

## Supporting Information

### *Electrochemical synthesis of Isobenzofuran-1-imines using Oxidative Halocyclization of o-Alkynylbenzamides*

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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 300MHz NMR spectrometer (300 MHz for  $^1\text{H}$  NMR and 75 MHz 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. Electrochemical studies were carried out using a Metrohm Autolab model AUT51540 (PGSTAT 204).

## 2. Reaction set-up for synthesis of Isobenzofuran-1-imines:

a)



b)

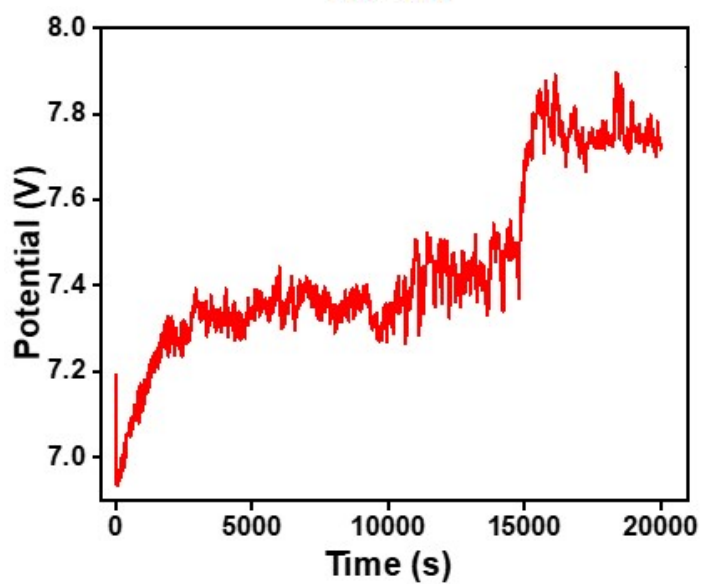
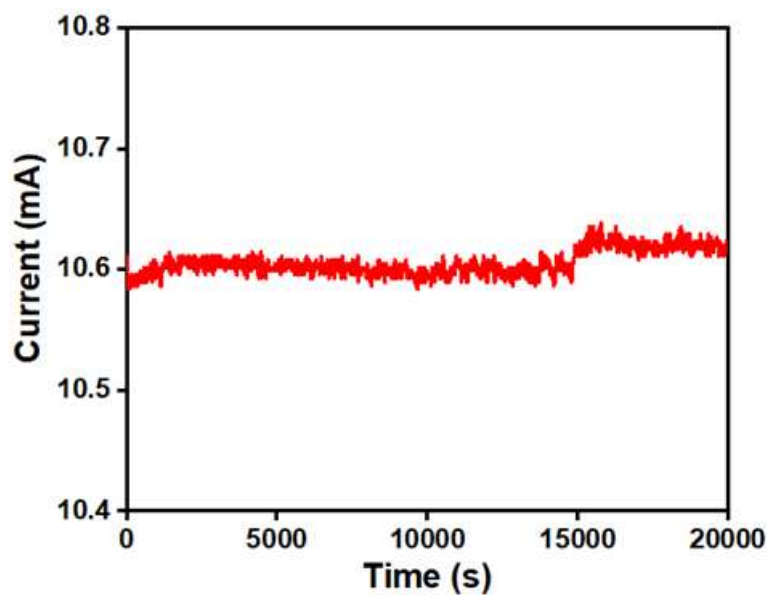
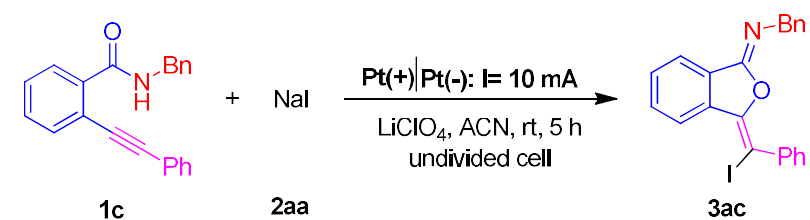


c)



**Fig S1:** a) Reaction set-up for synthesis of isobenzofuran-1-imines; b) before reaction; c) After completion of the reaction.

### 3. Current vs Time (i-t) and Potential vs Time (v-t) curve



**Figure S2:** Current vs Time and Potential vs Time during Electrolysis. 0.15 mmol (**1c**), 0.22 mmol (**2aa**), LiClO<sub>4</sub> (0.3 M), ACN (8.0 mL), Pt(+)|Pt(-), rt, 5h.



#### 4. General procedure A for synthesis of *o*-alkynylbenzamides:

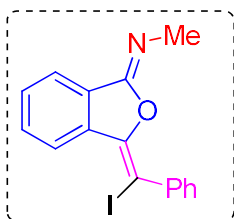
*o*-Alkynylbenzamides were synthesized using the literature procedure.<sup>1</sup>

To a solution of iodo compound (1 equiv.) in DCE, Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (2 mol%) and CuI (1 mol%) was added under nitrogen atmosphere. Triethylamine (4.0 equiv.) was added by a syringe and reaction mixture was stirred at rt. After 20 minutes, acetylene (1.2 equiv.) was added dropwise to the reaction mixture heated to 70 °C for 4h. The reaction completion was monitored by TLC, crude reaction mixture was passed through celite and solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using EtOAc/Hexane as eluent to furnish the corresponding *o*-alkynylbenzamides.

#### 5. General procedure B for synthesis of isobenzofuran-1-imines:

A 25 ml four-necked round-bottomed flask was charged with *o*-alkynylbenzamide **1** (0.15 mmol), sodium salt **2** (0.22 mmol), LiClO<sub>4</sub> (0.3 M) in MeCN (8 mL). The flask was equipped with a platinum disk anode and a platinum wire cathode. Electrolysis was carried out for 5h under open atmosphere. After the completion of the reaction solvent was evaporated and crude product was purified with basic alumina column chromatography using EtOAc/Hexane as eluent to furnish the corresponding isobenzofuran-1-imines. The reaction set-up pictures were shown in figure S1.

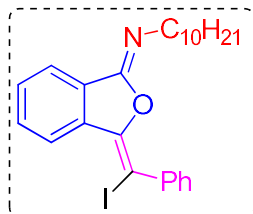
**(Z)-N-((E)-3-(iodo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)methanamine 3aa**<sup>2</sup>



**3aa** (43 mg) was obtained from **1a** (35 mg) following general procedure **B**; white solid; 81% yield (eluent: EtOAc/Hexanes= 2:98); mp: 124-126 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.17 (s, 3H), 7.27-7.32 (m, 1H), 7.38-7.42 (m, 2H), 7.53-7.58 (m, 1H), 7.63-7.71 (m, 3H), 7.88 (d, *J* = 7.5 Hz, 1H), 8.85 (d, *J* = 7.8 Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 34.9, 73.2, 123.0, 125.0, 127.9, 128.2, 130.1, 130.5, 131.1, 132.1, 136.1, 140.8, 147.7, 154.6.

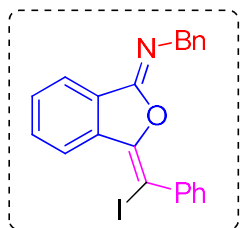
**(*Z*)-*N*-((*E*)-3-(iodo(phenyl)methylene)isobenzofuran-1(*3H*)-ylidene)decan-1-amine **3ab****



**3ab** (58 mg) was obtained from **1b** (54 mg) following general procedure **B**; colorless oily liquid; 80% yield (eluent: EtOAc/Hexanes = 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 0.90 (t, *J* = 6.9 Hz, 3H), 1.28-1.35 (m, 14H), 1.58-1.66 (m, 2H), 3.44 (t, *J* = Hz, 2H), 7.27-7.31 (m, 1H), 7.36-7.41 (m, 2H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.61-7.64 (m, 3H), 7.91 (d, *J* = 7.5 Hz, 1H), 8.84 (d, *J* = 8.1 Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 14.0, 22.7, 27.5, 29.3, 29.4, 29.6, 29.7, 30.7, 31.9, 48.1, 72.8, 123.2, 125.0, 127.9, 128.2, 130.2, 130.4, 131.0, 132.1, 136.1, 140.9, 147.6, 153.3; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>25</sub>H<sub>31</sub>INO: 488.1450, Found: 488.1474.

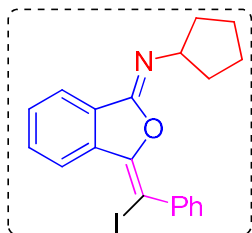
**(*Z*)-*N*-((*E*)-3-(iodo(phenyl)methylene)isobenzofuran-1(*3H*)-ylidene)-1-phenylmethanamine **3ac**<sup>2</sup>**



**3ac** (55 mg) was obtained from **1c** (47 mg) following general procedure **B**; colorless oily liquid; 84% yield (eluent: EtOAc/Hexanes = 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 4.65 (s, 2H), 7.24-7.34 (m, 6H), 7.39-7.44 (m, 2H), 7.54-7.64 (m, 4H), 7.97 (d, *J*= 7.75Hz, 1H), 8.85 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 51.8, 73.3, 123.4, 124.9, 126.6, 128.0, 128.1, 128.3, 130.1, 130.4, 131.2, 132.0, 136.1, 140.0, 140.8, 147.4, 154.0.

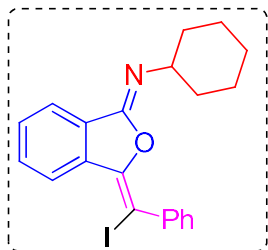
**(*Z*)-*N*-((*E*)-3-(iodo(phenyl)methylene)isobenzofuran-1(3*H*)-ylidene)cyclopentanamine 3ad**



**3ad** (51 mg) was obtained from **1d** (43 mg) following general procedure **B**; yellow liquid; 82% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 1.57-1.62 (m, 2H), 1.79-1.90 (m, 2H), 2.06-2.13 (m, 4H), 4.08-4.12 (m, 1H), 7.28-7.32 (m, 1H), 7.37-7.42 (m, 2H), 7.47-7.56 (m, 1H), 7.61-7.65 (m, 3H), 7.92 (d, *J*= 7.2Hz, 1H), 8.84 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 24.5, 34.5, 58.3, 72.5, 123.2, 124.9, 127.7, 128.1, 129.0, 130.3, 130.8, 132.3, 135.9, 140.9, 147.6, 152.3; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>20</sub>H<sub>19</sub>INO: 416.0511, Found: 416.0492.

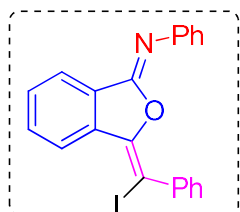
**(*Z*)-*N*-((*E*)-3-(iodo(phenyl)methylene)isobenzofuran-1(3*H*)-ylidene)cyclohexanamine 3ae**



**3ae** (51 mg) was obtained from **1e** (46 mg) following general procedure **B**; yellow liquid; 79% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 1.26-1.30 (m, 4H), 1.43-1.50 (m, 2H), 1.77-1.84 (m, 4H), 3.57-3.64 (m, 1H), 7.27-7.32 (m, 1H), 7.37-7.41 (m, 2H), 7.54 (t, *J*= 7.5Hz, 1H), 7.61-7.65 (m, 3H), 7.94 (d, *J*= 7.5Hz, 1H), 8.84 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 24.9, 25.8, 34.0, 56.7, 72.5, 123.3, 124.9, 127.7, 128.1, 130.3, 130.9, 132.2, 136.0, 140.7, 147.5, 151.9; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>21</sub>H<sub>21</sub>INO: 430.0668, Found: 430.0646.

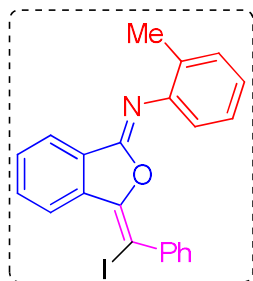
**(Z)-N-((E)-3-(iodo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)aniline 3af<sup>2</sup>**



**3af** (46 mg) was obtained from **1f** (45 mg) following general procedure **B**; white solid; 72% yield (eluent: EtOAc/Hexanes= 2:98); mp: 96-98 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 7.11-7.13 (m, 1H), 7.23-7.32 (m, 3H), 7.37-7.38 (m, 4H), 7.60-7.73 (m, 4H), 8.07 (d, *J*= 7.5Hz, 1H), 8.88 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 74.7, 123.9, 124.8, 124.9, 125.1, 127.9, 128.5, 130.2, 130.6, 131.6, 132.7, 135.6, 140.5, 144.9, 147.7, 151.7.

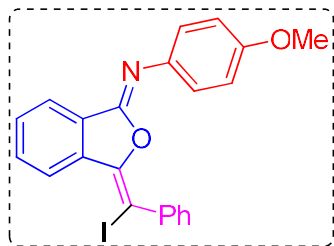
**(Z)-N-((E)-3-(iodo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)-2-methylaniline 3ag**



**3ag** (44 mg) was obtained from **1g** (47 mg) following general procedure **B**; white solid; 68% yield (eluent: EtOAc/Hexanes= 2:98); mp: 139-141 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.32 (m, 3H), 7.00-7.05 (m, 2H), 7.15-7.32 (m, 5H), 7.56-7.74 (m, 4H), 8.08 (d, *J* = 7.5Hz, 1H), 8.89 (d, *J* = 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 18.1, 74.8, 122.5, 123.8, 124.6, 125.0, 125.7, 127.7, 128.3, 129.8, 130.1, 130.2, 130.5, 131.6, 132.4, 135.8, 140.2, 143.8, 147.5, 151.1.

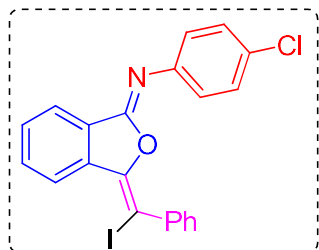
**(Z)-N-((E)-3-(iodo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)-4-methoxyaniline 3ah**



**3ah** (51 mg) was obtained from **1h** (50 mg) following general procedure **B**; white solid; 74% yield (eluent: EtOAc/Hexanes= 4:96); mp: 137-139 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.81 (s, 3H), 6.77 (d, *J* = 7.5Hz, 2H), 7.27-7.41 (m, 5H), 7.58-7.68 (m, 4H), 8.03 (d, *J* = 7.5Hz, 1H), 8.86 (d, *J* = 7.5Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 55.4, 73.7, 113.8, 123.6, 124.8, 126.8, 127.9, 128.4, 130.2, 130.5, 131.3, 133.1, 135.2, 138.0, 140.8, 148.0, 150.3, 157.5; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>22</sub>H<sub>17</sub>INO<sub>2</sub>: 454.0304, Found: 454.0304.

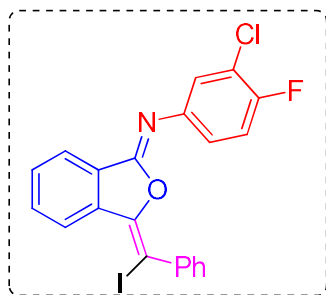
**(Z)-4-chloro-N-((E)-3-(iodo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)aniline 3ai**



**3ai** (49 mg) was obtained from **1i** (50 mg) following general procedure **B**; white solid; 71% yield (eluent: EtOAc/Hexanes= 2:98); mp: 138-140 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 7.17-7.19 (m, 2H), 7.29-7.41 (m, 5H), 7.58-7.74 (m, 4H), 8.05 (d, *J* = 6.9Hz, 1H), 8.86 (d, *J* = 7.5Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 75.1, 123.9, 124.9, 126.3, 127.9, 128.5, 128.6, 130.0, 130.5, 130.7, 131.8, 132.4, 135.5, 140.5, 143.3, 147.4, 152.2; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>21</sub>H<sub>14</sub>ClINO: 457.9809, Found: 457.9830.

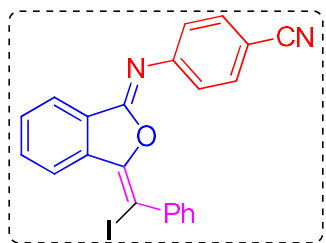
**(Z)-3-chloro-4-fluoro-N-((E)-3-(iodo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)aniline 3aj**



**3aj** (48 mg) was obtained from **1j** (53 mg) following general procedure **B**; white solid; 66% yield (eluent: EtOAc/Hexanes= 2:98); mp: 142-144 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 6.98-7.01 (m, 1H), 7.19-7.23 (m, 1H), 7.27-7.33 (m, 1H), 7.36-7.49 (m, 3H), 7.57-7.66 (m, 3H), 7.73 (t, *J* = 7.5Hz, 1H), 8.02 (d, *J* = 7.2Hz, 1H), 8.87 (d, *J* = 7.5Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 75.5, 115.9, 116.2, 120.4, 120.7, 123.9, 124.9, 125.2, 125.3, 126.6, 128.2, 128.7, 129.8, 130.7, 132.0, 132.3, 135.5, 140.4, 141.6, 147.5, 152.3, 154.0, 157.3; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>21</sub>H<sub>13</sub>FCIINO: 475.9714, Found: 475.9715.

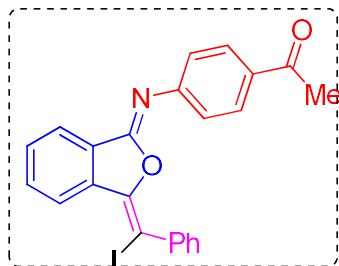
**4-((Z)-((E)-3-(iodo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)amino)benzonitrile 3ak**



**3ak** (43 mg) was obtained from **1k** (45 mg) following general procedure **B**; pale yellow solid; 70% yield (eluent: EtOAc/Hexanes= 2:98); mp: 170-172 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 7.31-7.36 (m, 5H), 7.48-7.54 (m, 4H), 7.66 (t, *J*= 7.5Hz, 1H), 7.75 (t, *J*= 7.5Hz, 1H), 8.04 (d, *J*= 7.2Hz, 1H), 8.87 (d, *J*= 8.1Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 77.2, 107.9, 119.1, 124.2, 125.0, 127.9, 128.8, 129.9, 130.8, 131.7, 132.4, 132.5, 135.8, 140.2, 147.2, 149.4, 153.7.

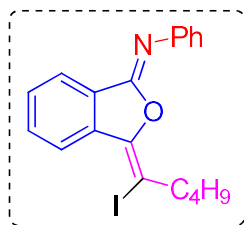
**1-(4-((*Z*)-((*E*)-3-(iodo(phenyl)methylene)isobenzofuran-1(3*H*)-ylidene)amino)phenyl)ethanone 3al**



**3al** (51 mg) was obtained from **1l** (51 mg) following general procedure **B**; pale yellow solid; 73% yield (eluent: EtOAc/Hexanes= 4:96); mp: 154-156°C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.57 (s, 3H), 7.27-7.37 (m, 5H), 7.55-7.66 (m, 3H), 7.73 (t, *J*= 7.5Hz, 1H), 7.84 (d, *J*= 8.1Hz, 2H), 8.05 (d, *J*= 6.6Hz, 1H), 8.87 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 26.3, 76.0, 124.1, 124.4, 124.9, 127.9, 128.7, 129.0, 129.8, 130.0, 130.7, 132.1, 133.7, 135.8, 140.2, 147.4, 149.6, 153.1, 197.0.

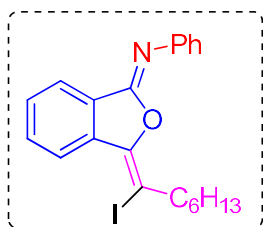
**(*Z*)-*N*-((*E*)-3-(1-iodopentylidene)isobenzofuran-1(3*H*)-ylidene)aniline 3am**



**3am** (43 mg) was obtained from **1m** (42 mg) following general procedure **B**; colorless oily liquid; 71% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  0.95 (t,  $J$ = 7.5Hz, 3H), 1.36-1.45 (m, 2H), 1.58-1.68 (m, 2H), 2.92 (t,  $J$ = 7.8Hz, 2H), 7.15-7.19 (m, 1H), 7.27-7.45 (m, 4H), 7.55-7.66 (m, 2H), 8.04 (d,  $J$ = 7.2Hz, 1H), 8.70 (d,  $J$ = 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  13.7, 21.6, 31.2, 39.5, 82.2, 123.8, 124.0, 124.7, 128.6, 129.9, 131.6, 132.5, 135.6, 145.7, 147.3, 152.2; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>19</sub>H<sub>19</sub>INO: 404.0511, Found: 404.0546.

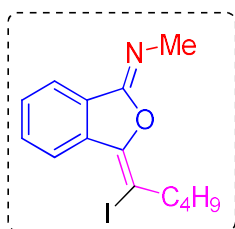
**(Z)-N-((E)-3-(1-iodoheptylidene)isobenzofuran-1(3H)-ylidene)aniline 3an**



**3an** (45 mg) was obtained from **1n** (46 mg) following general procedure **B**; colorless oily liquid; 70% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  0.90 (t,  $J$ = 7.5Hz, 3H), 1.29-1.39 (m, 6H), 1.62-1.66 (m, 2H), 2.92 (t,  $J$ = 7.5Hz, 2H), 7.18-7.20 (m, 1H), 7.36-7.47 (m, 4H), 7.57-7.66 (m, 2H), 8.04 (d,  $J$ = 7.2Hz, 1H), 8.71 (d,  $J$ = 7.5Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  13.9, 22.5, 28.1, 29.1, 31.5, 39.8, 82.3, 122.6, 123.8, 124.1, 124.7, 128.6, 130.0, 131.6, 132.5, 135.6, 145.7, 147.3, 152.3; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>21</sub>H<sub>23</sub>INO: 432.0824, Found: 432.0822.

**(Z)-N-((E)-3-(1-iodopentylidene)isobenzofuran-1(3H)-ylidene)methanamine 3ao<sup>3</sup>**

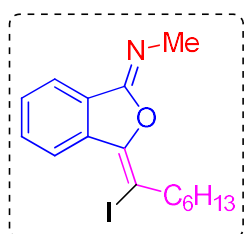




**3ao** (40 mg) was obtained from **1o** (32 mg) following general procedure **B**; colorless liquid; 78% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  0.99 (t,  $J$ = 7.2Hz, 3H), 1.39-1.46 (m, 2H), 1.62-1.67 (m, 2H), 2.98 (t,  $J$ = 7.5Hz, 2H), 3.29 (s, 3H), 7.47-7.60 (m, 2H), 7.83 (d,  $J$ = 7.5Hz, 1H), 8.67 (d,  $J$ = 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  13.8, 21.5, 31.2, 34.6, 39.0, 80.7, 122.9, 124.1, 129.8, 131.0, 132.0, 135.8, 147.1, 154.8.

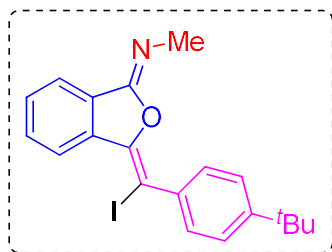
**(Z)-N-((E)-3-(1-iodoheptylidene)isobenzofuran-1(3H)-ylidene)methanamine 3ap**



**3ap** (42 mg) was obtained from **1p** (37 mg) following general procedure **B**; colorless liquid; 76% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  0.93 (t,  $J$ = 7.2Hz, 3H), 1.28-1.43 (m, 6H), 1.65-1.68 (m, 2H), 2.97 (t,  $J$ = 7.5Hz, 2H), 3.31 (s, 3H), 7.46-7.59 (m, 2H), 7.84 (d,  $J$ = 7.2Hz, 1H), 8.66 (d,  $J$ = 7.5Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  13.9, 22.5, 28.0, 28.9, 31.5, 34.6, 39.3, 80.8, 122.8, 124.1, 129.8, 130.9, 132.0, 135.8, 147.1, 154.8; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>16</sub>H<sub>21</sub>INO: 370.0668, Found: 370.0687.

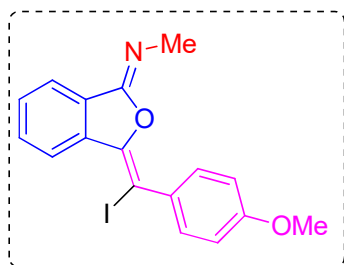
**(Z)-N-((E)-3-((4-(tert-butyl)phenyl)iodomethylene)isobenzofuran-1(3H)-ylidene)methanamine 3aq**



**3aq** (47 mg) was obtained from **1q** (44 mg) following general procedure **B**; yellow liquid; 74% yield (eluent: EtOAc/Hexanes= 2:98);

$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ ):  $\delta_{\text{H}}$  1.38 (s, 9H), 3.21 (s, 3H), 7.41 (d,  $J= 8.4\text{Hz}$ , 2H), 7.51-7.66 (m, 4H), 7.87 (d,  $J= 7.5\text{Hz}$ , 1H), 8.85 (d,  $J= 8.1\text{Hz}$ , 1H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ):  $\delta_{\text{C}}$  31.2, 34.6, 35.0, 74.1, 122.9, 124.8, 125.0, 130.0, 130.3, 131.0, 131.9, 136.2, 137.6, 147.1, 151.4, 154.6.

**(Z)-N-((E)-3-(iodo(4-methoxyphenyl)methylene)isobenzofuran-1(3H)-ylidene)methanamine**  
**3ar**



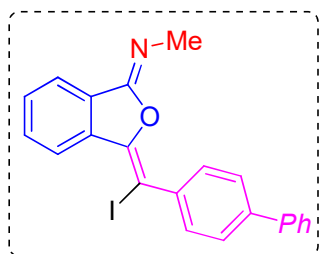
**3ar** (39 mg) was obtained from **1r** (35 mg) following general procedure **B**; colorless oily liquid; 72% yield (eluent: EtOAc/Hexanes= 4:96);

$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ ):  $\delta_{\text{H}}$  3.20 (s, 3H), 3.87 (s, 3H), 6.93 (d,  $J= 8.4\text{Hz}$ , 2H), 7.54-7.66 (m, 4H), 7.88 (d,  $J= 6.9\text{Hz}$ , 1H), 8.84 (d,  $J= 7.8\text{Hz}$ , 1H);  $^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ ):  $\delta_{\text{C}}$  34.9, 55.3, 73.9, 113.4, 123.1, 124.9, 130.3, 131.1, 131.6, 131.8, 133.2, 136.2, 146.9, 154.9, 159.5;

**HRMS:** (M+H) $^+$  calculated for  $\text{C}_{17}\text{H}_{15}\text{INO}_2$ : 392.0147, Found: 392.0173.

**(Z)-N-((E)-3-([1,1'-biphenyl]-4-yl iodomethylene)isobenzofuran-1(3H)-ylidene)methanamine**

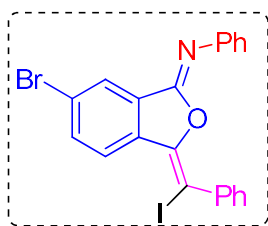
**3as**



**3as** (45 mg) was obtained from **1s** (47 mg) following general procedure **B**; white solid; 68% yield (eluent: EtOAc/Hexanes= 2:98); mp: 123-125 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.21 (s, 3H), 7.38-7.40 (m, 1H), 7.45-7.50 (m, 2H), 7.55-7.75 (m, 8H), 7.96 (d, *J*= 7.5Hz, 1H), 8.7 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 34.8, 77.2, 123.3, 125.1, 126.5, 127.1, 127.6, 12., 130.6, 130.7, 131.3, 131.6, 136.1, 139.5, 140.4, 141.1, 147.4, 155.1.

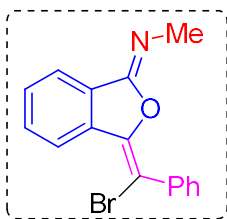
**(Z)-N-((E)-6-bromo-3-(iodo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)aniline 3at**



**3at** (51 mg) was obtained from **1t** (56 mg) following general procedure **B**; half white solid; 69% yield (eluent: EtOAc/Hexanes= 2:98); mp: 182-184 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 7.08-7.13 (m, 1H), 7.21-7.30 (m, 2H), 7.32-7.39 (m, 5H), 7.59 (d, *J*= 6.9Hz, 2H), 7.80 (d, *J*= 7.5Hz, 1H), 8.20 (s, 1H), 8.73 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 75.6, 124.9, 125.0, 125.5, 126.1, 126.8, 127.9, 128.5, 128.6, 130.1, 134.3, 134.5, 134.6, 140.2, 144.4, 147.2, 150.0.

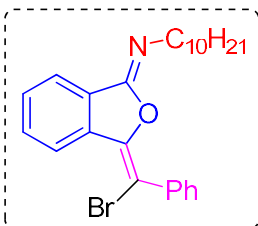
**(Z)-N-((E)-3-(bromo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)methanamine 3ba<sup>4</sup>**



**3ba** (35 mg) was obtained from **1a** (35 mg) following general procedure **B**; white solid; 74% yield (eluent: EtOAc/Hexanes= 2:98); mp: 86-88 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.25 (s, 3H), 7.32-7.37 (m, 1H), 7.42-7.46 (m, 2H), 7.53-7.58 (m, 1H), 7.64 (t, *J* = 7.8Hz, 1H), 7.78-7.80 (m, 2H), 7.89 (d, *J* = 7.5Hz, 1H), 8.63 (d, *J* = 7.5Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 35.0, 102.6, 122.9, 125.2, 128.0, 128.5, 129.7, 130.2, 131.4, 136.0, 137.3, 145.8, 154.8.

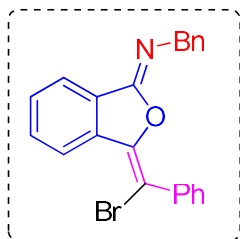
**(*Z*)-*N*-((*E*)-3-(bromo(phenyl)methylene)isobenzofuran-1(3*H*)-ylidene)decan-1-amine **3bb****



**3bb** (48 mg) was obtained from **1b** (54 mg) following general procedure **B**; white solid; 73% yield (eluent: EtOAc/Hexanes= 2:98); mp: 97-99 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 0.90 (t, *J* = 6.3Hz, 3H), 1.23-1.41 (m, 14H), 1.65-1.73 (m, 2H), 3.51-3.55 (m, 2H), 7.34-7.37 (m, 1H), 7.41-7.46 (m, 2H), 7.54 (t, *J* = 7.5Hz, 1H), 7.63 (t, *J* = 7.8Hz, 1H), 7.77-7.80 (m, 2H), 7.93 (d, *J* = 7.5Hz, 1H), 8.62 (d, *J* = 7.2Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 14.0, 22.6, 27.5, 29.3, 29.4, 29.6, 29.6, 30.7, 31.9, 48.2, 102.5, 123.3, 125.1, 128.0, 128.5, 129.7, 130.2, 131.4, 131.5, 136.1, 137.4, 145.9, 153.7; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>25</sub>H<sub>31</sub>BrNO: 440.1589, Found: 440.1576.

**(*Z*)-*N*-((*E*)-3-(bromo(phenyl)methylene)isobenzofuran-1(3*H*)-ylidene)-1-phenylmethanamine **3bc**<sup>4</sup>**

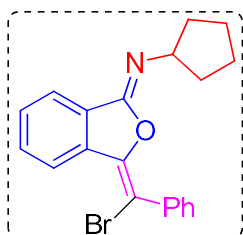


**3bc** (45 mg) was obtained from **1c** (47 mg) following general procedure **B**; white solid; 77% yield (eluent: EtOAc/Hexanes= 2:98); mp: 89-91 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  4.74 (s, 2H), 7.27-7.47 (m, 8H), 7.56 (t,  $J=7.5\text{Hz}$ , 1H), 7.65 (t,  $J=7.8\text{Hz}$ , 1H), 7.68-7.76 (m, 2H), 7.99 (d,  $J=7.5\text{Hz}$ , 1H), 8.63 (d,  $J=7.5\text{Hz}$ , 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  51.9, 102.9, 123.4, 125.1, 126.7, 127.9, 128.1, 128.3, 128.6, 129.7, 130.2, 131.4, 131.7, 136.1, 137.4, 140.1, 154.4.

**(Z)-N-((E)-3-(bromo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)cyclopentanamine**

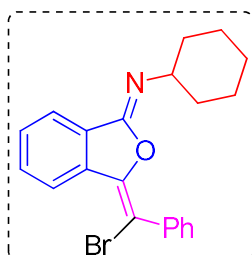
**3bd**



**3bd** (39 mg) was obtained from **1d** (43 mg) following general procedure **B**; colorless liquid; 72% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{H}}$  1.62-1.68 (m, 4H), 1.77-1.83 (m, 2H), 1.94-2.00 (m, 2H), 4.17-4.25 (m, 1H), 7.27-7.65 (m, 5H), 7.77-7.84 (m, 2H), 7.93 (d,  $J=7.5\text{Hz}$ , 1H), 8.61 (d,  $J=7.8\text{Hz}$ , 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):**  $\delta_{\text{C}}$  24.6, 34.6, 58.4, 102.2, 123.3, 125.1, 127.9, 128.4, 129.8, 130.1, 131.4, 131.6, 135.9, 137.4, 146.0, 152.7; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>20</sub>H<sub>19</sub>BrNO: 368.0650, Found: 368.0646.

