

## Supporting Information

### *Photoredox-catalyzed Chemoselective Aerobic C $\alpha$ -H Oxidation of Propargylamine: Synthesis of Substituted 2-Ynamide and Oxazolo[2,3-a]isoquinolinone derivatives*

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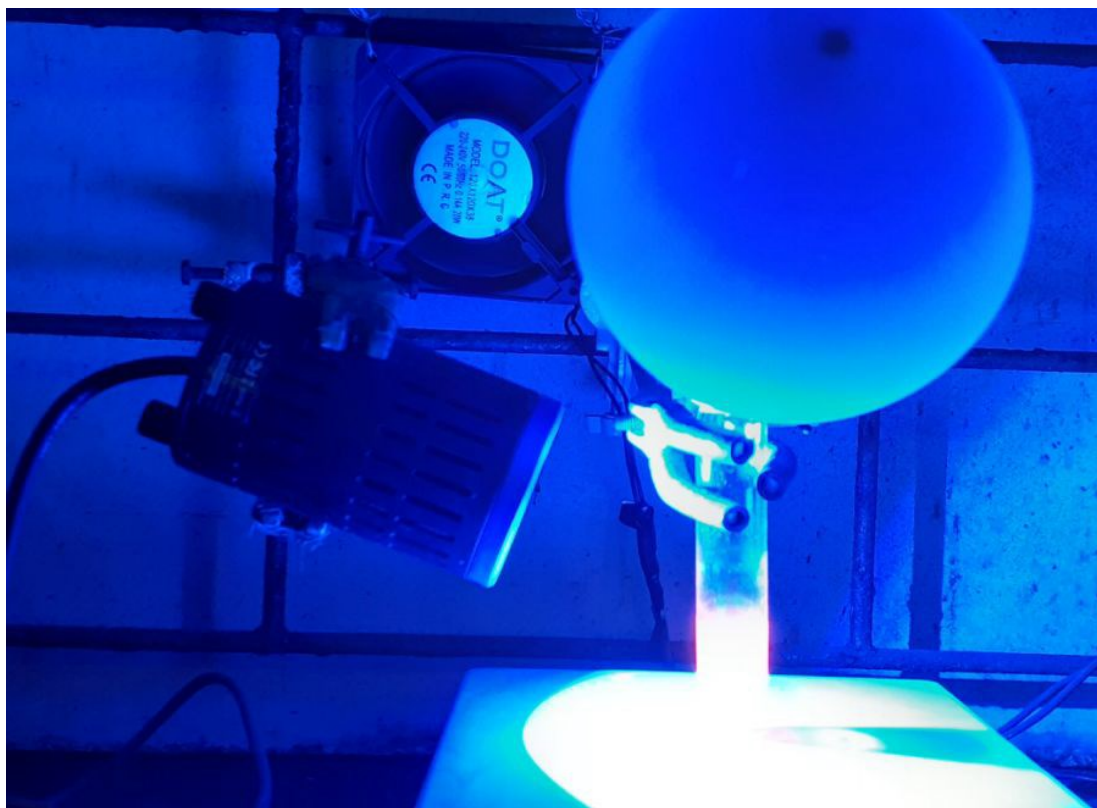
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## 1. General Experimental Details:

The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded in  $\text{CDCl}_3$  on Bruker spectrometers 300, 400MHz NMR spectrometer spectrometer (300, 400 MHz for  $^1\text{H}$  NMR and 75, 100MHz for  $^{13}\text{C}$  NMR) respectively with TMS as an internal standard. Mass spectra were recorded on Xevo G2S Q-TOF spectrometer. TLC was performed on using Merck pre-coated TLC plates (Merck 60 F254) and detected under UV light. Column chromatography was carried out with silica gel (100-200 mesh). Reagents and solvents were purified as per standard procedures.



**Fig 1:** Reaction setup for synthesis of 2-ynamides and Oxazolo[2,3-a]isoquinolinone.

## 2. General procedure A for synthesis of propargylamine

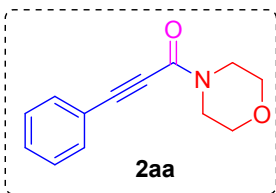
Propargylamine were synthesized using the modified literature procedure.<sup>1</sup>

Reaction tube was charged with amine (0.57 mmol), paraformaldehyde (0.62 mmol), alkyne (0.62 mmol) and CuI (5 mol%) in ACN. The reaction mixture was stirred at 70 °C for 6 hours. After the reaction completion, solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using EtOAc/Hexane as eluent to furnish the corresponding Propargylamine compounds.

## 3. General procedure B for synthesis of 2-ynamides

Reaction tube was charged with 2-propynyl-tertiary amines (0.5 mmol), DBU (0.5 mmol) and rose bengal (2 mol%) in ACN (4 mL). The reaction mixture was stirred in the presence of O<sub>2</sub> (balloon) under blue light for 3 hours. After the reaction completion, solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using EtOAc/Hexane as eluent to furnish the corresponding 2-ynamide compounds.

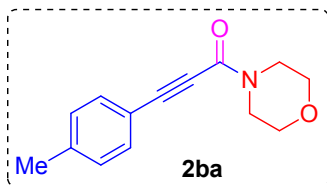
### 1-morpholino-3-phenylprop-2-yn-1-one **2aa**<sup>2</sup>



**2aa** (102 mg) was obtained from **1aa** (101 mg) following general procedure **B**; colorless oily liquid; 94% yield (eluent: EtOAc/Hexanes= 3:7);

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ<sub>H</sub> 3.69 (s, 4H), 3.72-3.75 (m, 2H), 3.81-3.84 (m, 2H), 7.33-7.41 (m, 3H), 7.51-7.55 (m, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ<sub>C</sub> 42.0, 47.3, 66.4, 66.8, 80.8, 91.0, 120.4, 128.5, 130.0, 132.3, 153.1.

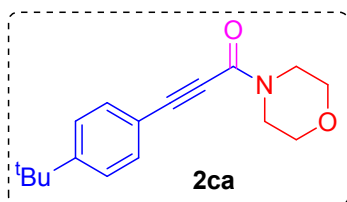
### 1-morpholino-3-(p-tolyl)prop-2-yn-1-one 2ba<sup>3</sup>



**2ba** (105 mg) was obtained from **1ba** (108 mg) following general procedure **B**; white solid; 91% yield (eluent: EtOAc/Hexanes= 3:7); mp: 87-89 °C;

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ<sub>H</sub> 2.36 (s, 3H), 3.68 (s, 4H), 3.71-3.74 (m, 2H), 3.81-3.84 (m, 2H), 7.16 (d, *J*= 7.8 Hz, 2H), 7.42 (d, *J*= 8.1 Hz, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ<sub>C</sub> 21.5, 42.0, 47.3, 66.4, 66.8, 80.4, 91.5, 117.3, 129.2, 132.3, 140.6, 153.3.

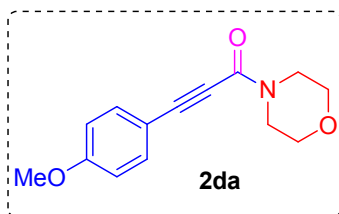
### 3-(4-(tert-butyl)phenyl)-1-morpholinoprop-2-yn-1-one 2ca<sup>2</sup>



**2ca** (123 mg) was obtained from **1ca** (129 mg) following general procedure **B**; yellow solid; 91% yield (eluent: EtOAc/Hexanes= 3:7); mp: 149-151 °C;

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ<sub>H</sub> 1.31 (s, 9H), 3.68 (s, 4H), 3.71-3.74 (m, 2H), 3.81-3.84 (m, 2H), 7.38 (d, *J*= 8.1 Hz, 2H), 7.47 (d, *J*= 8.4 Hz, 2H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>): δ<sub>C</sub> 31.0, 34.9, 42.0, 47.3, 66.4, 66.8, 80.4, 91.4, 117.2, 125.5, 132.1, 153.3, 153.8.

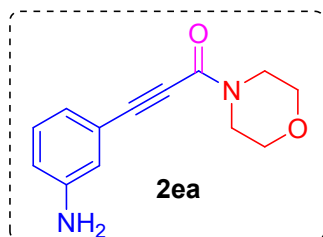
### 3-(4-methoxyphenyl)-1-morpholinoprop-2-yn-1-one 2da



**2da** (108 mg) was obtained from **1da** (116 mg) following general procedure **B**; colorless oily liquid; 88% yield (eluent: EtOAc/Hexanes= 3:7);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  3.68 (s, 4H), 3.71-3.74 (m, 2H), 3.80-3.86 (s, 5H), 6.87 (d,  $J=$  8.7 Hz, 2H), 7.47 (d,  $J=$  9.0 Hz, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$ 41.9, 47.3, 55.3, 66.5, 66.8, 80.1, 91.7, 112.2, 114.3, 134.1, 153.5, 161.2; **IR (KBr)  $\nu$ :** 2973, 2224, 1616, 1556, 1113, 1046; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>14</sub>H<sub>16</sub>NO<sub>3</sub>: 246.1130, Found: 246.1088.

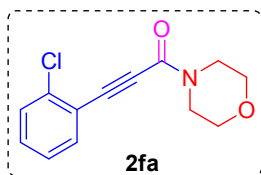
### 3-(3-aminophenyl)-1-morpholinoprop-2-yn-1-one **2ea**



**2ea** (86 mg) was obtained from **1ea** (108 mg) following general procedure **B**; yellow oily liquid; 75% yield (eluent: EtOAc/Hexanes= 1:1);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  3.68 (s, 4H), 3.70-3.74 (m, 2H), 3.79-3.82 (m, 2H), 6.69-6.73 (m, 1H), 6.82 (s, 1H), 6.91 (d,  $J=$  7.8Hz, 2H), 7.09-7.14 (m, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$ 42.0, 47.3, 66.4, 66.8, 80.2, 91.5, 117.0, 118.2, 120.9, 122.5, 129.4, 146.5, 153.3; **IR (KBr)  $\nu$ :** 3546, 2989, 2211, 1621, 1570, 1117, 1050; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>13</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>: 231.1133, Found: 231.1135.

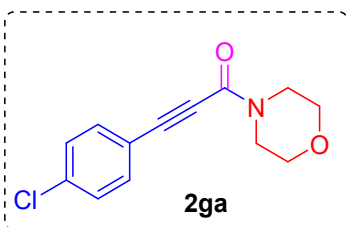
### 3-(2-chlorophenyl)-1-morpholinoprop-2-yn-1-one **2fa**



**2fa** (100 mg) was obtained from **1fa** (118 mg) following general procedure **B**; colorless oily liquid; 80% yield (eluent: EtOAc/Hexanes= 3:7);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.69 (s, 4H), 3.73-3.76 (m, 2H), 3.89-3.93 (m, 2H), 7.24-7.29 (m, 1H), 7.33 (dt, *J*= 1.8, 6.8 Hz, 1H), 7.43 (d, *J*= 7.5 Hz, 1H), 7.60 (dd, *J*= 1.2, 6.3 Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.0, 47.3, 66.4, 66.8, 85.4, 87.1, 120.6, 126.7, 129.4, 131.1, 134.4, 136.7, 152.8; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>13</sub>H<sub>13</sub>ClNO<sub>2</sub>: 250.0635, Found: 250.0593.

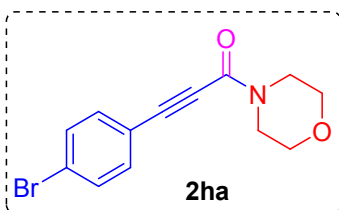
### 3-(4-chlorophenyl)-1-morpholinoprop-2-yn-1-one **2ga**<sup>2</sup>



**2ga** (112 mg) was obtained from **1ga** (118 mg) following general procedure **B**; white solid; 90% yield (eluent: EtOAc/Hexanes= 3:7); mp: 110-112 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.68 (s, 4H), 3.71-3.74 (m, 2H), 3.79-3.81 (m, 2H), 7.34 (d, *J*= 8.4 Hz, 2H), 7.46 (m, *J*= 8.4 Hz, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.0, 47.2, 66.4, 66.8, 81.7, 89.7, 118.8, 128.9, 133.5, 136.5, 152.8.

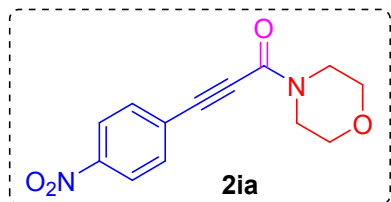
### 3-(4-bromophenyl)-1-morpholinoprop-2-yn-1-one **2ha**



**2ha** (129 mg) was obtained from **1ha** (140 mg) following general procedure **B**; pale yellow solid; 88% yield (eluent: EtOAc/Hexanes= 3:7); mp: 110-112 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub>3.69 (s, 4H), 3.71-3.75 (m, 2H), 3.79-3.82 (m, 2H), 7.39 (d, *J*= 8.4 Hz, 2H), 7.51 (m, *J*= 6.3 Hz, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.0, 47.3, 66.4, 66.8, 81.8, 89.8, 119.3, 124.8, 131.9, 133.6, 152.9; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>13</sub>H<sub>13</sub>BrNO<sub>2</sub>: 294.0129, Found: 294.0097.

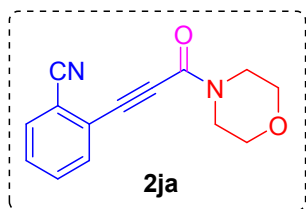
### 1-morpholino-3-(4-nitrophenyl)prop-2-yn-1-one **2ia**



**2ia** (108 mg) was obtained from **1ia** (123 mg) following general procedure **B**; yellow solid; 83% yield (eluent: EtOAc/Hexanes= 4:6); mp: 194-196 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.71 (s, 4H), 3.74-3.77 (m, 2H), 3.80-3.83 (m, 2H), 7.69 (d, *J*= 8.7Hz, 2H), 8.22 (d, *J*= 9Hz, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.1, 47.3, 66.4, 66.8, 84.6, 88.1, 123.6, 126.9, 133.0, 148.3, 152.2; **IR (KBr) v:** 2978, 2225, 1620, 1569, 1113, 1050; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>13</sub>H<sub>13</sub>N<sub>2</sub>O<sub>4</sub>: 261.0875, Found: 261.0835.

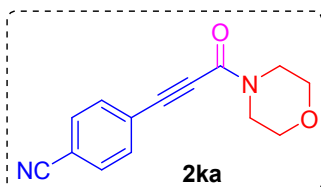
### 2-(3-morpholino-3-oxoprop-1-yn-1-yl)benzonitrile **2ja**<sup>2</sup>



**2ja** (98 mg) was obtained from **1ja** (113 mg) following general procedure **B**; pale yellow solid; 82% yield (eluent: EtOAc/Hexanes= 4:6); mp: 108-110 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.71 (s, 4H), 3.75-3.79 (m, 2H), 3.96-3.99 (m, 2H), 7.51-7.55 (m, 1H), 7.60-7.66 (m, 1H), 7.69-7.75 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>40.0, 47.3, 66.1, 66.7, 85.5, 85.9, 115.7, 116.9, 124.3, 130.0, 132.4, 133.5, 151.9.

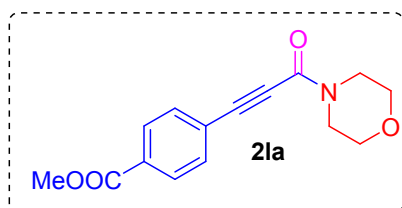
#### 4-(3-morpholino-3-oxoprop-1-yn-1-yl)benzonitrile **2ka**<sup>3</sup>



**2ka** (102 mg) was obtained from **1ka** (113 mg) following general procedure **B**; white solid; 85% yield (eluent: EtOAc/Hexanes= 4:6); mp: 197-199 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub>3.70 (s, 4H), 3.72-3.75 (m, 2H), 3.78-3.81 (m, 2H), 7.60-7.67 (m, 4H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.1, 47.3, 66.4, 66.7, 84.1, 88.5, 113.7, 117.7, 125.1, 132.1, 132.7, 152.3.

#### Methyl 4-(3-morpholino-3-oxoprop-1-yn-1-yl)benzoate **2la**<sup>3</sup>

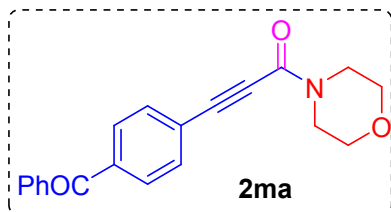


**2la** (109 mg) was obtained from **1la** (130 mg) following general procedure **B**; white solid; 80% yield (eluent: EtOAc/Hexanes= 4:6); mp: 124-126 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.69 (s, 4H), 3.73-3.76 (m, 2H), 3.81-3.84 (m, 2H), 3.92(s, 3H), 7.59 (d, *J*= 8.4Hz, 2H), 8.02 (d, *J*= 8.4Hz, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.0, 47.3, 52.3, 66.4, 66.8, 82.9, 89.7, 124.8, 129.5, 131.4, 132.1, 152.7, 165.9.

#### 3-(4-benzoylphenyl)-1-morpholinoprop-2-yn-1-one **2ma**

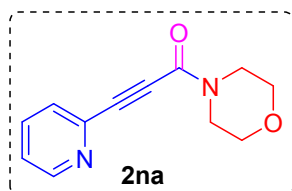




**2ma** (135 mg) was obtained from **1ma** (153 mg) following general procedure **B**; pale yellow oily liquid; 85% yield (eluent: EtOAc/Hexanes= 4:6);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.70 (s, 4H), 3.73-3.77 (m, 2H), 3.82-3.85 (m, 2H), 6.45-6.50 (m, 2H), 7.58 (d, *J*= 7.5Hz, 1H), 7.64 (d, *J*= 8.4Hz, 2H), 7.75-7.80 (m, 4H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.0, 47.3, 66.4, 66.8, 83.0, 89.8, 124.2, 128.4, 129.8, 132.1, 132.7, 137.0, 138.6, 152.7, 195.3; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>20</sub>H<sub>17</sub>NO<sub>3</sub>: 320.1287, Found: 320.1295.

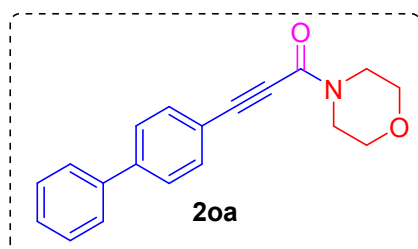
### 1-morpholino-3-(pyridin-2-yl)prop-2-yn-1-one **2na**



**2na** (76 mg) was obtained from **1na** (101 mg) following general procedure **B**; brown solid; 70% yield (eluent: EtOAc/Hexanes= 1:1); mp: 59-61 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.69 (s, 4H), 3.71-3.75 (m, 2H), 3.85-3.88 (m, 2H), 7.31-7.35 (m, 1H), 6.59 (d, *J*= 7.8Hz, 1H), 7.69-7.75 (m, 1H), 8.63 (d, *J*= 4.2Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.0, 47.3, 66.3, 66.8, 79.4, 89.1, 124.2, 128.3, 136.2, 141.0, 150.2, 152.4; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>12</sub>H<sub>13</sub>N<sub>2</sub>O<sub>2</sub>: 217.0977, Found: 217.0983.

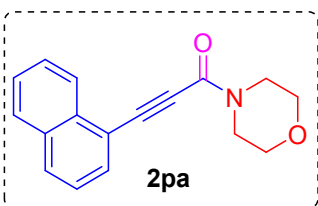
### 3-([1,1'-biphenyl]-4-yl)-1-morpholinoprop-2-yn-1-one **2oa**<sup>3</sup>



**2oa** (131 mg) was obtained from **1oa** (139 mg) following general procedure B; white solid; 90% yield (eluent: EtOAc/Hexanes= 3:7); mp: 128-130 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.69 (s, 4H), 3.72-3.75 (m, 2H), 3.83-3.85 (m, 2H), 7.36-7.46 (m, 3H), 7.56-7.59 (m, 6h); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.0, 47.3, 66.4, 66.8, 81.4, 91.0, 119.1, 127.0, 127.1, 128.0, 128.9, 132.8, 139.8, 143.0, 153.2.

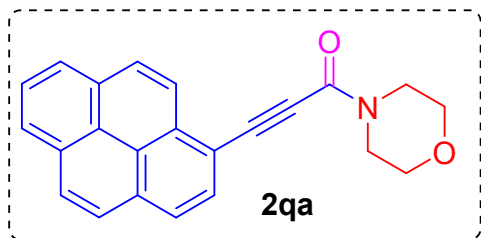
**1-morpholino-3-(naphthalen-1-yl)prop-2-yn-1-one 2pa<sup>2</sup>**



**2pa** (114 mg) was obtained from **1pa** (126 mg) following general procedure B; yellow solid; 86% yield (eluent: EtOAc/Hexanes= 3:7); mp: 133-135 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub>3.72 (s, 4H), 3.75-3.78 (m, 2H), 3.91-3.94 (m, 2H), 7.40-7.46 (m, 1H), 7.50-7.61 (m, 2H), 7.78 (d, *J*= 7.2Hz, 1H), 7.84-7.91 (m, 2H), 8.27 (d, *J*= 8.1Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.1, 47.4, 66.5, 66.8, 85.5, 89.5, 118.0, 125.0, 125.6, 126.7, 127.4, 128.4, 130.7, 132.0, 133.1, 133.3, 153.2.

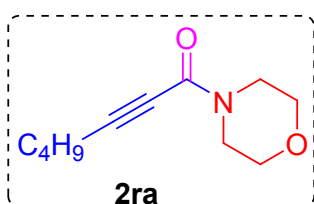
**1-morpholino-3-(pyren-1-yl)prop-2-yn-1-one 2qa**



**2qa** (121 mg) was obtained from **1qa** (164 mg) following general procedure B; brown solid; 71% yield (eluent: EtOAc/Hexanes= 3:7); mp: 138-140 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.67 (s, 4H), 3.68-3.75 (m, 2H), 3.90-3.93 (m, 2H), 7.88-7.97 (m, 4H), 8.01-7.12 (m, 4H), 8.37 (d, *J* = 9 Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 42.1, 47.5, 66.5, 66.9, 86.2, 90.7, 114.2, 124.0, 124.3, 124.4, 124.8, 126.1, 126.2, 126.4, 127.0, 129.1, 129.2, 130.2, 130.8, 131.1, 132.6, 132.9, 153.4; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>23</sub>H<sub>18</sub>NO<sub>2</sub>: 340.1337, Found: 340.1389.

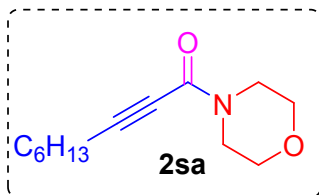
### 1-morpholinohept-2-yn-1-one 2ra



**2ra** (74 mg) was obtained from **1ra** (91 mg) following general procedure B; colorless oily liquid; 76% yield (eluent: EtOAc/Hexanes = 3:7);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 0.95 (t, *J* = 7.2 Hz, 3H), 1.42-1.44 (m, 2H), 1.54-1.57 (m, 2H), 2.35 (t, *J* = 6.9 Hz, 2H), 3.63 (s, 4H), 3.67-3.69 (m, 2H), 3.72-3.74 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 13.3, 18.5, 21.9, 29.80, 41.8, 47.1, 66.4, 66.8, 73.3, 94.0, 153.3; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>11</sub>H<sub>18</sub>NO<sub>2</sub>: 196.1337, Found: 196.1290.

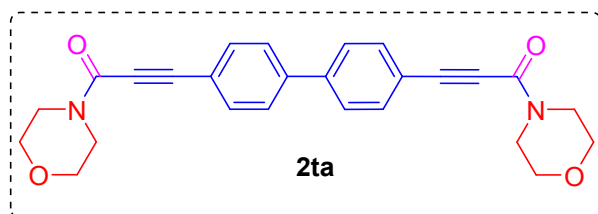
### 1-morpholinonon-2-yn-1-one 2sa



**2sa** (84 mg) was obtained from **1sa** (105 mg) following general procedure B; colorless oily liquid; 76% yield (eluent: EtOAc/Hexanes = 3:7);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 0.96 (t, *J*= 7.2Hz, 3H), 1.28-1.31 (m, 4H), 1.35-1.43 (m, 2H), 1.53-1.60 (m, 2H), 2.35 (t, *J*= 6.9Hz, 2H), 3.63 (s, 4H), 3.66-3.68 (m, 2H), 3.69-3.73 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>13.8, 18.8, 22.3, 27.7, 28.4, 31.1, 41.8, 47.1, 66.4, 66.8, 73.3, 94.0, 153.3; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>13</sub>H<sub>22</sub>NO<sub>2</sub>: 224.1650, Found: 224.1604.

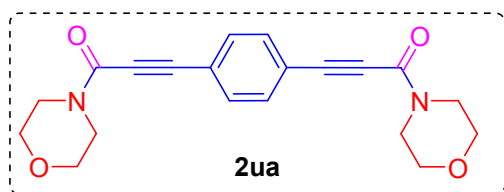
**3,3'-([1,1'-biphenyl]-4,4'-diyl)bis(1-morpholinoprop-2-yn-1-one) 2ta**



**2ta** (91 mg) was obtained from **1ta** (100 mg) following general procedure B; pale yellow solid; 85% yield (eluent: EtOAc/Hexanes= 1:1); mp: 231-233 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.70 (s, 8H), 3.73-3.76 (m, 4H), 3.83-3.86 (m, 4H), 7.61 (s, 8H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.1, 47.4, 66.5, 66.9, 81.9, 90.7, 120.1, 127.2, 133.0, 141.6, 153.1; **IR (KBr) v:** 2876, 2218, 1621, 1562, 1113, 1039; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>26</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>: 429.1814, Found: 429.1829.

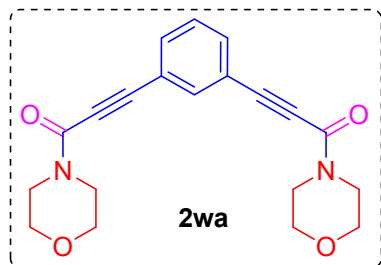
**3,3'-(1,4-phenylene)bis(1-morpholinoprop-2-yn-1-one) 2ua**



**2ua** (137 mg) was obtained from **1ua** (162 mg) following general procedure B; brown solid; 78% yield (eluent: EtOAc/Hexanes= 1:1); mp: 238-240 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.69 (s, 8H), 3.72-3.75 (m, 4H), 3.79-3.82 (m, 4H), 7.53 (s, 4H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>42.0, 47.3, 66.4, 66.8, 83.0, 89.7, 122.0, 132.3, 152.7; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>: 353.1501, Found: 353.1509.

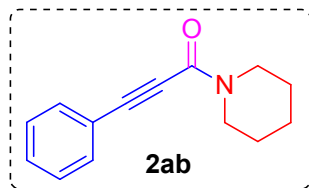
**3,3'-(1,3-phenylene)bis(1-morpholinoprop-2-yn-1-one) 2va**



**2va** (123 mg) was obtained from **1va** (162 mg) following general procedure B; colorless oily liquid; 75% yield (eluent: EtOAc/Hexanes= 1:1);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.62 (s, 8H), 3.66-3.69 (m, 4H), 3.73-3.76 (m, 4H), 7.29-7.34 (m, 1H), 7.51 (d, *J*= 7.8Hz, 2H), 7.63 (s, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 42.0, 47.3, 66.4, 66.8, 81.75, 89.25, 121.1, 128.9, 133.5, 135.8, 152.7; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>: 353.1501, Found: 353.1510.

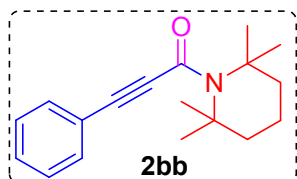
**3-phenyl-1-(piperidin-1-yl)prop-2-yn-1-one 2ab<sup>2</sup>**



**2ab** (97 mg) was obtained from **1ab** (100 mg) following general procedure B; white solid; 91% yield (eluent: EtOAc/Hexanes= 2:8); mp: 96-98 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 1.57-1.66 (m, 6H), 3.60-3.64 (m, 2H), 3.75-3.78 (m, 2H), 7.34-7.39 (m, 3H), 7.52-7.54 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>24.5, 25.3, 26.4, 42.3, 48.1, 81.6, 90.1, 120.8, 128.4, 129.7, 132.2, 152.9.

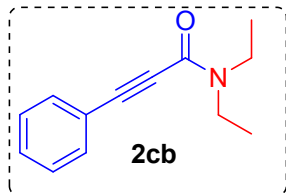
**3-phenyl-1-(2,2,6,6-tetramethylpiperidin-1-yl)prop-2-yn-1-one 2bb**



**2bb** (112 mg) was obtained from **1bb** (128 mg) following general procedure B; yellow liquid; 83% yield (eluent: EtOAc/Hexanes= 1:9);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 1.68 (s, 12H), 1.74-1.79 (m, 6H), 7.37-7.39 (m, 3H), 7.54-7.56 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>15.0, 29.8, 39.3, 57.0, 87.2, 88.5, 121.6, 128.2, 129.2, 131.6, 155.9; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>24</sub>NO: 270.1859, Found: 270.1819.

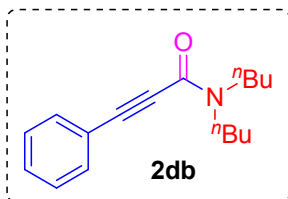
***N,N*-diethyl-3-phenylpropiolamide 2cb<sup>2</sup>**



**2cb** (60 mg) was obtained from **1cb** (94 mg) following general procedure B; yellow liquid; 60% yield (eluent: EtOAc/Hexanes= 1:9);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 1.10 (t, *J*= 6.9Hz, 3H), 1.21 (t, *J*= 6.9Hz, 3H), 3.37-3.44 (m, 2H), 3.55-3.62 (m, 2H), 7.25-7.33 (m, 3H), 7.44-7.47 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>12.7, 14.3, 39.3, 43.5, 82.0, 88.9, 120.9, 128.4, 129.7, 132.2, 153.9.

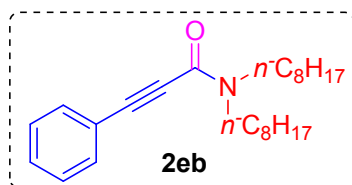
### ***N,N*-dibutyl-3-phenylpropiolamide **2db**<sup>4</sup>**



**2db** (83 mg) was obtained from **1db** (122 mg) following general procedure B; yellow liquid; 65% yield (eluent: EtOAc/Hexanes= 1:9);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  0.84-0.92 (m, 6H), 1.19-1.36 (m, 4H), 1.44-1.60 (m, 4H), 3.30-3.35 (m, 2H), 3.49-3.54 (m, 2H), 7.25-7.32 (m, 3H), 7.43-7.45 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  13.7, 19.9, 20.1, 29.6, 31.0, 44.6, 48.9, 82.3, 89.1, 120.9, 128.4, 129.7, 132.2, 154.4.

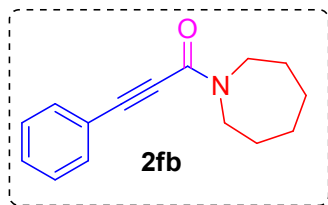
### ***N,N*-dinonyl-3-phenylpropiolamide **2eb****



**2eb** (102 mg) was obtained from **1eb** (179 mg) following general procedure B; colorless oily liquid; 55% yield (eluent: EtOAc/Hexanes= 1:9);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  0.76-0.82 (m, 6H), 1.14-1.31 (m, 20H), 1.48-1.61 (m, 4H), 3.29-3.34 (m, 2H), 3.48-3.53 (m, 2H), 7.24-7.32 (m, 3H), 7.43-7.45 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  13.9, 22.5, 22.6, 26.7, 26.9, 27.5, 28.9, 29.1, 29.2, 29.3, 31.7, 31.8, 44.9, 49.1, 82.3, 89.1, 121.0, 128.4, 129.7, 132.2, 154.3; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>25</sub>H<sub>40</sub>NO: 370.3109, Found: 370.3081.

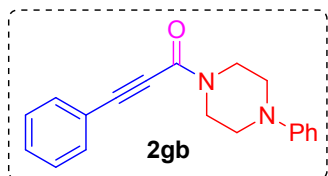
### **1-(azepan-1-yl)-3-phenylprop-2-yn-1-one **2fb**<sup>3</sup>**



**2fb** (100 mg) was obtained from **1fb** (107 mg) following general procedure B; colorless oily liquid; 88% yield (eluent: EtOAc/Hexanes= 1:9);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  1.90 (s, 4H), 2.06-2.11 (m, 4H), 3.86-3.90 (m, 2H), 4.04-4.08 (m, 2H), 7.63-7.68 (m, 3H), 7.80-7.8.3 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$ 26.9, 27.1, 27.2, 29.2, 45.3, 49.1, 82.1, 89.5, 120.9, 128.4, 129.7, 132.2, 154.4.

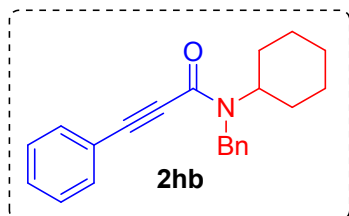
### 3-phenyl-1-(4-phenylpiperazin-1-yl)prop-2-yn-1-one **2gb**



**2gb** (134 mg) was obtained from **1gb** (138 mg) following general procedure B; pale yellow solid; 93% yield (eluent: EtOAc/Hexanes= 2:8); mp: 95-97 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  3.18 (t,  $J$ = 5.1Hz, 2H), 3.24 (t,  $J$ = 4.8Hz, 2H), 3.82-3.85 (m, 2H), 3.95-3.99 (m, 2H), 6.90-6.94 (m, 3H), 7.25-7.41 (m, 5H), 7.55 (d,  $J$ = 7.2Hz, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$ 41.5, 46.9, 49.3, 50.0, 81.1, 90.8, 116.9, 120.5, 120.7, 128.5, 129.2, 130.0, 132.3, 150.9, 153.0; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>19</sub>H<sub>18</sub>N<sub>2</sub>O: 291.1497, Found: 291.1501.

### *N*-benzyl-*N*-cyclohexyl-3-phenylpropiolamide **2hb**

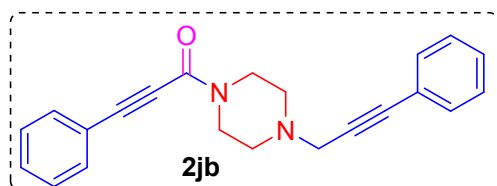




**2hb** (103 mg) was obtained from **1hb** (151 mg) following general procedure B; white solid; 65% yield (eluent: EtOAc/Hexanes= 1:9); mp: 88-90 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 1.26-1.45 (m, 5H), 1.57-1.82 (m, 5H), 4.34-4.35 (m, 1H), 4.65 (s, 1H), 4.83 (s, 1H), 7.24-7.41 (m, 9H), 7.53-7.56 (m, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 25.3, 25.5, 25.9, 26.2, 29.7, 30.7, 32.2, 44.8, 49.5, 54.8, 59.8, 82.2, 82.9, 89.5, 90.4, 115.9, 120.8, 121.0, 126.8, 126.9, 127.3, 127.4, 128.4, 128.5, 128.6, 129.8, 130.0, 132.3, 132.4, 138.7, 138.8, 155.2, 155.4; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>22</sub>H<sub>24</sub>NO: 318.1857, Found: 318.1824.

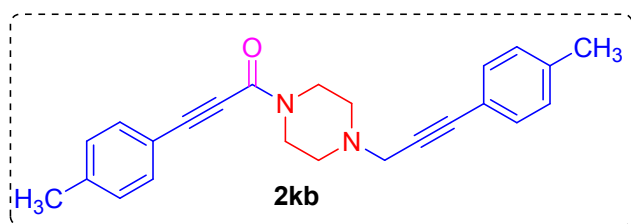
### 3-phenyl-1-(4-(3-phenylprop-2-yn-1-yl)piperazin-1-yl)prop-2-yn-1-one **2jb**



**2jb** (116 mg) was obtained from **1jb** (157 mg) following general procedure B; white solid; 71% yield (eluent: EtOAc/Hexanes= 2:8); mp: 86-88 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.58 (t, *J*= 5.1Hz, 2H), 2.64 (t, *J*= 5.1Hz, 2H), 3.50 (s, 2H), 3.67-3.71 (m, 2H), 3.81-3.84 (m, 2H), 7.18-7.24 (m, 3H), 7.27-7.36 (m, 5H), 7.44-7.47 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 41.3, 46.8, 47.6, 51.3, 52.1, 81.1, 83.4, 85.9, 90.7, 120.5, 122.8, 128.2, 128.4, 129.9, 131.7, 132.3, 153.0; **IR (KBr) v:** 2999, 2876, 2220, 1616, 1125, 1056; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>22</sub>H<sub>21</sub>N<sub>2</sub>O: 329.1653, Found: 329.1619.

### 3-(p-tolyl)-1-(4-(3-(p-tolyl)prop-2-yn-1-yl)piperazin-1-yl)prop-2-yn-1-one **2kb**



**2kb** (133 mg) was obtained from **1kb** (171 mg) following general procedure B; white

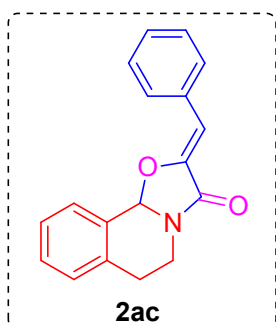
solid; 75% yield (eluent: EtOAc/Hexanes= 2:8); mp: 87-89 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.36 (s, 3H), 2.37 (s, 3H), 2.65 (t, *J*= 5.1Hz, 2H), 2.70 (t, *J*= 5.1Hz, 2H), 3.56 (s, 2H), 3.74-3.78 (m, 2H), 3.88-3.92 (m, 2H), 7.09 (d, *J*= 7.8Hz, 2H), 7.14-7.18 (m, 2H), 7.30 (d, *J*= 8.1HZ, 2H), 7.41-7.45 (m, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub>21.3, 21.5, 41.2, 48.8, 47.7, 51.4, 52.1, 80.7, 82.6, 88.1, 91.1, 117.4, 119.7, 128.9, 129.2, 131.5, 132.2, 138.3, 140.4, 153.1; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>24</sub>H<sub>25</sub>N<sub>2</sub>O: 357.1966, Found: 357.1962.

#### 4. General procedure C for synthesis of Oxazolo[2,3-a]isoquinolinone

Reaction tube was charged with phenylpropynyltetrahydroisoquinoline (0.3 mmol), DBU (0.3 mmol), Rose bengal (2 mol%) and Ag(OTf) (10 mol%) in ACN 4 mL. The reaction mixture was stirred in the presence of O<sub>2</sub> (balloon) under blue light for 2 hours. After the reaction completion, solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using EtOAc/Hexane as eluent to furnish the corresponding Oxazolo[2,3-a]isoquinolinone compounds.

**(Z)-2-benzylidene-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2ac**

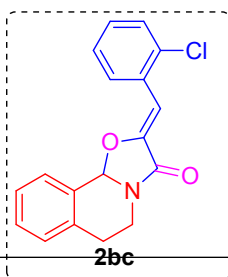


**2ac** (51 mg) was obtained from **1ac** (74 mg) following general procedure C; yellow liquid; 61% yield (eluent: EtOAc/Hexanes= 3:7);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  2.81-2.88 (m, 1H), 3.09-3.16 (m, 1H), 3.44-3.52 (m, 1H), 4.37-4.45 (m, 1H), 6.32 (s, 1H), 6.55 (s, 1H), 7.20 (d,  $J$ = 6.6Hz, 1H), 7.27-7.29 (m, 1H), 7.34-7.41 (m, 4H), 7.63-7.65 (m, 1H), 7.74 (d,  $J$ = 7.2Hz, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  27.5, 37.7, 87.1, 103.7, 125.8, 127.2, 127.4, 128.4, 128.8, 129.1, 129.2, 133.2, 133.8, 133.9, 144.1, 161.8;

**IR (KBr) v:** 2935, 1562, 1158, 967; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>16</sub>NO<sub>2</sub>: 278.1181, Found: 278.1184.

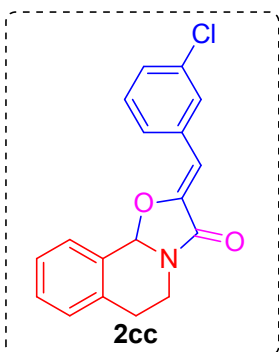
**(Z)-2-(2-chlorobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2bc**



**2bc** (52 mg) was obtained from **1bc** (85 mg) following general procedure C; white solid; 55% yield (eluent: EtOAc/Hexanes= 3:7); mp: 128-130 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.79-2.86 (m, 1H), 3.00-3.17 (m, 1H), 3.43-3.52 (m, 1H), 4.39-4.46 (m, 1H), 6.55 (s, 1H), 6.74 (s, 1H), 7.15-7.20 (m, 2H), 7.27-7.40 (m, 4H), 7.57-7.60 (m, 1H), 8.17 (d, *J*= 6Hz, 1H); **<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.6, 37.9, 87.3, 99.0, 125.9, 126.7, 127.3, 128.4, 129.0, 129.3, 129.6, 130.1, 131.7, 132.8, 133.6, 133.9, 145.5, 161.4; **IR (KBr) ν:** 2932, 2876, 1562, 1153, 973; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>15</sub>ClNO<sub>2</sub>: 312.0791, Found: 312.0795.

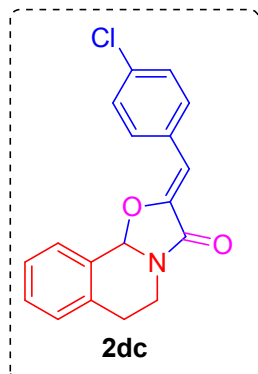
**(Z)-2-(3-chlorobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2cc**



**2cc** (42 mg) was obtained from **1cc** (85 mg) following general procedure C; white solid; 45% yield (eluent: EtOAc/Hexanes= 3:7); mp: 123-125 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.83-2.88 (m, 1H), 3.12-3.19 (m, 1H), 3.46-3.55 (m, 1H), 4.42-4.44 (m, 1H), 6.25 (s, 1H), 6.57 (s, 1H), 7.20-7.30 (m, 3H), 7.33-7.40 (m, 2H), 7.56 (d, *J*= 6.9Hz, 1H), 7.64 (d, *J*= 6.6Hz, 1H), 7.77 (s, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.6, 37.8, 87.4, 102.2, 125.8, 127.3, 127.4, 127.5, 128.9, 129.3, 129.6, 132.9, 133.9, 134.4, 134.6, 135.7, 145.1, 161.4; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>15</sub>ClNO<sub>2</sub>: 312.0791, Found: 312.0784.

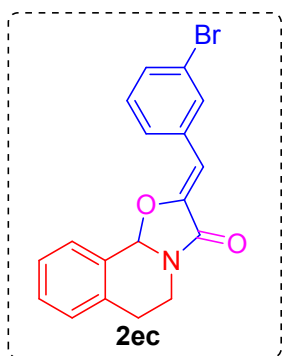
**(Z)-2-(4-chlorobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2dc**



**2dc** (61 mg) was obtained from **1dc** (85 mg) following general procedure C; white solid; 65% yield (eluent: EtOAc/Hexanes= 3:7); mp: 118-120 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  2.80-2.88 (m, 1H), 3.07-3.18 (m, 1H), 3.44-3.53 (m, 1H), 4.38-4.45 (m, 1H), 6.26 (s, 1H), 6.55 (s, 1H), 7.21 (d,  $J= 6.6\text{Hz}$ , 1H), 7.28-7.41 (m, 4H), 7.60-7.67 (m, 3H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  27.6, 37.8, 87.3, 102.4, 125.8, 127.3, 128.7, 128.9, 129.3, 130.3, 132.4, 133.0, 133.1, 133.9, 144.6, 161.5; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>15</sub>ClNO<sub>2</sub>: 312.0791, Found: 312.0789.

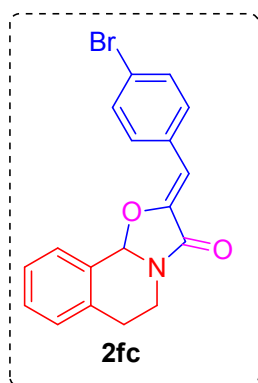
**(Z)-2-(3-bromobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2ec**



**2ec** (55 mg) was obtained from **1ec** (98 mg) following general procedure C; brown solid; 52% yield (eluent: EtOAc/Hexanes= 3:7); mp: 130-132 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.93-2.77 (m, 1H), 3.06-3.17 (m, 1H), 3.44-3.54 (m, 1H), 4.38-4.45 (m, 1H), 6.21 (s, 1H), 6.57 (s, 1H), 7.16-7.266 (m, 2H), 7.31-7.46 (m, 3H), 7.60 (d, *J*=7.4Hz, 2H), 7.90 (s, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** 27.6, 37.9, 87.4, 102.1, 122.6, 125.9, 127.3, 127.7, 129.9, 129.4, 130.0, 130.3, 131.8, 132.7, 133.8, 135.9, 145.1, 161.4; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>15</sub>BrNO<sub>2</sub>: 356.0286, Found: 356.0287.

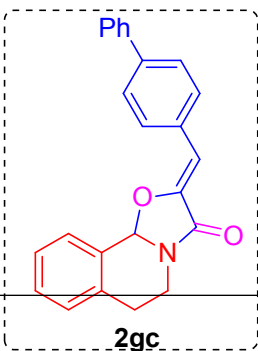
**(Z)-2-(4-bromobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2fc**



**2fc** (62 mg) was obtained from **1fc** (98 mg) following general procedure C; brown solid; 58% yield (eluent: EtOAc/Hexanes= 3:7); mp: 185-187 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.80-2.86 (m, 1H), 3.07-3.15 (m, 1H), 3.44-3.51 (m, 1H), 4.38-4.44 (m, 1H), 6.22 (s, 1H), 6.55 (s, 1H), 7.19 (d, *J* = 7.0Hz, 1H), 7.32-7.41 (m, 2H), 7.46-7.52 (m, 2H), 7.55-7.63 (m, 3H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.6, 37.8, 87.3, 102.4, 121.2, 125.9, 127.3, 129.0, 129.3, 130.6, 131.7, 132.7, 132.8, 133.9, 144.7, 161.6; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>15</sub>BrNO<sub>2</sub>: 356.0286, Found: 356.0286.

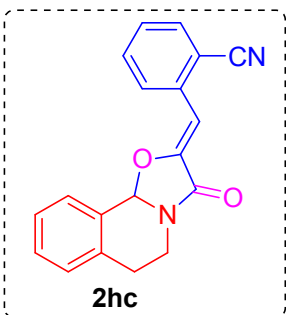
**(Z)-2-([1,1'-biphenyl]-4-ylmethylene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2gc**



**2gc** (51 mg) was obtained from **1gc** (97 mg) following general procedure C; white solid; 48% yield (eluent: EtOAc/Hexanes= 3:7); mp: 212-214 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.81-2.86 (m, 1H), 3.00-3.17 (m, 1H), 3.43-3.53 (m, 1H), 4.38-4.43 (m, 1H), 6.34 (s, 1H), 6.57 (s, 1H), 7.19 (d, *J*= 6.7Hz, 1H), 7.32-7.36 (m, 2H), 7.47-7.47 (m, 3H), 7.57-7.63 (m, 5H), 7.80 (d, *J*= 8Hz, 2H); **<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.6, 37.8, 87.2, 103.3, 125.9, 127.0, 127.2, 127.3, 127.4, 128.8, 128.9, 129.2, 129.6, 132.8, 133.0, 133.9, 140.1, 140.7, 144.3, 161.8; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>24</sub>H<sub>20</sub>NO<sub>2</sub>: 354.1494, Found: 354.1496.

**(Z)-2-((3-oxo-3,5,6,10b-tetrahydro-2H-oxazolo[2,3-a]isoquinolin-2-ylidene)methyl)benzonitrile 2hc**

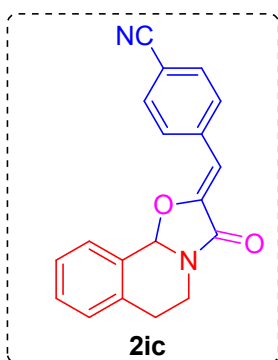


**2hc** (56 mg) was obtained from **1hc** (82 mg) following general procedure C; white solid; 62% yield (eluent: EtOAc/Hexanes= 3:7); mp: 155-157 °C;

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.74-2.79 (m, 1H), 3.00-3.07 (m, 1H), 3.37-3.45 (m, 1H), 4.30-4.40 (m, 1H), 6.52 (s, 1H), 6.58 (s, 1H), 7.13 (d, *J*= 4.8Hz, 1H), 7.18-7.29 (m, 3H), 7.50-7.56 (m,

3H), 8.18 (d,  $J$  = 6Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta_{\text{C}}$  27.6, 37.9, 87.7, 98.7, 111.7, 117.7, 125.9, 127.2, 127.3, 129.1, 129.2, 129.5, 132.3, 132.6, 133.1, 134.0, 136.9, 147.1, 160.7; IR (KBr)  $\nu$ : 2932, 2343, 1562, 1155, 961; HRMS: (M+H) $^+$  calculated for  $\text{C}_{19}\text{H}_{15}\text{N}_2\text{O}_2$ : 303.1133, Found: 303.1097.

**(Z)-4-((3-oxo-3,5,6,10b-tetrahydro-2H-oxazolo[2,3-a]isoquinolin-2-ylidene)methyl)benzonitrile 2ic**

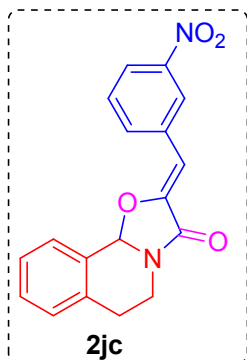


**2ic** (62 mg) was obtained from **1ic** (82 mg) following general procedure C; white solid; 69% yield (eluent: EtOAc/Hexanes = 3:7); mp: 195-197 °C;

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta_{\text{H}}$  2.83-2.91 (m, 1H), 3.09-3.20 (m, 1H), 3.47-3.57 (m, 1H), 4.41-4.48 (m, 1H), 6.30 (s, 1H), 6.61 (s, 1H), 7.23 (d,  $J$  = 6.6Hz, 1H), 7.35-7.43 (m, 2H), 7.63 (t,  $J$  = 7.2Hz, 3H), 7.79 (d,  $J$  = 6Hz, 2H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ):  $\delta_{\text{C}}$  27.2, 37.6, 87.4, 101.3, 110.0, 118.5, 125.5, 127.0, 128.7, 129.0, 129.1, 131.8, 132.1, 133.5, 138.2, 146.3, 160.6; HRMS: (M+H) $^+$  calculated for  $\text{C}_{19}\text{H}_{15}\text{N}_2\text{O}_2$ : 303.1133, Found: 303.1098.

