

## A Thermo-regulated Highly Regioselective Mono and Dihalogenations of Phenols and Anilines in Water Employing New Lewis Base Adducts (LBAs) [DBUBr]<sup>+</sup>Br<sup>-</sup> and [DBUI]<sup>+</sup>I<sup>-</sup> As Green Reagents; A Simple Approach

Vijayalaxmi Gavinolla,<sup>a</sup> Swathi Thangalipalli,<sup>a</sup> Siddarama Goud Bandalla,<sup>b</sup> Ramaraju Panduga<sup>b</sup> and Chandra Kiran Neella\*<sup>a</sup>

<sup>a</sup> Dept. of Chemistry, Palamuru University, Mahbubnagar, Telangana, India 509001.

<sup>b</sup>Dept. of Integrated Chemistry, Palamuru University, Mahbubnagar, Telangana, India 509001.

### Table of Contents

<b>General Information .....</b>	<b>2</b>
<b>Description of Products.....</b>	<b>.2</b>
<b>Copies of <sup>1</sup>H <sup>13</sup>C{<sup>1</sup>H} and IR Spectra of LBAs.....</b>	<b>19</b>
<b>IR spectra of LBAs 2 and 3 .....</b>	<b>90</b>

**General Considerations.** All solvents were treated according to standard methods. Commercial reagents were purchased from AVRA, Merck and TCCI and used without further purification unless otherwise stated. Solvents, unless otherwise specified, were reagent grade and distilled once prior to use. <sup>1</sup>H-NMR spectra were recorded at 400 MHz (Varian); <sup>13</sup>C NMR spectra were recorded at 100 MHz (Varian). <sup>1</sup>H-NMR chemical shifts are calibrated using residual undeuterated solvents CHCl<sub>3</sub> ( $\delta$  = 7.26 ppm), DMSO ( $\delta$  = 2.50 ppm) <sup>13</sup>C-NMR chemical shifts for <sup>13</sup>C-NMR are reported relative to the central CHCl<sub>3</sub> ( $\delta$  = 77.16 ppm) or DMSO ( $\delta$  = 39.52 ppm). Coupling constants are given in Hz. Elemental analyses was done using Elementar Vario EL Cube.

### **General Procedure for the preparation of 2 and 3:**

To an ice cold solution of DBU (1.0 equiv) in ethyl acetate (10 mL) was added a solution of reagent (1.1 equiv) in ethyl acetate (5 mL) slowly drop by drop through addition funnel. After addition the reaction mass was warmed to rt and stirred for 30 min. The resultant solid was filtered through Buchner funnel and washed successively with ethyl acetate (10 mL) and ether (10 mL). The solid thus obtained was thoroughly dried under vacuum to furnish different LBAs.

### **General Experimental procedure for monohalogenation:**

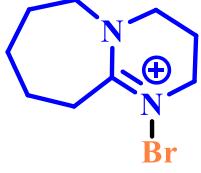
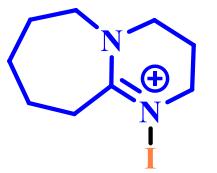
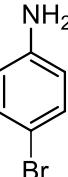
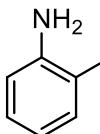
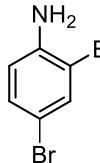
To a stirred solution/suspension of phenol/aniline derivative (5.0 mmol) in water (7 mL) at temperature mentioned in table was added reagent **5** (5.5 mmol) and stirred until completion (TLC). The resultant solid was filtered through syntered disc and washed thoroughly with water (5 mL) and dried under vacuum to produce solid products. The solids were recrystallised from ethanol/ether.

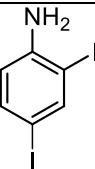
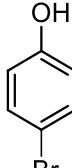
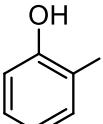
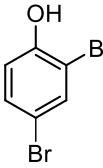
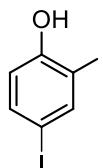
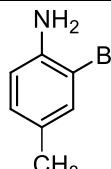
### **General Experimental procedure for dihalogenation:**

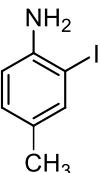
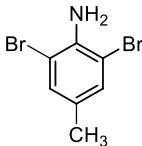
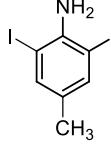
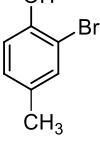
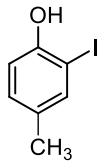
To a stirred solution/suspension of phenol/aniline derivative (5.0 mmol) in water (3 mL) at temperature mentioned in table was added reagent **2/3** (10.5 mmol) and stirred until completion (TLC). The resultant solid was filtered through syntered disc and washed thoroughly with water (5 mL) and dried under vacuum to produce solid products. The solids were recrystallised from ethanol/ether. For liquid products the aqueous layer was extracted into ethylacetate (2 x 10 mL). combined organic layers were dried using Na<sub>2</sub>SO<sub>4</sub> and evaporated under vacuum to furnish pure products.

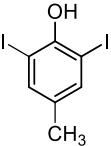
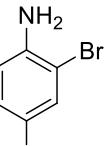
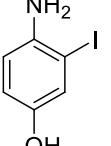
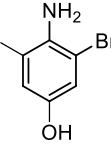
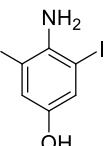
### **Procedure for recovery of DBU:**

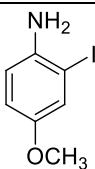
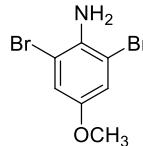
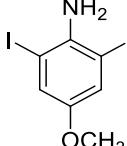
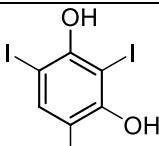
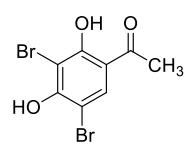
The aqueous layer was basified with aq. NaOH and extracted into ethyl acetate. The organic layers were evaporated under vacuum to obtain DBU which was reused again for preparation of LBAs.

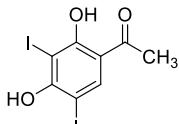
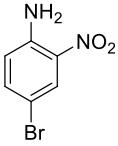
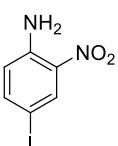
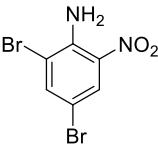
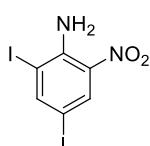
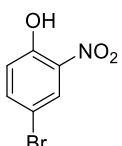
 2	<p><b>MP</b> = 140-143 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 3.73 – 3.43 (m, 6H), 3.02-2.93 (m, 2H), 2.16 (s, 2H), 1.90–1.66 (m, 6H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: δ 168.0, 167.8, 62.3, 55.6, 55.2, 49.6, 48.9, 29.3, 28.2, 25.7, 22.4, 20.0, 14.0.</p> <p><b>IR (film) ν<sub>max</sub></b> : 1193, 1253, 1325, 1627, 1724, 2935, 3446 cm<sup>-1</sup>. Mass (ESI-MS): 312.05 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>9</sub>H<sub>16</sub>Br<sub>2</sub>N<sub>2</sub>; C, 34.64; H, 5.17; N, 8.98; Br, 51.21; Found: C, 34.67; H, 5.15; N, 8.96; Br, 51.26.</p>
 3	<p><b>MP</b> = 161-164 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 3.64 (dd, <i>J</i> = 12.7, 7.2 Hz, 4H), 3.54 (s, 2H), 2.98 (s, 2H), 2.23 – 2.11 (m, 2H), 1.82 (d, <i>J</i> = 23.4 Hz, 6H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: δ 166.2, 55.3, 49.2, 38.4, 33.6, 28.9, 26.7, 24.0, 19.6.</p> <p><b>IR (film) ν<sub>max</sub></b> : 1319, 1481, 1643, 2935, 3118 cm<sup>-1</sup>.</p> <p><b>Mass (ESI-MS)</b>: 405.94 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>9</sub>H<sub>16</sub>I<sub>2</sub>N<sub>2</sub>; C, 26.62; H, 3.97; N, 8.78; I, 62.97; Found: C, 26.58; H, 3.92; N, 8.75; I, 62.96.</p>
 4a	<p><b>MP</b> = 62-64 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 7.23 (d, <i>J</i> = 8.8 Hz, 2H), 6.56 (d, <i>J</i> = 8.8 Hz, 2H), 3.69 (s, 2H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 145.4, 131.98, 116.68, 110.17.</p> <p><b>Mass (ESI-MS)</b>: 172.0 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>6</sub>BrN; C, 41.89; H, 3.52; Br, 46.45; N, 8.14; Found: C, 41.92; H, 3.58; Br, 46.50, N, 8.19.</p>
 4b	<p><b>MP</b> = 56-59 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 7.87 (d, <i>J</i> = 6.7 Hz, 1H), 7.28 (t, <i>J</i> = 5.9 Hz, 1H), 7.12 (t, <i>J</i> = 7.3 Hz, 1H), 7.07 (d, <i>J</i> = 7.8 Hz, 1H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 134.5, 129.4, 129.2, 125.6, 125.6, 118.7;</p> <p><b>Mass (ESI-MS)</b>: 218.95 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>6</sub>IN; C, 32.90; H, 2.76; I, 57.94; N, 6.40; Found: C, 32.47; H, 2.84; I, 57.57, N, 6.77.</p>
 4c	<p><b>MP</b> = 78-79 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 7.53 (d, <i>J</i> = 2.0 Hz, 1H), 7.19 (dd, <i>J</i> = 8.4 &amp; 2.0 Hz, 1H), 6.64 (d, <i>J</i> = 8.4 Hz, 1H), 4.10 (s, 2H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 149.8, 129.2, 128.0, 124.9, 113.5, 107.0.</p> <p><b>Mass (ESI-MS)</b>: 250.88 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>5</sub>Br<sub>2</sub>N; C, 41.89; H, 3.52; Br, 46.45; N, 8.14; Found: C, 41.92; H, 3.58; Br, 46.50, N, 8.19.</p>

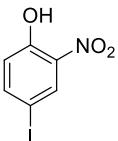
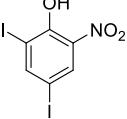
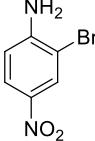
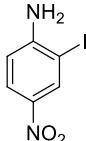
 4d	<b>MP</b> = 93-95 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b> : δ 7.53 (d, <i>J</i> = 2.2 Hz, 1H), 7.20 (dd, <i>J</i> = 8.5, 2.2 Hz, 1H), 6.24 (d, <i>J</i> = 8.5 Hz, 1H), 4.09 (s, 2H). <b><sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)</b> : δ 146.7, 139.4, 130.2, 119.7, 86.1, 85.3 <b>Mass (ESI-MS)</b> : 344.85 [M <sup>+</sup> ]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>5</sub> I <sub>2</sub> N; C, 20.89; H, 1.46; I, 73.58; N, 4.06; Found: C, 20.80; H, 1.49; I, 73.55; N, 4.55.
 5a	<b>MP</b> = 65-67 °C. <b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b> : 7.32 (d, <i>J</i> = 8.8 Hz, 2H), 6.72 (d, <i>J</i> = 8.8 Hz, 2H), 5.03 (s, 1H); <b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b> : 154.7, 132.5, 117.2, 112.8. <b>Mass (ESI-MS)</b> : 172.0 [M <sup>+</sup> ]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>5</sub> BrO; C, 41.65; H, 2.91; Br, 46.18; Found: C, 41.62; H, 2.94; Br, 46.15.
 5b	<b>MP</b> = 37-40 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b> : δ 7.66 (dd, <i>J</i> = 7.9, 1.4 Hz, 1H), 7.23 (d, <i>J</i> = 1.4 Hz, 1H), 7.00 (dd, <i>J</i> = 8.1, 1.4 Hz, 1H), 6.84 (m, 1H), 5.28 (s, 1H). <b><sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)</b> : δ 154.7, 138.2, 130.2, 122.4, 115.1, 85.7. <b>Mass [ESI-MS]</b> : 219.94 [M <sup>+</sup> ]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>5</sub> IO; C, 32.76; H, 2.29; I, 57.68; Found: C, 32.70; H, 2.30; I, 55.65.
 5c	<b>MP</b> = 38-40 °C. <b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b> : 7.59 (d, <i>J</i> = 2.0 Hz, 1H), 7.32 (dd, <i>J</i> = 8.8 & 2.0 Hz, 1H), 6.91 (d, <i>J</i> = 8.8 Hz, 1H), 5.49 (s, 1H). <b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b> : 152.7, 133.9, 129.2, 113.5, 110.3. <b>Mass (ESI-MS)</b> : 249.0 [M <sup>+</sup> ]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub> O; C, 28.61; H, 1.60; Br, 63.44; Found: C, 28.62; H, 1.64; Br, 63.38.
 5d	<b>MP</b> = 68-70 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b> : δ 7.85 (s, 1H), 7.53 (d, <i>J</i> = 6.2 Hz, 1H), 6.29 (d, <i>J</i> = 5.2 Hz, 1H), 5.25 (s, 1H). <b><sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)</b> : δ 153.5, 136.7, 128.8, 115.1, 85.7, 83.2. <b>Mass (ESI-MS)</b> : 345.84 [M <sup>+</sup> ]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>4</sub> I <sub>2</sub> O <sub>2</sub> ; C, 20.83; H, 1.17; I, 73.38; Found: C, 20.80; H, 1.19; I, 73.34.
 6a	<b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b> : 7.23 (s, 1H), 6.90 (d, <i>J</i> = 8.0 Hz, 1H), 6.67 (d, <i>J</i> = 8.0 Hz, 1H), 2.22 (s, 3H). <b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b> : 143.2, 134.5, 131.2, 129.3, 116.7, 109.6, 23.3. <b>Mass (ESI-MS)</b> : 186.1 [M <sup>+</sup> ]. <b>CHN</b> : Expected for C <sub>7</sub> H <sub>8</sub> BrN; C, 45.19; H, 4.33; Br, 42.95; N, 7.53; Found: C, 45.21; H, 4.36; Br, 42.98; N, 7.48.

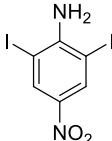
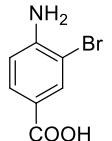
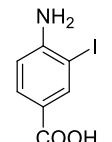
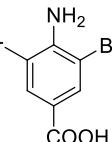
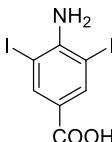
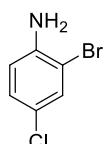
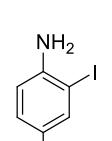
 6b	<p><b>MP</b> = 39-41 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.47 (s, 1H), 6.94 (d, <i>J</i> = 7.1 Hz, 1H), 6.66 (d, <i>J</i> = 8.1 Hz, 1H), 3.13(s, 2H), 2.20 (s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)</b>: δ 144.2, 139.0, 130.0, 129.5, 114.7, 84.3, 19.8.</p> <p><b>Mass (ESI-MS)</b>: 232.97 [M+].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>8</sub>IN; C, 36.08; H, 3.46; I, 54.45; N, 6.01; Found; C, 36.11; H, 3.40; I, 54.44; N, 6.06.</p>
 6c	<p><b>MP</b> = 74-75 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 7.19 (s, 2H), 4.38 (s, 2H), 2.20 (s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 151.7, 136.8, 133.9, 120.3, 18.7.</p> <p><b>Mass (ESI-MS)</b>: 264.9, [M+].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>7</sub>Br<sub>2</sub>N; C, 31.73; H, 2.66; Br, 60.32; N, 5.29; Found: C, 31.76; H, 2.64; Br, 60.28; N, 5.32.</p>
 6d	<p><b>MP</b> = 85-87 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.25 (s, 2H), 4.38 (s, 2H), 2.25 (s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)</b>: δ 139.6, 132.2, 129.4, 85.3, 19.8.</p> <p><b>Mass (ESI-MS)</b>: 358.87 [M+].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>7</sub>I<sub>2</sub>N; C, 23.42; H, 1.97; I, 70.71; N, 3.90; Found; C, 23.40; H, 1.95; I, 70.70; N, 3.94.</p>
 7a	<p><b>MP</b> = 210-214 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 7.26 (s, 1H), 7.00 (dd, <i>J</i> = 8.2, 1.2 Hz, 1H), 6.90 (d, <i>J</i> = 8.2 Hz, 1H), 5.33 (s, 1H), 2.26 (s, 3H);</p> <p><b>Mass (ESI-MS)</b>: 187.03 [M+].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>7</sub>BrO; C, 44.95; H, 3.77; Br, 42.72; Found: C, 44.98; H, 3.80; Br, 42.70.</p>
 7b	<p><b>MP</b> = 34-36 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.47 (s, 1H), 7.04 (d, <i>J</i> = 8.2 Hz, 1H), 6.87 (d, <i>J</i> = 8.2 Hz, 1H), 5.16 (s, 1H), 2.25 (s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 154.2, 144.2, 134.3, 130.0, 114.7, 84.3, 19.8.</p> <p><b>Mass (ESI-MS)</b>: 233.95 [M+].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>7</sub>IO; C, 35.92; H, 3.01; I, 54.22; Found: C, 35.90; H, 3.11; I, 54.20.</p>
 7c	<p><b>MP</b> = 46-48 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 7.49 (s, 2H), 5.57 (s, 1H), 2.25 (s, 3H).</p> <p><b>Mass (ESI-MS)</b>: 327.77 [M+].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>6</sub>OBr<sub>2</sub>; C, 31.62; H, 2.27; Br, 60.09; Found: 31.63; H, 2.24; Br, 60.10.</p>

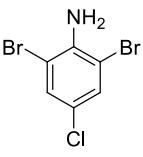
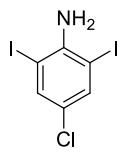
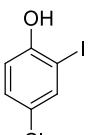
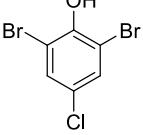
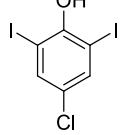
 7d	<p><b>MP</b> = 59-61 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.53 (s, 2H), 5.55 (s, 1H), 2.22 (s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 139.6, 132.2, 129.4, 82.0, 19.8.</p> <p><b>Mass (ESI-MS)</b>: 359.85 [M<sup>+ <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>6</sub>I<sub>2</sub>O; C, 23.36; H, 1.68; I, 70.52; Found; C, 23.32; H, 1.60; I, 70.55.</p> </sup></p>
 8a	<p><b>MP</b> = 151-153 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 7.31 (d, <i>J</i> = 2.4 Hz, 1H), 6.97 (d, <i>J</i> = 9.0 Hz, 1H), 6.83 (dd, <i>J</i> = 9.0, 2.4 Hz, 1H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 143.3, 134.5, 122.7, 119.8, 118.9, 116.7.</p> <p><b>Mass (ESI-MS)</b>: 188.0 [M<sup>+ <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>6</sub>BrNO; C, 38.33; H, 3.22; Br, 42.50; N, 7.45; Found: C, 38.36; H, 3.24; Br, 42.48, N, 7.41.</p> </sup></p>
 8b	<p><b>MP</b> = 143-146 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.40 (d, <i>J</i> = 2.3 Hz, 1H), 7.07 (dd, <i>J</i> = 8.6, 2.3 Hz, 1H), 6.68 (d, <i>J</i> = 8.6 Hz, 1H), 4.07 (s, 2H).</p> <p><b>Mass (ESI-MS)</b>: 234.95 [M<sup>+ <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>6</sub>I NO; C, 30.66; H, 2.57; I, 54.00; N, 5.96; Found; C, 30.62; H, 2.54; I, 54.08; N, 5.98.</p> </sup></p>
 8c	<p><b>MP</b> = 156-158 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 7.33 (s, 2H);</p> <p><b>Mass (ESI-MS)</b>: 266.92 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>5</sub>Br<sub>2</sub>NO; C, 27.00; H, 1.89; Br, 59.87; N, 5.25; Found: C, 27.04; H, 1.93; Br, 59.85, N, 5.28.</p>
 8d	<p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.23 (s, 2H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 153.1, 141.1, 122.6, 120.1.</p> <p><b>Mass (ESI-MS)</b>: 360.85 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>5</sub>I<sub>2</sub> NO; C, 19.97; H, 1.40; I, 70.32; N, 3.88; Found: C, 19.99; H, 1.42; I, 70.35; N, 3.89.</p>
 9a	<p><b>MP</b> = 62-64 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 6.99 (d, <i>J</i> = 1.8 Hz, 1H), 6.78 (dd, <i>J</i> = 7.1, 2.3 Hz, 1H), 6.45 (d, <i>J</i> = 8.1 Hz, 1H), 3.78(s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 151.7, 141.2, 120.7, 118.2, 117.8, 110.3, 51.0.</p> <p><b>Mass (ESI-MS)</b>: 202.05 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>8</sub>BrNO; C, 41.61; H, 3.99; Br, 39.55; N, 6.93; Found; C, 41.62; H, 3.95; Br, 39.56; N, 6.94.</p>

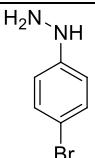
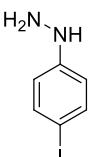
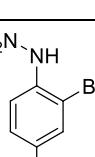
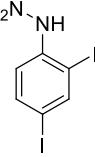
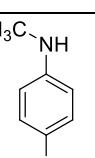
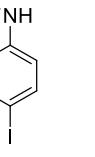
 9b	<p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 7.42 (s, 1H), 6.75 (d, <i>J</i> = 7.3 Hz, 1H), 6.47 (d, <i>J</i> = 7.3 Hz, 1H), 3.92 (s, 3H).</p> <p><b>Mass (ESI-MS):</b> 248.97 [M<sup>+ <p><b>CHN:</b> Expected for C<sub>7</sub>H<sub>8</sub>INO; C, 33.76; H, 3.24; I, 50.96; N, 5.62; Found: C, 33.77; H, 3.23; I, 50.90; N, 5.60.</p> </sup></p>
 9c	<p><b>MP</b> = 80-82 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 6.98 (s, 2H), 3.86 (s, 3H).</p> <p><b>Mass (ESI-MS):</b> 280.94 [M<sup>+ <p><b>CHN:</b> Expected for C<sub>7</sub>H<sub>7</sub>Br<sub>2</sub>NO; C, 29.93; H, 2.51; Br, 56.88; N, 4.99; Found; C, 29.91; H, 2.49; Br, 56.85; N, 4.97.</p> </sup></p>
 9d	<p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 7.26 (s, 2H), 3.82(s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 153.1, 141.0, 122.6, 85.5, 54.4.</p> <p><b>Mass (ESI-MS):</b> 374.86 [M<sup>+ <p><b>CHN:</b> Expected for C<sub>7</sub>H<sub>7</sub>I<sub>2</sub>NO; C, 22.426; H, 1.88; I, 67.69; N, 3.74; Found; C, 22.40; H, 1.84; I, 67.71; N, 3.72.</p> </sup></p>
 10a	<p><b>MP</b> = 112-115 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>):</b> δ 7.60 (d, <i>J</i> = 4.4 Hz, 1H), 5.94 (s, 2H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 150.6, 132.3, 115.5, 110.7.</p> <p><b>Mass (ESI-MS):</b> 343.77 [M<sup>+ <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>3</sub>O<sub>2</sub>Br<sub>3</sub>; C, 20.78; H, 0.87; Br, 69.12; Found, 20.80; H, 0.89; Br, 69.19.</p> </sup></p>
 10b	<p><b>MP</b> = 140-142 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 7.94 (s, 1H), 5.86 (s, 2H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 153.3, 146.6, 86.6, 80.6.</p> <p><b>Mass (ESI-MS):</b> 487.73 [M<sup>+</sup>].</p> <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>3</sub>I<sub>3</sub>O<sub>2</sub>; C, 14.77; H, 0.62; I, 78.05; Found: C, 14.78, H, 0.66; I, 78.09.</p>
 11a	<p><b>MP</b> = 96-99 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>):</b> δ 7.63 (s, 1H), 6.52 (s, 2H), 2.59 (s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> δ 201.92, 160.27, 155.51, 133.32, 115.21, 99.33, 98.87, 26.28.</p> <p><b>Mass (ESI-MS):</b> 307.87 [M<sup>+</sup>].</p> <p><b>CHN:</b> Expected for C<sub>8</sub>H<sub>6</sub>O<sub>3</sub>Br<sub>2</sub>; C, 31.00; H, 1.95; Br, 51.56; Found: C, 31.08; H, 1.98; Br, 51.50.</p>

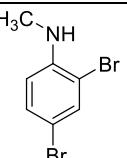
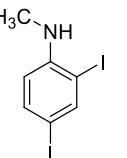
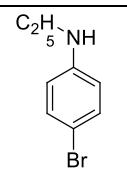
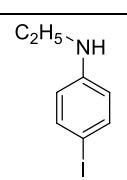
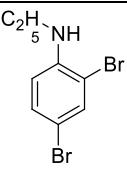
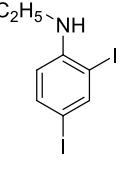
 11b	<p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 7.89 (s, 1H), 2.59 (S, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 201.9, 161.2, 160.3, 136.5, 116.9, 81.7, 80.6, 26.3.</p> <p><b>Mass (ESI-MS):</b> 403.84 [M+].</p> <p><b>CHN:</b> Expected for C<sub>8</sub>H<sub>6</sub>I<sub>2</sub>O<sub>3</sub>; C, 23.79; H, 1.50; I, 62.83; Found; C, 23.76; H, 1.50; I, 62.89.</p>
 12a	<p><b>MP = 108-110 °C.</b></p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>):</b> δ 8.27 (d, <i>J</i> = 2.3 Hz, 1H), 7.43 (dd, <i>J</i> = 8.9, 2.3 Hz, 1H), 6.73 (d, <i>J</i> = 8.9 Hz, 1H), 6.08 (s, 2H).</p> <p><b>Mass (ESI-MS):</b> 215.95 [M+].</p> <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>5</sub>N<sub>2</sub>O<sub>2</sub>Br; C, 33.21; H, 2.32; N, 12.91; Br, 36.82 Found: C, 33.29; H, 2.34; N, 12.96; Br, 36.93.</p>
 12b	<p><b>MP = 120-123 °C.</b></p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 8.17 (s, 1H), 7.78 (dd, <i>J</i> = 8.9, 2.3 Hz, 1H), 6.73 (d, <i>J</i> = 8.9 Hz, 1H), 6.08 (s, 2H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 141.3, 140.9, 132.9, 128.2, 112.8, 78.7.</p> <p><b>Mass (ESI-MS):</b> 263.94 [M+].</p> <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>5</sub>IN<sub>2</sub>O<sub>2</sub>; C, 27.29; H, 1.91; I, 48.07; N, 10.61; Found: C, 27.25; H, 1.90; I, 48.17; N, 10.60.</p>
 12c	<p><b>MP = 128-130 °C.</b></p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>):</b> δ 8.29 (d, <i>J</i> = 2.3 Hz, 1H), 7.81 (d, <i>J</i> = 2.3 Hz, 1H), 6.64 (s, 2H).</p> <p><b>Mass (ESI-MS):</b> 293.86 [M+]</p> <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>Br<sub>2</sub>; C, 24.35; H, 1.36; N, 9.47; Br, 54.00 Found: C, 24.40; H, 1.39; N, 9.90; Br, 54.30.</p>
 12d	<p><b>MP = 136-138 °C.</b></p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 8.16 (d, <i>J</i> = 2.3 Hz, 2H), 5.25 (s, 2H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 150.2, 149.4, 140.9, 134.2, 86.8, 86.1.</p> <p><b>Mass (ESI-MS):</b> 389.84 [M+].</p> <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>4</sub>I<sub>2</sub>N<sub>2</sub>O<sub>2</sub>; C, 18.48; H, 1.03; I, 65.09; N, 7.18; Found; C, 18.50; H, 1.05; I, 65.12; N, 7.17.</p>
 13a	<p><b>MP = 109-112 °C.</b></p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 8.52 (d, <i>J</i> = 2.2 Hz, 1H), 7.76 (dd, <i>J</i> = 8.7, 2.3 Hz, 1H), 6.73 (d, <i>J</i> = 8.9 Hz, 1H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 150.6, 138.7, 136.8, 128.3, 124.2, 117.2.</p> <p><b>Mass (ESI-MS):</b> 218.00[M+].</p> <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>4</sub>BrNO<sub>3</sub>; C, 33.06; H, 1.85; N, 9.47; Br, 36.65; N, 6.42; Found; C, 33.08; H, 1.83; N, 9.45; Br, 36.62; N, 6.45.</p>

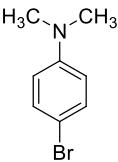
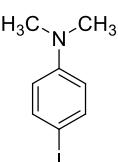
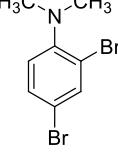
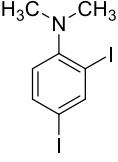
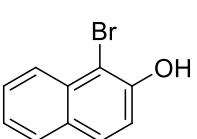
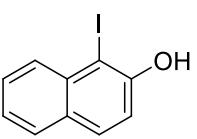
 13b	<p><b>MP</b> = 38-40 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 8.25 (s, 1H), 8.03 (d, <i>J</i> = 2.0 Hz, 1H), 6.93 (d, <i>J</i> = 2.0 Hz, 1H), 6.16 (s, 1H).</p> <p><b>Mass (ESI-MS)</b>: 262.94 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>4</sub>INO<sub>3</sub>; C, 27.19; H, 1.52; I, 47.89; N, 5.29; Found C, 27.20; H, 1.50; I, 47.85; N, 5.25.</p>
 13c	<p><b>MP</b> = 139-141 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 11.05 (s, 1H), 8.25 (d, <i>J</i> = 2.4 Hz, 1H), 7.99 (d, <i>J</i> = 2.4 Hz, 1H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 149.8, 141.3, 140.2, 128.0, 118.4, 116.6.</p> <p><b>Mass (ESI-MS)</b>: 296.9 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>3</sub>Br<sub>2</sub>NO<sub>3</sub>; C, 24.27; H, 1.02; Br, 53.83; N, 4.72; Found: C, 24.25; H, 1.05; Br, 53.86, N, 4.69.</p>
 13d	<p><b>MP</b> = 155-157 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 11.05 (s, 1H), 8.25 (t, <i>J</i> = 8.4 Hz, 2H).</p> <p><b>Mass (ESI-MS)</b>: 390.82 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>3</sub>I<sub>2</sub>NO<sub>3</sub>; C, 18.44; H, 0.77; I, 64.93; N, 3.58; Found: C, 18.40; H, 0.74; I, 64.98; N, 3.50.</p>
 14a	<p><b>MP</b> = 100-102 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 8.28 (d, <i>J</i> = 2.5 Hz, 1H), 7.93 (dd, <i>J</i> = 8.6, 2.5 Hz, 1H), 6.75 (d, <i>J</i> = 4.4 Hz, 1H), 4.83 (s, 2H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 153.1, 141.0, 131.3, 122.6, 119.6, 117.9.</p> <p><b>Mass (ESI-MS)</b>: 215.95 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>5</sub>N<sub>2</sub>O<sub>2</sub>Br; C, 33.21; H, 2.32; N, 12.91; Br, 36.82 Found: C, 33.29; H, 2.34; N, 12.96; Br, 36.93.</p>
 14b	<p><b>MP</b> = 91-93 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 8.37 (d, <i>J</i> = 2.5 Hz, 1H), 8.03 (dd, <i>J</i> = 8.9, 2.5 Hz, 1H), 6.74 (d, <i>J</i> = 4.6 Hz, 1H), 4.83 (s, 2H).</p> <p><b>Mass (ESI-MS)</b>: 264.92 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>5</sub>IN<sub>2</sub>O<sub>2</sub>; C, 27.19; H, 1.52; I, 47.89; N, 5.29; Found: C, 27.21; H, 1.54; I, 47.91; N, 5.32.</p>
 14c	<p><b>MP</b> = 203-206 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 8.34 (s, 2H), 5.29 (s, 2H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 155.7, 142.5, 129.0, 118.0</p> <p><b>Mass (ESI-MS)</b>: 293.86 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>Br<sub>2</sub>; C, 24.35; H, 1.362; N, 9.47; Br, 54.00; Found: C, 24.40; H, 1.39; N, 9.90; Br, 54.30.</p>

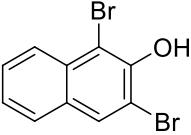
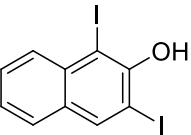
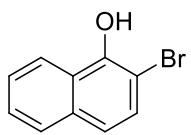
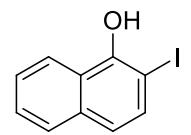
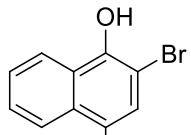
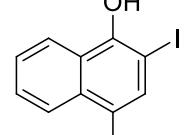
 14d	<p><b>MP</b> = 151-514 °C.</p> <p><b>1H NMR (400 MHz, in CDCl3):</b> δ 8.34 (s, 2H), 5.23 (s, 2H).</p> <p><b>Mass (ESI-MS):</b> 390.82 [M+].</p> <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>3</sub>I<sub>2</sub>N<sub>2</sub>O<sub>2</sub>; C, 18.44; H, 0.77; I, 64.93; N, 3.58; Found: C, 18.42; H, 0.76; I, 64.95; N, 3.61.</p>
 15a	<p><b>MP</b> = 210-212 °C.</p> <p><b>1H NMR (400 MHz, in CDCl3):</b> δ 8.18 (d, <i>J</i> = 1.9 Hz, 1H), 7.84 (dd, <i>J</i> = 8.4, 1.9 Hz, 1H), 6.75 (d, <i>J</i> = 8.4 Hz, 1H).</p> <p><b>Mass (ESI-MS):</b> 214.96 [M+].</p> <p><b>CHN:</b> Expected for C<sub>7</sub>H<sub>6</sub>NO<sub>2</sub>Br; C, 38.92; H, 2.80; N, 6.48; O, 14.81Br. 36.99 Found: C, 38.98; H, 2.90; N, 6.50;O, 14.98; Br, 37.00</p>
 15b	<p><b>MP</b> = 160-162 °C.</p> <p><b>1H NMR (400 MHz, CDCl3):</b> δ 8.28 (d, <i>J</i> = 1.9 Hz, 1H), 7.84 (dd, <i>J</i> = 8.4, 1.9 Hz, 1H), 6.65 (d, <i>J</i> = 8.4 Hz, 1H).</p> <p><b>Mass (ESI-MS):</b> 262.94 [M+].</p> <p><b>CHN:</b> Expected for C<sub>7</sub>H<sub>6</sub>INO<sub>2</sub>; C, 31.96; H, 2.30; I, 43.25; N; 5.33; Found; C, 31.91; H, 2.32; I, 43.20; N, 5.39.</p>
 15c	<p><b>MP</b> = 285-286 °C.</p> <p><b>1H NMR (400 MHz, in CDCl3):</b> δ 8.34 (s, 2H), 5.29 (s, 2H);</p> <p><b>Mass (ESI-MS):</b> 292.87 [M+].</p> <p><b>CHN:</b> Expected for C<sub>7</sub>H<sub>5</sub>NO<sub>2</sub>Br<sub>2</sub>; C, 28.51; H,1.71; N, 4.75; Br. 54.19 Found: 28.55; H,1.75; N, 4.72; Br, 54.21.</p>
 15d	<p><b>MP</b> = 201-203 °C.</p> <p><b>1H NMR (400 MHz, CDCl3):</b> δ 8.34 (s, 2H), 5.29 (s, 2H).</p> <p><b>Mass (ESI-MS):</b> 388.84 [M+].</p> <p><b>CHN:</b> Expected for C<sub>7</sub>H<sub>5</sub>I<sub>2</sub>NO<sub>2</sub>; C, 21.62; H, 1.30; I, 65.26; N; 3.60; Found: C; 21.66; H, 1.35; I, 65.22; N, 3.68.</p>
 16a	<p><b>MP</b> = 66-68 °C.</p> <p><b>1H NMR (400 MHz, in CDCl3):</b> 7.40 (d, <i>J</i> = 2.4 Hz, 1H), 7.07 (dd, <i>J</i> = 8.2 &amp; 2.4 Hz, 1H), 6.68 (d, <i>J</i> = 8.4 Hz, 1H), 4.07 (s, 2H);</p> <p><b>Mass (ESI-MS):</b> 206.4 [M+].</p> <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>5</sub>BrClN; C, 34.90; H, 2.44; Br, 38.70; Cl, 17.17; N, 6.78; Found: C, 34.86; H, 2.54; Br, 38.68, Cl, 17.19; N, 6.75.</p>
 16b	<p><b>MP</b> = 39-41 °C.</p> <p><b>1H NMR (400 MHz, CDCl3):</b> δ 7.40 (d, <i>J</i> = 2.3 Hz, 1H), 7.07 (dd, <i>J</i> = 8.6, 2.3 Hz, 1H), 6.68 (d, <i>J</i> = 8.6 Hz, 1H), 4.07 (s, 2H).</p> <p><b>13C NMR (100 MHz, in CDCl3):</b> 142.9, 131.8, 128.4, 123.0, 116.2, 85.1.</p> <p><b>Mass (ESI-MS):</b> 252.92 [M+].</p> <p><b>CHN:</b> Expected for C<sub>6</sub>H<sub>5</sub>INCl; C, 28.43; H, 1.99; I, 50.07; N; 5.53;</p>

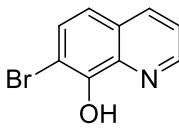
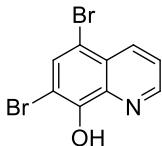
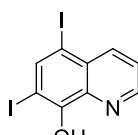
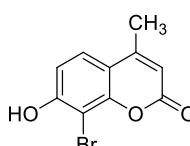
	Found: C, 28.40; H, 1.90; I, 50.55; N; 5.50; Cl.
 16c	<b>MP</b> = 94-95 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b> : δ 7.39 (s, 2H), 4.54 (s, 2H); <b>Mass (ESI-MS)</b> : 285.4 [M+]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>4</sub> Br <sub>2</sub> ClN; C, 25.25; H, 1.41; Br, 56.00; Cl, 12.42; N, 4.91; Found: C, 25.26; H, 1.44; Br, 55.98; Cl, 12.39; N, 4.88.
 16d	<b>MP</b> = 60-62 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b> : δ 7.26 (s, 2H), 4.54 (s, 2H). <b><sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)</b> : 141.0, 131.3, 122.6, 86.6. <b>Mass (ESI-MS)</b> : 378.81 [M+]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>4</sub> I <sub>2</sub> NCl; C, 19.00; H, 1.06; I, 66.90; N; 3.69; Found; C, 19.04; H, 1.10 I, 66.94; N; 3.60; Cl; 9.39.
 17a	<b>MP</b> = 32-36 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b> : δ 7.68 (d, <i>J</i> = 2.1 Hz, 1H), 7.21 (dd, <i>J</i> = 8.2, 2.3 Hz, 1H), 6.65 (d, <i>J</i> = 8.5 Hz, 1H). <b>Mass (ESI-MS)</b> : 207.45 [M+]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>4</sub> BrClO; C, 34.74; H, 1.94; Br, 38.52; Cl, 17.09; Found: C, 34.73; H, 1.96; Br, 38.50; Cl, 17.07.
 17b	<b>MP</b> = 75-79 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b> : δ 7.47 (s, 1H), 7.35(d, <i>J</i> = 8.2 Hz, 1H), 6.82 (d, <i>J</i> = 8.2 Hz, 1H), 5.16 (s, 1H). <b>Mass (ESI-MS)</b> : 253.90 [M+]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>4</sub> ClIO; C, 28.32; H, 1.58; I, 49.87; Found: C, 28.30 H, 1.60; I, 49.90.
 17c	<b>MP</b> = 90-92 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b> : δ 7.61 (s, 2H). <b>Mass (ESI-MS)</b> : 286.35 [M+]. <b>CHN</b> : Expected for C <sub>6</sub> H <sub>3</sub> Br <sub>2</sub> ClO; C, 25.17; H, 1.06; Br, 55.81; Cl, 12.38; Found: C, 25.18; H, 1.04; Br, 55.83; Cl, 12.35;
 17d	<b>MP</b> = 102-104 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b> : δ 7.66 (s, 2H), 5.71 (s, 1H). <b>Mass (ESI-MS)</b> : 379.80 [M+]; <b>CHN</b> : Expected for C <sub>6</sub> H <sub>3</sub> ClI <sub>2</sub> O; C, 18.95; H, 0.80; I, 66.7; Found: C, 18.90; H, 0.88; I, 66.74.

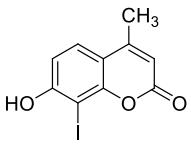
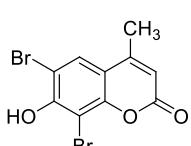
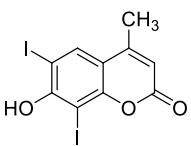
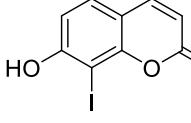
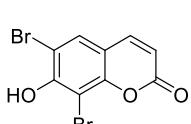
 18a	<p><b>MP</b> = 105-107 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 7.24 (d, <i>J</i> = 2.0 Hz, 2H), 6.58 (d, <i>J</i> = 3.1 Hz, 2H), 3.66 (s, 2H);</p> <p><b>Mass (ESI-MS)</b>: 185.98 [M<sup>+</sup>];</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>7</sub>N<sub>2</sub>Br; C, 38.53; H, 3.77; N, 14.98; Br, 42.72; Found: C, 38.65; H, 3.70; N, 14.97; Br, 42.79.</p>
 18b	<p><b>MP</b> = 102-106 °C.</p> <p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.24 – 7.21 (m, 2H), 6.58 – 6.55 (m, 2H), 3.68 (s, 2H). <b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 156.2, 137.6, 113.4.</p> <p><b>Mass (ESI-MS)</b>: 233.97 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>7</sub>IN<sub>2</sub>; C, 30.79; H, 3.01; I, 54.22; N, 11.97; Found: C, 30.81; H, 3.05; I, 54.21; N, 11.90.</p>
 18c	<p><b>MP</b> = 57-60 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 7.53 (d, <i>J</i> = 2.2 Hz, 1H), 7.20 (dd, <i>J</i> = 8.5, 2.2 Hz, 1H), 6.64 (d, <i>J</i> = 8.5 Hz, 1H), 4.09 (s, 2H);</p> <p><b>Mass (ESI-MS)</b>: 263.89 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>Br<sub>2</sub>; C, 27.10; H, 2.27; N, 10.53; Br, 60.09; Found: C, 27.19; H, 2.30; N, 10.56; Br, 60.11.</p>
 18d	<p><b>MP</b> = 110-112 °C.</p> <p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.52 (dd, <i>J</i> = 10.8, 2.4 Hz, 1H), 7.20 (dt, <i>J</i> = 8.5, 4.3 Hz, 1H), 6.64 (d, <i>J</i> = 8.5 Hz, 1H), 4.09 (s, 2H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 148.6, 140.1, 137.6, 118.5, 85.6, 81.8.</p> <p><b>Mass (ESI-MS)</b>: 359.86 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>6</sub>H<sub>6</sub>I<sub>2</sub>N<sub>2</sub>; C, 20.02; H, 1.68; I, 70.52; N, 7.78; Found: C, 20.10; H, 1.66; I, 70.55; N, 7.55.</p>
 19a	<p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 7.43 (d, <i>J</i> = 8.8 Hz, 2H), 6.40 (d, <i>J</i> = 8.7 Hz, 2H), 2.81 (s, 3H);</p> <p><b>Mass (ESI-MS)</b>: 184.96 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>8</sub>NBr; C, 45.19; H, 4.33; N, 7.53; Br, 42.95; Found: C, 45.15; H, 4.30; N, 7.54; Br, 42.90.</p>
 19b	<p><b>MP</b> = 30-33 °C.</p> <p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.43 (d, <i>J</i> = 8.8 Hz, 2H), 6.40 (d, <i>J</i> = 8.7 Hz, 2H), 2.81 (s, 3H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 148.6, 140.1, 118.5, 77.7, 31.4.</p> <p><b>Mass (ESI-MS)</b>: 232.97 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>8</sub>IN; C, 36.08; H, 3.46; I, 54.45; N, 6.01 Found: C, 36.10; H, 3.43; I, 54.47; N, 6.10.</p>

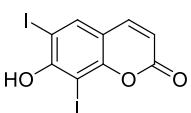
 19c	<p><b>MP</b> = 42-44 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 7.53 (d, <i>J</i> = 2.3 Hz, 1H), 7.26 (s, 1H), 6.48 (d, <i>J</i> = 8.7 Hz, 1H), 4.36 (s, 1H), 2.87 (s, 3H);</p> <p><b>Mass (ESI-MS)</b>: 262.89 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>7</sub>NBr<sub>2</sub>; C, 31.73; H, 2.66; N, 5.29; Br. 60.32; Found: C, 31.70; H, 2.65; N, 5.30; Br. 60.34.</p>
 19d	<p><b>MP</b> = 80-82 °C.</p> <p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.75 (d, <i>J</i> = 2.3 Hz, 1H), 7.30 (dd, <i>J</i> = 8.7, 2.3 Hz, 1H), 6.47 (d, <i>J</i> = 8.2 Hz, 1H), 4.36(s, 1H), 2.87 (s, 3H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 149.2, 145.1, 137.2, 116.3, 84.7, 82.8, 29.7.</p> <p><b>Mass (ESI-MS)</b>: 358.87 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>7</sub>H<sub>7</sub>I<sub>2</sub>N; C, 23.42; H, 1.97; I, 70.71; N; 3.90; Found: C, 23.40; H, 1.94; I, 70.70; N; 3.94.</p>
 20a	<p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.39 (d, <i>J</i> = 8.7 Hz, 2H), 6.51 (d, <i>J</i> = 8.7 Hz, 2H), 3.12 (q, <i>J</i> = 7.1 Hz, 2H), 1.24 (t, <i>J</i> = 7.1 Hz, 3H).</p> <p><b>Mass (ESI-MS)</b>: 200.08 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>8</sub>H<sub>10</sub>BrN; C, 48.02; H, 5.04; N, 7.00; Br. 39.94; N; 7.00; Found: C, 48.39; H, 5.06; N, 7.02; Br. 39.96.</p>
 20b	<p><b>MP</b> = 50-52 °C.</p> <p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.41 (d, <i>J</i> = 8.7 Hz, 2H), 6.40 (d, <i>J</i> = 8.7 Hz, 2H), 3.12 (q, <i>J</i> = 7.1 Hz, 2H), 1.24 (t, <i>J</i> = 7.1 Hz, 3H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 143.3, 134.5, 116.7, 45.9, 29.7.</p> <p><b>Mass (ESI-MS)</b>: 246.99 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>8</sub>H<sub>10</sub>IN; C, 38.89; H, 4.08; I, 51.36; N; 5.97; Found: C; 38.92; H, 4.10; I, 51.30; N; 5.95.</p>
 20c	<p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.78 (d, <i>J</i> = 2.1 Hz, 1H), 7.20 (dd, <i>J</i> = 8.2, 2.3 Hz, 1H), 6.38 (d, <i>J</i> = 8.7 Hz, 1H), 3.12 (q, <i>J</i> = 7.1 Hz, 2H), 1.24 (t, <i>J</i> = 7.1 Hz, 3H).</p> <p><b>Mass (ESI-MS)</b>: 278.97 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>8</sub>H<sub>9</sub>Br<sub>2</sub>N; C, 34.44; H, 3.25; N, 7.00; Br. 57.28; N; 5.02; Found: C, 34.45; H, 3.22; N, 6.96; Br. 57.31.</p>
 20d	<p><b>MP</b> = 65-67 °C.</p> <p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.53 (d, <i>J</i> = 2.3 Hz, 1H), 7.29 (dd, <i>J</i> = 8.7, 2.3 Hz, 1H), 6.48 (d, <i>J</i> = 8.7 Hz, 1H), 3.12 (q, <i>J</i> = 7.1 Hz, 2H), 1.24 (t, <i>J</i> = 7.1 Hz, 3H).</p> <p><b>Mass (ESI-MS)</b>: 372.88 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>8</sub>H<sub>9</sub>I<sub>2</sub>N; C, 25.76; H, 2.43; I, 68.05; N, 3.76; Found: C, 25.79; H, 2.40; I, 68.10; N; 3.79.</p>

