

## Supporting Information

# Synthesis of (*E*)-2-(1-(Methoxyimino)ethyl)-2-phenylbenzofuran-3(2*H*)-ones from (*E*)-1-(Benzofuran-2-yl)ethan-1-one *O*-methyl Oximes and Iodobenzenes via a Palladium-catalyzed Dearomative Arylation/Oxidation Reaction

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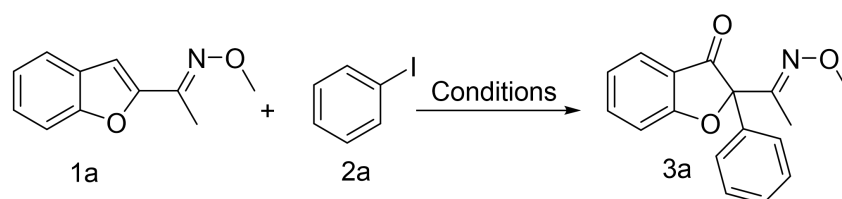
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## 1. General Experiment Information

All the chemicals were obtained commercially and used without any prior purification.  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and  $^{19}\text{F}$  NMR spectra were recorded on a BrukerAvanceII 400 spectrometer. MS spectra were recorded on an Agilent 6546 LC/Q-TOF. All products were isolated by short chromatography on a silica gel (200–300 mesh) column using petroleum ether (60–90 °C) and ethyl acetate. Unless otherwise noted. All compounds were characterized by  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRLC- HRMS, which are consistent with those reported in the literature.

## 2. Optimization of Experimental Conditions



Entry	Solvent	Catalyst	T (°C)	Time (h)	Yield (%) <sup>b</sup>
1	Acetone	Pd(OAc) <sub>2</sub>	80	8	nr
2	DMSO	Pd(OAc) <sub>2</sub>	80	8	nr
3	CH <sub>3</sub> CN	Pd(OAc) <sub>2</sub>	80	8	nr
4	CH <sub>3</sub> OH	Pd(OAc) <sub>2</sub>	80	8	nr
5	EtOH	Pd(OAc) <sub>2</sub>	80	8	nr
6	DMF	Pd(OAc) <sub>2</sub>	80	8	nr
7	HFIP / H <sub>2</sub> O (1:1)	Pd(OAc) <sub>2</sub>	80	8	66
<b>8</b>	<b>HFIP</b>	<b>Pd(OAc)<sub>2</sub></b>	<b>80</b>	<b>8</b>	<b>82</b>
9	HFIP	Cu(OAc) <sub>2</sub>	80	8	nr
10	HFIP	Co(NO <sub>3</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	80	8	nr
11	HFIP	PdCl <sub>2</sub>	80	8	nr
12	HFIP	Pd(CH <sub>3</sub> CN) <sub>2</sub> Cl <sub>2</sub>	80	8	nr
13	HFIP	Pd(Ph <sub>3</sub> P) <sub>2</sub> Cl <sub>2</sub>	80	8	nr
14	HFIP	(DBA) <sub>3</sub> Pd <sub>2</sub>	80	8	nr
15	HFIP	-	80	8	nr <sup>c</sup>
16	HFIP	Pd(OAc) <sub>2</sub>	0	8	nr
17	HFIP	Pd(OAc) <sub>2</sub>	25	8	41

18	HFIP	Pd(OAc) <sub>2</sub>	60	8	65
19	HFIP	Pd(OAc) <sub>2</sub>	110	8	72
20	HFIP	Pd(OAc) <sub>2</sub>	80	1	54
21	HFIP	Pd(OAc) <sub>2</sub>	80	2	62
22	HFIP	Pd(OAc) <sub>2</sub>	80	4	69
23	HFIP	Pd(OAc) <sub>2</sub>	80	12	76
24	HFIP	Pd(OAc) <sub>2</sub>	80	8	80 <sup>c</sup> , 62 <sup>d</sup>

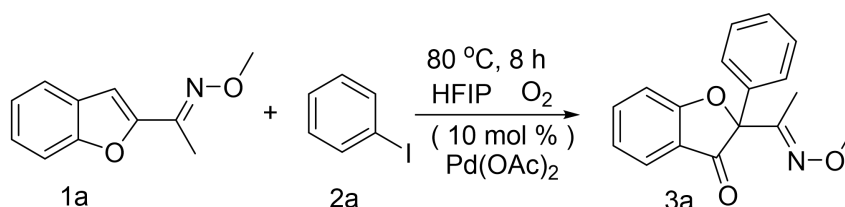
<sup>a</sup>Reaction conditions: **1a** (0.2 mmol), **2** (0.24 mmol), Pd(OAc)<sub>2</sub> (10 mol %) and HFIP (2.0 mL), O<sub>2</sub>, sealed tube, 80 °C, 8 h. <sup>b</sup>Isolated yield. <sup>c</sup>Air. <sup>d</sup>N<sub>2</sub>.

### 3. Experimental Section

#### General procedure for Synthesis of (*E*)-1-(benzofuran-2-yl)ethan-1-one *O*-methyl oxime

A combination of substrate **1aa** (1.00 g, 6.25 mmol), **1ab** (1.30 g, 12.50 mmol), and **1ac** (2.00 g, 25.00 mmol) was added to a round-bottom flask containing 20 mL of EtOH. The mixture was stirred and refluxed under 70 °C in an oil bath for 10 minutes. When the raw material was transformed into the product by LC-MS, the reaction mixture was extracted 3 times with 20 mL of H<sub>2</sub>O / CH<sub>2</sub>Cl<sub>2</sub>. Brown liquid **1a** with a yield of 95 % was obtained by evaporating the solvent.

#### General procedure for Synthesis of (*E*)-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2*H*)-one.



A mixture of substrate **1a** (37.80 mg, 0.20 mmol), **2a** iodobenzene (48.72 mg, 0.24 mmol), and Pd(OAc)<sub>2</sub> (4.48 mg, 10 mol %) in hexafluoroisopropanol (HFIP) (2.0 mL) within a glass sealed-tube. The mixture was then stirred under an O<sub>2</sub> atmosphere and heated using an oil bath at 80 °C for 8 hours. Upon completion of the transformation of the raw material into the final product, as verified by LC-MS, the reaction mixture was treated with H<sub>2</sub>O/CH<sub>2</sub>Cl<sub>2</sub> and the organic layer was extracted and subsequently dried with Na<sub>2</sub>SO<sub>4</sub>. The purified product **3a**, a colorless liquid, was obtained with a yield of 82 % through silica gel chromatography (silica gel, PE / EA).

#### Mechanistic Studies (Scheme 3)

##### General procedure for Mechanistic Studies a

A mixture of substrate **1a** (37.80 mg, 0.20 mmol), **2a** iodobenzene, (48.72 mg, 0.24 mmol), Pd(OAc)<sub>2</sub> (4.48 mg, 10 mol %), in HFIP/H<sub>2</sub>O<sup>18</sup> (100:1) (2.0 mL) was charged in a glass sealed-tube and stirred under O<sub>2</sub> atmosphere (after adding raw materials, close all interfaces, rotate the three-way interface, connect the reaction bottle and vacuum, and extract the air in the reaction bottle. Then rotate the three-way interface, connect the reaction bottle and oxygen, and fill the bottle with oxygen. Repeating air pumping - oxygen filling, after several times, oxygen protection could be formed.) was heated using an oil bath under 80 °C for 8 h. When the raw material is basically transformed into product monitored by LC-MS, the reaction mixture was extracted with H<sub>2</sub>O/CH<sub>2</sub>Cl<sub>2</sub>. Then the organic layer was dried with Na<sub>2</sub>SO<sub>4</sub>. The brown product was purified by silica gel chromatography (silica gel, PE/EA) to afford the product **3a'** as colorless liquid.

#### **General procedure for Mechanistic Studies b-c**

A mixture of substrate **4** (32.00 mg, 0.20 mmol), **2a** iodobenzene, (48.72 mg, 0.24 mmol), Pd(OAc)<sub>2</sub> (4.48 mg, 10 mol %), in hexafluoroisopropanol (HFIP) (2.0 mL) was charged in a glass sealed-tube and stirred under O<sub>2</sub> atmosphere was heated using an oil bath under 80 °C for 8 h. Monitor the reaction by LC-MS.

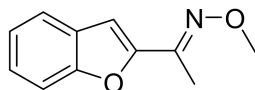
A mixture of substrate **5** (34.60 mg, 0.20 mmol), **2a** iodobenzene, (48.72 mg, 0.24 mmol), Pd(OAc)<sub>2</sub> (4.48 mg, 10 mol %), in hexafluoroisopropanol (HFIP) (2.0 mL) was charged in a glass sealed-tube and stirred under O<sub>2</sub> atmosphere was heated using an oil bath under 80 °C for 8 h. Monitor the reaction by LC-MS.

#### **Observation of intermediate D, E, F**

A mixture of substrate **1a** (37.80 mg, 0.20 mmol), **2a** iodobenzene, (48.72 mg, 0.24 mmol), Pd(OAc)<sub>2</sub> (4.48 mg, 10 mol %), in HFIP (2.0 mL) was charged in a glass sealed-tube and stirred under O<sub>2</sub> atmosphere was heated using an oil bath under 80 °C. Monitor the reaction solution of 0.5 hour, 1 hour, 1.5 hour, 2 hours, 2.5 hours, 3 hours, etc. by LC-MS.

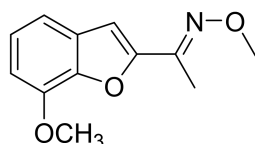
## 4. Characterization data of the products

### (*E*)-1-(benzofuran-2-yl)ethan-1-one *O*-methyl oxime (1a)



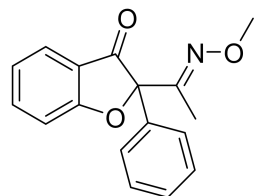
CAS Registry Number: 1447826-76-7: brown liquid, 1.12 g, 95 % yield;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.49 (t,  $J = 8.2$  Hz, 2H), 7.28 – 7.21 (m, 1H), 7.18 – 7.13 (m, 1H), 6.90 (s, 1H), 4.01 (s, 3H), 2.17 (s, 3H).

### (*E*)-1-(7-methoxybenzofuran-2-yl)ethan-1-one *O*-methyl oxime (1aa).



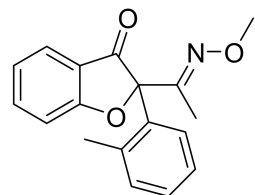
Yellow liquid, 1.06 g, 92 % yield.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.21 – 7.10 (m, 2H), 6.97 (s, 1H), 6.86 – 6.78 (m, 1H), 4.05 (s, 3H), 4.00 (s, 3H), 2.25 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  152.20, 147.12, 145.49, 144.47, 129.71, 123.81, 113.50, 107.27, 106.05, 62.49, 55.92, 11.89. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{12}\text{H}_{13}\text{NO}_3\text{Na}$  242.0787; Found 242.0796.

### (*E*)-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2*H*)-one (3a)



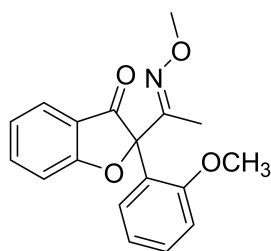
Colorless liquid, 46.10 mg, 82 % yield (eluent: ethyl acetate/petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.84 (t,  $J = 7.8$  Hz, 1H), 7.70 (d,  $J = 7.6$  Hz, 1H), 7.65 – 7.30 (m, 6H), 7.24 (t,  $J = 7.4$  Hz, 1H), 3.77 (s, 3H), 1.74 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  196.0, 170.5, 154.0, 138.0, 134.6, 128.63, 128.60, 125.7, 125.3, 122.5, 120.4, 113.4, 91.7, 62.2, 11.9. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{17}\text{H}_{15}\text{NO}_3\text{Na}$  304.0944; Found 304.0951.

### (*E*)-2-(1-(methoxyimino)ethyl)-2-(*o*-tolyl)benzofuran-3(2*H*)-one (3b)



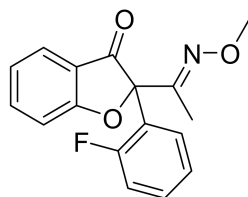
Colorless liquid, 43.68 mg, 74 % yield (eluent: ethyl acetate / petroleum ether = 1:50); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.71 (dd, *J* = 7.7, 0.7 Hz, 1H), 7.68 – 7.63 (m, 1H), 7.41 (d, *J* = 7.7 Hz, 1H), 7.27 – 7.24 (m, 1H), 7.24 – 7.20 (m, 2H), 7.18 (dd, *J* = 6.9, 4.7 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 3.84 (s, 3H), 2.47 (s, 3H), 1.87 (s, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (101 MHz, CDCl<sub>3</sub>) δ 197.1, 170.4, 154.2, 138.2, 137.9, 132.7, 132.5, 128.9, 127.0, 125.8, 125.1, 122.4, 120.6, 113.5, 93.1, 62.2, 21.0, 12.1. HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calculated for C<sub>18</sub>H<sub>17</sub>NO<sub>3</sub>Na 318.1100; Found 318.1093.

