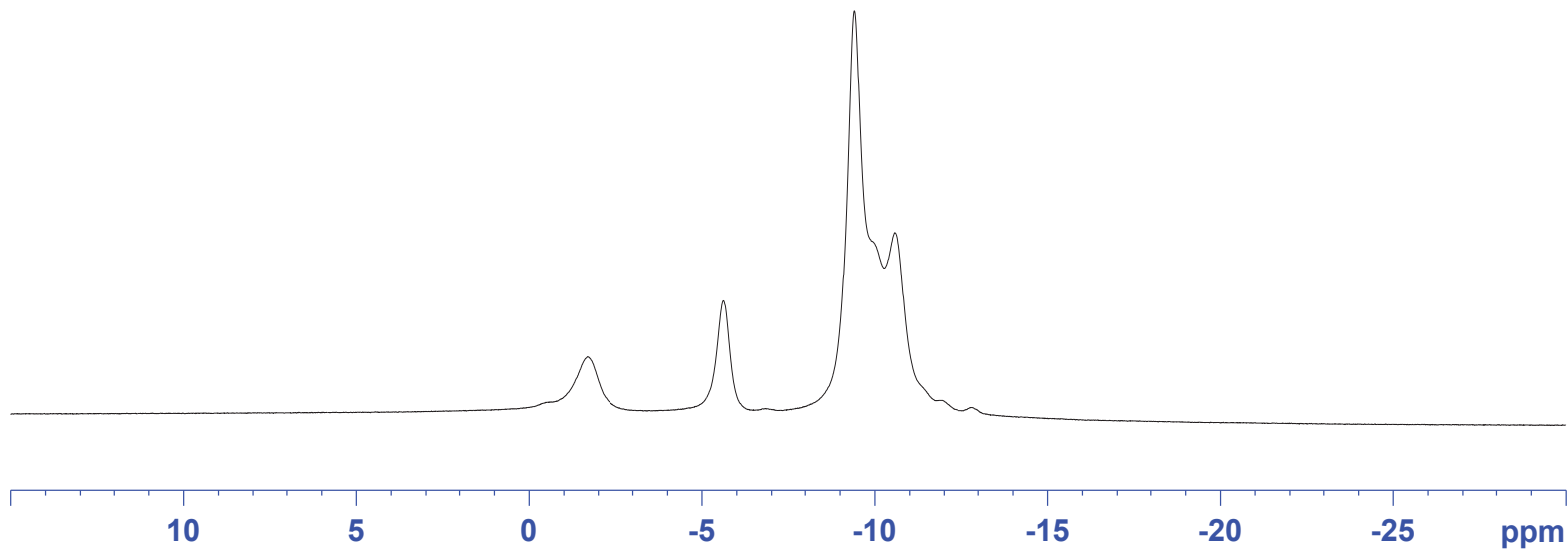


— -1.68  
— -5.62  
— -9.41  
— -10.57

Current Data Parameters  
NAME I hr-B-cassm764  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180124  
Time 9.48 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl 3  
NS 20  
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 1.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4615790 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

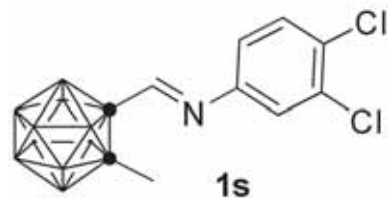
F2 - Processing parameters  
SI 16384  
SF 160.4615999 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.06  
1.13  
8.00

I hr-B-CASSM764(C)

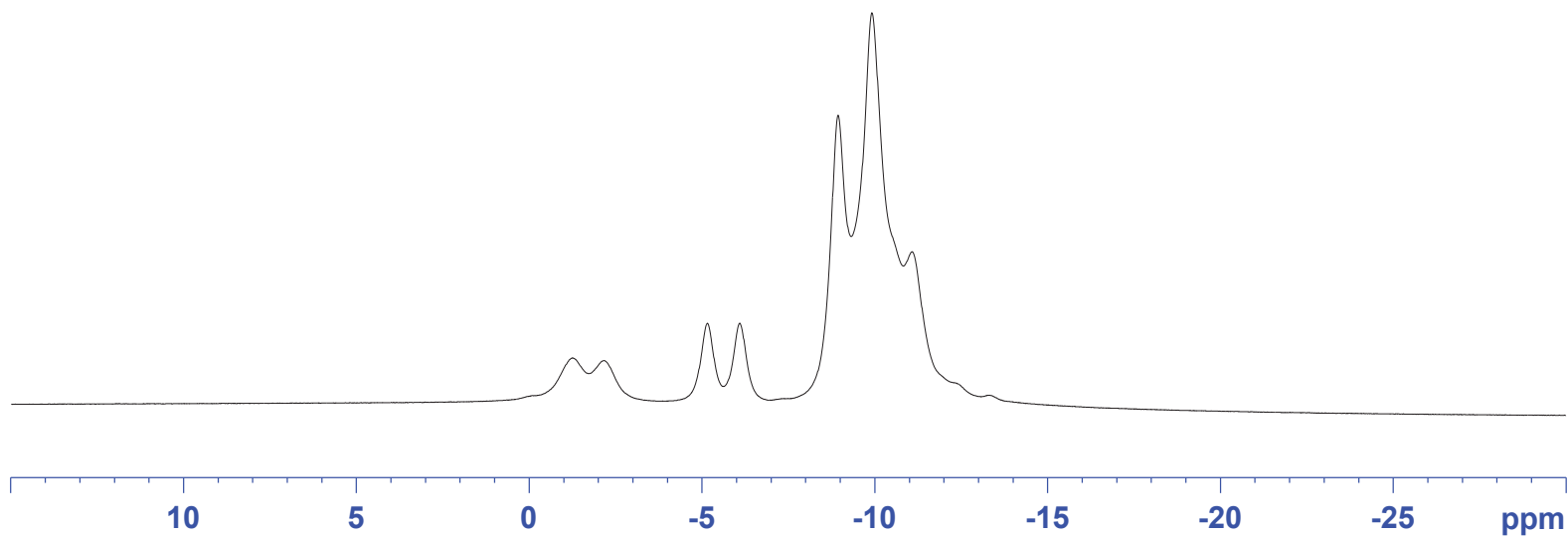
-1.24  
-2.15  
-5.15  
-6.09  
-8.93  
-9.91  
-11.08



Current Data Parameters  
NAME I hr-B-cassm764(c)  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180124  
Time 9.49 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 20  
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 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

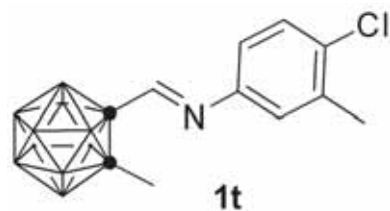
F2 - Processing parameters  
SI 16384  
SF 160.4615997 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



7.808  
7.359  
7.338  
7.260  
7.008  
6.918  
6.897

2.400  
2.111

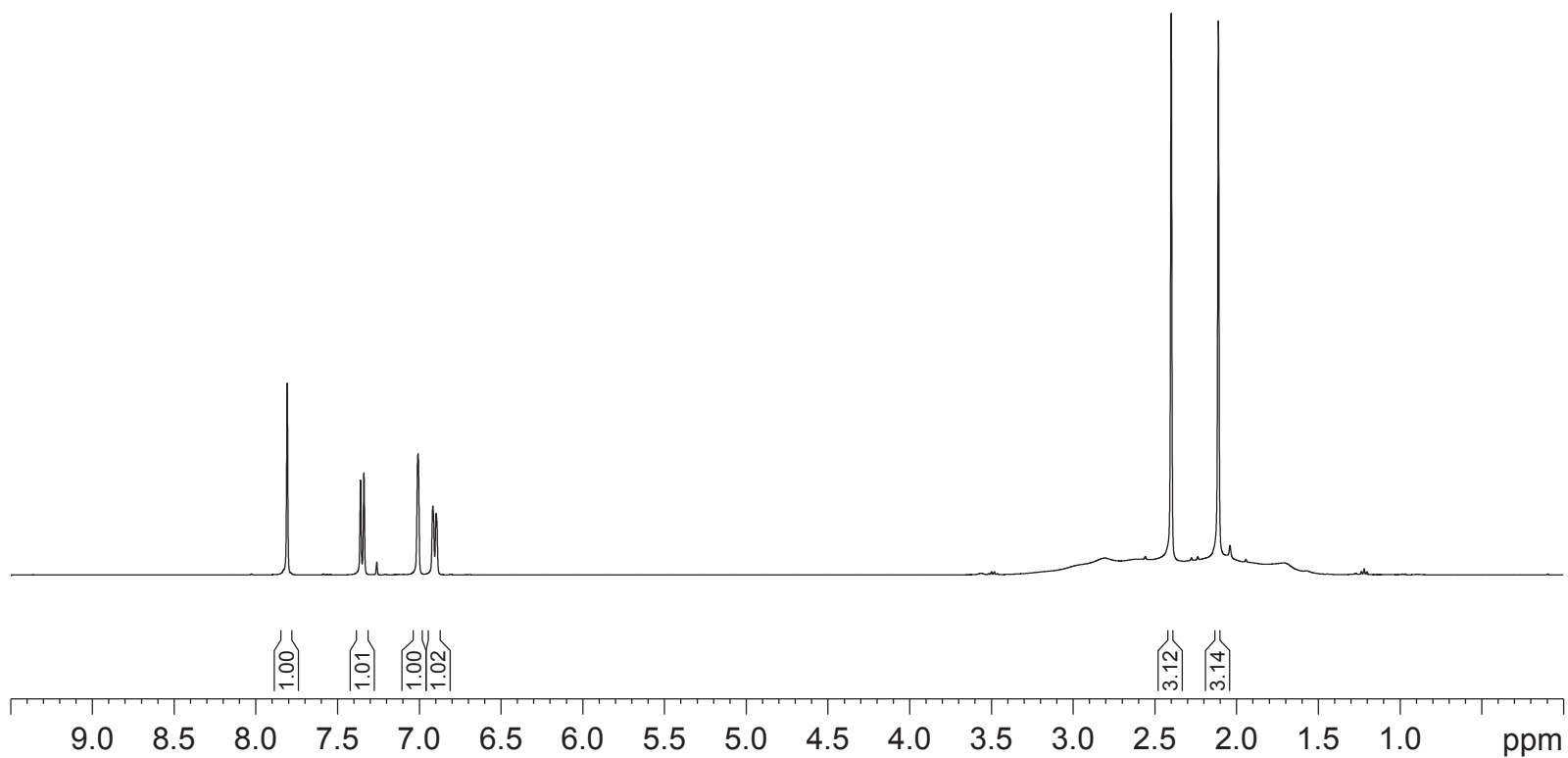
[1hr-H-cassm-783-cdc]

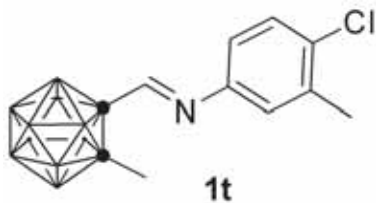


Current Data Parameters  
NAME 1hr-H-cassm-783-cdc  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171209  
Time 16.38 h  
INSTRUM spect  
PROBHD Z108618\_0257 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 9  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 28.5  
DW 62.400 usec  
DE 6.50 usec  
TE 297.1 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 400.2300101 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





— 151.92  
 — 146.99  
 — 137.49  
 — 134.10  
 — 130.00  
 — 123.54  
 — 119.43

77.48  
 77.16  
 76.93  
 76.84  
 75.44

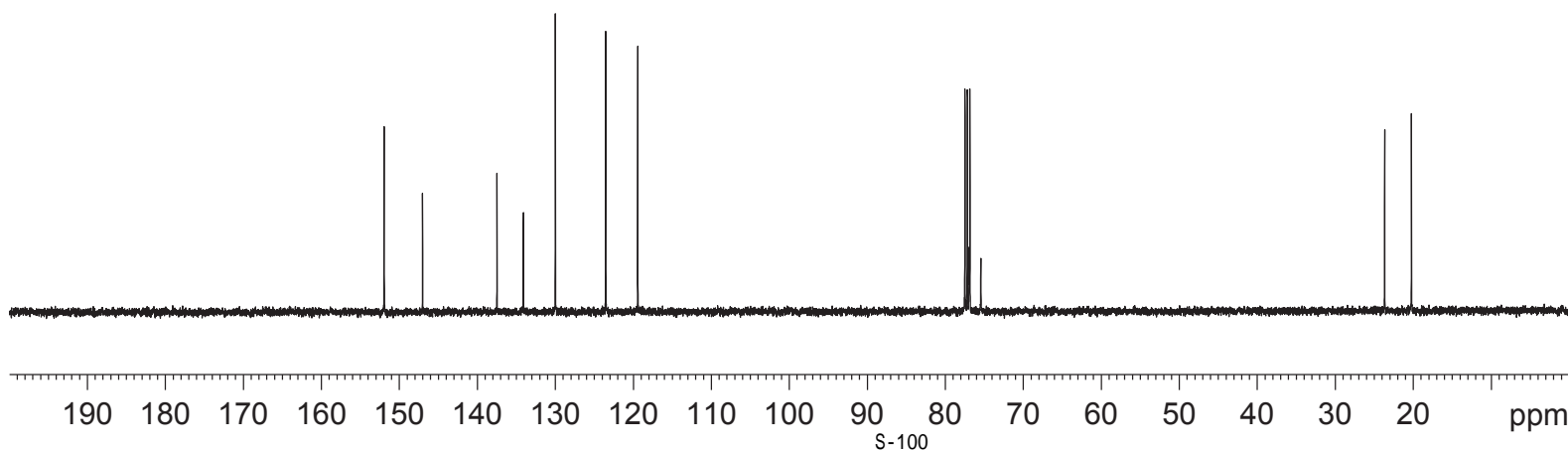
— 23.66  
 — 20.22

lhr-C-cassm-783-cdcl3

Current Data Parameters  
 NAME lhr-C-cassm-783-cdcl3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20171209  
 Time 16.41 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 60  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.454131 Hz  
 AQ 1.1010048 sec  
 RG 203  
 DW 16.800 usec  
 DE 6.50 usec  
 TE 297.4 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 100.6379043 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





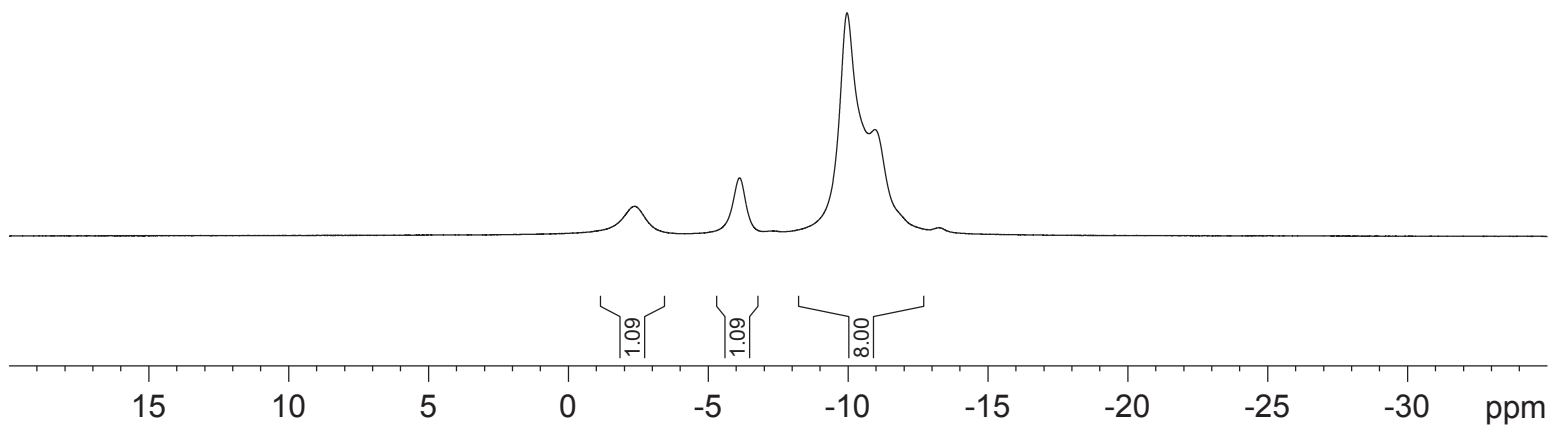
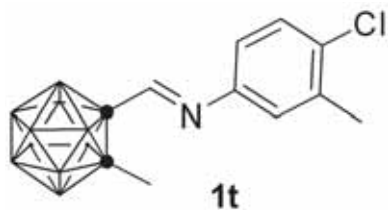
1hr-B-cassm-783-cdcl3

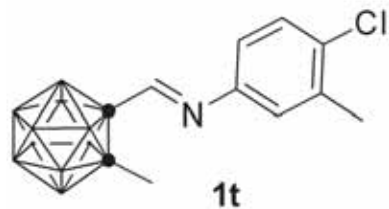
Current Data Parameters  
NAME 1hr-B-cassm-783-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171209  
Time 17.00 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 6  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 203  
DW 20.800 usec  
DE 6.50 usec  
TE 297.1 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

— -2.38  
— -6.12  
— -9.97  
— -10.97





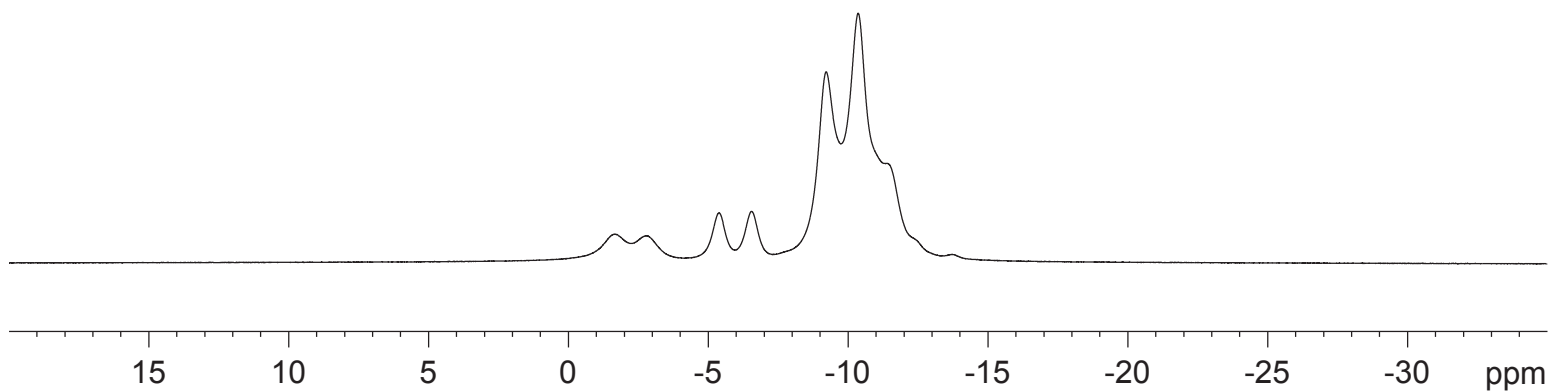
| -1.69  
 | -2.78  
 | -5.38  
 | -6.54  
 | -9.21  
 | -10.36  
 | -11.37

1hr-B-cassm-783-cdcl3 (c)

Current Data Parameters  
 NAME 1hr-B-cassm-783-cdcl3 (c)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20171209  
 Time\_ 17.01 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 10  
 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 296.8 K  
 D1 2.0000000 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

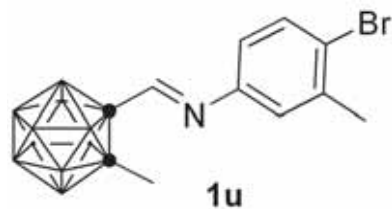


1 hr-H-cassm794

Current Data Parameters  
NAME 1 hr-H-cassm794  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171214  
Time 11.42  
INSTRUM spect  
PROBHD Z149001\_0010 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 16.5  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300126  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00



7.809  
7.542  
7.525  
7.260  
7.003  
6.998  
6.830  
6.825  
6.814  
6.809

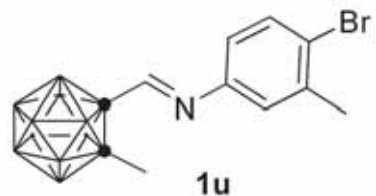
2.421  
2.110

1.00  
1.01  
1.01  
1.02

3.18  
3.17

S-103

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



152.03  
147.67  
139.37  
133.28  
124.33  
123.38  
119.58

77.41  
77.16  
76.91  
75.40

23.66  
23.07

1 hr-C-cassm794

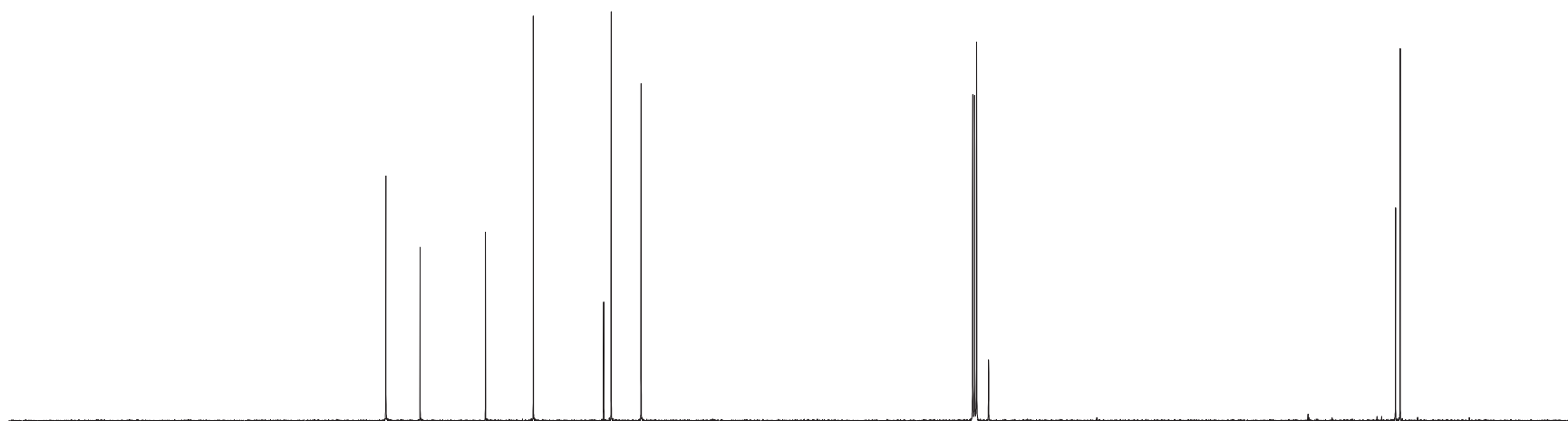
Current Data Parameters  
NAME 1 hr-C-cassm794  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20171214  
Time 11.48 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters

SI 32768  
SF 125.7577783 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

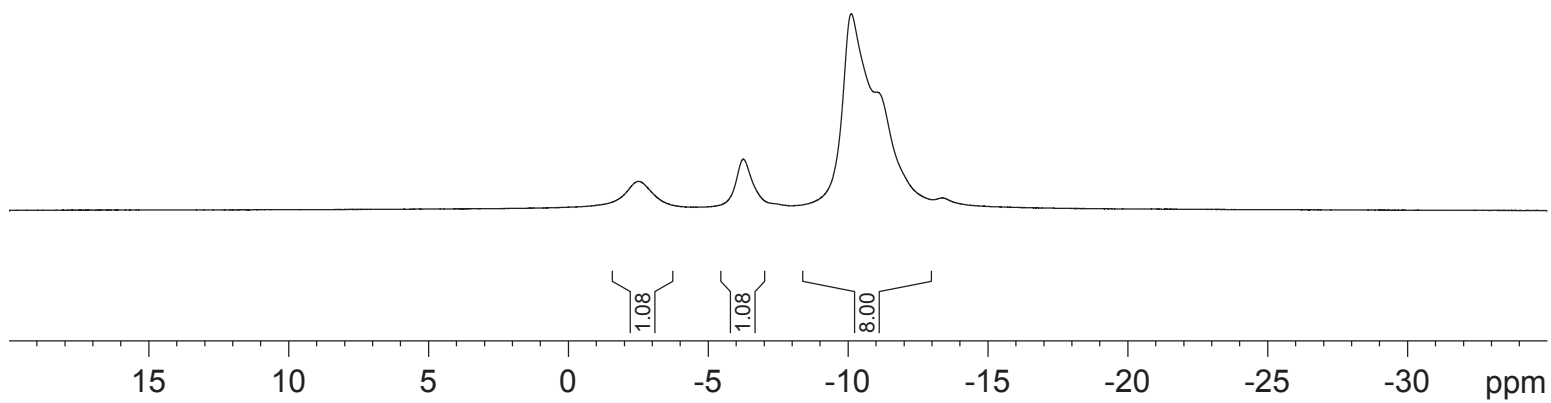
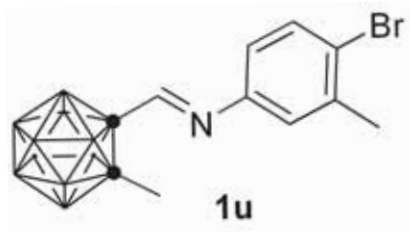
lhr-B-cassm-794-cdcl3

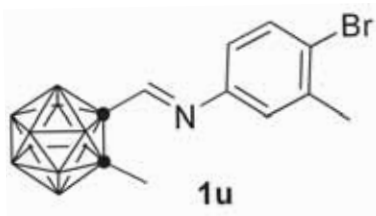
Current Data Parameters  
NAME lhr-B-cassm-794-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171214  
Time 11.37 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT THF  
NS 36  
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 296.5 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

— -2.49  
— -6.25  
— -10.11  
— -11.06





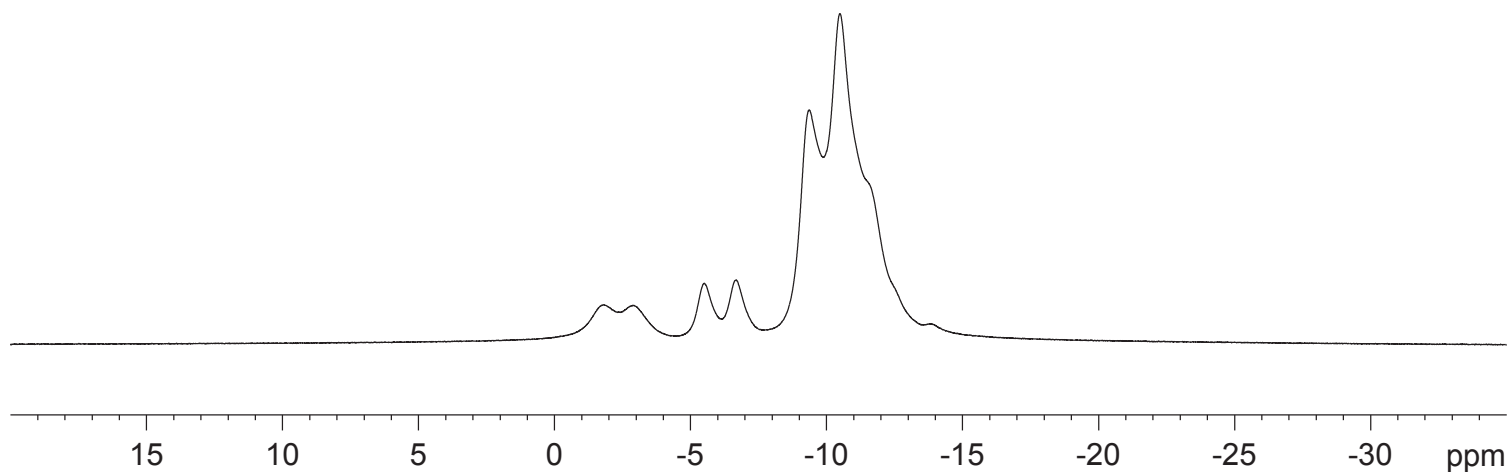
| -1.84  
 | -2.91  
 | -5.51  
 | -6.67  
 | -9.35  
 | -10.50  
 | -11.57

lhr-B-cassm-794-cdcl3 (C)

Current Data Parameters  
 NAME lhr-B-cassm-794-cdcl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20171214  
 Time\_ 11.38 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT THF  
 NS 16  
 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 296.0 K  
 D1 2.00000000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 11B  
 P1 7.50 usec  
 PLW1 55.09999847 W

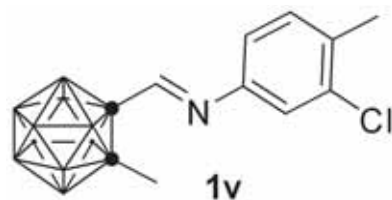
F2 - Processing parameters  
 SI 32768  
 SF 128.4097430 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



7.815  
7.267  
7.247  
7.149  
6.970  
6.950

2.395  
2.111

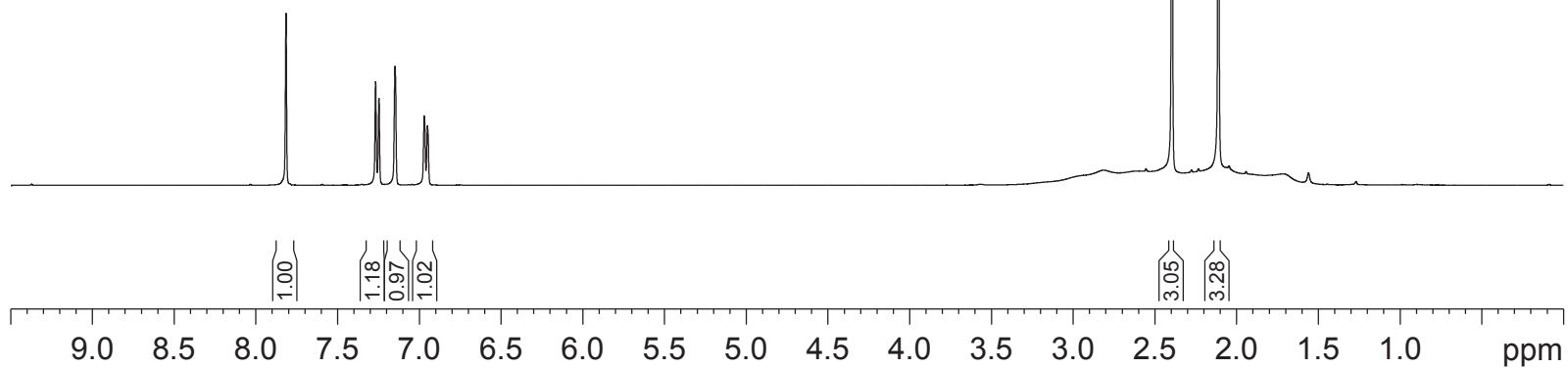
[hr-H-cassm-795-cdc]

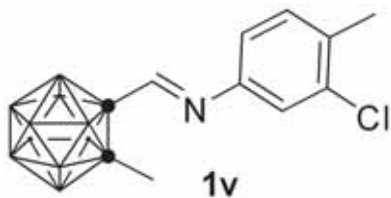


Current Data Parameters  
NAME hr-H-cassm-795-cdc  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171209  
Time 16.48 h  
INSTRUM spect  
PROBHD Z108618\_0257 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 13  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 64  
DW 62.400 usec  
DE 6.50 usec  
TE 296.9 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 400.2300068 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





152.14  
147.35  
136.19  
135.18  
131.67  
121.57  
119.42

77.48  
77.16  
76.96  
76.84  
75.36

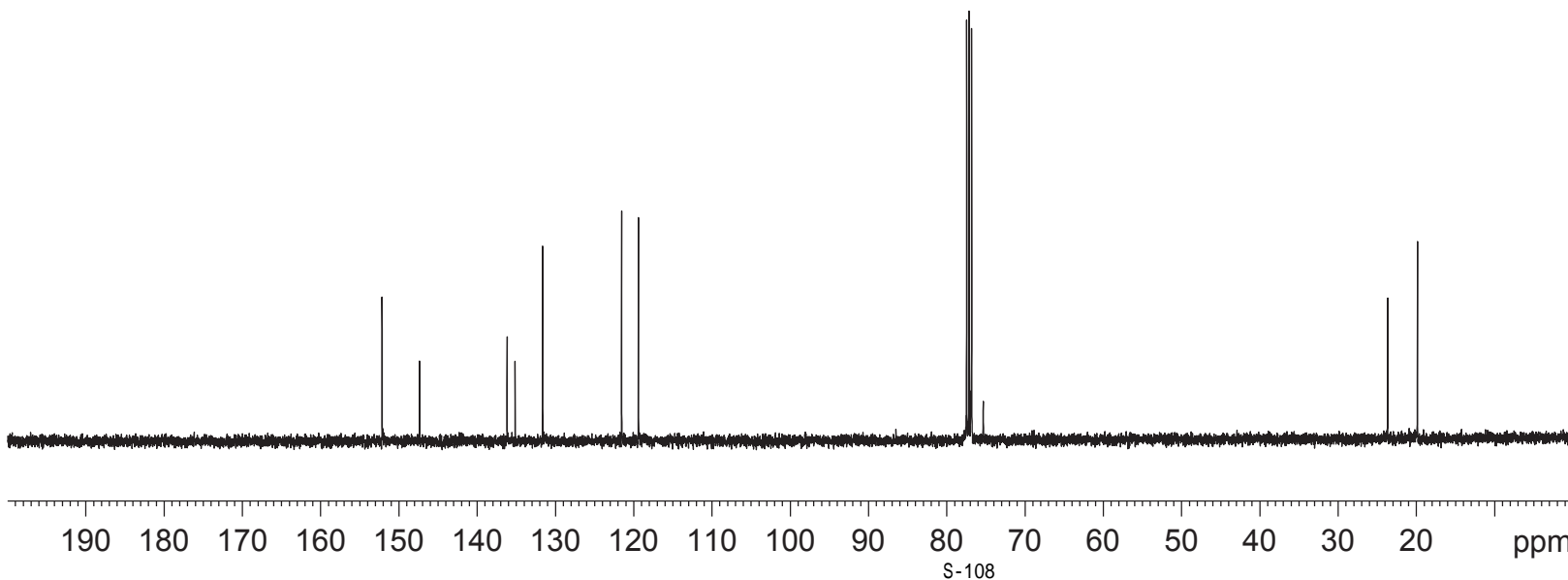
23.69  
19.87

lhr-C-cassm-795-cd

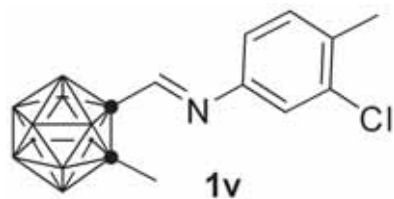
Current Data Parameters  
NAME lhr-C-cassm-795-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171209  
Time 16.53 h  
INSTRUM spect  
PROBHD Z108618\_0257 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 100  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010048 sec  
RG 203  
DW 16.800 usec  
DE 6.50 usec  
TE 297.3 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 100.6379010 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







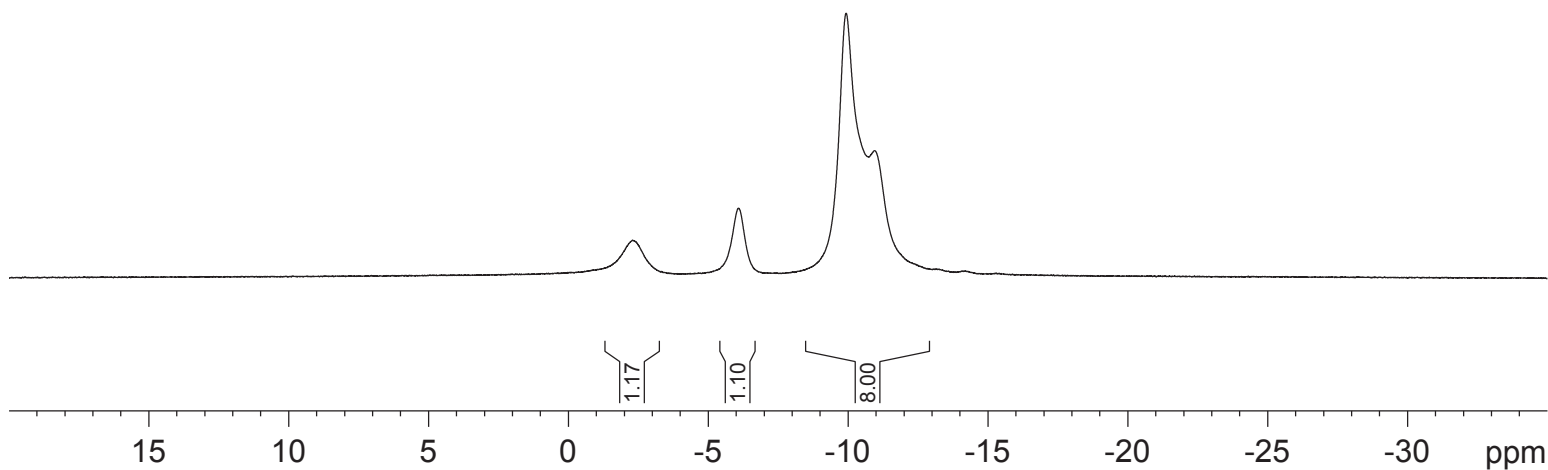
— 2.29  
 — 6.09  
 — 9.93  
 — 10.95

1hr-B-cassm-795-cdcl3

Current Data Parameters  
 NAME 1hr-B-cassm-795-cdcl3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20171209  
 Time 16.57 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 228  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.1 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



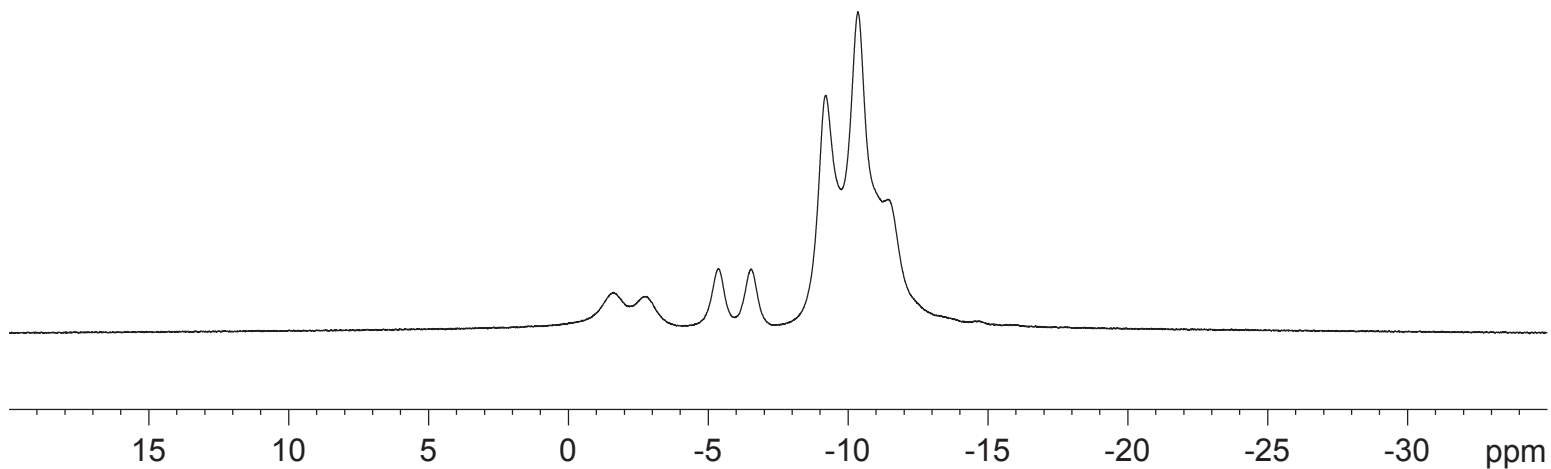
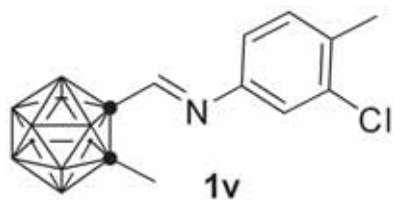
lhr-B-cassm-795-cdcl3 (c)

Current Data Parameters  
NAME lhr-B-cassm-795-cdcl3 (c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171209  
Time\_ 16.58 h  
INSTRUM spect  
PROBHD Z108618\_0257 ( )  
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 228  
DW 20.800 usec  
DE 6.50 usec  
TE 297.0 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

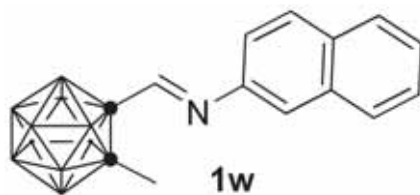
— -1.61  
— -2.77  
— -5.35  
— -6.53  
— -9.21  
— -10.35  
— -11.42



7.967  
7.888  
7.871  
7.859  
7.559  
7.556  
7.546  
7.543  
7.531  
7.529  
7.517  
7.514  
7.503  
7.500  
7.331  
7.327  
7.314  
7.309  
7.260

— 2.174

I hr-H-cassm735-nap



Current Data Parameters  
NAME I hr-H-cassm735-  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170816  
Time 10.22  
INSTRUM spect  
PROBHD Z149001\_0010 (   
PULPROG zg30  
TD 65536  
SOLVENT CDCl 3  
NS 12  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 17.56  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

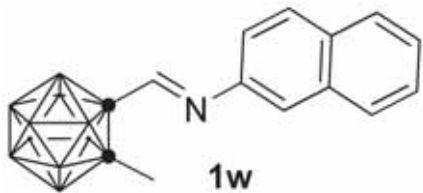
F2 - Processing parameters  
SI 65536  
SF 500.1300125  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00

1.02  
3.05  
3.00  
1.00

3.18



S-111



151.74  
146.00  
133.73  
132.96  
129.57  
128.32  
127.94  
127.11  
126.62  
119.68  
119.38

77.41  
77.16  
77.03  
76.91  
75.71

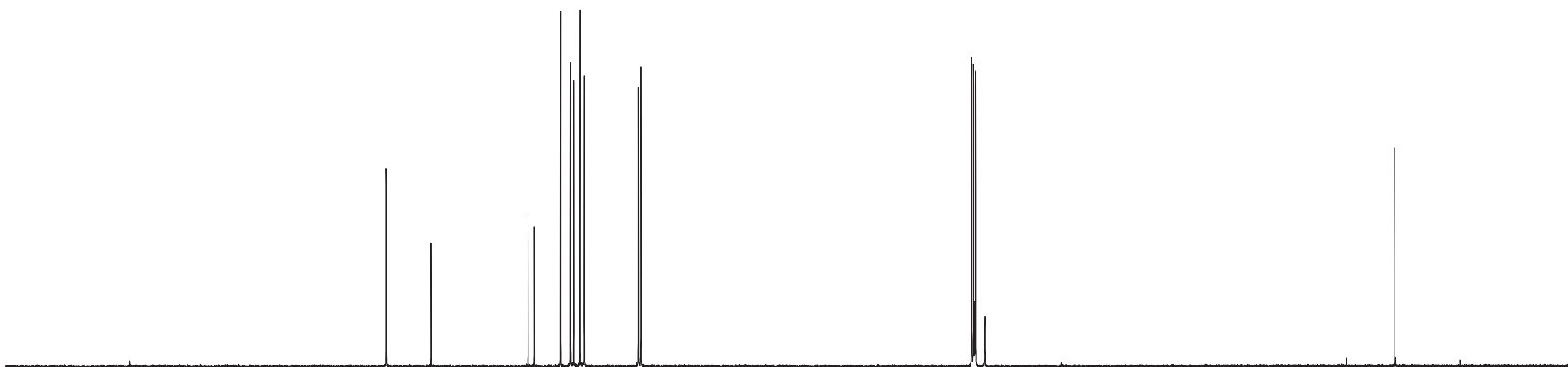
23.70

I hr-C-cassm735-nap

Current Data Parameters  
NAME I hr-C-cassm735-nap  
EXPNO 1  
PROCNO 1

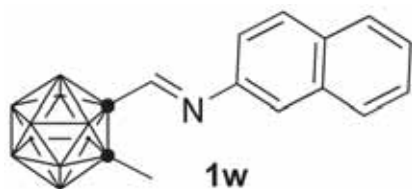
F2 - Acquisition Parameters  
Date\_ 20170816  
Time 10.30 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 120  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters  
SI 32768  
SF 125.7577791 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

1 hr-B-cassm735-nap

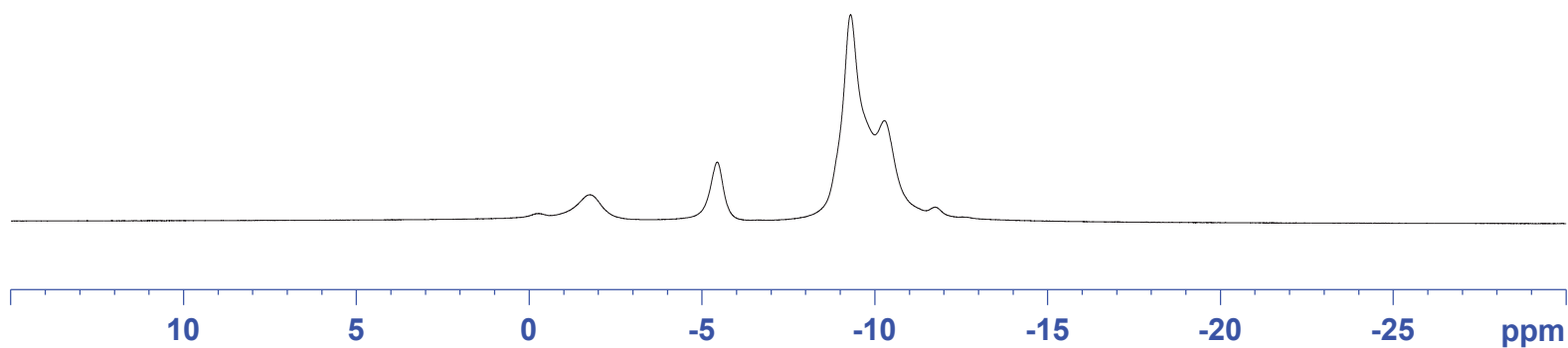


-1.75  
-5.43  
-9.29  
-10.27

Current Data Parameters  
NAME 1 hr-B-cassm735-nap  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170816  
Time 10.33 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 4  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 102.6  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

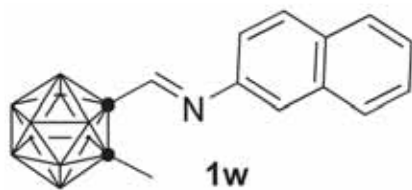


1.01  
1.15  
8.00

S-113

I hr-B-cassm735-nap(C)

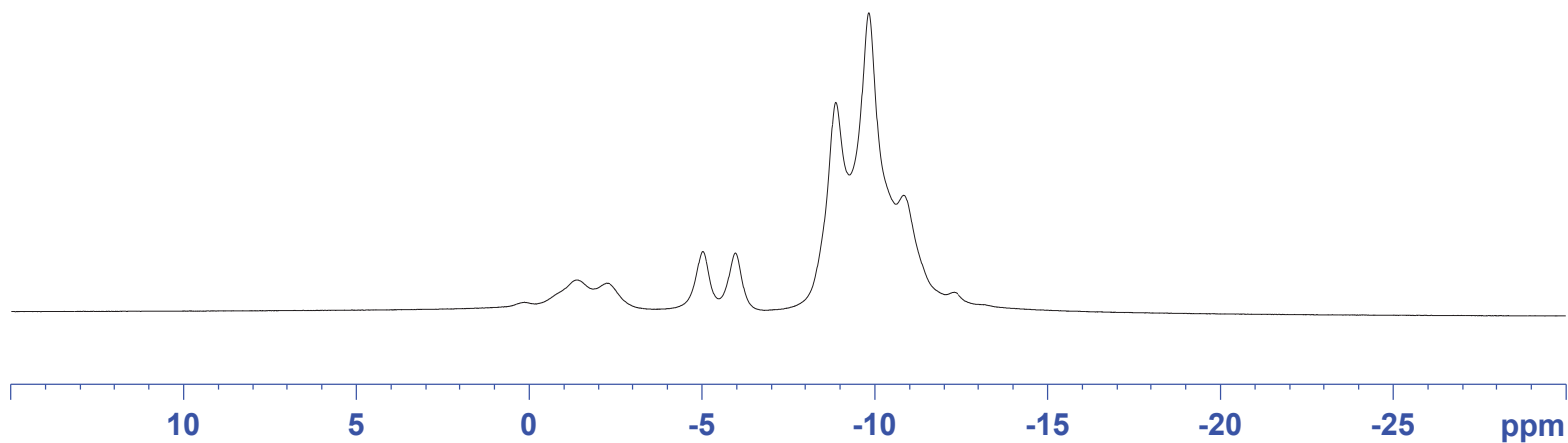
-1.35  
-2.23  
-5.01  
-5.95  
-8.87  
-9.82  
-10.82



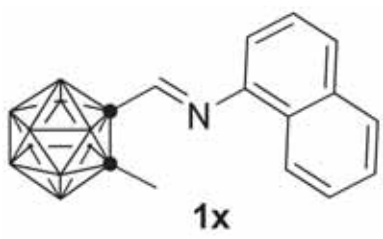
Current Data Parameters  
NAME I hr-B-cassm735-nap(C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170816  
Time 10.34 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 12  
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 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



8.136  
8.121  
8.112  
7.949  
7.875  
7.864  
7.857  
7.852  
7.816  
7.796  
7.570  
7.564  
7.560  
7.557  
7.552  
7.546  
7.456  
7.436  
7.417  
7.260  
6.950  
6.932



2.201  
1.558

Current Data Parameters  
NAME I hr-H-0748sm-cd  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170821  
Time 10.26  
INSTRUM spect  
PROBHD Z108618\_0257 (   
PULPROG zg30  
TD 65536  
SOLVENT CDCl 3  
NS 10  
DS 2  
SWH 8012.820  
FIDRES 0.122266  
AQ 4.0894465  
RG 181  
DW 62.400  
DE 6.50  
TE 295.1  
D1 1.00000000  
TDO 1  
SF01 400.2324714  
NUC1 1H  
P1 12.80  
PLW1 13.56000042

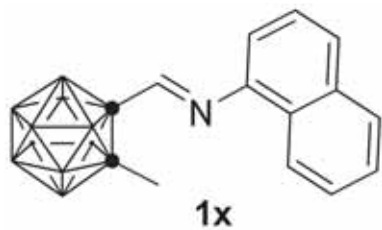
F2 - Processing parameters  
SI 65536  
SF 400.230098  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00



9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

1.03  
1.06  
1.07  
1.06  
2.04  
1.06  
1.00

3.03



151.96  
145.81  
134.05  
128.50  
128.26  
127.96  
127.08  
126.80  
125.73  
123.43  
112.69

77.41  
77.16  
76.91  
76.77  
75.80

23.91

I hr-0748-cassm-C

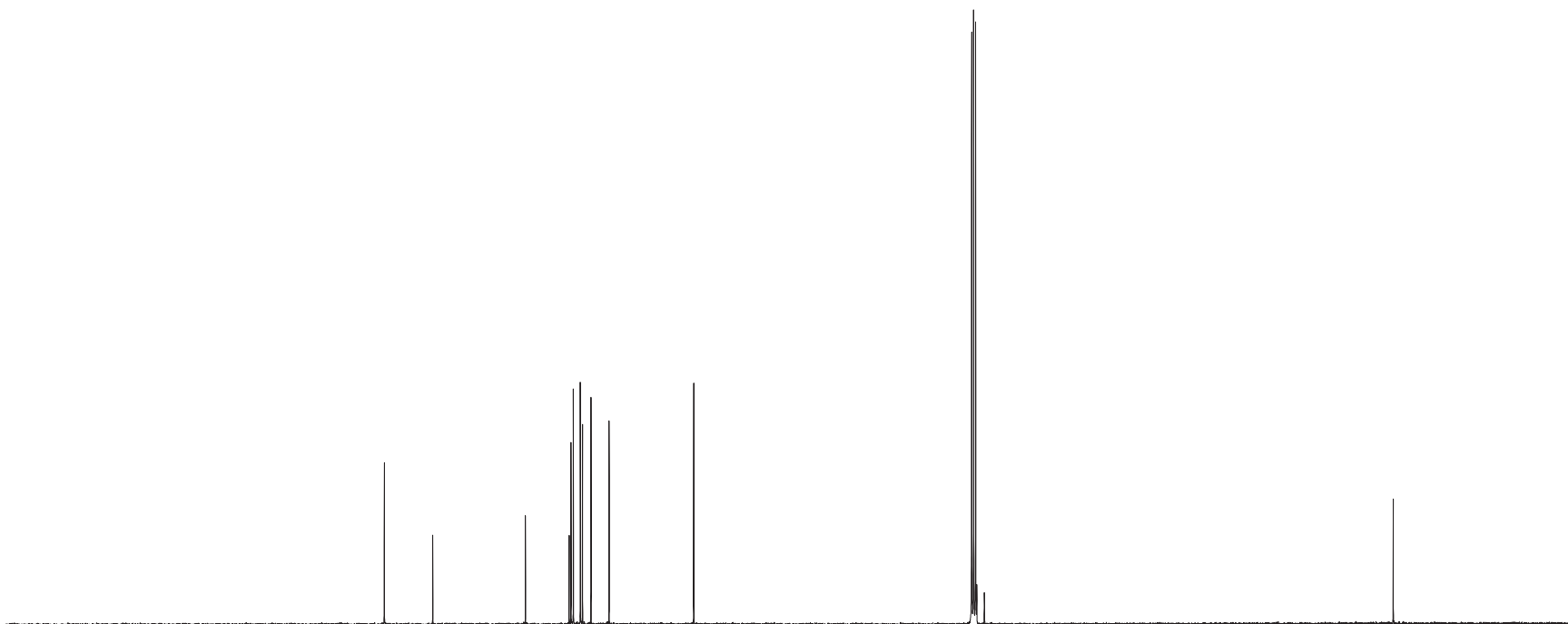
Current Data Parameters  
NAME I hr-0748-cassm-C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170821  
Time 19.10 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 300  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters

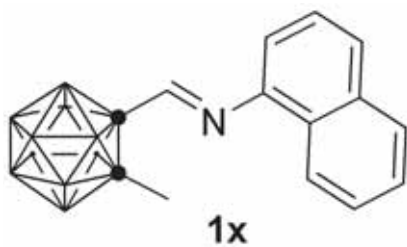
SI 32768  
SF 125.7577740 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



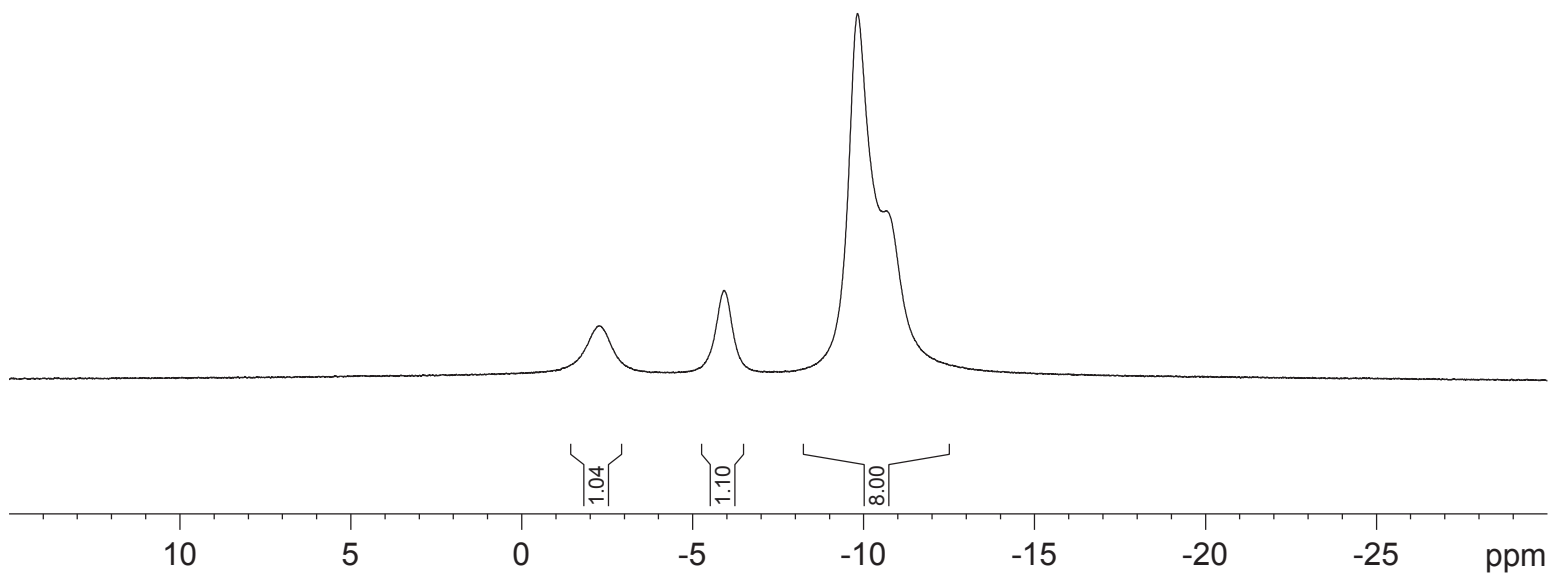
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



1hr-B-0748-2napcassm-cdcl3



— -2.27  
— -5.91  
— -9.82  
— -10.69



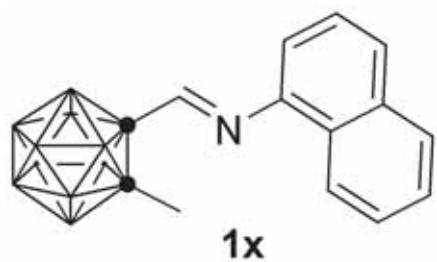
S-117

Current Data Parameters  
NAME 1hr-B-0748-2napcassm-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170822  
Time 9.48 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 228  
DW 20.800 usec  
DE 6.50 usec  
TE 295.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 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

1hr-B-0748-2napcassm-cdcl3 (C)

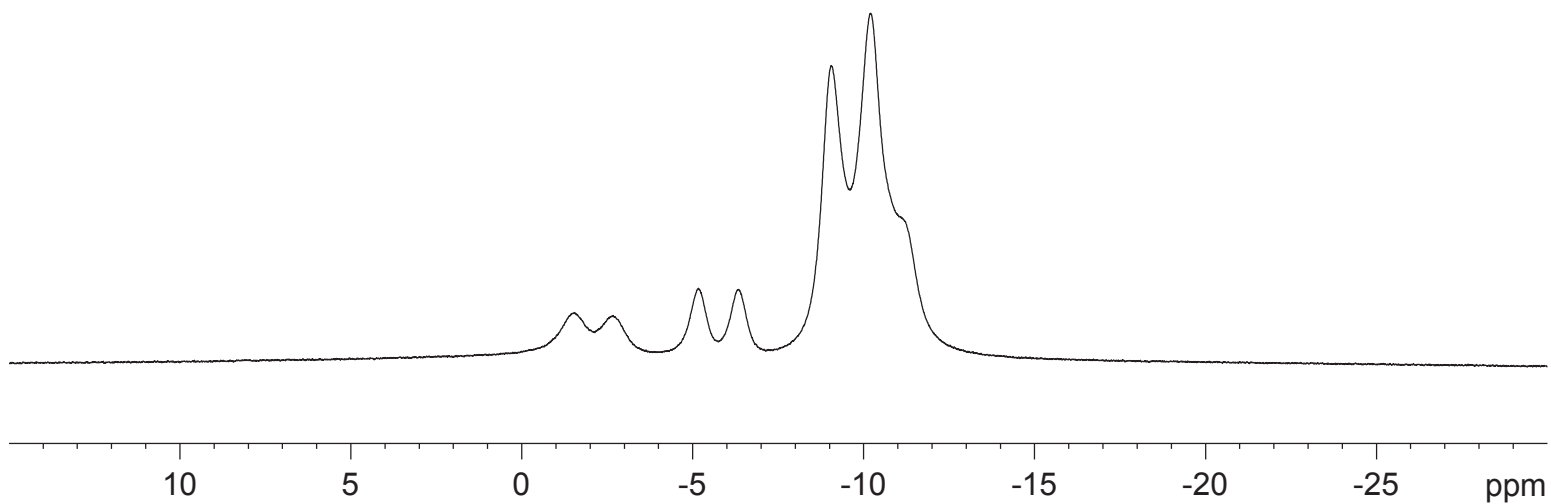


— 1.54  
— 2.67  
— 5.17  
— 6.35  
— 9.05  
— 10.21  
— 11.14

Current Data Parameters  
NAME 1hr-B-0748-2napcassm-cdcl3 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170822  
Time 9.50 h  
INSTRUM spect  
PROBHD Z108618\_0257 (Z108618\_0257)  
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 15  
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 295.1 K  
D1 2.0000000 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

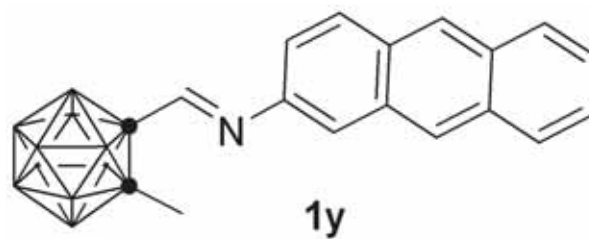


I hr-H-756cassm

Current Data Parameters  
NAME I hr-H-756cassm  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170907  
Time 11.03  
INSTRUM spect  
PROBHD Z149001\_0010 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 30.85  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300125  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00



8.437  
8.427  
8.037  
8.015  
8.011  
8.005  
8.000  
7.706  
7.703  
7.524  
7.514  
7.505  
7.495  
7.486  
7.336  
7.332  
7.318  
7.314  
7.260

2.183

1.568



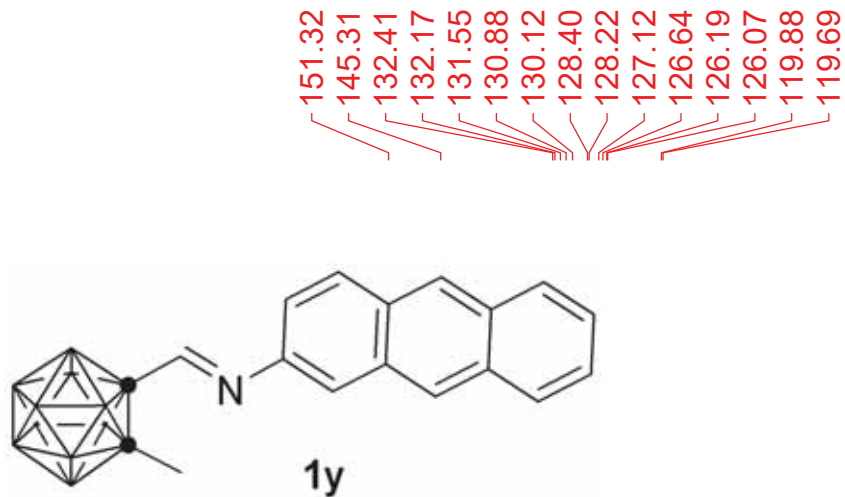
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

2.04  
4.08  
1.00  
2.01  
1.01

S-119

3.14

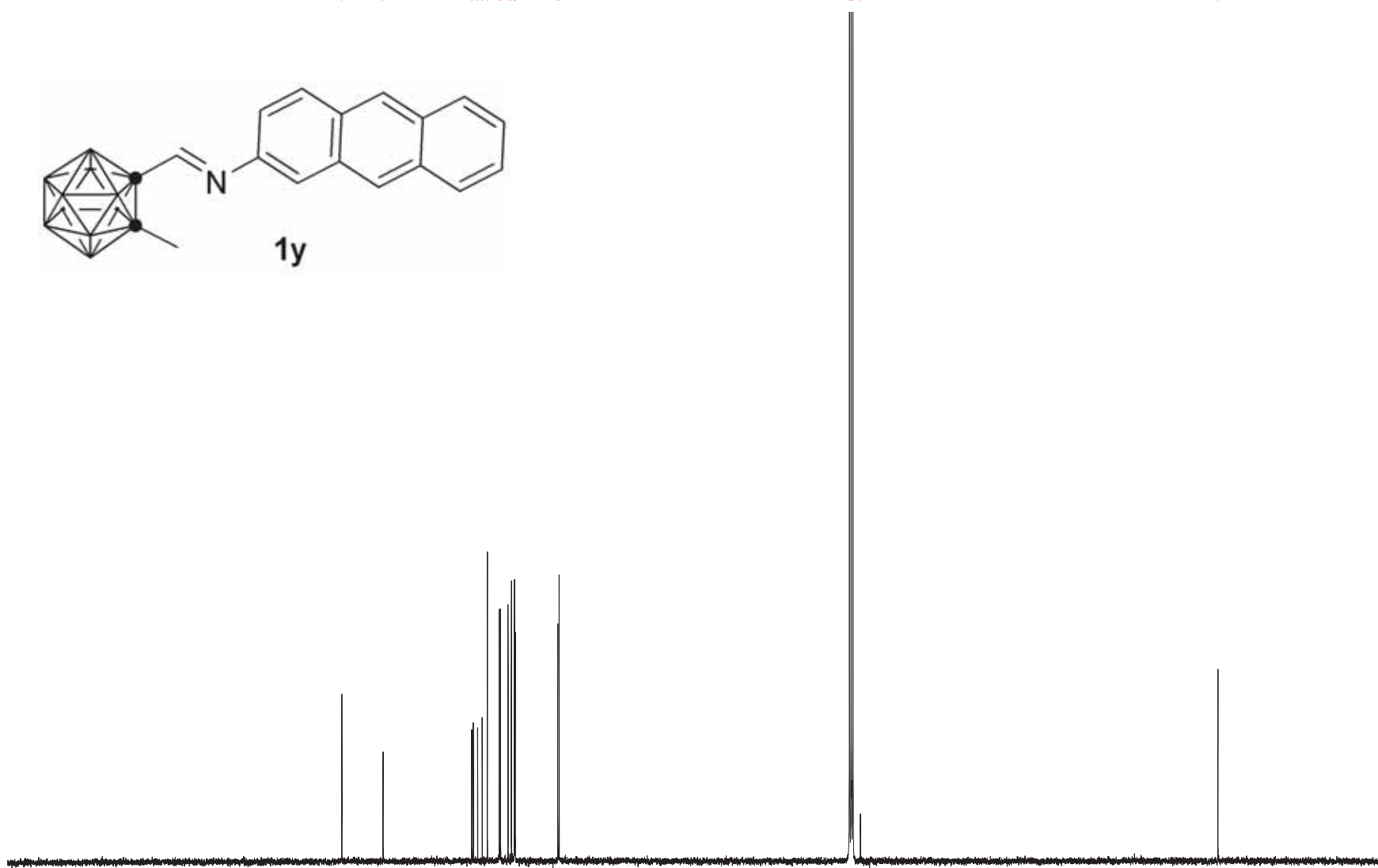
1 hr-C-756cassm



151.32  
145.31  
132.41  
132.17  
131.55  
130.88  
130.12  
128.40  
128.22  
127.12  
126.64  
126.19  
126.07  
119.88  
119.69