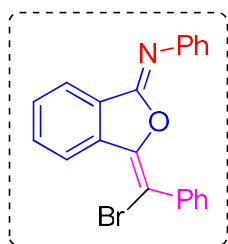
**(Z)-N-((E)-3-(bromo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)cyclohexanamine 3be**



**3be** (41 mg) was obtained from **1e** (46 mg) following general procedure **B**; colorless liquid; 71% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 1.26-1.44 (m, 4H), 1.47-1.54 (m, 2H), 1.68-1.88 (m, 4H), 3.69-3.76 (m, 1H), 7.34-7.65 (m, 5H), 7.78-7.81 (m, 2H), 7.95 (d, *J*= 7.5Hz, 1H), 8.61 (t, *J*= 8.1Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 25.0, 25.8, 34.0, 56.9, 102.1, 123.3, 125.1, 127.9, 128.4, 129.7, 130.1, 131.3, 133.6, 136.0, 137.3, 146.0, 152.2; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>21</sub>H<sub>21</sub>BrNO: 382.0806, Found: 382.0805.

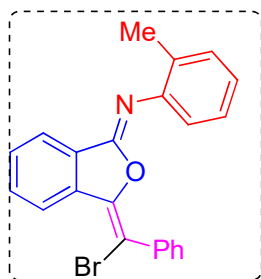
**(Z)-N-((E)-3-(bromo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)aniline 3bf<sup>4</sup>**



**3bf** (37 mg) was obtained from **1f** (45 mg) following general procedure **B**; white solid; 65% yield (eluent: EtOAc/Hexanes= 2:98); mp: 109-111 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 7.45 (d, *J*= Hz, 1H), 7.27-7.39 (m, 7H), 7.60-7.76 (m, 4H), 8.09 (d, *J*= 6.9Hz, 1H), 8.66 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 104.1, 123.9, 124.4, 125.0, 125.1, 127.9, 128.5, 128.8, 129.8, 130.3, 131.9, 132.1, 135.7, 136.9, 145.1, 146.1, 152.2.

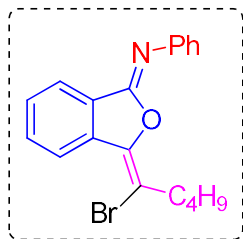
**(Z)-N-((E)-3-(bromo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)-2-methylaniline 3bg**



**3bg** (36 mg) was obtained from **1g** (47 mg) following general procedure **B**; half white solid; 61% yield (eluent: EtOAc/Hexanes= 2:98); mp: 114-116 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 2.32 (s, 3H), 7.04-7.32 (m, 7H), 7.62-7.72 (m, 4H), 8.10 (d, *J*=6.9Hz, 1H), 8.67 (d, *J*=7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 18.1, 104.1, 122.2, 123.8, 124.5, 125.3, 125.8, 127.8, 128.6, 128.9, 129.1, 129.8, 130.3, 132.1, 132.3, 136.0, 136.7, 144.2, 145.9, 151.8.

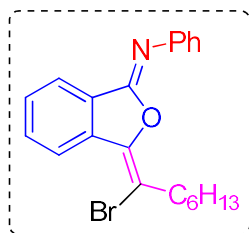
**(*Z*)-*N*-((*E*)-3-(1-bromopentylidene)isobenzofuran-1(3*H*)-ylidene)aniline 3bh**



**3bh** (36 mg) was obtained from **1m** (42 mg) following general procedure **B**; colorless liquid; 68% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 0.95 (t, *J*=7.5Hz, 3H), 1.37-1.44 (m, 2H), 1.65-1.70 (m, 2H), 2.84 (t, *J*=7.8Hz, 2H), 7.17-7.19 (m, 1H), 7.27-7.41 (m, 4H), 7.52-7.66 (m, 2H), 8.04 (d, *J*=7.5Hz, 1H), 8.47 (d, *J*=7.5Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 13.6, 21.7, 30.1, 35.9, 109.5, 123.7, 124.0, 124.2, 124.7, 128.6, 129.7, 132.0, 133.9, 135.2, 145.6, 145.9, 152.6; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>19</sub>H<sub>19</sub>BrNO: 356.0650, Found: 356.0649.

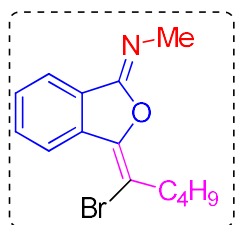
**(*Z*)-*N*-((*E*)-3-(1-bromopentylidene)isobenzofuran-1(3*H*)-ylidene)aniline 3bi**



**3bi** (38 mg) was obtained from **1n** (46 mg) following general procedure **B**; colorless liquid; 66% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 0.89 (t, *J*= 7.8Hz, 3H), 1.27-1.43 (m, 6H), 1.66-1.70 (m, 2H), 2.83 (t, *J*= 7.5Hz, 2H), 7.17-7.19 (m, 1H), 7.36-7.41 (m, 4H), 7.54-7.66 (m, 2H), 8.04 (d, *J*= 7.5Hz, 1H), 8.47 (d, *J*= 7.5Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 13.9, 22.5, 279, 28.2, 31.4, 36.2, 109.7, 123.8, 124.0, 124.2, 124.7, 125.8, 128.6, 129.8, 132.0, 135.3, 145.6, 146.0, 152.6; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>21</sub>H<sub>23</sub>BrNO: 384.0963, Found: 384.0953.

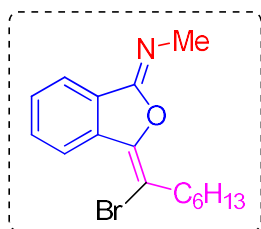
**(Z)-N-((E)-3-(1-bromopentylidene)isobenzofuran-1(3H)-ylidene)methanamine 3bj**



**3bj** (31 mg) was obtained from **1o** (32 mg) following general procedure **B**; colorless liquid; 71% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 0.99 (t, *J*= 7.5Hz, 3H), 1.40-1.47 (m, 2H), 1.67-1.74 (m, 2H), 2.90 (t, *J*= 7.2Hz, 2H), 3.31 (s, 3H), 7.48-7.58 (m, 2H), 7.84 (d, *J*= 7.5Hz, 1H), 8.43 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 13.7, 21.6, 30.0, 34.6, 35.6, 108.0, 122.8, 124.3, 129.6, 131.3, 131.6, 135.5, 145.7, 155.0; **HRMS:** (M+H)<sup>+</sup> calculated for C<sub>14</sub>H<sub>17</sub>BrNO: 294.0493, Found: 294.0516.

**(Z)-N-((E)-3-(1-bromoheptylidene)isobenzofuran-1(3H)-ylidene)methanamine 3bk**

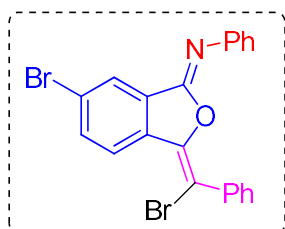


**3bk** (33 mg) was obtained from **1p** (37 mg) following general procedure **B**; colorless liquid; 69% yield (eluent: EtOAc/Hexanes= 2:98);



**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 0.91 (t, *J*= 7.5Hz, 3H), 1.28-1.44 (m, 6H), 1.65-1.73 (m, 2H), 2.89 (t, *J*= 7.5Hz, 2H), 3.31 (s, 3H), 7.46-7.58 (m, 2H), 7.84 (d, *J*= 7.5Hz, 1H), 8.43 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 13.9, 22.5, 27.8, 28.2, 31.5, 34.6, 35.9, 108.2, 122.9, 124.3, 129.6, 131.4, 131.5, 135.5, 145.7, 155.2; HRMS: (M+H)<sup>+</sup> calculated for C<sub>16</sub>H<sub>21</sub>BrNO: 322.0806, Found: 322.0813.

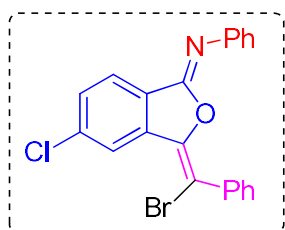
**(Z)-N-((E)-6-bromo-3-(bromo(phenyl)methylene)isobenzofuran-1(3H)-ylidene)aniline 3bl**



**3bl** (44 mg) was obtained from **1t** (56 mg) following general procedure **B**; white solid; 64% yield (eluent: EtOAc/Hexanes= 2:98); mp: 163-165 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 7.14-7.17 (m, 1H), 7.27-7.40 (m, 7H), 7.72-7.80 (m, 3H), 8.21 (s, 1H), 8.50 (d, *J*= 8.7Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 104.8, 124.6, 124.7, 125.5, 126.3, 126.9, 128.0, 128.6, 129.0, 129.7, 133.8, 134.4, 135.1, 136.7, 144.6, 145.5, 150.6.

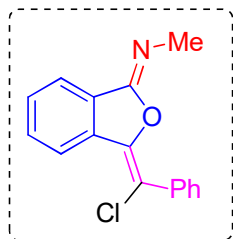
**(Z)-N-((E)-3-(bromo(phenyl)methylene)-5-chloroisobenzofuran-1(3H)-ylidene)aniline 3bm**



**3bm** (40 mg) was obtained from **1w** (50 mg) following general procedure **B**; pale yellow solid; 65% yield (eluent: EtOAc/Hexanes= 2:98); mp: 162-164 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 7.14-7.16 (m, 1H), 7.27-7.39 (m, 7H), 7.59 (d, *J*= 8.1Hz, 1H), 7.74 (d, *J*= 7.2Hz, 2H), 7.99 (d, *J*= 6.6Hz, 1H), 8.66 (s, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 105.5, 124.5, 124.9, 125.1, 125.3, 128.0, 128.6, 129.1, 129.4, 129.8, 130.4, 130.8, 136.6, 137.1, 138.5, 144.8, 151.1.

**(Z)-N-((E)-3-(chloro(phenyl)methylene)isobenzofuran-1(3H)-ylidene)methanamine 3ca**

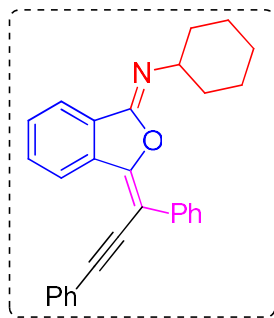


**3ca** (16 mg) was obtained from **1a** (35 mg) following general procedure **B**; colorless oily liquid; 41% yield (eluent: EtOAc/Hexanes= 2:98);

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 3.32 (s, 3H), 7.39 (d, *J*= 8.1Hz, 1H), 7.44-7.56 (m, 3H), 7.63 (t, *J*= 7.2Hz, 1H), 7.89-7.92 (m, 3H), 8.44 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 35.1, 113.3, 123.0, 125.1, 128.1, 128.6, 128.7, 130.1, 130.2, 131.7, 135.7, 135.9, 145.4, 155.1;

**HRMS:** (M+H)<sup>+</sup> calculated for C<sub>16</sub>H<sub>13</sub>ClNO: 270.0686, Found: 270.0681.

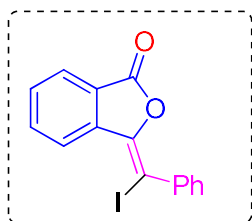
**(Z)-N-((E)-3-(1,3-diphenylprop-2-yn-1-ylidene)isobenzofuran-1(3H)-ylidene)cyclohexanamine 4**



**4** (54 mg) was obtained from **3ae** (65 mg) following literature procedure; pale yellow solid; 89% yield (eluent: EtOAc/Hexanes= 5:95); mp: 138-140 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 1.38-1.97 (m, 10H), 3.90-3.97 (m, 1H), 7.36-7.55 (m, 7H), 7.59-7.64 (m, 3H), 7.97 (d, *J*= 7.5Hz, 1H), 8.05 (d, *J*= 7.5Hz, 2H), 8.65 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 25.0, 26.0, 34.2, 57.3, 88.2, 96.5, 100.1, 123.3, 123.8, 124.1, 127.6, 128.1, 128.3, 128.5, 128.6, 129.1, 130.0, 131.1, 131.5, 135.9, 136.7, 152.1, 152.5; (M+H)<sup>+</sup> calculated for C<sub>29</sub>H<sub>26</sub>NO: 404.2014, Found: 404.2024.

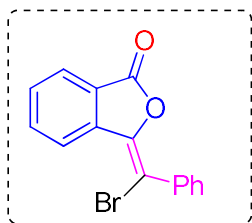
**(*E*)-3-(iodo(phenyl)methylene)isobenzofuran-1(3*H*)-one 5<sup>3</sup>**



**5** (43 mg) was obtained from **3ae** (64 mg) following literature procedure; white solid; 82% yield (eluent: EtOAc/Hexanes= 5:95); mp: 164-166 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 7.27-7.43 (m, 3H), 7.57 (d, *J*= 7.2Hz, 2H), 7.66 (t, *J*= 7.5Hz, 1H), 7.83 (t, *J*= 7.5Hz, 1H), 7.98 (d, *J*= 7.5Hz, 1H), 8.96 (d, *J*= 8.1Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 79.8, 125.0, 125.8, 126.6, 128.1, 128.9, 130.1, 130.7, 134.0, 138.8, 140.4, 144.7, 165.0.

**(*E*)-3-(bromo(phenyl)methylene)isobenzofuran-1(3*H*)-one 6<sup>4</sup>**



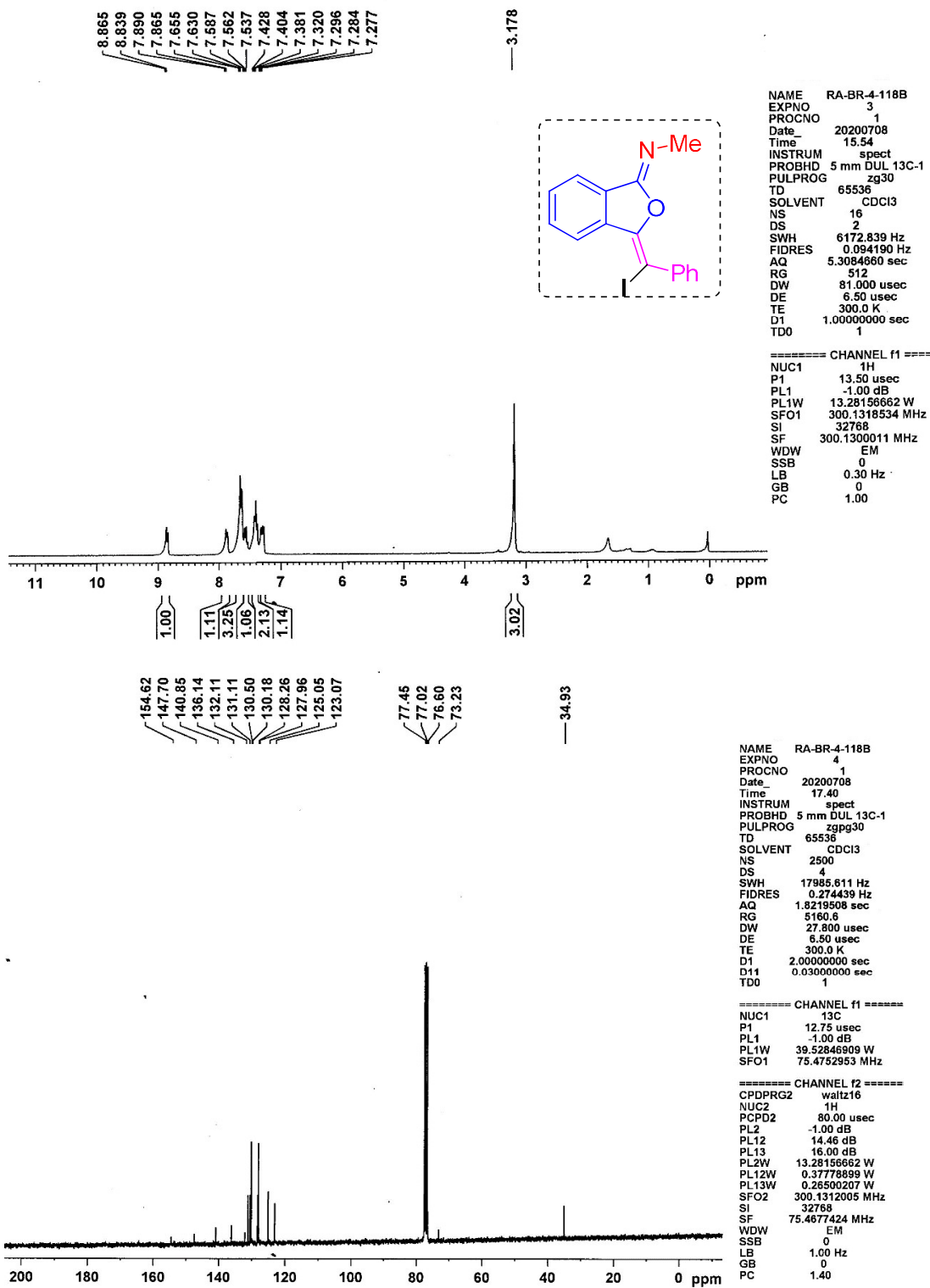
**6** (36 mg) was obtained from **3be** (57 mg) following literature procedure **B**; white solid; 81% yield (eluent: EtOAc/Hexanes= 5:95); mp: 119-121 °C;

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):** δ<sub>H</sub> 7.39-7.52 (m, 3H), 7.67 (d, *J*= 7.2Hz, 1H), 7.73-7.85 (m, 3H), 7.99 (d, *J*= 7.2Hz, 1H), 8.71 (d, *J*= 7.8Hz, 1H); **<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>):** δ<sub>C</sub> 108.4, 125.3, 125.7, 125.8, 128.2, 129.4, 130.1, 130.5, 134.5, 136.5, 1385, 142.8, 165.7.

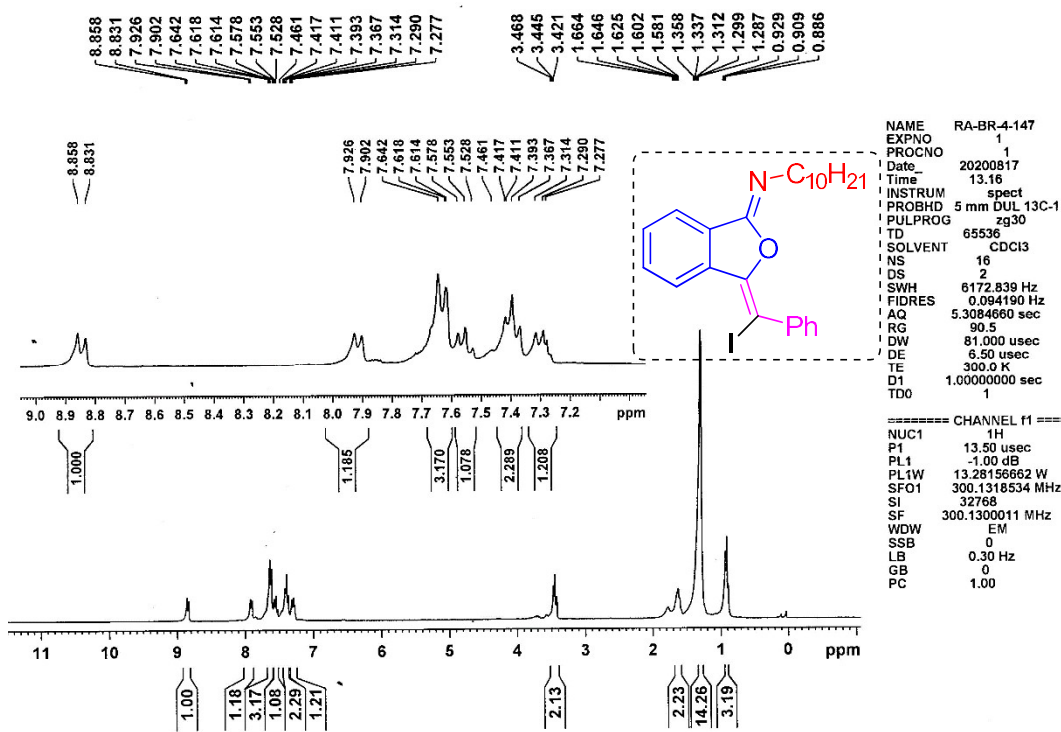
## 6. References:

1. D. Brahmchari, A. K. Verma and S. Mehta, *J. Org. Chem.*, 2018, **83**, 3339–3347.
2. S. Mehta, T. Yao and R. C. Larock, *J. Org. Chem.*, 2012, **77**, 10938–10944.
3. Y. H. Wang, J. B. Liu, B. Ouyang, H. Zhou and G. Qiu, *Tetrahedron*, 2018, **74**, 4429–4434.
4. R. X. Wang, S. T. Yuan, J. B. Liu, J. Wu and G. Qiu, *Org. Biomol. Chem.*, 2018, **16**, 4501–4508.

## 7. Spectral data



<sup>1</sup>H & <sup>13</sup>C spectra of compound 3aa

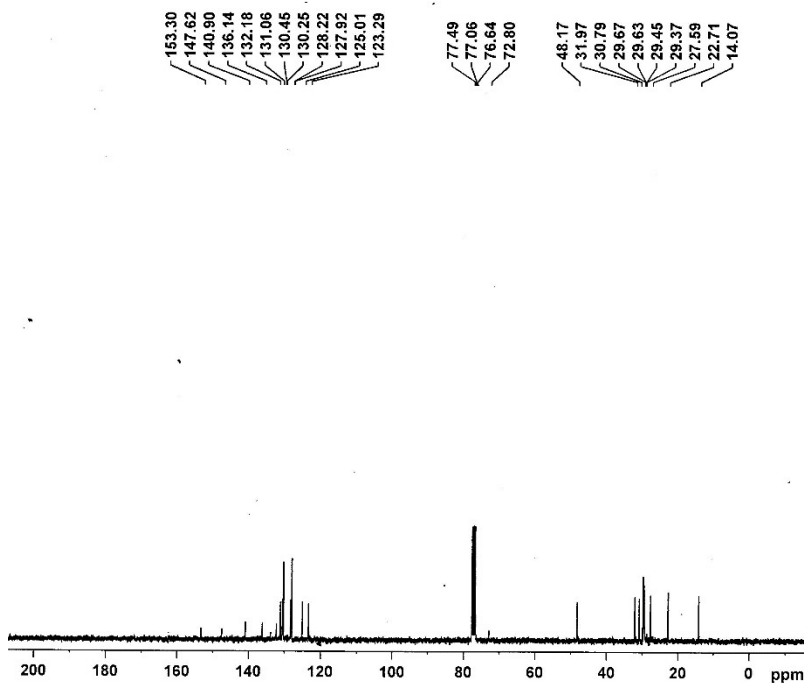


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PULPROG zg30
TD 65536
SOLVENT CDCI3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 90.5
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

===== 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

```



```

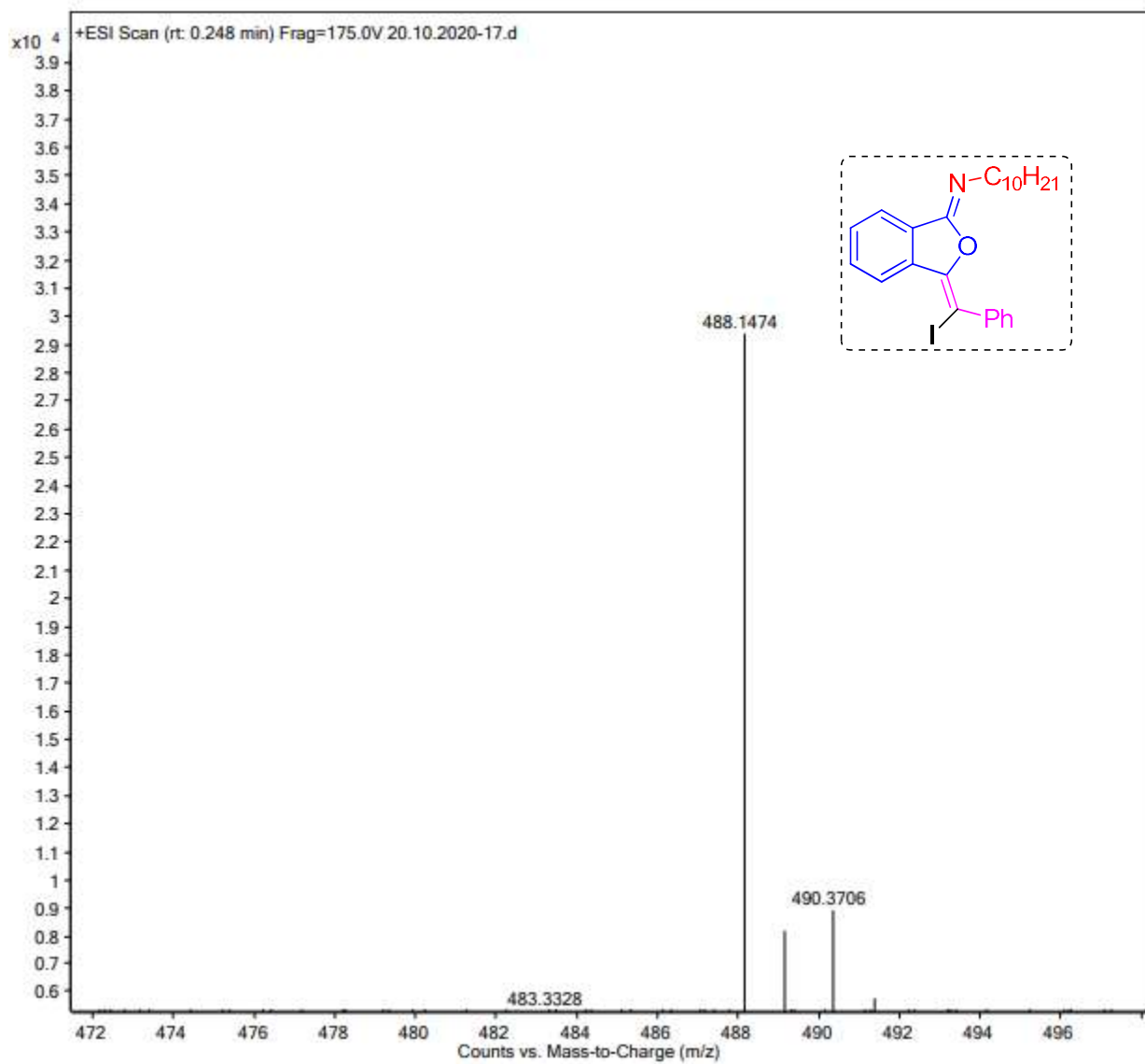
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PULPROG zgpg30
TD 65536
SOLVENT CDCI3
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2580.3
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== 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 0.3778899 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677409 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

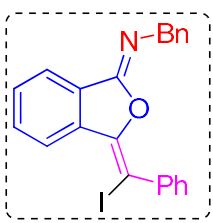
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<sup>1</sup>H & <sup>13</sup>C spectra of compound 3ab

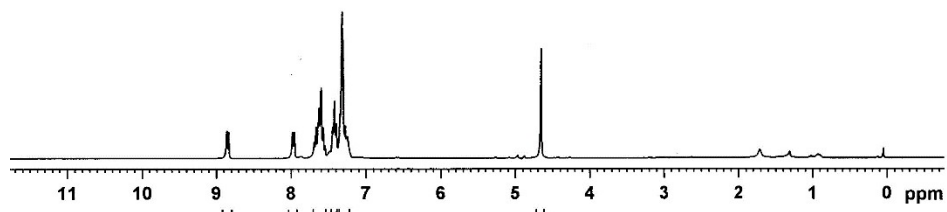


HRMS spectrum of compound 3ab

8.864  
8.838  
7.982  
7.957  
7.691  
7.667  
7.640  
7.635  
7.626  
7.622  
7.598  
7.570  
7.545  
7.446  
7.443  
7.419  
7.398  
7.394  
7.345  
7.321  
7.309  
7.277  
7.264  
7.254  
7.243  
4.652

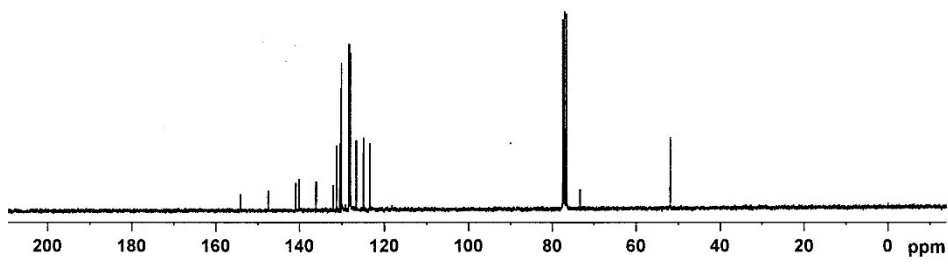


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PROCNO 1  
Date\_ 20200712  
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INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 161  
DW 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

164.08  
147.45  
140.87  
140.08  
136.11  
132.08  
131.26  
130.47  
130.13  
128.31  
128.04  
128.00  
126.66  
124.96  
123.44  
77.45  
77.03  
76.60  
73.30  
51.87



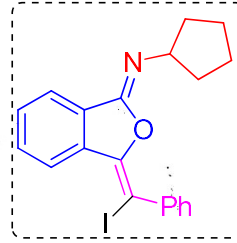
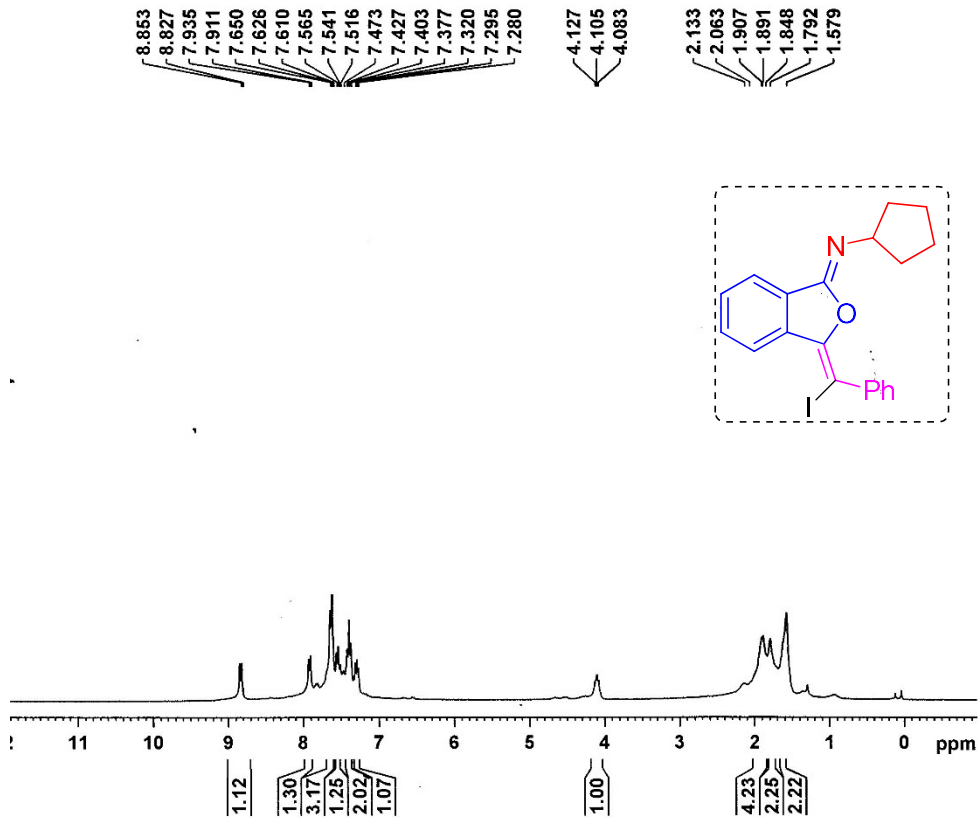
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PROCNO 1  
Date\_ 20200712  
Time 13.37  
INSTRUM spect  
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 713  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 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 75.4677449 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