**(Z)-2-(3-nitrobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2jc**



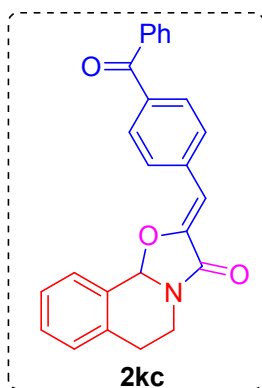


**2jc** (62 mg) was obtained from **1jc** (88 mg) following general procedure C; yellow liquid; 65% yield (eluent: EtOAc/Hexanes= 4:6);

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  2.84-2.91 (m, 1H), 3.09-3.20 (m, 1H), 3.47-3.53 (m, 1H), 4.41-4.48 (m, 1H), 6.34 (s, 1H), 6.62 (s, 1H), 7.22 (d,  $J=7.2\text{Hz}$ , 1H), 7.34-7.44 (m, 2H), 7.52 (t,  $J=7.8\text{Hz}$ , 1H), 7.66 (d,  $J=7.5\text{Hz}$ , 1H), 7.90 (d,  $J=7.5\text{Hz}$ , 1H), 8.09 (d,  $J=7.5\text{Hz}$ , 1H), 8.70 (s, 1H);

**<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  27.6, 37.9, 87.7, 101.1, 121.8, 123.4, 125.9, 127.5, 129.0, 129.3, 129.5, 132.6, 133.8, 134.6, 135.6, 146.3, 148.7, 160.9; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>15</sub>N<sub>2</sub>O<sub>4</sub>: 323.1031, Found: 323.0996.

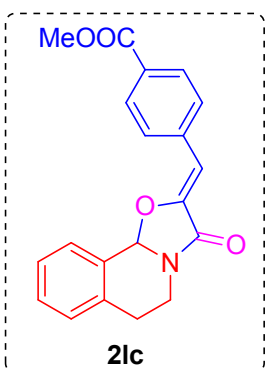
**(Z)-2-(4-benzoylbenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2kc**



**2kc** (58 mg) was obtained from **1kc** (105 mg) following general procedure C; yellow liquid; 51% yield (eluent: EtOAc/Hexanes= 4:6);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.85-2.90 (m, 1H), 3.13-3.20 (m, 1H), 3.48-3.56 (m, 1H), 4.41-4.48 (m, 1H), 6.37 (s, 1H), 6.60 (s, 1H), 7.23 (d, *J* = 6.6Hz, 1H), 7.37-7.39 (m, 2H), 7.47-7.52 (m, 2H), 7.57-7.64 (m, 2H), 7.80-7.84 (m, 6H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.6, 37.9, 87.5, 102.5, 125.8, 127.3, 128.2, 128.8, 128.9, 129.3, 129.8, 130.3, 132.1, 132.8, 133.9, 136.0, 137.9, 138.1, 145.9, 161.3, 195.9; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>25</sub>H<sub>20</sub>NO<sub>3</sub>: 382.1443, Found: 382.1412.

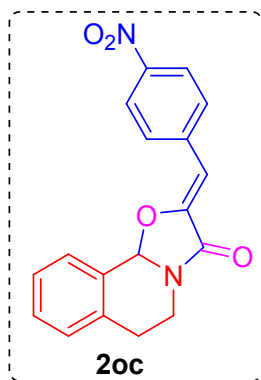
**(Z)-methyl 4-((3-oxo-3,5,6,10b-tetrahydro-2H-oxazolo[2,3-a]isoquinolin-2-ylidene)methyl)benzoate 2lc**



**2lc** (67 mg) was obtained from **1lc** (91 mg) following general procedure C; white solid; 67% yield (eluent: EtOAc/Hexanes = 4:6); mp: 202-204 °C;

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.75-2.78 (m, 1H), 3.00-3.07 (m, 1H), 3.38-3.44 (m, 1H), 4.32-4.36 (m, 1H), 6.23 (s, 1H), 6.50 (s, 1H), 7.10 (d, *J* = 6.6Hz, 1H), 7.26-7.32 (m, 2H), 7.54 (d, *J* = 3Hz, 1H), 7.68 (d, *J* = 6Hz, 2H), 7.95 (d, *J* = 6Hz, 2H); **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.6, 37.9, 52.1, 87.5, 102.4, 125.9, 127.3, 128.5, 128.9, 129.0, 129.4, 129.7, 132.6, 133.8, 138.4, 145.8, 161.3, 166.8; **IR (KBr) ν:** 2847, 1712, 1556, 1153, 954; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>20</sub>H<sub>18</sub>NO<sub>4</sub>: 336.1236, Found: 336.1234.

**(Z)-2-(4-nitrobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2oc**

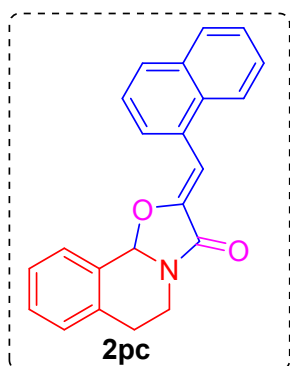


**2oc** (68 mg) was obtained from **1oc** (88 mg) following general procedure B; yellow solid; 71% yield (eluent: EtOAc/Hexanes= 4:6); mp: 220-222 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.85-2.90 (m, 1H), 3.10-3.25 (m, 1H), 3.52-3.56 (m, 1H), 4.43-4.49 (m, 1H), 6.35 (s, 1H), 6.63 (s, 1H), 7.23 (d, *J*= 6.6Hz, 1H), 7.36-7.41 (m, 2H), 7.62-7.65 (m, 1H), 7.85 (d, *J*= 8.7Hz, 2H), 8.23 (d, *J*= 8.7Hz, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.6, 38.0, 87.8, 101.2, 123.8, 125.8, 127.4, 129.0, 129.4, 129.5, 132.4, 133.9, 140.5, 146.4, 147.1, 160.8; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>15</sub>N<sub>2</sub>O<sub>4</sub>: 323.1031, Found: 323.1031.

**(Z)-2-(naphthalen-1-ylmethylene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one**

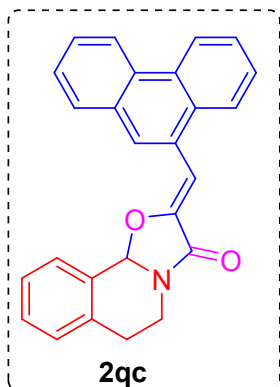
**2pc**



**2pc** (51 mg) was obtained from **1pc** (89 mg) following general procedure C; yellow liquid; 52% yield (eluent: EtOAc/Hexanes= 3:7);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.82-2.91 (m, 1H), 3.11-3.22 (m, 1H), 3.47-3.57 (m, 1H), 4.42-4.50 (m, 1H), 6.58 (s, 1H), 7.08 (s, 1H), 7.20-7.23 (m, 1H), 7.35-7.41 (m, 2H), 7.50-7.58 (m, 3H), 7.62-7.65 (m, 1H), 7.79-7.88 (m, 2H), 8.26 (d, *J* = 7.2Hz, 2H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.6, 37.8, 87.1, 99.3, 123.8, 125.4, 125.7, 125.9, 126.2, 127.2, 127.3, 128.0, 128.6, 128.9, 129.2, 129.8, 131.6, 133.2, 133.8, 133.9, 145.1, 161.8; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>22</sub>H<sub>18</sub>NO<sub>2</sub>: 328.1337, Found: 328.1335.

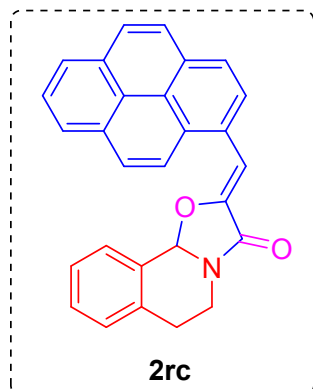
**(Z)-2-(phenanthren-9-ylmethylene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one**  
**2qc**



**2qc** (57 mg) was obtained from **1qc** (104 mg) following general procedure C; yellow liquid; 50% yield (eluent: EtOAc/Hexanes= 3:7);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.85-2.91 (m, 1H), 3.16-3.24 (m, 1H), 3.49-3.59 (m, 1H), 4.44-4.51 (m, 1H), 6.62 (s, 1H), 7.07 (s, 1H), 7.21-7.39 (m, 3H), 7.60-7.68 (m, 5H), 7.95 (d, *J* = 6.9Hz, 1H), 8.31 (d, *J* = 7.2Hz, 1H), 8.49 (s, 1H), 8.68 (d, *J* = 7.5Hz, 1H), 8.75 (d, *J* = 8.4Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.6, 37.9, 87.2, 99.5, 122.5, 123.08, 124.5, 125.9, 126.4, 126.6, 126.7, 126.8, 127.3, 128.2, 128.4, 128.7, 128.9, 129.2, 130.2, 130.6, 130.1, 131.7, 133.3, 134.0, 145.6, 161.7; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>26</sub>H<sub>20</sub>NO<sub>2</sub>: 378.1494, Found: 378.1466.

**(Z)-2-(pyren-1-ylmethylene)-6,10b-dihydro-5H-oxazolo[2,3-a]isoquinolin-3(2H)-one 2rc**

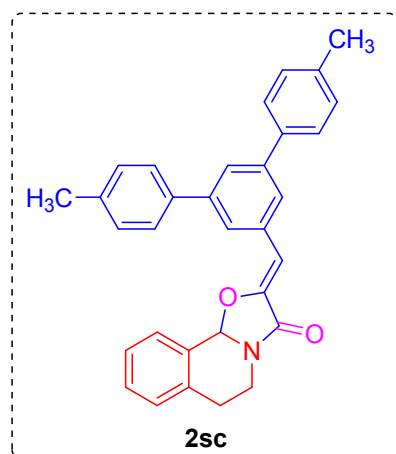


**2rc** (61 mg) was obtained from **1rc** (111 mg) following general procedure C; brown semi solid; 49% yield (eluent: EtOAc/Hexanes= 3:7);

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  2.77-2.96 (m, 1H), 3.13-3.22 (m, 1H), 3.50-3.57 (m, 1H), 4.37-4.55 (m, 1H), 6.64 (s, 1H), 7.21 (d,  $J= 7.3\text{Hz}$ , 1H), 7.30-7.44 (m, 3H), 7.69 (d,  $J= 7.3\text{Hz}$ , 1H), 7.96-8.07 (m, 3H), 8.10-8.23 (m, 4H), 8.51 (d,  $J= 9.3\text{ Hz}$ , 1H), 8.78 (d,  $J= 8.2\text{Hz}$ , 1H); **<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  27.7, 37.9, 87.2, 99.9, 123.2, 124.8, 124.9, 125.2, 125.3, 126.0, 126.9, 127.3, 127.4, 127.5, 127.6, 127.7, 128.9, 129.3, 130.7, 130.9, 131.4, 133.1, 134.0, 145.1, 161.9;

**HRMS:** (M+H)<sup>+</sup> calculated for C<sub>28</sub>H<sub>20</sub>NO<sub>2</sub>: 402.1494, Found: 402.1486

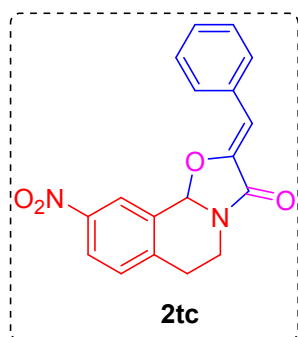
**(Z)-2-((4,4''-dimethyl-[1,1':3',1''-terphenyl]-5'-yl)methylene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2sc**



**2sc** (61 mg) was obtained from **1sc** (128 mg) following general procedure B; yellow liquid; 45% yield (eluent: EtOAc/Hexanes= 3:7);

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.45 (s, 6H), 2.83-2.90 (m, 1H), 3.10-3.19 (m, 1H), 3.47-3.56 (m, 1H), 4.39-4.47 (m, 1H), 6.44 (s, 1H), 6.58 (s, 1H), 7.21 (d, *J*= 7.2Hz, 1H), 7.28-7.38 (m, 6H), 7.59-7.61 (m, 5H), 7.69 (s, 1H), 7.94 (d, *J*= 1.2Hz, 2H); **<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 21.1, 27.6, 37.8, 87.2, 103.8, 125.0, 125.7, 126.6, 127.1, 127.3, 128.9, 129.2, 129.5, 133.3, 134.0, 134.6, 137.2, 138.4, 141.9, 144.6, 161.8; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>32</sub>H<sub>28</sub>NO<sub>2</sub>: 458.2120, Found: 458.2101.

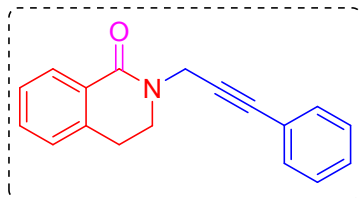
**(Z)-2-benzylidene-9-nitro-6,10b-dihydro-5H-oxazolo[2,3-a]isoquinolin-3(2H)-one 2tc**



**2tc** (56 mg) was obtained from **1tc** (88 mg) following general procedure B; yellow liquid; 59% yield (eluent: EtOAc/Hexanes= 3:7);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.94-3.00 (m, 1H), 3.15-3.26 (m, 1H), 3.47-3.57 (m, 1H), 4.45-4.51 (m, 1H), 6.37 (s, 1H), 6.58 (s, 1H), 7.32 (d, *J*= 7.5Hz, 1H), 7.38-7.44 (m, 3H), 7.73 (d, *J*= 1.2Hz, 2H), 8.21 (d, *J*= 8.4Hz, 1H), 8.50 (s, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 27.7, 37.1, 86.1, 105.1, 121.5, 124.0, 128.0, 128.7, 129.4, 130.2, 133.2, 134.8, 141.3, 143.2, 147.4, 161.6; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>15</sub>N<sub>2</sub>O<sub>4</sub>: 323.1032, Found: 323.1039.

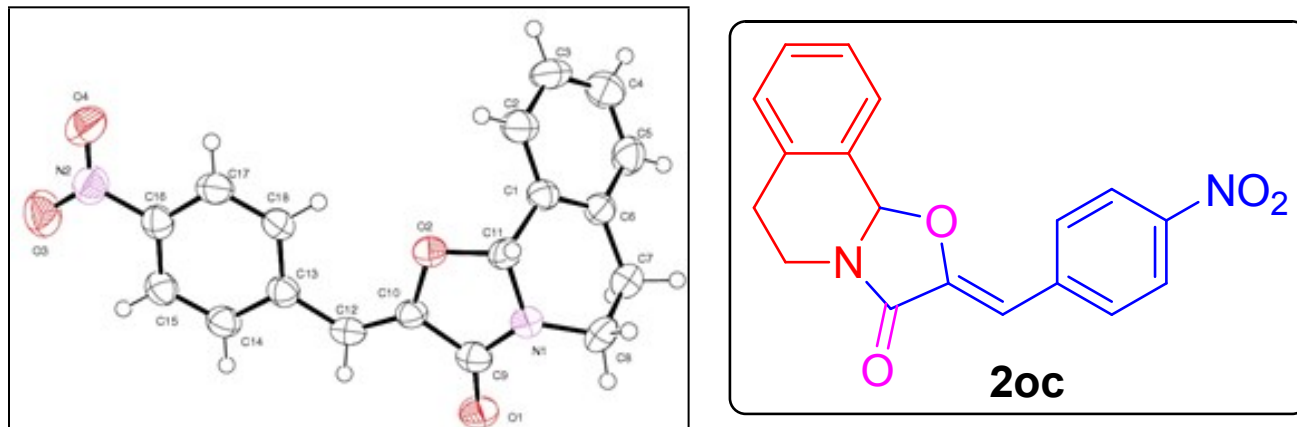
**2-(3-phenylprop-2-yn-1-yl)-3,4-dihydroisoquinolin-1(2H)-one 2ad**



**2ad** (20 mg) was obtained from **1ad** (74 mg) following general procedure B; yellow liquid; 25% yield (eluent: EtOAc/Hexanes= 1:9);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  3.04 (t,  $J= 6.6\text{Hz}$ , 2H), 3.74 (t,  $J= 6.6\text{Hz}$ , 2H), 4.65 (s, 2H), 7.17 (d,  $J= 6.6\text{Hz}$ , 1H), 7.24-7.38 (m, 4H), 7.40-7.43 (m, 3H), 8.11 (d,  $J= 7.8\text{Hz}$ , 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  28.0, 36.6, 45.1, 83.8, 84.0, 122.8, 126.9, 127.0, 128.2, 128.3, 128.5, 129.2, 129.8, 131.7, 138.1, 164.1; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>18</sub>H<sub>16</sub>NO: 262.1231, Found: 262.1248.

## 5. X-Ray Crystallographic Studies of compound 2oc



**Figure 2.** ORTEP structure of compound **2oc** (CCDC 1988860).

**Table 1.** Crystal data and structure refinement for Compound **2oc**.

<b>Identification code</b>	2oc	
<b>Chemical formula</b>	$C_{18}H_{14}N_2O_4$	
<b>Formula weight</b>	322.31 g/mol	
<b>Temperature</b>	296(2) K	
<b>Wavelength</b>	0.71073 Å	
<b>Crystal size</b>	0.100 x 0.110 x 0.150 mm	
<b>Crystal habit</b>	clear light yellow Block	
<b>Crystal system</b>	Monoclinic	
<b>Space group</b>	P 1 n 1	
<b>Unit cell dimensions</b>	a = 6.3537(8) Å	$\alpha = 90^\circ$
	b = 5.0200(6) Å	$\beta = 90.173(4)^\circ$
	c = 23.596(3) Å	$\gamma = 90^\circ$
<b>Volume</b>	752.60(16) Å <sup>3</sup>	
<b>Z</b>	2	
<b>Density (calculated)</b>	1.422 g/cm <sup>3</sup>	
<b>Absorption coefficient</b>	0.102 mm <sup>-1</sup>	
<b>F(000)</b>	336	



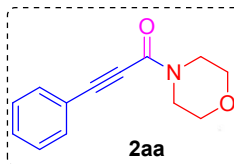
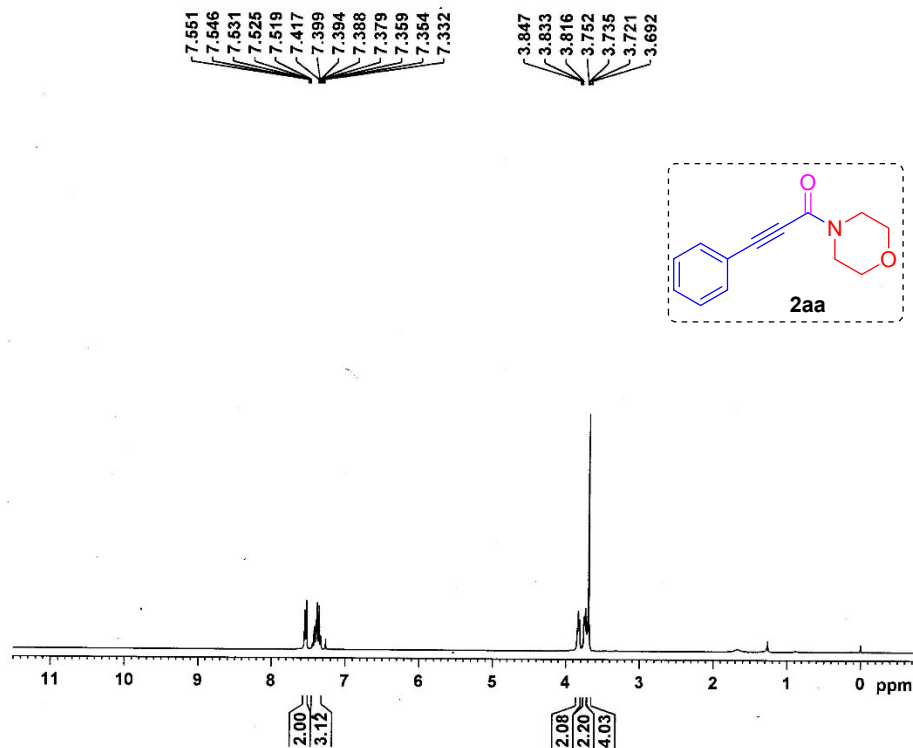
<b>Theta range for data collection</b>	3.32 to 24.70°
<b>Index ranges</b>	-5<=h<=7, -5<=k<=5, -27<=l<=27
<b>Reflections collected</b>	3980
<b>Independent reflections</b>	2005 [R(int) = 0.0421]
<b>Coverage of independent reflections</b>	99.8%
<b>Absorption correction</b>	multi-scan
<b>Max. and min. transmission</b>	0.9900 and 0.9850
<b>Refinement method</b>	Full-matrix least-squares on F <sup>2</sup>
<b>Refinement program</b>	SHELXL-2014/7 (Sheldrick, 2014)
<b>Function minimized</b>	$\Sigma w(F_o^2 - F_c^2)^2$
<b>Data / restraints / parameters</b>	2005 / 2 / 218
<b>Goodness-of-fit on F<sup>2</sup></b>	1.032
<b>Final R indices</b>	1414 data; I>2σ(I) R1 = 0.0420, wR2 = 0.0778
	all data R1 = 0.0730, wR2 = 0.0913
<b>Weighting scheme</b>	w=1/[σ <sup>2</sup> (F <sub>o</sub> <sup>2</sup> )+(0.0305P) <sup>2</sup> +0.0216P] where P=(F <sub>o</sub> <sup>2</sup> +2F <sub>c</sub> <sup>2</sup> )/3
<b>Absolute structure parameter</b>	-0.8(10)
<b>Extinction coefficient</b>	0.0310(40)
<b>Largest diff. peak and hole</b>	0.161 and -0.164 eÅ <sup>-3</sup>
<b>R.M.S. deviation from mean</b>	0.039 eÅ <sup>-3</sup>

---

## 6. References:

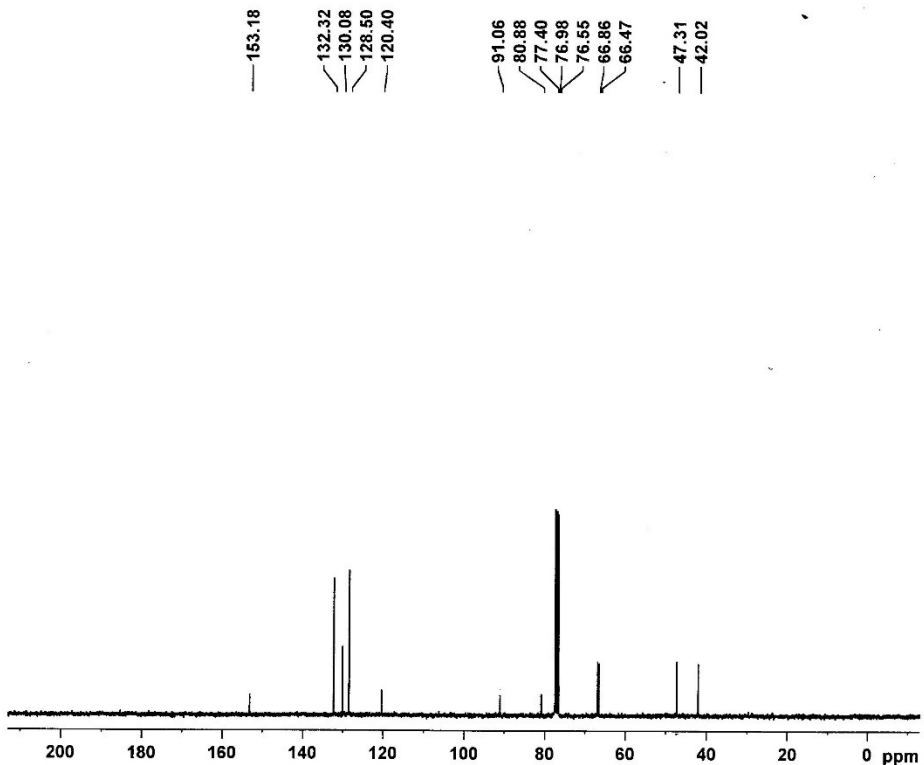
1. L. W. Bieber and M. F. da Silva, Mild and efficient synthesis of propargylamines by copper-catalyzed Mannich reaction, *Tetrahedron Lett.*, 2004, **45**, 8281-8283.
2. Y. Dong, S. Sun, F. Yang, Y. Zhu, W. Zhu, H. Qiao, Y. Wu and Y. Wu, Pd-catalyzed aminocarbonylation of alkynes with amines using  $\text{Co}_2(\text{CO})_8$  as a carbonyl source, *Org. Chem. Front.*, 2016, **3**, 720-724.
3. J. Hwang, J. Choi, K. Park, W. Kim, K. H. Song and S. Lee, Palladium-Catalyzed Oxidative Aminocarbonylation by Decarboxylative Coupling: Synthesis of Alkynyl Amides, *Eur. J. Org. Chem.*, 2015, **2015**, 2235-2243.
4. R. S. Mane and B. M. Bhanage, Palladium-Catalyzed Oxidative N-Dealkylation/Carbonylation of Tertiary Amines with Alkynes to  $\alpha,\beta$ -Alkynylamides, *J. Org. Chem.*, 2016, **81**, 4974-4980.

## 7. Spectral data:



NAME RA-BR-3-20  
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 PROCNO 1  
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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 181  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300058 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

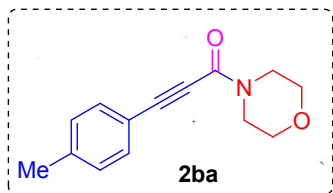
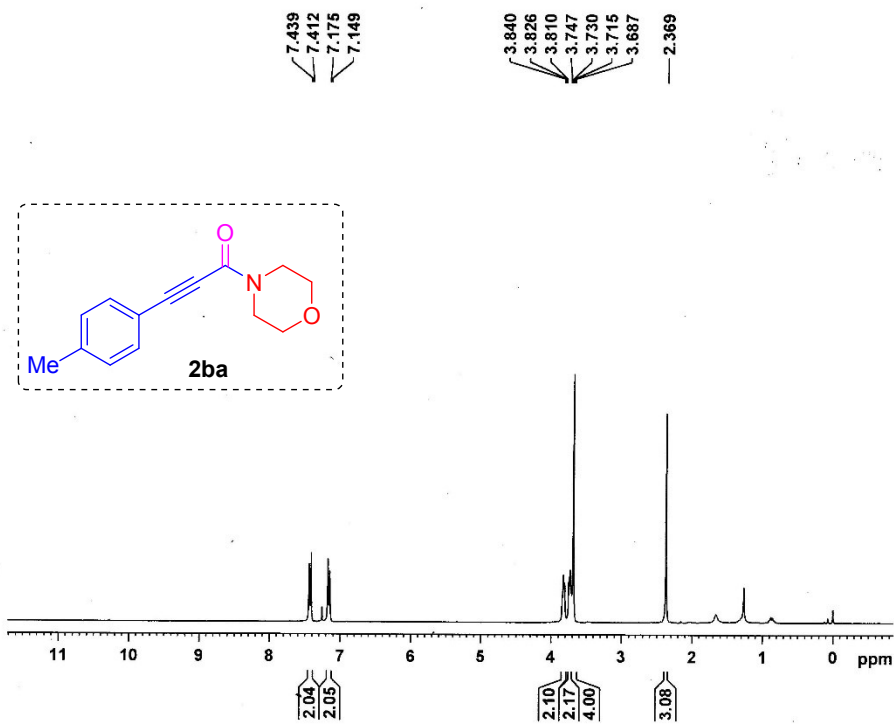


NAME RA-BR-3-20  
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 PROCNO 1  
 Date\_ 20181201  
 Time 16.10  
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 512  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 5160.6  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39858055 W  
 SFO1 75.4752953 MHz

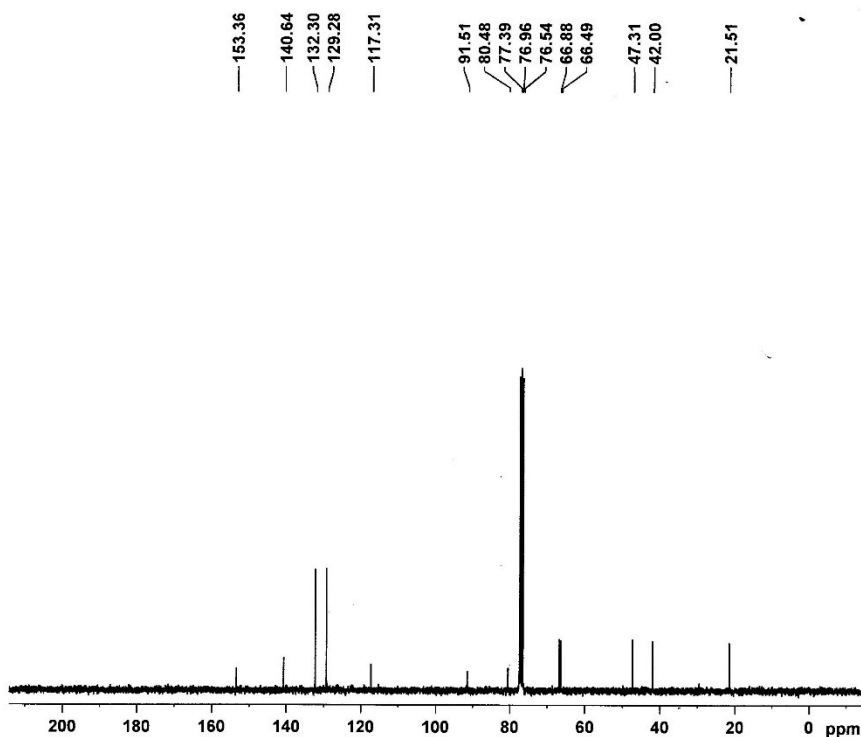
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 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.29870972 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2aa



NAME RA-BR-3-23  
 EXPNO 4  
 PROCNO 1  
 Date\_ 20181204  
 Time 20.59  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 181  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.2815662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300075 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

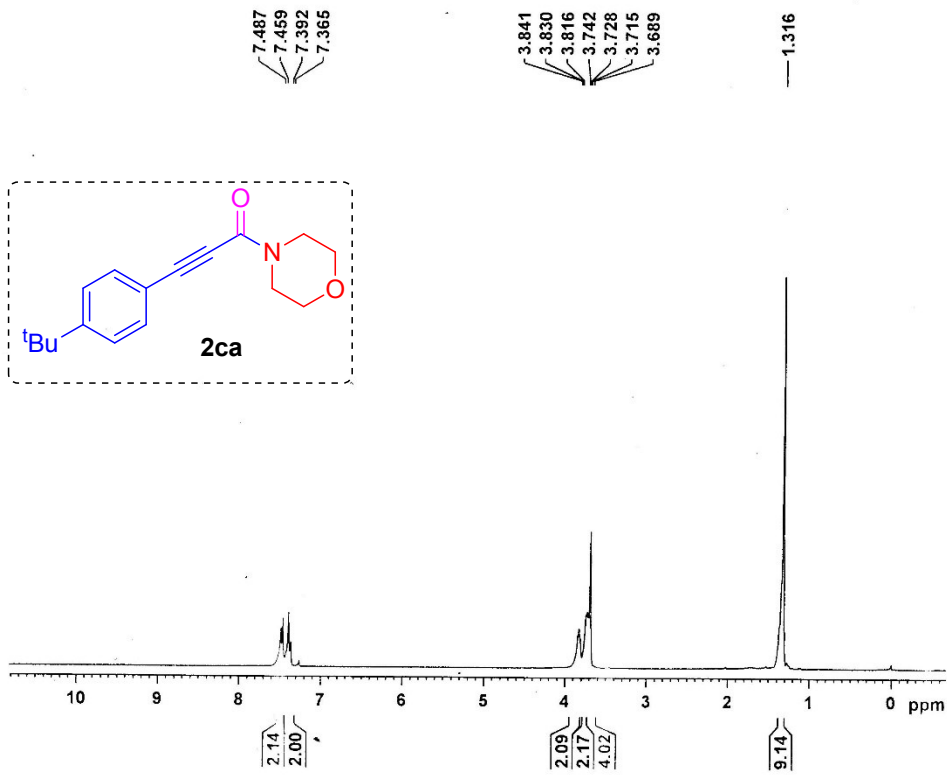


NAME RA-BR-3-23  
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 PROCNO 1  
 Date\_ 20181204  
 Time 20.48  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 512  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 7298.2  
 DW 27.600 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
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 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39858055 W  
 SFO1 75.4752953 MHz

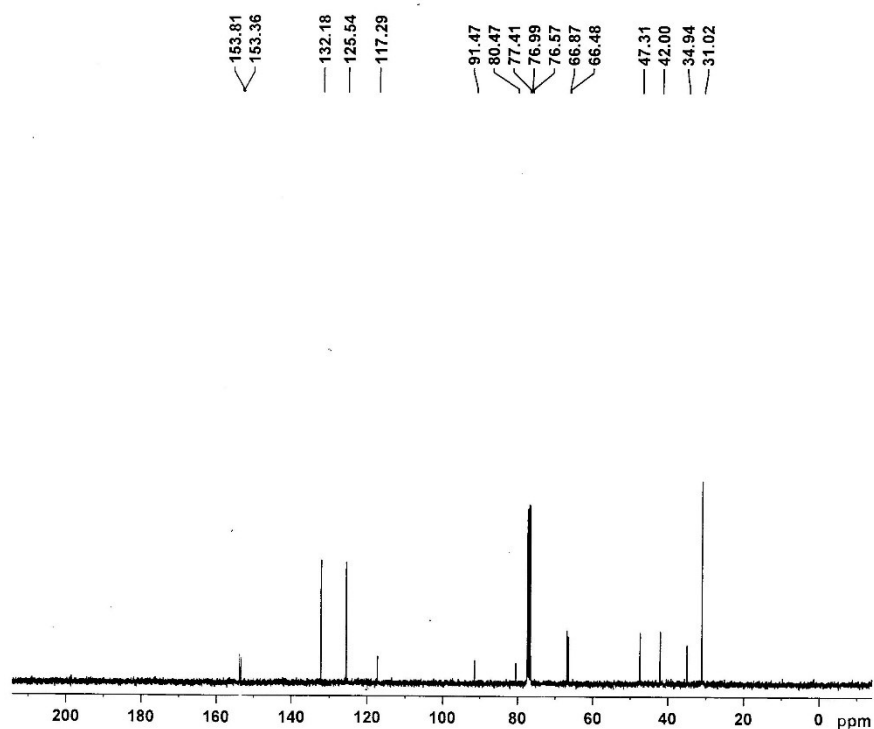
===== CHANNEL f2 =====  
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 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.2815662 W  
 PL12W 0.29870972 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2ba



NAME RA-BR-3-301B  
 EXPNO 7  
 PROCNO 1  
 Date\_ 20191015  
 Time 16.44  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084560 sec  
 RG 128  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300054 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

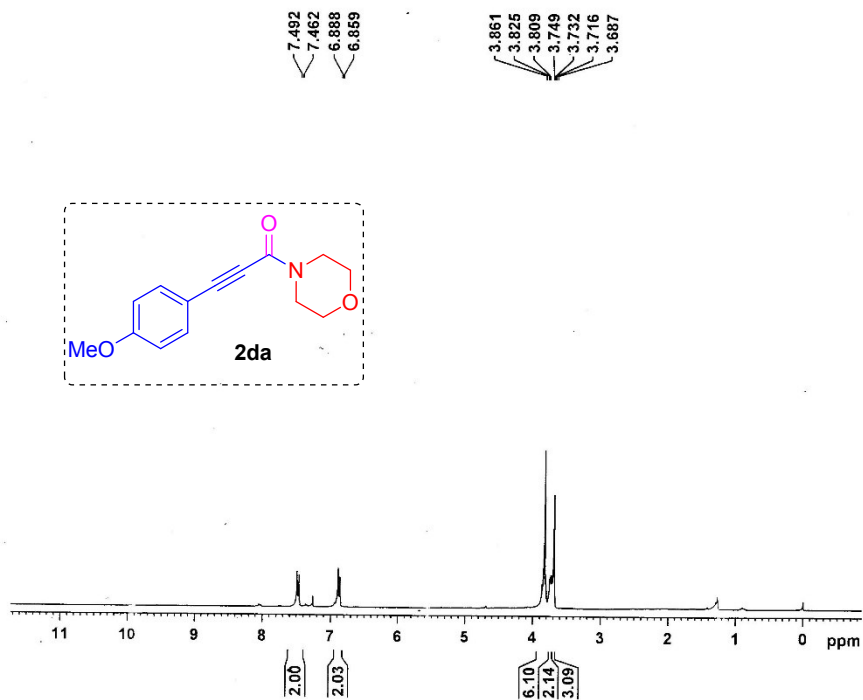
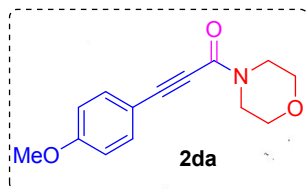


NAME RA-BR-3-301B  
 EXPNO 6  
 PROCNO 1  
 Date\_ 20191015  
 Time 16.25  
 INSTRUM spect  
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 310  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 5160.8  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39858055 W  
 SFO1 75.4752953 MHz

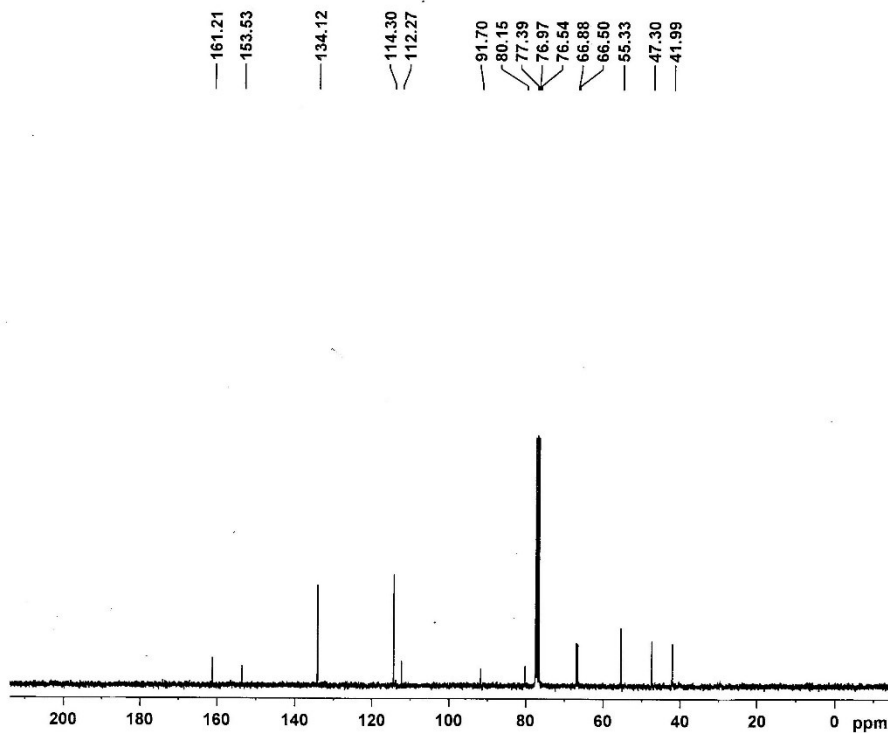
===== CHANNEL f2 =====  
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 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.29870972 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ca



NAME RA-BR-3-296B  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20190922  
 Time 13.14  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 181  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300061 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME RA-BR-3-296B  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20190922  
 Time 12.36  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 817  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 2048  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39858055 W  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.29870972 W  
 PL13W 0.28500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

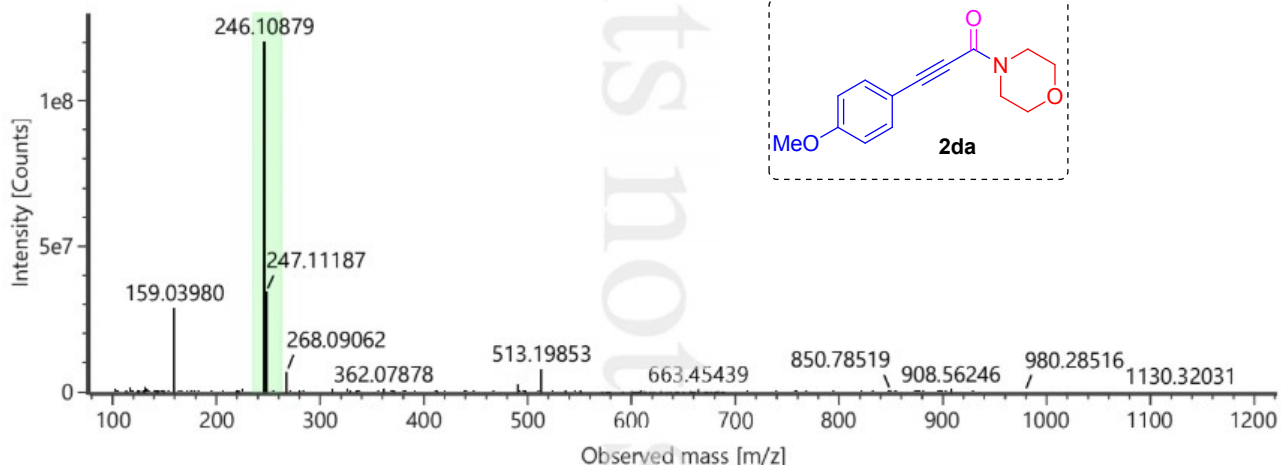
$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2da

**Component name: C<sub>14</sub>H<sub>15</sub>NO<sub>3</sub>**

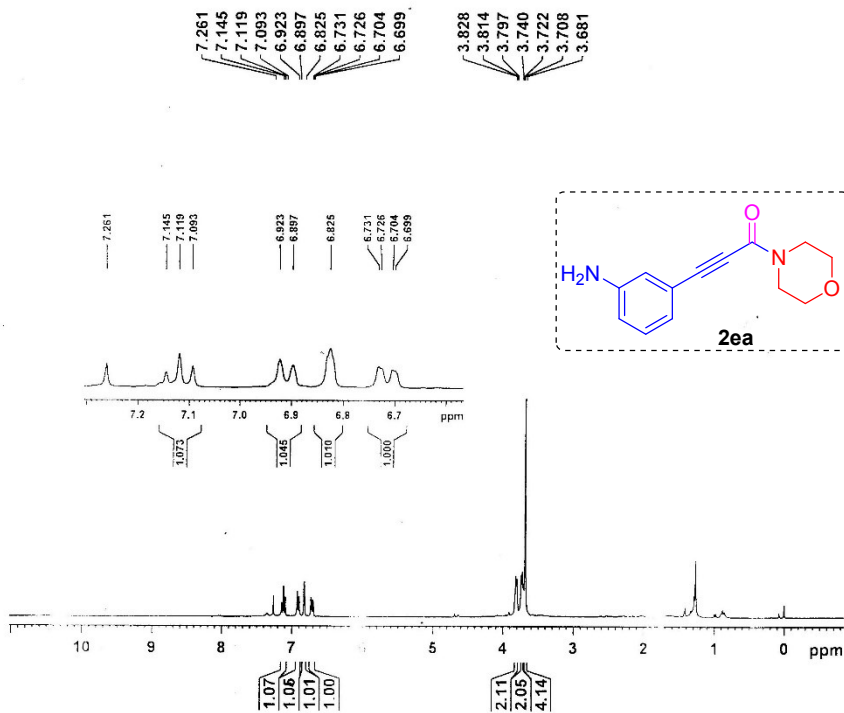
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Item description:

Channel name: Low energy : Time 0.3310 +/- 0.1833 minutes

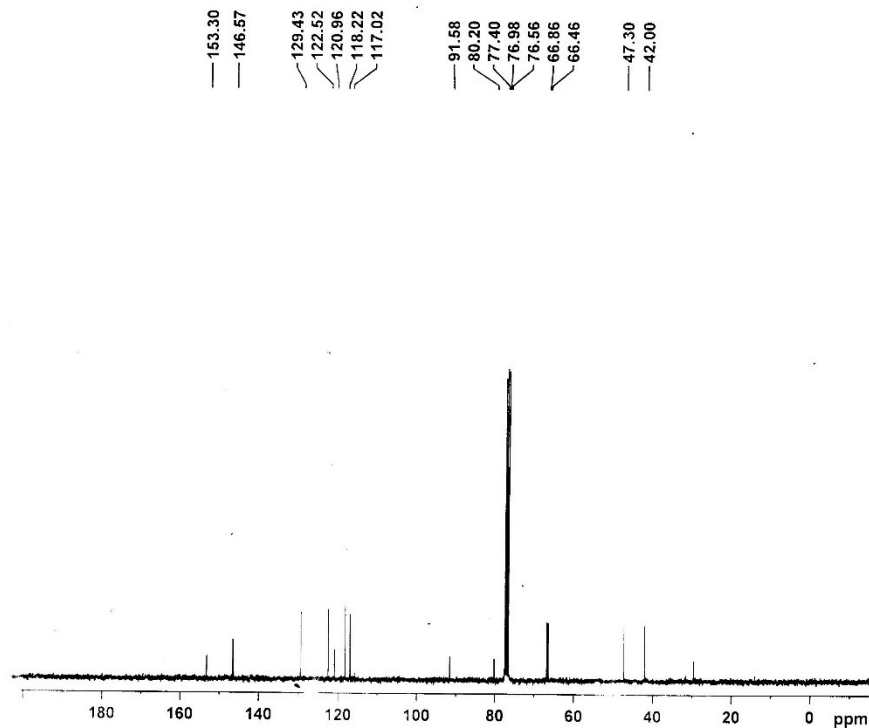


### HRMS Spectrum of Compound 2da



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 PROCNO 1  
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 Time 16.31  
 INSTRUM spect  
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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 15  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 181  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32.68  
 SF 300.1000065 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



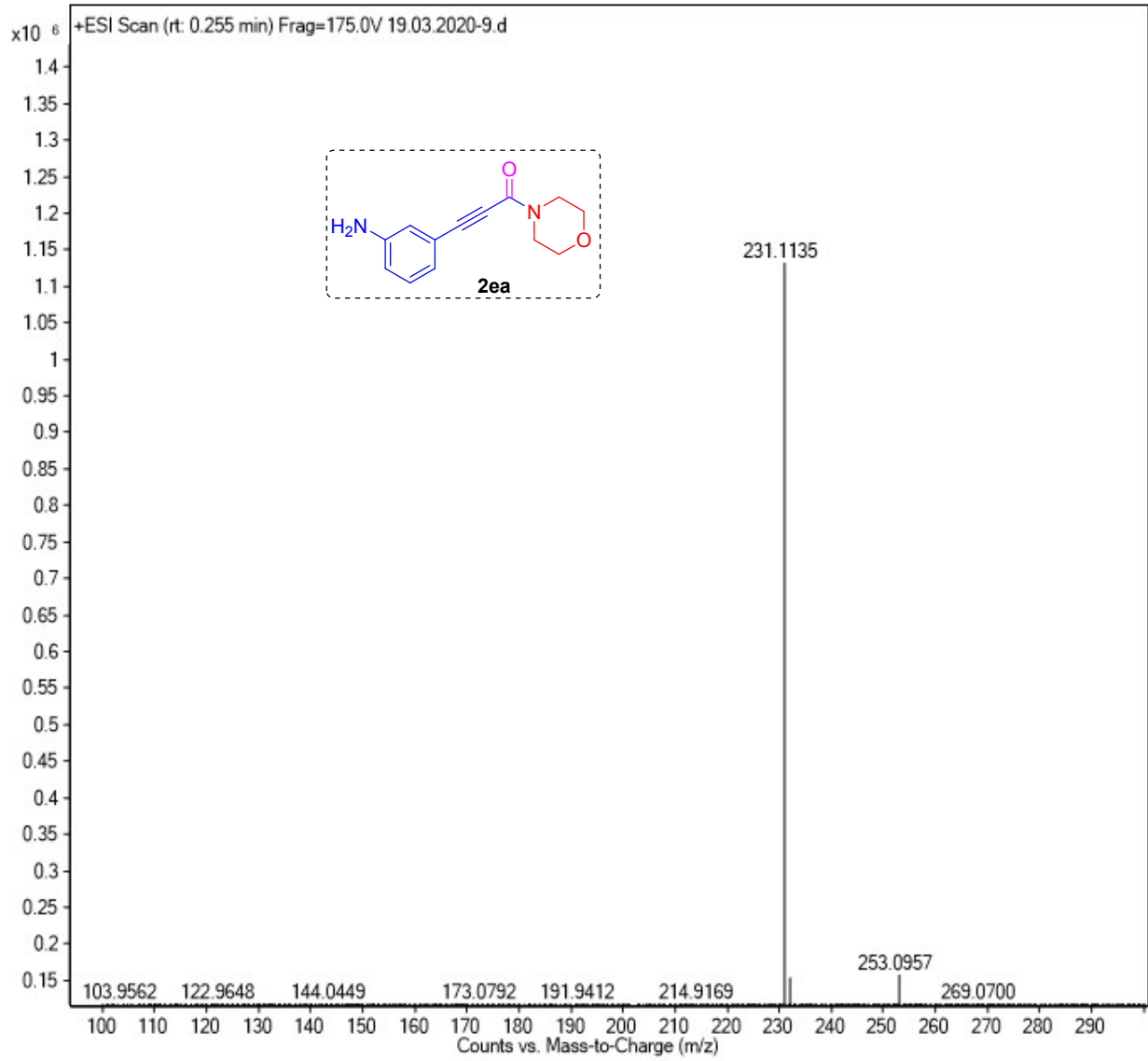
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 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 539  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 2298.8  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39888055 W  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.29870972 W  
 PL13W 0.28500207 W  
 SFO2 300.1312005 MHz  
 SI 32.768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ea



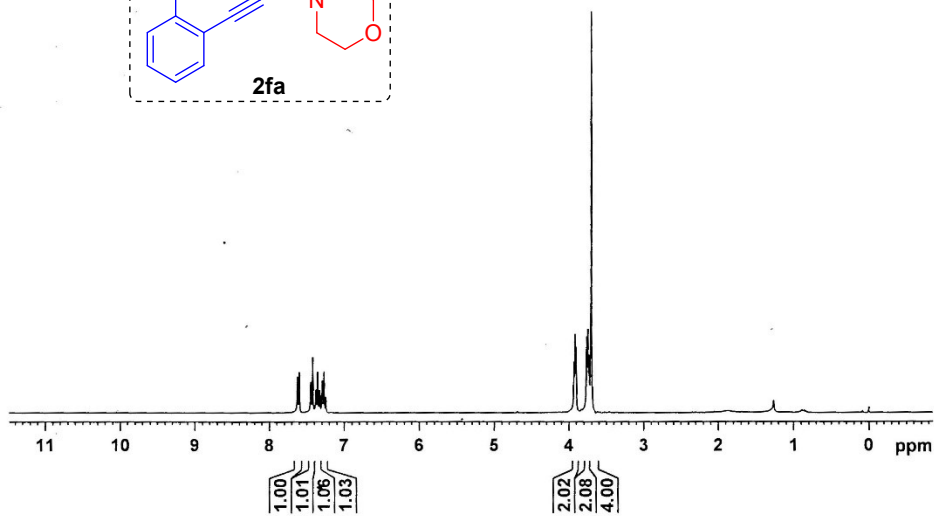
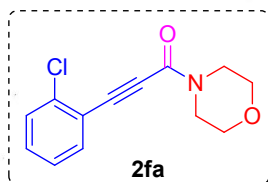