77.41  
77.16  
77.08  
76.91  
75.81

23.76



Current Data Parameters  
NAME 1 hr-C-756cassm  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170907  
Time 11.15 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 200  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

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

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

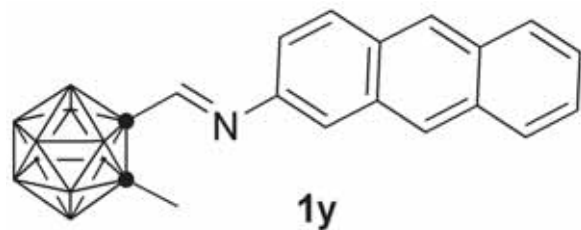
S-120

I hr-B-756cassm

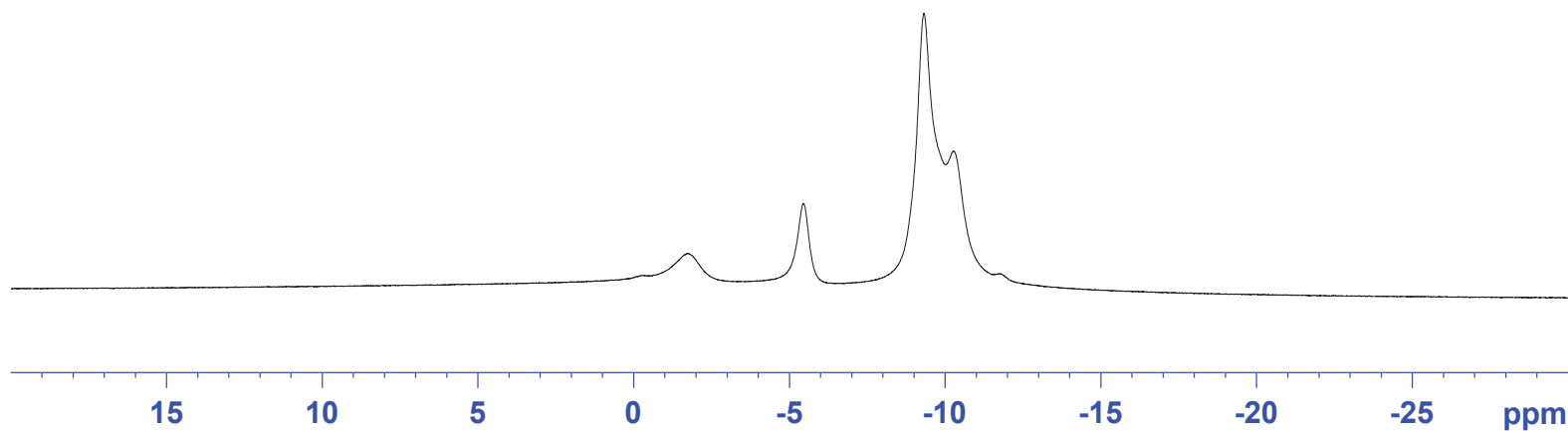
Current Data Parameters  
NAME I hr-B-756cassm  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170907  
Time 11.19 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 16  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 163.99  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TDO 1  
SFO1 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SFO2 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



---1.73  
---5.45  
---9.31  
---10.26



1.15  
1.16  
8.00  
3-121

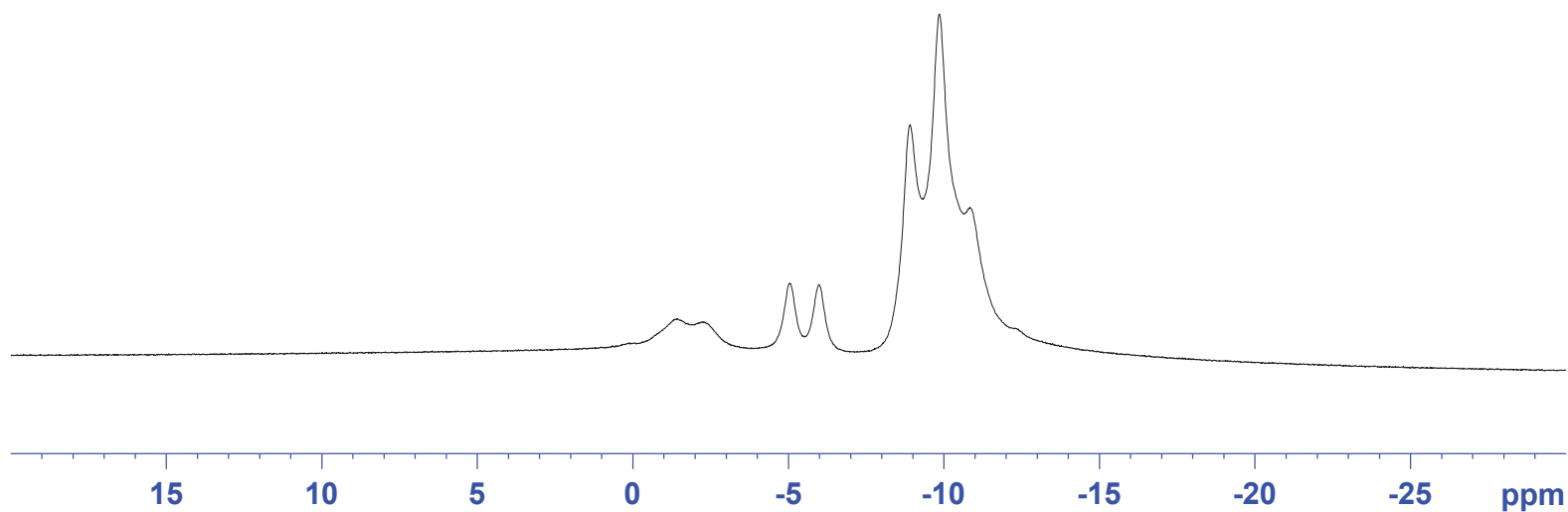
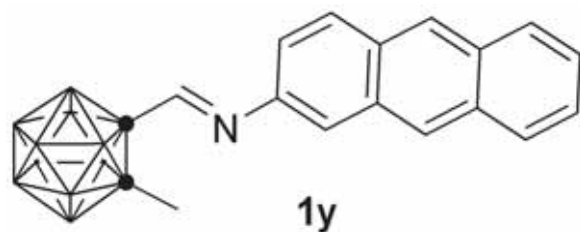
I hr-B-756cassm(c)

Current Data Parameters  
NAME I hr-B-756cassm(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170907  
Time 11.20 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl 3  
NS 16  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 163.99  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

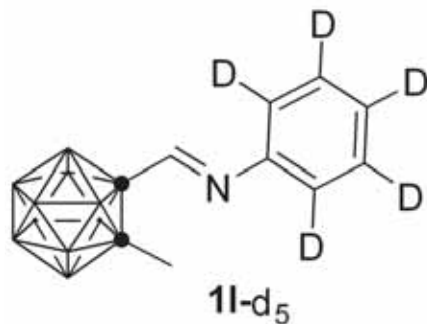
1.43  
2.27  
5.03  
5.98  
8.90  
9.85  
10.81



7.817  
7.260

2.117  
1.545

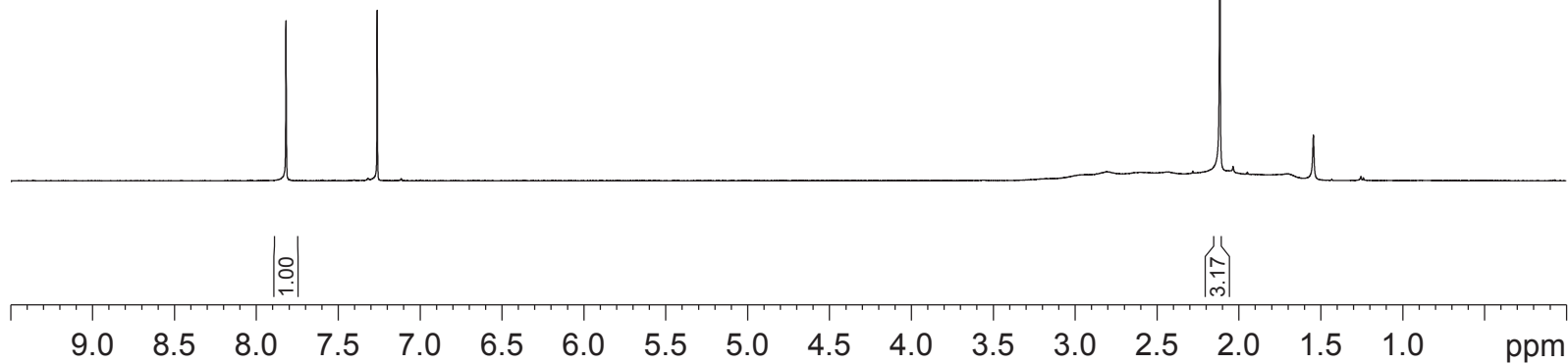
1hr-H-d5-cassmcdcl3



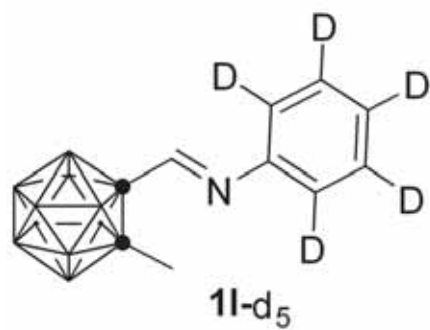
Current Data Parameters  
NAME 1hr-H-d5-cassmcdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171110  
Time 19.45 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 295.3 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 400.2300099 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



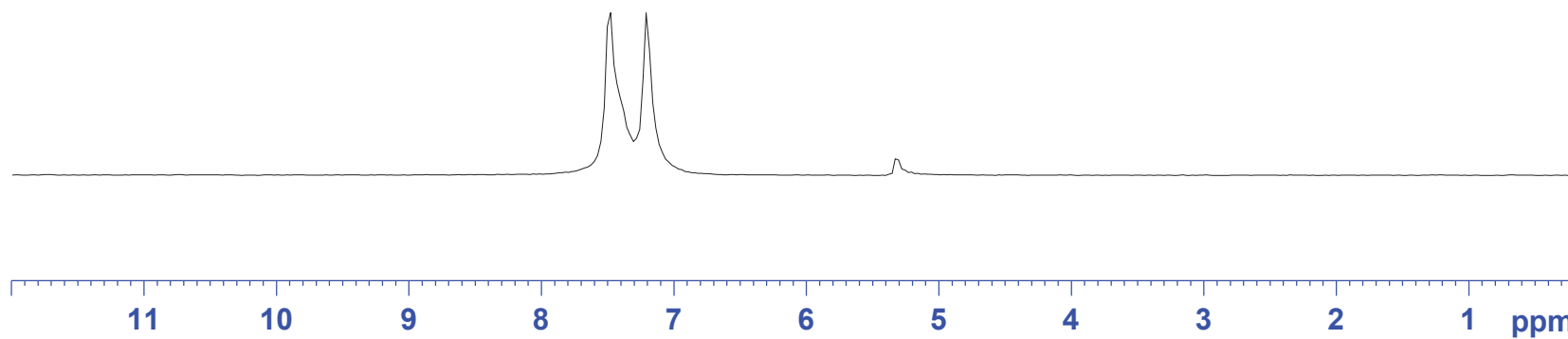
— 7.471  
 — 7.192  
  
 — 5.306



Current Data Parameters  
 NAME 1hr-2H-cassmd5-chloroform  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180602  
 Time 15.47 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zg2h  
 TD 4096  
 SOLVENT CDCl3  
 NS 420  
 DS 0  
 SWH 6142.506 Hz  
 FIDRES 2.999271 Hz  
 AQ 0.3334144 sec  
 RG 0.5  
 DW 81.400 usec  
 DE 6.50 usec  
 TE 297.3 K  
 D1 0.05000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 61.4226981 MHz  
 NUC1 2H  
 P1 300.00 usec  
 PLW1 3.00000000 W

F2 - Processing parameters  
 SI 4096  
 SF 61.4223850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00



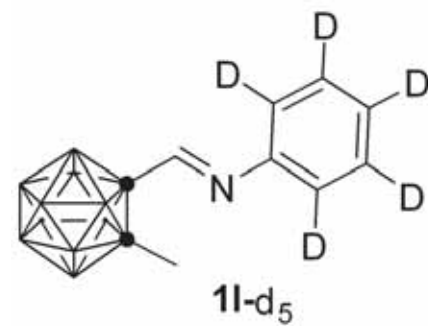


I hr-C-d5cassm-r

Current Data Parameters  
NAME I hr-C-d5cassm-r  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171111  
Time 10.30 h  
INSTRUM spect  
PROBHD Z149001\_0010 (   
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 300  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters  
SI 32768  
SF 125.7577728 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

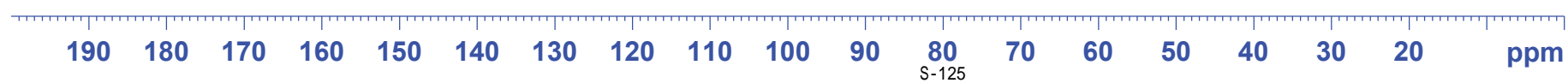
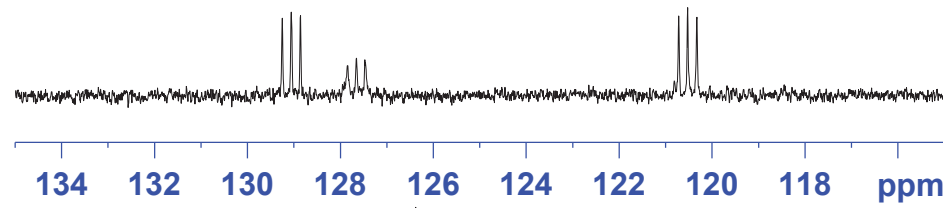


129.25  
129.06  
128.86  
127.85  
127.66  
127.47

151.91  
148.59  
129.25  
129.06  
128.86  
127.85  
127.66  
127.47  
120.72  
120.53  
120.33

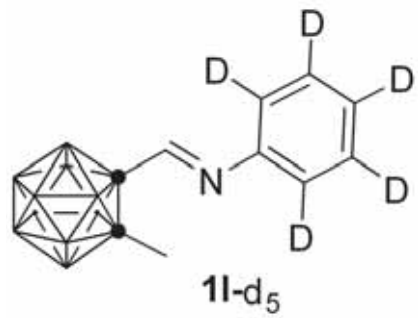
77.41  
77.16  
76.91  
75.54

23.68



S-125

1 hr-B-d5cassm-r

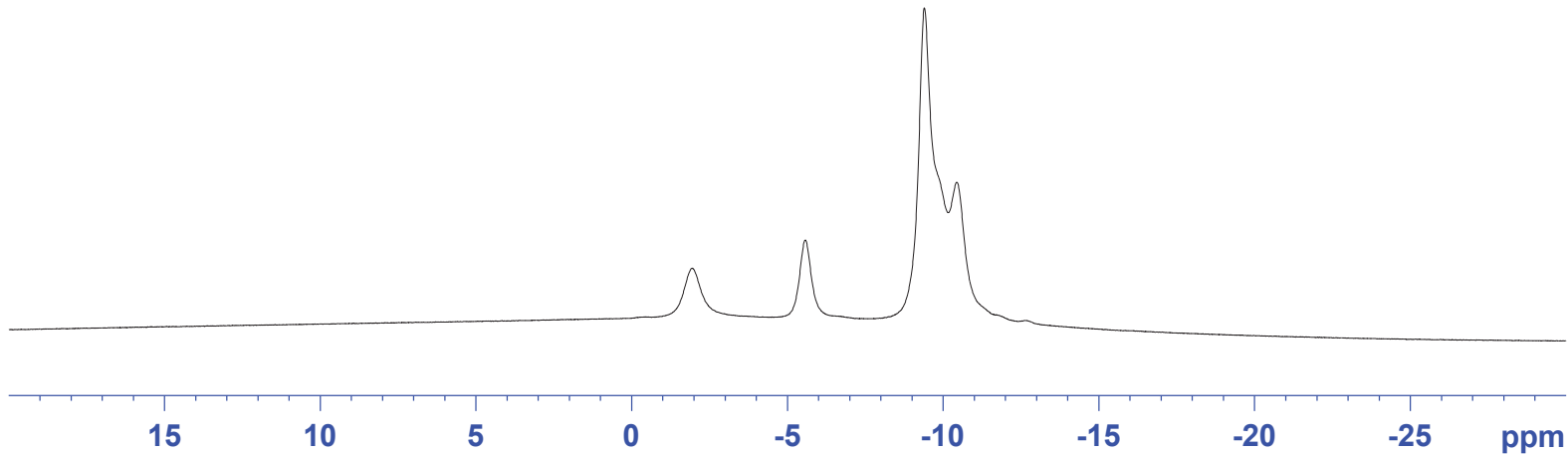


-1.94  
-5.57  
-9.39  
-9.84  
-10.43

Current Data Parameters  
NAME 1 hr-B-d5cassm-r  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171111  
Time 11.12 h  
INSTRUM spect  
PROBHD Z149001\_0010 (   
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 163.99  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4615790 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

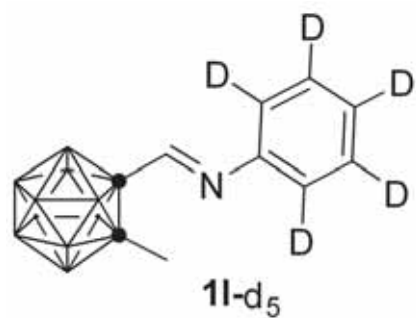
F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.13  
1.18  
8.00<sup>126</sup>

l hr-B-d5cassm-r(C)

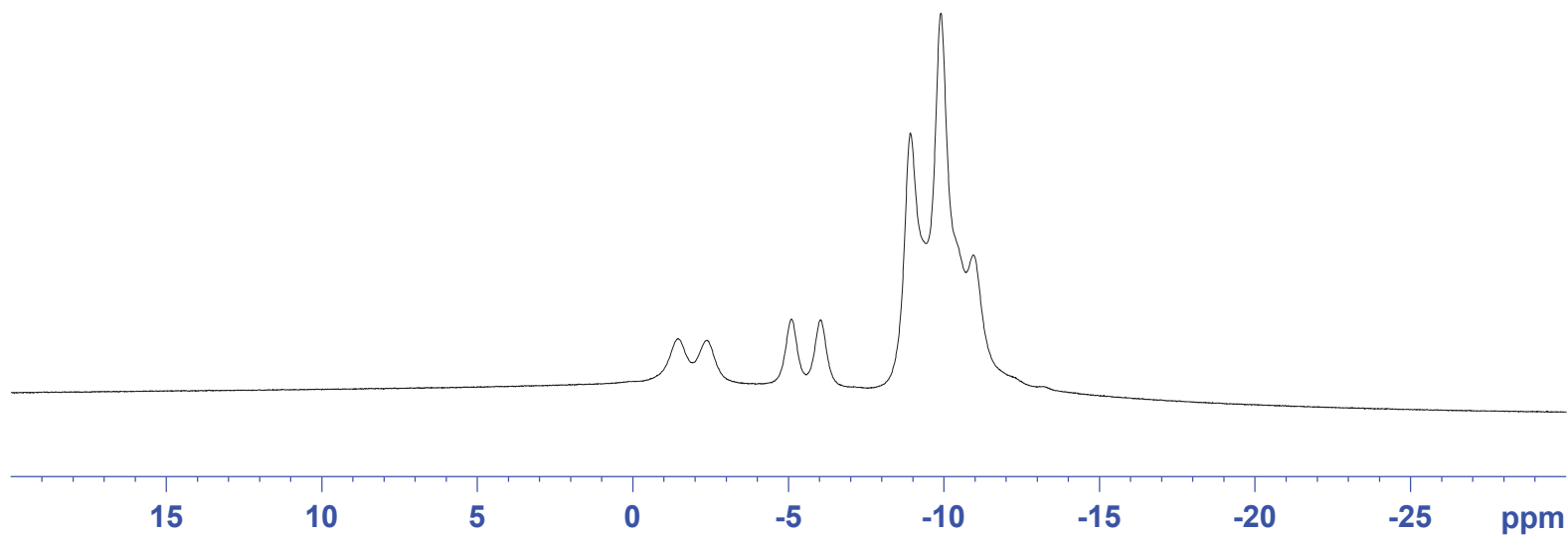
-1.44  
-2.38  
-5.09  
-6.04  
-8.92  
-9.89  
-10.41  
-10.93



Current Data Parameters  
NAME l hr-B-d5cassm-r(C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171111  
Time 11.14 h  
INSTRUM spect  
PROBHD Z149001\_0010 (   
PULPROG zg  
TD 32768  
SOLVENT CDCl 3  
NS 17  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 163.99  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

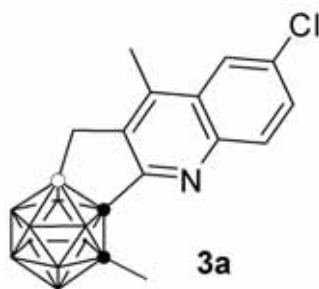
F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



7.970  
7.964  
7.948  
7.626  
7.621  
7.604  
7.599  
7.260

2.619  
2.590  
2.544  
2.509  
2.462  
2.418

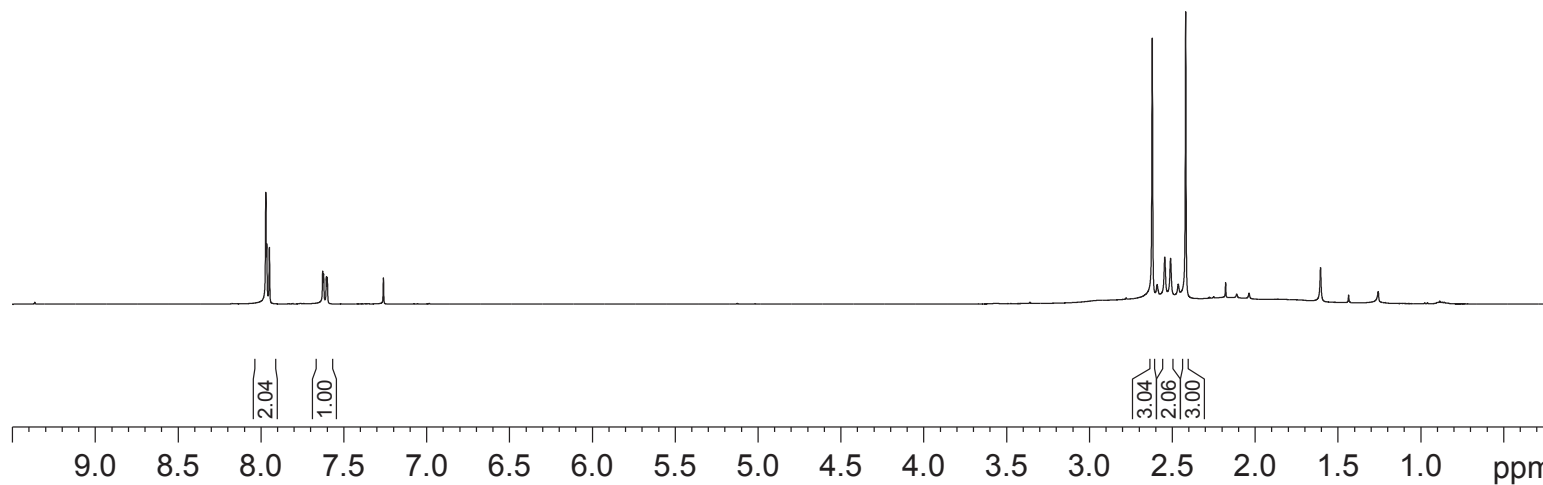
1hr-H-casCl-0427-1-CD

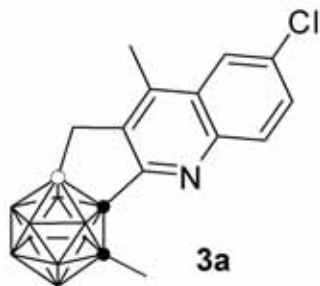


Current Data Parameters  
NAME 1hr-H-casCl-0427-1-CD  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160803  
Time 13.33 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 64  
DW 62.400 usec  
DE 6.50 usec  
TE 294.7 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters  
SI 65536  
SF 400.2300106 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





— 156.854

144.159  
142.124  
140.726

133.122  
131.868  
129.929  
128.340  
122.910

82.969  
77.477  
77.160  
76.842  
75.392

— 22.258

— 15.094

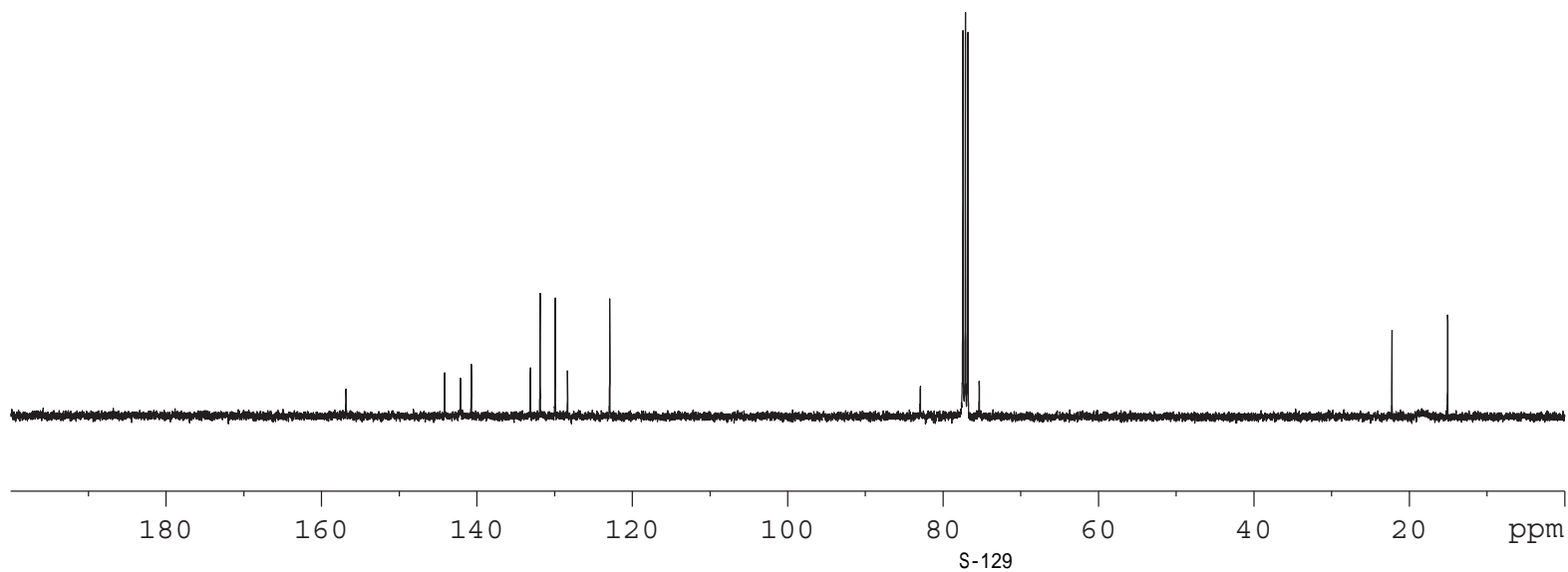
lhr-C-casCl-0427-1-CDCl3

Bruker Advance III 400

Current Data Parameters  
NAME lhr-C-casCl-0427-1-CDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160803  
Time\_ 12.41 h  
INSTRUM spect  
PROBHD Z824601\_0021 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 438  
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  
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

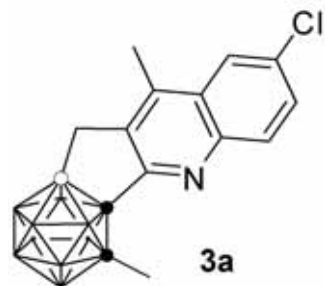


lhr-B-casCl-0427-1-CDCl3

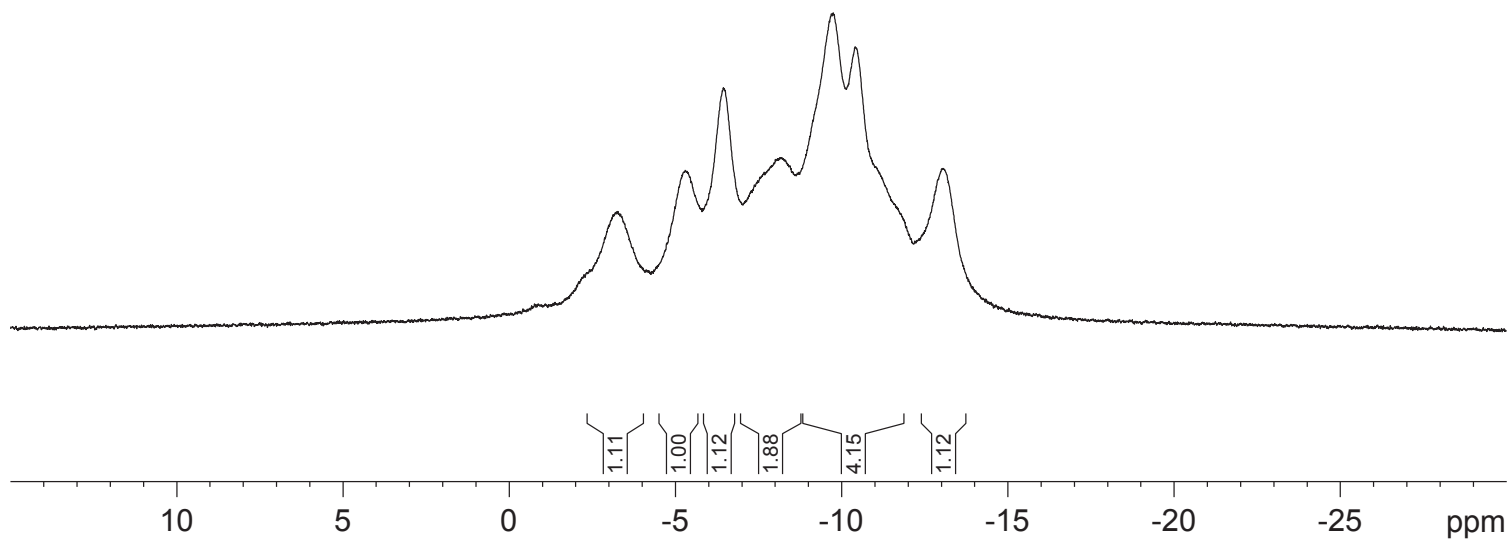
Current Data Parameters  
NAME lhr-B-casCl-0427-1-CDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160803  
Time\_ 13.35 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 9  
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

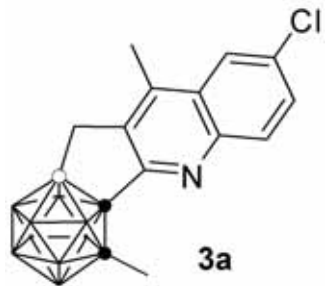
F2 - Processing parameters  
SI 32768  
SF 128.4097615 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



— -3.28  
— -5.29  
— -6.45  
— -8.19  
— -9.75  
— -10.41  
— -13.05



S-130



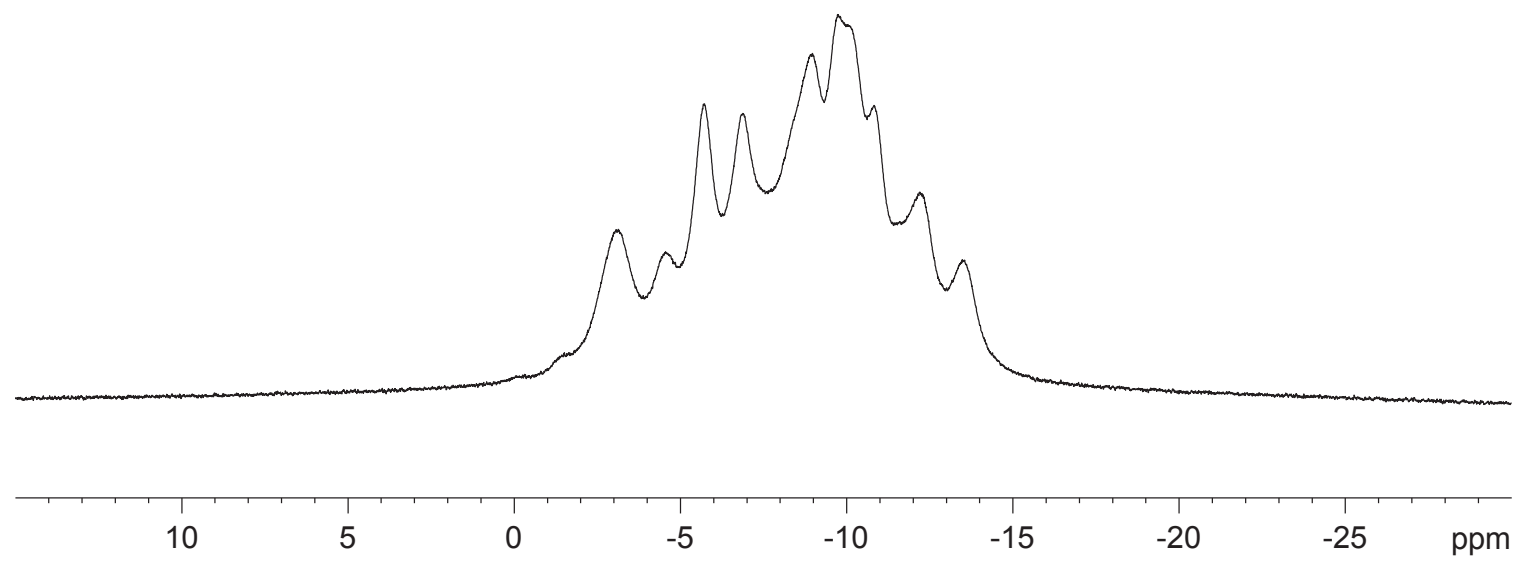
— 3.14  
 — 4.56  
 — 5.73  
 — 6.89  
 — 8.98  
 — 9.74  
 — 10.09  
 — 10.83  
 — 12.21  
 — 13.47

1hr-B-casCl-0427-1-CDC13

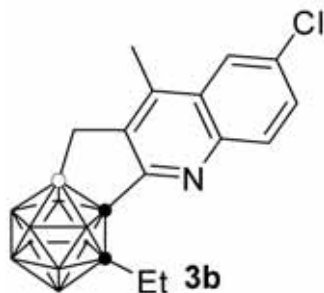
Current Data Parameters  
 NAME 1hr-B-casCl-0427-1-CDC13(C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160803  
 Time\_ 13.37 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zg  
 TD 65536  
 SOLVENT CDC13  
 NS 17  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 287  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 2.00000000 sec  
 TD0 1  
 SF01 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



7.967  
7.961  
7.938  
7.625  
7.620  
7.603  
7.598  
7.260



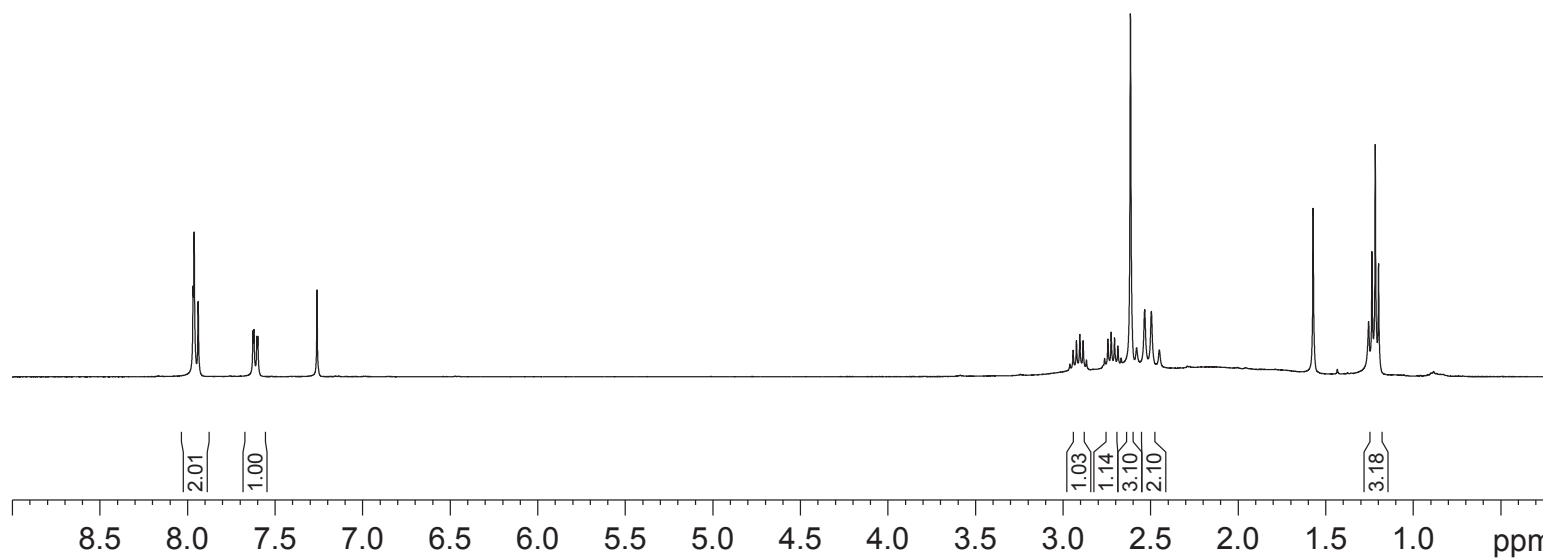
2.960  
2.941  
2.922  
2.903  
2.884  
2.865  
2.761  
2.743  
2.724  
2.705  
2.686  
2.614  
2.579  
2.533  
2.494  
2.449  
1.571  
1.234  
1.216  
1.197

lhr-H-0716-cascdcl3

Current Data Parameters  
NAME lhr-H-0716-cascdcl  
EXPNO 1  
PROCNO 1

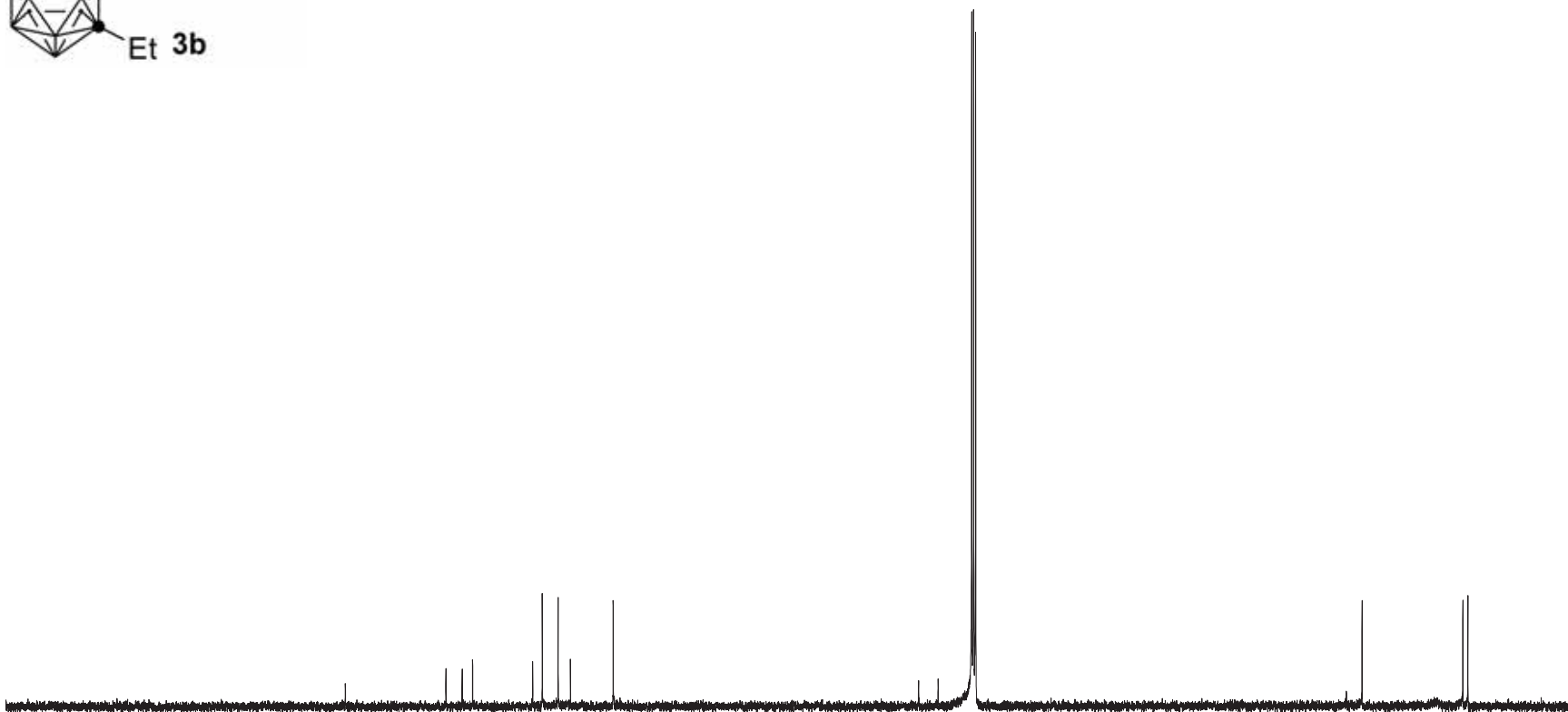
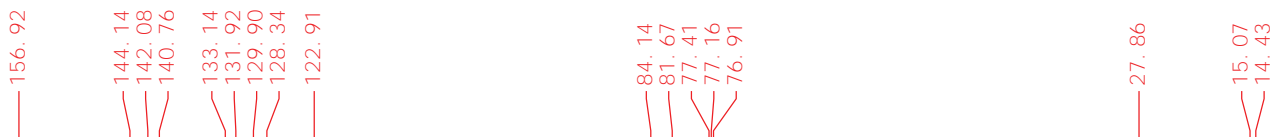
F2 - Acquisition Parameters  
Date\_ 20170704  
Time\_ 22.06 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 13  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 295.6 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MH;  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

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





I hr-0716-4cl cetcascddl 3



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

S-133

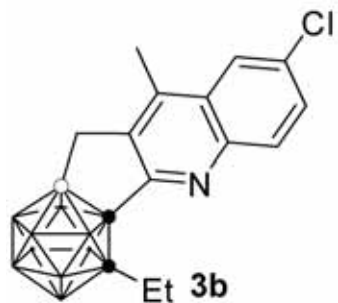
Current Data Parameters  
NAME I hr-0716-4cl cetcascddl 3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170705  
Time\_ 20.33 h  
INSTRUM spect  
PROBHD Z119470\_0283 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 647  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 6.50 usec  
TE 299.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 94.0000000 W  
SFO2 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 25.0000000 W  
PLW12 0.39063001 W  
PLW13 0.19648001 W

F2 - Processing parameters

SI 32768  
SF 125.7577711 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



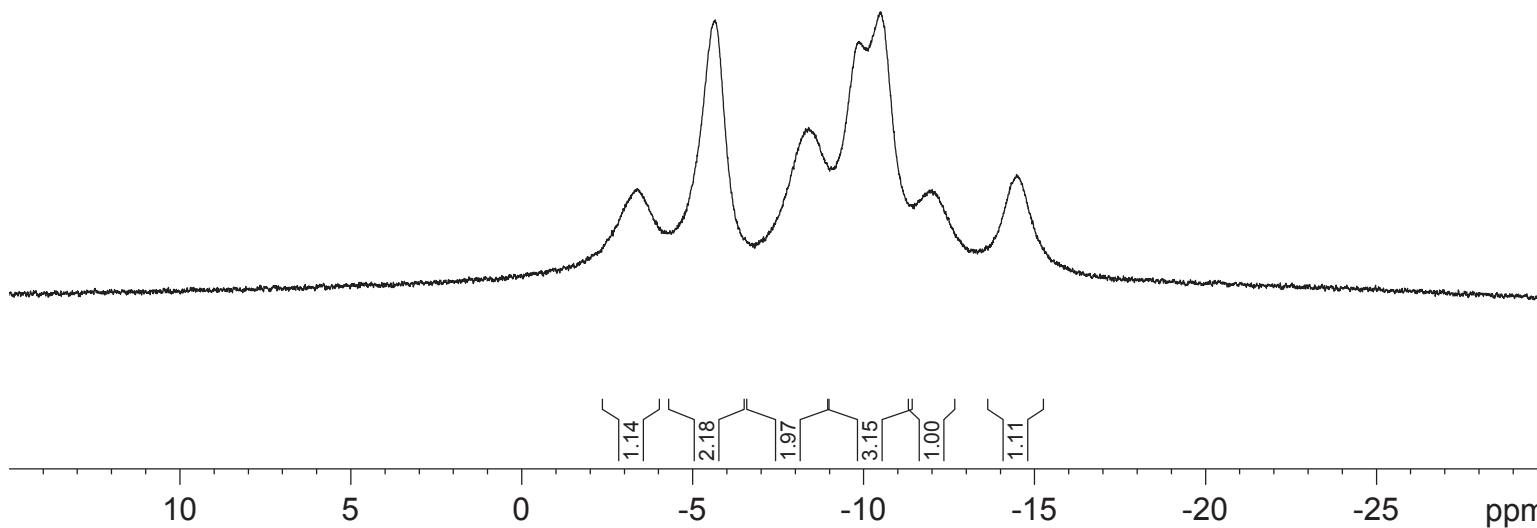
— 3.39  
 — 5.65  
 — 8.39  
 — 9.83  
 — 10.50  
 — 12.01  
 — 14.48

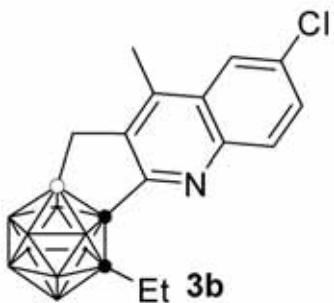
lhr-B-0716-cascdcl3

Current Data Parameters  
 NAME lhr-B-0716-cascdcl3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170705  
 Time\_ 20.58 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 362  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.9 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





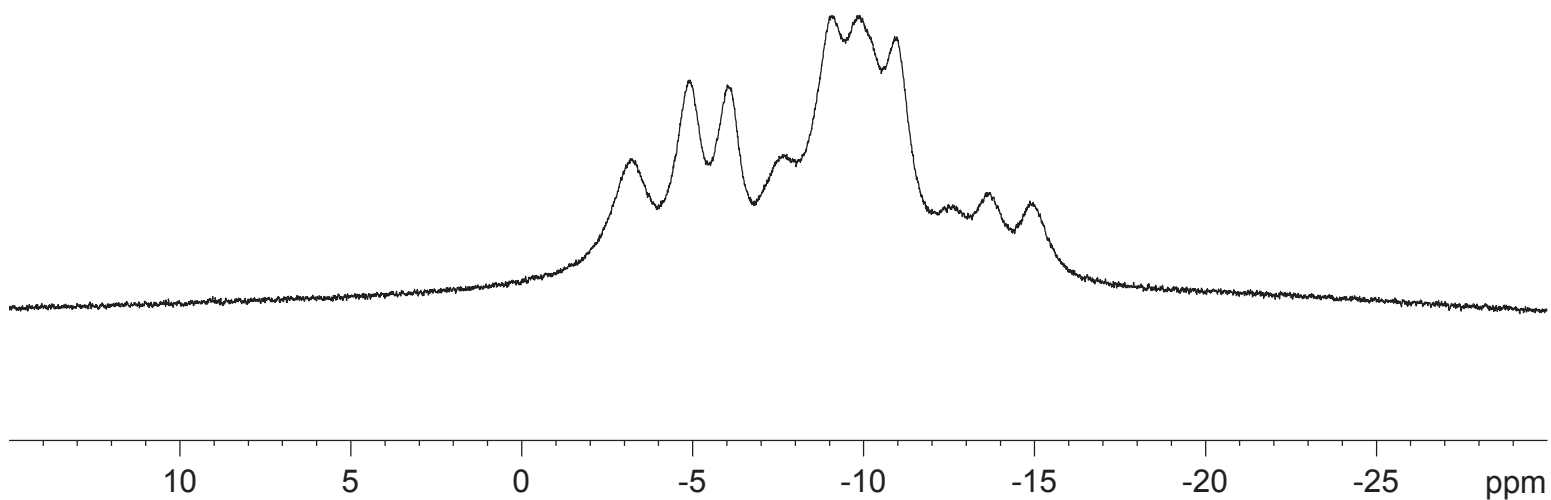
| 3.23  
 | 4.92  
 | 6.01  
 | 7.60  
 | 9.08  
 | 9.89  
 | 10.91  
 | 12.57  
 | 13.59  
 | 14.87

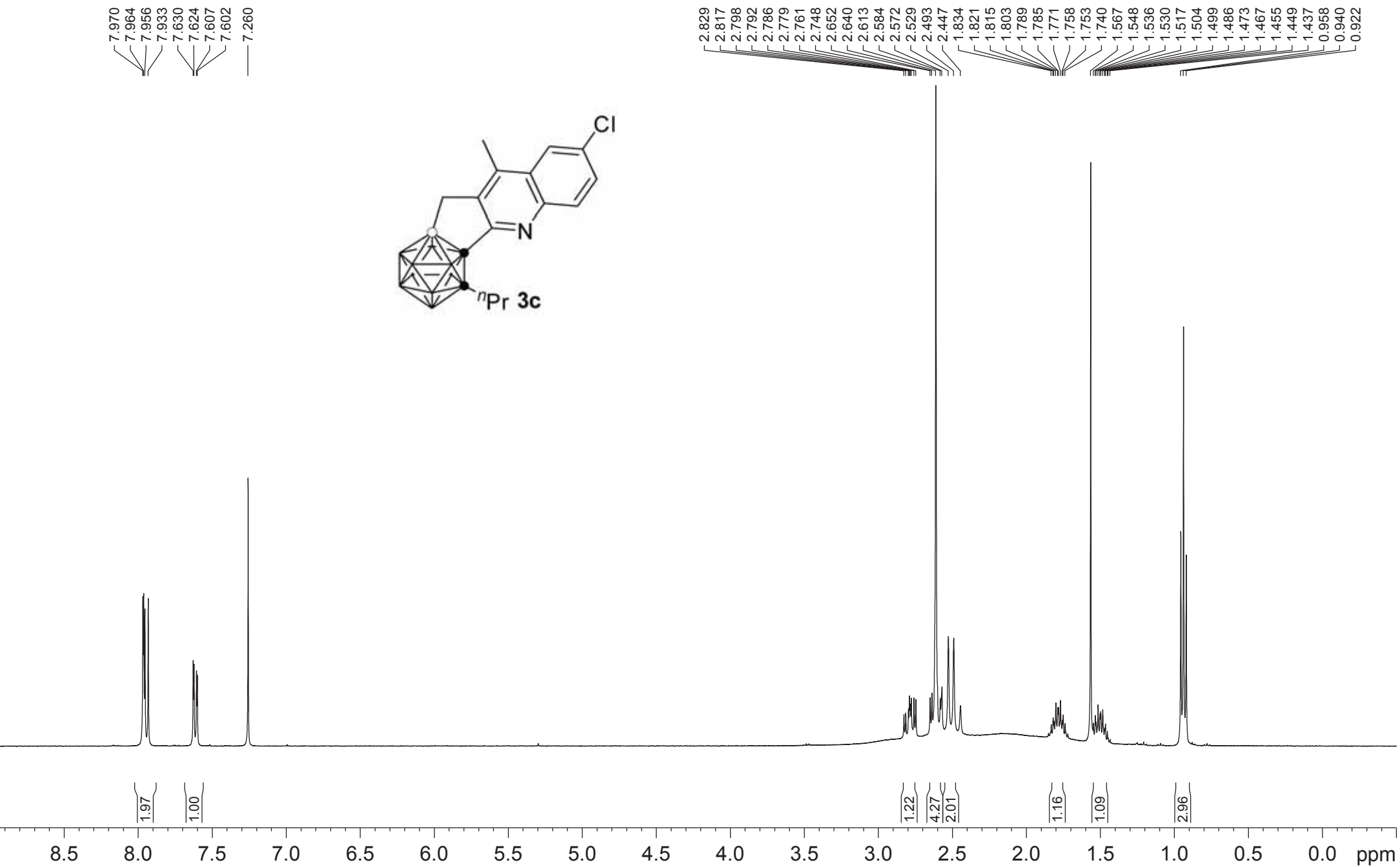
1hr-B-0716-cascdcl3 (C)

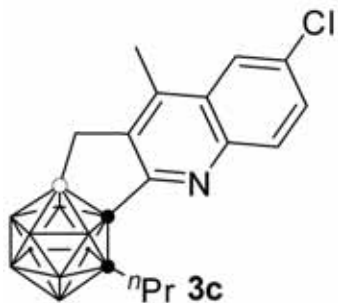
Current Data Parameters  
 NAME 1hr-B-0716-cascdcl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170705  
 Time 21.00 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 24  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 362  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.4 K  
 D1 2.00000000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 11B  
 P1 7.50 usec  
 PLW1 55.09999847 W

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







156.92  
 144.14  
 142.07  
 140.75  
 133.12  
 131.90  
 129.92  
 128.34  
 122.91  
 83.92  
 80.75  
 77.48  
 77.16  
 76.84  
 36.18  
 23.49  
 15.08  
 13.92

lhr-C-0728-4cl-ccc:

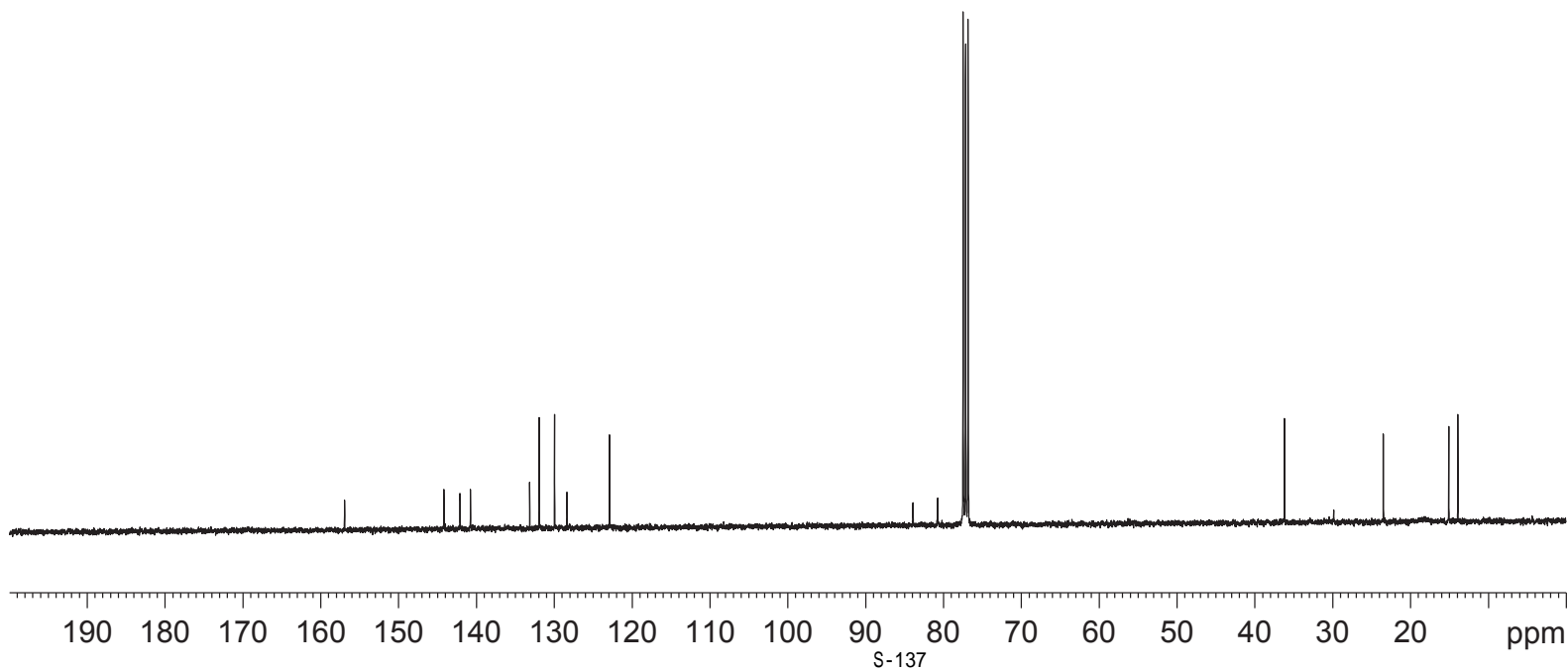
Current Data Parameters  
 NAME lhr-C-0728-4cl-cccscdcl3-NPR  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170716  
 Time 16.27 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 900  
 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 2.0000000 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

F2 - Processing parameters

SI 32768  
 SF 100.6379007 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



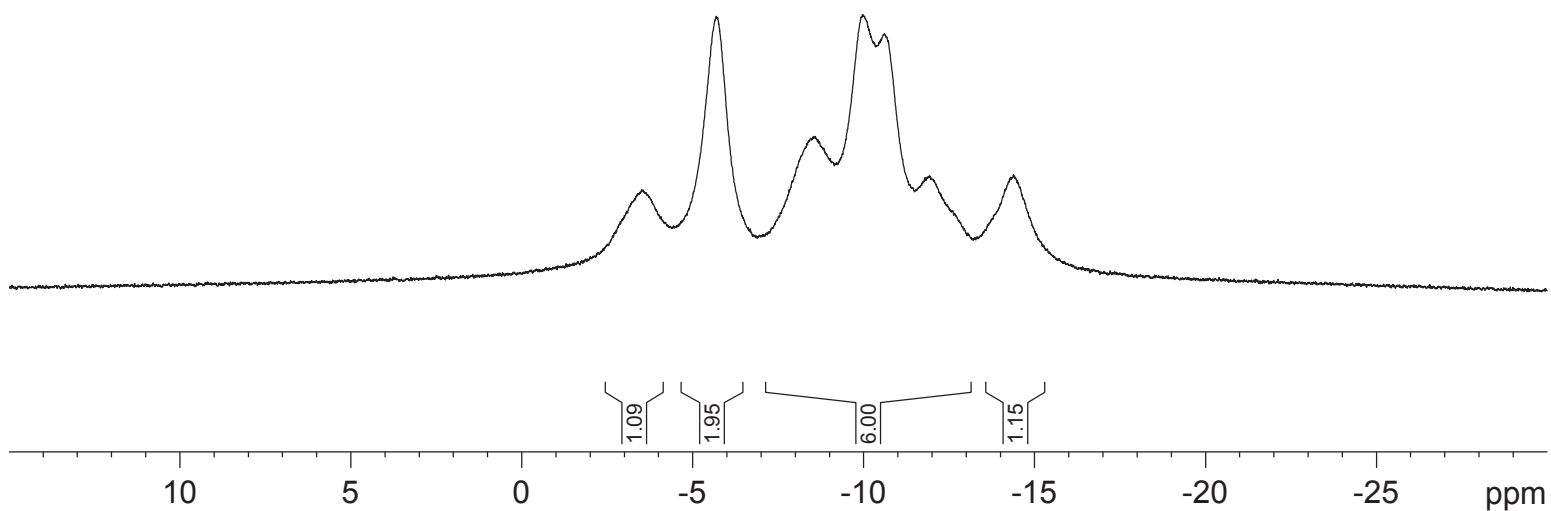
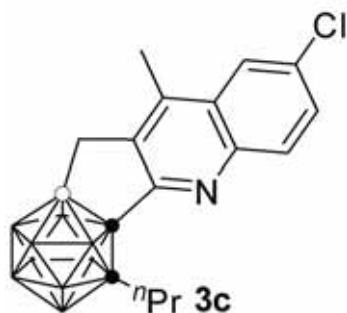
1hr-B-0728-4cl-cccascdcl3-NPR

Current Data Parameters  
NAME 1hr-B-0728-4cl-cccascdcl3-NPR  
EXPNO 1  
PROCNO 1

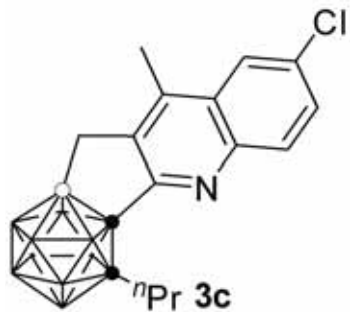
F2 - Acquisition Parameters  
Date\_ 20170716  
Time 17.12 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 24  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 406  
DW 20.800 usec  
DE 6.50 usec  
TE 295.3 K  
D1 2.0000000 sec  
D11 0.0300000 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

— 3.50  
— 5.69  
— 8.56  
— 9.98  
— 10.62  
— 11.93  
— 14.39



S-138



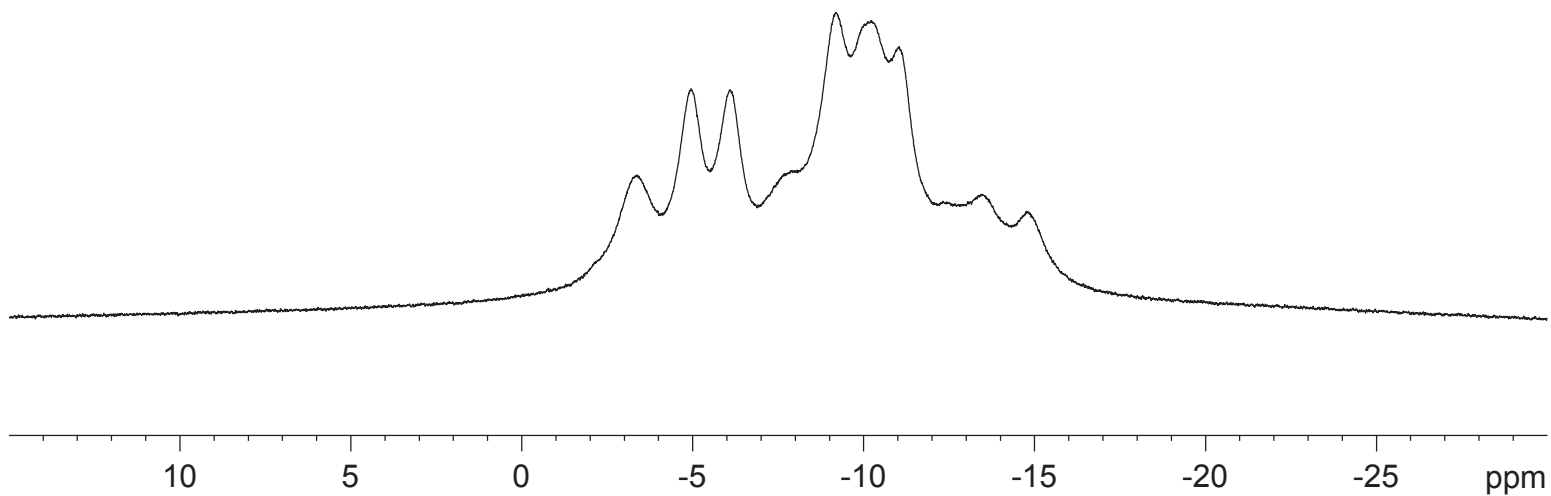
— 3.37  
 — 4.95  
 — 6.09  
 — 7.74  
 — 9.18  
 — 10.04  
 — 10.22  
 — 11.04  
 — 12.38  
 — 13.53  
 — 14.79

1hr-B-0728-4cl-cccasccl3-NPR(C)

Current Data Parameters  
 NAME 1hr-B-0728-4cl-cccasccl3-NPR(C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170716  
 Time 17.18 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 63  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 362  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.9 K  
 D1 2.0000000 sec  
 TD0 1  
 SF01 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



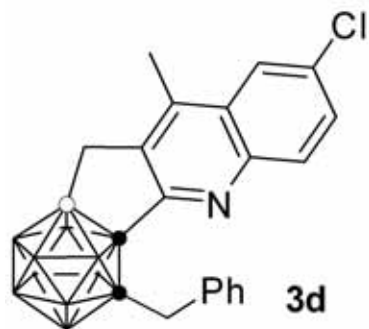
8.058  
8.040  
8.011  
8.006  
7.671  
7.667  
7.653  
7.649  
7.299  
7.260

4.282  
4.252  
3.978  
3.948

2.644  
2.583  
2.546  
2.510  
2.474

1.561

I hr-H-0723-RE



Current Data Parameters  
NAME I hr-H-0723-RE  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170719  
Time 19.36  
INSTRUM spect  
PROBHD Z119470\_0283 (Z1194700283)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 117.01  
DW 50.000  
DE 6.50  
TE 297.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 10.00  
PLW1 25.00000000

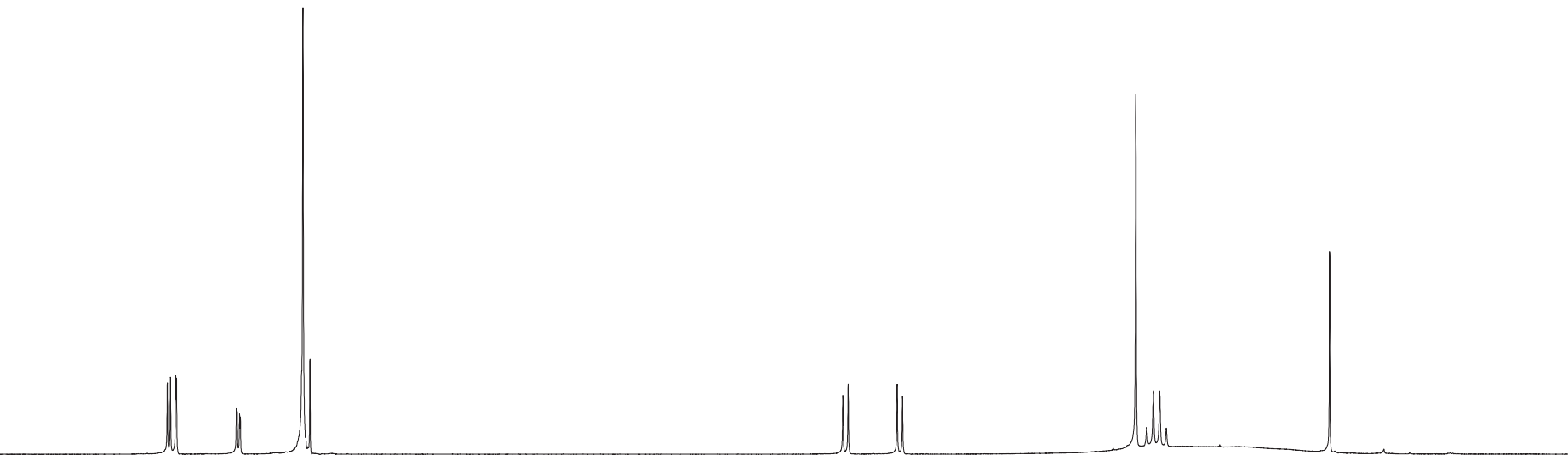
F2 - Processing parameters  
SI 65536  
SF 500.1300126  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00