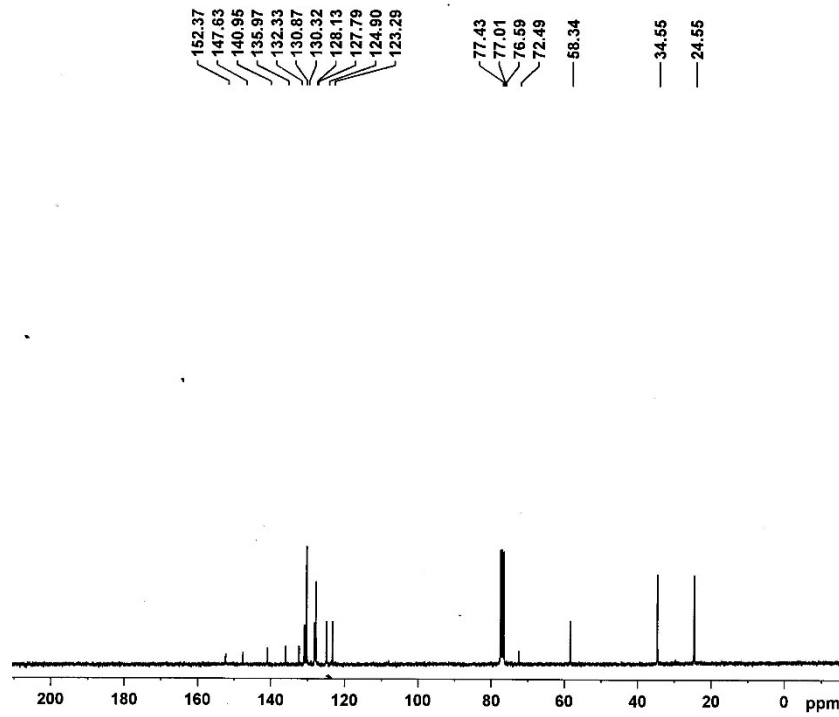
<sup>1</sup>H & <sup>13</sup>C spectra of compound 3ac





NAME RA-BR-4-119  
EXPNO 1  
PROCNO 1  
Date\_ 20200709  
Time\_ 15.12  
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 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



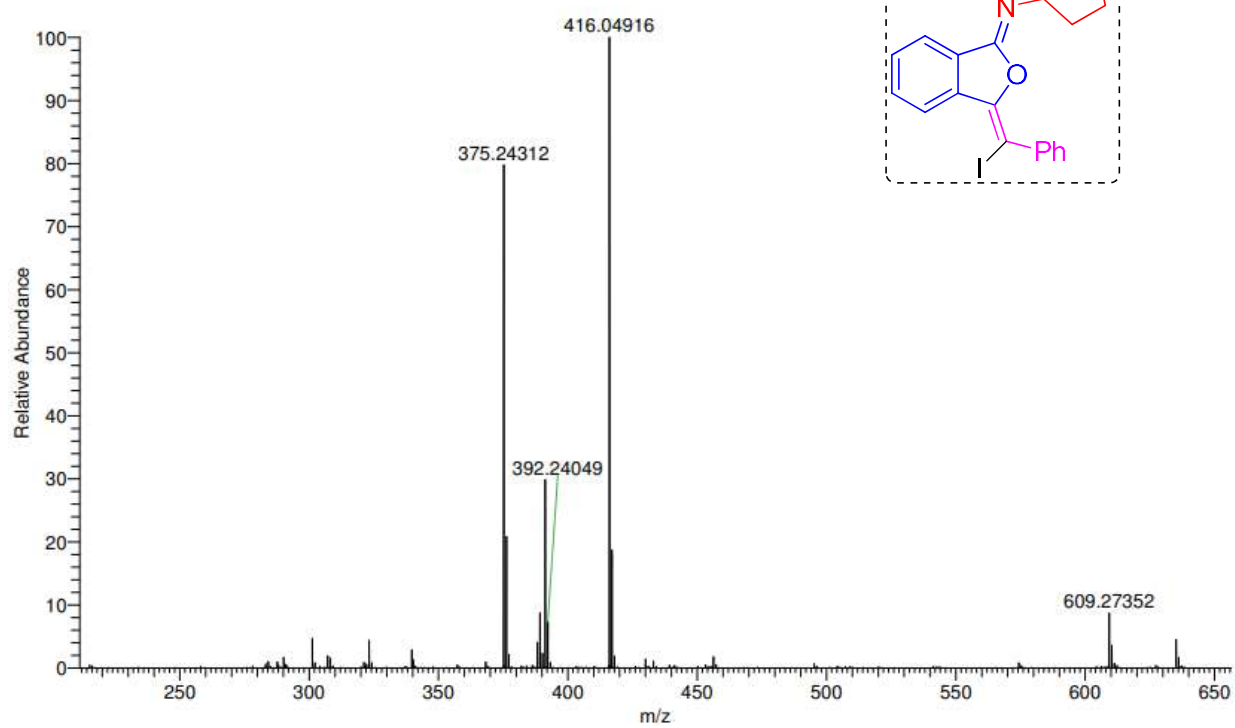
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Date\_ 20201215  
Time\_ 18.42  
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 822  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 456.1  
DW 27.900 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

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

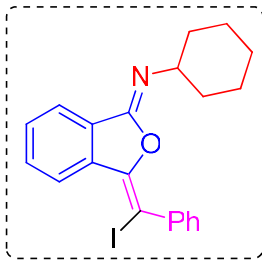
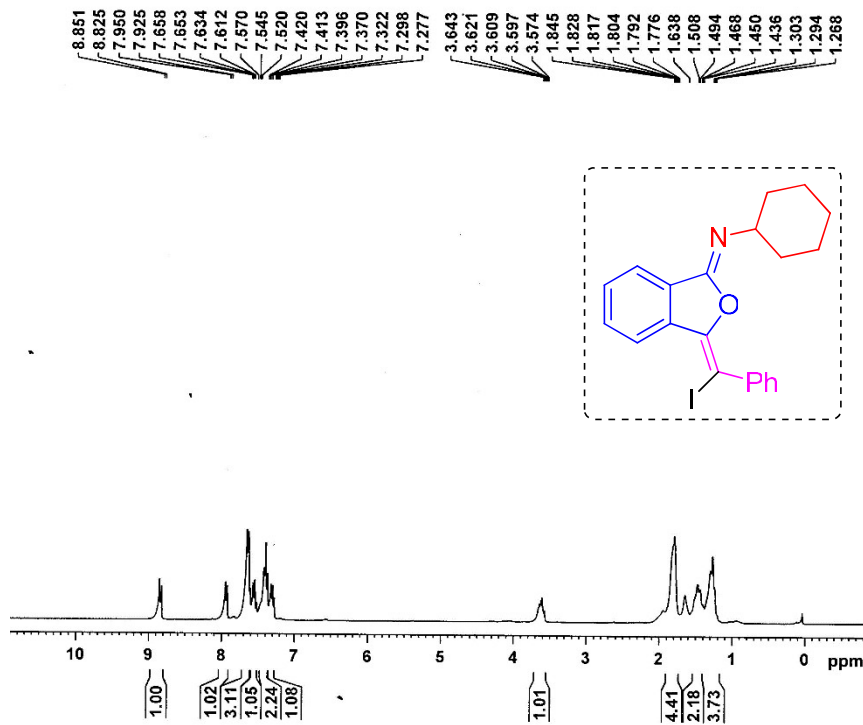
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NUC2 1H  
PCPD2 80.00 usec  
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PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677465 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3ad

SR-119A #6-15 RT: 0.05-0.11 AV: 10 NL: 1.52E8  
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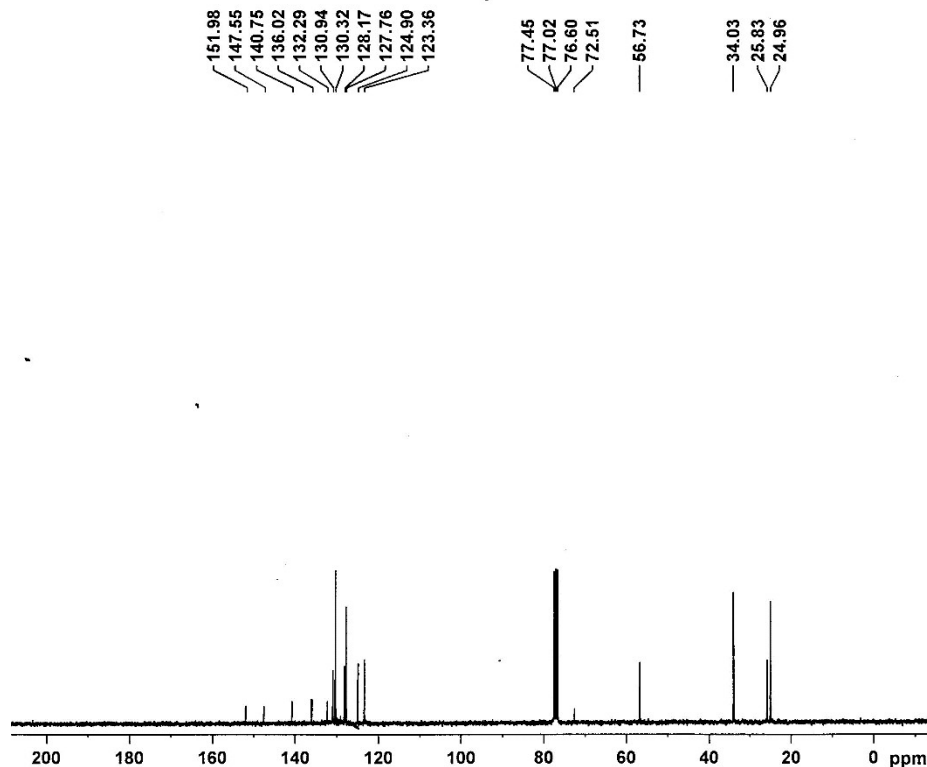


**HRMS spectrum of compound 3ad**



NAME RA-BR-4-124A  
EXPNO 1  
PROCNO 1  
Date\_ 20200714  
Time 12.04  
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 181  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 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



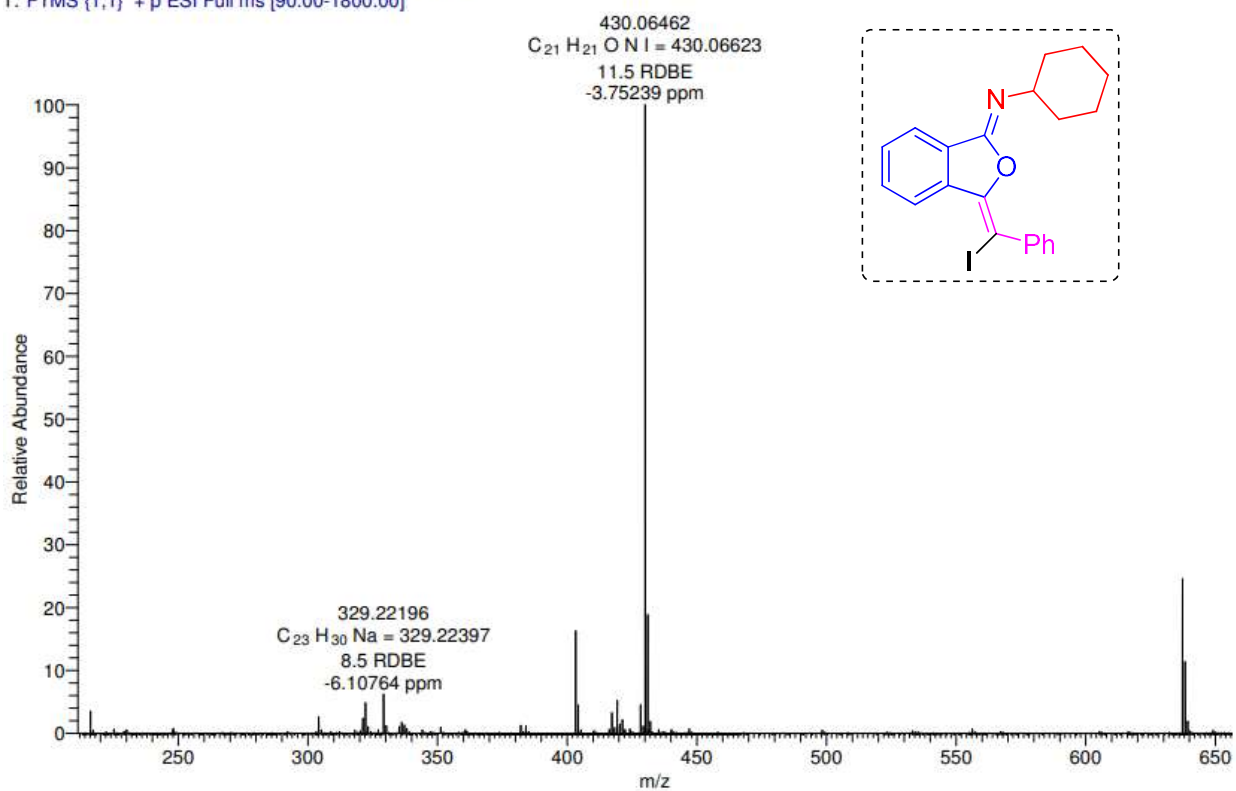
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 656  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 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 0.37778699 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677452 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

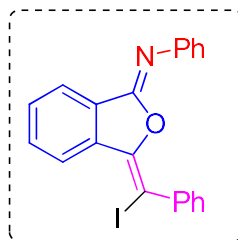
$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 3ae

SR-124A #4-16 RT: 0.03-0.12 AV: 13 NL: 8.12E7  
T: FTMS (1,1) + p ESI Full ms [90.00-1800.00]



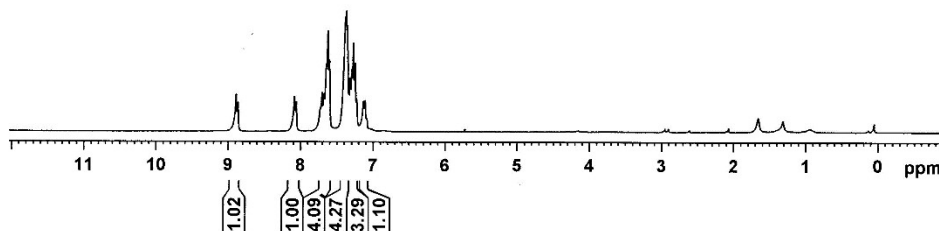
HRMS spectrum of compound 3ae

8.893  
8.867  
8.088  
8.063  
7.734  
7.710  
7.684  
7.650  
7.629  
7.608  
7.386  
7.376  
7.322  
7.298  
7.277  
7.254  
7.231  
7.136  
7.112



NAME RA-BR-4-133  
EXPNO 4  
PROCNO 1  
Date\_ 20200802  
Time 13.00  
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 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 13.28156682 W  
SFO1 300.1318534 MHz  
SI 32768  
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GB 0  
PC 1.00

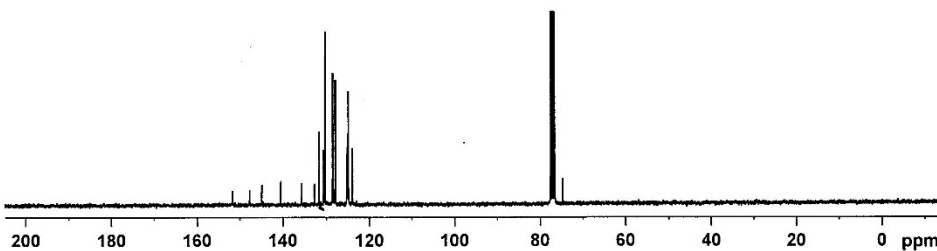


151.73  
147.74  
144.95  
140.54  
135.66  
132.72  
131.68  
130.63  
130.25  
128.50  
127.90  
125.15  
124.94  
124.87  
123.94  
77.47  
77.05  
76.82  
74.76

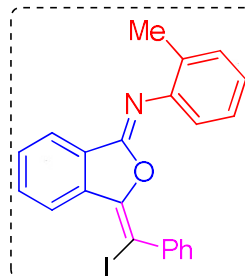
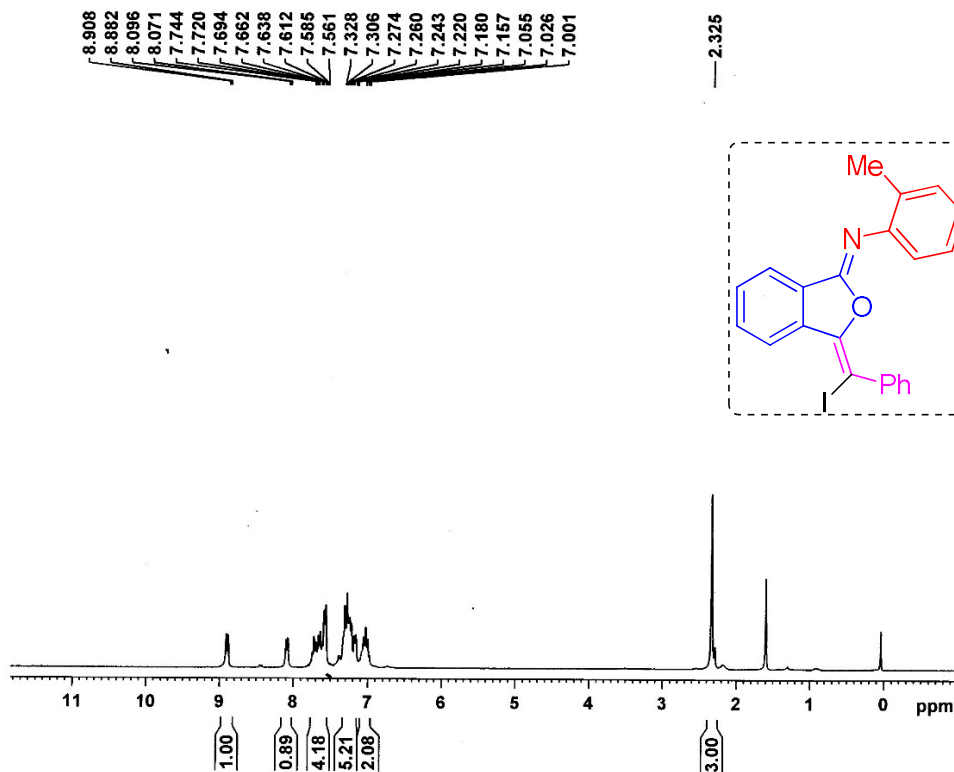
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 874  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== 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 75.4677442 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



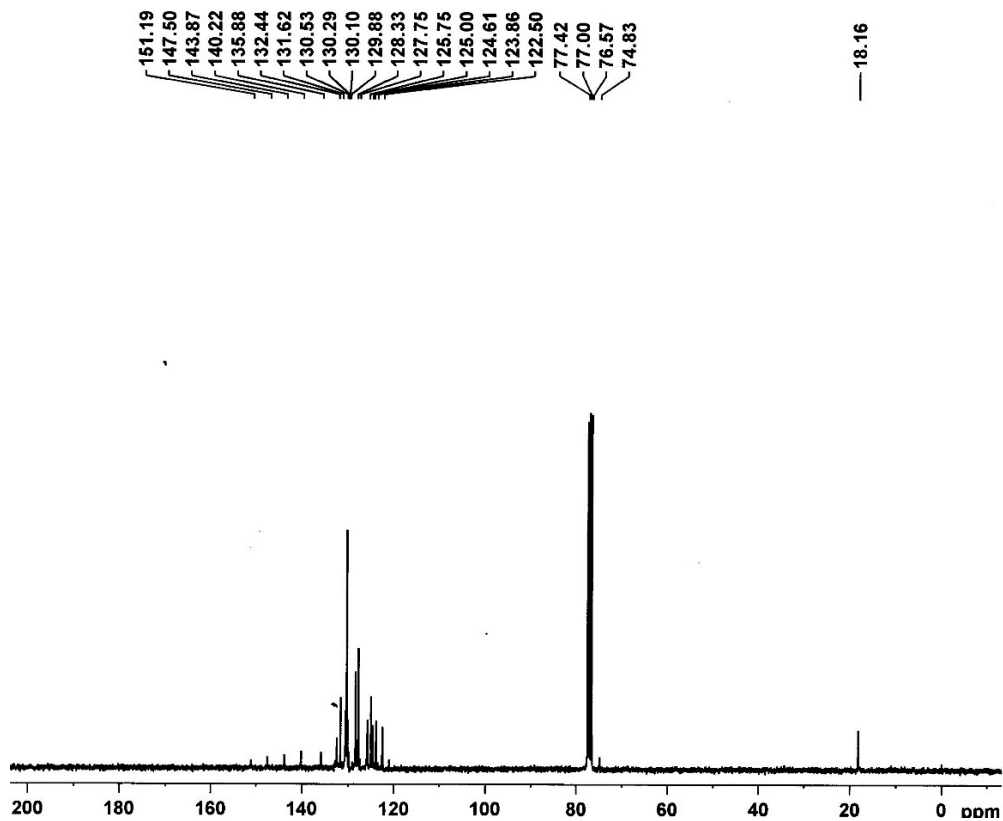
<sup>1</sup>H & <sup>13</sup>C spectra of compound 3af



```

NAME RA-BR-4-239A
EXPNO 2
PROCNO 1
Date_ 20210424
Time 19.17
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
D0 1
===== CHANNEL f1 =====
NUC1 13C
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

```

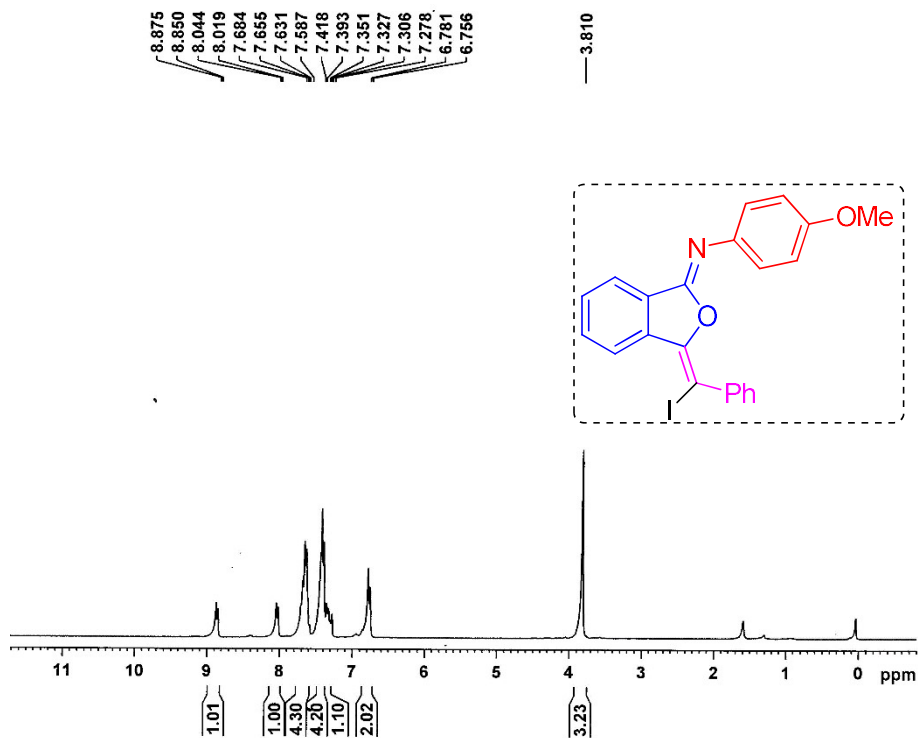


```

NAME RA-BR-4-239A
EXPNO 4
PROCNO 1
Date_ 20210425
Time 10.13
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 2298.8
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D0 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 0.37778999 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677471 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

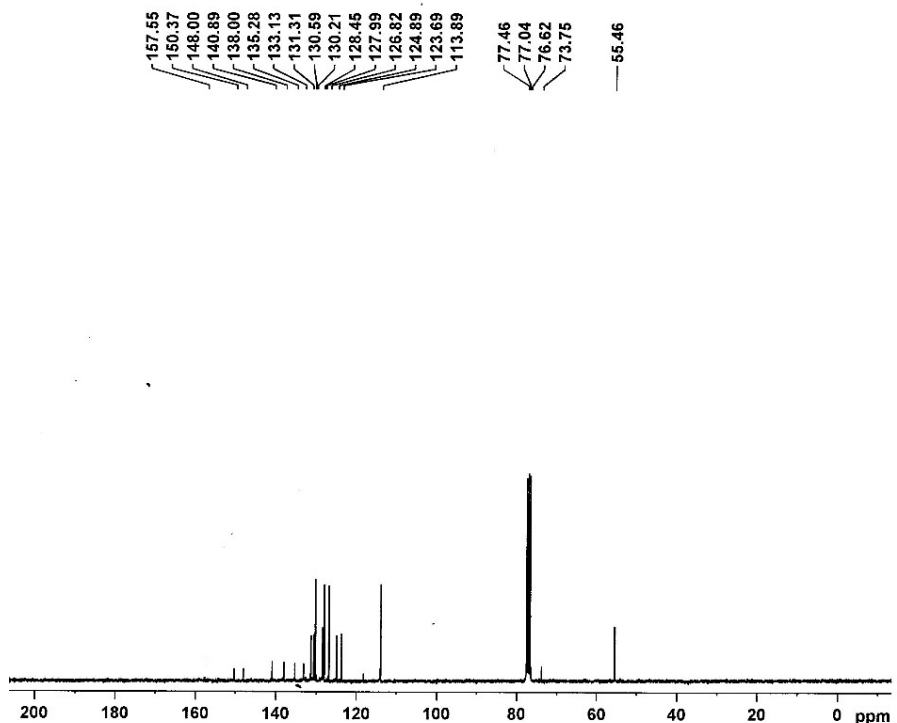
```

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3ag



NAME RA-BR-4-125A  
 EXPNO 1  
 PROCNO 1  
 Date 20200716  
 Time 8.52  
 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 13.28158662 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-4-125A  
 EXPNO 4  
 PROCNO 1  
 Date 20200717  
 Time 20.18  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 62538  
 SOLVENT CDCl3  
 NS 2500  
 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  
 P1 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.46 dB  
 PL13 16.00 dB  
 PL2W 13.28158662 W  
 PL12W 0.37778899 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677422 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 3ah

Item name: SR-125-A-454, Sample position: 1:A,3, Replicate number: 1

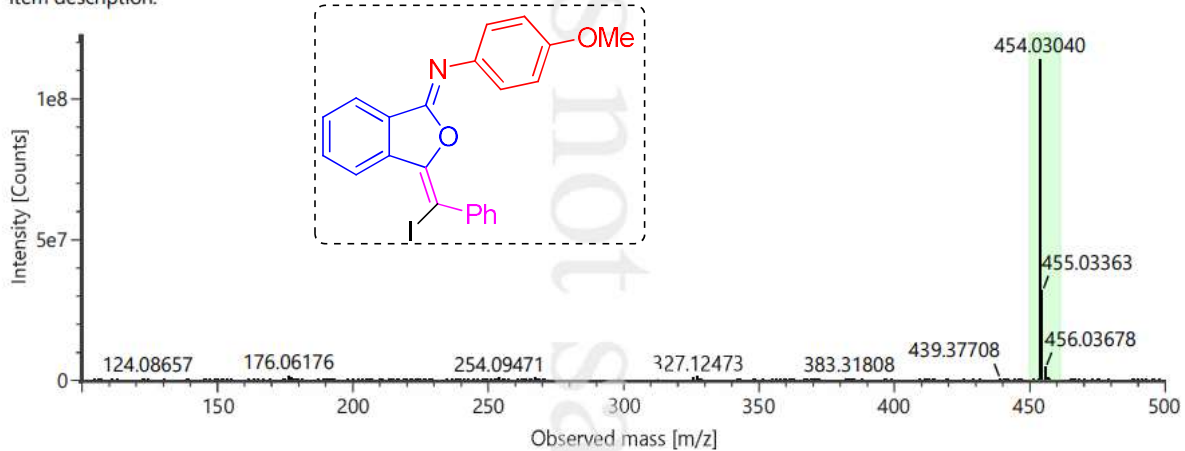
	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C22H16INO2	453.0231	453.02257	454.0304	1.2	+H

**Component name: C22H16INO2**

Item name: MSR-125-A-454

Channel name: Low energy : Time 0.6001 +/- 0.1937 minutes

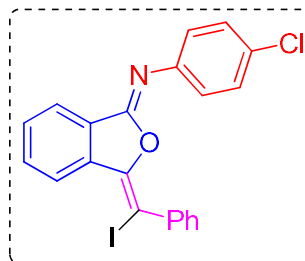
Item description:



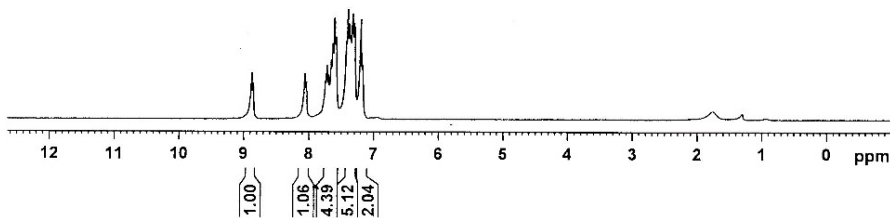
**HRMS spectrum of compound 3ah**



8.879  
8.854  
8.062  
8.039  
7.745  
7.722  
7.696  
7.667  
7.631  
7.604  
7.580  
7.419  
7.398  
7.372  
7.355  
7.330  
7.320  
7.292  
7.195  
7.173

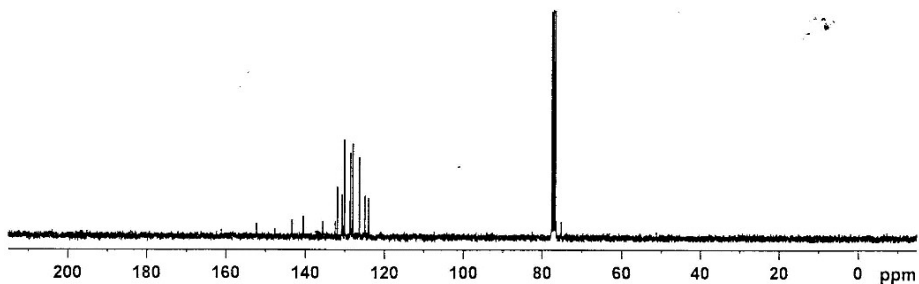


NAME RA-BR-4-136A  
EXPNO 1  
PROCNO 1  
Date\_ 20201020  
Time 15.04  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 362  
DW 61.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1  $^1\text{H}$   
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

152.23  
147.49  
143.33  
140.53  
135.57  
132.45  
131.89  
130.71  
130.59  
130.06  
128.66  
128.57  
127.98  
126.32  
124.92  
123.99  
77.43  
77.01  
76.58  
75.17

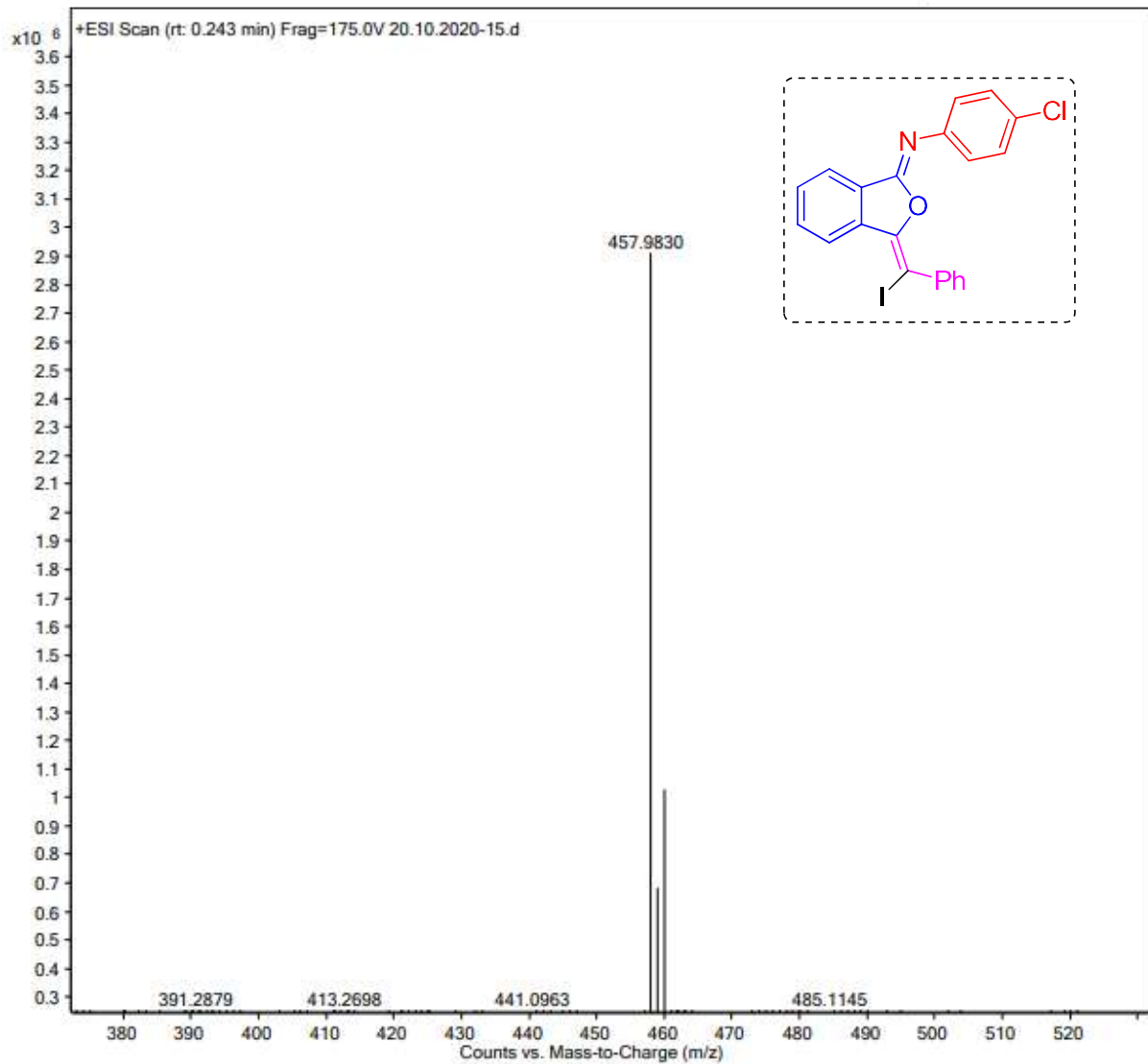


NAME RA-BR-4-136A  
EXPNO 2  
PROCNO 1  
Date\_ 20201020  
Time 15.51  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 736  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 4597.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