HRMS spectrum of compound 2ea

7.624  
7.619  
7.598  
7.594  
7.443  
7.418  
7.378  
7.374  
7.354  
7.349  
7.328  
7.322  
7.293  
7.290  
7.268  
7.243  
3.930  
3.915  
3.898  
3.762  
3.745  
3.730  
3.699



NAME RA-BR-3-269A  
EXPNO 2  
PROCNO 1  
Date\_ 20190902  
Time\_ 15.13  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 114  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
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WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

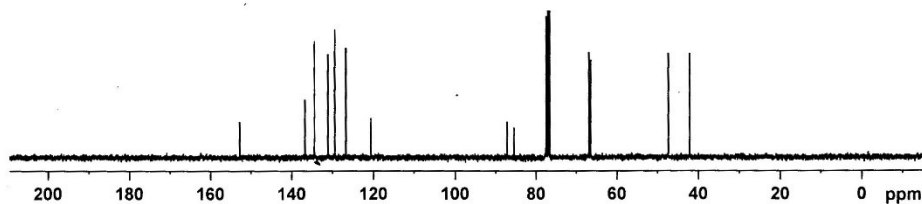
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76.61  
66.88  
66.43  
47.33  
42.09



NAME RA-BR-3-269A  
EXPNO 1  
PROCNO 1  
Date\_ 20190902  
Time\_ 15.04  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 148  
DS 4  
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FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 3649.1  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.23870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



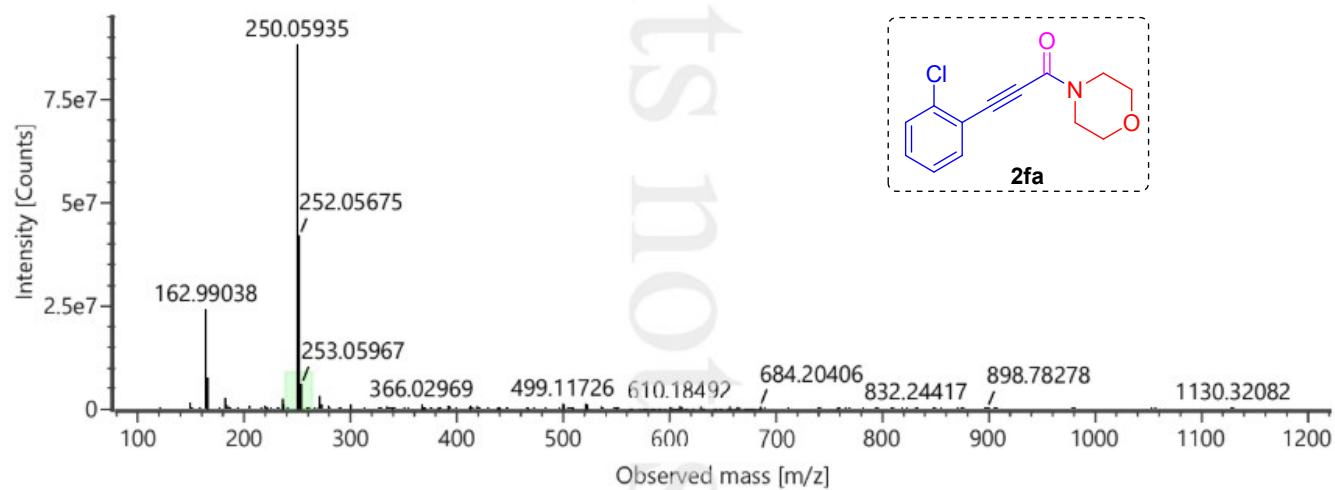
$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2fa

Component name: C<sub>13</sub>H<sub>12</sub>ClNO<sub>2</sub>

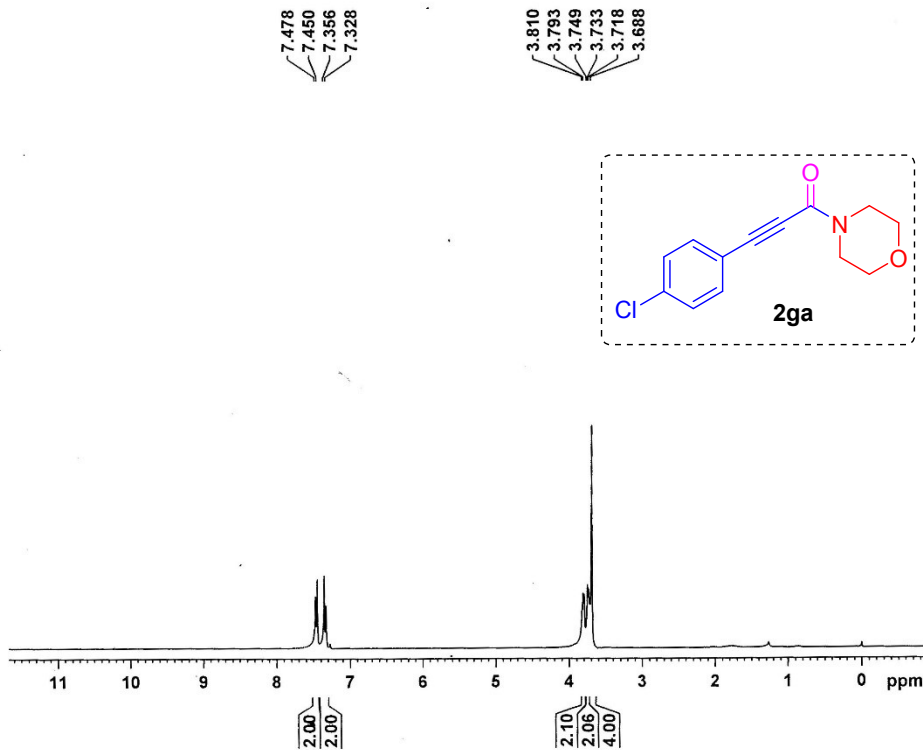
Item name: MSR\_376\_250

Item description:

Channel name: Low energy : Time 0.3157 +/- 0.0647 minutes

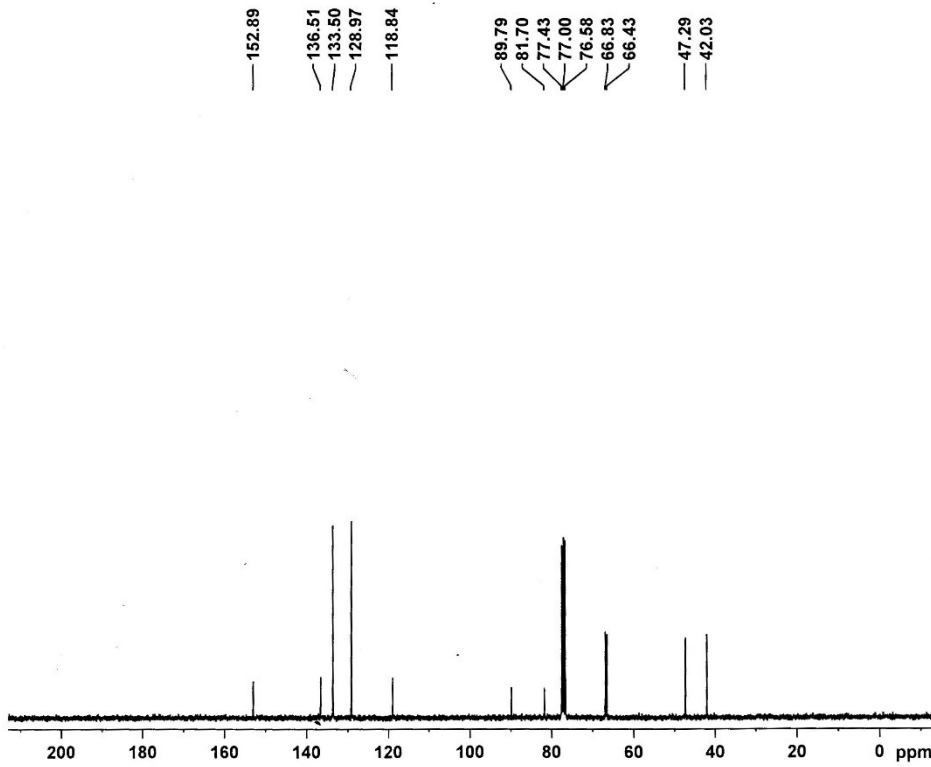


HRMS Spectrum of Compound 2fa



NAME RA-BR-3-261A  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20190830  
 Time\_ 18.36  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 128  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300025 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

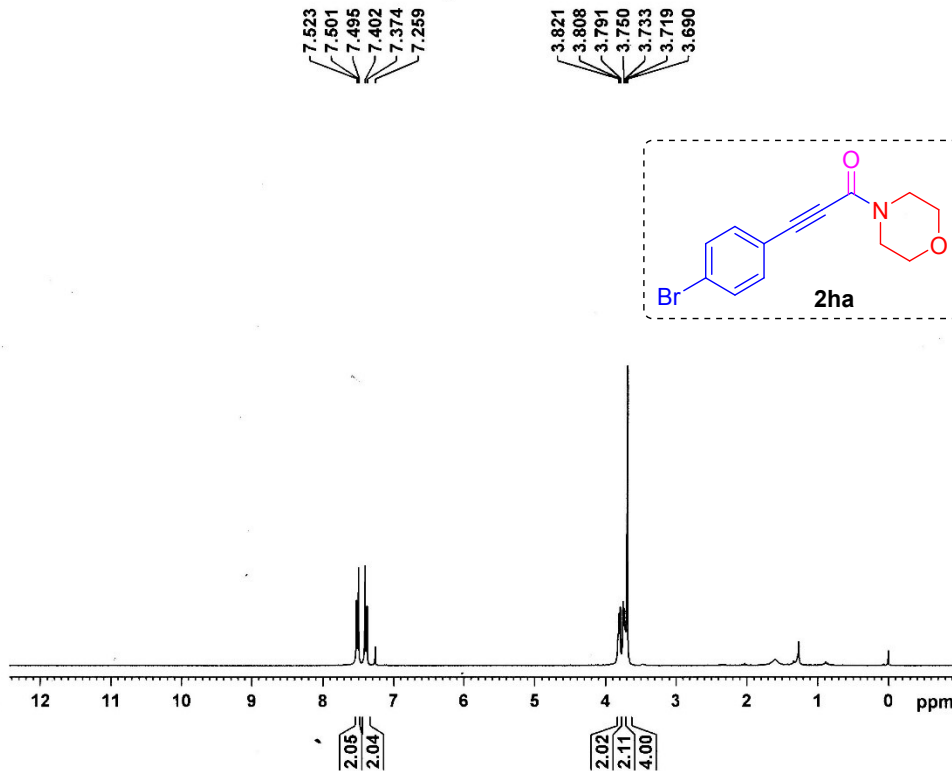


NAME RA-BR-3-261A  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20190830  
 Time\_ 18.07  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 466  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 2580.3  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

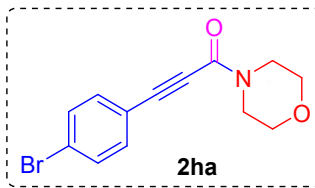
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39858055 W  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.29870972 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

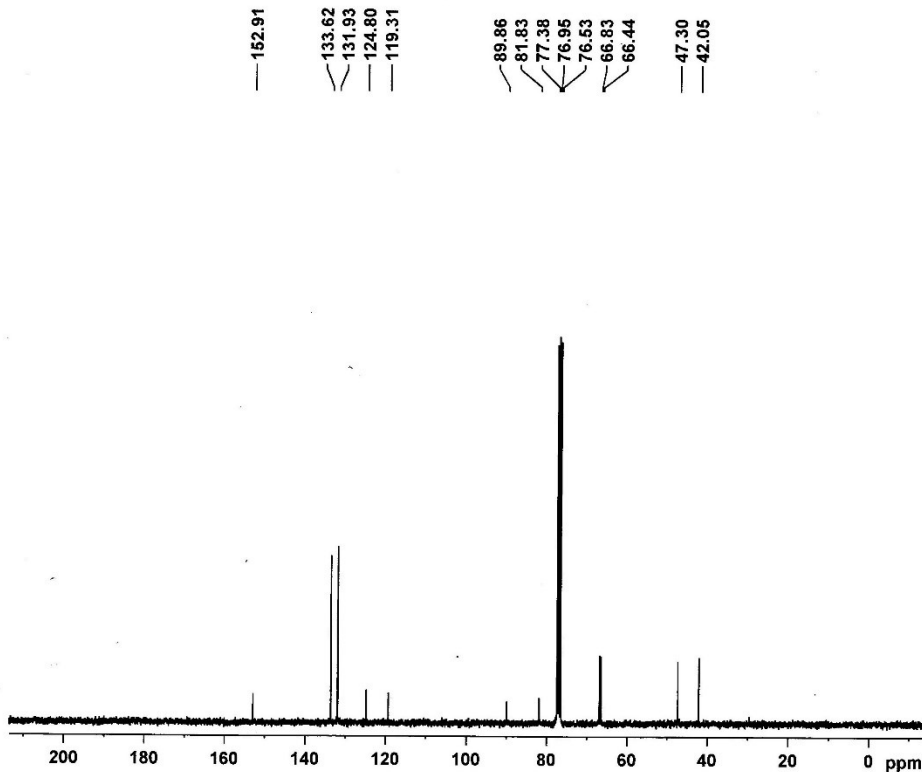
<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ga



NAME RA-BR-3-151  
EXPNO 13  
PROCNO 1  
Date\_ 20190502  
Time 23.33  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 256  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
TDO 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28158662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300067 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



NAME RA-BR-3-151  
EXPNO 12  
PROCNO 1  
Date\_ 20190502  
Time 22.34  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 6502  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28158662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

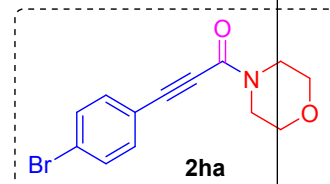
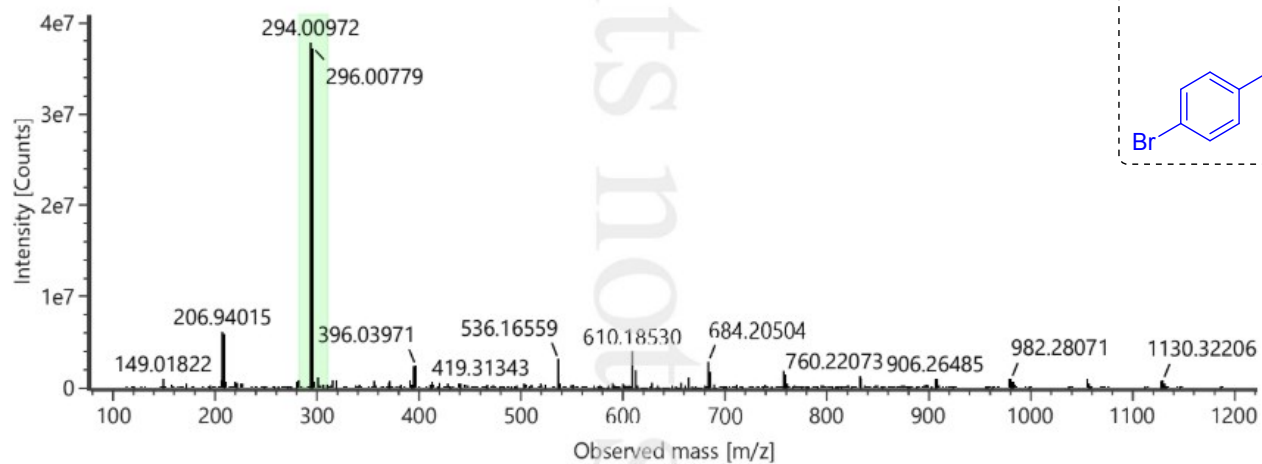
$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2ha

Component name: C<sub>13</sub>H<sub>12</sub>BrNO<sub>2</sub>

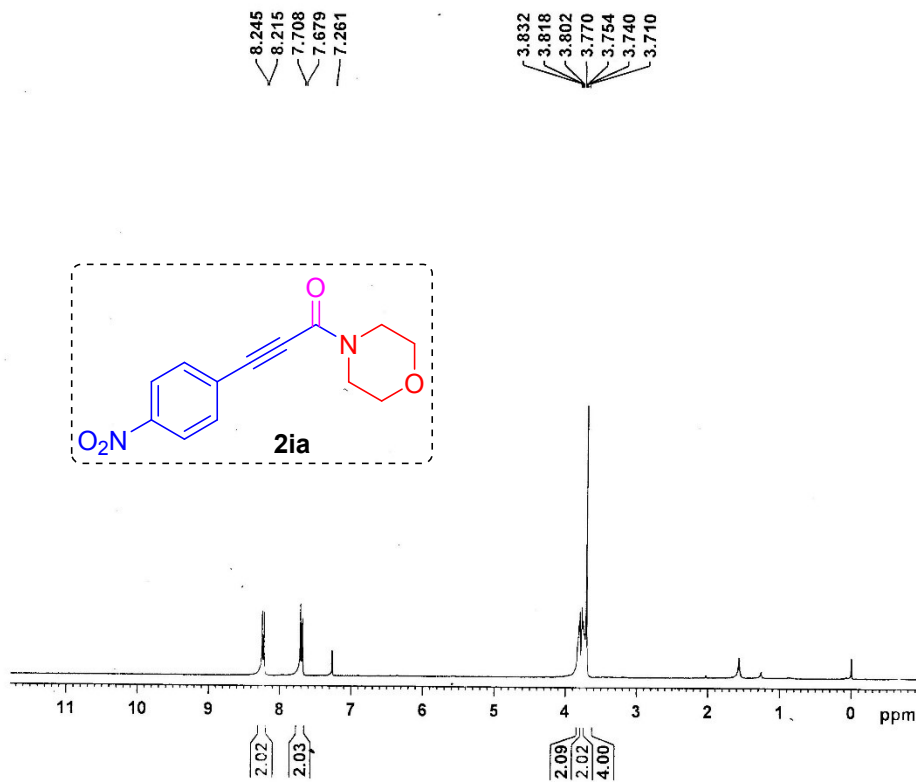
Item name: MSR\_151\_294

Item description:

Channel name: Low energy : Time 0.3218 +/- 0.0600 minutes

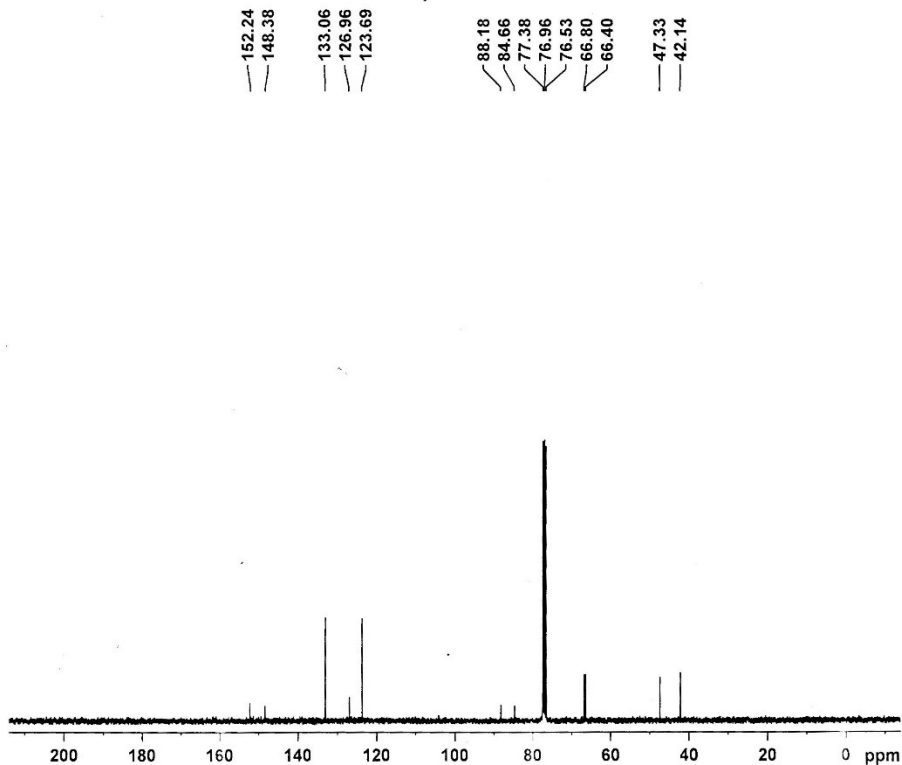


HRMS Spectrum of Compound 2ha



NAME RA-BR-3-302B  
 EXPNO 7  
 PROCNO 1  
 Date\_ 20191015  
 Time 14.09  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 322.5  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300060 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME RA-BR-3-302B  
 EXPNO 6  
 PROCNO 1  
 Date\_ 20191015  
 Time 14.00  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 587  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 4597.6  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39858055 W  
 SFO1 75.4752953 MHz

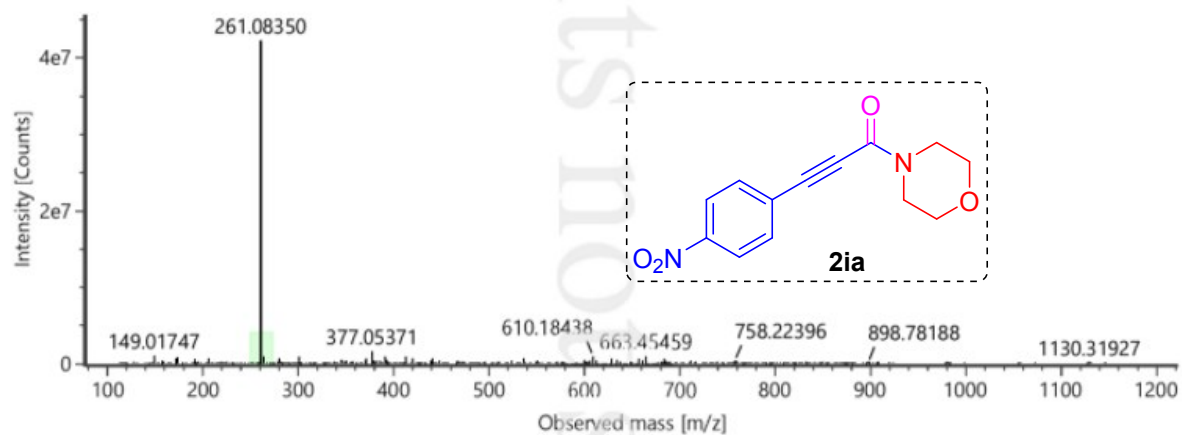
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.29870972 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound **2ia**

Component name: C13H12N2O4

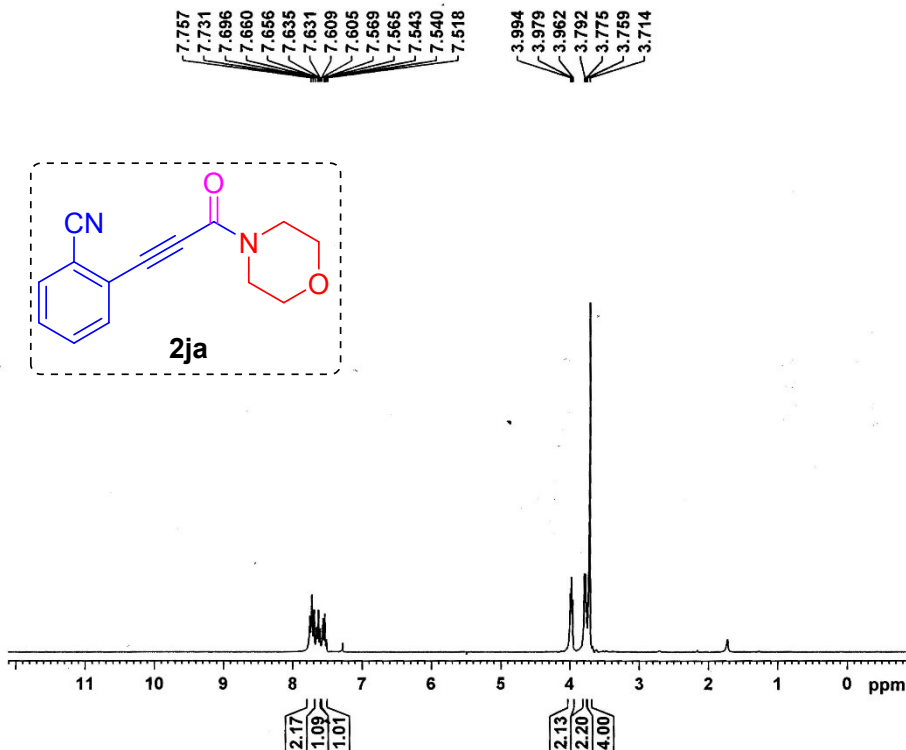
Item name: MSR\_302\_B\_260  
Item description:

Channel name: Low energy : Time 0.3237 +/- 0.0633 minutes



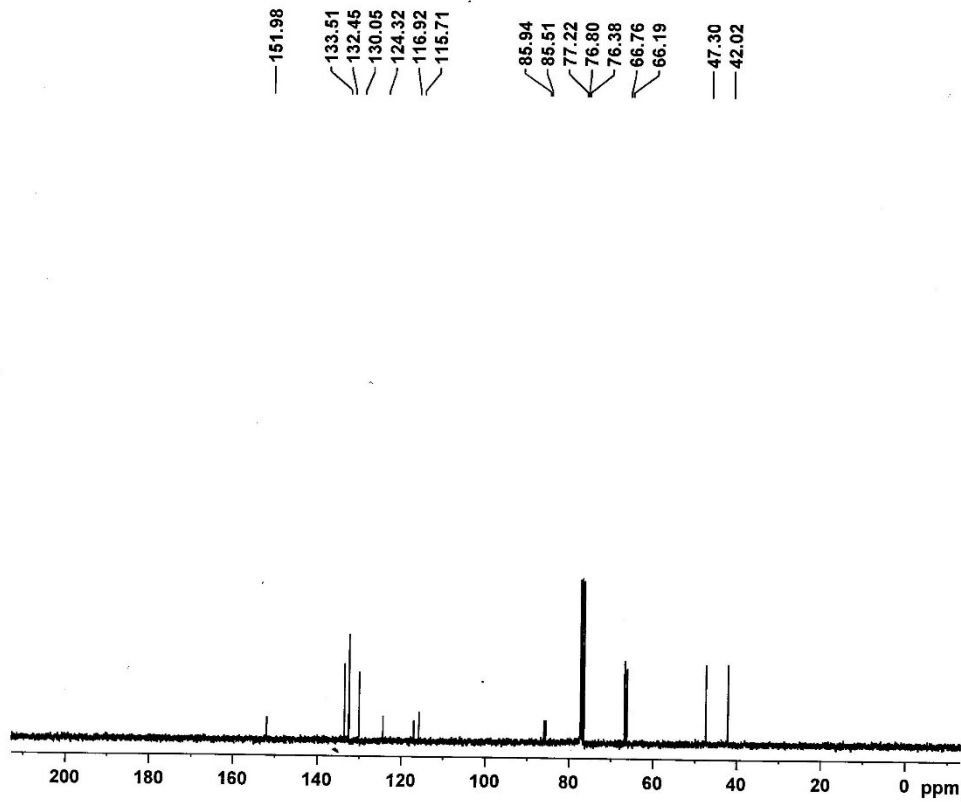
HRMS spectrum of compound 2ia





NAME RA-BR-3-374  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20200324  
 Time 17.32  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 228.1  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 -1.00 dB  
 PL1W 13.2815662 W  
 SFO1 300.1316534 MHz  
 SI 32768  
 SF 300.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME RA-BR-3-374  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20200324  
 Time 17.40  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 302  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 5160.6  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.75 usec  
 PL1 -1.00 dB  
 PL1W 39.52846909 W  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.46 dB  
 PL13 16.00 dB  
 PL2W 13.2815662 W  
 PL12W 0.37778899 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677643 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

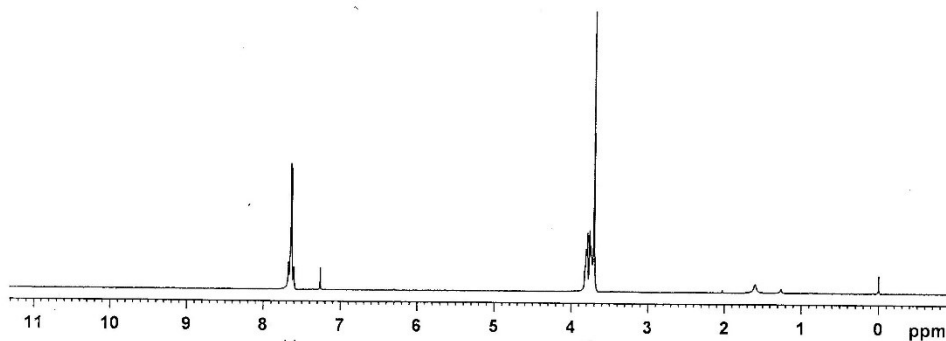
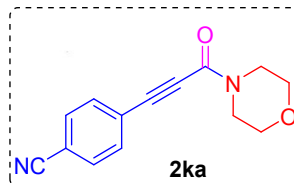
$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2ja

7.676  
7.648  
7.633  
7.605  
7.264

3.817  
3.805  
3.789  
3.769  
3.743  
3.729  
3.702



NAME RA-BR-3-300B  
EXPNO 2  
PROCNO 1  
Date\_ 20191012  
Time 20.48  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 256  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1

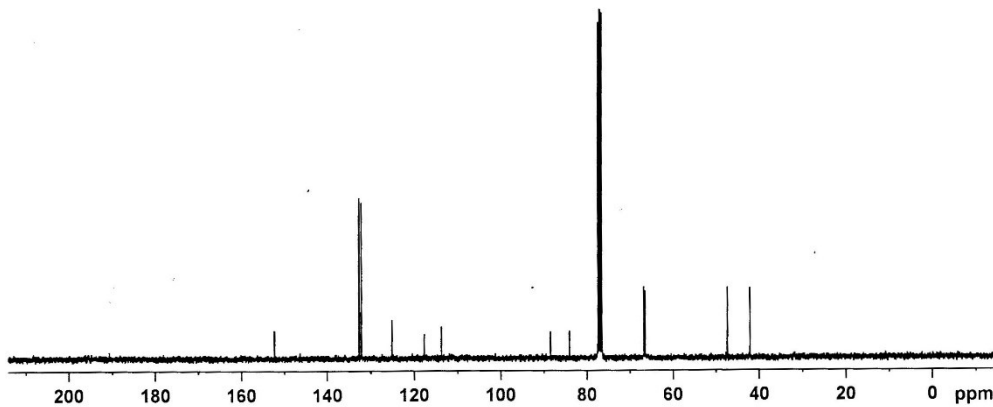


=====  
CHANNEL f1  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300054 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

152.33  
132.70  
132.16  
125.13  
117.73  
113.72  
88.51  
84.11  
77.39  
76.97  
76.54  
66.79  
66.40  
47.31  
42.12

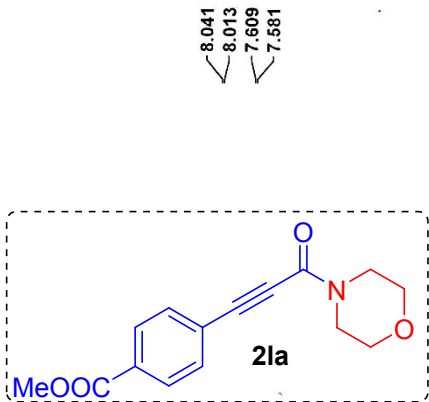


NAME RA-BR-3-300B  
EXPNO 1  
PROCNO 1  
Date\_ 20191012  
Time 20.29  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 729  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 4096  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

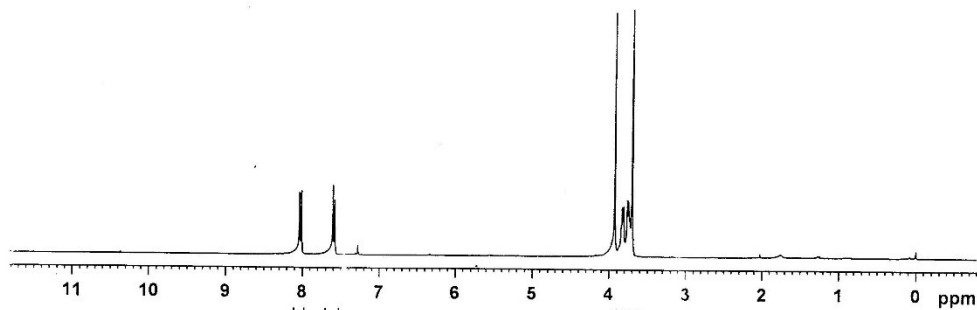


=====  
CHANNEL f1  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz  
=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

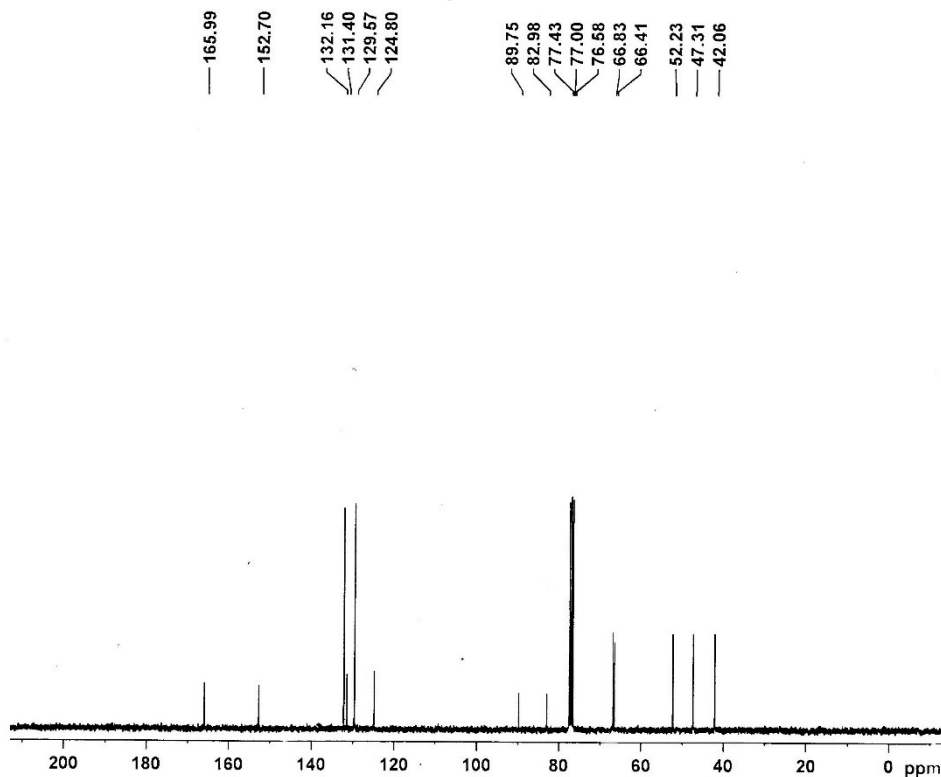
$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2ka



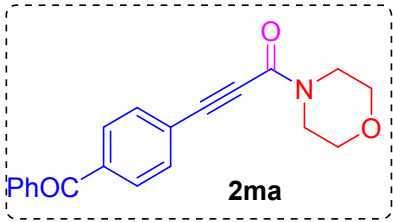
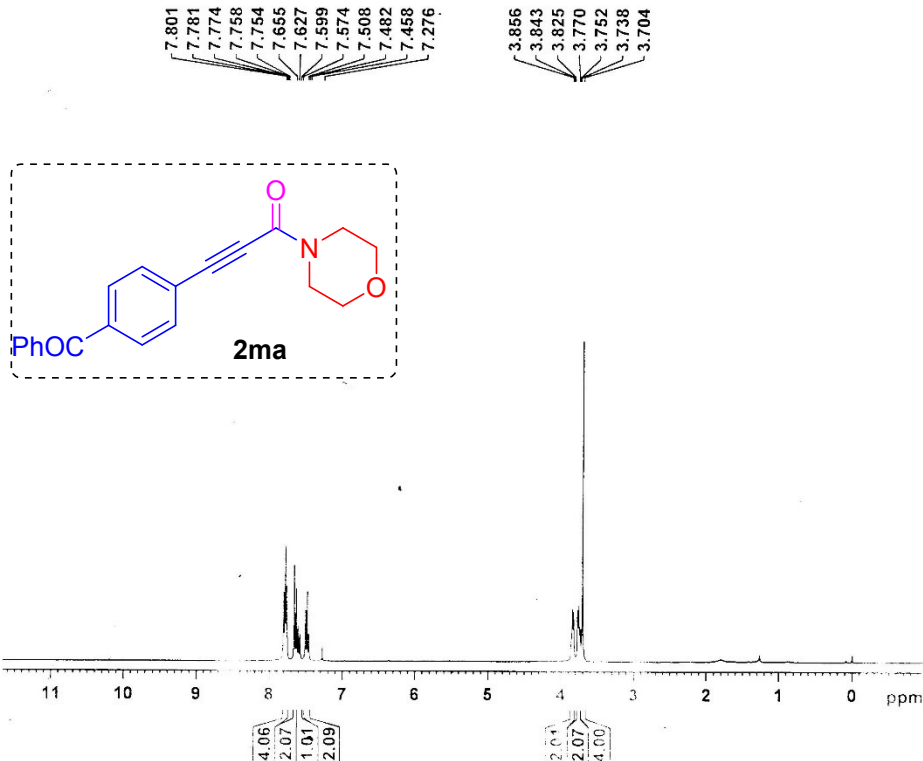
NAME RA-BR-303B  
EXPNO 7  
PROCNO 1  
Date\_ 20191015  
Time 14.56  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 128  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



NAME RA-BR-303B  
EXPNO 6  
PROCNO 1  
Date\_ 20191015  
Time 14.49  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 401  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 2580.3  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

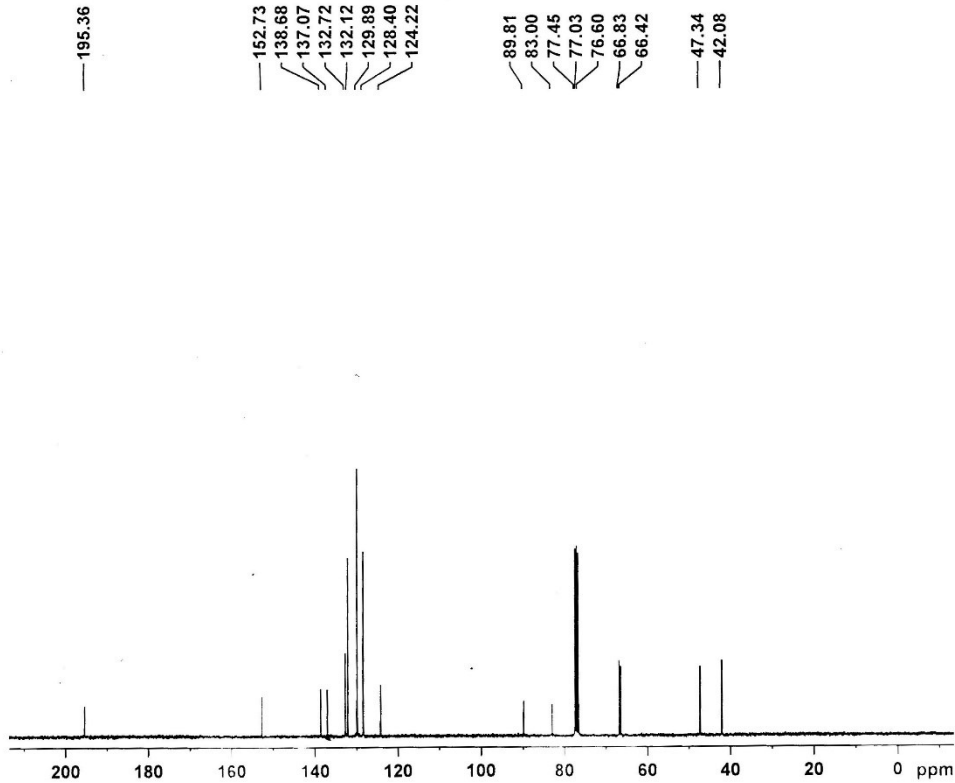


<sup>1</sup>H & <sup>13</sup>C spectra of compound 2la



NAME RA-BR-3-316  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20191106  
 Time 11.38  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 128  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.2815662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300020 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

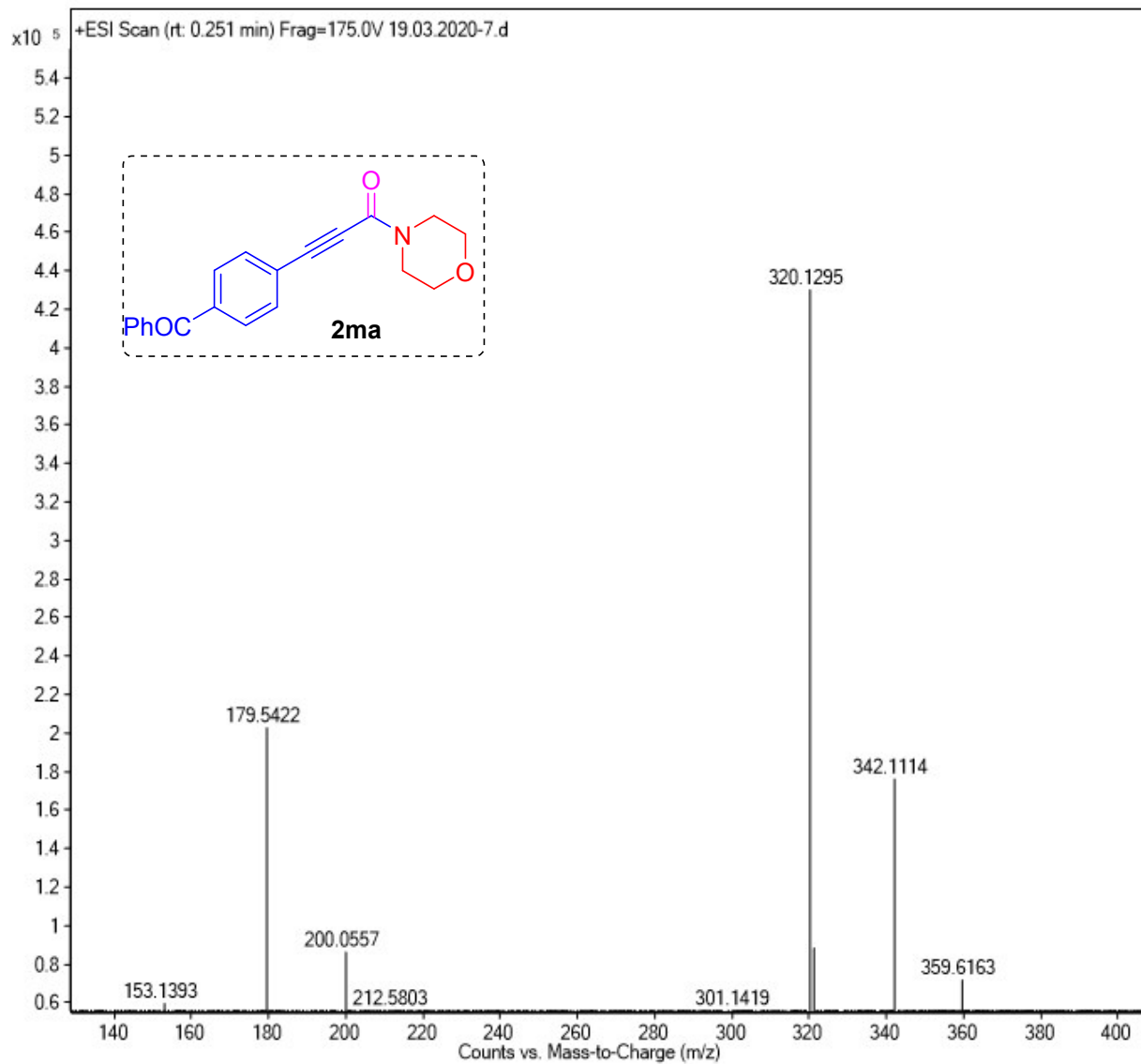


NAME RA-BR-3-316  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20191106  
 Time 11.36  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 700  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 4096  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39858055 W  
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.29870972 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ma

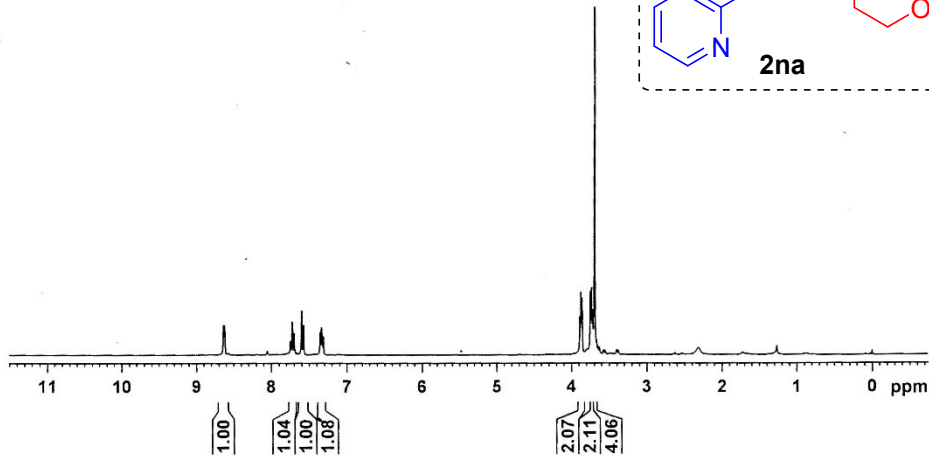
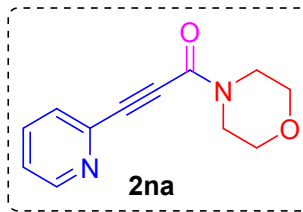


HRMS spectrum of compound 2ma

8.637  
8.623  
7.754  
7.749  
7.729  
7.723  
7.703  
7.697  
7.602  
7.576  
7.359  
7.355  
7.342  
7.339  
7.334  
7.330  
7.317  
7.314  
3.888  
3.874  
3.857  
3.751  
3.735  
3.719  
3.692



NAME RA-BR-3-260A  
EXPNO 2  
PROCNO 1  
Date\_ 20190830  
Time 19.06  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 71.8  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.2815662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1299820 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

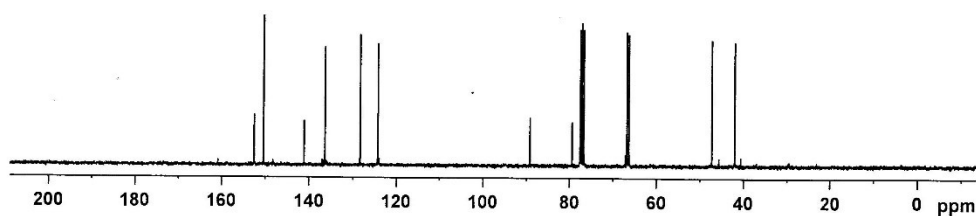
152.43  
150.27  
141.07  
136.29  
128.30  
124.27  
89.17  
79.43  
77.54  
77.12  
76.69  
66.82  
66.32  
47.30  
42.01



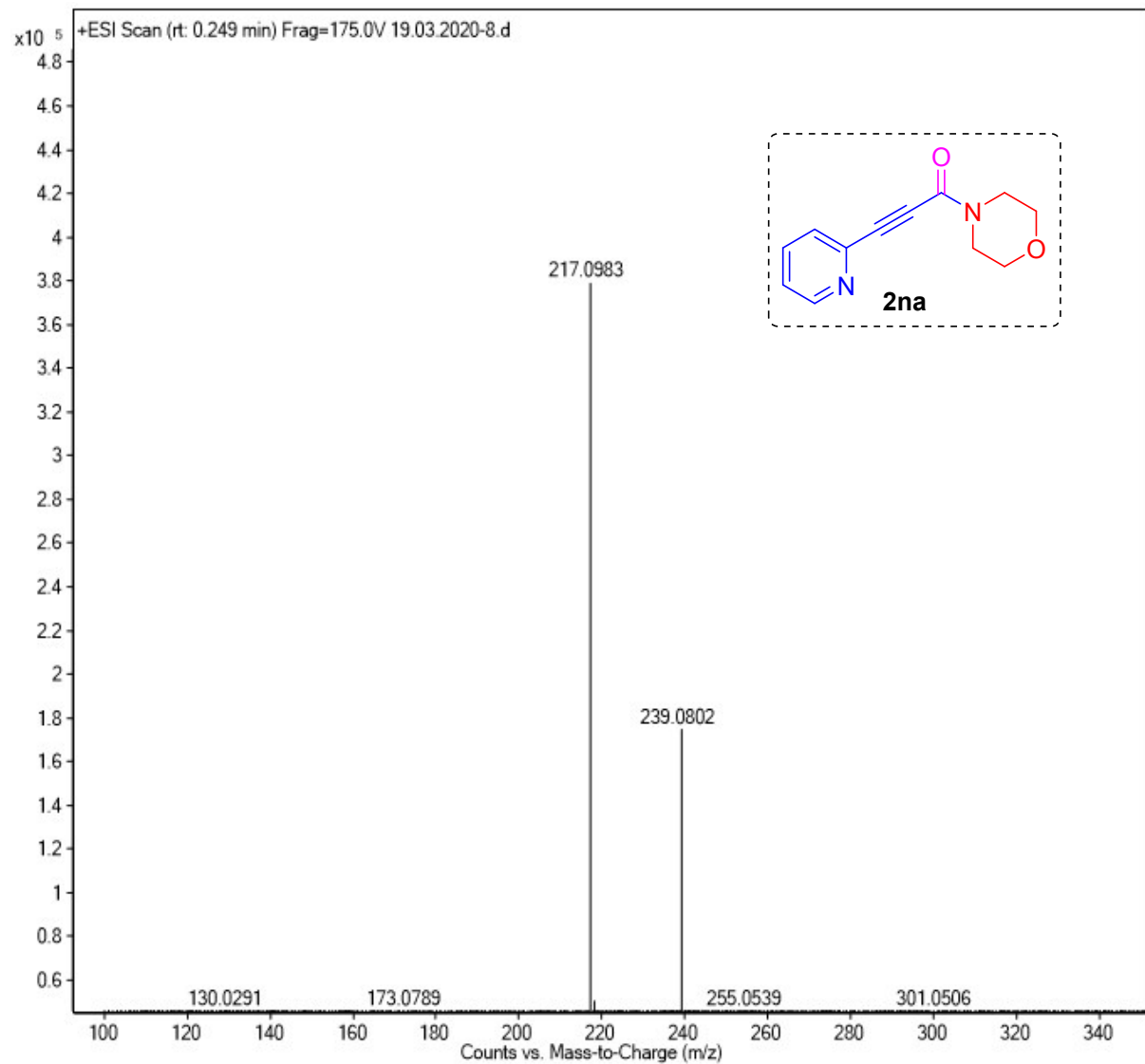
NAME RA-BR-3-260A  
EXPNO 1  
PROCNO 1  
Date\_ 20190830  
Time 19.03  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 260  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5792.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