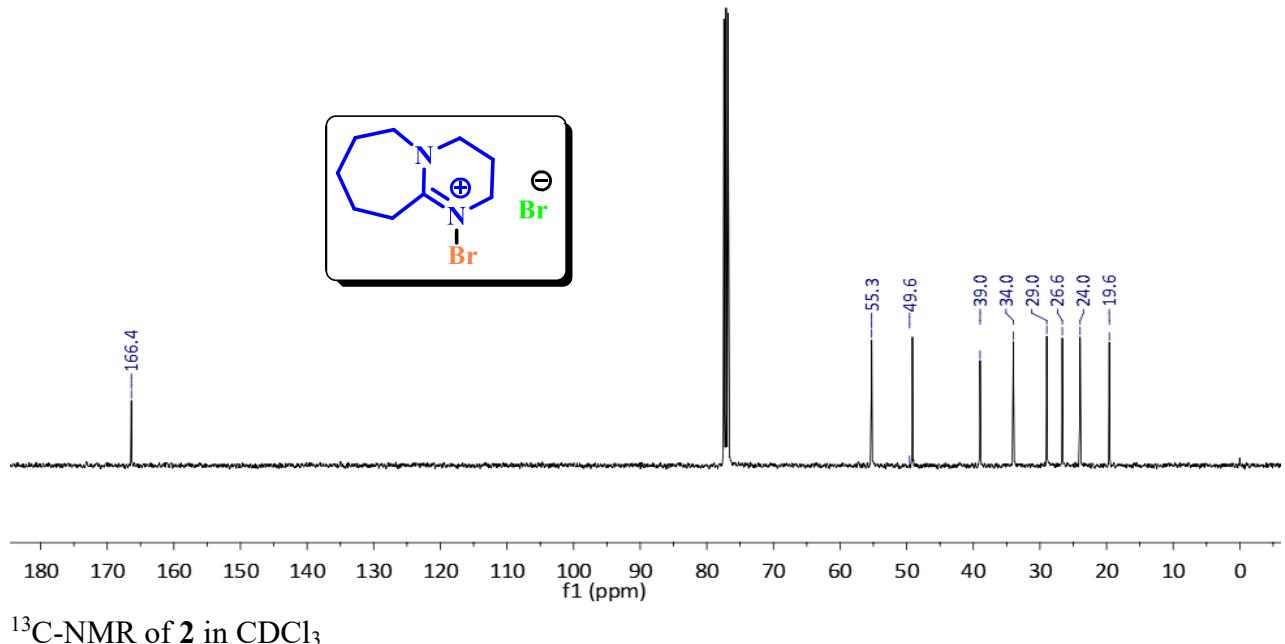
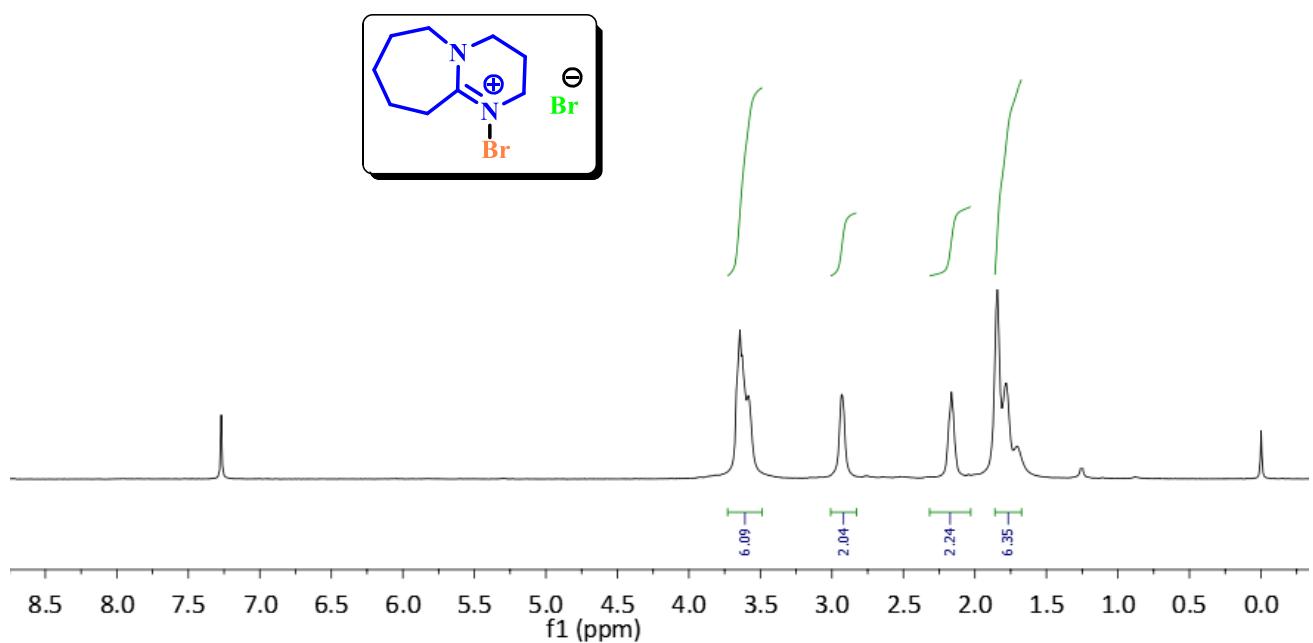
 21a	<p><b>MP</b> = 52-54 °C.</p> <p><b>1H NMR (400 MHz, in CDCl3):</b> δ 7.43 (d, <i>J</i> = 2.1 Hz, 2H), 6.65 (d, <i>J</i> = 9.0 Hz, 2H), 2.92 (s, 6H);</p> <p><b>Mass (ESI-MS):</b> 199.00 [M+].</p> <p><b>CHN:</b> Expected for CHN: Expected for C<sub>8</sub>H<sub>10</sub>NBr; C, 48.02; H, 5.04; N, 7.00; Br, 39.94; Found: C, 48.05; H, 5.06; N, 7.10; Br, 39.99.</p>
 21b	<p><b>MP</b> = 63-65 °C.</p> <p><b>1H NMR (400 MHz, in CDCl3):</b> δ 7.47 (d, <i>J</i> = 2.1 Hz, 2H), 6.49 (d, <i>J</i> = 9.0 Hz, 2H), 2.92 (s, 6H);</p> <p><b>13C NMR (100 MHz, in CDCl3):</b> 150.0, 137.5, 114.7, 77.4, 40.3.</p> <p><b>Mass (ESI-MS):</b> 246.99 [M+].</p> <p><b>CHN:</b> Expected for C<sub>8</sub>H<sub>10</sub>IN; C, 38.89; H, 4.08; I, 51.36; N, 5.67; Found: C, 38.80; H, 4.08; I, 51.39; N, 5.60.</p>
 21c	<p><b>MP</b> = 52-54 °C.</p> <p><b>1H NMR (400 MHz, in CDCl3):</b> δ 7.31 – 7.28 (m, 1H), 6.93 (d, <i>J</i> = 8.6 Hz, 1H), 6.60 – 6.56 (m, 1H), 2.92 (s, 6H);</p> <p><b>Mass (ESI-MS):</b> 199.00 [M+].</p> <p><b>CHN:</b> Expected for C<sub>8</sub>H<sub>9</sub>NBr<sub>2</sub>; C, 48.02; H, 5.04; N, 7.00; Br, 39.94; Found: C, 48.05; H, 5.06; N, 7.10; Br, 39.99.</p>
 21d	<p><b>MP</b> = 70-72 °C.</p> <p><b>1H NMR (400 MHz, in CDCl3):</b> 7.53 (d, <i>J</i> = 2.2 Hz, 1H), 7.29 (dd, <i>J</i> = 5.2, 2.6 Hz, 1H), 6.48 (d, <i>J</i> = 8.7 Hz, 1H), 2.87 (s, 6H);</p> <p><b>Mass (ESI-MS):</b> 372.88 [M+].</p> <p><b>CHN:</b> Expected for C<sub>8</sub>H<sub>9</sub>I<sub>2</sub>N; C, 25.76; H, 2.43; I, 68.05; N, 3.76; Found: C, 25.74; H, 2.40; I, 68.15; N, 3.70.</p>
 25a	<p><b>MP</b> = 79-80 °C.</p> <p><b>1H NMR (400 MHz, in CDCl3):</b> δ 7.92 (dd, <i>J</i> = 14.7, 5.3 Hz, 2H), 7.69 – 7.57 (m, 3H), 7.28 (d, <i>J</i> = 5.7 Hz, 1H), 5.93 (s, 1H);</p> <p><b>Mass (ESI-MS):</b> 223.1 [M+].</p> <p><b>CHN:</b> Expected for C<sub>10</sub>H<sub>7</sub>BrO; C, 53.84; H, 3.16; Br, 35.82; Found: C, 53.87; H, 3.14; Br, 35.78.</p>
 25b	<p><b>MP</b> = 108-110 °C.</p> <p><b>1H NMR (400 MHz, CDCl3):</b> δ 7.93 (d, <i>J</i> = 8.5 Hz, 1H), 7.76 – 7.72 (m, 2H), 7.55 (t, <i>J</i> = 7.7 Hz, 1H), 7.38 (t, <i>J</i> = 7.5 Hz, 1H), 7.26 (d, <i>J</i> = 1.5 Hz, 1H), 5.79 (s, 1H);</p> <p><b>13C NMR (100 MHz, in CDCl3):</b> 153.7, 134.7, 131.6, 130.2, 129.66, 128.2, 124.1, 116.4, 86.2.</p> <p><b>Mass (ESI-MS):</b> 269.95 [M+].</p> <p><b>CHN:</b> Expected for C<sub>10</sub>H<sub>7</sub>IO; C, 44.47; H, 2.61; I, 46.99; Found: C, 44.44; H, 2.69; I, 46.90.</p>

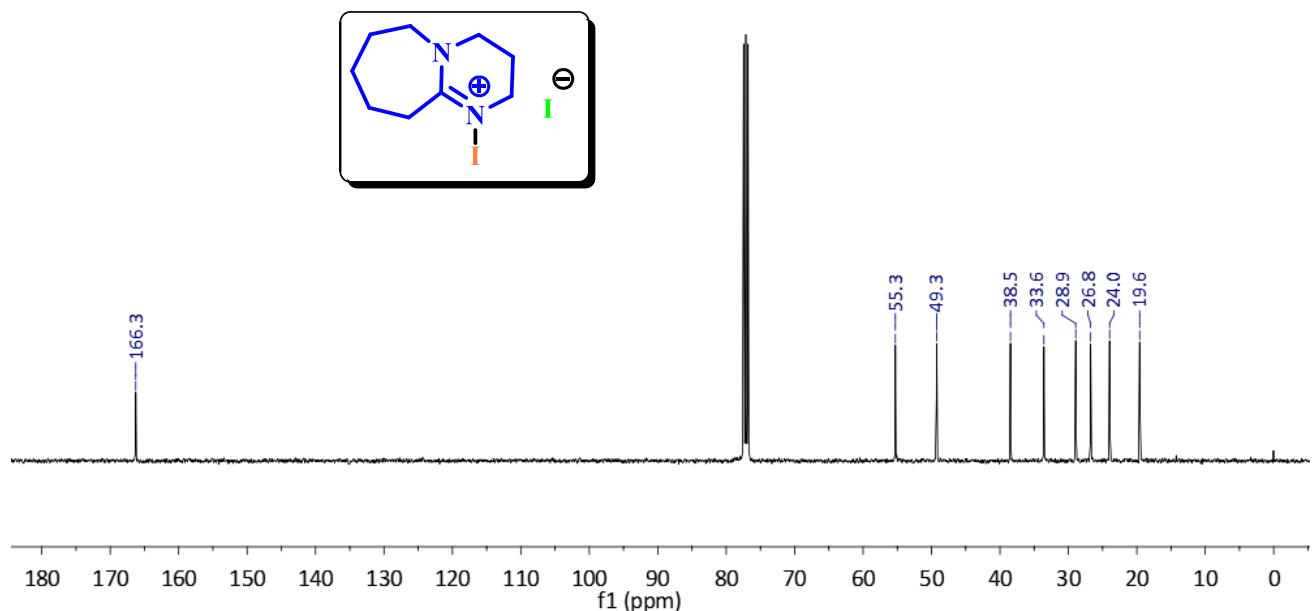
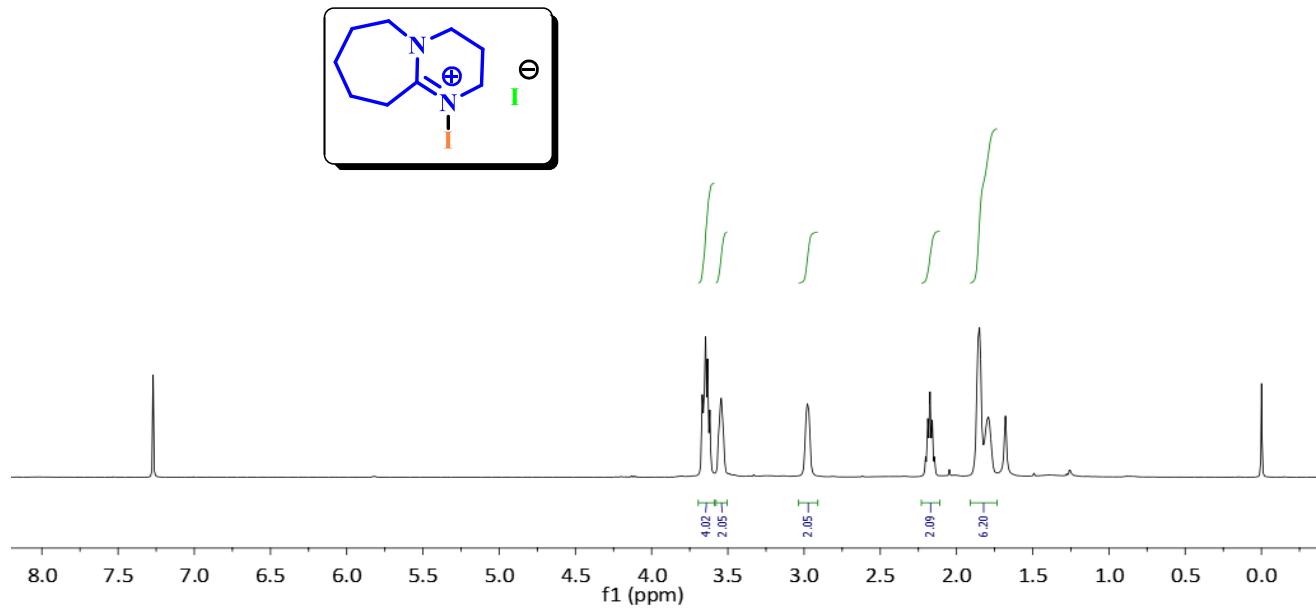
 25c	<p><b>MP</b> = 105-106 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 8.16 (d, <i>J</i> = 1.6 Hz, 1H), 7.81-7.79 (m, 2H), 7.65-7.61 (m, 2H), 5.93 (s, 1H);</p> <p><b>Mass (ESI-MS)</b>: 301.9 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>10</sub>H<sub>6</sub>Br<sub>2</sub>O; C, 39.78; H, 2.00; Br, 52.92; Found: C, 39.81; H, 2.04; Br, 52.89.</p>
 25d	<p><b>MP</b> = 120-123 °C.</p> <p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.92 (dd, <i>J</i> = 14.7, 5.3 Hz, 2H), 7.69-7.62 (m, 2H), 7.29 (s, 1H), 5.93 (s, 1H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 150.6, 132.3, 129.7, 129.4, 127.9, 125.4, 124.2, 85.2, 82.3.</p> <p><b>Mass (ESI-MS)</b>: 395.85 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>10</sub>H<sub>6</sub>I<sub>2</sub>O; C, 30.33; H, 1.53; I, 64.10; Found: C, 30.37; H, 1.55; I, 64.08.</p>
 26a	<p><b>MP</b> = 43-45 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 8.03 (d, <i>J</i> = 8.5 Hz, 1H), 7.79 – 7.73 (m, 2H), 7.57 (t, <i>J</i> = 7.7 Hz, 1H), 7.39 (t, <i>J</i> = 7.5 Hz, 1H), 7.27 (d, <i>J</i> = 7.5 Hz, 1H), 5.92 (s, 1H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 150.6, 134.1, 132.3, 128.3, 127.9, 126.8, 124.2, 122.6, 121.3, 106.2.</p> <p><b>Mass (ESI-MS)</b>: 221.97 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>10</sub>H<sub>7</sub>OB<sub>r</sub>; C, 53.84; H, 3.16; O, 7.17; Br, 35.82; Found: C, 53.88; H, 3.11; O, 7.19; Br, 35.80.</p>
 26b	<p><b>MP</b> = 92-96 °C.</p> <p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 8.23 (d, <i>J</i> = 8.5 Hz, 1H), 8.06 (dd, <i>J</i> = 15.8, 8.5 Hz, 2H), 7.57 (t, <i>J</i> = 7.7 Hz, 1H), 7.39 (t, <i>J</i> = 7.5 Hz, 1H), 7.27 (d, <i>J</i> = 4.8 Hz, 1H), 5.91 (s, 1H).</p> <p><b>Mass (ESI-MS)</b>: 269.95 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>10</sub>H<sub>7</sub>IO; C, 44.47; H, 2.61; I, 46.99; Found: C, 44.44; H, 2.69; I, 46.90.</p>
 26c	<p><b>MP</b> = 105-107 °C.</p> <p><b>1H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: δ 8.25 (d, <i>J</i> = 8.4 Hz, 1H), 8.13 (d, <i>J</i> = 8.4 Hz, 1H), 7.80 (s, 1H), 7.61-7.56 (m, 2H), 5.97 (s, 1H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 150.6, 132.3, 129.7, 129.4, 127.9, 125.4, 124.2, 119.9, 114.2, 106.2.</p> <p><b>Mass (ESI-MS)</b>: 299.88 [M<sup>+</sup>]; 301.88 (M+2) 303.88 (M+4);</p> <p><b>CHN</b>: Expected for C<sub>10</sub>H<sub>6</sub>OB<sub>r</sub><sub>2</sub>; C, 39.78; H, 2.00; O, 5.30; Br, 52.9; Found: C, 39.80; H, 2.10; O, 5.35; Br, 52.99.</p>
 26d	<p><b>MP</b> = 110-112 °C.</p> <p><b>1H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 8.25 (d, <i>J</i> = 8.4 Hz, 1H), 8.13 (d, <i>J</i> = 8.4 Hz, 1H), 7.80 (s, 1H), 7.59 (dd, <i>J</i> = 14.3, 3.6 Hz, 2H), 5.97 (s, 1H).</p> <p><b>13C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 163.7, 148.3, 136.9, 132.3, 129.7, 129.4, 128.3, 123.4, 92.8, 76.7.</p> <p><b>Mass (ESI-MS)</b>: 395.85 [M<sup>+</sup>].</p> <p><b>CHN</b>: Expected for C<sub>10</sub>H<sub>6</sub>I<sub>2</sub>O; C, 30.33; H, 1.53; I, 64.10; Found: C,</p>

	30.37; H, 1.55; I, 64.08.
27a 	<b>MP</b> = 140-142 °C. <b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>):</b> δ 8.77 (dd, <i>J</i> = 4.3, 1.5 Hz, 1H), 8.15 (dd, <i>J</i> = 8.3, 1.5 Hz, 1H), 7.79 (d, <i>J</i> = 4.4 Hz, 1H), 7.48 (dd, <i>J</i> = 8.3, 4.3 Hz, 1H), 7.14 (d, <i>J</i> = 8.8 Hz, 1H). <b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 152.5, 150.6, 140.2, 132.3, 129.4, 125.4, 124.2, 121.7, 106.2. <b>Mass (ESI-MS):</b> 222.96 [M+]. <b>CHN:</b> Expected for C <sub>9</sub> H <sub>6</sub> NBrO; C, 48.25; H, 2.70; N, 6.25; Br. 35.66; Found: C, 48.30; H, 2.69; N, 6.24; Br. 35.62.
27b 	<b>MP</b> = 150-153 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 8.77 (dd, <i>J</i> = 4.3, 1.5 Hz, 1H), 8.15 (dd, <i>J</i> = 8.3, 1.5 Hz, 1H), 7.82 (m, 1H), 7.48 (dd, <i>J</i> = 8.3, 4.3 Hz, 1H), 7.14 (d, <i>J</i> = 8.8 Hz, 1H). <b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 153.0, 148.6, 137.5, 136.2, 135.2, 128.1, 122.3, 119.3, 77.5. <b>Mass (ESI-MS):</b> 270.95 [M+]. <b>CHN:</b> Expected for C <sub>9</sub> H <sub>6</sub> ION; C, 39.88; H, 2.23; I, 46.82; N, 5.17; Found: C, 39.80; H, 2.25; I, 46.79; N, 5.11.
27c 	<b>MP</b> = 197-199 °C. <b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>):</b> 8.82 (dd, <i>J</i> = 4.0, 1.2 Hz, 1H), 8.47 (dd, <i>J</i> = 8.2, 1.2 Hz, 1H), 7.91 (s, 1H), 7.59 (dd, <i>J</i> = 8.2, 4.0 Hz, 1H). <b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 153.1, 150.6, 135.0, 132.3, 129.7, 129.4, 124.2, 121.0, 120.4. <b>Mass (ESI-MS):</b> 302.9 [M+]. <b>CHN:</b> Expected for C <sub>9</sub> H <sub>5</sub> Br <sub>2</sub> NO; C, 35.68; H, 1.66; Br, 52.75; N, 4.62; O, 5.28; Found: C, 35.71; H, 1.65; Br, 52.78, N, 4.60, O, 5.25.
27d 	<b>MP</b> = 202-205 °C. <b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 8.74 (d, <i>J</i> = 4.2 Hz, 1H), 8.32 (s, 1H), 8.29 (d, <i>J</i> = 1.2 Hz, 1H), 7.56 (dd, <i>J</i> = 8.5, 4.2 Hz, 1H). <b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 153.0, 147.8, 146.1, 137.5, 136.2, 128.2, 85.7, 80.7. <b>Mass (ESI-MS):</b> 396.8 [M+]. <b>CHN:</b> Expected for C <sub>9</sub> H <sub>5</sub> I <sub>2</sub> ON; C, 27.23; H, 1.27; I, 63.94; N, 3.53; Found: C, 27.24; H, 1.20; I, 63.89; N, 3.59.
28a 	<b>MP</b> = 215-217 °C. <b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>):</b> δ 7.51 (d, <i>J</i> = 8.7 Hz, 1H), 7.00 (d, <i>J</i> = 5.1 Hz, 1H), 6.16 (s, 1H), 5.95 (s, 1H), 2.42 (S, 3H). <b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>):</b> 162.3, 157.0, 152.9, 148.8, 130.8, 114.2, 112.8, 107.8, 21.4. <b>Mass (ESI-MS):</b> 254.99 [M+]. <b>CHN:</b> Expected for C <sub>10</sub> H <sub>7</sub> O <sub>3</sub> Br; C, 46.90; H, 3.94; N, 5.47; Br, 31.20; Found: C, 46.96; H, 3.90; N, 5.49; Br, 31.25.

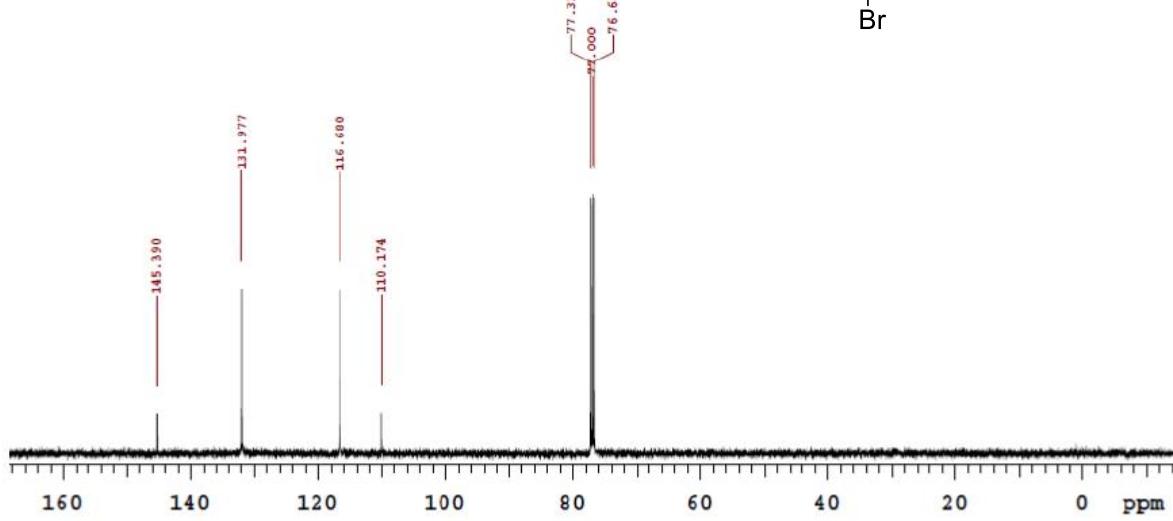
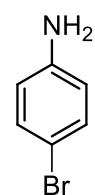
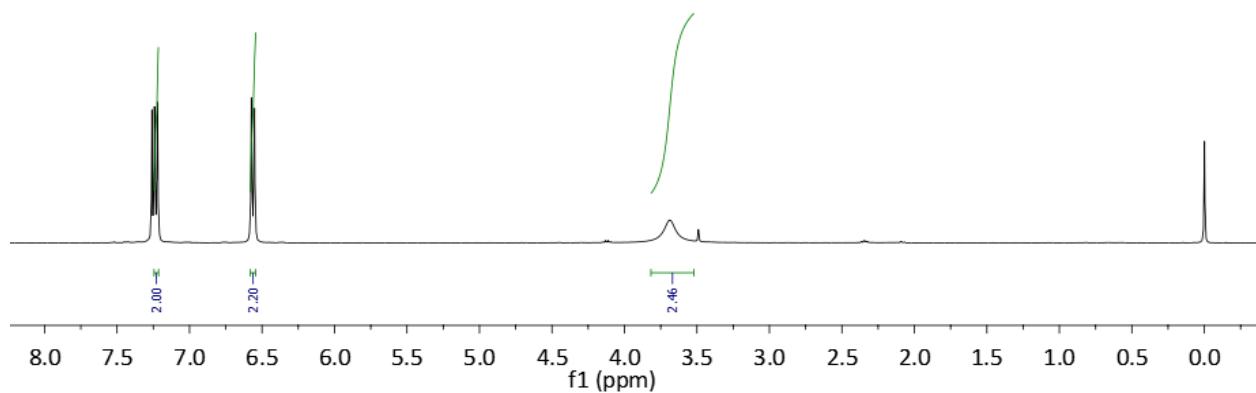
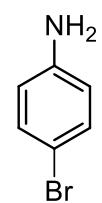
 28b	<p><b>MP</b> = 234-236 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.51 (d, <i>J</i> = 8.7 Hz, 1H), 7.00 (d, <i>J</i> = 8.7 Hz, 1H), 6.15 (d, <i>J</i> = 9.0 Hz, 1H), 5.94 (s, 1H), 2.42 (s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 162.1, 161.0, 155.2, 151.7, 133.9, 113.5, 110.3, 108.1, 82.1, 18.7.</p> <p><b>Mass (ESI-MS)</b>: 301.94 [M+].</p> <p><b>CHN</b>: Expected for C<sub>10</sub>H<sub>7</sub>IO<sub>3</sub>; C, 39.76; H, 2.34; I, 42.01; Found C, 39.79; H, 2.30; I, 42.41.</p>
 28c	<p><b>MP</b> = 279-280 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, in CDCl<sub>3</sub>)</b>: 7.94 (s, 1H), 6.16 (s, 1H), 2.41 (s, 3H).</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 162.6, 152.2, 150.0, 148.5, 130.9, 129.4, 114.2, 122.8, 107.8, 19.2.</p> <p><b>Mass (ESI-MS)</b>: 333.9 [M+].</p> <p><b>CHN</b>: Expected for C<sub>10</sub>H<sub>6</sub>Br<sub>2</sub>O<sub>3</sub>; C, 35.97; H, 1.81; Br, 47.85; Found: C, 35.99; H, 1.84; Br, 47.82.</p>
 28d	<p><b>MP</b> = 252-254 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: δ 7.94 (s, 1H), 6.16 (s, 1H), 2.41 (s, 3H)</p> <p><b><sup>13</sup>C NMR (100 MHz, in CDCl<sub>3</sub>)</b>: 162.2, 161.1, 151.7, 148.2, 133.9, 116.3, 113.5, 85.2, 82.8, 18.7.</p> <p><b>Mass (ESI-MS)</b>: 427.84 [M+].</p> <p><b>CHN</b>: Expected for C<sub>10</sub>H<sub>6</sub>I<sub>2</sub>O<sub>3</sub>; C, 28.06; H, 1.41; I, 59.31; Found: C, 28.23; H, 1.38; I, 59.45.</p>
 29a	<p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: 7.79 (d, <i>J</i>=8.4 Hz, 1H), 7.51 (d, <i>J</i> = 8.7 Hz, 1H), 6.85 (d, <i>J</i> = 3.7 Hz, 1H), 6.13 (d, <i>J</i> = 1.1 Hz, 1H).</p> <p><b>Mass (ESI-MS)</b>: 241.04 [M+].</p> <p><b>CHN</b>: Expected for C<sub>9</sub>H<sub>5</sub>BrO<sub>3</sub>; C, 44.85; H, 2.09; Br, 33.15; Found: C, 44.82; H, 2.11; Br, 33.17.</p>
 29b	<p><b>MP</b> = 140-142 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: 7.68 (d, <i>J</i>=8.41 Hz, 1H), 7.51 (d, <i>J</i> = 8.7 Hz, 1H), 6.99 (d, <i>J</i> = 3.7 Hz, 1H), 6.16 (d, <i>J</i> = 1.1 Hz, 1H).</p> <p><b>Mass (ESI-MS)</b>: 287.93 [M+].</p> <p><b>CHN</b>: Expected for C<sub>9</sub>H<sub>5</sub>IO<sub>3</sub>; C, 37.53; H, 1.75; I, 44.06; Found: C, 37.50; H, 1.74; I, 44.10.</p>
 29c	<p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)</b>: 7.96 (s, 1H), 7.78 (d, <i>J</i> = 8.7 Hz, 1H), 6.25 (d, <i>J</i> = 1.1 Hz, 1H).</p> <p><b>Mass (ESI-MS)</b>: 319.93 [M+].</p> <p><b>CHN</b>: Expected for C<sub>9</sub>H<sub>4</sub>Br<sub>2</sub>O<sub>3</sub>; C, 33.79; H, 1.26; Br, 49.95; Found: C, 33.81; H, 1.28; Br, 49.93.</p>

 29d	<p><b>MP</b> = 165-167 °C.</p> <p><b><sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):</b> δ 7.85 (s, 2H), 7.53 (d, <i>J</i> = 9.5 Hz, 2H), 6.29 (d, <i>J</i> = 5.0 Hz, 1H).</p> <p><b>Mass (ESI-MS):</b> 413.82 [M+].</p> <p><b>CHN:</b> Expected) for C<sub>9</sub>H<sub>4</sub>I<sub>2</sub>O<sub>3</sub>; C, 26.11; H, 0.97; I, 61.32; Found: C, 26.15; H, 0.95; I, 61.30.</p>
--	---

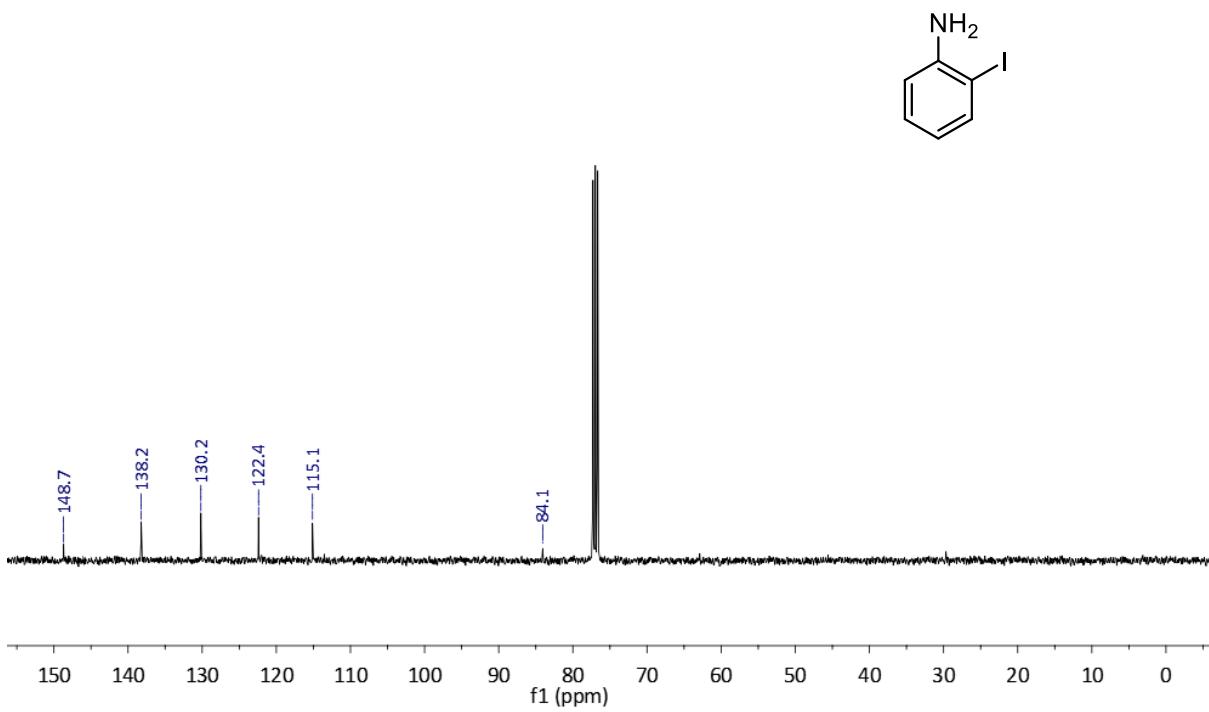
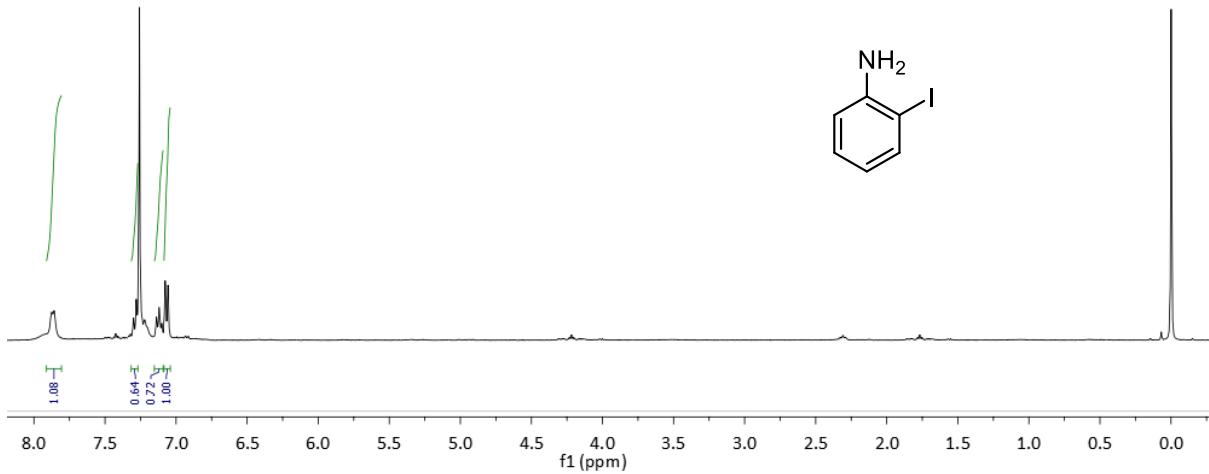


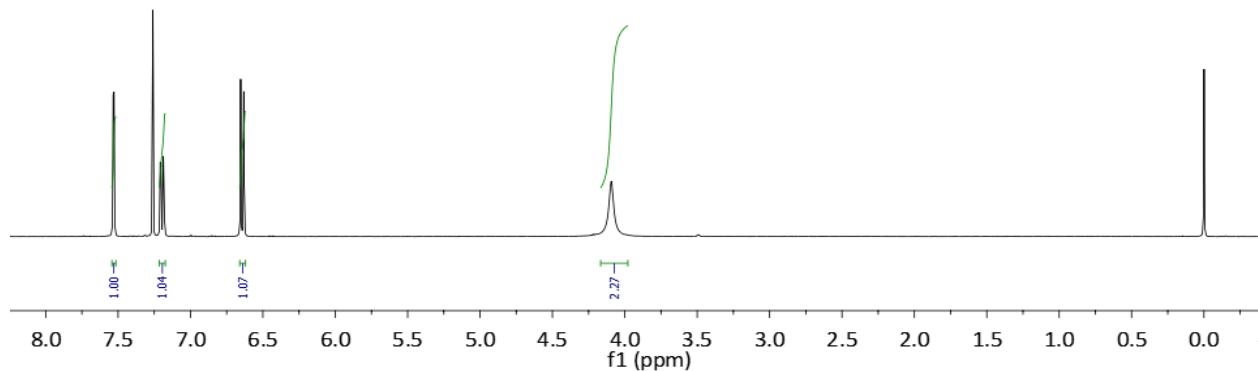
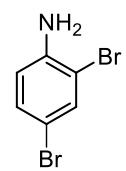


<sup>13</sup>C-NMR of **3** in CDCl<sub>3</sub>

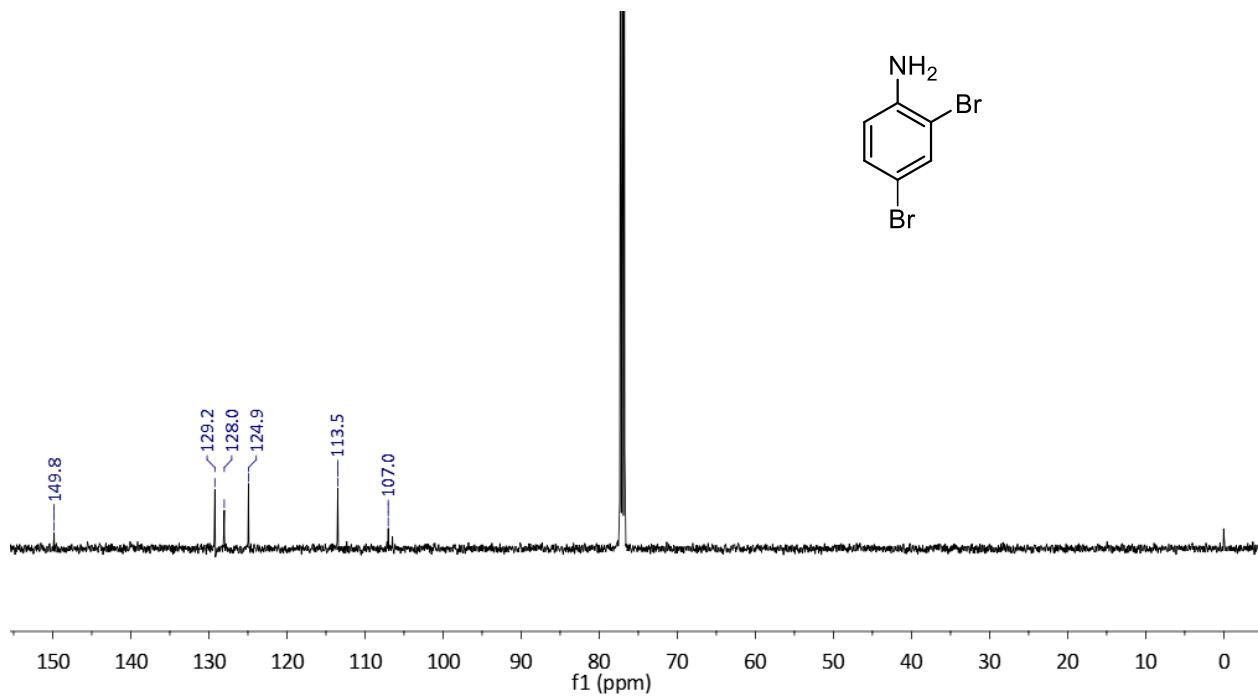


<sup>13</sup>C-NMR of 4a in CDCl<sub>3</sub>

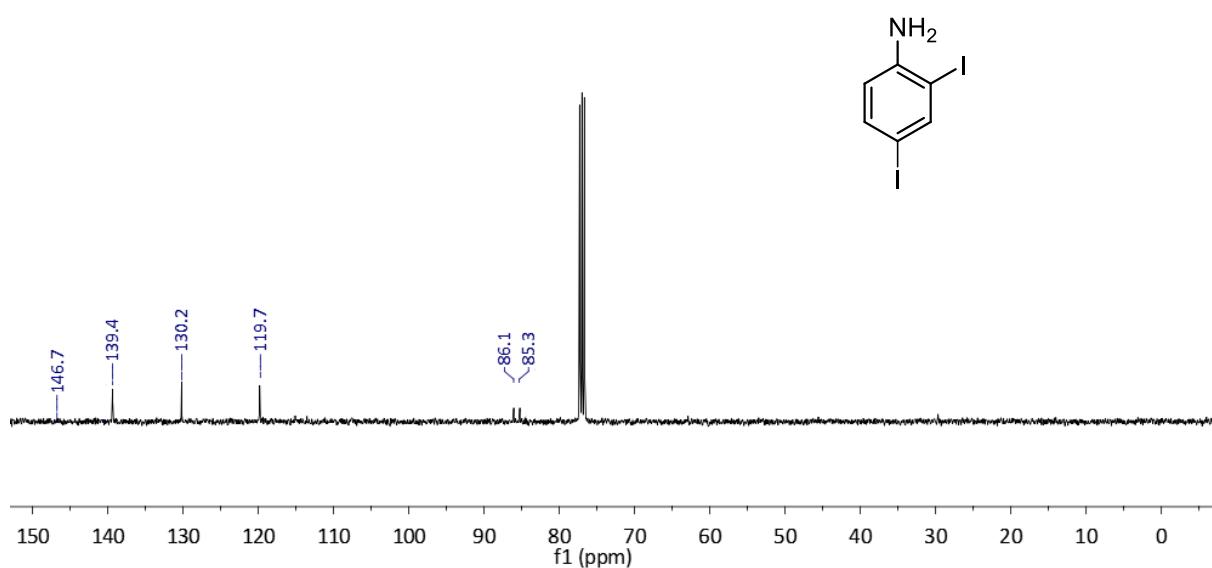
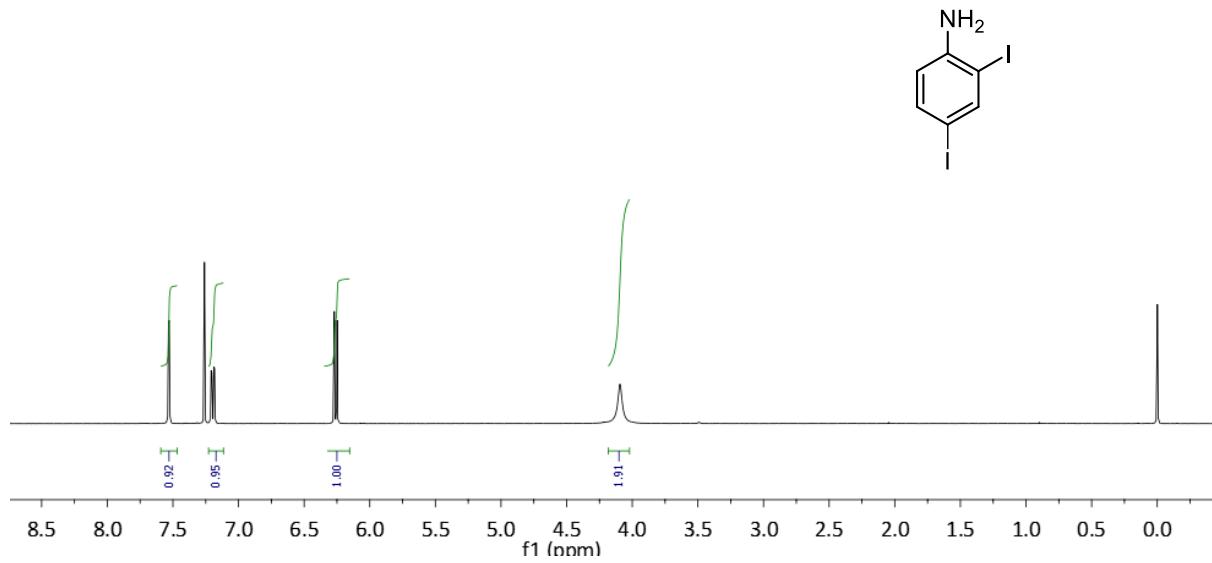


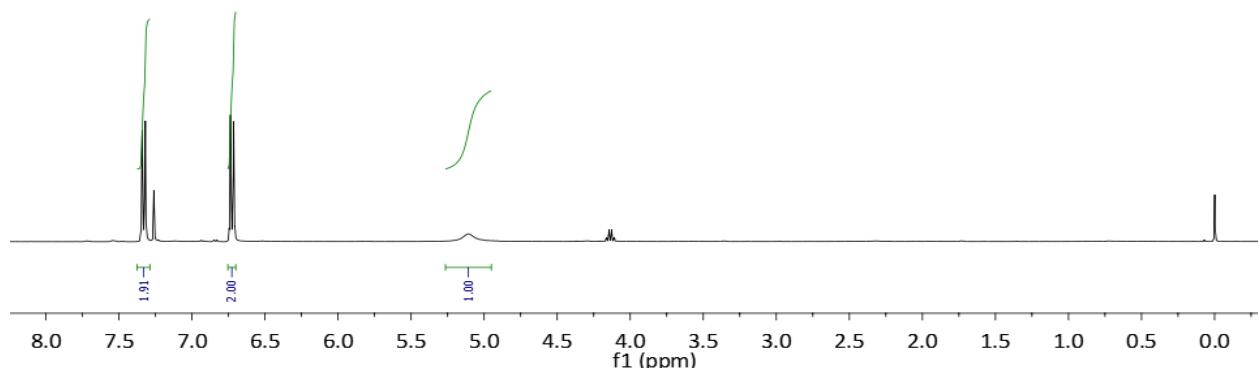
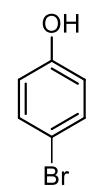


<sup>1</sup>H-NMR of 4c in CDCl<sub>3</sub>

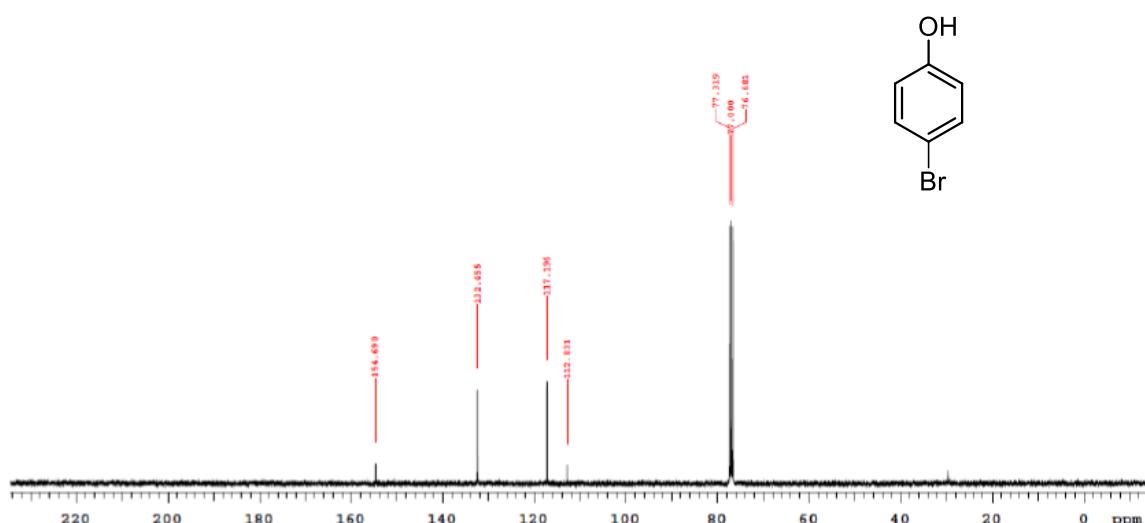


<sup>13</sup>C NMR of 4c in CDCl<sub>3</sub>

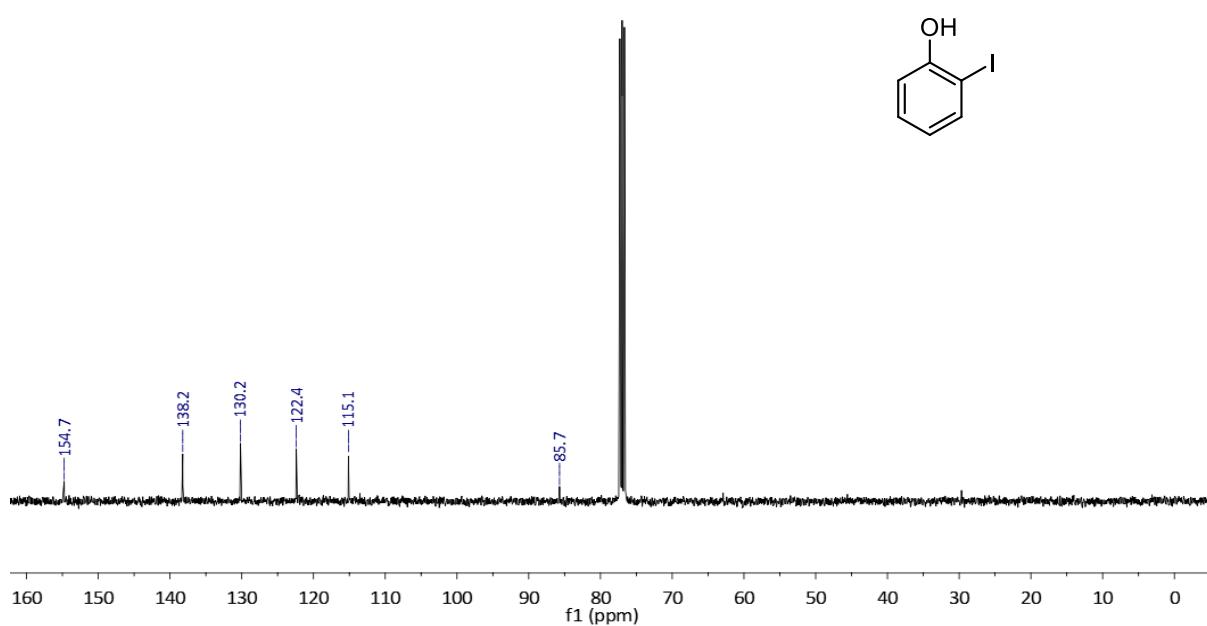
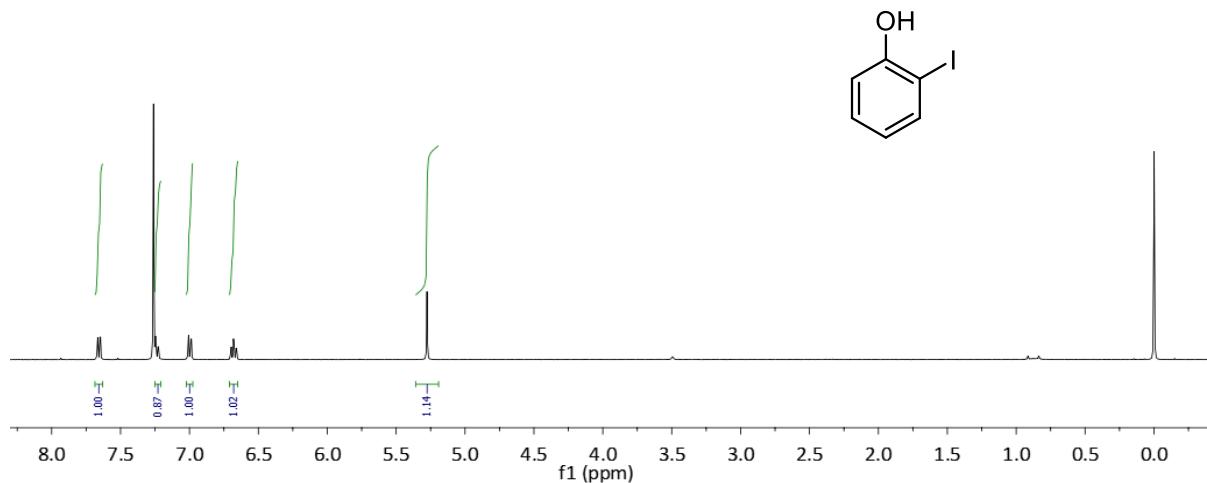