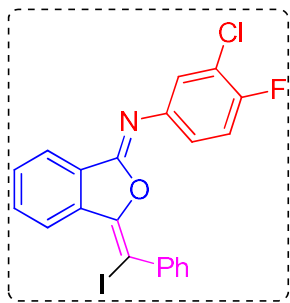
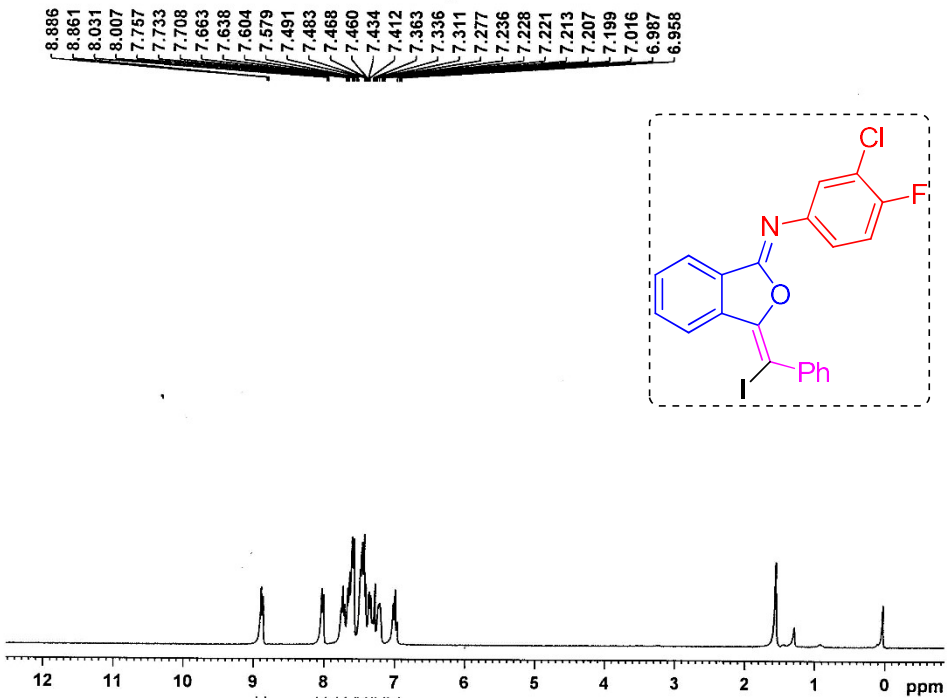
===== CHANNEL f1 =====  
NUC1  $^{13}\text{C}$   
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2  $^1\text{H}$   
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 75.4677448 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 3ai

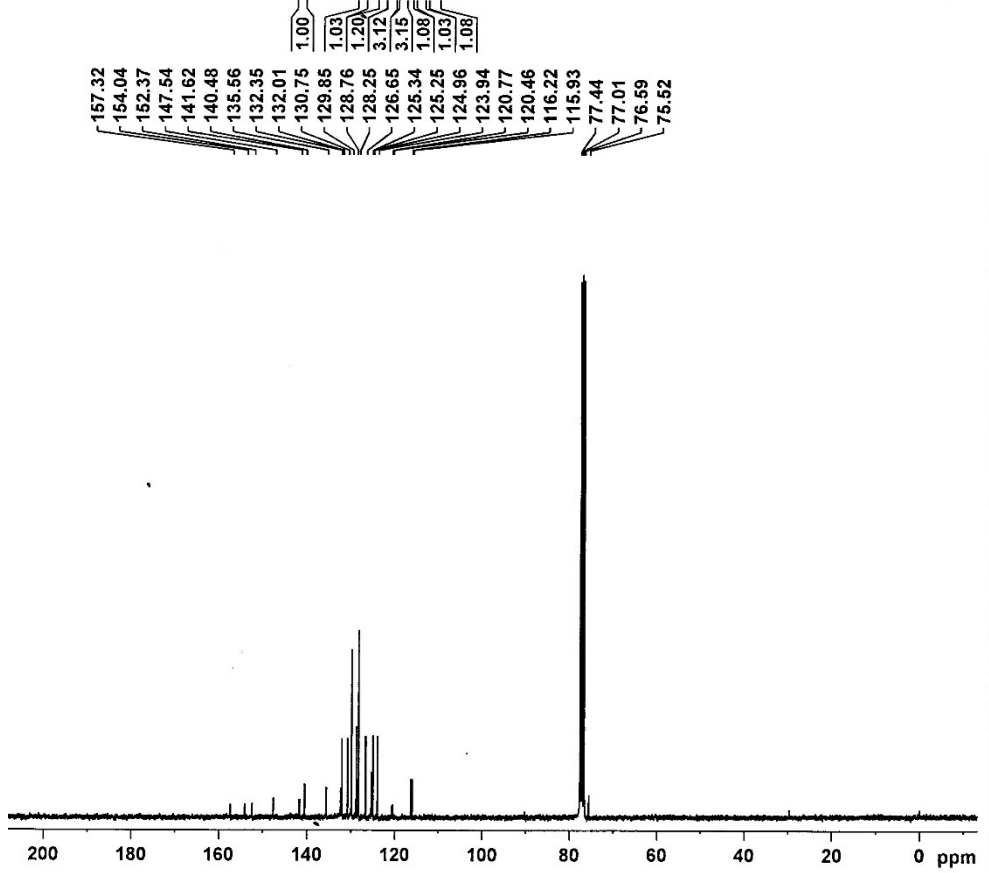


HRMS spectrum of compound 3ai



NAME RA-BR-4-121A  
EXPNO 1  
PROCNO 1  
Date\_ 20200711  
Time 21.12  
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 512  
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



NAME RA-BR-4-121A  
EXPNO 2  
PROCNO 1  
Date\_ 20200711  
Time 22.33  
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 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  
WDW 75.4677432 MHz  
SSB EM  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3aj

Item name: SR-121-A-475, Sample position: 1:A,4, Replicate number: 1

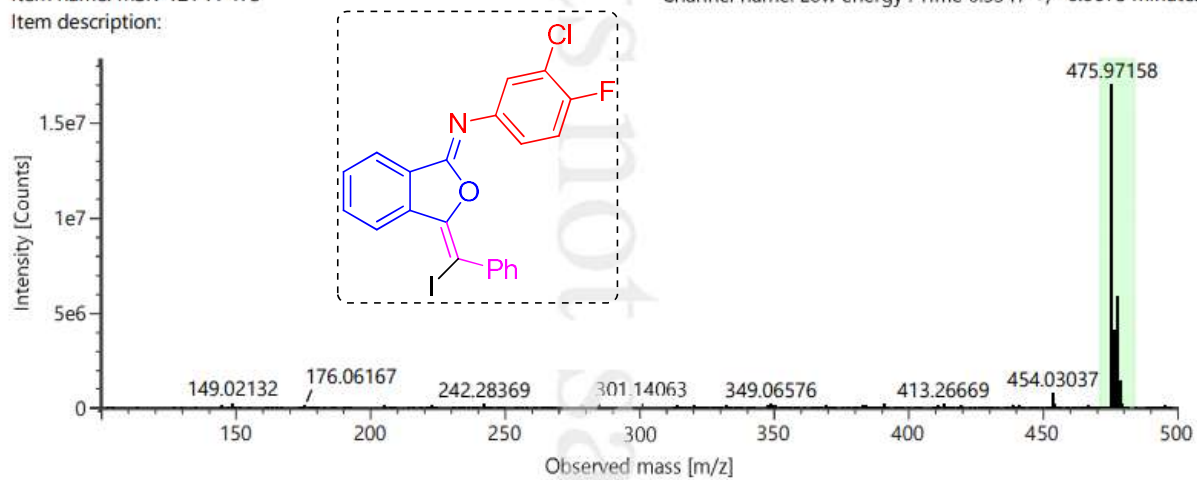
	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C <sub>21</sub> H <sub>12</sub> ClFINO	474.9643	474.96361	475.9716	1.4	+H

**Component name: C<sub>21</sub>H<sub>12</sub>ClFINO**

Item name: MSR-121-A-475

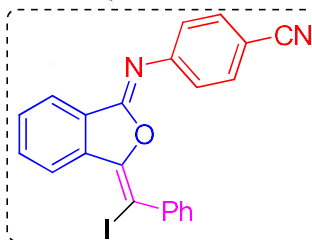
Item description:

Channel name: Low energy : Time 0.5347 +/- 0.0675 minutes

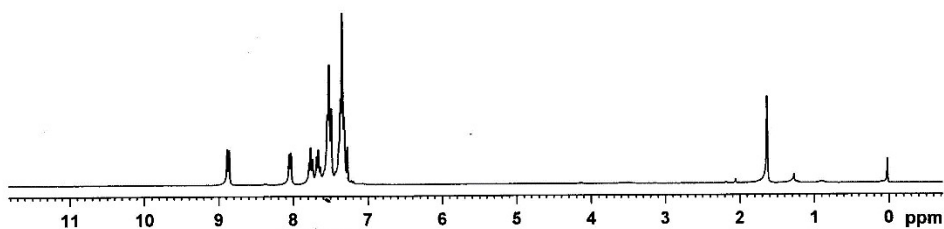


**HRMS spectrum of compound 3aj**

8.888  
8.861  
8.055  
8.031  
7.791  
7.766  
7.741  
7.689  
7.664  
7.639  
7.541  
7.518  
7.489  
7.435  
7.366  
7.343  
7.316  
7.275



NAME RA-BR-4-239B  
EXPNO 1  
PROCNO 1  
Date\_ 20210425  
Time 17.04  
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

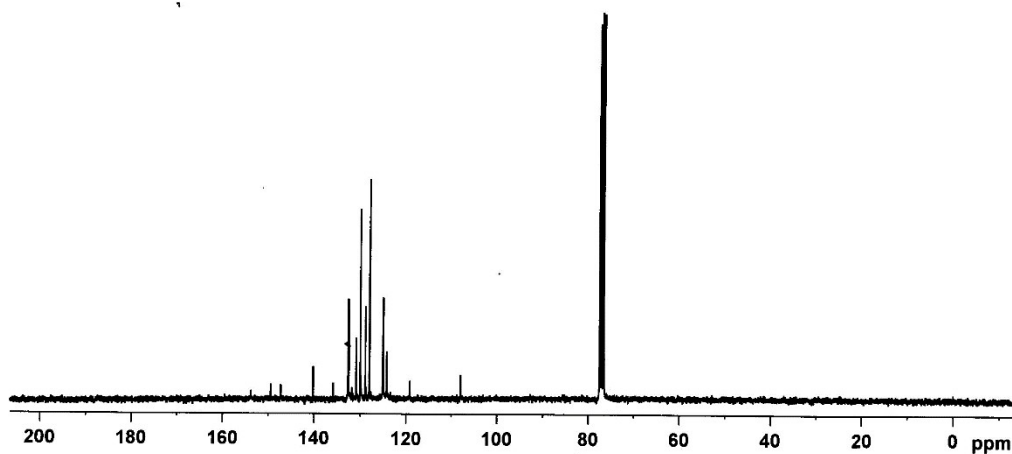


===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1.01  
1.00  
1.18  
1.20  
4.22  
6.17

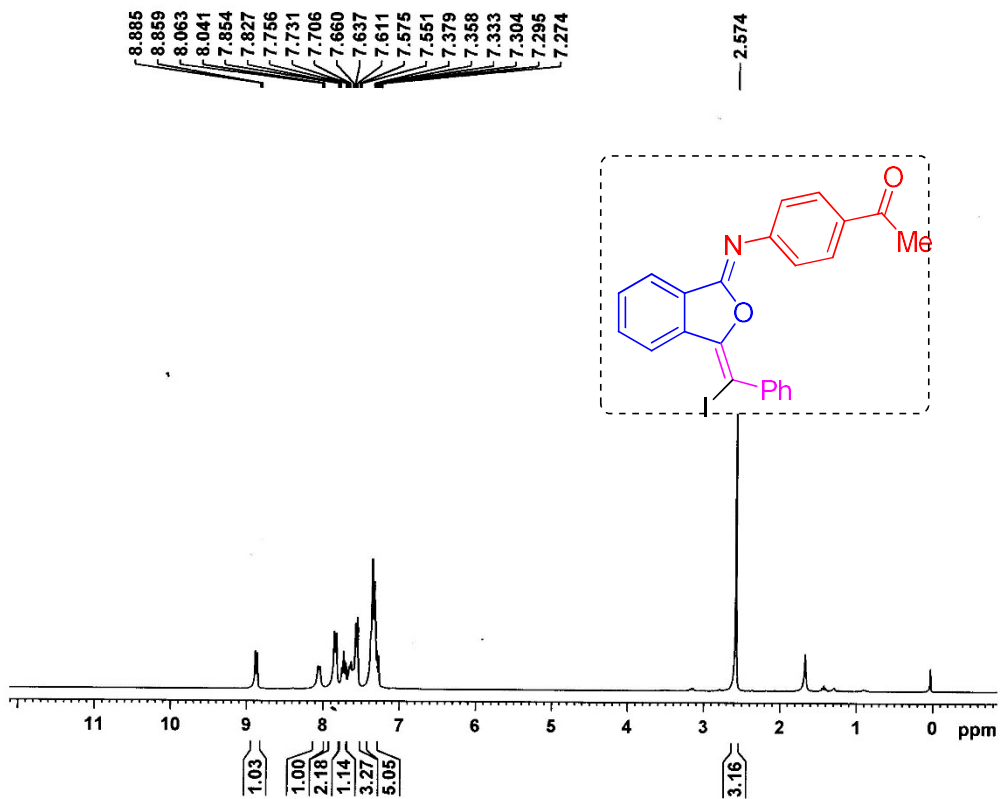
153.77  
149.44  
147.29  
140.21  
135.88  
132.58  
132.49  
131.79  
130.84  
129.97  
128.86  
127.97  
125.02  
124.22  
119.16  
107.97  
77.44  
77.21  
77.01  
76.59

NAME RA-BR-4-239B  
EXPNO 2  
PROCNO 1  
Date\_ 20210425  
Time 18.17  
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 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 75.4677447 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 3ak



```

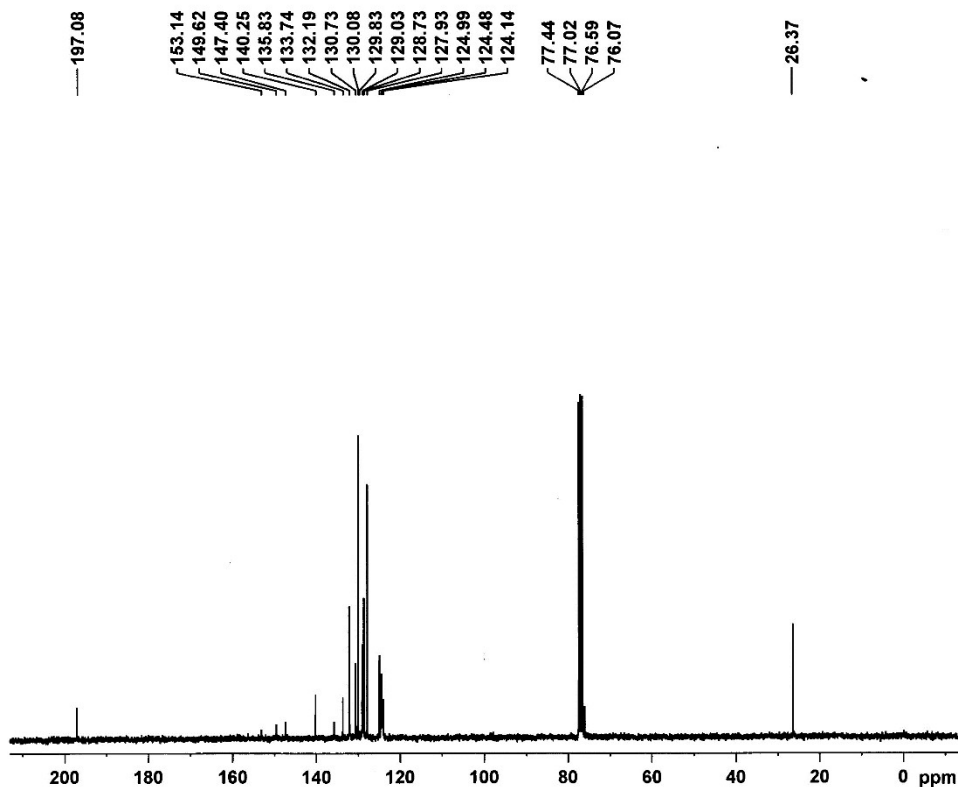
NAME RA-BR-4-239C
EXPNO 1
PROCNO 1
Date_ 20210426
Time 13.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

```

```

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

```



```

NAME RA-BR-4-239C
EXPNO 2
PROCNO 1
Date_ 20210426
Time 14.11
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 12.75 usec
PL1 -1.00 dB
PL1W 39.52848909 W
SFO1 75.4752953 MHz

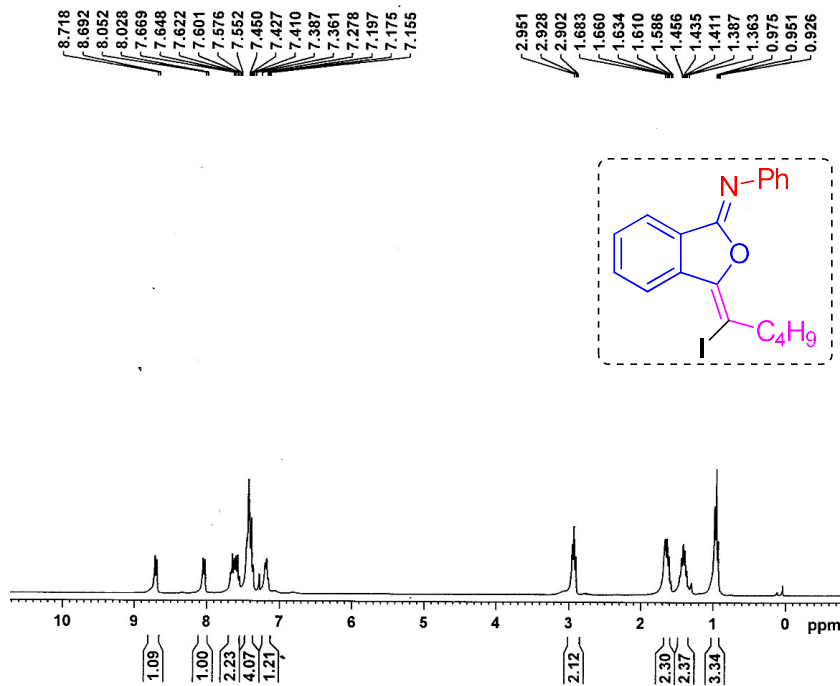
```

```

===== 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 75.4677457 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

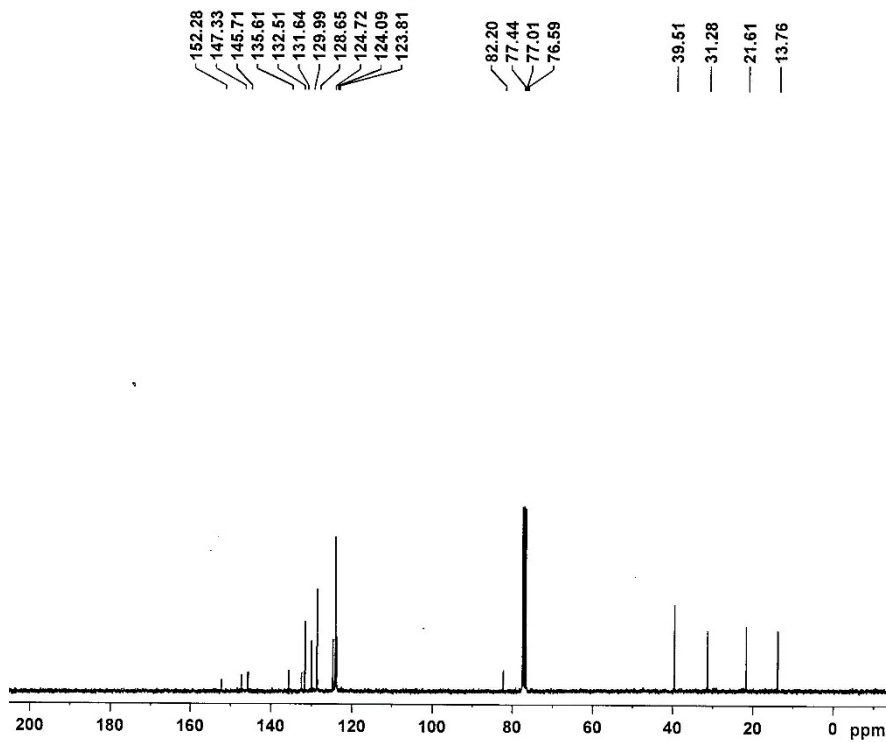
```

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3al



NAME RA-BR-4-144A  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20200809  
 Time\_ 13.16  
 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 181  
 DW 81.000 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 <sup>1</sup>H  
 P1 13.50 usec  
 PL1 -1.00 dB  
 PL1W 13.2815662 W  
 SFO1 300.1318534 MHz  
 SI 32768  
 SF 300.1300011 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

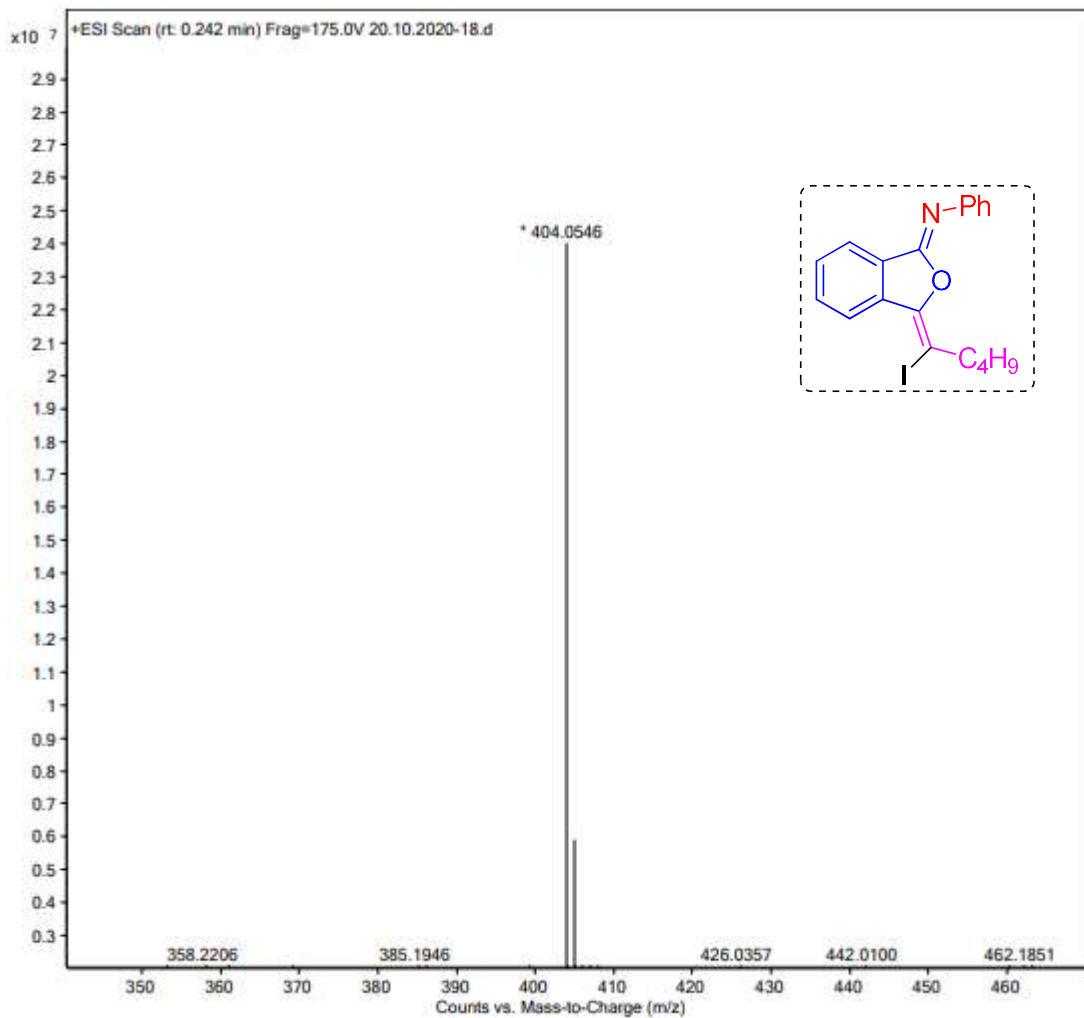


NAME RA-BR-4-144A  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20200809  
 Time\_ 14.03  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 822  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 5160.6  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 12.75 usec  
 PL1 -1.00 dB  
 PL1W 39.52848909 W  
 SFO1 75.4752953 MHz

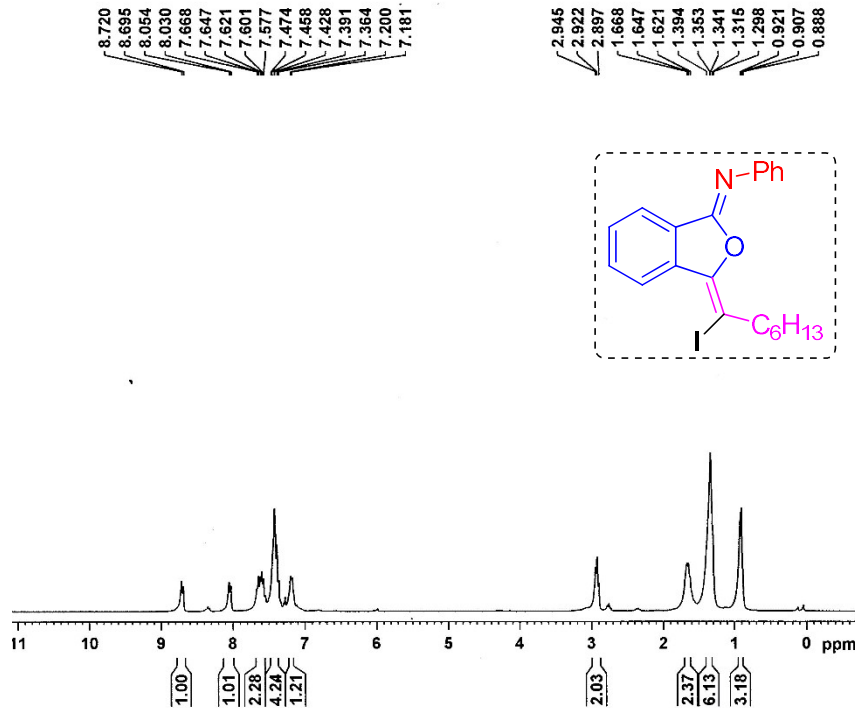
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 80.00 usec  
 PL2 -1.00 dB  
 PL12 14.46 dB  
 PL13 16.00 dB  
 PL2W 13.2815662 W  
 PL12W 0.37778899 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677451 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3a



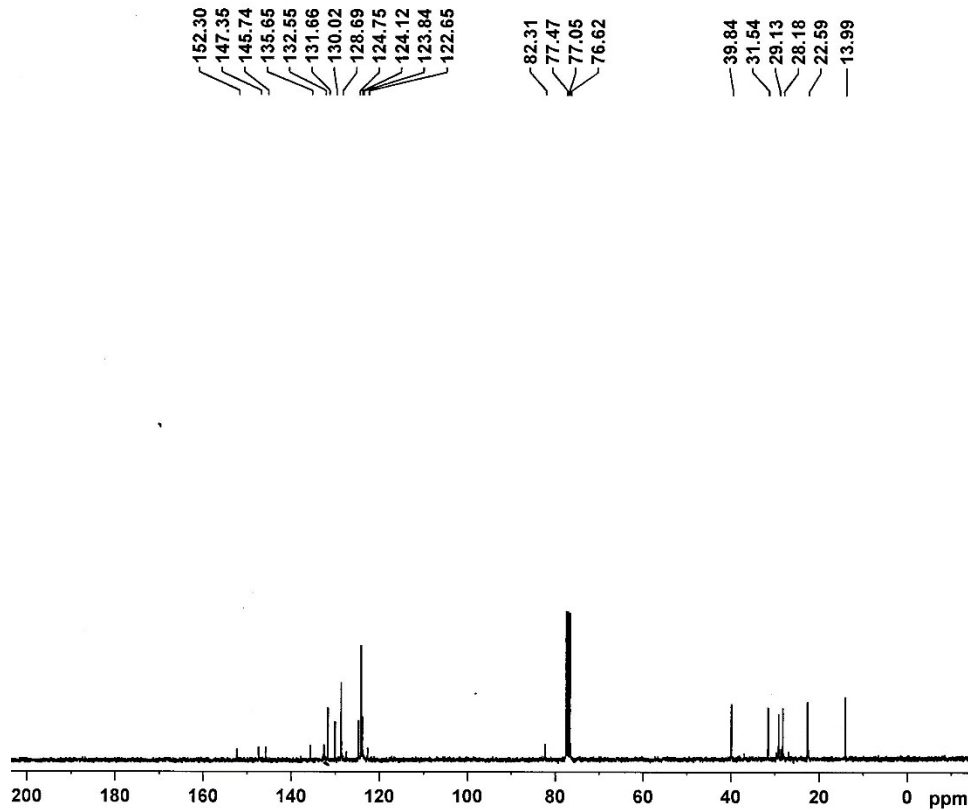
HRMS spectrum of compound 3am





NAME RA-BR-4-143B  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20200805  
 Time 18.44  
 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 5.3084660 sec  
 RG 181  
 DE 81.000 usec  
 DW 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 13.50 usec  
 PL1 -1.00 dB  
 PL1W 13.2815662 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-4-143B  
 EXPNO 2  
 PROCNO 1  
 Date\_ 20200805  
 Time 18.51  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 462  
 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 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 75.4677431 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 3a

Item name: SR-143-B-432, Sample position: 1:A2, Replicate number: 1

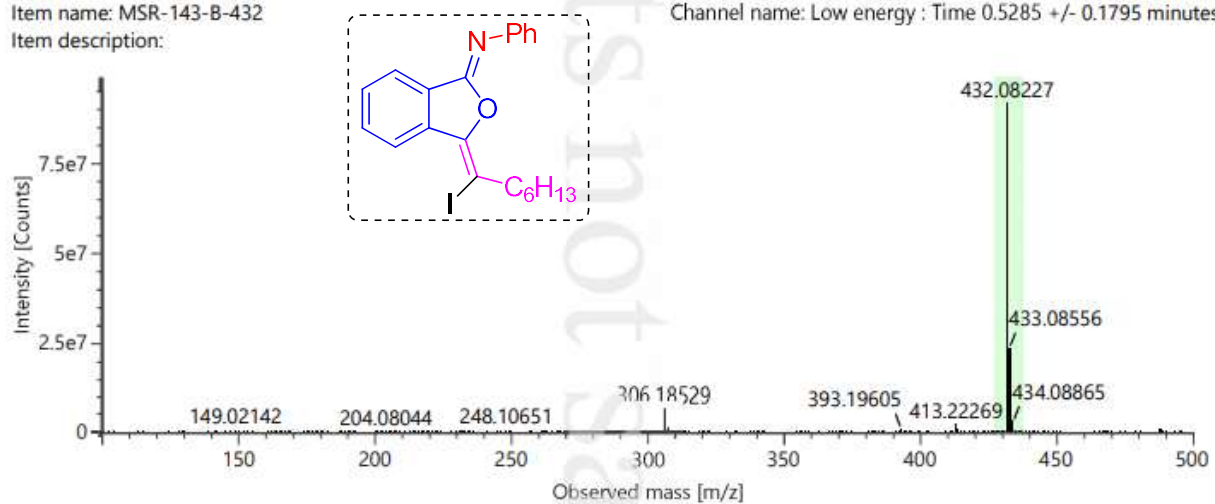
	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C <sub>21</sub> H <sub>22</sub> INO	431.0750	431.07461	432.0823	0.9	+H