1.12  
1.00  
1.08  
5.19

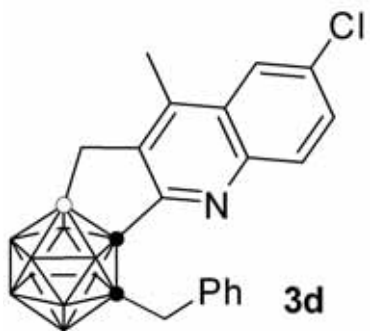
1.10  
1.10 S-140

3.18  
2.05

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







156.97  
144.08  
142.36  
140.91  
136.29  
133.30  
131.84  
130.82  
130.12  
128.47  
128.43  
127.85  
123.02

84.27  
80.22  
77.41  
77.16  
76.91

39.38

15.15

I hr-C-0723-RE

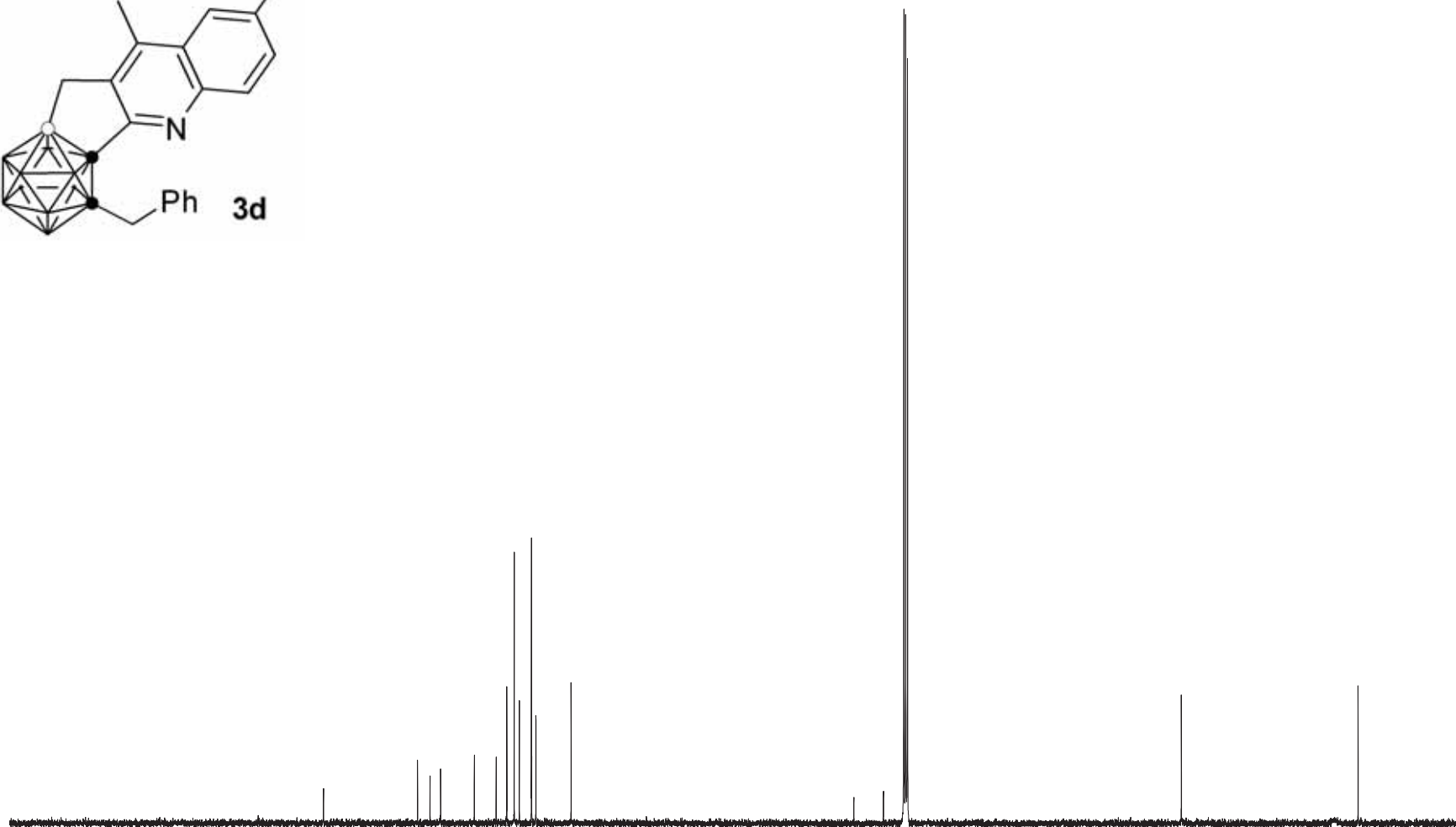
Current Data Parameters  
NAME I hr-C-0723-RE  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170719  
Time 20.11 h  
INSTRUM spect  
PROBHD Z119470\_0283 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 636  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 6.50 usec  
TE 297.8 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 94.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 25.0000000 W  
PLW12 0.39063001 W  
PLW13 0.19648001 W

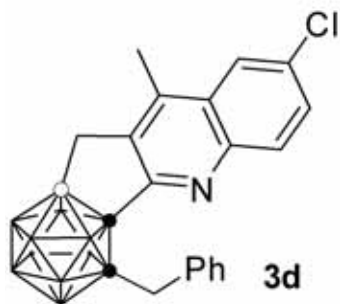
F2 - Processing parameters

SI 32768  
SF 125.7577719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

S-141



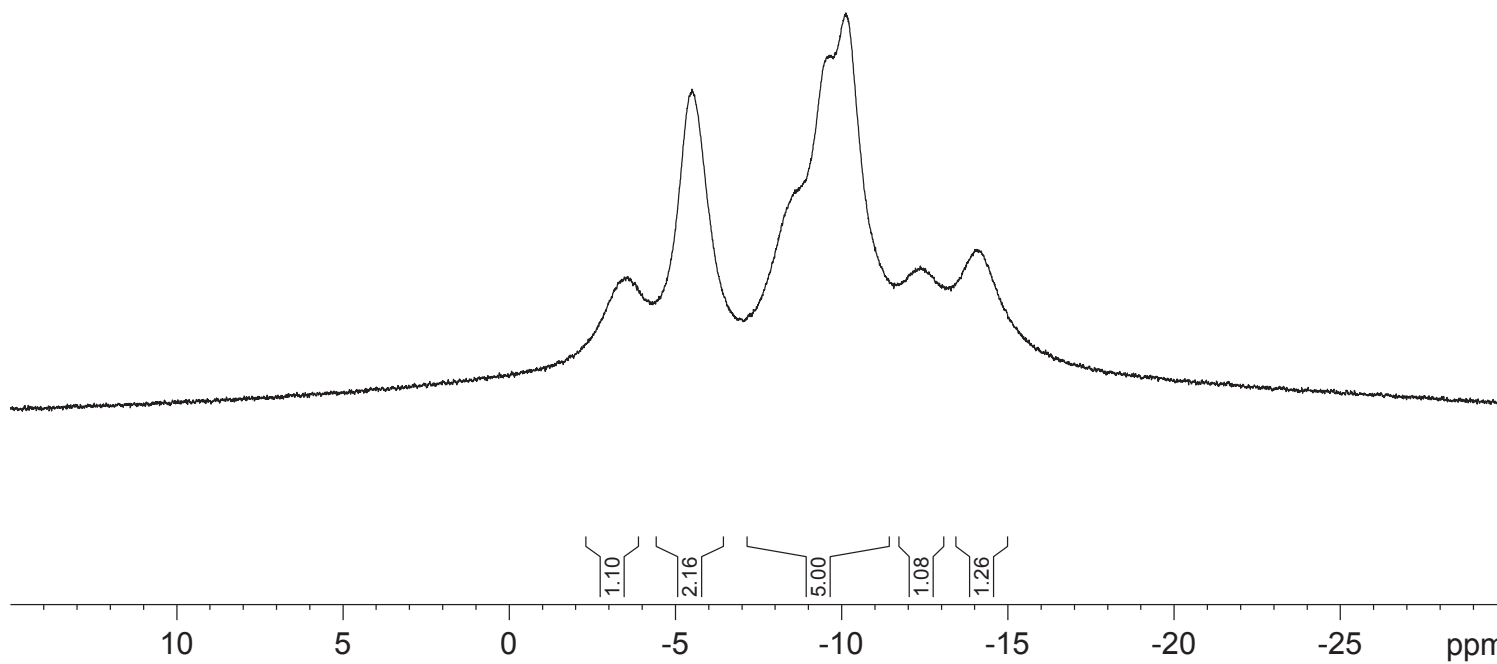
— -3.57  
 — -5.49  
 — -8.60  
 — -9.61  
 — -10.12  
 — -12.36  
 — -14.07

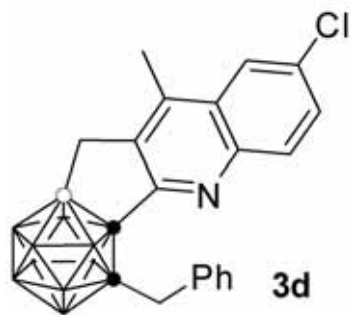
lhr-B-0723-4cl-cccascdcl

Current Data Parameters  
 NAME lhr-B-0723-4cl-cccascdcl3-bn  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170714  
 Time\_ 18.33 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 44  
 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 295.6 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





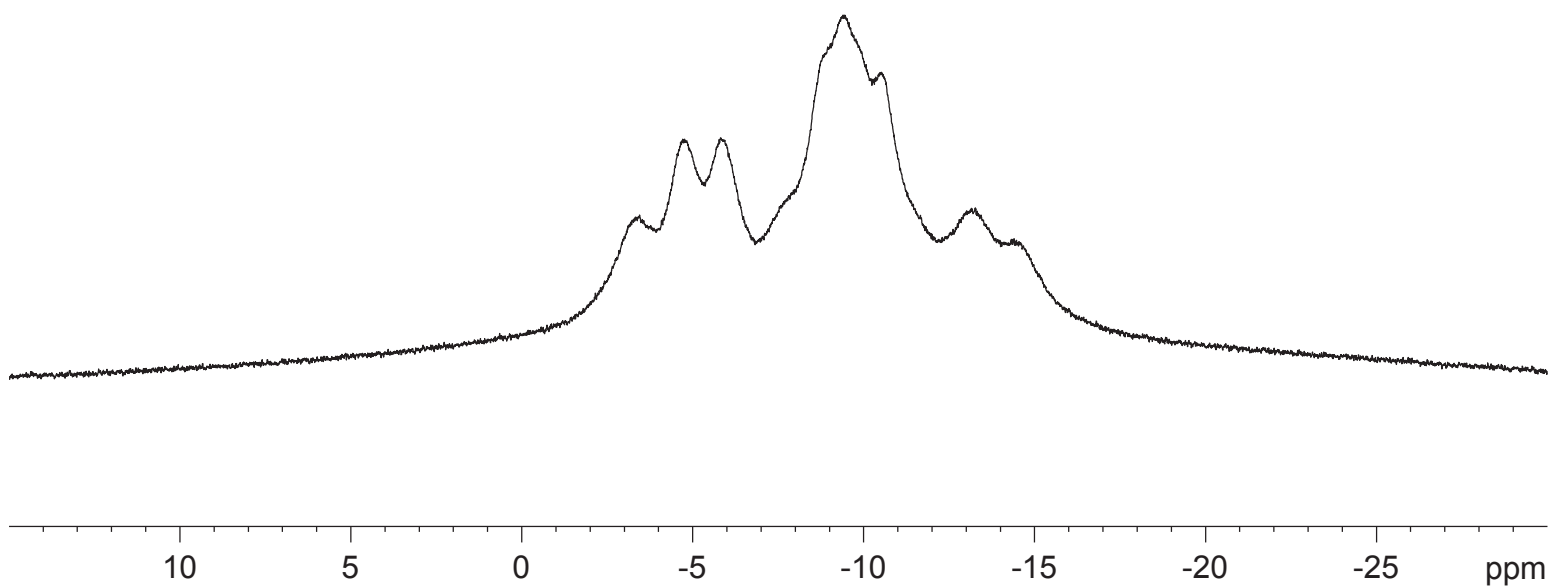
| 3.45  
 | 4.76  
 | 5.82  
 | 7.77  
 | 8.86  
 | 9.45  
 | 10.52  
 | 13.27  
 | 14.42

1hr-B-0723-4cl-cccascdcl3-bn(C)

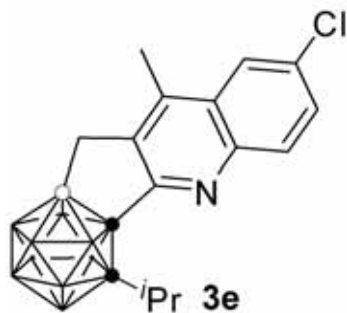
Current Data Parameters  
 NAME 1hr-B-0723-4cl-cccascdcl3-bn(C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170714  
 Time 18.35 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 37  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 362  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.1 K  
 D1 2.0000000 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



7.965  
7.961  
7.951  
7.933  
7.621  
7.616  
7.603  
7.598  
7.260



3.414  
3.400  
3.386  
3.372  
3.358  
2.611  
2.560  
2.523  
2.477  
2.441

1.568  
1.462  
1.449  
1.088  
1.074

I hr-0734-casH

Current Data Parameters  
NAME I hr-0734-casH  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170729  
Time 18.28  
INSTRUM spect  
PROBHD Z119470\_0283 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 102.6  
DW 50.000  
DE 6.50  
TE 297.3  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 10.00  
PLW1 25.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300127  
WDW EM  
SSB 0  
LB 0.30  
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

2.01

1.00

S-144

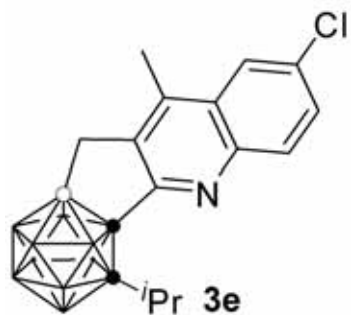
1.05

3.05

2.02

3.06

3.03



— 157.01  
 / 144.09  
 / 142.08  
 / 140.80  
 / 133.14  
 / 131.95  
 / 129.87  
 / 128.33  
 / 122.90

< 87.08  
 < 85.51  
 < 77.41  
 < 77.16  
 < 76.91

— 30.89  
 < 24.57  
 < 24.53  
 — 15.06

I hr-0734-casC

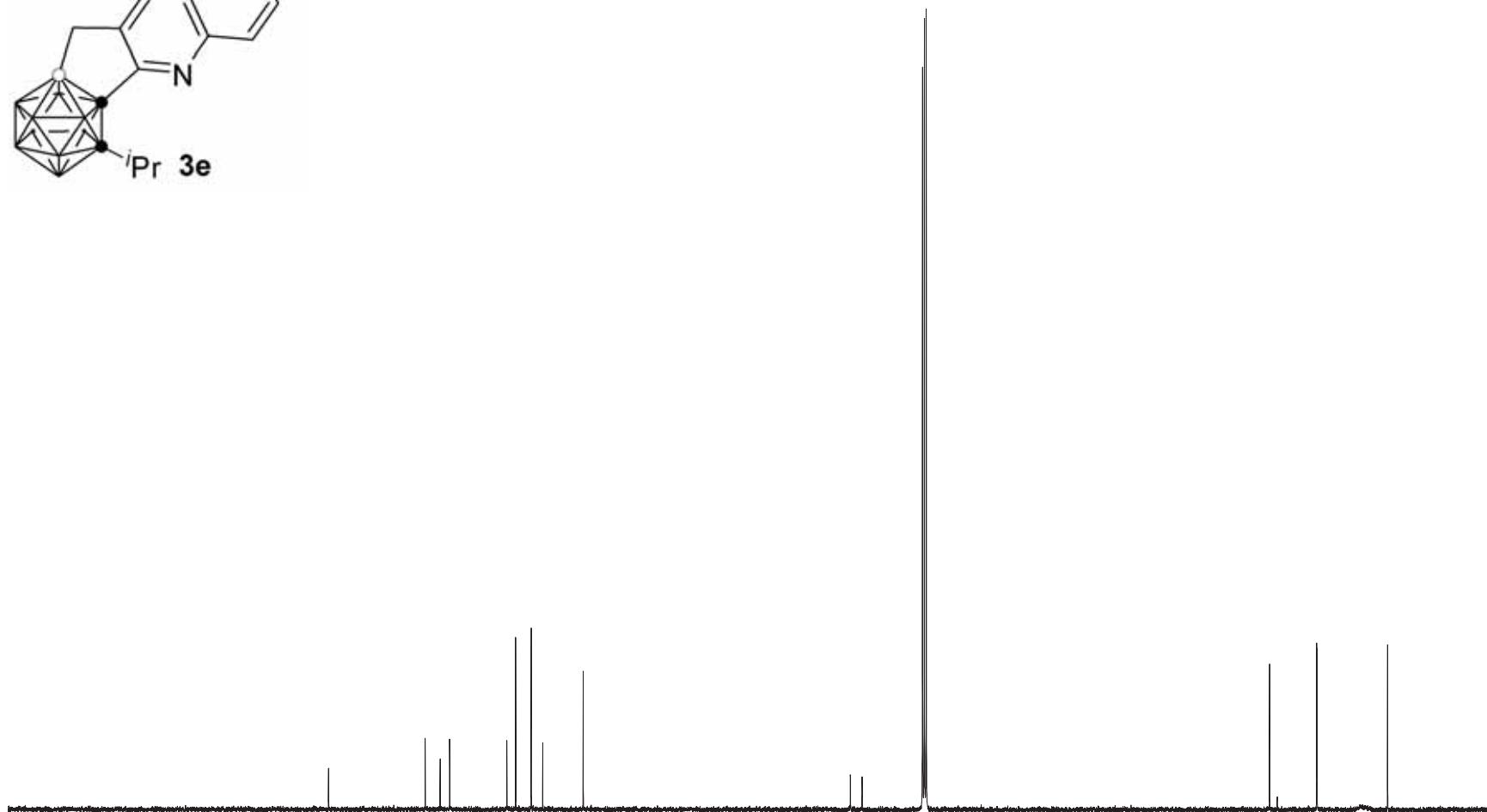
Current Data Parameters  
 NAME I hr-0734-casC  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170729  
 Time 19.10 h  
 INSTRUM spect  
 PROBHD Z119470\_0283 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 800  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 1.1010048 sec  
 RG 206.72  
 DW 16.800 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1  
 SF01 125.7703643 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 94.0000000 W  
 SF02 500.1320005 MHz  
 NUC2 1H  
 CPDPRG[2] wal tz16  
 PCPD2 80.00 usec  
 PLW2 25.0000000 W  
 PLW12 0.39063001 W  
 PLW13 0.19648001 W

F2 - Processing parameters

SI 32768  
 SF 125.7577714 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



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

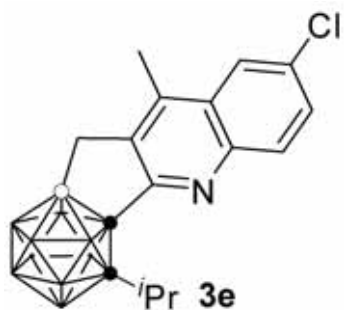
S-145

1hr-B-0734-cascdcl3-IPR

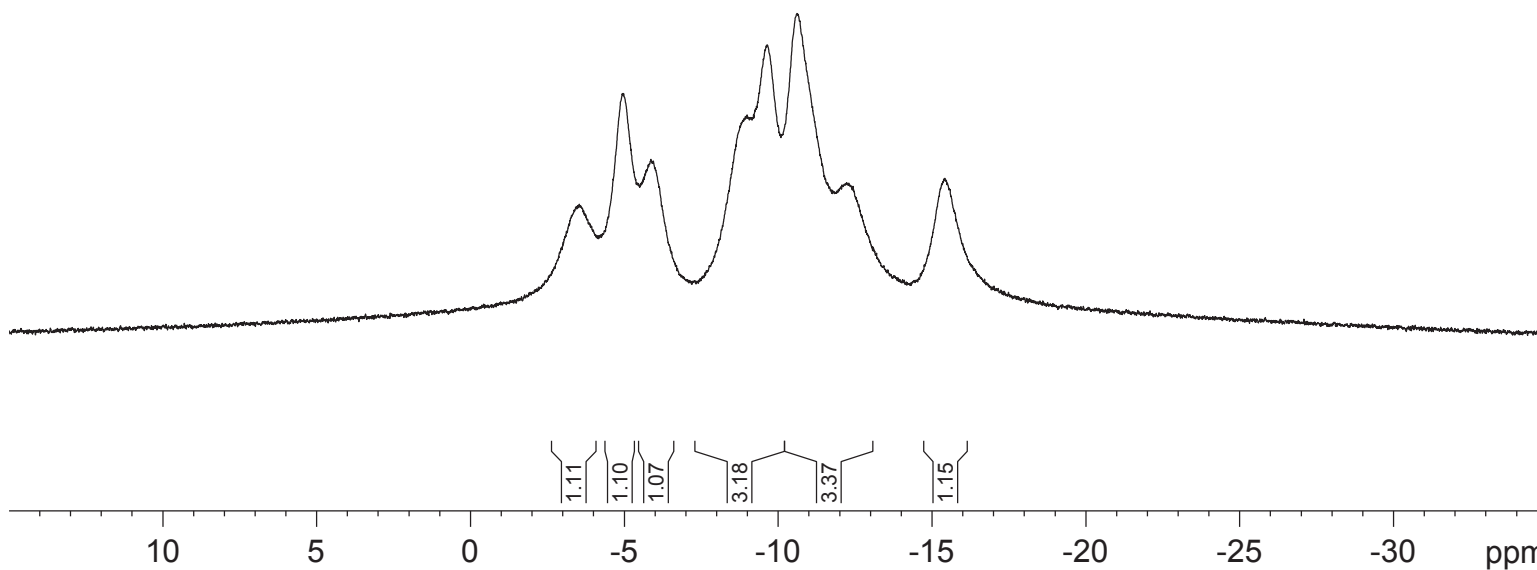
Current Data Parameters  
NAME 1hr-B-0734-cascdcl3-IPR  
EXPNO 1  
PROCNO 1

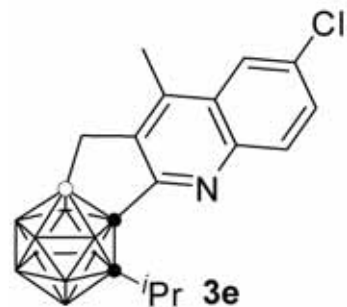
F2 - Acquisition Parameters  
Date\_ 20170729  
Time\_ 19.55 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 24  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 322  
DW 20.800 usec  
DE 6.50 usec  
TE 295.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W  
SFO2 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.56000042 W  
PLW12 0.27428001 W

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



— 3.54  
— 4.95  
— 5.87  
— 8.90  
— 9.64  
— 10.62  
— 12.23  
— 15.42





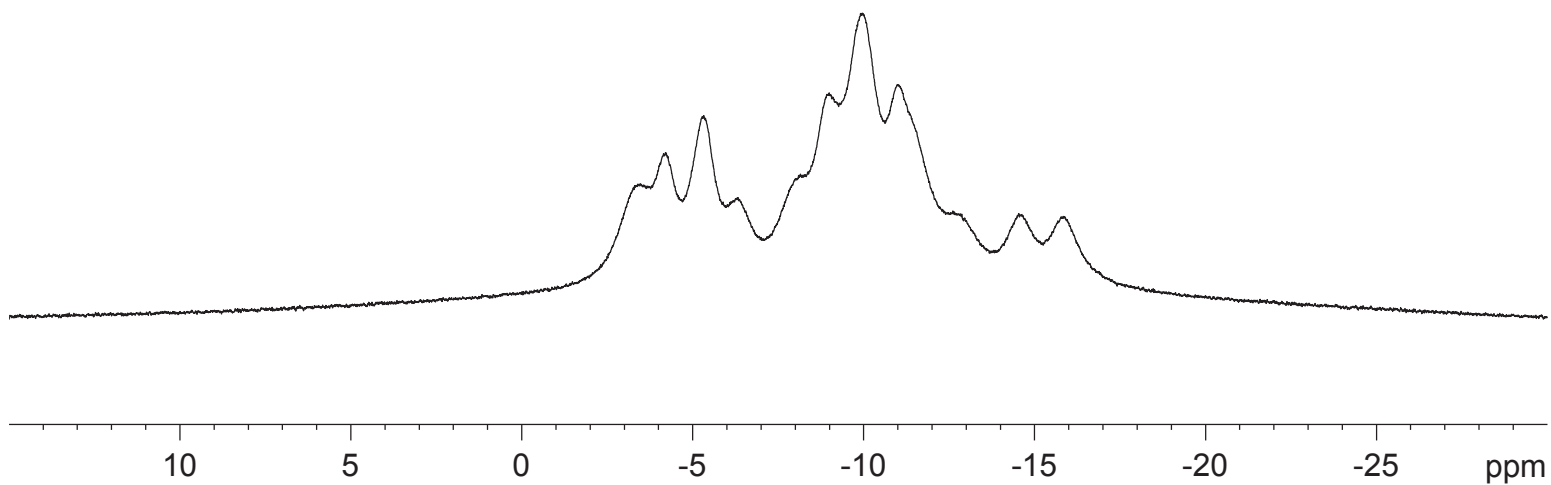
| 3.45  
 | 4.21  
 | 5.33  
 | 6.26  
 | 8.07  
 | 8.95  
 | 9.96  
 | 10.99  
 | 11.49  
 | 12.81  
 | 14.54  
 | 15.84

1hr-B-0734-cascdcl3-IPR(C)

Current Data Parameters  
 NAME 1hr-B-0734-cascdcl3-IPR(C)  
 EXPNO 1  
 PROCNO 1

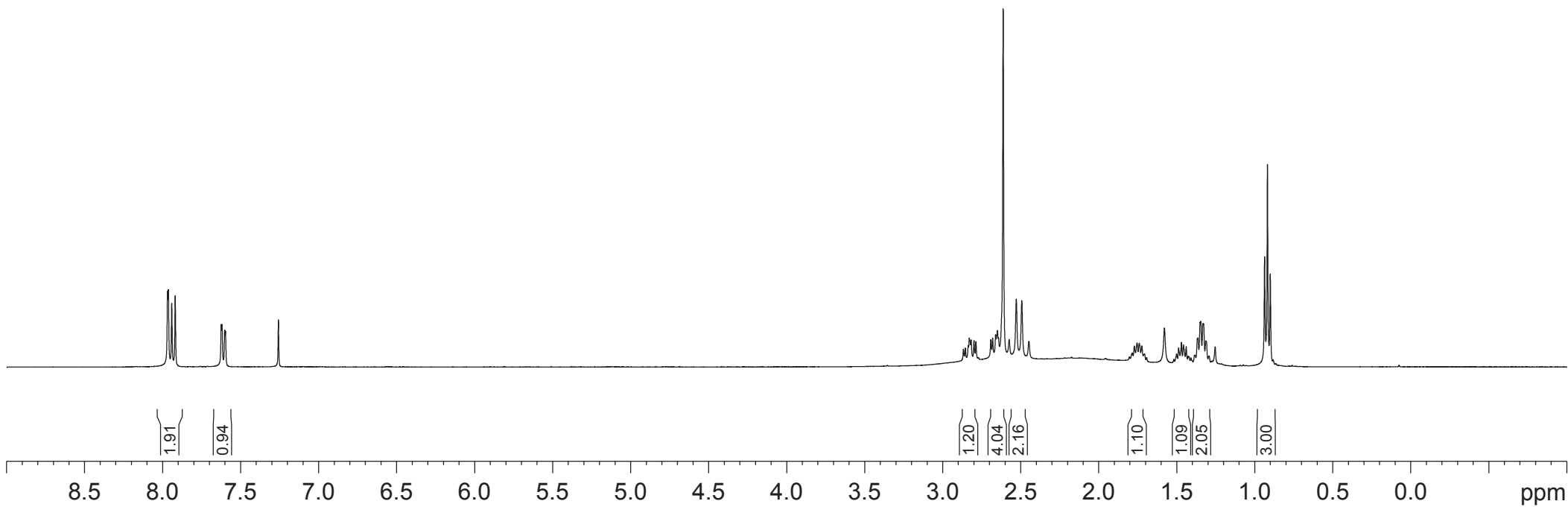
F2 - Acquisition Parameters  
 Date\_ 20170729  
 Time\_ 19.58 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 36  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 362  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.8 K  
 D1 2.0000000 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



7.969  
7.964  
7.942  
7.920  
7.625  
7.620  
7.603  
7.598  
7.260

2.869  
2.857  
2.838  
2.831  
2.819  
2.801  
2.789  
2.693  
2.682  
2.662  
2.651  
2.644  
2.614  
2.576  
2.530  
2.495  
2.449  
1.805  
1.786  
1.773  
1.756  
1.741  
1.725  
1.709  
1.694  
1.580  
1.520  
1.502  
1.489  
1.471  
1.458  
1.441  
1.428  
1.422  
1.411  
1.387  
1.369  
1.365  
1.351  
1.347  
1.333  
1.329  
1.315  
1.294  
1.276  
0.938  
0.920







156.93  
 144.12  
 142.07  
 140.75  
 133.11  
 131.84  
 129.94  
 128.34  
 122.92

83.99  
 80.91  
 77.48  
 77.16  
 76.84

33.82  
 32.05  
 22.45  
 15.08  
 13.81

lhr-C-0731-cascdcl:

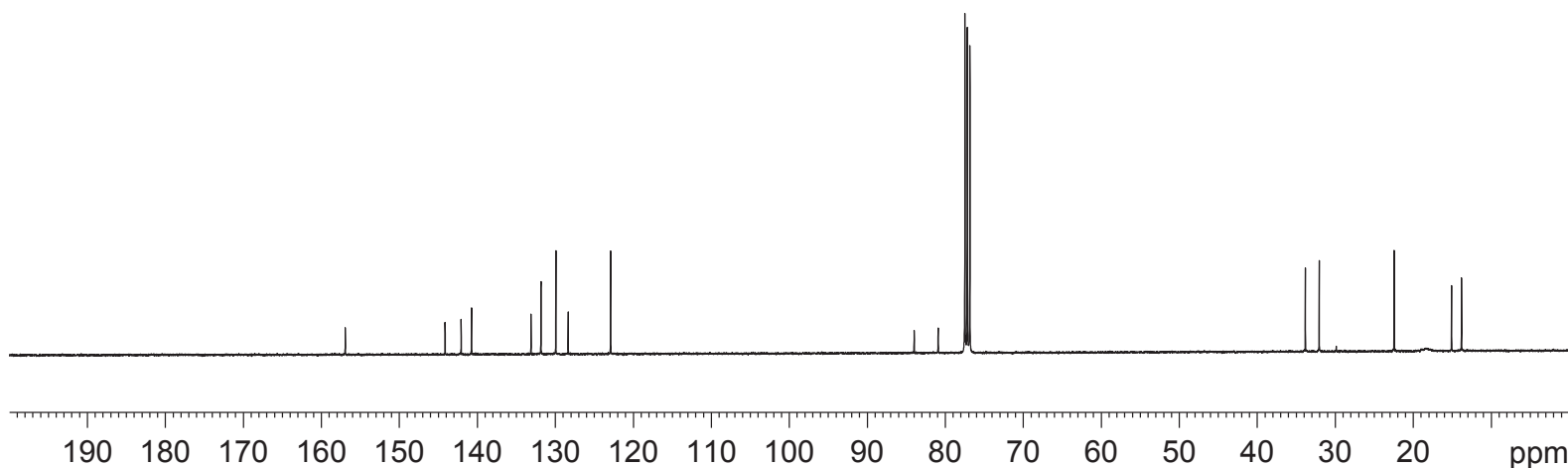
Current Data Parameters  
 NAME lhr-C-0731-cascdcl3-b  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170722  
 Time\_ 18.56 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 3072  
 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 295.4 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 100.6379005 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



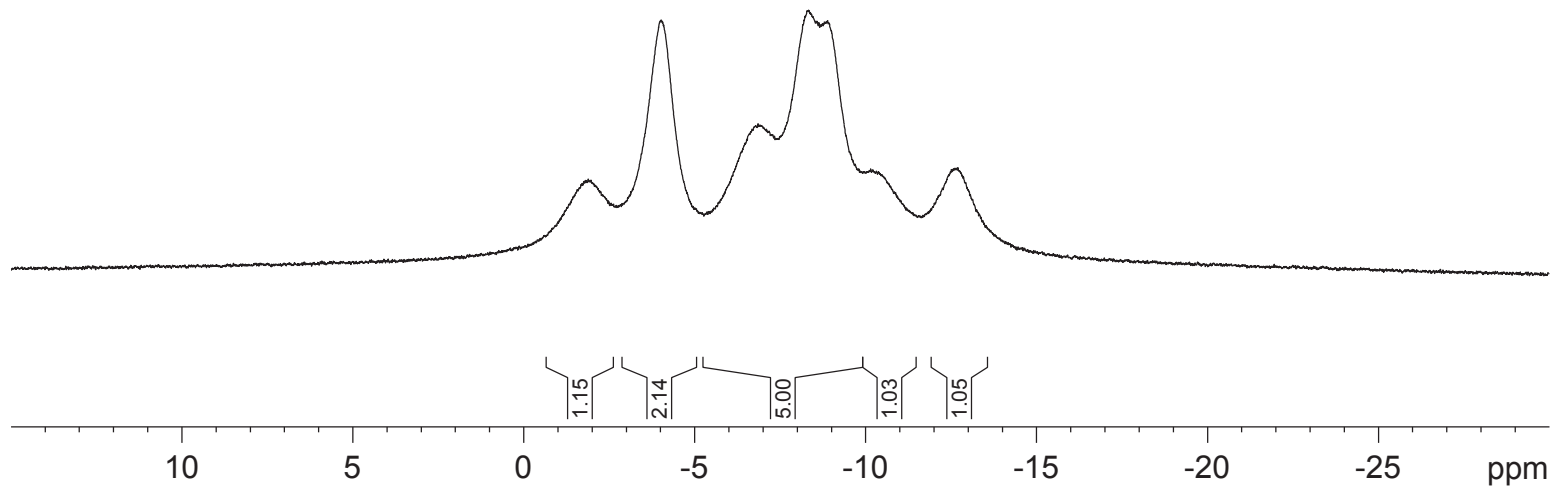
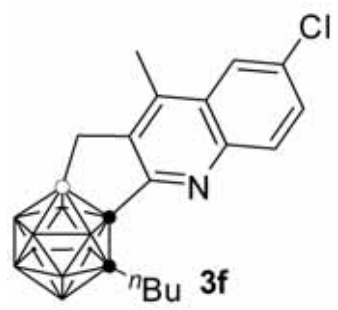
1hr-B-0735-cascdcl3-bu

Current Data Parameters  
NAME 1hr-B-0735-cascdcl3-bu  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170722  
Time 18.45 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 287  
DW 20.800 usec  
DE 6.50 usec  
TE 295.2 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

-1.89  
-4.02  
-6.86  
-8.34  
-8.92  
-10.26  
-12.71



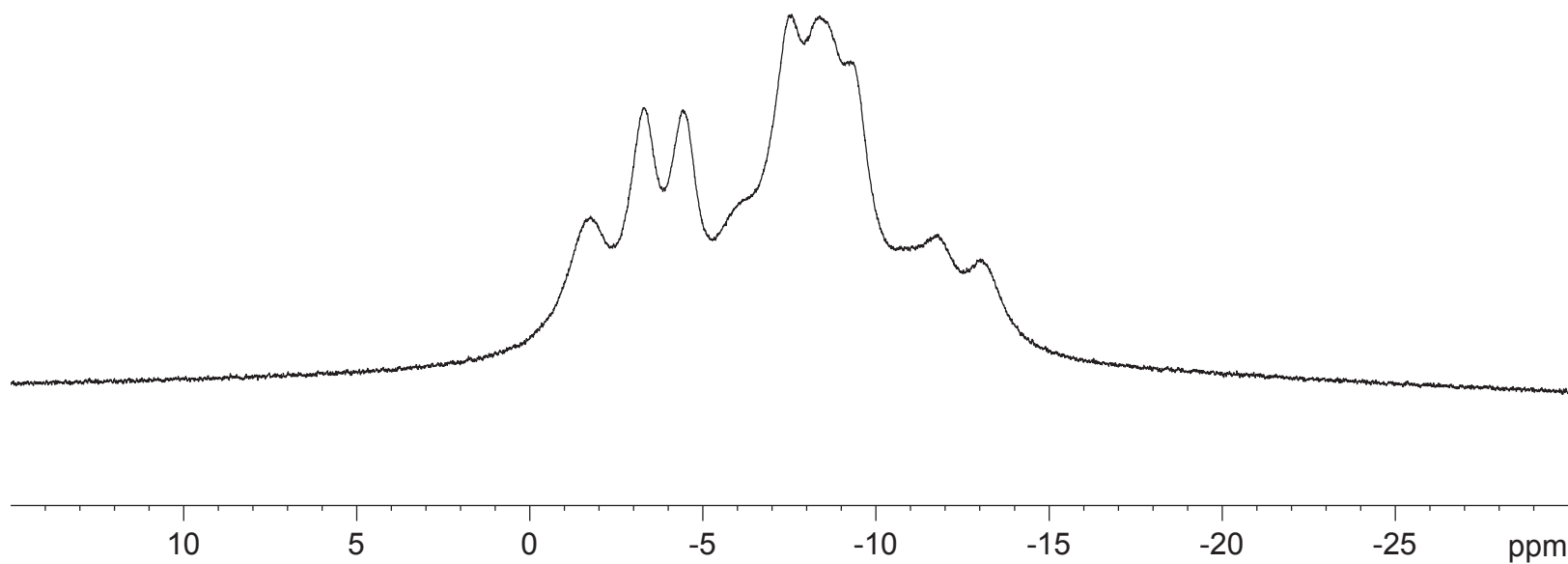
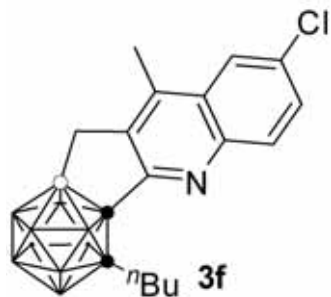
1hr-B-0735-cascdcl3-bu(C)

Current Data Parameters  
NAME 1hr-B-0735-cascdcl3-bu(C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170722  
Time 18.47 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 25  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 362  
DW 20.800 usec  
DE 6.50 usec  
TE 295.1 K  
D1 2.00000000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W

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

— 1.76  
— 3.28  
— 4.43  
— 6.09  
— 7.57  
— 8.38  
— 8.58  
— 9.31  
— 10.91  
— 11.76  
— 12.99



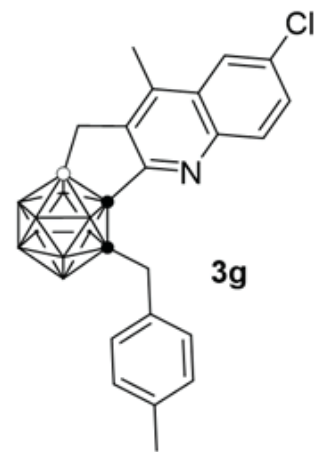
8.053  
8.031  
8.006  
8.001  
7.669  
7.663  
7.647  
7.641  
7.260  
7.179  
7.159  
7.115  
7.095

4.229  
4.191  
3.941  
3.903

2.639  
2.582  
2.537  
2.505  
2.459  
2.333

1.564

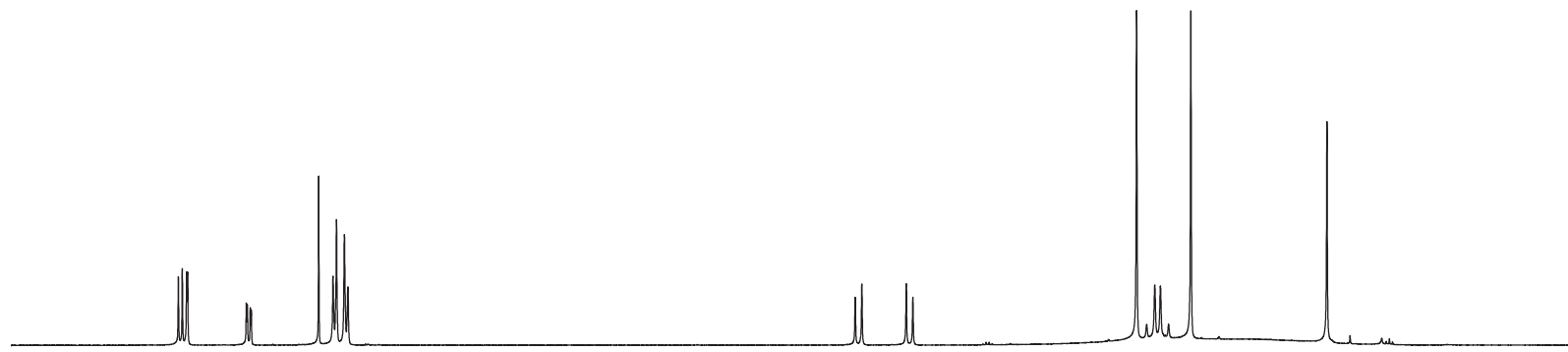
lhr-H-0740-cascdcl3-



Current Data Parameters  
 NAME lhr-H-0740-cascdcl3-bnch3  
 EXPNO 2  
 PROCNO 1

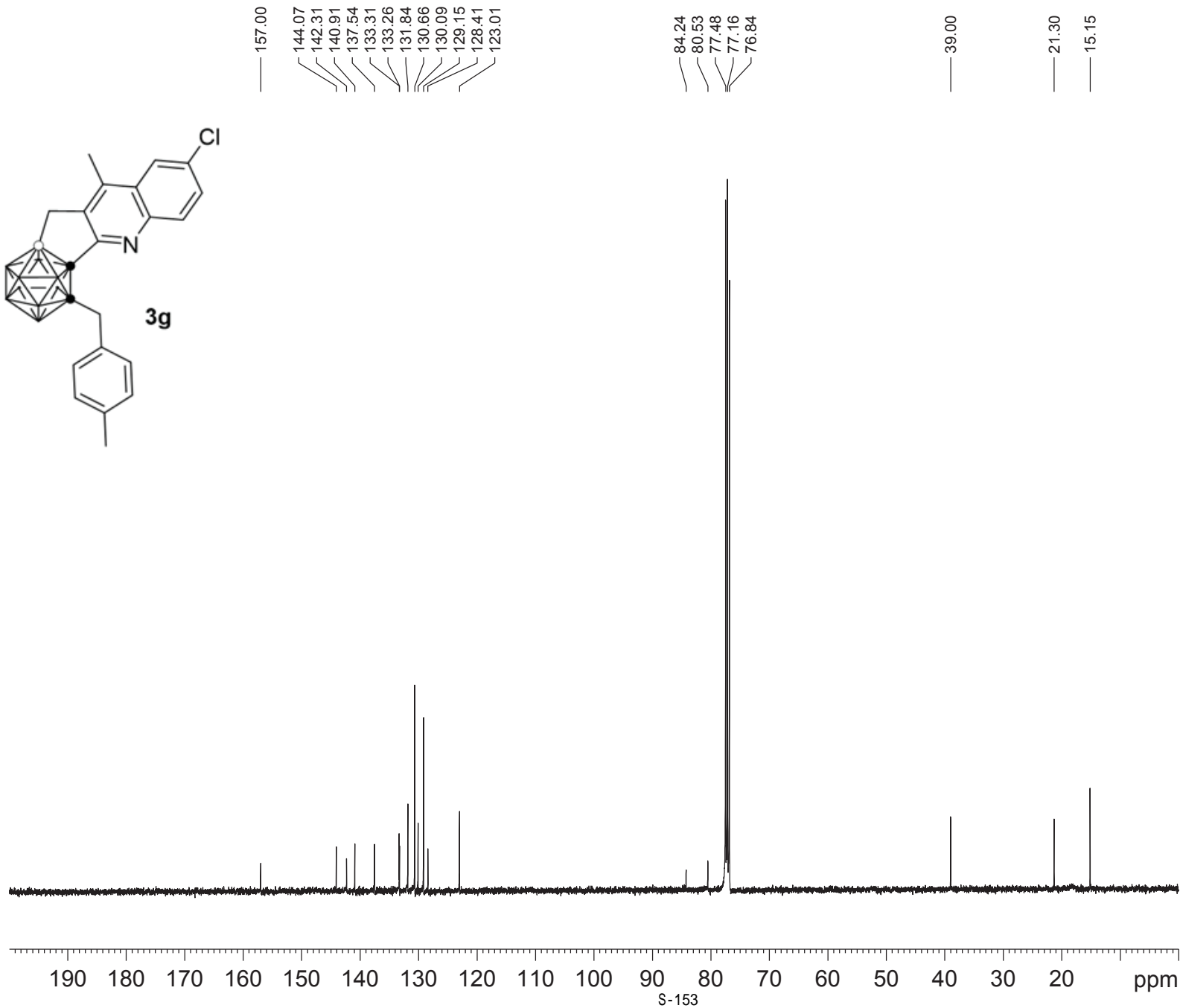
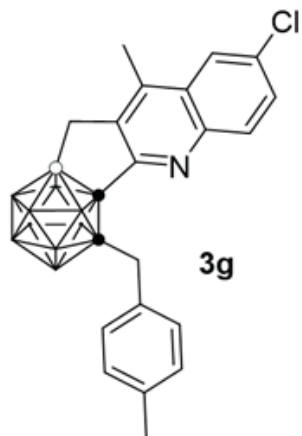
F2 - Acquisition Parameters  
 Date\_ 20170809  
 Time 16.49 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (zg30)  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 12  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.7 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

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



1.01  
0.94  
1.00  
2.05  
1.97  
1.04  
1.05  
3.02  
2.00  
3.08

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



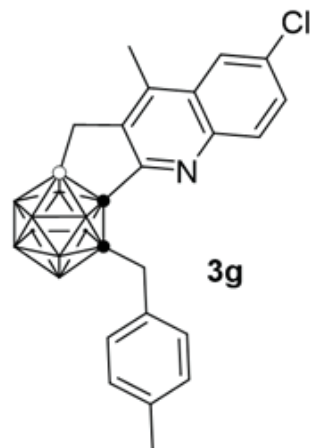
lhr-c-0740-cascdcl:

Current Data Parameters  
 NAME lhr-C-0740-cascdcl3-bnch:  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170804  
 Time\_ 17.45 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1486  
 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 100.6379004 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1hr-B-0740-cascdcl3-bnch3

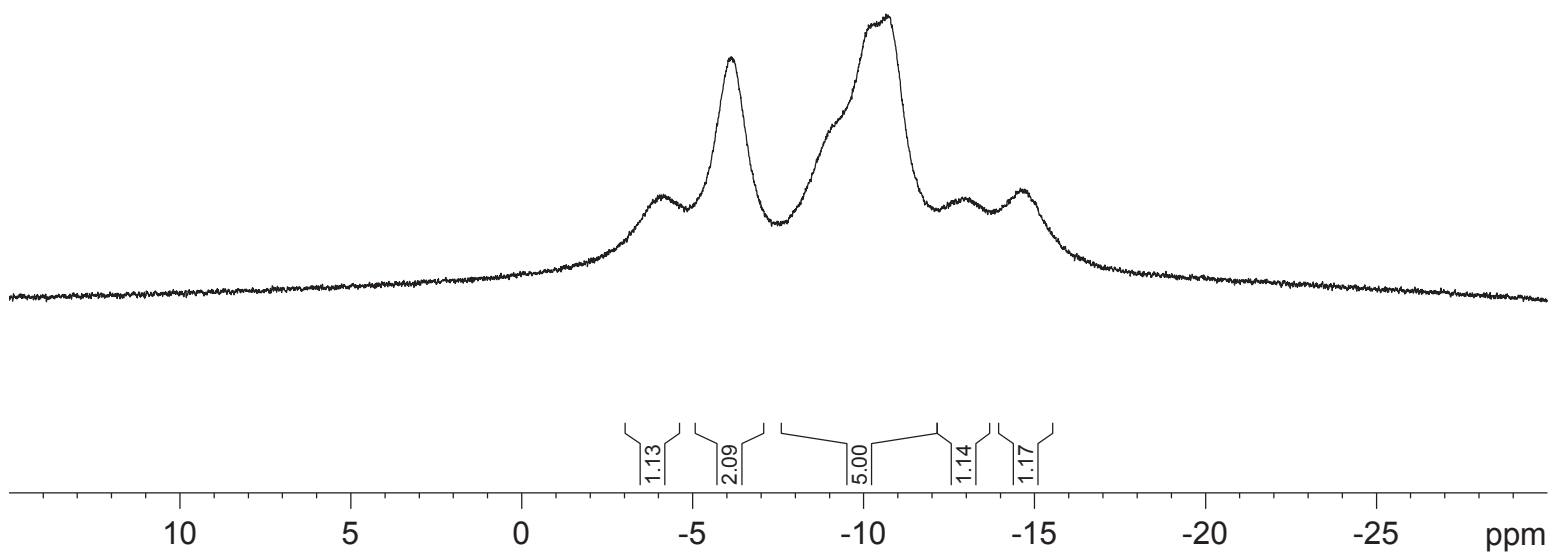


— 4.14  
— 6.13  
— 9.12  
— 10.10  
— 10.65  
— 12.97  
— 14.58

Current Data Parameters  
NAME 1hr-B-0740-cascdcl3-bnch3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170804  
Time 17.33 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CD3CN  
NS 32  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 322  
DW 20.800 usec  
DE 6.50 usec  
TE 295.2 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



S-154

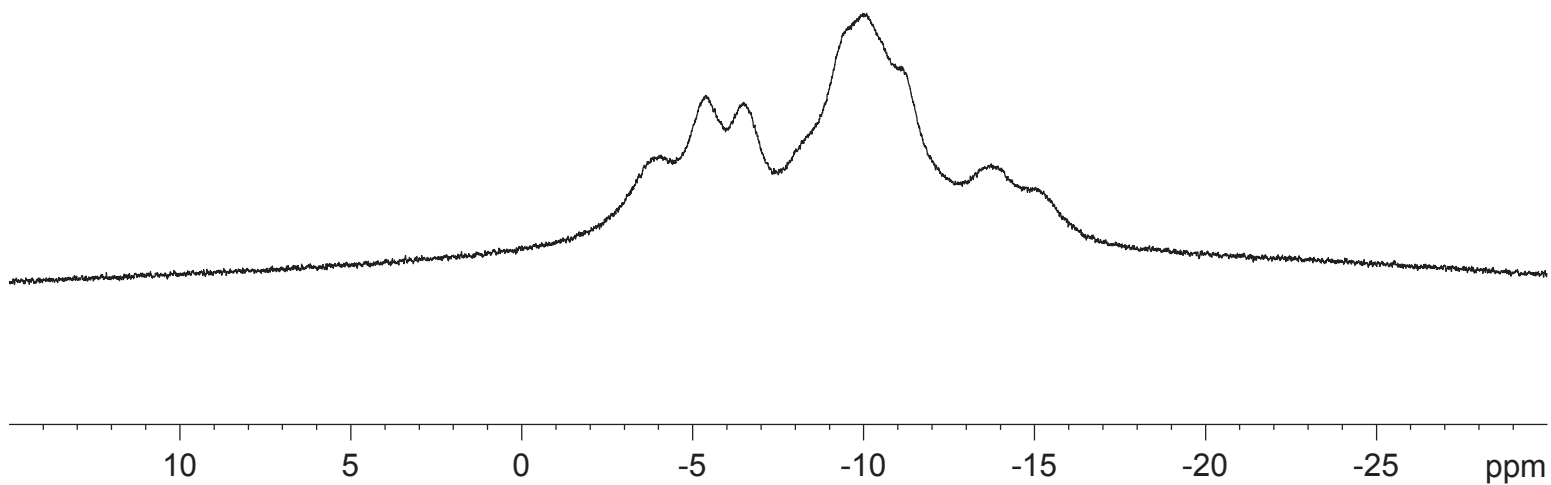
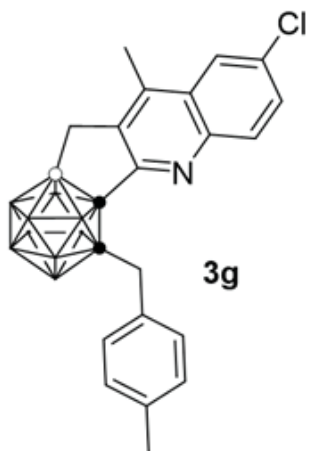
lhr-B-0740-cascdcl3-bnch3 (C)

Current Data Parameters  
NAME lhr-B-0740-cascdcl3-bnch3 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170804  
Time\_ 17.37 h  
INSTRUM spect  
PROBHD Z108618\_0257 (Z)  
PULPROG zg  
TD 65536  
SOLVENT CD3CN  
NS 44  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 322  
DW 20.800 usec  
DE 6.50 usec  
TE 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

— 4.07  
— 5.38  
— 6.50  
— 8.24  
— 9.43  
— 9.97  
— 11.12  
— 13.74  
— 15.05

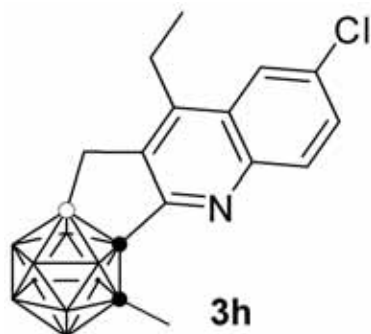


7.984  
7.976  
7.970  
7.962  
7.629  
7.624  
7.607  
7.601  
7.260

3.086  
3.067  
3.048  
3.029  
2.591  
2.545  
2.510  
2.464  
2.416

1.567  
1.315  
1.296  
1.277

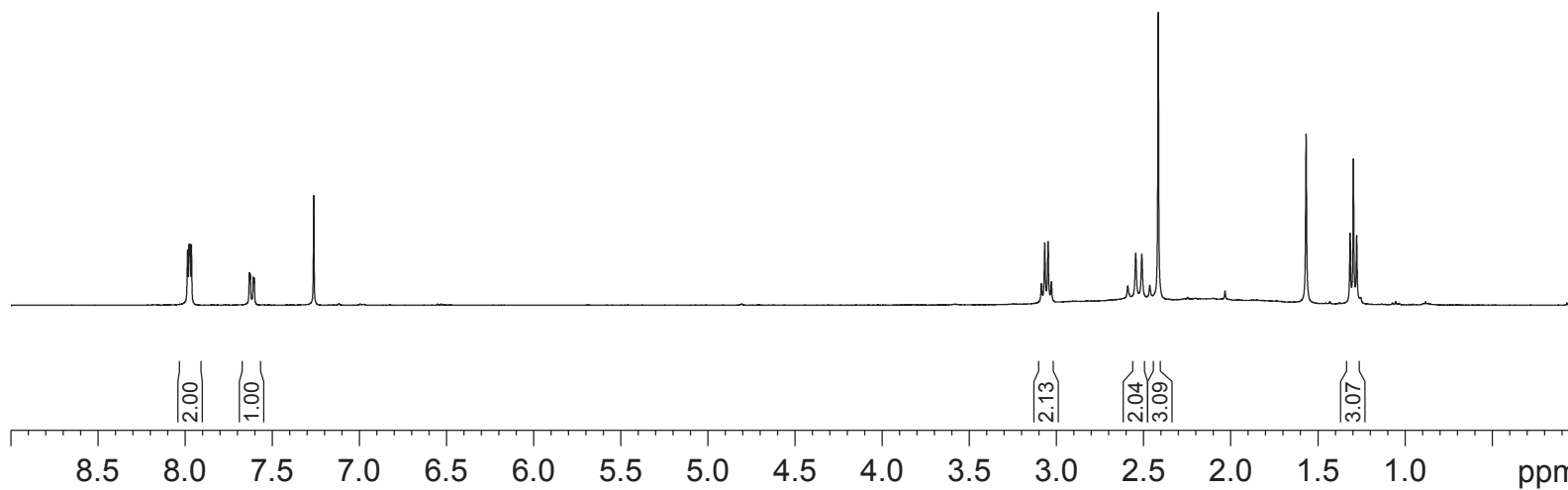
lhr-H-0710-pclet-cas



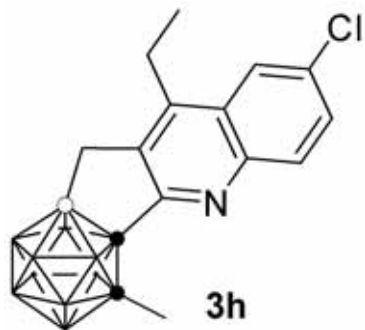
Current Data Parameters  
NAME lhr-H-0710-pclet-cascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170702  
Time 19.53 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCI3  
NS 12  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 295.2 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 400.2300100 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00







157.10  
147.88  
144.66  
139.90  
133.22  
132.10  
129.93  
127.32  
122.67

82.97  
77.41  
77.16  
76.91  
75.40

22.48  
22.26  
13.85

I hr-C-0710

Current Data Parameters  
NAME I hr-C-0710cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170703  
Time 20.26 h  
INSTRUM spect  
PROBHD Z119470\_0283 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1005  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 6.50 usec  
TE 297.8 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 94.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 25.0000000 W  
PLW12 0.39063001 W  
PLW13 0.19648001 W

F2 - Processing parameters

SI 32768  
SF 125.7577709 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

S-157

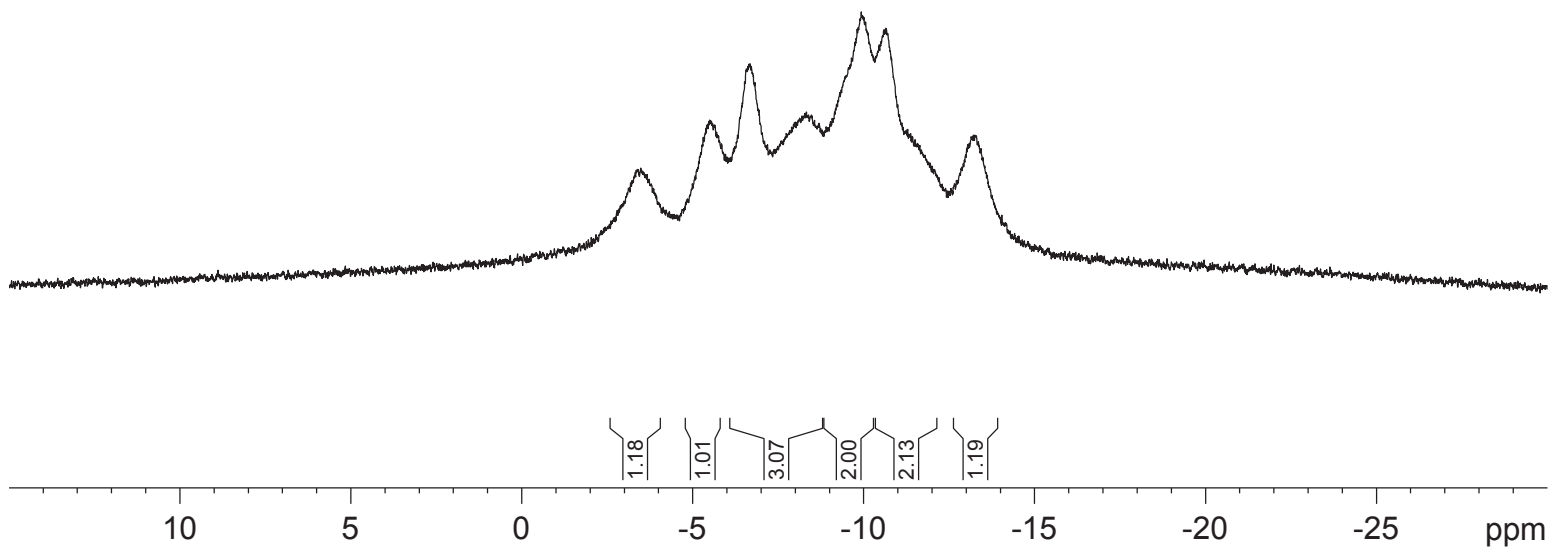
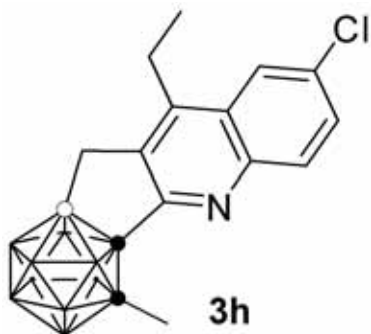
lhr-B-0710-pclet-cascdcl3

Current Data Parameters  
NAME lhr-B-0710-pclet-cascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170702  
Time 19.40 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT THF  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 287  
DW 20.800 usec  
DE 6.50 usec  
TE 295.8 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

— 3.48  
— 5.50  
— 6.68  
— 8.33  
— 9.93  
— 10.65  
— 11.52  
— 13.22



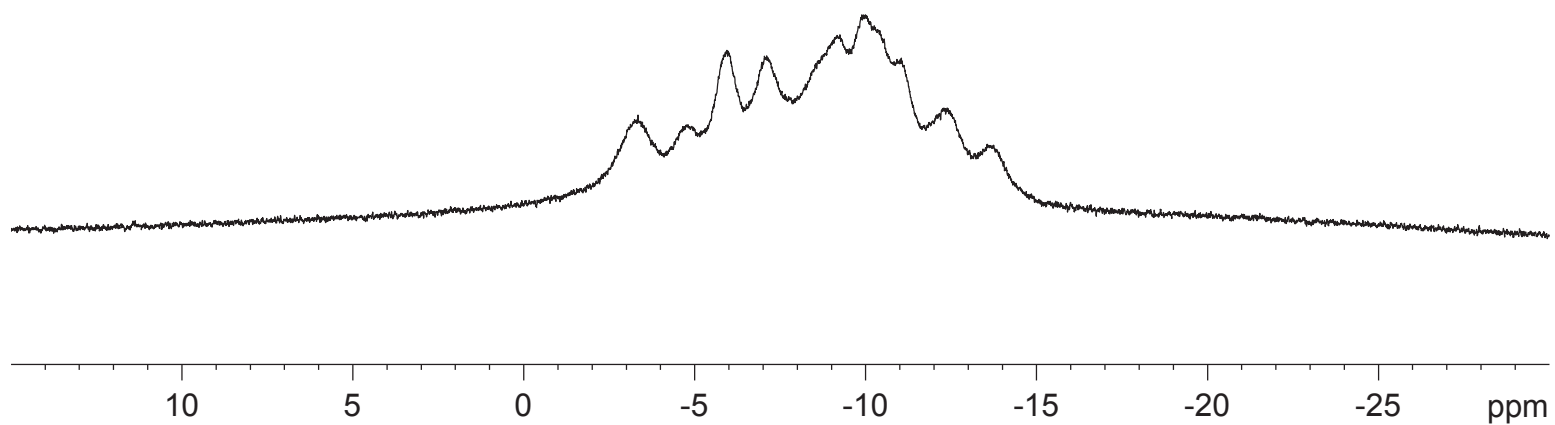
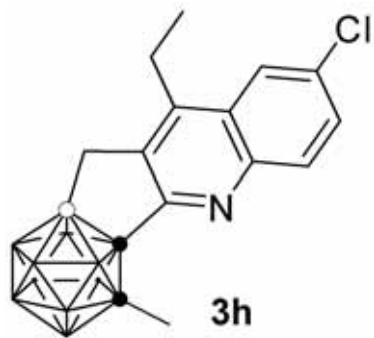
lhr-B-0710-pclet-cascdcl3(C)

Current Data Parameters  
NAME lhr-B-0710-pclet-cascdcl3(C)  
EXPNO 1  
PROCNO 1

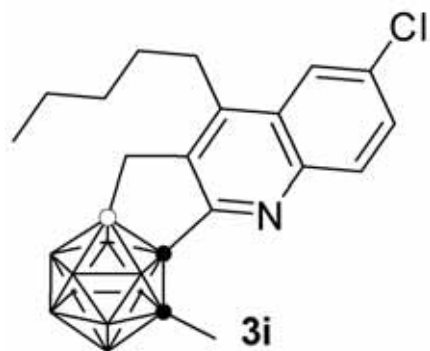
F2 - Acquisition Parameters  
Date\_ 20170702  
Time 19.42 h  
INSTRUM spect  
PROBHD Z108618\_0257 ( )  
PULPROG zg  
TD 65536  
SOLVENT THF  
NS 28  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 287  
DW 20.800 usec  
DE 6.50 usec  
TE 295.4 K  
D1 2.00000000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W