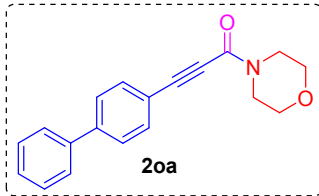
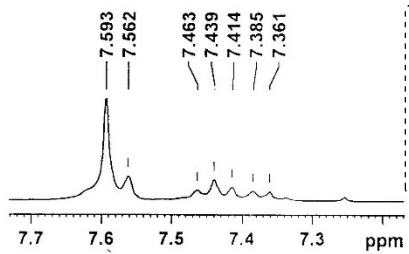
$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2na



HRMS spectrum of compound 2na

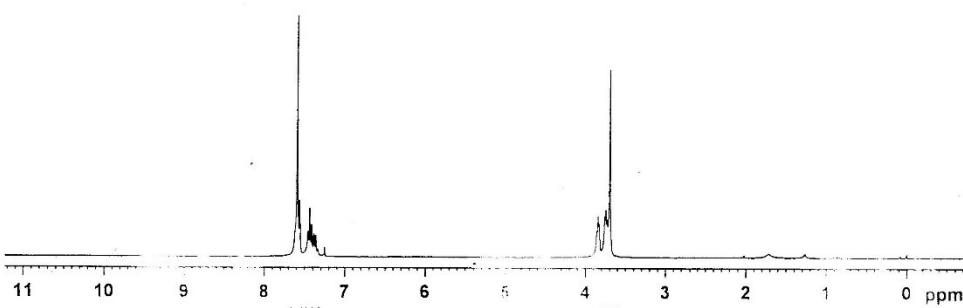
7.593  
7.562  
7.463  
7.439  
7.414  
7.385  
7.361

3.858  
3.845  
3.830  
3.758  
3.743  
3.728  
3.695



NAME RA-BR-3-319B  
EXPNO 3  
PROCNO 1  
Date 20191107  
Time 7.09  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 128  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300088 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



153.22  
143.03  
139.88  
132.80  
128.91  
128.04  
127.18  
127.05  
119.11

91.09  
81.49  
77.44  
77.02  
76.59  
66.89  
66.48

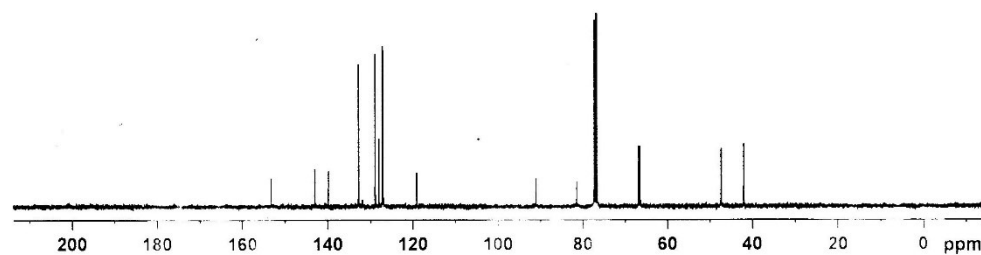
47.35  
42.04



NAME RA-BR-3-319B  
EXPNO 2  
PROCNO 1  
Date 20191107  
Time 7.04  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 432  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 3649.1  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

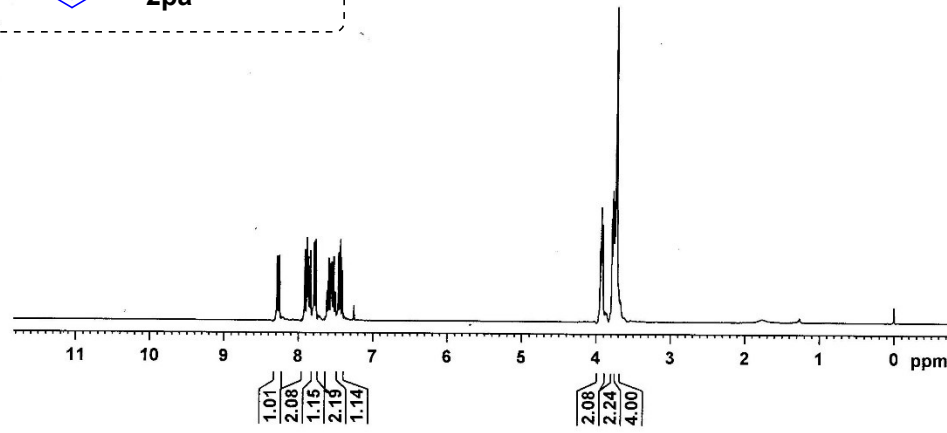
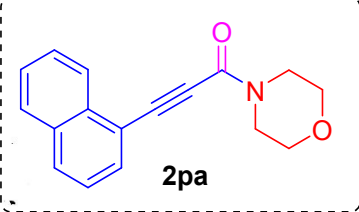
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 20a



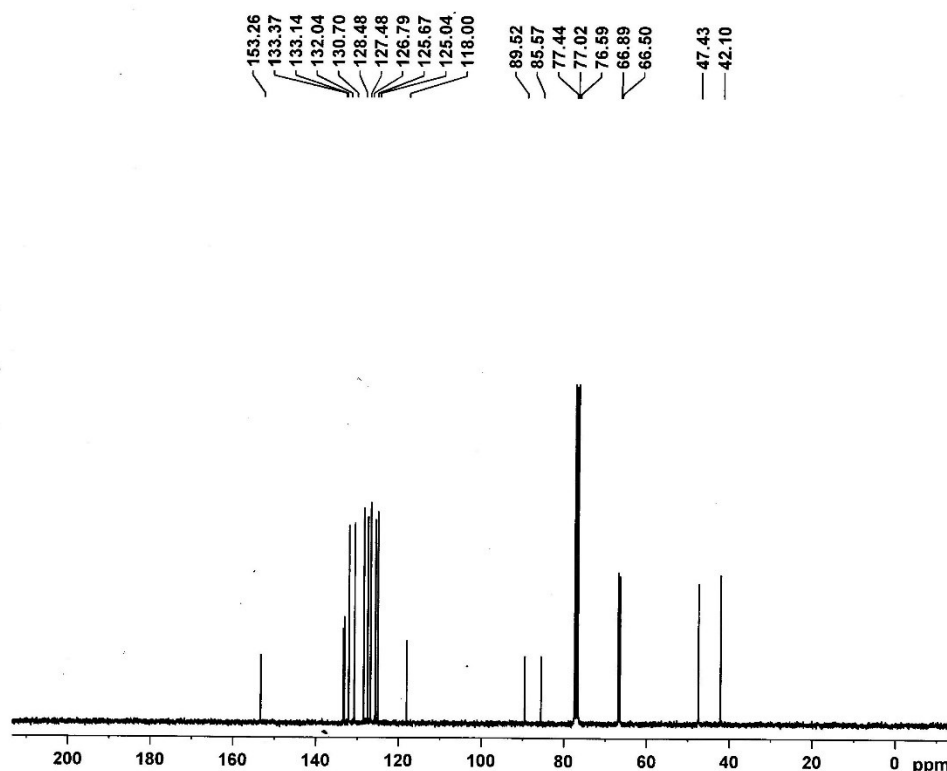
8.284  
8.257  
7.913  
7.885  
7.867  
7.841  
7.809  
7.790  
7.766  
7.619  
7.616  
7.596  
7.593  
7.570  
7.565  
7.555  
7.551  
7.528  
7.505  
7.461  
7.435  
7.409  
7.254  
3.942  
3.927  
3.910  
3.786  
3.769  
3.754  
3.728



NAME RA-BR-3-163  
EXPNO 3  
PROCNO 1  
Date\_ 20190515  
Time 12.59  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 114  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300085 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

153.26  
133.37  
133.14  
132.04  
130.70  
128.48  
127.48  
126.79  
125.67  
125.04  
118.00  
89.52  
85.57  
77.44  
77.02  
76.59  
66.89  
66.50  
47.43  
42.10



NAME RA-BR-3-163  
EXPNO 2  
PROCNO 1  
Date\_ 20190515  
Time 12.45  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 7298.2  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

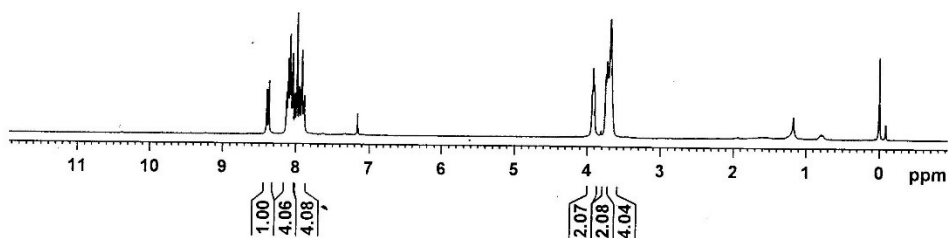
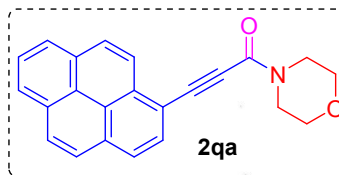
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL12W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2pa

8.391  
8.361  
8.123  
8.101  
8.076  
8.064  
8.043  
8.038  
8.010  
7.979  
7.951  
7.942  
7.915  
7.912  
7.890  
7.881  
7.155  
3.932  
3.918  
3.902  
3.750  
3.734  
3.718  
3.688  
3.678



NAME RA-BR-3-296B  
EXPNO 4  
PROCNO 1  
Date\_ 20190928  
Time 18.28  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 181  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

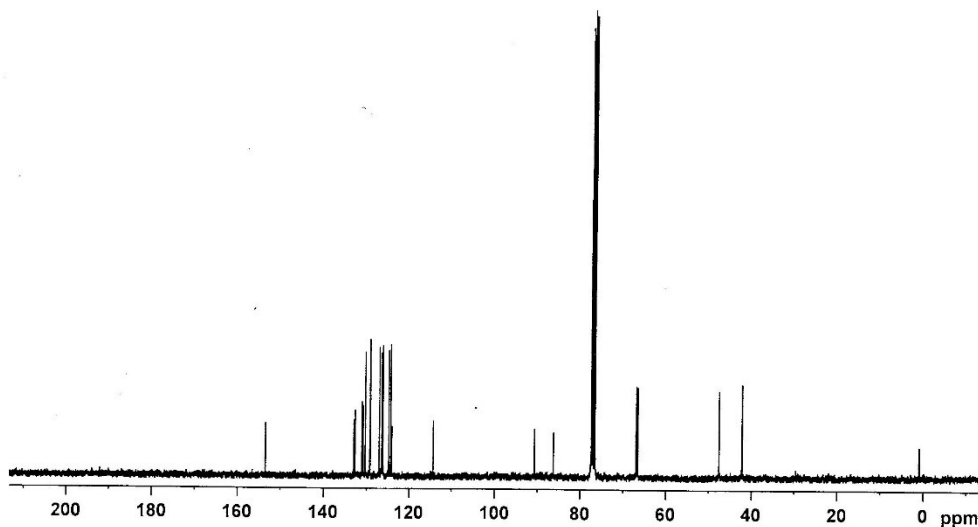


===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300382 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

153.47  
132.96  
132.61  
131.10  
130.86  
130.26  
129.20  
129.16  
127.02  
126.45  
126.20  
126.14  
124.81  
124.36  
124.30  
124.03  
114.29  
90.70  
86.27  
77.41  
76.99  
76.56  
66.97  
66.56  
47.52  
42.17



NAME RA-BR-3-296B  
EXPNO 3  
PROCNO 1  
Date\_ 20190928  
Time 17.35  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 2298.8  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

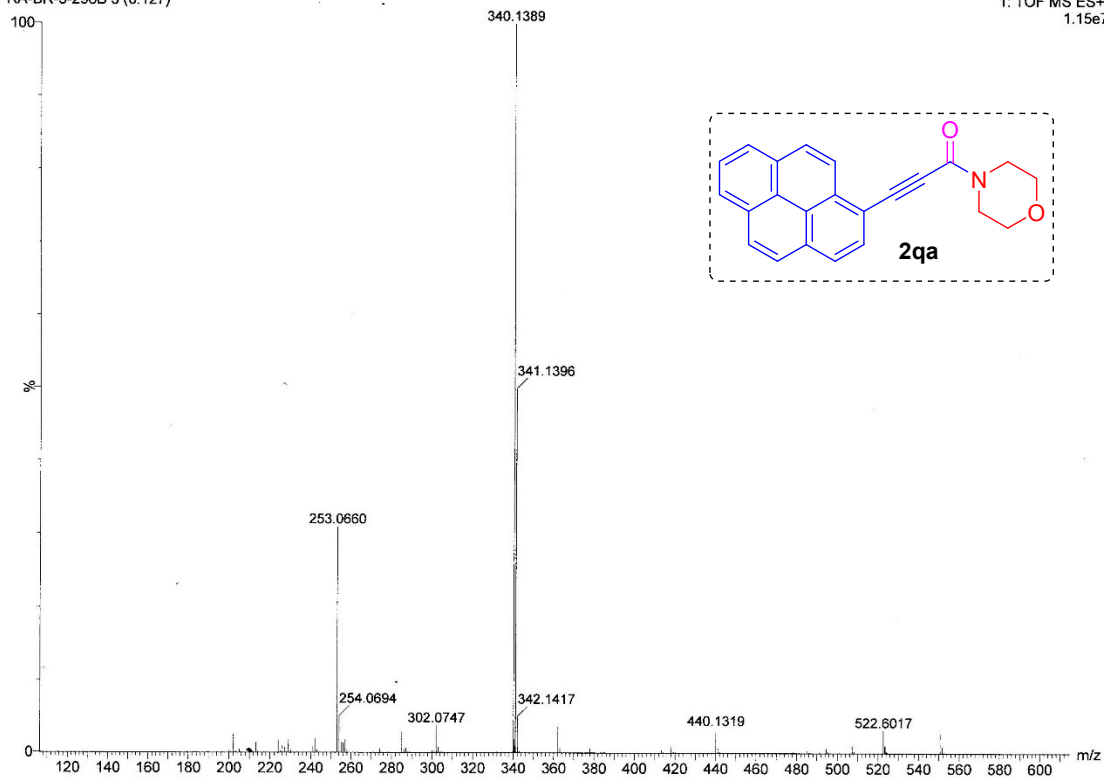


===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz  
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.28500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2qa

DRRA  
RA-BR-3-296B 3 (0.127)

1: TOF MS ES+  
1.15e7



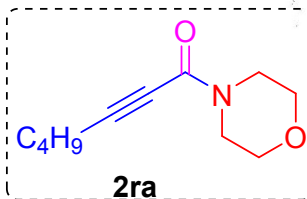
HRMS spectrum of compound 2qa

7.281

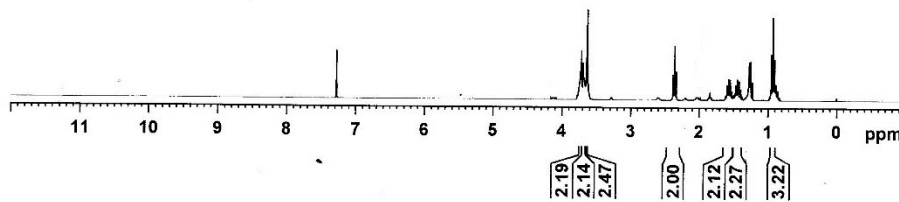
3.746  
3.732  
3.720  
3.698  
3.684  
3.676  
3.636  
2.382  
2.369  
2.335  
1.573  
1.549  
1.446  
1.420  
1.274  
1.263  
1.250  
1.227  
0.951  
0.927



NAME RA-BR-3-33  
EXPNO 8  
PROCNO 1  
Date\_ 20181218  
Time 19.26  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 71.8  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300002 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



153.31

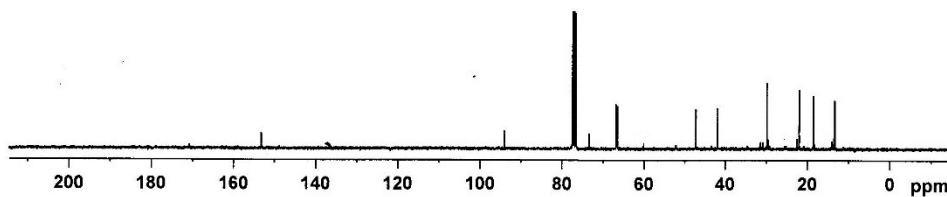
94.00  
77.41  
76.98  
76.56  
73.37  
66.81  
66.42  
47.18  
41.84  
29.80  
21.92  
18.53  
13.31



NAME RA-BR-3-33  
EXPNO 7  
PROCNO 1  
Date\_ 20181218  
Time 19.22  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 476  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 9195.2  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waitz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



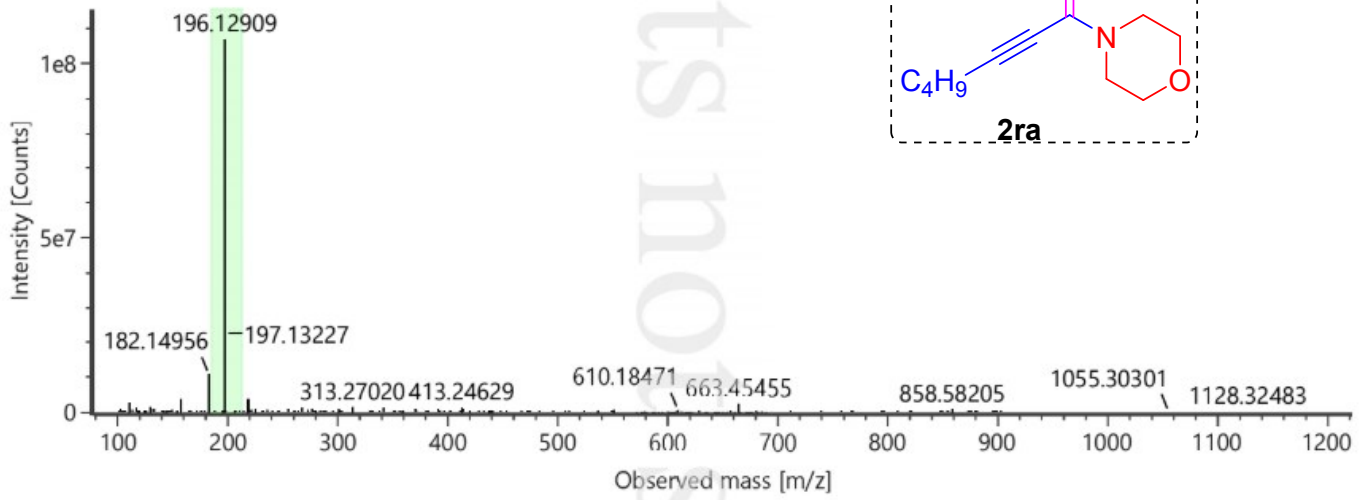
<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ra

Component name: C<sub>11</sub>H<sub>17</sub>NO<sub>2</sub>

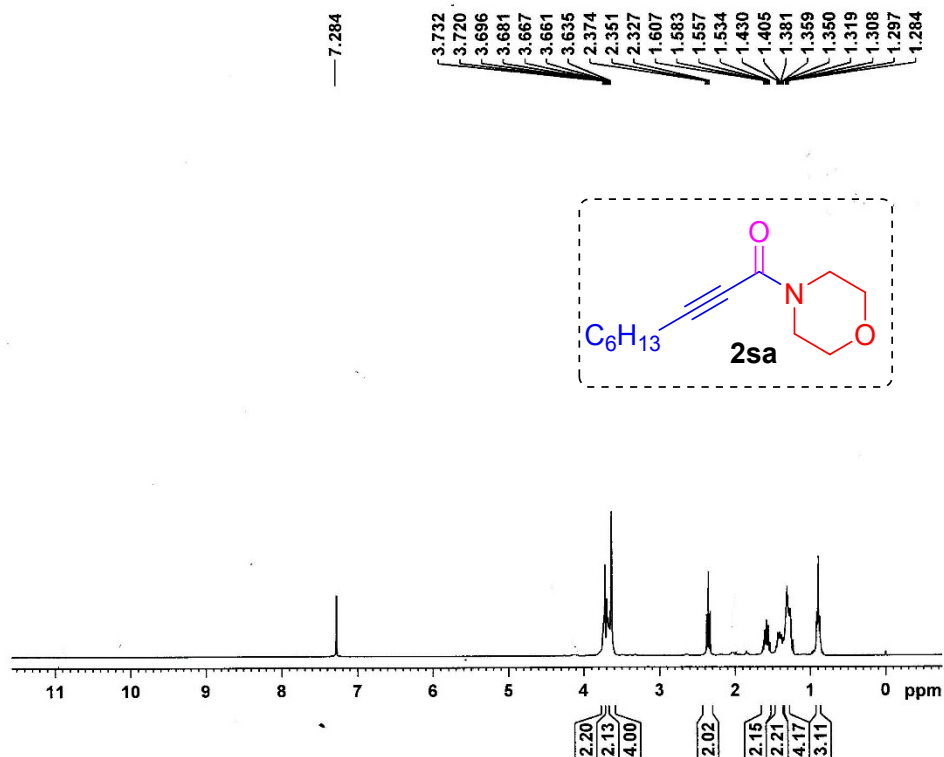
Item name: MSR\_33\_196

Item description:

Channel name: Low energy : Time 0.3279 +/- 0.1852 minutes

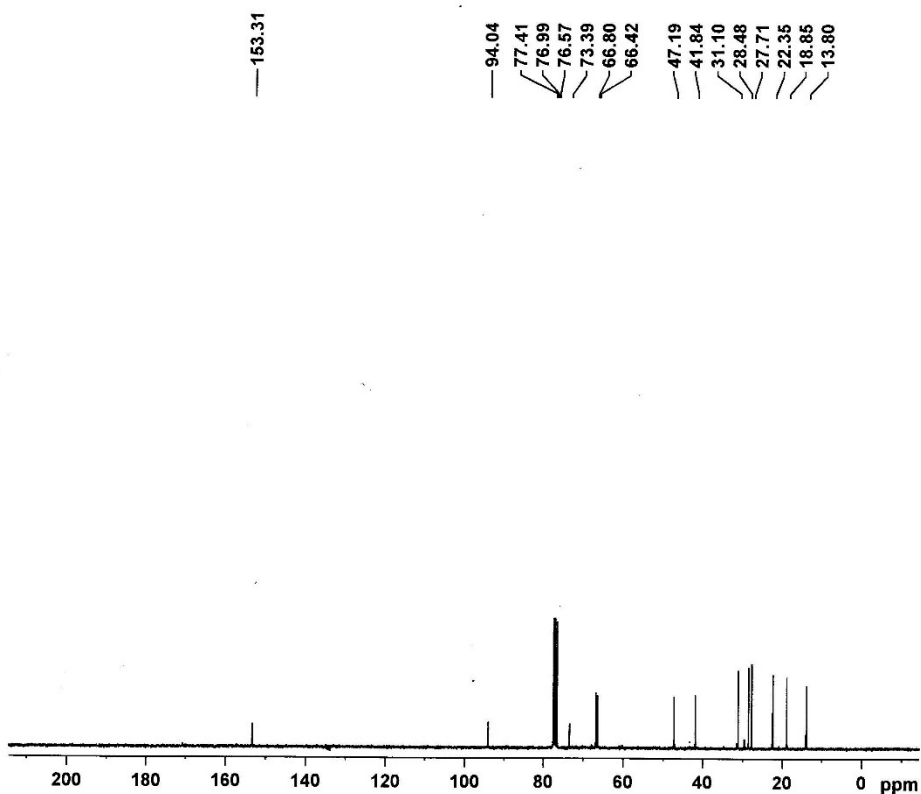


HRMS Spectrum of Compound 2ra



NAME RA-BR-3-37  
EXPNO 2  
PROCNO 1  
Date\_ 20181220  
Time\_ 15.16  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 64  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1299993 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



NAME RA-BR-3-37  
EXPNO 1  
PROCNO 1  
Date\_ 20181220  
Time\_ 15.13  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 511  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 4096  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

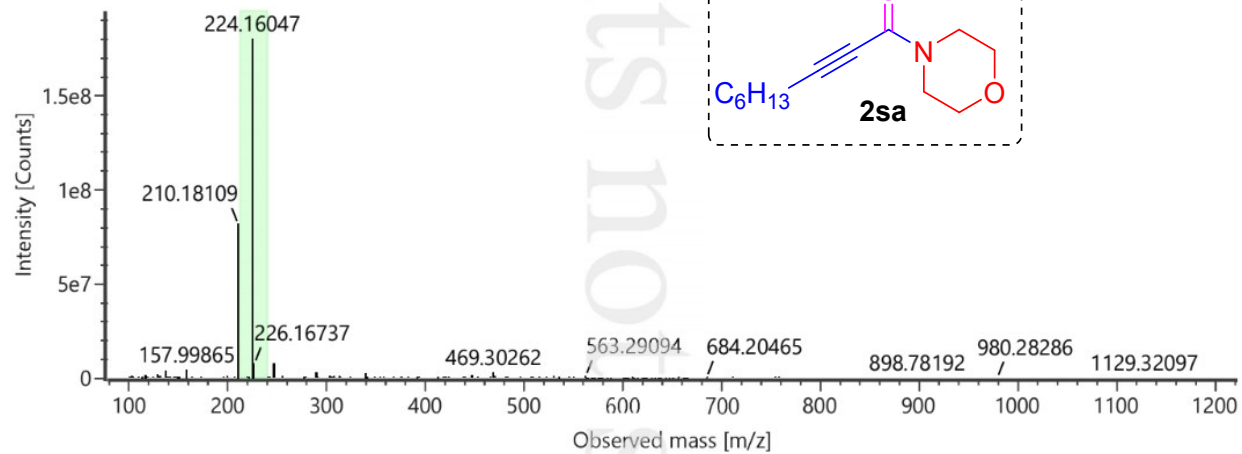
$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2sa

Component name: **C13H21NO2**

Item name: MSR\_37\_224

Item description:

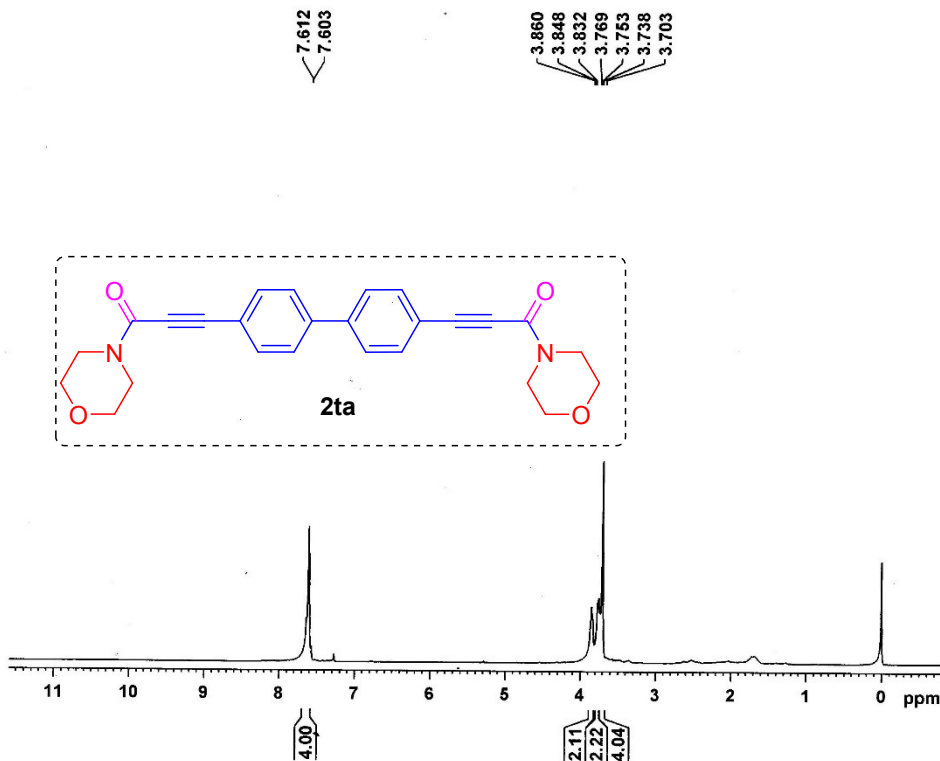
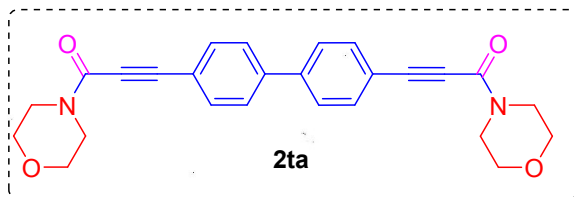
Channel name: Low energy : Time 0.3370 +/- 0.1825 minutes



**HRMS Spectrum of Compound 2sa**



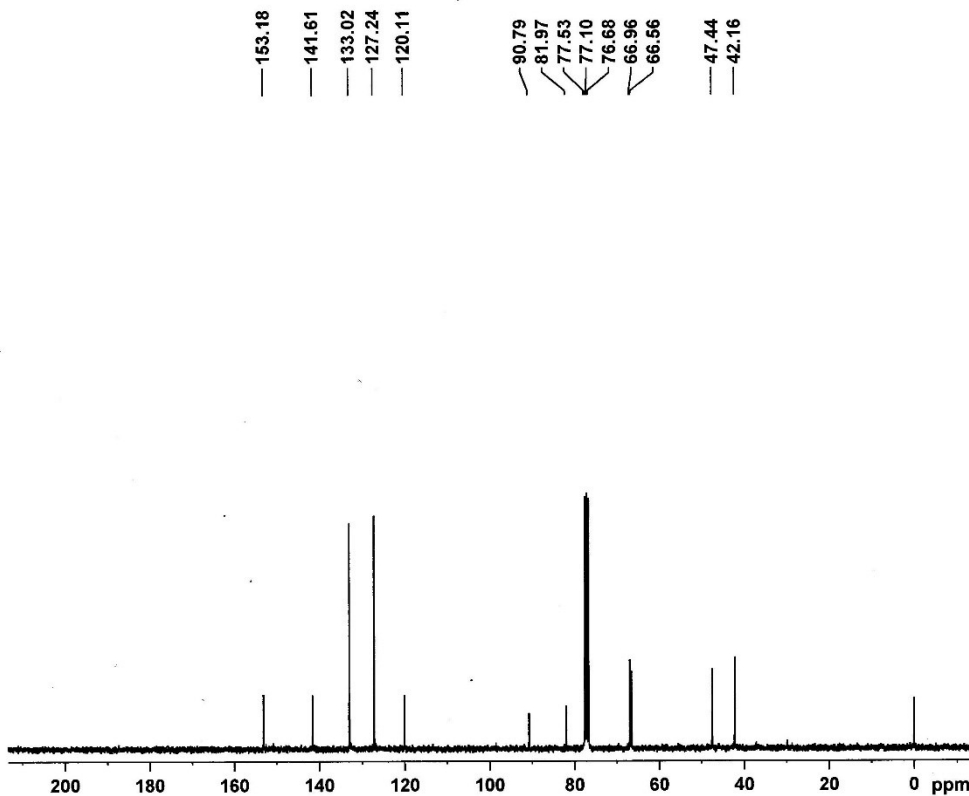
NAME RA-BR-3-53  
EXPNO 2  
PROCNO 1  
Date\_ 20190319  
Time\_ 21.55  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 128  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300020 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



NAME RA-BR-3-53  
EXPNO 1  
PROCNO 1  
Date\_ 20190319  
Time\_ 21.51  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1069  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 9195.2  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

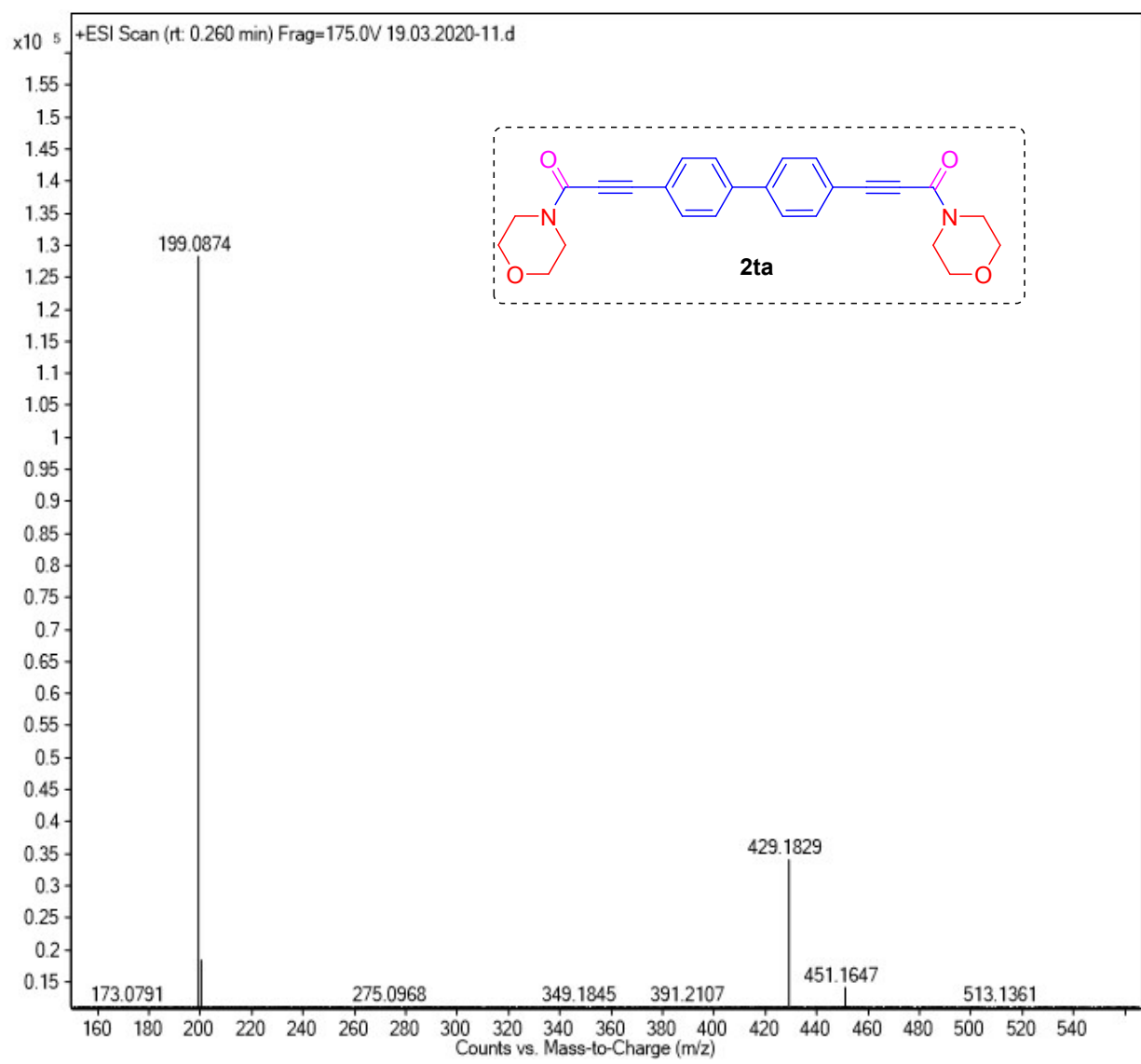


===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

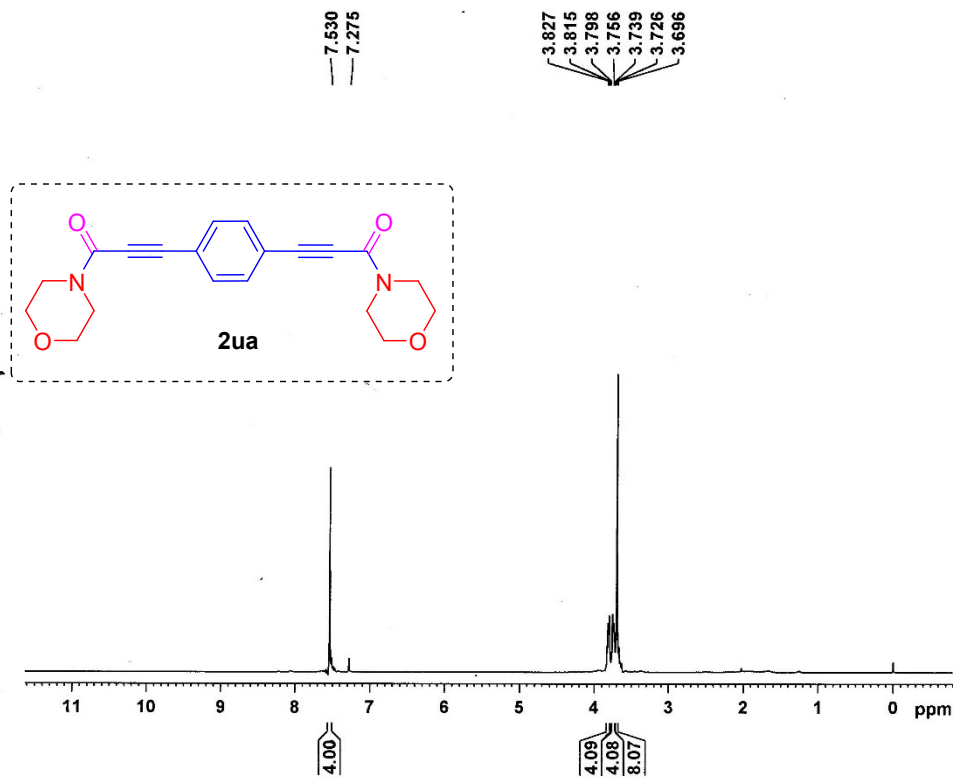
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 18.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.28500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4877412 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ta



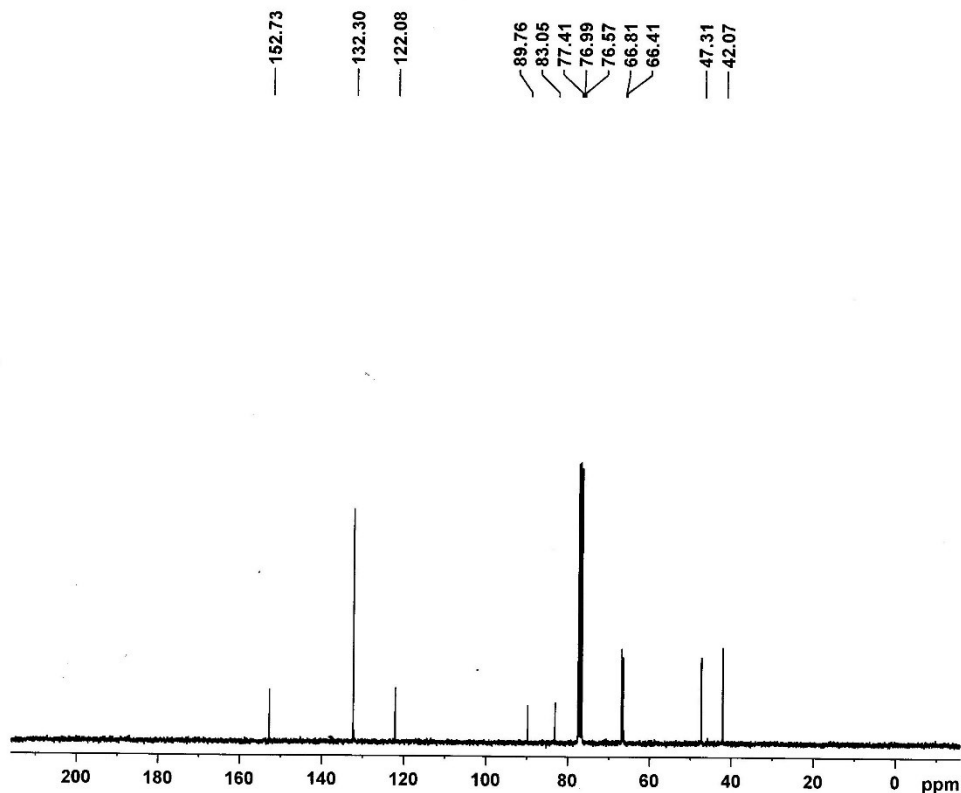


HRMS spectrum of compound 2ua



NAME RA-BR-3-164  
 EXPNO 3  
 PROCNO 1  
 Date\_ 20190515  
 Time 11.40  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 161.3  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300019 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

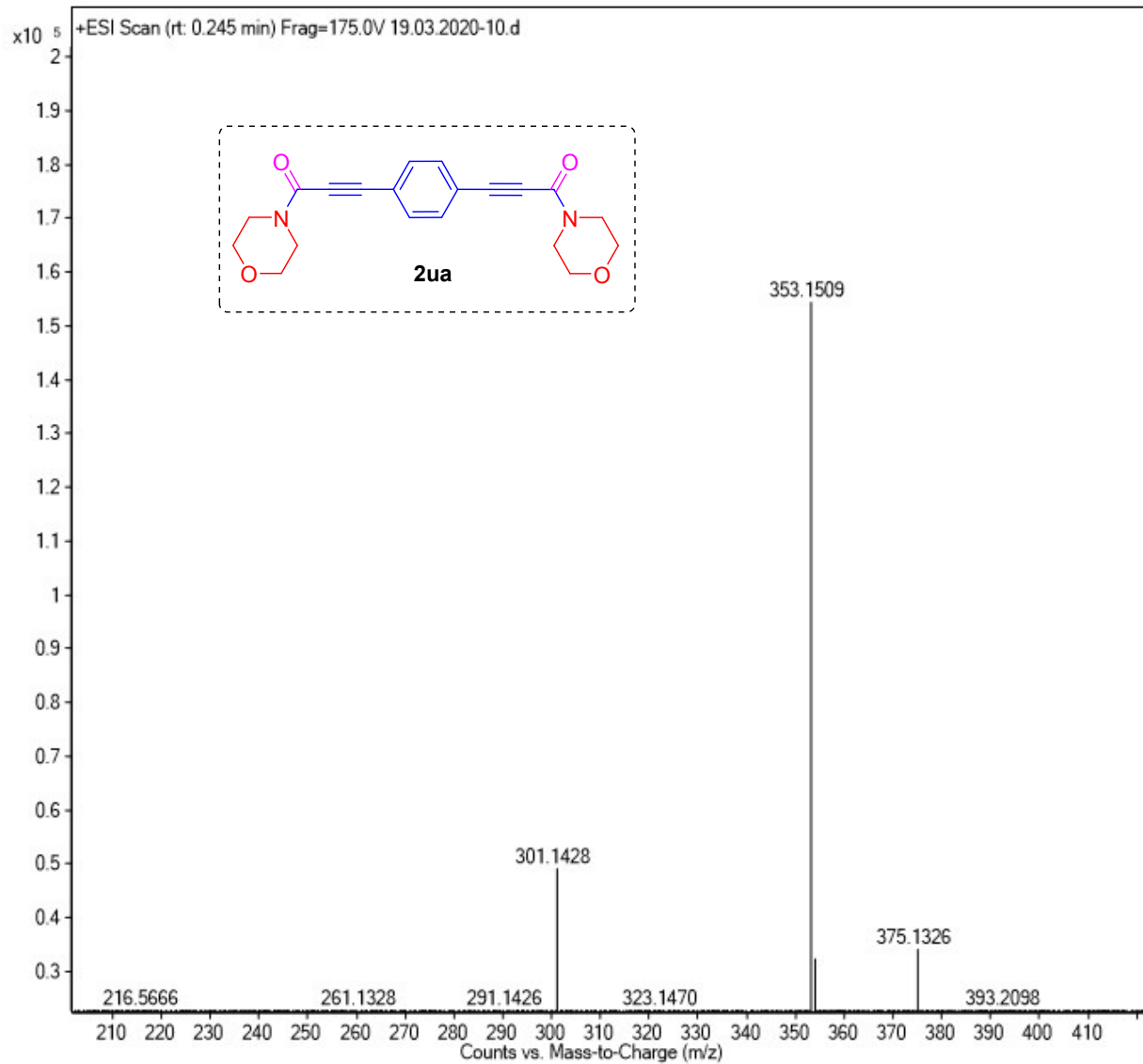


NAME RA-BR-3-164  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20190515  
 Time 11.37  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 701  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 8192  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39858055 W  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.29870972 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

**<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ua**



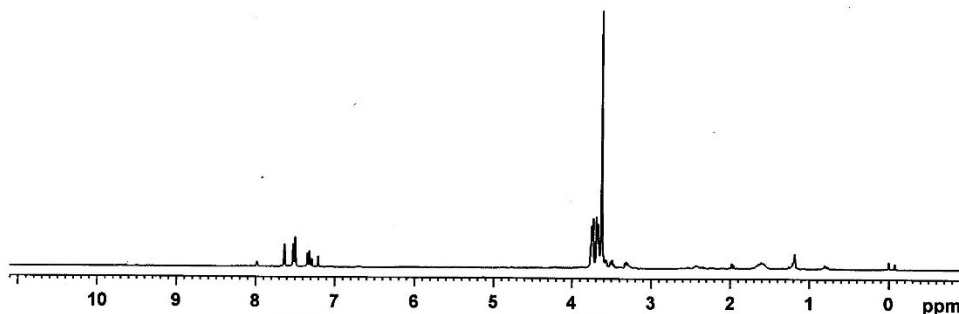
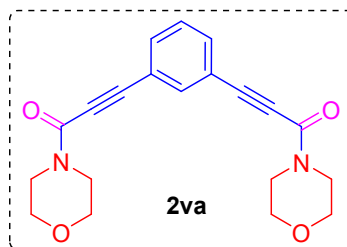
HRMS spectrum of compound 2ua

7.634  
7.525  
7.499  
7.344  
7.318  
7.292  
7.209

3.764  
3.749  
3.732  
3.691  
3.674  
3.660  
3.624



NAME RA-BR-3-331A  
EXPNO 8  
PROCNO 1  
Date\_ 20191126  
Time 16.14  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 128  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300222 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1.00  
2.06  
1.17

4.08  
4.07  
8.28

152.71  
135.82  
133.59  
128.96  
121.18

89.25  
81.75  
77.44  
77.01  
76.59  
66.82  
66.41

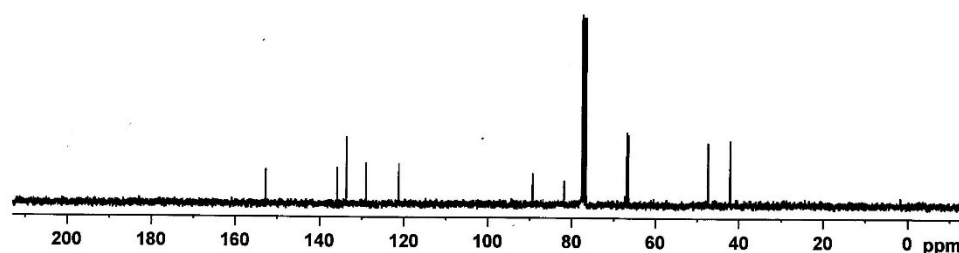
47.32  
42.06



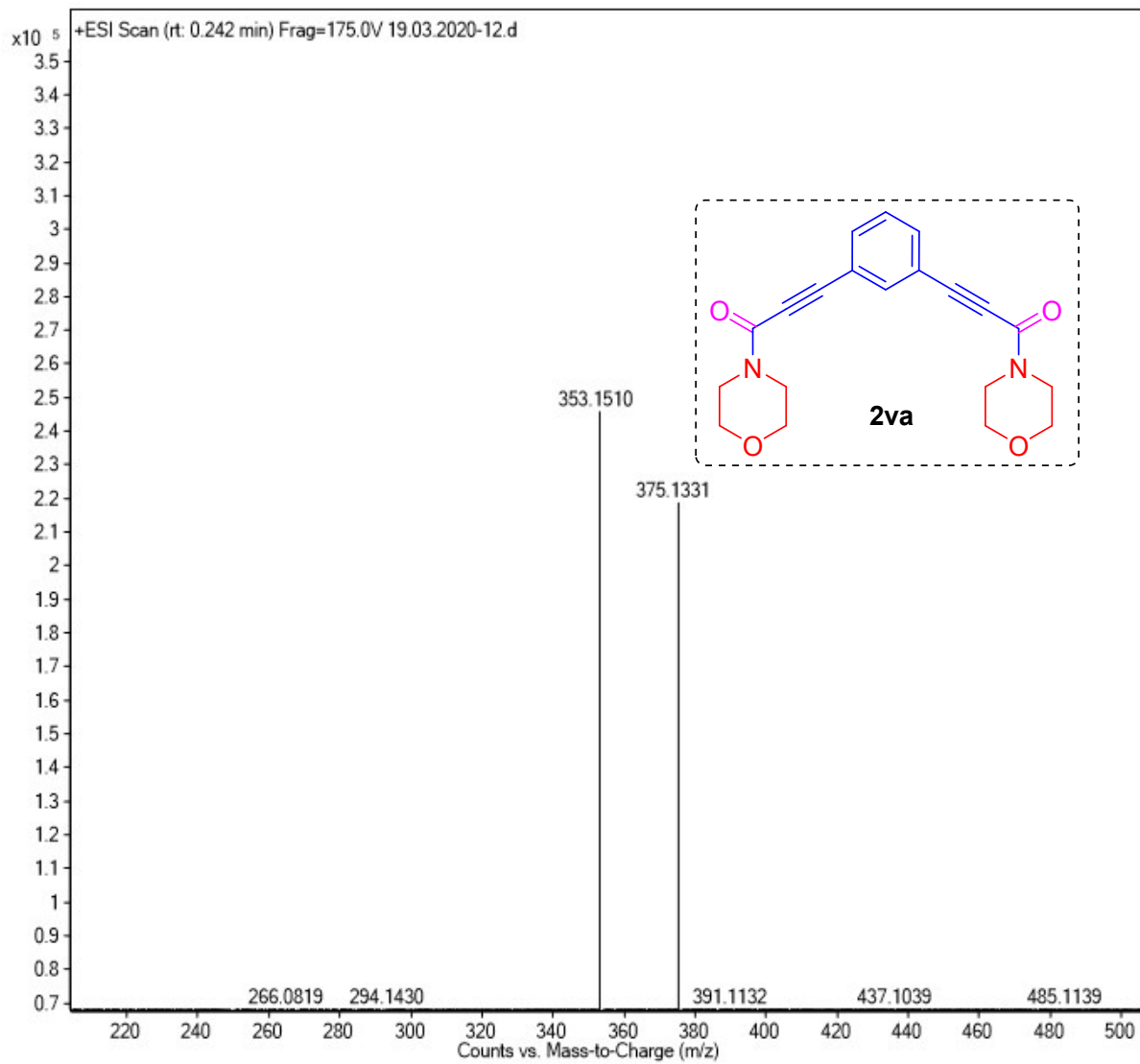
NAME RA-BR-3-331A  
EXPNO 9  
PROCNO 1  
Date\_ 20191126  
Time 16.23  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 109  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5792.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