**Component name: C<sub>21</sub>H<sub>22</sub>INO**

Item name: MSR-143-B-432

Item description:

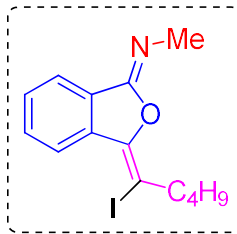
Channel name: Low energy : Time 0.5285 +/- 0.1795 minutes



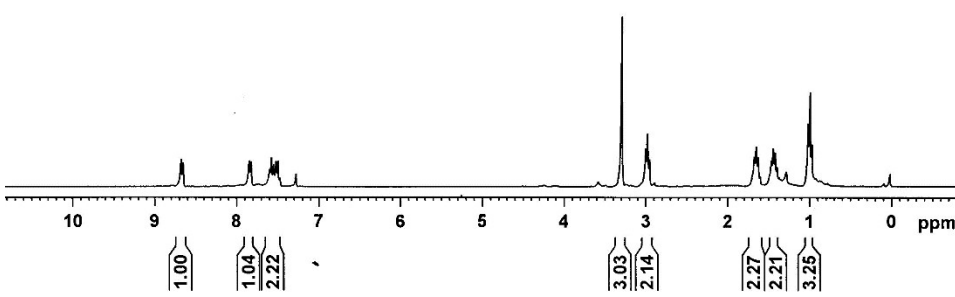
**HRMS spectrum of compound 3a**

8.680  
8.654  
7.848  
7.823  
7.600  
7.576  
7.550  
7.520  
7.496  
7.471  
7.276

3.293  
3.004  
2.981  
2.956  
1.675  
1.652  
1.627  
1.466  
1.444  
1.420  
1.396  
1.015  
0.991  
0.967



NAME RA-BR-4-129A  
EXPNO 1  
PROCNO 1  
Date 20200719  
Time 22.22  
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



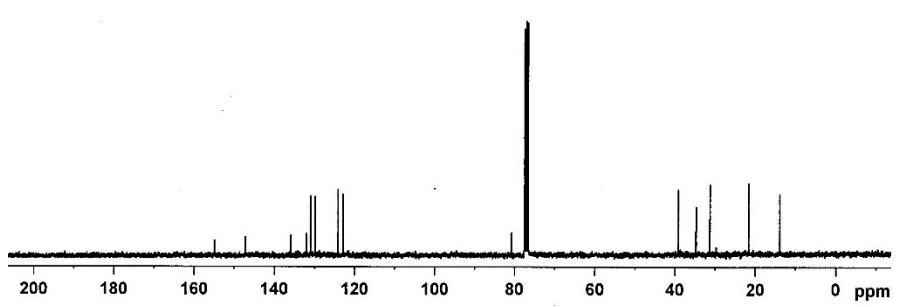
===== CHANNEL f1 =====  
NUC1 1H  
P1 13.50 usec  
PL1 -1.00 dB  
PL1W 13.28156662 W  
SFO1 300.1318534 MHz  
SI 32768  
SF 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

154.87  
147.15  
135.88  
132.03  
131.01  
129.86  
124.17  
122.90

80.78  
77.45  
77.03  
76.60

39.08  
34.66  
31.20  
21.53  
13.81

NAME RA-BR-4-129A  
EXPNO 2  
PROCNO 1  
Date 20200719  
Time 22.30  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 506  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5180.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1



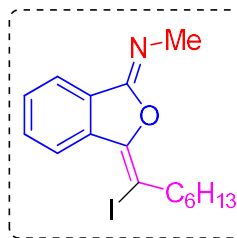
===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52646909 W  
SFO1 75.4752953 MHz

===== 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 75.4677432 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 3ao

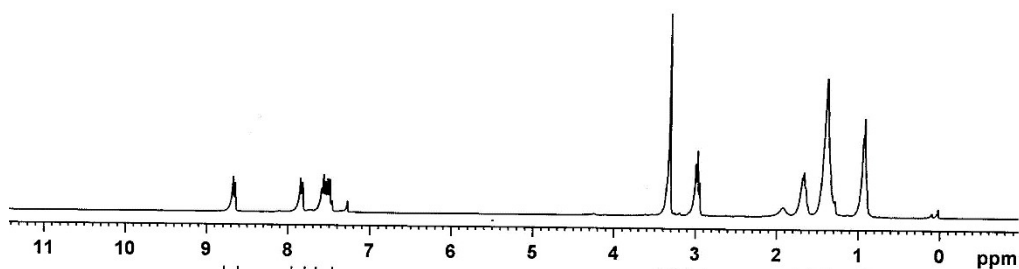
8.677  
8.652  
7.850  
7.826  
7.596  
7.571  
7.545  
7.516  
7.492  
7.467  
7.277

3.310  
2.995  
2.972  
2.947  
1.685  
1.664  
1.651  
1.433  
1.376  
1.285  
0.951  
0.936  
0.914



NAME RA-BR-4-135  
EXPNO 1  
PROCNO 1  
Date\_ 20200724  
Time 19.16  
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 181  
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

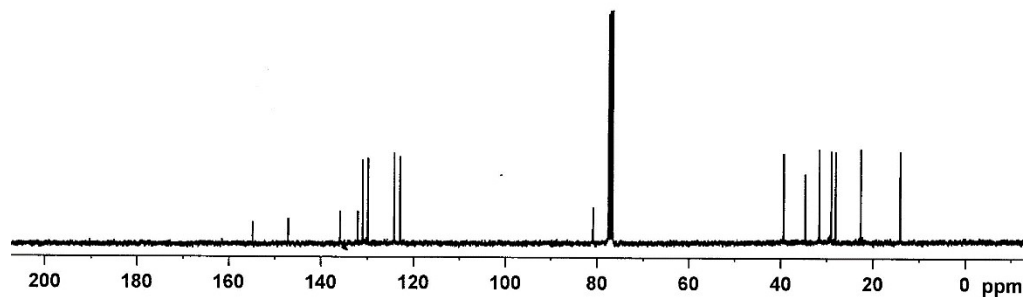


1.00  
1.09  
2.24  
3.19  
2.18  
2.23  
6.12  
3.27

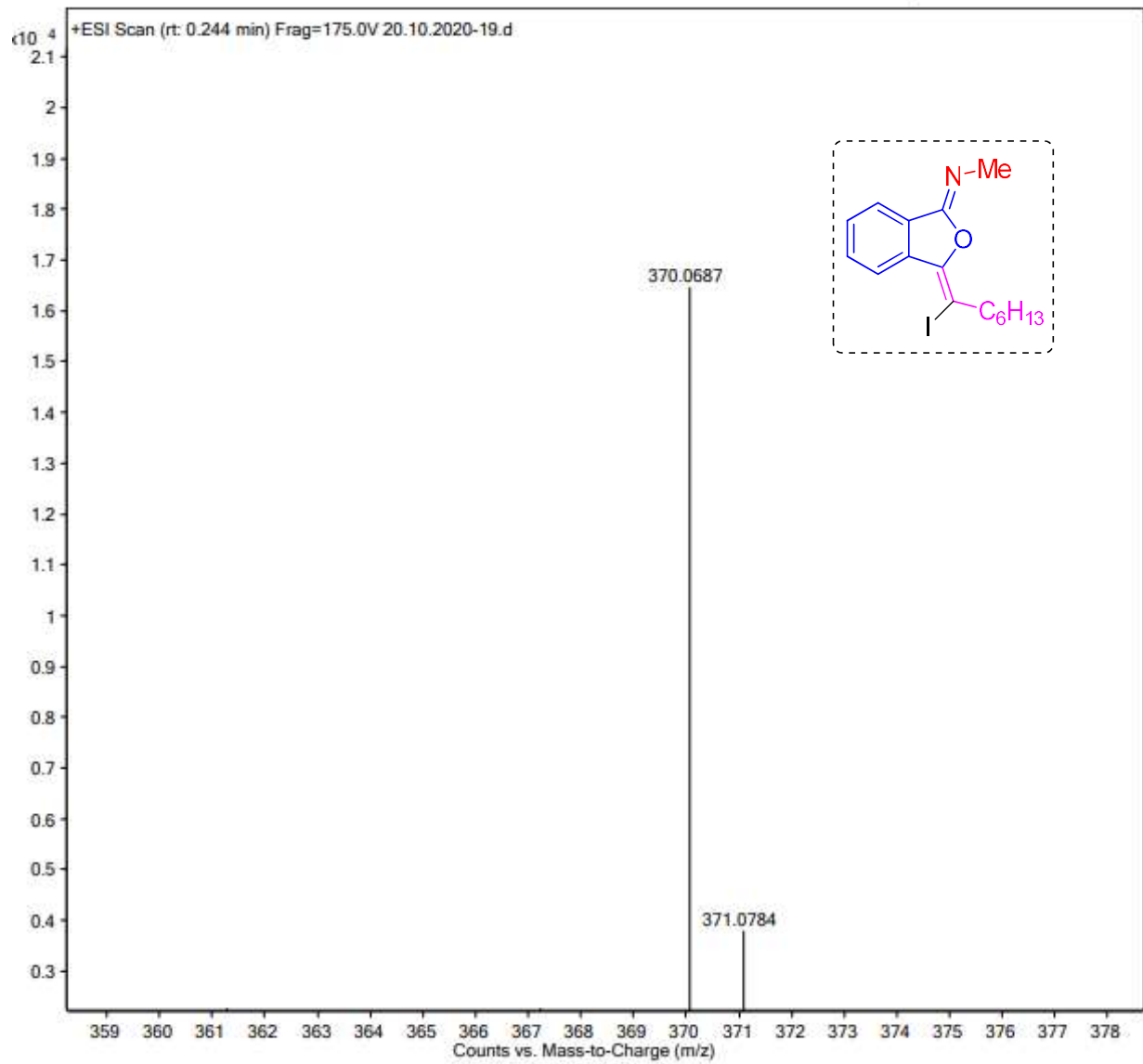
NAME RA-BR-4-135  
EXPNO 3  
PROCNO 1  
Date\_ 20200728  
Time 21.50  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 828  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

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

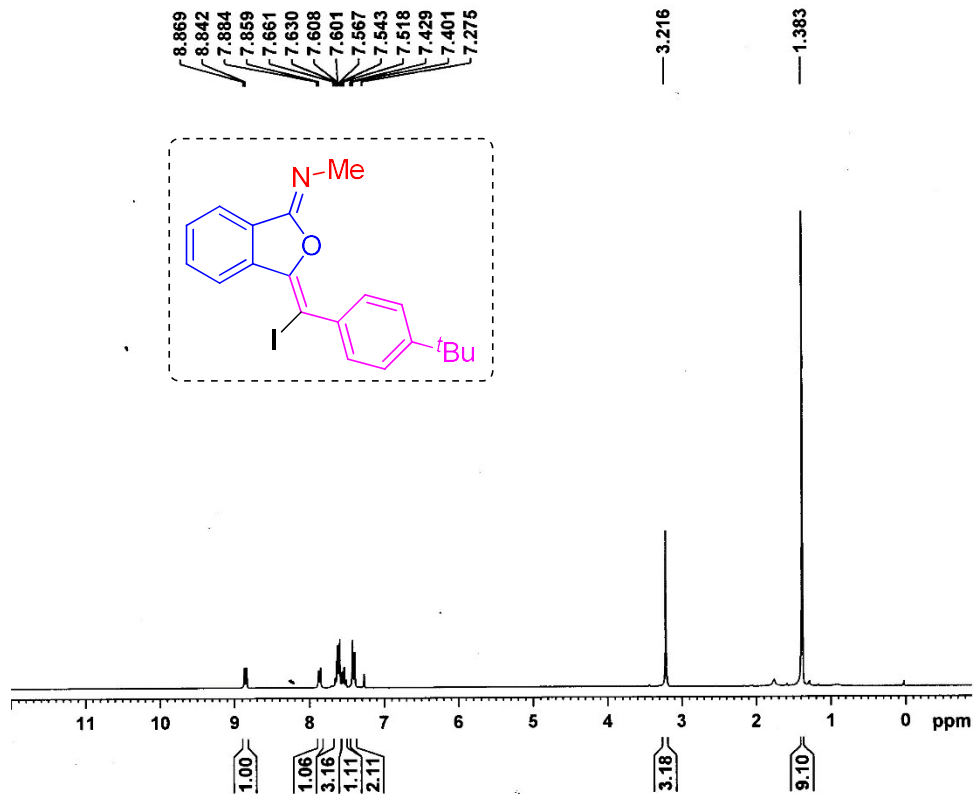
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677440 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>H & <sup>13</sup>C spectra of compound 3ap



HRMS spectrum of compound 3ap



```

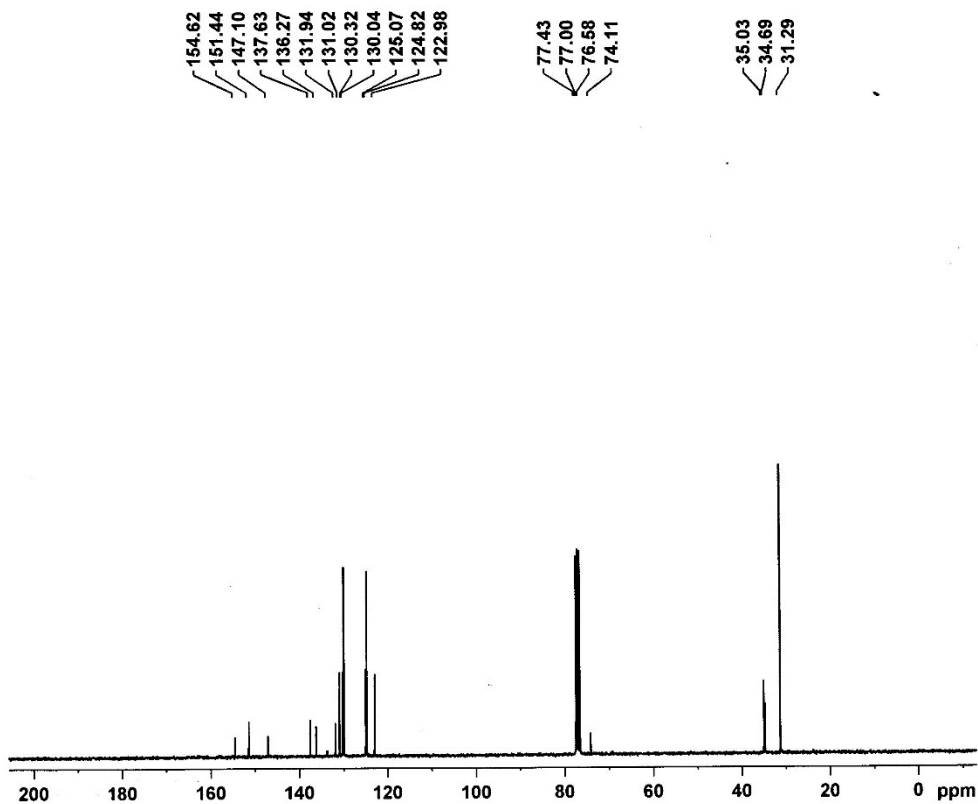
NAME RA-BR-4-244
EXPNO 1
PROCNO 1
Date_ 20210625
Time 18.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

```

```

===== CHANNEL f1 =====
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
PL1W 13.2815662 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-4-244
EXPNO 2
PROCNO 1
Date_ 20210625
Time 19.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1147
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
TD0 1

```

```

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

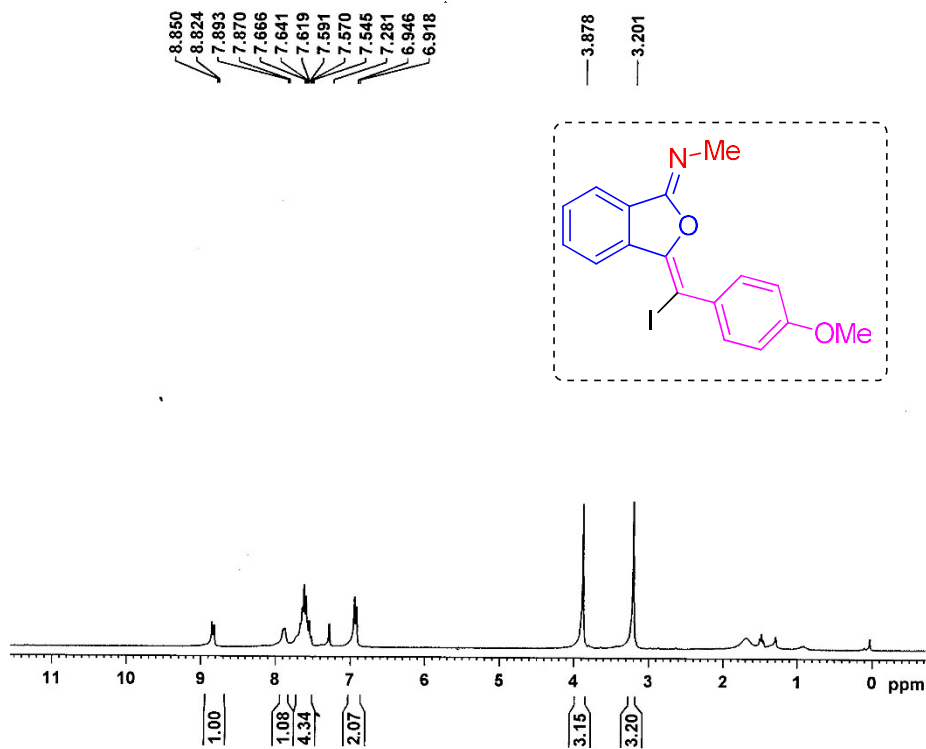
```

```

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.45 dB
PL13 16.00 dB
PL2W 13.2815662 W
PL12W 0.37778899 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677450 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 3aq



```

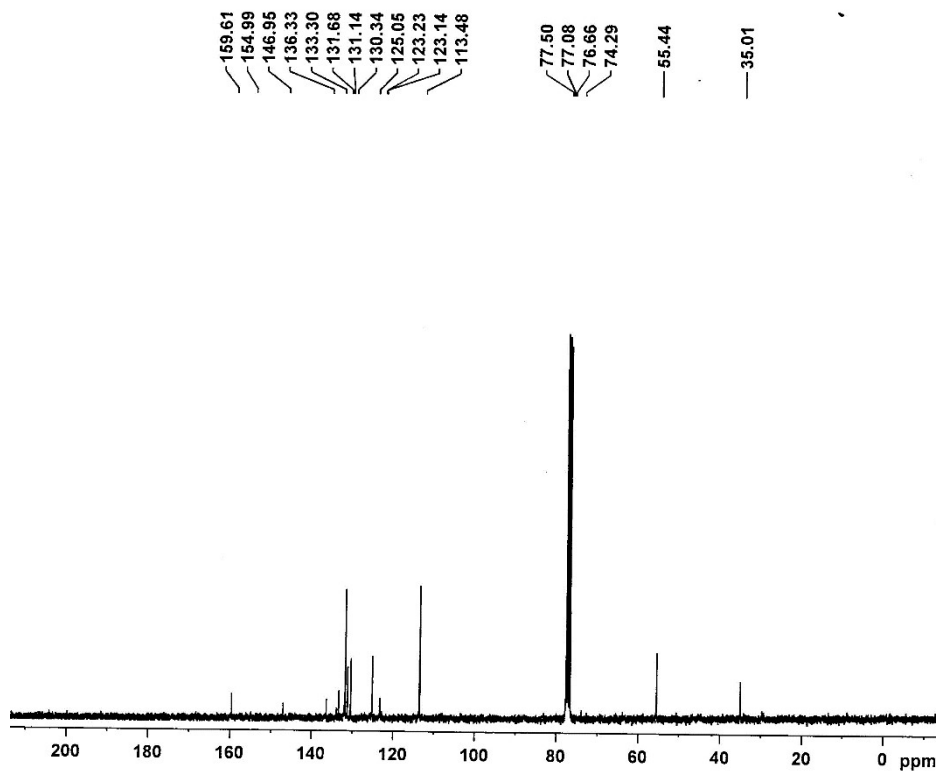
NAME RA-BR-4-132
EXPNO 2
PROCNO 1
Date_ 20200804
Time 15.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

```

```

===== 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

```



```

NAME RA-BR-4-132
EXPNO 3
PROCNO 1
Date_ 20200804
Time 17.59
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

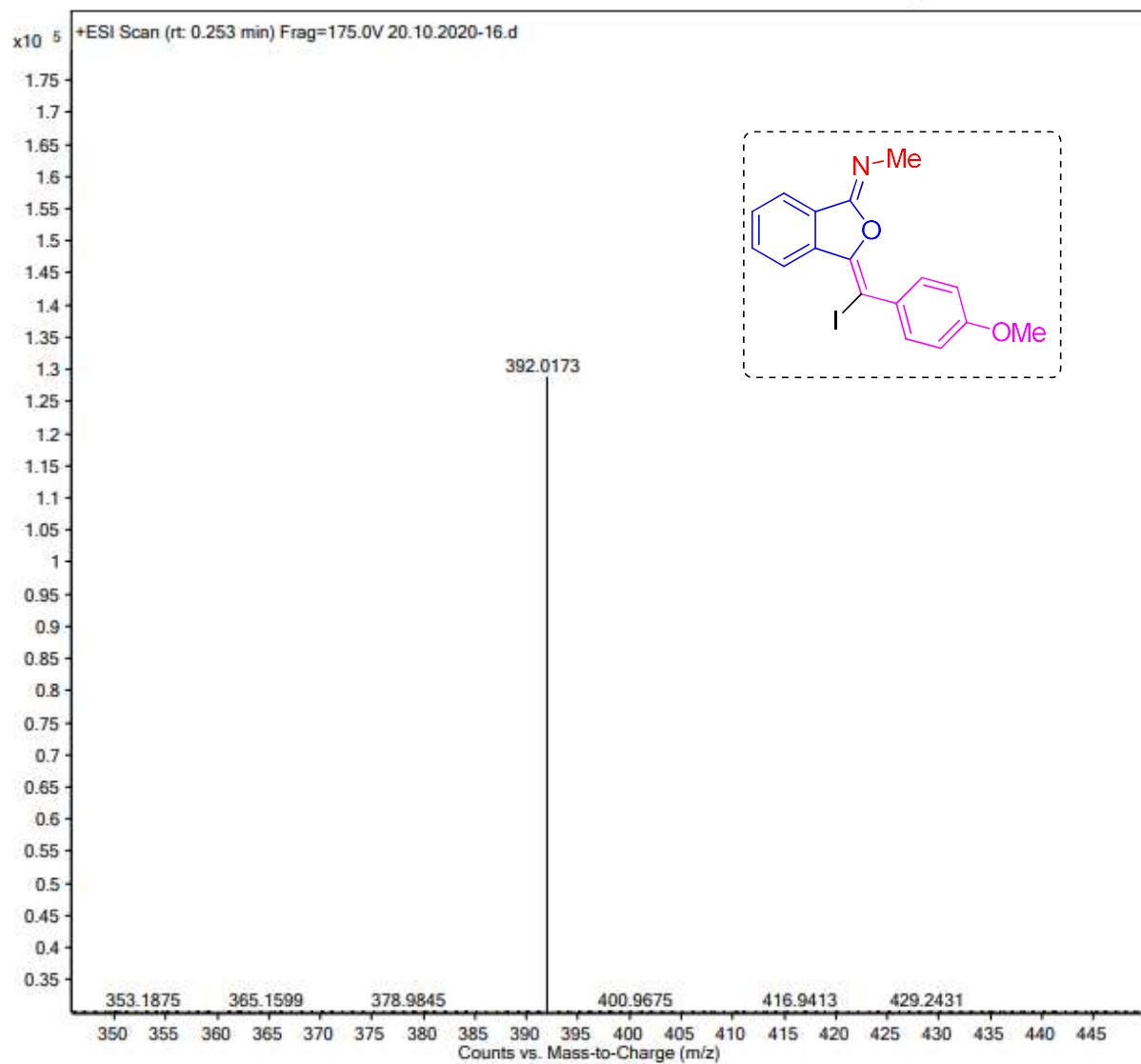
```

```

===== 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 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677378 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

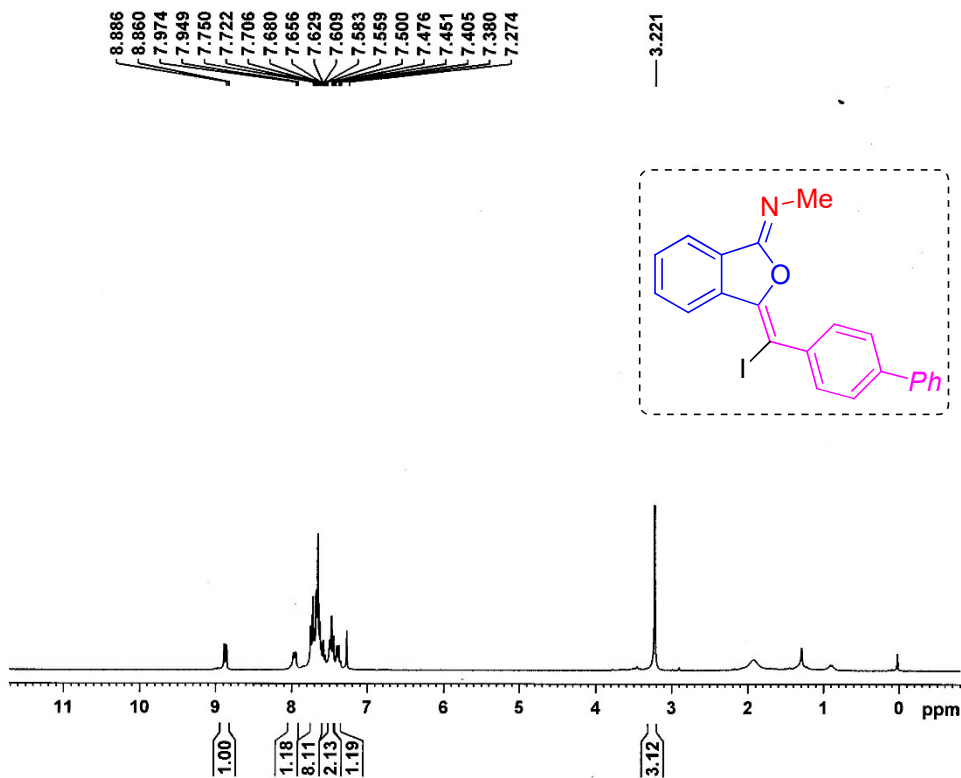
```

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3ar



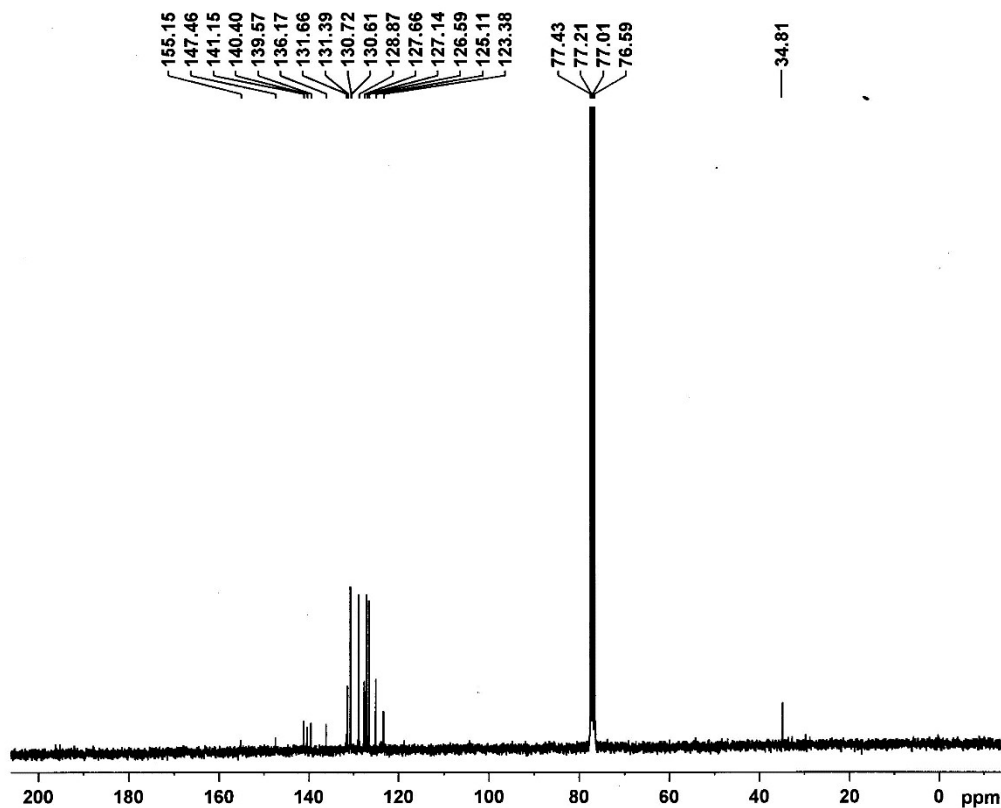
HRMS spectrum of compound 3ar





NAME RA-BR-4-243B  
EXPNO 3  
PROCNO 1  
Date\_ 20210624  
Time 21.40  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084680 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 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

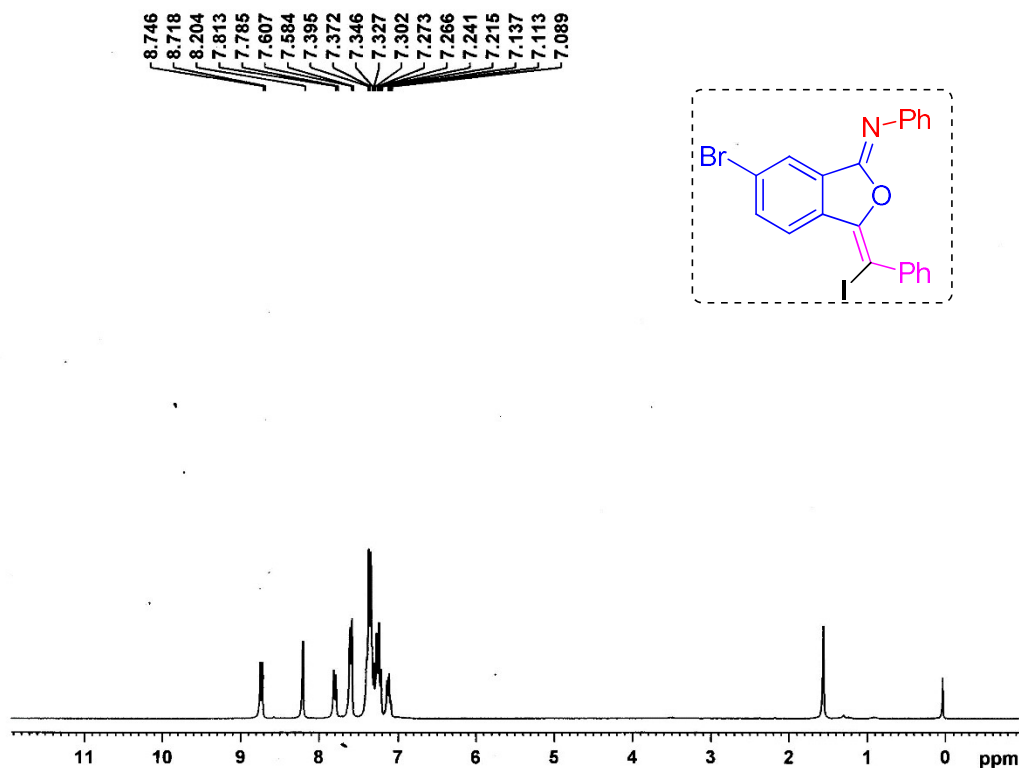


NAME RA-BR-4-243B  
EXPNO 2  
PROCNO 1  
Date\_ 20210624  
Time 19.32  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65538  
SOLVENT CDCl3  
NS 2500  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 3649.1  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52848909 W  
SFO1 75.4752953 MHz

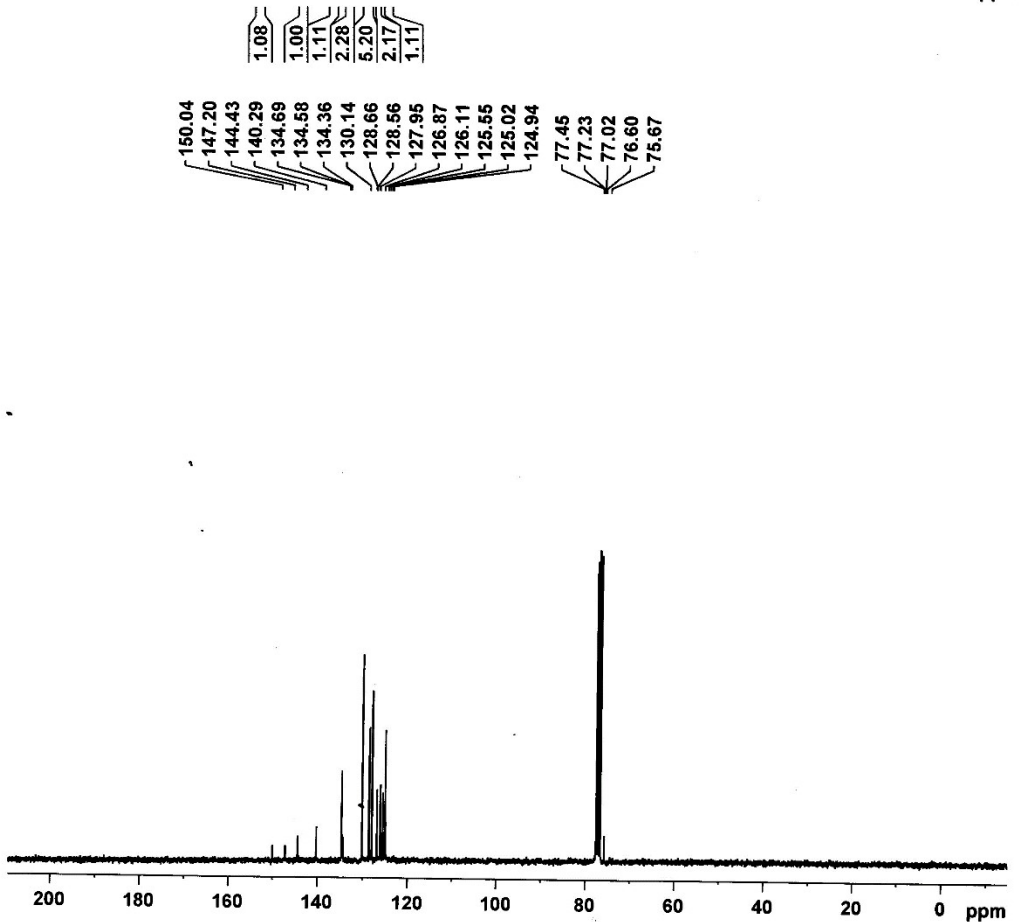
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677432 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3as



NAME RA-BR-4-240A  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20210428  
 Time 14.11  
 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 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 300.1300011 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

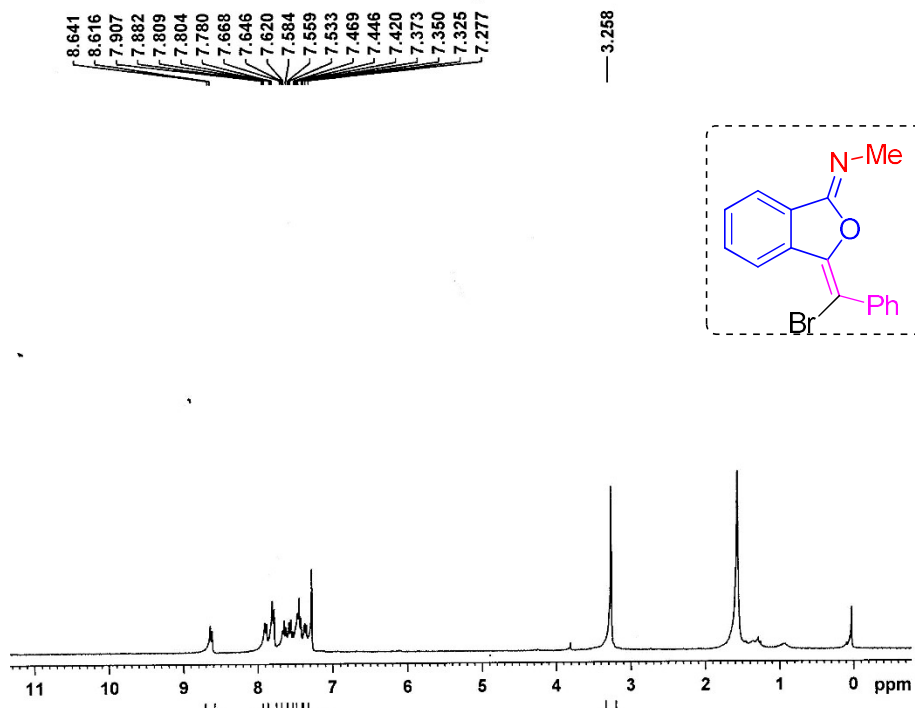


NAME RA-BR-4-240A  
 EXPNO 3  
 PROCNO 1  
 Date\_ 20210428  
 Time 18.01  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 2298.8  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 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 75.4677436 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 3at