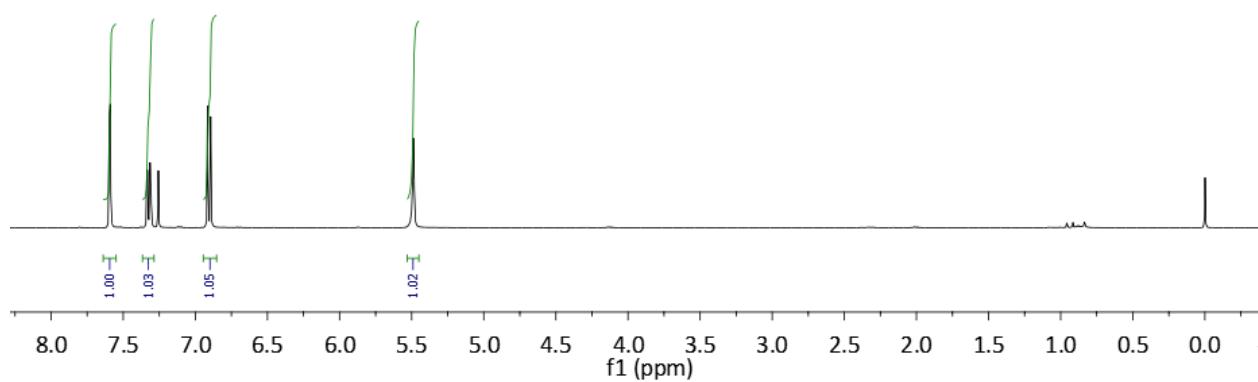
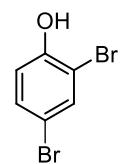


<sup>1</sup>H-NMR of 5a in CDCl<sub>3</sub>

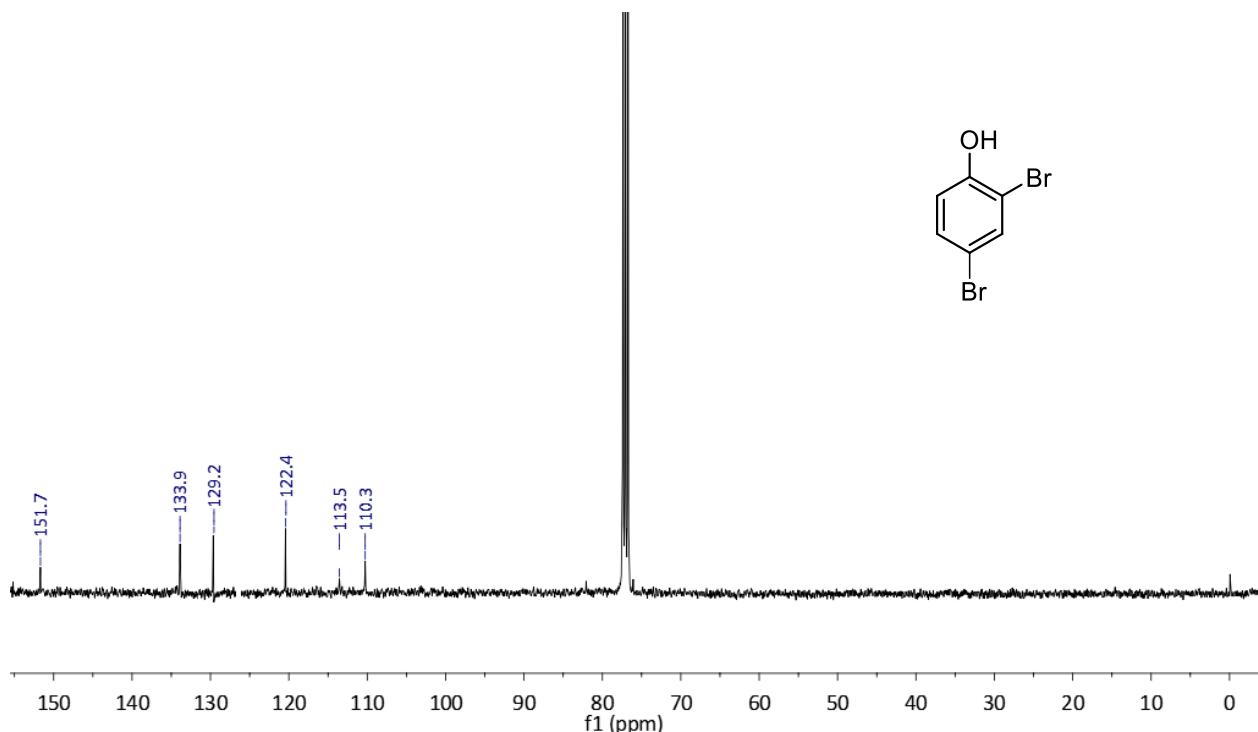


<sup>13</sup>C NMR of 5a in CDCl<sub>3</sub>

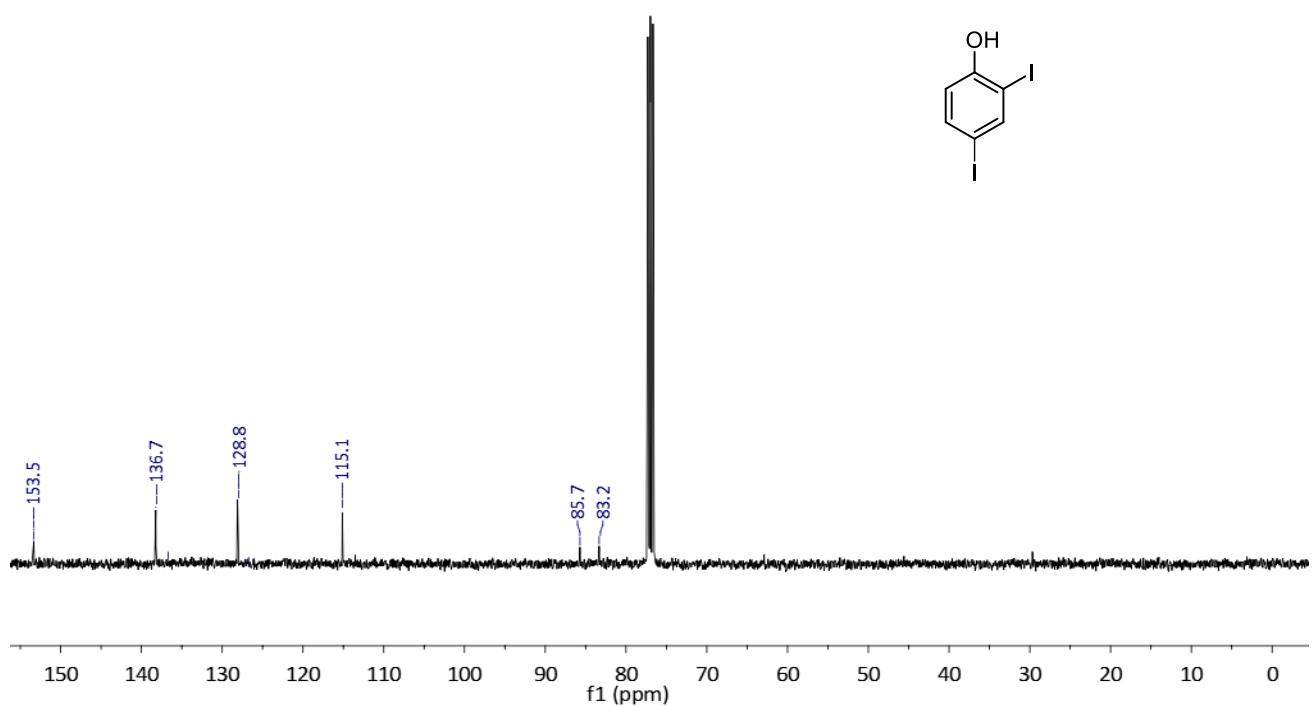
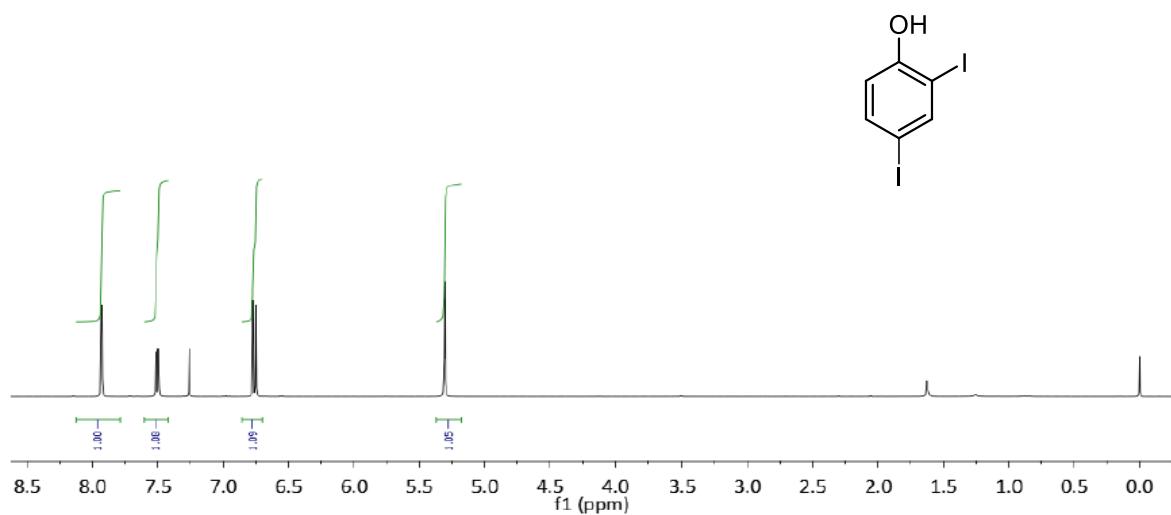


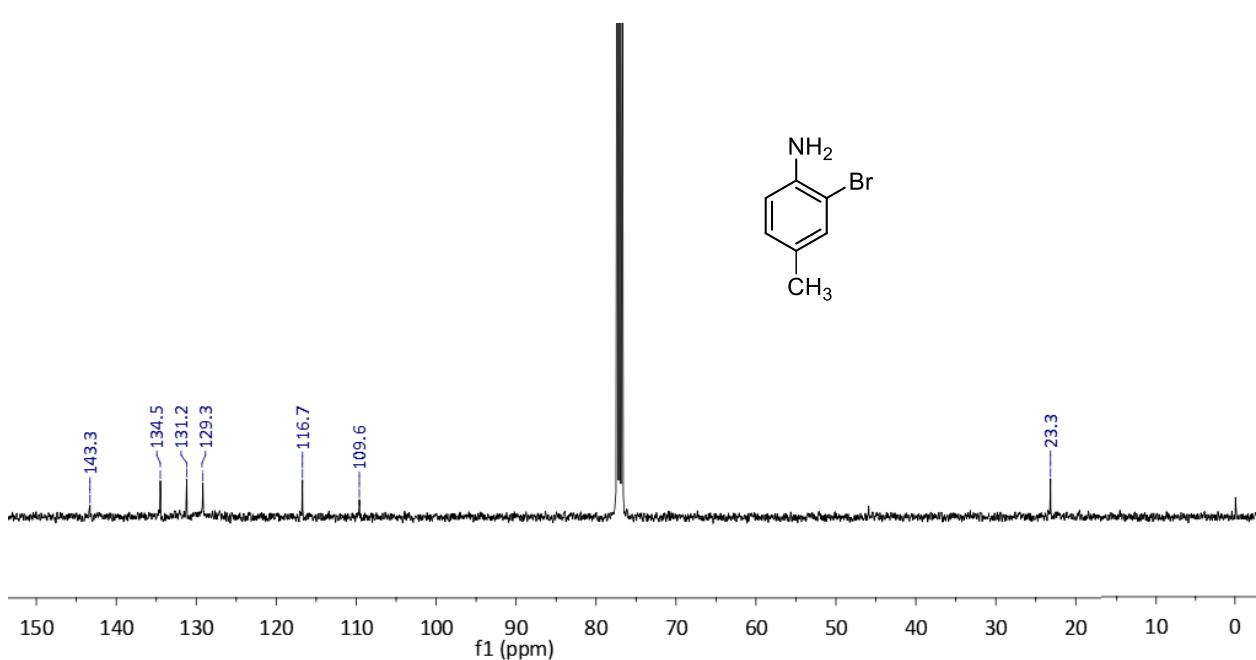
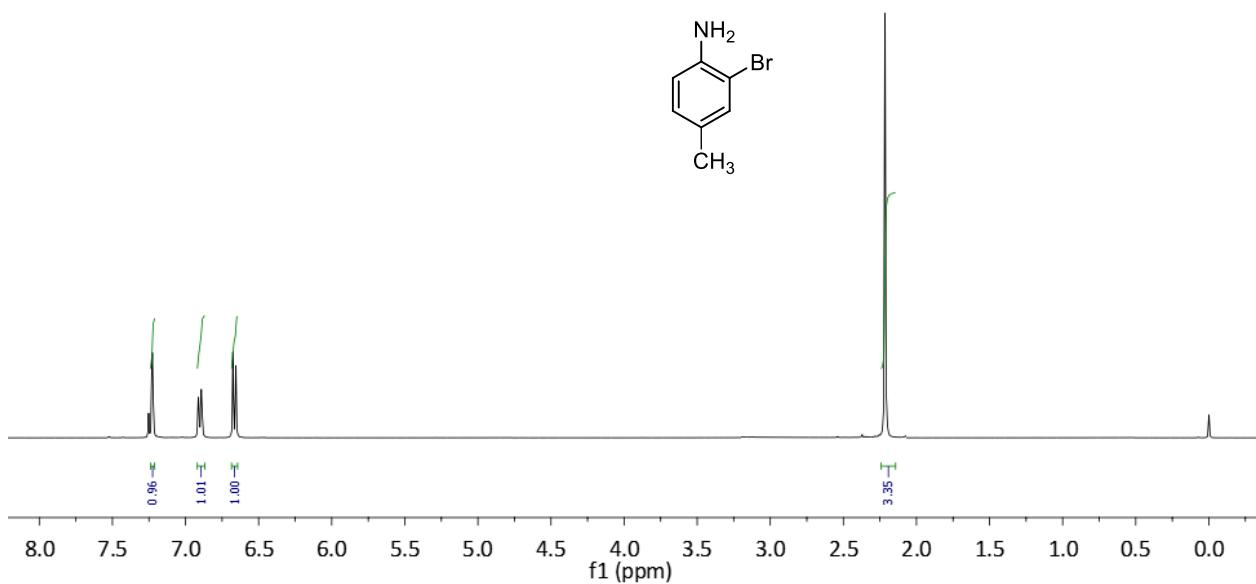


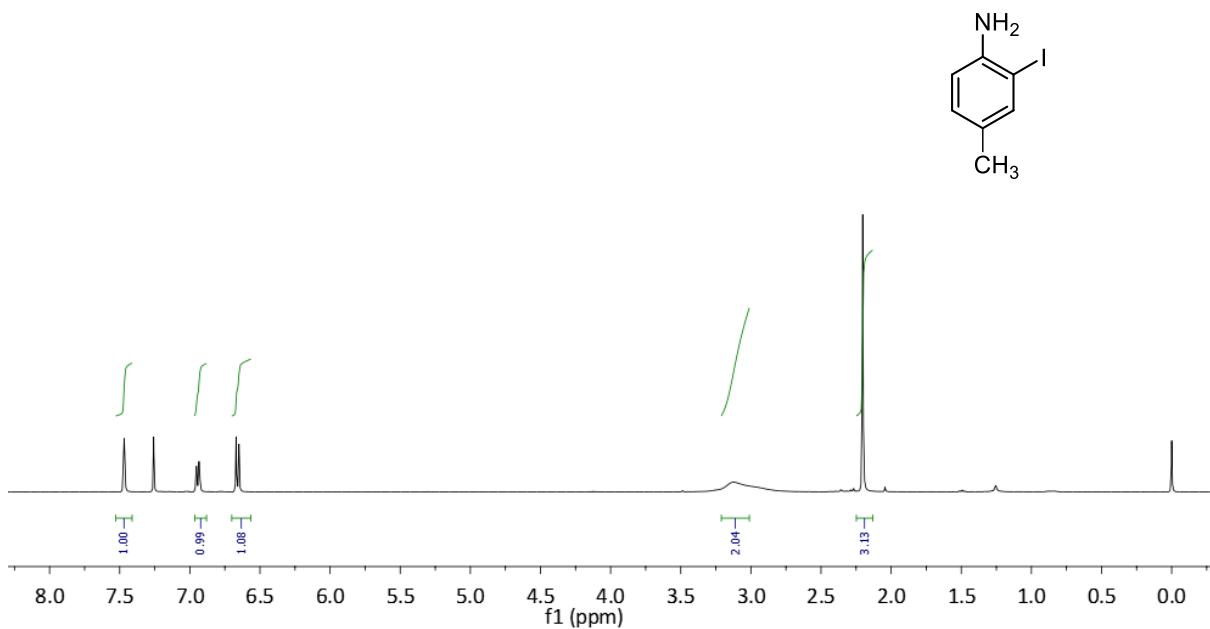
<sup>1</sup>H-NMR of 5c in CDCl<sub>3</sub>



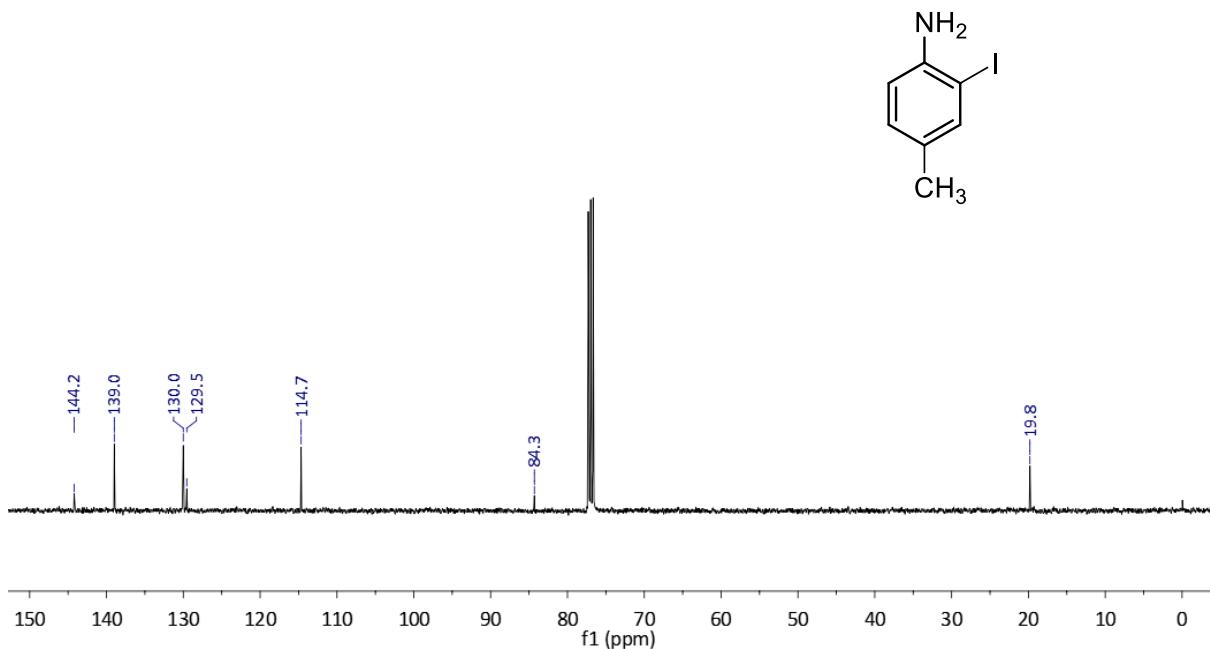
<sup>13</sup>C NMR of 5c in CDCl<sub>3</sub>



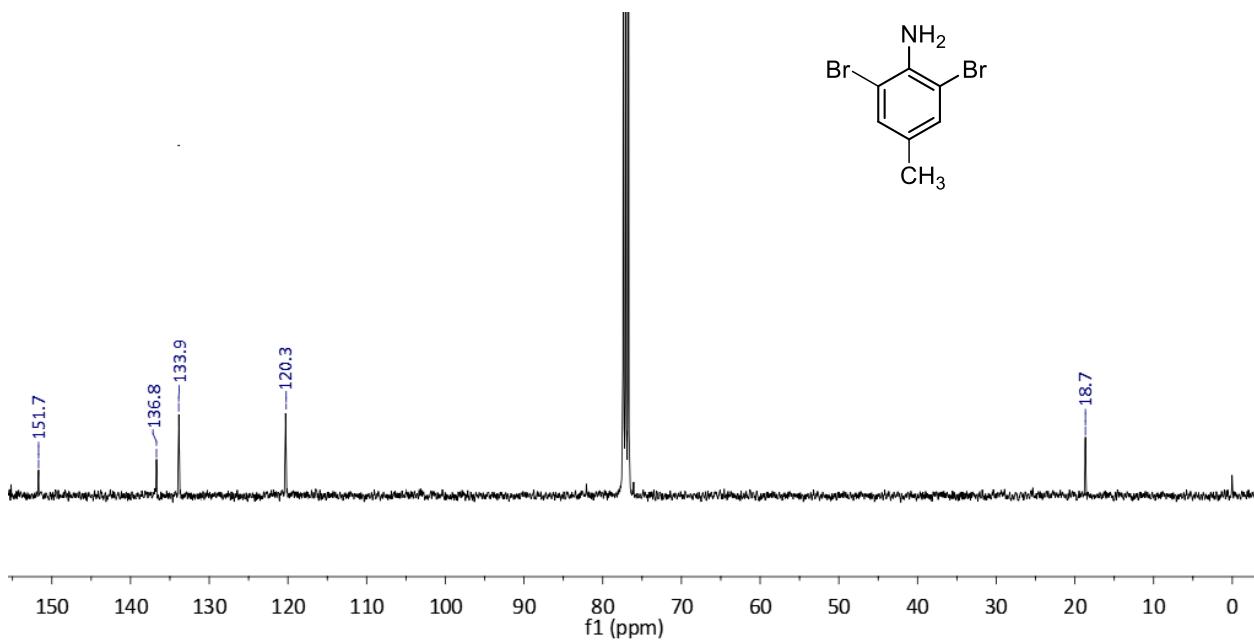
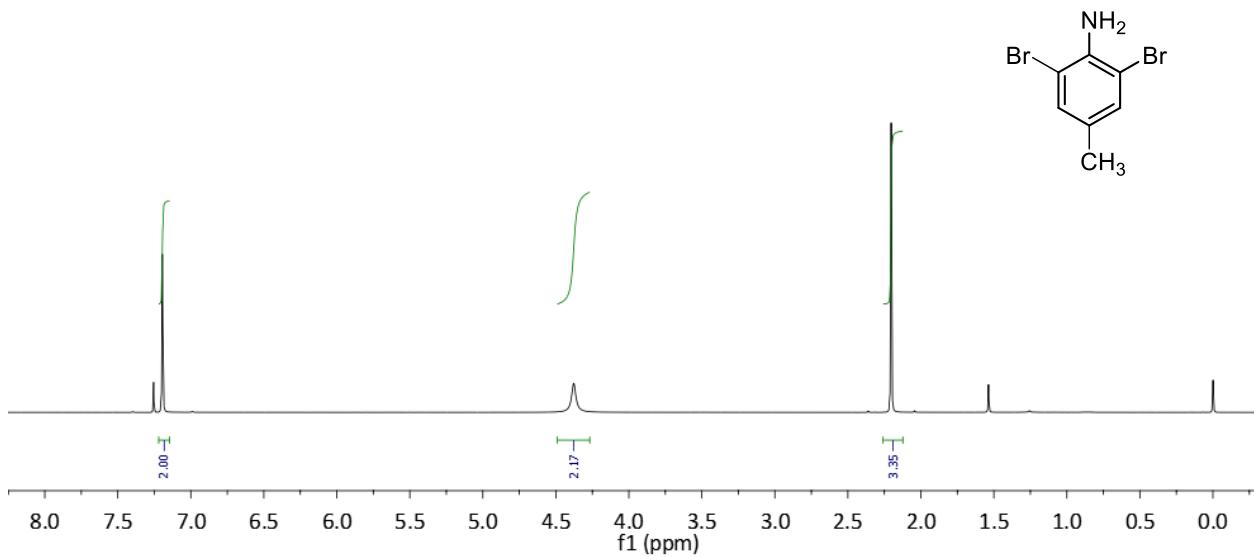


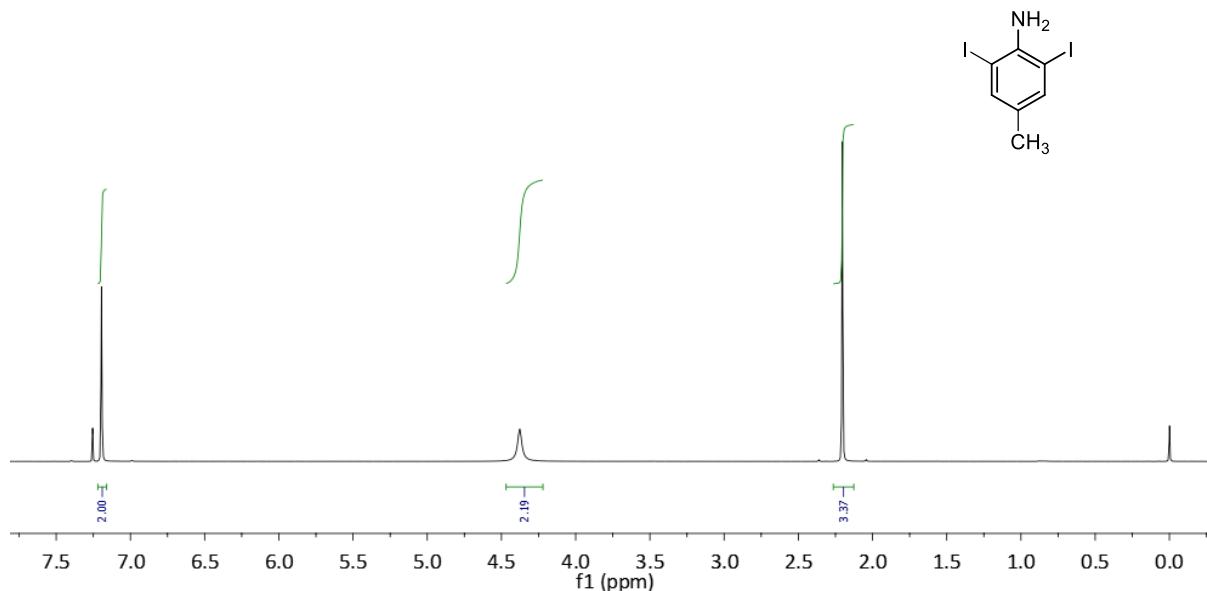


<sup>1</sup>H-NMR of 6b in CDCl<sub>3</sub>

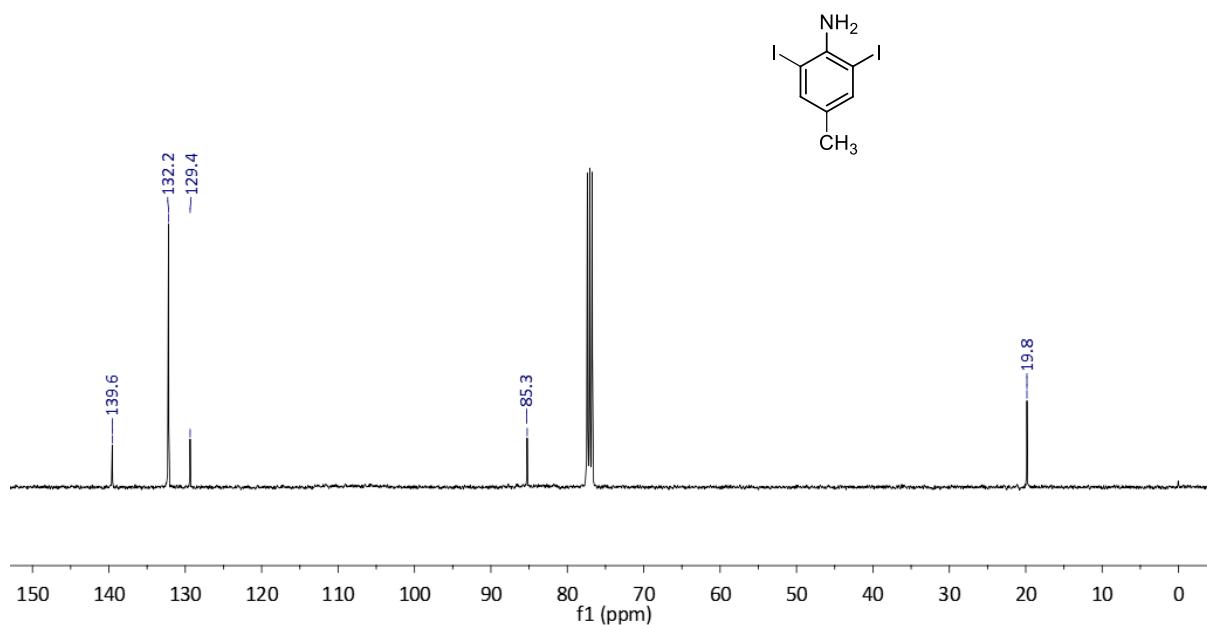


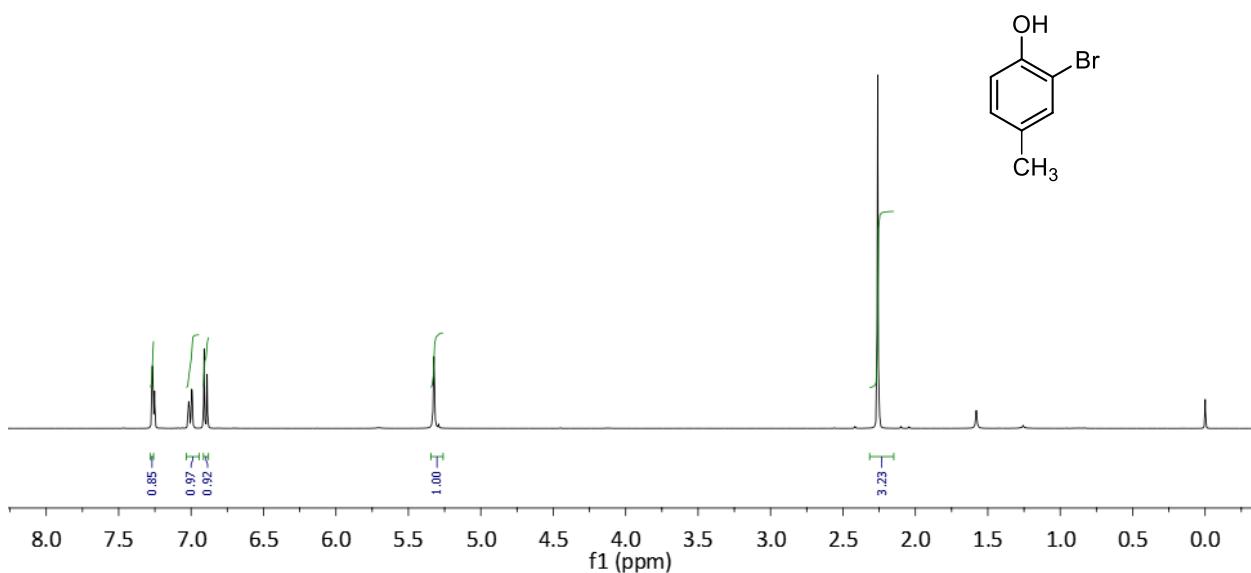
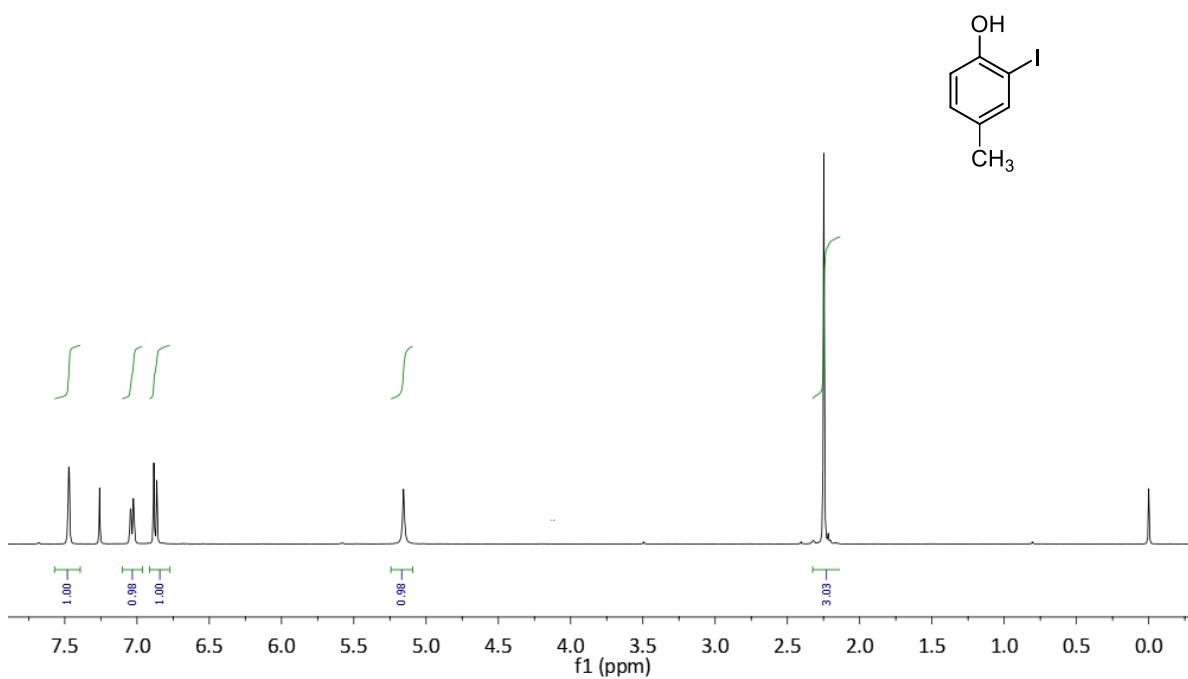
<sup>13</sup>C NMR of 6b in CDCl<sub>3</sub>

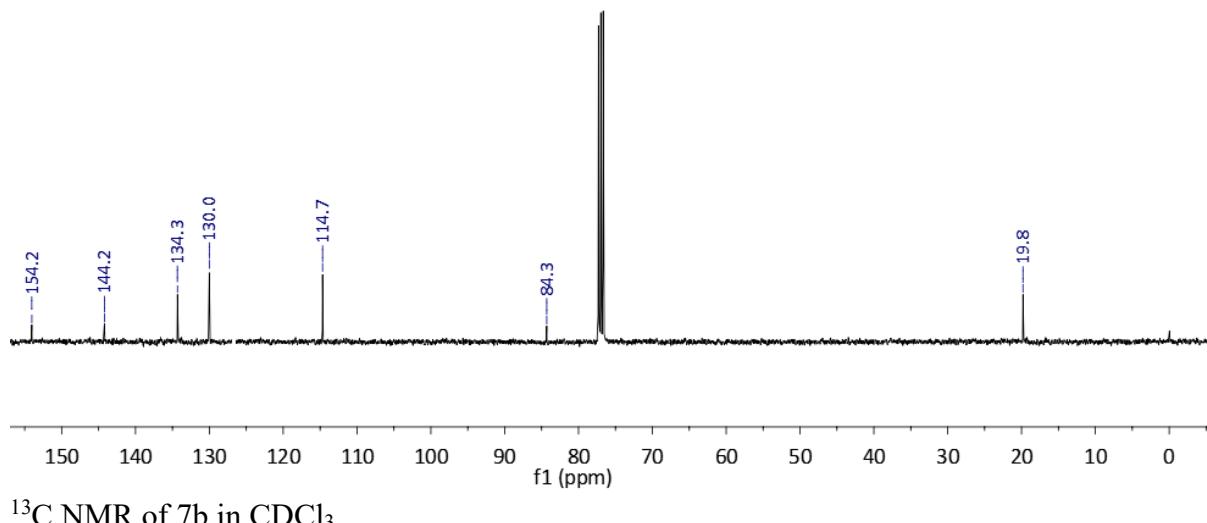
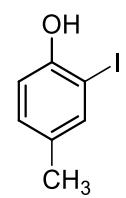




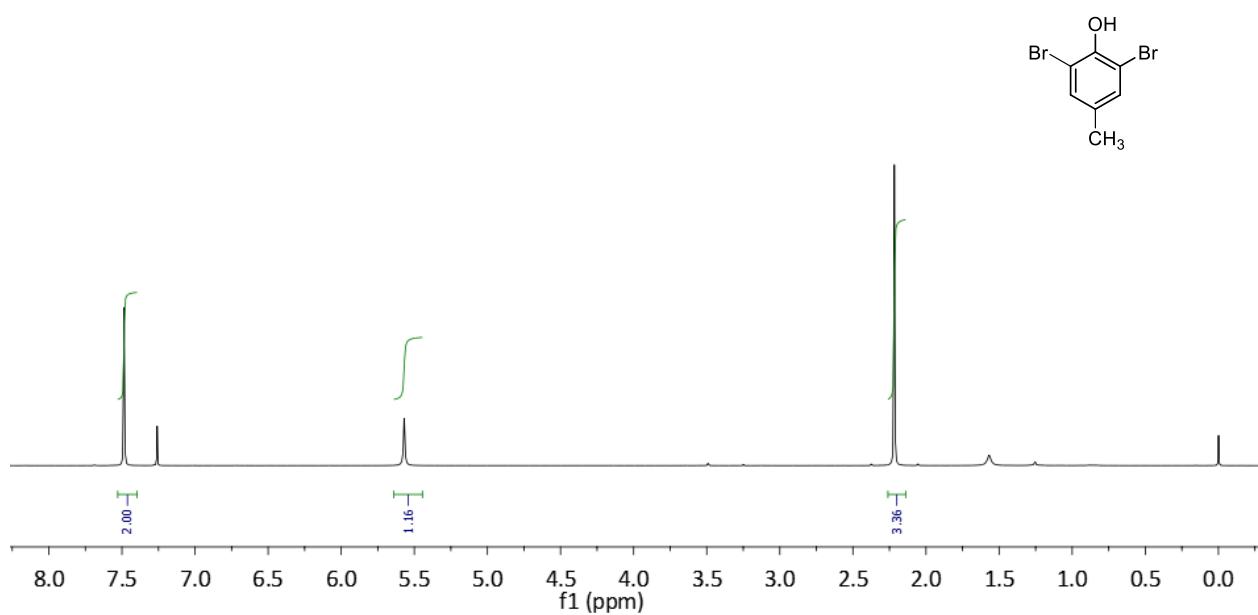
<sup>1</sup>H-NMR of 6d in CDCl<sub>3</sub>



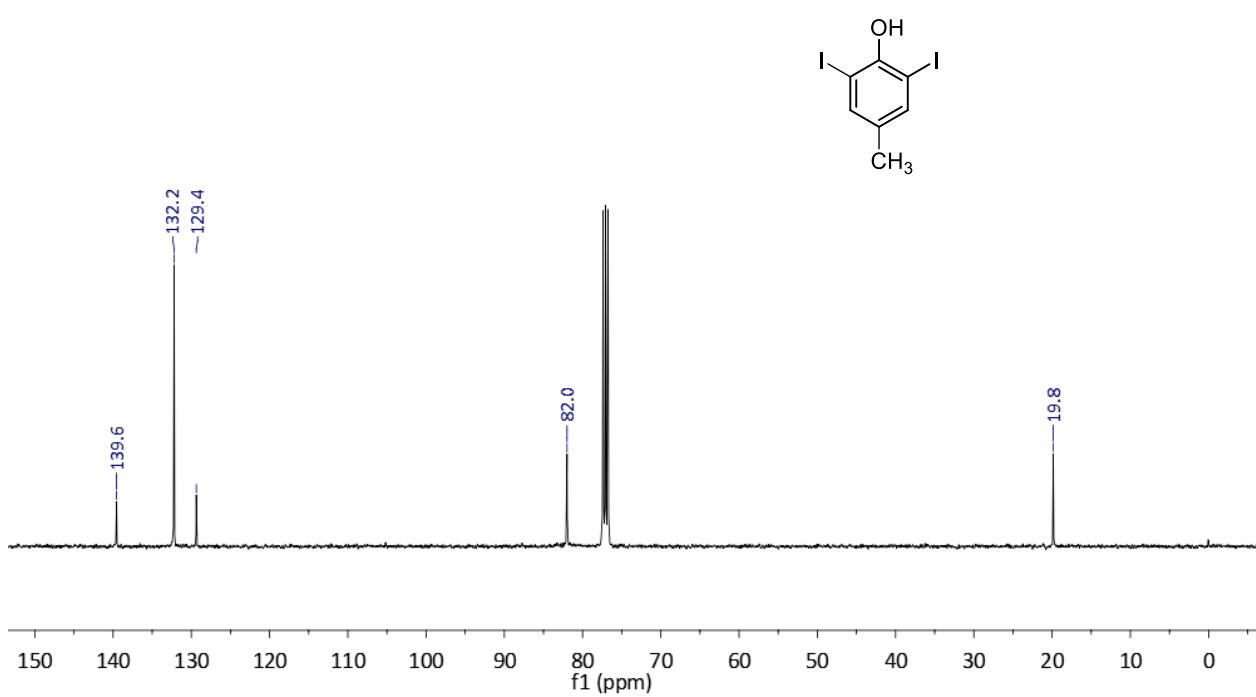
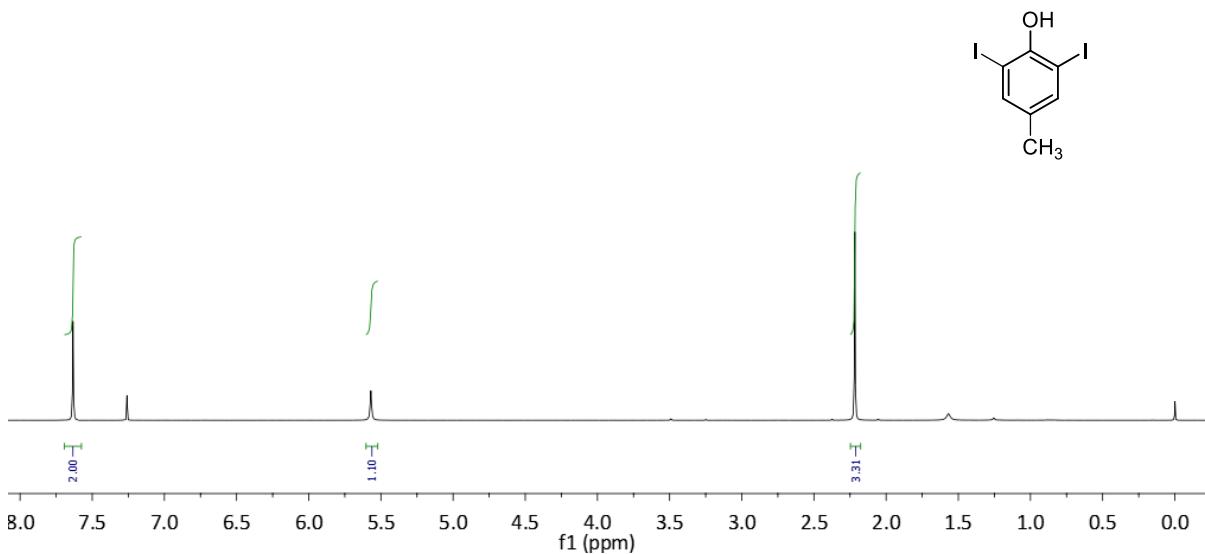
<sup>1</sup>H-NMR of 7a in CDCl<sub>3</sub><sup>1</sup>H-NMR of 7b in CDCl<sub>3</sub>

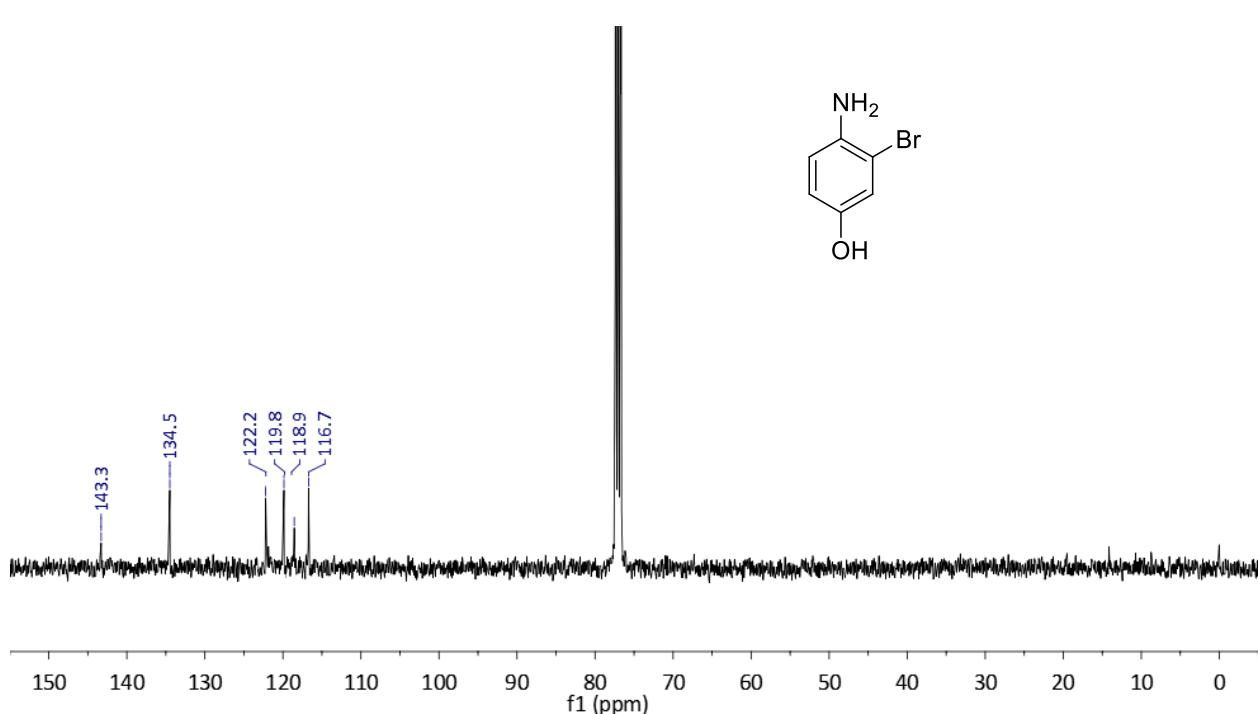
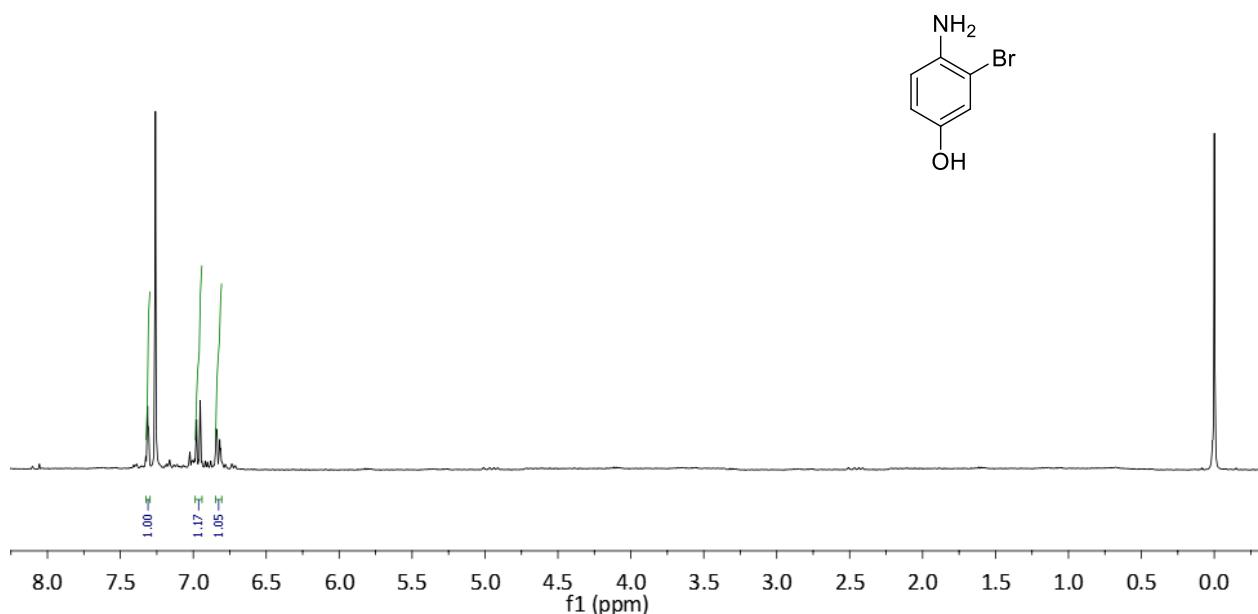