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

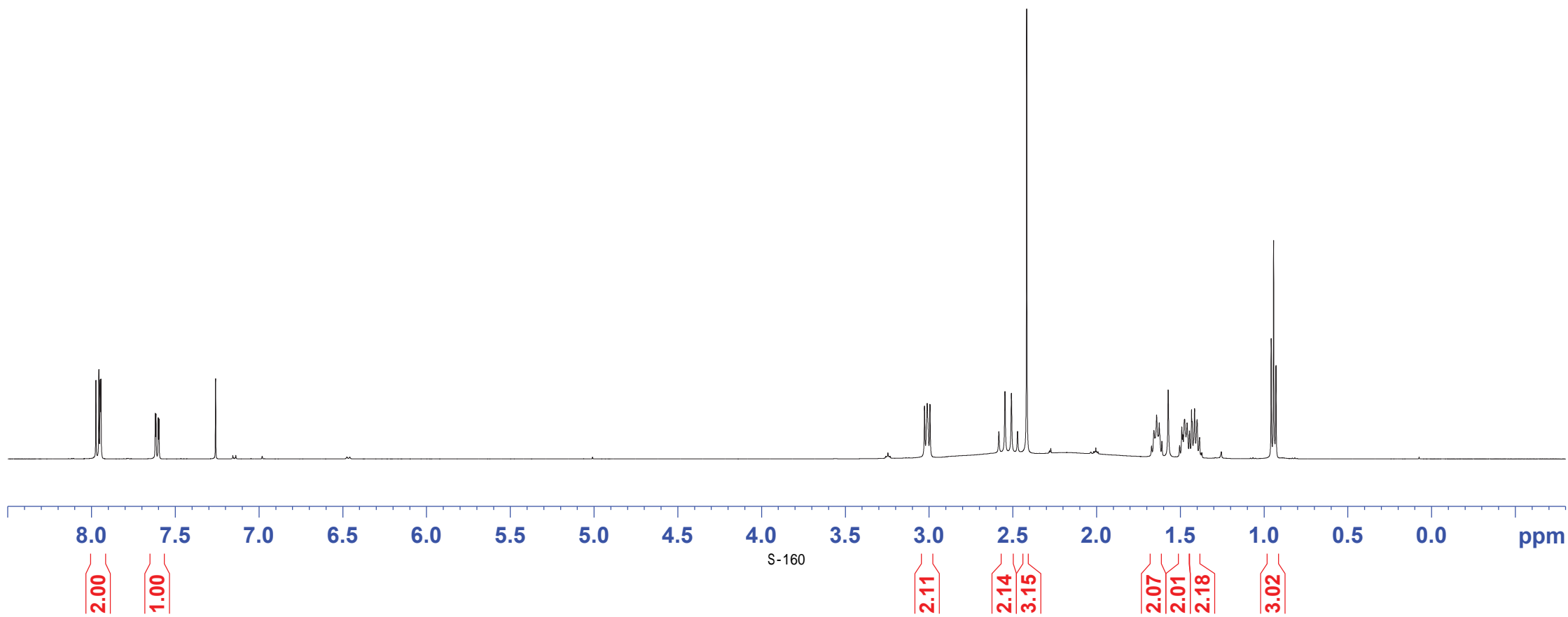
3.34  
4.80  
5.94  
7.11  
8.60  
9.25  
10.00  
10.37  
11.00  
12.29  
13.56

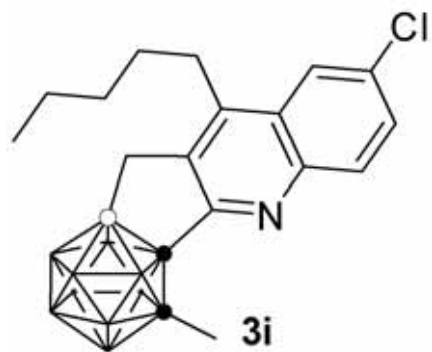


7.974  
7.957  
7.949  
7.944  
7.620  
7.615  
7.602  
7.598  
7.260



3.027  
3.011  
2.995  
2.584  
2.547  
2.509  
2.472  
2.418  
1.672  
1.658  
1.642  
1.632  
1.626  
1.610  
1.573  
1.505  
1.491  
1.485  
1.474  
1.460  
1.446  
1.434  
1.430  
1.415  
1.400  
1.385  
0.958  
0.944  
0.929





157.00  
146.82  
144.61  
140.23  
133.12  
132.05  
129.89  
127.59  
122.80

82.97  
77.41  
77.16  
76.91  
75.40

32.37  
29.49  
29.33  
22.63  
22.25  
14.15

I hr-C-0754

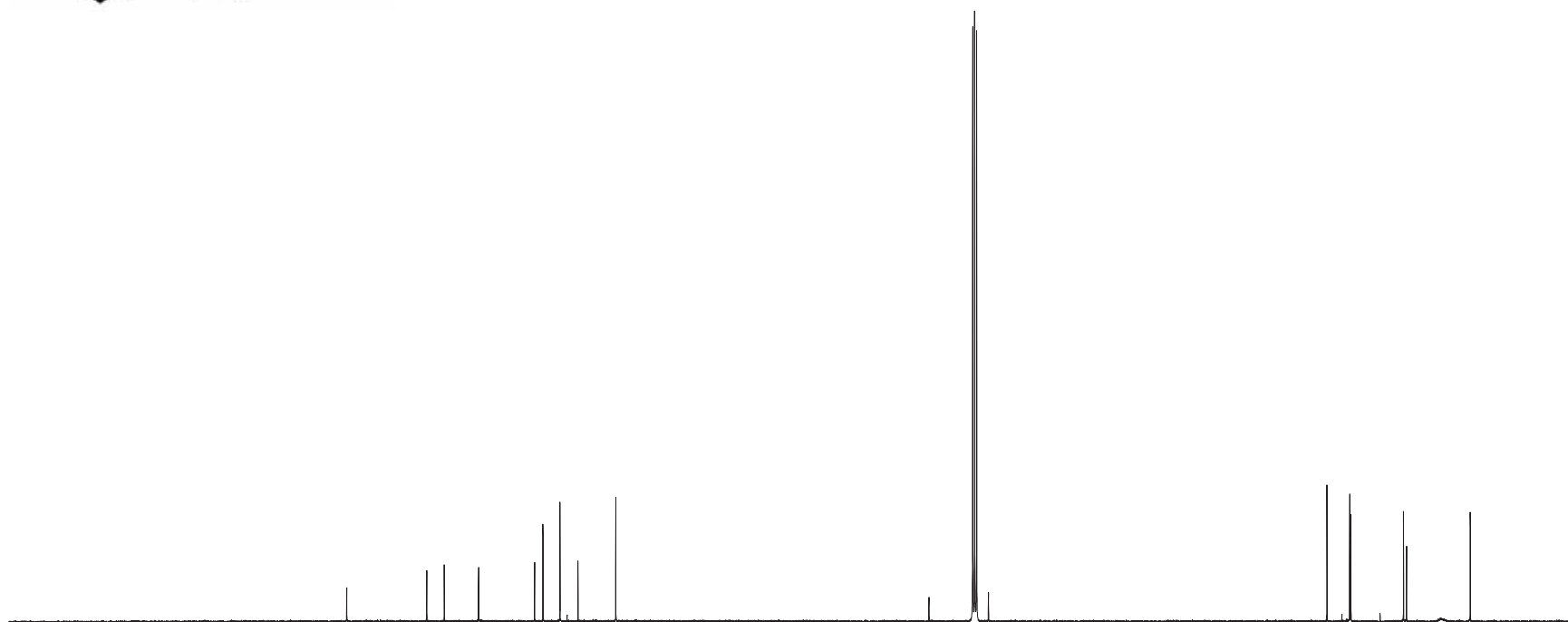
Current Data Parameters  
NAME I hr-C-0754  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170908  
Time 9.56 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 400  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters

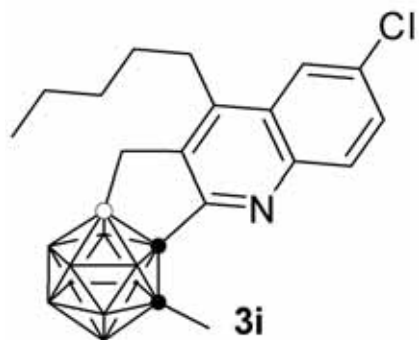
SI 32768  
SF 125.7577721 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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

S-161

I hr-B-0754-cascdcl 3

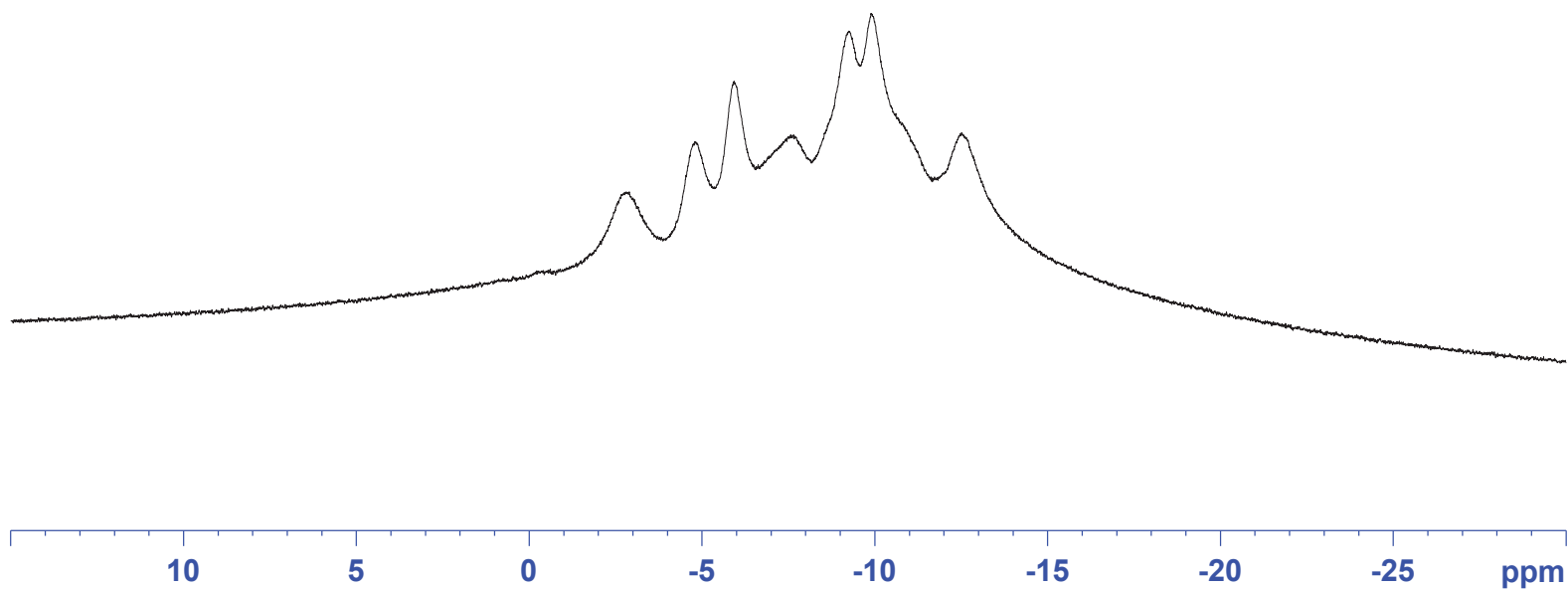


-2.89  
-4.81  
-5.92  
-7.58  
-9.24  
-9.90  
-10.88  
-12.50

Current Data Parameters  
NAME I hr-B-0754-cascdcl 3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170828  
Time 18.58 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 24  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 163.99  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

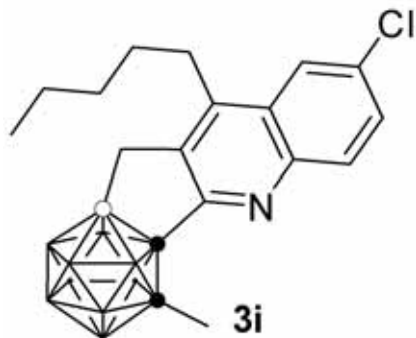
F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.14  
1.05  
1.07  
2.00  
4.00  
1.17  
S 162

1 hr-B-0754-cascdcl 3(C)

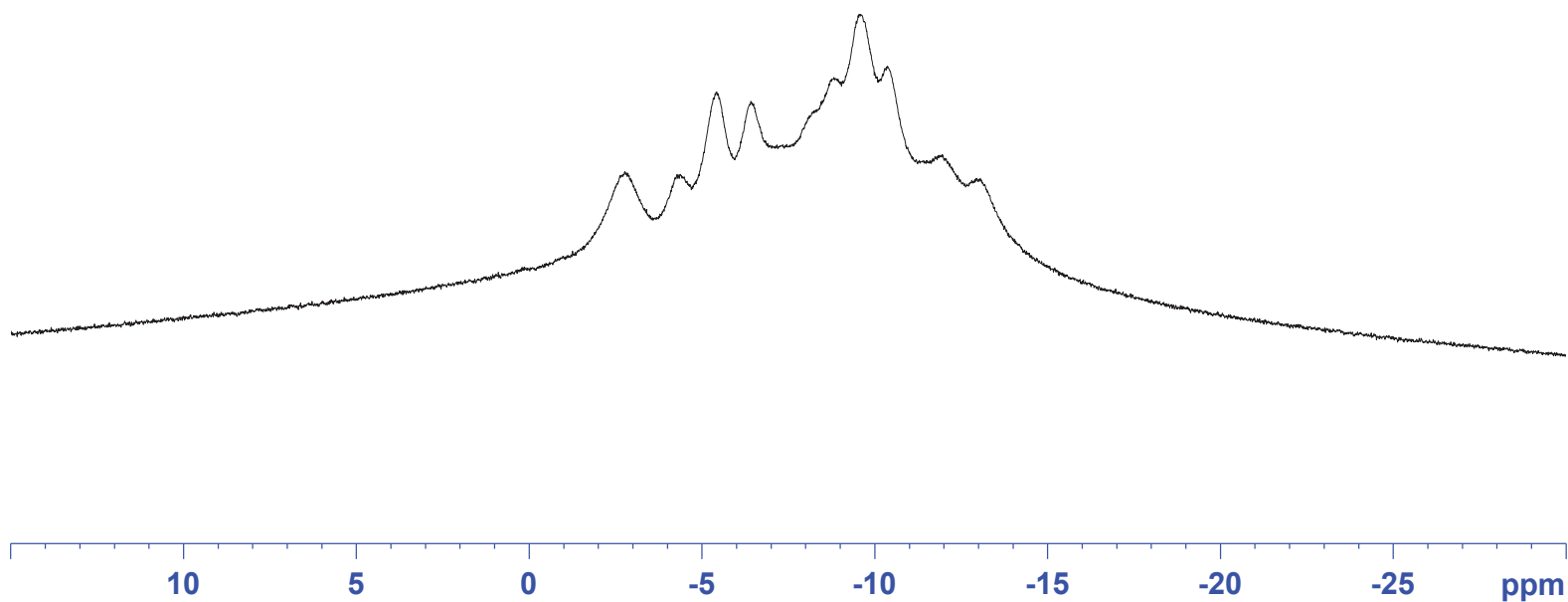
-2.76  
-4.36  
-5.41  
-6.41  
-8.14  
-8.78  
-9.54  
-10.36  
-11.90  
-12.99



Current Data Parameters  
NAME 1 hr-B-0754-cascdcl 3(C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170828  
Time\_ 19.00 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 24  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.00000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

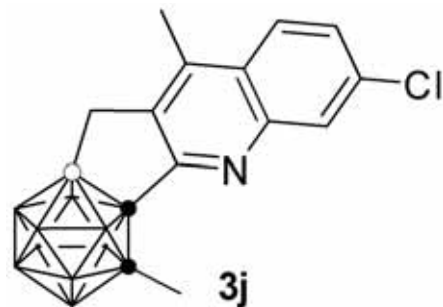


8.042  
8.037  
7.952  
7.930  
7.542  
7.537  
7.519  
7.514  
7.260

2.643  
2.575  
2.529  
2.495  
2.449  
2.414

1.573

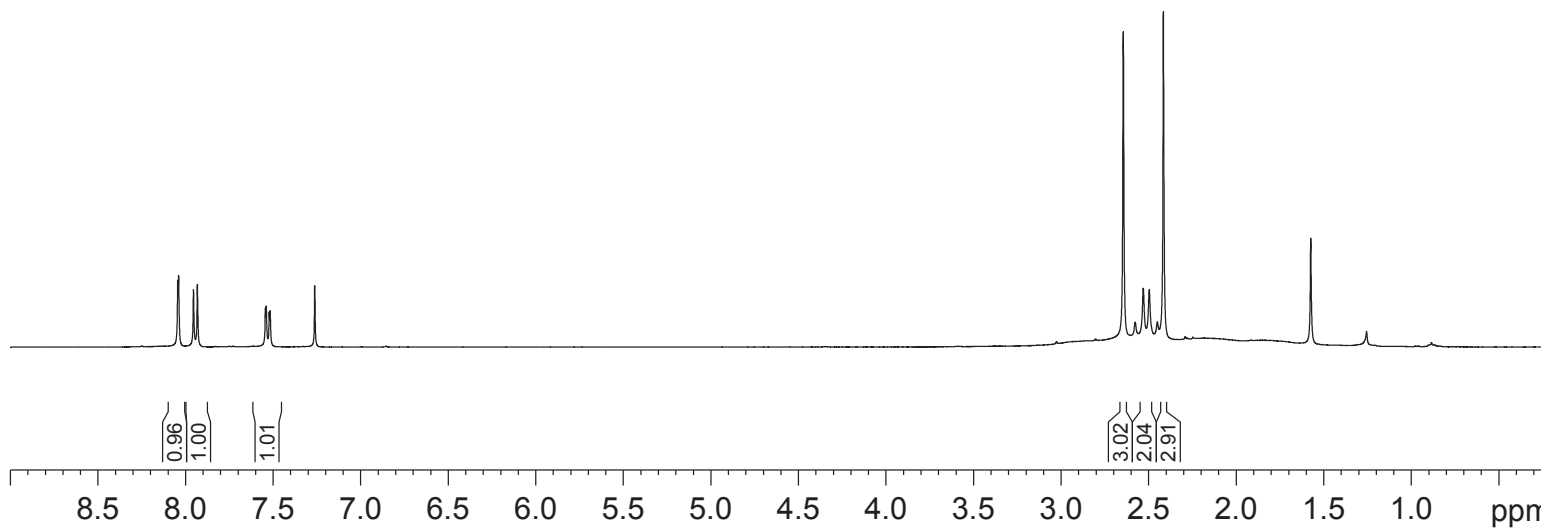
1hr-H-0712-3cl-casc



Current Data Parameters  
NAME 1hr-H-0712-3cl-casc  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170704  
Time\_ 10.22 h  
INSTRUM spect  
PROBHD Z108618\_0257 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 296.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

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





I hr-0712

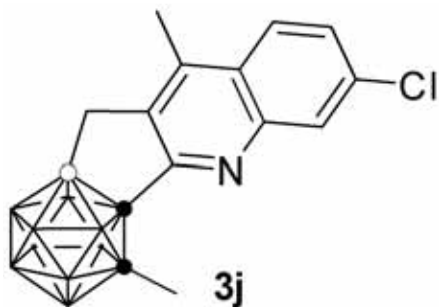
Current Data Parameters  
NAME I hr-0712-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170704  
Time 15.48 h  
INSTRUM spect  
PROBHD Z119470\_0283 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 300  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 6.50 usec  
TE 297.9 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 94.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 25.0000000 W  
PLW12 0.39063001 W  
PLW13 0.19648001 W

F2 - Processing parameters

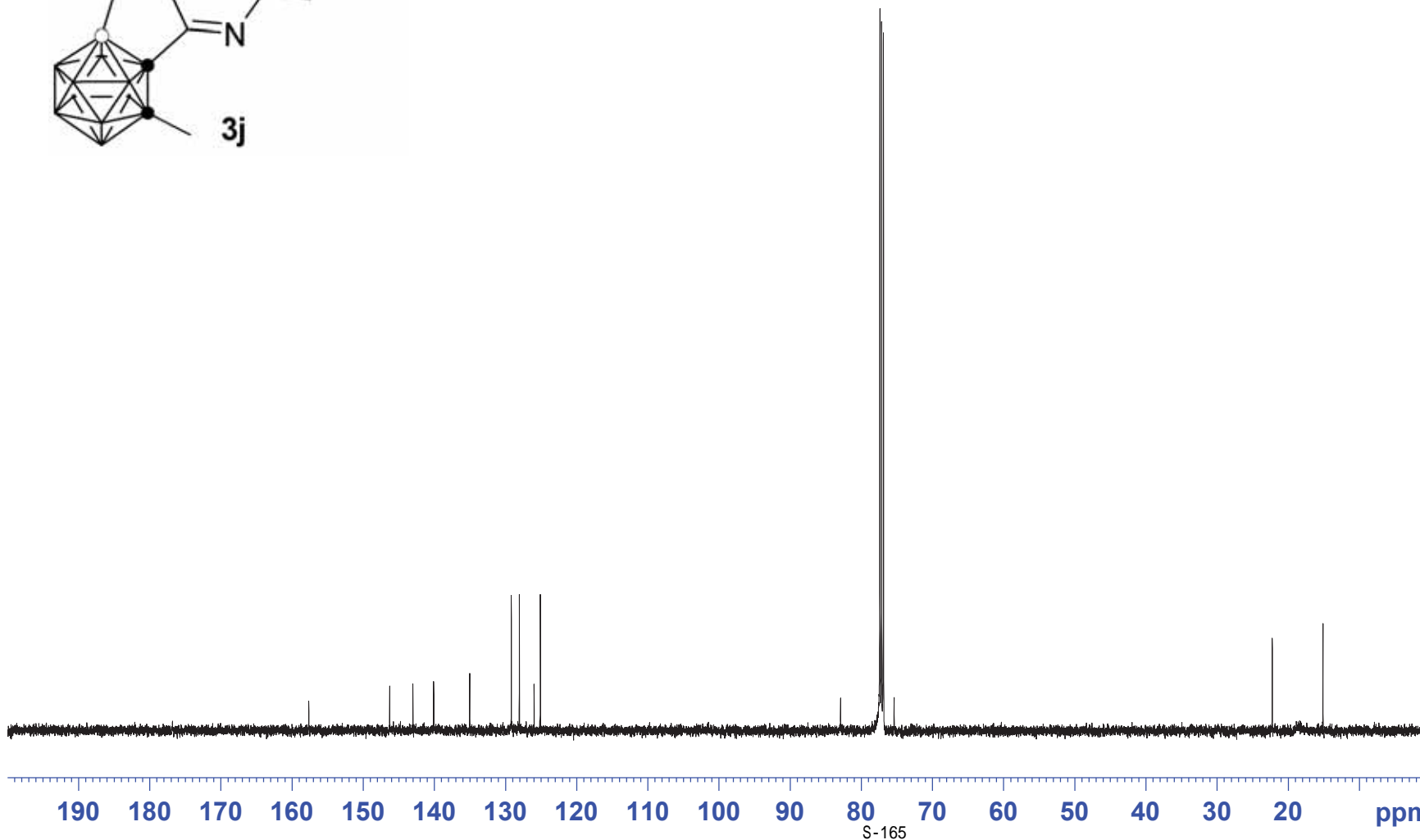
SI 32768  
SF 125.7577717 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



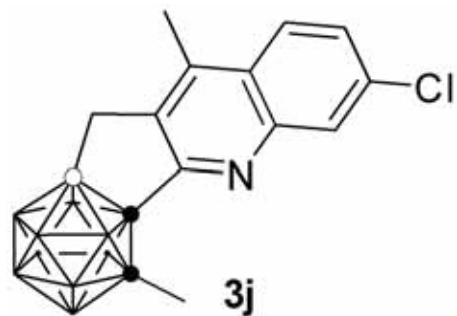
157.69  
146.31  
143.05  
140.13  
135.06  
129.22  
128.10  
126.02  
125.13

82.93  
77.41  
77.16  
76.91  
75.41

22.26  
15.14



1hr-B-0712-3cl-cascdcl3

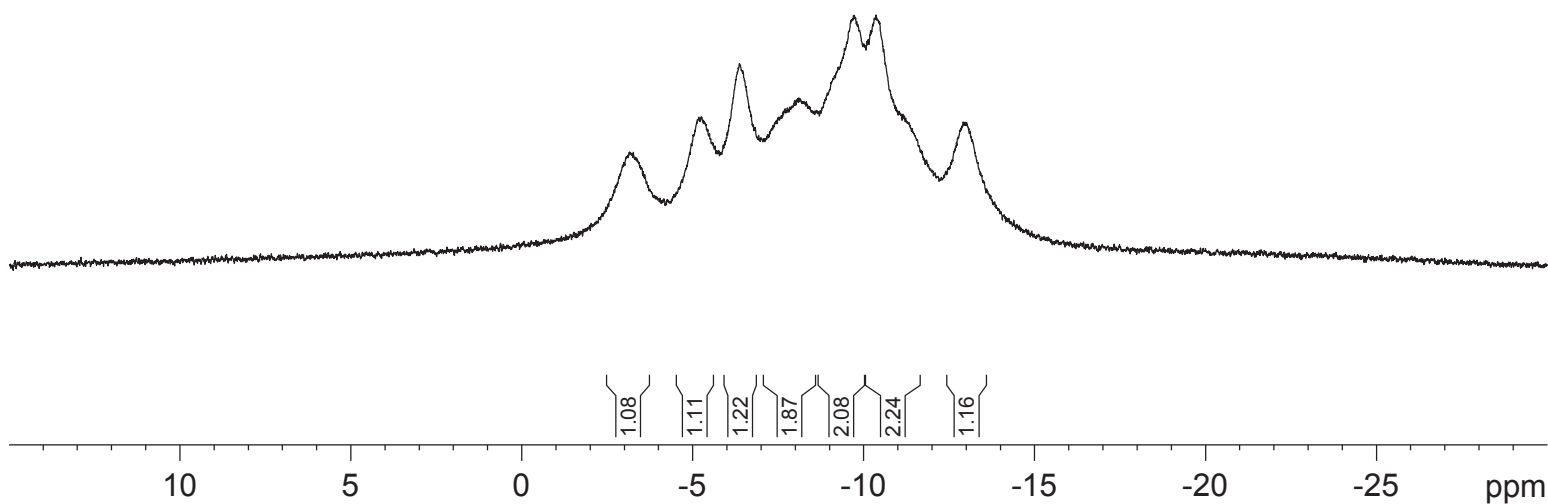


— 3.16  
— 5.25  
— 6.37  
— 7.58  
— 8.11  
— 9.17  
— 9.72  
— 10.36  
— 11.31  
— 12.91

Current Data Parameters  
NAME 1hr-B-0712-3cl-cascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170704  
Time\_ 10.04 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 287  
DW 20.800 usec  
DE 6.50 usec  
TE 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



1.08 1.11 1.22 1.87 2.08 2.24 1.16

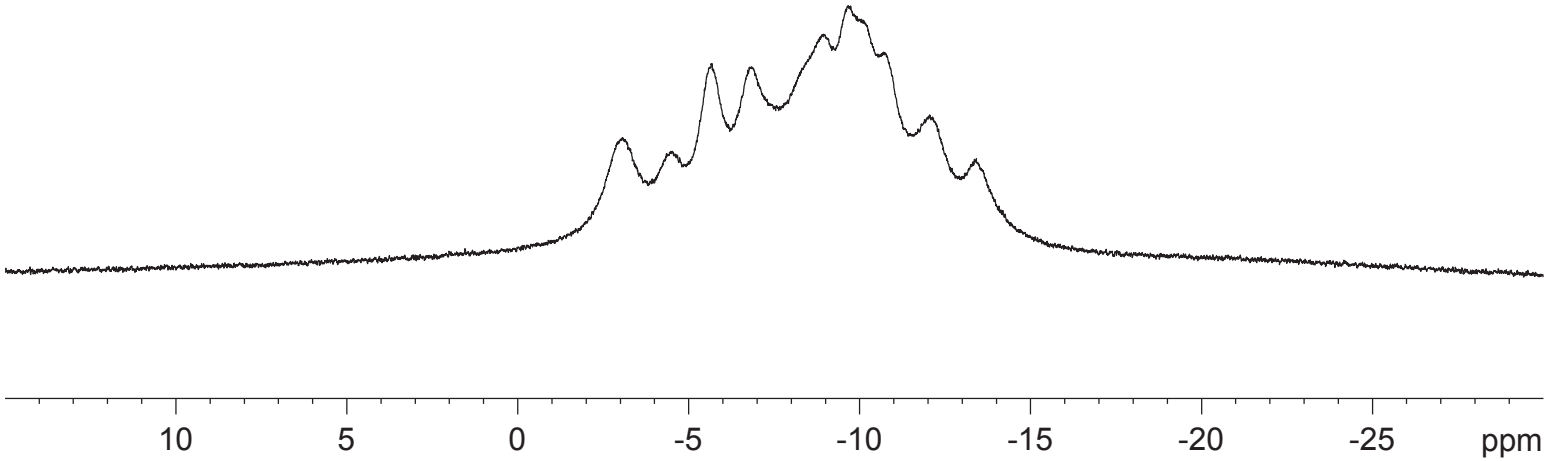
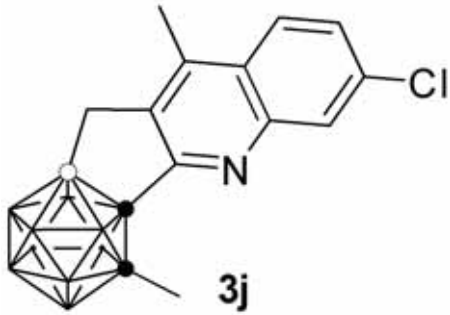
1hr-B-0712-3cl-cascdcl3 (C)

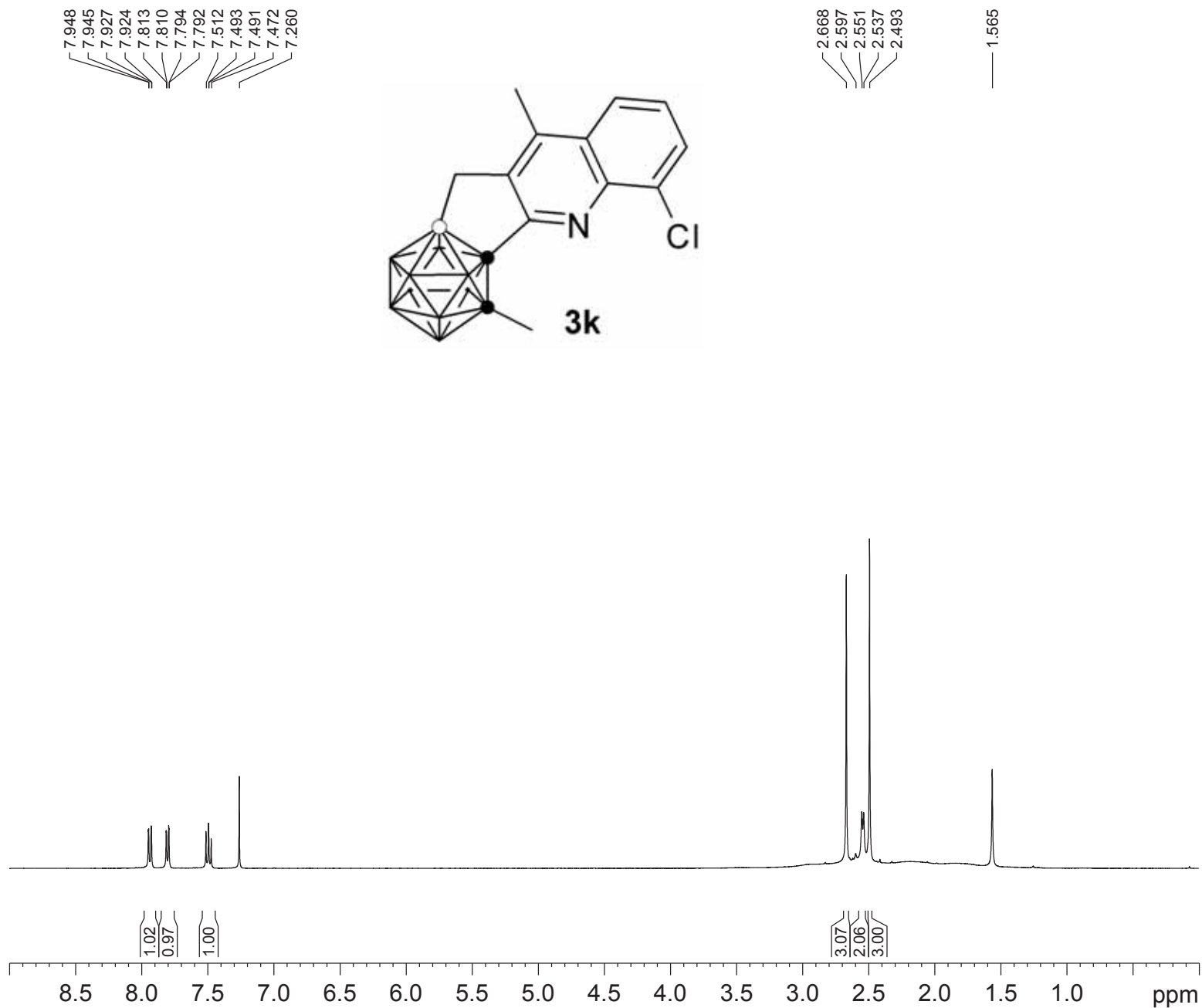
Current Data Parameters  
 NAME 1hr-B-0712-3cl-cascdcl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170704  
 Time 10.07 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 287  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.6 K  
 D1 2.0000000 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

- 3.07
- 4.45
- 5.67
- 6.84
- 8.18
- 8.95
- 9.67
- 10.12
- 10.68
- 12.05
- 13.41





lhr-H-0713-2cl-ccca:

Current Data Parameters  
 NAME lhr-H-0713-2cl-ccca  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170713  
 Time 15.09 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (zg30)  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 128  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.1 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

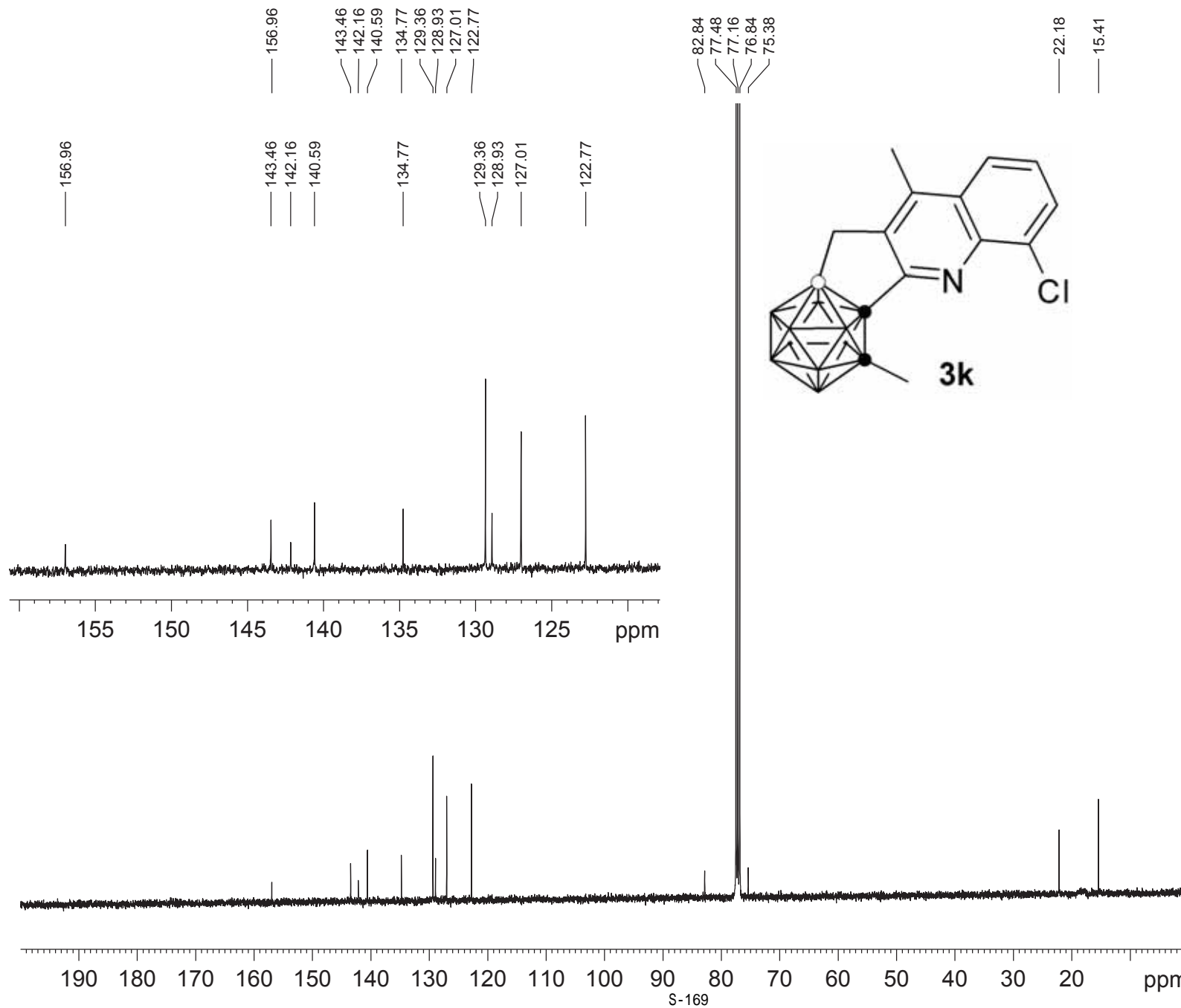
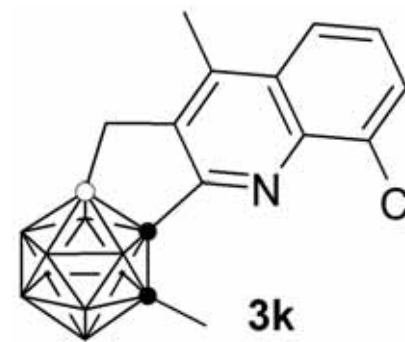
F2 - Processing parameters  
 SI 65536  
 SF 400.2300107 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

lhr-C-0713-2cl-ccc:

Current Data Parameters  
NAME lhr-C-0713-2cl-cccscdcl:  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170713  
Time 15.13 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1300  
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 2.0000000 sec  
D11 0.0300000 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 100.6379003 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



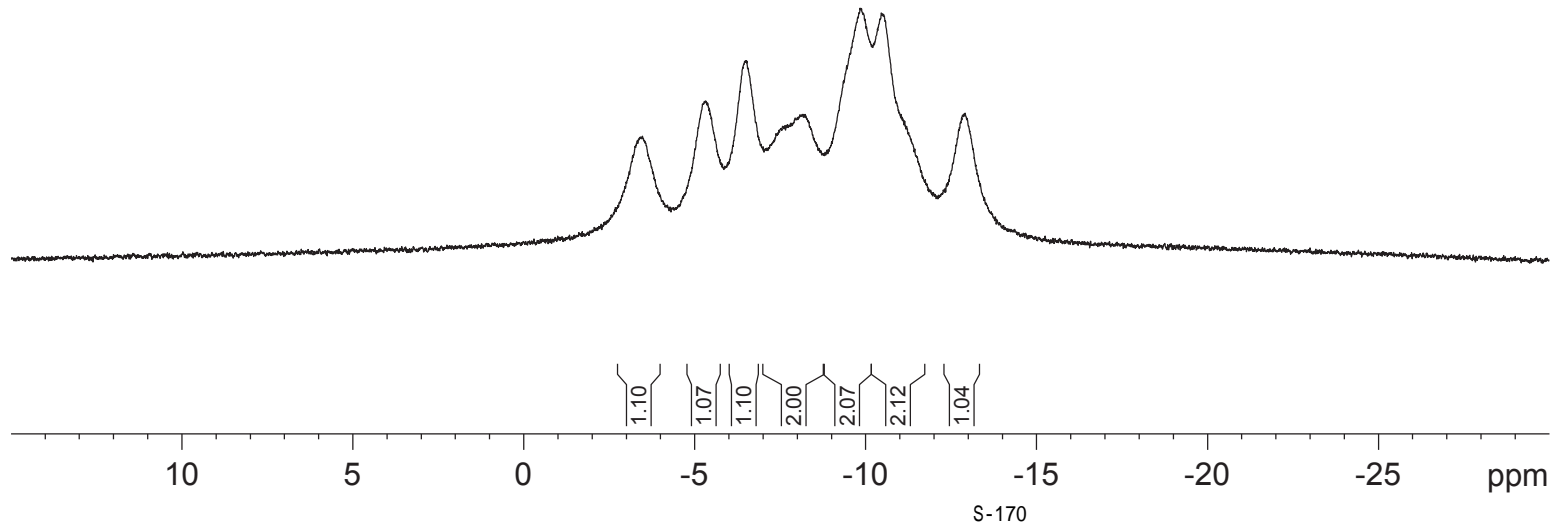
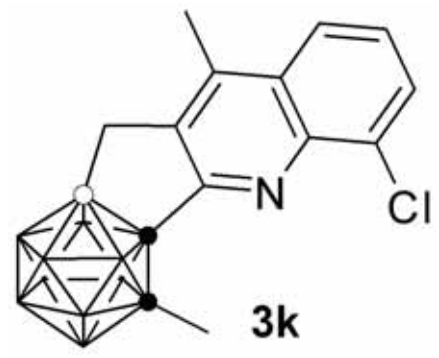
1hr-B-0713-2cl-cccasccl3

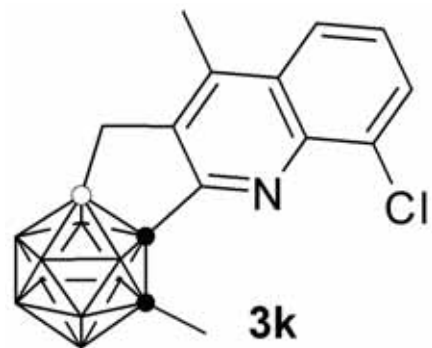
Current Data Parameters  
NAME 1hr-B-0713-2cl-cccasccl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170713  
Time 16.26 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 406  
DW 20.800 usec  
DE 6.50 usec  
TE 295.7 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

— 3.47  
— 5.31  
— 6.51  
— 7.52  
— 8.15  
— 9.38  
— 9.84  
— 10.46  
— 11.11  
— 12.91





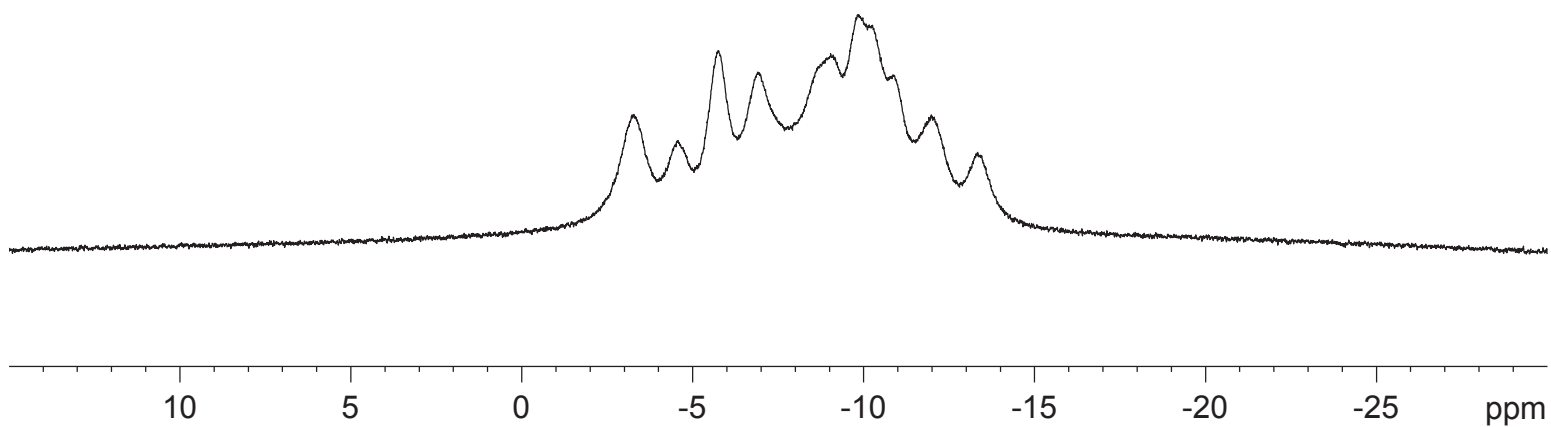
| -3.28  
 | -4.57  
 | -5.74  
 | -6.92  
 | -8.67  
 | -9.04  
 | -9.86  
 | -10.25  
 | -10.86  
 | -11.98  
 | -13.34

lhr-B-0713-2cl-cccasccl3(C)

Current Data Parameters  
 NAME lhr-B-0713-2cl-cccasccl3(C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170713  
 Time\_ 16.29 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 24  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 362  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.4 K  
 D1 2.00000000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 11B  
 P1 7.50 usec  
 PLW1 55.09999847 W

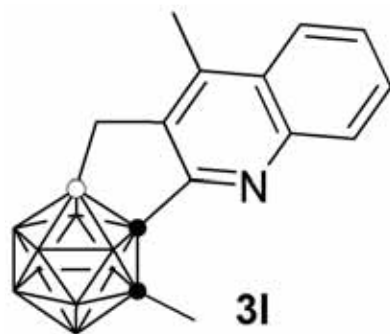
F2 - Processing parameters  
 SI 32768  
 SF 128.4097430 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



8.059  
8.040  
8.029  
8.027  
8.008  
8.006  
7.713  
7.710  
7.696  
7.693  
7.675  
7.672  
7.612  
7.609  
7.595  
7.592  
7.588  
7.574  
7.571  
7.260

2.665  
2.599  
2.554  
2.517  
2.471  
2.445

1hr-H-cas-0367-CDCl3



Current Data Parameters  
NAME 1hr-H-cas-0367-CDCl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160509  
Time 9.56 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 20  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 57  
DW 62.400 usec  
DE 6.50 usec  
TE 294.7 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

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

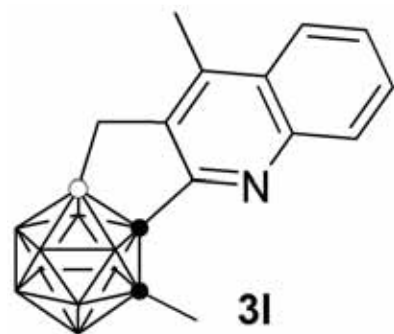


1.95  
1.00  
0.97

3.02  
2.01  
2.95

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





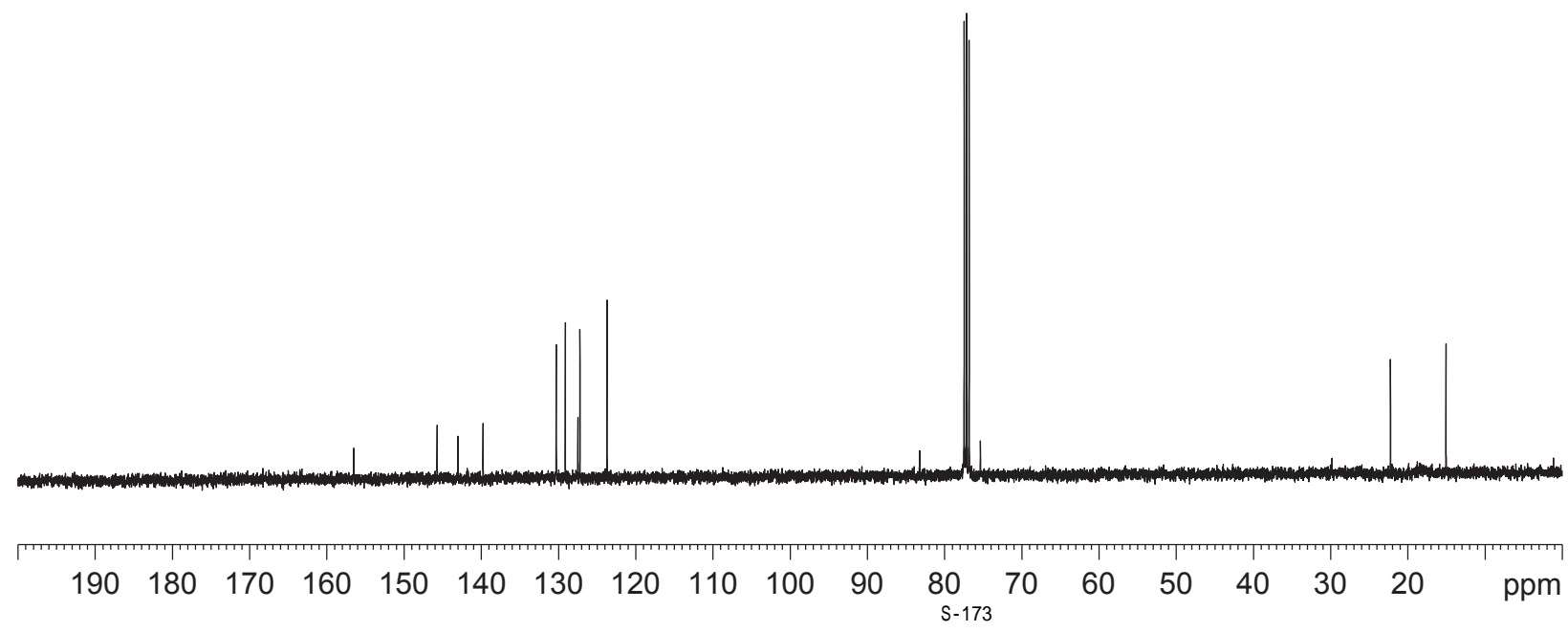
156.50  
 145.69  
 143.00  
 139.75  
 130.31  
 129.13  
 127.52  
 127.25  
 123.74  
 83.26  
 77.48  
 77.16  
 76.84  
 75.38  
 22.27  
 15.08

lhr-C-cas-0367-CDC13

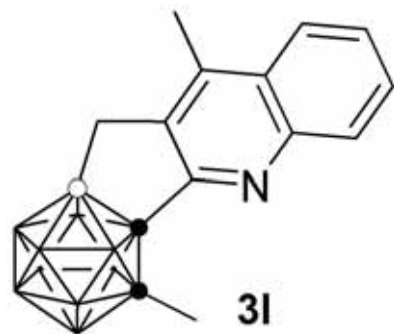
Current Data Parameters  
 NAME lhr-C-cas-0367-CDC13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160509  
 Time\_ 10.02 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 100  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.454131 Hz  
 AQ 1.1010048 sec  
 RG 90.5  
 DW 16.800 usec  
 DE 6.50 usec  
 TE 295.3 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 100.6379019 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



1hr-B-cas-0367-CDC13

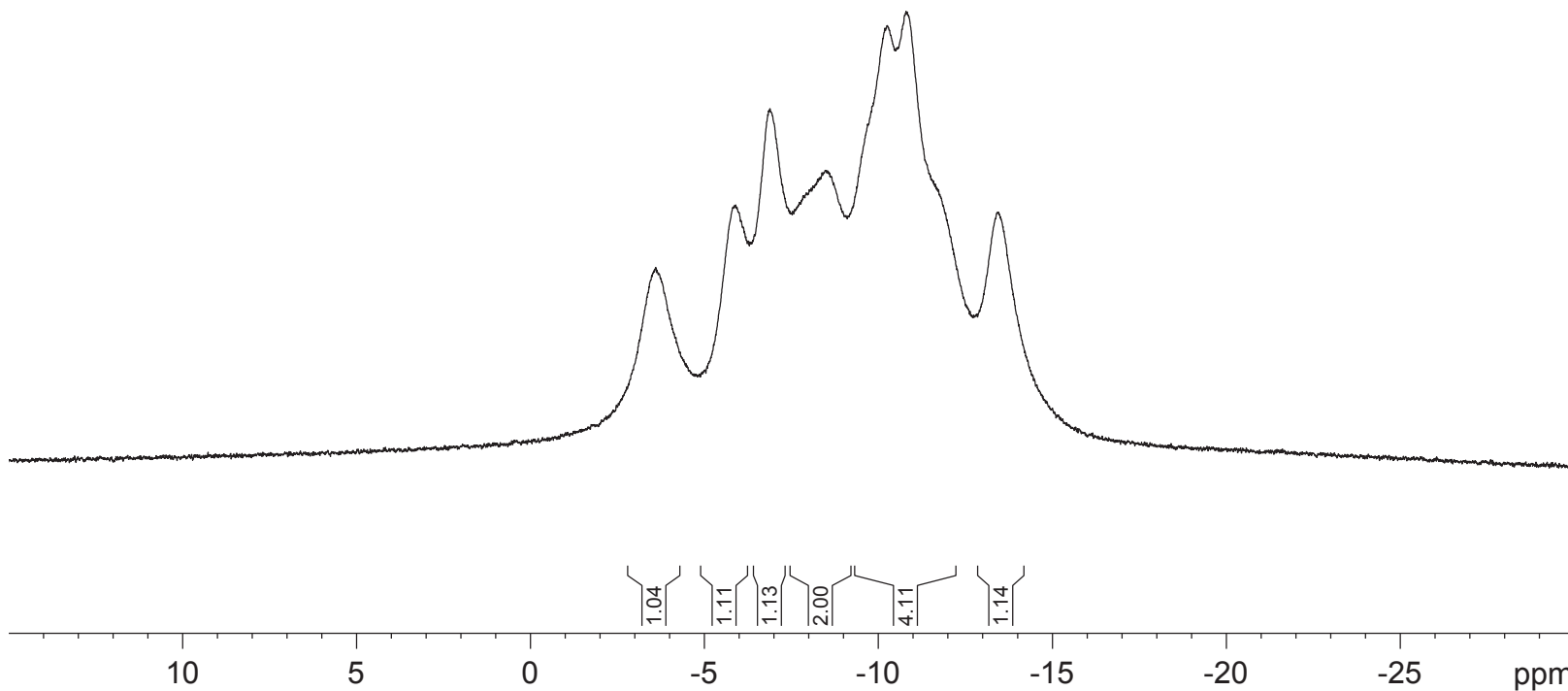


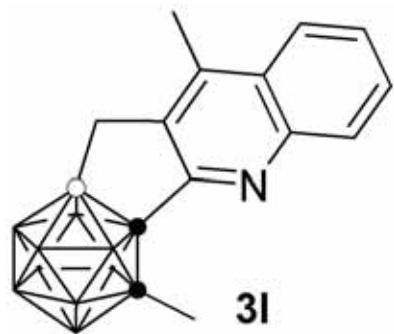
— 3.60  
— 5.90  
— 6.89  
— 8.49  
— 10.25  
— 10.79  
— 11.67  
— 13.43

Current Data Parameters  
NAME 1hr-B-cas-0367-CDC13  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160509  
Time\_ 9.45 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT THF  
NS 22  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 287  
DW 20.800 usec  
DE 6.50 usec  
TE 296.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W  
SFO2 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.56000042 W  
PLW12 0.27428001 W

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





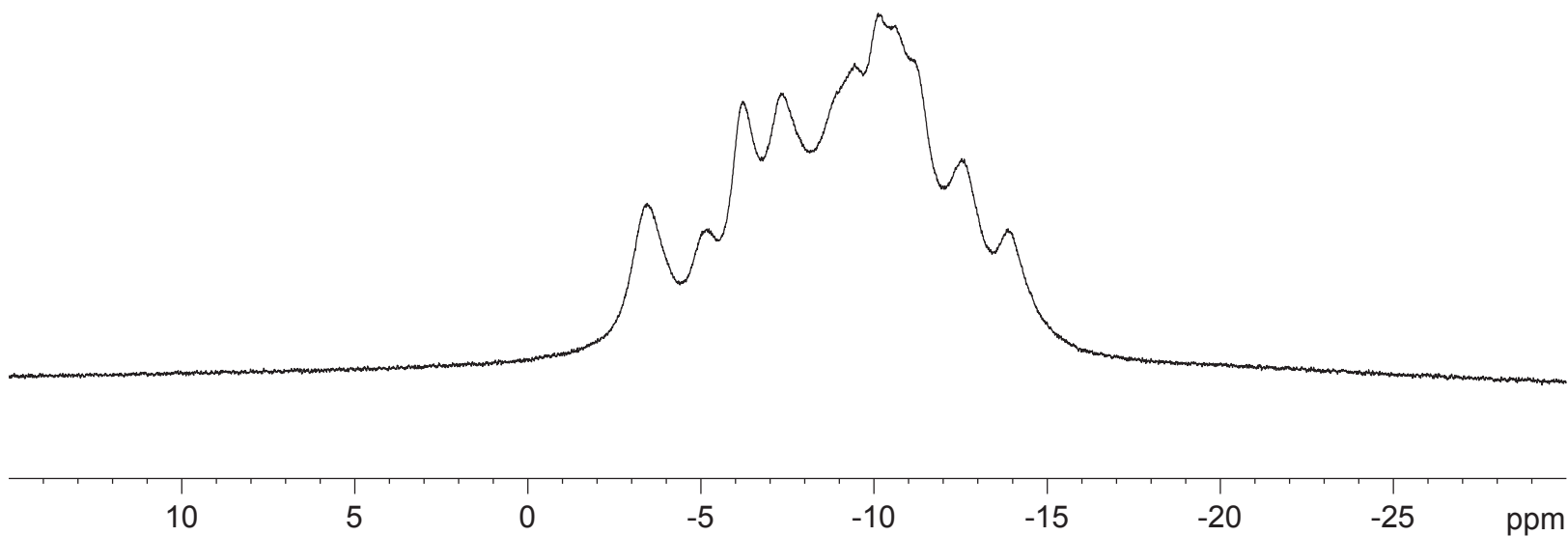
— 3.44  
 — 5.10  
 — 6.20  
 — 7.31  
 — 8.82  
 — 9.44  
 — 10.12  
 — 10.56  
 — 11.12  
 — 12.54  
 — 13.88

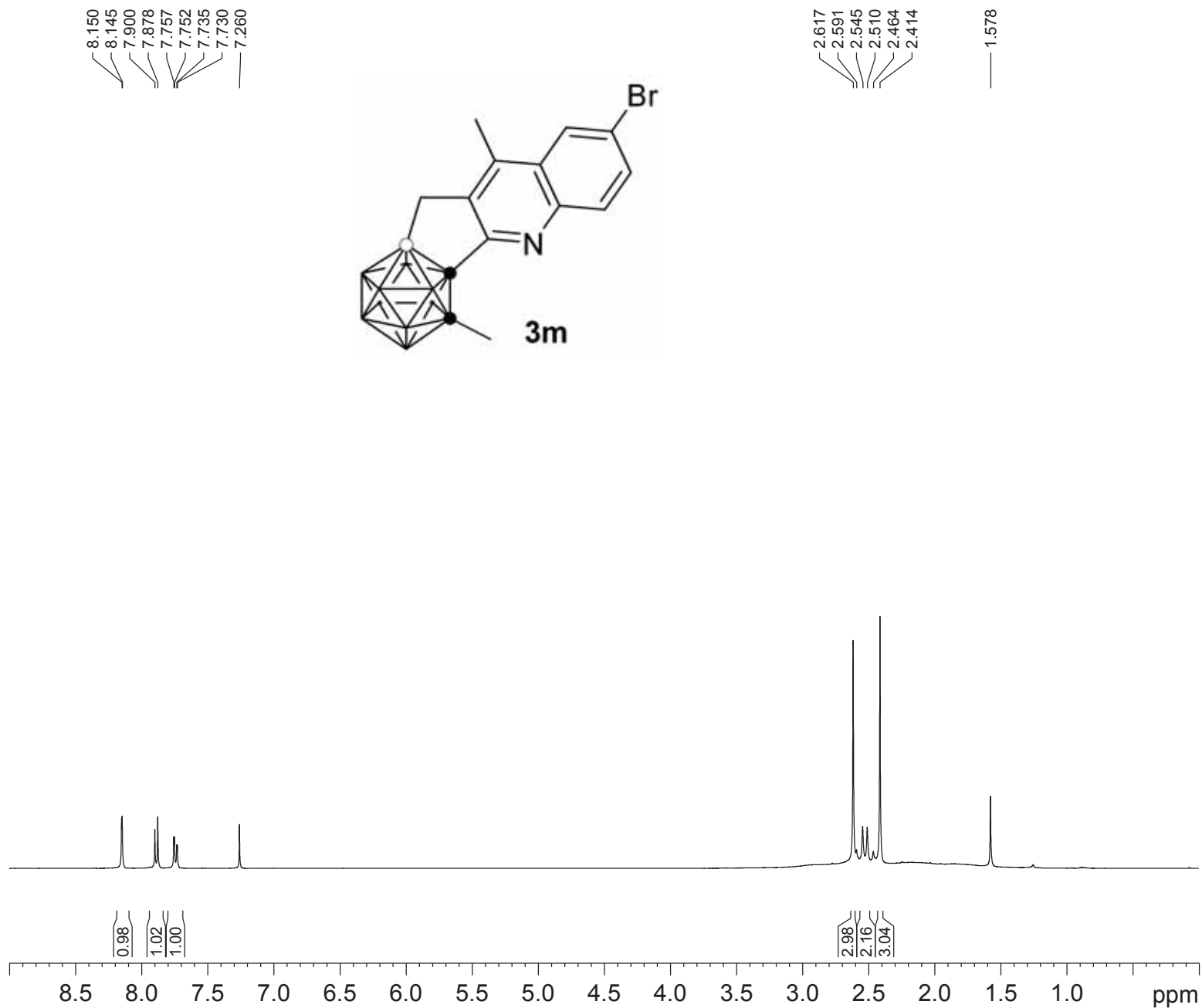
1hr-B-cas-0367-CDCl3 (C)

Current Data Parameters  
 NAME 1hr-B-cas-0367-CDCl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160509  
 Time 9.46 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 ( )  
 PULPROG zg  
 TD 65536  
 SOLVENT THF  
 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 295.6 K  
 D1 2.0000000 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





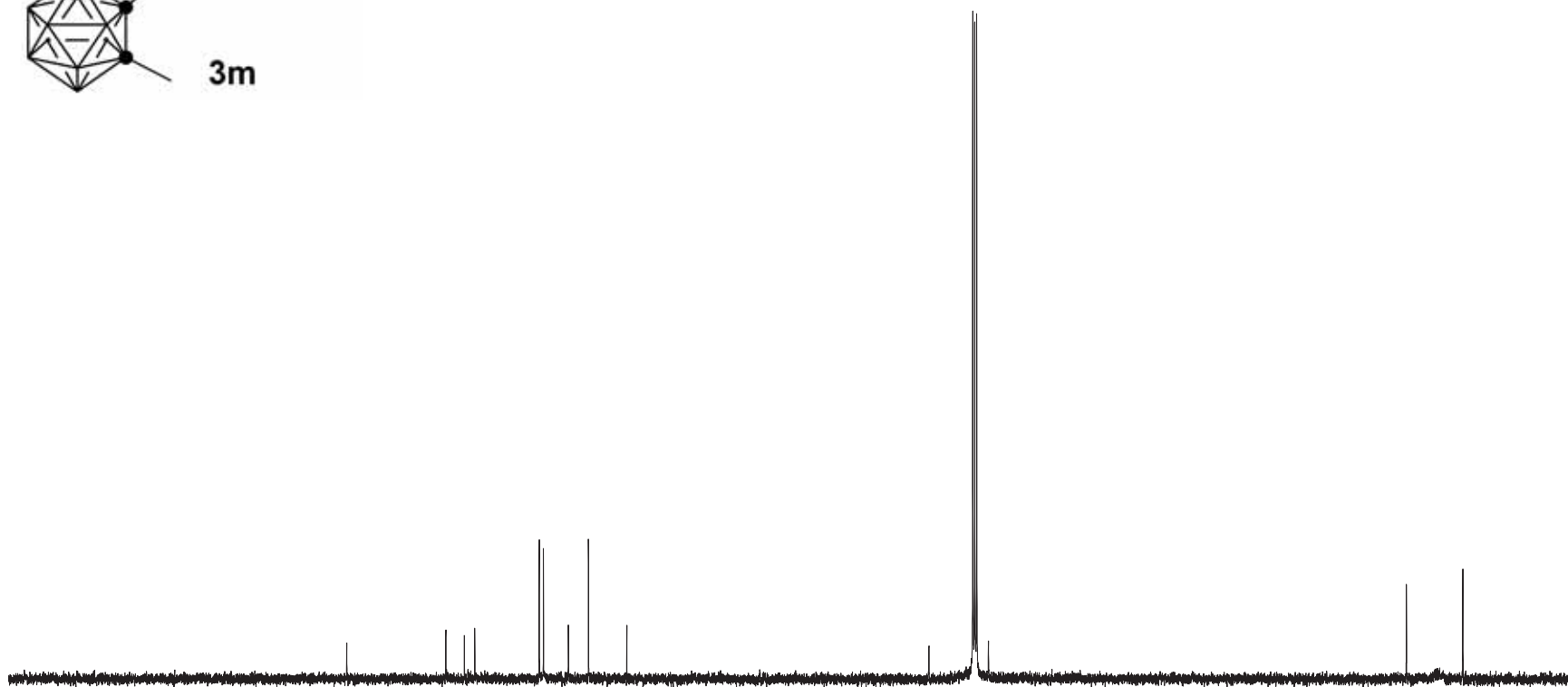
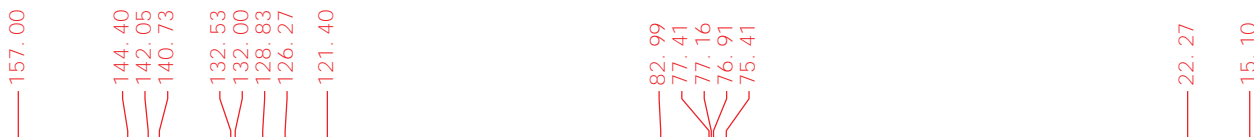
lhr-H-0715-4brcascd:

Current Data Parameters  
 NAME lhr-H-0715-4brcasc  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170705  
 Time 16.51 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (zg30)  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 12  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.4 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 400.2300109 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

I hr-0715-4brcascdcl 3



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

S-177

Current Data Parameters  
NAME I hr-0715-4brcascdcl 3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170705  
Time 19.54 h  
INSTRUM spect  
PROBHD Z119470\_0283 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl 3  
NS 400  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 6.50 usec  
TE 299.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 94.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 25.0000000 W  
PLW12 0.39063001 W  
PLW13 0.19648001 W