```

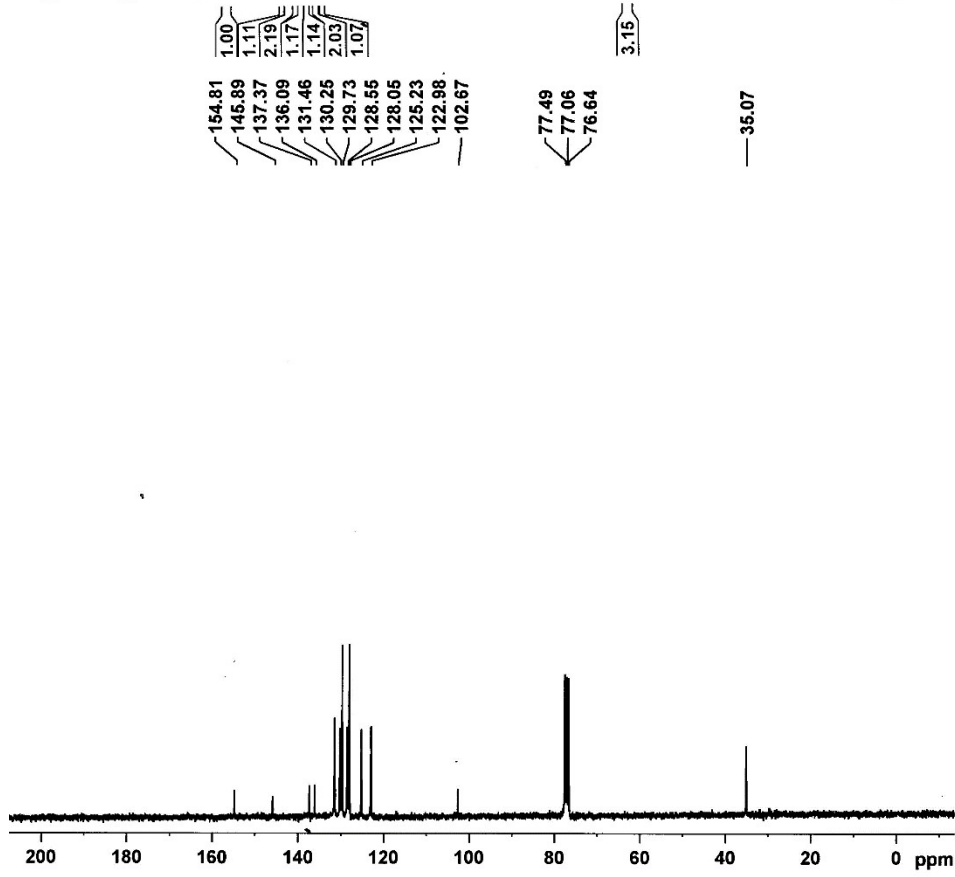
NAME RA-BR-4-118D
EXPNO 2
PROCNO 1
Date_ 20200820
Time 19.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 812.7
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

```

```

===== 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-4-133D
EXPNO 2
PROCNO 1
Date_ 20201224
Time 22.52
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 364.1
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

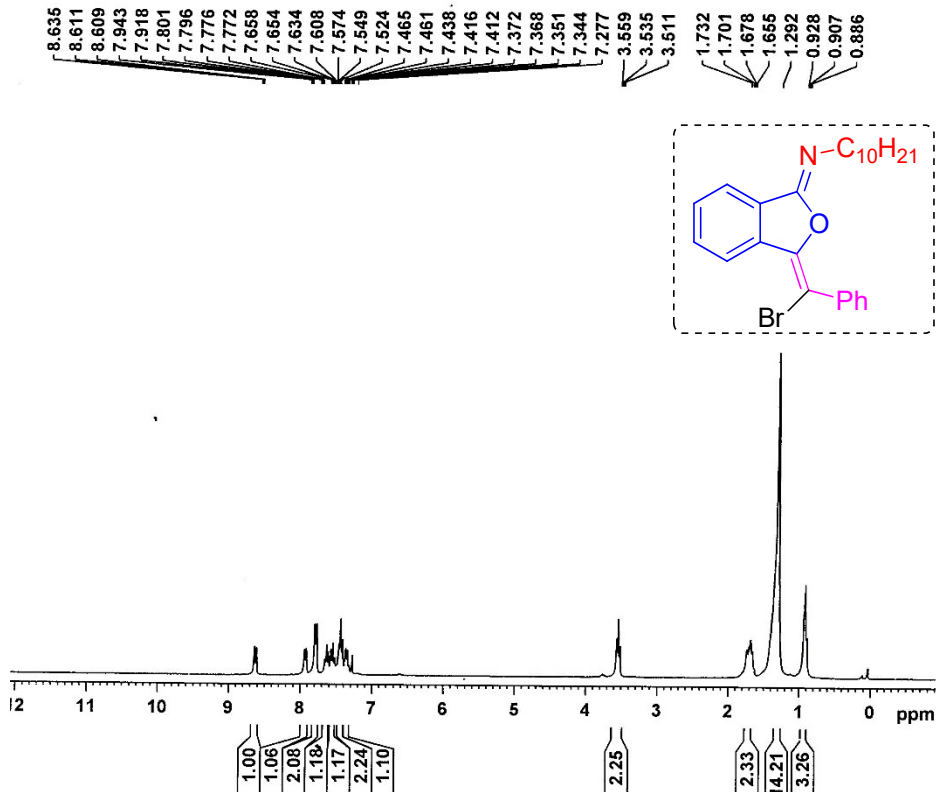
```

```

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.46 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.37778999 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677493 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

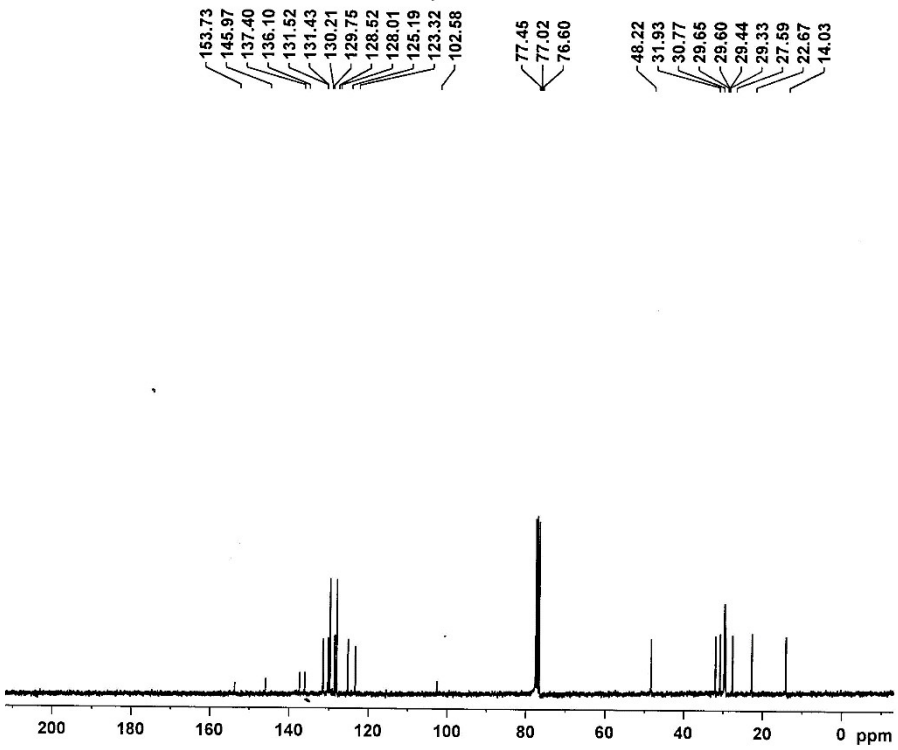
```

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3ba



NAME RA-BR-4-147B  
EXPNO 1  
PROCNO 1  
Date\_ 20200818  
Time 12.48  
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 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 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



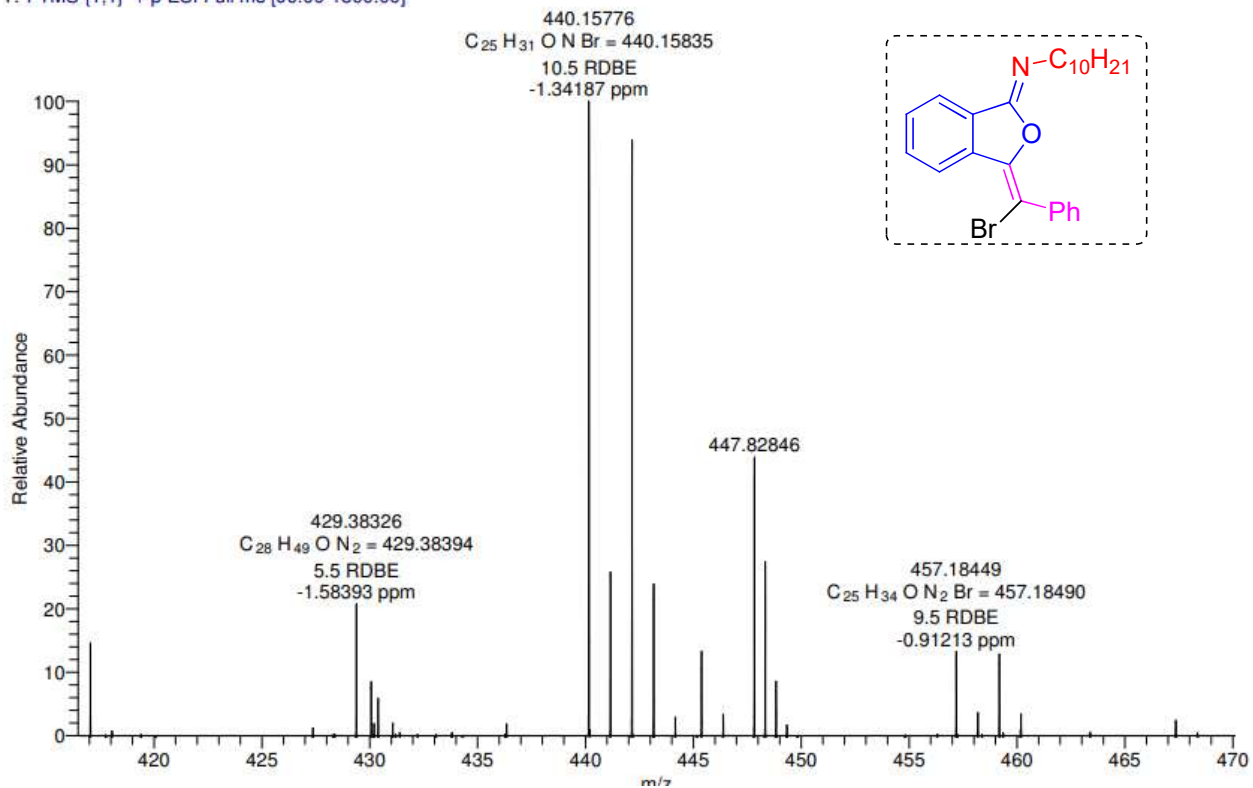
NAME RA-BR-4-147B  
EXPNO 3  
PROCNO 1  
Date\_ 20200819  
Time 18.22  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 2896.3  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52848909 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 0.37778889 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677437 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

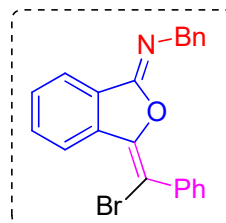
<sup>1</sup>H & <sup>13</sup>C spectra of compound 3bb

SR-147B #8-18 RT: 0.06-0.13 AV: 11 NL: 2.72E6  
T: FTMS (1,1) + p ESI Full ms [90.00-1800.00]



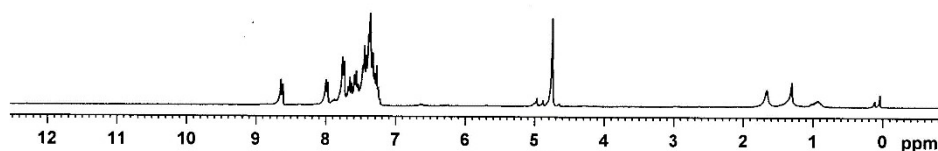
HRMS spectrum of compound 3bb

8.643  
8.617  
8.000  
7.975  
7.765  
7.760  
7.753  
7.741  
7.736  
7.682  
7.657  
7.631  
7.591  
7.567  
7.542  
7.475  
7.471  
7.448  
7.422  
7.392  
7.388  
7.383  
7.368  
7.355  
7.331  
7.305  
7.277  
7.258  
7.251  
4.742



NAME RA-BR-4-122B  
EXPNO 1  
PROCNO 1  
Date\_ 20200712  
Time\_ 13.46  
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 5.3084660 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 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

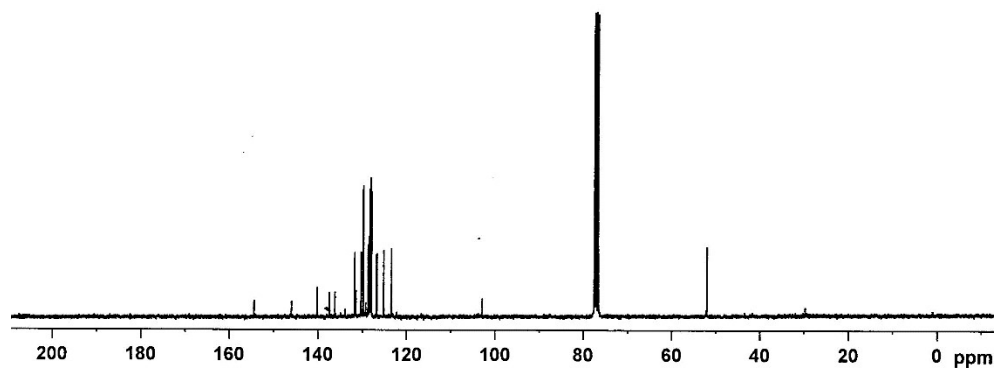


154.42  
140.13  
137.40  
136.14  
131.71  
131.48  
130.27  
129.79  
128.65  
128.37  
128.10  
127.94  
126.72  
125.19  
123.45  
102.92  
77.45  
77.03  
76.61  
51.94

NAME RA-BR-4-122B  
EXPNO 2  
PROCNO 1  
Date\_ 20200712  
Time\_ 16.40  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2629  
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

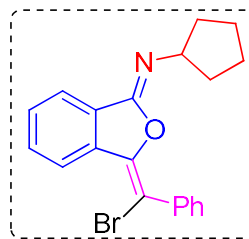
===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== 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 75.4677433 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



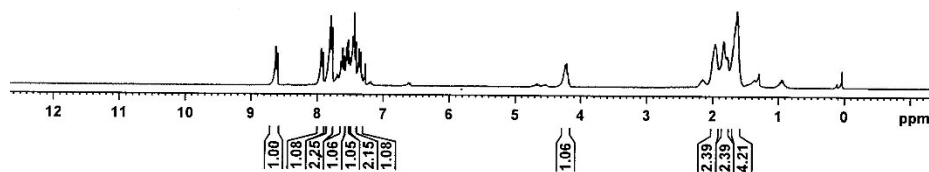
$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 3bc

8.627  
8.601  
7.944  
7.919  
7.840  
7.830  
7.806  
7.801  
7.777  
7.646  
7.643  
7.622  
7.596  
7.592  
7.562  
7.559  
7.537  
7.524  
7.512  
7.466  
7.460  
7.442  
7.416  
7.369  
7.352  
7.345  
7.277  
4.253  
4.234  
4.212  
4.190  
4.173  
2.001  
1.983  
1.967  
1.953  
1.946  
1.834  
1.825  
1.796  
1.784  
1.776  
1.686  
1.672  
1.659  
1.644  
1.628



NAME RA-BR-4-120  
EXPNO 1  
PROCNO 1  
Date\_ 20200710  
Time 11.07  
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 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 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

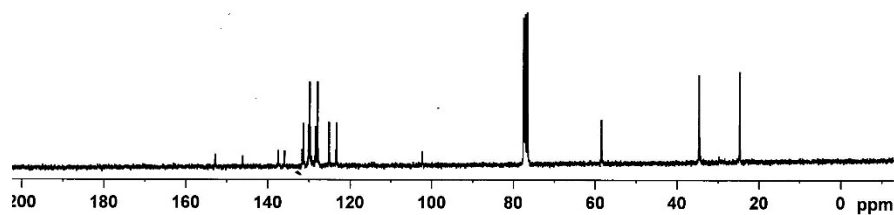


152.75  
146.05  
137.40  
135.97  
131.68  
131.40  
130.16  
129.85  
128.49  
127.98  
125.17  
123.36  
102.25  
77.47  
77.05  
76.63  
58.49  
34.61  
24.63

NAME RA-BR-4-192B  
EXPNO 3  
PROCNO 1  
Date\_ 20201219  
Time 9.51  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65336  
SOLVENT CDCl3  
NS 2048  
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

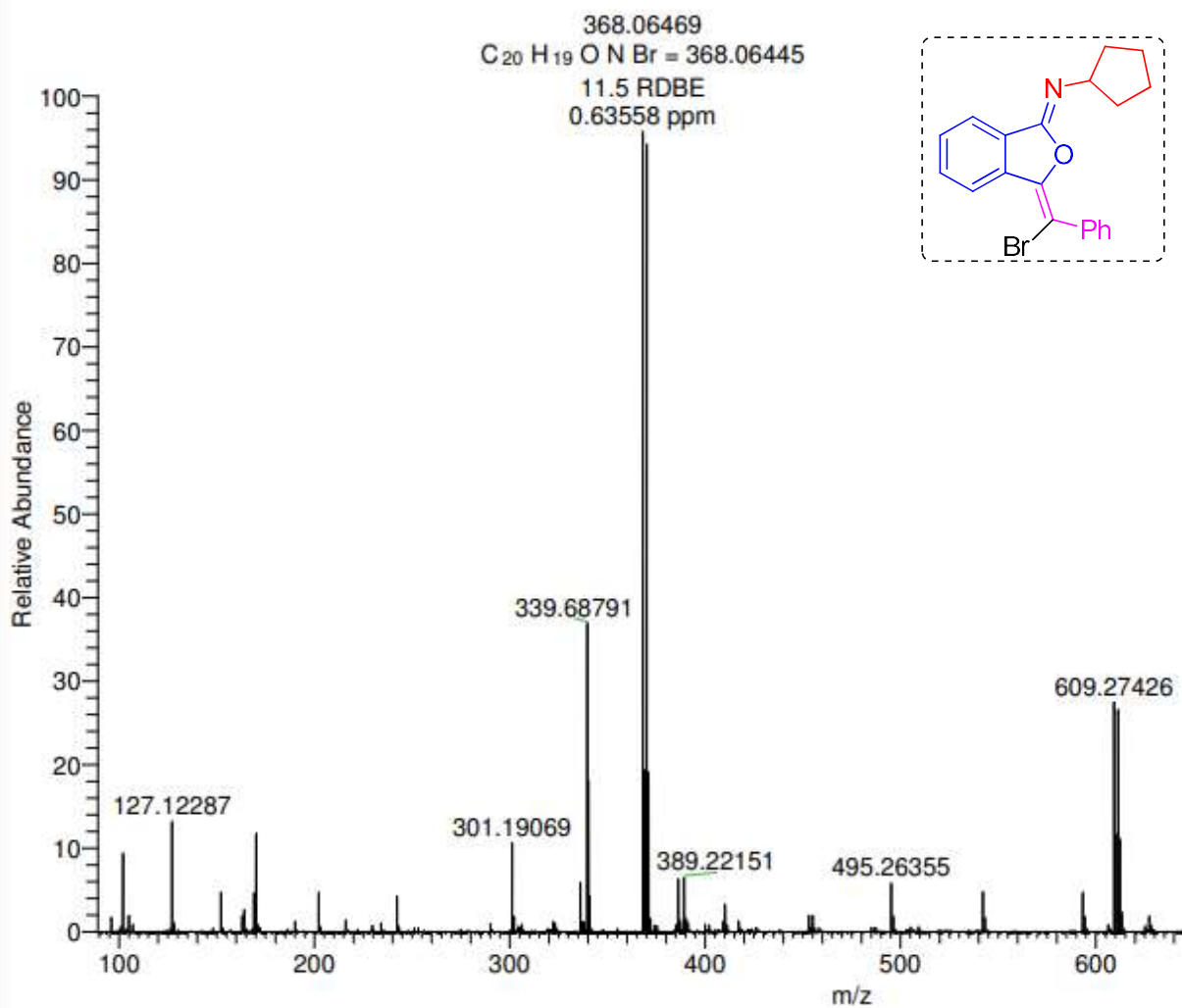
===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52848909 W  
SFO1 75.4752953 MHz

===== 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



<sup>1</sup>H & <sup>13</sup>C spectra of compound 3bd

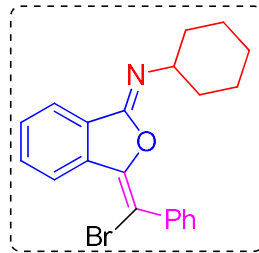
SR-120A #5-13 RT: 0.04-0.10 AV: 9 NL: 4.39E7  
T: FTMS {1,1} + p ESI Full ms [90.00-1800.00]



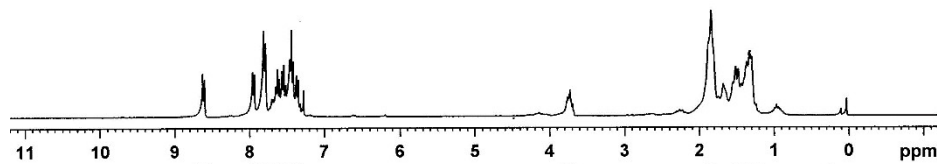
HRMS spectrum of compound 3bd



8.628  
8.601  
7.961  
7.936  
7.813  
7.809  
7.785  
7.651  
7.647  
7.626  
7.600  
7.566  
7.540  
7.516  
7.463  
7.456  
7.439  
7.413  
7.372  
7.355  
7.348  
7.277  
3.761  
3.739  
3.727  
3.714  
3.692  
1.881  
1.842  
1.819  
1.788  
1.681  
1.646  
1.510  
1.475  
1.441  
1.430  
1.383  
1.363  
1.323  
1.296  
1.260



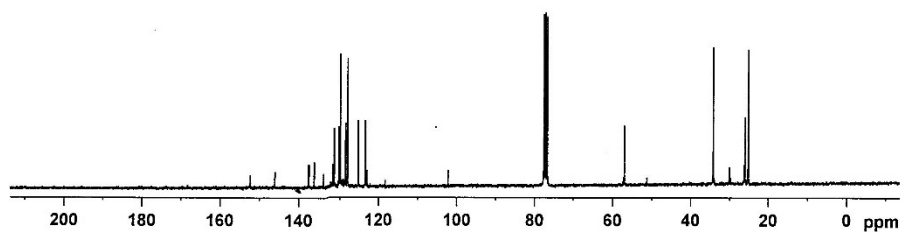
NAME RA-BR-4-124B  
EXPNO 5  
PROCNO 1  
Date 20200718  
Time 8.16  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65538  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 181  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1



1.00  
1.13  
1.13  
2.32  
1.19  
1.22  
2.21  
1.04  
1.05  
4.24  
2.12  
4.28

===== 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

152.26  
146.01  
137.39  
136.04  
133.66  
131.36  
130.11  
129.77  
128.46  
127.91  
125.15  
123.34  
102.12  
77.44  
77.02  
76.60  
56.90  
34.06  
25.87  
25.01



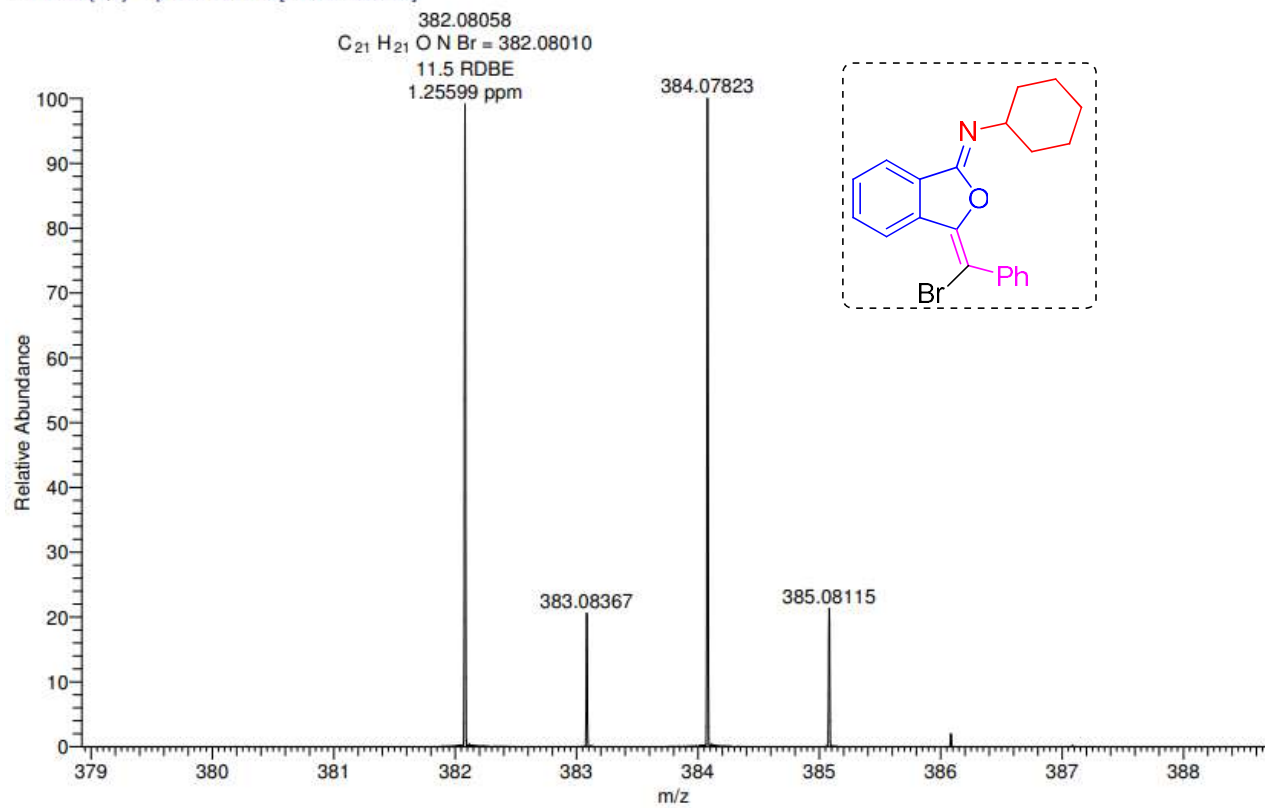
NAME RA-BR-4-124B  
EXPNO 6  
PROCNO 1  
Date 20200718  
Time 12.39  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65538  
SOLVENT CDCl3  
NS 4000  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 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 75.4677440 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

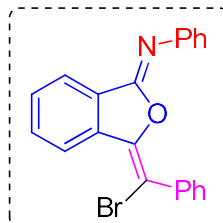
<sup>1</sup>H & <sup>13</sup>C spectra of compound 3be

T: FTMS (1,1) + p ESI Full ms [90.00-1800.00]

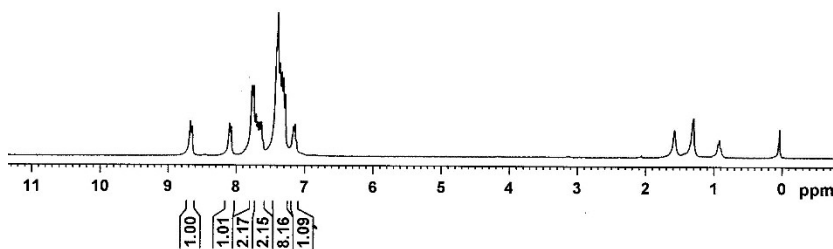


HRMS spectrum of compound 3be

8.676  
8.650  
8.099  
8.076  
7.768  
7.745  
7.707  
7.682  
7.653  
7.629  
7.605  
7.390  
7.362  
7.331  
7.307  
7.279  
7.164  
7.141.

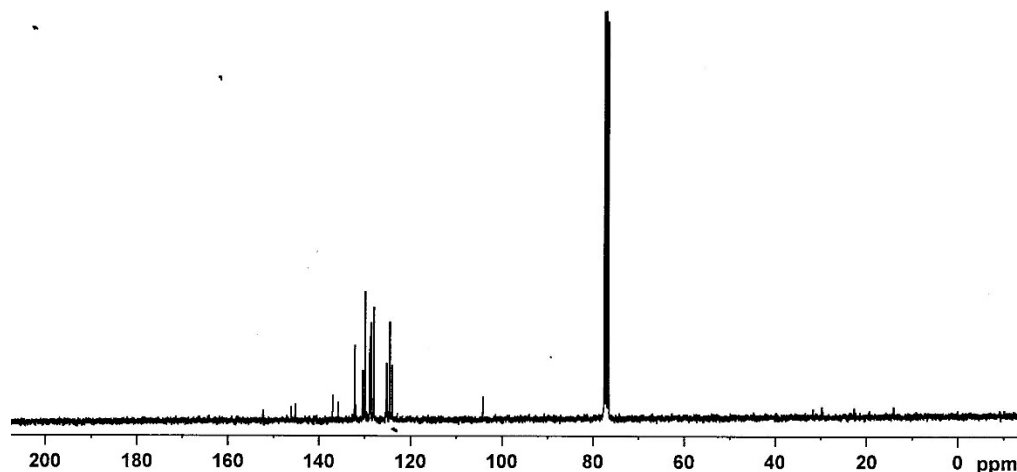


NAME RA-BR-4-133B  
EXPNO 1  
PROCNO 1  
Date\_ 20200729  
Time 14.47  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 18  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 456.1  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
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

152.25  
146.10  
145.17  
136.98  
135.77  
132.13  
131.97  
130.39  
129.86  
128.80  
128.58  
127.95  
125.18  
125.09  
124.46  
123.92  
104.15  
77.44  
77.01  
76.59

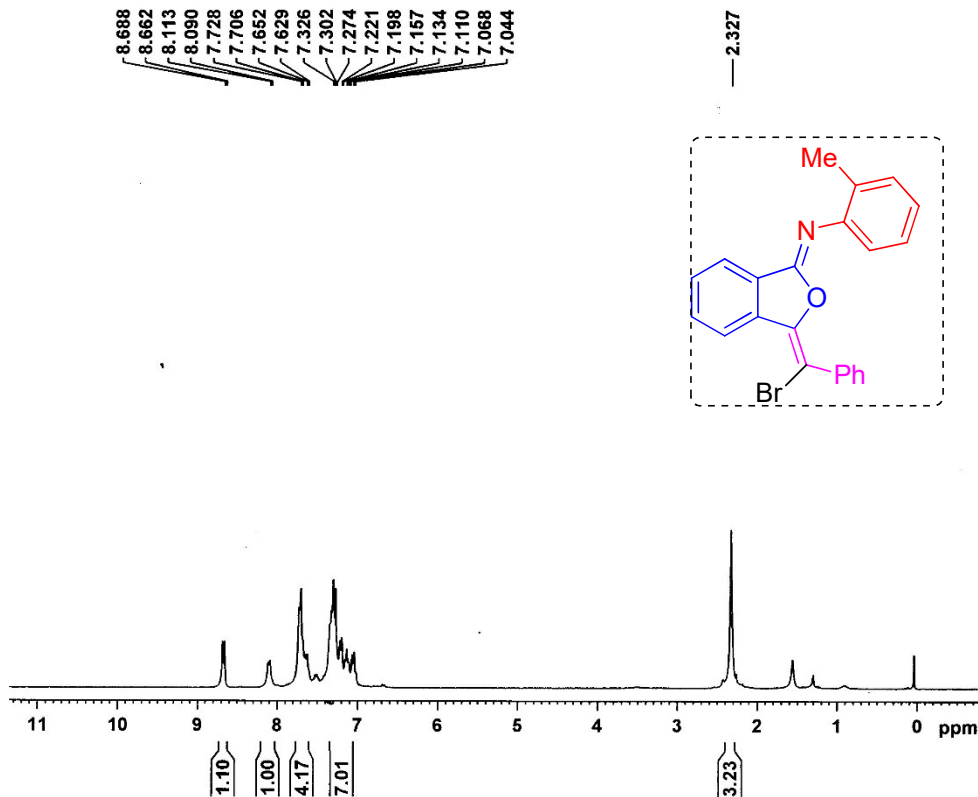


NAME RA-BR-4-133B  
EXPNO 2  
PROCNO 1  
Date\_ 20200729  
Time 15.20  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2048  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 5160.6  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 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 75.4677434 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 3bf