**(*E*)-2-(1-(methoxyimino)ethyl)-2-(2-methoxyphenyl)benzofuran-3(2*H*)-one (3c)**



Colorless liquid, 43.56 mg, 70 % yield (eluent: ethyl acetate / petroleum ether = 1:35); <sup>1</sup>H NMR (400 MHz, DMSO) δ 7.75 (ddd, *J* = 8.5, 7.3, 1.4 Hz, 1H), 7.72 – 7.66 (m, 1H), 7.43 (td, *J* = 8.3, 1.6 Hz, 1H), 7.28 (d, *J* = 8.3 Hz, 1H), 7.23 – 7.14 (m, 2H), 7.09 (d, *J* = 7.8 Hz, 1H), 7.01 (td, *J* = 7.6, 0.9 Hz, 1H), 3.77 (s, 3H), 3.51 (s, 3H), 1.91 (s, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (101 MHz, DMSO) δ 196.9, 170.2, 158.3, 153.3, 138.7, 131.6, 129.7, 124.1, 122.8, 121.2, 120.4, 113.6, 113.3, 90.9, 62.3, 56.2, 13.3. HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calculated for C<sub>18</sub>H<sub>17</sub>NO<sub>4</sub>Na 334.1050; Found 334.1060.

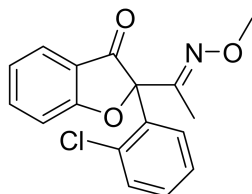
**(*E*)-2-(2-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2*H*)-one (3d)**



Colorless liquid, 43.67 mg, 73 % yield (eluent: ethyl acetate / petroleum ether = 1:50); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.73 (dd, *J* = 7.7, 0.7 Hz, 1H), 7.66 (ddd, *J* = 8.5, 7.3, 1.4 Hz, 1H), 7.42 – 7.31 (m, 2H), 7.21 (d, *J* = 8.4 Hz, 1H), 7.14 (d, *J* = 8.2 Hz, 2H), 7.12 – 7.08 (m, 1H), 3.86 (s, 3H), 1.93 (s, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (101 MHz, CDCl<sub>3</sub>) δ 196.2, 170.7, 162.3 (d, *J* = 252.5 Hz), 159.8 (d, *J* = 252.5 Hz), 152.7, 138.3, 131.1 (d, *J* = 10.1 Hz), 131.0 (d, *J* = 10.1 Hz), 128.6 (d, *J* = 10.1 Hz), 128.5 (d, *J* = 10.1 Hz), 125.2, 124.11 (d, *J* = 3.0 Hz), 124.08 (d, *J* = 3.0 Hz), 122.7 (d, *J* = 20.2 Hz), 122.6, 122.5 (d, *J* = 20.2 Hz), 120.2, 116.8 (d, *J* = 20.2 Hz), 116.6 (d, *J* = 20.2 Hz), 113.5, 90.3, 62.3, 11.9. <sup>19</sup>F NMR (377 MHz, CDCl<sub>3</sub>) δ -110.64. HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calculated for C<sub>17</sub>H<sub>14</sub>FNO<sub>3</sub>Na 322.0850; Found

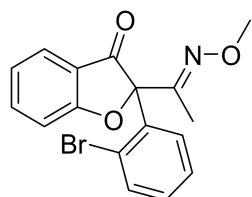
322.0855.

**(E)-2-(2-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3e)**



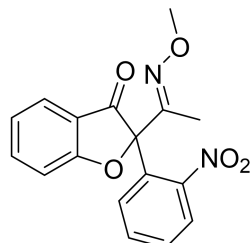
Colorless liquid, 45.37 mg, 72 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.83 (ddd,  $J$  = 8.5, 7.2, 1.4 Hz, 1H), 7.75 (dd,  $J$  = 7.7, 0.8 Hz, 1H), 7.56 (dd,  $J$  = 7.9, 1.0 Hz, 1H), 7.47 (ddd,  $J$  = 7.9, 6.9, 2.3 Hz, 1H), 7.43 – 7.35 (m, 3H), 7.30 – 7.17 (m, 1H), 3.75 (s, 3H), 1.87 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, DMSO)  $\delta$  195.7, 170.3, 153.6, 139.7, 133.6, 132.6, 132.0, 131.6, 130.1, 127.9, 125.2, 123.7, 120.2, 114.1, 91.7, 62.4, 12.8. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{17}\text{H}_{14}\text{ClNO}_3\text{Na}$  338.0554; Found 338.0561.

**(E)-2-(2-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3f)**



Colorless liquid, 53.85 mg, 75 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.86 (ddd,  $J$  = 8.5, 7.3, 1.4 Hz, 1H), 7.72 (dd,  $J$  = 7.7, 0.8 Hz, 1H), 7.67 – 7.55 (m, 2H), 7.58 – 7.47 (m, 2H), 7.43 (t,  $J$  = 7.9 Hz, 1H), 7.27 (dd,  $J$  = 11.1, 3.8 Hz, 1H), 3.78 (s, 3H), 1.75 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, DMSO)  $\delta$  195.2, 170.4, 154.1, 139.9, 136.8, 132.3, 131.6, 128.2, 125.5, 125.2, 124.0, 122.4, 119.5, 114.4, 90.7, 62.5, 12.4. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{17}\text{H}_{14}\text{BrNO}_3\text{Na}$  382.0049; Found 382.0049.

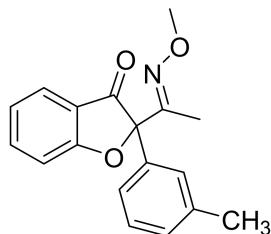
**(E)-2-(1-(methoxyimino)ethyl)-2-(2-nitrophenyl)benzofuran-3(2H)-one (3g)**



Colorless liquid, 47.61 mg, 73 % yield (eluent: ethyl acetate / petroleum ether = 1:20);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.86 (dd,  $J$  = 7.9, 1.2 Hz, 1H), 7.84 – 7.74 (m, 3H), 7.69 (td,  $J$  = 7.7, 1.2 Hz, 1H), 7.58 (dd,  $J$  = 7.8, 1.2 Hz, 1H), 7.36 – 7.23 (m, 2H), 3.76 (s, 3H), 1.79 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,

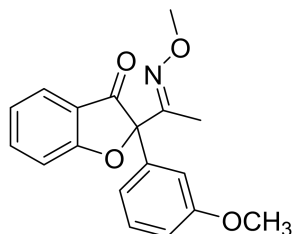
DMSO)  $\delta$  194.7, 169.7, 153.9, 149.2, 139.5, 132.8, 131.2, 130.2, 126.4, 125.3, 125.0, 124.3, 119.7, 113.9, 90.7, 62.5, 12.6. HRMS (ESI)  $m/z$ :  $[M+H]^+$  Calculated for  $C_{17}H_{15}N_2O_5$  327.0976; Found 327.0982.

**(E)-2-(1-(methoxyimino)ethyl)-2-(m-tolyl)benzofuran-3(2H)-one (3h)**



Colorless liquid, 44.27 mg, 75 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1H$  NMR (400 MHz, DMSO)  $\delta$  7.84 (ddd,  $J$  = 8.5, 7.2, 1.4 Hz, 1H), 7.69 (dd,  $J$  = 7.7, 0.8 Hz, 1H), 7.47 (d,  $J$  = 8.4 Hz, 1H), 7.36 – 7.30 (m, 1H), 7.23 (dt,  $J$  = 8.2, 5.0 Hz, 4H), 3.78 (s, 3H), 2.32 (s, 3H), 1.75 (s, 3H).  $^{13}C$   $\{^1H\}$  NMR (101 MHz, DMSO)  $\delta$  195.5, 170.3, 154.5, 139.6, 138.7, 134.4, 130.0, 129.2, 126.1, 125.4, 123.7, 123.0, 119.8, 114.2, 91.6, 62.4, 21.5, 12.6. HRMS (ESI)  $m/z$ :  $[M+Na]^+$  Calculated for  $C_{18}H_{17}NO_3Na$  318.1100; Found 318.1106.

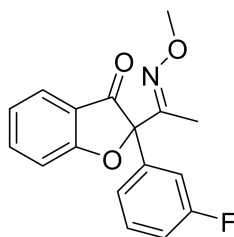
**(E)-2-(1-(methoxyimino)ethyl)-2-(3-methoxyphenyl)benzofuran-3(2H)-one (3i)**



Colorless liquid, 46.05 mg, 74 % yield (eluent: ethyl acetate / petroleum ether = 1:30);  $^1H$  NMR (400 MHz, DMSO)  $\delta$  7.84 (ddd,  $J$  = 8.5, 7.2, 1.4 Hz, 1H), 7.70 (dd,  $J$  = 7.7, 0.8 Hz, 1H), 7.47 (d,  $J$  = 8.4 Hz, 1H), 7.38 (t,  $J$  = 8.0 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.06 – 7.02 (m, 1H), 7.01 – 6.95 (m, 2H), 3.78 (s, 3H), 3.76 (s, 3H), 1.76 (s, 3H).  $^{13}C$   $\{^1H\}$  NMR (101 MHz, DMSO)  $\delta$  195.3, 170.3, 159.9, 154.4, 139.6, 135.9, 130.6, 125.4, 123.7, 119.8, 118.0, 114.4, 114.2, 111.7, 91.4, 62.4, 55.7, 12.5. HRMS (ESI)  $m/z$ :  $[M+Na]^+$  Calculated for  $C_{18}H_{17}NO_4Na$  334.1050; Found 334.1057.

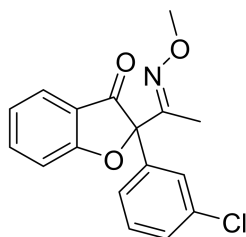
**(E)-2-(3-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3j)**





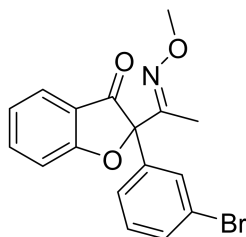
Colorless liquid, 43.67 mg, 73 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.86 (ddd,  $J$  = 8.5, 7.3, 1.4 Hz, 1H), 7.71 (dd,  $J$  = 7.7, 0.8 Hz, 1H), 7.57 – 7.45 (m, 2H), 7.38 – 7.31 (m, 1H), 7.31 – 7.21 (m, 3H), 3.78 (s, 3H), 1.76 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  195.5, 170.4, 164.1 (d,  $J$  = 252.5 Hz), 161.6 (d,  $J$  = 252.5 Hz), 153.6, 138.3, 137.04 (d,  $J$  = 7.1 Hz), 136.97 (d,  $J$  = 7.1 Hz), 130.2 (d,  $J$  = 10.1 Hz), 130.1 (d,  $J$  = 10.1 Hz), 125.4, 122.7, 121.6 (d,  $J$  = 10.1 Hz), 121.5 (d,  $J$  = 10.1 Hz), 120.2, 115.7 (d,  $J$  = 20.2 Hz), 115.5 (d,  $J$  = 20.2 Hz), 113.5, 113.2 (d,  $J$  = 20.2 Hz), 113.0 (d,  $J$  = 20.2 Hz), 91.1, 62.3, 11.8.  $^{19}\text{F}$  NMR (377 MHz,  $\text{CDCl}_3$ )  $\delta$  -112.05 HRMS (ESI+): Calculated for  $\text{C}_{17}\text{H}_{14}\text{FNO}_3\text{Na}$  322.0850; Found 322.0853.

**(E)-2-(3-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3k)**



Colorless liquid, 45.37 mg, 72 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 – 7.64 (m, 2H), 7.60 – 7.59 (m, 1H), 7.50 (ddd,  $J$  = 5.7, 3.7, 1.7 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.27 – 7.24 (m, 1H), 7.16 – 7.10 (m, 1H), 3.87 (s, 3H), 1.81 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  195.4, 170.4, 153.6, 138.3, 136.5, 134.6, 129.9, 128.9, 125.8, 125.4, 124.2, 122.8, 120.2, 113.5, 91.0, 62.3, 11.8. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{17}\text{H}_{14}\text{ClNO}_3\text{Na}$  338.0554; Found 338.0554.