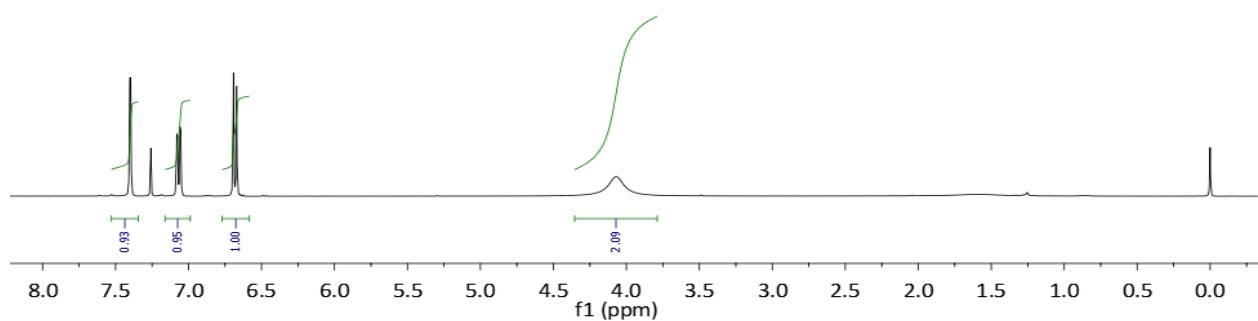
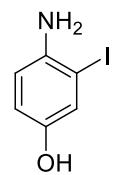
<sup>13</sup>C NMR of 7b in  $\text{CDCl}_3$



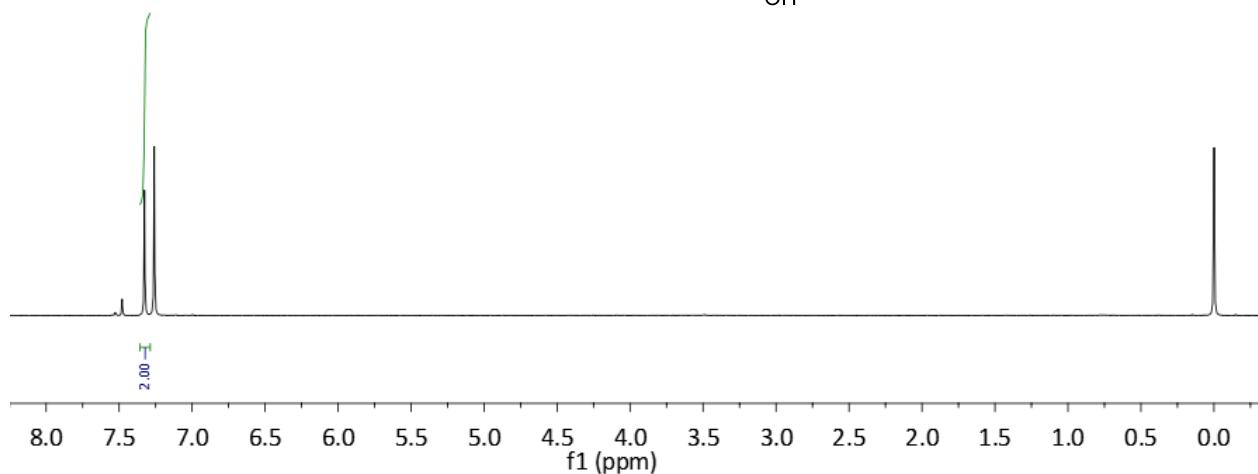
<sup>1</sup>H-NMR of 7c in  $\text{CDCl}_3$



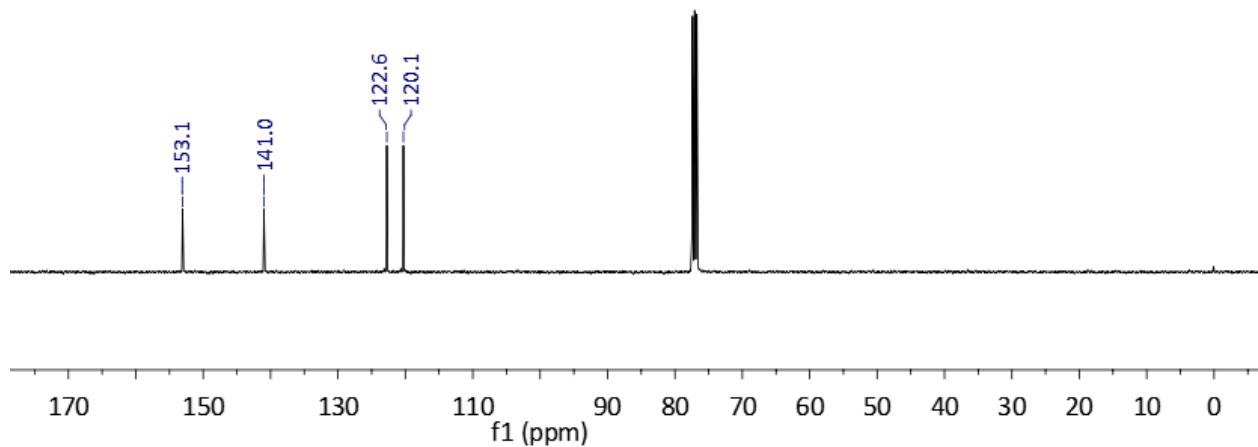
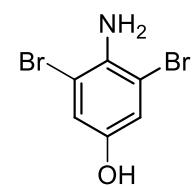




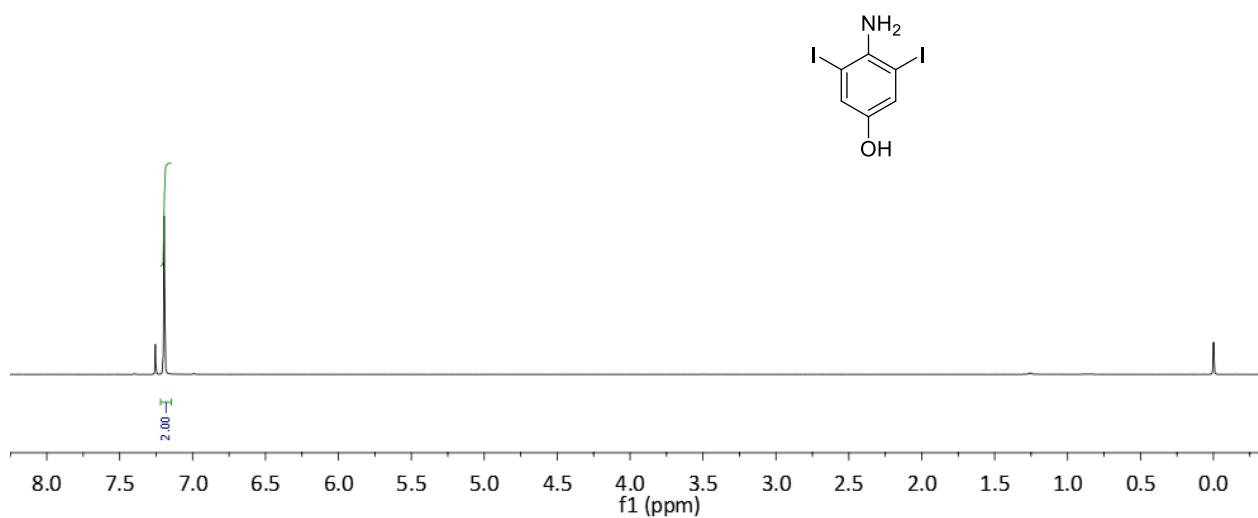
$^1\text{H-NMR}$  of 8b in  $\text{CDCl}_3$



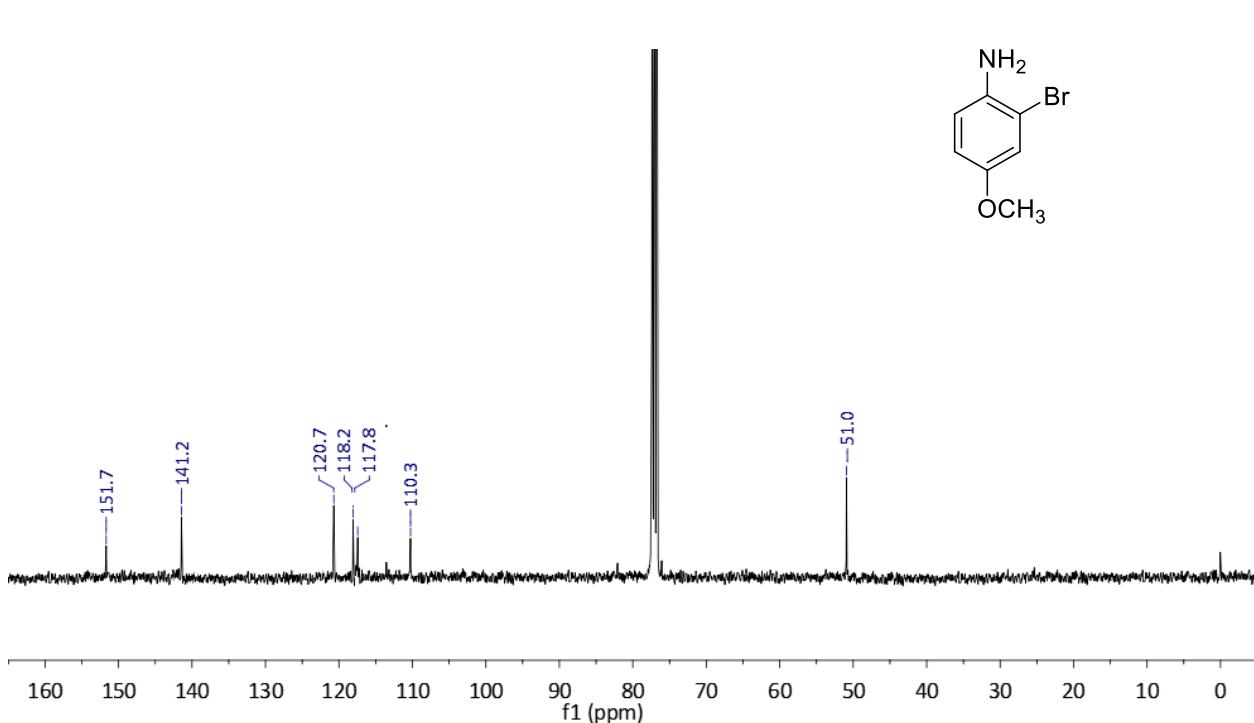
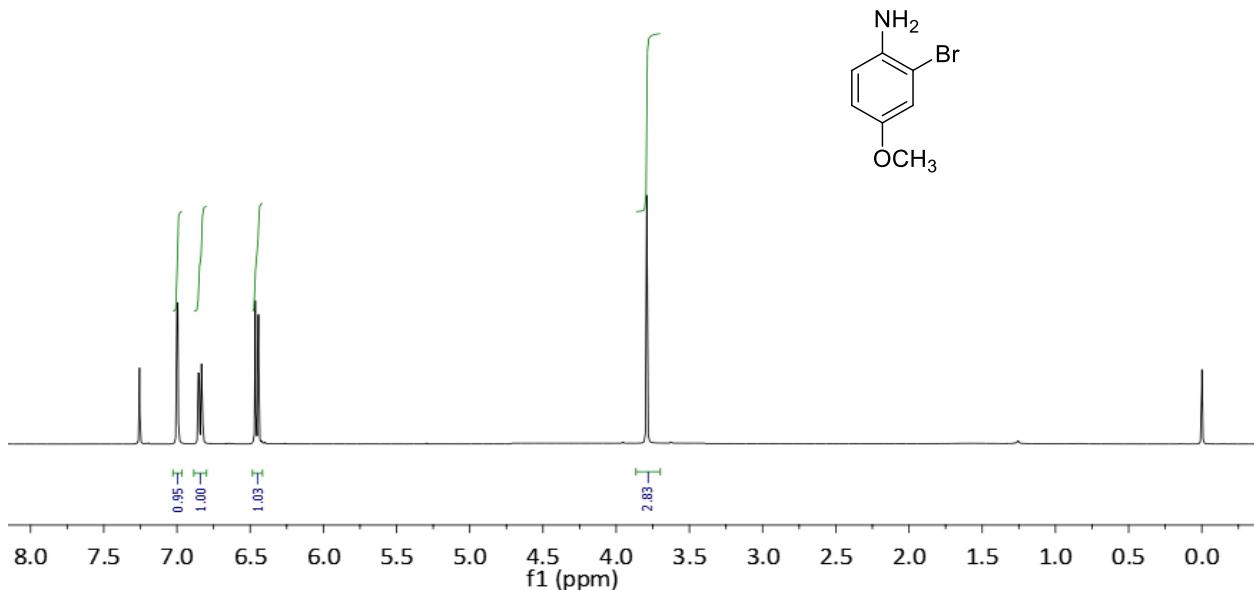
$^1\text{H-NMR}$  of 8c in  $\text{CDCl}_3$

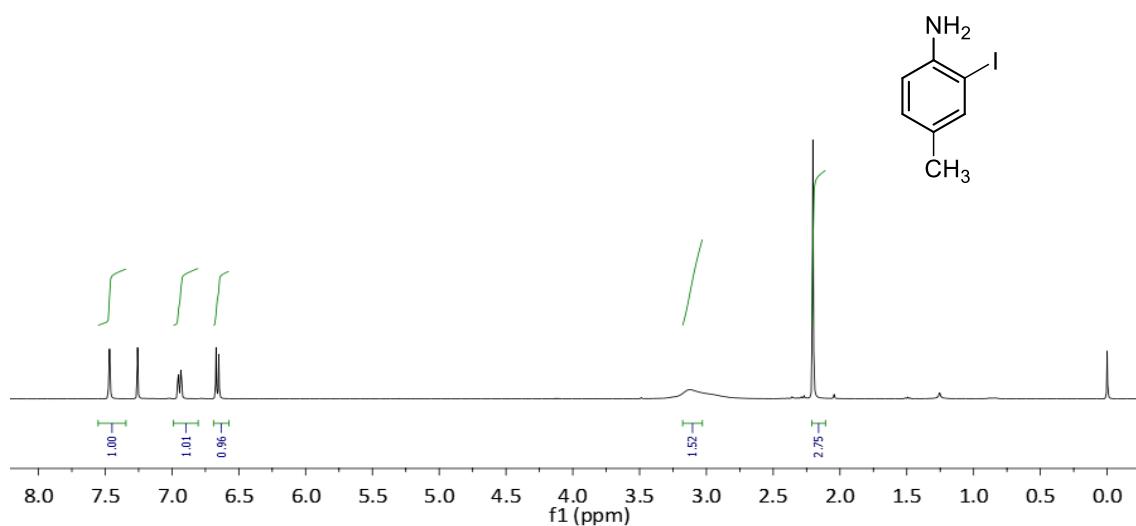
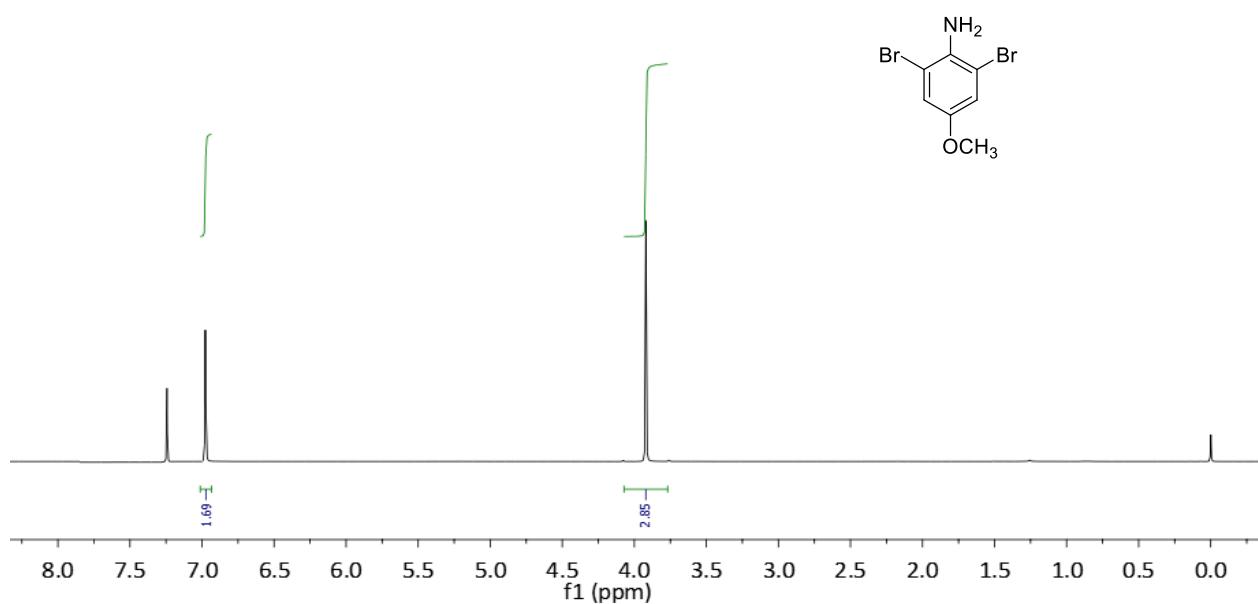


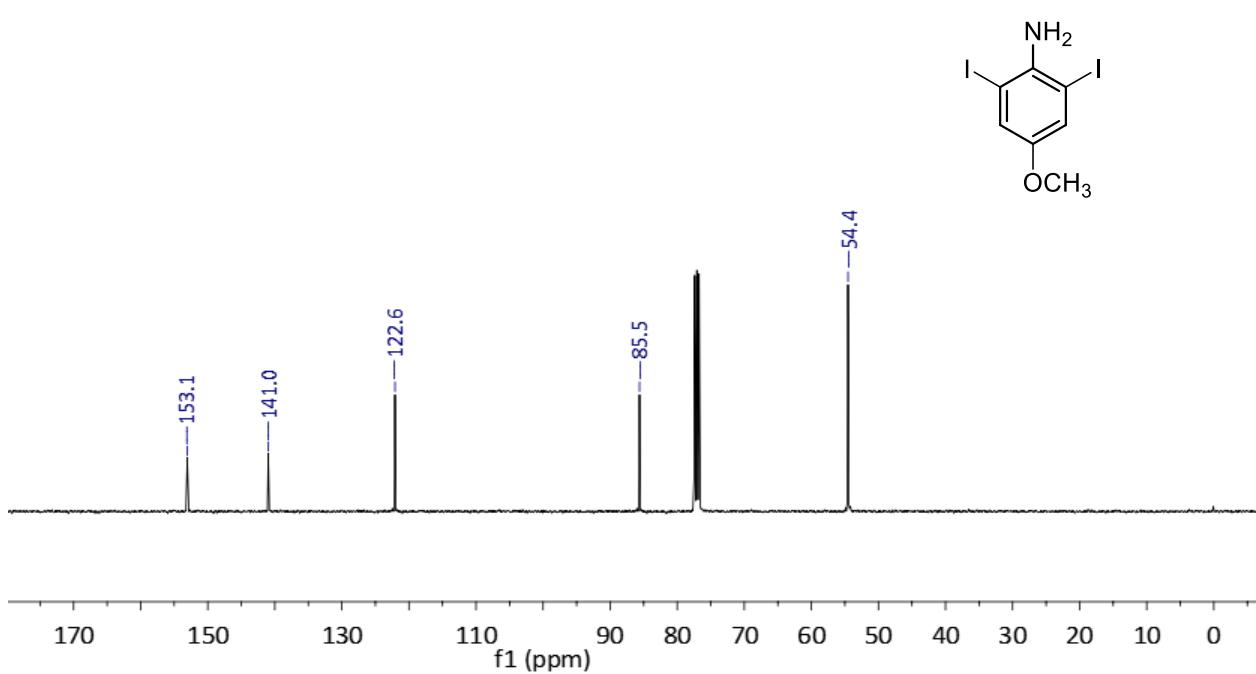
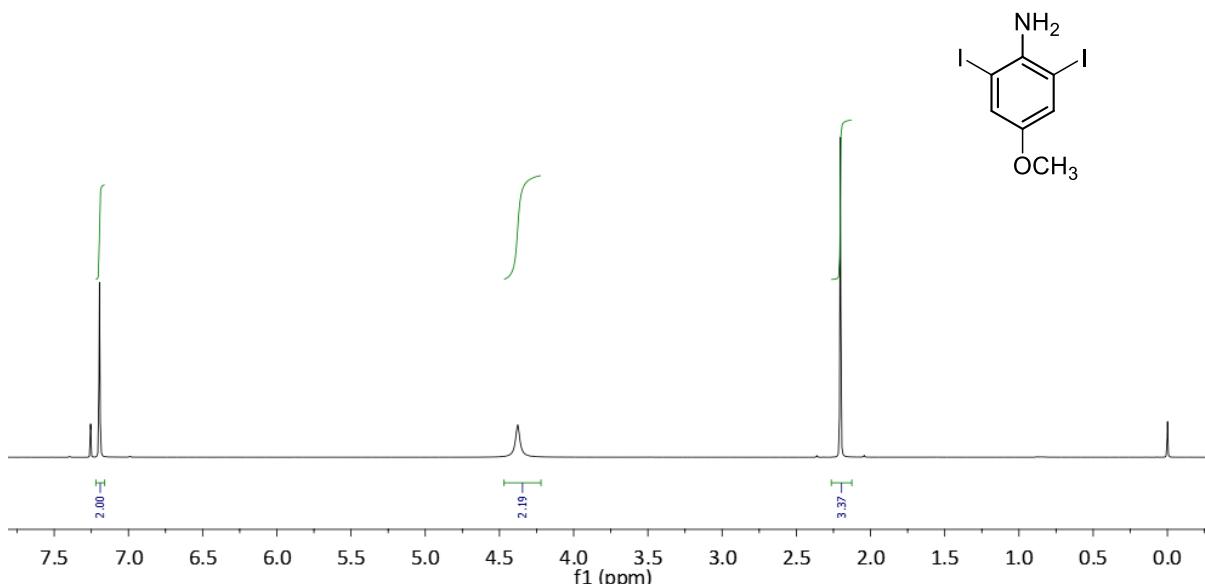
$^{13}\text{C}$  NMR of 8c in  $\text{CDCl}_3$

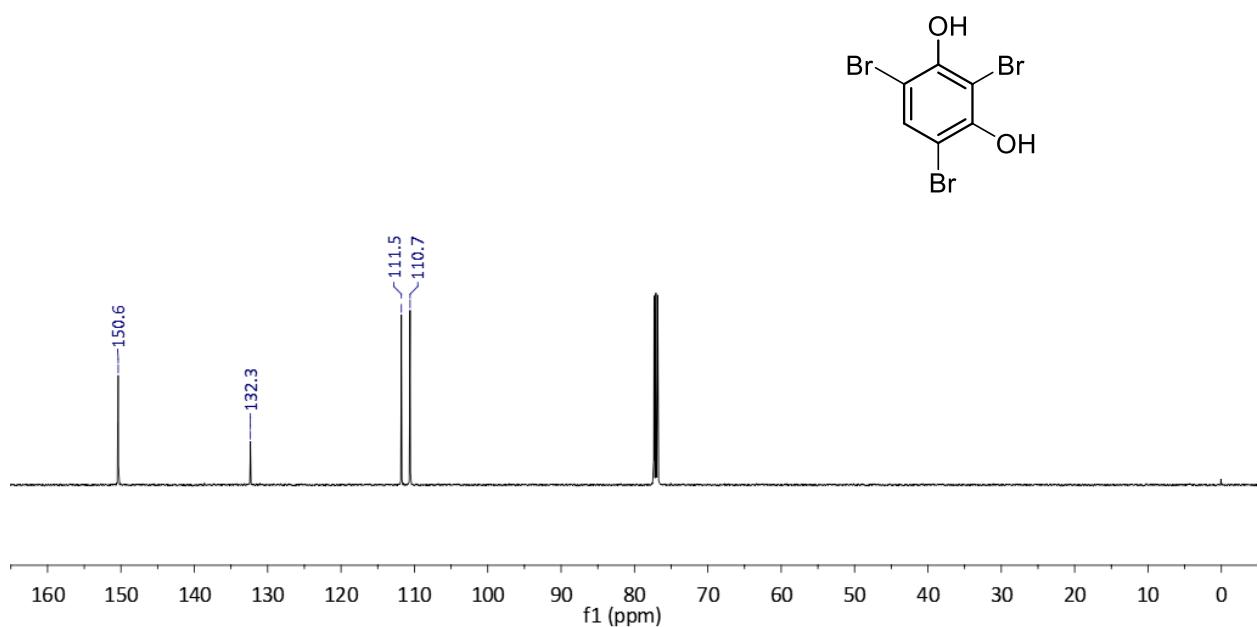
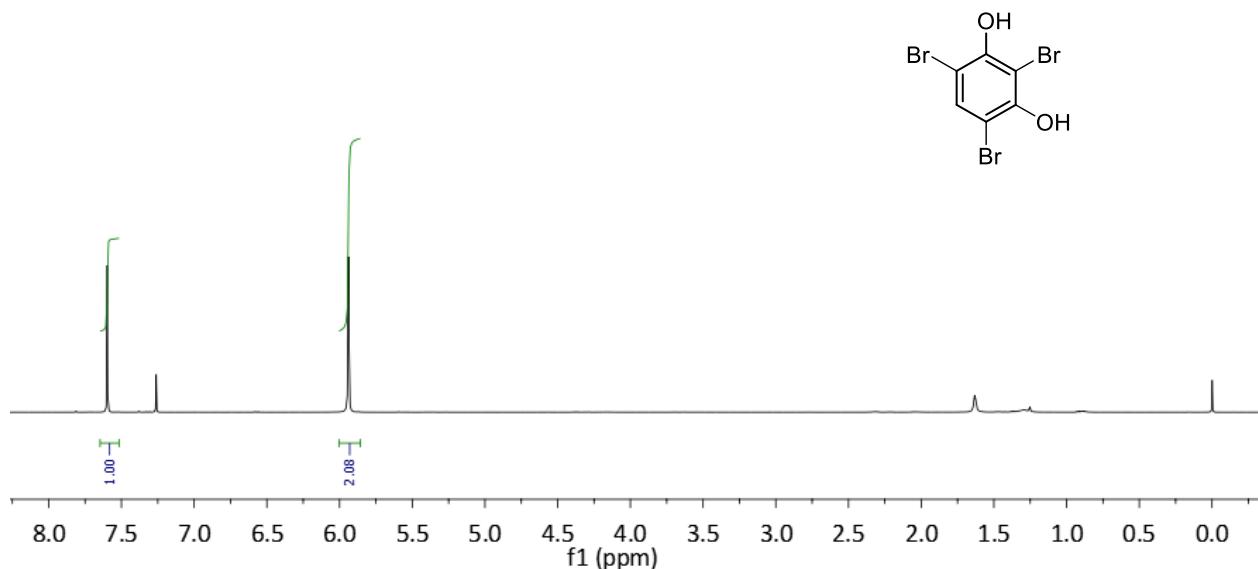


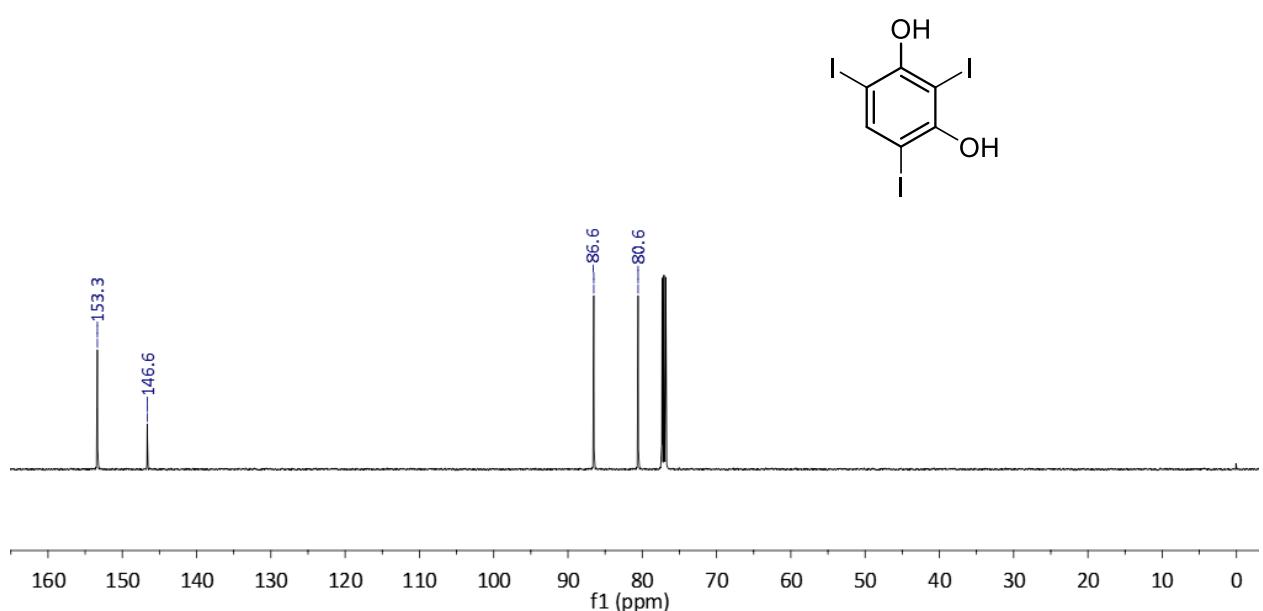
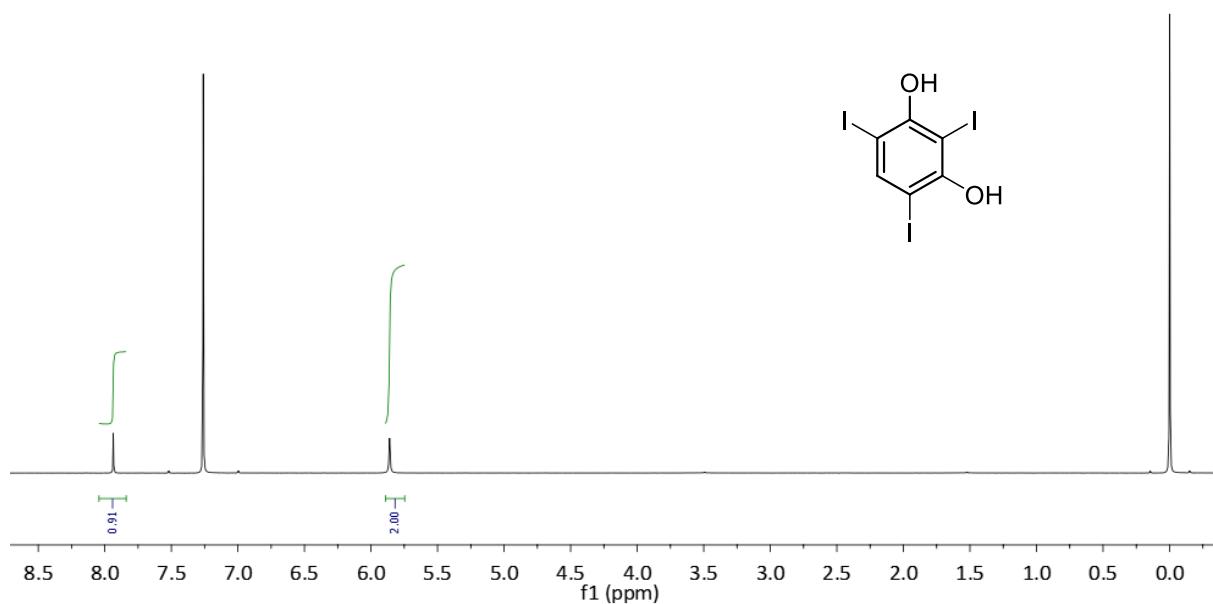
$^1\text{H}$ -NMR of 8d in  $\text{CDCl}_3$

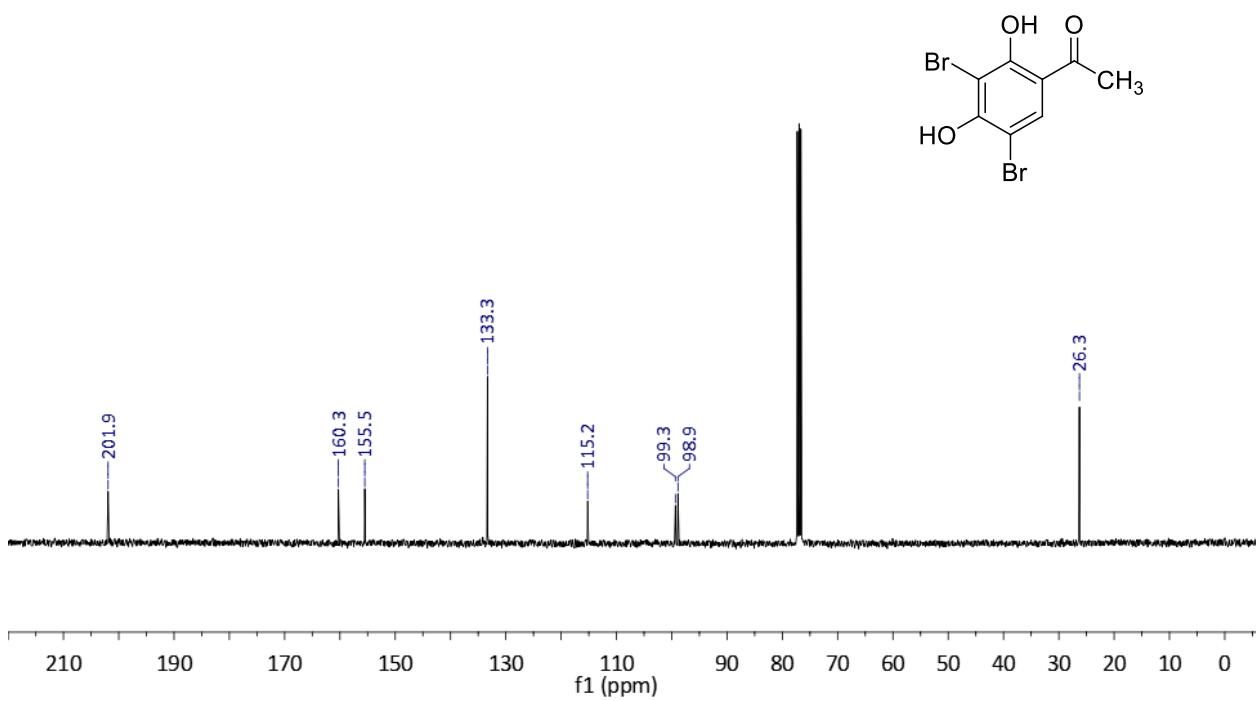
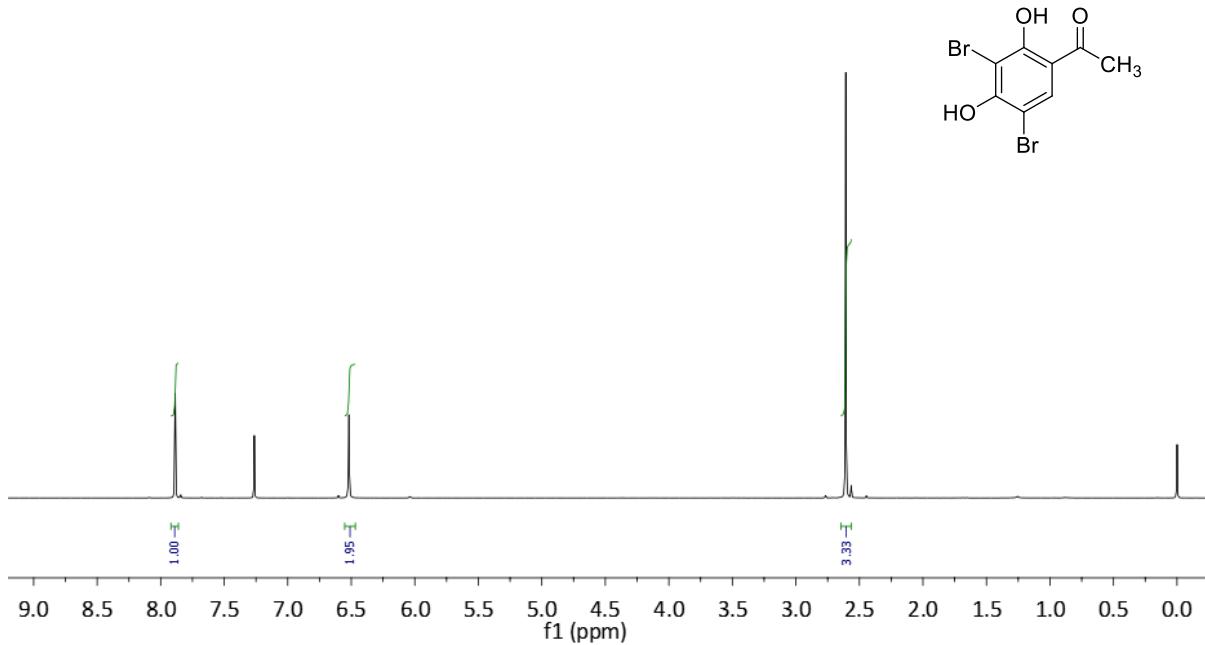


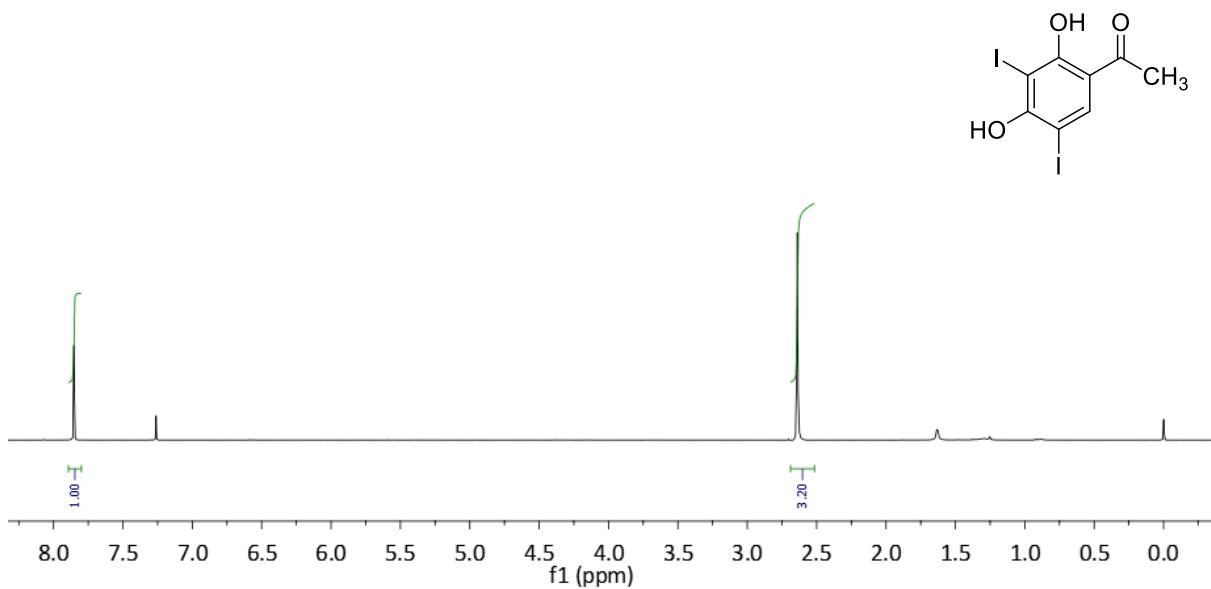
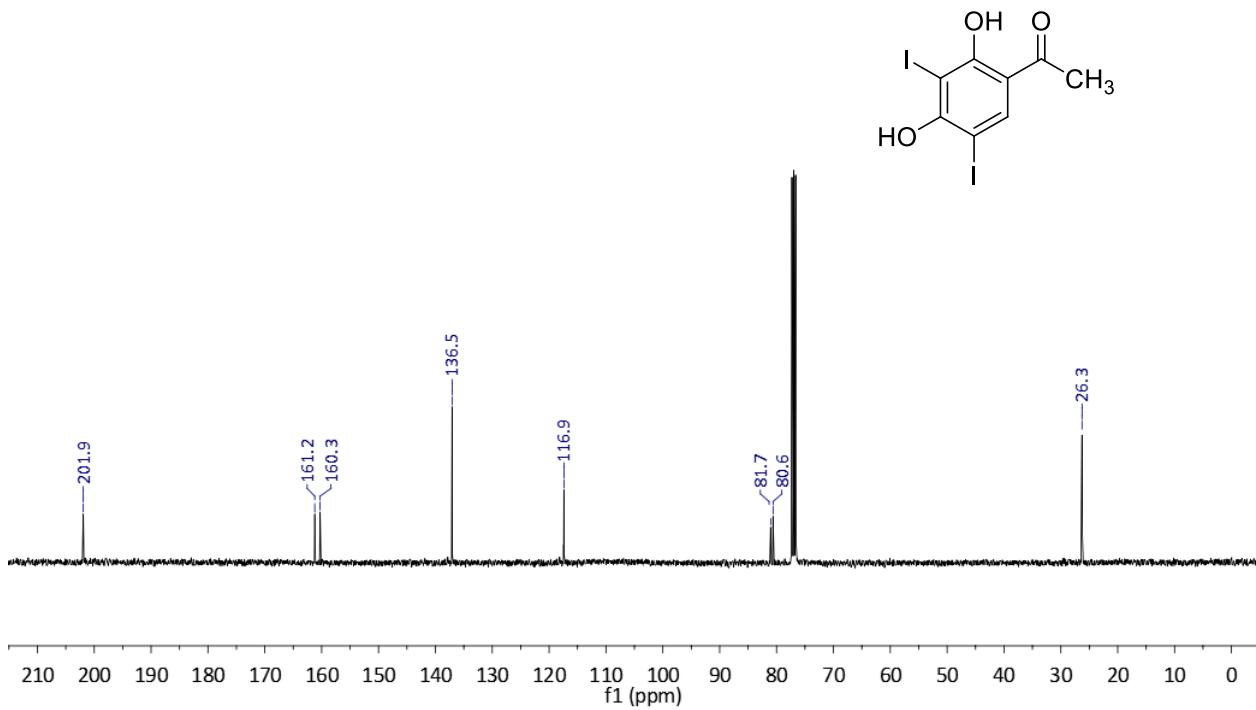
<sup>1</sup>H-NMR of 9b in  $\text{CDCl}_3$ <sup>1</sup>H-NMR of 9c in  $\text{CDCl}_3$

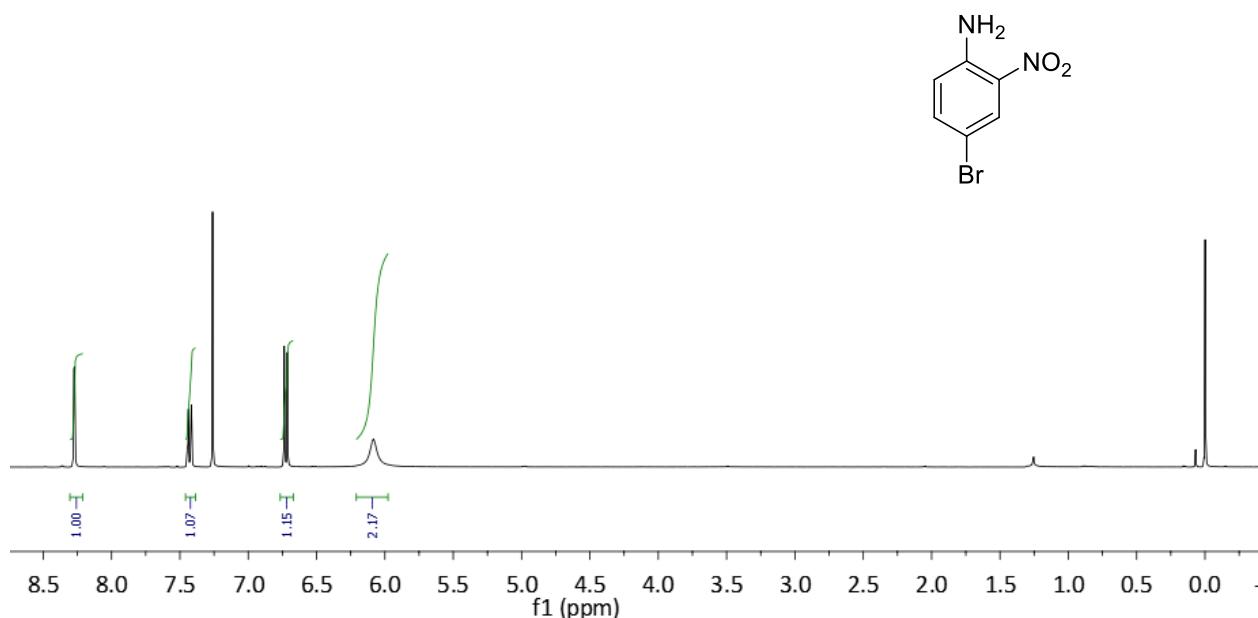




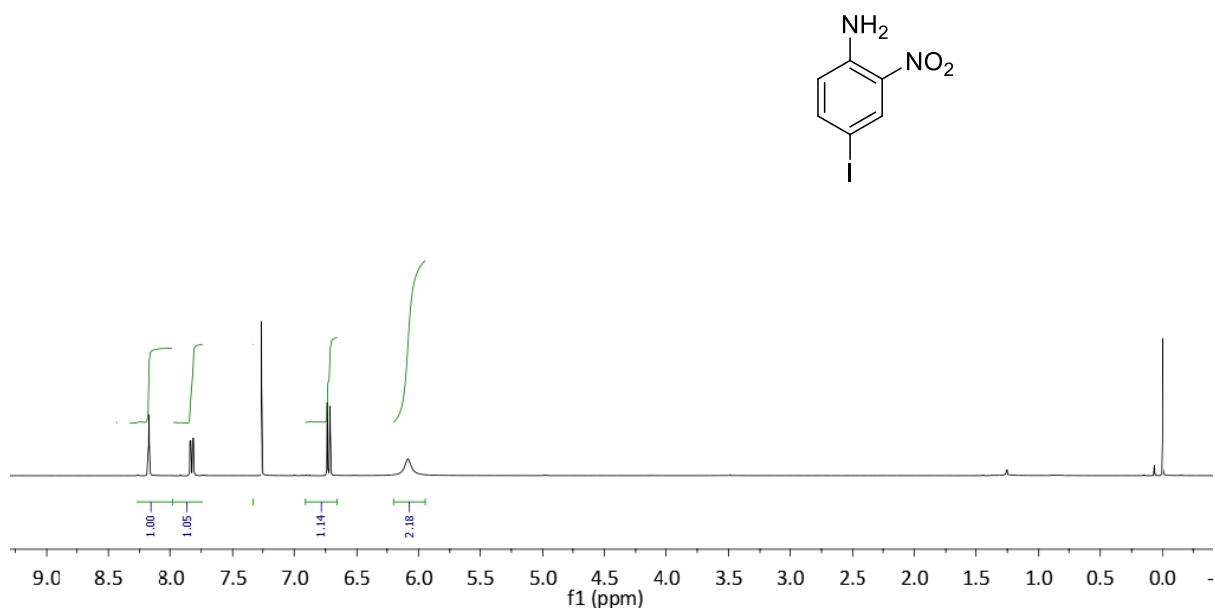




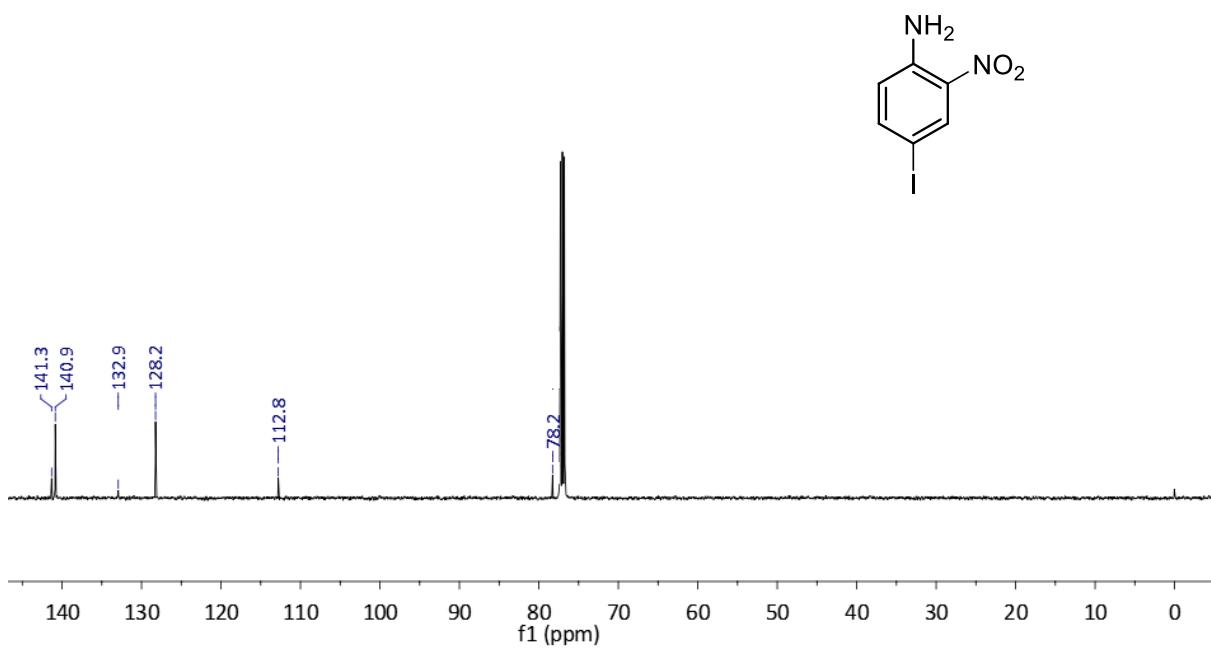
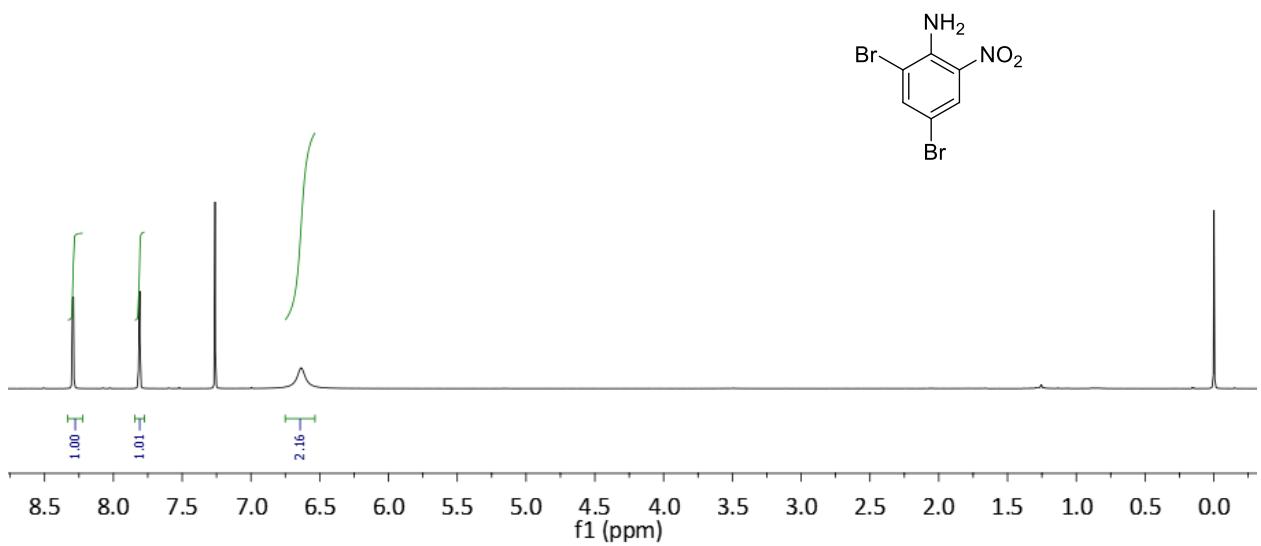
<sup>1</sup>H-NMR of 11b in CDCl<sub>3</sub><sup>13</sup>C NMR of 11b in CDCl<sub>3</sub>