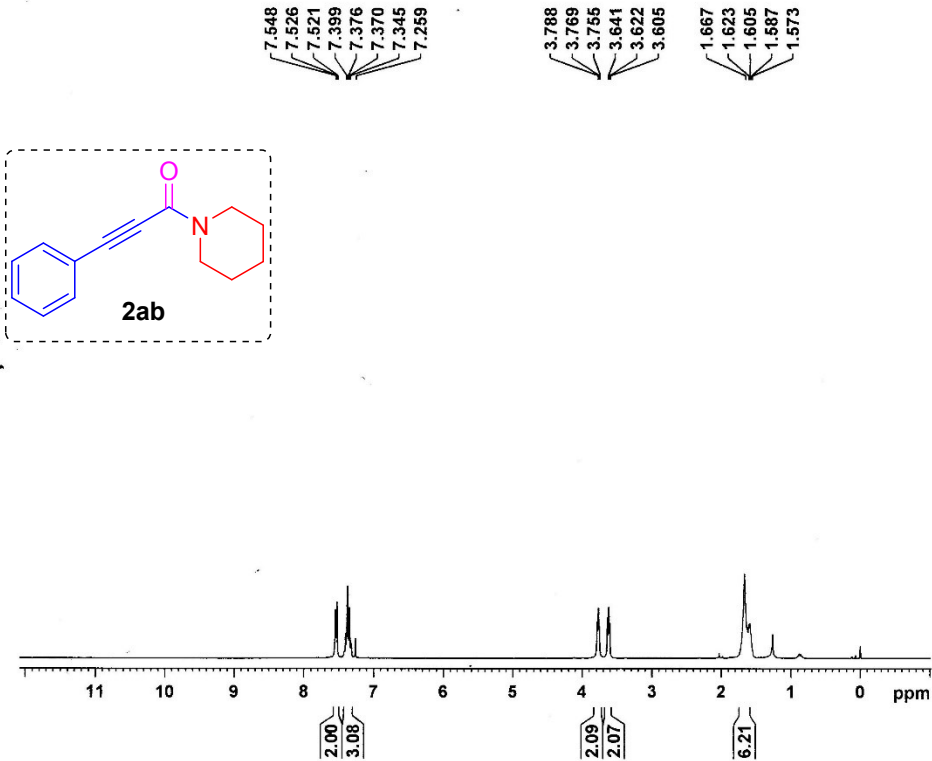
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 2va

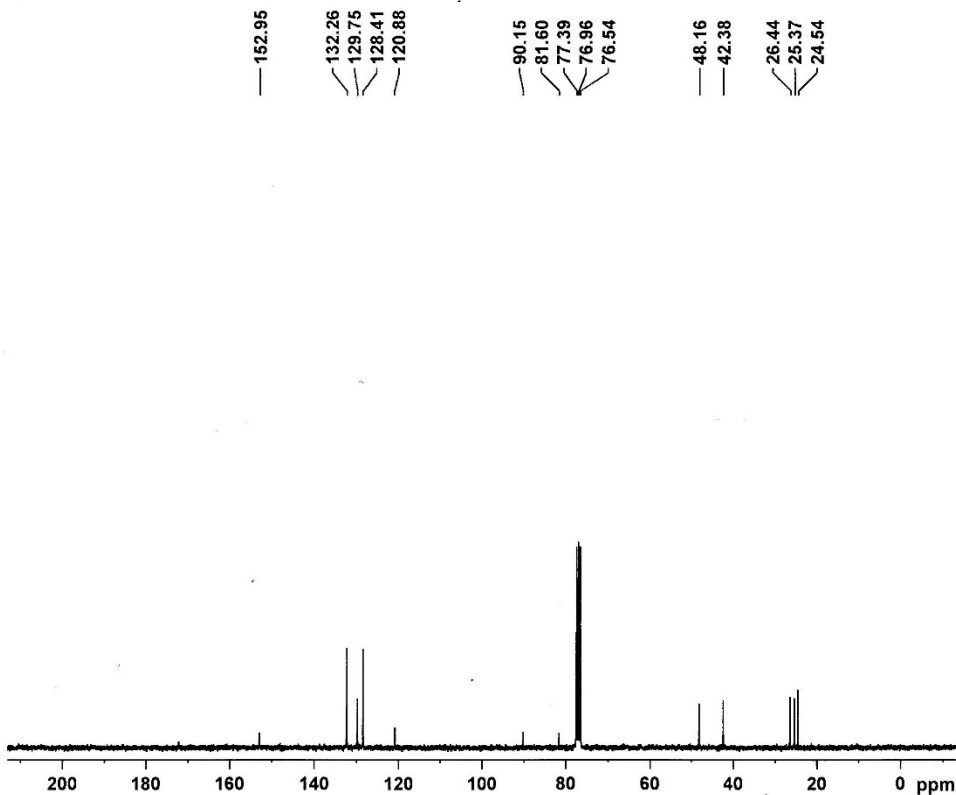


HRMS spectrum of compound 2va



NAME RA-BR-3-27  
 EXPNO 4  
 PROCNO 1  
 Date\_ 20181214  
 Time 16.14  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 181  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.00 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300069 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

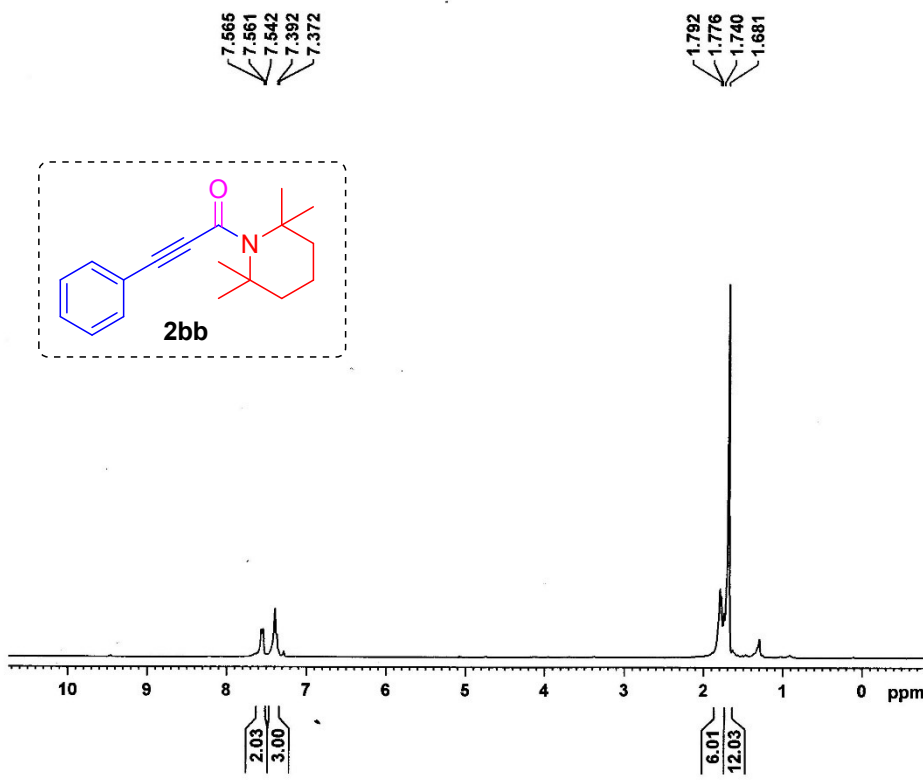


NAME RA-BR-3-27  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20181214  
 Time 13.59  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 5792.6  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.68 usec  
 PL1 0.00 dB  
 PL1W 31.39858055 W  
 SFO1 75.4752953 MHz

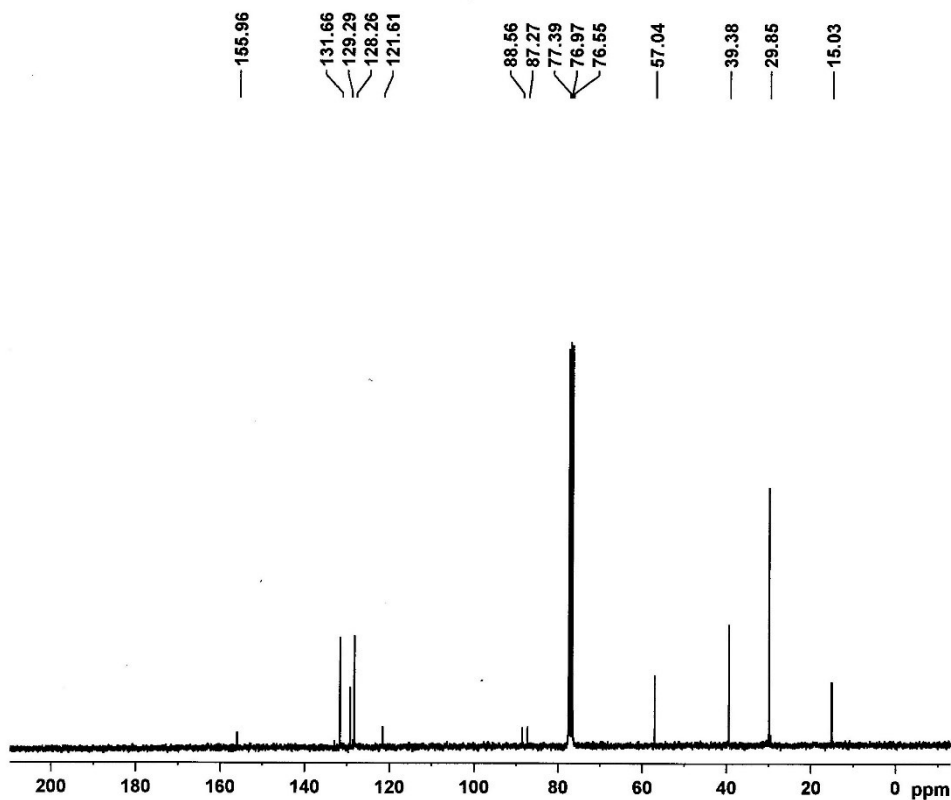
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 15.48 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.29870972 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ab



NAME RA-BR-3-354  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20200111  
 Time 11.02  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 161.3  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 <sup>1</sup>H  
 P1 13.50 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME RA-BR-3-354  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20200111  
 Time 11.08  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 504  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 5160.6  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 12.75 usec  
 PL1 -1.00 dB  
 PL1W 39.52846909 W  
 SFO1 75.4752953 MHz

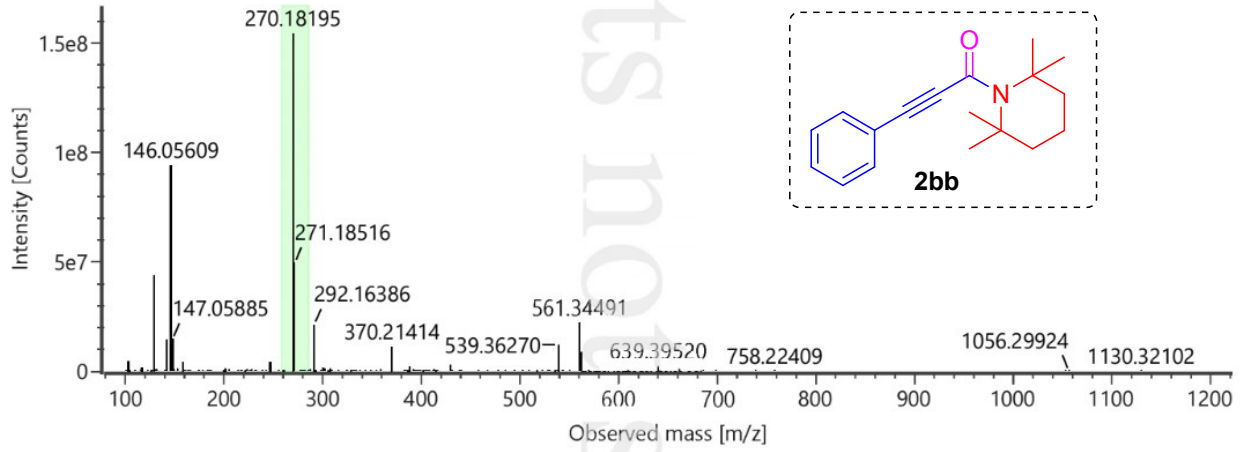
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.46 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.37778899 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677601 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2bb

Component name: **C18H23NO**

Item name: MSR\_354\_270  
Item description:

Channel name: Low energy : Time 0.3322 +/- 0.1810 minutes



**HRMS Spectrum of compound 2bb**



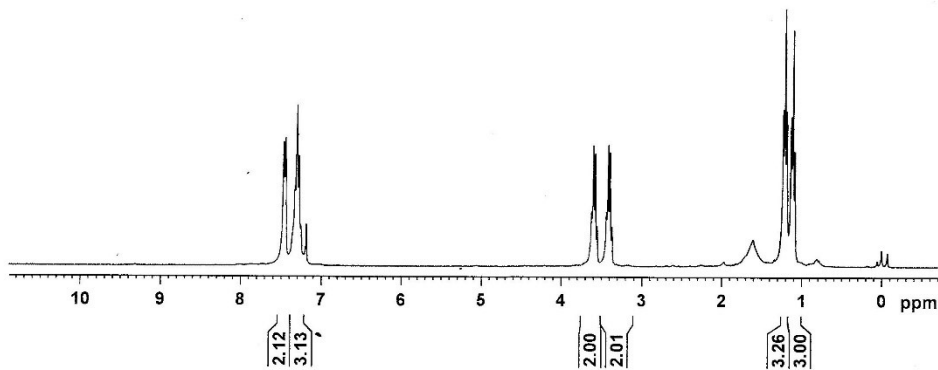
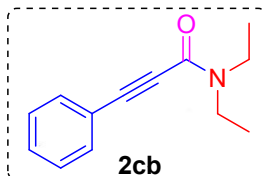
7.470  
7.447  
7.330  
7.301  
7.277  
7.255  
7.187

3.626  
3.603  
3.579  
3.556  
3.441  
3.418  
3.394  
3.371

1.233  
1.210  
1.187  
1.133  
1.109  
1.086



NAME RA-BR-3-75A  
EXPNO 1  
PROCNO 1  
Date\_ 20190304  
Time\_ 9.11  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 228.1  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1316534 MHz  
SI 32768  
SF 300.1300291 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

153.97  
132.27  
129.75  
128.43  
120.91

88.95  
82.08  
77.37  
76.95  
76.53

43.55  
39.33

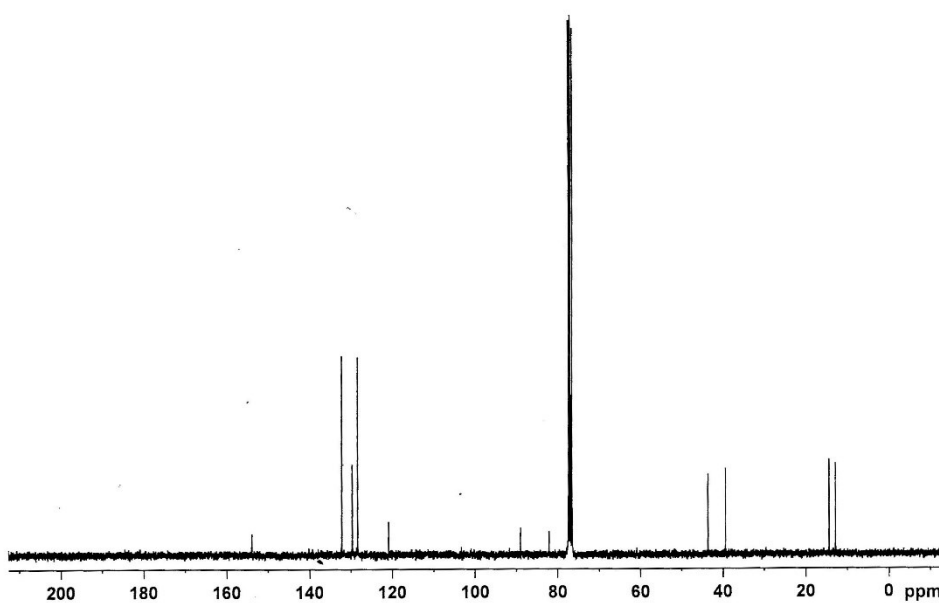
14.33  
12.79



NAME RA-BR-3-75A  
EXPNO 2  
PROCNO 1  
Date\_ 20190304  
Time\_ 10.06  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1200  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 4096  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2cb

7.457  
7.431  
7.322  
7.295  
7.271  
7.250  
7.184  
3.548  
3.523  
3.499  
3.356  
3.332  
3.307  
1.605  
1.581  
1.556  
1.526  
1.497  
1.474  
1.447  
1.361  
1.337  
1.313  
1.289  
1.265  
1.240  
1.214  
1.190  
0.923  
0.897  
0.872  
0.846

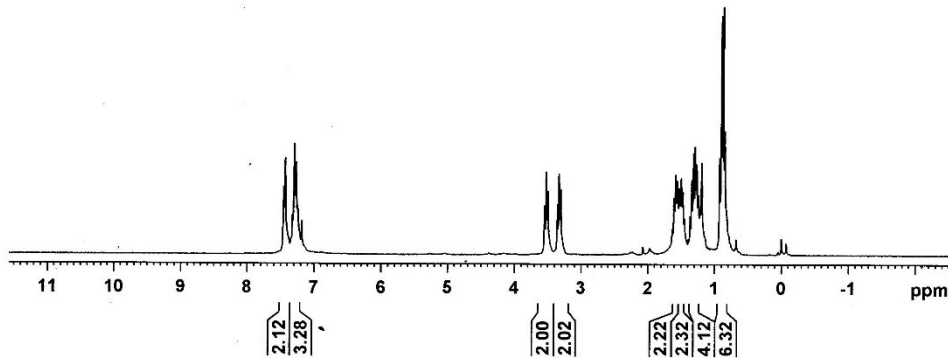
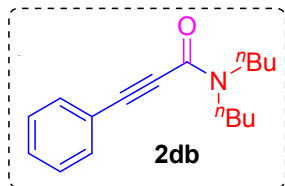


Current Data Parameters  
NAME RA-BR-3-75B  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20190301  
Time 14.46  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3064680 sec  
RG 181  
DW 81.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300296 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



154.41  
132.23  
129.73  
128.44  
120.97  
89.19  
82.30  
77.37  
76.95  
76.53  
48.92  
44.63  
31.05  
29.61  
20.17  
19.97  
13.70



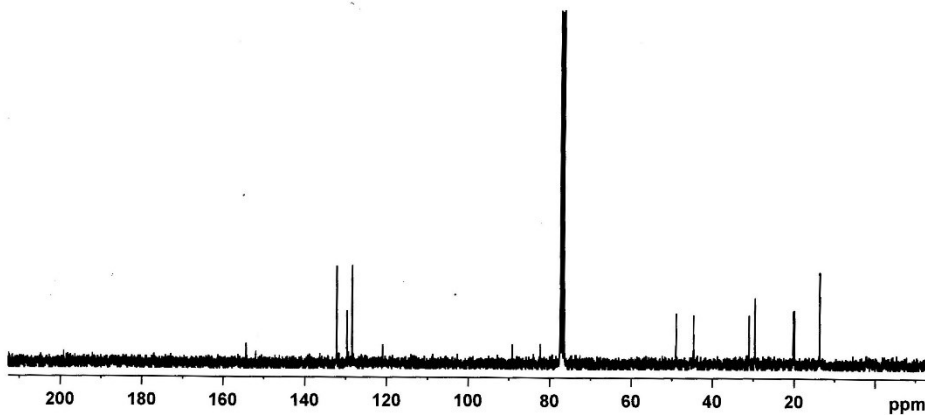
Current Data Parameters  
NAME RA-BR-3-75B  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20190301  
Time 14.07  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 394  
DS 4  
SWH 17965.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 1149.4  
DW 27.800 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

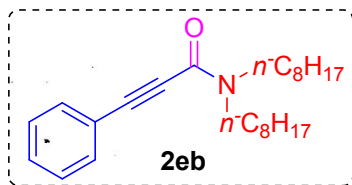
===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.46 dB  
PL13 16.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 2db

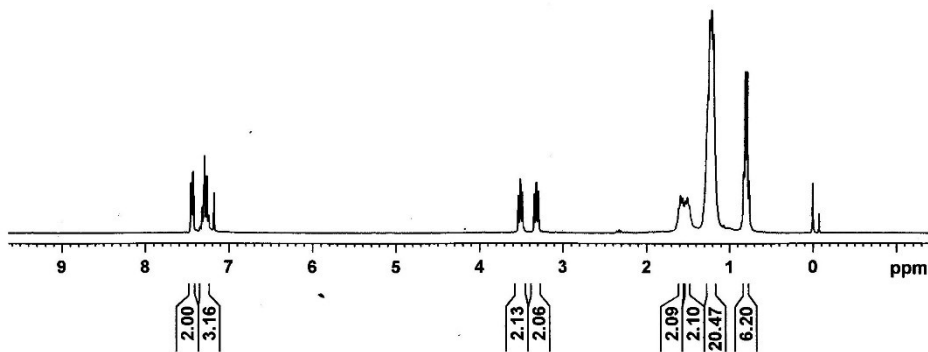


7.459  
7.437  
7.432  
7.326  
7.304  
7.296  
7.271  
7.250  
7.242  
7.185

3.537  
3.513  
3.487  
3.343  
3.318  
3.292  
1.611  
1.587  
1.563  
1.528  
1.504  
1.482  
1.378  
1.256  
1.235  
1.223  
1.210  
1.190  
1.140  
0.829  
0.810  
0.786  
0.762



NAME RA-BR-3-340B  
EXPNO 3  
PROCNO 1  
Date\_ 20191205  
Time 21.15  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 128  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300294 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

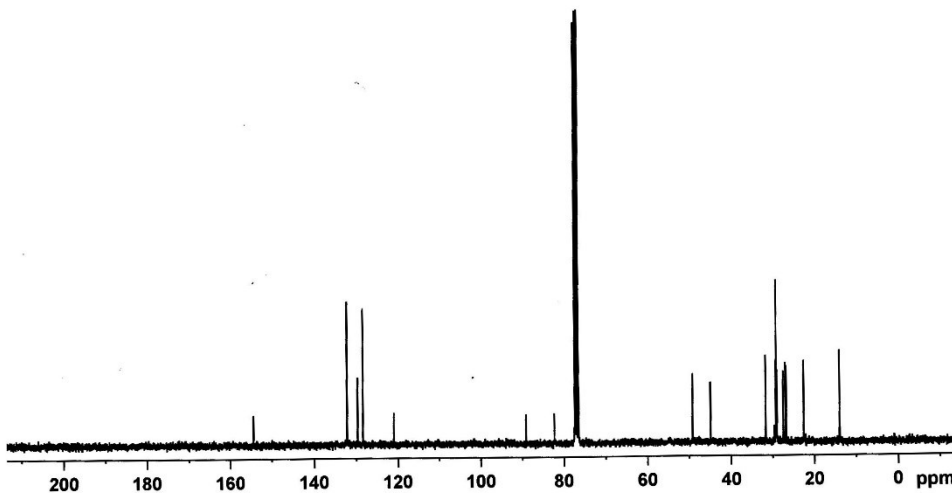
154.38

132.23  
129.71  
128.42  
121.00

89.16  
82.35  
77.37  
76.94  
76.52  
49.19  
44.92  
31.74  
31.70  
29.29  
29.23  
29.14  
28.95  
27.51  
26.98  
26.77  
22.54  
22.51  
13.92  
13.90



NAME RA-BR-3-340A  
EXPNO 2  
PROCNO 1  
Date\_ 20191205  
Time 19.48  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 831  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 8192  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

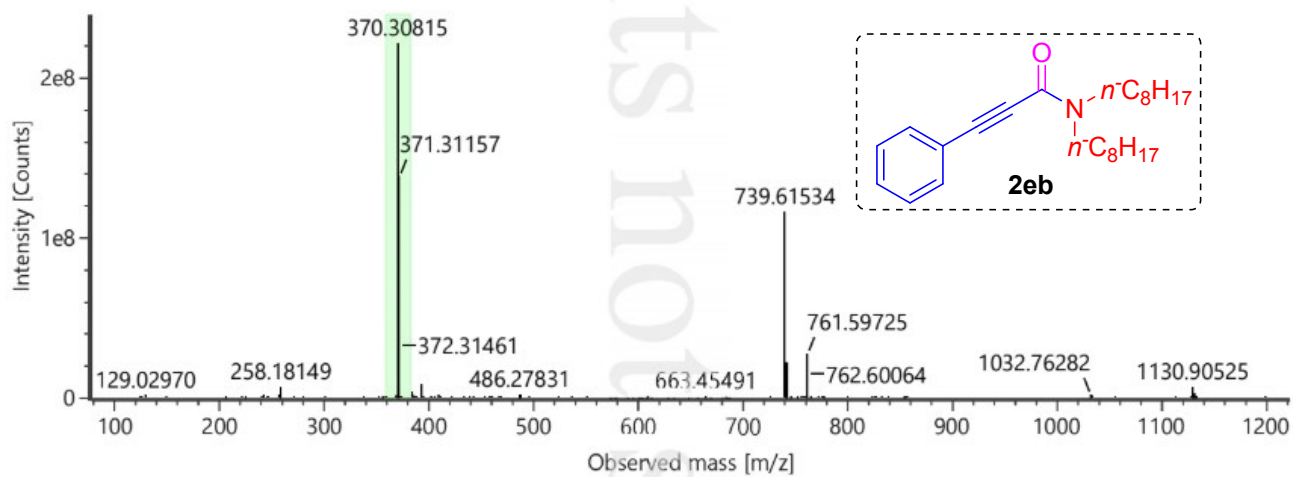
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677480 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2eb

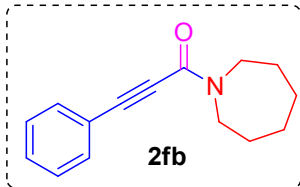
Component name: C<sub>25</sub>H<sub>39</sub>NO

Item name: MSR\_340B\_370  
Item description:

Channel name: Low energy : Time 0.3367 +/- 0.1894 minutes



HRMS spectrum of compound 2eb



7.831  
7.807  
7.686  
7.662  
7.657  
7.634  
7.544

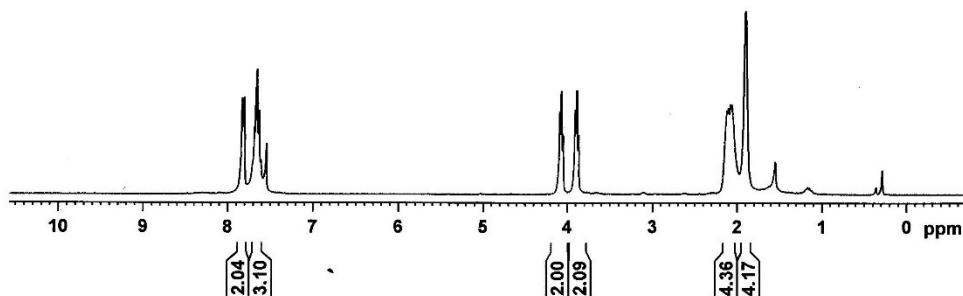
4.088  
4.069  
4.049  
3.906  
3.888  
3.867

2.117  
2.099  
2.078  
2.062  
1.901



NAME RA-BR-3-337A  
EXPNO 6  
PROCNO 1  
Date\_ 20191128  
Time 18.07  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 256  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156682 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



154.49

132.29  
129.74  
128.42  
120.94

89.52  
82.10  
77.37  
76.95  
76.53

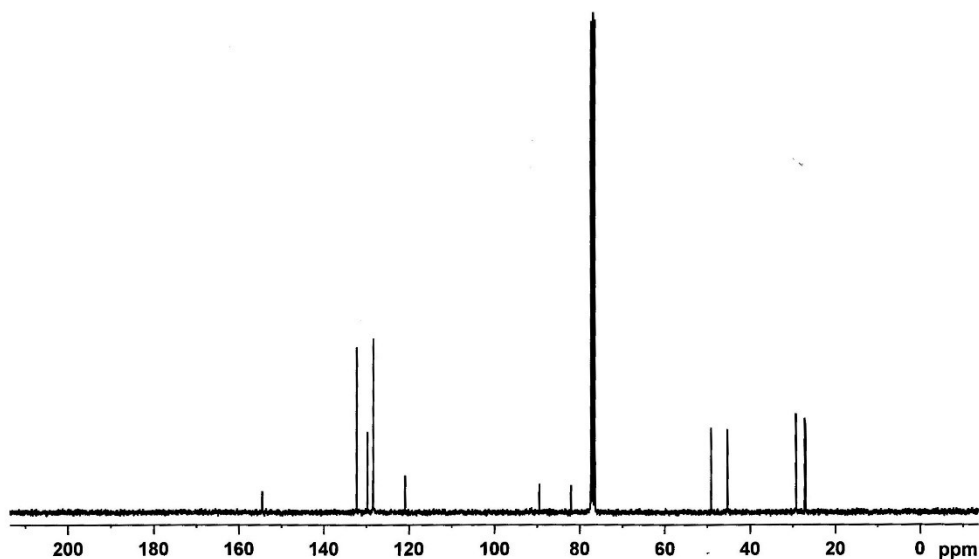
49.17  
45.37  
29.27  
27.25  
27.15  
26.99



NAME RA-BR-3-337A  
EXPNO 7  
PROCNO 1  
Date\_ 20191128  
Time 22.25  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2048  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 9195.2  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156682 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

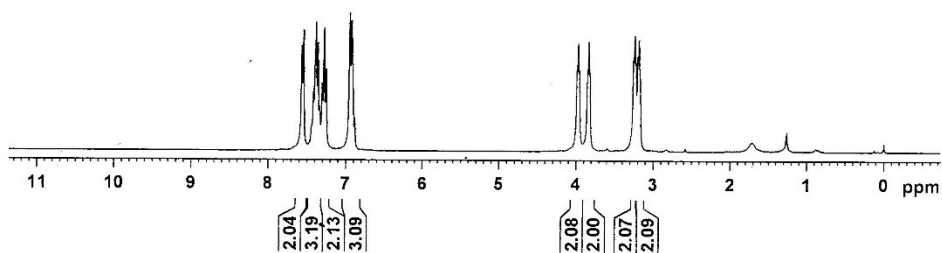
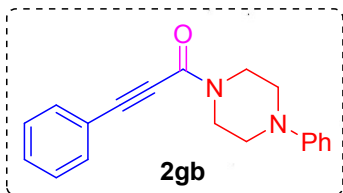


$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2fb

7.567  
7.543  
7.417  
7.384  
7.359  
7.337  
7.303  
7.278  
7.252  
6.947  
6.921  
6.908  
3.990  
3.975  
3.959  
3.853  
3.838  
3.822  
3.260  
3.244  
3.228  
3.205  
3.188  
3.173



NAME RA-BR-3-68  
EXPNO 3  
PROCNO 1  
Date\_ 20190303  
Time 19.34  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084680 sec  
RG 114  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

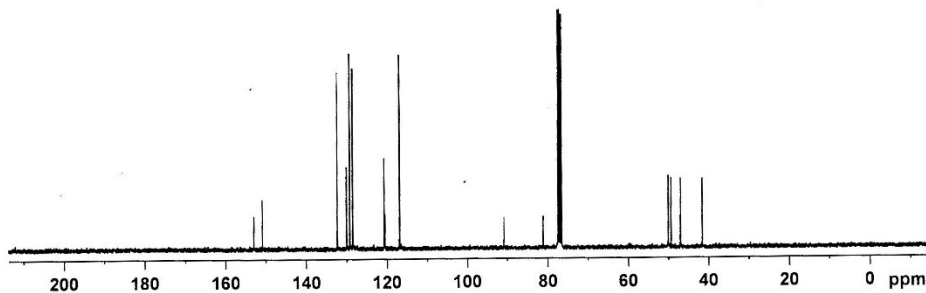


===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300115 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

153.06  
150.94  
132.35  
130.04  
129.25  
128.52  
120.71  
120.53  
116.90  
90.86  
81.17  
77.42  
77.00  
76.58  
50.02  
49.37  
46.92  
41.53



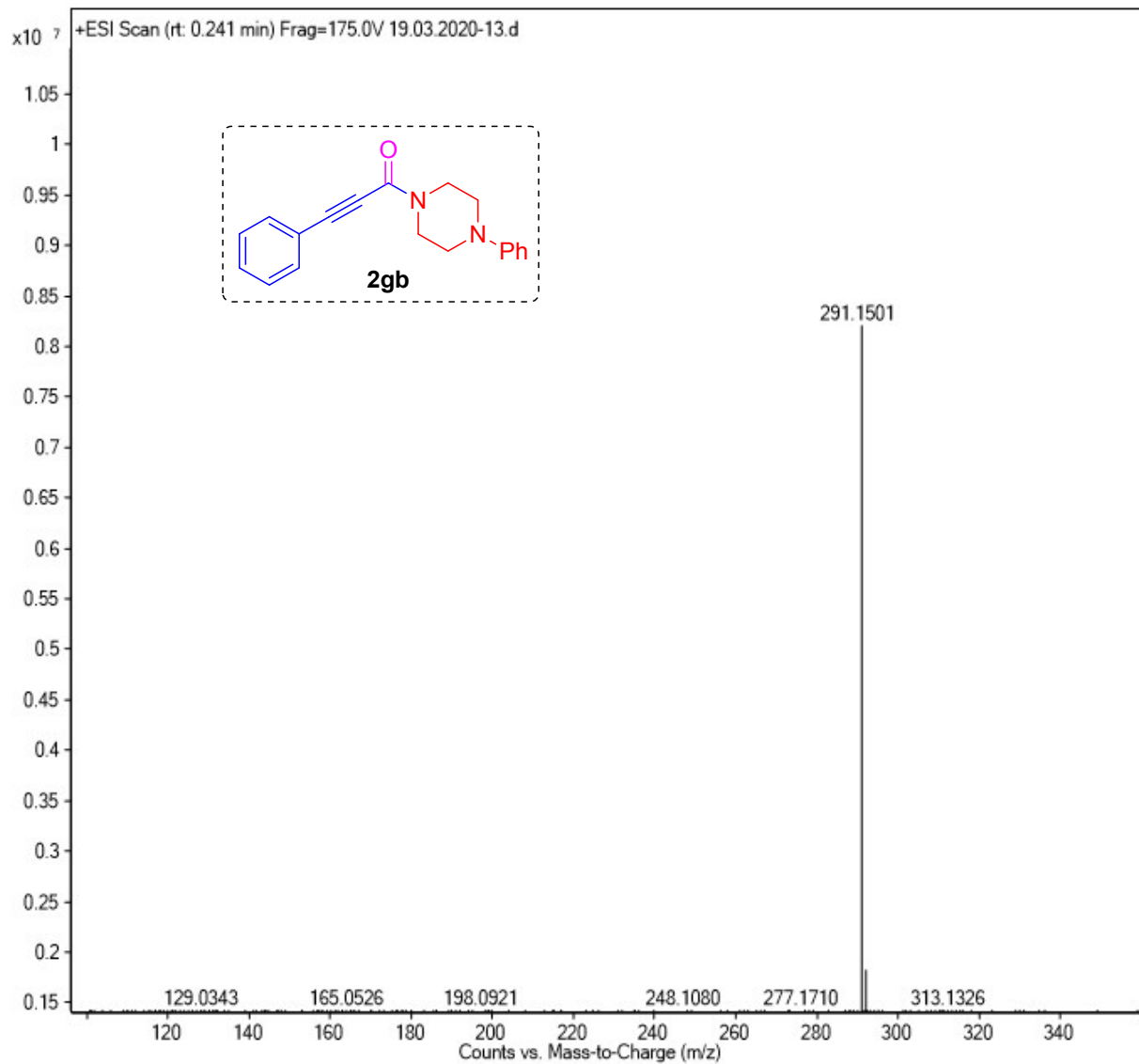
NAME RA-BR-3-68  
EXPNO 4  
PROCNO 1  
Date\_ 20190303  
Time 20.32  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 877  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1



===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2gb

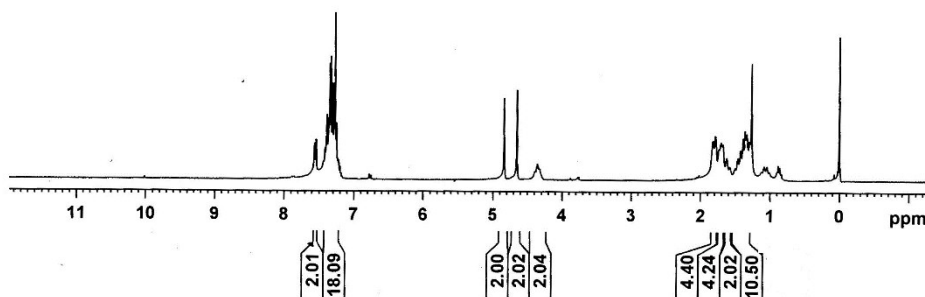
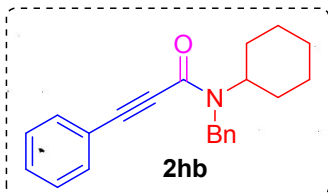


**HRMS spectrum of compound 2gb**

7.569  
7.565  
7.544  
7.538  
7.414  
7.398  
7.392  
7.386  
7.362  
7.344  
7.329  
7.315  
7.305  
7.283  
7.270  
7.252  
7.248  
4.836  
4.651  
4.356  
4.345  
1.823  
1.788  
1.733  
1.703  
1.690  
1.677  
1.620  
1.575  
1.458  
1.426  
1.387  
1.358  
1.332  
1.301  
1.292  
1.285  
1.263  
1.082  
1.043  
0.880  
0.856



NAME RA-BR-3-117A  
EXPNO 4  
PROCNO 1  
Date\_ 20190324  
Time 21.19  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 90.5  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

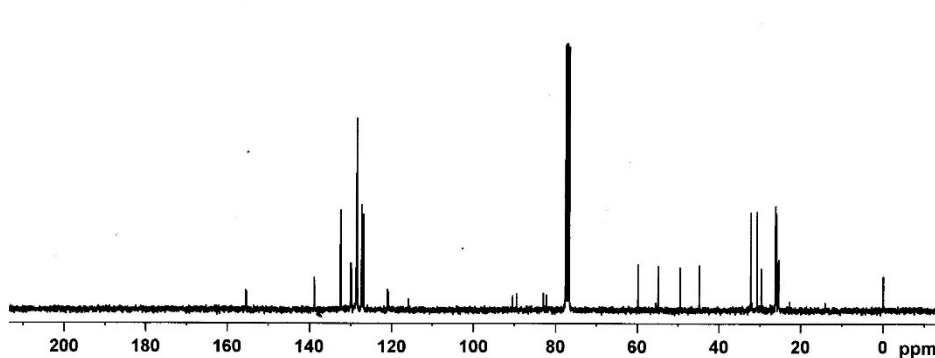


===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300100 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

155.41  
155.25  
138.86  
138.77  
132.47  
132.39  
132.31  
130.00  
129.83  
128.61  
128.41  
127.38  
127.31  
126.95  
126.87  
121.02  
120.81  
115.90  
90.45  
89.53  
82.97  
82.21  
77.07  
77.07  
76.65  
59.82  
54.85  
49.52  
44.82  
32.26  
30.72  
29.72  
26.21  
25.94  
25.54  
25.37



NAME RA-BR-3-117A  
EXPNO 2  
PROCNO 1  
Date\_ 20190324  
Time 20.27  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 7298.2  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 13C  
P1 10.88 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677418 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 2hb

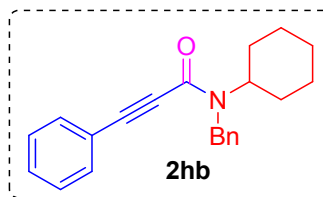
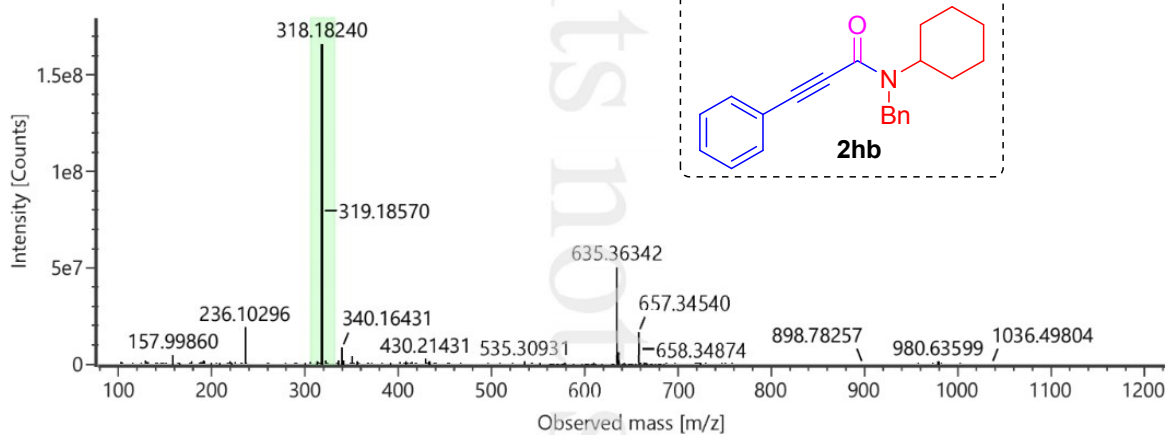


**Component name: C<sub>22</sub>H<sub>23</sub>NO**

Item name: MSR\_117A\_318

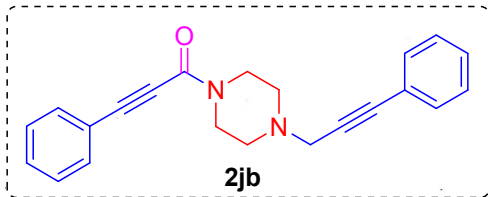
Item description:

Channel name: Low energy : Time 0.3360 +/- 0.1779 minutes

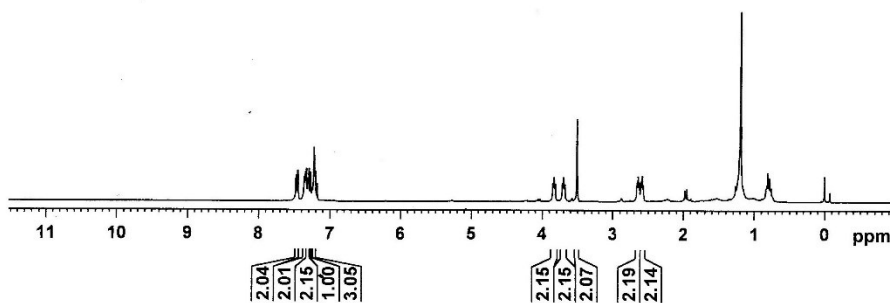


**HRMS Spectrum of compound 2hb**

7.478  
7.474  
7.452  
7.447  
7.366  
7.358  
7.346  
7.333  
7.321  
7.314  
7.308  
7.296  
7.271  
7.249  
7.238  
7.226  
7.217  
7.211  
7.205  
7.180  
3.848  
3.832  
3.815  
3.713  
3.697  
3.679  
3.506  
2.657  
2.640  
2.623  
2.601  
2.584  
2.567



NAME RA-BR-3-26  
EXPNO 3  
PROCNO 1  
Date\_ 20181213  
Time 13.40  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 114  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

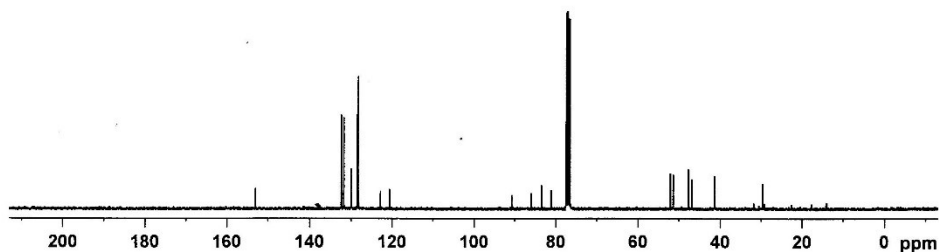


===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300304 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

153.02  
132.32  
131.71  
129.97  
128.46  
128.23  
122.84  
120.57  
90.72  
85.98  
83.47  
81.18  
77.39  
76.97  
76.55  
52.11  
51.39  
47.67  
46.85  
41.33



NAME RA-BR-3-26  
EXPNO 4  
PROCNO 1  
Date\_ 20181214  
Time 15.51  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 8192  
DW 27.900 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

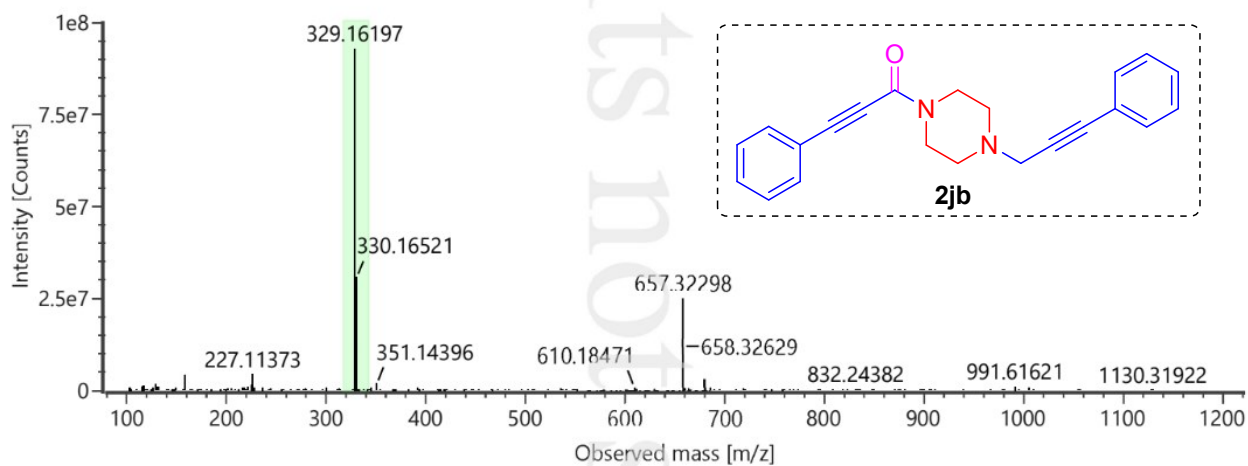
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2jb

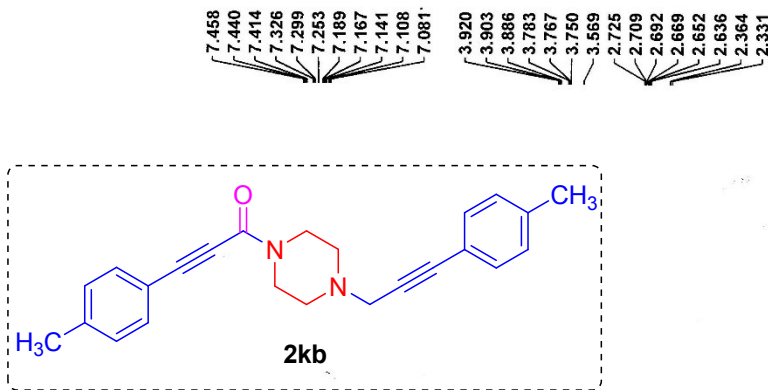
Component name: C<sub>22</sub>H<sub>20</sub>N<sub>2</sub>O

Item name: MSR\_26\_329  
Item description:

Channel name: Low energy : Time 0.3176 +/- 0.1939 minutes

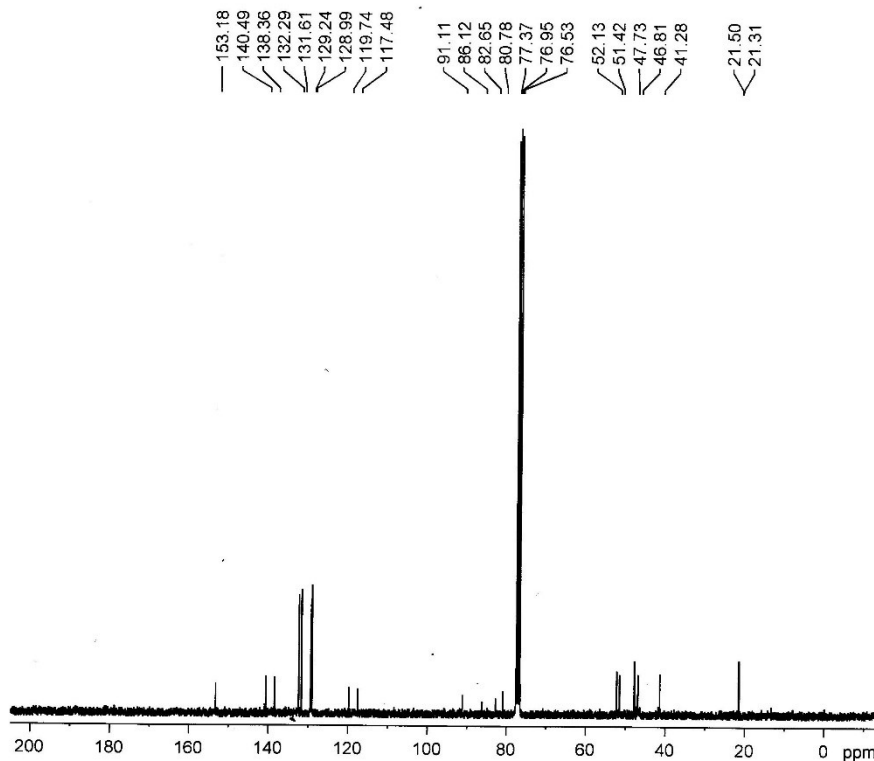
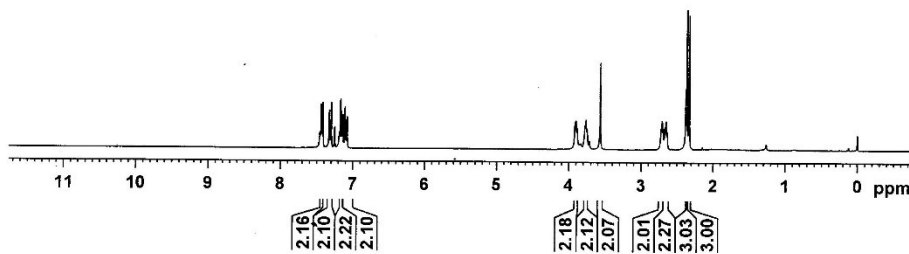