```

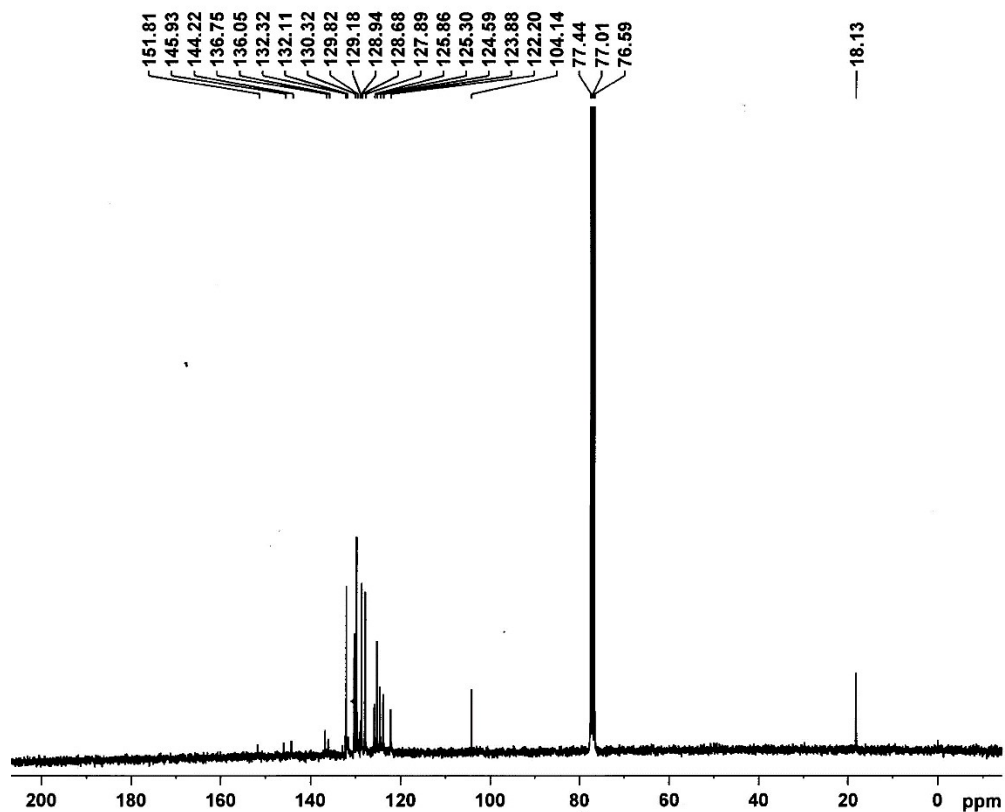
NAME RA-BR-4-239D
EXPNO 4
PROCNO 1
Date_ 20210426
Time 19.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 228.1
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

```

```

===== 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-4-239D
EXPNO 2
PROCNO 1
Date_ 20210426
Time 17.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1957
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

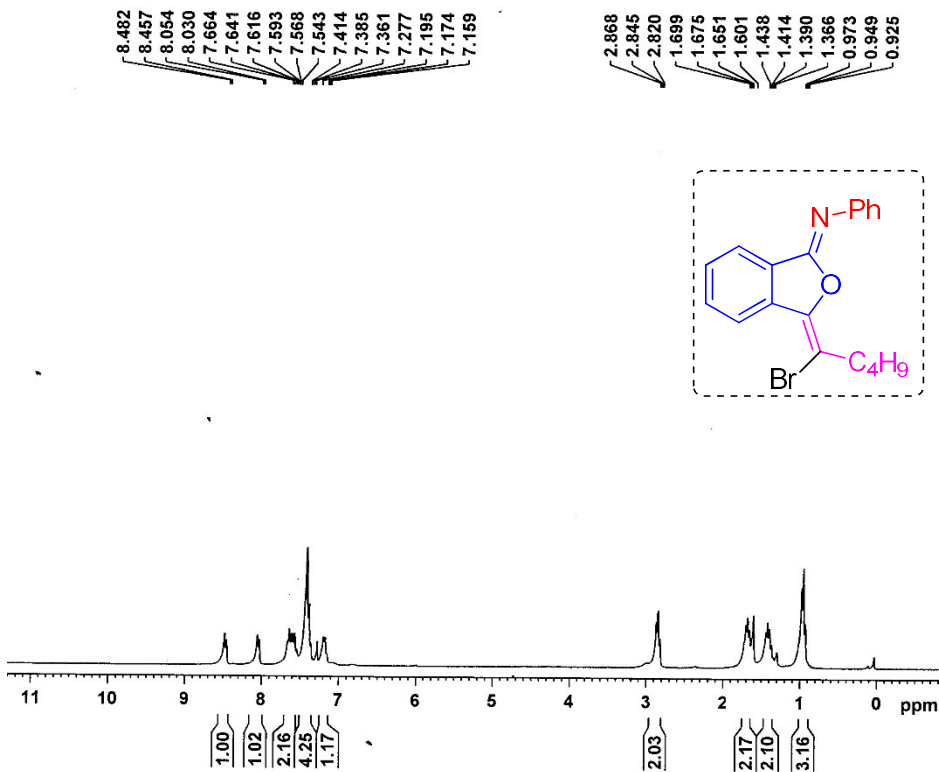
```

```

===== 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 75.4677441 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

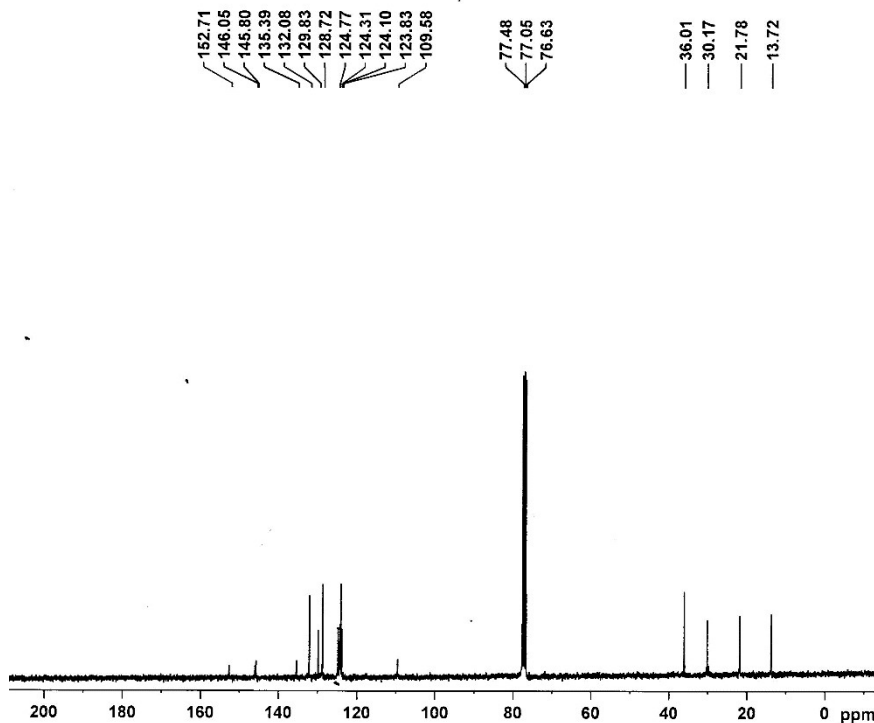
```

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3bg



NAME RA-BR-4-144B  
 EXPNO 1  
 PROCNO 4  
 Date\_ 20200813  
 Time\_ 12.57  
 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  
 TDO 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-4-144B  
 EXPNO 5  
 PROCNO 1  
 Date\_ 20200813  
 Time\_ 14.28  
 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 5180.6  
 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 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 0.2850207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677403 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 3bh

&

Item name: SR-144-B-356, Sample position: 1:A,7, Replicate number: 1

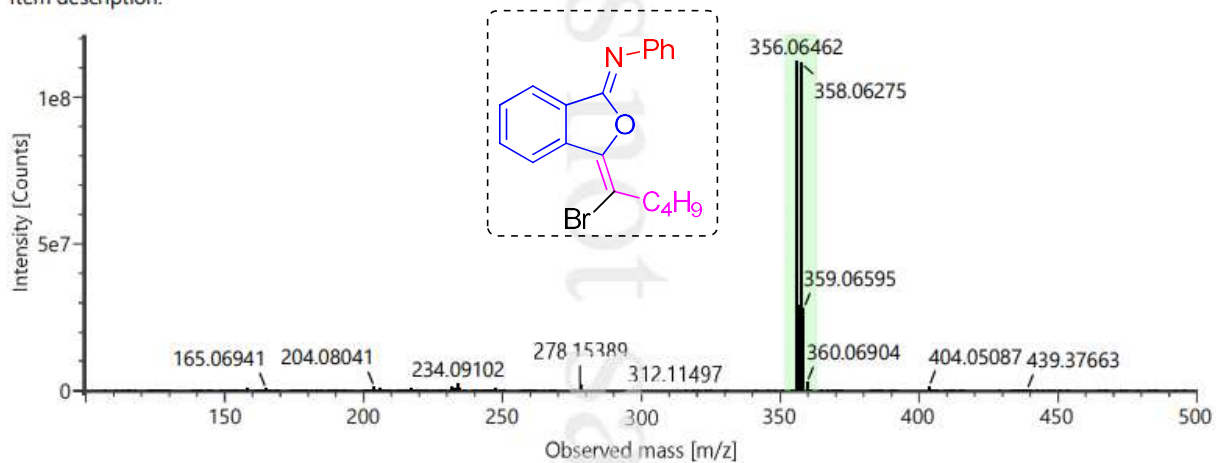
	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C <sub>19</sub> H <sub>18</sub> BrNO	355.0573	355.05718	356.0646	0.5	+H

**Component name: C<sub>19</sub>H<sub>18</sub>BrNO**

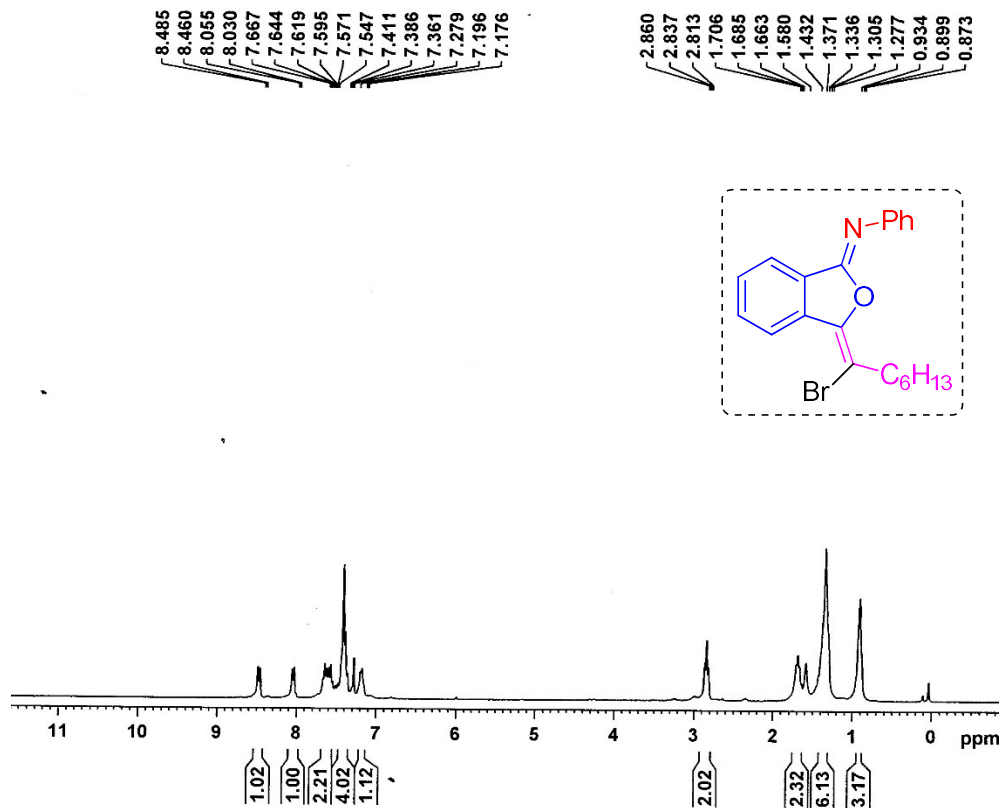
Item name: MSR-144-B-356

Channel name: Low energy : Time 0.6212 +/- 0.1787 minutes

Item description:

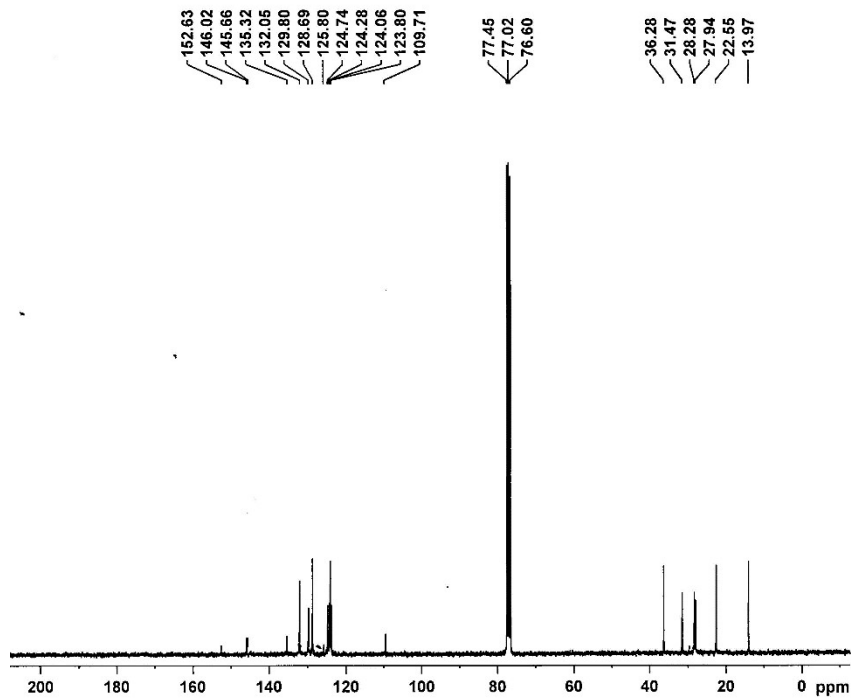


**HRMS spectrum of compound 3bh**



NAME RA-BR-4-142  
EXPNO 3  
PROCNO 1  
Date\_ 20200803  
Time 22.16  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 32  
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



NAME RA-BR-4-142  
EXPNO 4  
PROCNO 1  
Date\_ 20200804  
Time 5.22  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 6580  
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

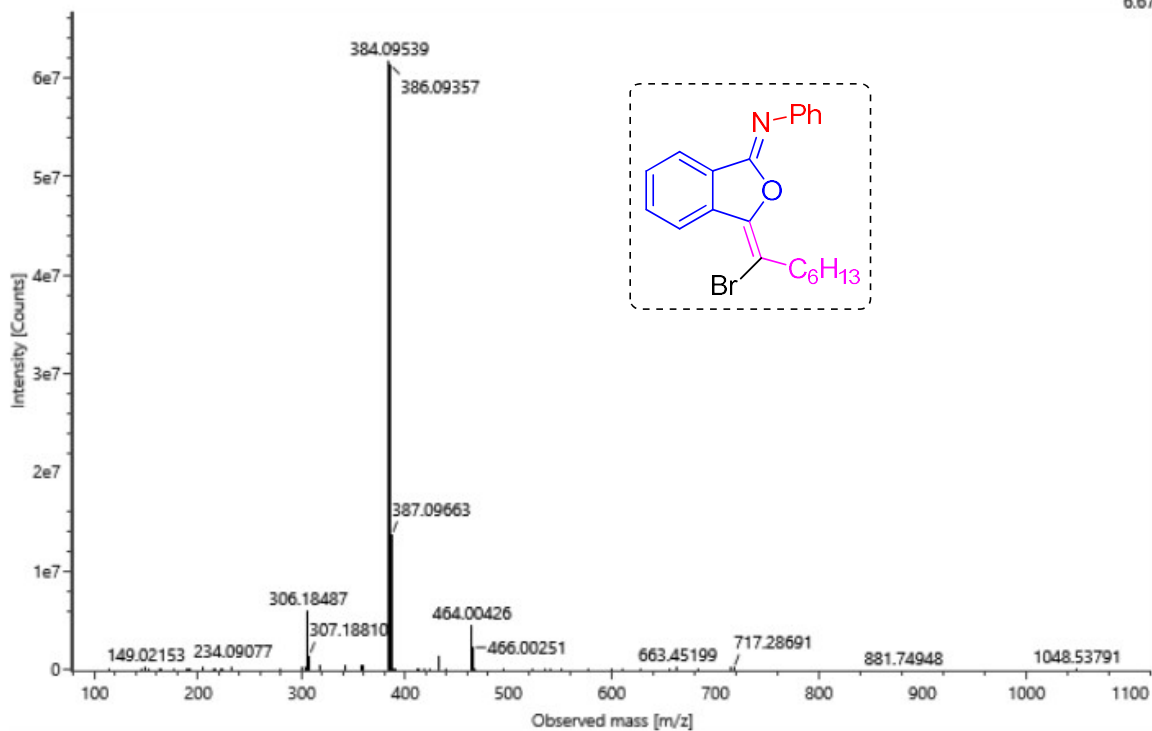
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677422 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>1</sup>H & <sup>13</sup>C spectra of compound 3bi

Item name: SR-142-1-356  
Item description:

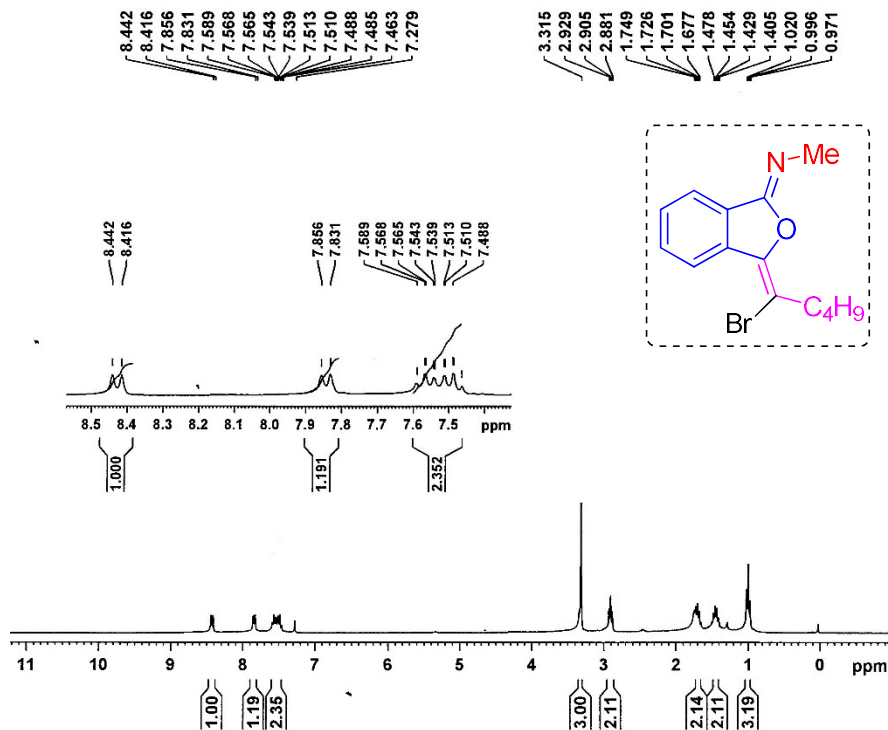
Channel name: Low energy : Time 0.6427 +/- 0.0615 minutes

6.67e7



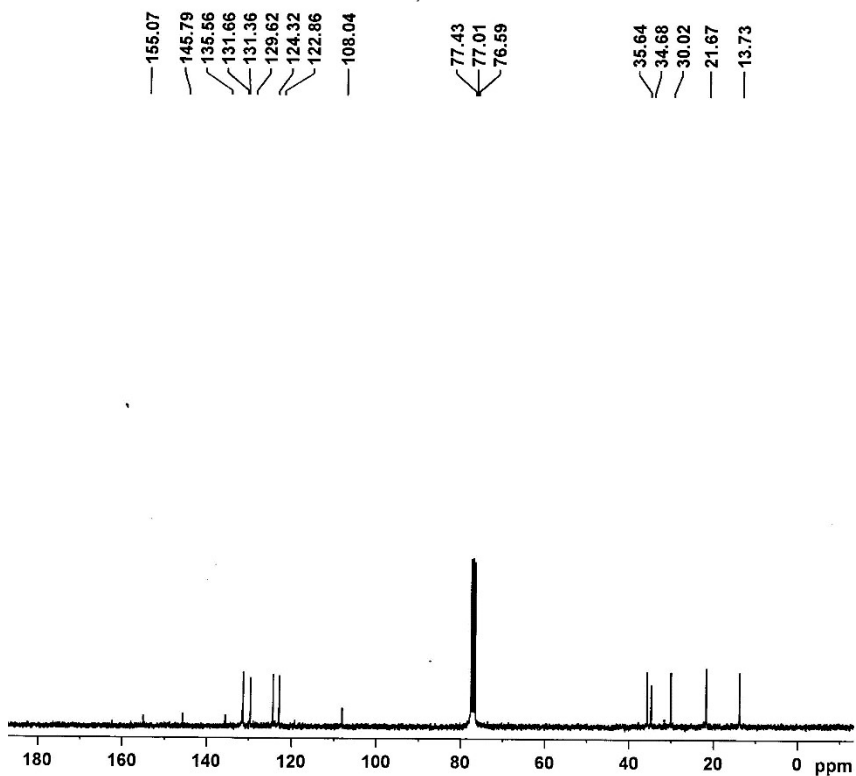
HRMS spectrum of compound 3bi





NAME RA-BR-4-129B  
 EXPNO 1  
 PROCNO 1  
 Date\_ 20200719  
 Time 18.43  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 32  
 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

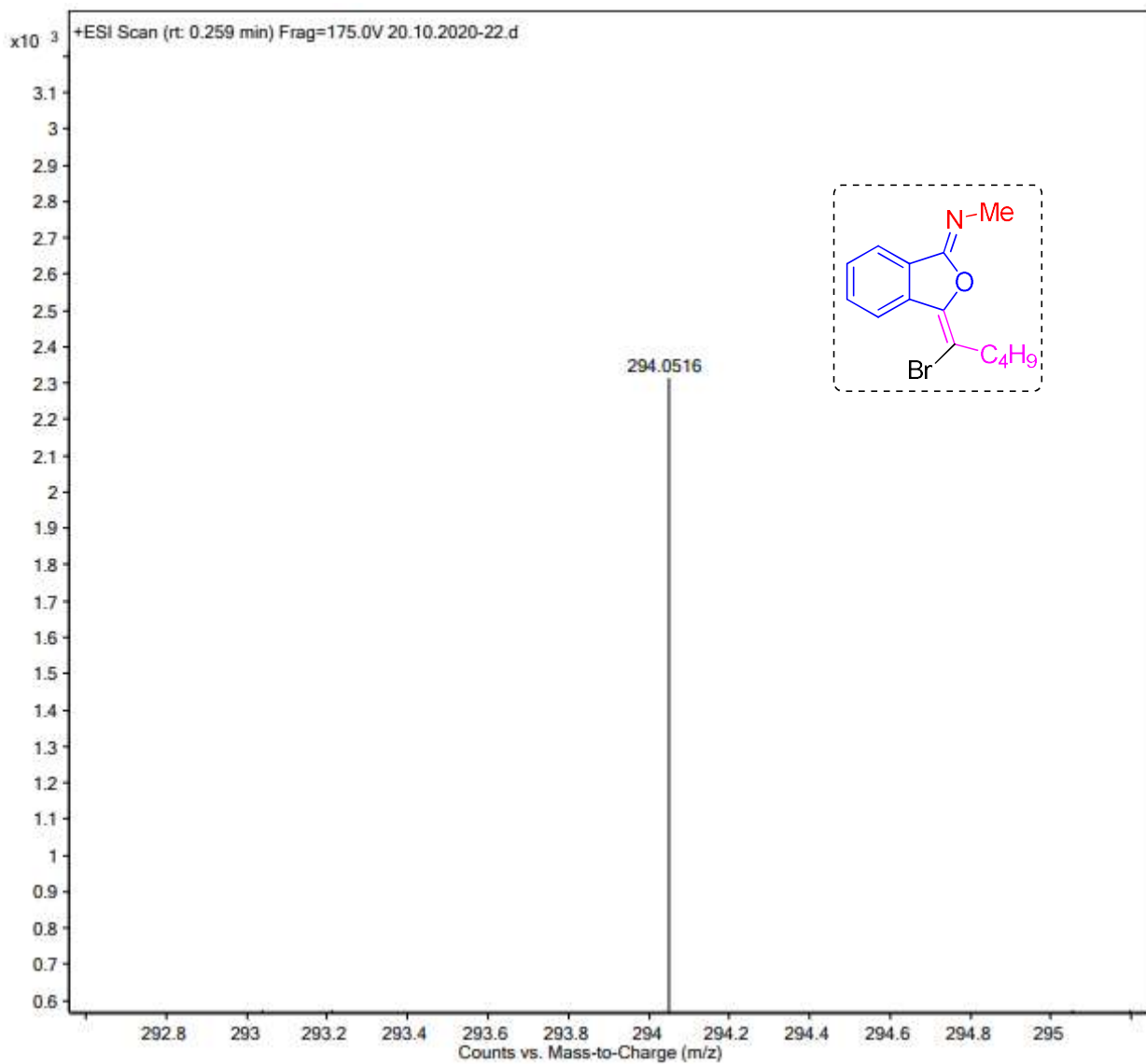


NAME RA-BR-4-129B  
 EXPNO 3  
 PROCNO 1  
 Date\_ 20200719  
 Time 19.28  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 3250  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 5160.6  
 DW 27.800 usec  
 DE 6.50 usec  
 TE 300.0 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  
 PL13W 13.28156662 W  
 PL12W 0.37778899 W  
 PL13W 0.26500207 W  
 SFO2 300.1312005 MHz  
 SI 32768  
 SF 75.4677426 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

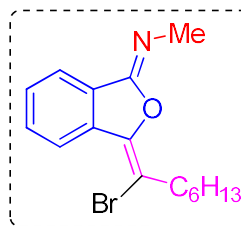
<sup>1</sup>H & <sup>13</sup>C spectra of compound 3bj



**HRMS spectrum of compound 3bj**

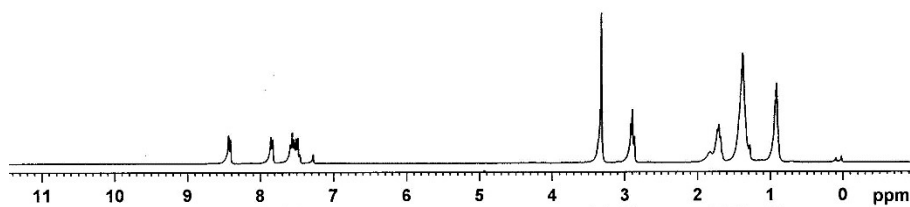
8.440  
8.414  
7.855  
7.830  
7.588  
7.564  
7.538  
7.509  
7.484  
7.460  
7.277

3.314  
2.914  
2.891  
2.867  
1.730  
1.709  
1.686  
1.651  
1.447  
1.377  
1.343  
1.286  
0.935  
0.915  
0.890



NAME RA-BR-4-135B  
EXPNO 1  
PROCNO 1  
Date\_ 20200725  
Time 12.48  
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 181  
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



1.00  
1.01  
2.17

3.20  
2.15

2.16  
6.12  
3.27

155.23  
145.79  
135.58  
131.55  
131.43  
129.65  
124.34  
122.93  
108.25

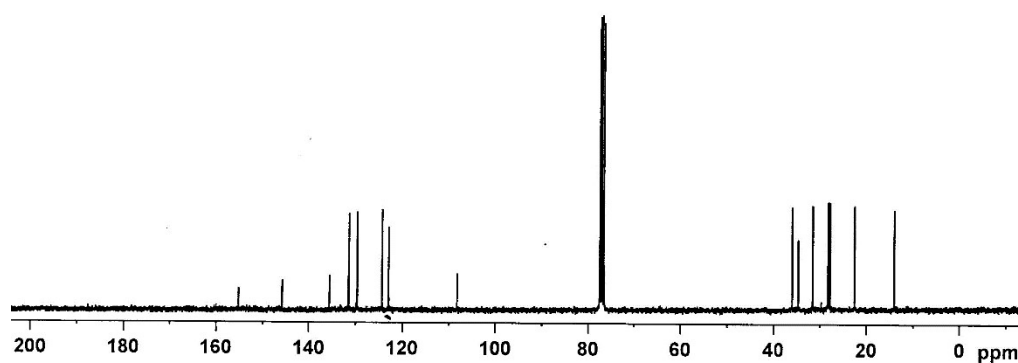
77.47  
77.04  
76.62

35.96  
34.66  
31.55  
28.24  
27.84  
22.56  
13.99

NAME RA-BR-4-135B  
EXPNO 2  
PROCNO 1  
Date\_ 20200728  
Time 20.53  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1214  
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 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 75.4677412 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

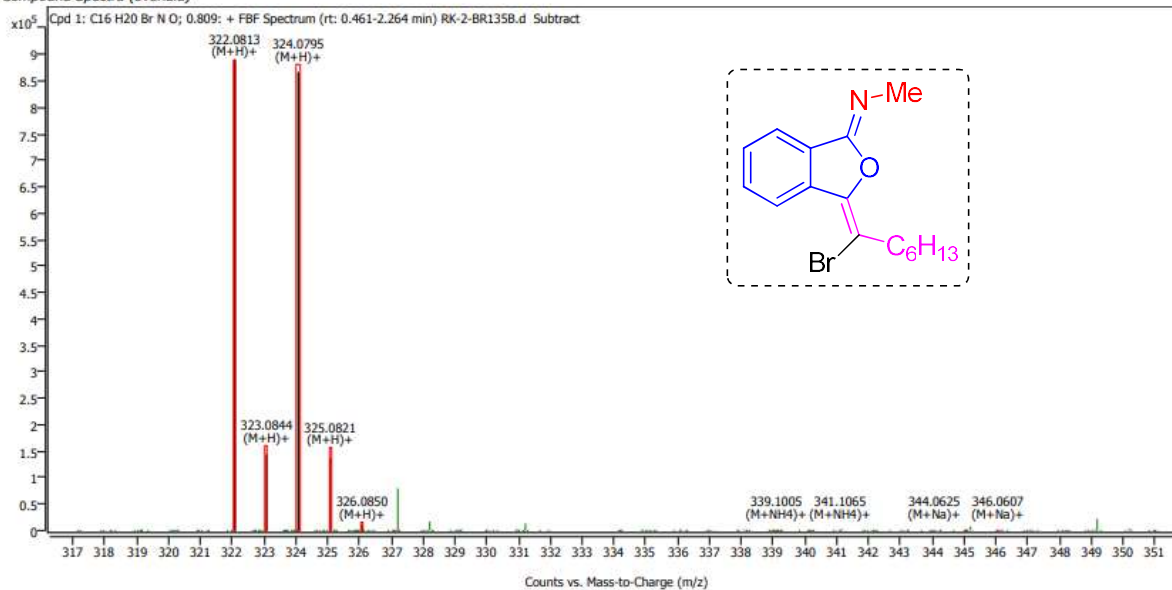


<sup>1</sup>H & <sup>13</sup>C spectra of compound 3bk

### Compound Details

Cpd. 1: C<sub>16</sub>H<sub>20</sub>BrNO

Compound Spectra (overlaid)

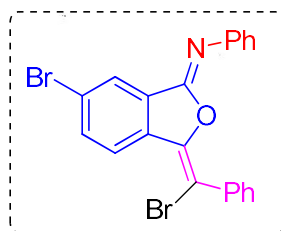


Compound ID Table

Cpd	Formula	Mass (Tgt)	Calc. Mass	Mass	Species	Diff(Tgt.ppm)	mDa
1	C <sub>16</sub> H <sub>20</sub> BrNO	321.0728	321.0740	322.0813	(M+H)+	3.72	1.19
				339.1005	(M+NH <sub>4</sub> )+		
				344.0625	(M+Na)+		

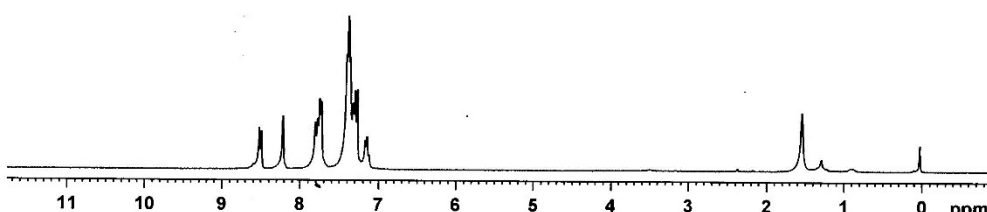
HRMS spectrum of compound 3bk

8.518  
8.489  
8.217  
7.806  
7.777  
7.750  
7.726  
7.408  
7.388  
7.366  
7.338  
7.324  
7.300  
7.273  
7.171  
7.147



NAME RA-BR-4-240B  
EXPNO 1  
PROCNO 1  
Date\_ 20210428  
Time 15.40  
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 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 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



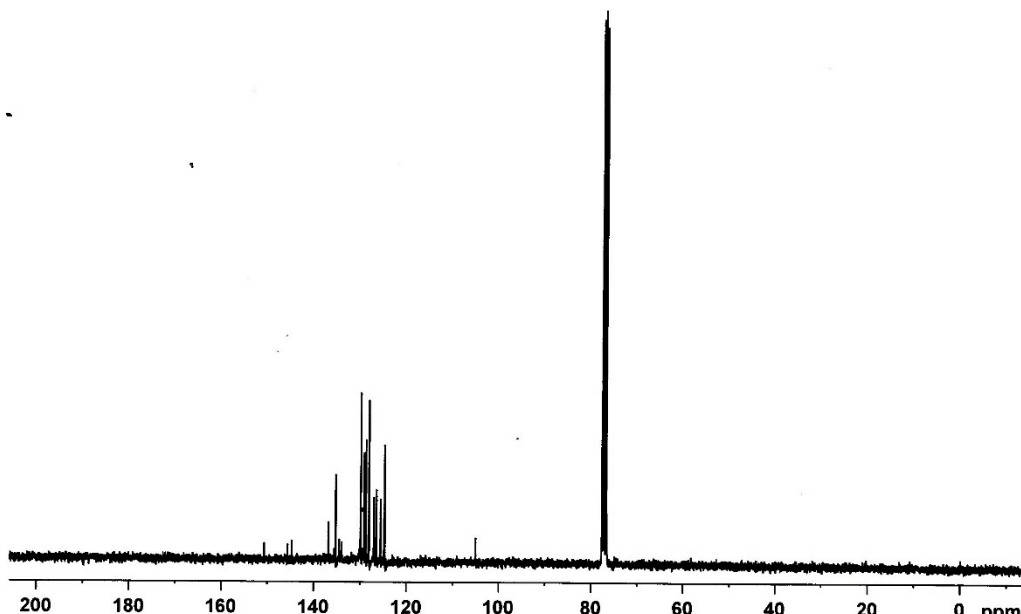
1.12  
1.00  
3.16  
7.19  
1.05

150.60  
145.51  
144.63  
136.71  
135.18  
134.42  
133.83  
129.78  
129.04  
128.65  
128.02  
126.90  
126.35  
125.50  
124.70  
124.62  
104.87  
77.43  
77.00  
76.58

NAME RA-BR-4-240B  
EXPNO 3  
PROCNO 1  
Date\_ 20210428  
Time 20.13  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1781  
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

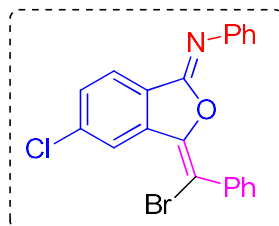
===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== 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 75.4677437 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



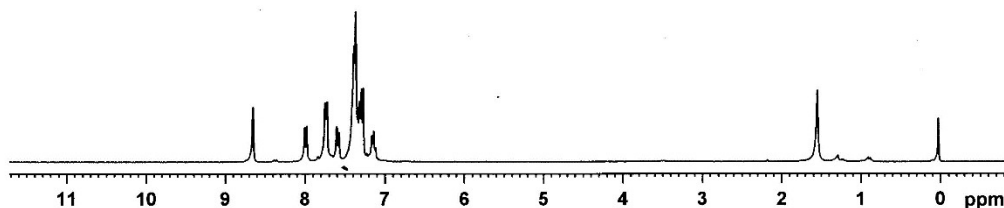
<sup>1</sup>H & <sup>13</sup>C spectra of compound 3bl

8.655  
8.005  
7.978  
7.751  
7.727  
7.605  
7.578  
7.391  
7.368  
7.340  
7.320  
7.296  
7.273  
7.165  
7.141



NAME RA-BR-4-242  
EXPNO 2  
PROCNO 1  
Date\_ 20210429  
Time 13.15  
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 458.1  
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  
SF 32768  
SF 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 9  
PC 1.00

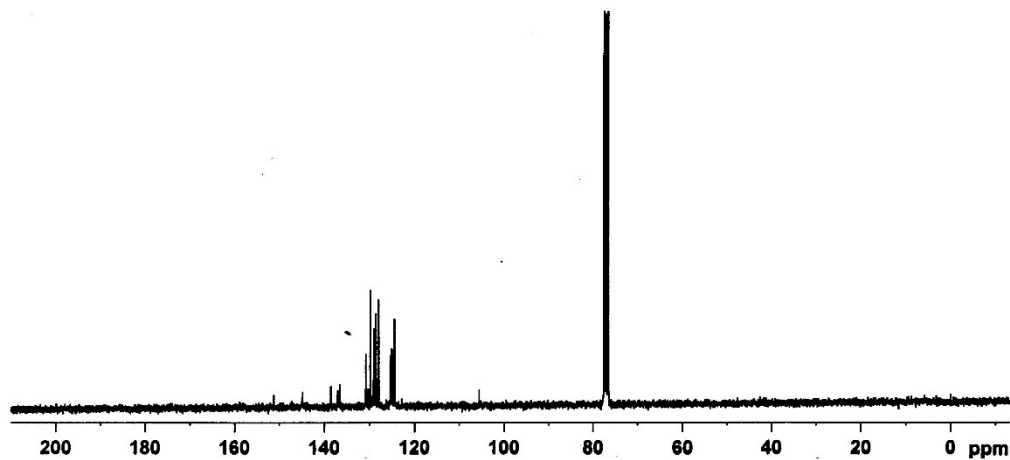


1.00  
1.06  
2.08  
1.03  
7.38  
1.10  
151.17  
144.82  
138.55  
137.13  
136.65  
130.87  
130.40  
129.84  
129.49  
129.13  
128.65  
128.04  
125.37  
125.13  
124.97  
124.52  
105.50  
77.45  
77.03  
76.61

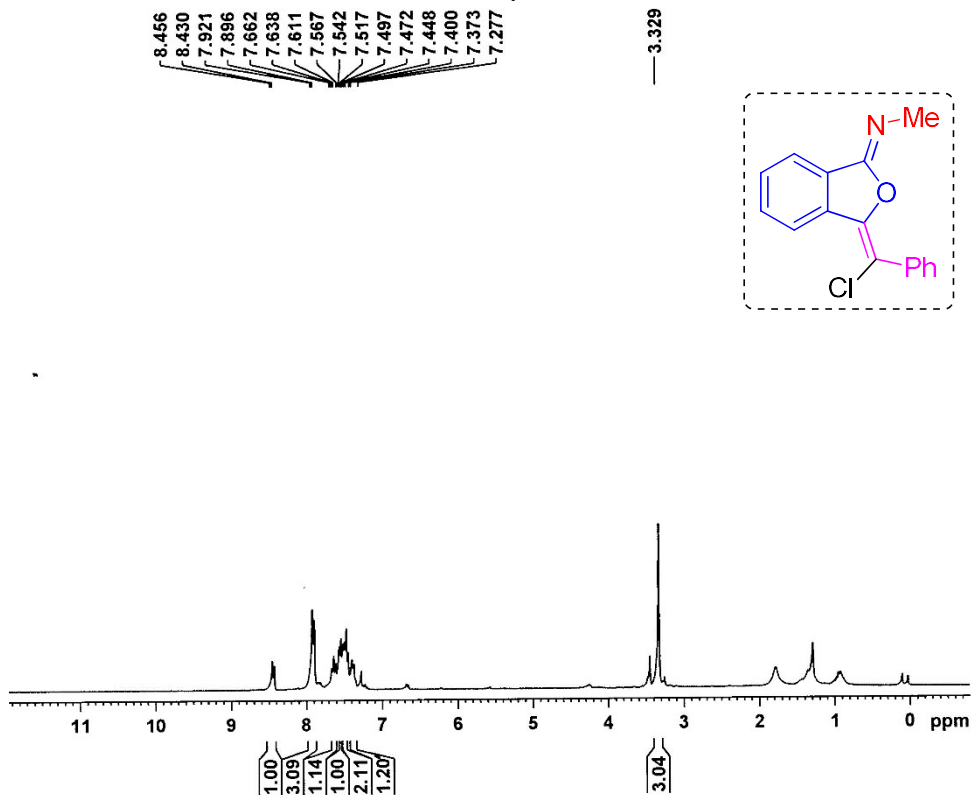
NAME RA-BR-4-242  
EXPNO 4  
PROCNO 1  
Date\_ 20210429  
Time 18.47  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1890  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 2298.8  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.0300000 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 14.48 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677416 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 3bm