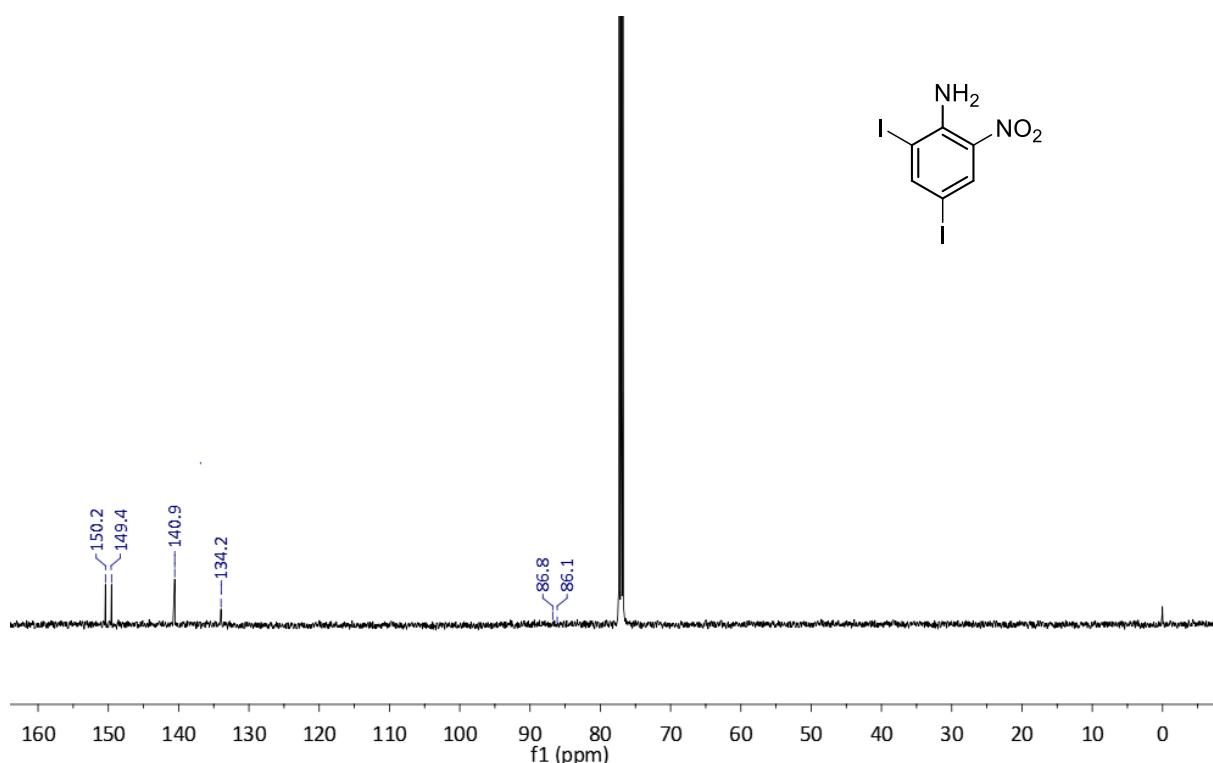
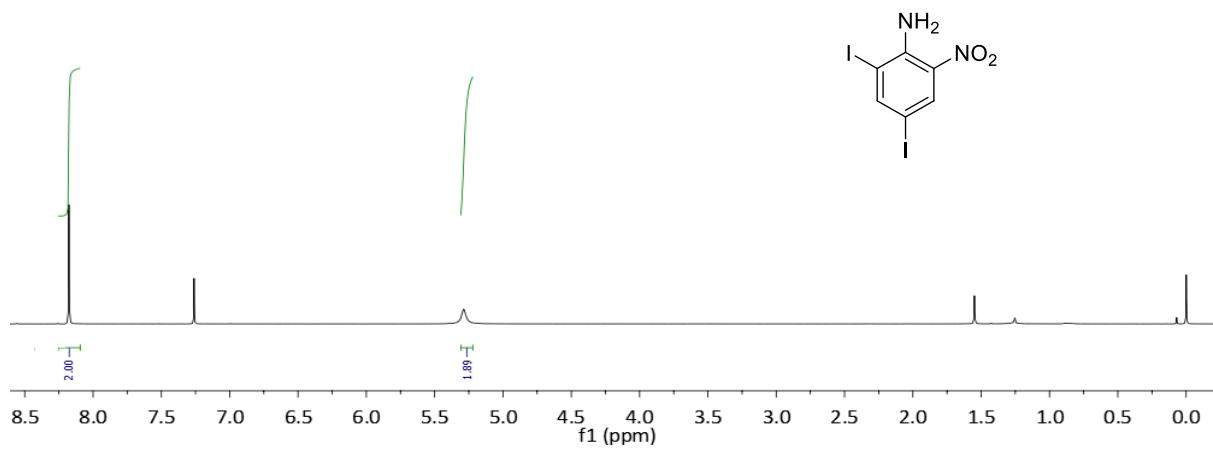


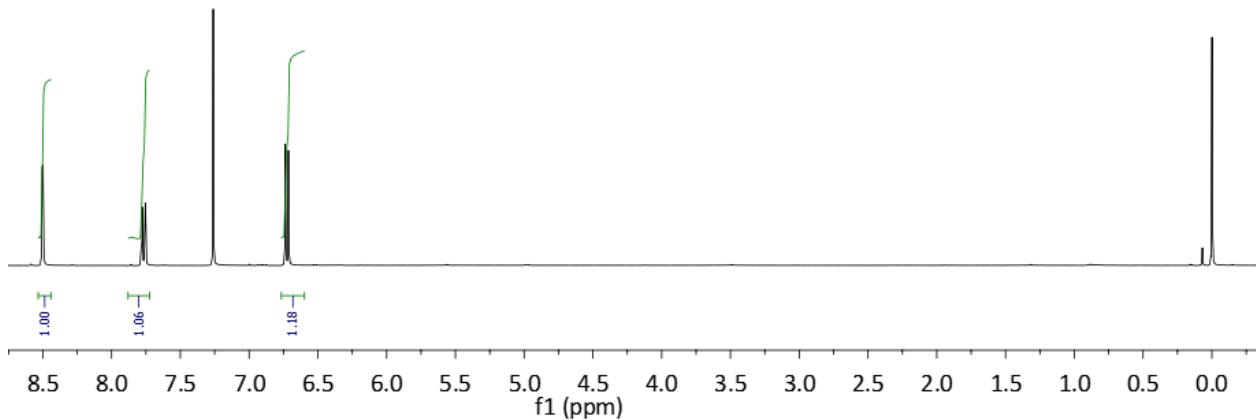
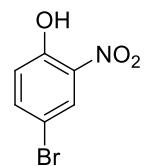
$^1\text{H}$ -NMR of 12a in  $\text{CDCl}_3$



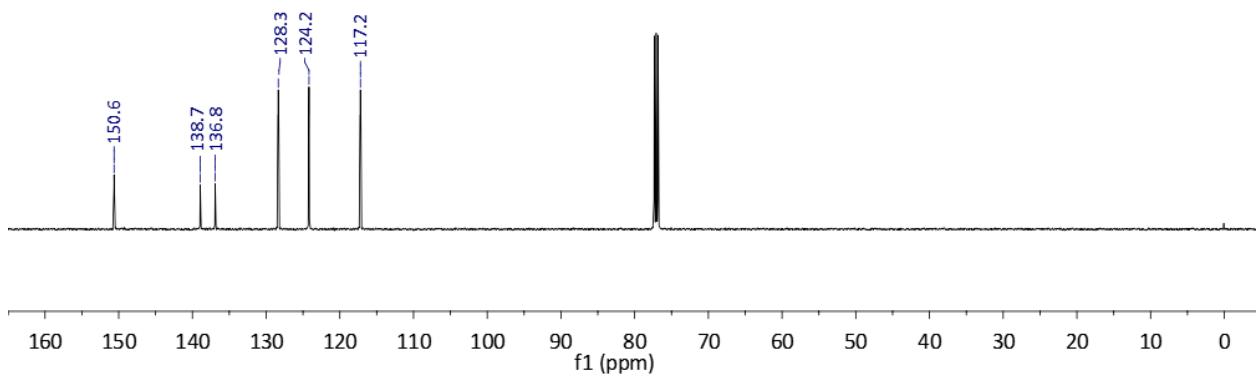
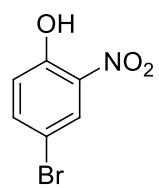
$^1\text{H}$ -NMR of 12b in  $\text{CDCl}_3$

<sup>13</sup>C NMR of 12b in  $\text{CDCl}_3$ <sup>1</sup>H-NMR of 12c in  $\text{CDCl}_3$

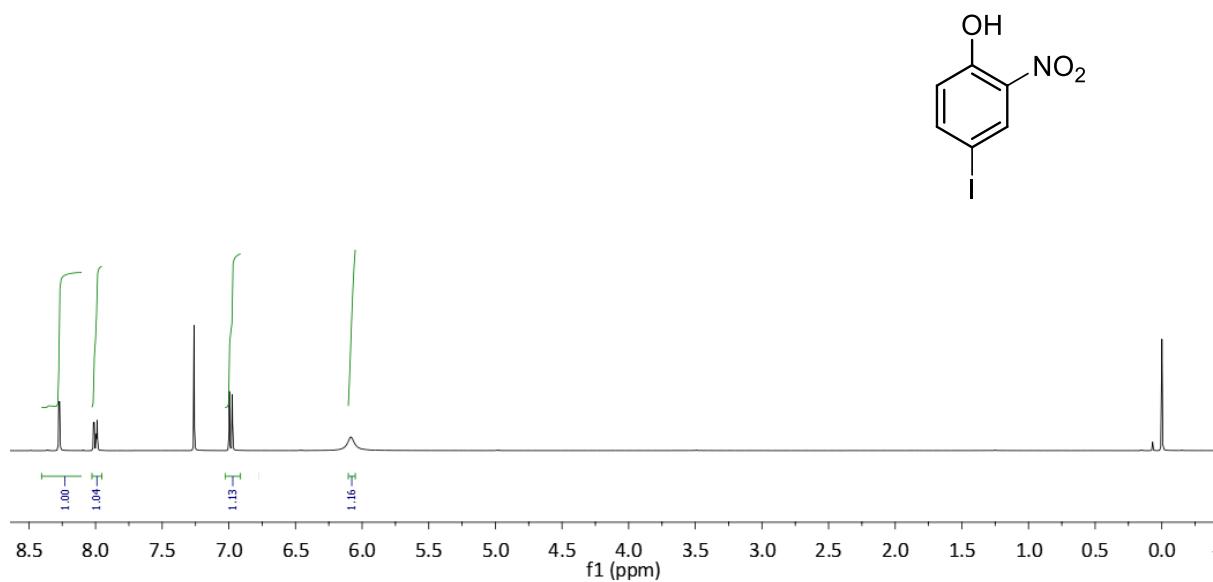




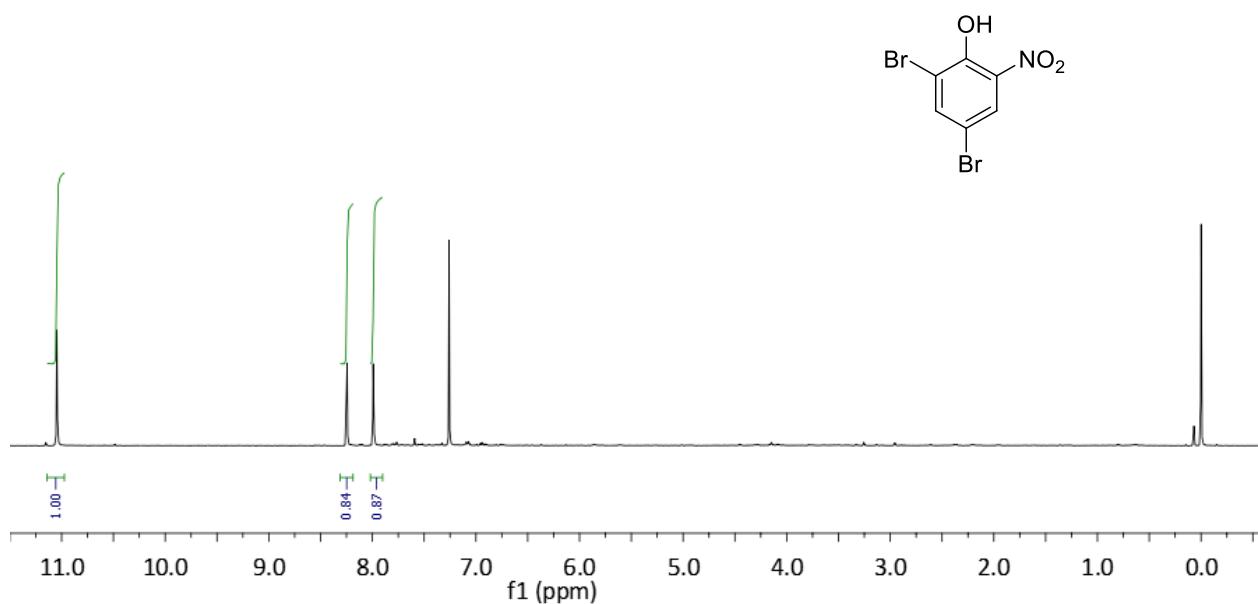
<sup>1</sup>H-NMR of 13a in CDCl<sub>3</sub>



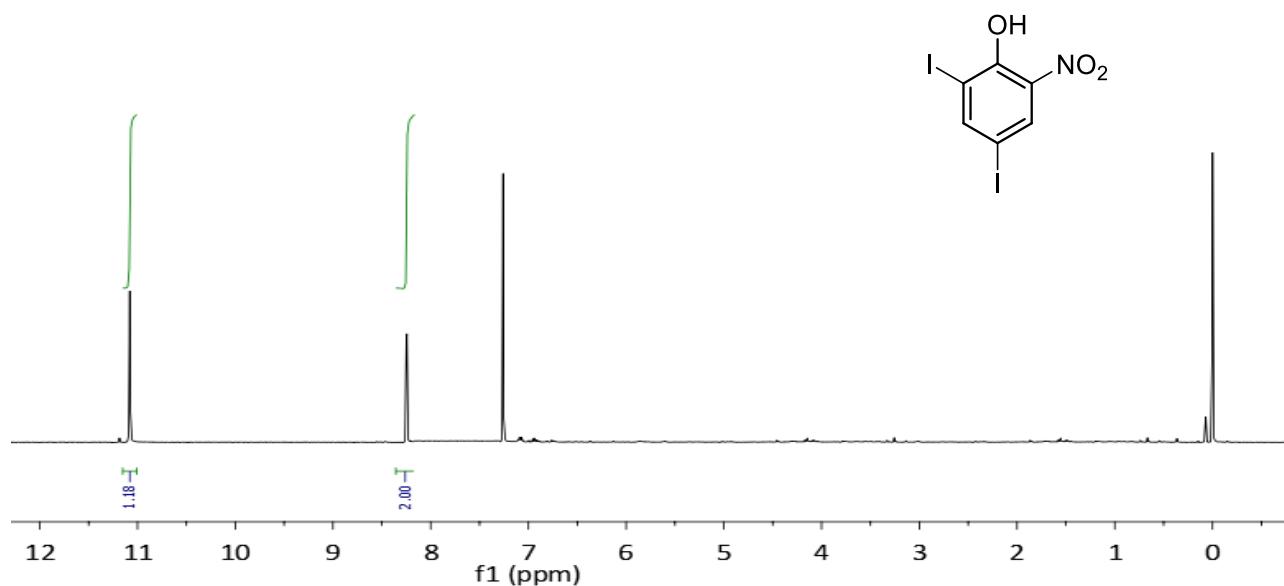
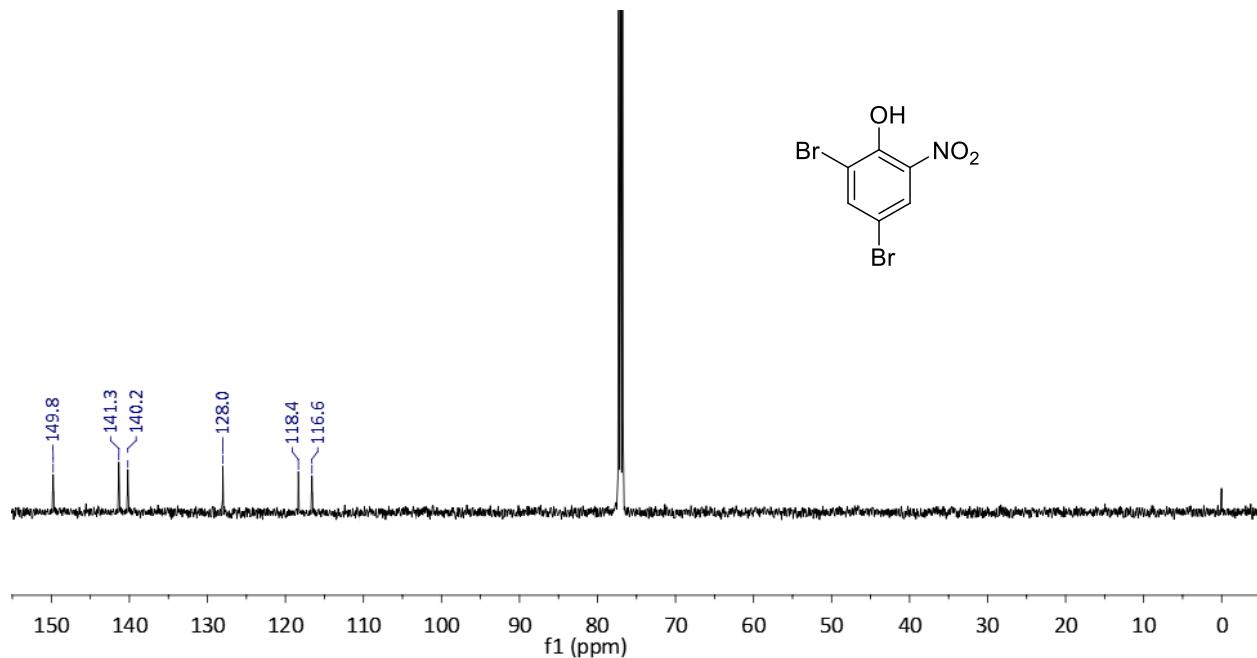
<sup>13</sup>C NMR of 13a in CDCl<sub>3</sub>

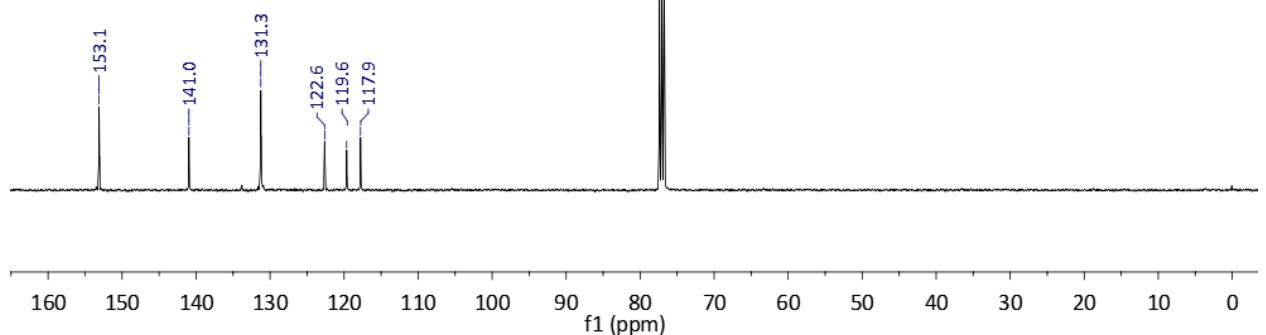
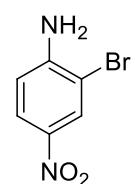
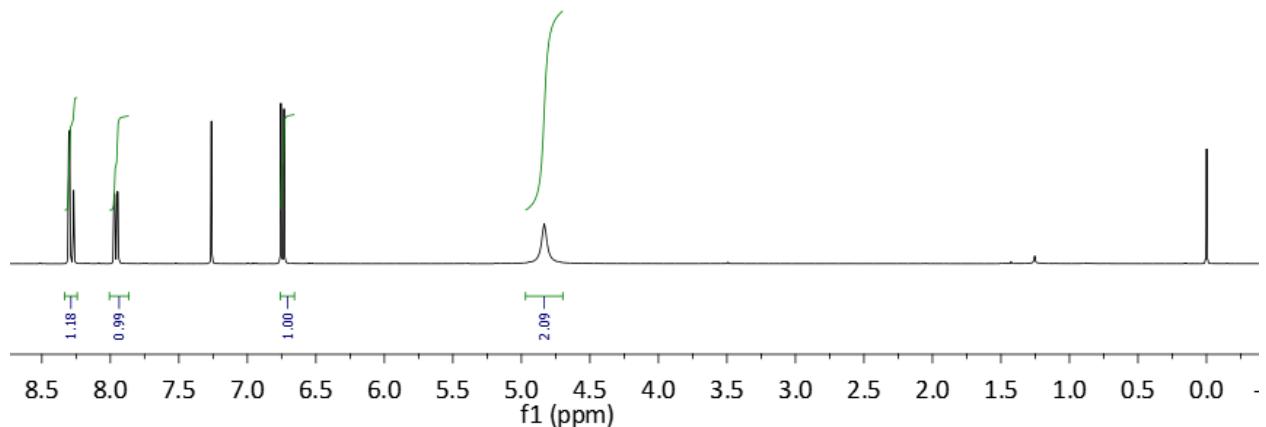
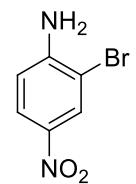


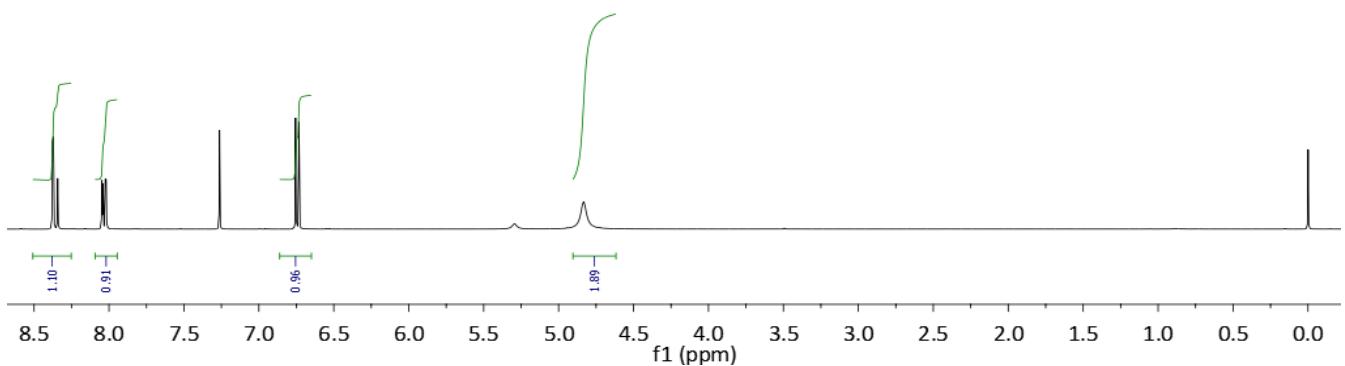
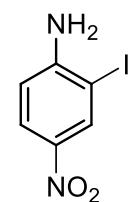
<sup>1</sup>H-NMR of 13b in CDCl<sub>3</sub>



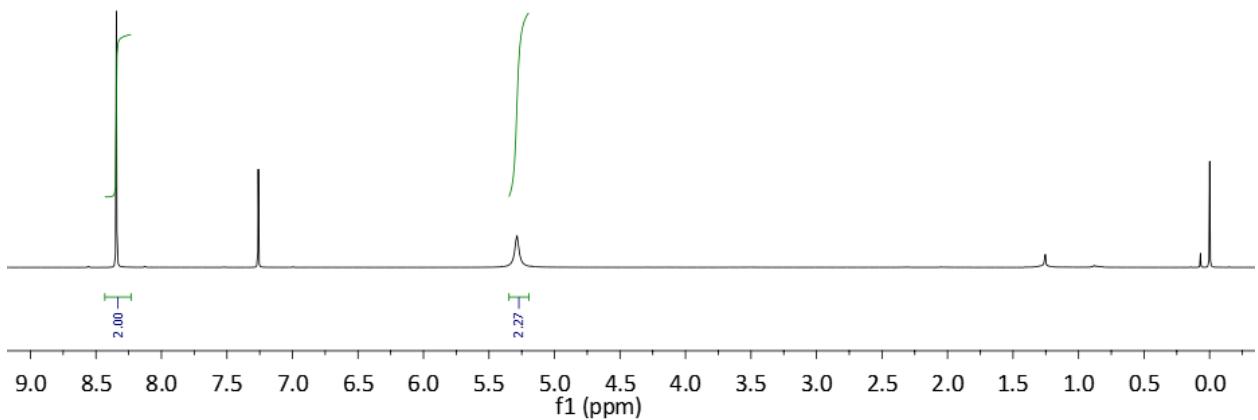
<sup>1</sup>H-NMR of 13c in CDCl<sub>3</sub>



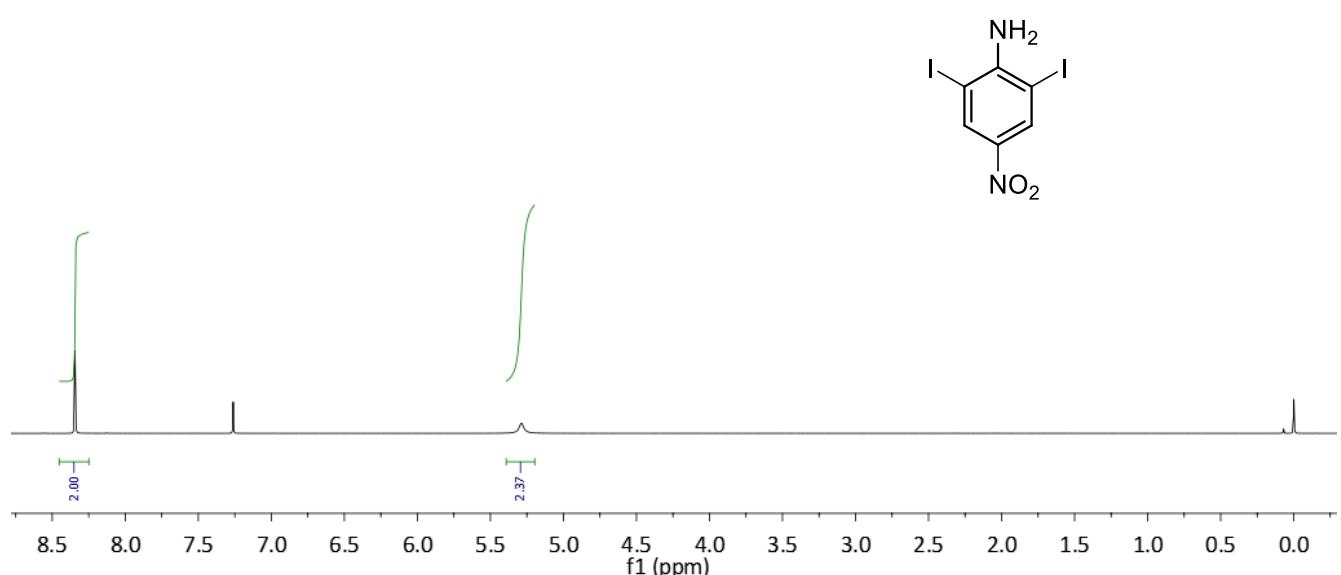
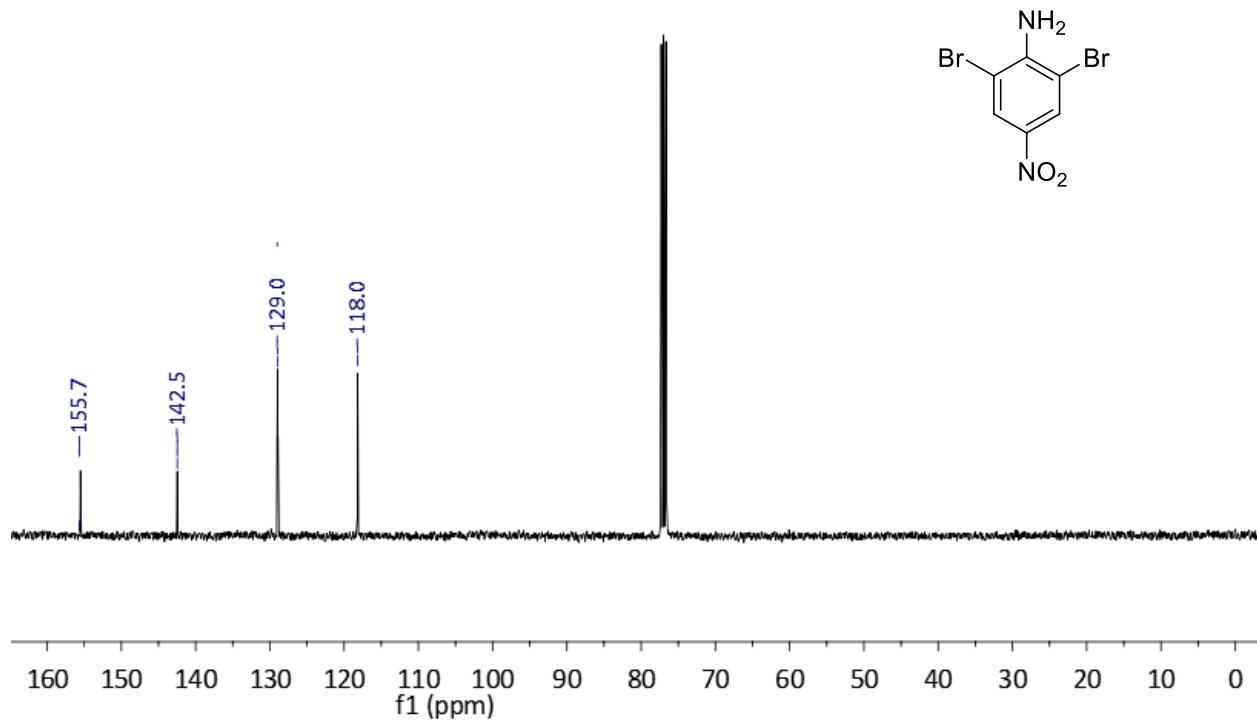




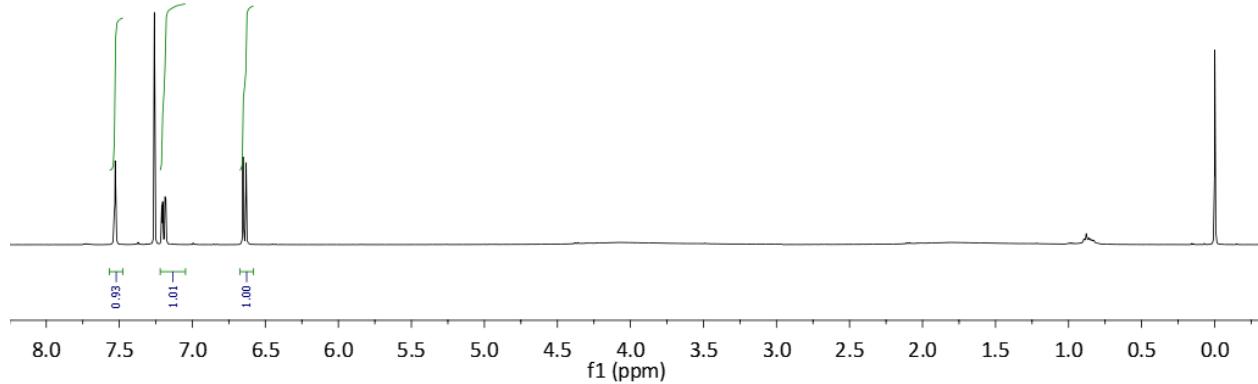
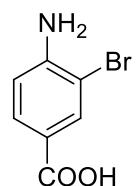
$^1\text{H-NMR}$  of 14b in  $\text{CDCl}_3$



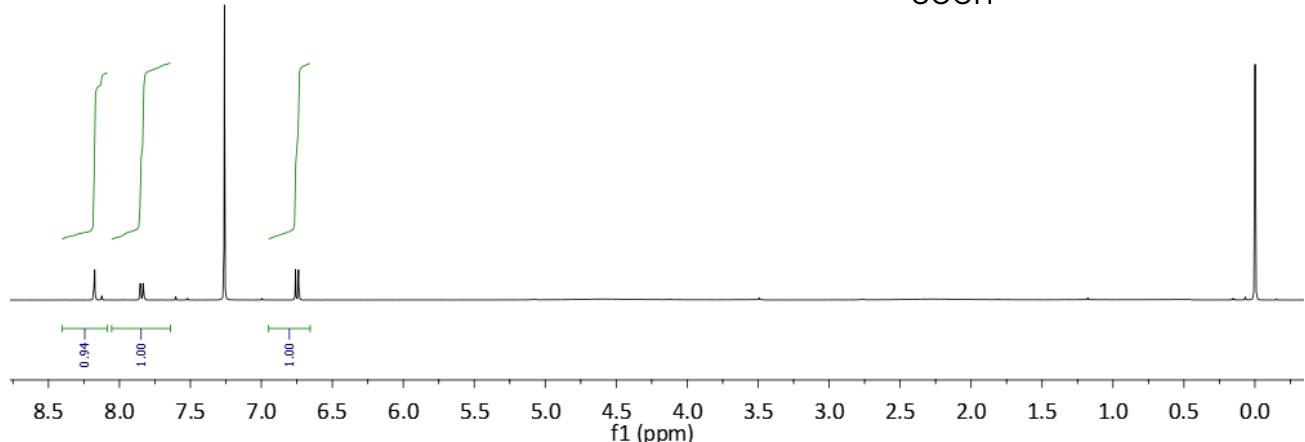
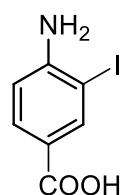
$^1\text{H-NMR}$  of 14c in  $\text{CDCl}_3$



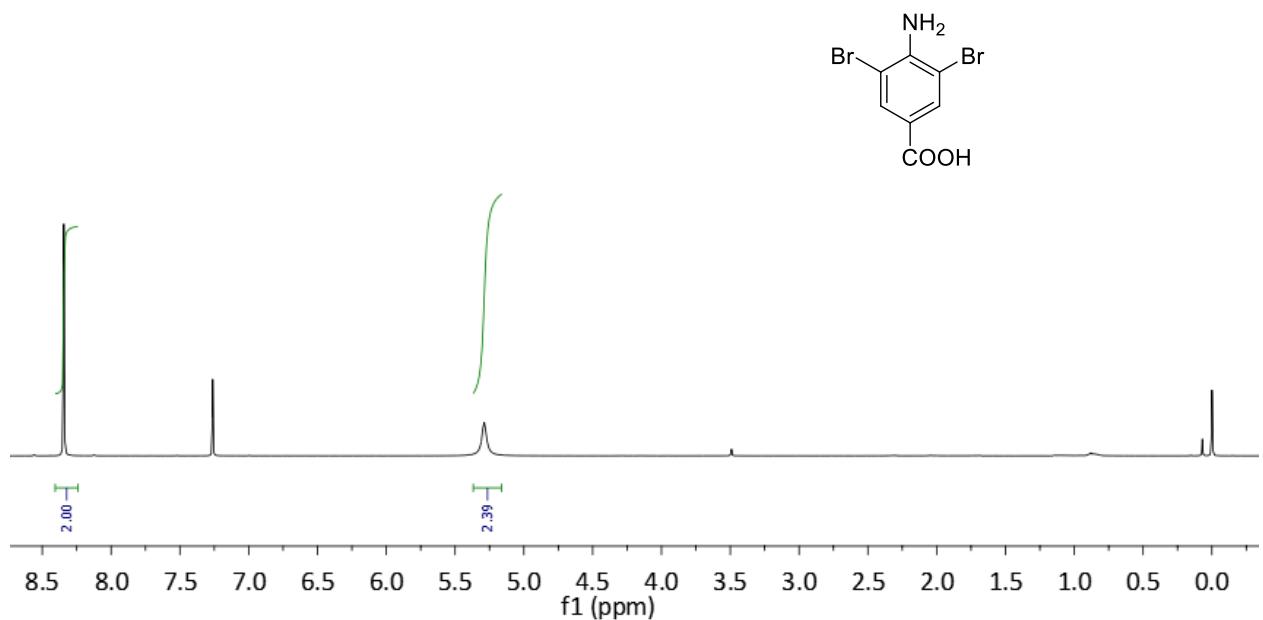
<sup>1</sup>H-NMR of 14d in CDCl<sub>3</sub>



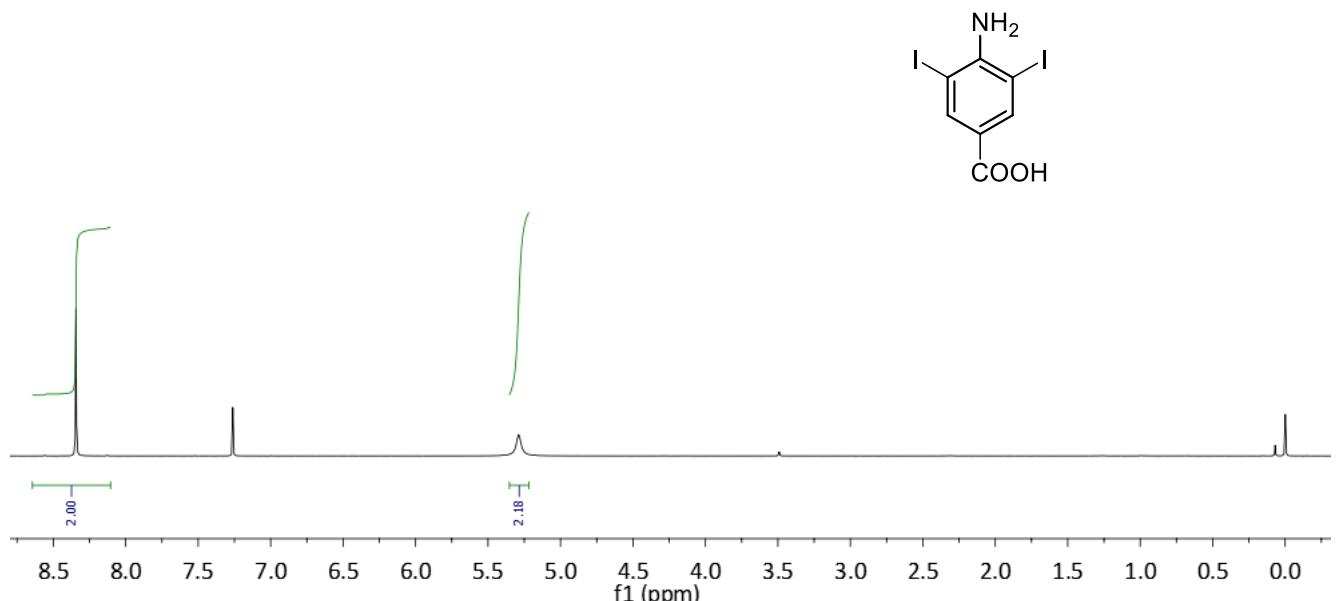
<sup>1</sup>H-NMR of 15a in CDCl<sub>3</sub>



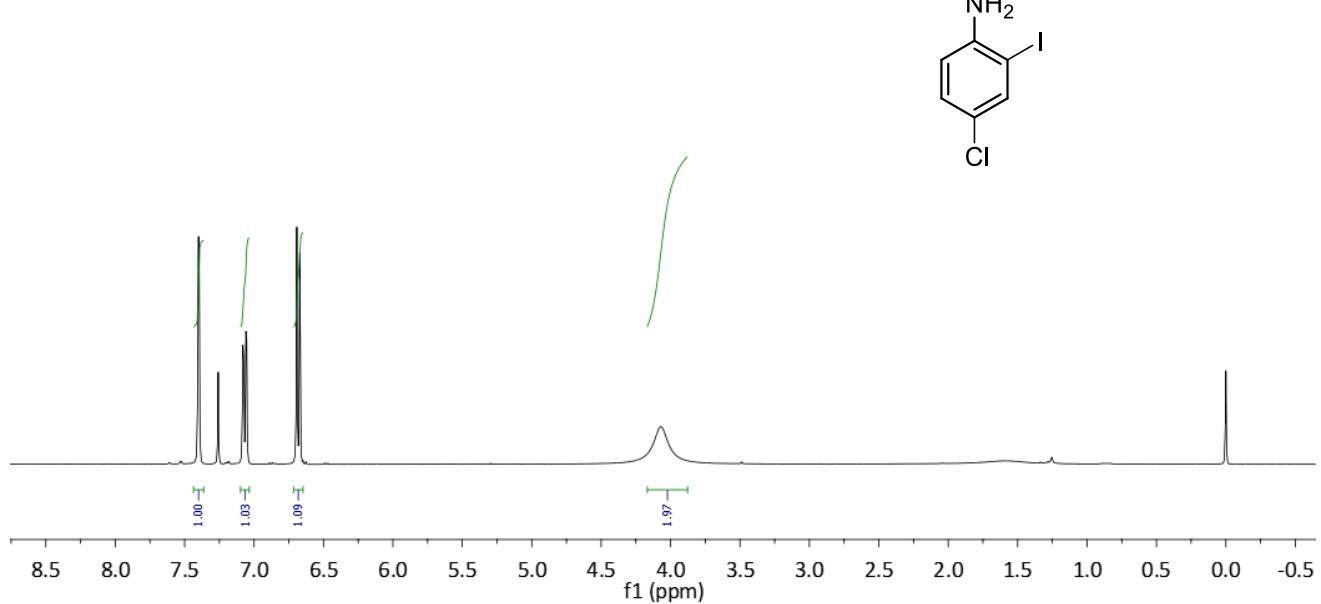
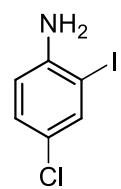
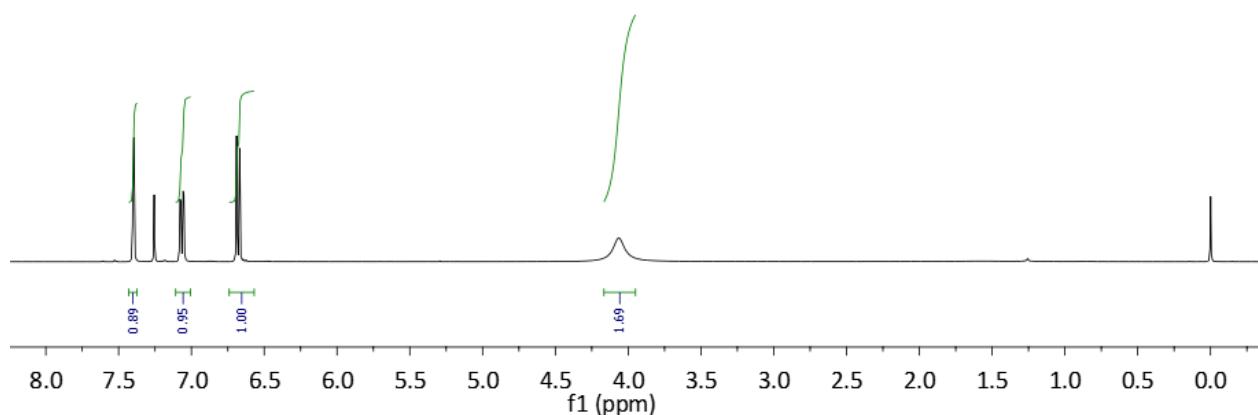
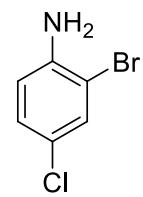
<sup>1</sup>H-NMR of 15b in CDCl<sub>3</sub>

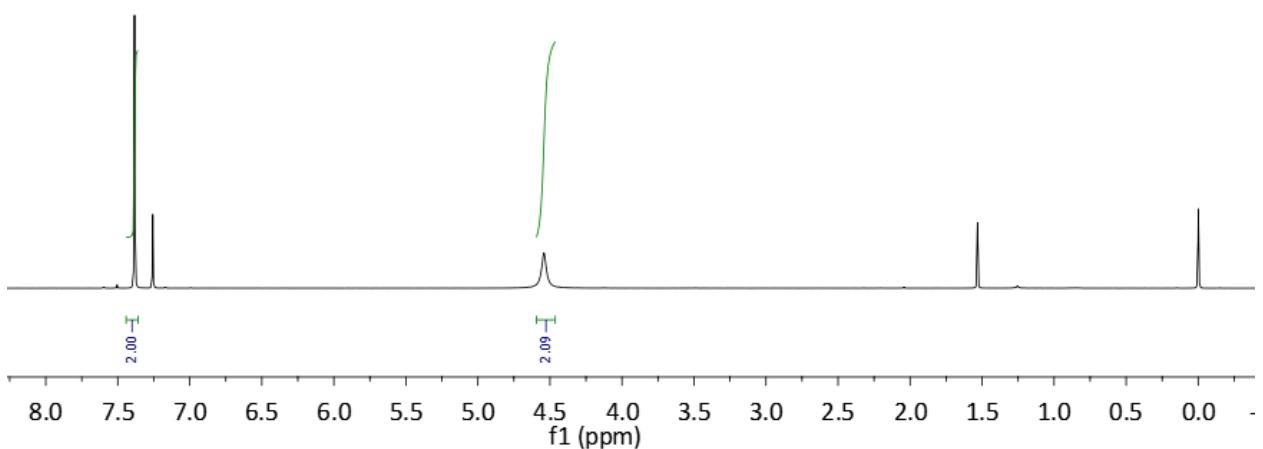
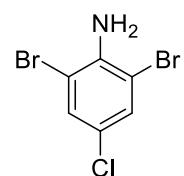
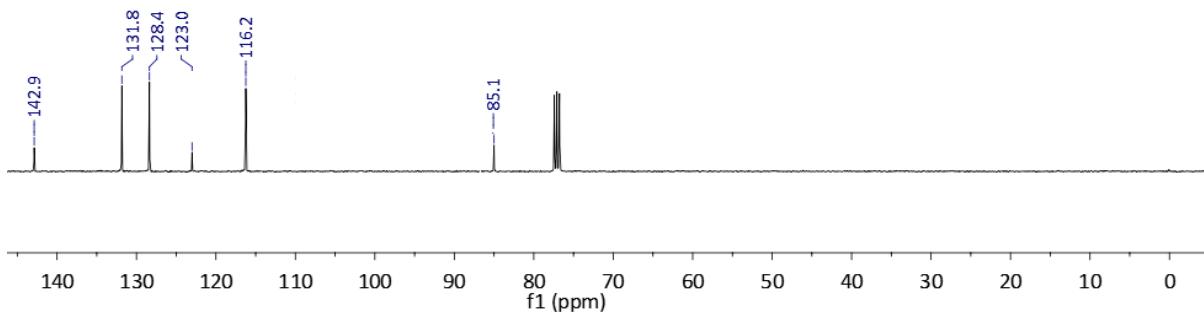
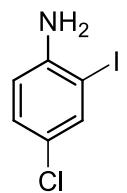