HRMS Spectrum of compound 2jb



NAME RA-BR-3-56  
EXPNO 4  
PROCNO 1  
Date\_ 20181228  
Time 22.02  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT C CDCI3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 181  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300087 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



NAME RA-BR-3-56  
EXPNO 1  
PROCNO 1  
Date\_ 20181228  
Time 17.41  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 4  
SOLVENT C CDCI3  
NS 1024  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 6502  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

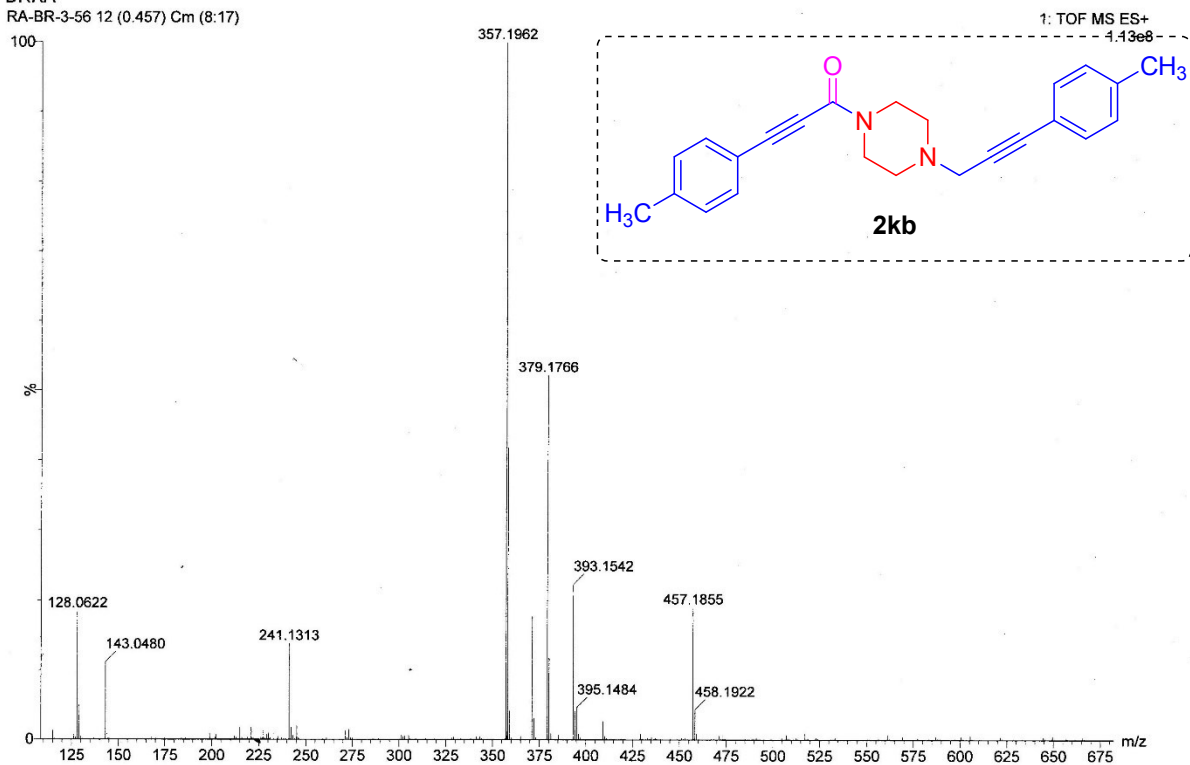
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2kb

DEPARTMENT OF ORGANIC CHEMISTRY  
UNIVERSITY OF MADRAS  
DRRA  
RA-BR-3-56 12 (0.457) Cm (8:17)

XEVO-G2SQTOF#NotSet

01-Feb-2019  
11:30:20

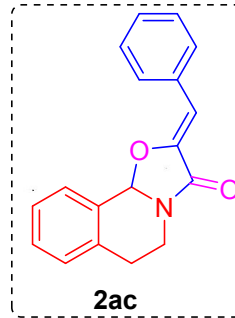


HRMS spectrum of compound 2kb

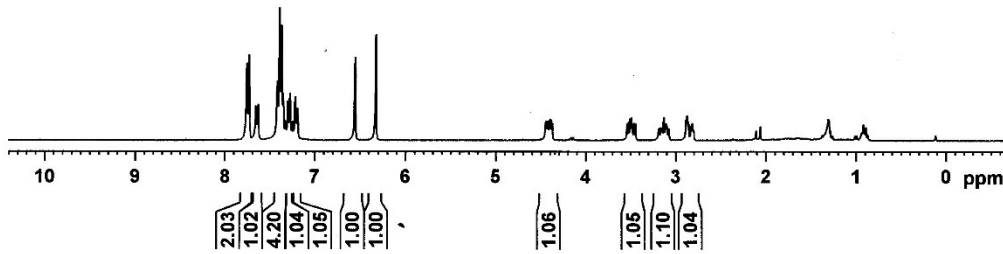
7.756  
7.732  
7.658  
7.652  
7.630  
7.418  
7.393  
7.369  
7.353  
7.348  
7.298  
7.281  
7.274  
7.217  
7.195  
6.555  
6.326  
4.452  
4.441  
4.431  
4.420  
4.407  
4.397  
4.386  
4.375  
3.540  
3.523  
3.506  
3.495  
3.489  
3.478  
3.462  
3.444  
3.165  
3.132  
3.110  
3.099  
2.885  
2.873  
2.858  
2.831  
2.819



NAME RA-BR-3-170  
EXPNO 1  
PROCNO 1  
Date\_ 20200107  
Time 19.58  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCI3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 256  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



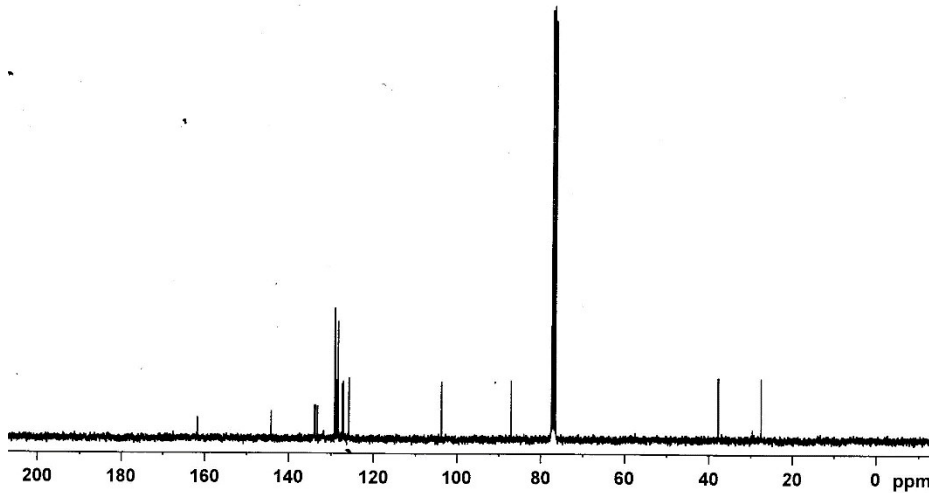
161.82  
144.18  
133.93  
133.83  
133.21  
129.20  
129.16  
128.83  
128.44  
127.40  
127.20  
125.83  
103.70  
87.10  
77.36  
76.94  
76.52  
37.77  
27.55



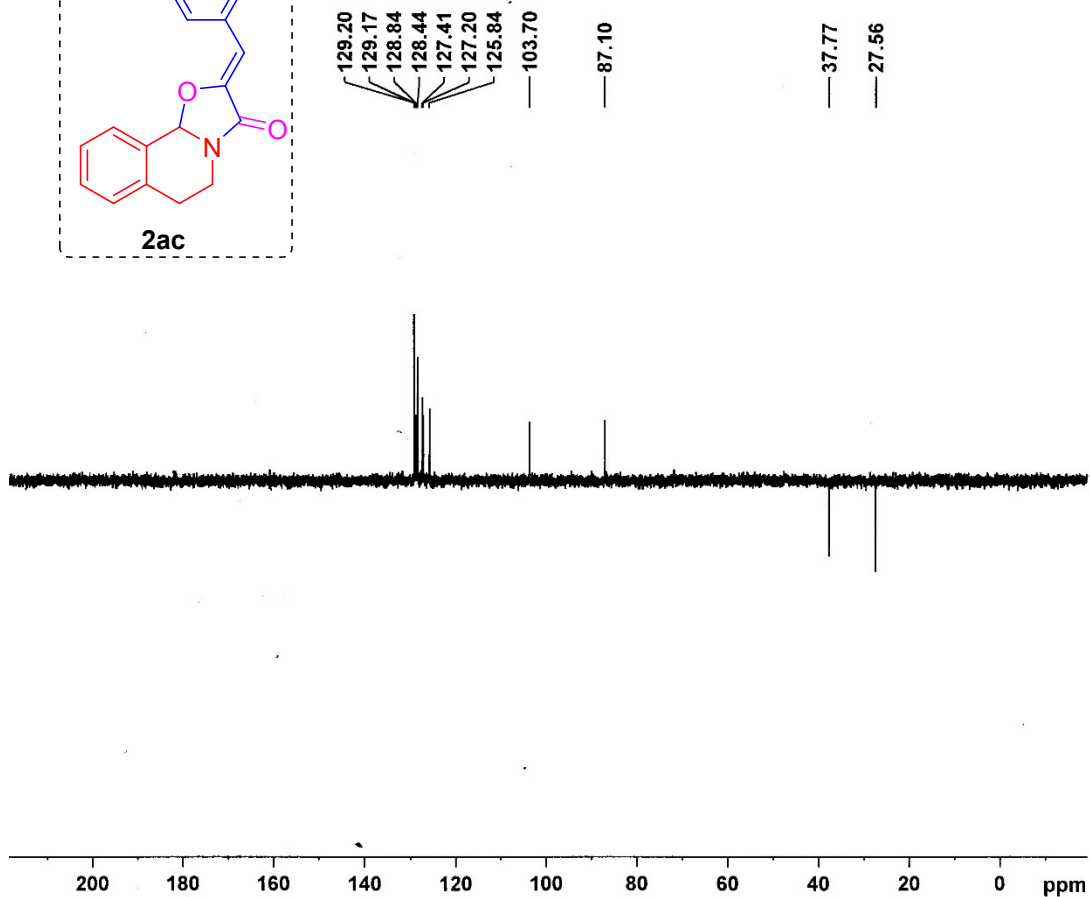
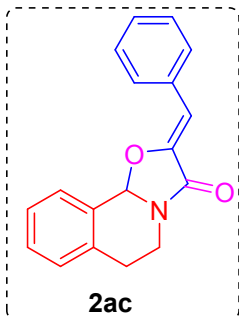
NAME RA-BR-3-170B  
EXPNO 4  
PROCNO 1  
Date\_ 20190525  
Time 20.52  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCI3  
NS 1200  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 4597.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waitz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ac



NAME RA-BR-3-170B  
EXPNO 5  
PROCNO 1  
Date\_ 20190525  
Time 21.43  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG dept135  
TD 65536  
SOLVENT CDCI3  
NS 306  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 23170.5  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
CNST2 145.000000  
D1 2.00000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD0 1

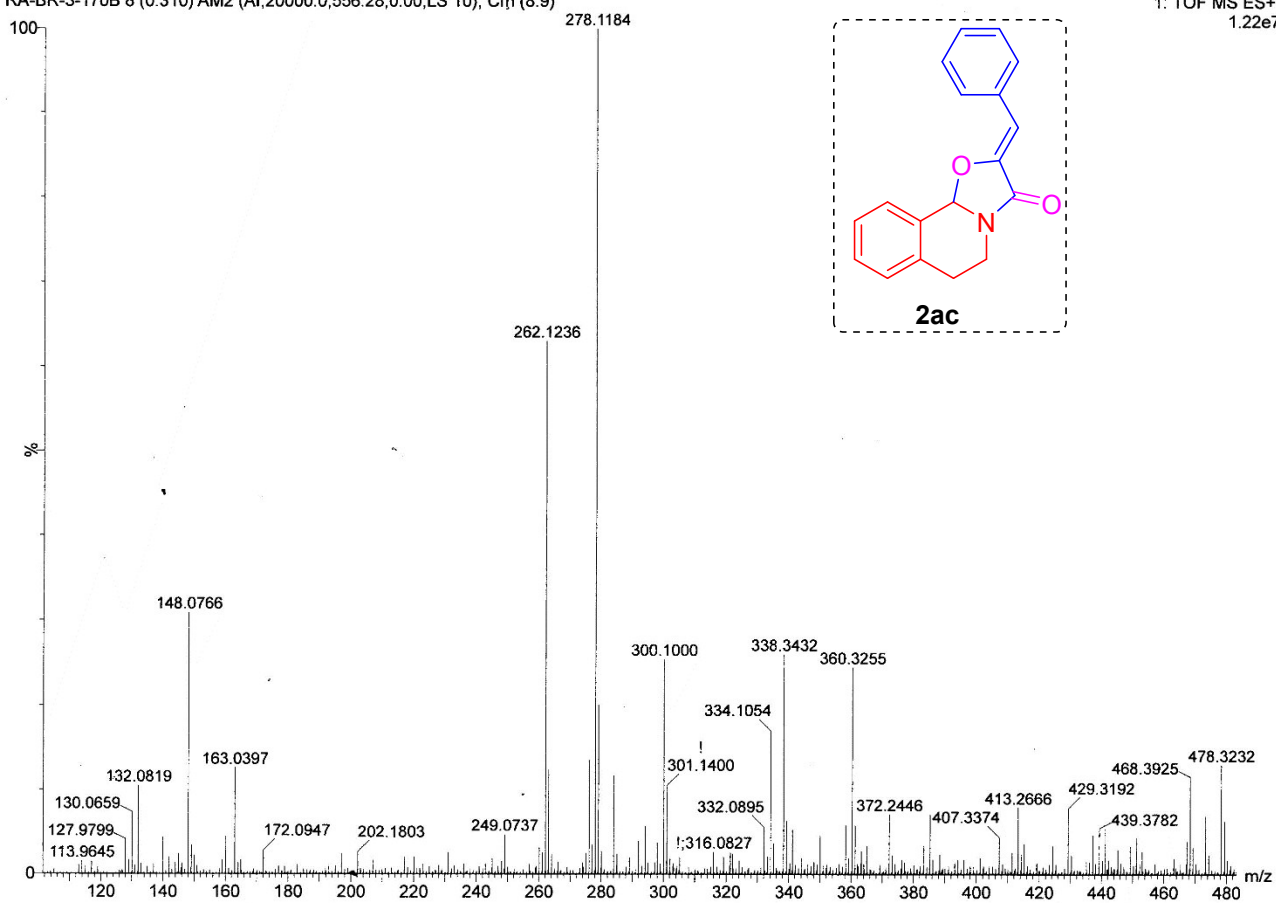
===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
P2 21.36 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
P3 12.00 usec  
P4 24.00 usec  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

DEPT-135 spectra of compound 2ac

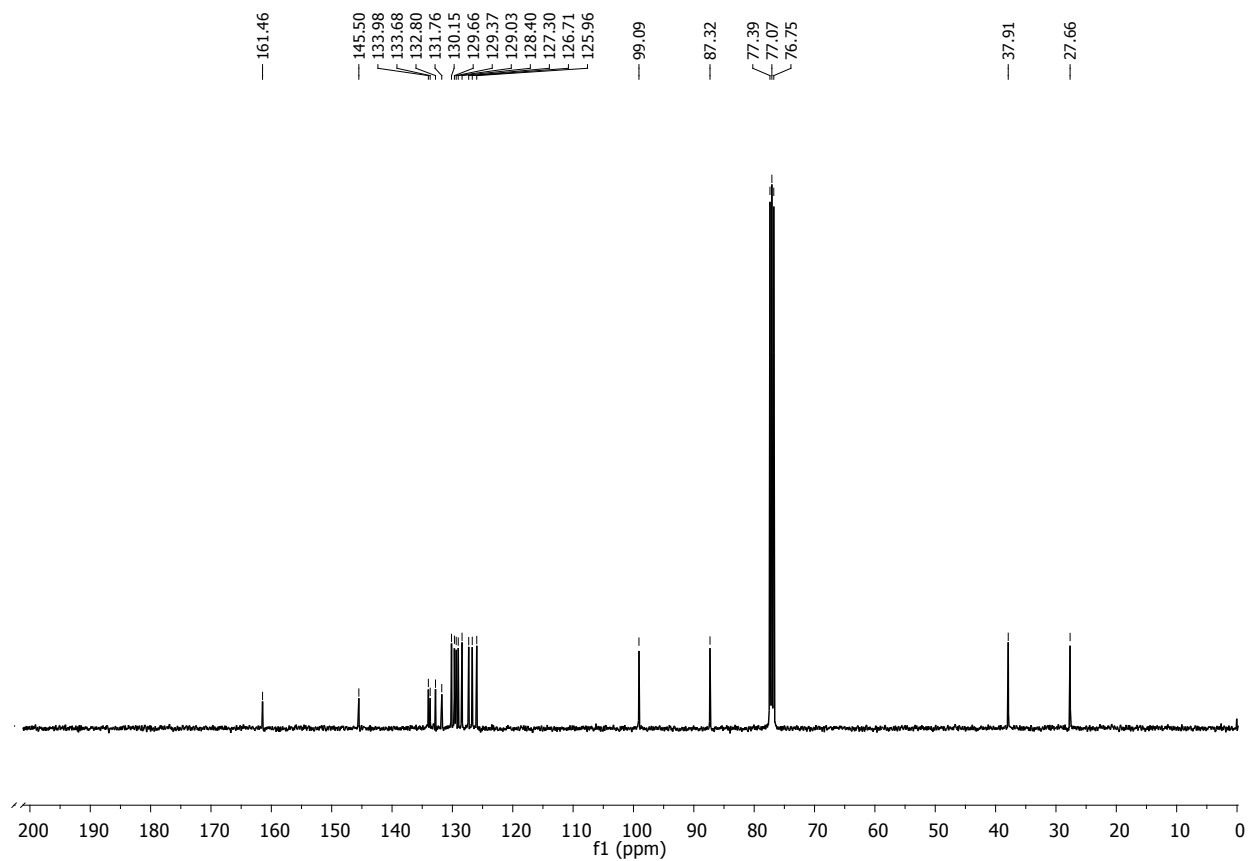
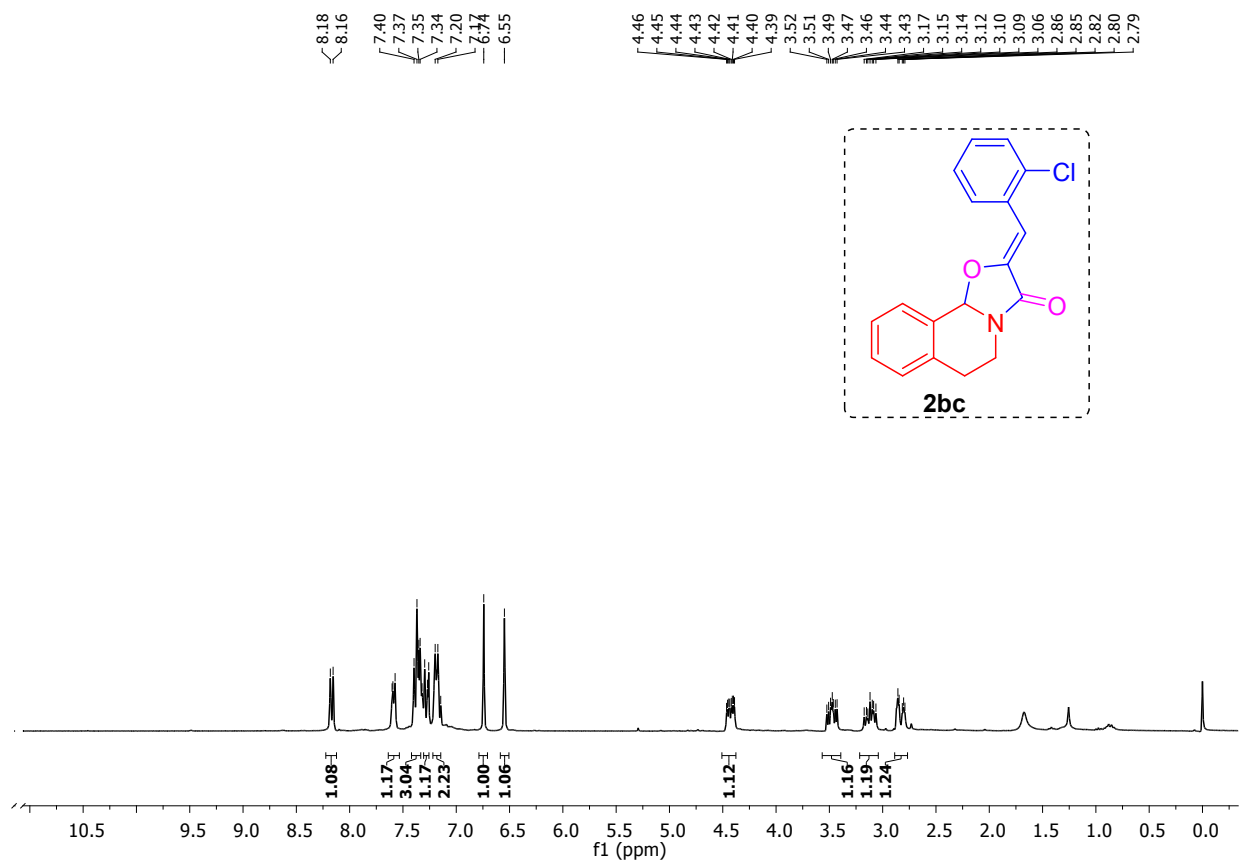
DRRA  
RA-BR-3-170B 8 (0.310) AM2 (Ar,20000.0,556.28,0.00,LS 10); Cm (8:9)

1: TOF MS ES+  
1.22e7



HRMS spectrum of compound 2ac

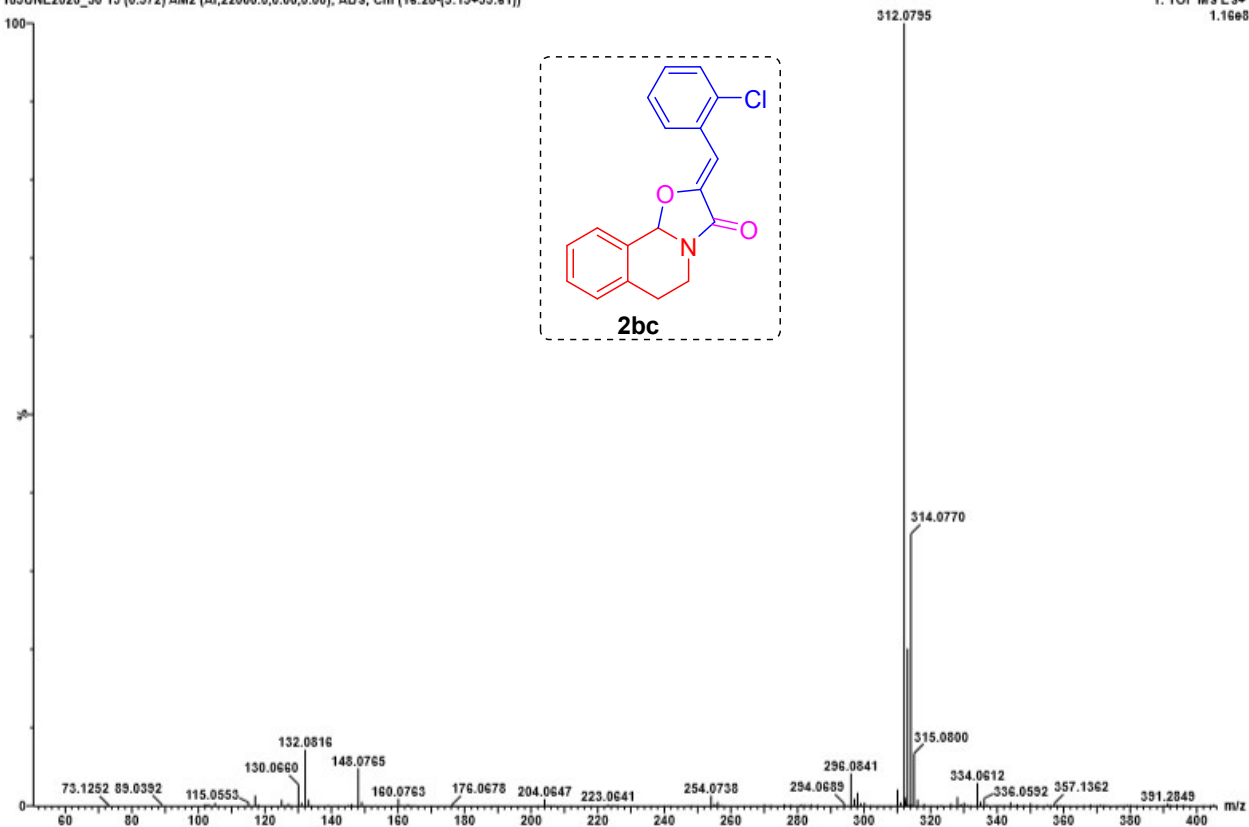




**<sup>1</sup>H & <sup>13</sup>C spectra of compound 2bc**

MSR\_370B\_311  
18JUNE2020\_50 19 (0.372) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (16:28-[3:13+33:61])

XEVO-G2-XS-QToF  
1: TOF MS ES+  
1.16e8

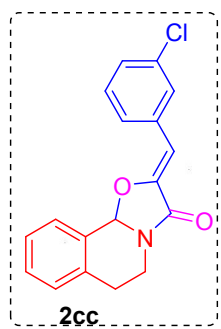


HRMS spectrum of compound 2bc

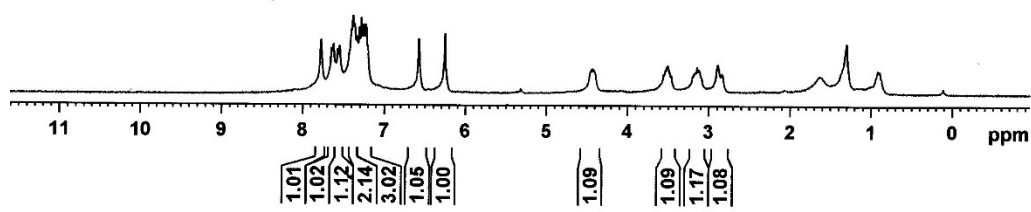
7.779  
7.648  
7.626  
7.574  
7.551  
7.407  
7.387  
7.368  
7.338  
7.309  
7.297  
7.285  
7.257  
7.231  
7.208  
6.578  
6.256  
4.444  
4.433  
4.422  
3.556  
3.539  
3.507  
3.478  
3.461  
3.197  
3.144  
3.122  
2.889  
2.835



NAME RA-BR-3-355B  
EXPNO 3  
PROCNO 1  
Date\_ 20200110  
Time 21.36  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 30  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 456.1  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

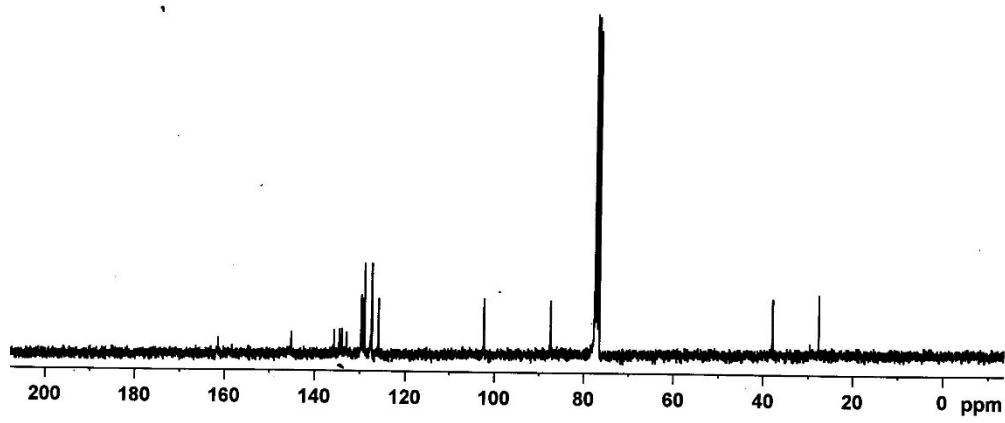


161.44  
145.16  
135.72  
134.67  
134.46  
133.95  
132.96  
129.66  
129.36  
128.94  
127.39  
127.38  
127.30  
125.89  
102.27  
87.41  
77.42  
76.99  
76.57  
37.89  
27.61

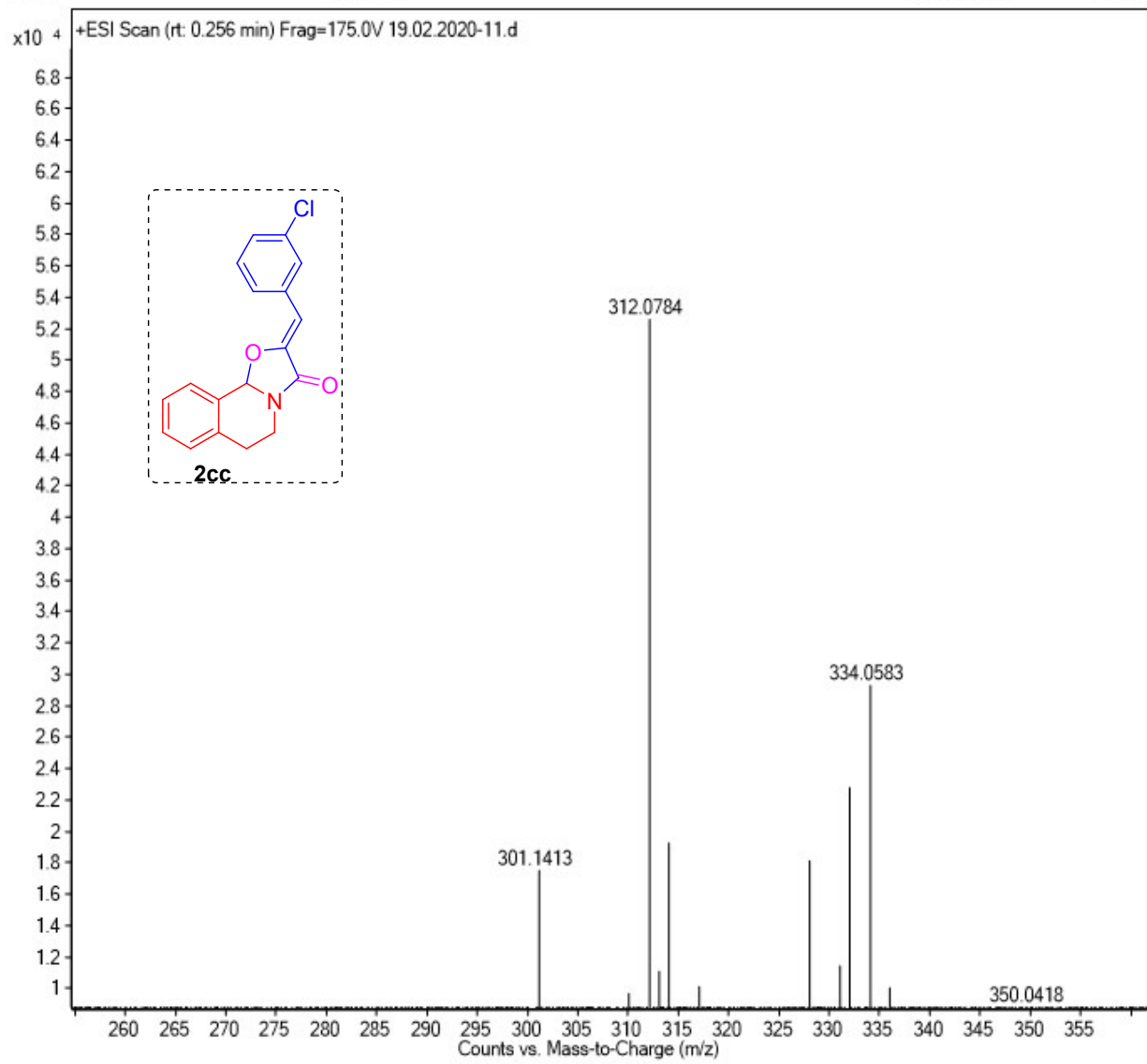


NAME RA-BR-3-355B  
EXPNO 2  
PROCNO 1  
Date\_ 20200110  
Time 19.23  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2048  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz  
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.28800207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677447 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 2cc  
S91

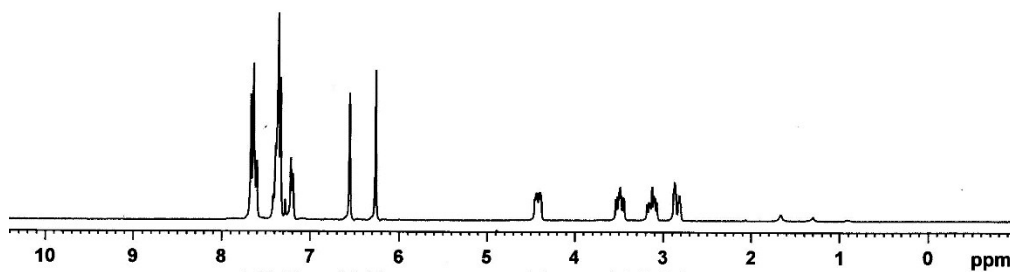
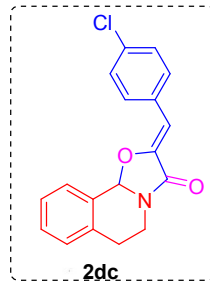


HRMS spectrum of compound 2cc

7.675  
7.647  
7.606  
7.417  
7.393  
7.375  
7.365  
7.337  
7.284  
7.220  
7.198  
6.556  
6.266  
4.455  
4.445  
4.435  
4.424  
4.412  
4.401  
4.390  
4.380  
3.537  
3.520  
3.503  
3.487  
3.477  
3.459  
3.442  
3.183  
3.162  
3.150  
3.129  
3.108  
3.096  
3.074  
2.884  
2.872  
2.860  
2.830  
2.818  
2.806



NAME RA-BR-3-353B  
EXPNO 1  
PROCNO 1  
Date\_ 20200109  
Time 19.05  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 181  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.13000000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

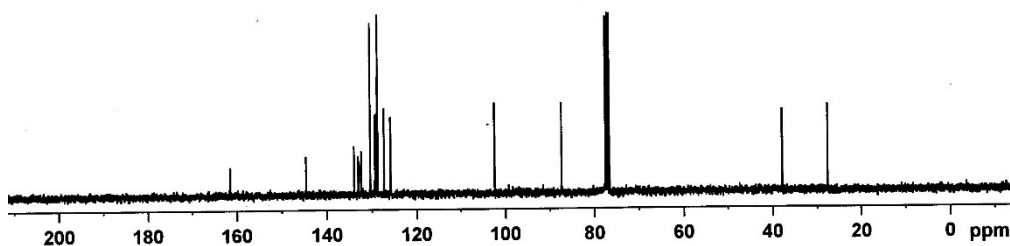
161.56  
144.64  
133.99  
133.10  
133.03  
132.43  
130.37  
129.33  
128.97  
128.73  
127.31  
125.87  
102.45  
87.34  
77.47  
77.04  
76.62  
37.87  
27.62



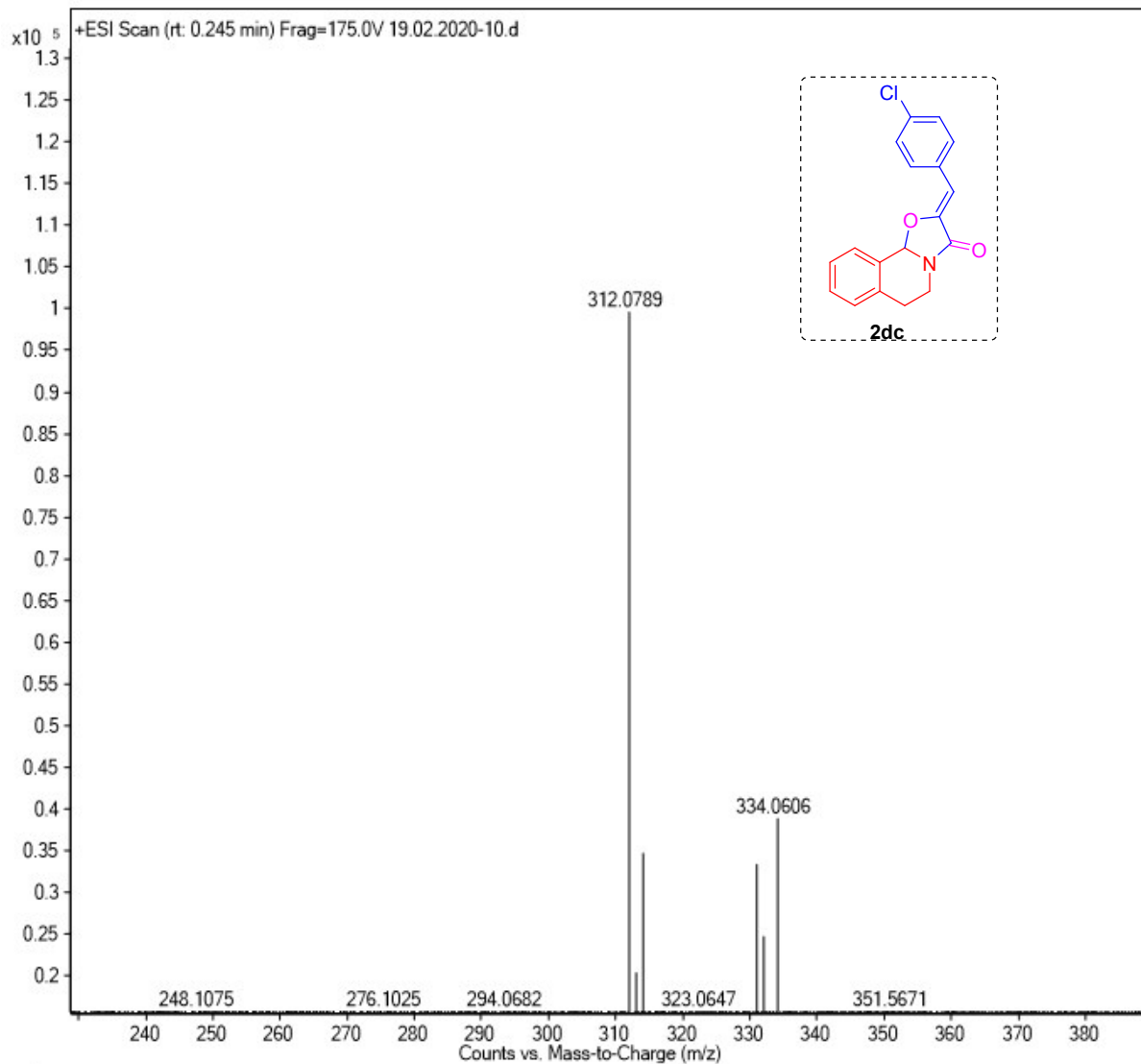
NAME RA-BR-3-353B  
EXPNO 2  
PROCNO 1  
Date\_ 20200109  
Time 19.14  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 150  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 2048  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677447 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 2dc



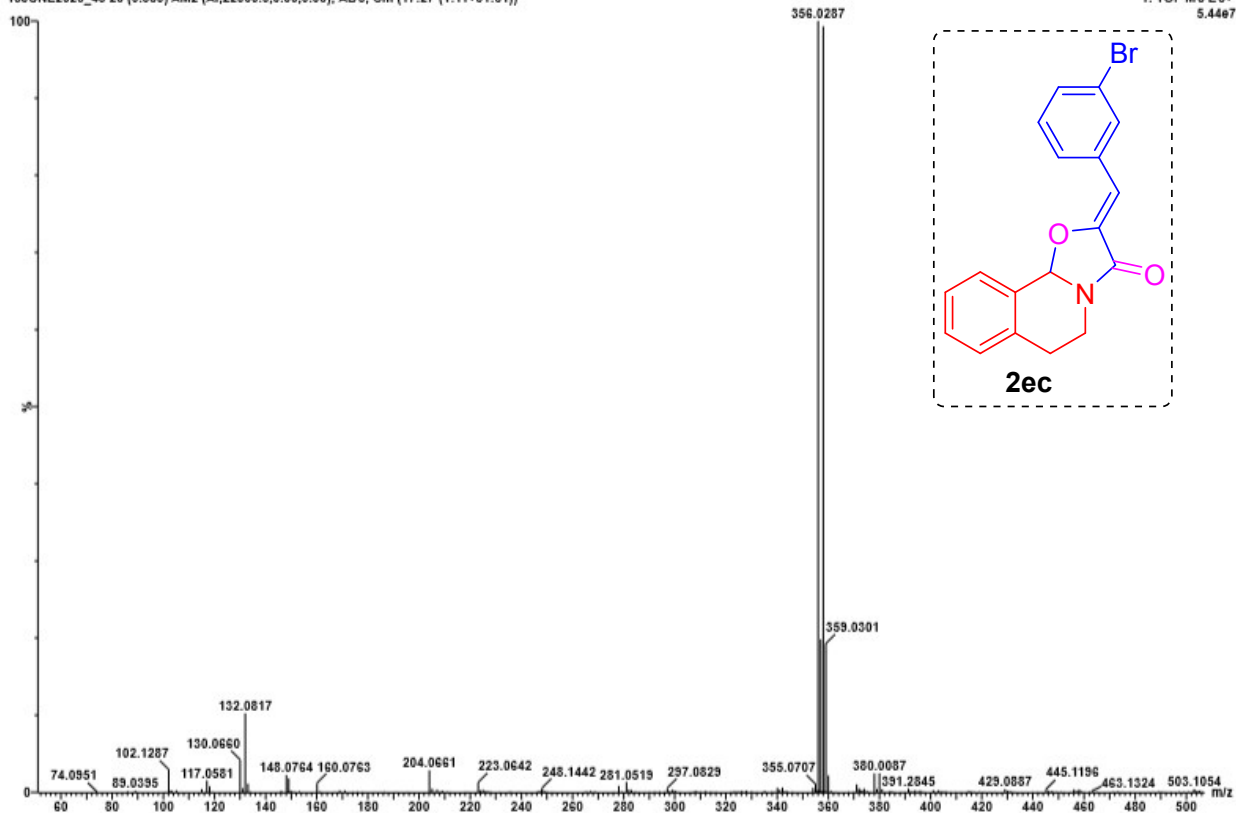
HRMS spectrum of compound 2dc



**<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ec**

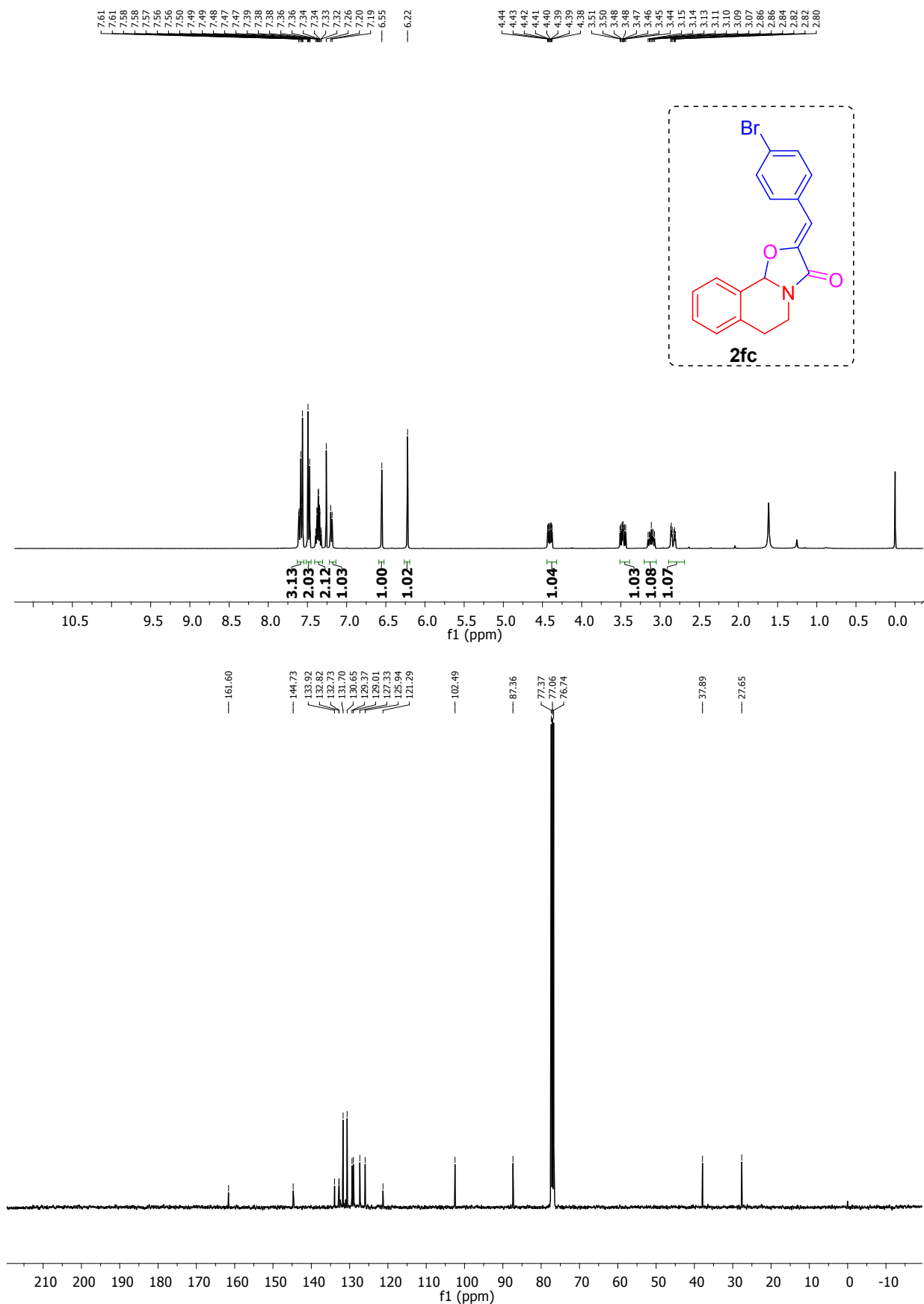
MSR\_369B2\_355  
18JUNE2020\_48 20 (0.389) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (17:27-(1:11+31:61))

XEVO-G2-XS-QToF  
1: TOF MS ES+  
5.44e7



HRMS spectrum of compound 2ec





**<sup>1</sup>H & <sup>13</sup>C spectra of compound 2fc**  
S97

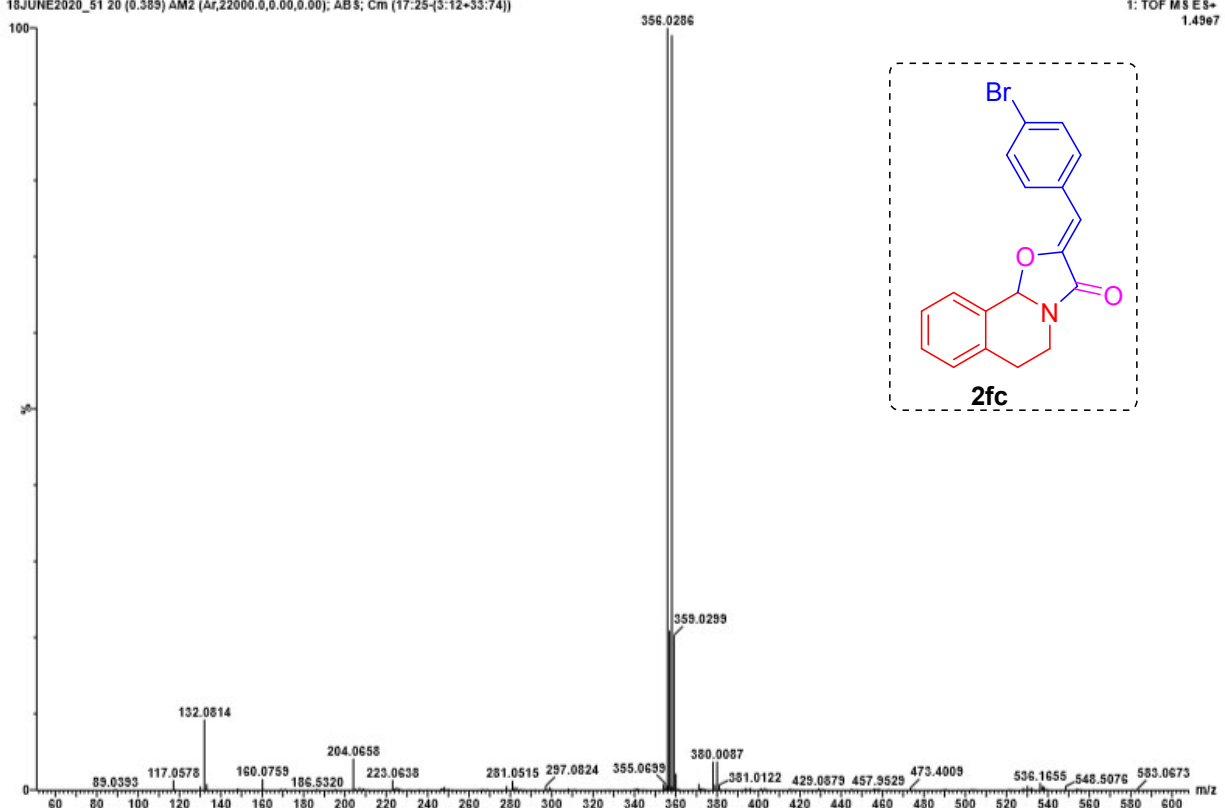
MSR\_369B1\_355

18JUNE2020\_51 20 (0.389) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (17:25-(3:12+33:74))