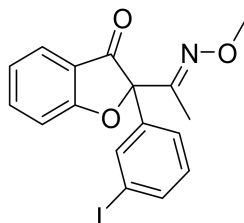
**(E)-2-(3-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3l)**



Colorless liquid, 56.01 mg, 78 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.86 (ddd,  $J$  = 8.5, 7.2, 1.4 Hz, 1H), 7.72 (dd,  $J$  = 7.7, 0.8 Hz, 1H), 7.66 – 7.58 (m,

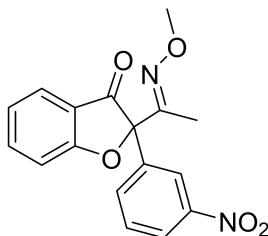
2H), 7.51 (ddd,  $J = 8.4, 3.5, 2.1$  Hz, 2H), 7.43 (t,  $J = 7.9$  Hz, 1H), 7.29 – 7.23 (m, 1H), 3.78 (s, 3H), 1.75 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  195.4, 170.4, 153.5, 138.3, 136.7, 131.8, 130.1, 128.6, 125.4, 124.7, 122.8, 122.7, 120.2, 113.5, 90.9, 62.3, 11.8. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{17}\text{H}_{14}\text{BrNO}_3\text{Na}$  382.0049; Found 382.0051.

**(*E*)-2-(3-iodophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2*H*)-one (3m)**



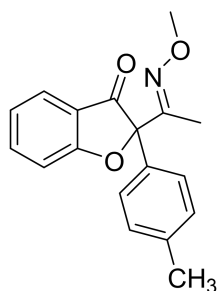
Colorless liquid, 59.42 mg, 73 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.86 (ddd,  $J = 8.5, 7.3, 1.4$  Hz, 1H), 7.82 – 7.73 (m, 2H), 7.71 (dd,  $J = 7.7, 0.8$  Hz, 1H), 7.54 – 7.46 (m, 2H), 7.27 (td,  $J = 7.6, 3.5$  Hz, 2H), 3.78 (s, 3H), 1.74 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, DMSO)  $\delta$  195.2, 170.3, 154.1, 139.9, 138.1, 136.6, 133.9, 131.5, 125.53, 125.48, 124.0, 119.6, 114.4, 95.6, 90.6, 62.5, 12.4. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{17}\text{H}_{14}\text{INO}_3\text{Na}$  429.9910; Found 429.9921.

**(*E*)-2-(1-(methoxyimino)ethyl)-2-(3-nitrophenyl)benzofuran-3(2*H*)-one (3n)**



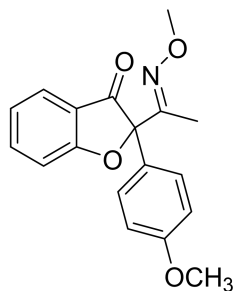
Colorless liquid, 46.96 mg, 72 % yield (eluent: ethyl acetate / petroleum ether = 1:20);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.49 (t,  $J = 2.0$  Hz, 1H), 8.21 (ddd,  $J = 8.2, 2.3, 1.0$  Hz, 1H), 8.02 (ddd,  $J = 7.9, 1.7, 1.1$  Hz, 1H), 7.76 – 7.66 (m, 2H), 7.58 (t,  $J = 8.0$  Hz, 1H), 7.32 (d,  $J = 8.2$  Hz, 1H), 7.21 – 7.13 (m, 1H), 3.86 (s, 3H), 1.81 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  195.4, 170.7, 153.0, 148.3, 138.7, 136.6, 132.5, 129.4, 125.4, 123.6, 123.1, 121.0, 120.0, 113.7, 90.7, 62.4, 11.6. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calculated for  $\text{C}_{17}\text{H}_{15}\text{N}_2\text{O}_5$  349.0795; Found 349.0806.

**(*E*)-2-(1-(methoxyimino)ethyl)-2-(*p*-tolyl)benzofuran-3(2*H*)-one (3o)**



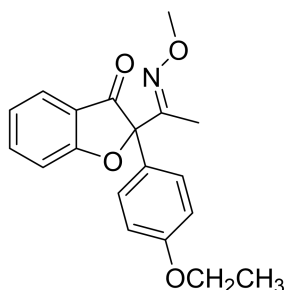
Colorless liquid, 43.68 mg, 74 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 – 7.57 (m, 2H), 7.48 – 7.40 (m, 2H), 7.23 (d,  $J$  = 8.4 Hz, 1H), 7.18 (d,  $J$  = 8.0 Hz, 2H), 7.14 – 7.05 (m, 1H), 3.87 (s, 3H), 2.33 (s, 3H), 1.82 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  196.3, 170.5, 154.1, 138.6, 138.0, 131.6, 129.4, 125.6, 125.3, 122.4, 120.4, 113.4, 91.8, 62.2, 21.2, 12.0. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calculated for  $\text{C}_{18}\text{H}_{18}\text{NO}_3$  296.1281; Found 296.1287.

**(E)-2-(1-(methoxyimino)ethyl)-2-(4-methoxyphenyl)benzofuran-3(2H)-one (3p)**



Colorless liquid, 47.91 mg, 77 % yield (eluent: ethyl acetate/petroleum ether = 1:30);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79 – 7.55 (m, 2H), 7.57 – 7.32 (m, 2H), 7.23 (d,  $J$  = 8.4 Hz, 1H), 7.10 (t,  $J$  = 7.4 Hz, 1H), 6.98 – 6.83 (m, 2H), 3.87 (s, 3H), 3.79 (s, 3H), 1.82 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  196.5, 170.5, 159.9, 154.0, 138.0, 127.2, 126.6, 125.3, 122.4, 120.5, 114.0, 113.4, 91.6, 62.2, 55.3, 11.8. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calculated for  $\text{C}_{18}\text{H}_{18}\text{NO}_4$  334.1050; Found 334.1045.

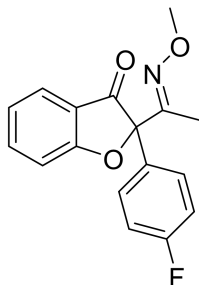
**(E)-2-(4-ethoxyphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3q)**



Colorless liquid, 49.42 mg, 76 % yield (eluent: ethyl acetate / petroleum ether = 1:35);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.71 – 7.58 (m, 2H), 7.54 – 7.41 (m, 2H), 7.22 (d,  $J$  = 8.4 Hz, 1H), 7.10 (t,  $J$  = 7.4 Hz, 1H), 6.92 – 6.84 (m, 2H), 4.01 (q,  $J$  = 7.0 Hz, 2H), 3.86 (s, 3H), 1.82 (s, 3H), 1.39 (t,  $J$  = 7.0 Hz, 3H).

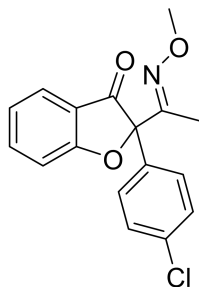
$^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  196.5, 170.5, 159.3, 154.1, 138.0, 127.1, 126.4, 125.3, 122.4, 120.5, 114.6, 113.4, 91.6, 63.5, 62.2, 14.8, 11.8. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{19}\text{H}_{19}\text{NO}_4\text{Na}$  348.1206; Found 348.1206.

**(E)-2-(4-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3r)**



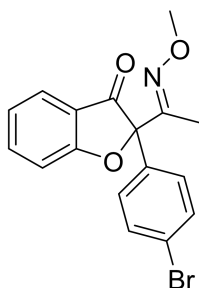
Colorless liquid, 43.67 mg, 73 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 – 7.62 (m, 2H), 7.62 – 7.49 (m, 2H), 7.25 (d,  $J$  = 8.4 Hz, 1H), 7.13 (t,  $J$  = 7.4 Hz, 1H), 7.10 – 6.93 (m, 2H), 3.86 (s, 3H), 1.81 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  196.1, 170.5, 164.2 (d,  $J$  = 252.5 Hz), 161.7 (d,  $J$  = 252.5 Hz), 153.8, 138.2, 130.29 (d,  $J$  = 3.0 Hz), 130.26 (d,  $J$  = 3.0 Hz), 127.8 (d,  $J$  = 10.1 Hz), 127.7 (d,  $J$  = 10.1 Hz), 125.4, 122.7, 120.3, 115.7 (d,  $J$  = 20.2 Hz), 115.5 (d,  $J$  = 20.2 Hz), 113.5, 91.2, 62.3, 11.8.  $^{19}\text{F}$  NMR (377 MHz, DMSO)  $\delta$  -113.20. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{17}\text{H}_{14}\text{FNO}_3\text{Na}$  322.0850; Found 322.0840.

**(E)-2-(4-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3s)**



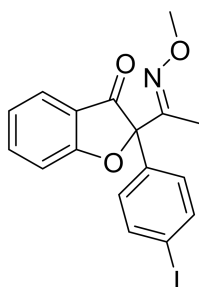
Colorless liquid, 47.26 mg, 75 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.94 – 7.79 (m, 1H), 7.71 (d,  $J$  = 7.5 Hz, 1H), 7.57 – 7.51 (m, 2H), 7.48 (d,  $J$  = 9.0 Hz, 3H), 7.26 (t,  $J$  = 7.4 Hz, 1H), 3.77 (s, 3H), 1.74 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, DMSO)  $\delta$  195.4, 170.4, 154.1, 139.8, 134.2, 133.3, 129.3, 127.9, 125.5, 123.9, 119.6, 114.3, 91.1, 62.4, 12.4. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{17}\text{H}_{14}\text{ClNO}_3\text{Na}$  338.0554; Found 338.0544.

**(E)-2-(4-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3t)**



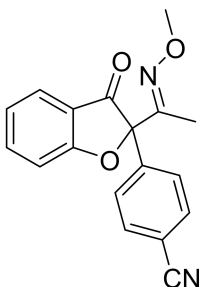
Colorless liquid, 51.70 mg, 72 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.85 (ddd,  $J = 8.5, 7.3, 1.4$  Hz, 1H), 7.71 (dd,  $J = 7.7, 0.8$  Hz, 1H), 7.68 – 7.56 (m, 2H), 7.47 (t,  $J = 7.3$  Hz, 1H), 7.46 – 7.37 (m, 2H), 7.29 – 7.21 (m, 1H), 3.78 (s, 3H), 1.74 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, DMSO)  $\delta$  195.3, 170.4, 154.0, 139.8, 133.7, 132.2, 128.2, 125.4, 123.9, 122.8, 119.6, 114.3, 91.1, 62.4, 12.4. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{17}\text{H}_{14}\text{BrNO}_3\text{Na}$  382.0049; Found 382.0044.

**(E)-2-(4-iodophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3u)**



Colorless liquid, 61.05 mg, 75 % yield (eluent: ethyl acetate/petroleum ether = 1:10);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 – 7.71 (m, 1H), 7.71 – 7.62 (m, 3H), 7.39 – 7.30 (m, 2H), 7.24 (d,  $J = 8.3$  Hz, 1H), 7.16 – 7.06 (m, 1H), 3.86 (s, 3H), 1.80 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, DMSO)  $\delta$  195.3, 170.4, 154.0, 139.8, 138.1, 134.2, 128.1, 125.4, 123.9, 119.6, 114.3, 96.1, 91.3, 62.4, 12.4. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calculated for  $\text{C}_{17}\text{H}_{15}\text{INO}_3$  429.9910; Found 429.9914.

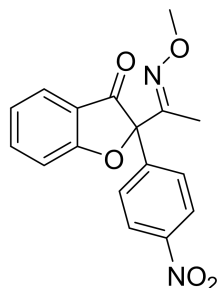
**(E)-4-(2-(1-(methoxyimino)ethyl)-3-oxo-2,3-dihydrobenzofuran-2-yl)benzotrile (3v)**



Colorless liquid, 46.53 mg, 76 % yield (eluent: ethyl acetate/petroleum ether = 1:10);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  8.00 – 7.90 (m, 2H), 7.87 (ddd,  $J = 8.5, 7.2, 1.4$  Hz, 1H), 7.72 (dd,  $J = 7.7, 0.8$  Hz, 1H), 7.71 – 7.64 (m, 2H), 7.51 (d,  $J = 8.4$  Hz, 1H), 7.31 – 7.25 (m, 1H), 3.78 (s, 3H), 1.74 (d,  $J = 5.7$

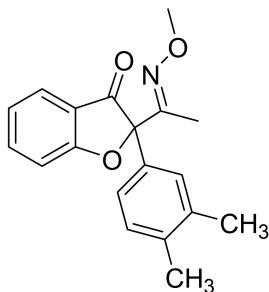
Hz, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, DMSO)  $\delta$  194.9, 170.5, 153.9, 140.0, 139.4, 133.2, 127.0, 125.5, 124.1, 119.5, 118.8, 114.4, 112.2, 91.1, 62.5, 12.4. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calculated for  $\text{C}_{18}\text{H}_{15}\text{N}_2\text{O}_3$  307.1077; Found 307.1078.