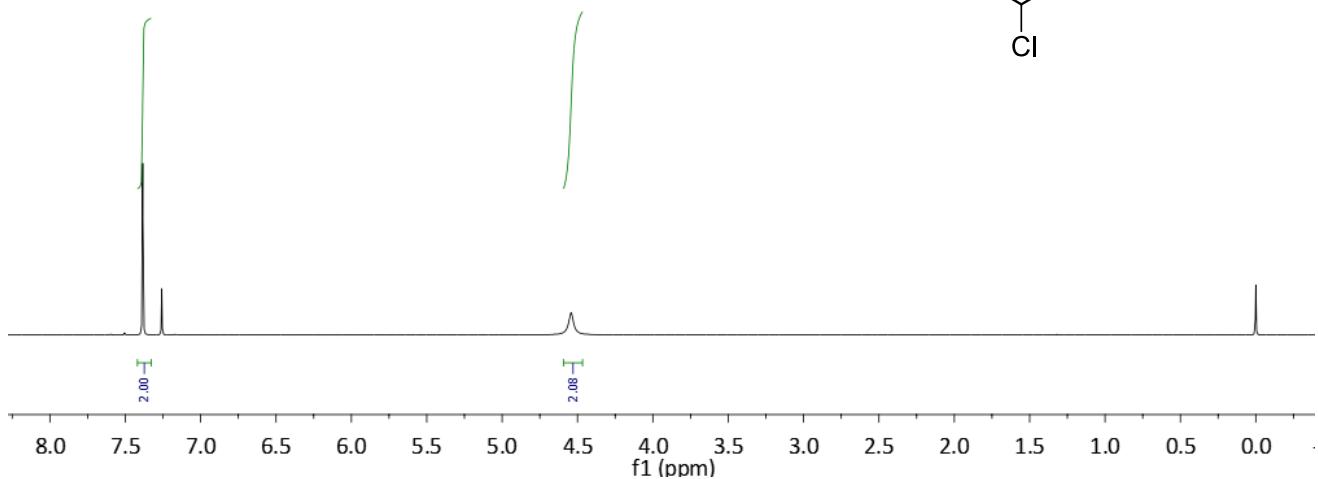
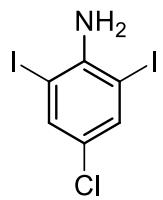
$^1\text{H}$ -NMR of 15c in  $\text{CDCl}_3$



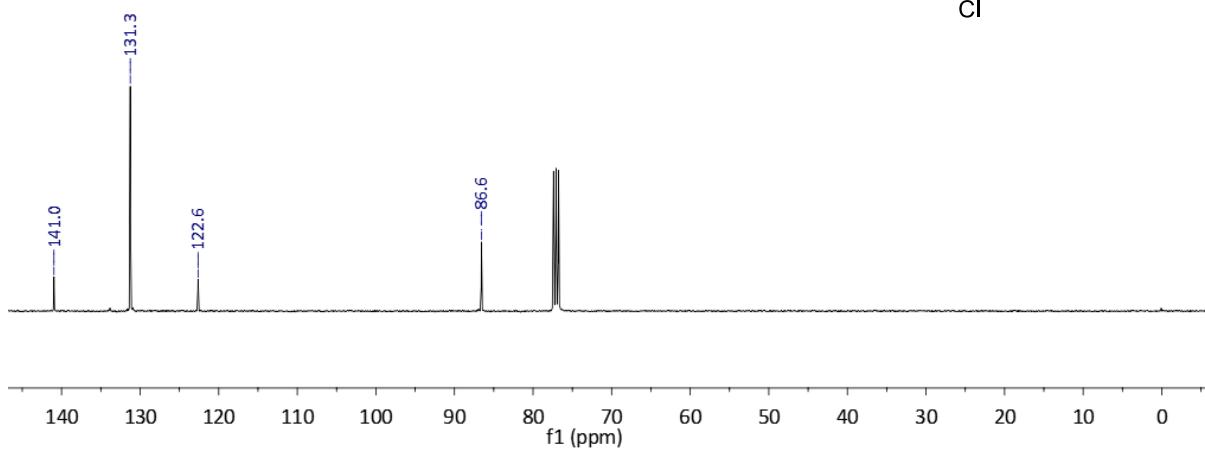
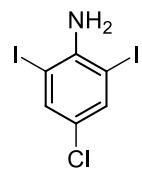
$^1\text{H}$ -NMR of 15d in  $\text{CDCl}_3$



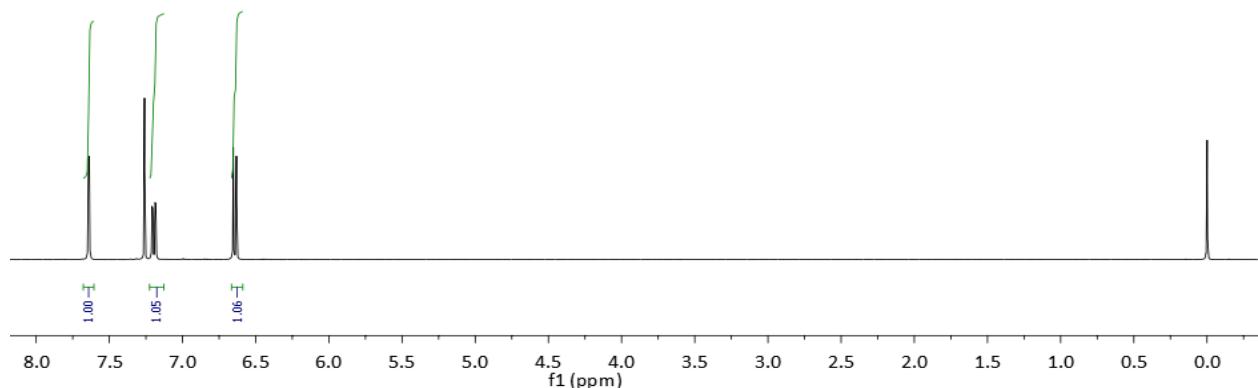
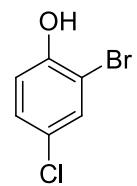




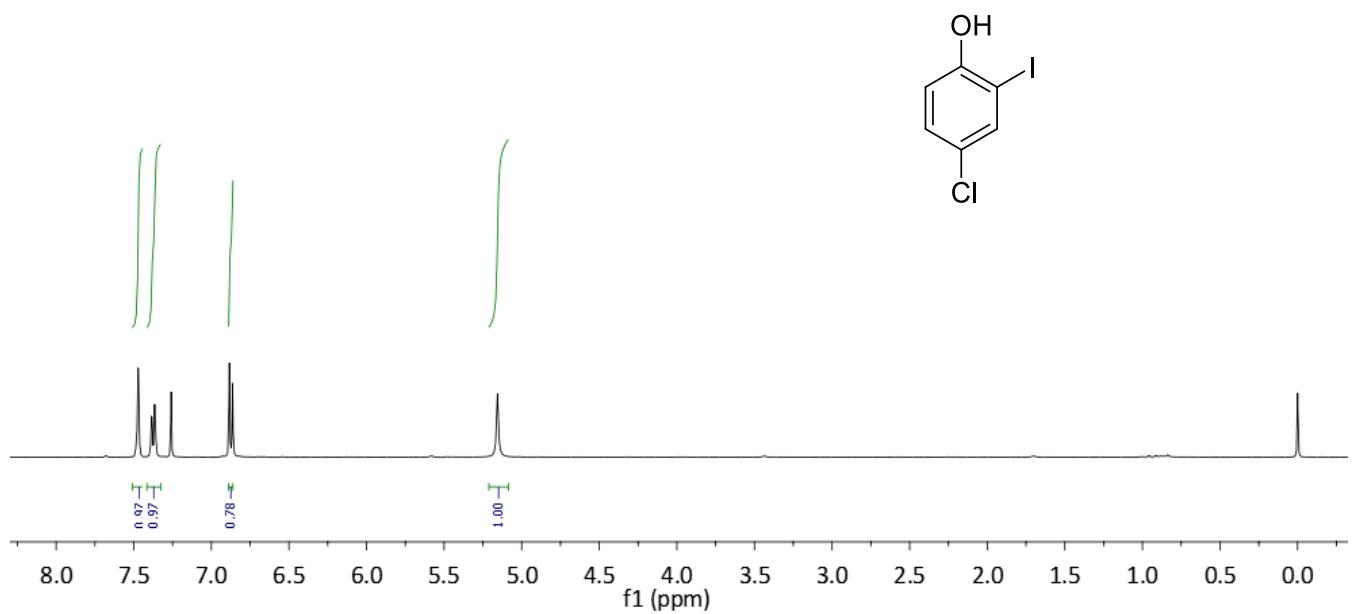
<sup>1</sup>H-NMR of 16d in CDCl<sub>3</sub>



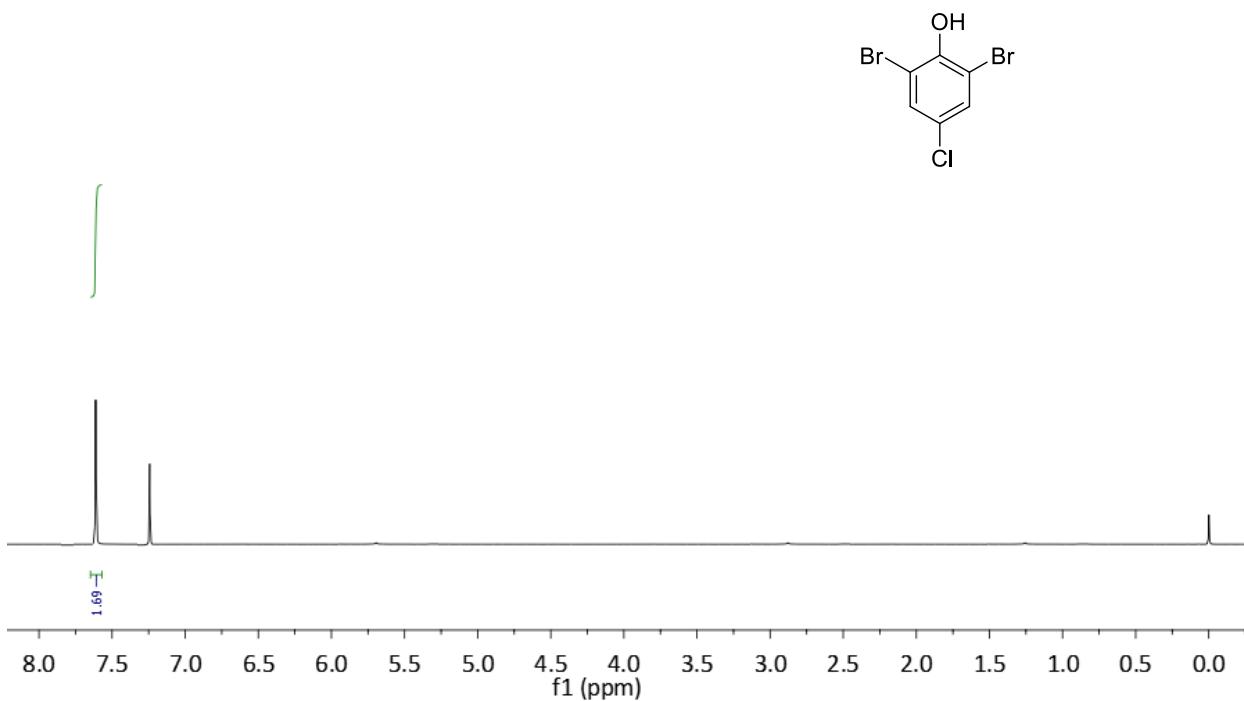
<sup>13</sup>C NMR of 16d in CDCl<sub>3</sub>



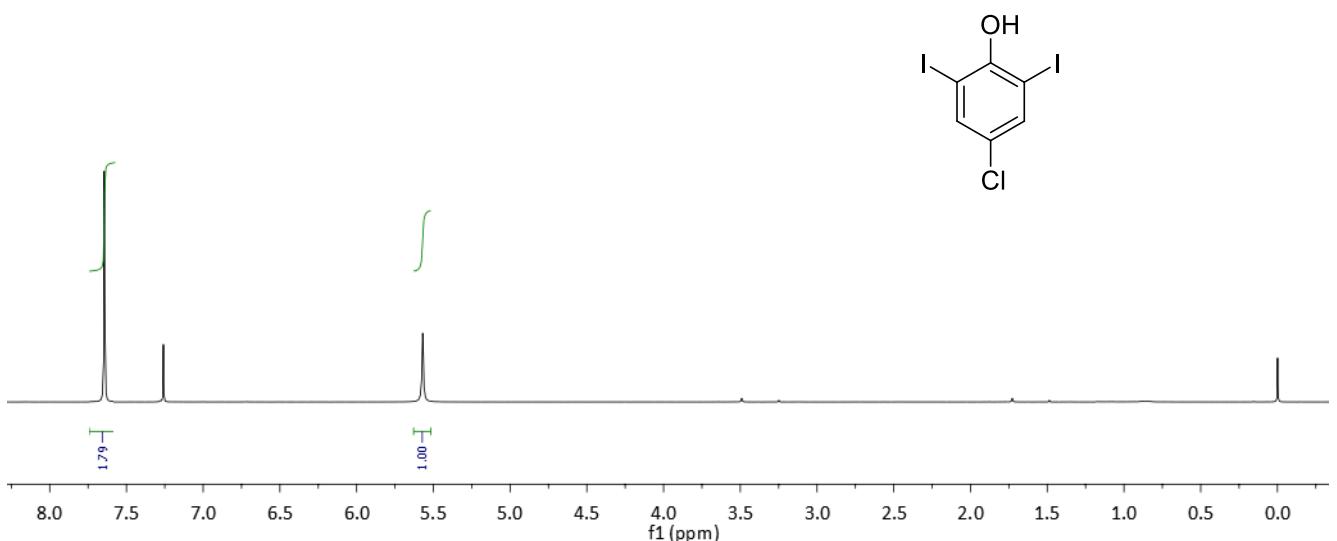
<sup>1</sup>H-NMR of 17a in CDCl<sub>3</sub>



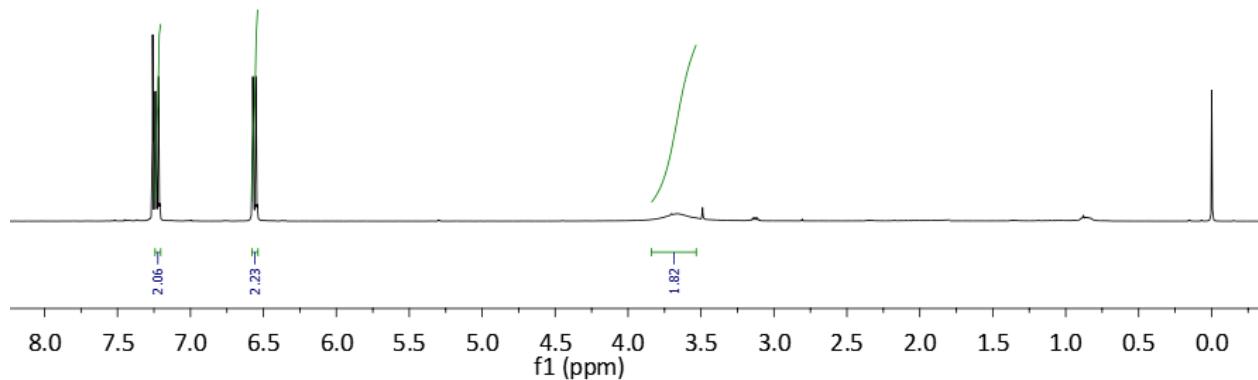
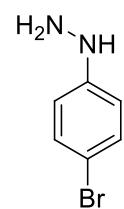
<sup>1</sup>H-NMR of 17b in CDCl<sub>3</sub>



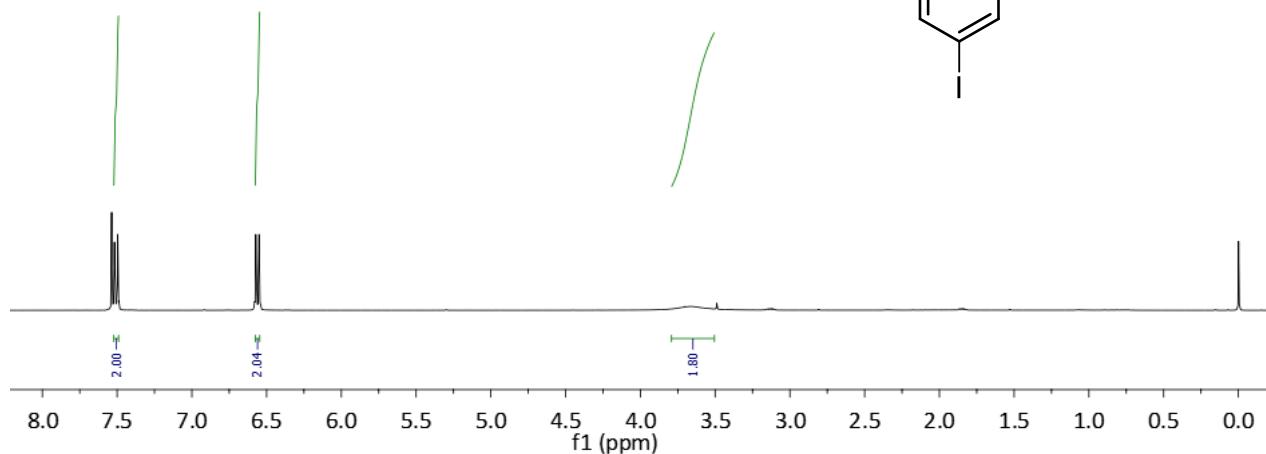
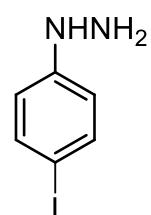
<sup>1</sup>H-NMR of 17c in CDCl<sub>3</sub>



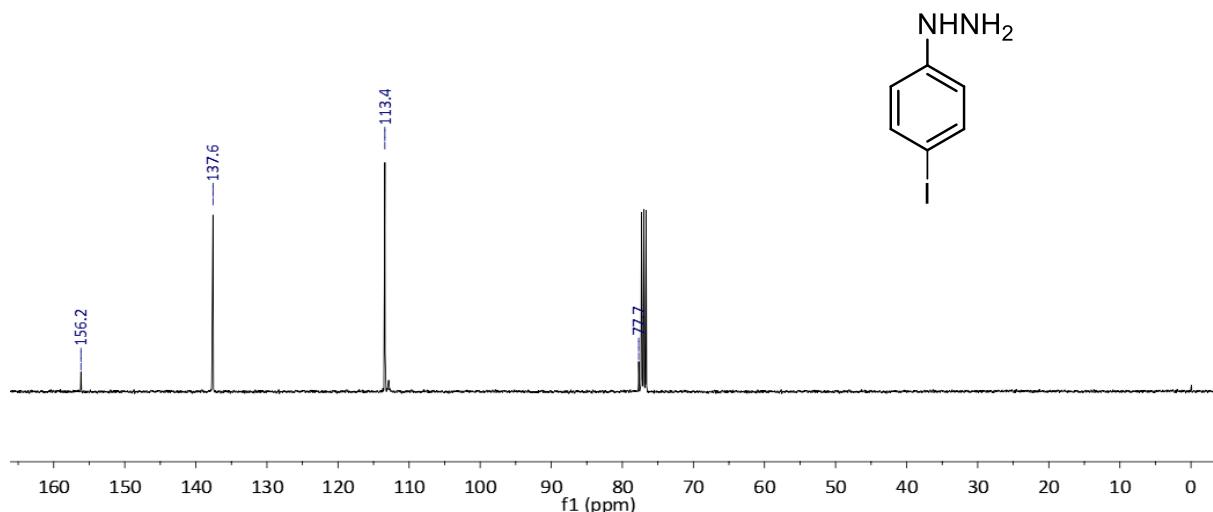
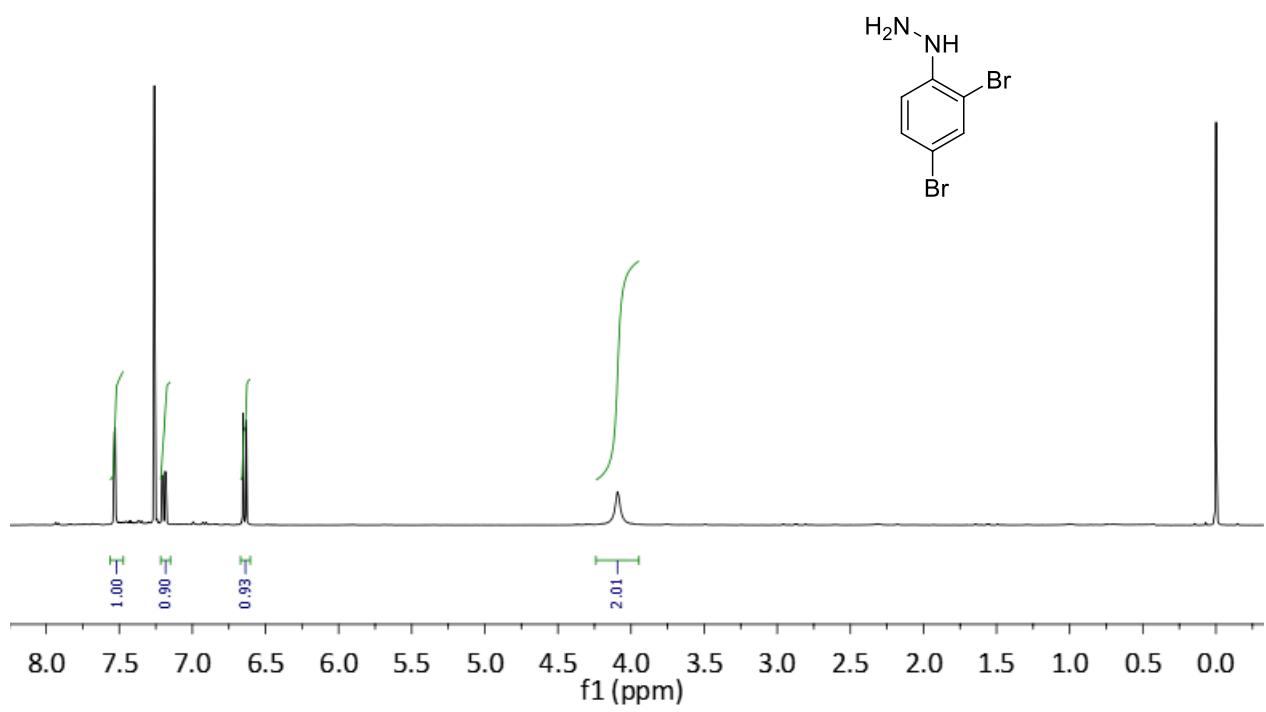
<sup>1</sup>H-NMR of 17d in CDCl<sub>3</sub>

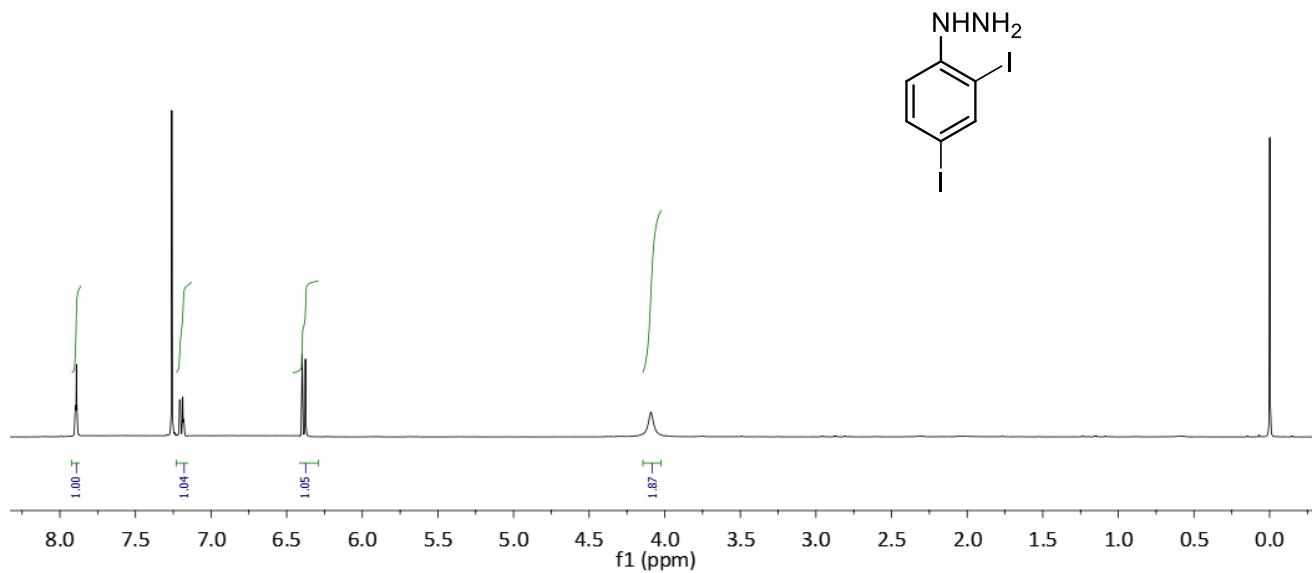


<sup>1</sup>H-NMR of 18a in CDCl<sub>3</sub>

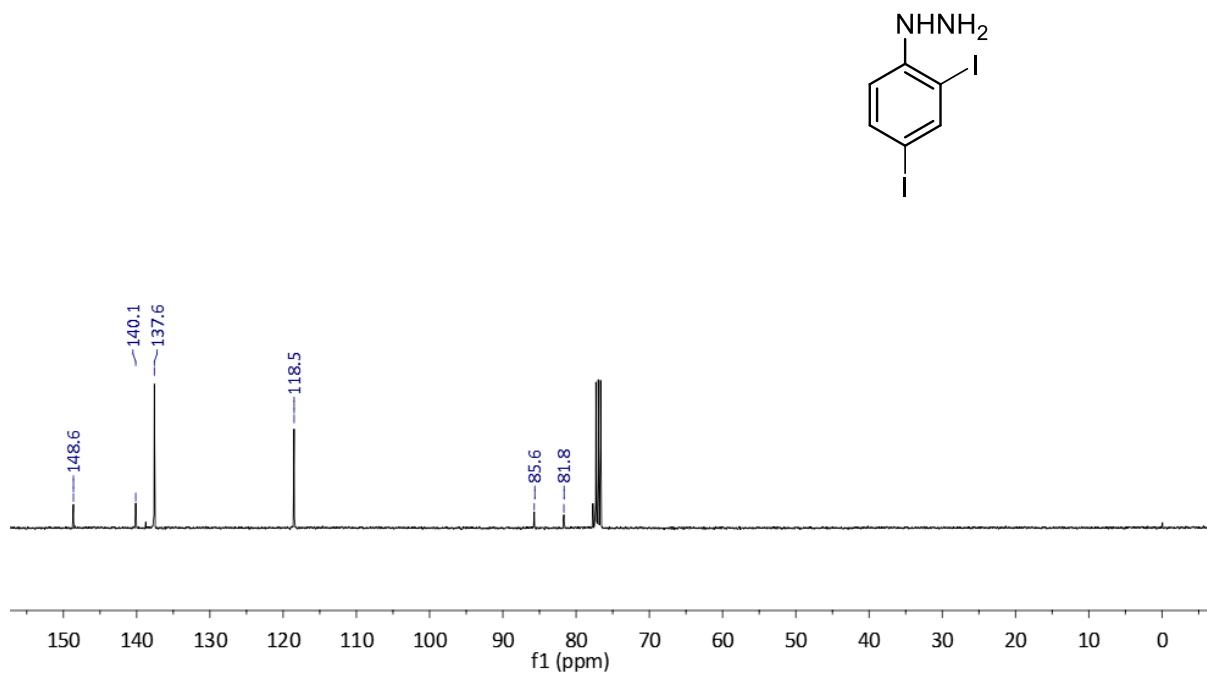


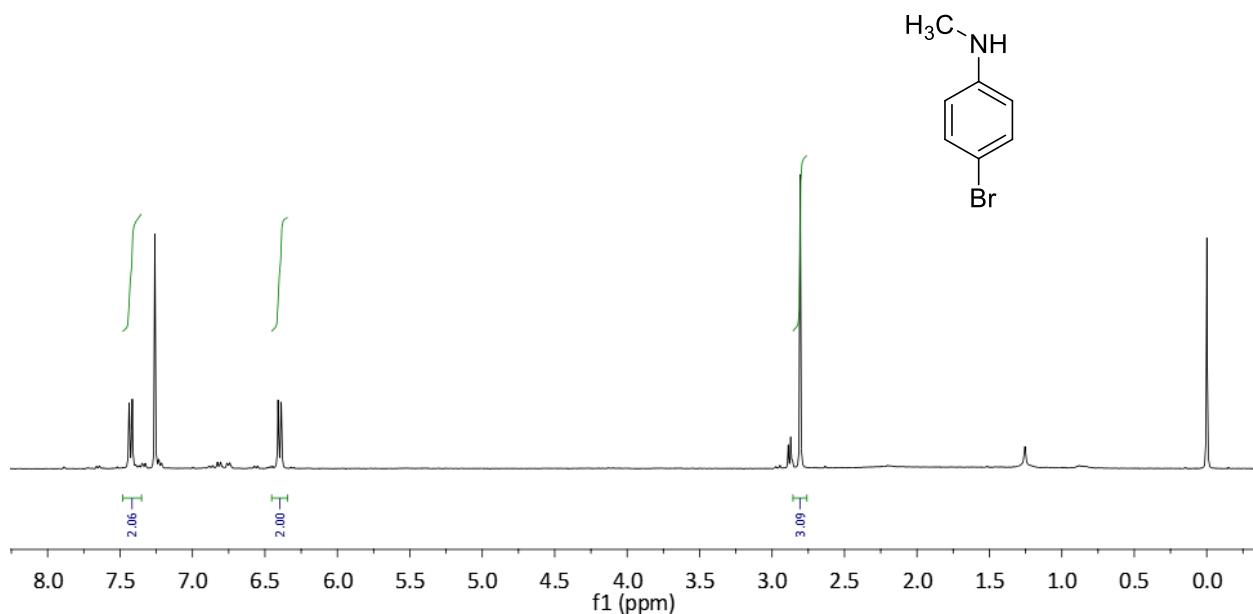
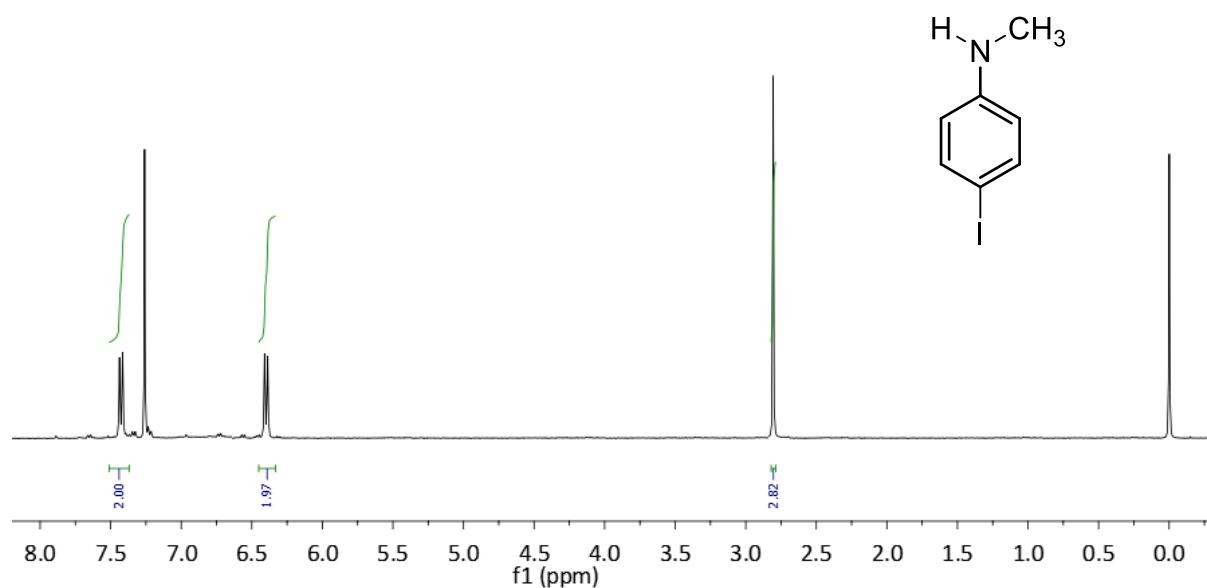
<sup>1</sup>H-NMR of 18b in CDCl<sub>3</sub>

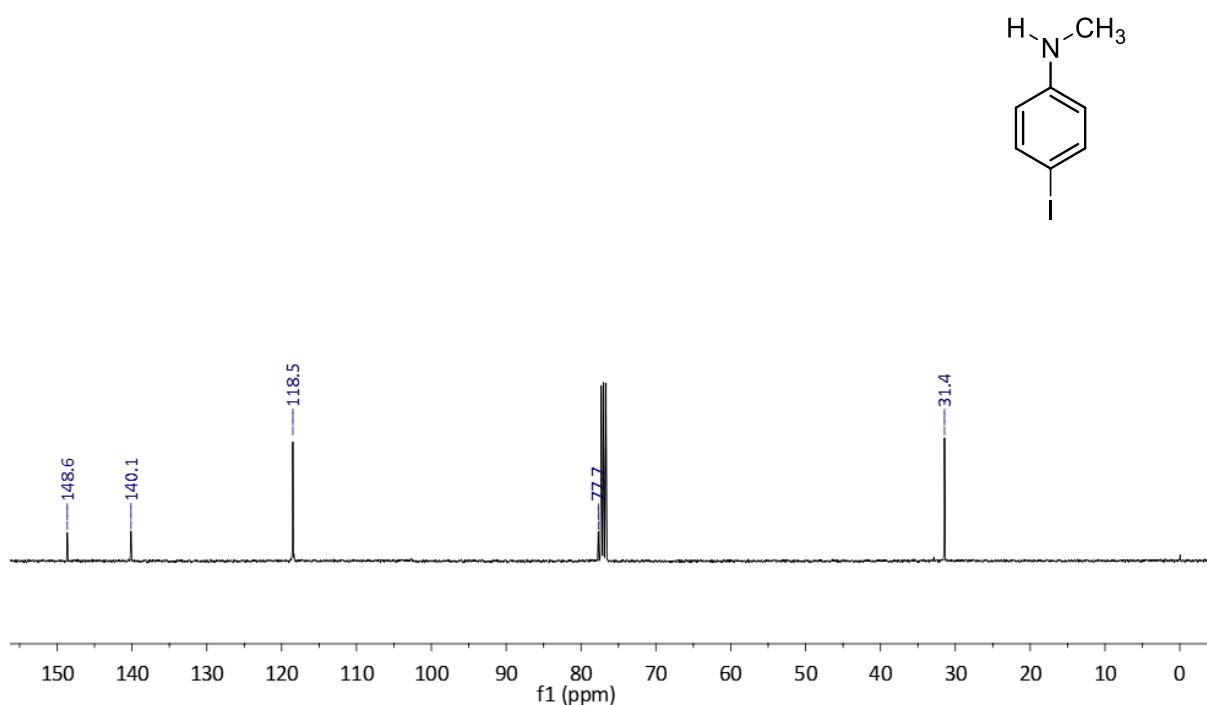
<sup>13</sup>C NMR of 18b in  $\text{CDCl}_3$ <sup>1</sup>H-NMR of 18c in  $\text{CDCl}_3$



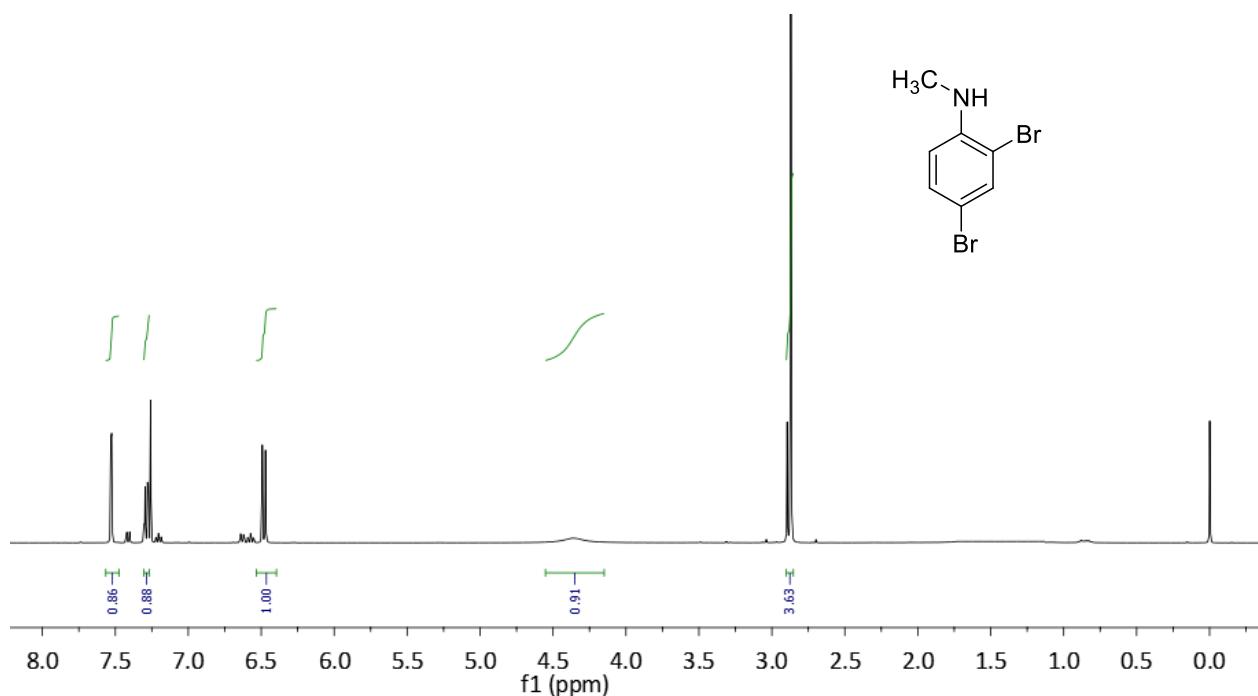
<sup>1</sup>H-NMR of 18d in CDCl<sub>3</sub>



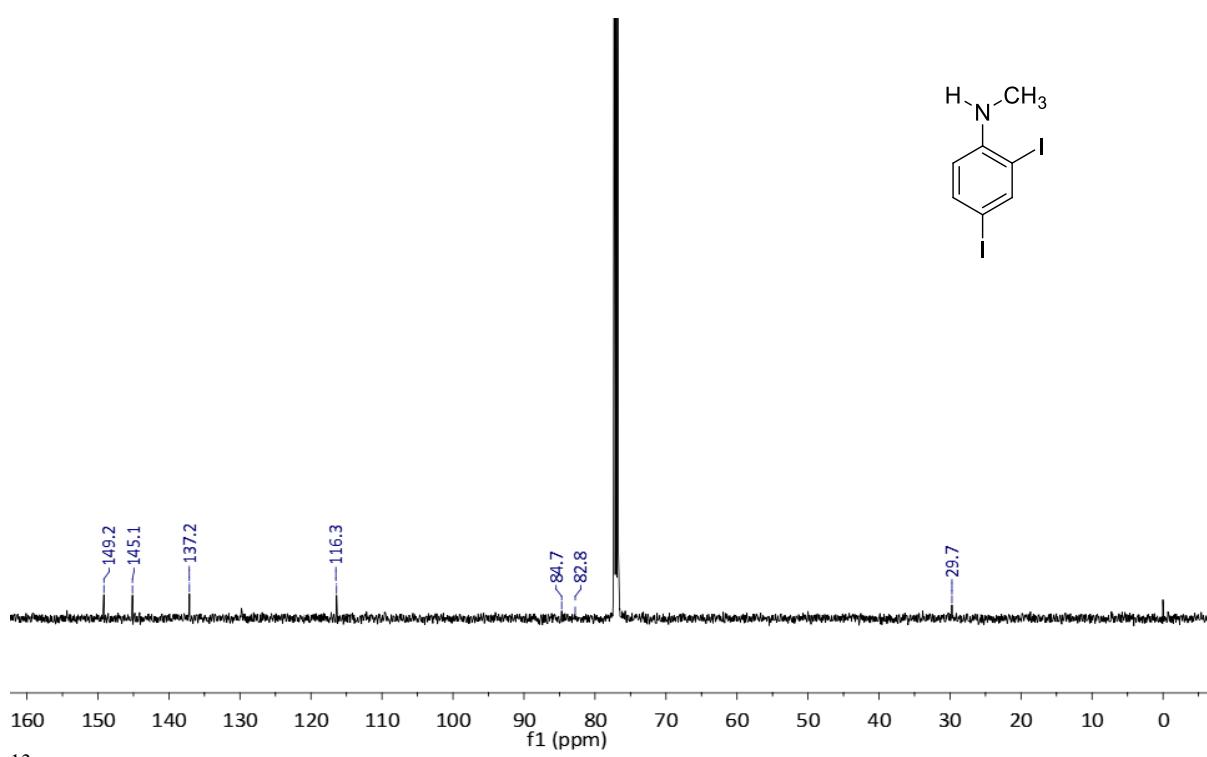
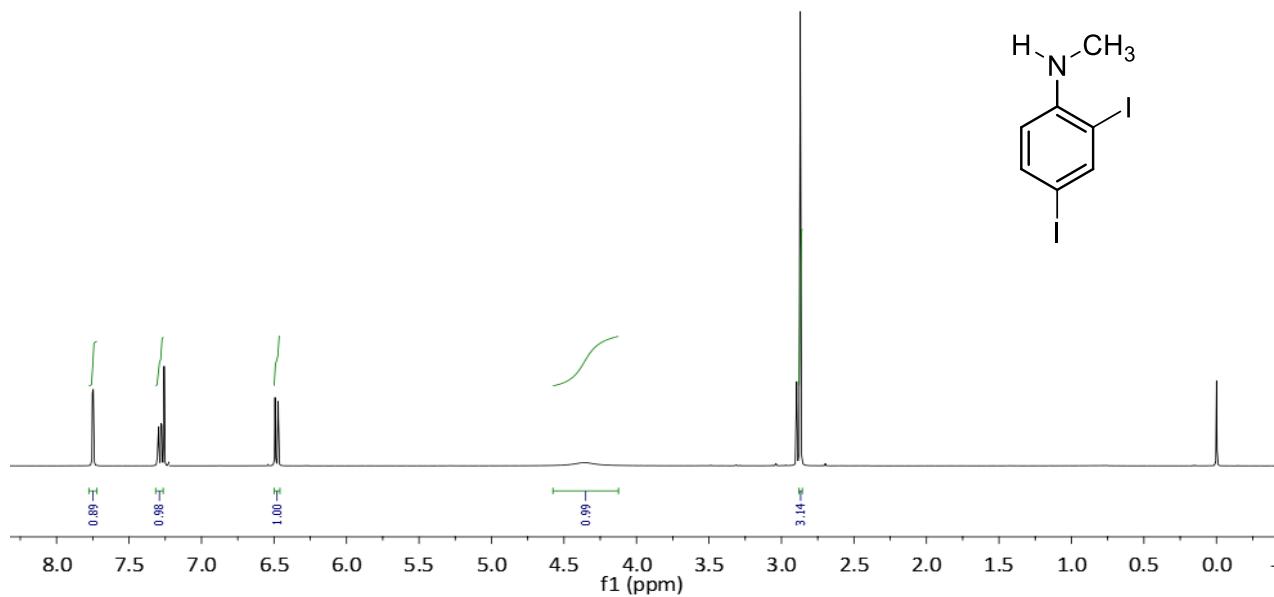
<sup>1</sup>H-NMR of 19a in CDCl<sub>3</sub><sup>1</sup>H-NMR of 19b in CDCl<sub>3</sub>

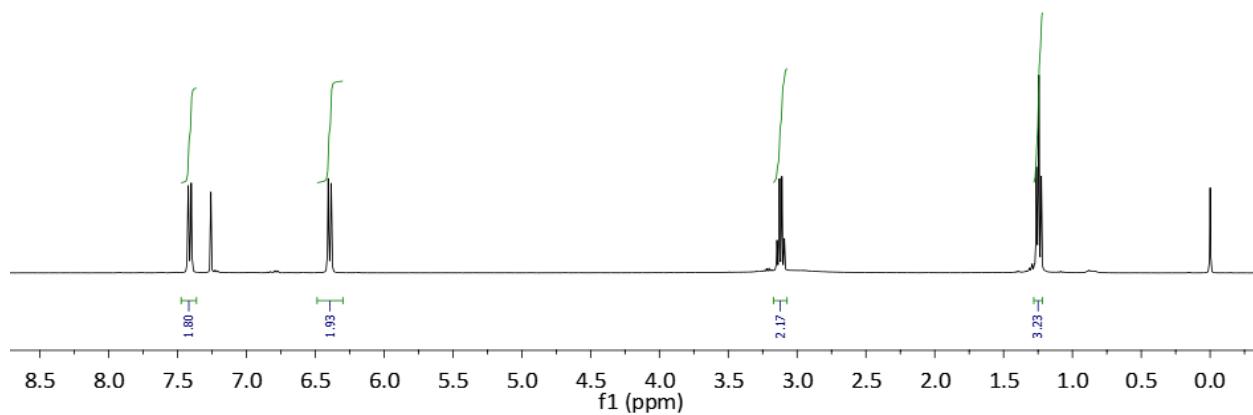
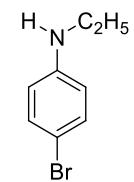