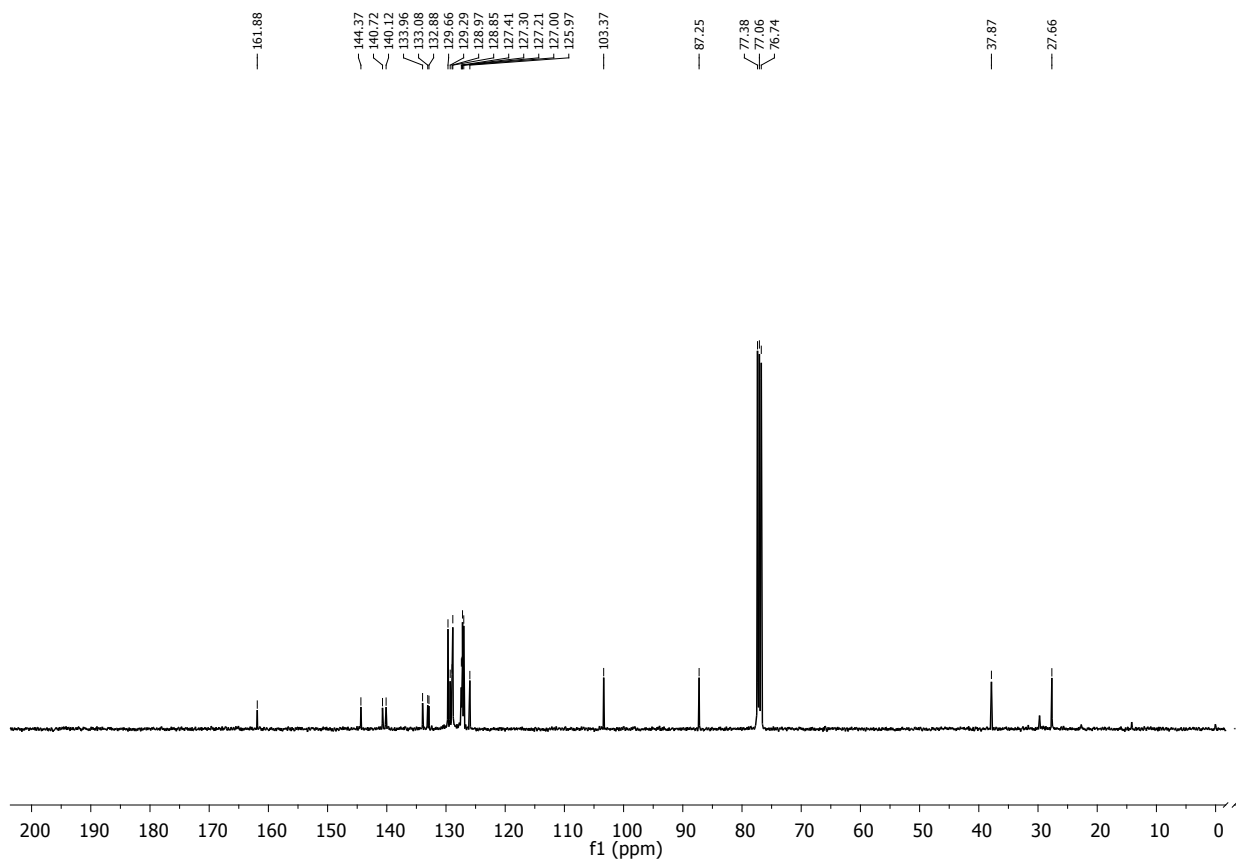
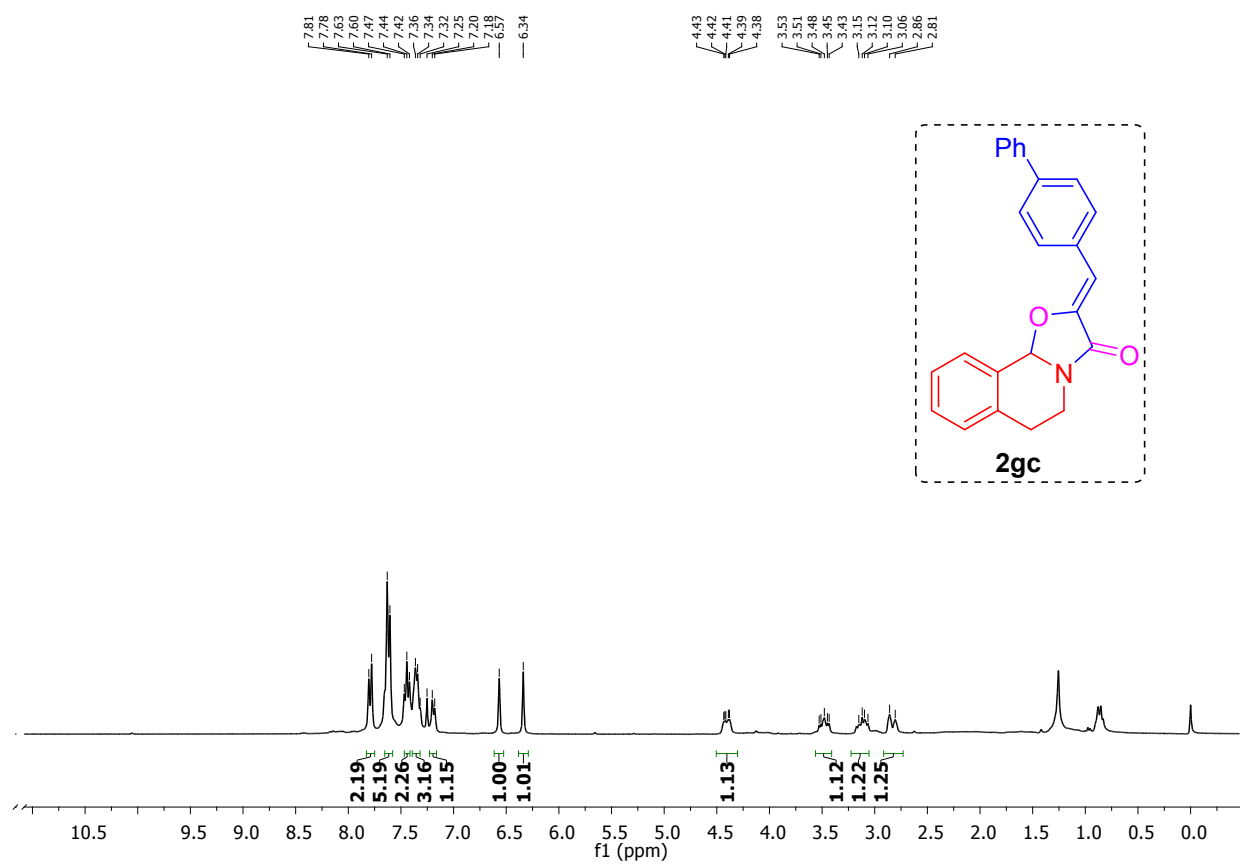
XEVO-G2-XS-QToF

1: TOF MS ES+

1.49e7



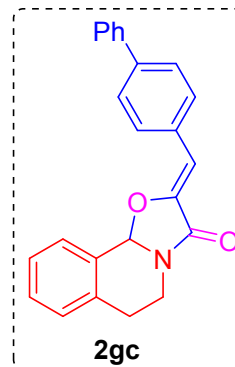
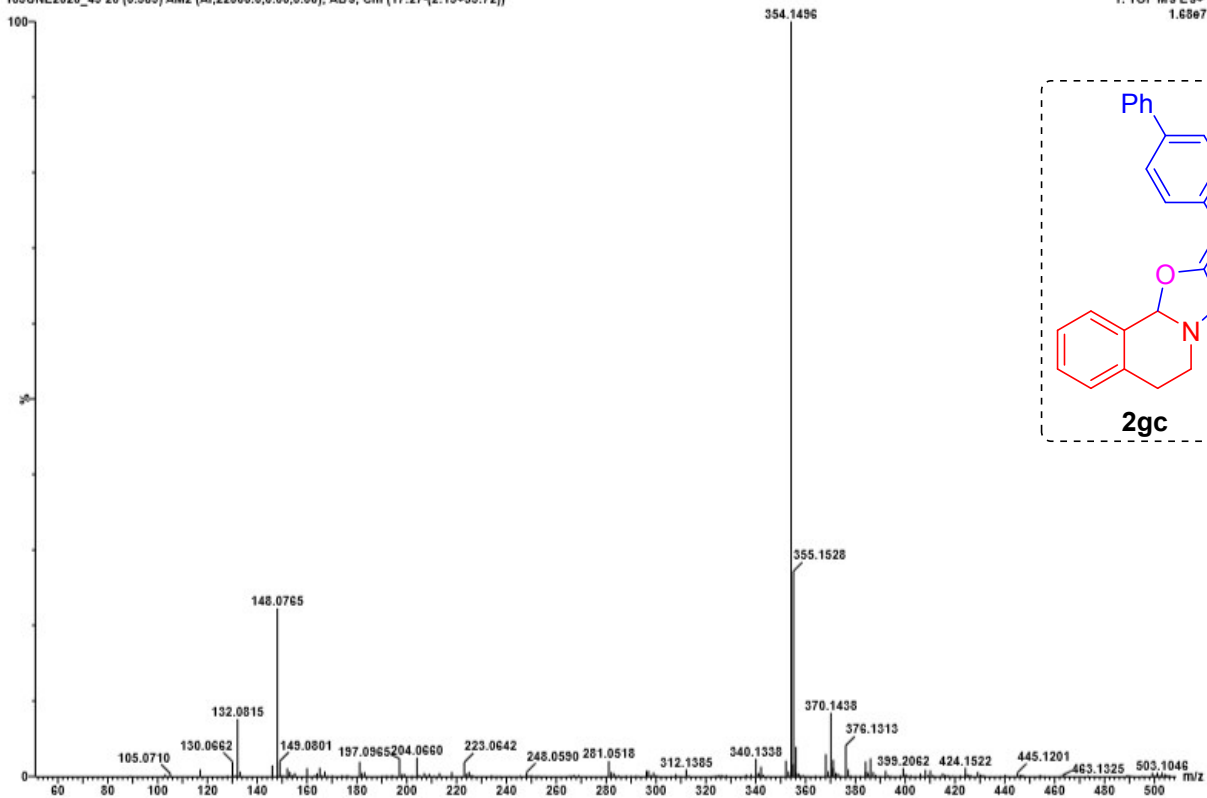
HRMS spectrum of compound 2fc



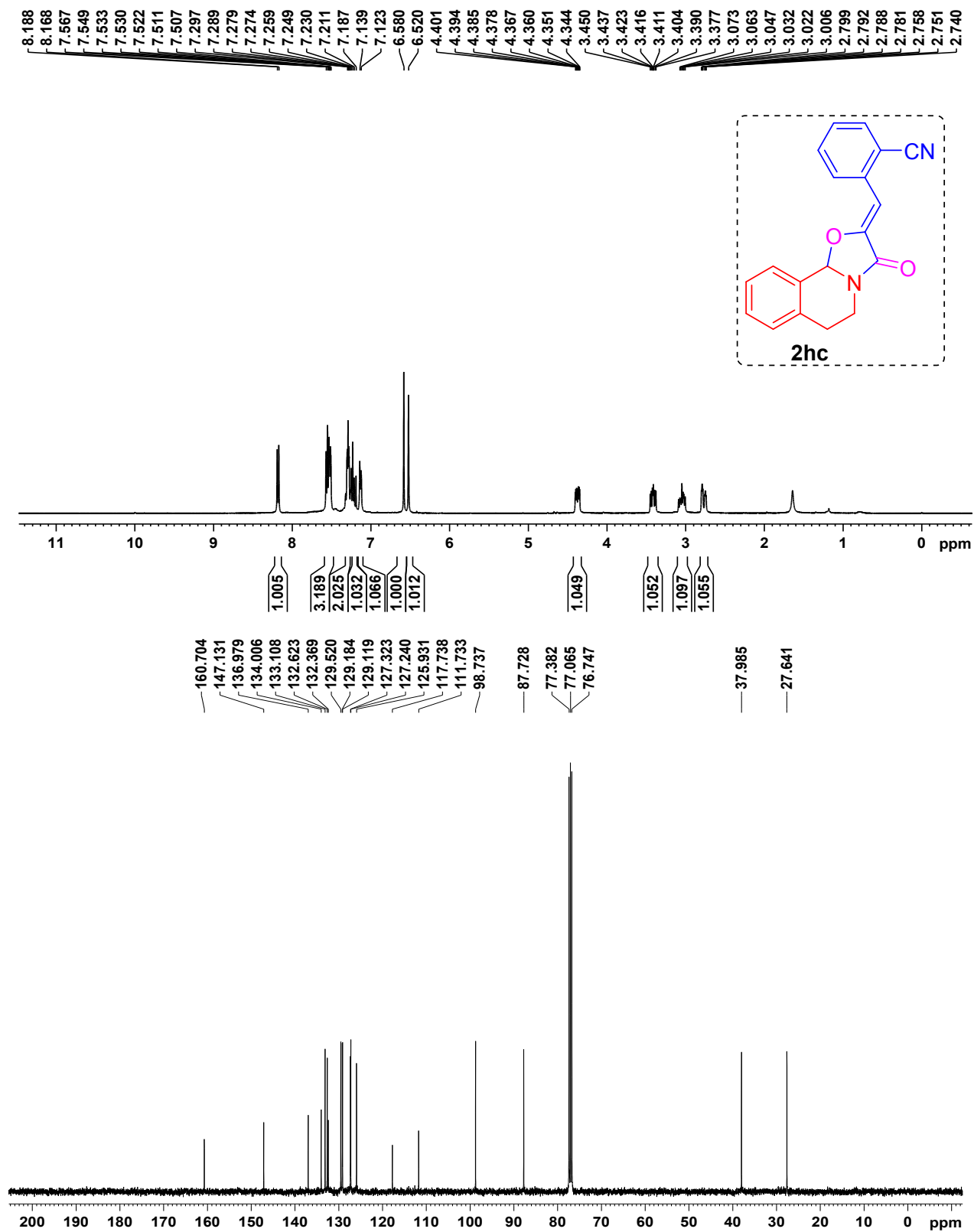
**<sup>1</sup>H & <sup>13</sup>C spectra of compound 2gc**

MSR\_363B\_353  
15JUNE2020\_49 20 (0.385) AM2 (Ar,22000.0,0.00,0.00); ABS; Cm (17:27-[2:13+33:72])

XEVO-G2-XS-QToF  
1: TOF MS ES+  
1.6867



HRMS spectrum of compound 2gc



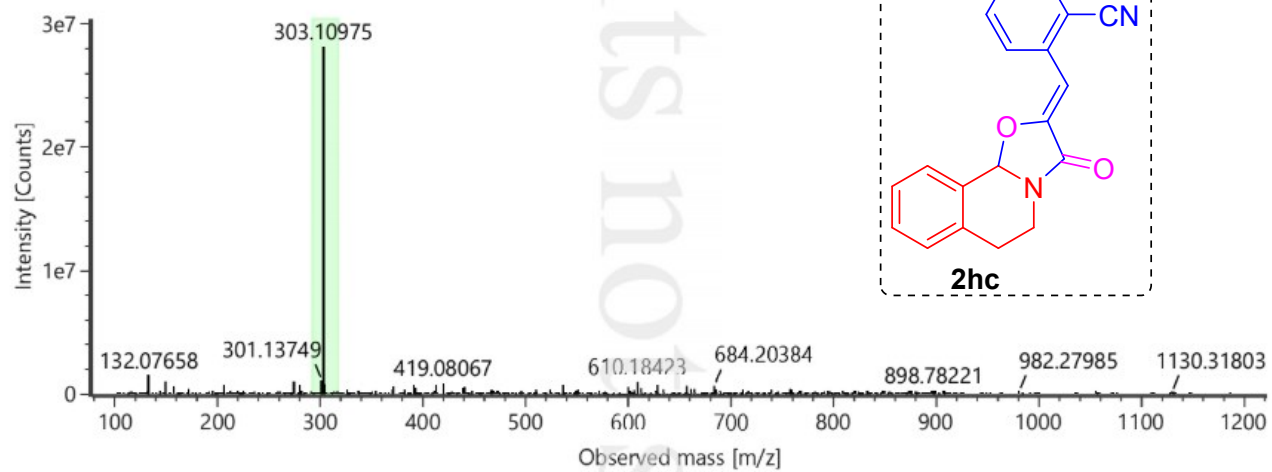
**<sup>1</sup>H & <sup>13</sup>C spectra of compound 2hc**

Component name: C19H14N2O2

Item name: MSR\_373\_B\_303

Item description:

Channel name: Low energy : Time 0.3263 +/- 0.0644 minutes

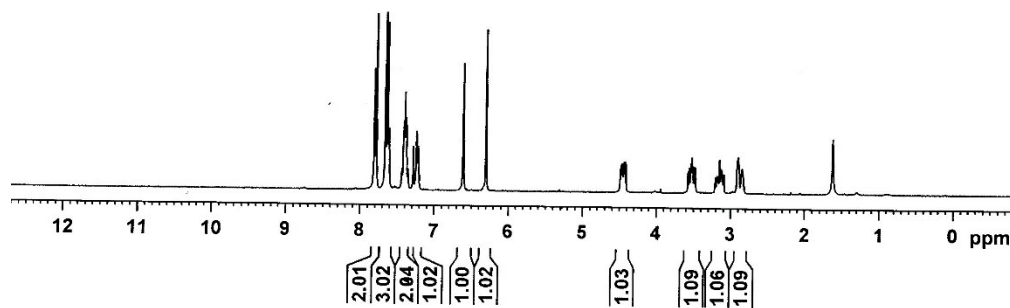
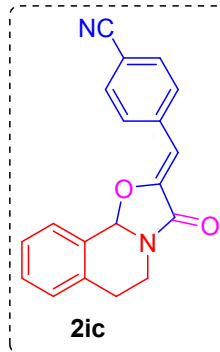


HRMS Spectrum of compound 2hc

7.814  
7.786  
7.664  
7.636  
7.612  
7.438  
7.414  
7.408  
7.399  
7.389  
7.384  
7.378  
7.359  
7.287  
7.243  
7.221  
6.611  
6.302  
4.489  
4.479  
4.468  
4.458  
4.445  
4.435  
4.424  
4.414  
3.572  
3.555  
3.538  
3.527  
3.521  
3.511  
3.493  
3.476  
3.150  
3.129  
3.117  
2.914  
2.899  
2.888  
2.860  
2.848



NAME PROTON\_UOM  
EXPNO 1  
PROCNO 1  
Date\_ 20200320  
Time 15.51  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 362  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

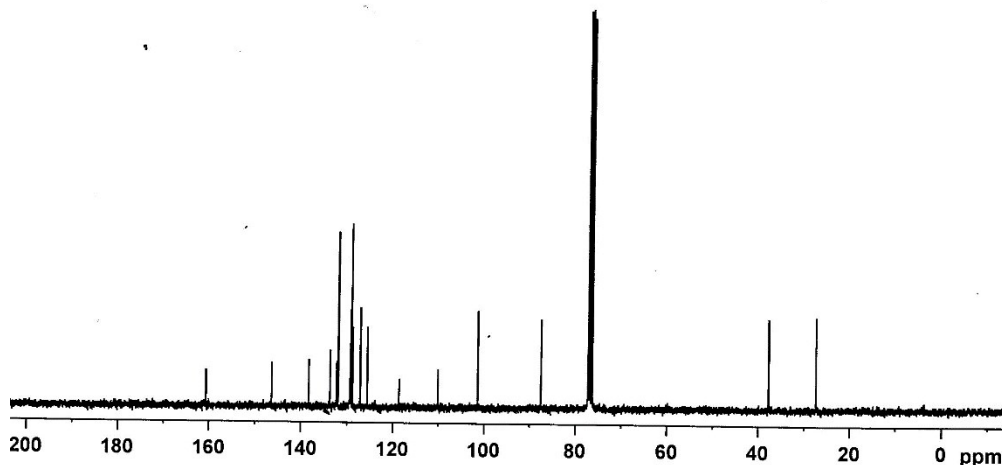
160.66  
146.30  
138.21  
133.59  
132.16  
131.87  
129.19  
129.01  
128.71  
127.05  
125.51  
118.58  
110.05  
101.33  
87.44  
77.08  
76.65  
76.23  
37.66  
27.27



NAME RA-BR-3-373 B  
EXPNO 1  
PROCNO 1  
Date\_ 20200320  
Time 15.43  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 737  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

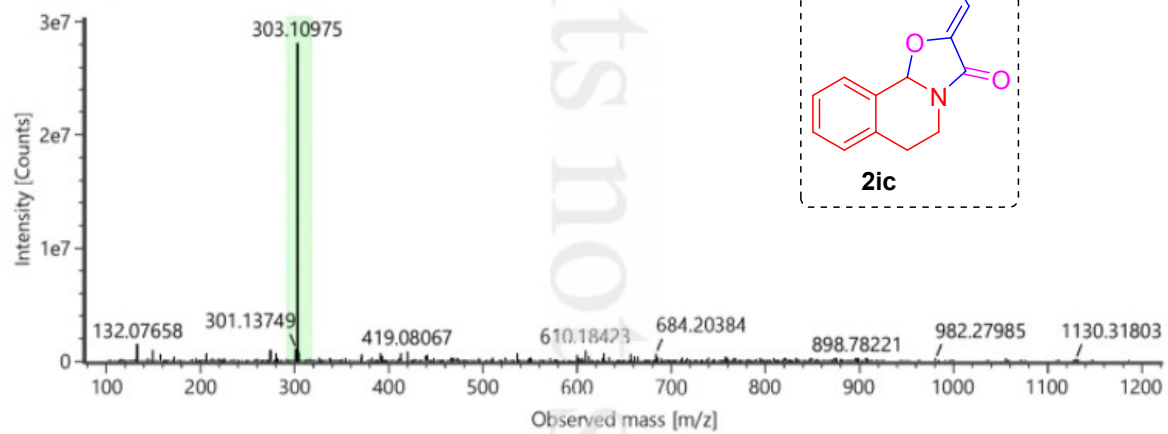
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677728 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ic  
S103

Component name: C<sub>19</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>

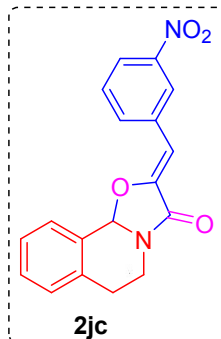
Item description:



MS Spectrum of Compound 2ic

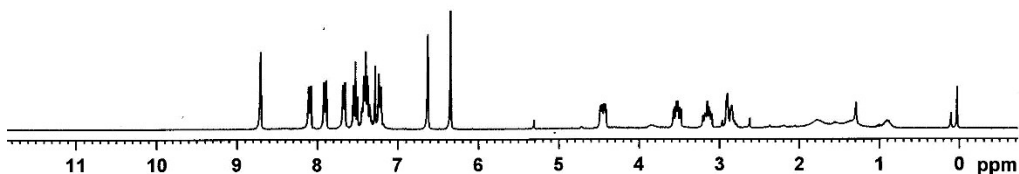


8.710  
8.704  
8.107  
8.082  
7.913  
7.888  
7.679  
7.654  
7.648  
7.522  
7.495  
7.442  
7.419  
7.395  
7.389  
7.371  
7.346  
7.277  
7.231  
7.207  
6.626  
6.344  
4.483  
4.473  
4.462  
4.452  
4.439  
4.428  
4.418  
3.555  
3.538  
3.527  
3.521  
3.511  
3.494  
3.477  
3.149  
3.128  
2.910  
2.900  
2.895  
2.856  
2.846



NAME RA-BR-4-84B  
EXPNO 3  
PROCNO 1  
Date\_ 20200514  
Time\_ 14.19  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 322.5  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



1.01  
1.08  
1.08  
1.09  
1.14  
2.05  
1.14  
1.00  
1.02  
1.09  
1.17  
1.16  
1.22

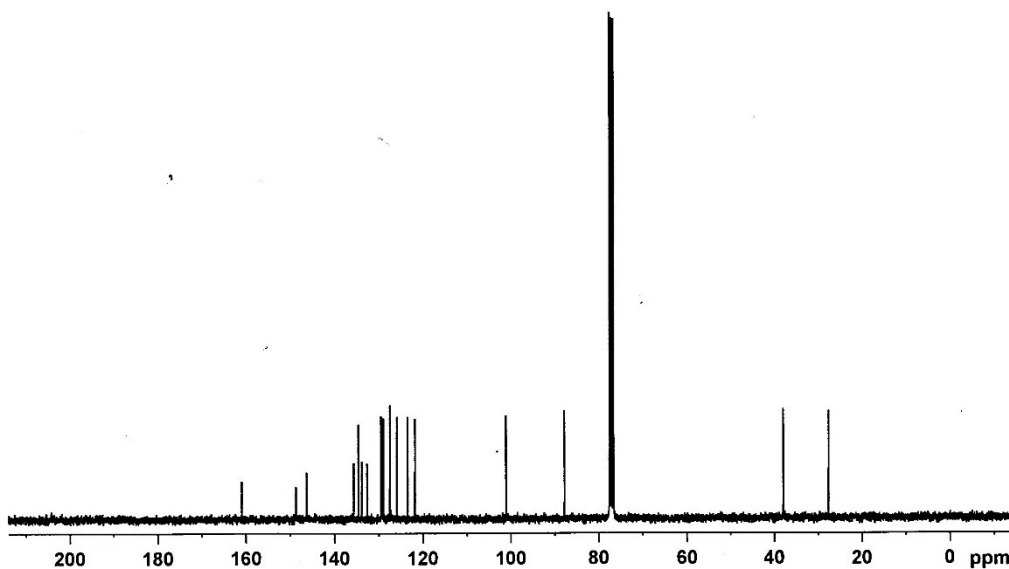
160.99  
148.75  
146.32  
135.69  
134.62  
133.88  
132.64  
129.52  
129.31  
129.00  
127.52  
125.93  
123.49  
121.81  
101.11  
87.74  
77.44  
77.02  
76.60  
37.97  
27.62



NAME RA-BR-4-84B  
EXPNO 2  
PROCNO 1  
Date\_ 20200514  
Time\_ 13.45  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1068  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waitz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677441 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



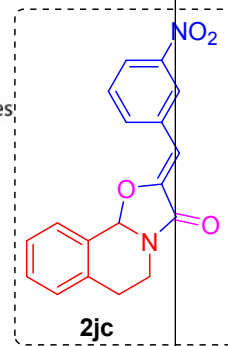
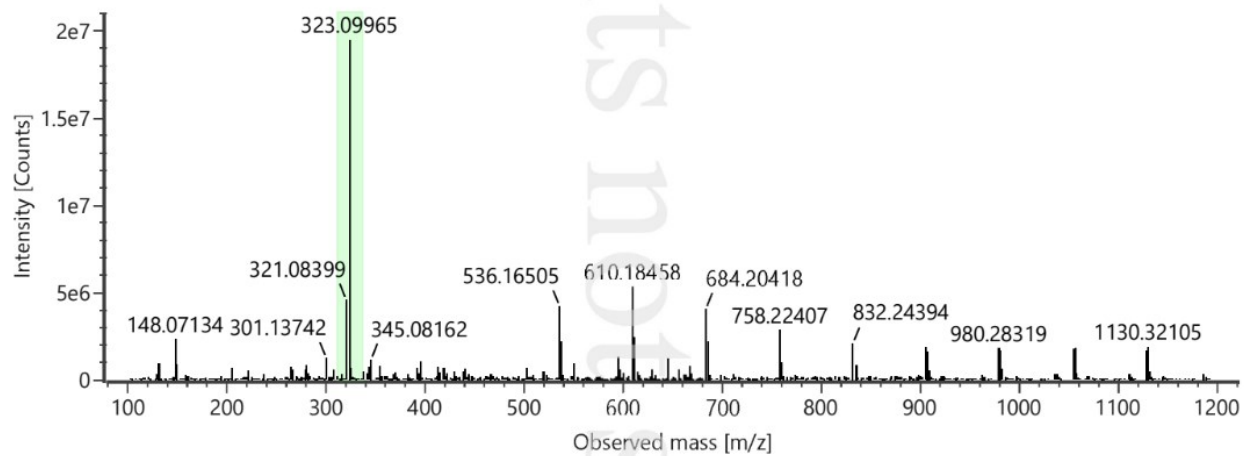
<sup>1</sup>H & <sup>13</sup>C spectra of compound 2jc

Component name: C<sub>18</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>

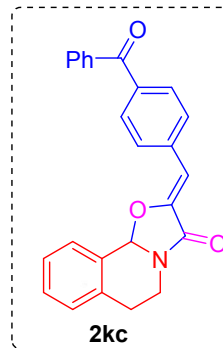
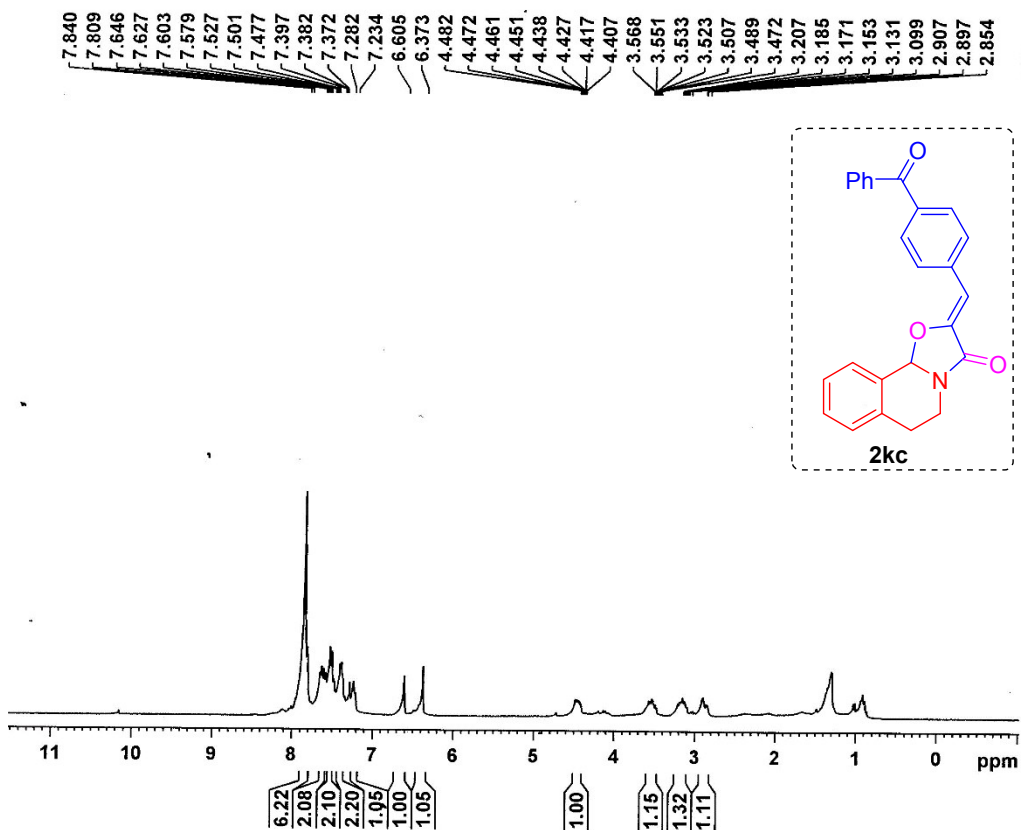
Item name: MSR\_84\_B\_323

Item description:

Channel name: Low energy : Time 0.3210 +/- 0.0622 minutes

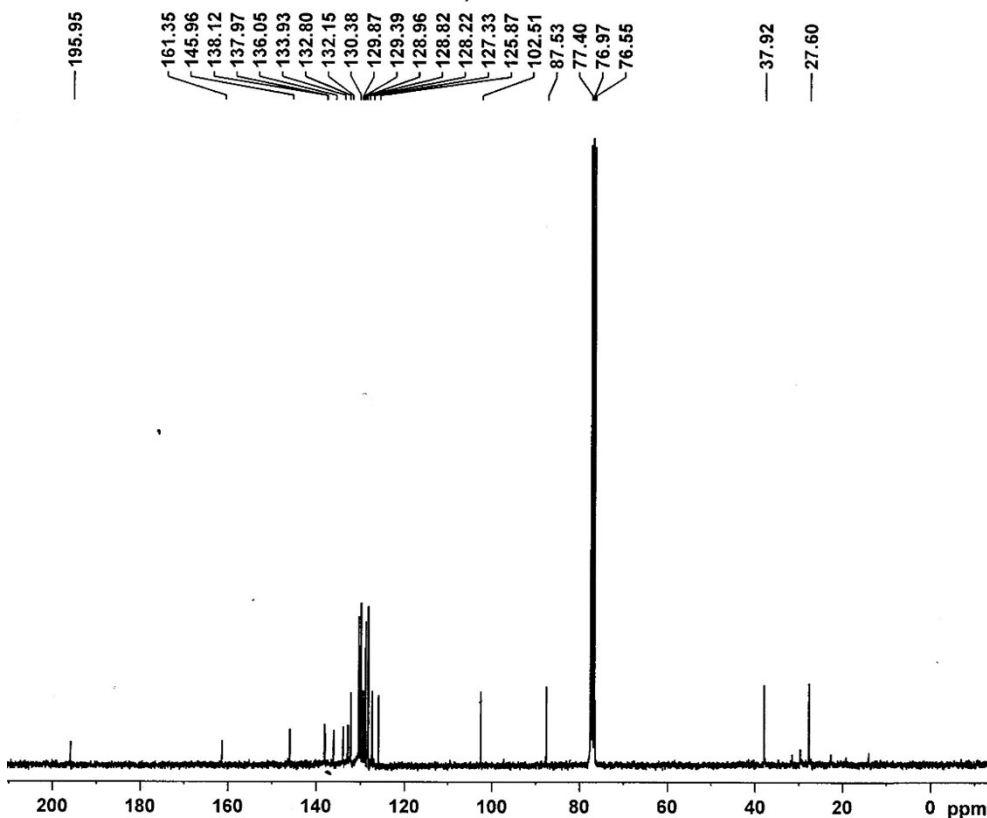


HRMS Spectrum of Compound 2jc



NAME RA-BR-3-364B  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20200321  
 Time 4.51  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 362  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 -1.00 dB  
 PL1W 13.28156662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME RA-BR-3-364 B  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20200320  
 Time 23.44  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 5920  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 2580.3  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

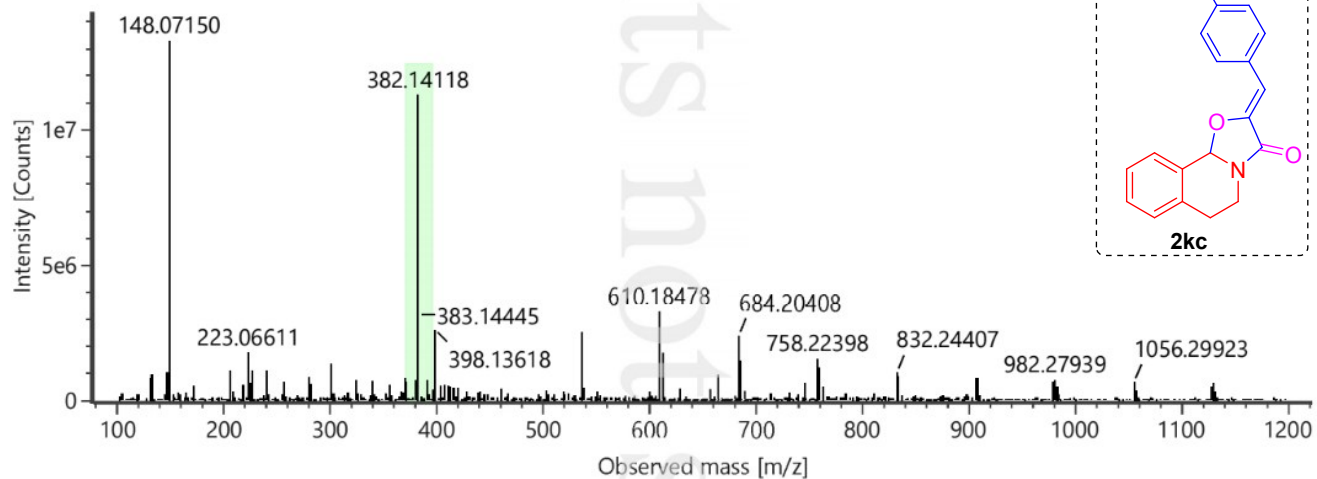
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 12.75 usec  
 PL1 -1.00 dB  
 PL1W 39.52846909 W  
 SFO1 75.4752953 MHz  
 ===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.46 dB  
 PL13 16.00 dB  
 PL2W 13.28156662 W  
 PL12W 0.37778899 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677477 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1H & 13C spectra of compound 2kc  
 S107

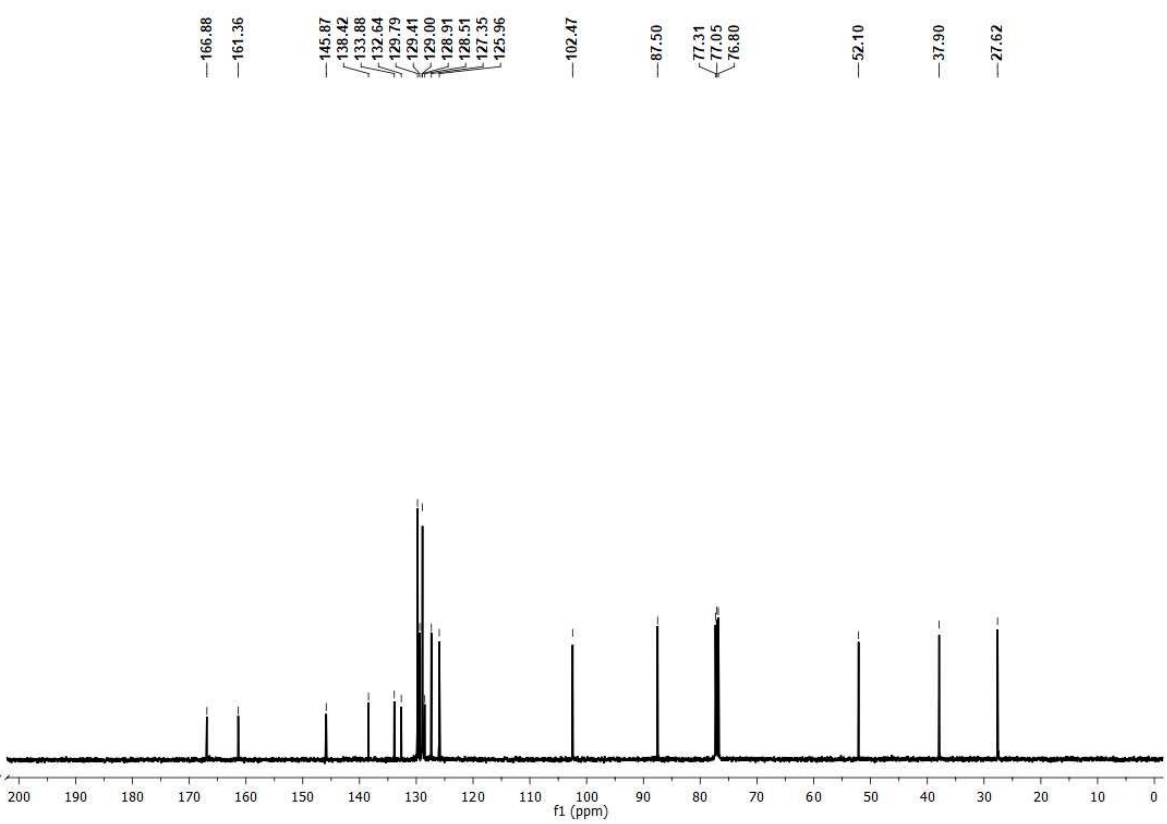
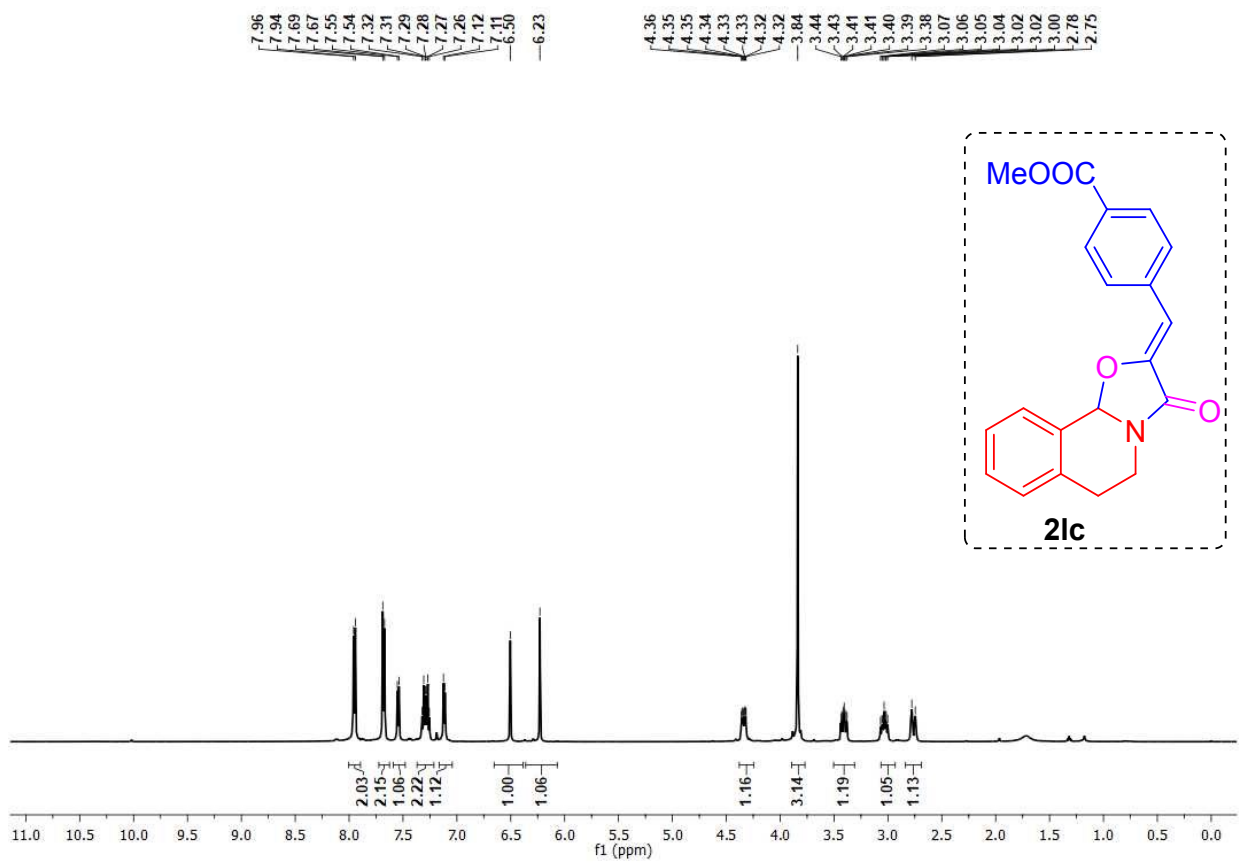
**Component name: C<sub>25</sub>H<sub>19</sub>NO<sub>3</sub>**

Item name: MSR\_364\_B\_382  
Item description:

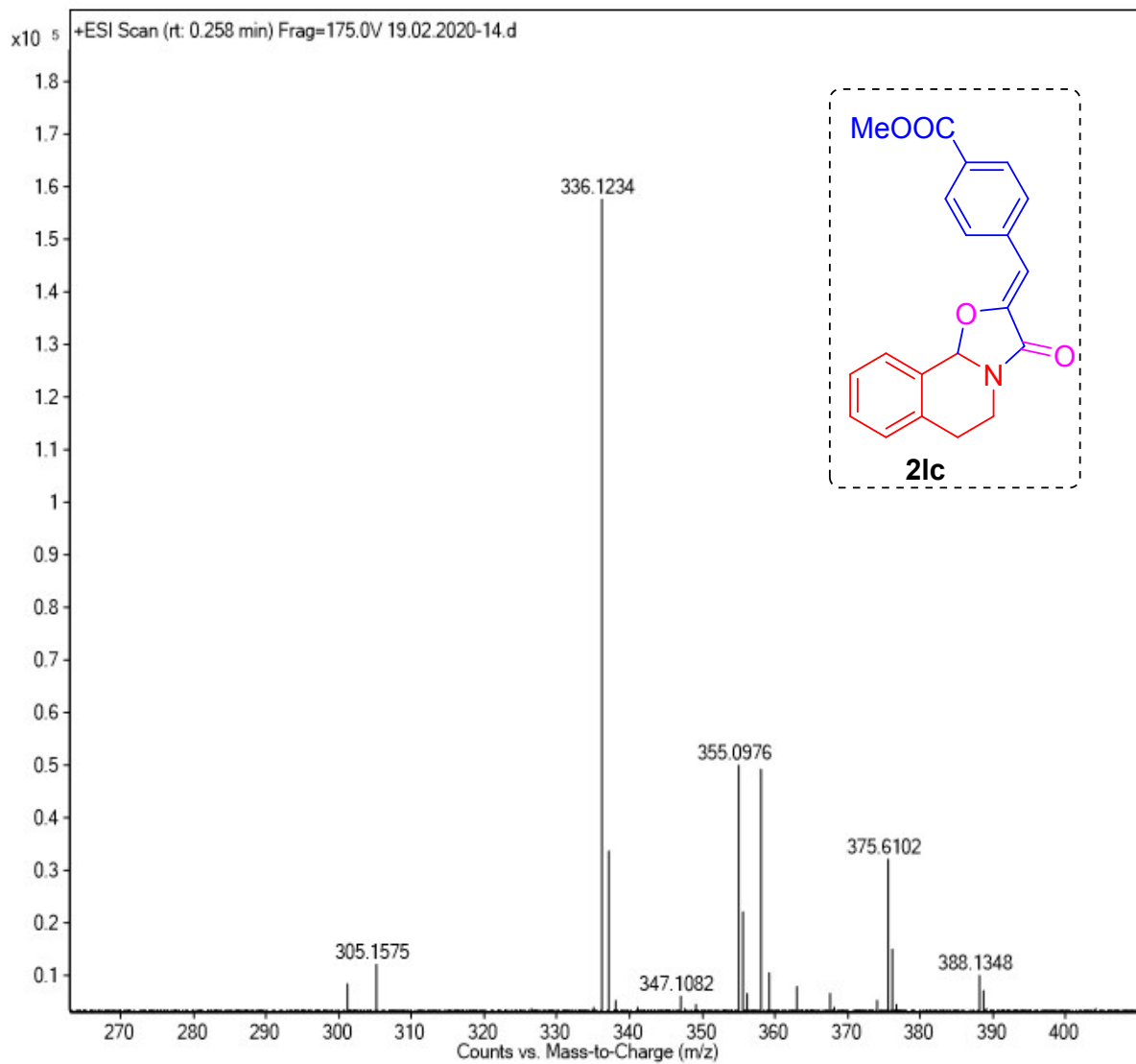
Channel name: Low energy : Time 0.3328 +/- 0.0613 minutes



**HRMS Spectrum of Compound 2kc**



**<sup>1</sup>H & <sup>13</sup>C spectra of compound 2lc**

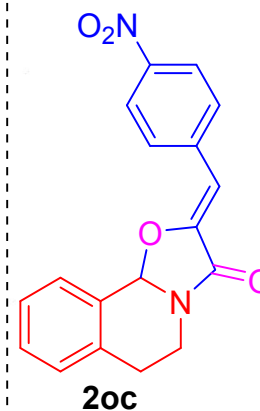


**HRMS spectrum of compound 2lc**

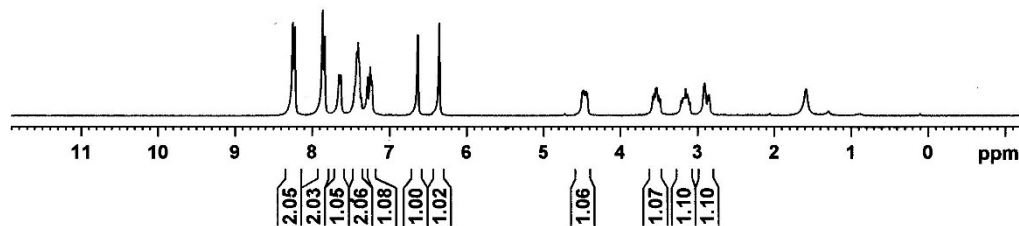
8.247  
8.218  
7.861  
7.832  
7.650  
7.626  
7.418  
7.410  
7.402  
7.362  
7.282  
7.245  
7.223  
6.631  
6.352  
4.497  
4.487  
4.476  
4.466  
4.453  
4.443  
4.431  
3.578  
3.561  
3.543  
3.533  
3.527  
3.517  
3.499  
3.482  
3.210  
3.188  
3.174  
3.155  
3.134  
3.101  
2.909  
2.854



NAME RA-BR-3-356B  
EXPNO 3  
PROCNO 1  
Date\_ 20200111  
Time\_ 19.23  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 362  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



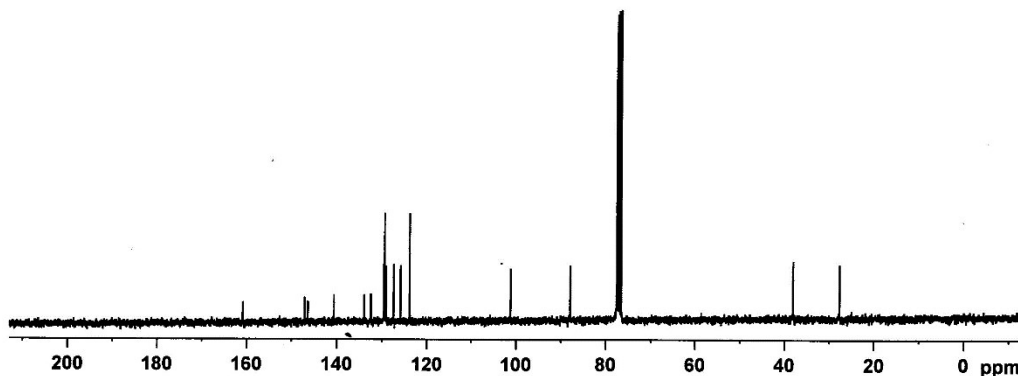
160.88  
147.10  
146.41  
140.59  
133.94  
132.43  
129.58  
129.41  
129.07  
127.43  
125.88  
123.83  
101.23  
87.89  
77.41  
76.99  
76.56  
38.03  
27.63