**(E)-2-(1-(methoxyimino)ethyl)-2-(4-nitrophenyl)benzofuran-3(2H)-one (3w)**



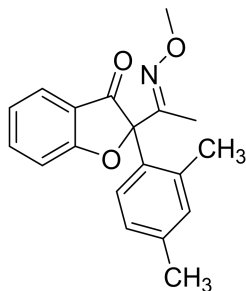
Colorless liquid, 50.87 mg, 78 % yield (eluent: ethyl acetate / petroleum ether = 1:20);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  8.36 – 8.25 (m, 2H), 7.92 – 7.85 (m, 1H), 7.81 – 7.76 (m, 2H), 7.75 – 7.71 (m, 1H), 7.53 (d,  $J$  = 8.4 Hz, 1H), 7.35 – 7.18 (m, 1H), 3.79 (s, 3H), 1.76 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  195.0, 170.6, 153.1, 148.0, 141.4, 138.7, 127.1, 125.5, 124.9, 123.6, 123.2, 119.9, 113.6, 91.2, 62.4, 11.7. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  Calculated for  $\text{C}_{17}\text{H}_{15}\text{N}_2\text{O}_5$  327.0976; Found 327.0983.

**(E)-2-(3,4-dimethylphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3x)**



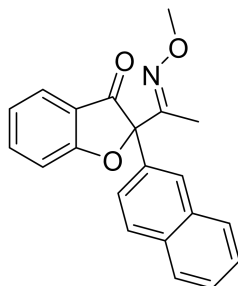
Colorless liquid, 43.28 mg, 70 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.72 – 7.54 (m, 2H), 7.31 – 7.21 (m, 3H), 7.16 – 7.06 (m, 2H), 3.88 (s, 3H), 2.25 (d,  $J$  = 9.2 Hz, 6H), 1.84 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  196.3, 170.5, 154.1, 138.0, 137.3, 137.1, 131.9, 129.9, 126.7, 125.3, 123.2, 122.4, 120.5, 113.4, 91.8, 62.2, 20.0, 19.6, 12.0. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{19}\text{H}_{19}\text{NO}_3\text{Na}$  332.1257; Found 332.1260.

**(E)-2-(2,4-dimethylphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3y)**



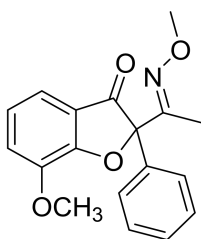
Colorless liquid, 44.52 mg, 72 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  7.82 (ddd,  $J$  = 8.5, 7.3, 1.4 Hz, 1H), 7.70 (t,  $J$  = 9.3 Hz, 1H), 7.40 (d,  $J$  = 8.4 Hz, 1H), 7.23 (t,  $J$  = 7.4 Hz, 1H), 7.16 (d,  $J$  = 8.0 Hz, 1H), 7.10 (s, 1H), 7.01 (d,  $J$  = 8.0 Hz, 1H), 3.76 (d,  $J$  = 11.6 Hz, 3H), 2.34 (s, 3H), 2.26 (d,  $J$  = 9.3 Hz, 3H), 1.79 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, DMSO)  $\delta$  196.8, 170.0, 154.7, 139.7, 138.9, 137.3, 133.7, 129.9, 127.0, 126.9, 125.2, 123.5, 120.2, 114.2, 92.8, 62.3, 20.9, 20.8, 12.7. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{19}\text{H}_{19}\text{NO}_3\text{Na}$  332.1257; Found 332.1264.

**(E)-7-methoxy-2-(1-(methoxyimino)ethyl)-2-(naphthalen-2-yl)benzofuran-3(2H)-one (3z)**



Colorless liquid, 43.05 mg, 65 % yield (eluent: ethyl acetate / petroleum ether = 1:50);  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  8.01 (d,  $J$  = 9.2 Hz, 3H), 7.96 – 7.91 (m, 1H), 7.87 (t,  $J$  = 7.8 Hz, 1H), 7.72 (d,  $J$  = 7.6 Hz, 1H), 7.60 – 7.51 (m, 4H), 7.26 (t,  $J$  = 7.4 Hz, 1H), 3.80 (s, 3H), 1.79 (s, 3H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz, DMSO)  $\delta$  195.7, 170.4, 154.5, 139.7, 133.2, 133.0, 131.9, 129.1, 128.7, 128.1, 127.4, 127.2, 125.4, 124.8, 123.8, 123.6, 119.8, 114.3, 91.8, 62.4, 12.6. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{Na}]^+$  Calculated for  $\text{C}_{22}\text{H}_{19}\text{NO}_4\text{Na}$  354.1100; Found 354.1101.

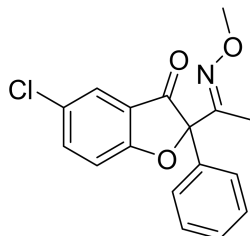
**(E)-7-methoxy-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one (3aa)**



Colorless liquid, 38.58 mg, 62 % yield (eluent: ethyl acetate / petroleum ether = 1:35);  $^1\text{H}$  NMR (400

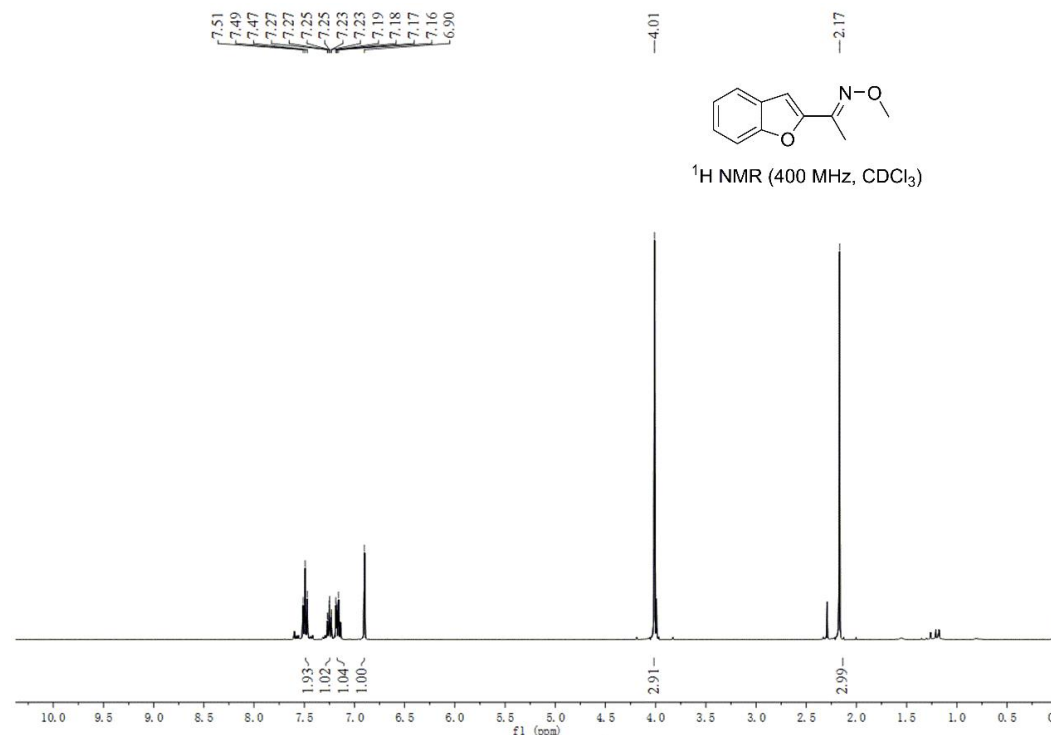
MHz, CDCl<sub>3</sub>) δ 7.59 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.42 – 7.30 (m, 3H), 7.29 – 7.23 (m, 1H), 7.18 – 7.13 (m, 1H), 7.03 (dd, *J* = 10.1, 5.5 Hz, 1H), 4.01 (s, 3H), 3.86 (s, 3H), 1.84 (s, 3H). <sup>13</sup>C{<sup>1</sup>H} NMR (101 MHz, CDCl<sub>3</sub>) δ 196.2, 160.5, 154.0, 146.7, 134.4, 128.63, 128.56, 125.8, 123.0, 121.7, 118.8, 116.3, 92.3, 62.2, 56.3, 12.1. HRMS (ESI) *m/z*: [M+Na]<sup>+</sup> Calculated for C<sub>18</sub>H<sub>17</sub>NO<sub>4</sub>Na 334.1050; Found 334.1059.

**(*E*)-5-chloro-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2*H*)-one (3ab)**



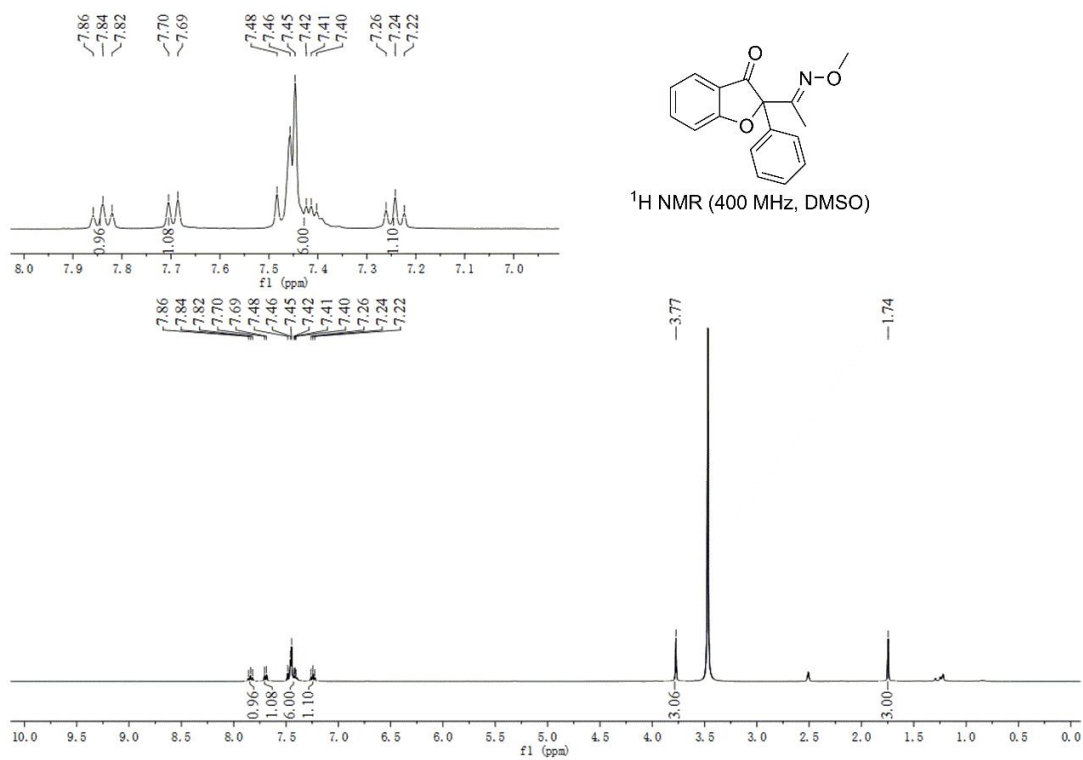
Colorless liquid, 39.70 mg, 63 % yield (eluent: ethyl acetate / petroleum ether = 1:35); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.64 (d, *J* = 2.3 Hz, 1H), 7.59 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.56 – 7.47 (m, 2H), 7.44 – 7.31 (m, 3H), 7.20 (d, *J* = 8.8 Hz, 1H), 3.87 (s, 3H), 1.80 (s, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 194.76, 168.72, 153.83, 137.87, 134.10, 128.83, 128.71, 128.01, 125.61, 124.65, 121.65, 114.77, 92.80, 62.27, 11.86. HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calculated for C<sub>17</sub>H<sub>15</sub>ClNO<sub>3</sub> 316.0735; Found 316.0744.