<sup>13</sup>C NMR of 19b in CDCl<sub>3</sub>

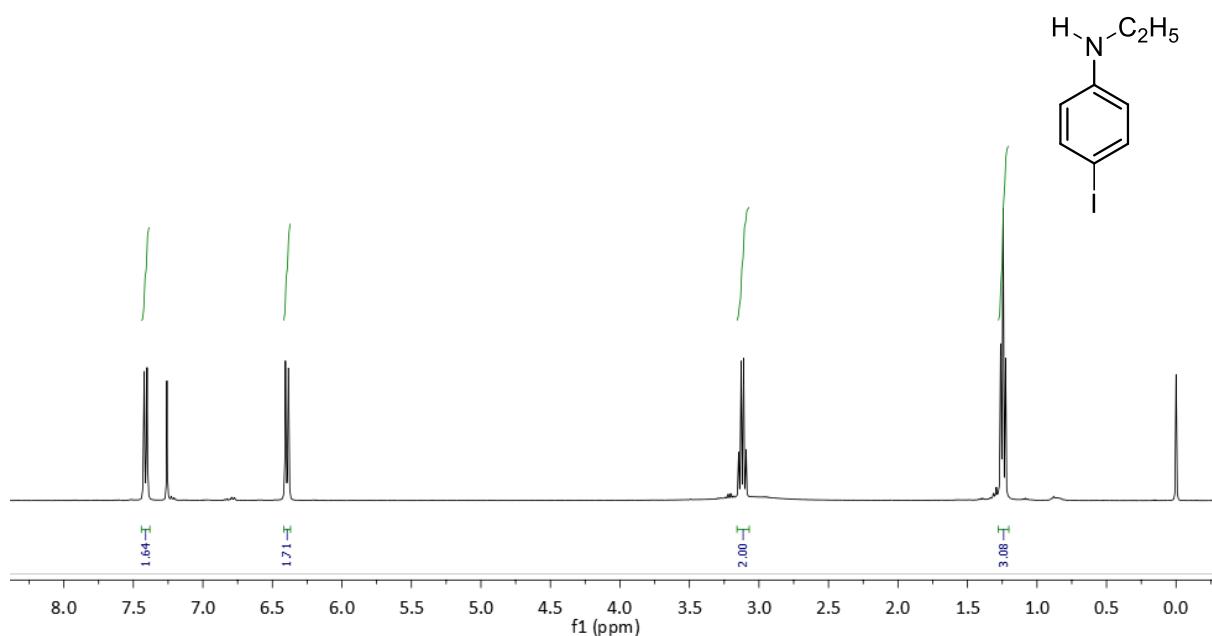


<sup>1</sup>H-NMR of 19c in CDCl<sub>3</sub>

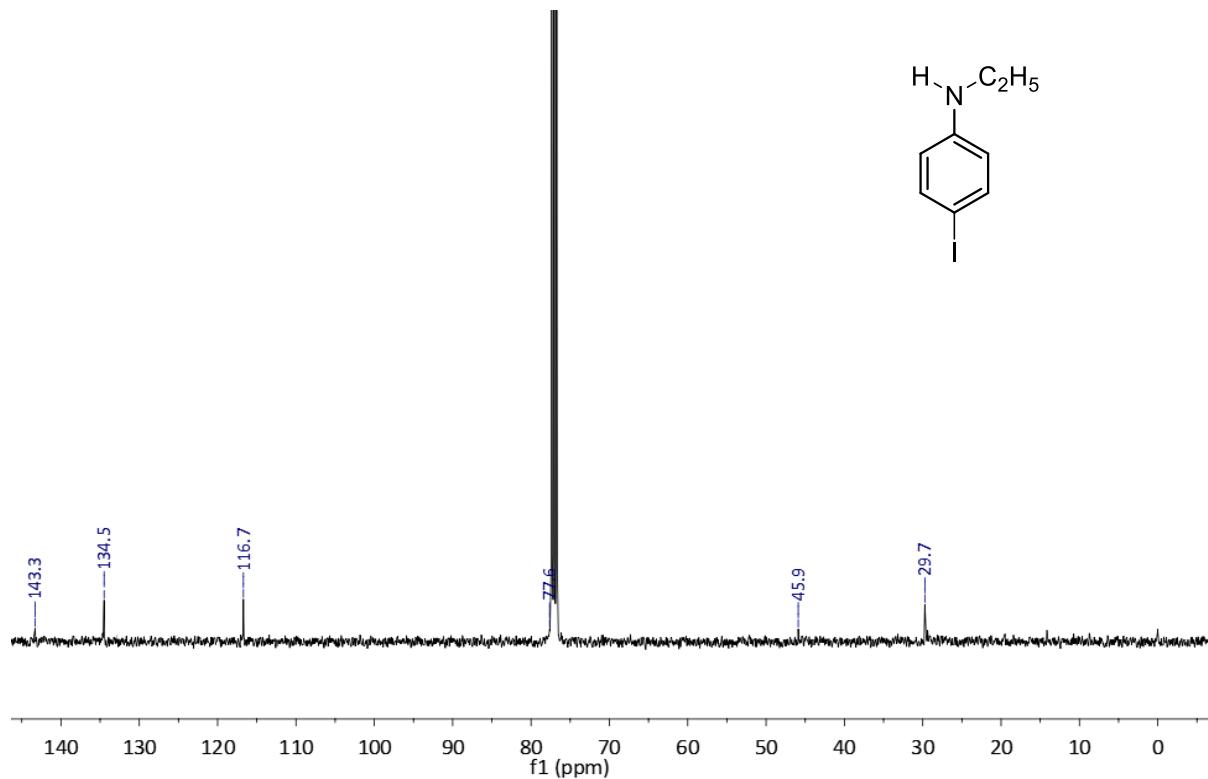
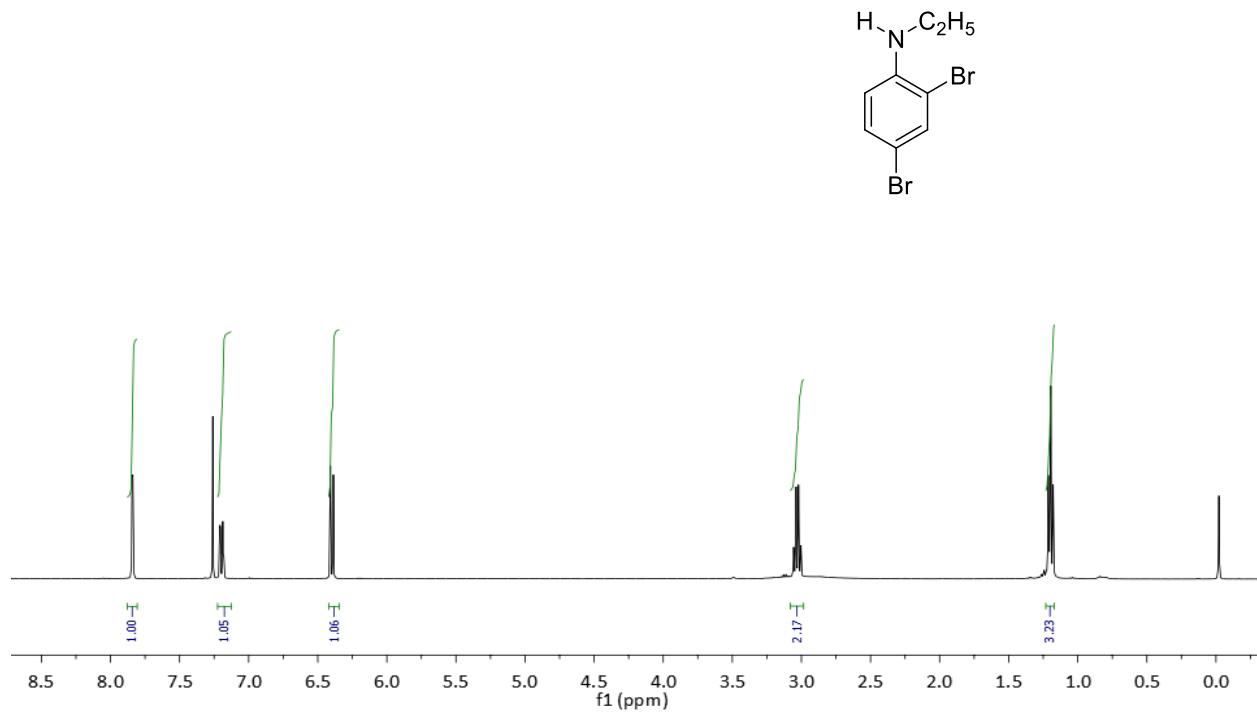


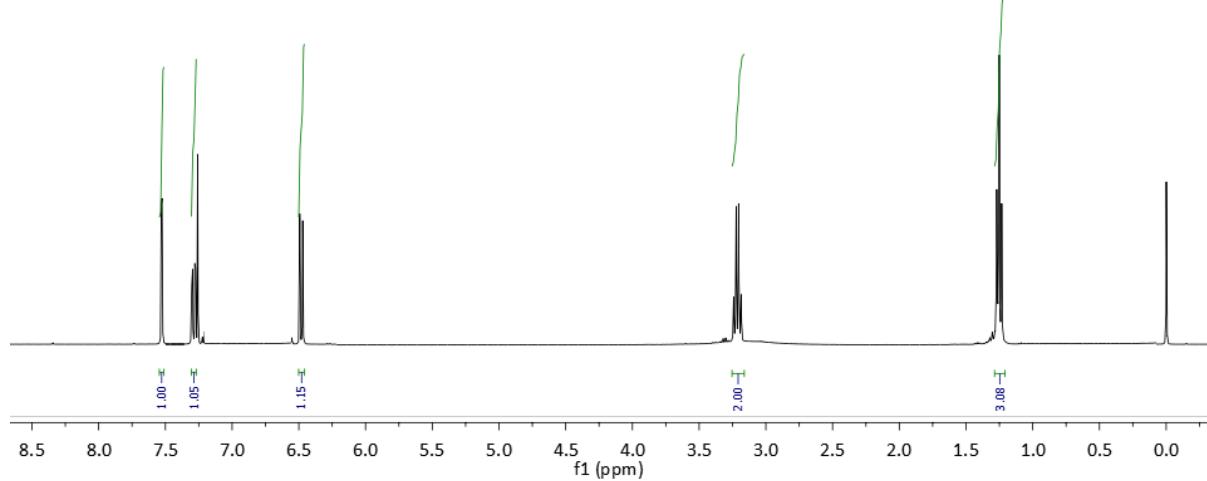
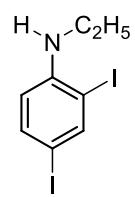


<sup>1</sup>H-NMR of 20a in CDCl<sub>3</sub>

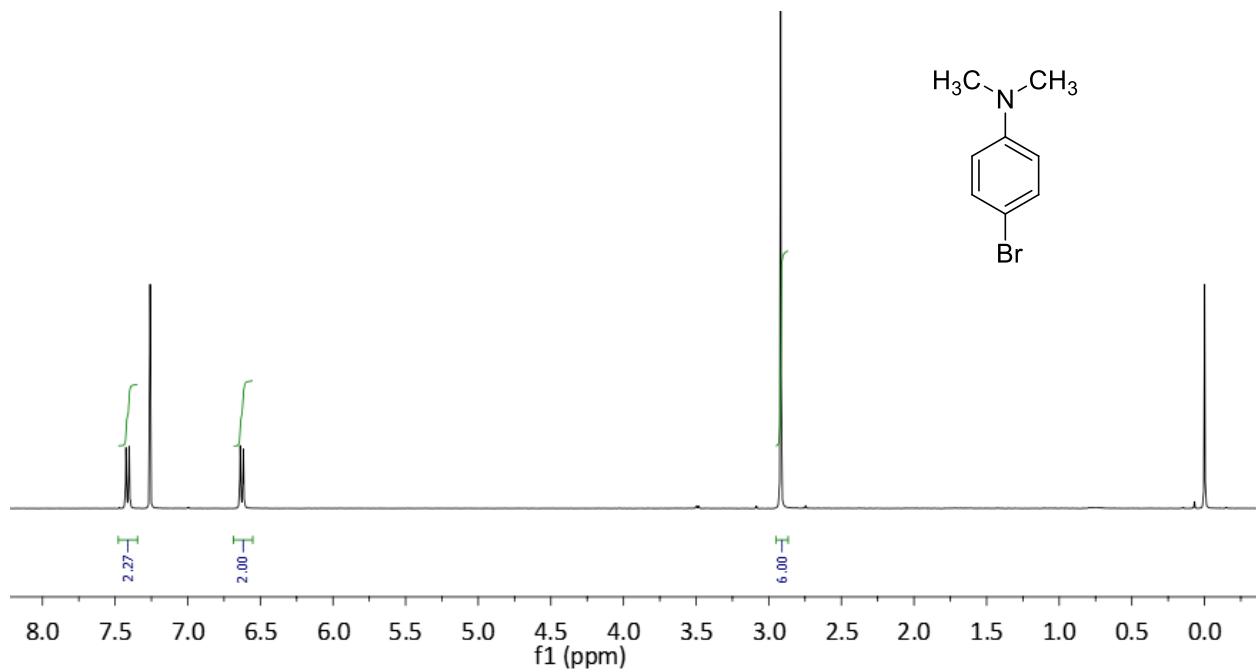


<sup>1</sup>H-NMR of 20b in CDCl<sub>3</sub>

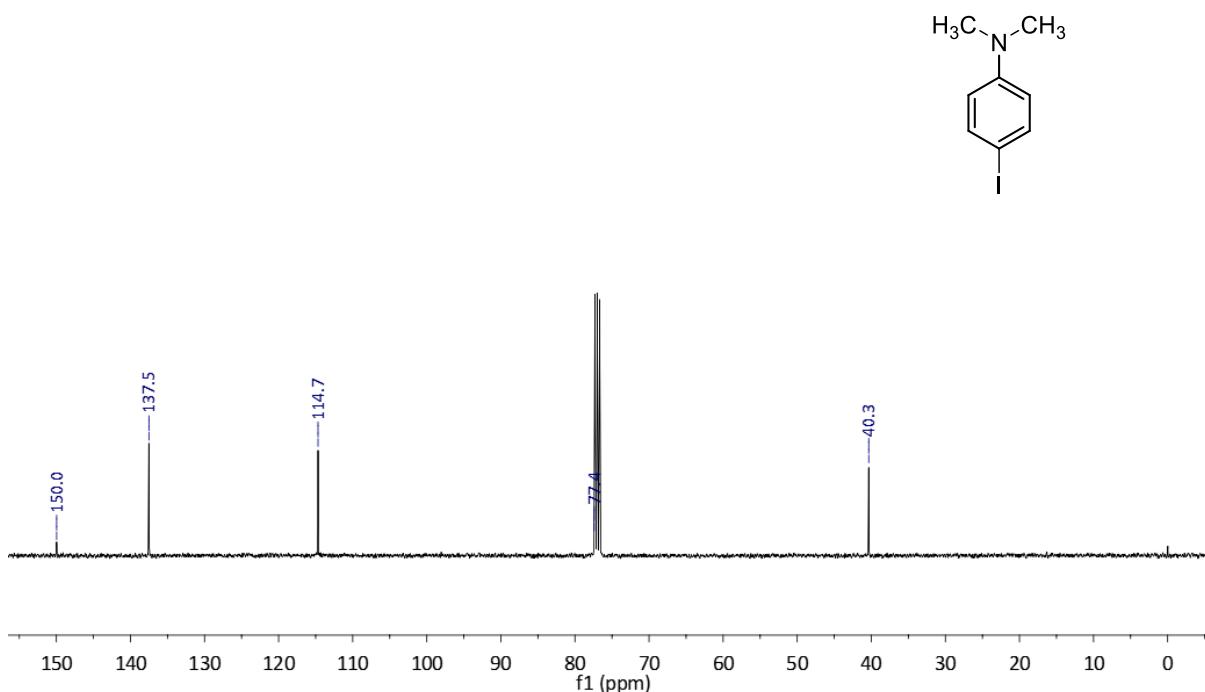
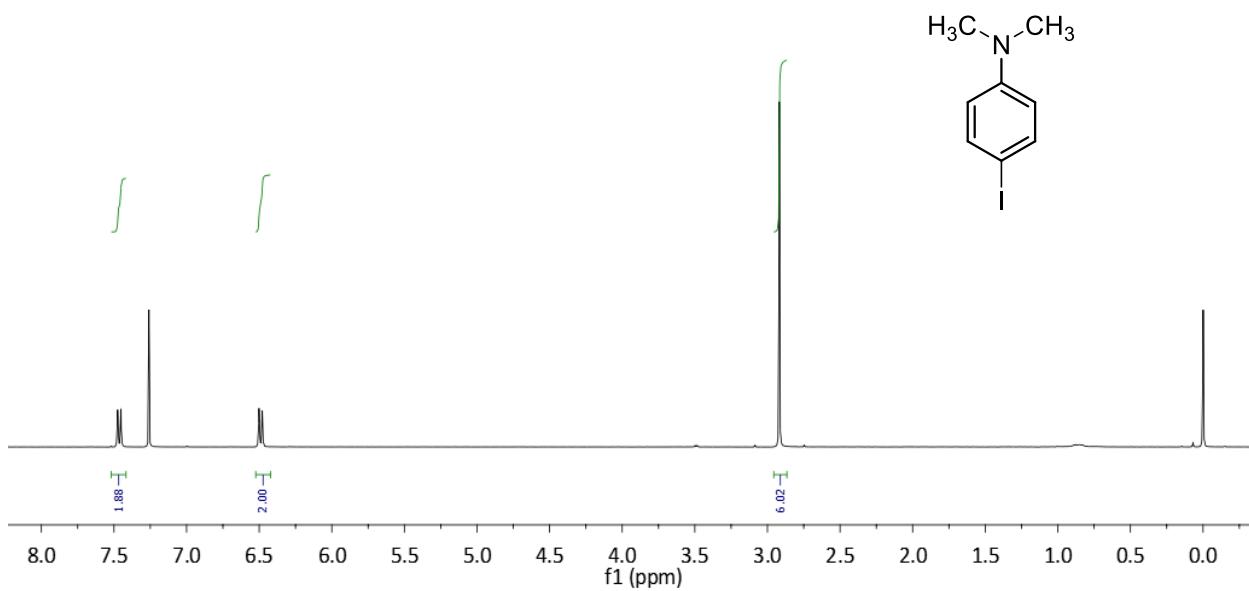
<sup>13</sup>C NMR of 20b in  $\text{CDCl}_3$ <sup>1</sup>H-NMR of 20C in  $\text{CDCl}_3$

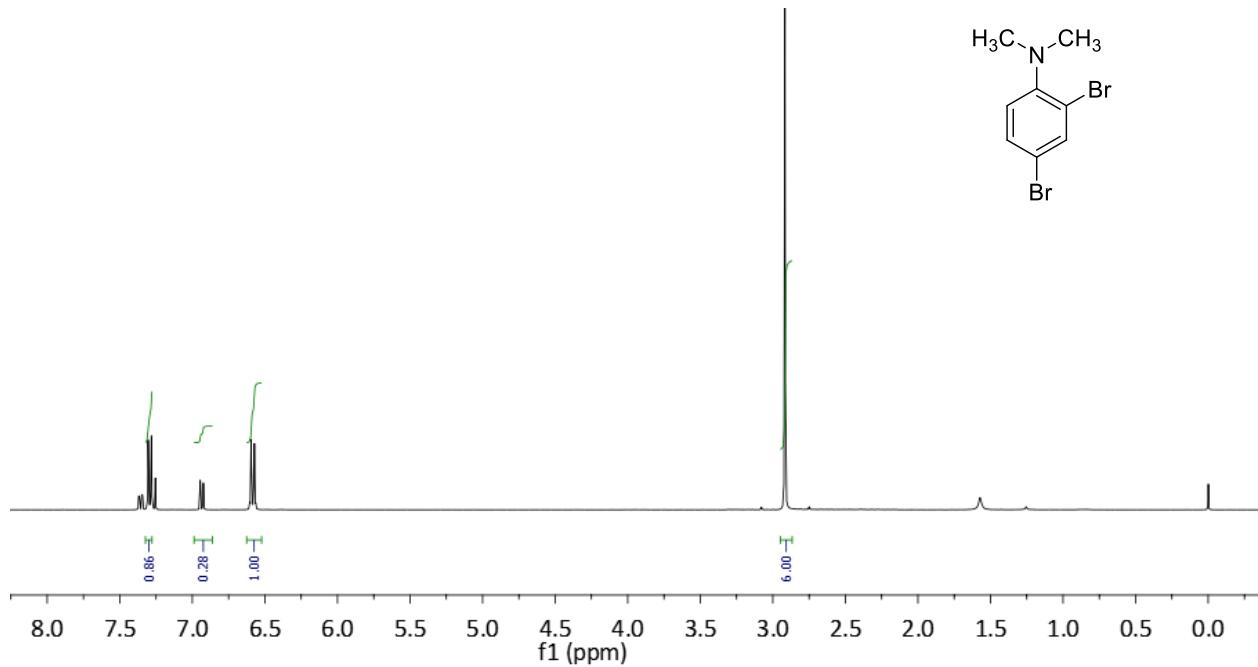


<sup>1</sup>H-NMR of 20d in CDCl<sub>3</sub>

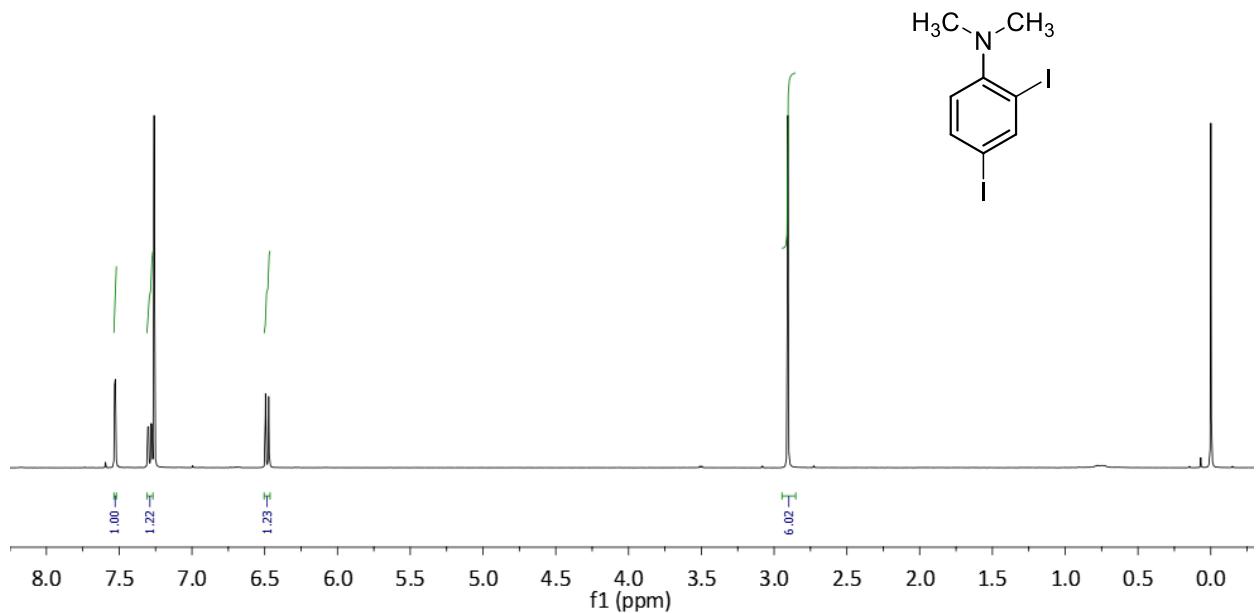


<sup>1</sup>H-NMR of 21a in CDCl<sub>3</sub>

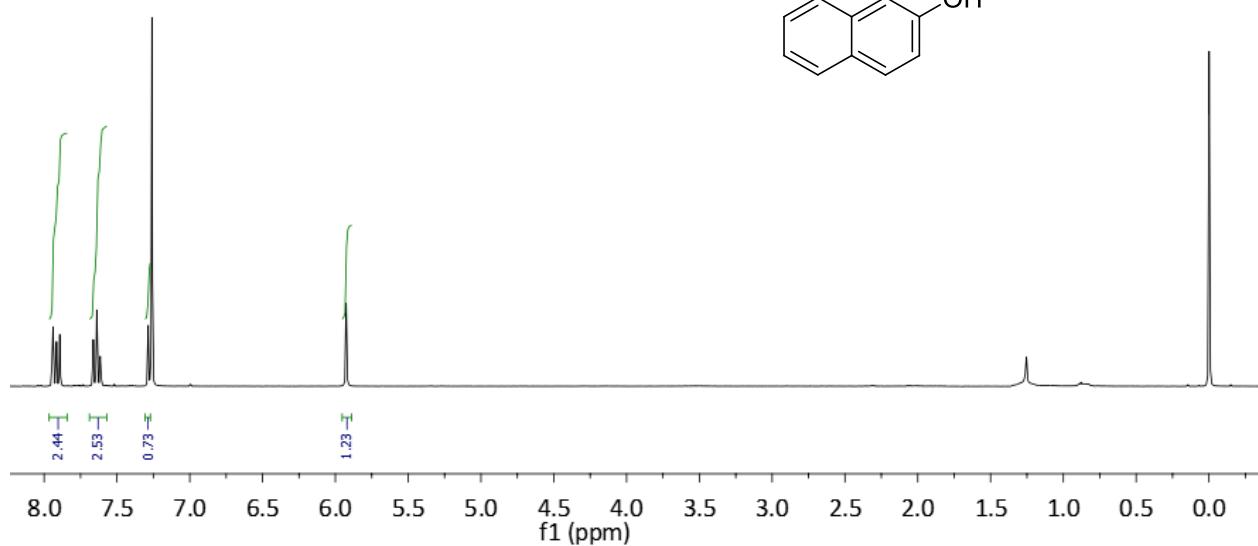
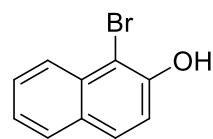




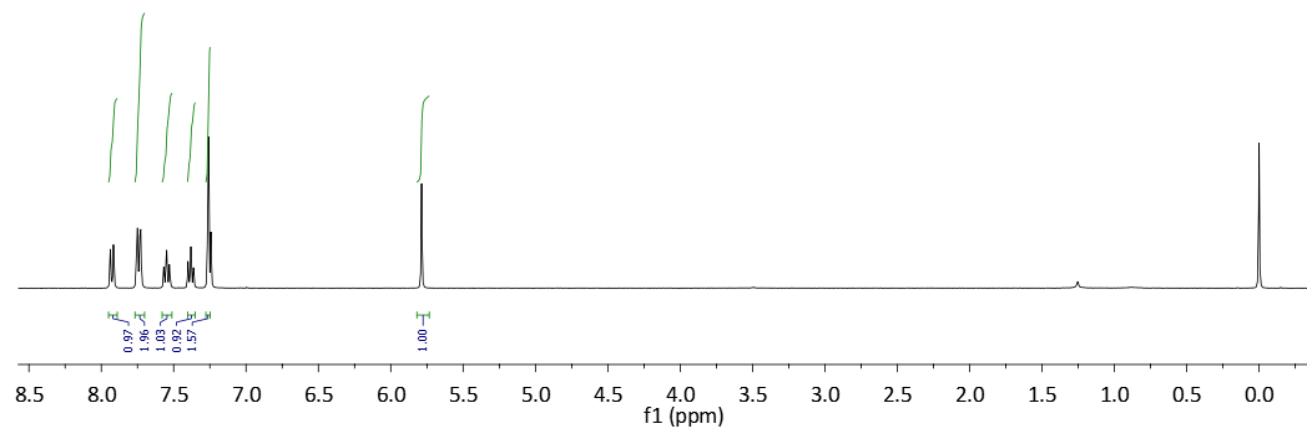
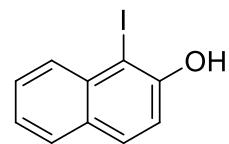
$^1\text{H}$ -NMR of 21c in  $\text{CDCl}_3$



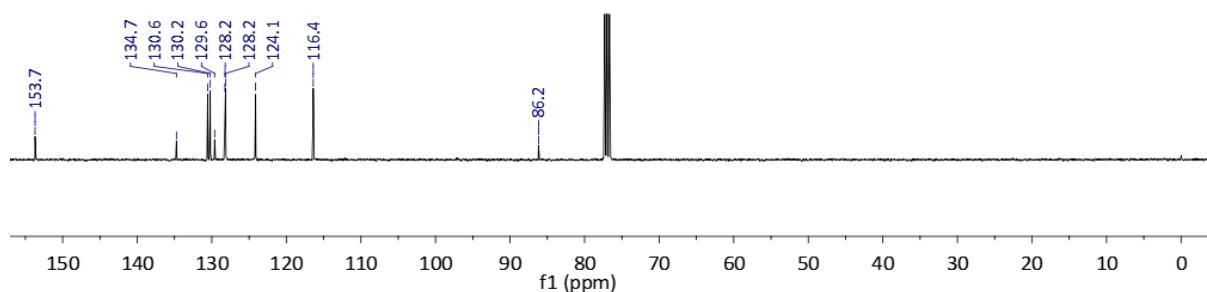
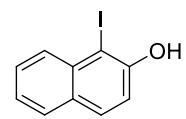
$^1\text{H}$ -NMR of 21d in  $\text{CDCl}_3$



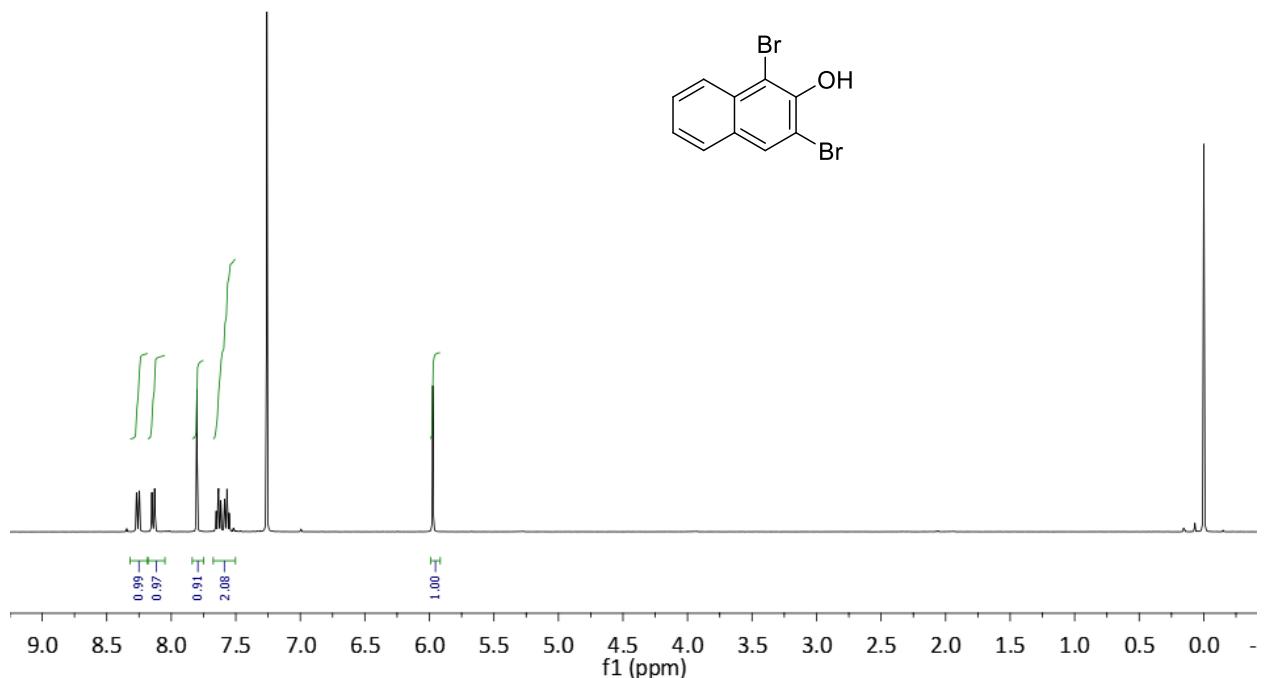
<sup>1</sup>H-NMR of 25a in CDCl<sub>3</sub>



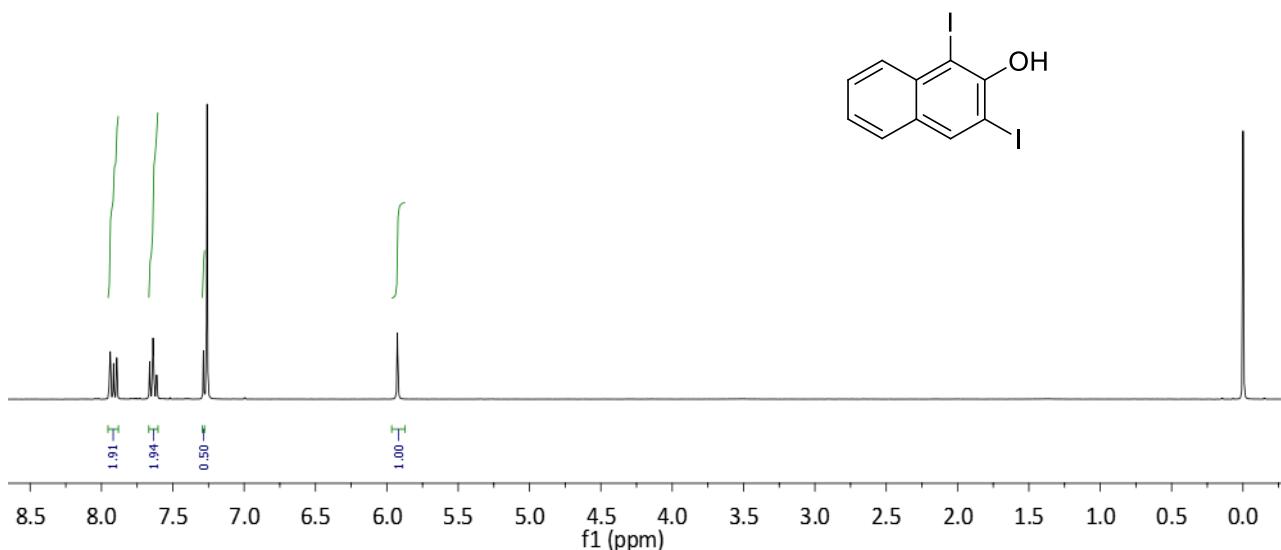
<sup>1</sup>H-NMR of 25b in CDCl<sub>3</sub>



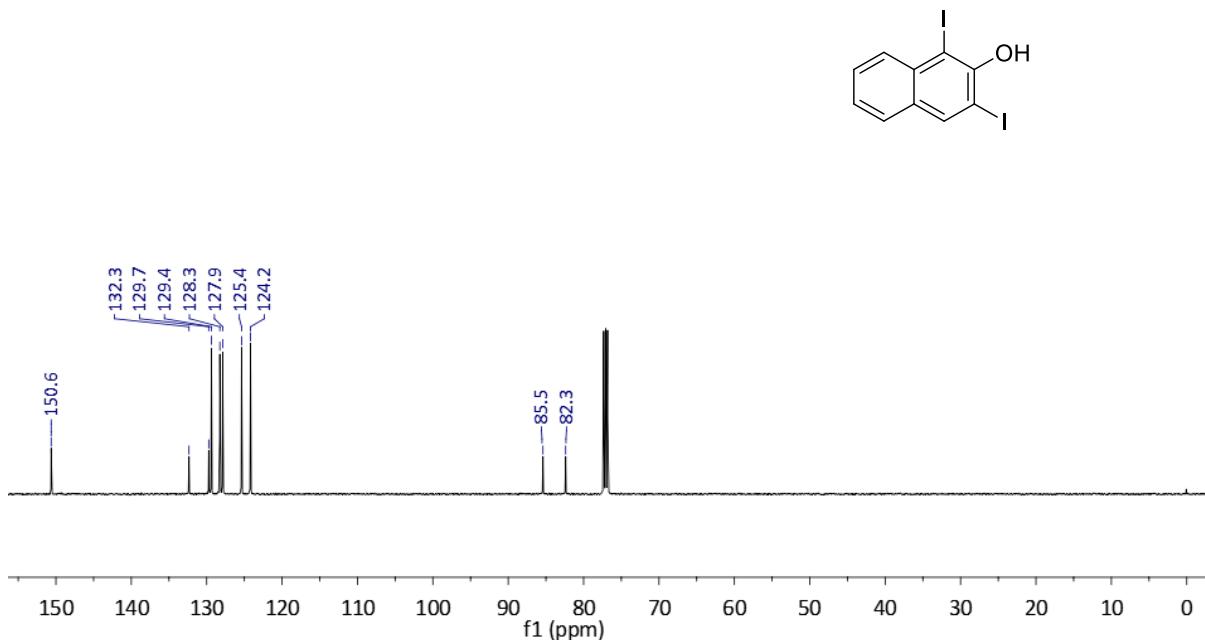
<sup>13</sup>C NMR of 25b in CDCl<sub>3</sub>

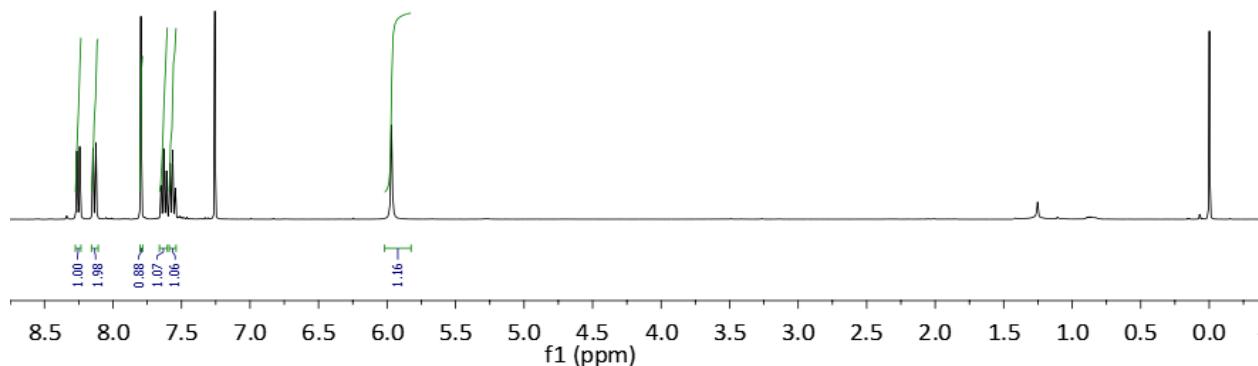
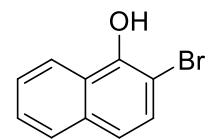


<sup>1</sup>H-NMR of 25c in CDCl<sub>3</sub>

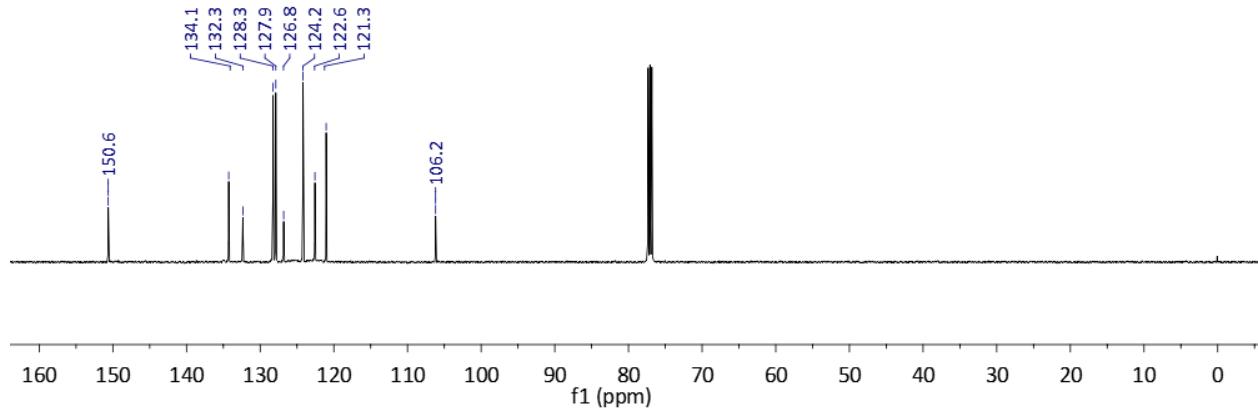
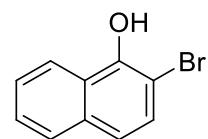


<sup>1</sup>H-NMR of 25d in CDCl<sub>3</sub>

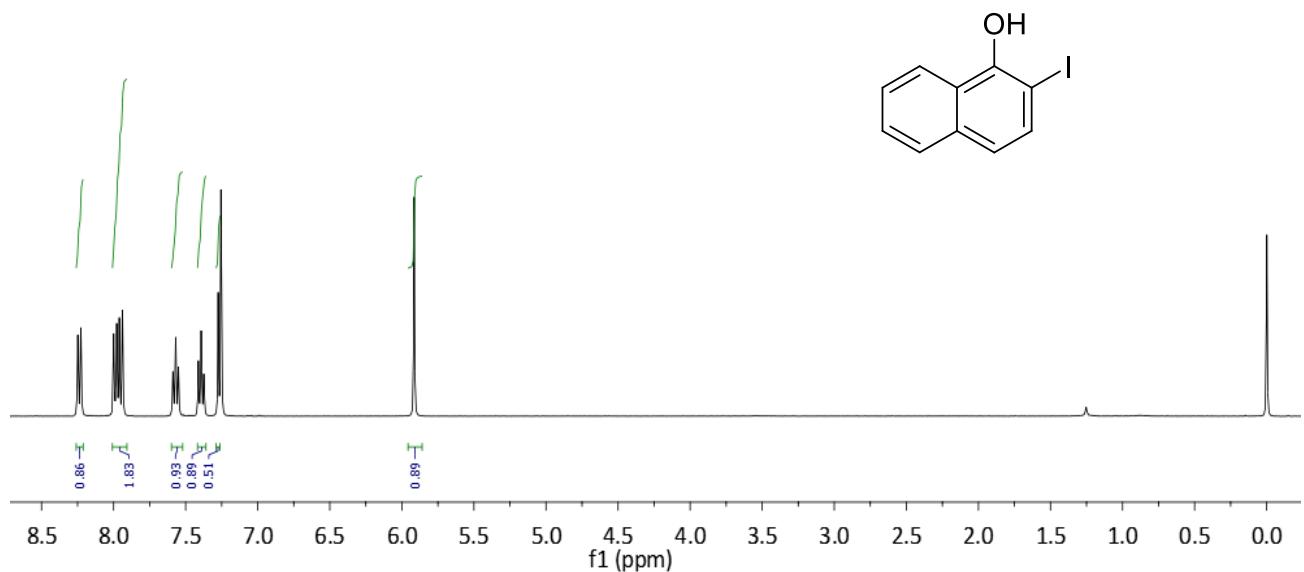




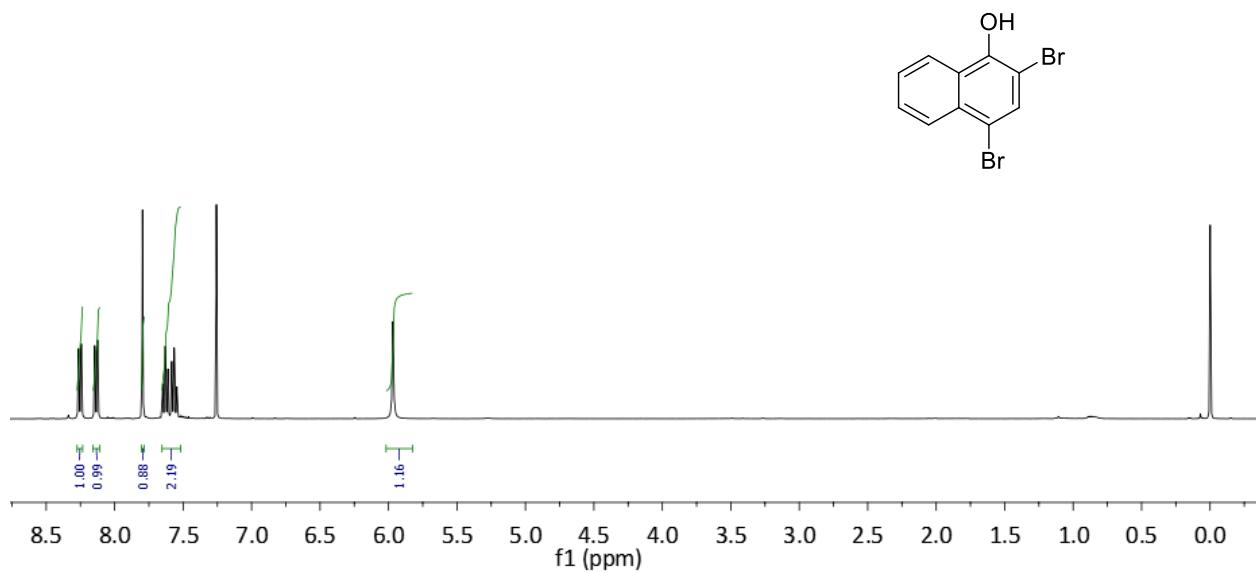
<sup>1</sup>H-NMR of 26a in  $\text{CDCl}_3$



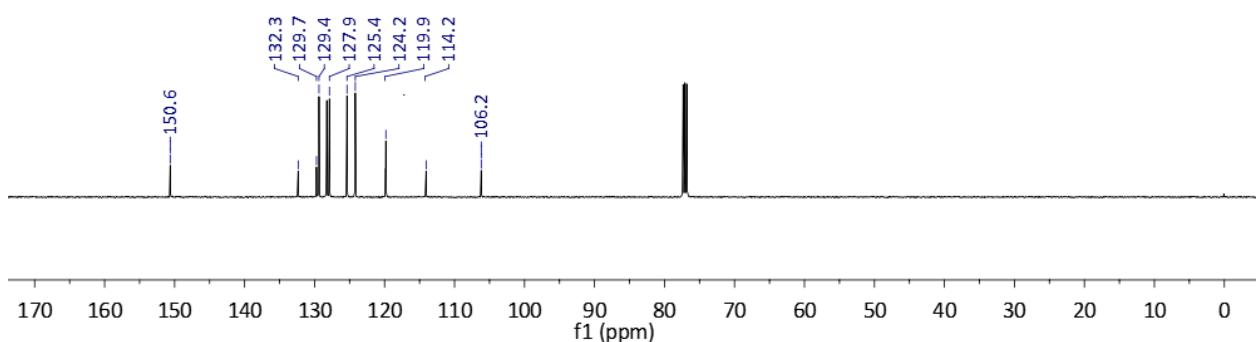
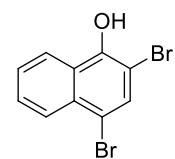
<sup>13</sup>C-NMR of 26a in  $\text{CDCl}_3$



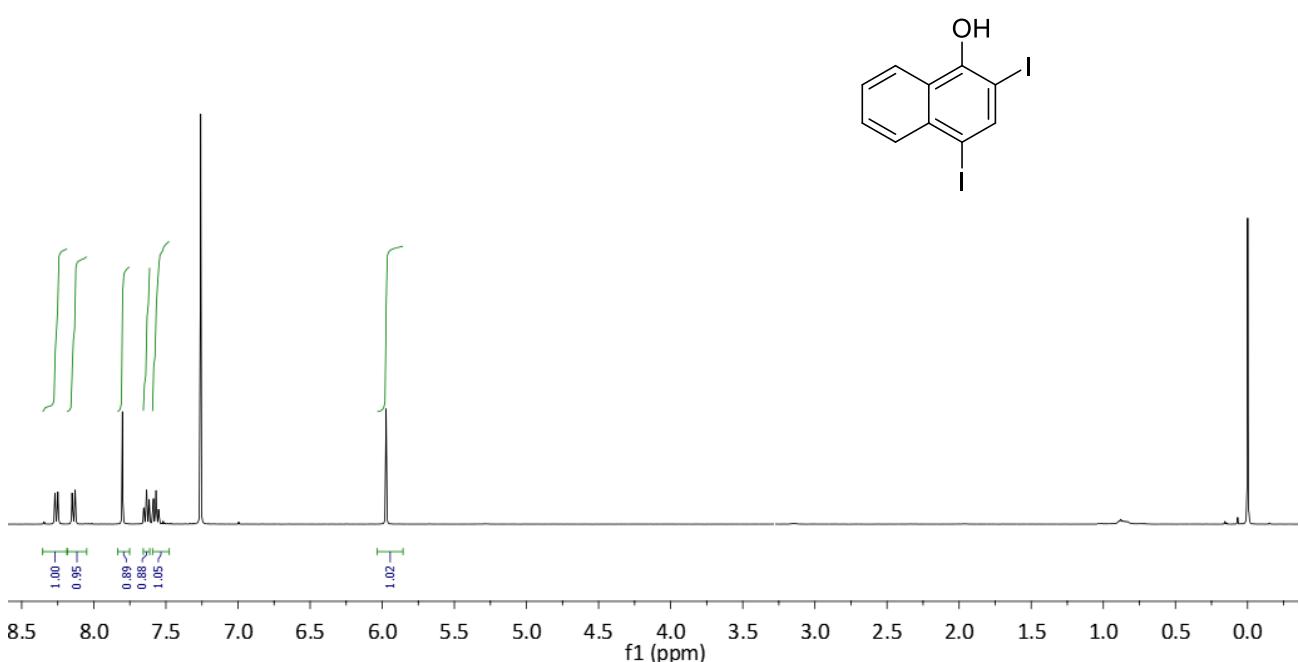
<sup>1</sup>H-NMR of 26b in CDCl<sub>3</sub>



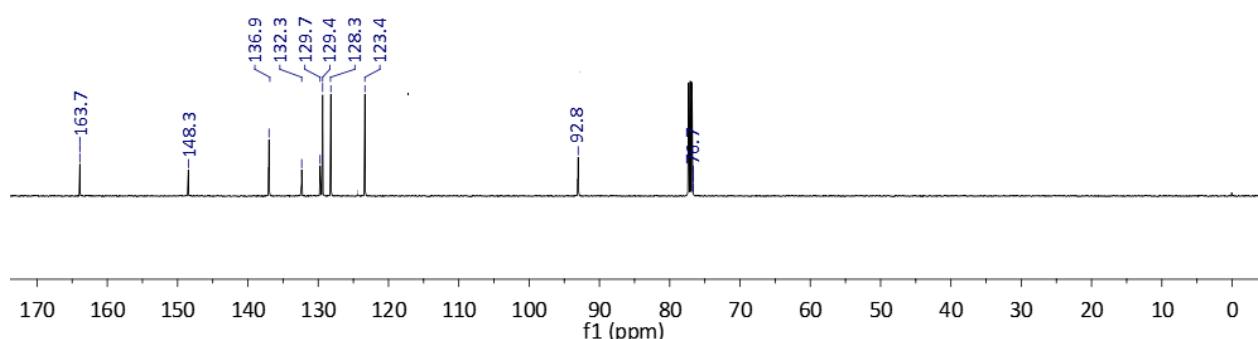
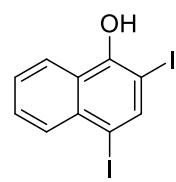
<sup>1</sup>H-NMR of 26c in CDCl<sub>3</sub>



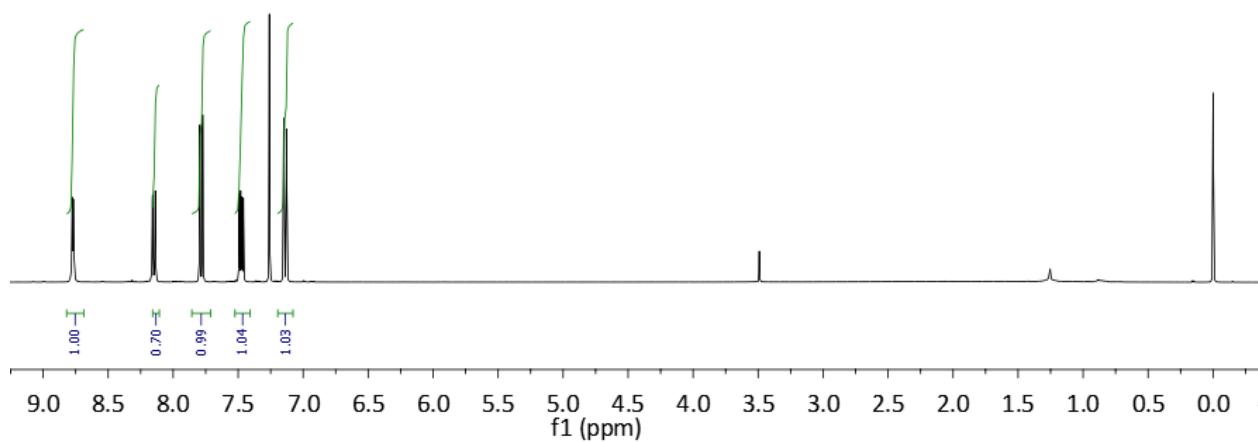
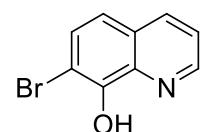
<sup>13</sup>C-NMR of 26c in CDCl<sub>3</sub>