F2 - Processing parameters

SI 32768  
SF 125.7577717 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

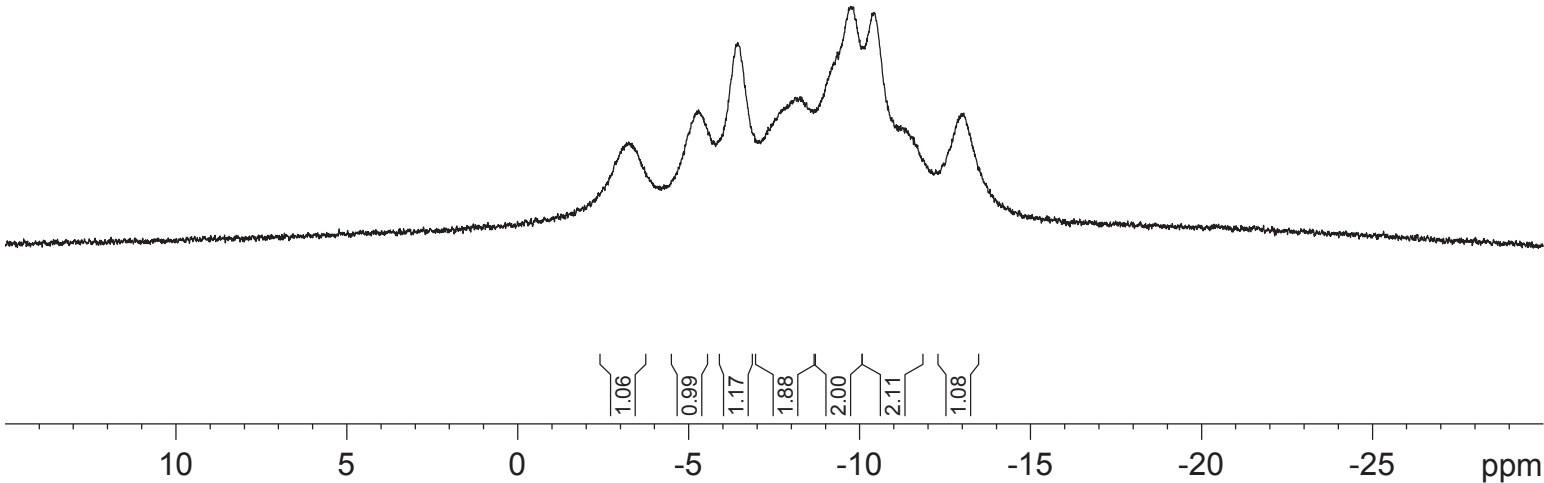
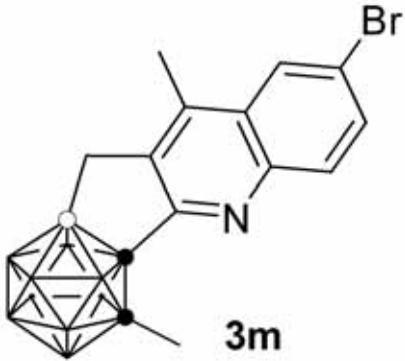
1hr-B-0715-4brcascdcl3

Current Data Parameters  
NAME 1hr-B-0715-4brcascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170705  
Time 16.54 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 24  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 512  
DW 20.800 usec  
DE 6.50 usec  
TE 295.6 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

— 3.25  
— 5.29  
— 6.43  
— 8.27  
— 9.21  
— 9.74  
— 10.41  
— 11.27  
— 13.05



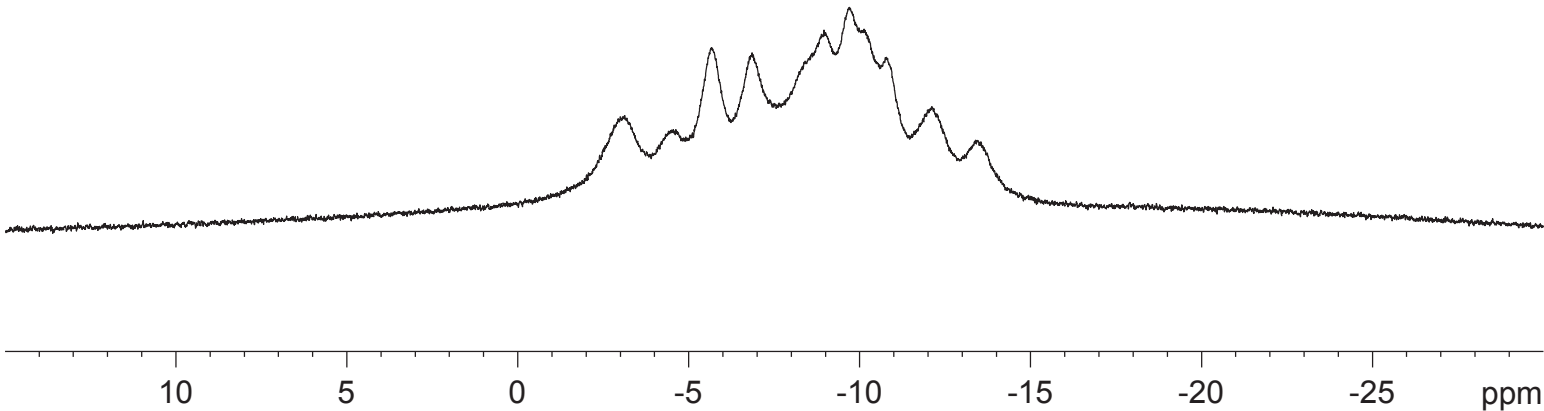
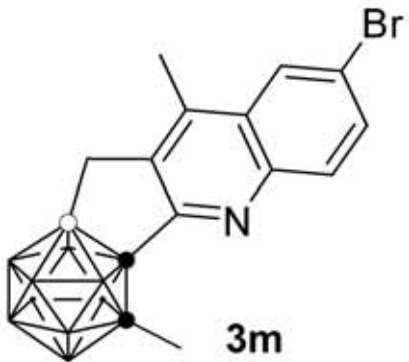
1hr-B-0715-4brcascdcl3 (C)

Current Data Parameters  
NAME 1hr-B-0715-4brcascdcl3 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170705  
Time 16.57 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 512  
DW 20.800 usec  
DE 6.50 usec  
TE 295.3 K  
D1 2.00000000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 13C  
P1 7.50 usec  
PLW1 55.09999847 W

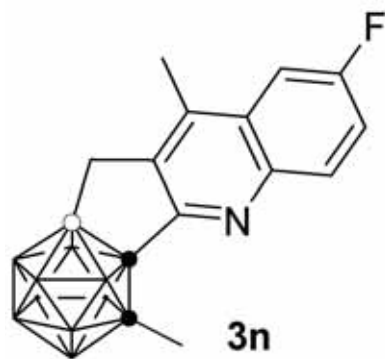
F2 - Processing parameters  
SI 32768  
SF 128.4097430 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

— 3.13  
— 4.63  
— 5.68  
— 6.85  
— 8.47  
— 8.96  
— 9.70  
— 10.15  
— 10.79  
— 12.11  
— 13.40



8.042  
8.028  
8.020  
8.005  
7.607  
7.601  
7.582  
7.576  
7.471  
7.464  
7.448  
7.445  
7.428  
7.422  
7.260

2.605  
2.544  
2.509  
2.462  
2.421  
1.587



lhr-H-0704-4F-cascd3

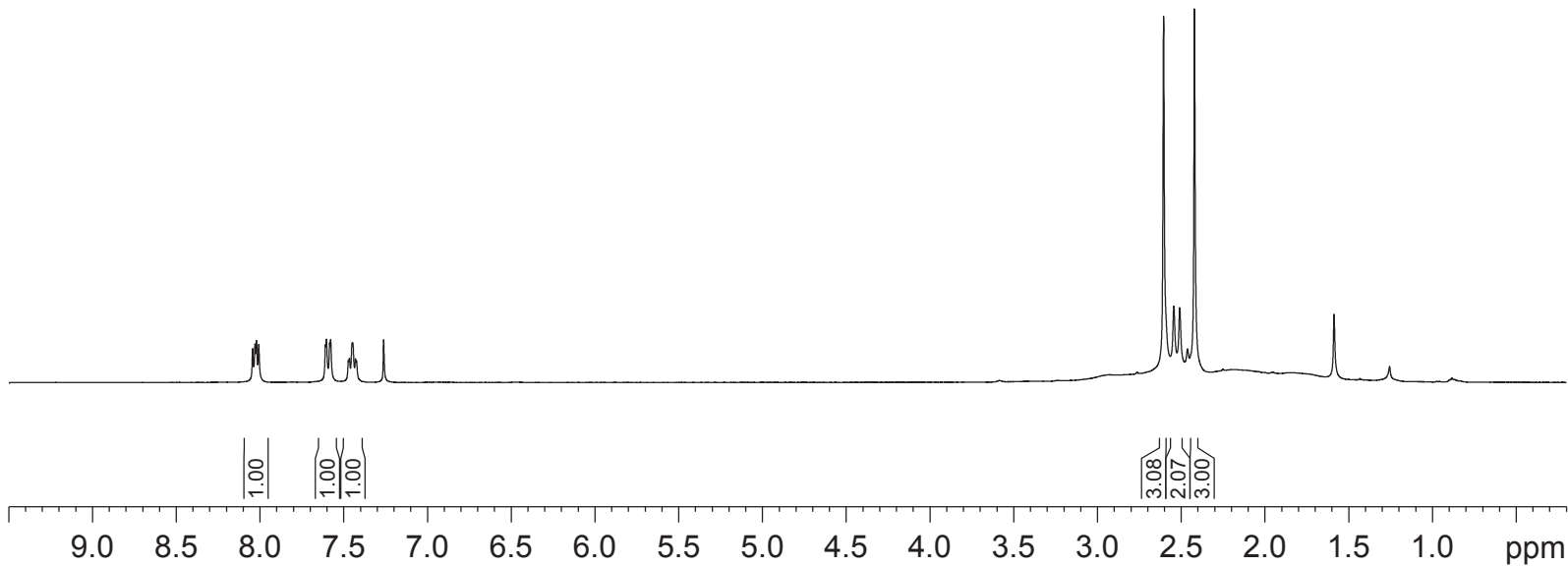
Current Data Parameters  
NAME lhr-H-0704-4F-cascd3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

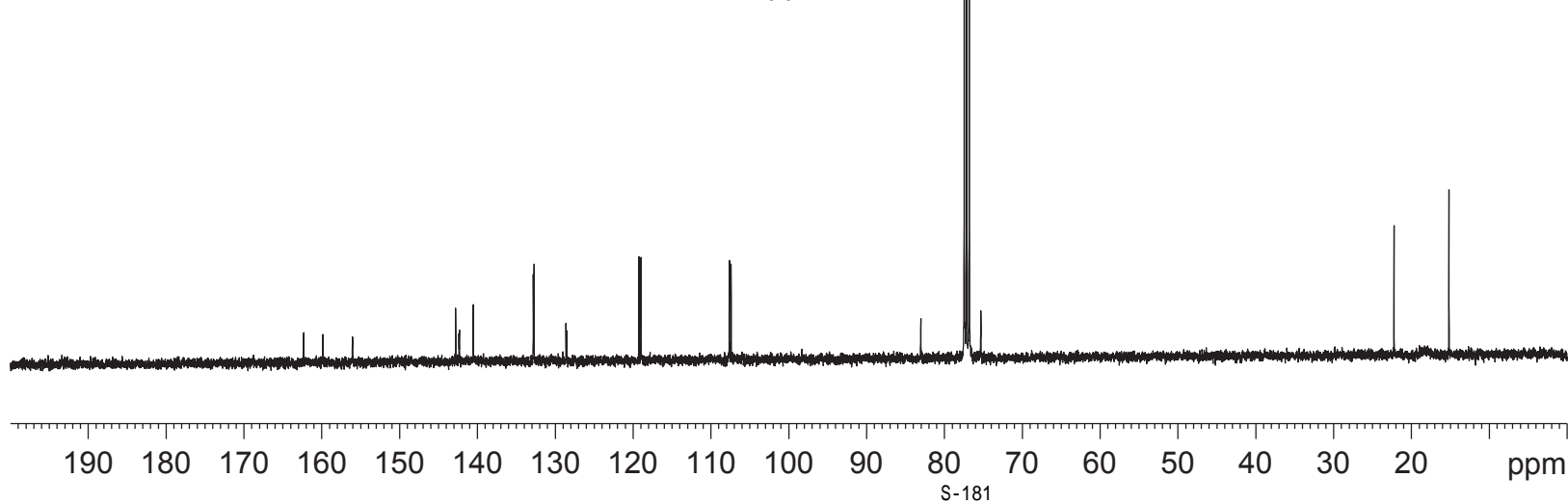
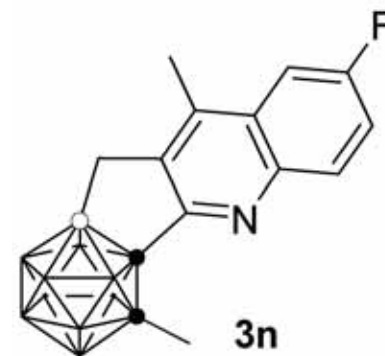
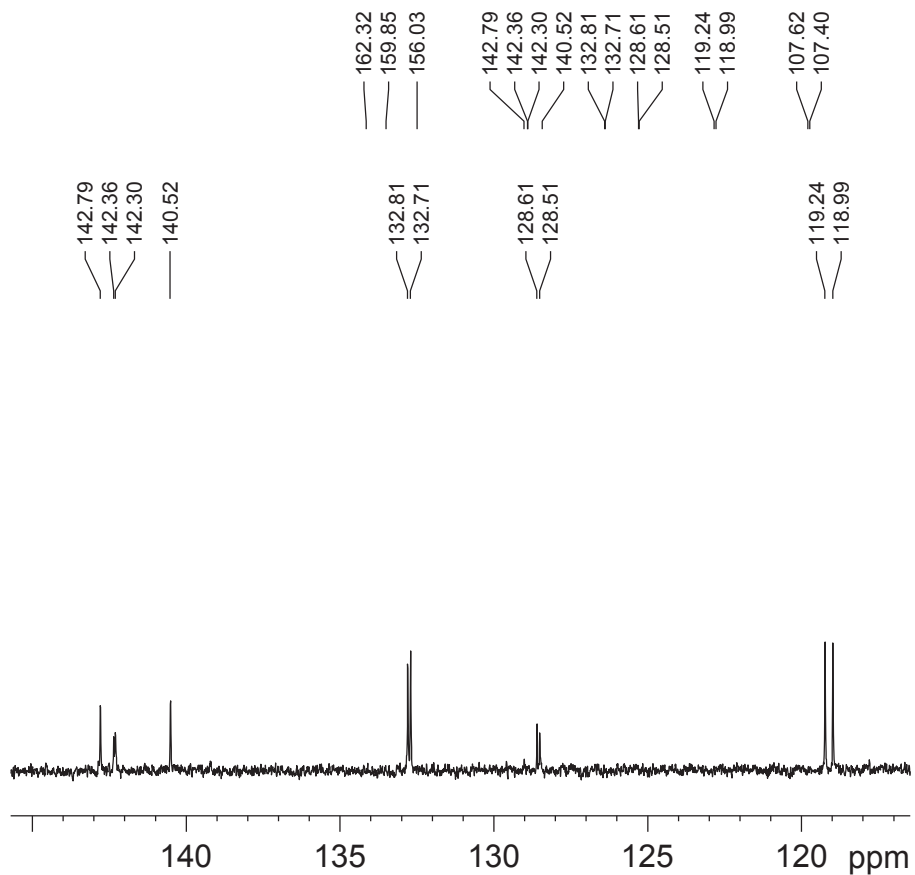
Date\_ 20170629  
Time 10.15 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 295.4 K  
D1 1.0000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters

SI 65536  
SF 400.2300108 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00







lhr-C-0704-4F-casc

Current Data Parameters  
NAME lhr-C-0704-4F-cascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170629  
Time 10.19 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 440  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.1010048 sec  
RG 203  
DW 16.800 usec  
DE 6.50 usec  
TE 295.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6479773 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 55.34000015 W  
SFO2 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.56000042 W  
PLW12 0.27428001 W  
PLW13 0.13796000 W

F2 - Processing parameters

SI 32768  
SF 100.6379007 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

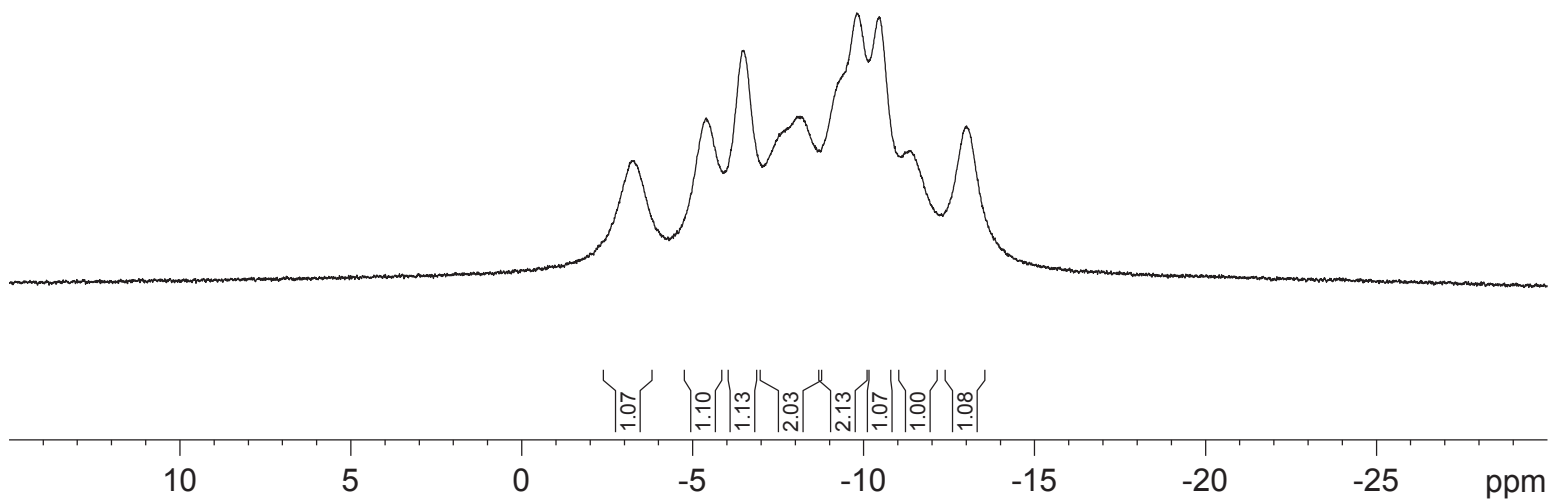
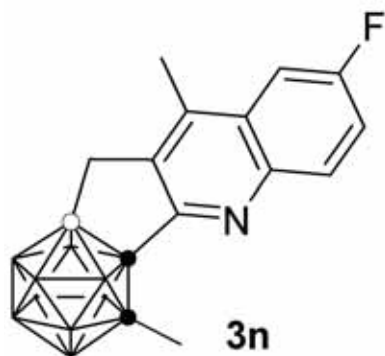
1hr-B-0704-4F-cascdcl3

Current Data Parameters  
NAME 1hr-B-0704-4F-cascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170629  
Time 10.43 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 295.9 K  
D1 2.0000000 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

— 3.27  
— 5.39  
— 6.49  
— 7.66  
— 8.11  
— 9.31  
— 9.80  
— 10.46  
— 11.34  
— 13.01



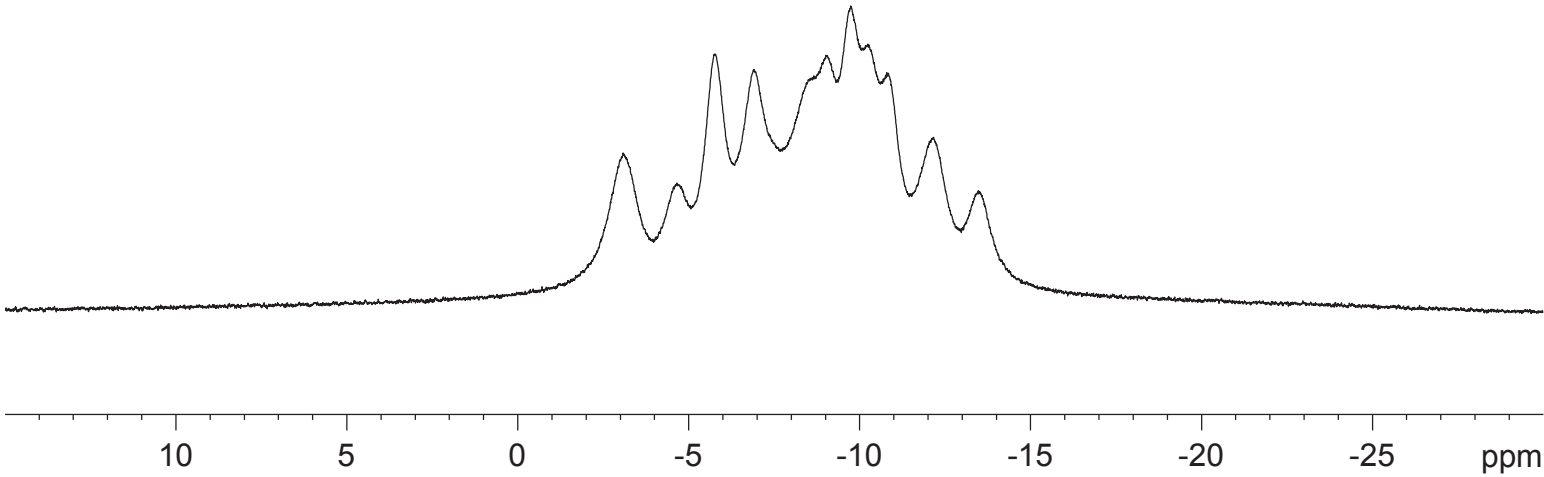
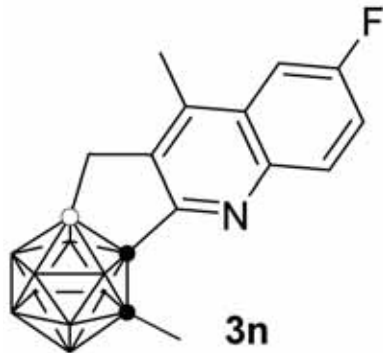
1hr-B-0704-4F-cascdcl3 (C)

Current Data Parameters  
 NAME 1hr-B-0704-4F-cascdcl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170629  
 Time 10.45 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 287  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 2.00000000 sec  
 TD0 1  
 SFO1 128.4096890 MHz  
 NUC1 11B  
 P1 7.50 usec  
 PLW1 55.09999847 W

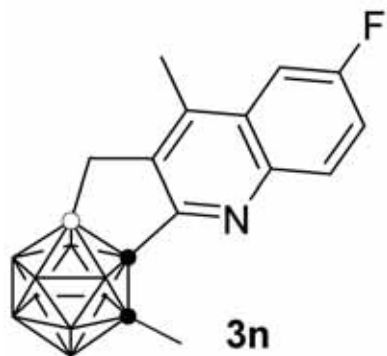
F2 - Processing parameters  
 SI 32768  
 SF 128.4097430 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

- 3.08
- 4.66
- 5.77
- 6.91
- 8.51
- 9.01
- 9.74
- 10.21
- 10.80
- 12.16
- 13.47



lhr-F-0704-4F-cascdcl3

-111.43



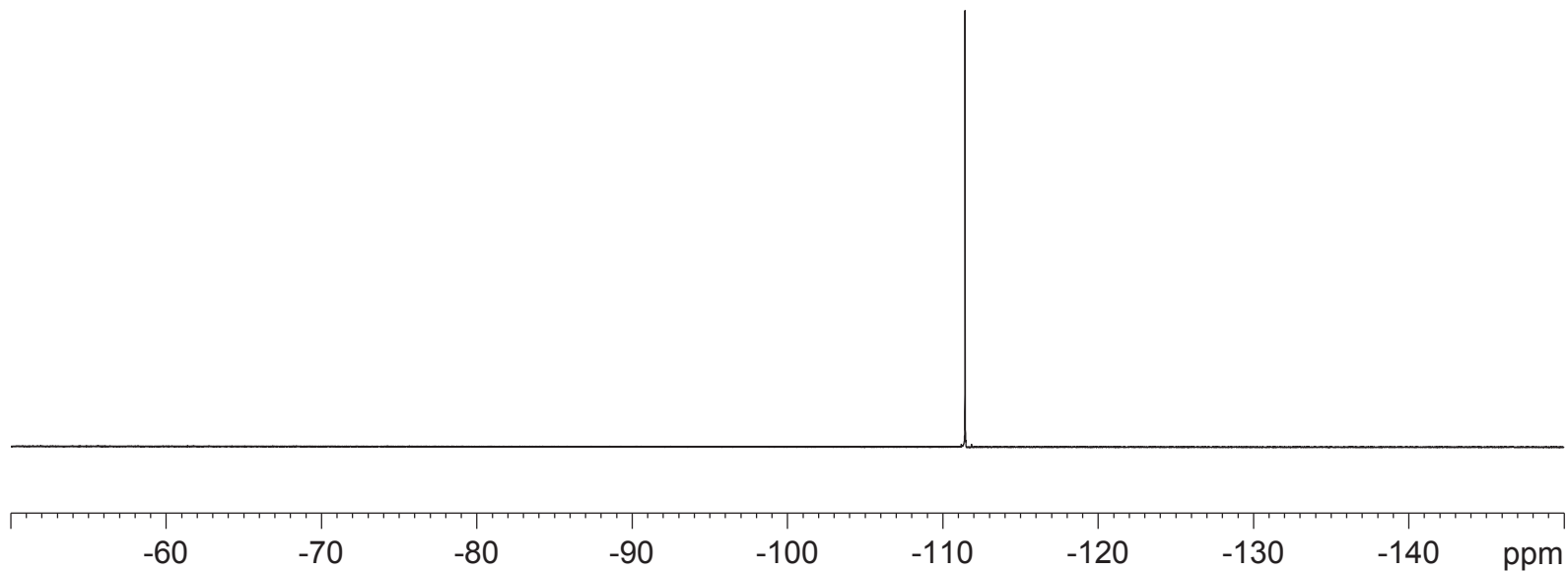
Current Data Parameters  
NAME lhr-F-0704-4F-cascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

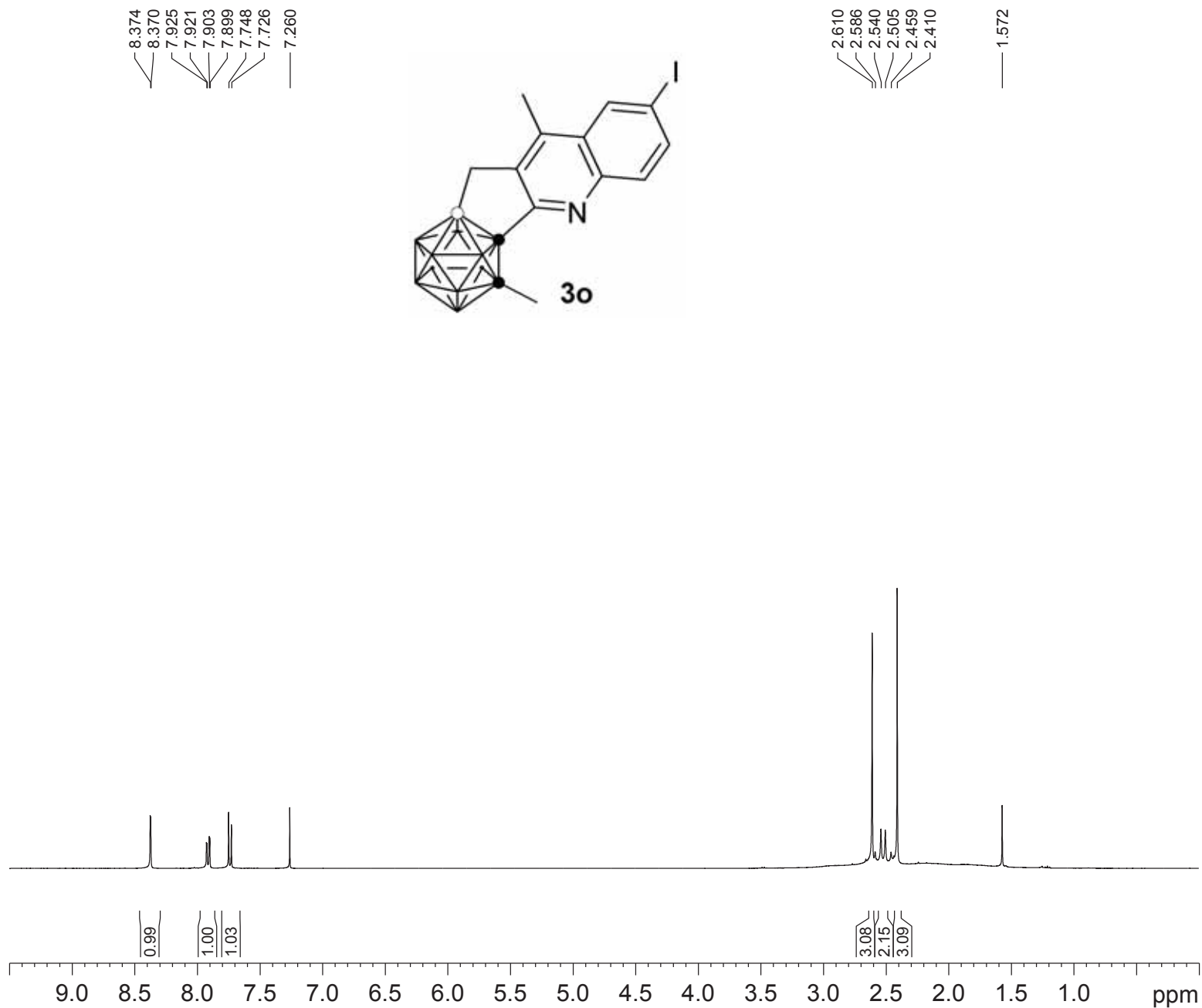
Date\_ 20170629  
Time\_ 10.47 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgfhigqn.2  
TD 131072  
SOLVENT CDCl3  
NS 11  
DS 4  
SWH 89285.711 Hz  
FIDRES 0.681196 Hz  
AQ 0.7340032 sec  
RG 645  
DW 5.600 usec  
DE 6.50 usec  
TE 295.7 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
D12 0.00002000 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



S-184

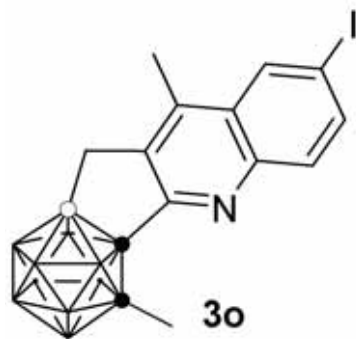


lhr-H-0739-i-cascdc:

Current Data Parameters  
 NAME lhr-H-0739-i-cascdc  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170810  
 Time\_ 20.14 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (zg30)  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 12  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.4 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 400.2300100 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



157.12  
144.76  
141.80  
140.58  
137.85  
132.96  
131.94  
129.31

93.17  
82.99  
77.41  
77.16  
76.91  
75.40

22.27  
18.21  
15.08

I hr-C-0739-I cas

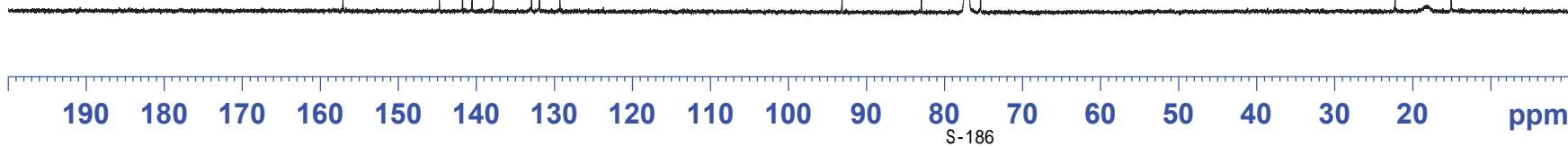
Current Data Parameters  
NAME I hr-C-0739-I cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170811  
Time 10.06 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 683  
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  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters

SI 32768  
SF 125.7577725 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

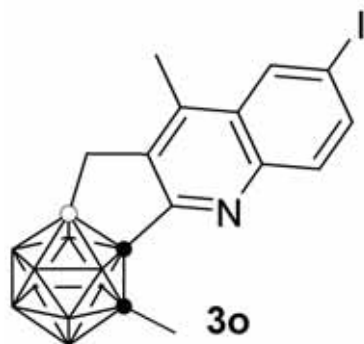


lhr-B-0739-i-cascdcl3

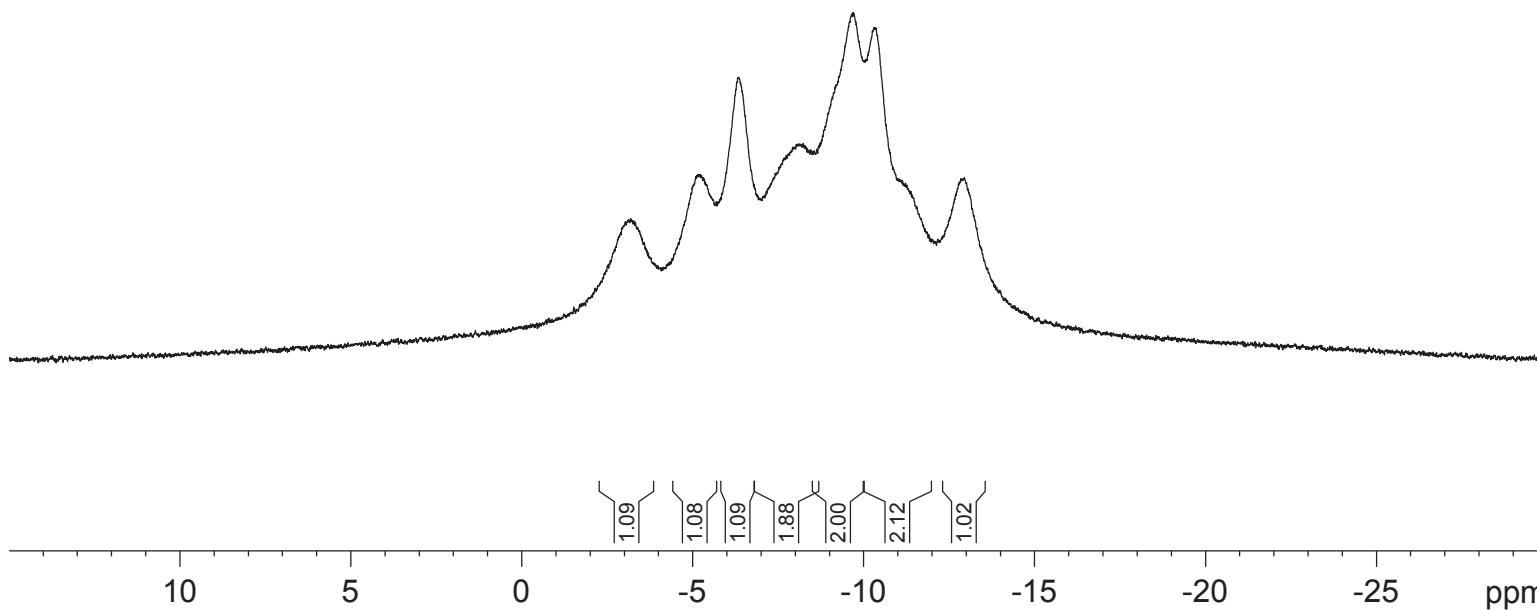
Current Data Parameters  
NAME lhr-B-0739-i-cascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170811  
Time 18.39 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 28  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 322  
DW 20.800 usec  
DE 6.50 usec  
TE 295.7 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



— -3.19  
— -5.16  
— -6.35  
— -8.07  
— -9.15  
— -9.69  
— -10.31  
— -11.19  
— -12.95



1.09 1.08 1.09 1.88 2.00 2.12 1.02

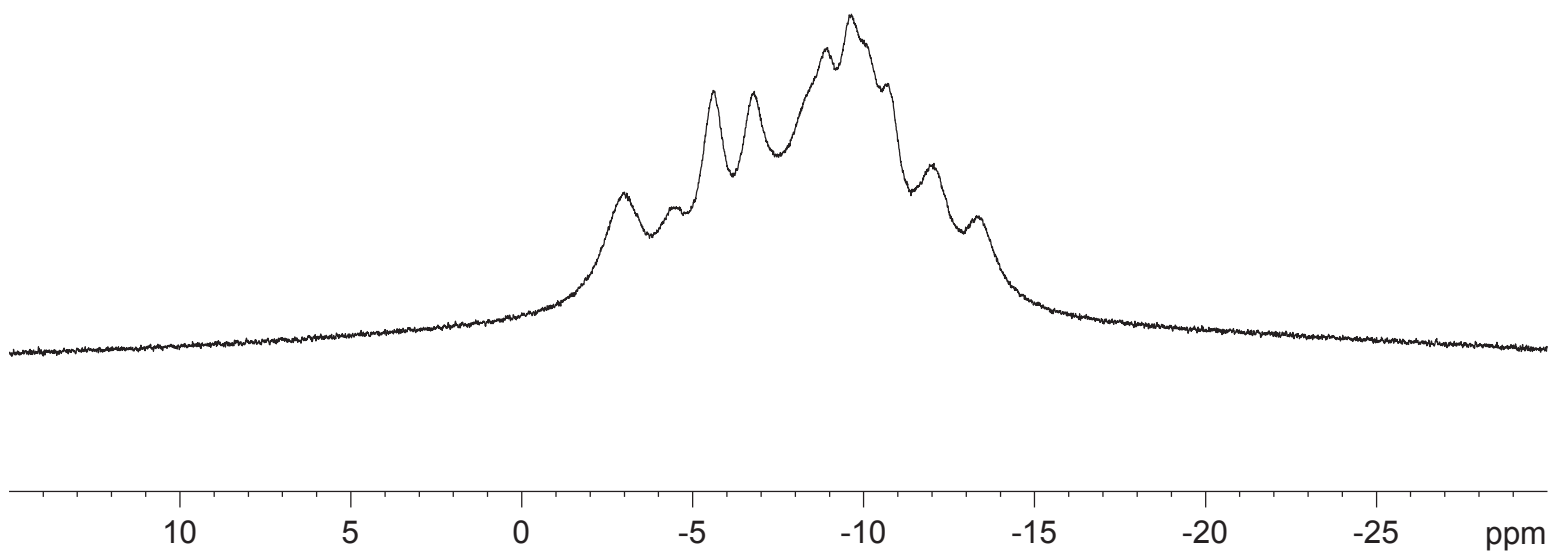
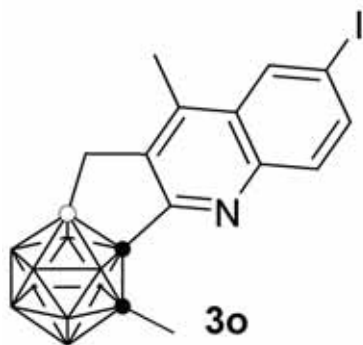
1hr-B-0739-i-cascdcl3 (C)

Current Data Parameters  
NAME 1hr-B-0739-i-cascdcl3 (C)  
EXPNO 1  
PROCNO 1

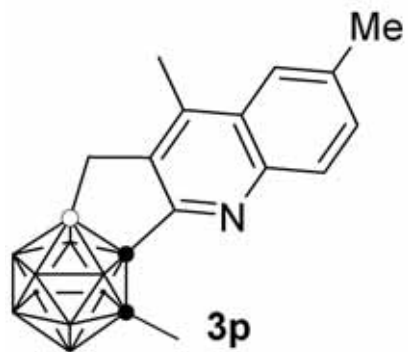
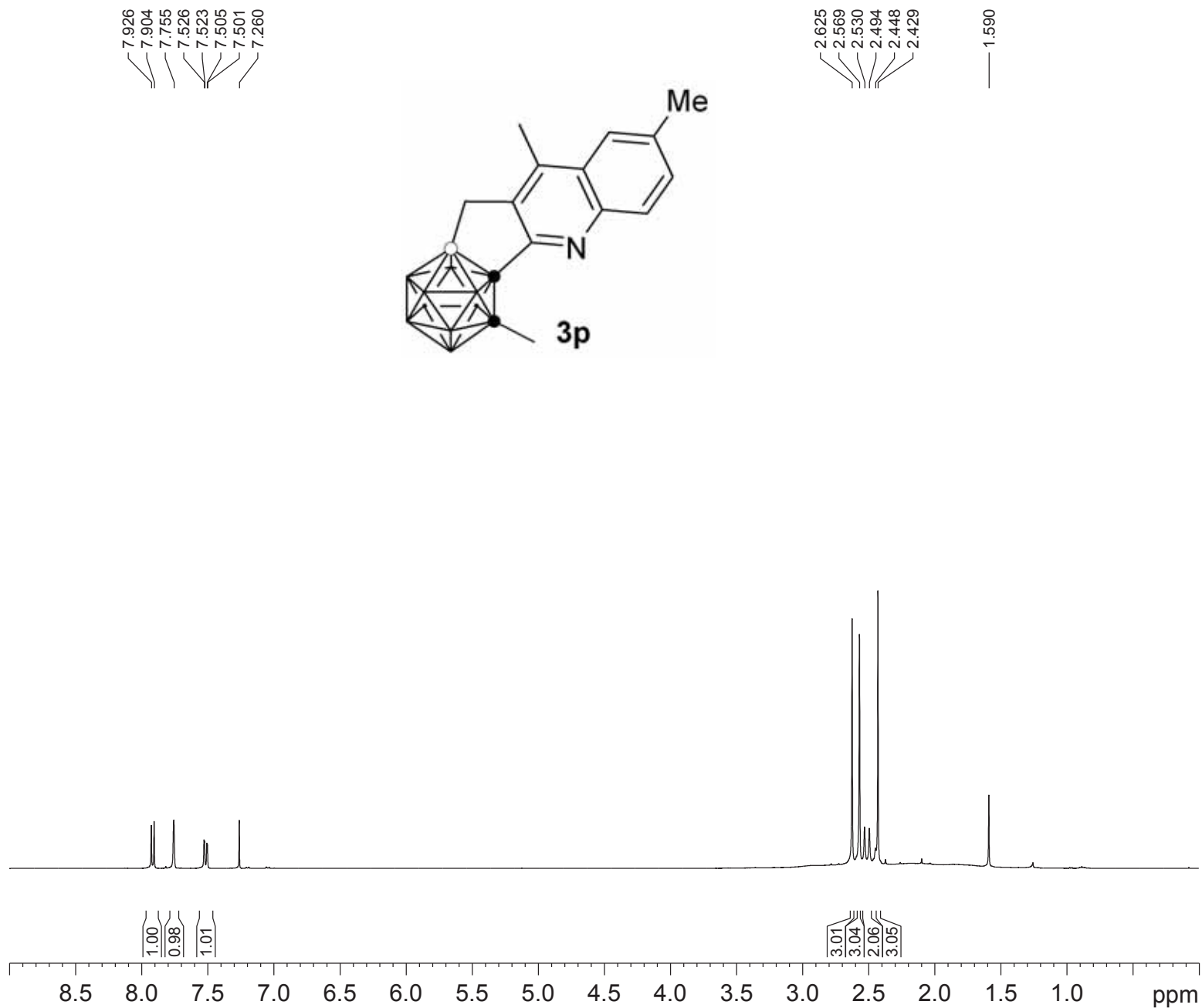
F2 - Acquisition Parameters  
Date\_ 20170811  
Time\_ 18.42 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 28  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 322  
DW 20.800 usec  
DE 6.50 usec  
TE 295.3 K  
D1 2.0000000 sec  
TD0 1  
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

— 3.00  
— 4.52  
— 5.60  
— 6.80  
— 8.22  
— 8.94  
— 9.64  
— 10.00  
— 10.71  
— 12.05  
— 13.37







1hr-H-0732-ch3cascd

Current Data Parameters

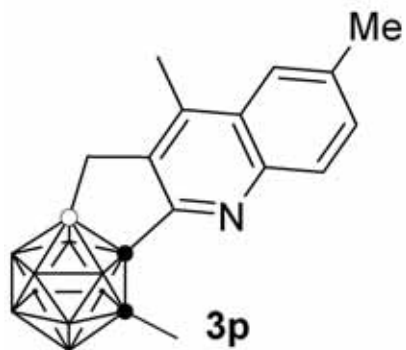
NAME 1hr-H-0732-ch3cascd  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170729  
Time 18.36 h  
INSTRUM spect  
PROBHD Z108618\_0257 (zg30)  
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 294.7 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters

SI 65536  
SF 400.2300098 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



155.65  
 144.26  
 142.15  
 139.70  
 137.19  
 131.25  
 130.03  
 127.48  
 122.75

83.44  
 77.48  
 77.16  
 76.84  
 75.30

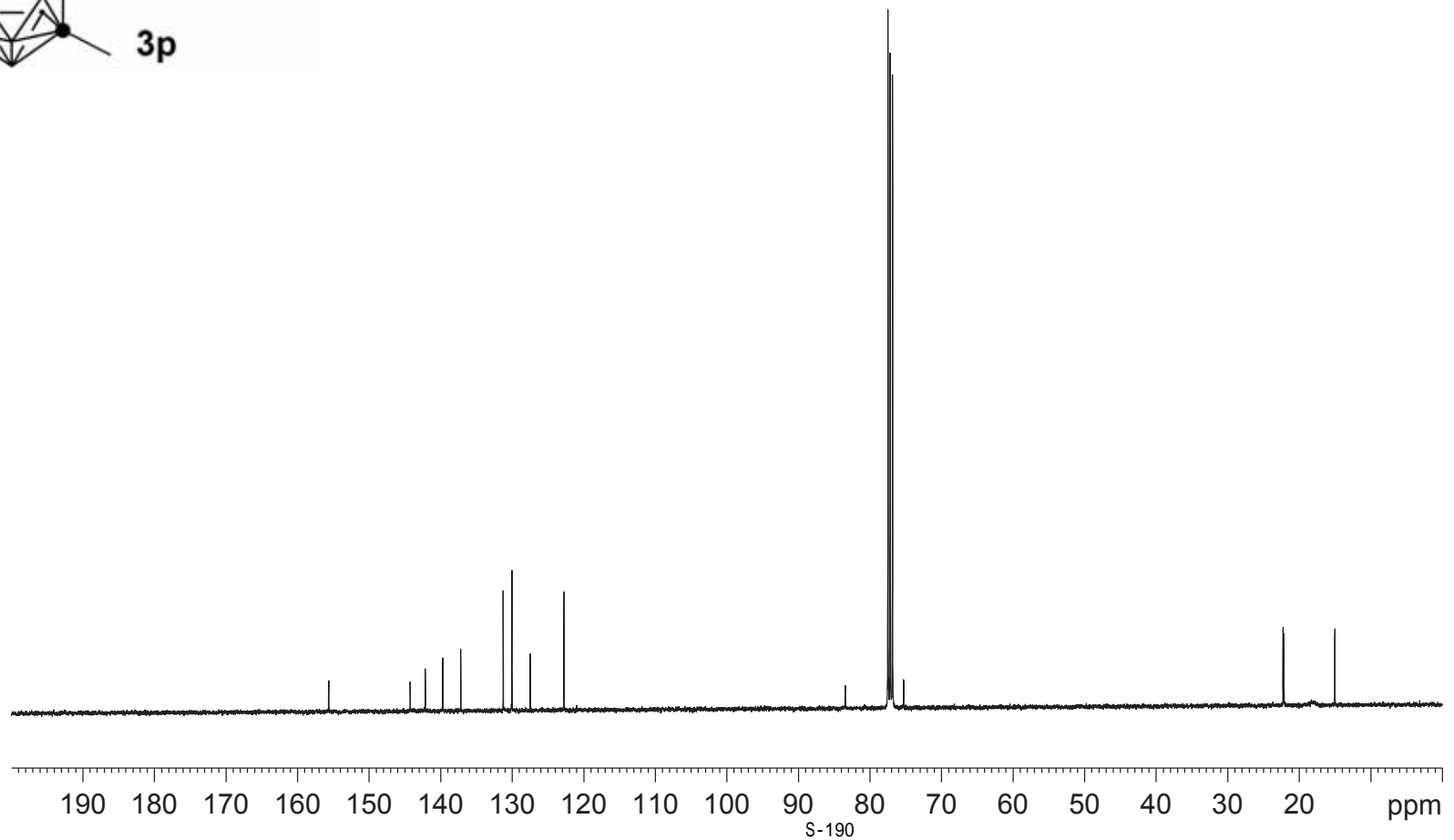
22.25  
 22.13  
 15.01

1hr-C-0732-ch3casdc

Current Data Parameters  
 NAME 1hr-C-0732-ch3casdc1:  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170729  
 Time\_ 18.41 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1412  
 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 100.6379006 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



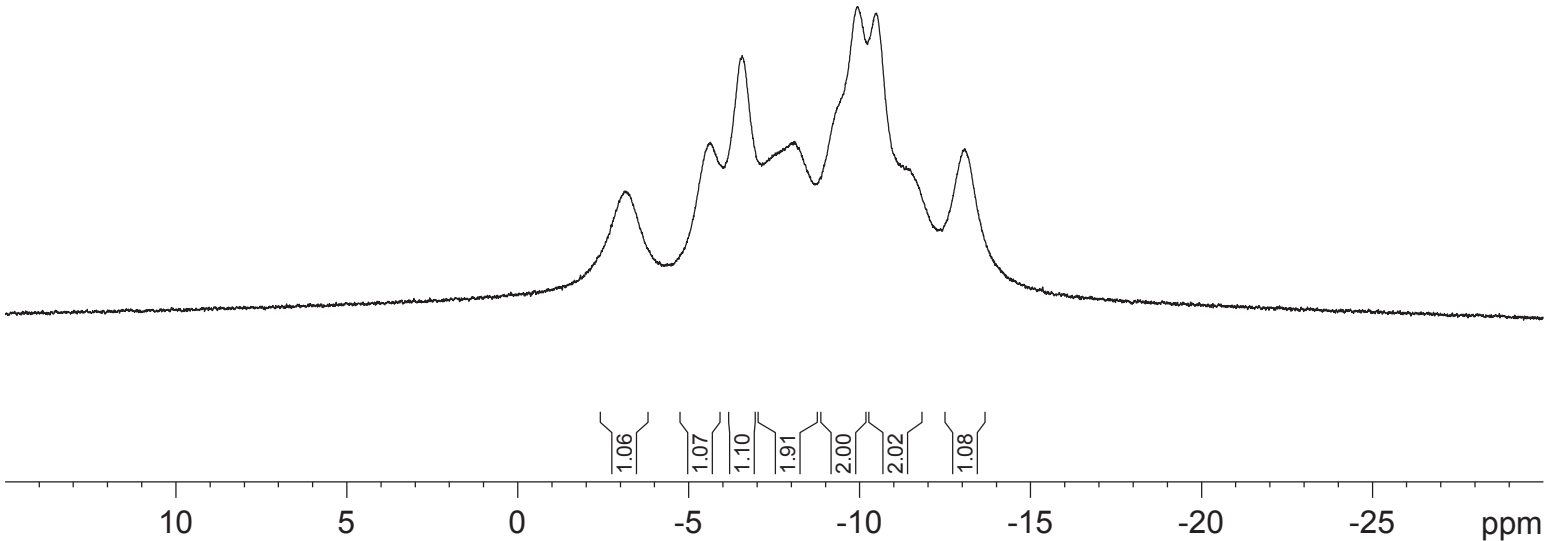
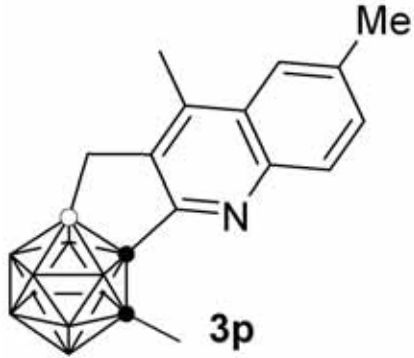
1hr-B-0732-ch3cascdcl3

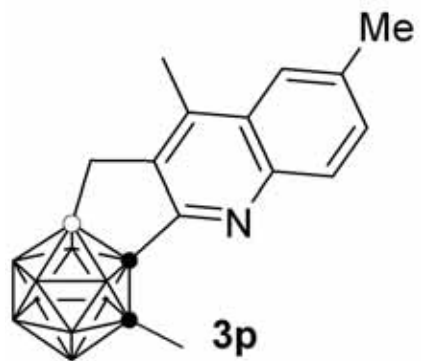
Current Data Parameters  
NAME 1hr-B-0732-ch3cascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170729  
Time 19.50 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 322  
DW 20.800 usec  
DE 6.50 usec  
TE 295.2 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

3.12  
5.64  
6.56  
7.52  
8.08  
9.36  
9.93  
10.48  
11.48  
13.08





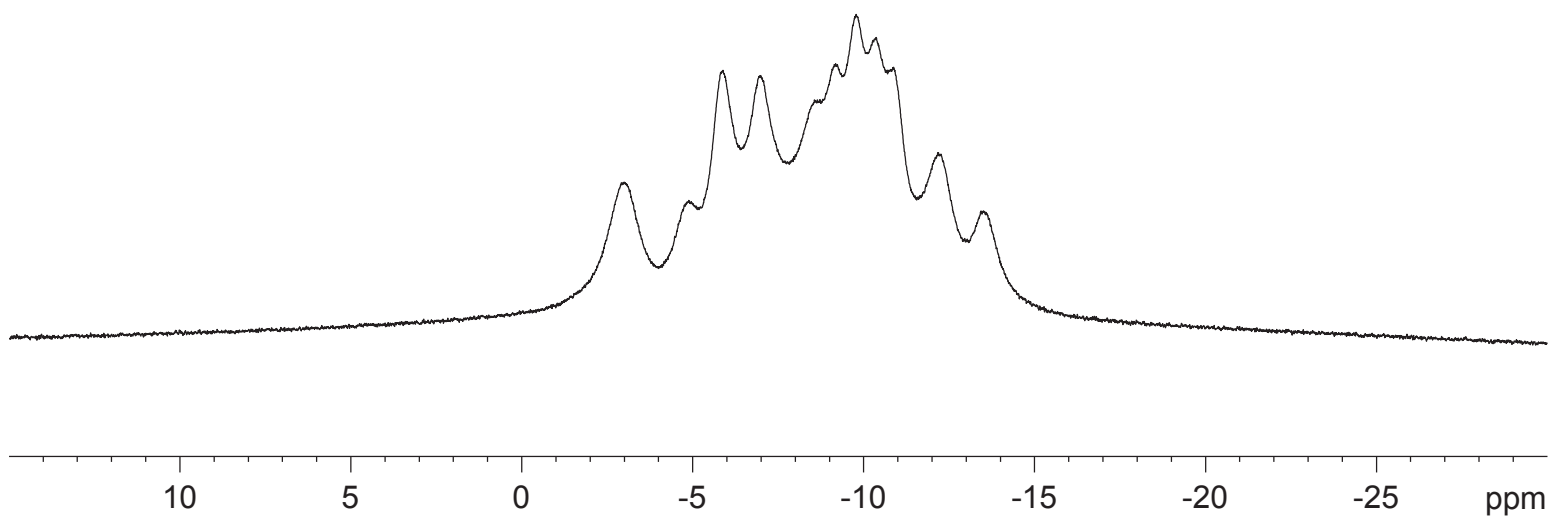
| 3.00  
 | 4.84  
 | 5.88  
 | 6.99  
 | 8.55  
 | 9.15  
 | 9.78  
 | 10.33  
 | 10.87  
 | 12.17  
 | 13.51

1hr-B-0732-ch3cascdcl3 (C)

Current Data Parameters  
 NAME 1hr-B-0732-ch3cascdcl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170729  
 Time 19.53 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 35  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 362  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 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



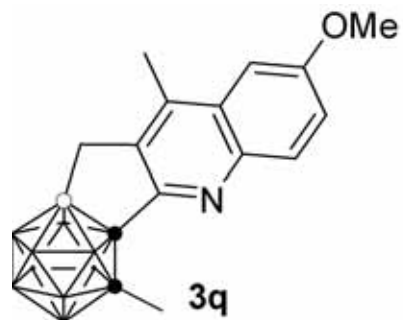
7.934  
7.911  
7.350  
7.343  
7.327  
7.320  
7.260  
7.196  
7.189

3.959

2.603  
2.576  
2.530  
2.494  
2.448  
2.420

1.567

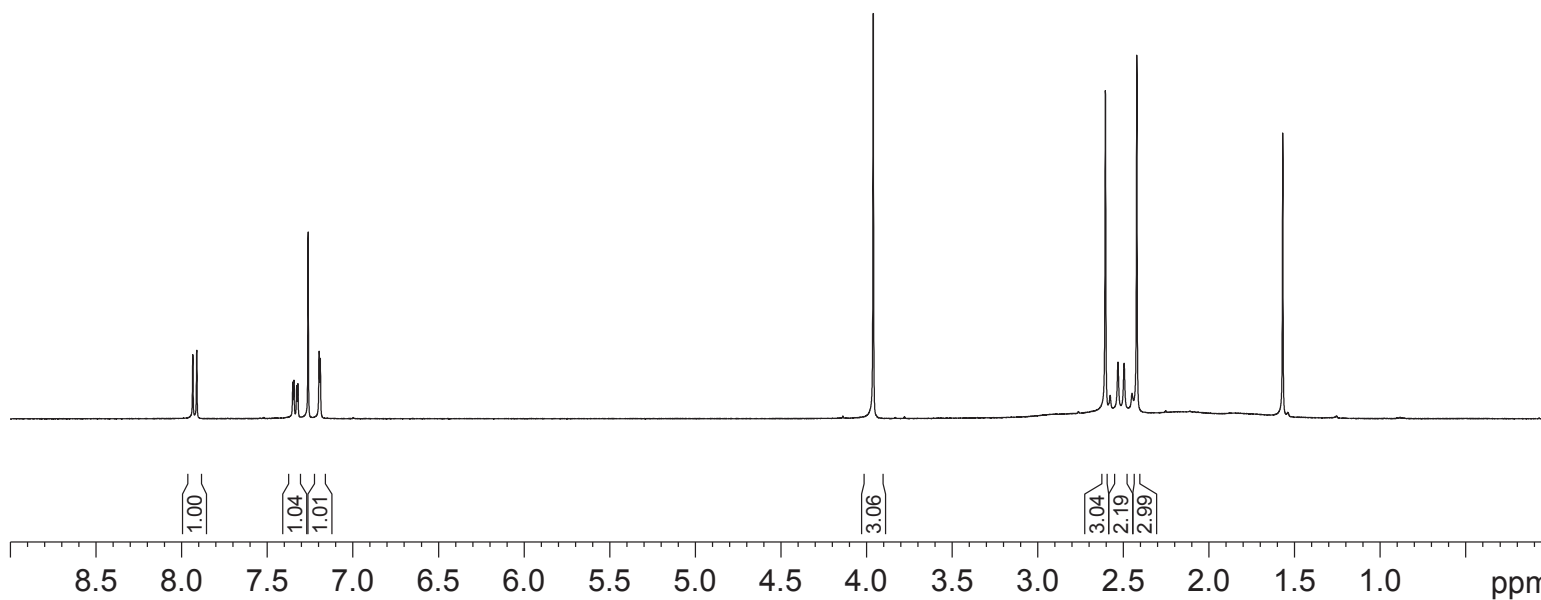
1hr-H-0722-3-ome-ca:



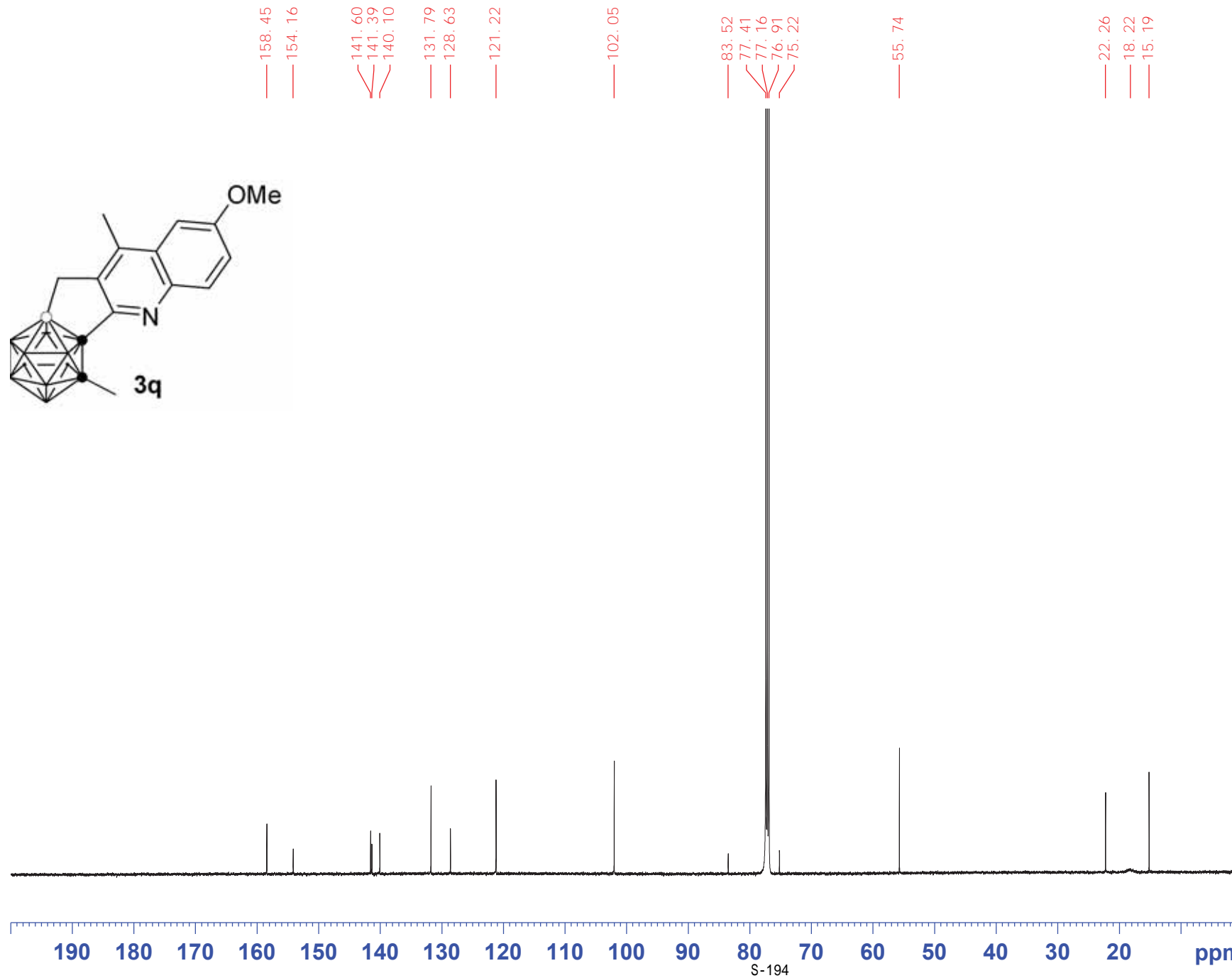
Current Data Parameters  
NAME 1hr-H-0722-3-ome-casc  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170812  
Time 10.30 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 11  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 203  
DW 62.400 usec  
DE 6.50 usec  
TE 294.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters  
SI 65536  
SF 400.2300102 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



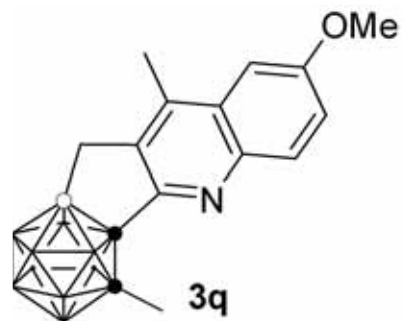
I hr-0722-3-C



Current Data Parameters  
NAME I hr-0722-3-C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170812  
Time 12.23 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2100  
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  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters  
SI 32768  
SF 125.7577716 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



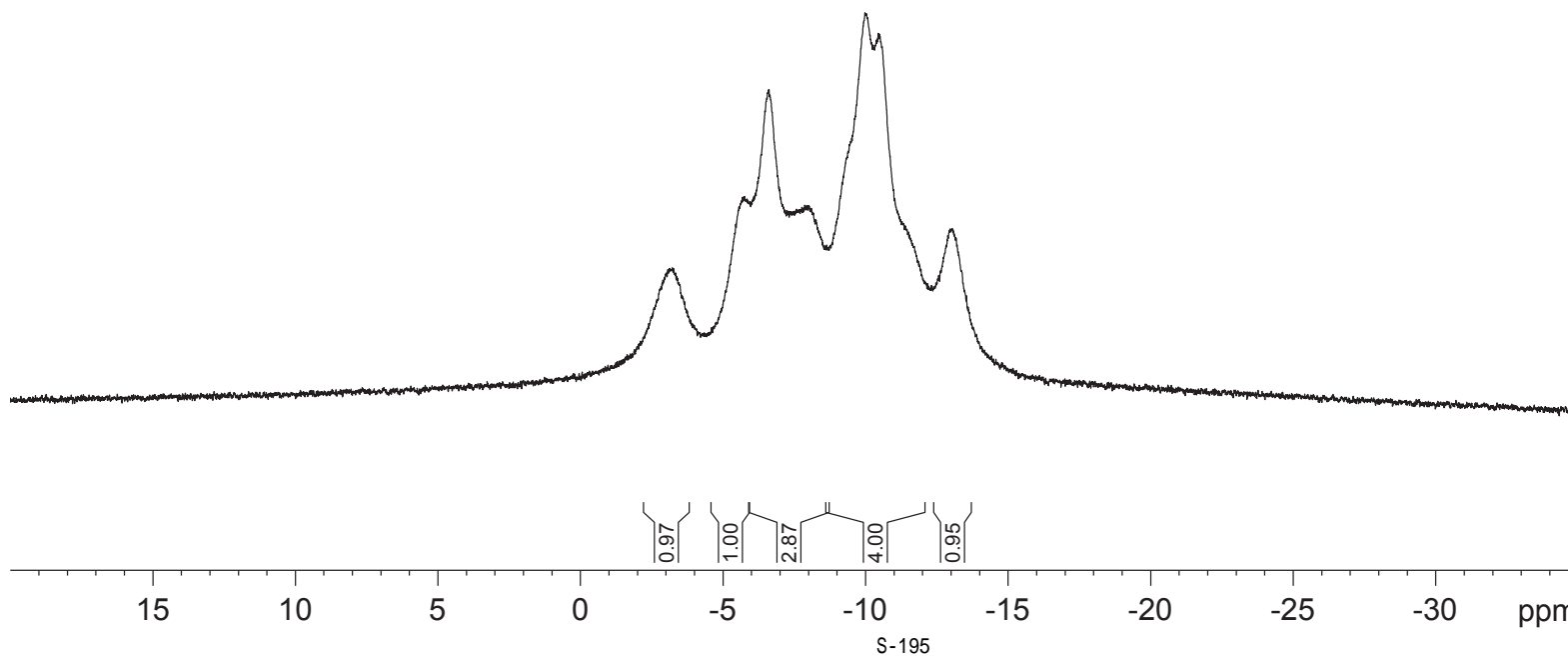
— -3.22  
 — -5.65  
 — -6.61  
 — -7.99  
 — -9.98  
 — -10.45  
 — -13.04