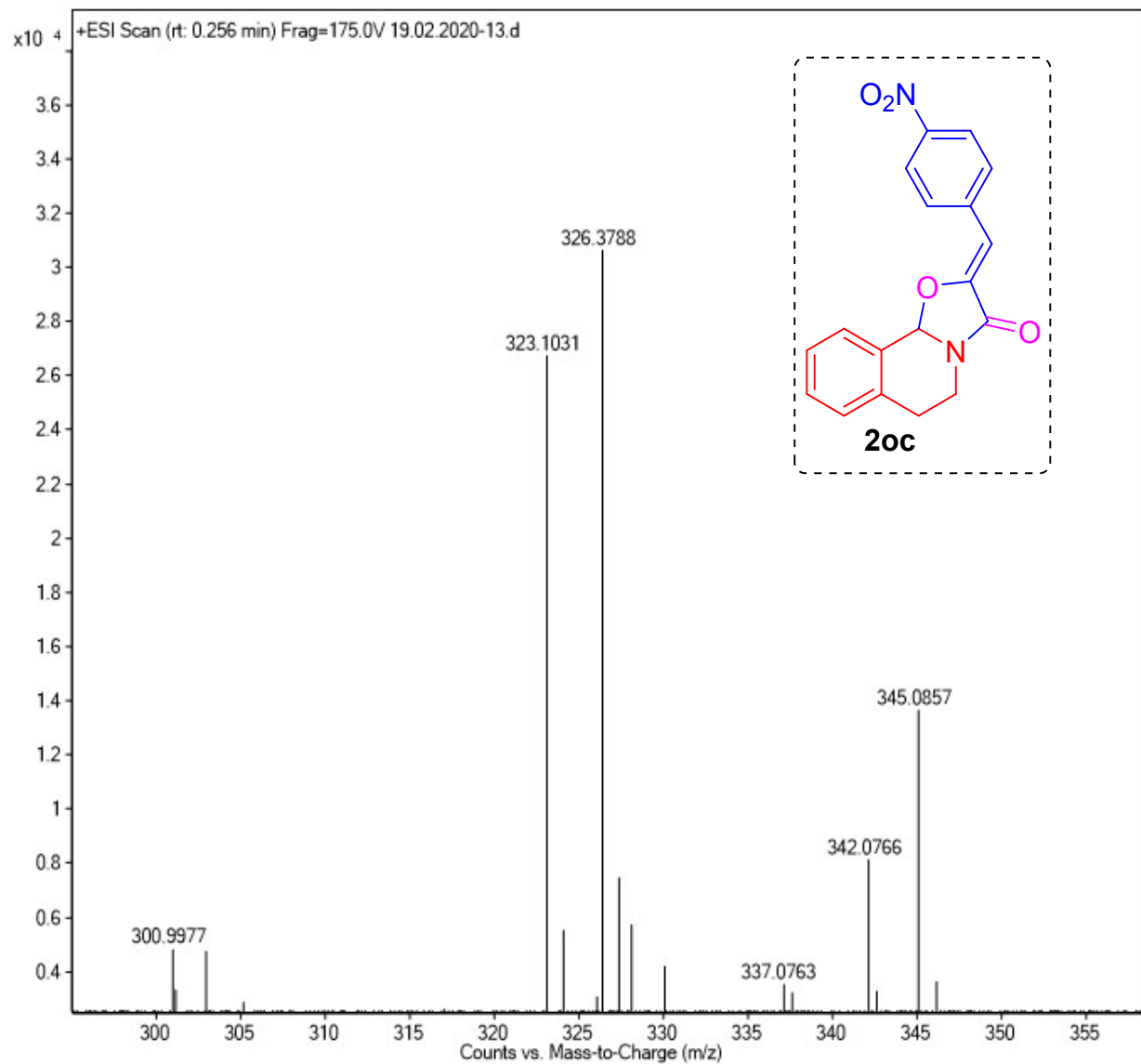
NAME RA-BR-3-356B  
EXPNO 2  
PROCNO 1  
Date\_ 20200111  
Time\_ 19.13  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 811  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 3251  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677462 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 20c



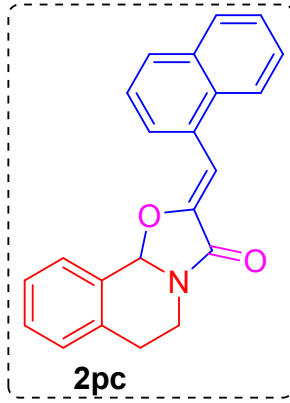
HRMS spectrum of compound **2oc**



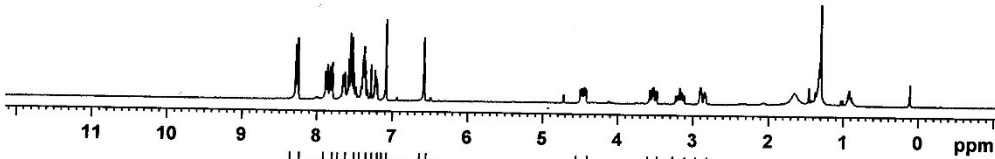
8.276  
8.252  
7.883  
7.859  
7.852  
7.821  
7.793  
7.656  
7.647  
7.626  
7.580  
7.553  
7.533  
7.528  
7.509  
7.505  
7.410  
7.391  
7.385  
7.372  
7.360  
7.352  
7.282  
7.230  
7.209  
7.085  
6.582  
4.491  
4.481  
4.470  
4.458  
4.447  
4.437  
3.574  
3.557  
3.540  
3.529  
3.523  
3.496  
3.172  
2.910  
2.898



NAME RA-BR-3-346  
EXPNO 1  
PROCNO 1  
Date\_ 20200103  
Time 16.01  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 256  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.13000000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



2.00  
2.16  
1.19  
3.00  
2.13  
1.02  
0.97  
0.94  
1.04  
1.06  
1.05  
1.05

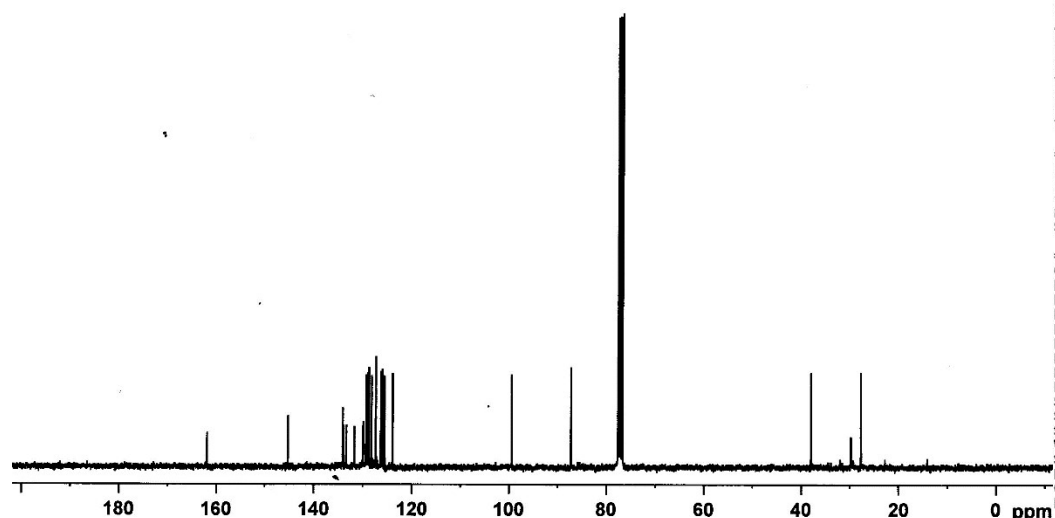
161.83  
145.16  
133.99  
133.84  
133.25  
131.61  
129.82  
129.24  
128.90  
128.64  
128.09  
127.25  
127.22  
126.22  
125.94  
125.75  
125.46  
123.83  
98.34  
87.13  
77.42  
77.00  
76.58  
37.86  
27.62



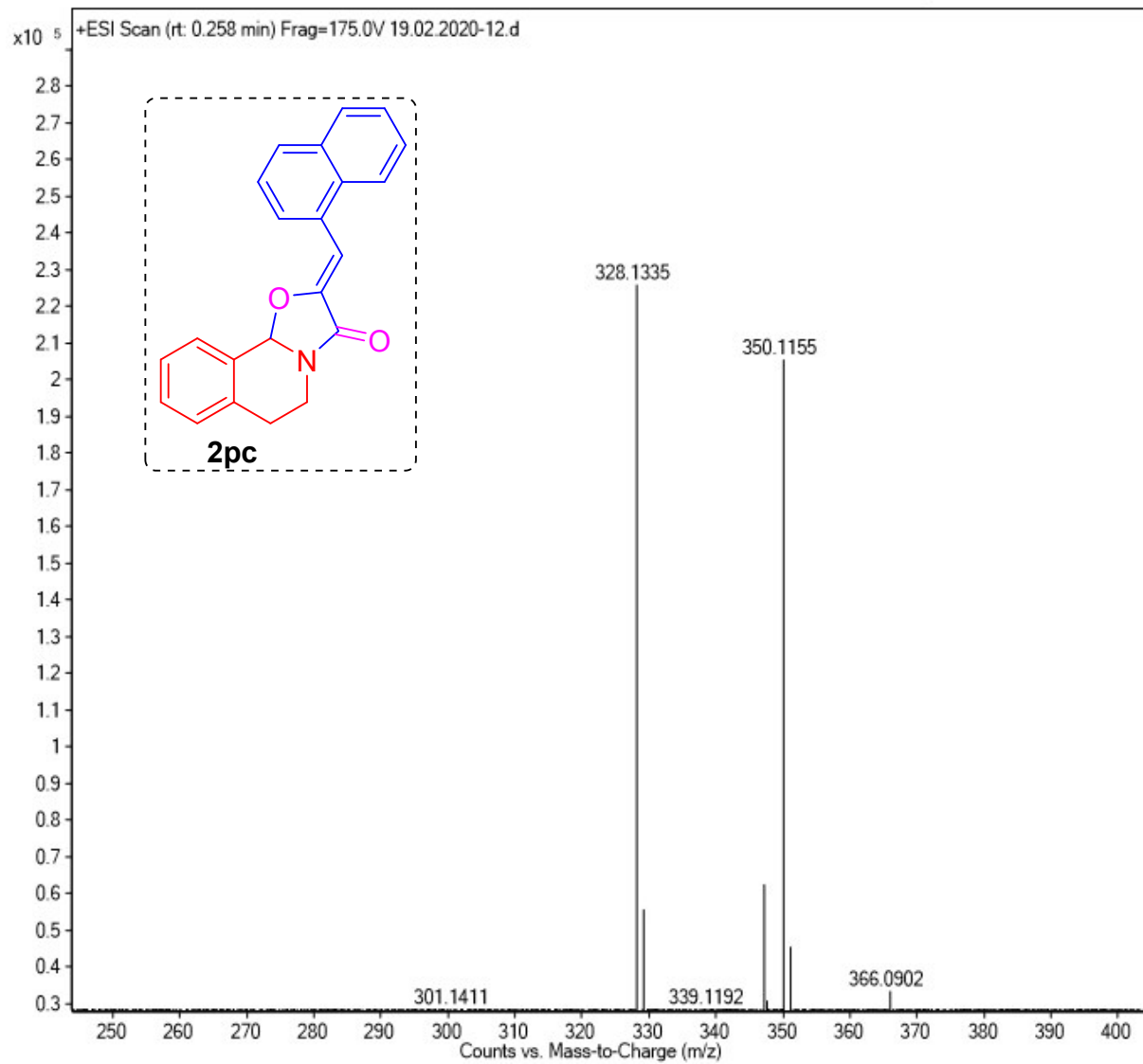
NAME RA-BR-3-346  
EXPNO 2  
PROCNO 1  
Date\_ 20200104  
Time 12.09  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1500  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 3649.1  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waitz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL12W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677454 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 2pc

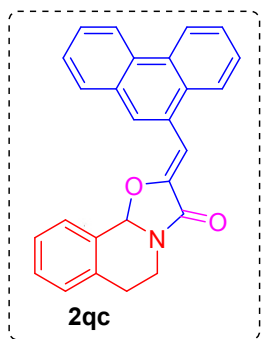


**HRMS spectrum of compound 2pc**

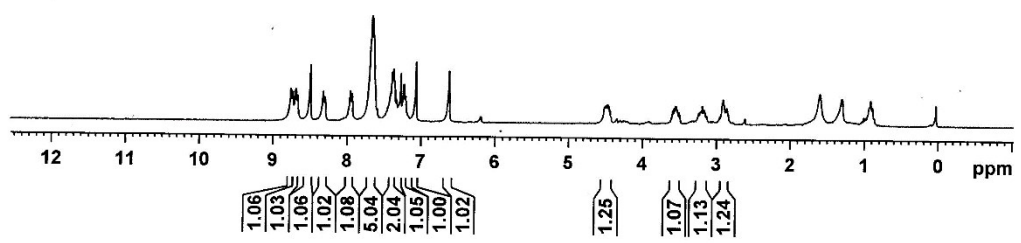
8.763  
8.735  
8.696  
8.671  
8.499  
8.328  
8.304  
7.964  
7.941  
7.683  
7.673  
7.665  
7.650  
7.643  
7.600  
7.394  
7.379  
7.339  
7.277  
7.238  
7.216  
7.070  
6.620  
4.517  
4.507  
4.497  
4.485  
4.473  
4.463  
4.452  
4.441  
3.593  
3.575  
3.569  
3.547  
3.515  
3.211  
3.191  
3.168  
2.911  
2.898  
2.869  
2.858



NAME RA-BR-3-371B  
EXPNO 1  
PROCNO 1  
Date\_ 20200614  
Time 15.16  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084650 sec  
RG 322.5  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



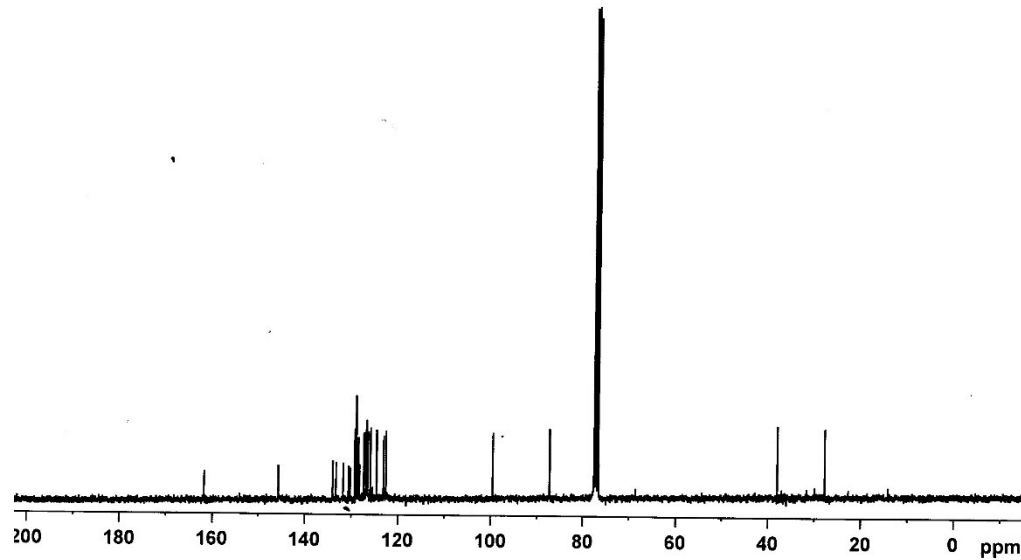
161.77  
145.68  
134.04  
133.31  
131.77  
130.64  
130.60  
130.22  
129.29  
128.95  
128.76  
128.49  
128.25  
127.31  
126.84  
126.78  
126.72  
126.48  
125.91  
124.59  
123.08  
122.57  
99.50  
87.20  
77.44  
77.01  
76.59  
37.91  
27.66



NAME RA-BR-3-371B  
EXPNO 1  
PROCNO 1  
Date\_ 20200614  
Time 16.50  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2576  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 2298.8  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677435 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

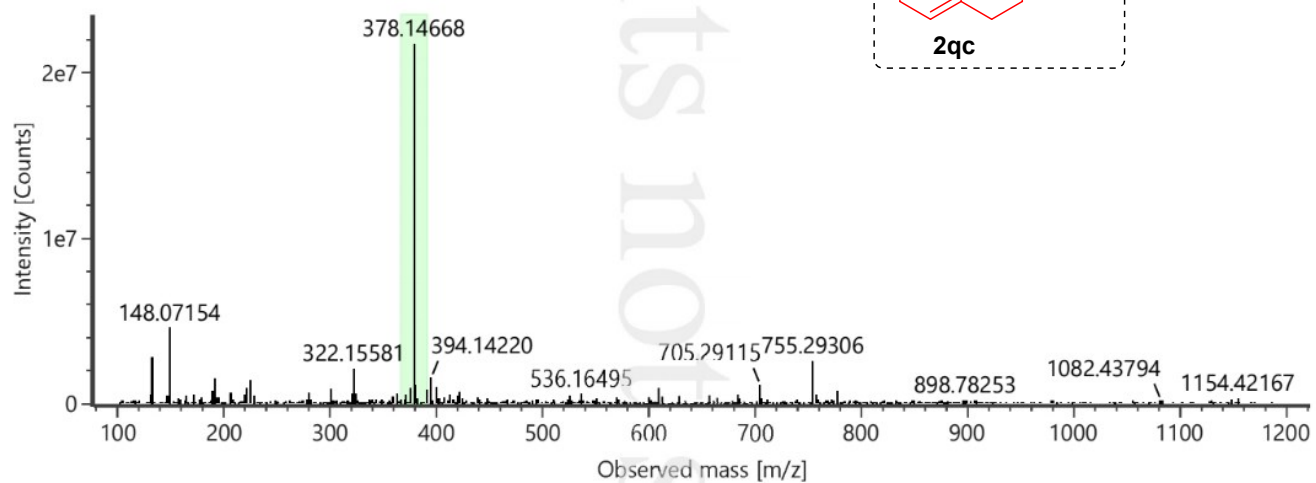
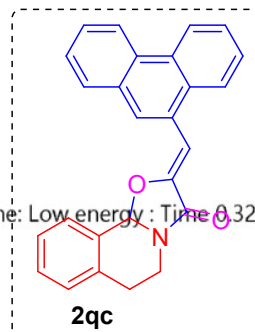


<sup>1</sup>H & <sup>13</sup>C spectra of compound 2qc

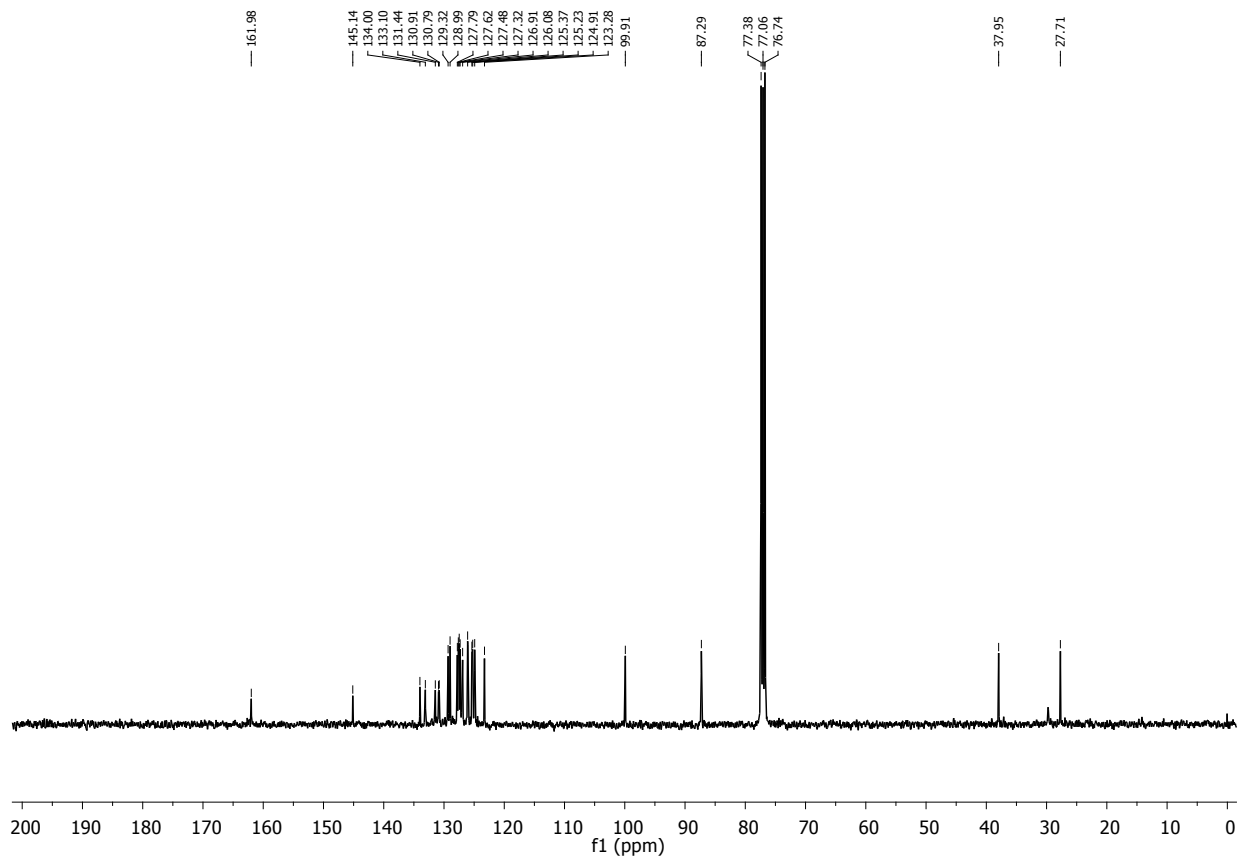
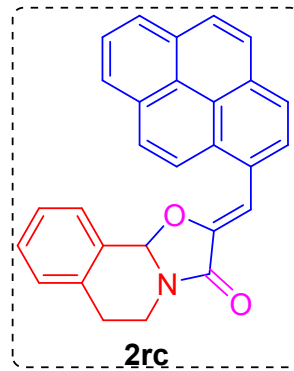
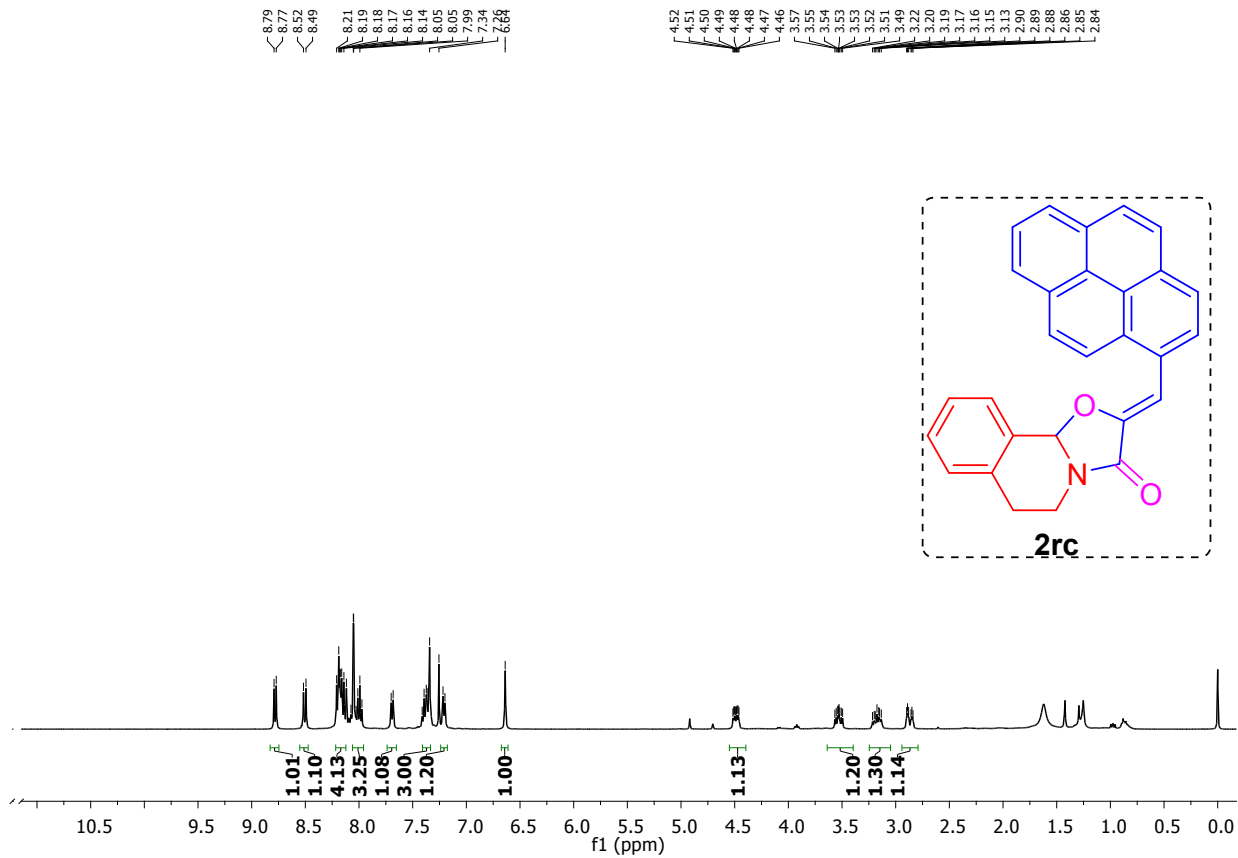
Component name: C<sub>26</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub>

Item name: MSR\_37B\_378  
Item description:

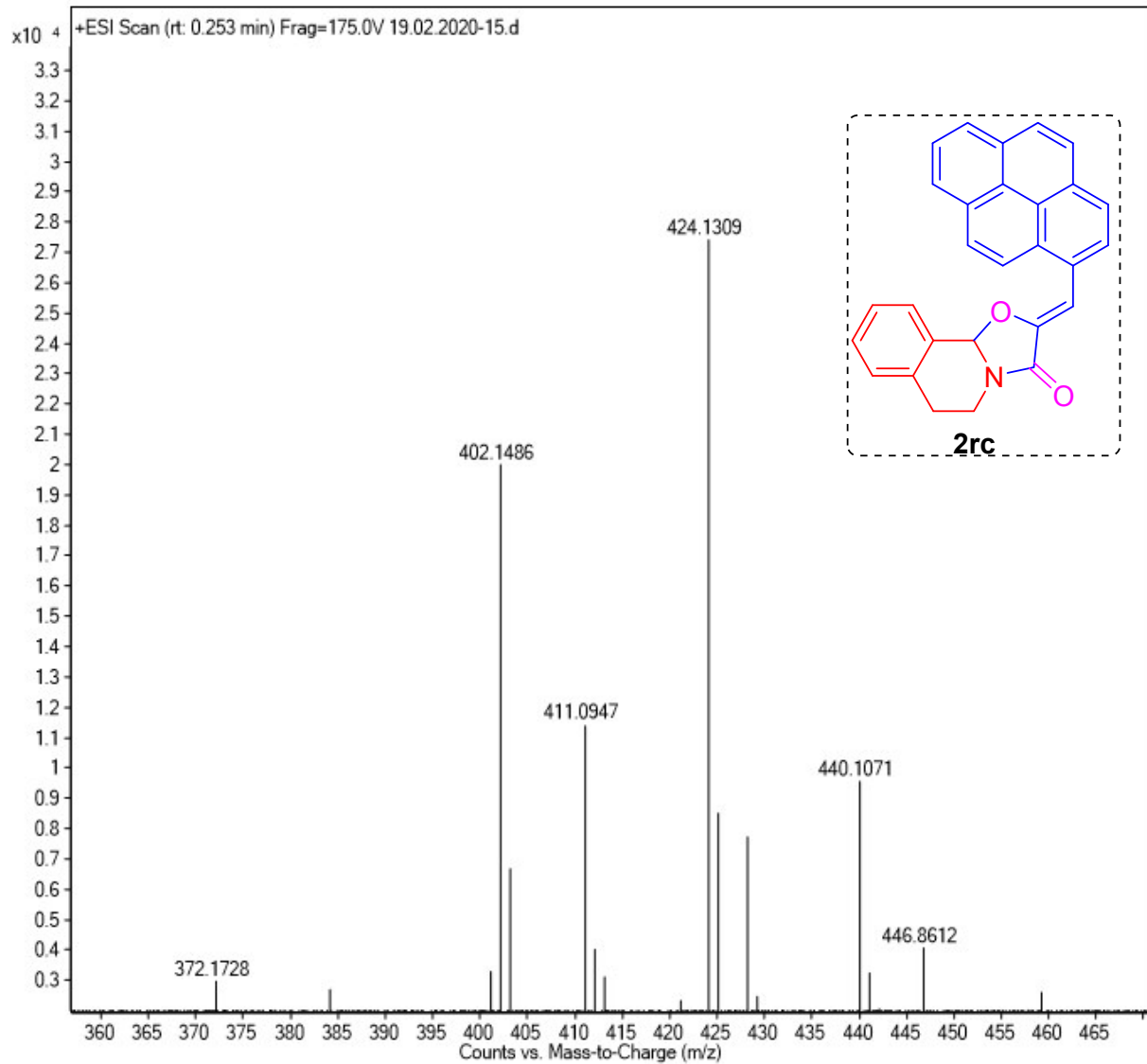
Channel name: Low energy : Time 0.3291 +/- 0.0613 minutes

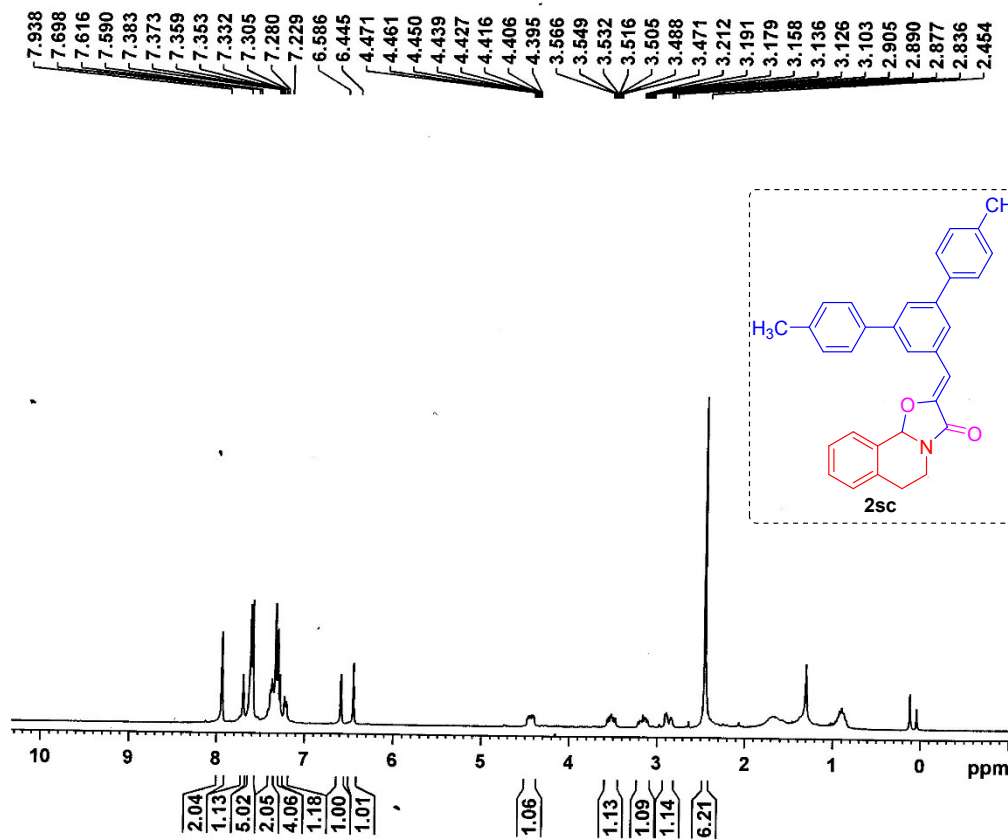


HRMS Spectrum of compound 2qc



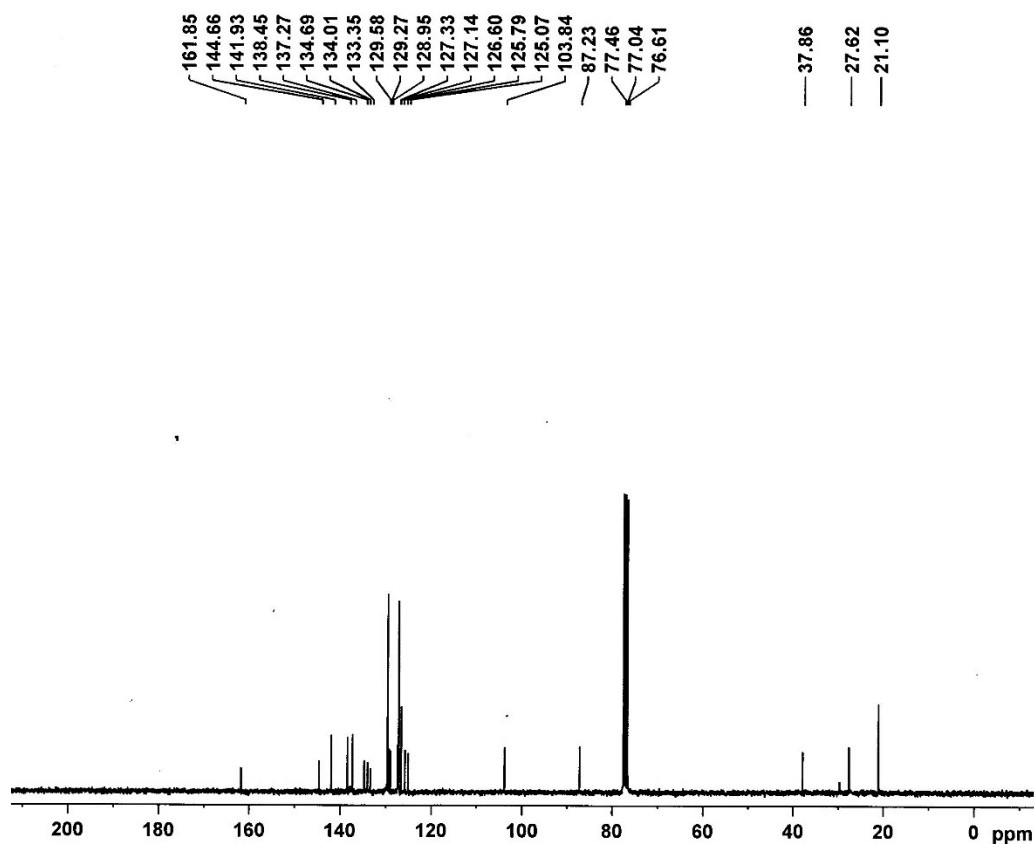
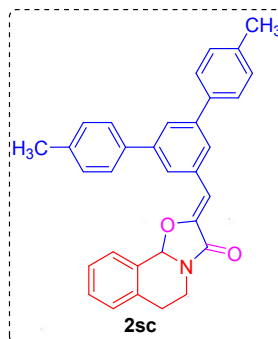
**<sup>1</sup>H & <sup>13</sup>C spectra of compound 2rc**  
S117





NAME RA-BR-4-86B  
EXPNO 3  
PROCNO 1  
Date\_ 20200515  
Time 21.35  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 228.1  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



NAME RA-BR-4-86B  
EXPNO 4  
PROCNO 1  
Date\_ 20200515  
Time 21.49  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1281  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

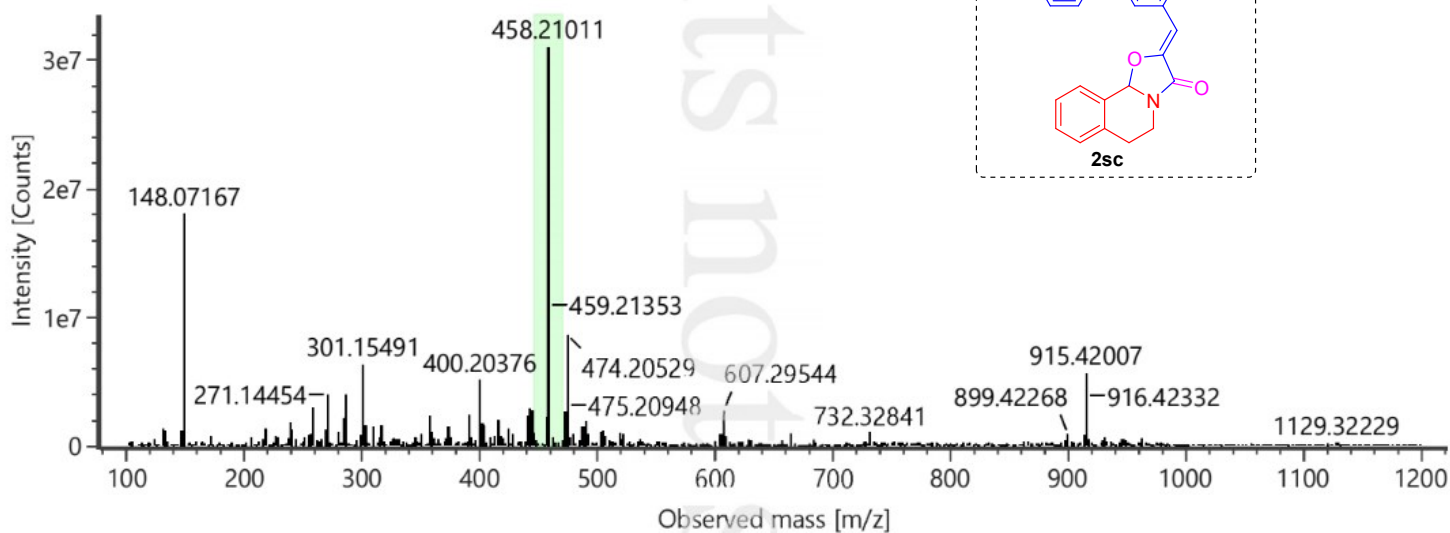
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677427 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2sc  
S119

Component name: C32H27NO2

Item name: MSR\_86B\_438

Item description:



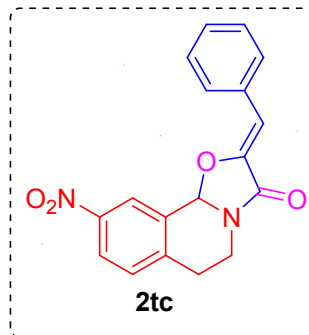
HRMS Spectrum of Compound 2sc



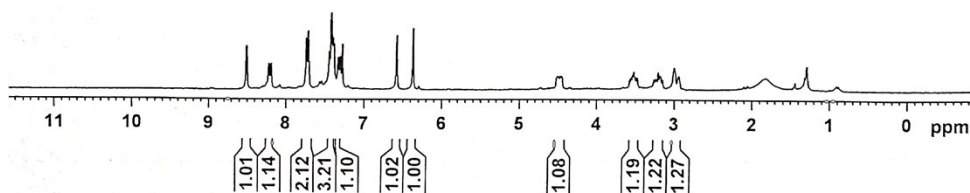
8.509  
8.225  
8.197  
7.741  
7.716  
7.448  
7.422  
7.398  
7.388  
7.332  
7.308  
7.281  
6.580  
6.370  
4.515  
4.503  
4.494  
4.478  
4.470  
4.458  
3.573  
3.556  
3.539  
3.524  
3.494  
3.478  
3.264  
3.244  
3.208  
3.185  
3.153  
3.000  
2.945



NAME RA-BR-4-170C  
EXPNO 3  
PROCNO 1  
Date\_ 20201025  
Time 22.00  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 574.7  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



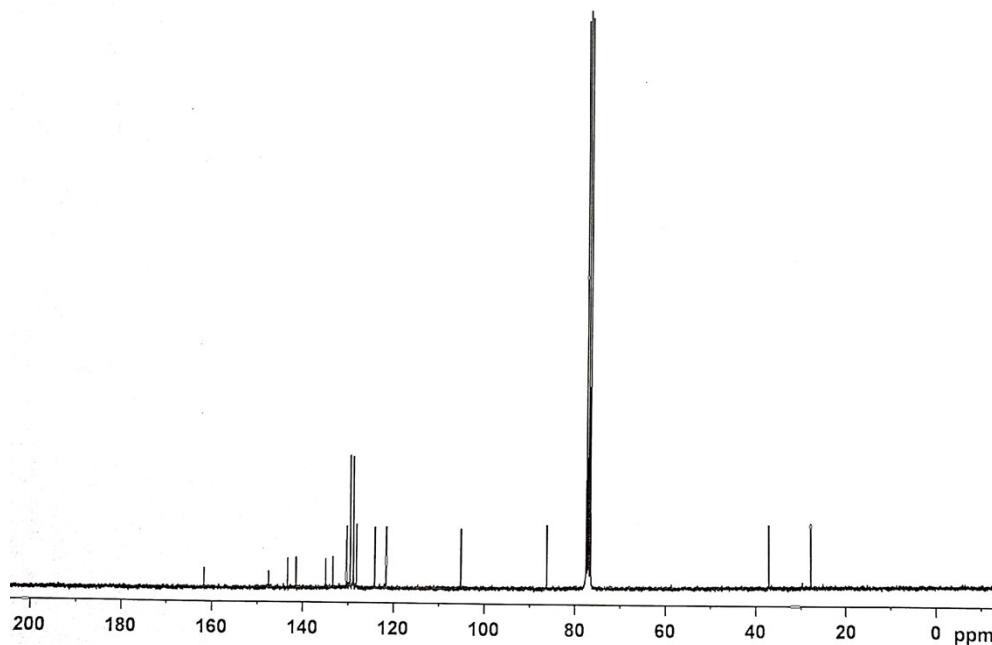
161.66  
147.45  
143.27  
141.35  
134.88  
133.23  
130.23  
129.42  
128.73  
128.03  
124.05  
121.52  
105.11  
86.14  
77.45  
77.02  
76.60  
37.13  
27.78



NAME RA-BR-4-170C  
EXPNO 4  
PROCNO 1  
Date\_ 20201026  
Time 4.31  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 6000  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 456.1  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677424 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

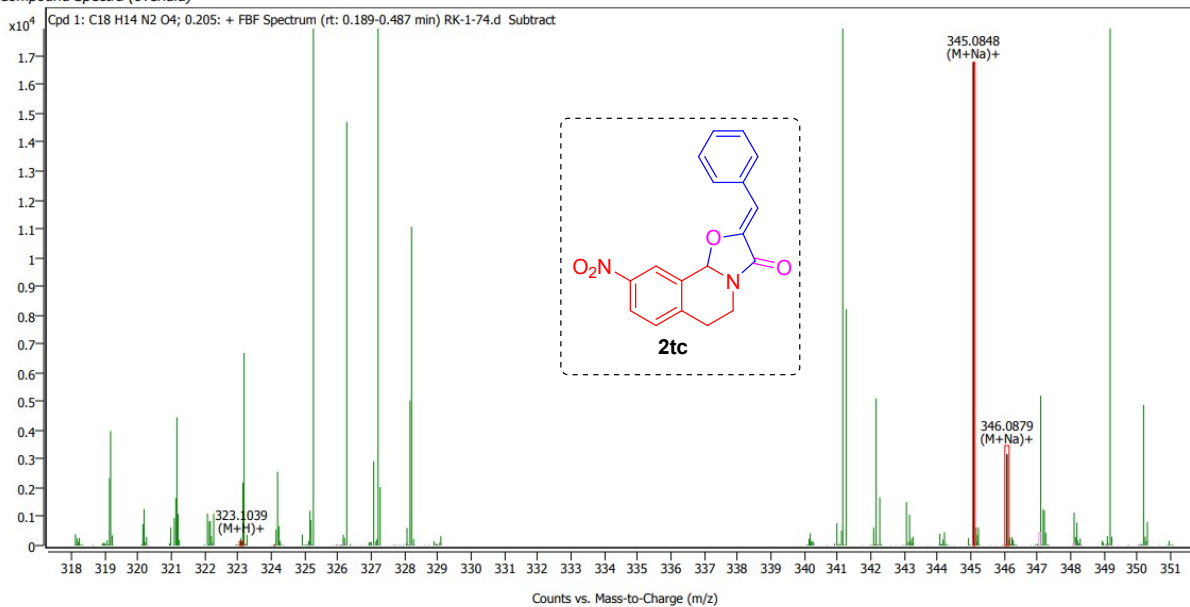


<sup>1</sup>H & <sup>13</sup>C spectra of compound 2tc

### Compound Details

Cpd. 1: C<sub>18</sub> H<sub>14</sub> N<sub>2</sub> O<sub>4</sub>

Compound Spectra (overlaid)

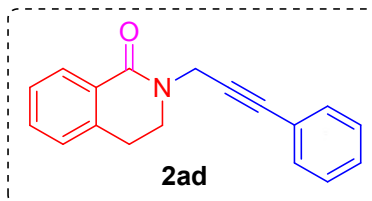


Compound ID Table

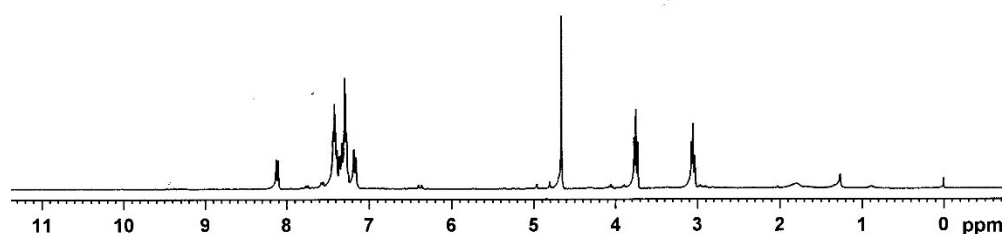
Cpd	Formula	Mass (Tgt)	Calc. Mass	Mass	Species	Diff(Tgt.ppm)	mDa
1	C <sub>18</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>	322.0954	322.0956	323.1039 345.0848	(M+H)+ (M+Na)+	0.79	0.25

## HRMS Spectrum of Compound 2tc

8.126  
8.100  
7.431  
7.424  
7.412  
7.400  
7.386  
7.350  
7.326  
7.287  
7.280  
7.270  
7.253  
7.247  
7.180  
7.155  
— 4.655  
3.769  
3.748  
3.725  
3.071  
3.049  
3.027



NAME RA-BR-3-170A  
EXPNO 4  
PROCNO 1  
Date\_ 20190525  
Time 19.58  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 181  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
TD0 1



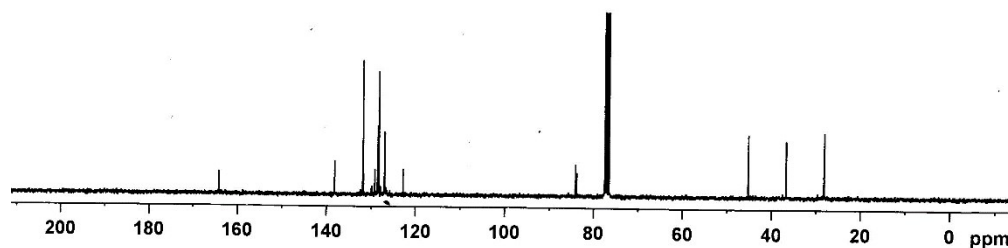
===== CHANNEL f1 =====  
NUC1 1H  
P1 12.00 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300105 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1.00  
3.04  
1.16  
3.16  
1.08  
2.03  
2.00  
2.10

— 164.17  
138.17  
131.78  
129.83  
129.21  
128.51  
128.29  
128.22  
127.02  
126.91  
122.81  
84.08  
83.87  
77.41  
76.98  
76.56  
— 45.17  
— 36.65  
— 28.07



NAME RA-BR-3-170A  
EXPNO 3  
PROCNO 1  
Date\_ 20190525  
Time 19.52  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 679  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1



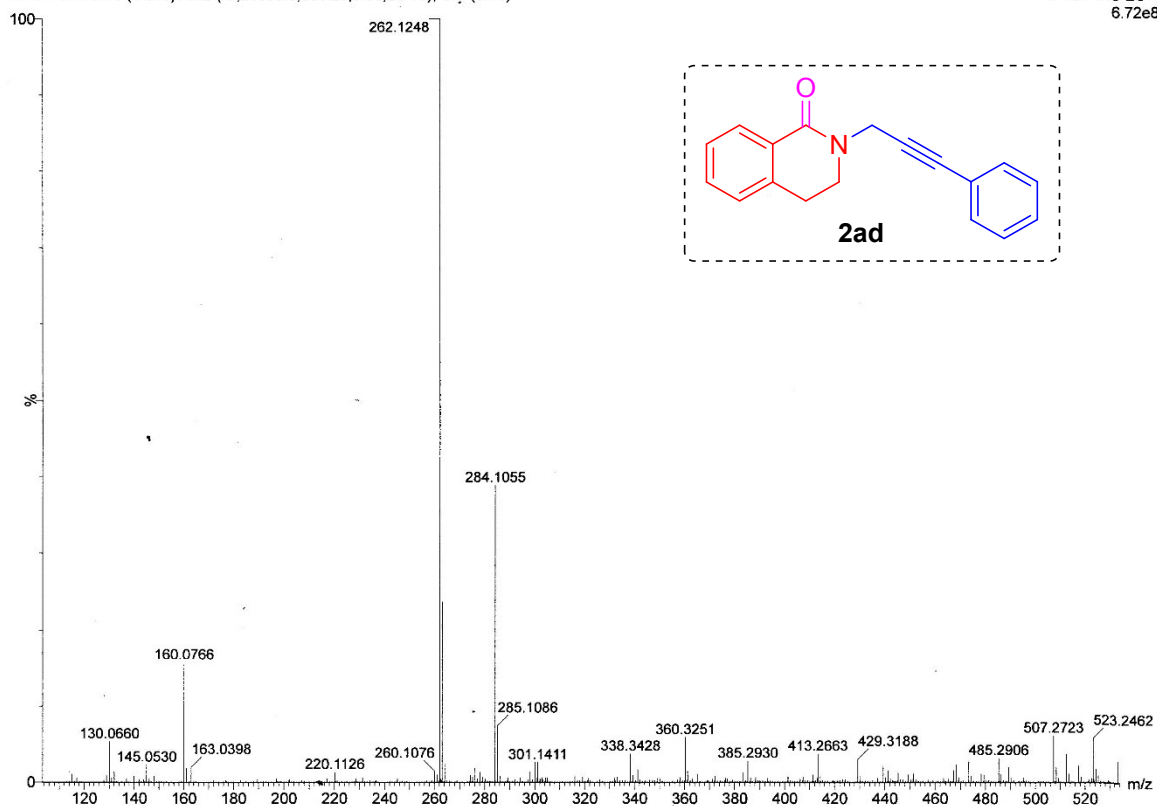
===== CHANNEL f1 =====  
NUC1 13C  
P1 10.68 usec  
PL1 0.00 dB  
PL1W 31.39858055 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 15.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.29870972 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 2ad

DRRA  
RA-BR-3-170A 8 (0.310) AM2 (Ar,20000.0,556.28,0.00,LS 10); Cm (8:40)

1: TOF MS ES+  
6.72e8



HRMS spectrum of compound 2ad