```

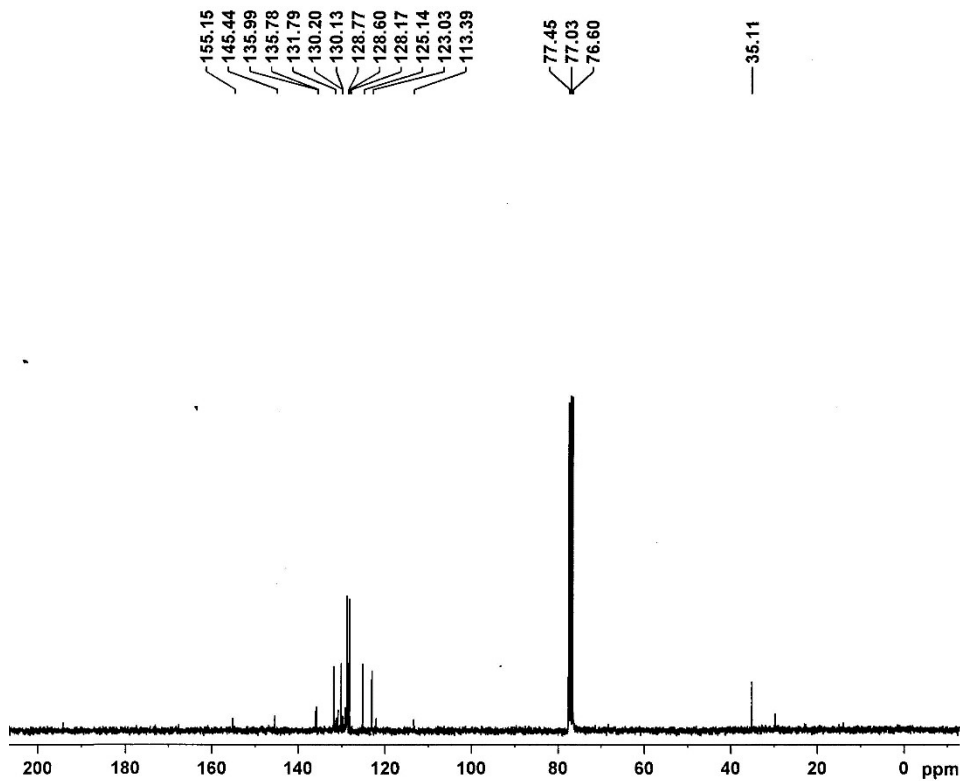
NAME RA-BR-4-138
EXPNO 2
PROCNO 1
Date_ 20200730
Time 16.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

```

```

===== 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

```



```

NAME RA-BR-4-138
EXPNO 3
PROCNO 1
Date_ 20200730
Time 16.30
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 2580.3
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 75.4677428 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 3ca

0

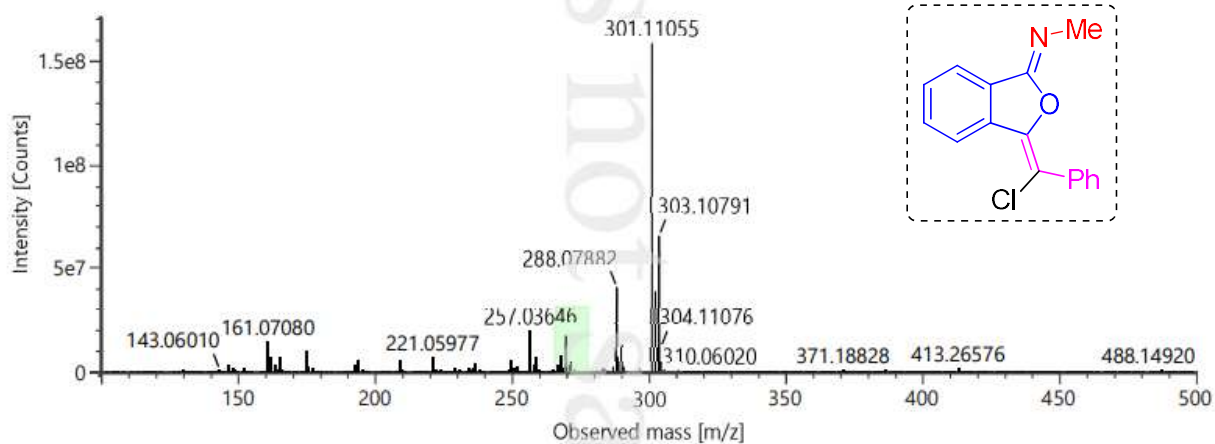
Item name: SR-138-A-270, Sample position: 1:A,1, Replicate number: 1

	Component name	Observed neutral mass (Da)	Neutral mass (Da)	Observed m/z	Mass error (ppm)	Adducts
1	C16H12ClNO	269.0608	269.06074	270.0681	0.3	+H

**Component name: C16H12ClNO**

Item name: MSR-138-A-270  
Item description:

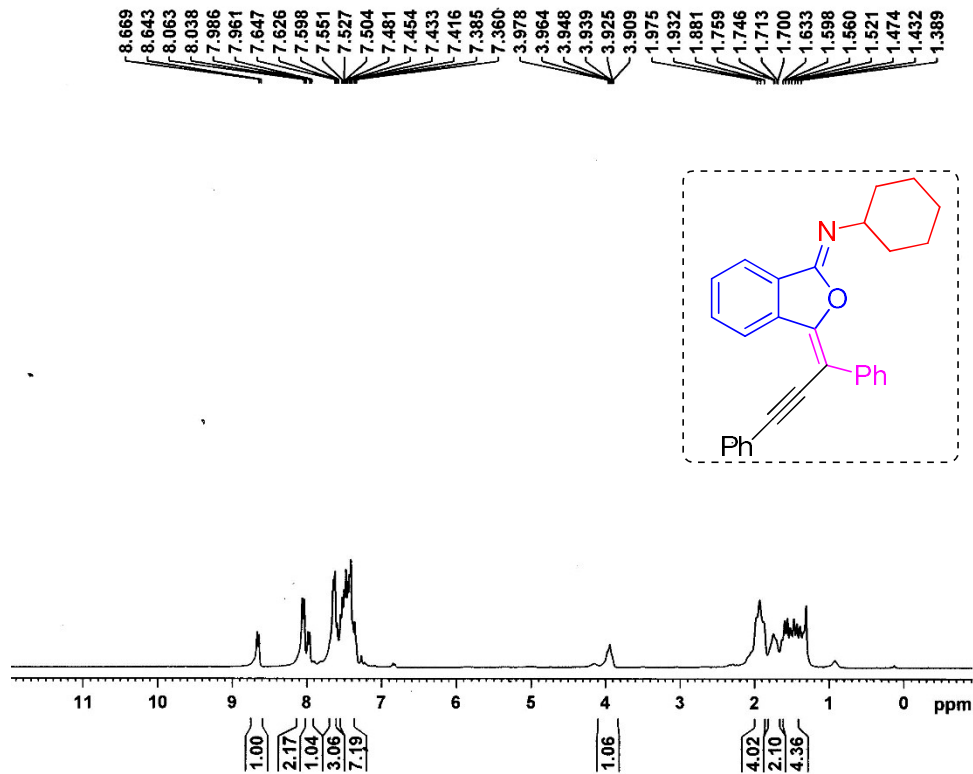
Channel name: Low energy : Time 0.4330 +/- 0.0574 minutes



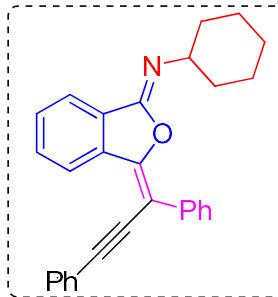
lylh6

**HRMS spectrum of compound 3ca**

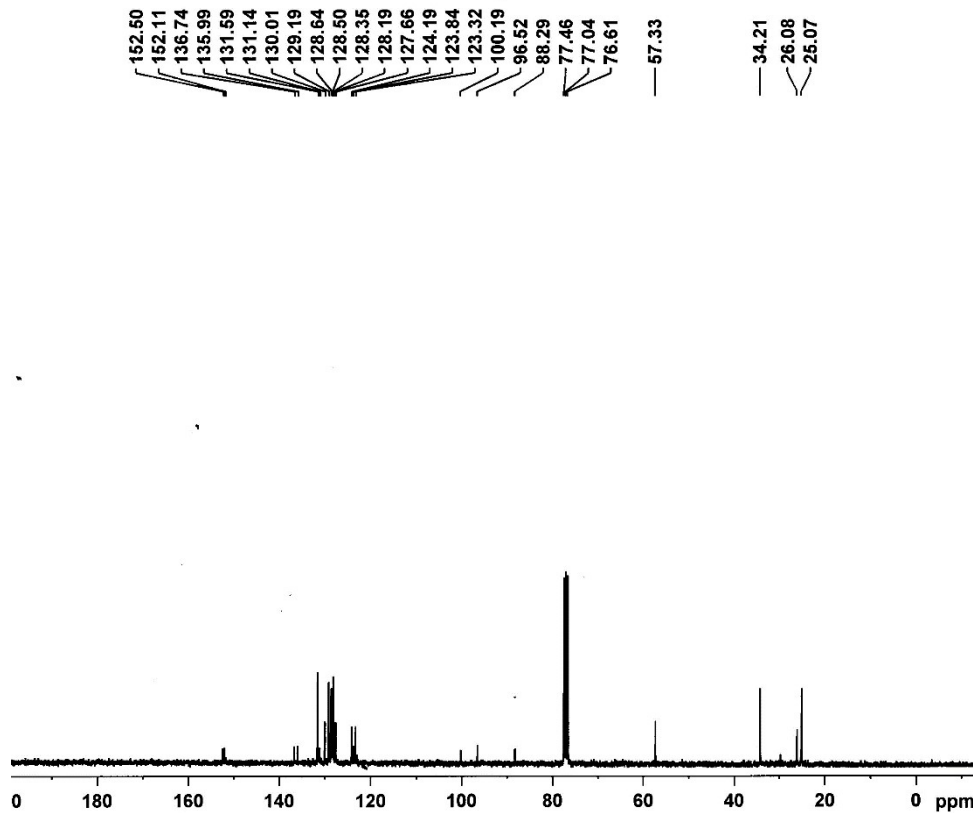




NAME RA-BR-4-198B  
EXPNO 1  
PROCNO 1  
Date\_ 20210214  
Time 9.46  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084660 sec  
RG 90.5  
DW 81.000 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 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-4-198B  
EXPNO 2  
PROCNO 1  
Date\_ 20210214  
Time 10.52  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 988  
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  
TDO 1

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

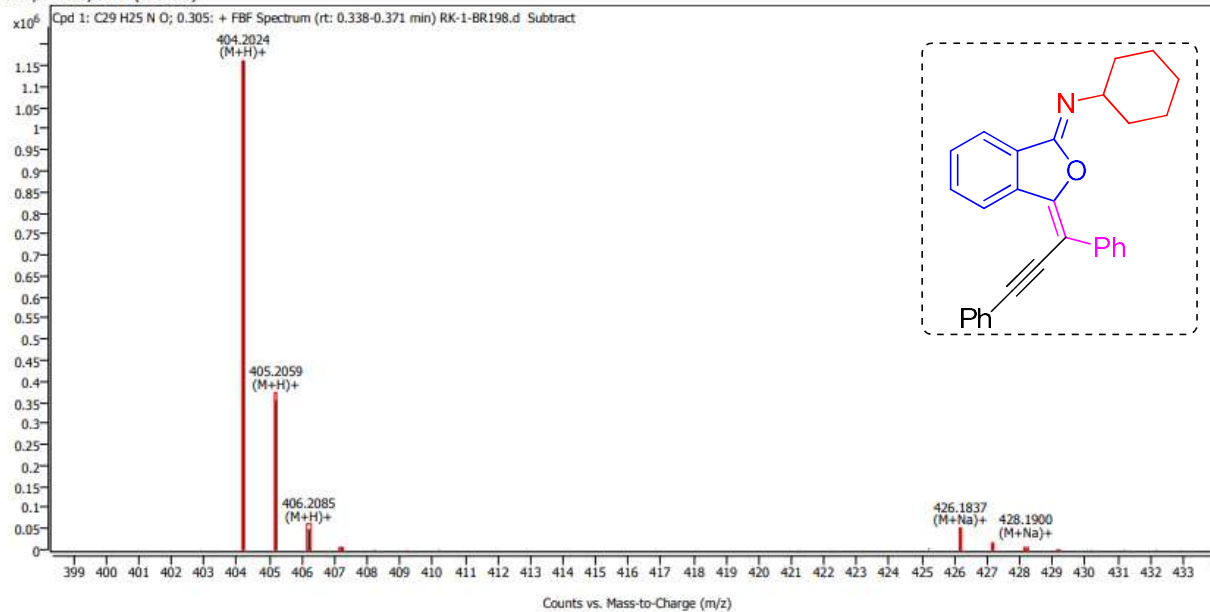
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.46 dB  
PL13 16.00 dB  
PL2W 13.28156662 W  
PL12W 0.37778899 W  
PL13W 0.26500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4677336 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

$^1\text{H}$  &  $^{13}\text{C}$  spectra of compound 4

**Compound Details**

**Cpd. 1: C<sub>29</sub> H<sub>25</sub> N O**

Compound Spectra (overlaid)

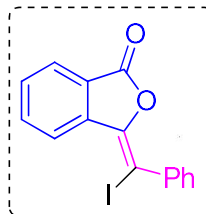


Compound ID Table

Cpd	Formula	Mass (Tgt)	Calc. Mass	Mass	Species	Diff(Tgt.ppm)	mDa
1	C <sub>29</sub> H <sub>25</sub> N O	403.1936	403.1951	404.2024 426.1837	(M+H) <sup>+</sup> (M+Na) <sup>+</sup>	3.74	1.51

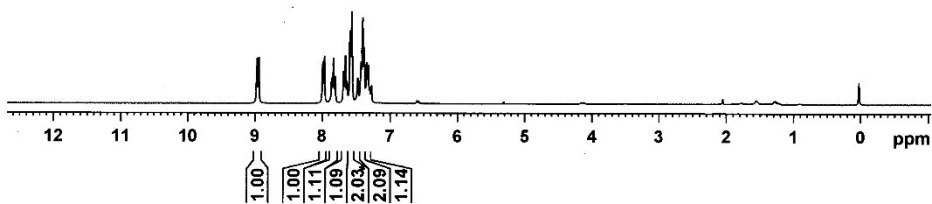
**HRMS spectrum of compound 4**

8.971  
8.944  
7.992  
7.967  
7.859  
7.834  
7.808  
7.685  
7.660  
7.635  
7.589  
7.565  
7.476  
7.430  
7.406  
7.381  
7.345  
7.321  
7.297  
7.274



NAME RA-BR-4-198C  
EXPNO 1  
PROCNO 1  
Date\_ 20210215  
Time 16.38  
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 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 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

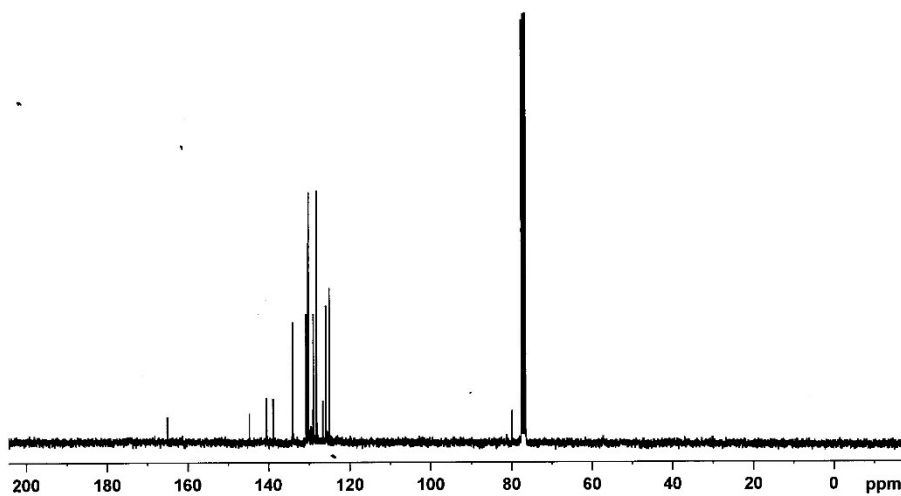


165.09  
144.73  
140.45  
138.82  
134.04  
130.72  
130.16  
128.94  
128.17  
126.63  
125.86  
125.06  
79.83  
77.43  
77.01  
76.59

NAME RA-BR-4-198C  
EXPNO 2  
PROCNO 1  
Date\_ 20210215  
Time 18.24  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1609  
DS 4  
SWH 17985.611 Hz  
FIDRES 0.274439 Hz  
AQ 1.8219508 sec  
RG 13004  
DW 27.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

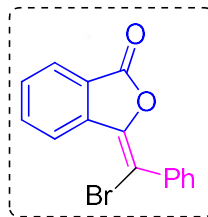
===== CHANNEL f1 =====  
NUC1 13C  
P1 12.75 usec  
PL1 -1.00 dB  
PL1W 39.52846909 W  
SFO1 75.4752953 MHz

===== 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 0.28500207 W  
SFO2 300.1312005 MHz  
SI 32768  
SF 75.4877358 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



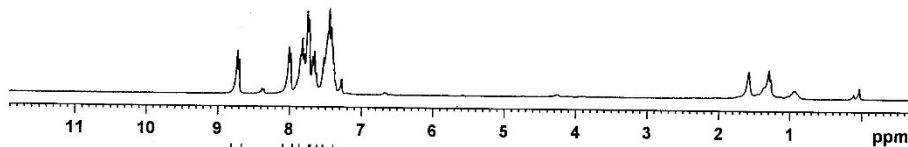
<sup>1</sup>H & <sup>13</sup>C spectra of compound 5

8.725  
8.699  
8.012  
7.988  
7.850  
7.826  
7.800  
7.756  
7.733  
7.681  
7.657  
7.527  
7.472  
7.452  
7.426  
7.411  
7.391



NAME RA-BR-4-118c  
EXPNO 1  
PROCNO 1  
Date\_ 20200731  
Time 21.56  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6172.838 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 13.2815662 W  
SF01 300.1318534 MHz  
SI 32768  
SF 300.1300011 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



1.00  
1.20  
3.04  
1.04  
3.38

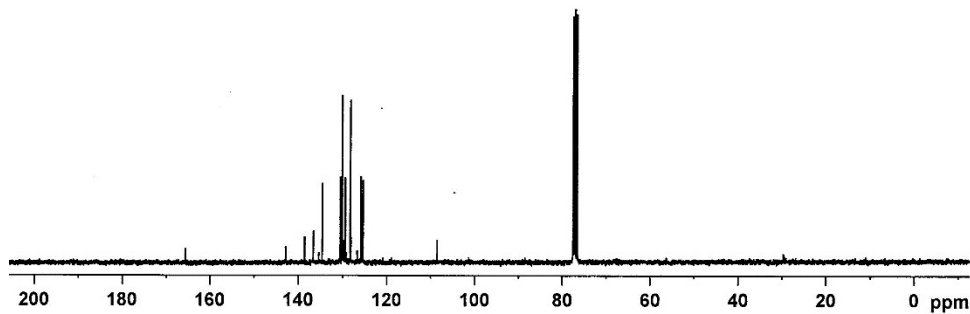
165.72  
142.83  
138.54  
136.57  
134.59  
130.57  
130.10  
129.41  
128.26  
125.85  
125.79  
125.38  
108.49

77.47  
77.04  
76.62

NAME RA-BR-4-118c  
EXPNO 2  
PROCNO 1  
Date\_ 20200731  
Time 23.21  
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 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  
SF01 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  
SF02 300.1312005 MHz  
SI 32768  
SF 75.4677425 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 6