1hr-B-cas-0396-OMe-CDCl3

Current Data Parameters  
 NAME 1hr-B-cas-0396-OMe-CDCl  
 EXPNO 1  
 PROCNO 1

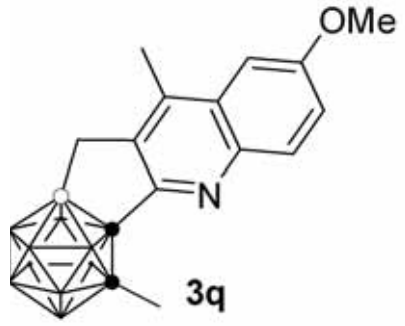
F2 - Acquisition Parameters  
 Date\_ 20160622  
 Time 14.45 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (   
 PULPROG zgdc  
 TD 65536  
 SOLVENT CDCl3  
 NS 12  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 287  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 2.00000000 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



| -3.00  
 | -5.00  
 | -5.90  
 | -7.03  
 | -8.53  
 | -9.23  
 | -9.80  
 | -10.35  
 | -10.91  
 | -12.16  
 | -13.44

1hr-B-cas-0396-OMe-CDCl3 (C)

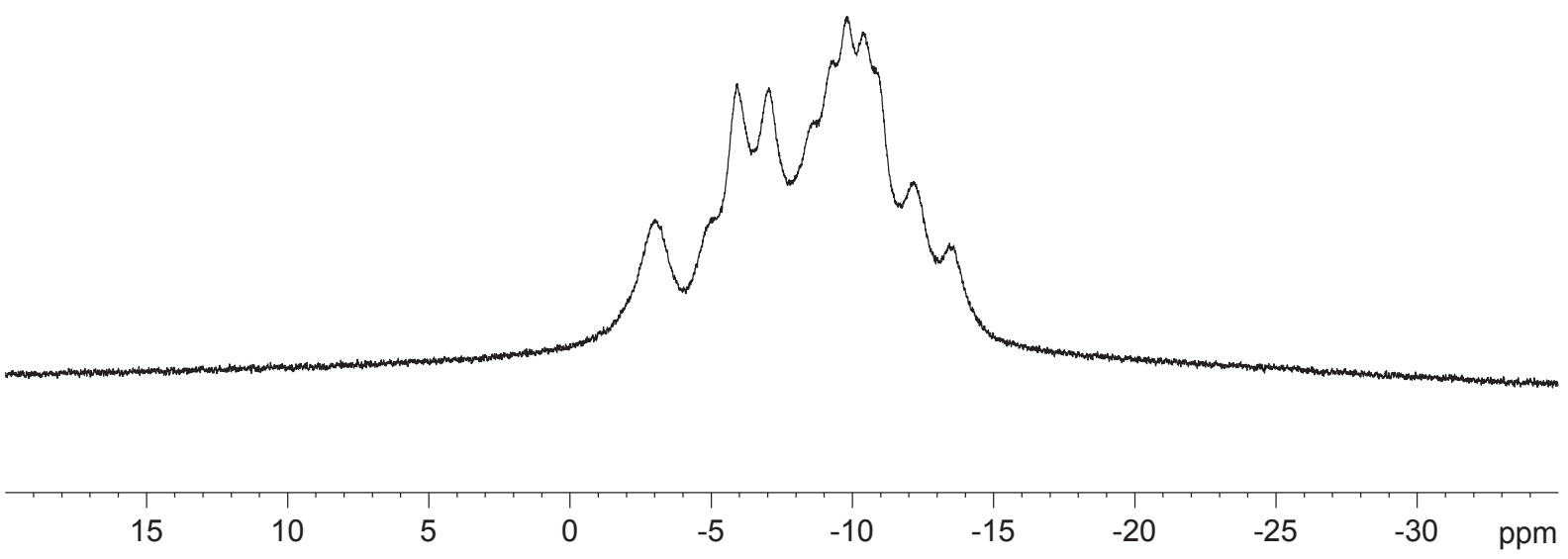


```

Current Data Parameters
NAME      1hr-B-cas-0396-OMe-CDCl3 (C)
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20160622
Time      14.46 h
INSTRUM   spect
PROBHD    Z108618_0257 (
PULPROG   zg
TD         65536
SOLVENT   CDCl3
NS         15
DS         2
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ         1.3631488 sec
RG         406
DW         20.800 usec
DE         6.50 usec
TE         294.7 K
D1         2.0000000 sec
TD0        1
SFO1      128.4096890 MHz
NUC1       13C
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
  
```



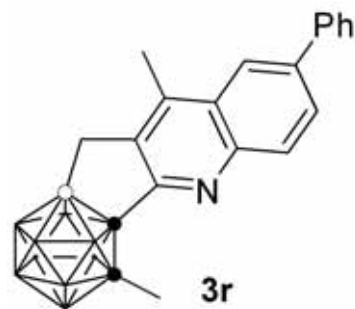


8.161  
8.157  
8.108  
8.086  
7.954  
7.951  
7.932  
7.929  
7.725  
7.706  
7.536  
7.517  
7.498  
7.444  
7.426  
7.408  
7.260

2.708  
2.614  
2.568  
2.532  
2.487  
2.453

1.572

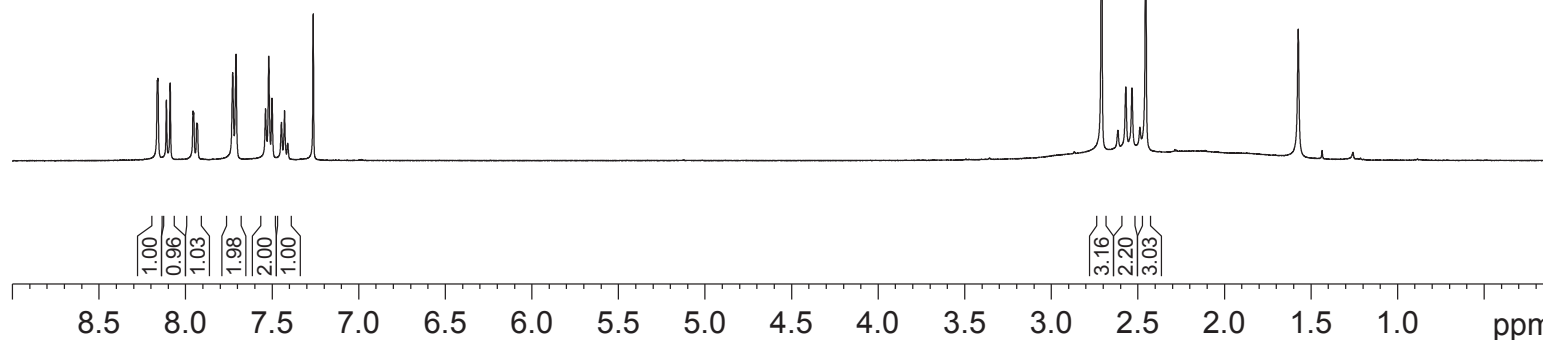
lhr-H-0746-phcccasc

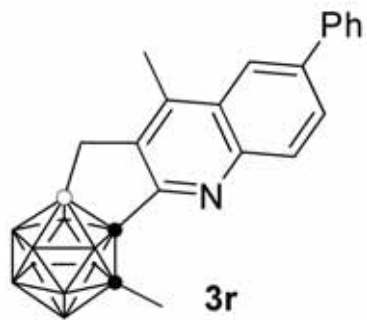


Current Data Parameters  
NAME lhr-H-0746-phcccasc  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170811  
Time 18.30 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 203  
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 400.2300102 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





156.51  
145.14  
143.00  
140.84  
140.17  
140.14  
130.78  
129.16  
128.88  
128.00  
127.74  
127.71  
121.69

83.32  
77.41  
77.16  
76.91  
75.38

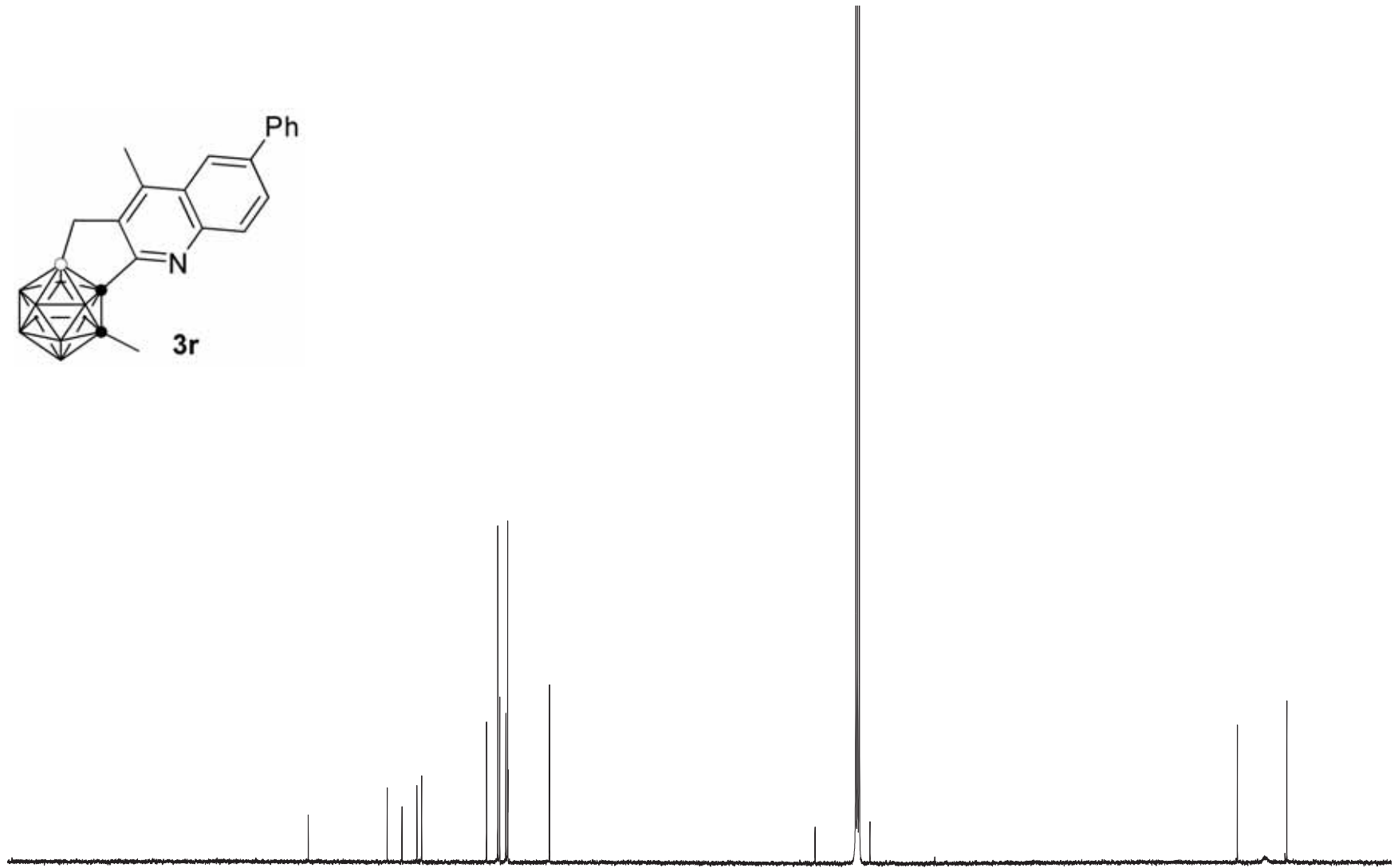
22.29  
15.15

I hr-C-0746

Current Data Parameters  
NAME I hr-C-0746  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170810  
Time 11.29 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

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



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

S-198

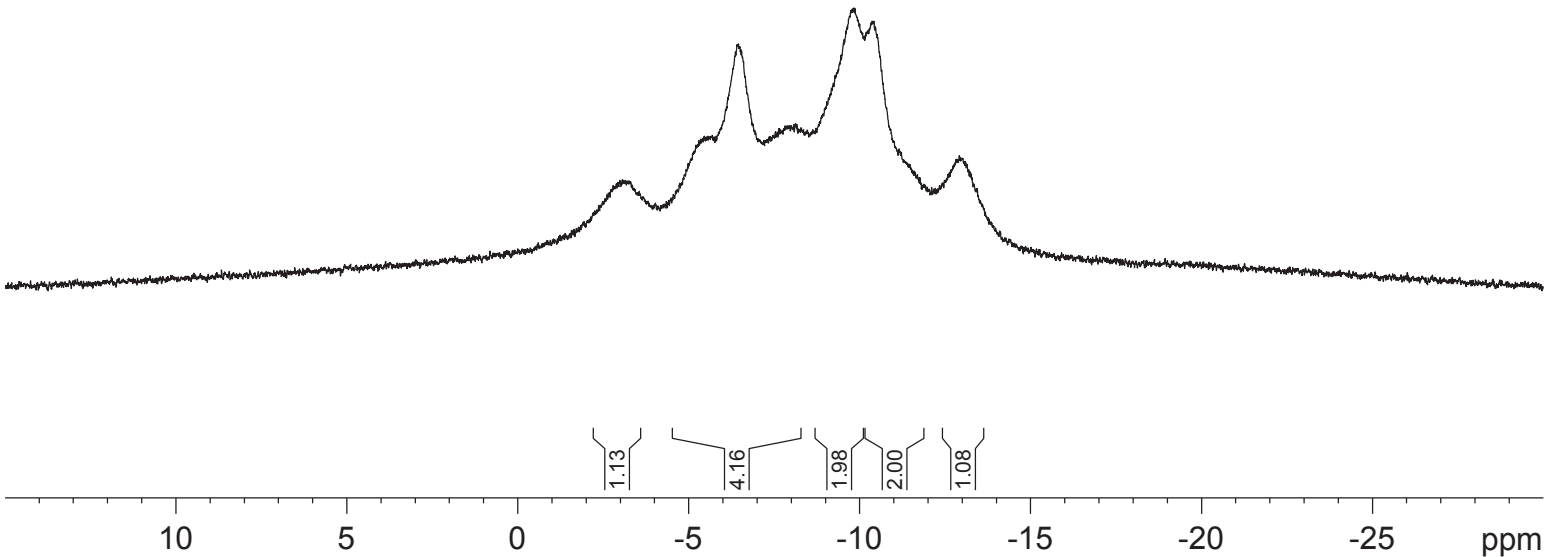
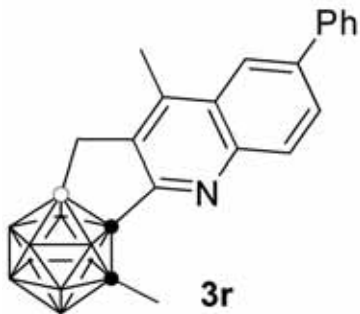
1hr-B-0746-phccasccl3

Current Data Parameters  
NAME 1hr-B-0746-phccasccl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170811  
Time\_ 18.34 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 36  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 322  
DW 20.800 usec  
DE 6.50 usec  
TE 295.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W  
SFO2 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.56000042 W  
PLW12 0.27428001 W

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

— 3.06  
— 5.43  
— 6.46  
— 8.12  
— 9.84  
— 10.37  
— 12.92



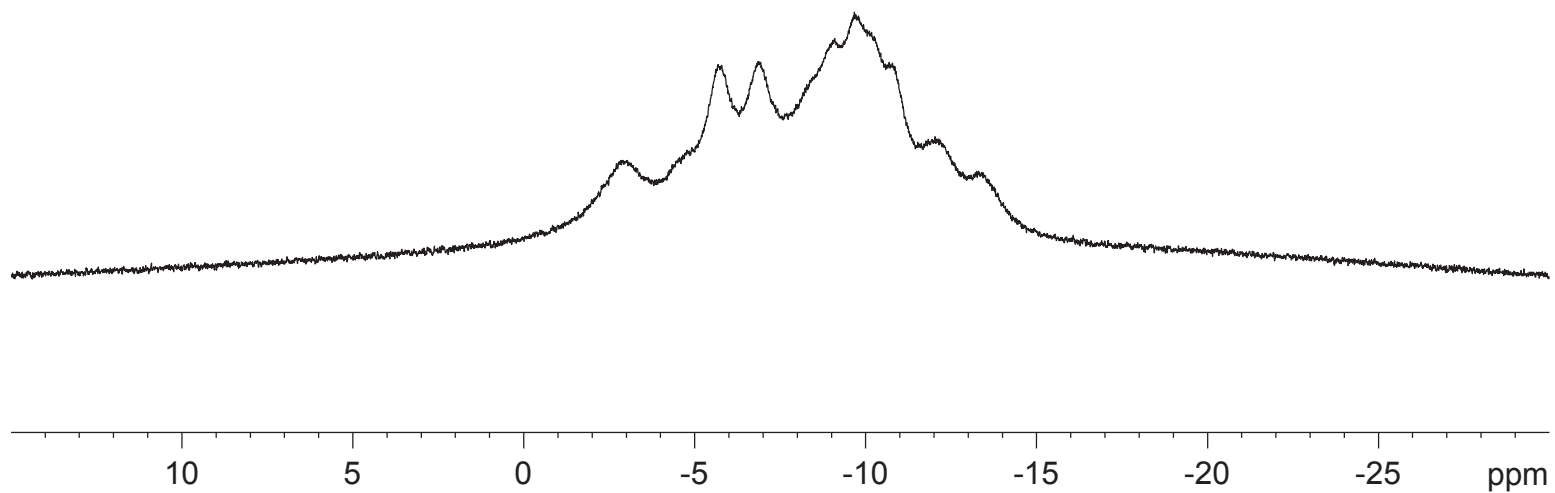
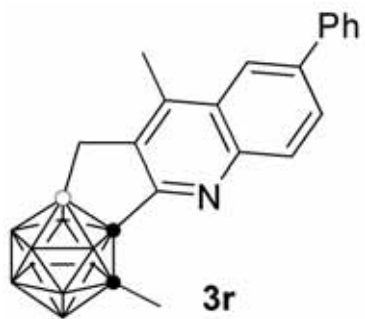
1hr-B-0746-phccasccl3 (C)

Current Data Parameters  
NAME 1hr-B-0746-phccasccl3 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170811  
Time 18.37 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 322  
DW 20.800 usec  
DE 6.50 usec  
TE 295.2 K  
D1 2.0000000 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

— 2.88  
— 4.69  
— 5.69  
— 6.84  
— 8.40  
— 9.04  
— 9.67  
— 10.74  
— 12.03  
— 13.36

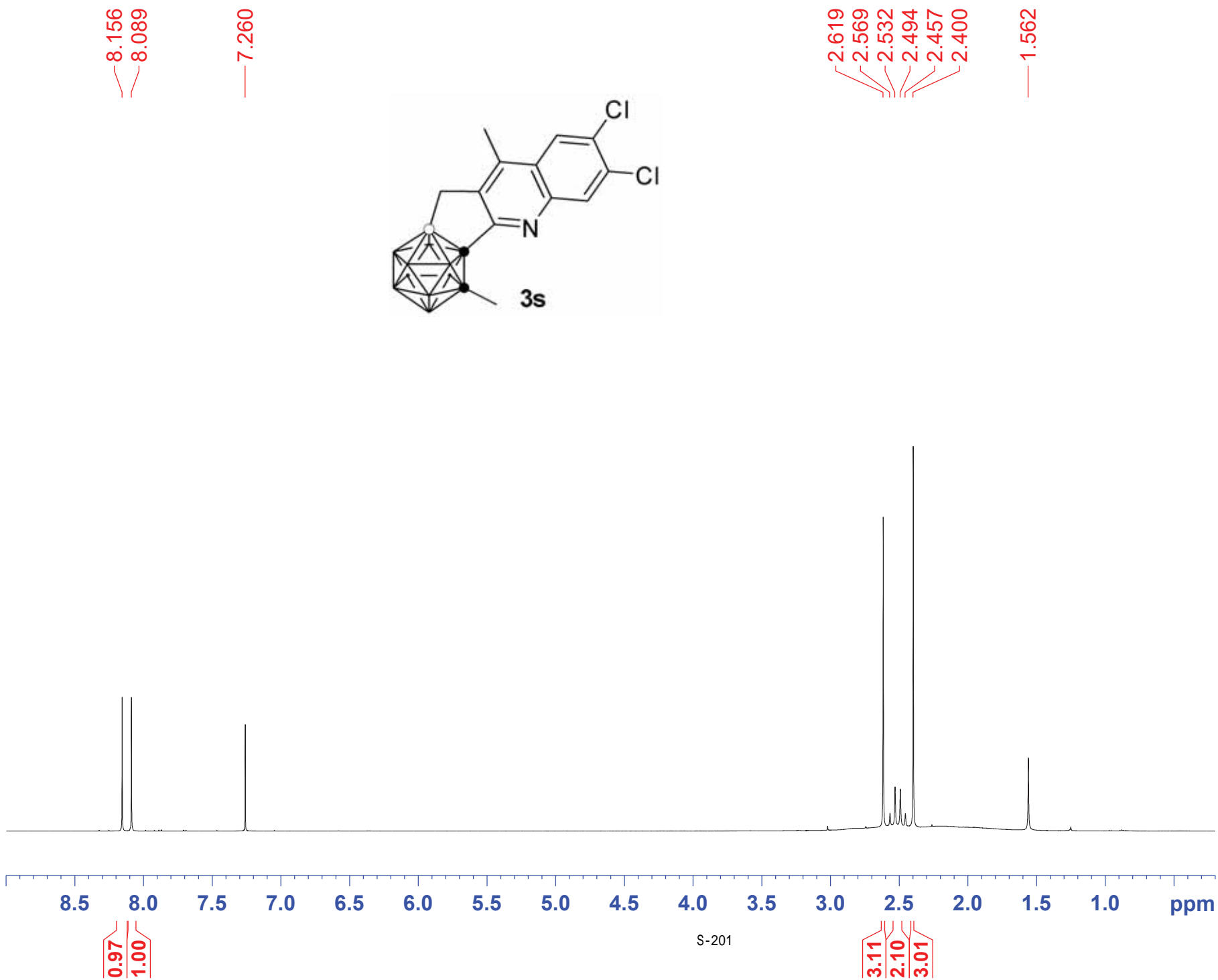
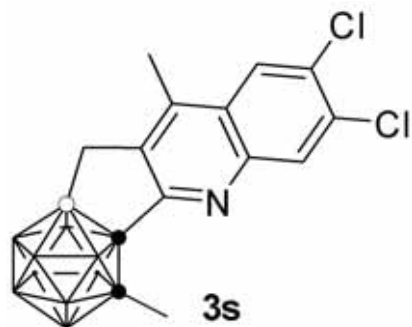


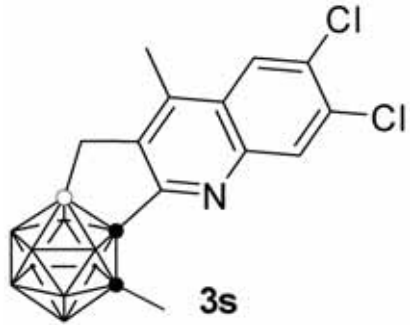
I hr-H-0764-cas

Current Data Parameters  
NAME I hr-H-0754-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170922  
Time 9.29  
INSTRUM spect  
PROBHD Z149001\_0010 (   
PULPROG zg30  
TD 65536  
SOLVENT CDCl 3  
NS 12  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 30.85  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300124  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00





157.96  
144.56  
142.16  
140.92  
133.64  
131.79  
131.21  
126.90  
124.84

82.69  
77.41  
77.16  
76.91  
75.45

22.27  
15.17

1 hr-C-0754-cas

Current Data Parameters  
NAME 1 hr-C-0754-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170922  
Time 9.55 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 450  
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  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters  
SI 32768  
SF 125.7577718 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

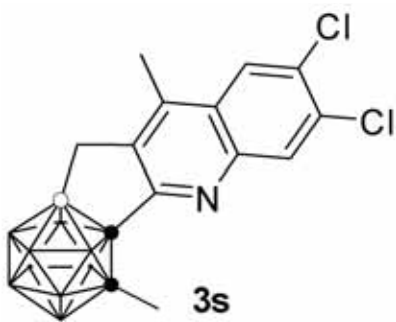


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

S-202

1 hr-B-0754-cas

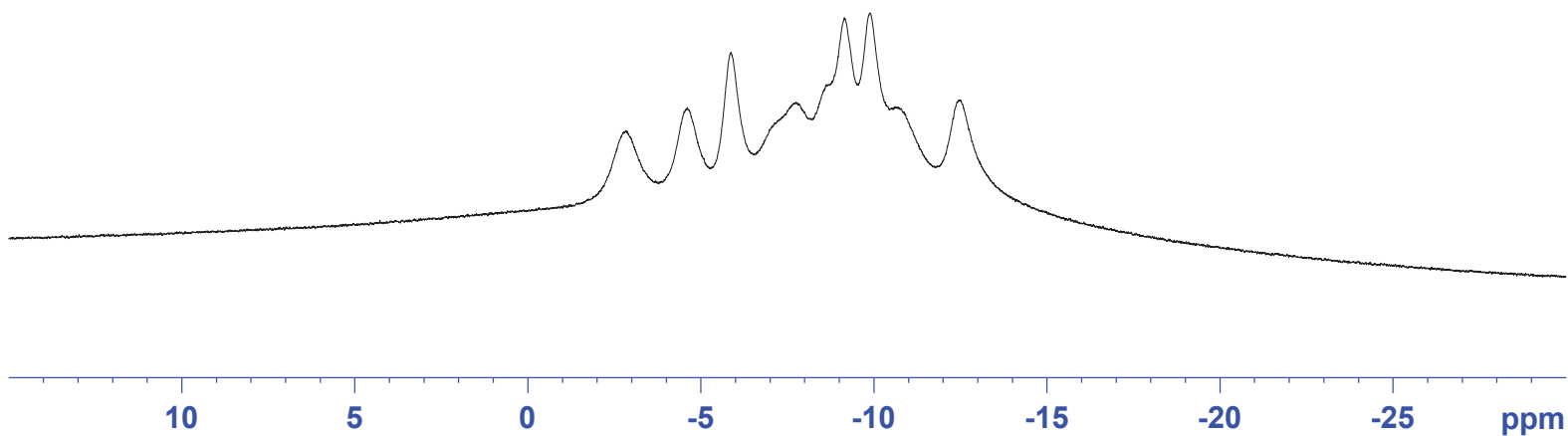
--2.82  
--4.60  
--5.85  
--7.10  
--7.73  
--8.60  
--9.14  
--9.87  
--10.70  
--12.48



Current Data Parameters  
NAME 1 hr-B-0754-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170922  
Time 9.58 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 20  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 186.15  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

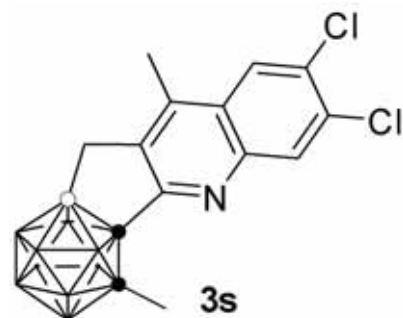
F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.06  
1.10  
1.11  
1.82  
3.94  
1.03

I hr-B-0754-cas(c)

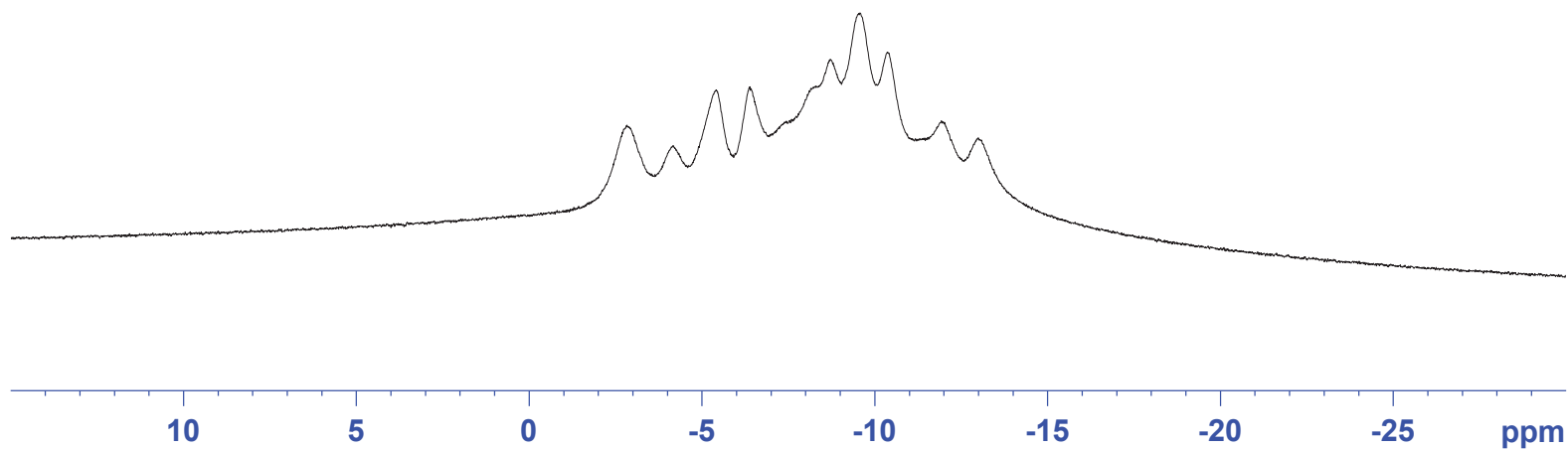
2.82  
4.11  
5.40  
6.38  
7.39  
8.16  
8.69  
9.57  
10.36  
11.33  
11.92  
12.98



Current Data Parameters  
NAME I hr-B-0754-cas(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170922  
Time 9.59 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl 3  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



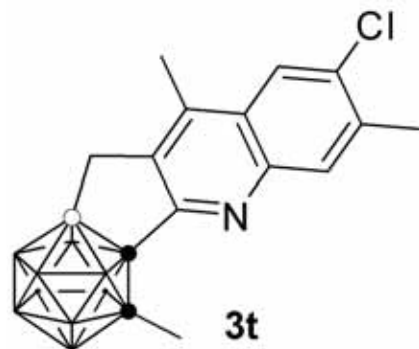


I hr-H-0783-cas

Current Data Parameters  
NAME I hr-H-0783-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171021  
Time 10.22  
INSTRUM spect  
PROBHD Z149001\_0010 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 30.85  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300125  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00



7.976  
7.893

7.260

2.601  
2.552  
2.523  
2.483  
2.446  
2.413

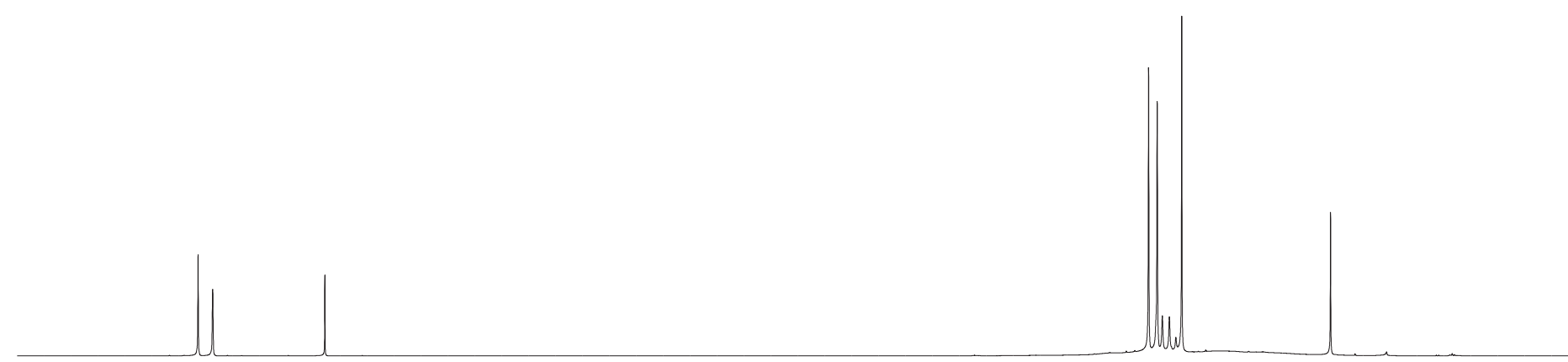
1.572

1.01  
1.00

3.16  
3.22  
2.18  
3.13

S-205

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

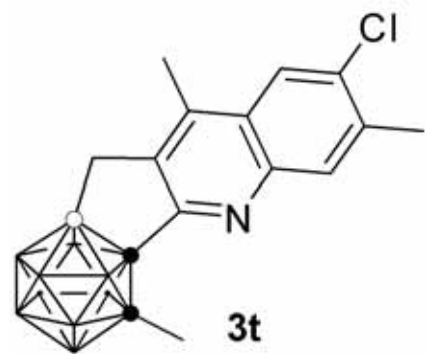


1 hr-C-0783-cas

156.80  
144.47  
141.85  
139.77  
137.77  
134.52  
131.39  
126.79  
123.24

83.13  
77.41  
77.16  
76.91  
75.32

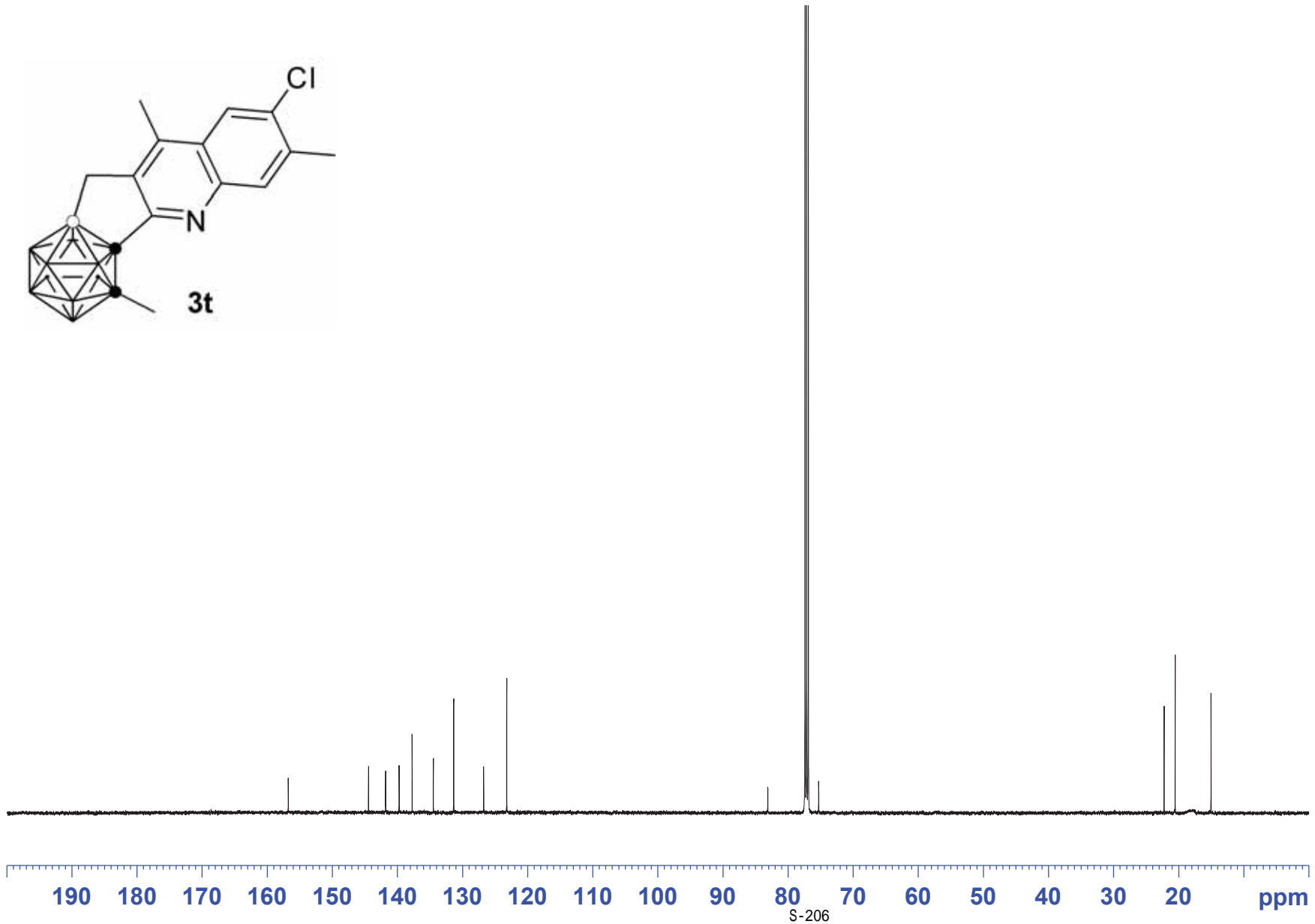
22.26  
20.55  
15.05



Current Data Parameters  
NAME 1 hr-C-0783-cas  
EXPNO 1  
PROCNO 1

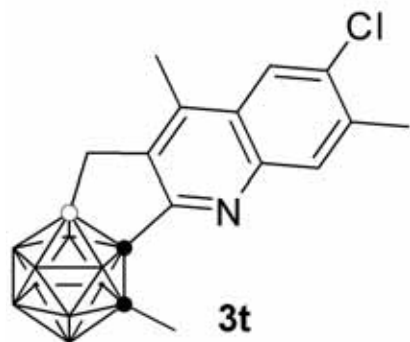
F2 - Acquisition Parameters  
Date\_ 20171021  
Time 10.41 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 360  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters  
SI 32768  
SF 125.7577721 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



S-206

I hr-B-0783-cas

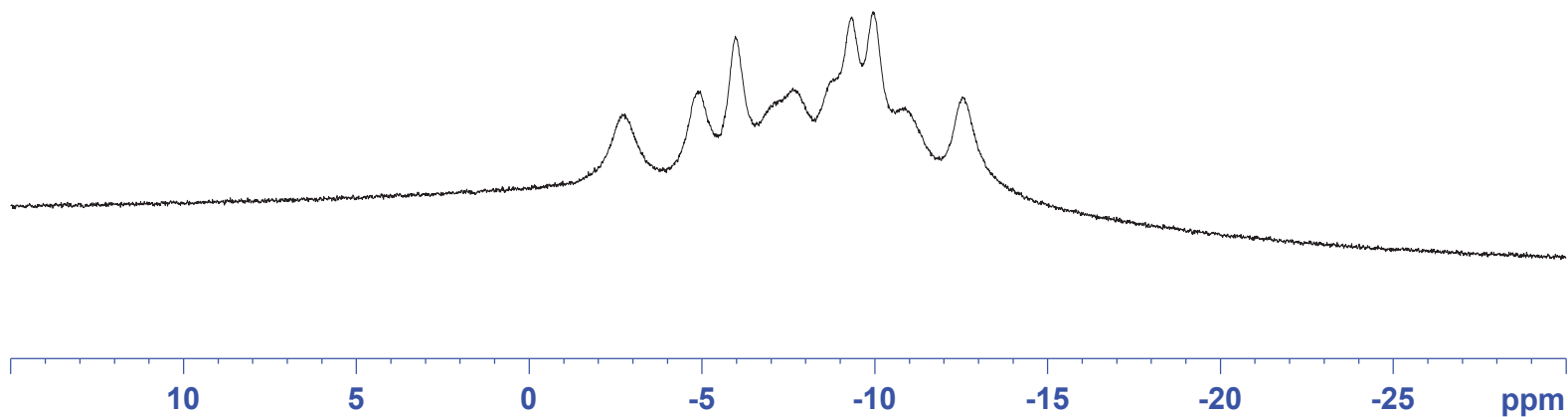


-2.75  
-4.94  
-5.96  
-7.06  
-7.62  
-8.69  
-9.32  
-9.94  
-10.85  
-12.53

Current Data Parameters  
NAME I hr-B-0783-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171021  
Time 10.43 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl 3  
NS 20  
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  
TDO 1  
SF01 160.4615790 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.00000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.00000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

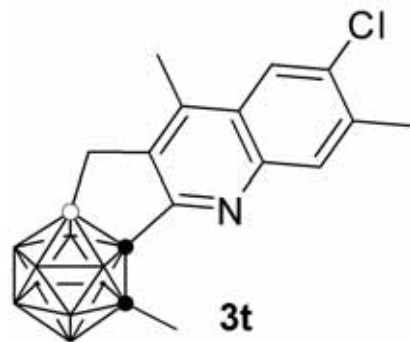
F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.20  
1.07  
0.99  
2.11  
3.00  
1.01  
1.10

I hr-B-0783-cas(c)

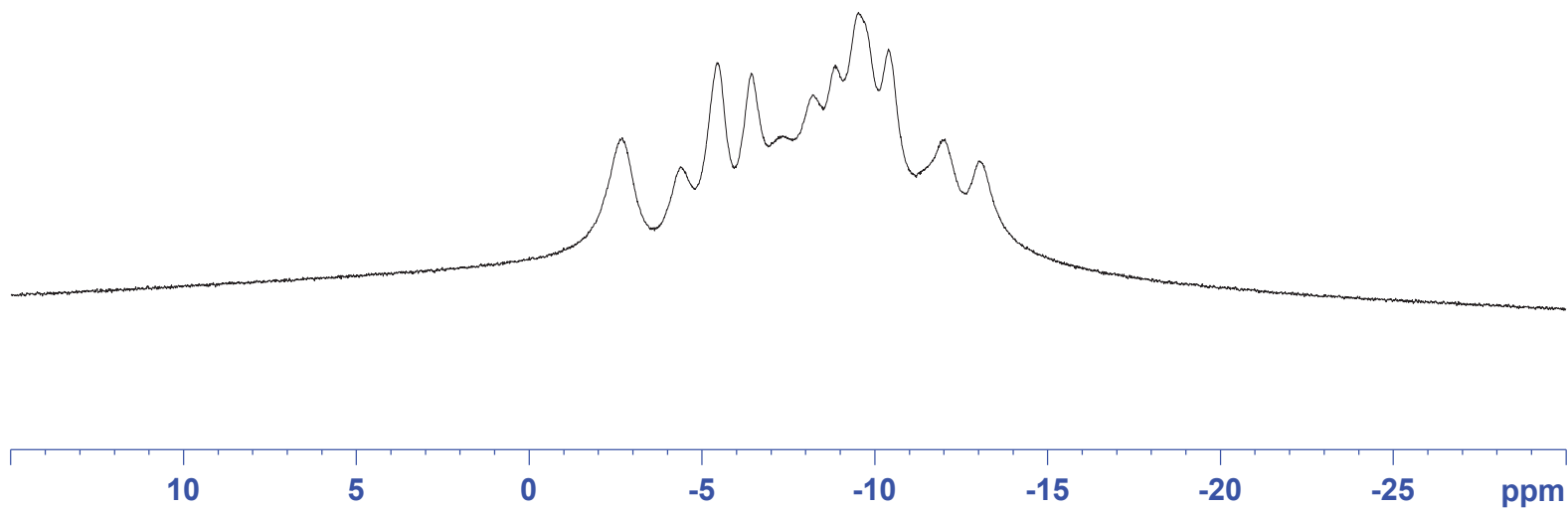
-2.69  
-4.37  
-5.43  
-6.42  
-7.19  
-8.21  
-8.85  
-9.52  
-10.39  
-12.03  
-13.00



Current Data Parameters  
NAME I hr-B-0783-cas(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171021  
Time 10.44 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl 3  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

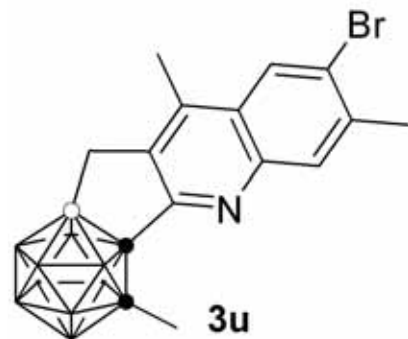


1 hr-H-784-cas

Current Data Parameters  
NAME 1 hr-H-784-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171025  
Time 9.26  
INSTRUM spect  
PROBHD Z149001\_0010 (   
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 30.85  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300127  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00



8.191  
7.890  
7.260

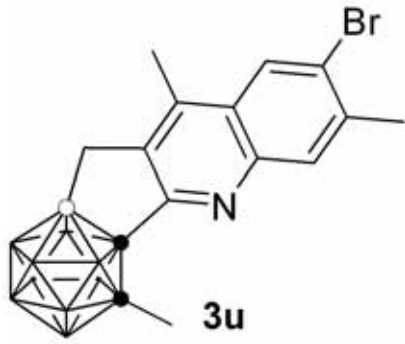
2.599  
2.575  
2.563  
2.526  
2.486  
2.450  
2.412  
1.571



1.00  
1.01

S-209

3.04  
2.99  
2.11  
3.02



156.96  
144.88  
141.76  
139.79  
139.20  
131.10  
127.10  
126.92  
125.08

83.13  
77.41  
77.16  
76.91  
75.33

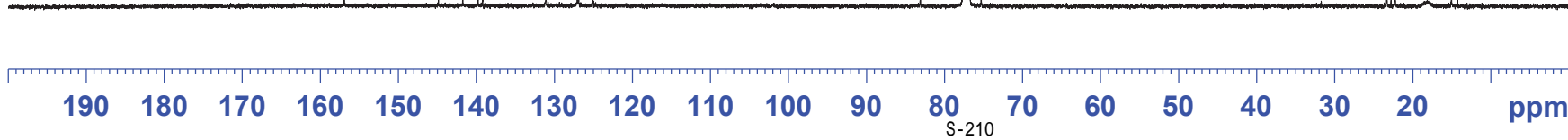
23.33  
22.26  
15.05

I hr-C-784-cas

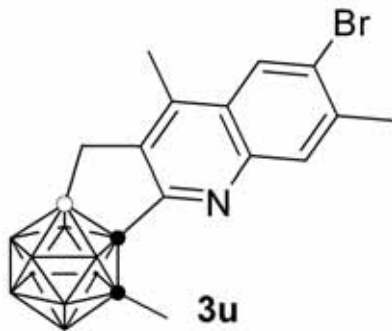
Current Data Parameters  
NAME I hr-C-784-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171025  
Time 10.11 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 800  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters  
SI 32768  
SF 125.7577720 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



I hr-B-784-cas

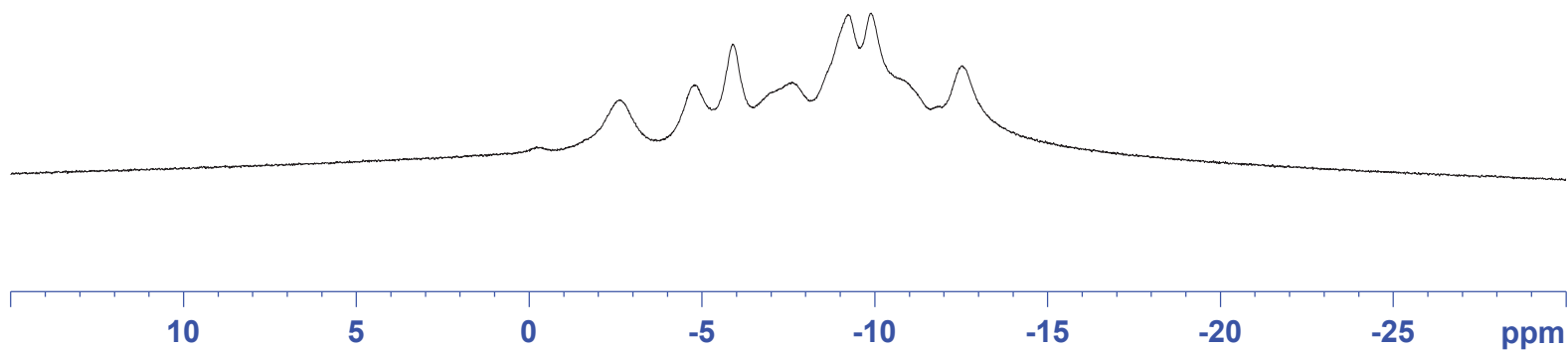


— -2.60  
— -4.79  
— -5.88  
— -6.98  
— -7.59  
— -9.22  
— -9.89  
— -10.93  
— -12.53

Current Data Parameters  
NAME I hr-B-784-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171025  
Time 9.21 h  
INSTRUM spect  
PROBHD Z149001\_0010 (g)  
PULPROG zgpg  
TD 32768  
SOLVENT None  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4615790 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

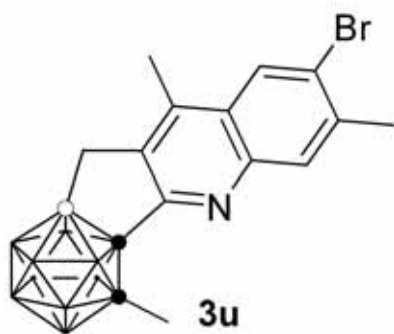
F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.11  
1.01  
0.98  
1.93  
4.00  
1.19

l hr-B-784-cas(c)

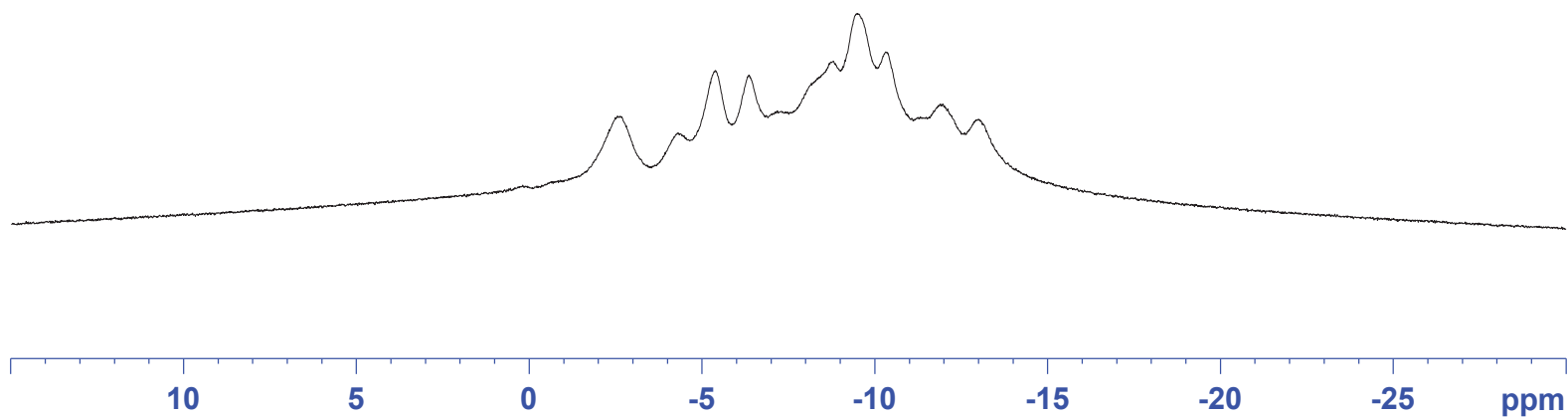
-2.55  
-4.32  
-5.38  
-6.35  
-7.18  
-8.17  
-8.72  
-9.49  
-10.31  
-11.89  
-13.00



Current Data Parameters  
NAME l hr-B-784-cas(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171025  
Time 9.22 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT None  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

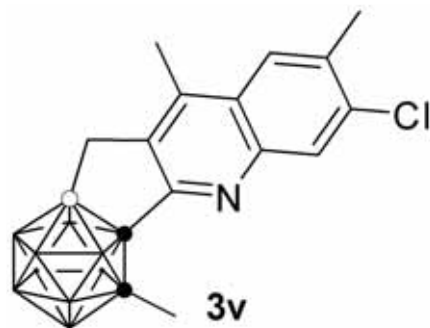
F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





8.045  
7.820  
7.260

2.619  
2.578  
2.563  
2.516  
2.481  
2.434  
2.409  
1.577

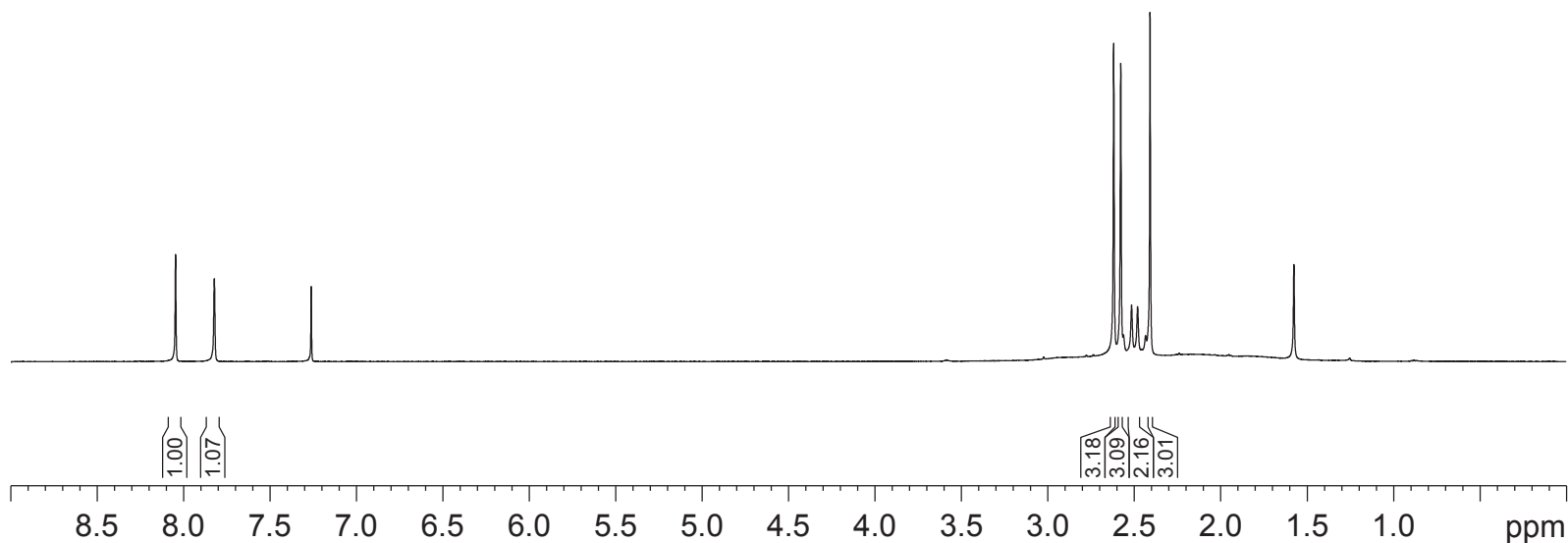


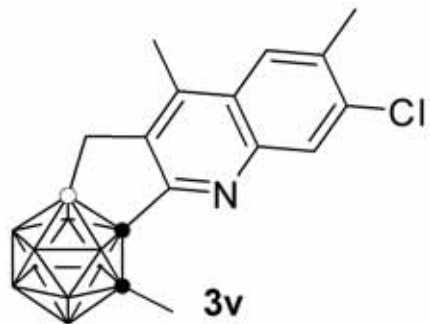
[1hr-H-0795-cccasccl3]

Current Data Parameters  
NAME 1hr-H-0795-cccasccl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171026  
Time\_ 21.32 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 203  
DW 62.400 usec  
DE 6.50 usec  
TE 294.4 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 400.2300104 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

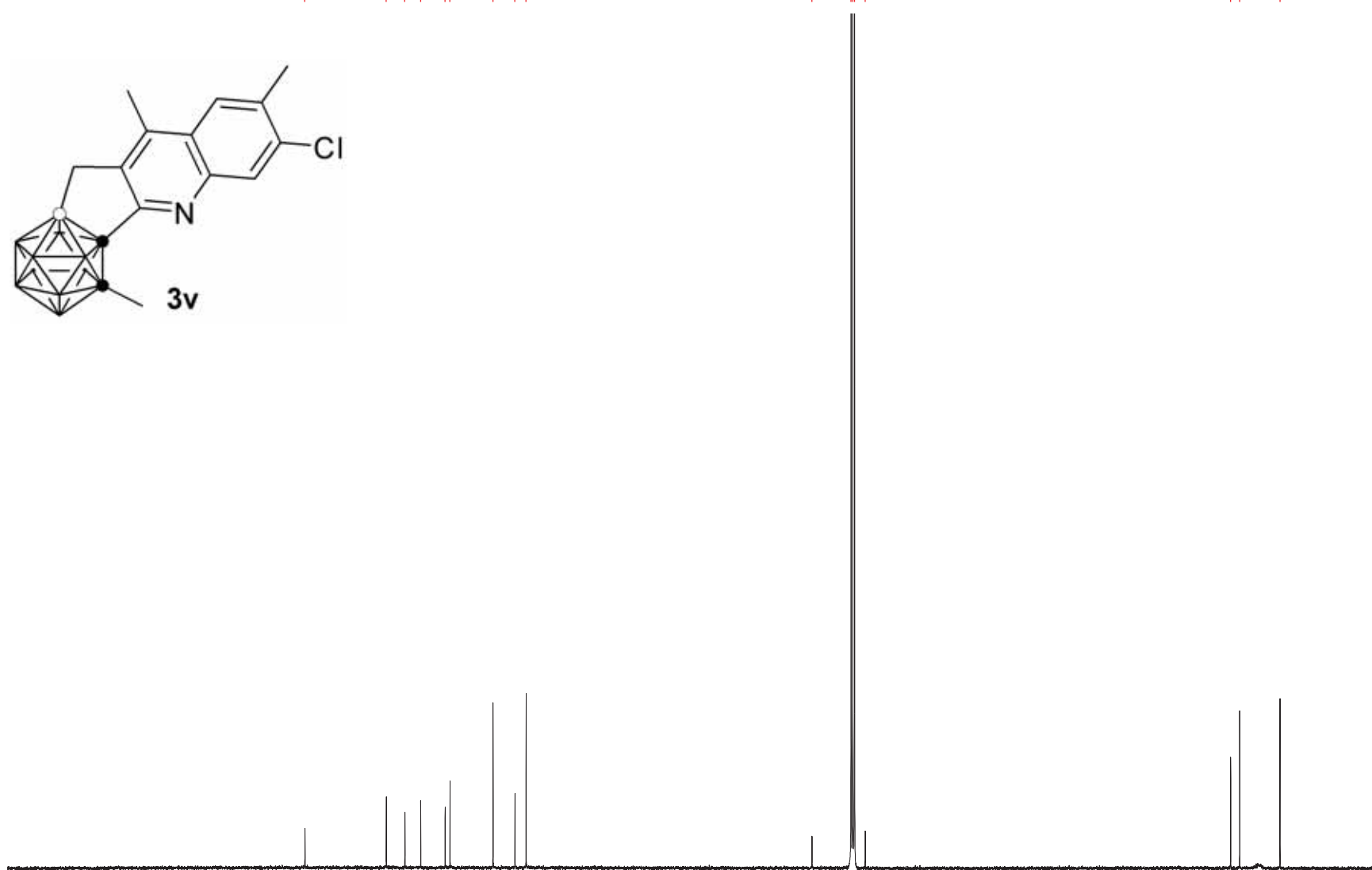




156.77  
 144.95  
 142.25  
 139.95  
 136.40  
 135.69  
 129.44  
 126.25  
 124.64

83.09  
 77.41  
 77.16  
 76.91  
 75.35

22.26  
 20.95  
 15.09



Current Data Parameters  
 NAME 1hr-795  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

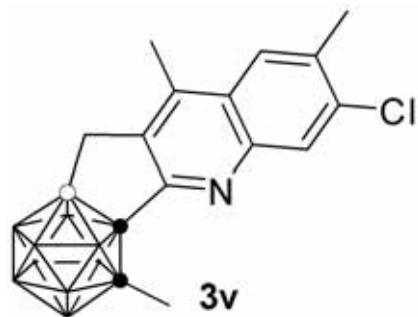
Date\_ 20171027  
 Time 2.26 h  
 INSTRUM spect  
 PROBHD Z149001\_0010 ( )  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 600  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 1.1010048 sec  
 RG 206.72  
 DW 16.800 usec  
 DE 18.00 usec  
 TE 298.0 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1  
 SF01 125.7703643 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 61.0000000 W  
 SF02 500.1320005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.33750001 W  
 PLW13 0.16976000 W

F2 - Processing parameters

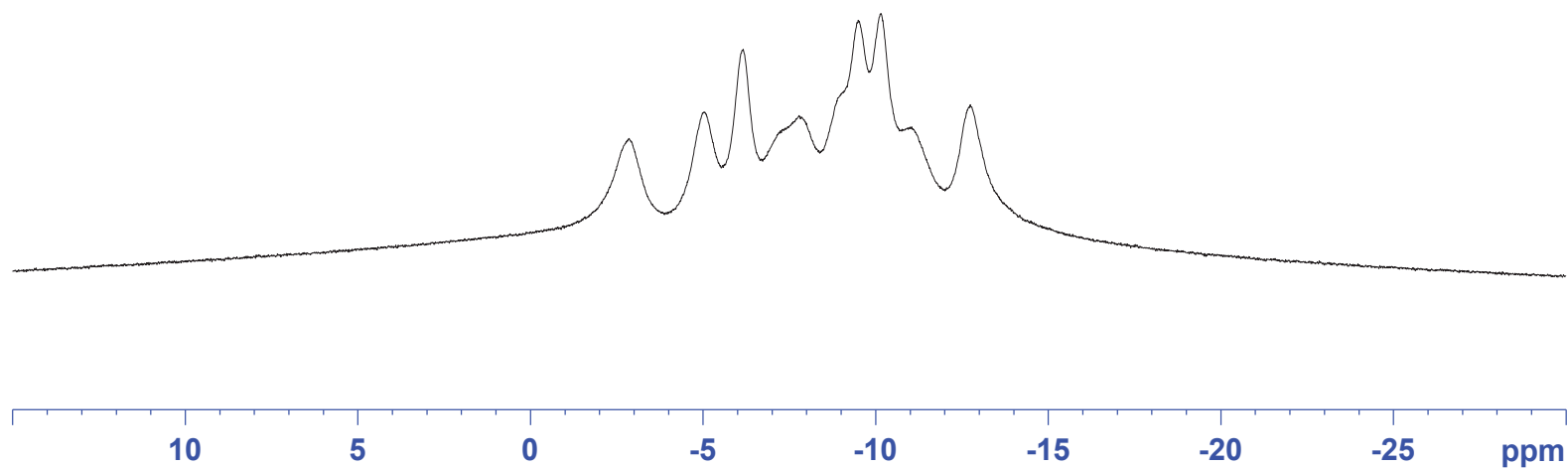
SI 32768  
 SF 125.7577721 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

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

I hr-B-795-cas



-2.85  
-5.04  
-6.15  
-7.28  
-7.78  
-8.89  
-9.49  
-10.14  
-11.01  
-12.73



1.09  
1.04  
1.06  
1.91  
4.00  
S -11.5  
1.16

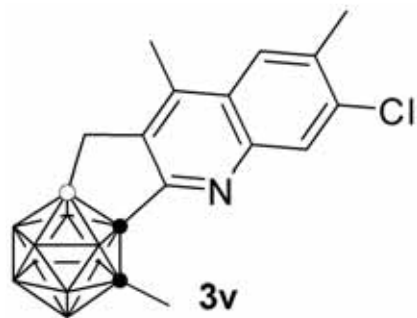
Current Data Parameters  
NAME I hr-B-795-cas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171027  
Time 9.18 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg  
TD 32768  
SOLVENT None  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4615790 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

l hr-B-795-cas(c)

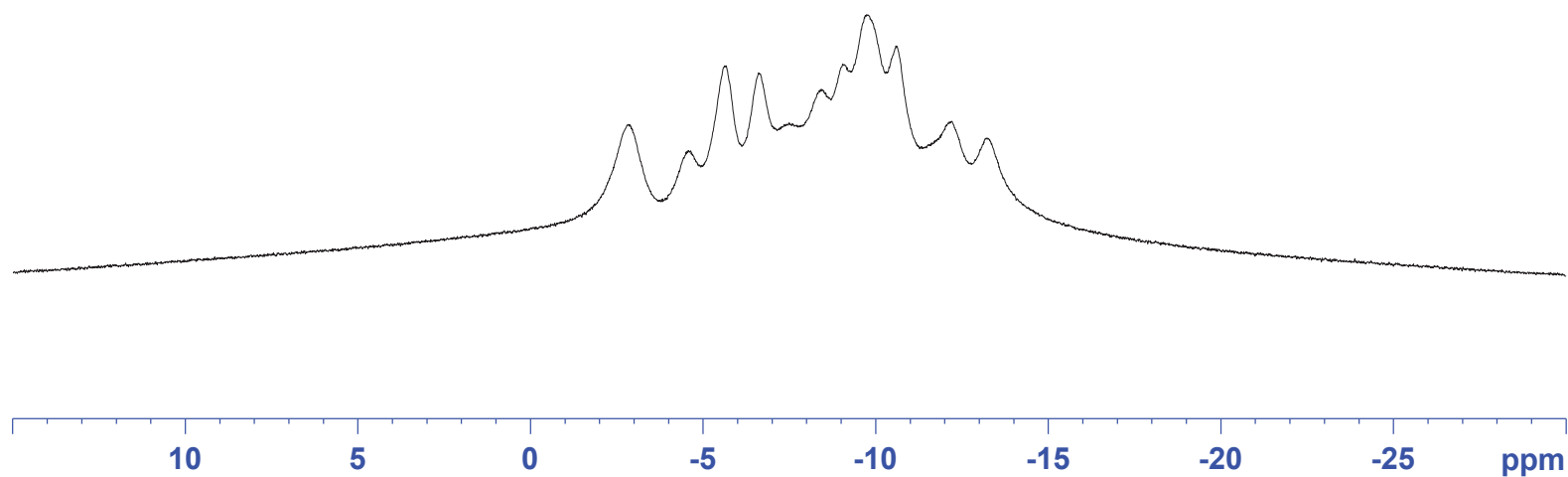
-2.81  
-4.51  
-5.62  
-6.61  
-7.41  
-8.37  
-9.01  
-9.73  
-10.58  
-12.20  
-13.23