**(*E*)-1-(benzofuran-2-yl)ethan-1-one *O*-methyl oxime (1a): <sup>1</sup>H NMR**

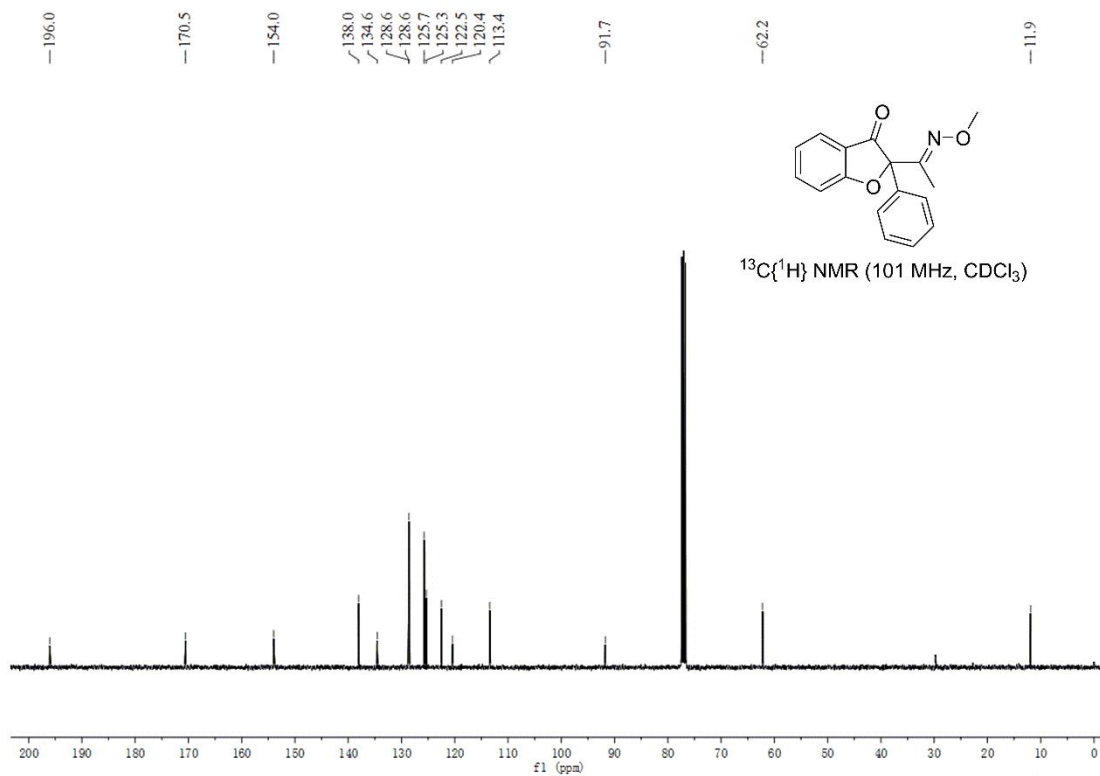




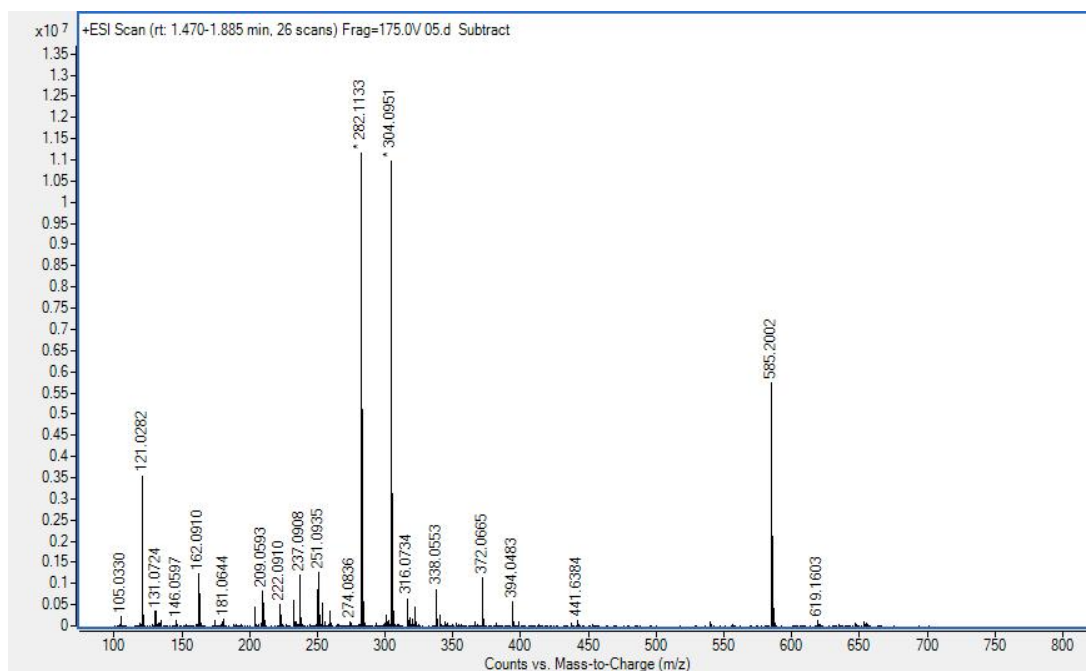
**(E)-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one (3a): <sup>1</sup>H NMR**



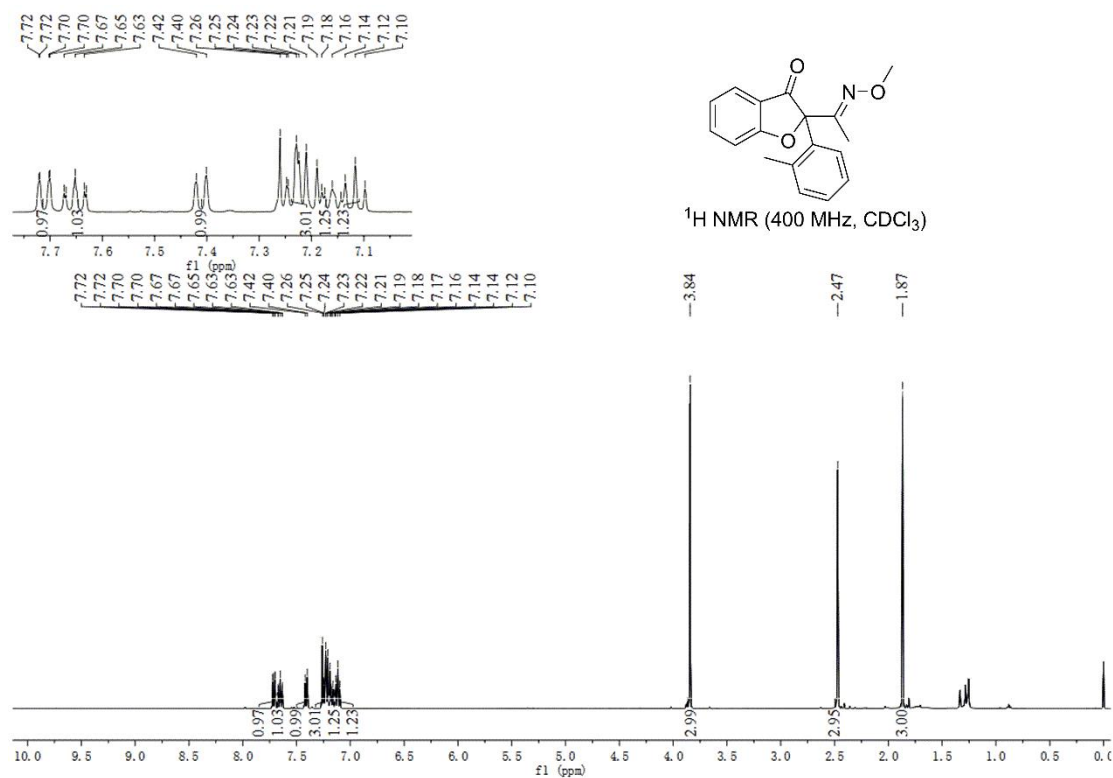
**(E)-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one (3a): <sup>13</sup>C NMR**



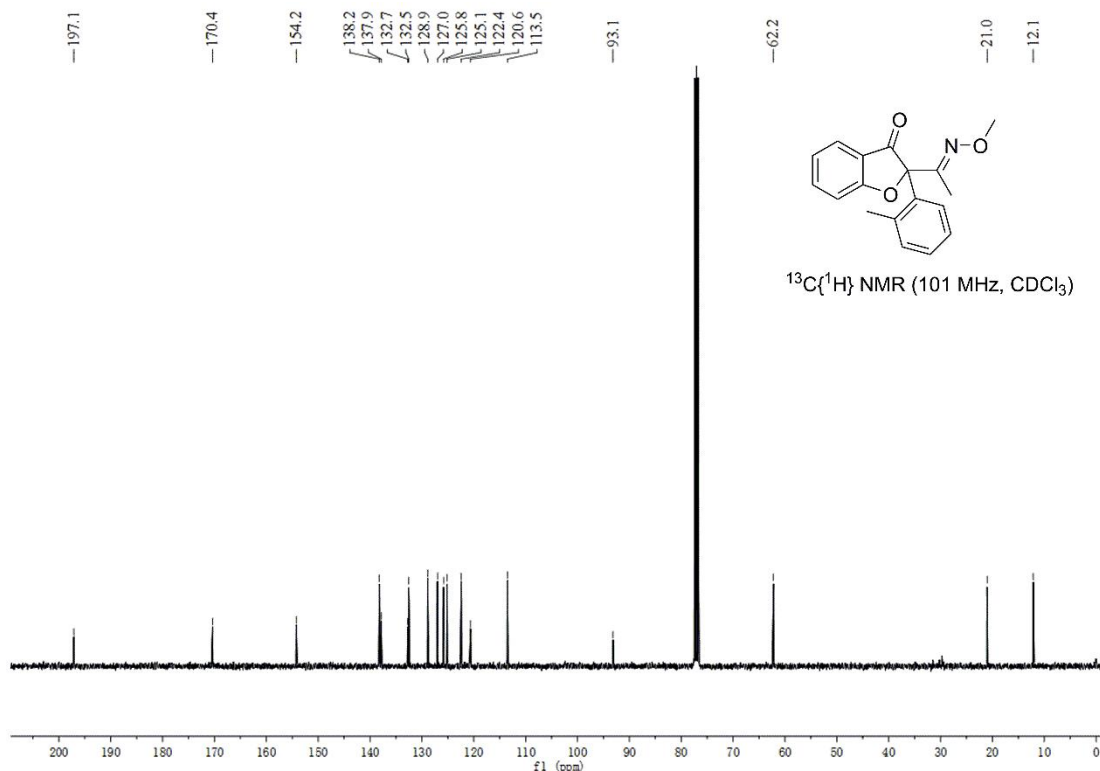
**(E)-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one (3a): MS**



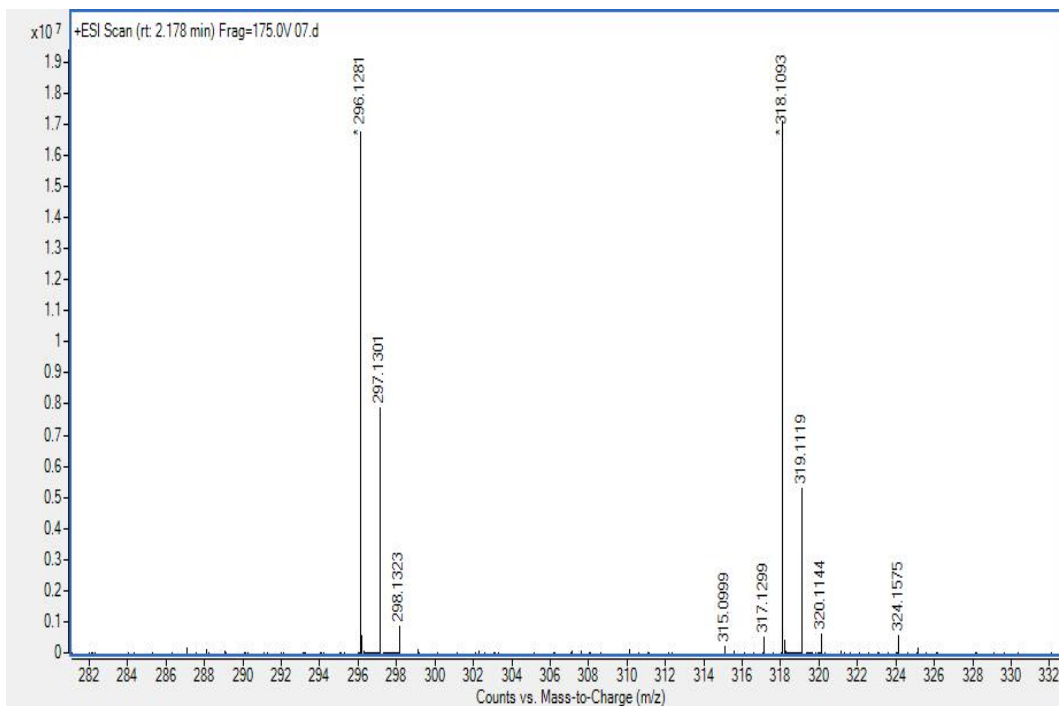
**(E)-2-(1-(methoxyimino)ethyl)-2-(o-tolyl)benzofuran-3(2H)-one (3b): <sup>1</sup>H NMR**