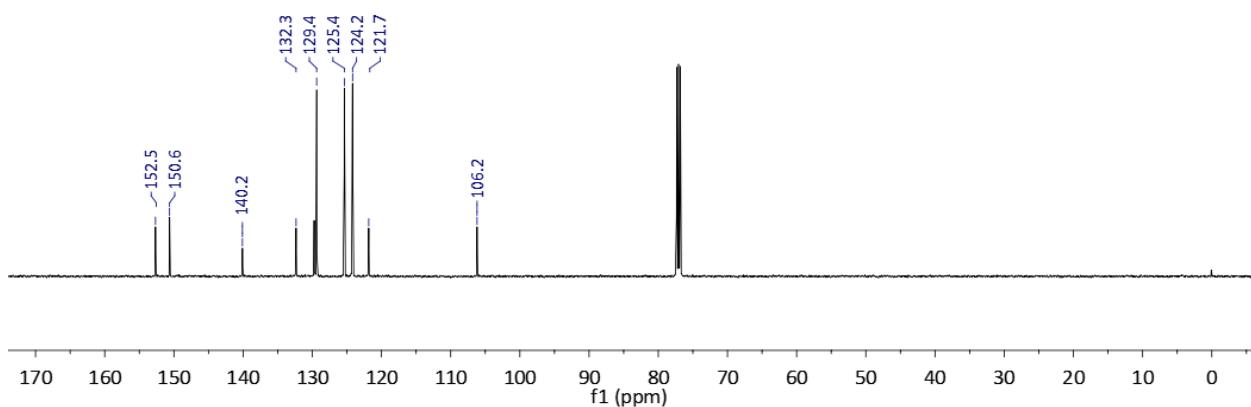
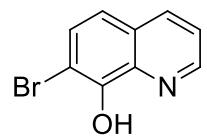
<sup>1</sup>H-NMR of 26d in CDCl<sub>3</sub>



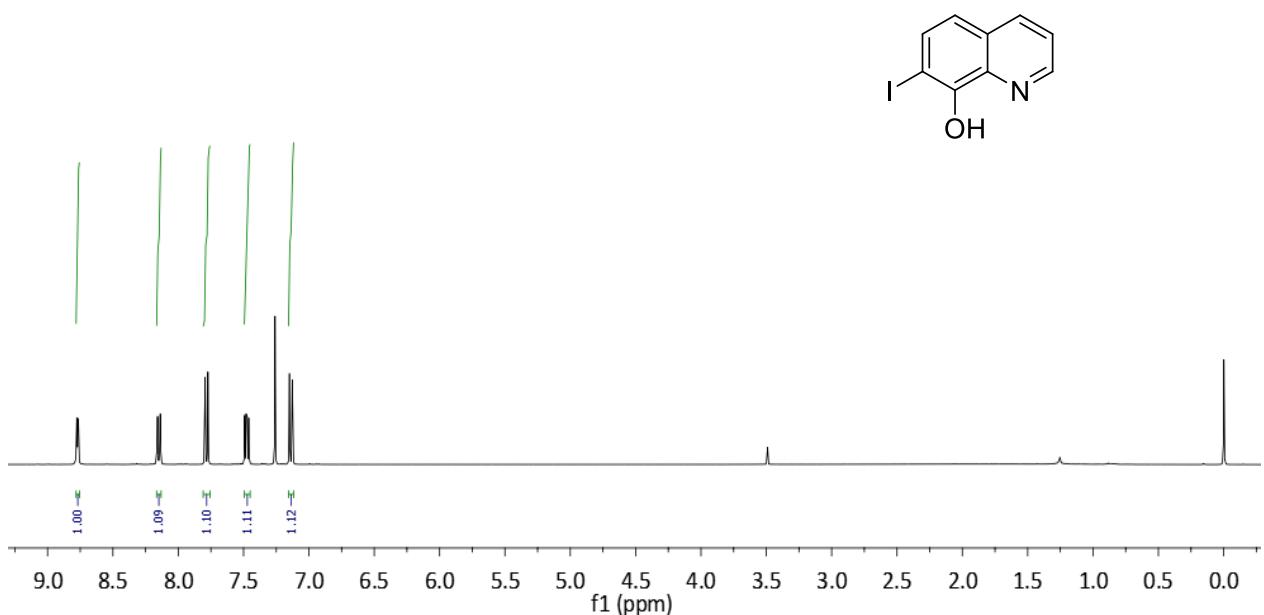
<sup>13</sup>C-NMR of 26d in  $\text{CDCl}_3$



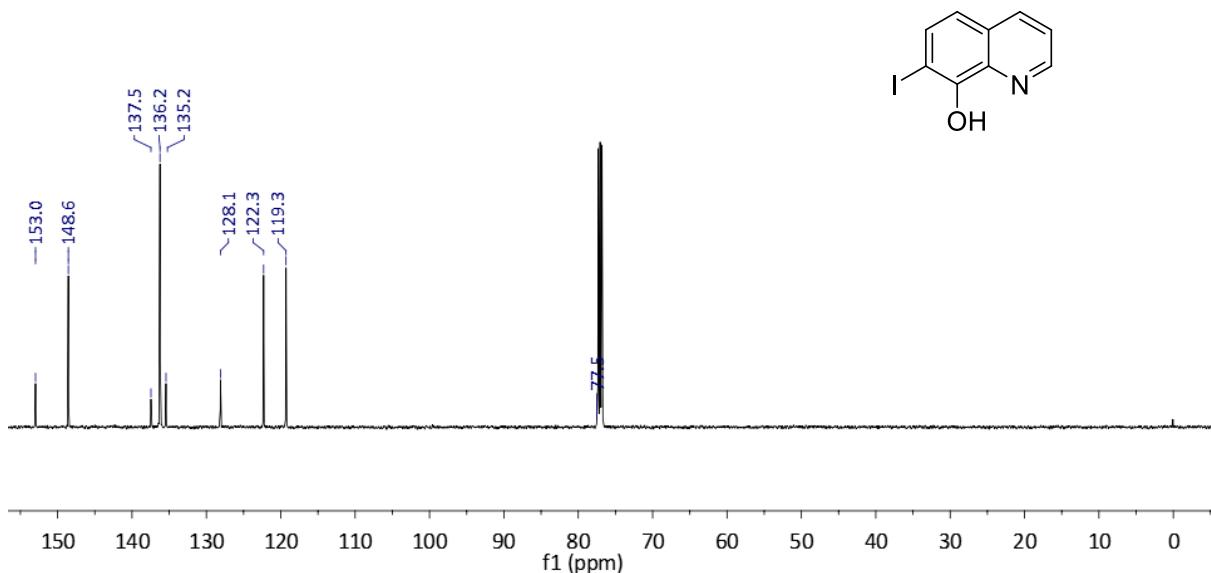
<sup>1</sup>H-NMR of 27a in  $\text{CDCl}_3$



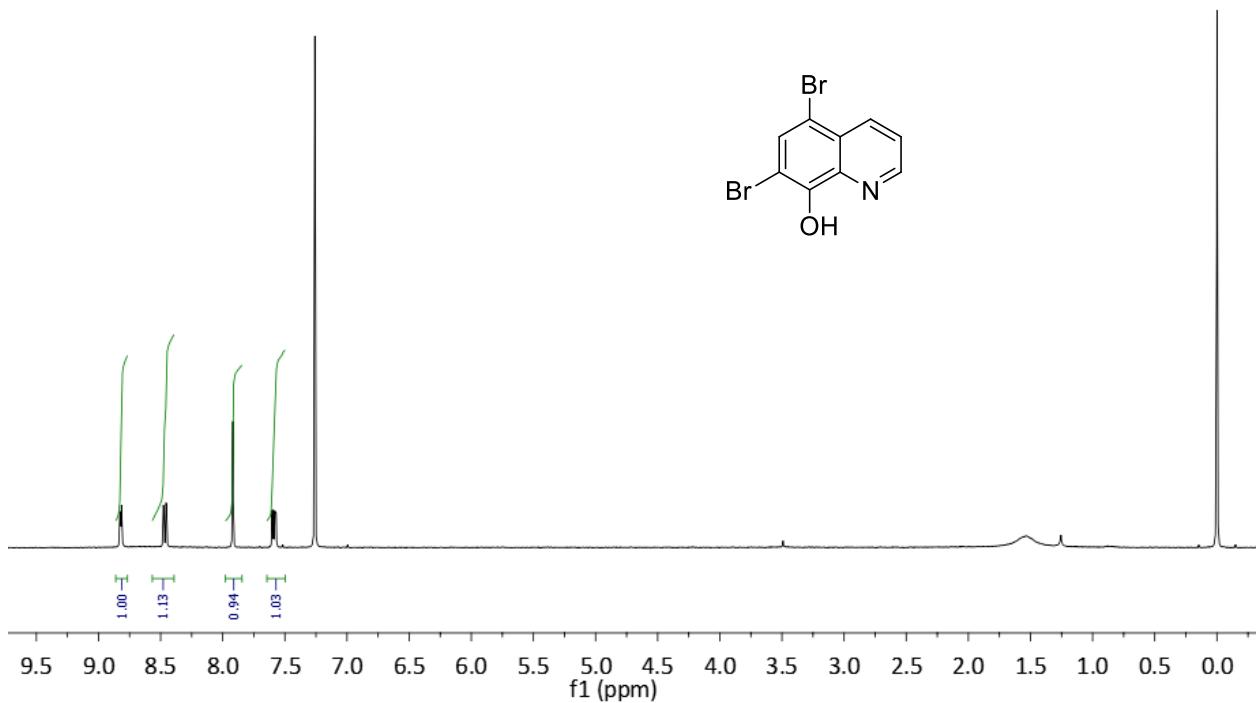
$^{13}\text{C}$ -NMR of 27a in  $\text{CDCl}_3$



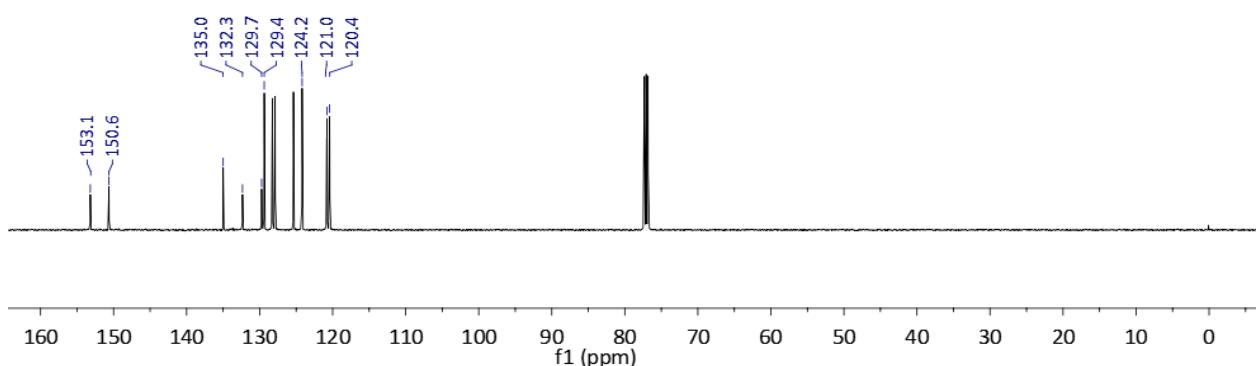
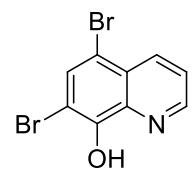
$^1\text{H}$ -NMR of 27b in  $\text{CDCl}_3$



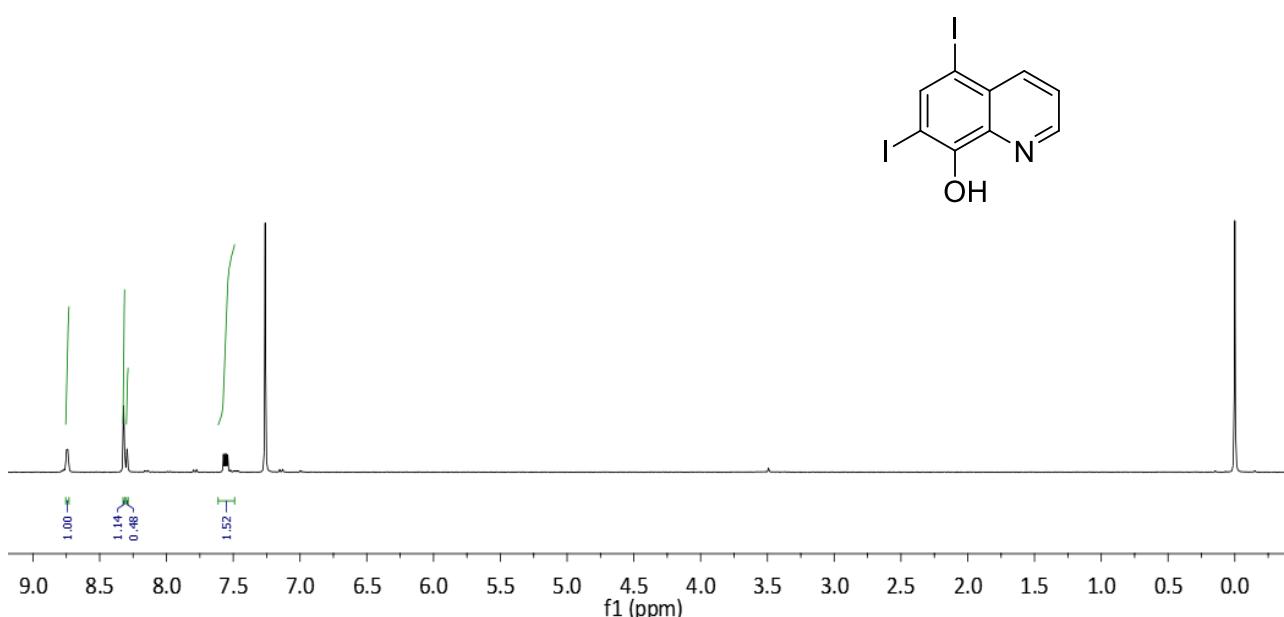
<sup>13</sup>C NMR of 27b in  $\text{CDCl}_3$



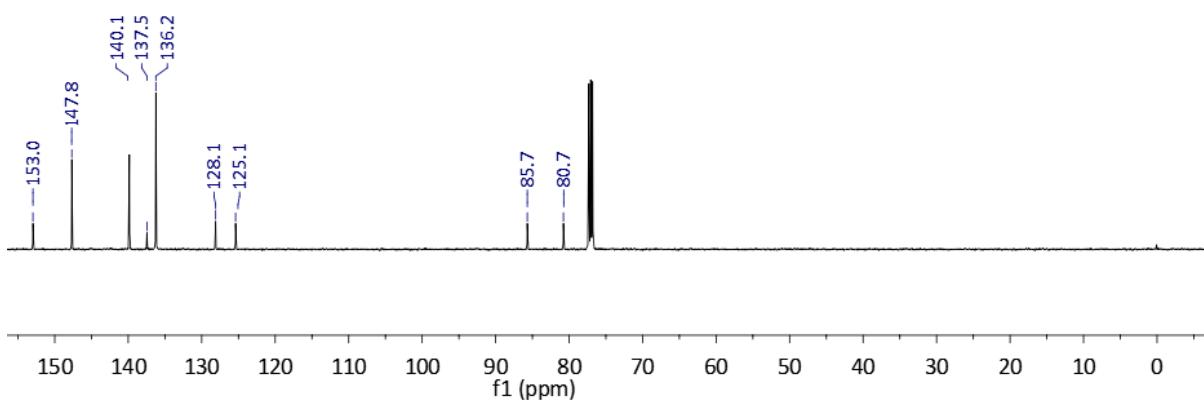
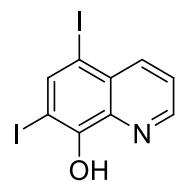
<sup>1</sup>H-NMR of 27c in  $\text{CDCl}_3$



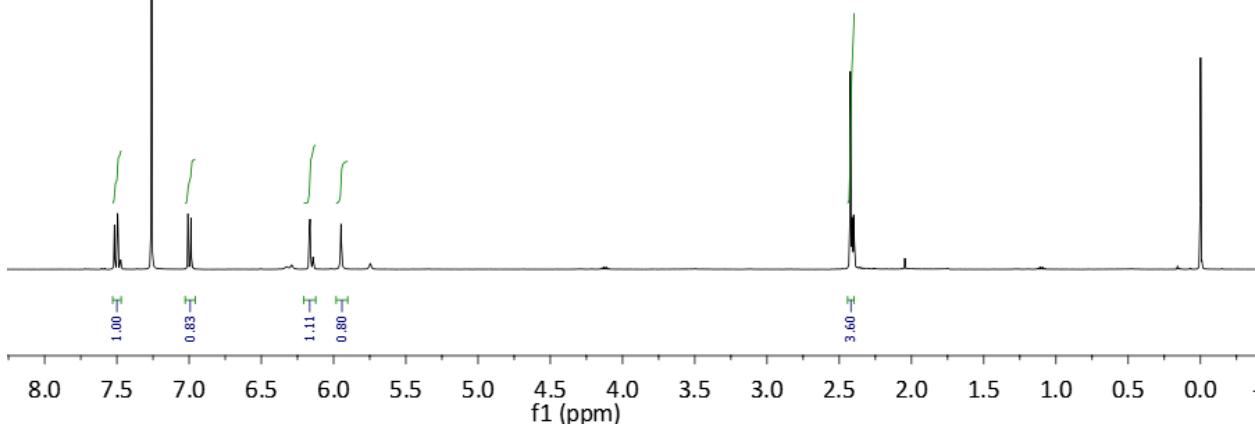
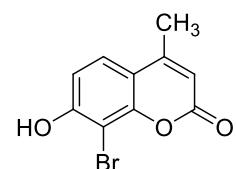
$^{13}\text{C}$ -NMR of 27c in  $\text{CDCl}_3$



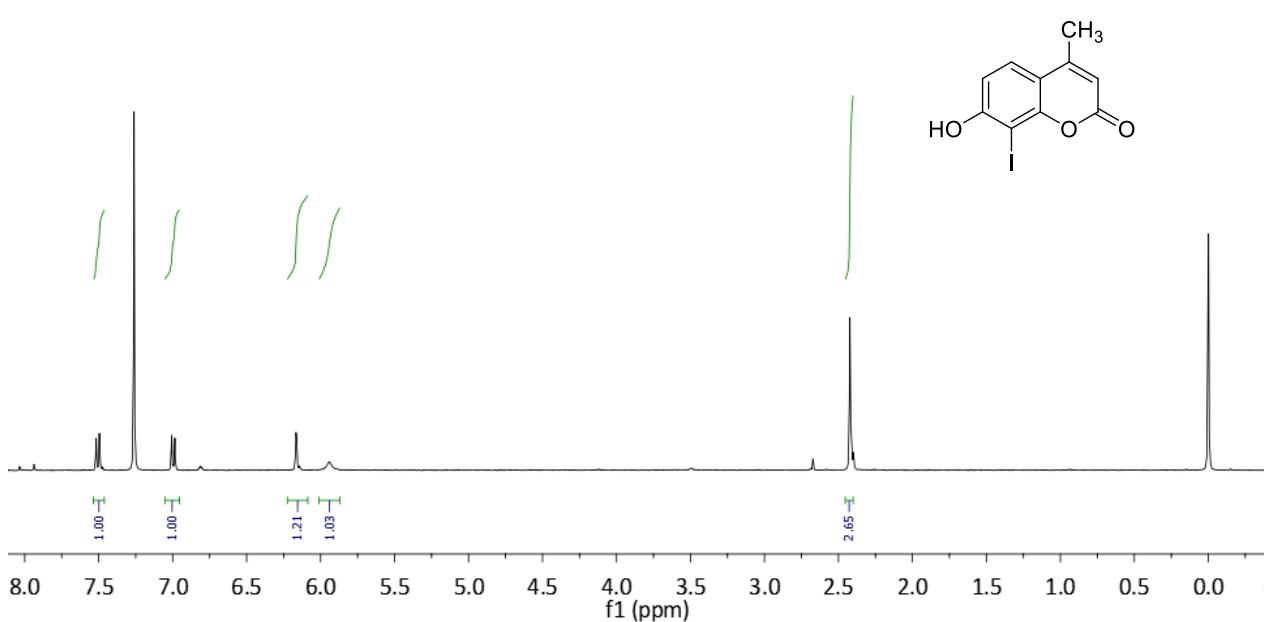
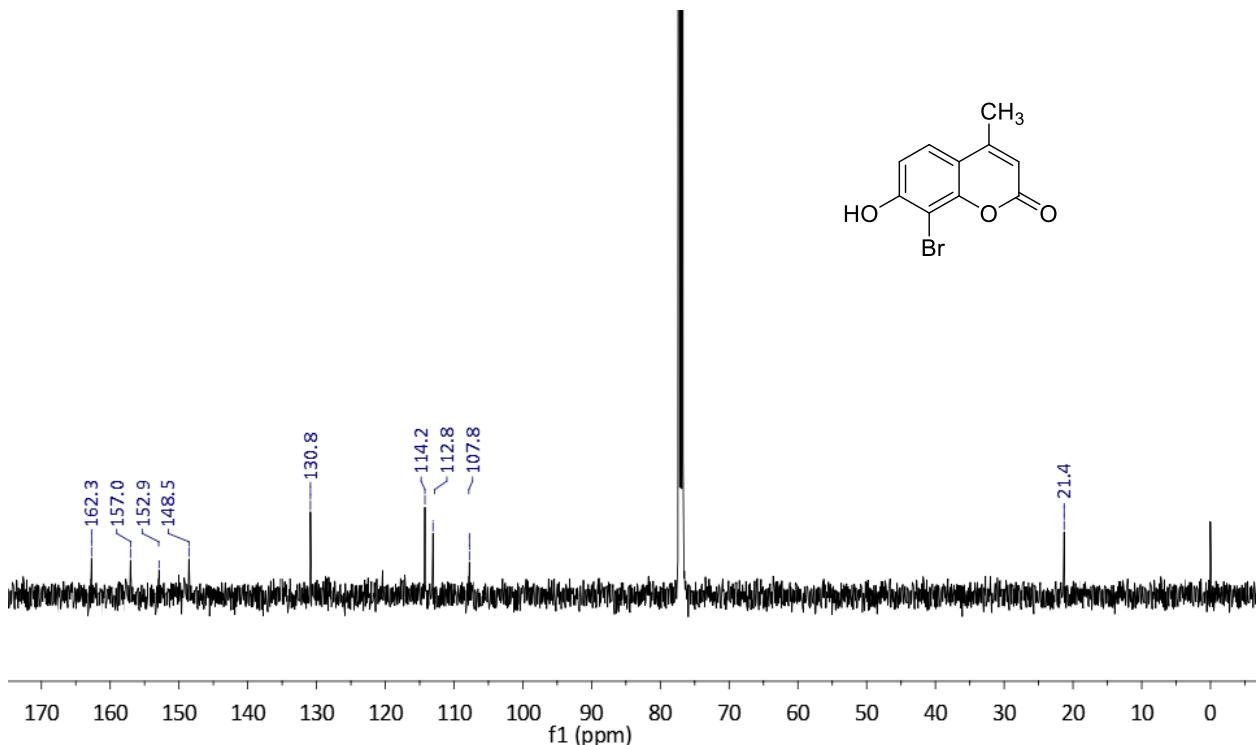
$^1\text{H}$ -NMR of 27d in  $\text{CDCl}_3$



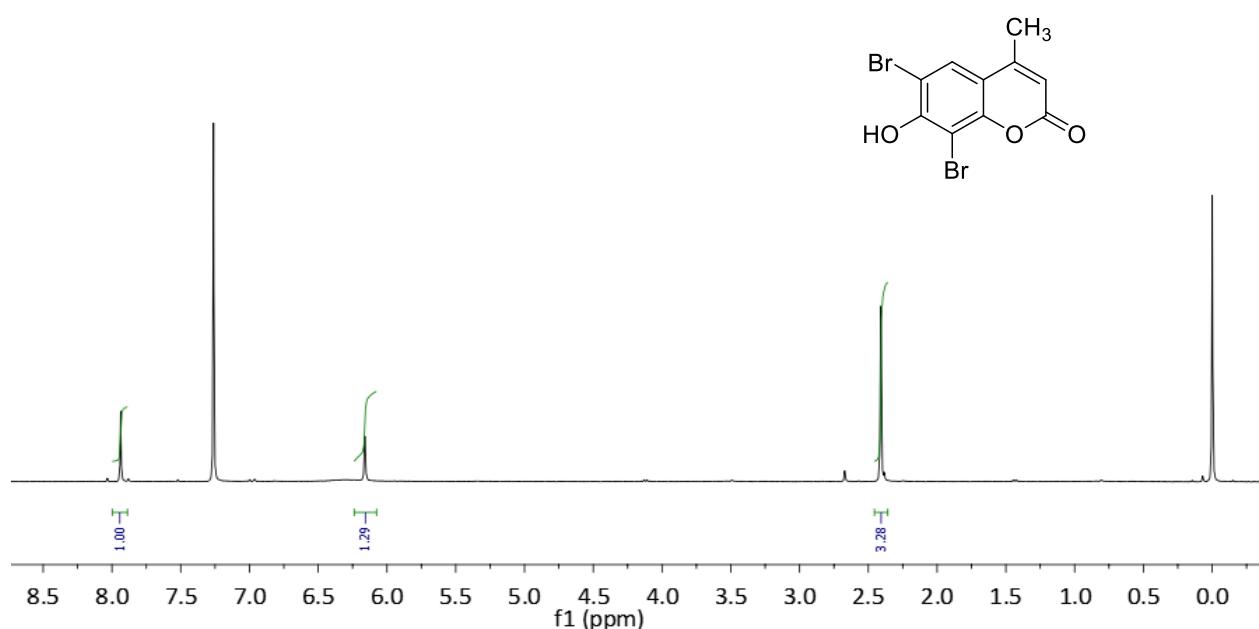
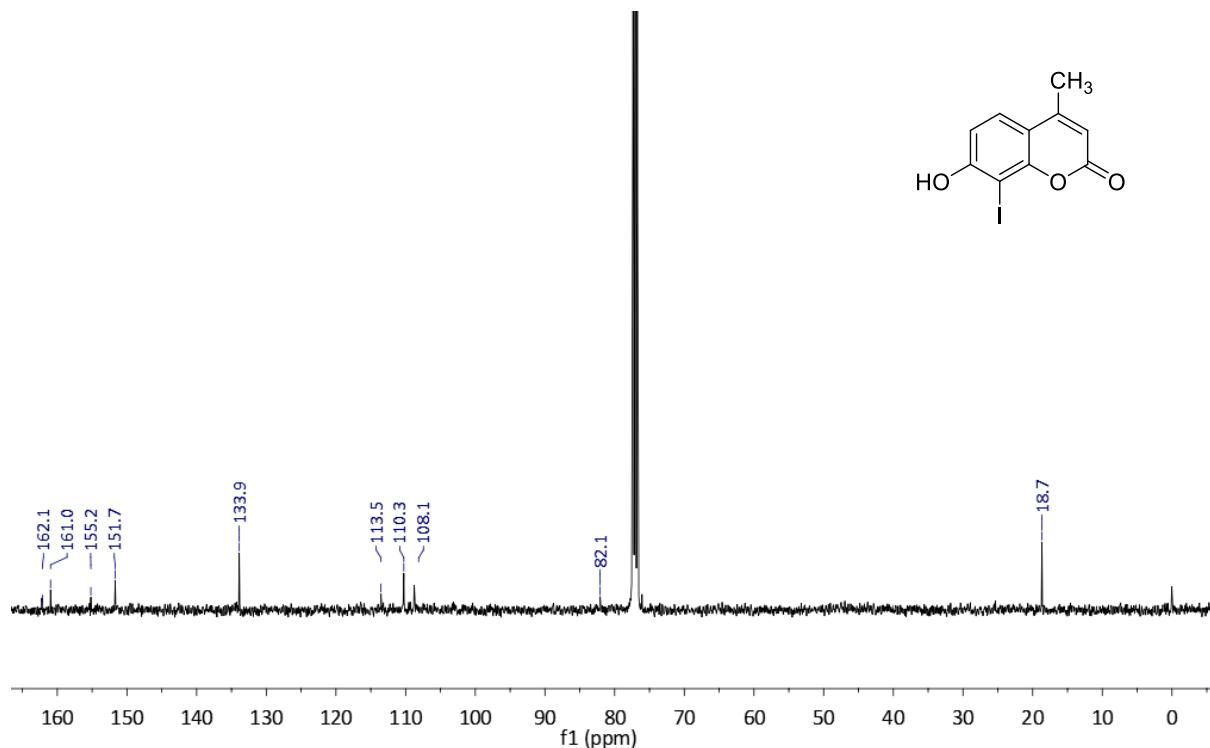
<sup>13</sup>C NMR of 27d in  $\text{CDCl}_3$

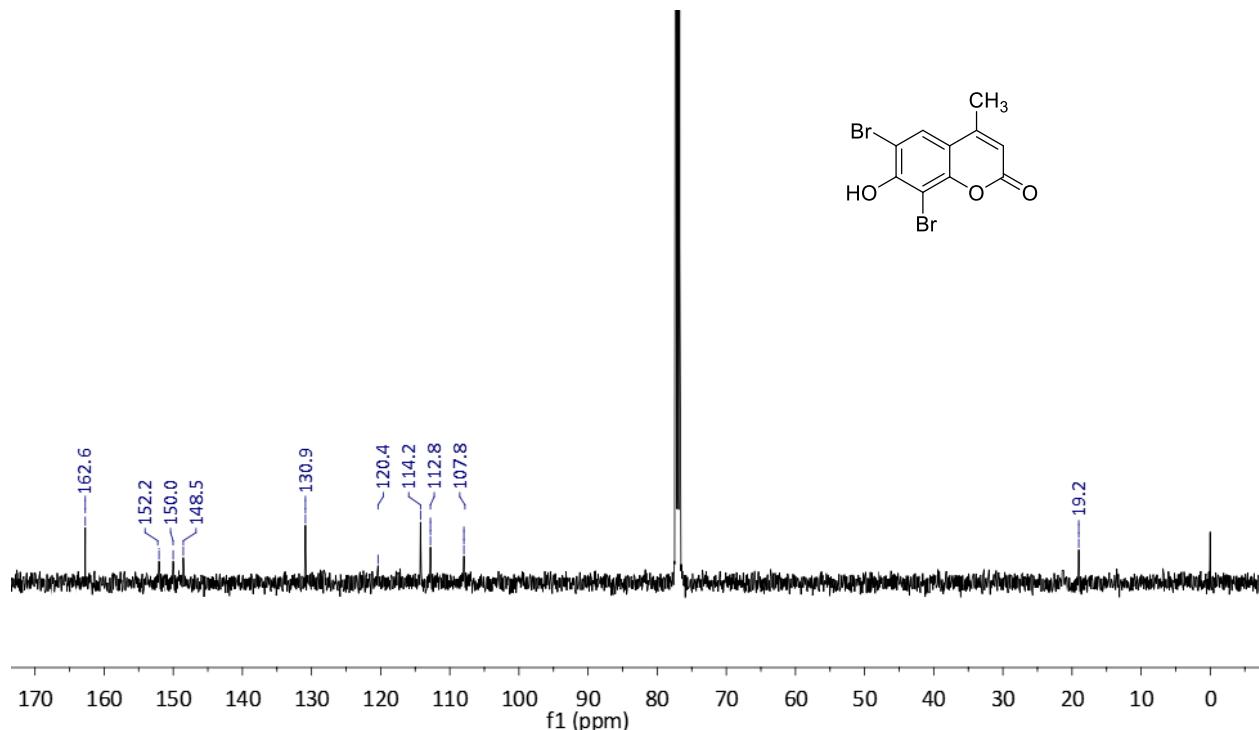
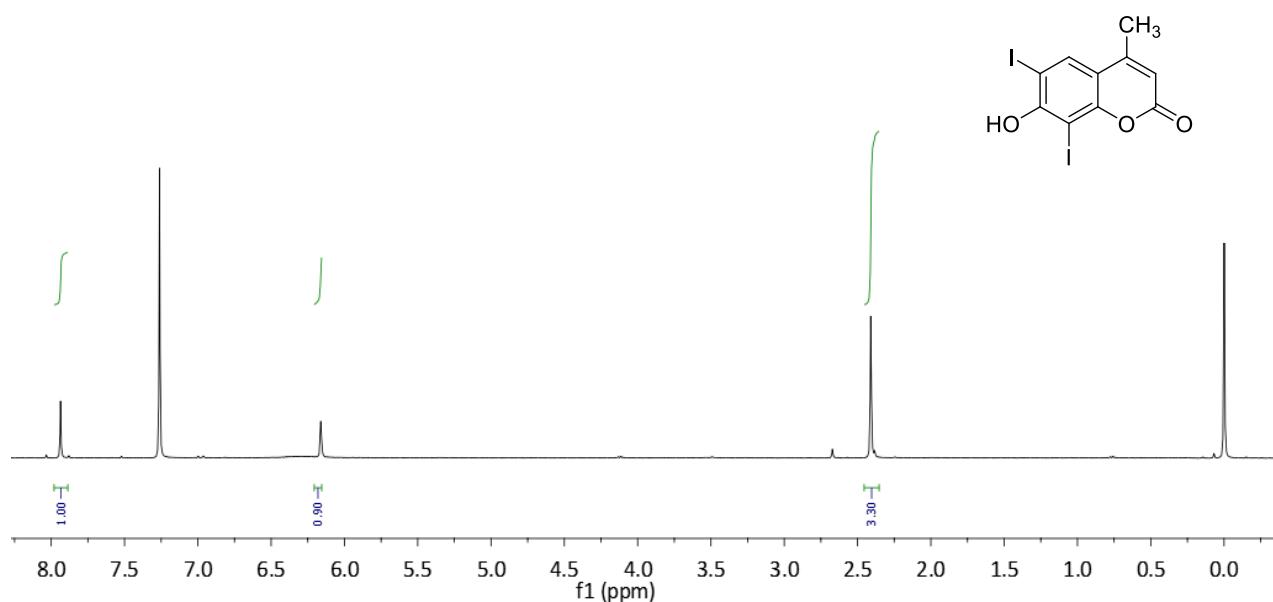


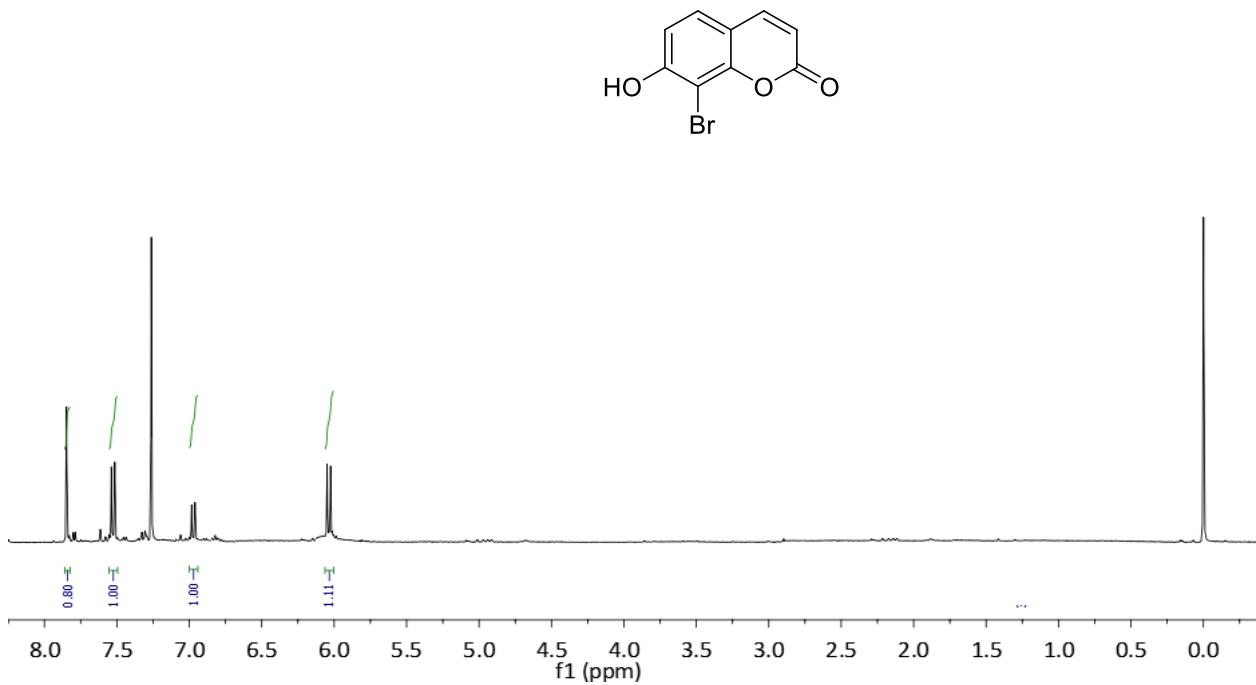
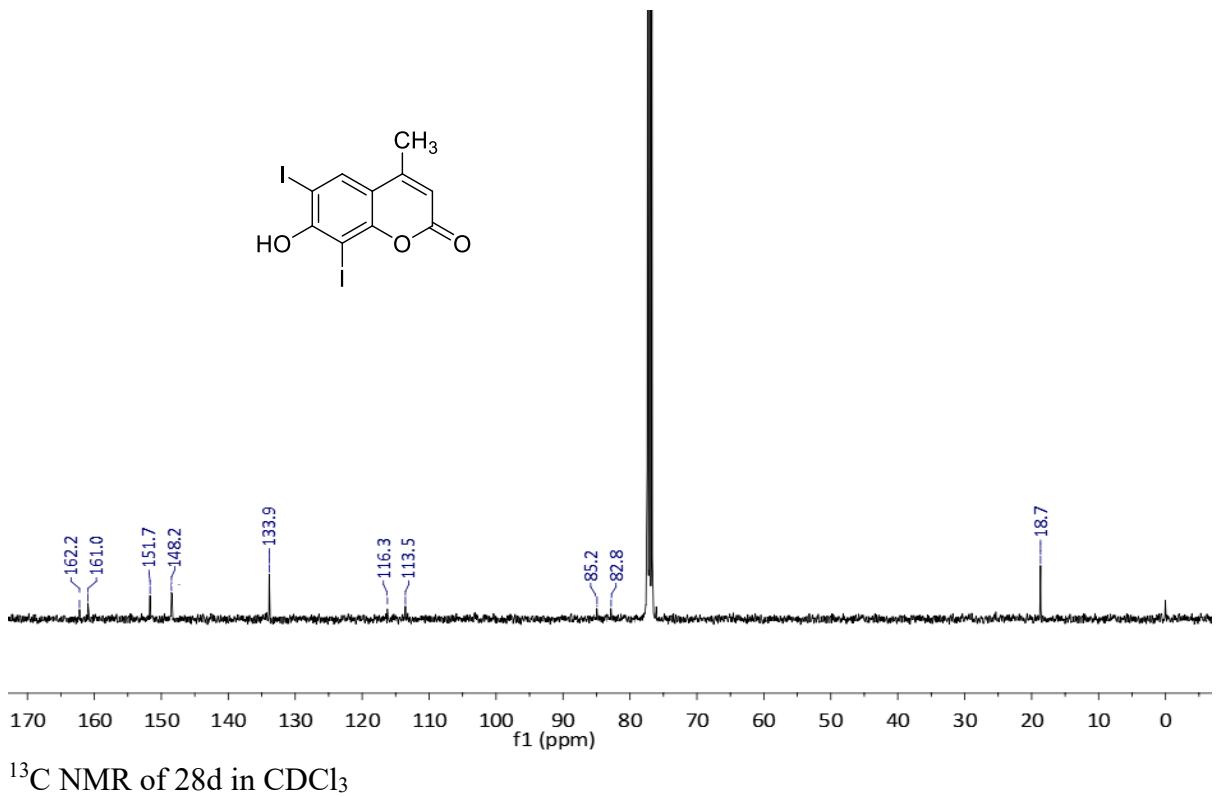
<sup>1</sup>H-NMR of 28a in  $\text{CDCl}_3$



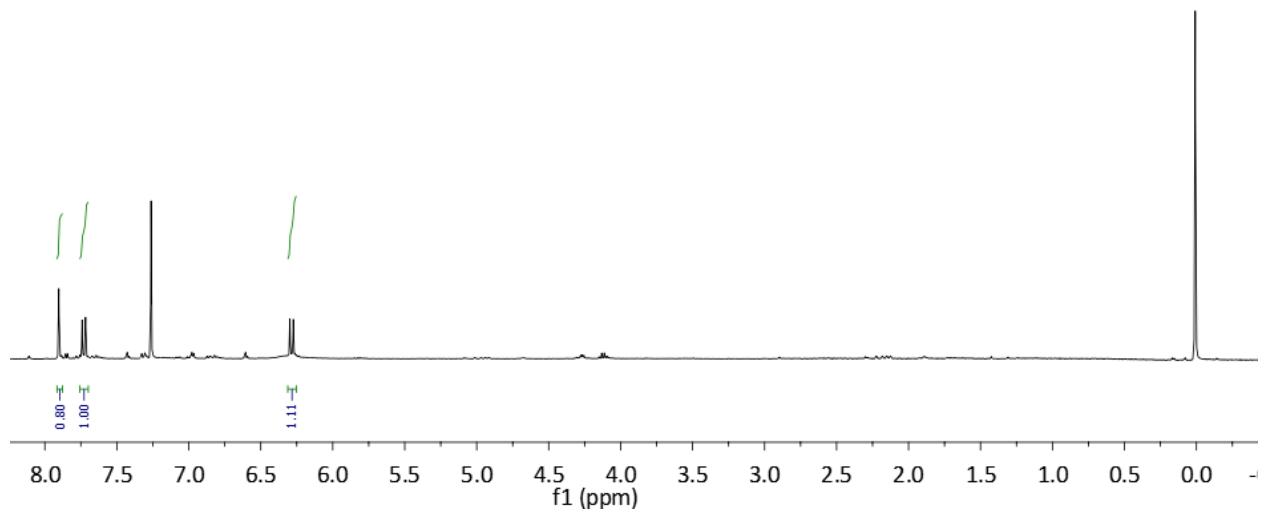
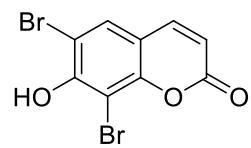
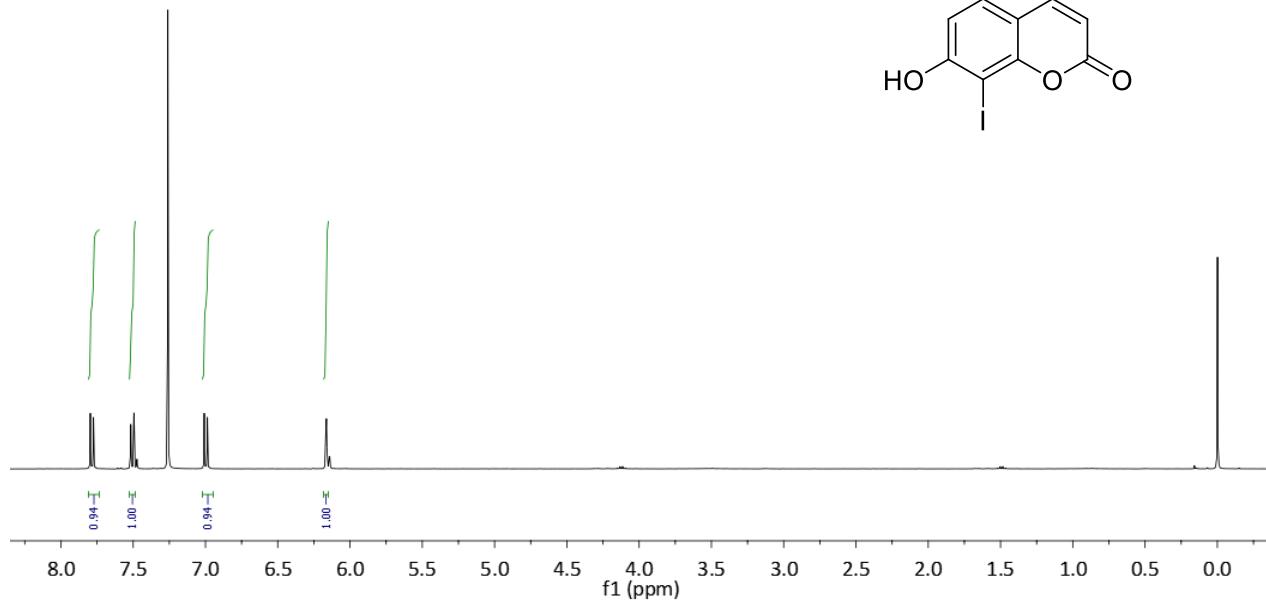
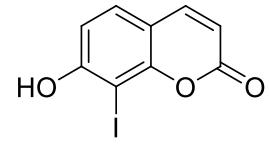
<sup>1</sup>H-NMR of 28b in CDCl<sub>3</sub>



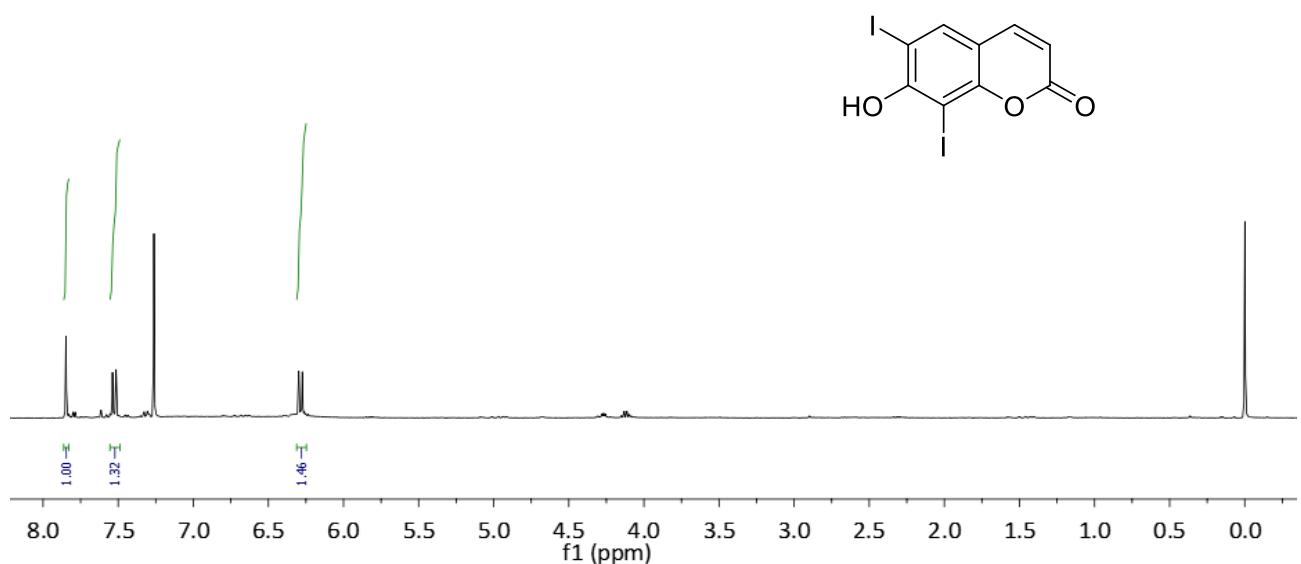
<sup>13</sup>C-NMR of 28c in  $\text{CDCl}_3$ <sup>1</sup>H-NMR of 28d in  $\text{CDCl}_3$



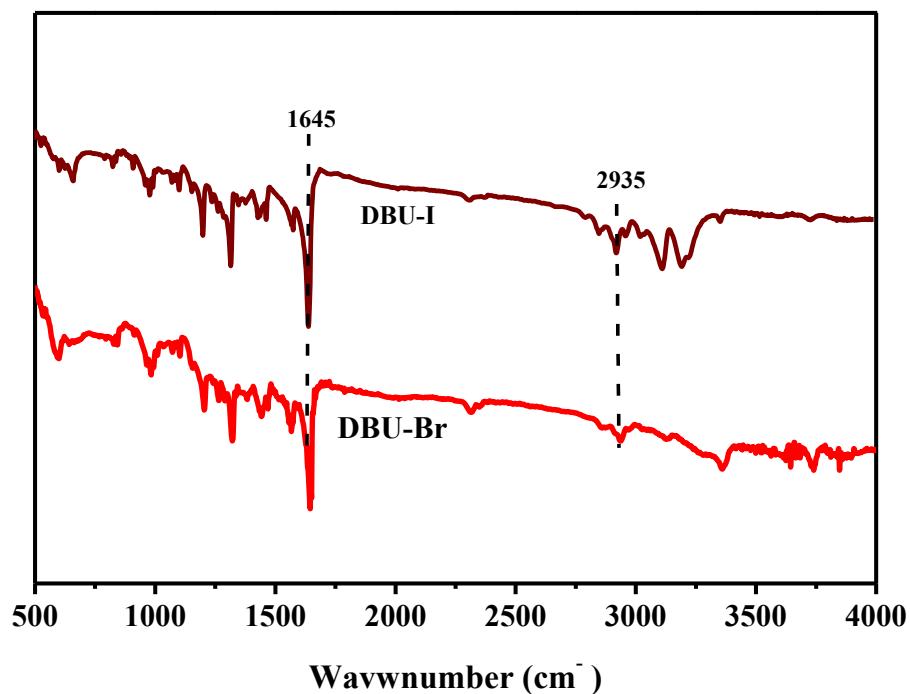
<sup>1</sup>H-NMR of 29a in CDCl<sub>3</sub>



<sup>1</sup>H-NMR of 29c in CDCl<sub>3</sub>



<sup>1</sup>H-NMR of 29d in CDCl<sub>3</sub>



FT-IR spectrum of LBAs of DBU-Br and DBU-I