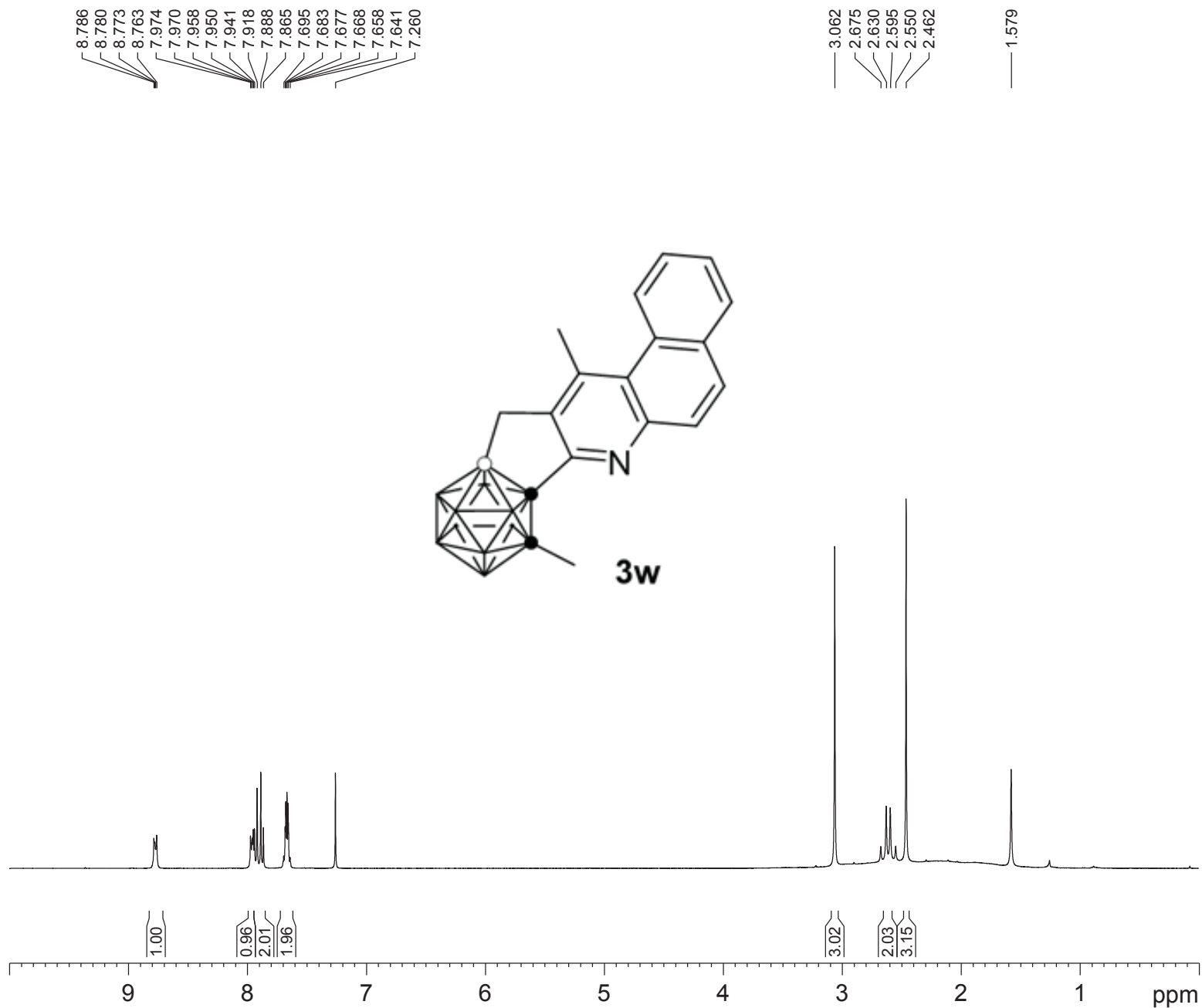


Current Data Parameters  
NAME l hr-B-795-cas(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171027  
Time 9.19 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT None  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





1hr-H-0735-napcascd

Current Data Parameters

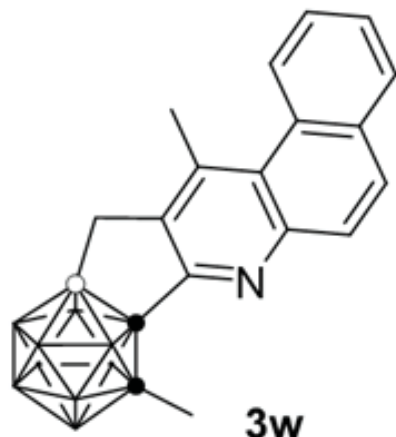
NAME 1hr-H-0735-napcascd  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170724  
 Time 21.21 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 144  
 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 400.2300106 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



154.80  
147.30  
144.16  
142.54  
133.51  
131.03  
130.46  
129.08  
129.01  
128.12  
126.98  
126.34  
125.67

83.50  
77.48  
77.16  
76.84  
75.14

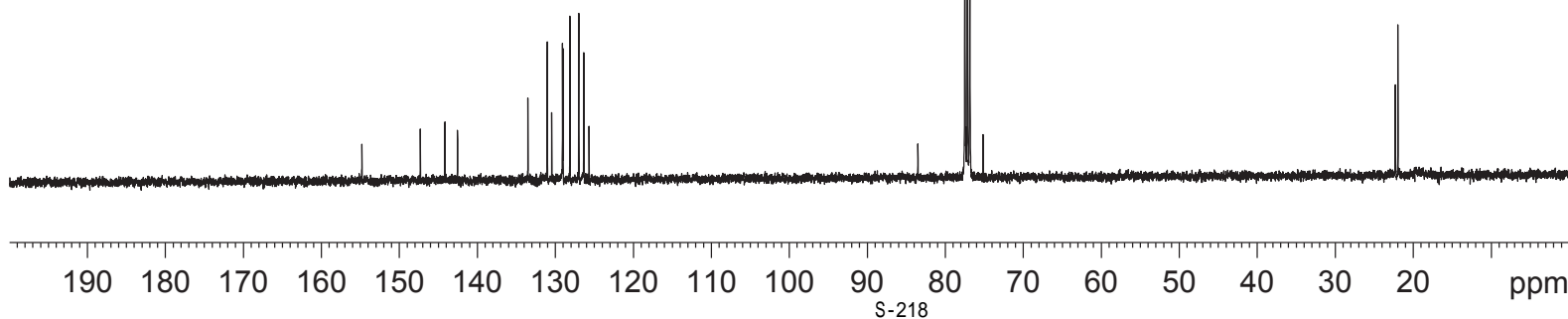
22.30  
21.96

1hr-C-0735-napcasdc

Current Data Parameters  
NAME 1hr-C-0735-napcasdc1:  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170725  
Time\_ 8.37 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1000  
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 295.3 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 100.6379005 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



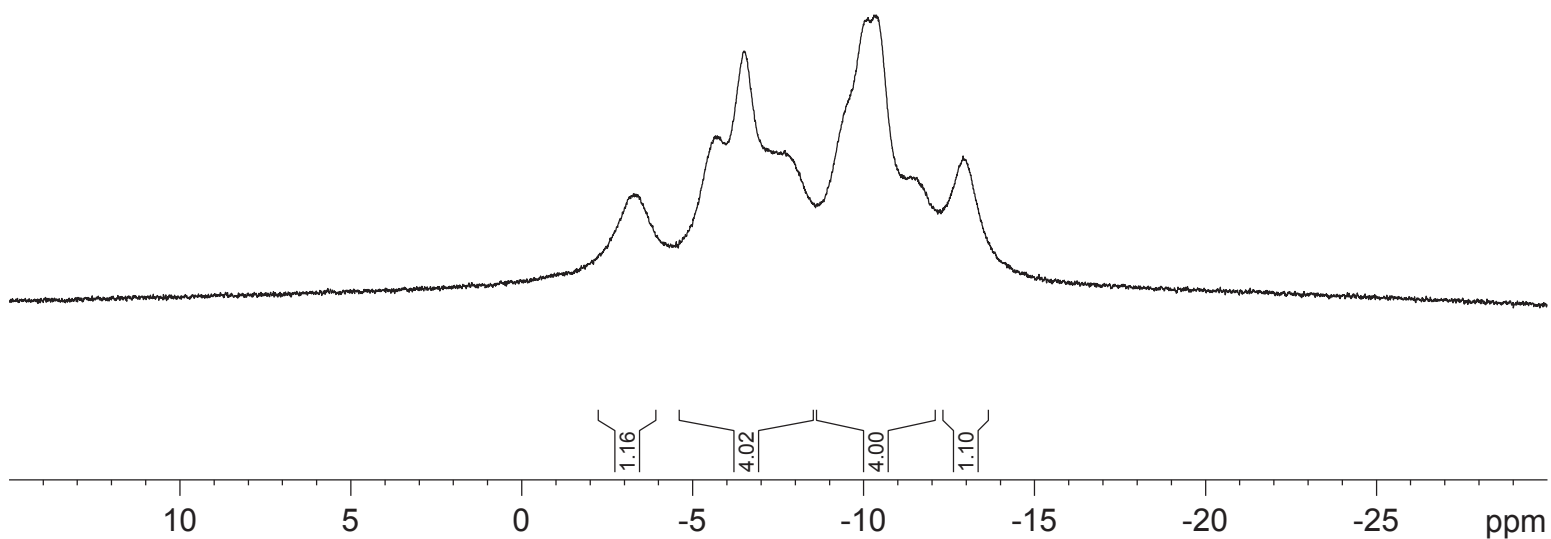
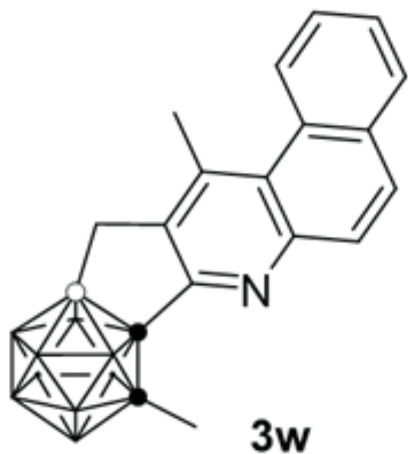
1hr-B-0735-napcascdcl3

Current Data Parameters  
NAME 1hr-B-0735-napcascdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170724  
Time 21.25 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 28  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 322  
DW 20.800 usec  
DE 6.50 usec  
TE 295.7 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 13C  
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

— -3.27  
— -5.67  
— -6.52  
— -7.75  
— -9.53  
— -10.08  
— -10.30  
— -11.51  
— -12.91



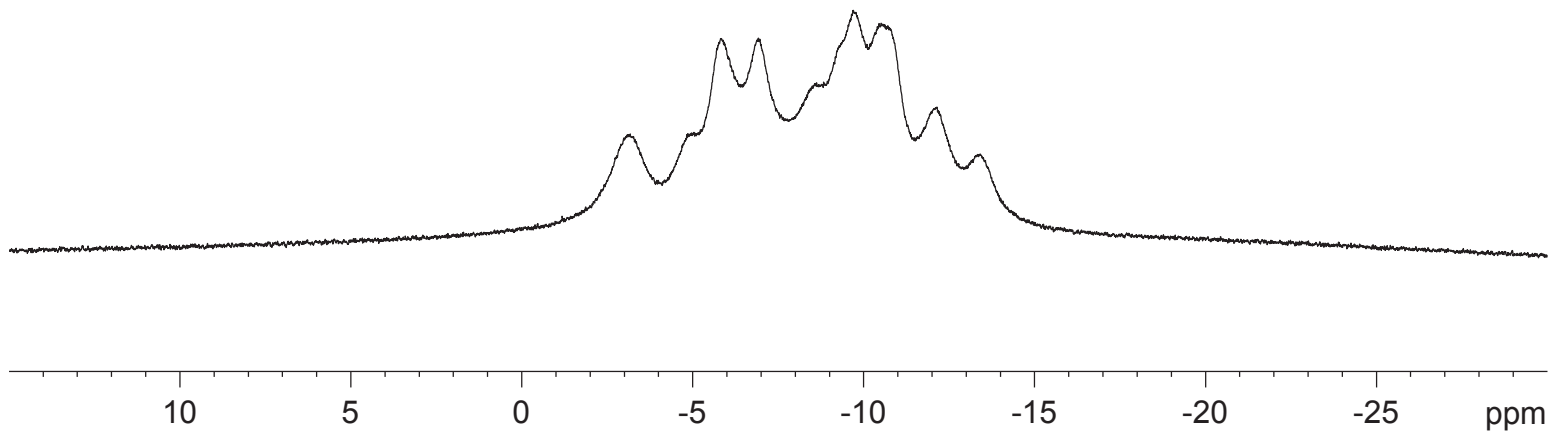
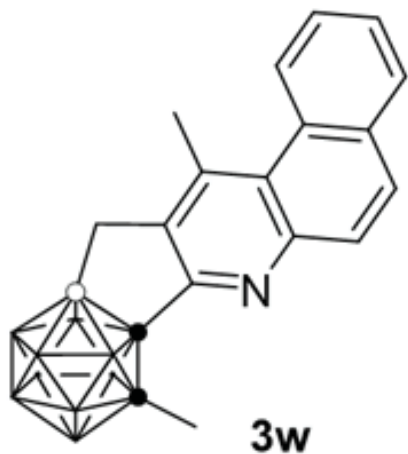
1hr-B-0735-napcascdcl3 (C)

Current Data Parameters  
NAME 1hr-B-0735-napcascdcl3 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170724  
Time 21.27 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 362  
DW 20.800 usec  
DE 6.50 usec  
TE 295.3 K  
D1 2.0000000 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

— 3.18  
— 4.86  
— 5.84  
— 6.92  
— 8.54  
— 9.21  
— 9.69  
— 10.52  
— 10.72  
— 12.15  
— 13.36





I hr-H-0748-cas1np

Current Data Parameters

NAME I hr-H-0748-cas1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170817  
Time 10.38  
INSTRUM spect  
PROBHD Z149001\_0010 (   
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 30.85  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

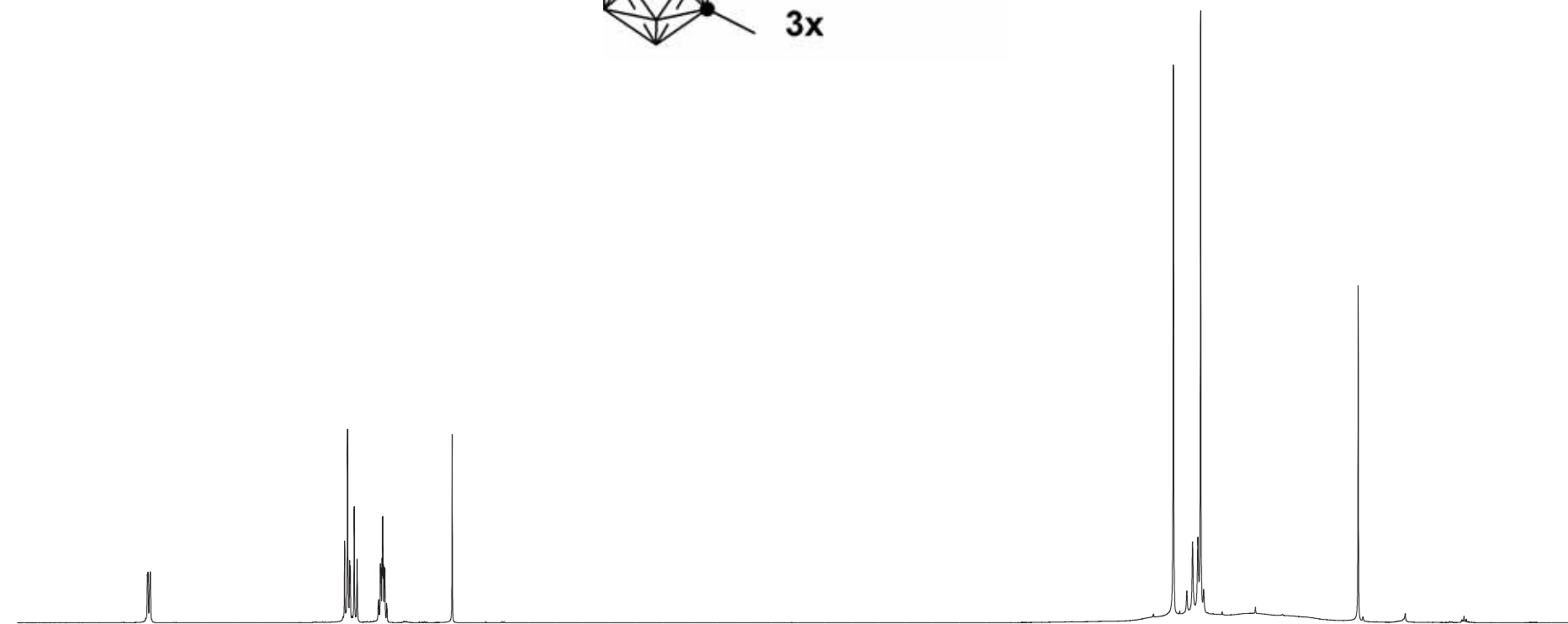
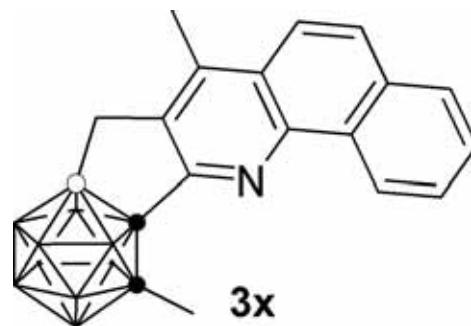
F2 - Processing parameters

SI 65536  
SF 500.1300126  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00

9.175  
9.160  
7.938  
7.919  
7.906  
7.902  
7.877  
7.859  
7.726  
7.723  
7.713  
7.709  
7.702  
7.698  
7.694  
7.687  
7.684  
7.673  
7.670  
7.260

2.717  
2.633  
2.596  
2.563  
2.546  
2.527

1.553



1.02

3.00

2.00

3.03

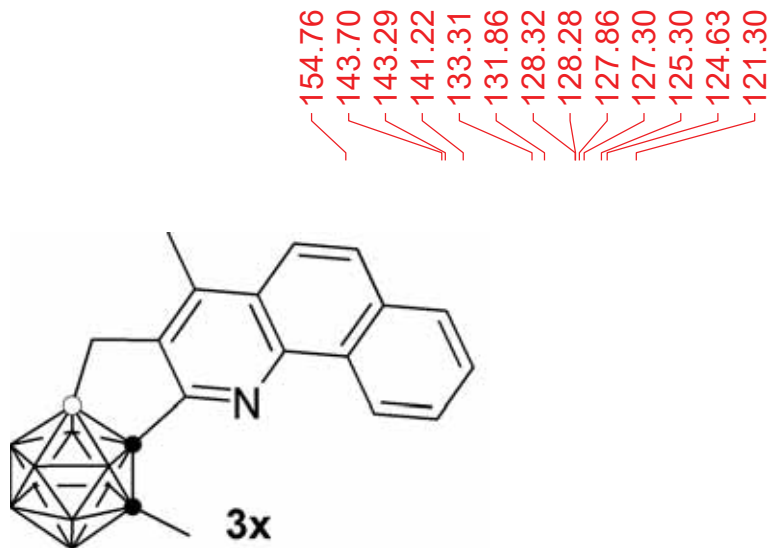
2.13

2.97

S-221

ppm

I hr-C-0748-cas1np



154.76  
143.70  
143.29  
141.22  
133.31  
131.86  
128.32  
128.28  
127.86  
127.30  
125.30  
124.63  
121.30

83.77  
77.41  
77.16  
76.91  
74.82

22.40  
15.43

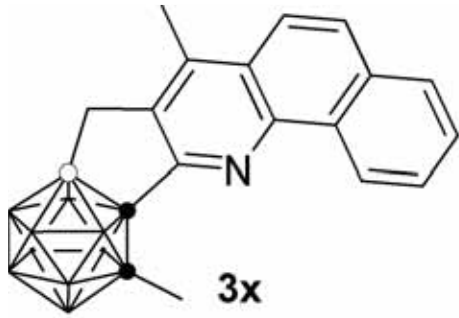
Current Data Parameters  
NAME I hr-C-0748-cas1np  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170817  
Time 11.26 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 900  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

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



I hr-B-0748-cas1np

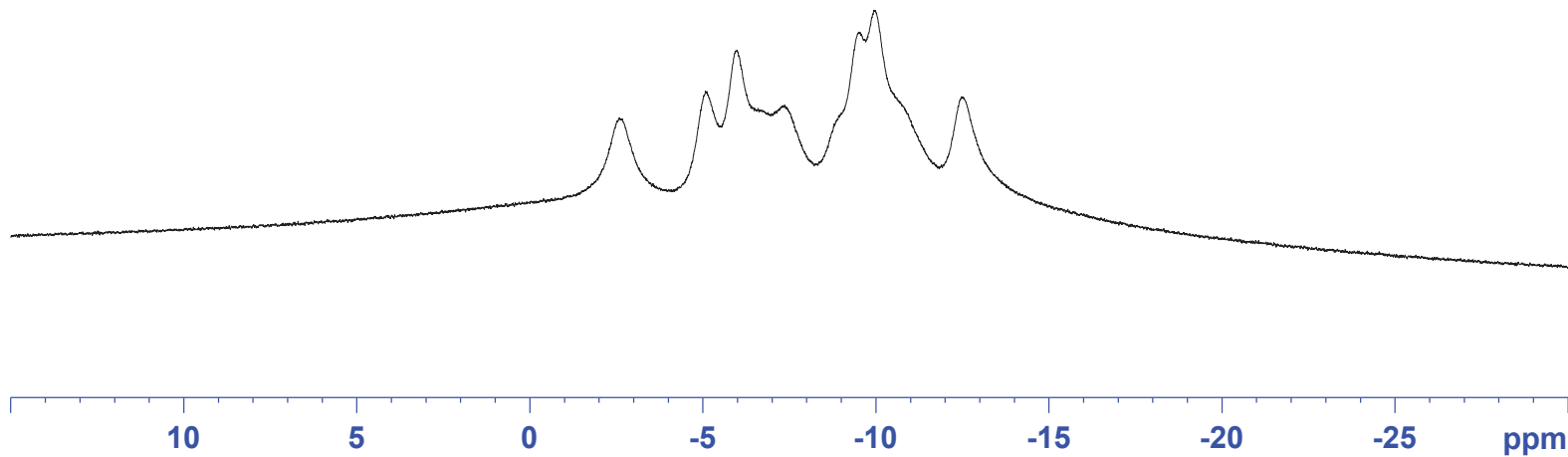


-2.57  
-5.06  
-5.98  
-6.69  
-7.32  
-8.89  
-9.93  
-10.76  
-12.47

Current Data Parameters  
NAME I hr-B-0748-cas1np  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170817  
Time 11.30 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 18  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 163.99  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

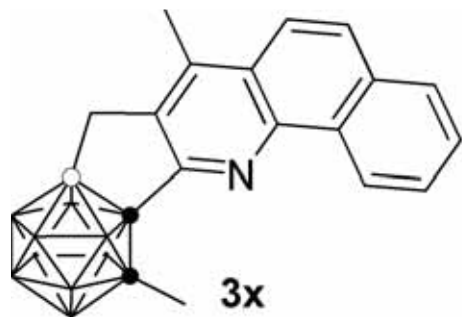
F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.03  
1.08  
2.94  
4.00  
1.04  
5.223

I hr-B-0748-cas1np(c)

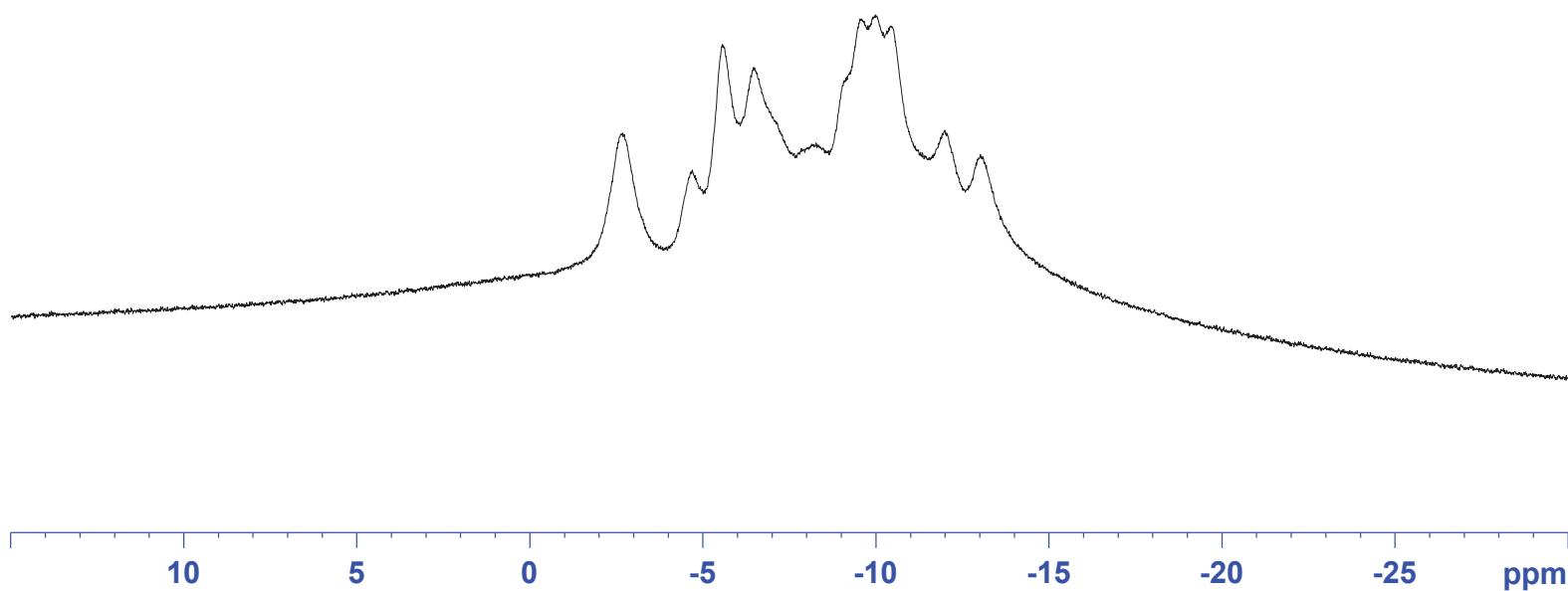
-2.68  
-4.67  
-5.56  
-6.46  
-7.09  
-7.85  
-8.26  
-9.08  
-9.53  
-9.99  
-10.44  
-12.00  
-13.01



Current Data Parameters  
NAME I hr-B-0748-cas1np(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170817  
Time 11.31 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



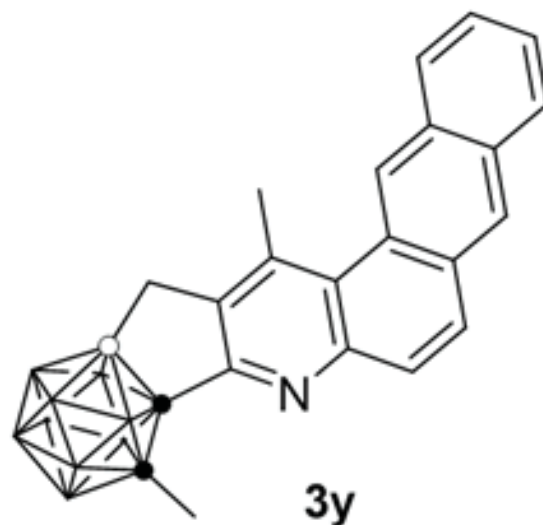
9.257  
8.445  
8.169  
8.156  
8.146  
8.103  
8.093  
8.081  
8.010  
7.987  
7.738  
7.715  
7.640  
7.628  
7.617

5.320

3.159  
2.720  
2.675  
2.632  
2.586  
2.474

1.539  
1.261

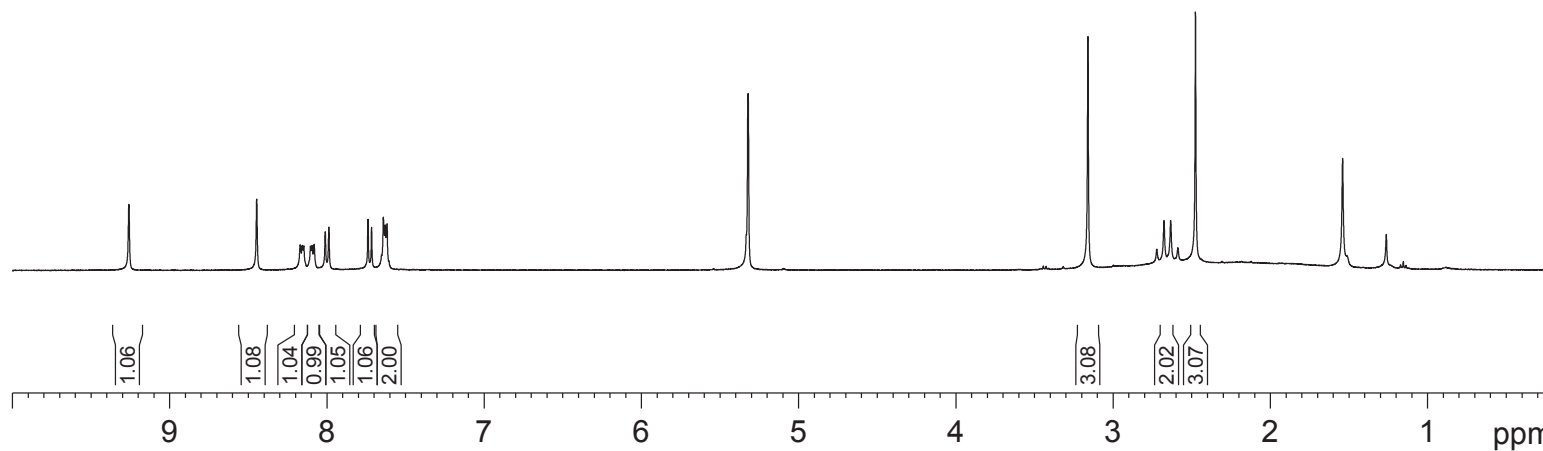
lhr-H-0756-cascdcl3



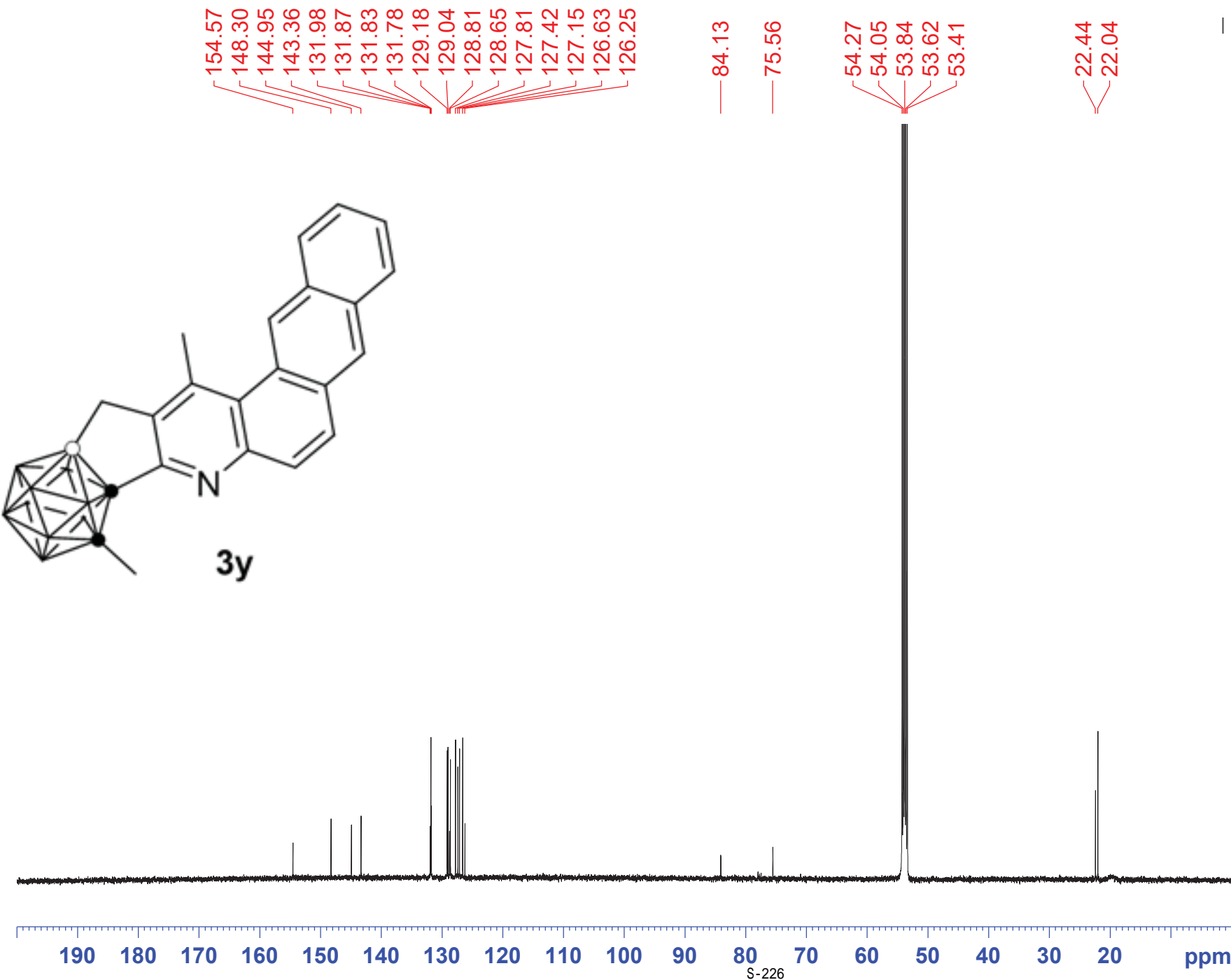
Current Data Parameters  
NAME lhr-H-0756-cascdcl3-cd  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170906  
Time\_ 9.39 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CD2Cl2  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 144  
DW 62.400 usec  
DE 6.50 usec  
TE 295.1 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters  
SI 65536  
SF 400.2300158 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



l hr-0756-re-c

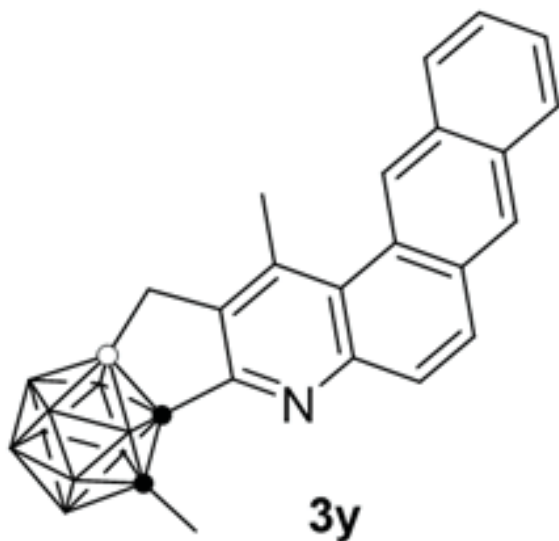


Current Data Parameters  
NAME l hr-0756-re-c  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170916  
Time 11.19 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2235  
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  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters  
SI 32768  
SF 125.7579786 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1hr-B-0756-cascdcl3-cd2cl2

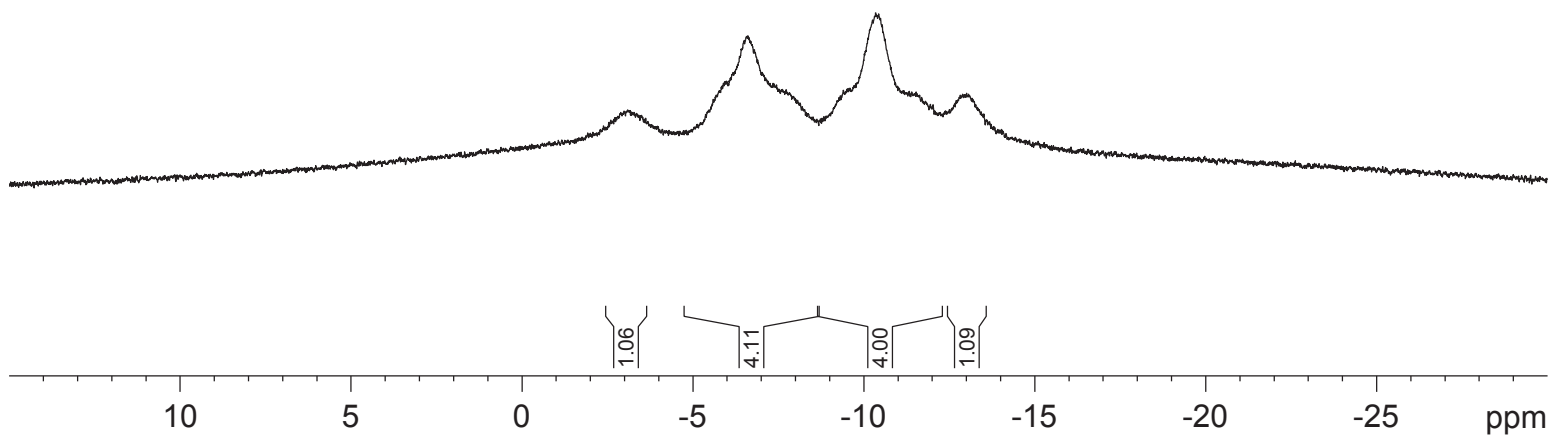


— 3.10  
— 5.94  
— 6.62  
— 7.82  
— 9.48  
— 10.35  
— 11.55  
— 13.01

Current Data Parameters  
NAME 1hr-B-0756-cascdcl3-cd2cl2  
EXPNO 1  
PROCNO 1

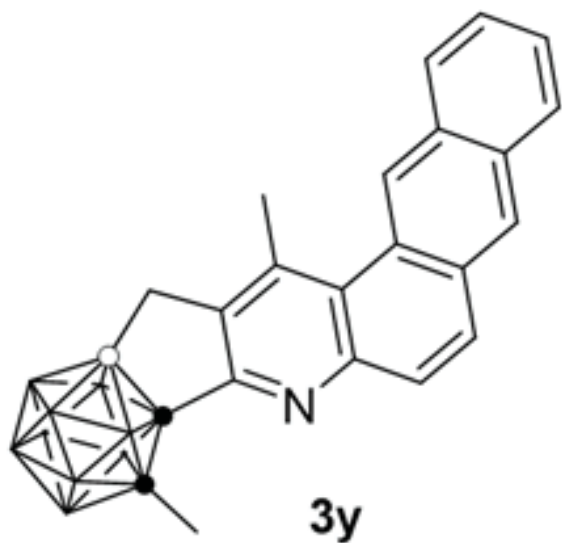
F2 - Acquisition Parameters  
Date\_ 20170830  
Time 17.05 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 40  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 575  
DW 20.800 usec  
DE 6.50 usec  
TE 295.7 K  
D1 2.0000000 sec  
D11 0.0300000 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



1hr-B-0756-cascdcl3-cd2cl2 (C)

— -2.95  
— -5.17  
— -5.97  
— -6.99  
— -8.54  
— -9.74  
— -10.79  
— -12.20  
— -13.36



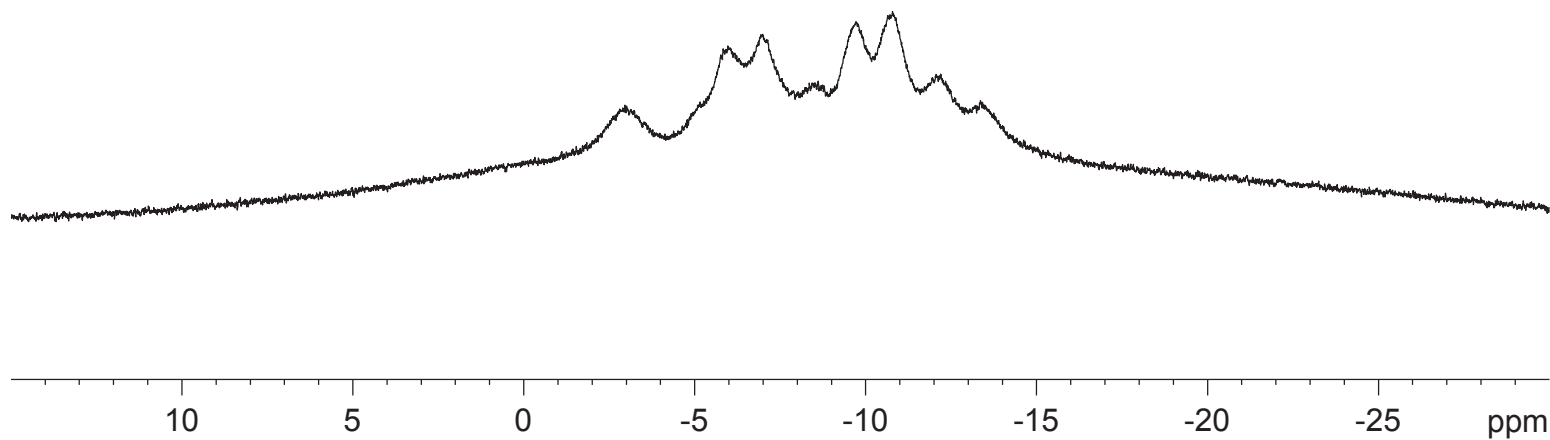
Current Data Parameters  
NAME 1hr-B-0756-cascdcl3-cd2cl2 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170830  
Time 17.09 h  
INSTRUM spect  
PROBHD Z108618\_0257 (   
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 52  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 575  
DW 20.800 usec  
DE 6.50 usec  
TE 295.5 K  
D1 2.00000000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W

F2 - Processing parameters

SI 32768  
SF 128.4097430 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



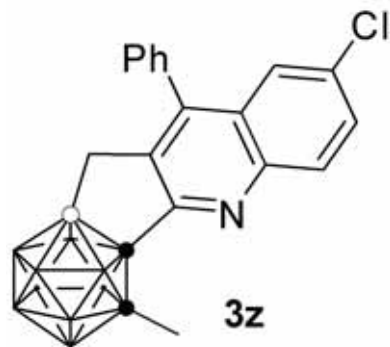


8.040  
8.018  
7.636  
7.613  
7.591  
7.584  
7.567  
7.550  
7.540  
7.536  
7.533  
7.526  
7.520  
7.500  
7.317  
7.310  
7.305  
7.296  
7.293  
7.290  
7.260

2.465  
2.401  
2.353  
2.328  
2.280  
— 1.579

Current Data Parameters  
NAME lhr-H-0889-1-cas-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180602  
Time\_ 15.42 h  
INSTRUM spect  
PROBHD Z824601\_0021 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 19  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 4.0894465 sec  
RG 161  
DW 62.400 usec  
DE 6.50 usec  
TE 297.3 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P1 15.00 usec  
PLW1 8.31000042 W



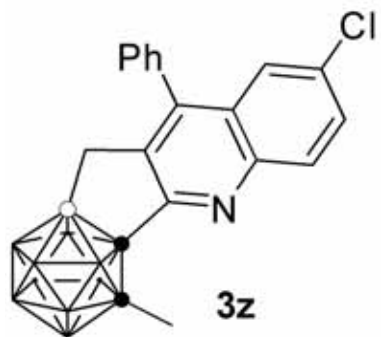
F2 - Processing parameters  
SI 65536  
SF 400.1300098 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

1.00  
1.03  
4.02  
2.02

3.13  
2.11



3z

157.139  
 146.837  
 144.635  
 140.494  
 135.436  
 133.376  
 131.422  
 130.272  
 129.122  
 129.080  
 128.819  
 127.894  
 124.911

82.826  
 77.477  
 77.160  
 76.842  
 75.444

22.317

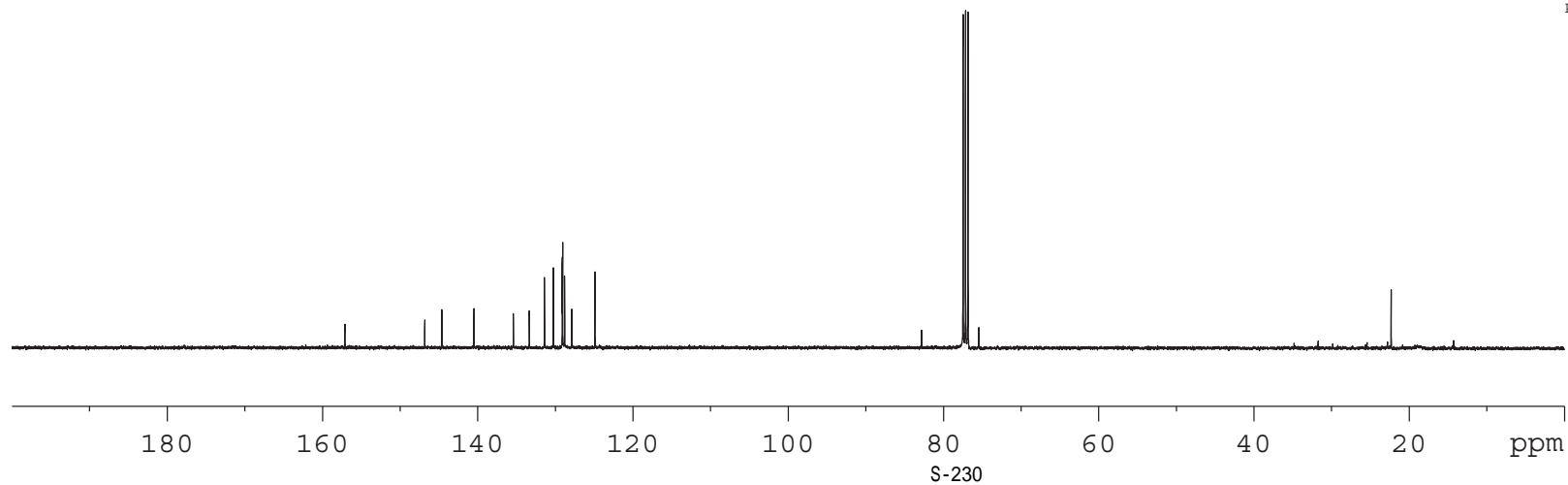
1hr-C-0889-1-cas-cdcl3

Bruker Advance III 400

Current Data Parameters  
 NAME 1hr-C-0889-1-cas-cdcl3  
 EXPNO 1  
 PROCNO 1

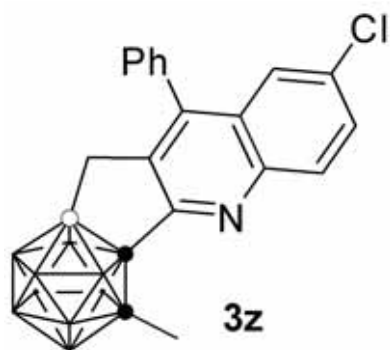
F2 - Acquisition Parameters  
 Date\_ 20180602  
 Time 17.07 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1330  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 203  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P1 9.50 usec  
 PLW1 41.25000000 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 8.31000042 W  
 PLW12 0.23083000 W  
 PLW13 0.11611000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127551 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



1hr-B-0889-1-cas-cdcl3

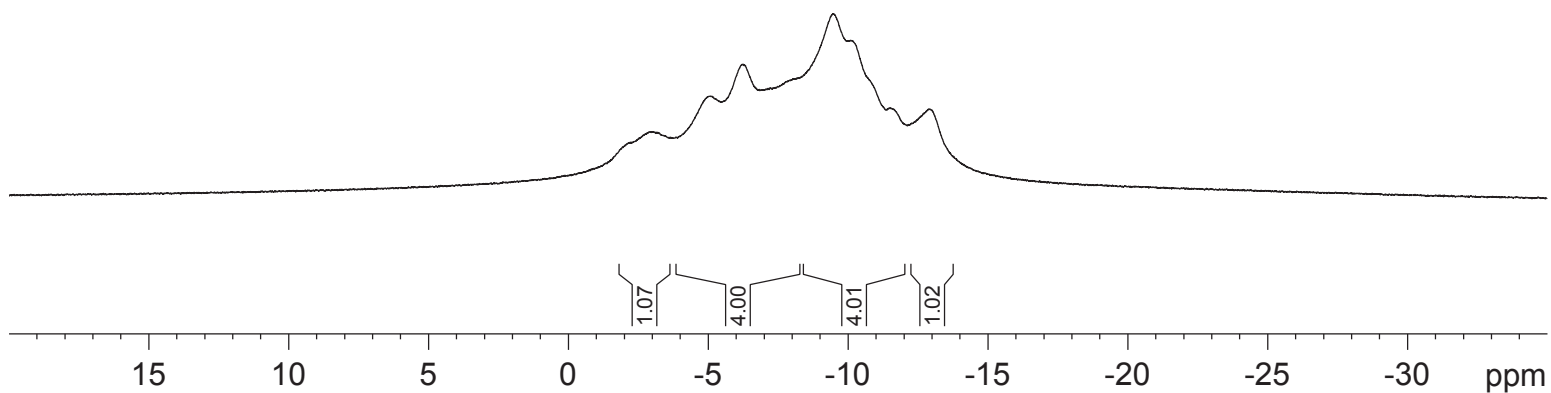
— 2.96  
— 5.00  
— 6.26  
— 7.87  
— 9.47  
— 10.17  
— 10.75  
— 11.50  
— 12.93



Current Data Parameters  
NAME 1hr-B-0889-1-cas-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180603  
Time 16.26 h  
INSTRUM spect  
PROBHD Z108618\_0257 ( )  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 68  
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 294.5 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



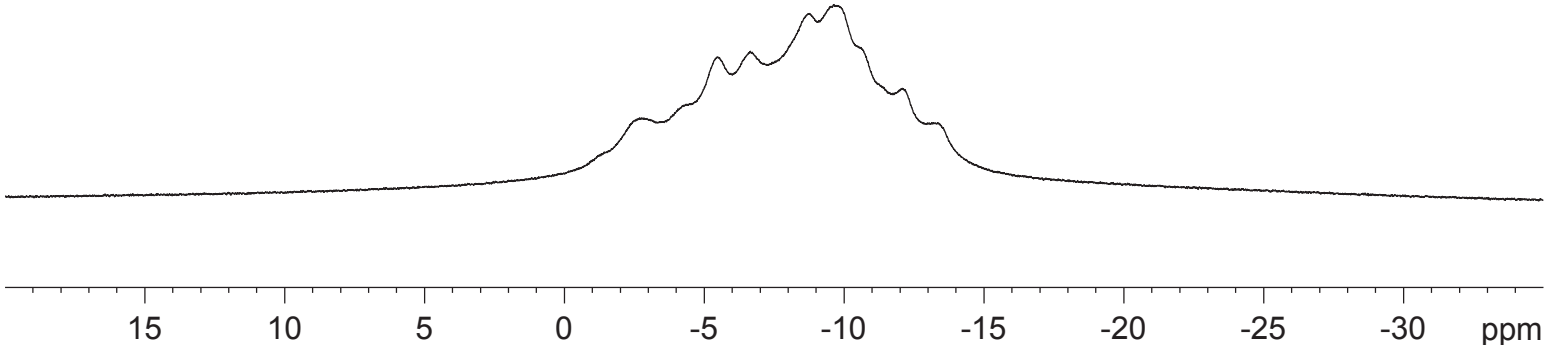
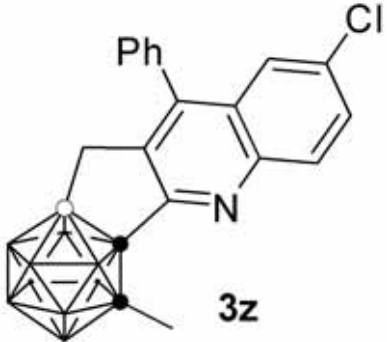
1hr-B-0889-1-cas-cdcl3 (C)

Current Data Parameters  
NAME 1hr-B-0889-1-cas-cdcl3 (C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180603  
Time 16.32 h  
INSTRUM spect  
PROBHD Z108618\_0257 ( )  
PULPROG zg  
TD 65536  
SOLVENT CDCl3  
NS 51  
DS 2  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 322  
DW 20.800 usec  
DE 6.50 usec  
TE 294.4 K  
D1 2.00000000 sec  
TD0 1  
SFO1 128.4096890 MHz  
NUC1 11B  
P1 7.50 usec  
PLW1 55.09999847 W

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

— -2.55  
— -4.29  
— -5.48  
— -6.65  
— -8.70  
— -9.64  
— -10.67  
— -12.00  
— -13.28

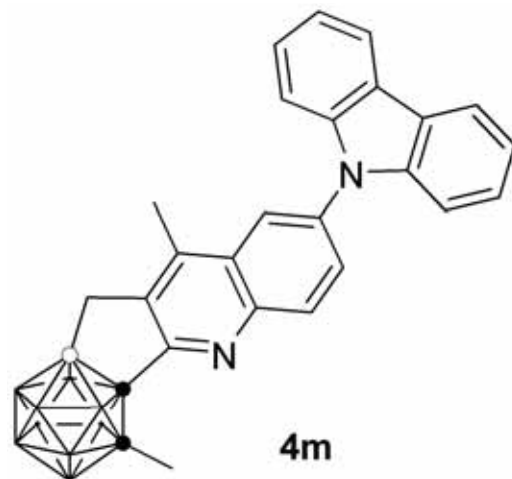


8.283  
8.266  
8.230  
8.204  
8.188  
7.911  
7.893  
7.469  
7.453  
7.440  
7.424  
7.357  
7.343  
7.329  
7.260

2.661  
2.642  
2.605  
2.565  
2.529  
2.494

1.601

I hr-H-0770-2



Current Data Parameters  
NAME I hr-H-0770-2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170928  
Time 10.36  
INSTRUM spect  
PROBHD Z149001\_0010 (4  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 30.85  
DW 50.000  
DE 10.00  
TE 288.5  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300126  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00



1.03  
0.97  
2.01  
1.00  
4.06  
2.02

3.12  
2.11  
3.06

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

I hr-C-0770-2

157.14  
144.62  
142.84  
140.94  
140.69  
136.41  
132.31  
128.45  
128.39  
126.32  
123.68  
121.47  
120.66  
120.51  
109.60

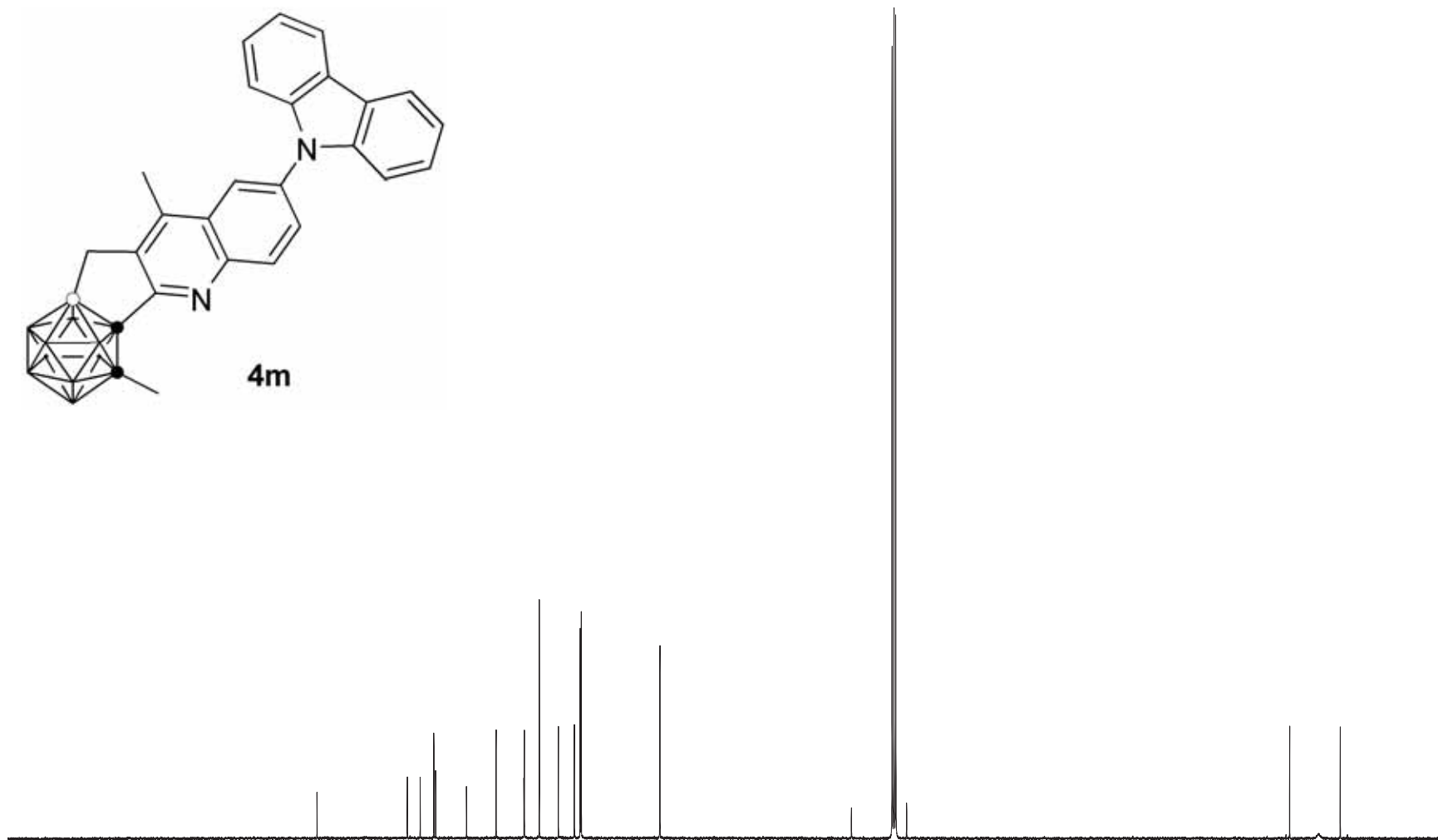
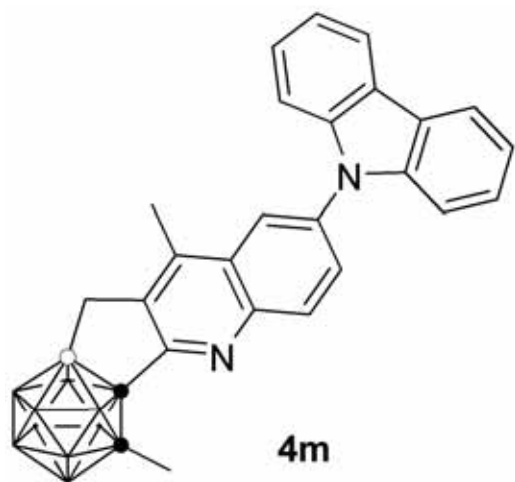
83.05  
77.41  
77.16  
76.91  
75.40

22.30  
18.29  
15.28

Current Data Parameters  
NAME I hr-C-0770-2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170928  
Time 10.56 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 360  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 288.5 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

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



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

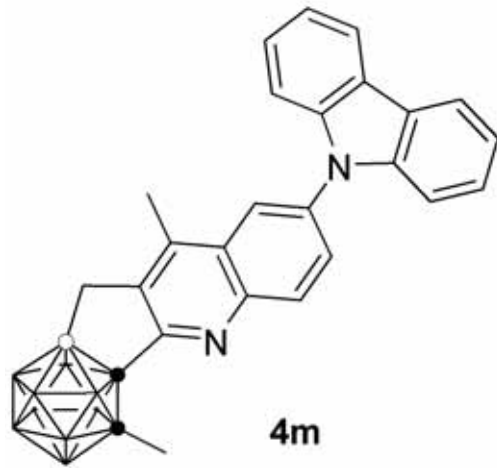
S-234

1 hr-B-0770-2

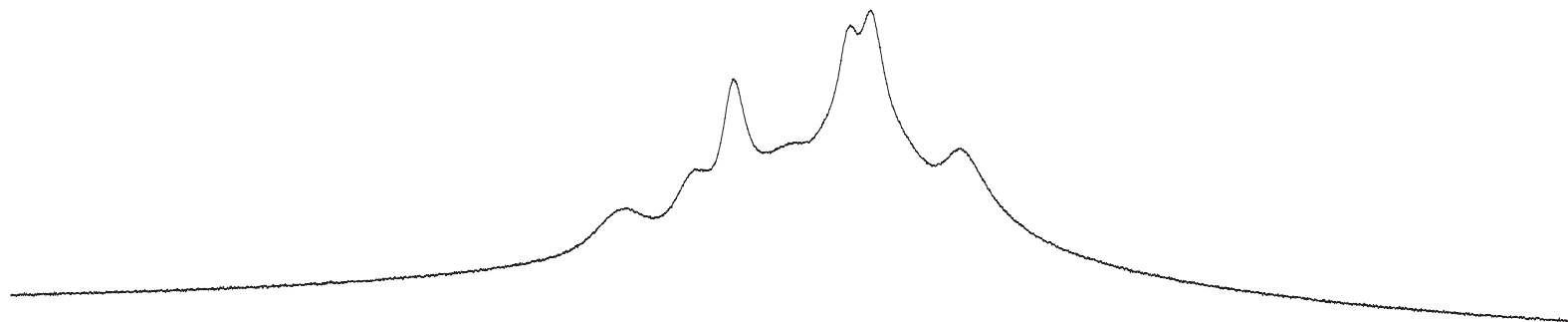
Current Data Parameters  
NAME 1 hr-B-0770-2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170928  
Time 10.59 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 20  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 163.99  
DW 21.000 usec  
DE 18.00 usec  
TE 288.5 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



-2.64  
-4.72  
-5.88  
-7.49  
-9.20  
-9.84  
-12.44



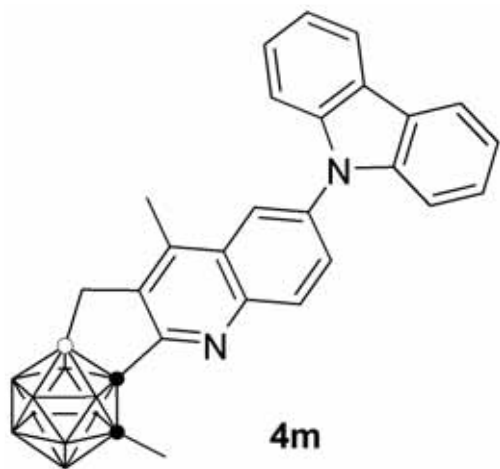
10 5 0 -5 -10 -15 -20 -25 ppm

1.19 4.02 4.00 1.09

S 235

l hr-B-0770-2(c)

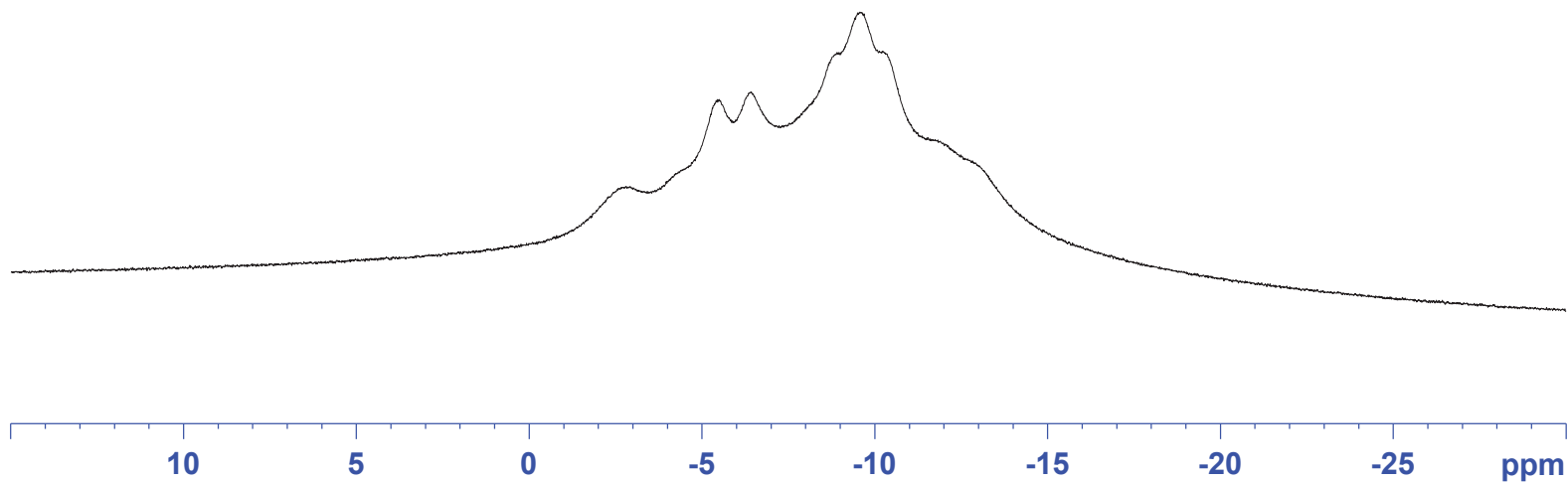
-2.71  
-4.23  
-5.44  
-6.42  
-8.00  
-8.76  
-9.56  
-10.32  
-11.85  
-12.90



Current Data Parameters  
NAME l hr-B-0770-2(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170928  
Time 11.00 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 288.5 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



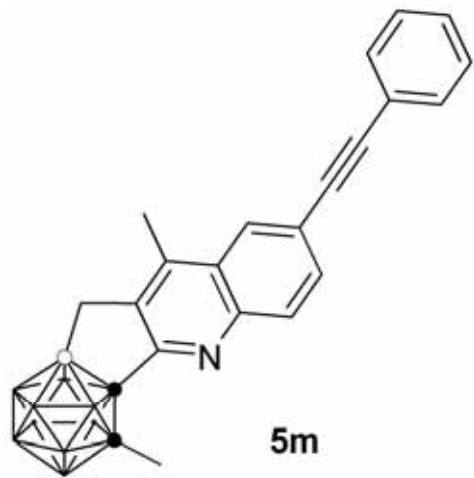


8.193  
8.190  
7.998  
7.977  
7.796  
7.792  
7.774  
7.770  
7.610  
7.600  
7.591  
7.586  
7.406  
7.396  
7.392  
7.384  
7.379  
7.260