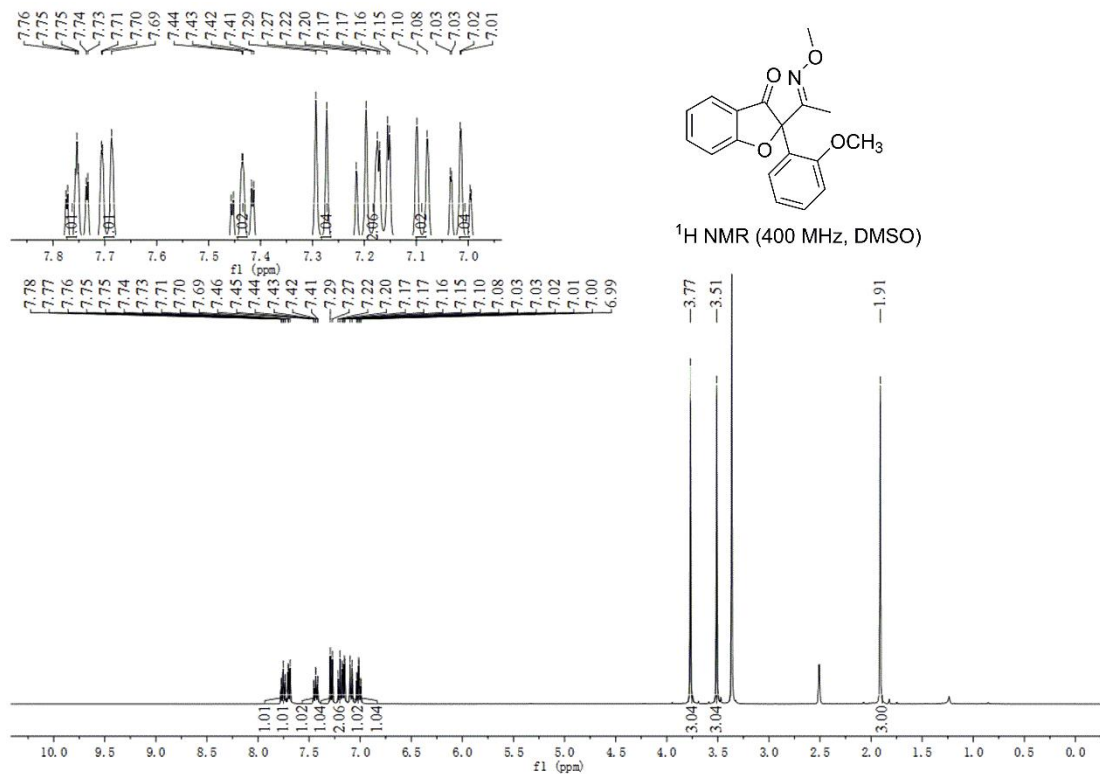
**(E)-2-(1-(methoxyimino)ethyl)-2-(o-tolyl)benzofuran-3(2H)-one (3b): <sup>13</sup>C NMR**



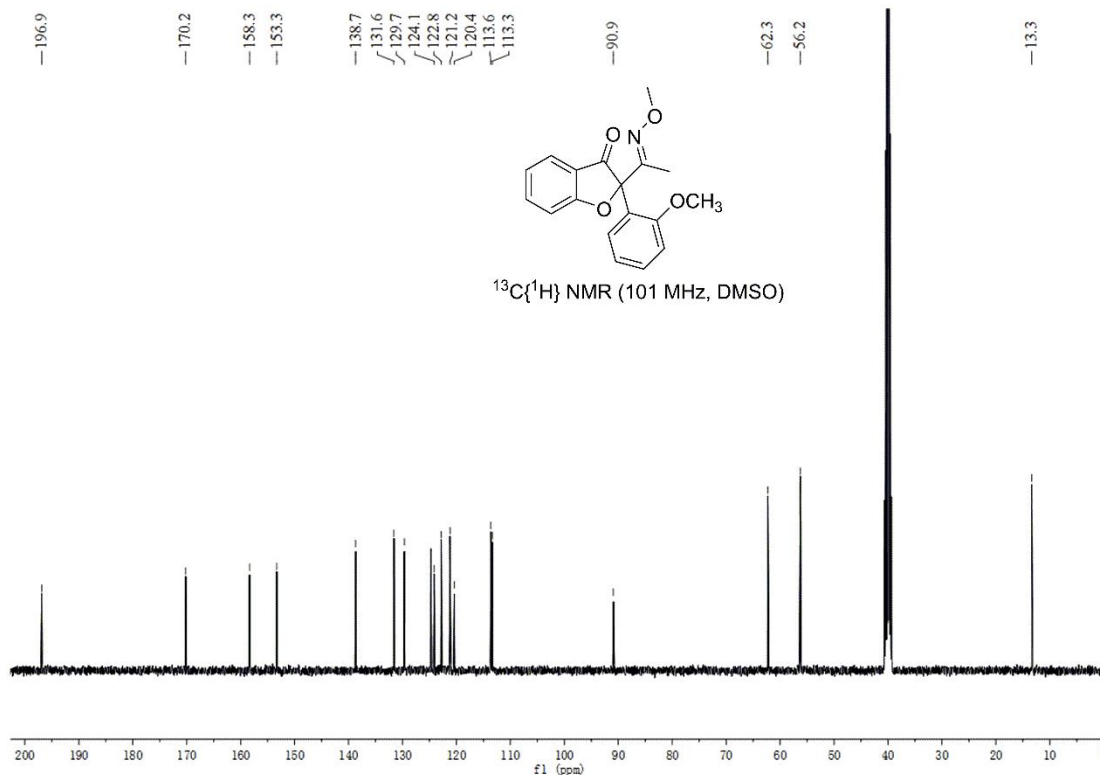
**(E)-2-(1-(methoxyimino)ethyl)-2-(o-tolyl)benzofuran-3(2H)-one (3b): MS**



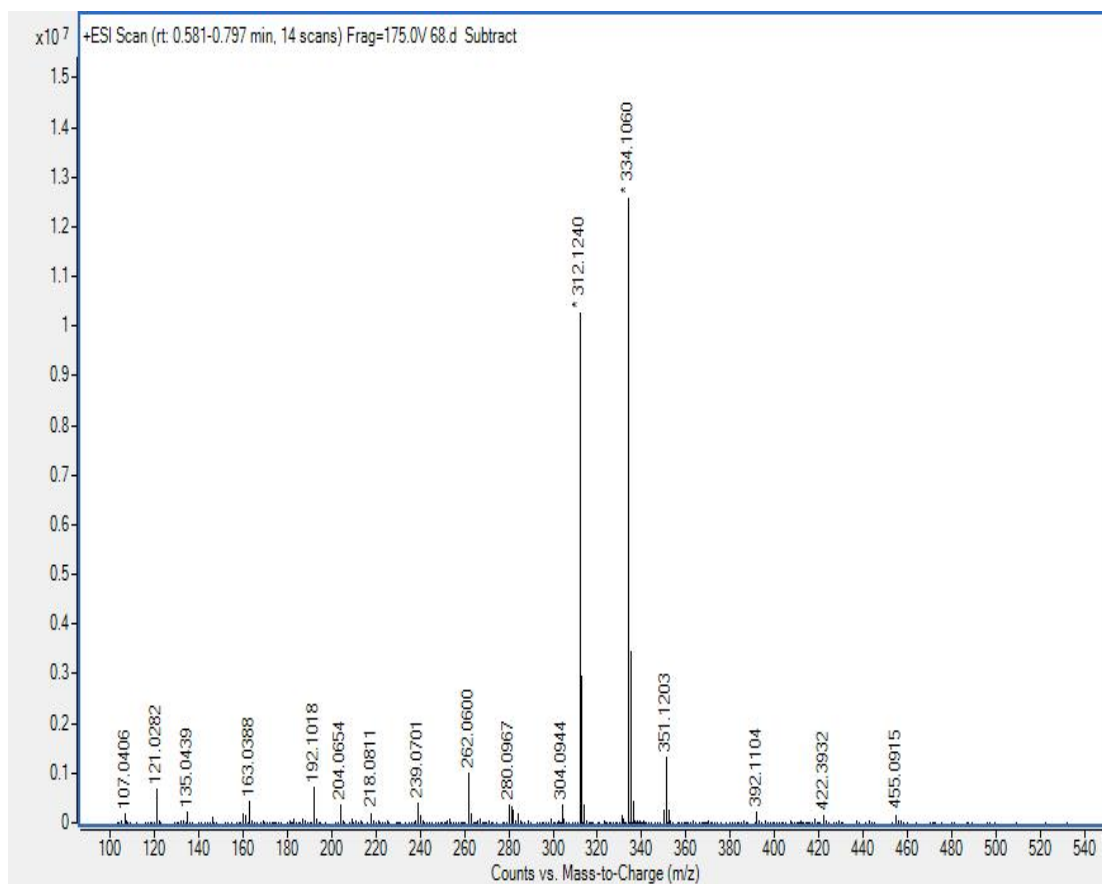
**(E)-2-(1-(methoxyimino)ethyl)-2-(2-methoxyphenyl)benzofuran-3(2H)-one (3c): <sup>1</sup>H NMR**



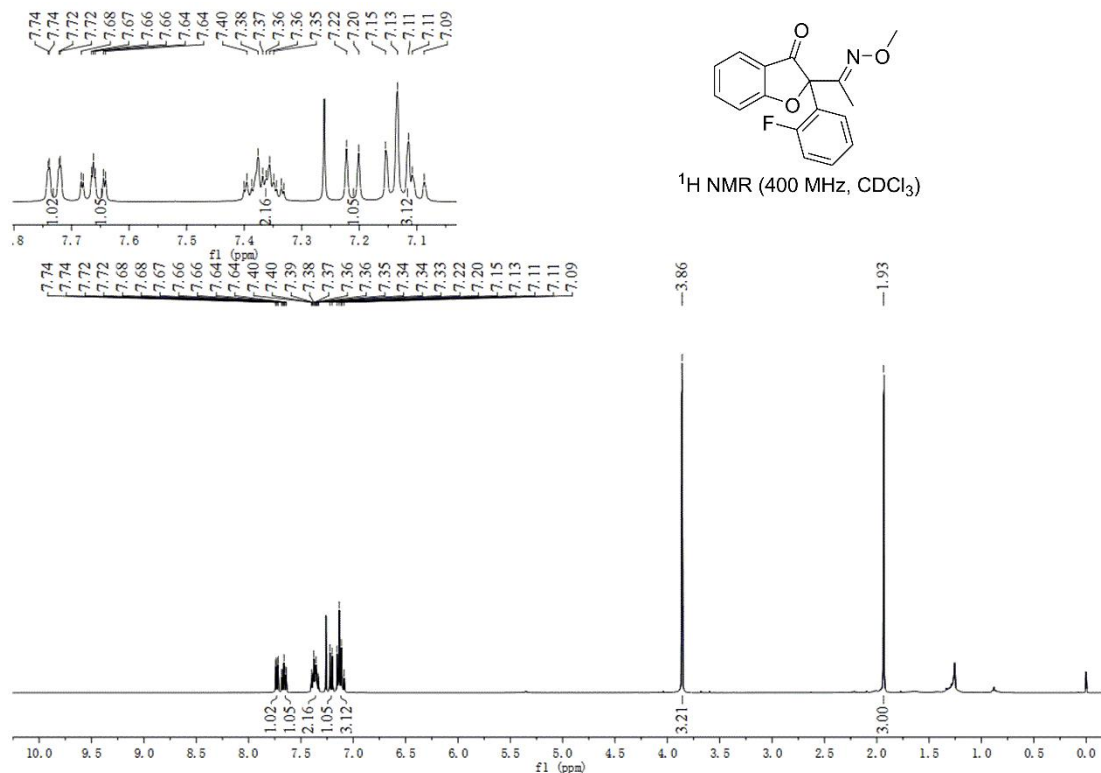
**(E)-2-(1-(methoxyimino)ethyl)-2-(2-methoxyphenyl)benzofuran-3(2H)-one (3c): <sup>13</sup>C NMR**



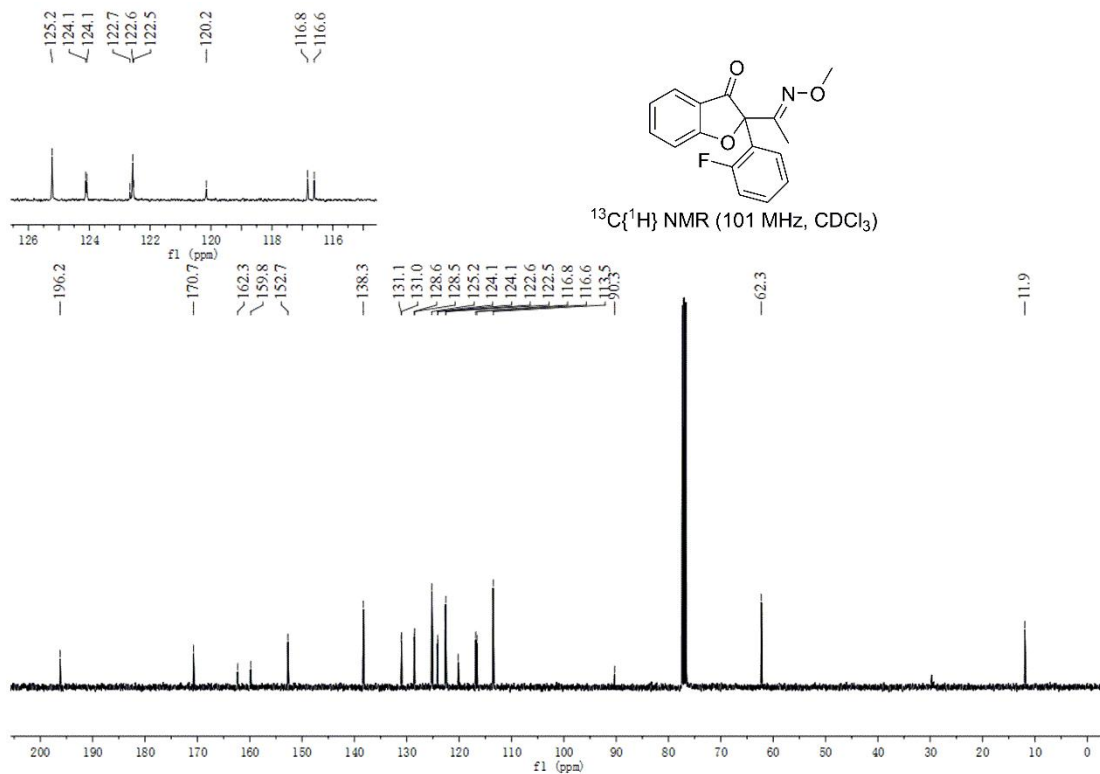
**(E)-2-(1-(methoxyimino)ethyl)-2-(2-methoxyphenyl)benzofuran-3(2H)-one (3c): MS**



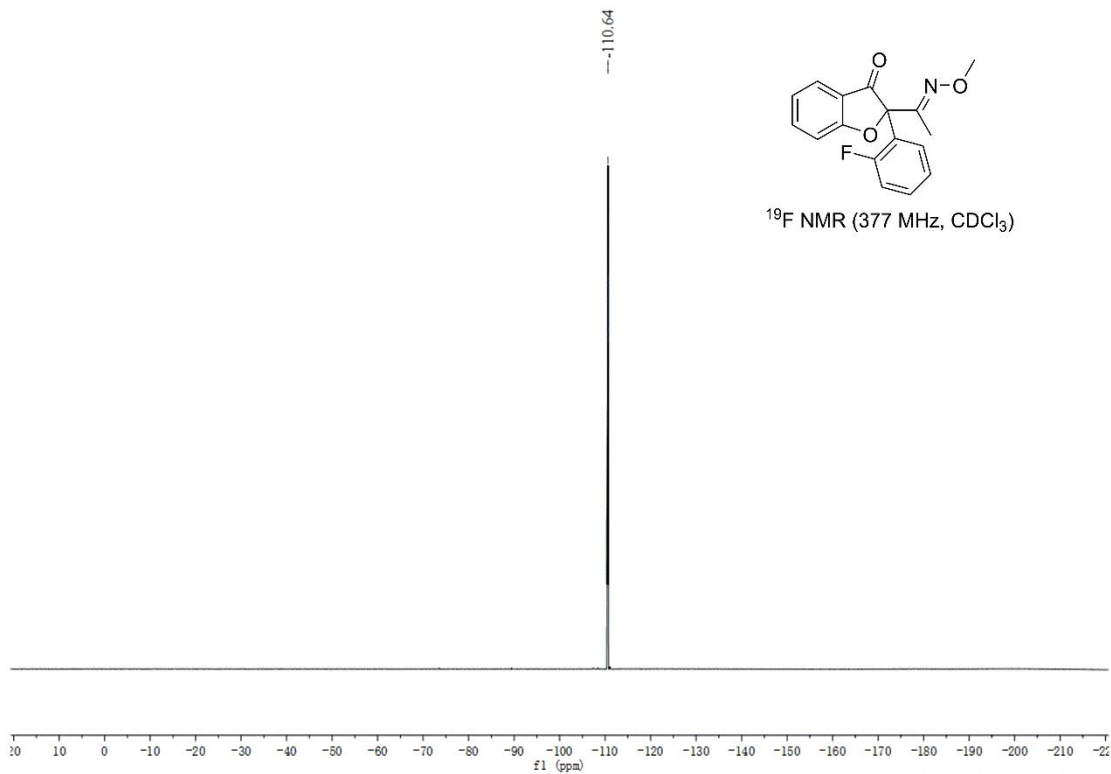
**(E)-2-(2-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3d): <sup>1</sup>H NMR**



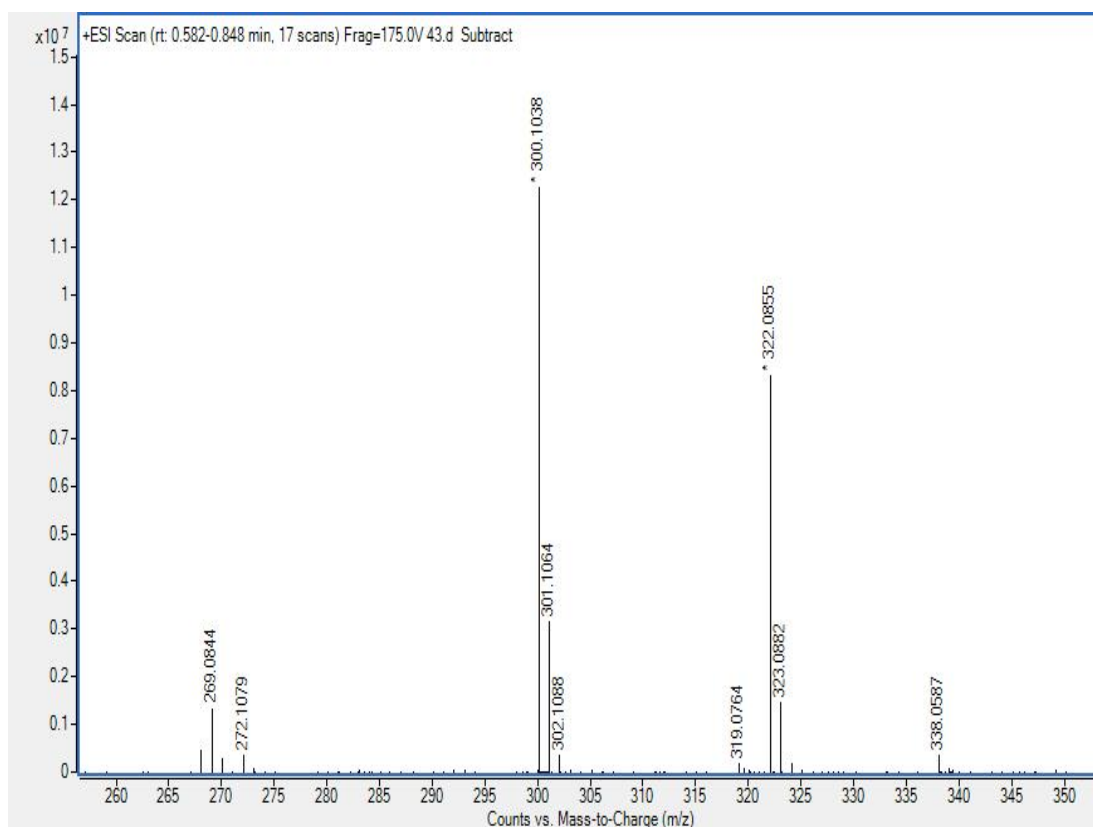
**(E)-2-(2-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3d):  $^{13}\text{C}$  NMR**



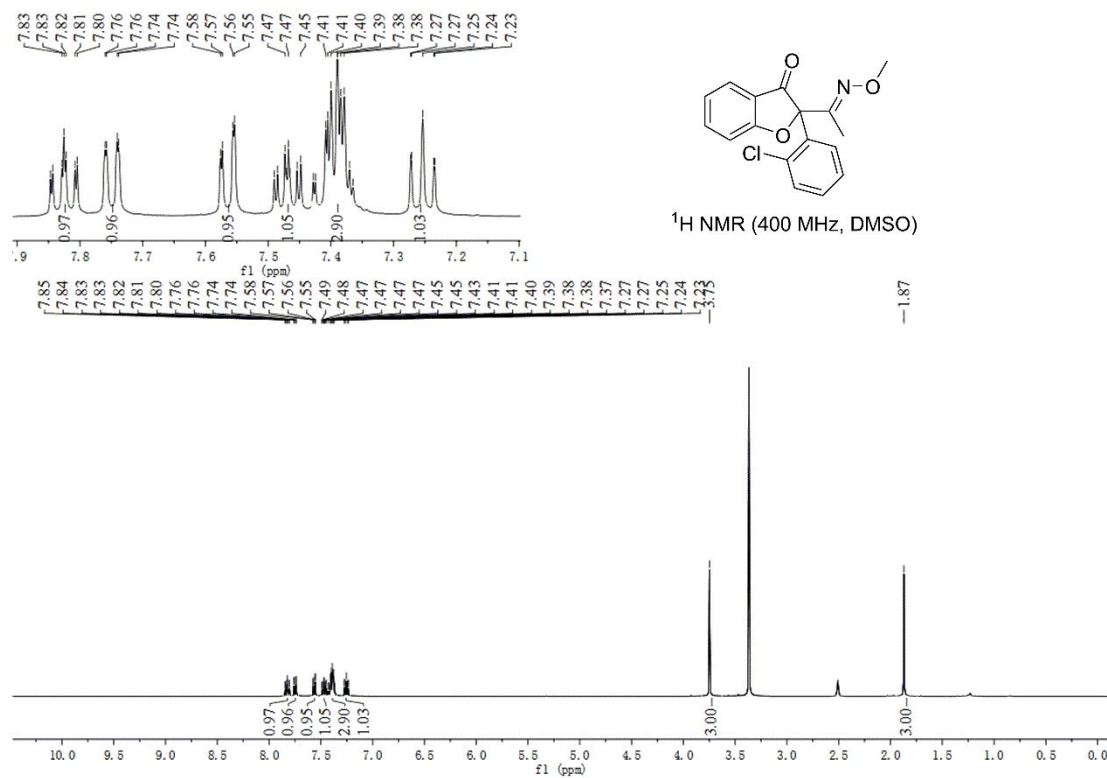
**(E)-2-(2-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3d):  $^{19}\text{F}$  NMR**