2.667  
2.597  
2.551  
2.517  
2.471  
2.437

1.571

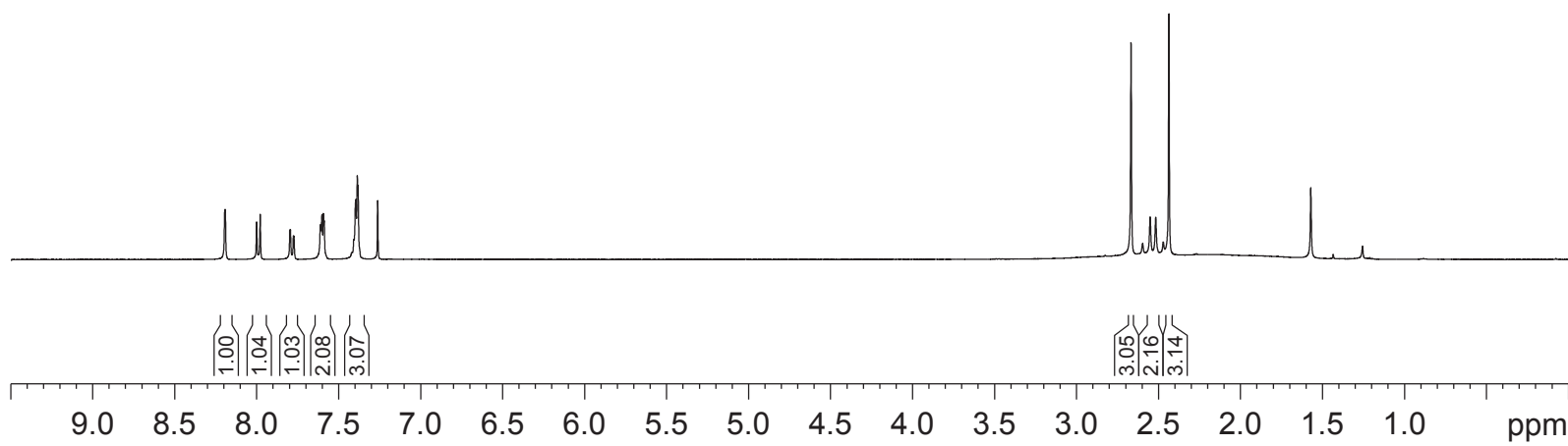
lhr-H-0770-3-cdcl3

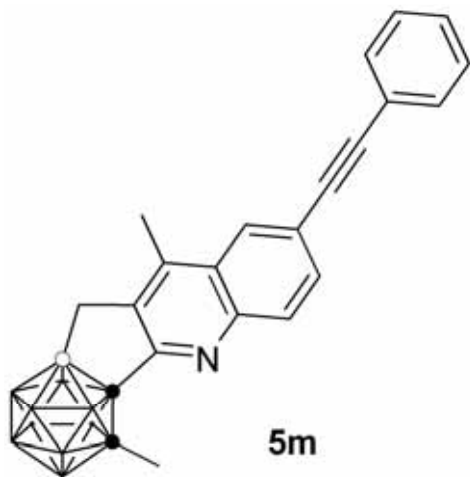


Current Data Parameters  
NAME lhr-H-0770-3-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170930  
Time\_ 19.10 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 203  
DW 62.400 usec  
DE 6.50 usec  
TE 295.3 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 400.2300098 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





157.08  
 145.23  
 142.67  
 140.49  
 131.86  
 131.79  
 130.45  
 128.82  
 128.62  
 127.40  
 127.26  
 122.98  
 122.18

91.01  
 89.44  
 83.13  
 77.48  
 77.16  
 76.84  
 75.41

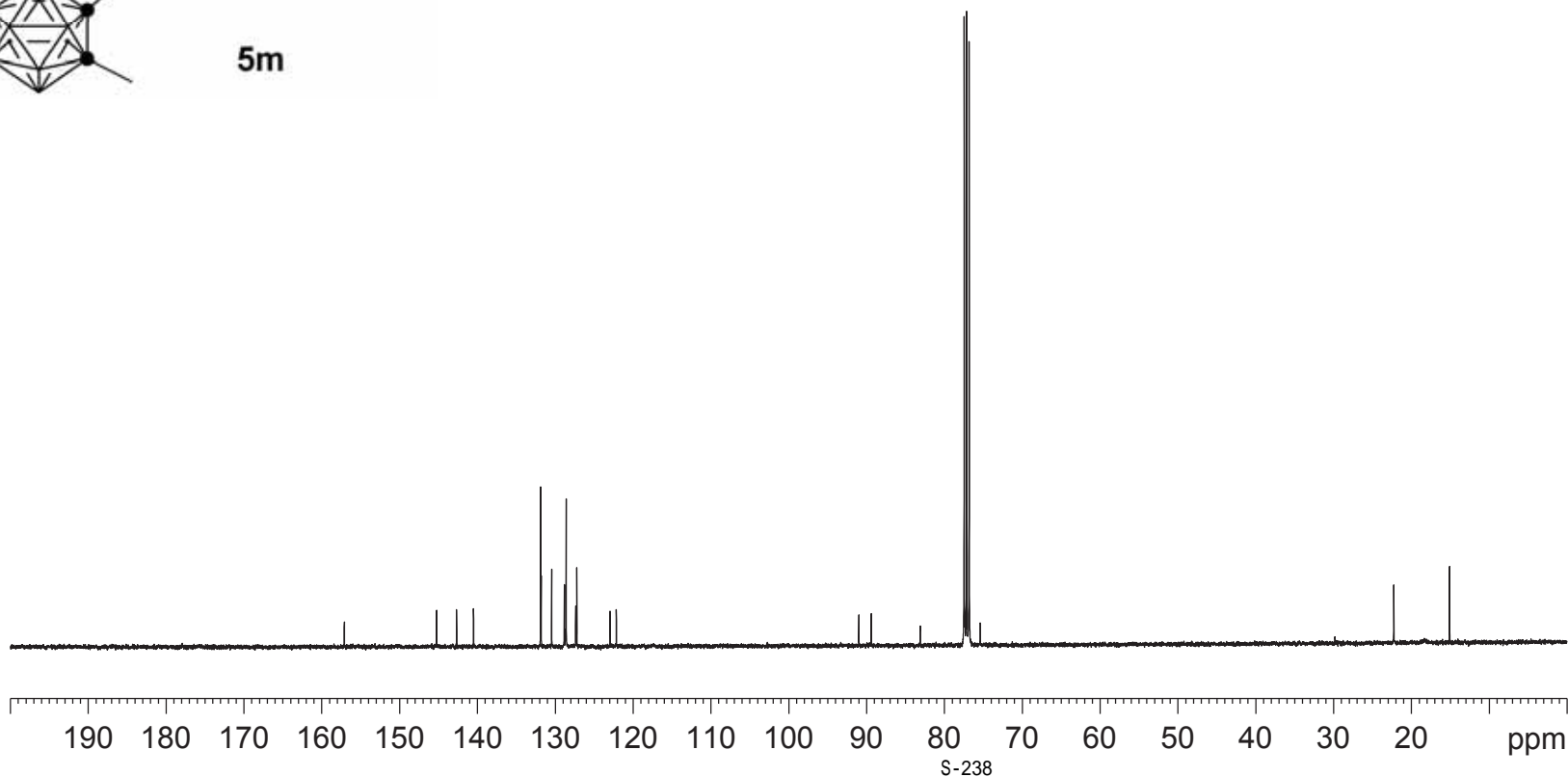
22.28  
 15.11

lhr-C-0770-3-cdcl3

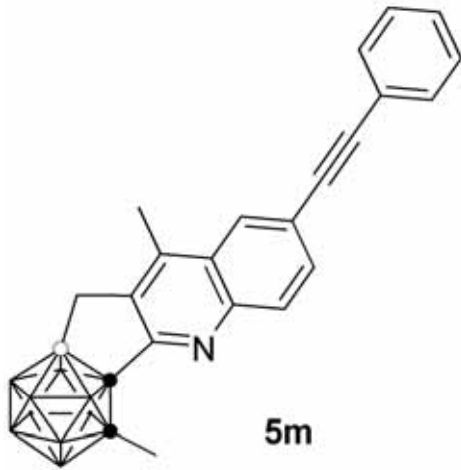
Current Data Parameters  
 NAME lhr-C-0770-3-cdcl3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170930  
 Time 19.13 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1467  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.454131 Hz  
 AQ 1.1010048 sec  
 RG 203  
 DW 16.800 usec  
 DE 6.50 usec  
 TE 295.5 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 100.6379009 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



I hr-B-0770-3

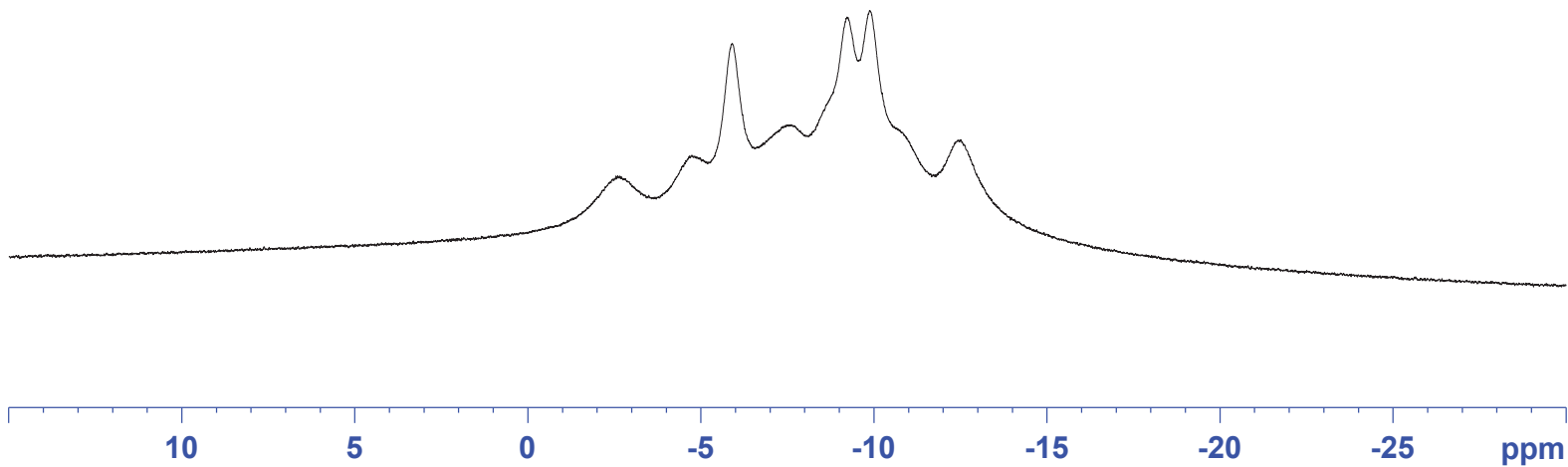


-2.60  
-4.70  
-5.88  
-7.52  
-8.67  
-9.21  
-9.86  
-10.71  
-12.48

Current Data Parameters  
NAME I hr-B-0770-3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170930  
Time 10.35 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 163.99  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

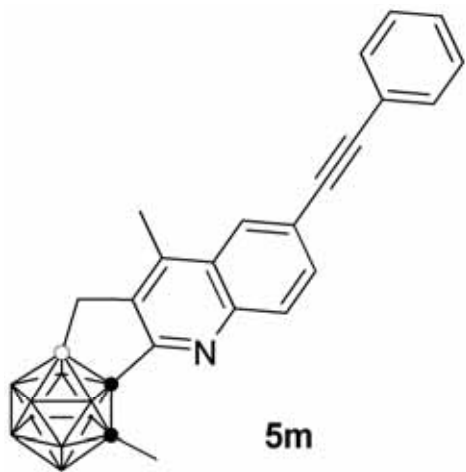
F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



1.08  
1.01  
3.00  
1.94  
2.20  
1.34  
5.239

I hr-B-0770-3(c)

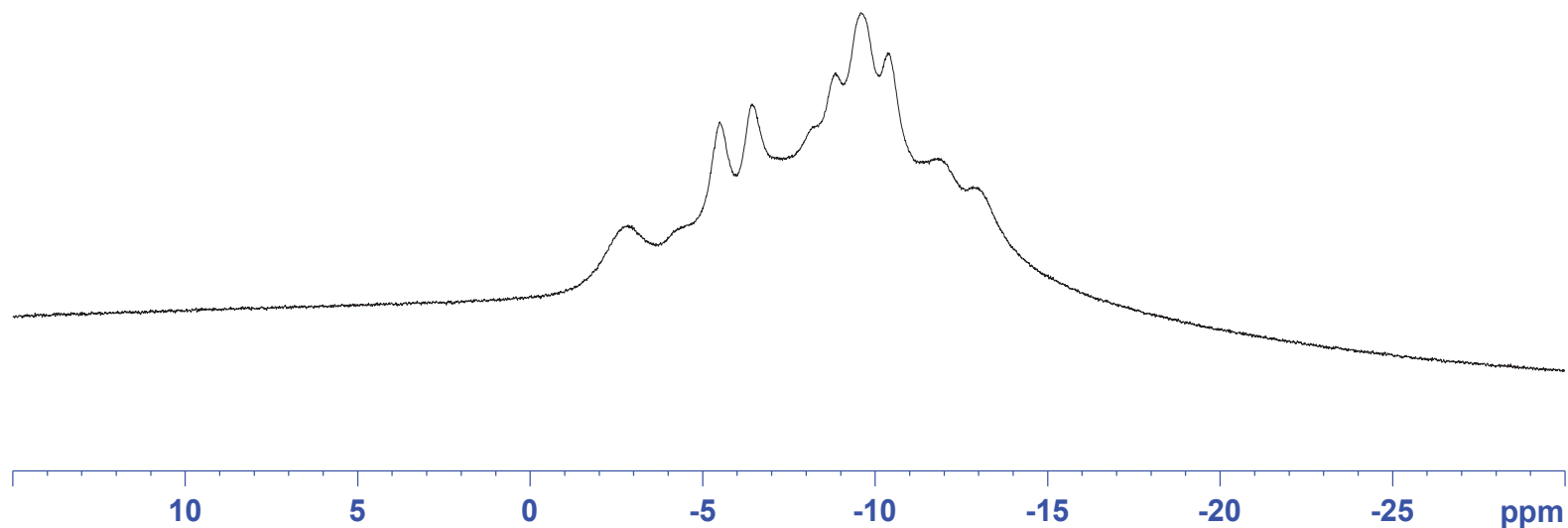
-2.83  
-4.19  
-5.49  
-6.43  
-8.10  
-8.86  
-9.59  
-10.36  
-11.89  
-12.92



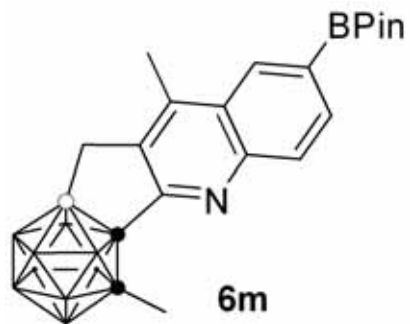
Current Data Parameters  
NAME I hr-B-0770-3(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170930  
Time 10.36 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



8.497  
8.053  
8.036  
8.001  
7.984  
7.260



2.710  
2.580  
2.543  
2.505  
2.469  
2.435  
1.579  
1.399

I hr-0770-1-H

Current Data Parameters  
NAME I hr-0770-1-H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170926  
Time 15.01  
INSTRUM spect  
PROBHD Z149001\_0010 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 12  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 56.83  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300125  
WDW EM  
SSB 0  
LB 0.30  
GB 0  
PC 1.00



1.02

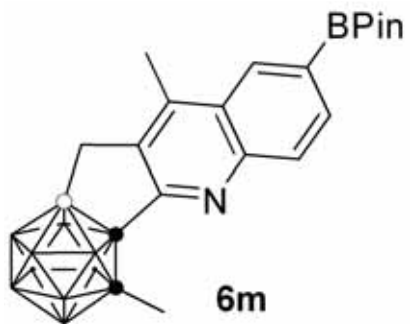
2.04

3.00

2.10

3.07

12.00



157.40  
147.36  
143.75  
139.75  
134.03  
131.76  
129.37  
126.82

84.37  
83.27  
77.41  
77.16  
76.91  
75.41

25.07  
22.28  
15.21

I hr-0770-1-C

Current Data Parameters  
NAME I hr-0770-1-C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170926  
Time 15.22 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 400  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 206.72  
DW 16.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

F2 - Processing parameters

SI 32768  
SF 125.7577717 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



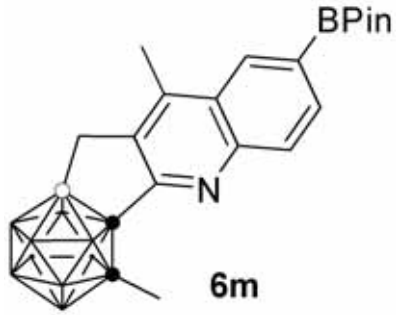
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

S-242

31.62

-2.73  
-4.90  
-5.97  
-7.56  
-8.61  
-9.27  
-9.95  
-10.84  
-12.55

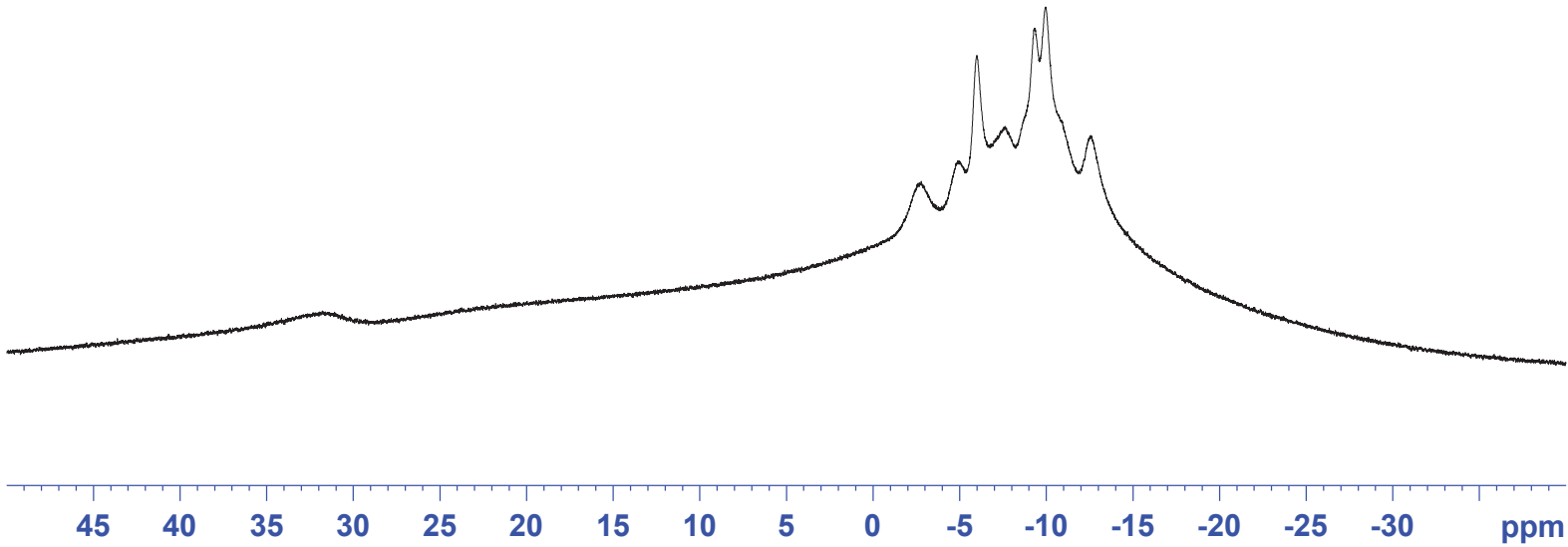
I hr-0770-1-B



Current Data Parameters  
NAME I hr-0770-1-B  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170926  
Time 15.25 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 20  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 186.15  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



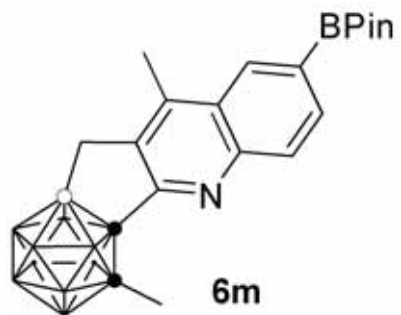
1.19

1.13  
1.02  
2.92  
4.00  
1.02

— 32.07

-2.69  
-4.46  
-5.55  
-6.49  
-8.21  
-8.92  
-9.74  
-10.40  
-11.91  
-13.05

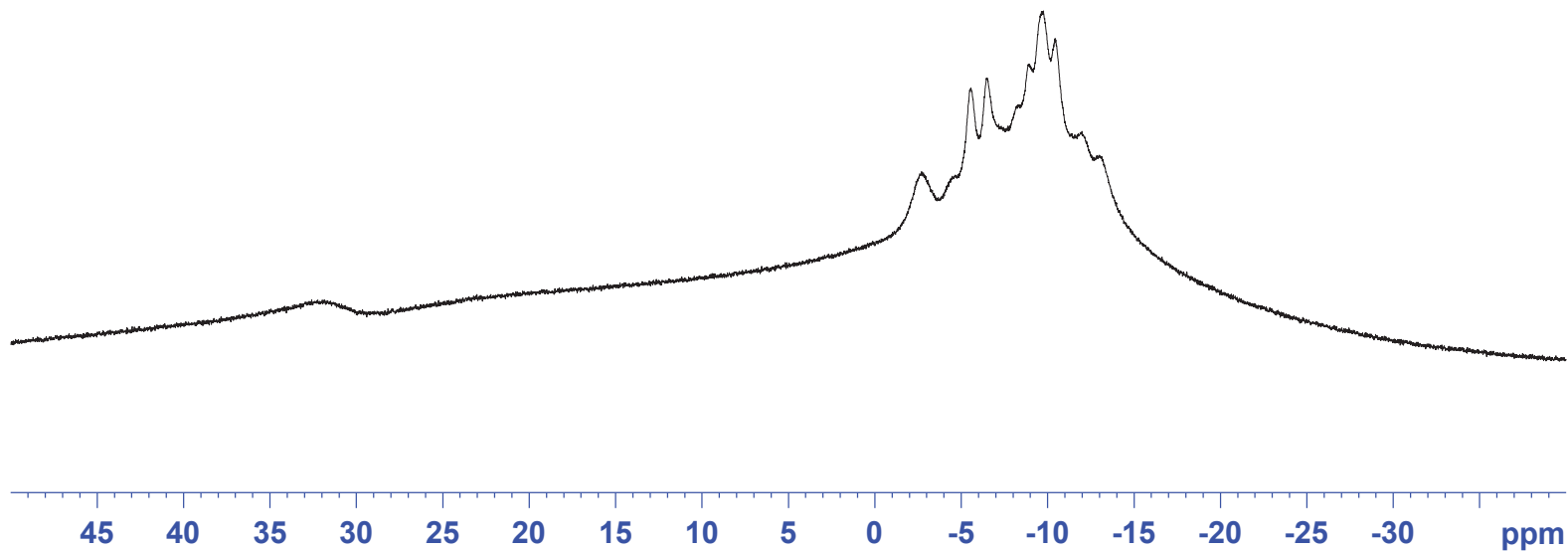
I hr-0770-1-B(c)



Current Data Parameters  
NAME I hr-0770-1-B(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170926  
Time 15.26 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



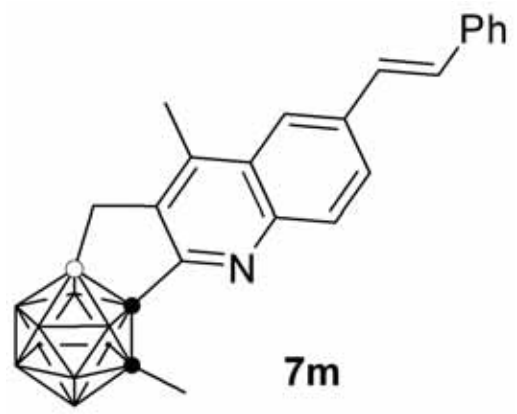


8.011  
7.990  
7.970  
7.947  
7.593  
7.574  
7.422  
7.403  
7.384  
7.342  
7.326  
7.307  
7.301  
7.285  
7.260  
7.244

2.679  
2.595  
2.549  
2.514  
2.467  
2.442

1.577

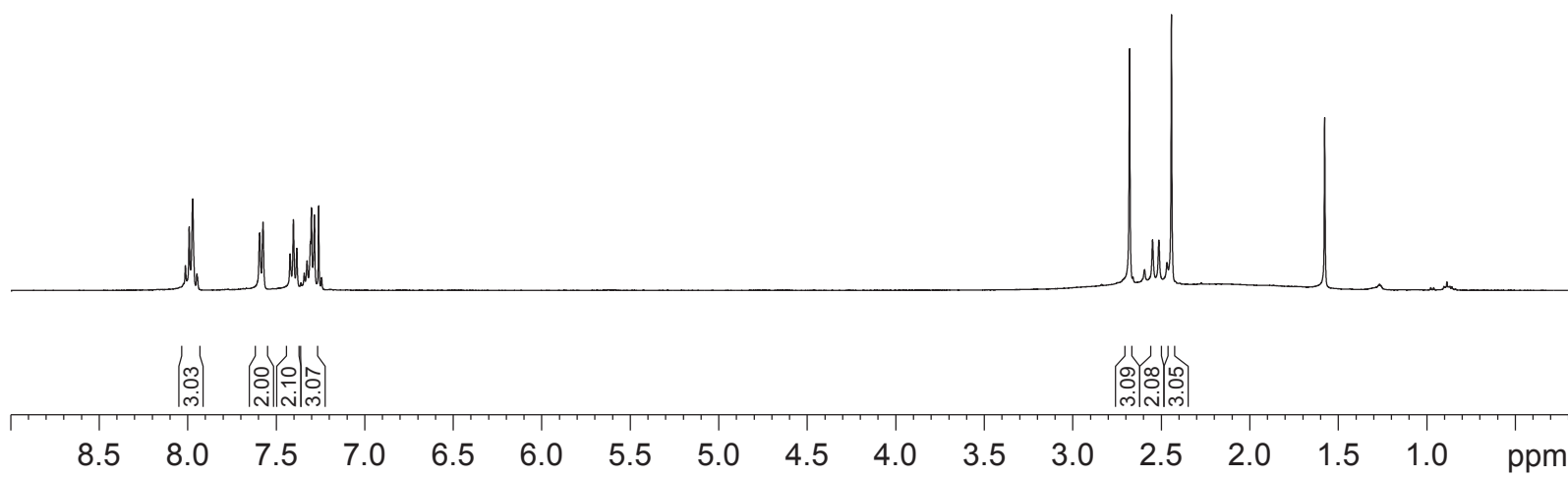
lhr-H-0770-10-cc-cdc

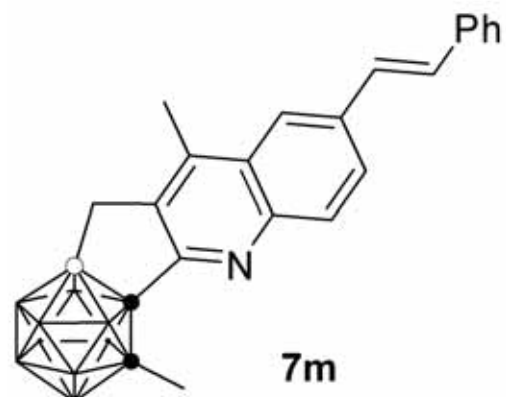


Current Data Parameters  
NAME lhr-H-0770-10-cc-cdcl3  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171009  
Time 14.25 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 144  
DW 62.400 usec  
DE 6.50 usec  
TE 294.8 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 400.2300103 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





156.21  
145.55  
142.72  
140.25  
137.07  
136.22  
130.68  
130.45  
128.96  
128.29  
128.23  
127.84  
126.82  
126.60  
122.30

83.36  
77.41  
77.16  
76.91  
75.34

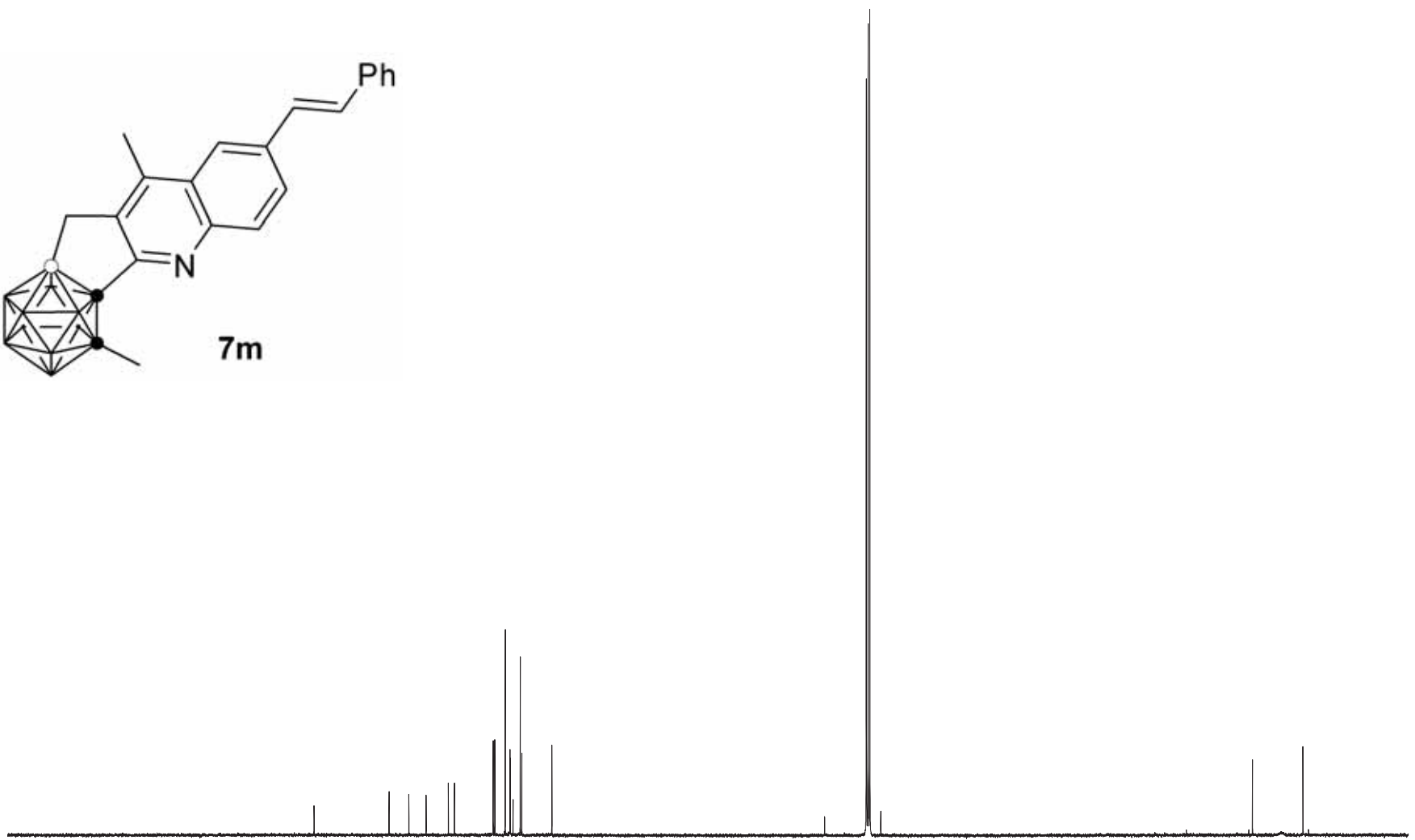
22.29  
15.09

I hr-C-0770-10

Current Data Parameters  
NAME I hr-C-0770-10  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171009  
Time 19.17 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 396  
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  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

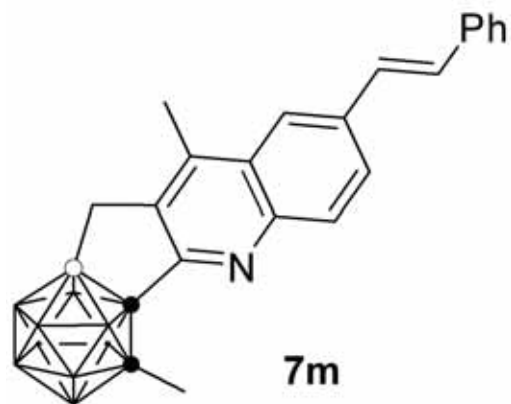
F2 - Processing parameters  
SI 32768  
SF 125.7577723 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



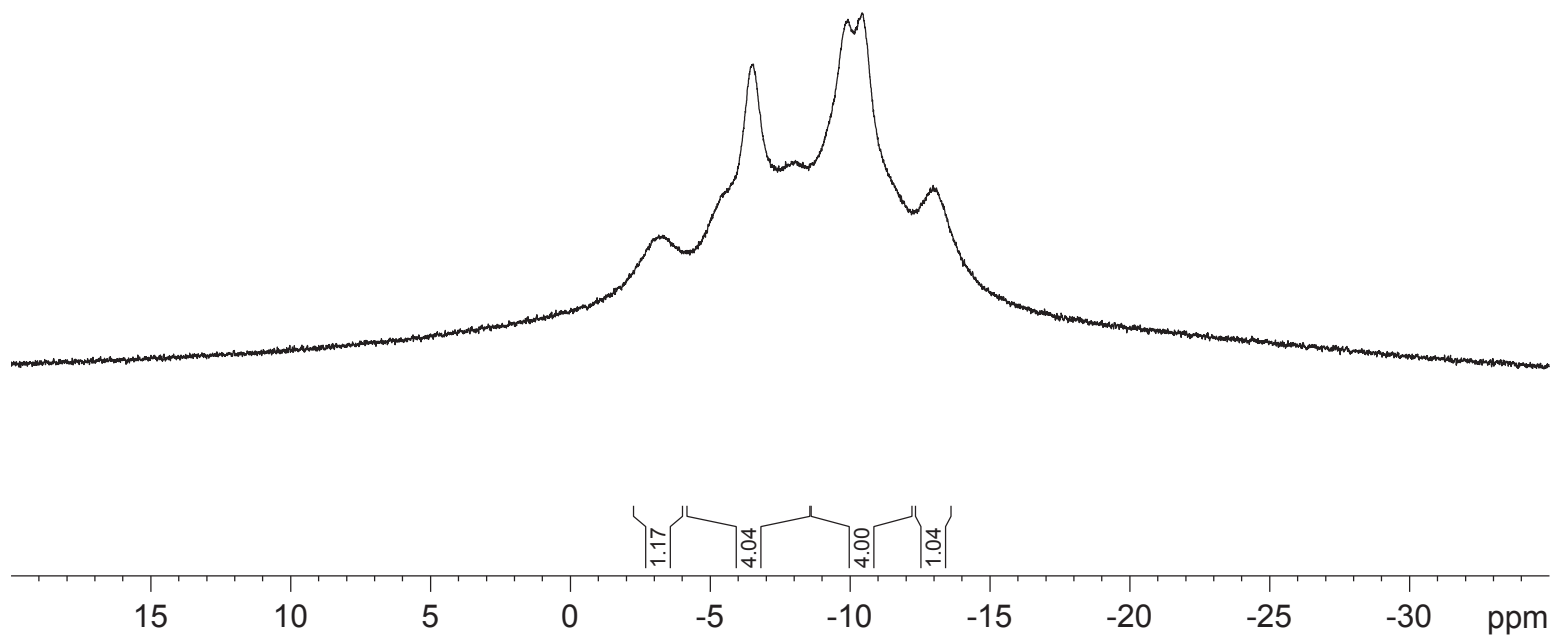
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

S-246

1hr-B-0770-10-cc-cdcl3



— 3.13  
— 5.43  
— 6.54  
— 8.01  
— 9.87  
— 10.43  
— 11.54  
— 12.97

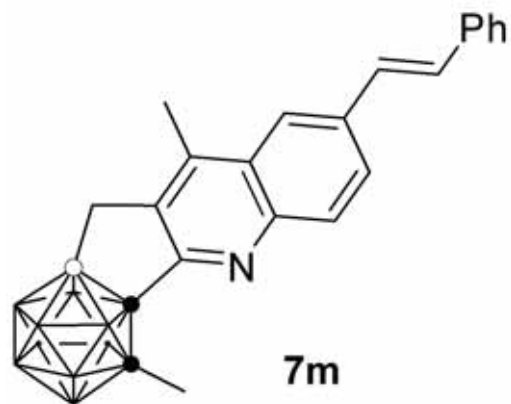


S-247

Current Data Parameters  
NAME 1hr-B-0770-10-cc-cdcl3  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171009  
Time 14.29 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 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



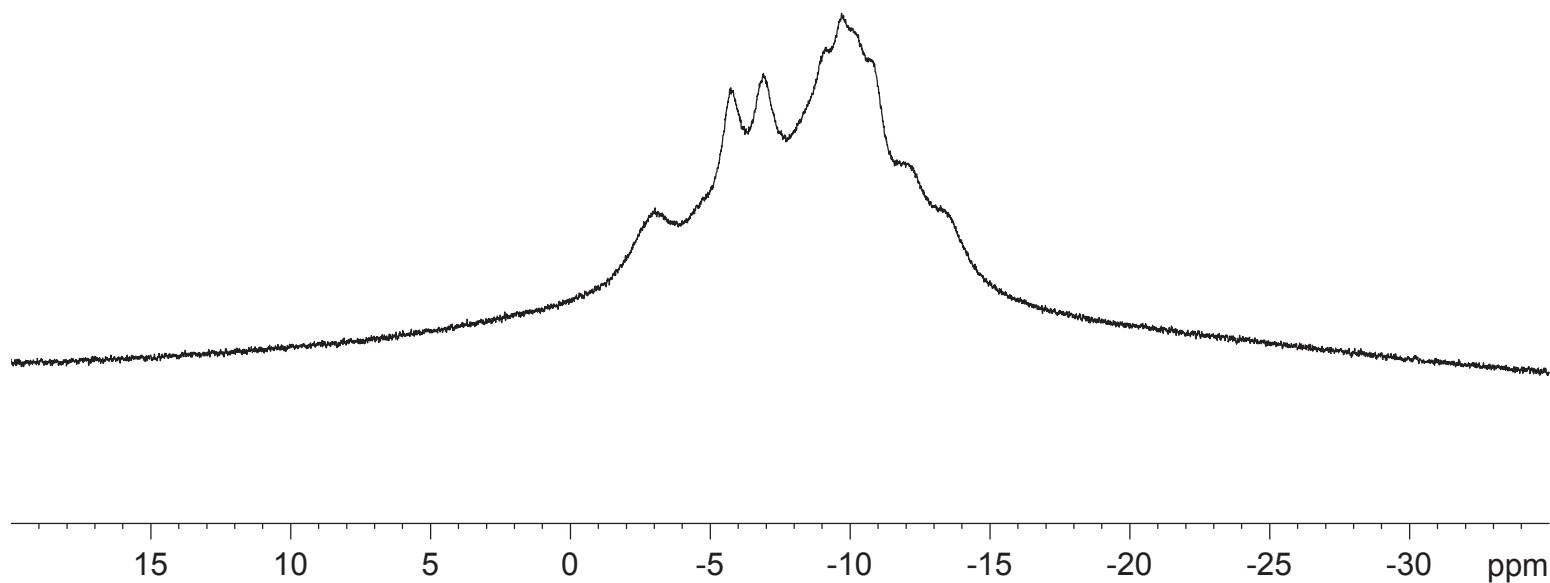
| 3.01  
 | 4.63  
 | 5.74  
 | 6.90  
 | 8.28  
 | 9.07  
 | 9.70  
 | 10.25  
 | 10.79  
 | 12.12  
 | 13.42

1hr-B-0770-10-cc-cdcl3 (C)

Current Data Parameters  
 NAME 1hr-B-0770-10-cc-cdcl3 (C)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20171009  
 Time 14.34 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (  
 PULPROG zg  
 TD 65536  
 SOLVENT CDCl3  
 NS 60  
 DS 2  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 456  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 294.9 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



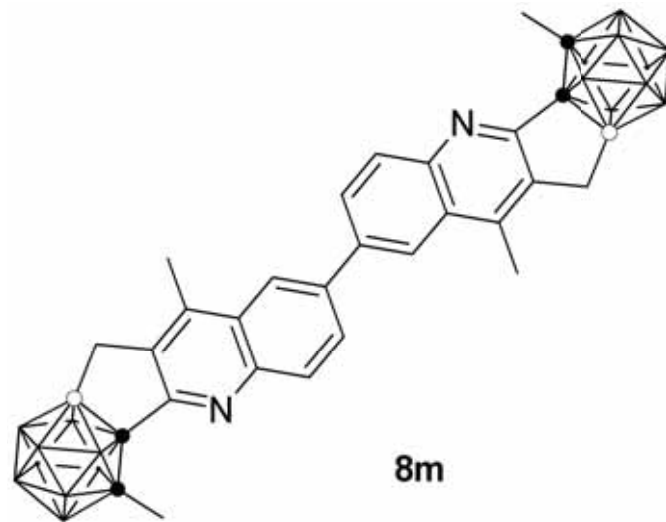
8.257  
8.168  
8.151  
8.054  
8.037

7.260

2.748  
2.627  
2.591  
2.551  
2.515  
2.464

1.562

I hr-H-0773-cc



Current Data Parameters  
NAME I hr-H-0773-cc  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171011  
Time 9.41  
INSTRUM spect  
PROBHD Z149001\_0010 (   
PULPROG zg30  
TD 65536  
SOLVENT CDCl 3  
NS 12  
DS 2  
SWH 10000.000  
FIDRES 0.305176  
AQ 3.2767999  
RG 56.83  
DW 50.000  
DE 10.00  
TE 298.0  
D1 1.00000000  
TDO 1  
SF01 500.1330883  
NUC1 1H  
P1 12.00  
PLW1 15.00000000

F2 - Processing parameters  
SI 65536  
SF 500.1300123  
WDW EM  
SSB 0  
LB 0.30  
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  
2.02  
2.03

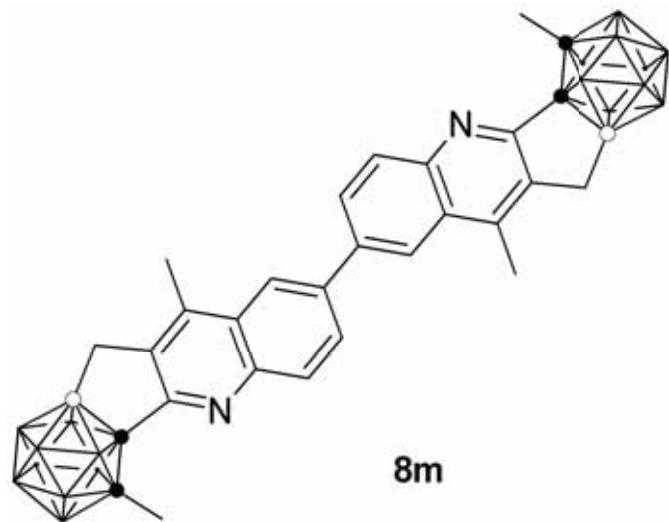
6.13  
4.06  
6.19

I hr-C-0773-cc

156.91  
145.34  
143.05  
140.49  
139.55  
131.12  
128.94  
127.79  
122.32

83.22  
77.41  
77.16  
76.91  
75.42

22.32  
15.23



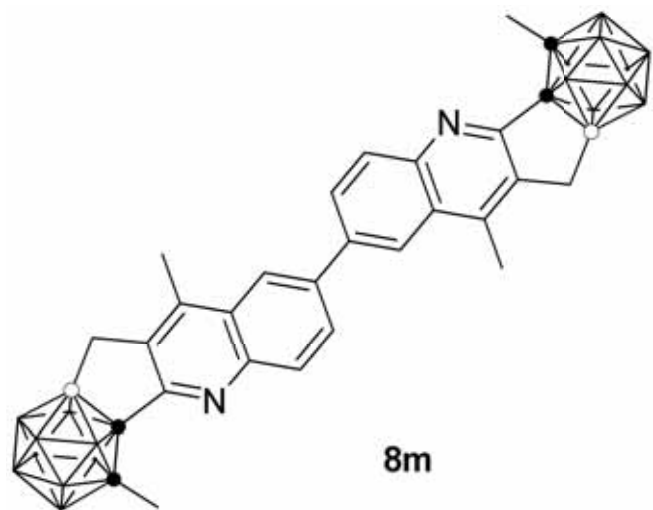
Current Data Parameters  
NAME I hr-C-0773-cc  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171011  
Time 10.24 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 781  
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  
TDO 1  
SF01 125.7703643 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 61.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] wal tz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W  
PLW13 0.16976000 W

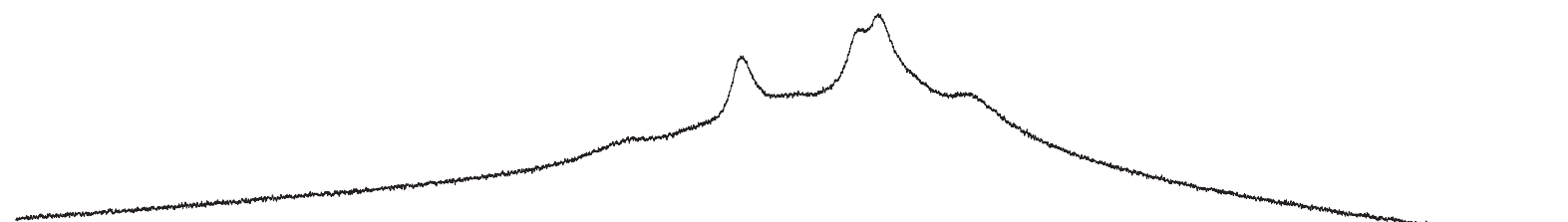
F2 - Processing parameters  
SI 32768  
SF 125.7577714 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



I hr-B-0773-cc



-2.67  
-4.36  
-5.91  
-7.49  
-9.88  
-12.17



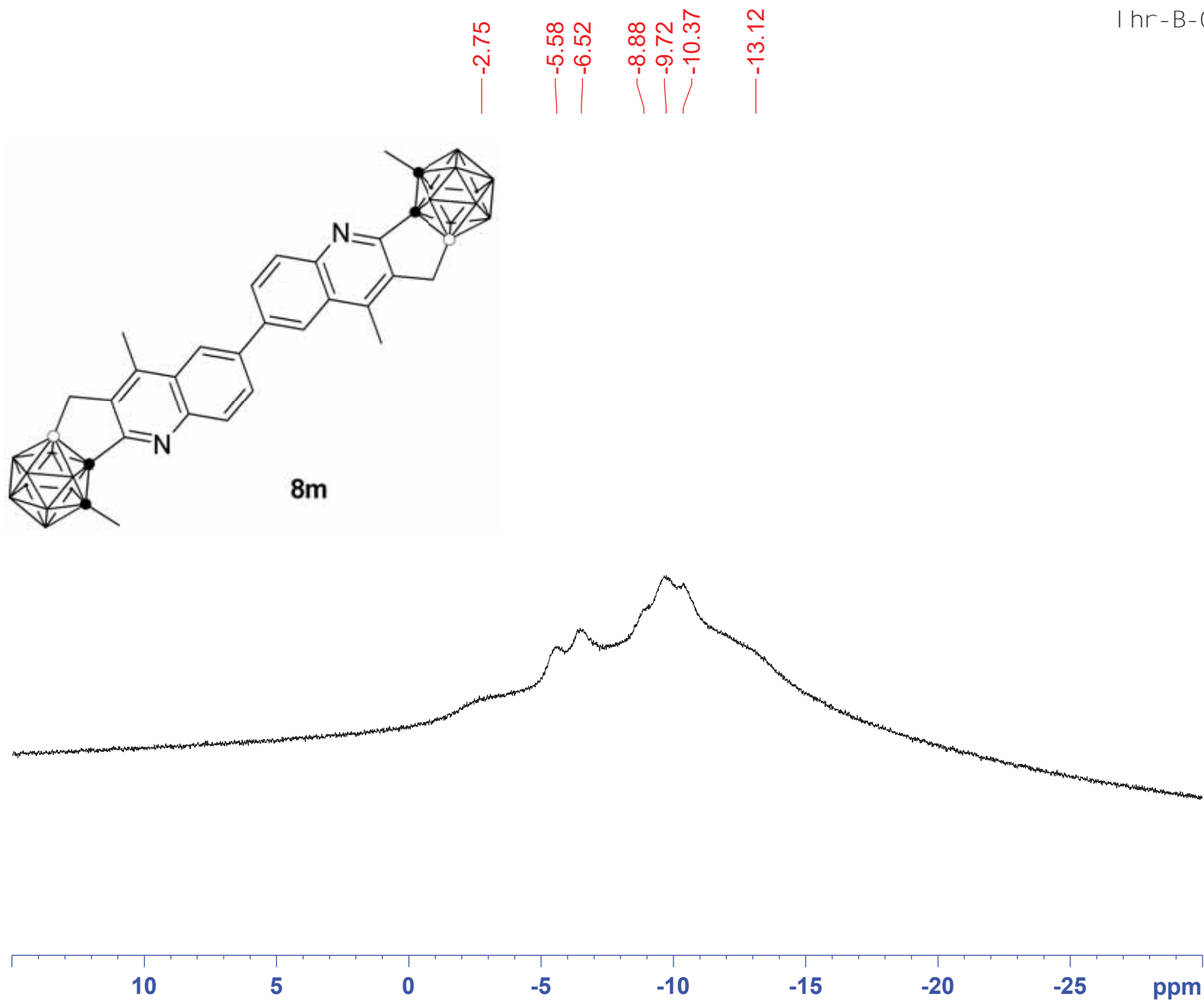
2.24  
8.09  
8.00  
2.11

Current Data Parameters  
NAME I hr-B-0773-cc  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171011  
Time 10.27 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl 3  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.733596 Hz  
AQ 1.3631488 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters  
SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

I hr-B-0773-cc(c)



Current Data Parameters  
NAME I hr-B-0773-cc(c)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171011  
Time 10.28 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 20  
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 1.0000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W

F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

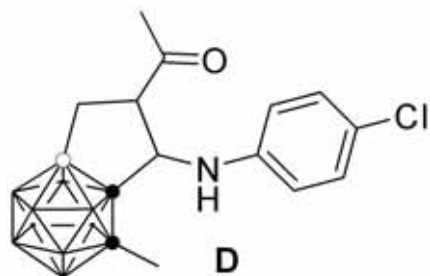


l hr-H-0759-10-p2-mc

Current Data Parameters  
NAME l hr-H-0759-10-p2-m  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170913  
Time 9.22 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  
TDO 1  
SF01 500.1330883 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300129 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



7.260  
7.151  
7.134

6.588  
6.572

5.223  
5.205  
5.188

3.493  
3.476  
3.258  
3.239  
3.220  
3.200

2.190  
1.950  
1.754  
1.734  
1.726  
1.707  
1.565  
1.248  
1.225  
1.198

1.96

2.02

1.07

1.00

1.06

2.99

3.02

1.13

1.13

S-253

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

— 205.48

— 143.94

— 129.77

— 124.04

— 113.96

82.78

77.84

77.41

77.16

76.91

67.37

60.95

— 28.59

— 23.45

I hr-C-0759-10-p2-mcas

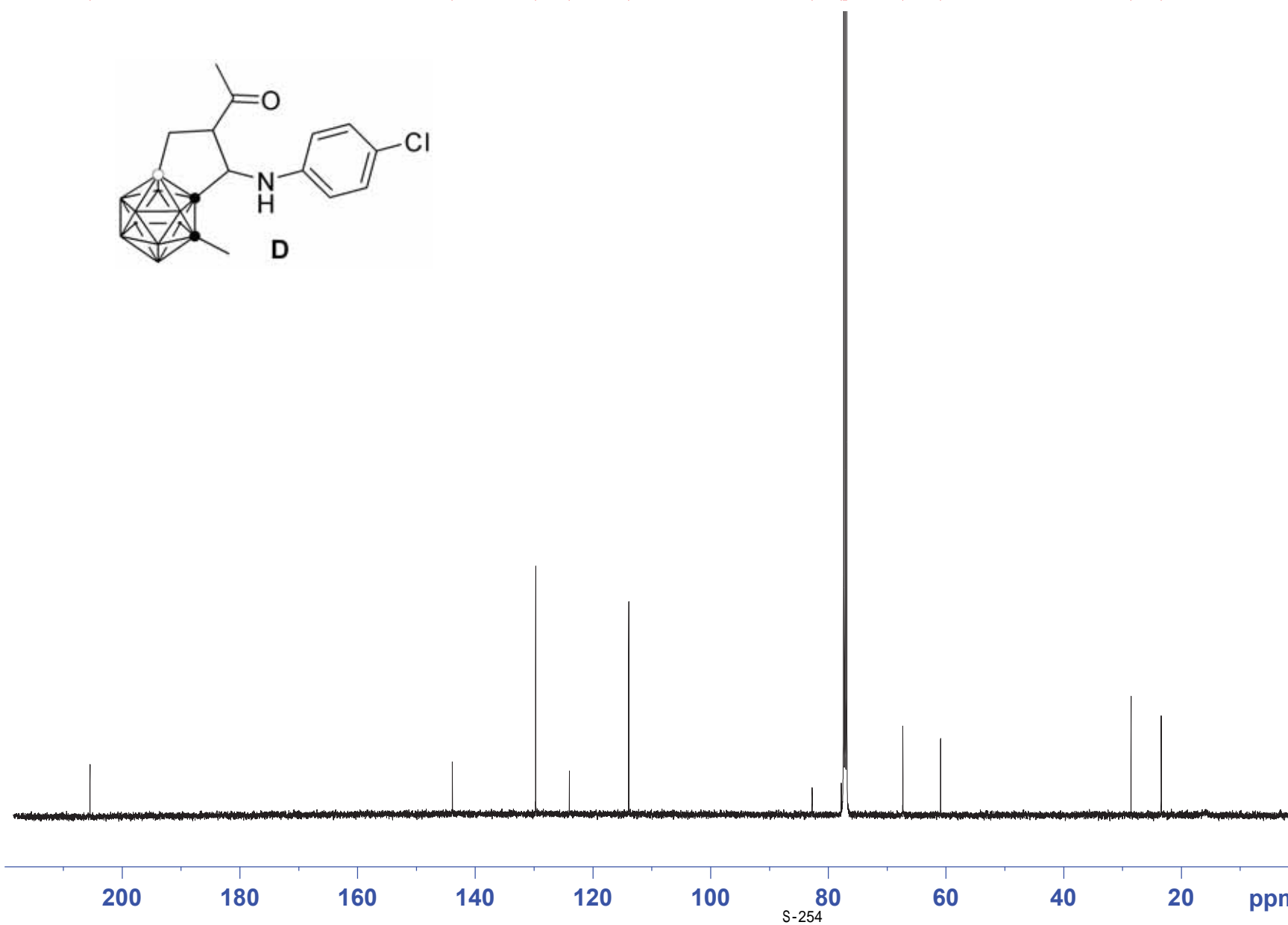
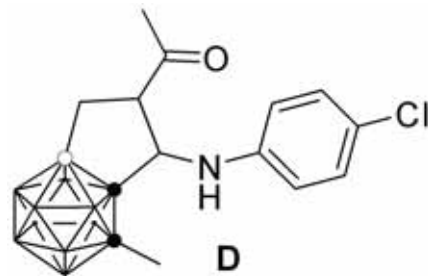
Current Data Parameters  
 NAME I hr-C-0759-10-p2-mcas  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20170913  
 Time 9.58 h  
 INSTRUM spect  
 PROBHD Z149001\_0010 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 680  
 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  
 TDO 1  
 SF01 125.7703643 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 61.0000000 W  
 SF02 500.1320005 MHz  
 NUC2 1H  
 CPDPRG[2] wal tz16  
 PCPD2 80.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.33750001 W  
 PLW13 0.16976000 W

F2 - Processing parameters

SI 32768  
 SF 125.7577717 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



I hr-B-0759-10-p2-mcas

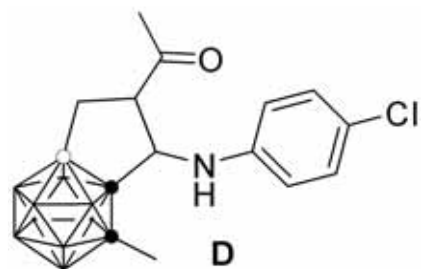
Current Data Parameters  
NAME I hr-B-0759-10-p2-mcas  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

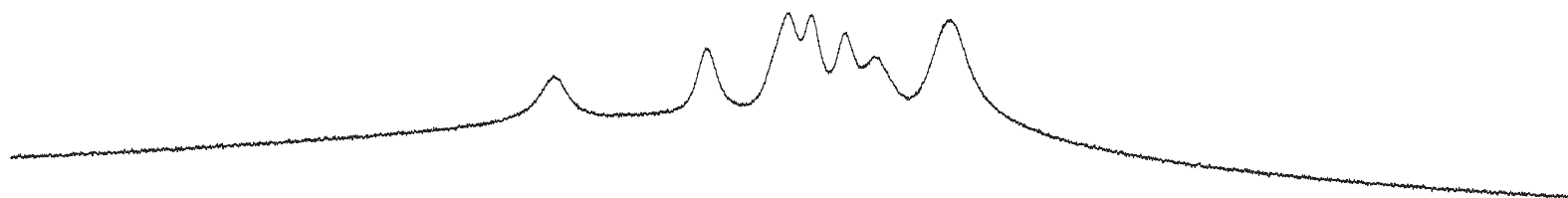
Date\_ 20170913  
Time 10.02 h  
INSTRUM spect  
PROBHD Z149001\_0010 (  
PULPROG zgdc  
TD 65536  
SOLVENT CDCl3  
NS 20  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 186.15  
DW 21.000 usec  
DE 18.00 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TDO 1  
SF01 160.4599621 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 15.0000000 W  
PLW12 0.33750001 W

F2 - Processing parameters

SI 32768  
SF 160.4615719 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



-0.68  
-5.07  
-7.49  
-8.14  
-9.14  
-9.99  
-12.16

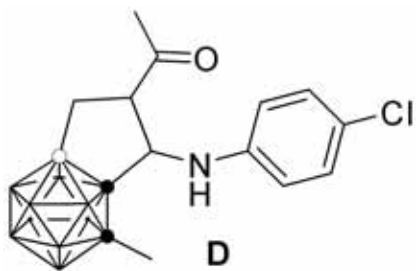


10 5 0 -5 -10 -15 -20 -25 ppm

1.18  
1.04  
2.99  
1.00  
1.09  
3.00  
8.255

I hr-B-0759-10-p2-mcas(C)

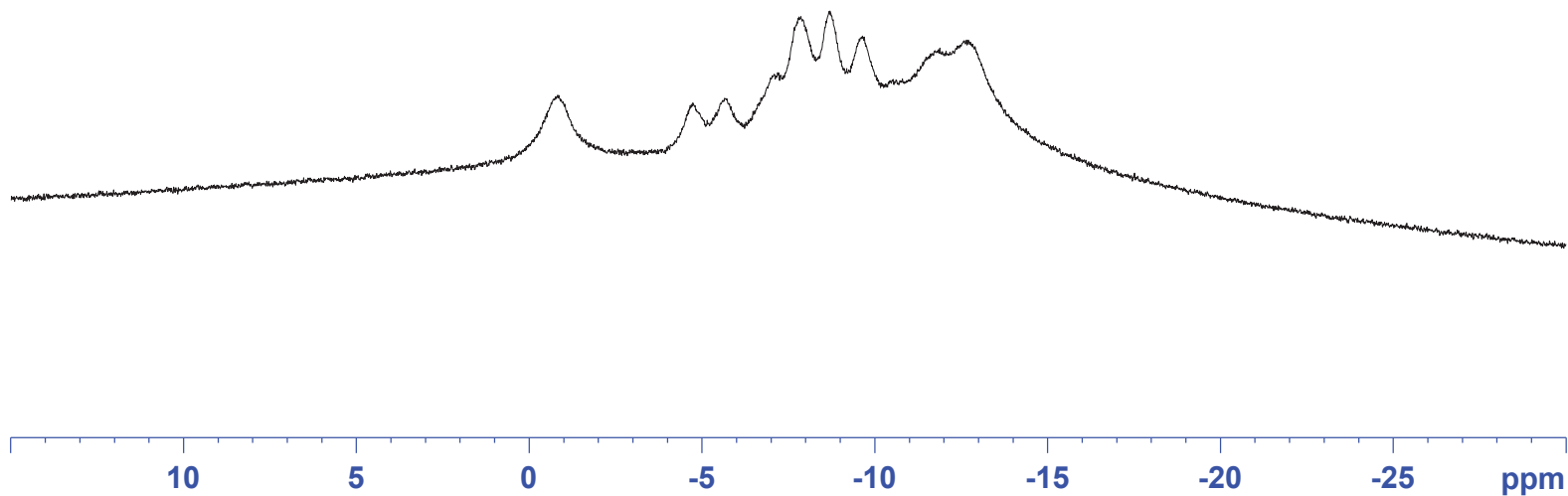
-0.82  
-4.73  
-5.65  
-7.10  
-7.86  
-8.70  
-9.63  
-10.60  
-11.74  
-12.70



Current Data Parameters  
NAME I hr-B-0759-10-p2-mcas(C)  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170913  
Time 10.03 h  
INSTRUM spect  
PROBHD Z149001\_0010 ( )  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 20  
DS 4  
SWH 24038.461 Hz  
FIDRES 1.467191 Hz  
AQ 0.6815744 sec  
RG 186.15  
DW 20.800 usec  
DE 18.00 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1  
SF01 160.4615792 MHz  
NUC1 11B  
P1 10.00 usec  
PLW1 50.00000000 W

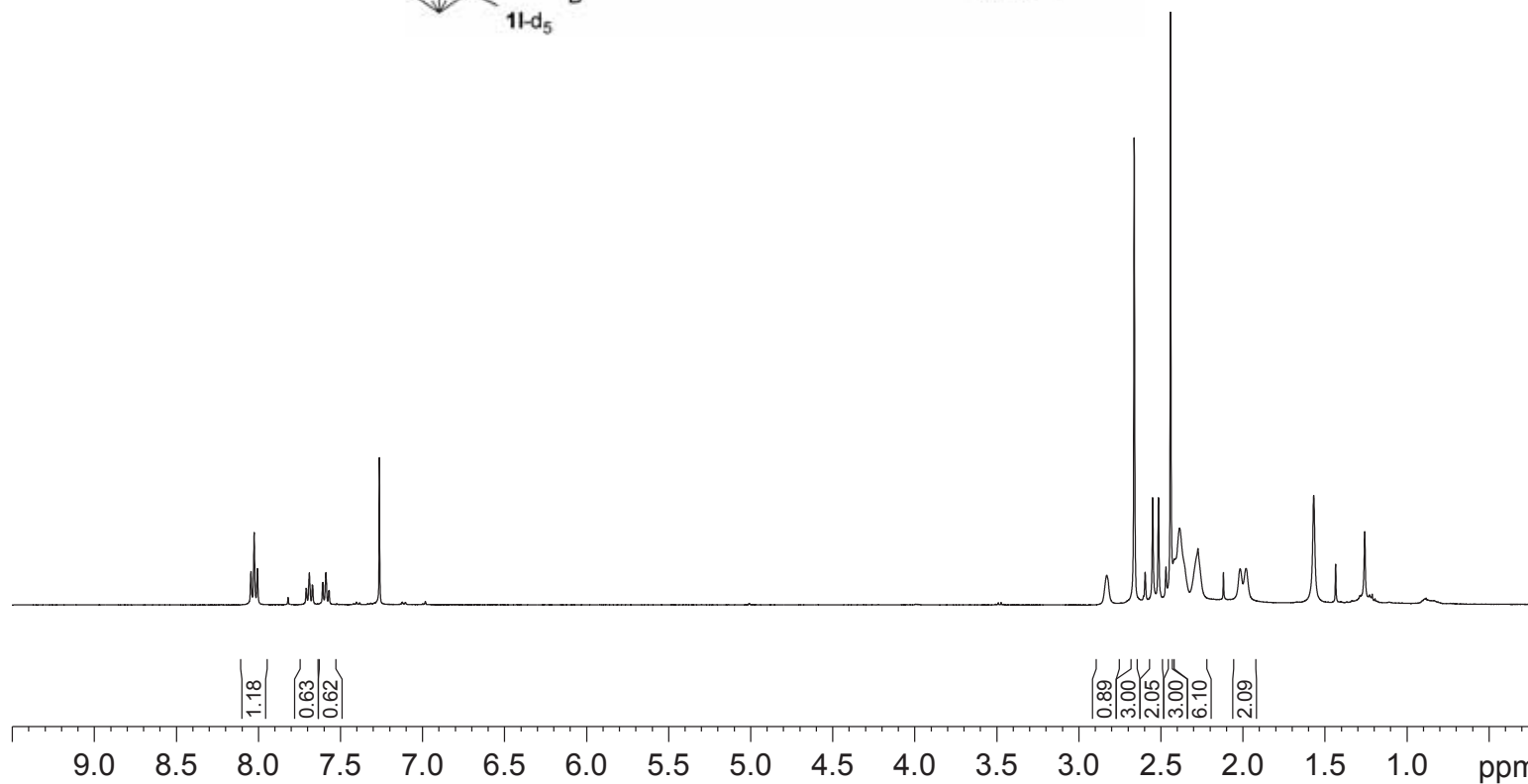
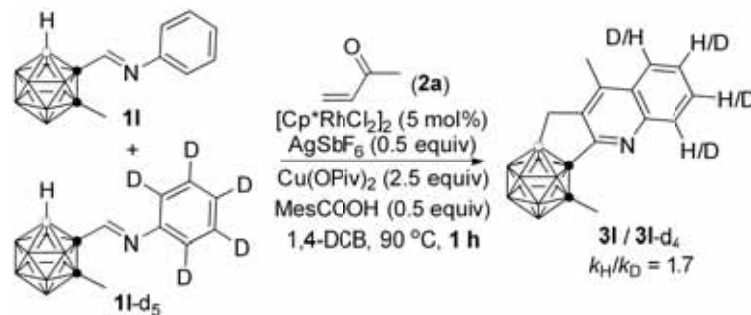
F2 - Processing parameters  
SI 16384  
SF 160.4615792 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



8.043  
8.023  
8.004  
7.707  
7.687  
7.669  
7.607  
7.604  
7.586  
7.566  
7.260

2.829  
2.661  
2.594  
2.548  
2.513  
2.467  
2.439  
2.384  
2.272  
2.015  
1.979  
1.566

1hr-H-decoB-d5cc-co



Current Data Parameters  
NAME 1hr-H-decoB-d5cc-com-product-c  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20171117  
Time 19.34 h  
INSTRUM spect  
PROBHD Z108618\_0257 (PULPROG zgig)  
TD 65536  
SOLVENT CDCl3  
NS 13  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 71.8  
DW 62.400 usec  
DE 6.50 usec  
TE 295.9 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W  
SFO2 128.4068641 MHz  
NUC2 11B  
CPDPRG2 waltz16  
PCPD2 80.00 usec  
PLW2 55.09999847 W  
PLW12 0.48427999 W

F2 - Processing parameters  
SI 32768  
SF 400.2300103 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Current Data Parameters  
 NAME 1hr-2H-casd5-chloroform  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180529  
 Time\_ 16.30 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (  
 PULPROG zg2h  
 TD 4096  
 SOLVENT CDCl3  
 NS 18190  
 DS 0  
 SWH 6142.506 Hz  
 FIDRES 2.999271 Hz  
 AQ 0.3334144 sec  
 RG 0.5  
 DW 81.400 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 0.05000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 61.4226981 MHz  
 NUC1 2H  
 P1 300.00 usec  
 PLW1 3.00000000 W

F2 - Processing parameters  
 SI 4096  
 SF 61.4223898 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

— 8.109  
 — 7.762

— 5.319