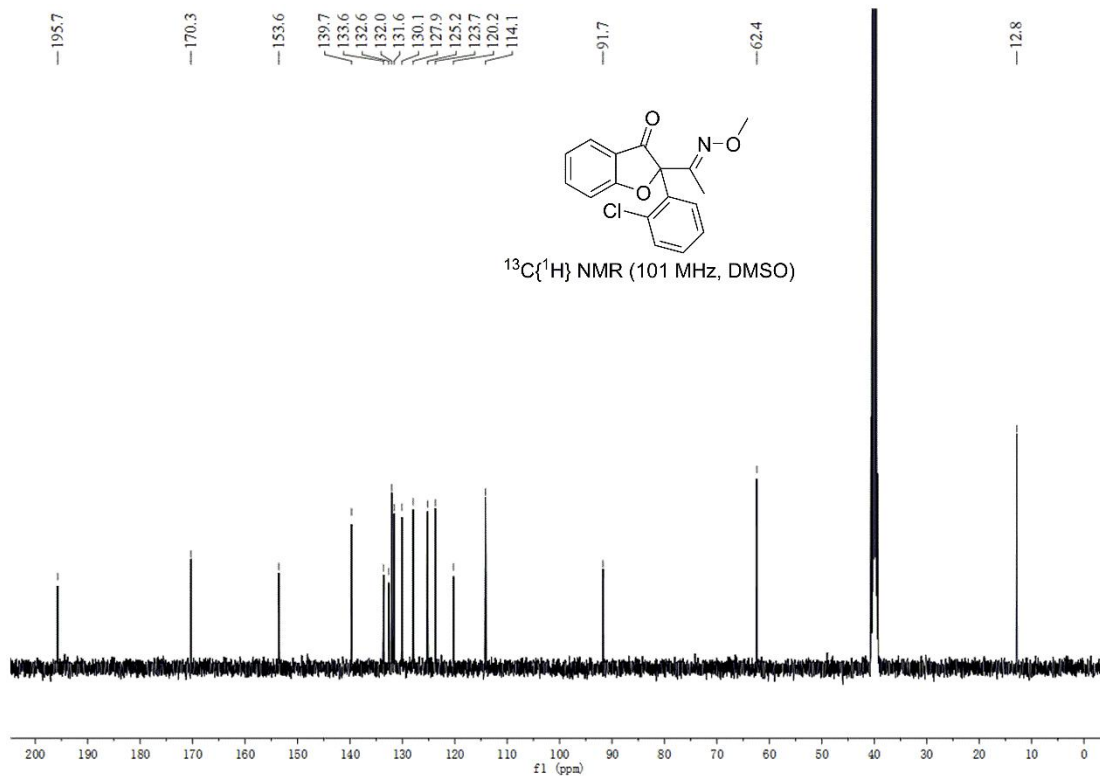
**(E)-2-(2-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3d): MS**



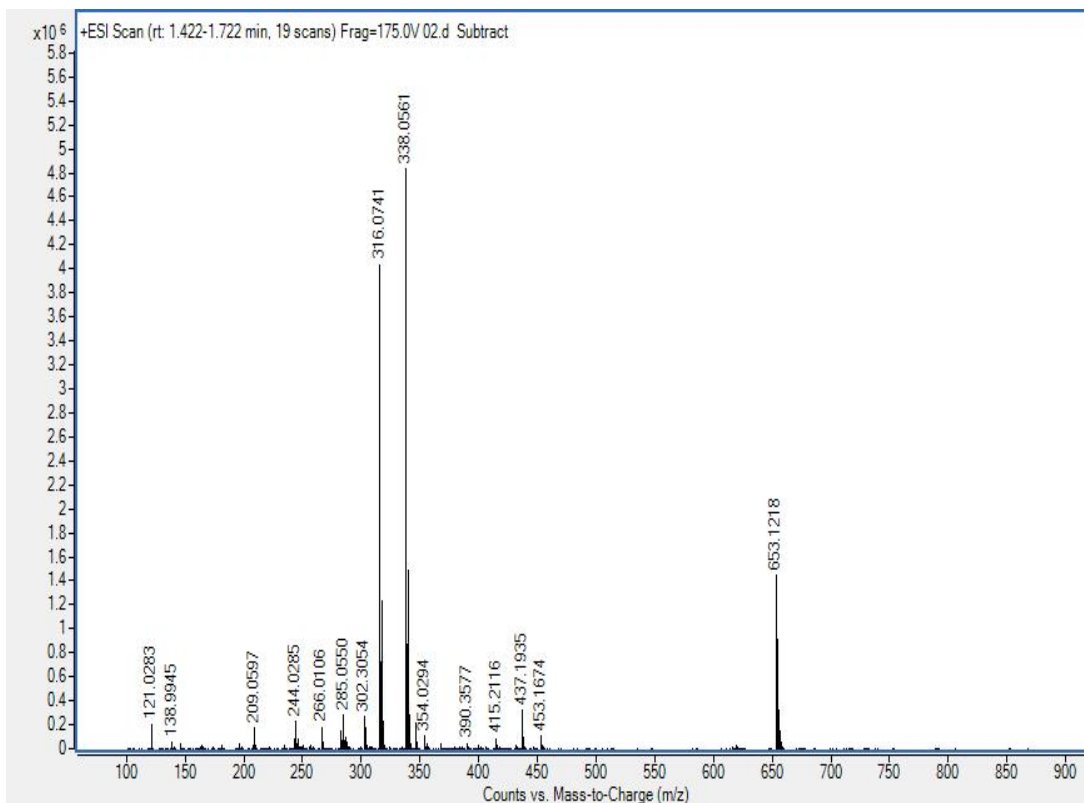
**(E)-2-(2-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3e): <sup>1</sup>H NMR**



**(E)-2-(2-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3e):  $^{13}\text{C}$  NMR**

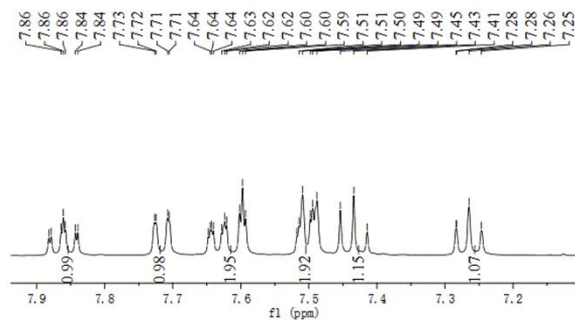


**(E)-2-(2-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3e): MS**

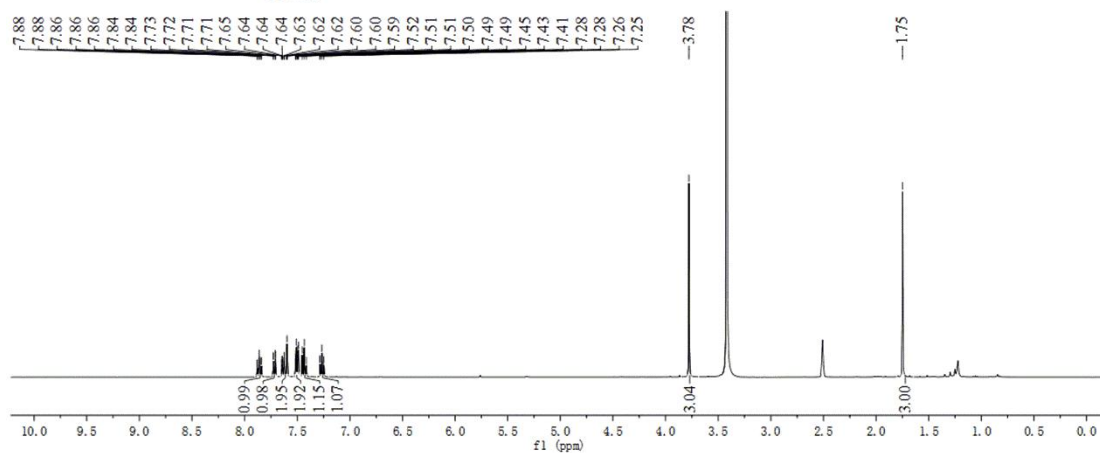




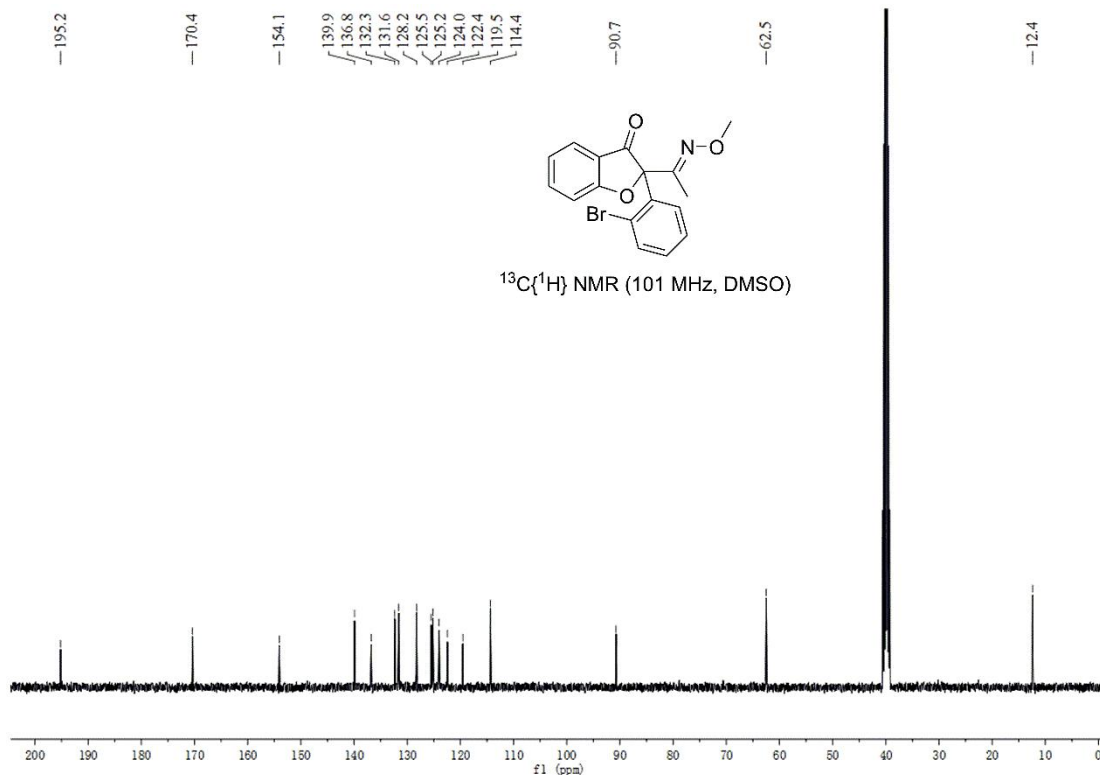
**(E)-2-(2-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3f): <sup>1</sup>H NMR**



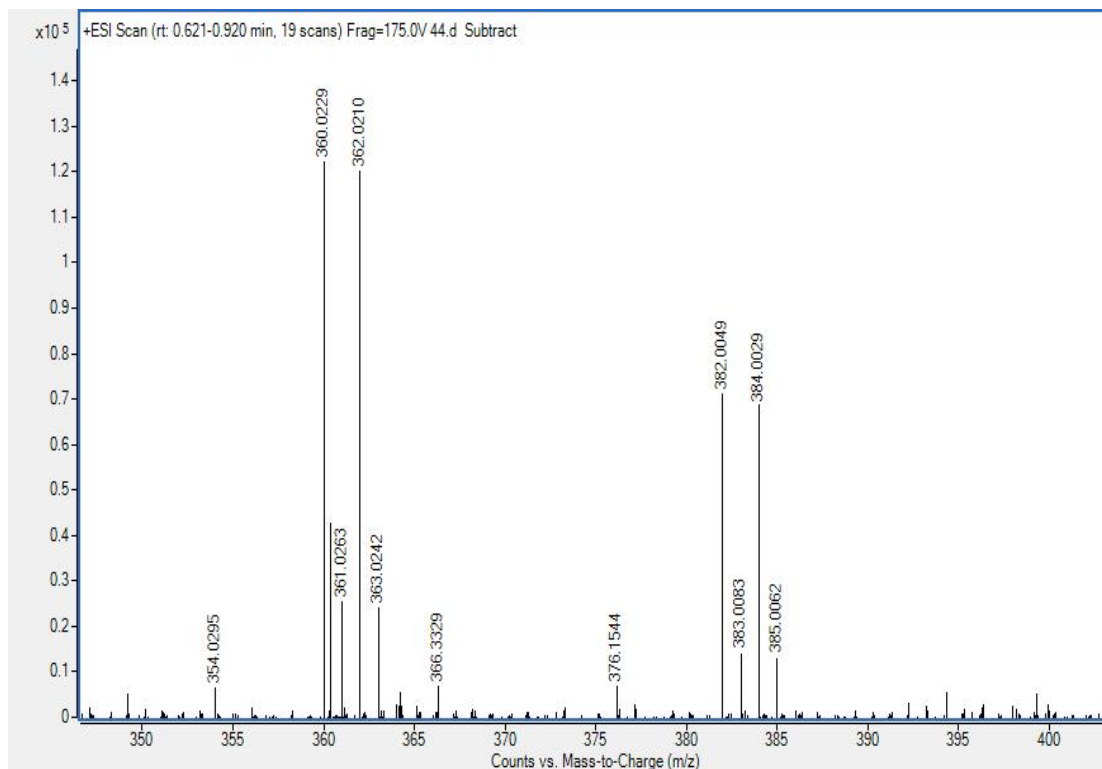
<sup>1</sup>H NMR (400 MHz, DMSO)



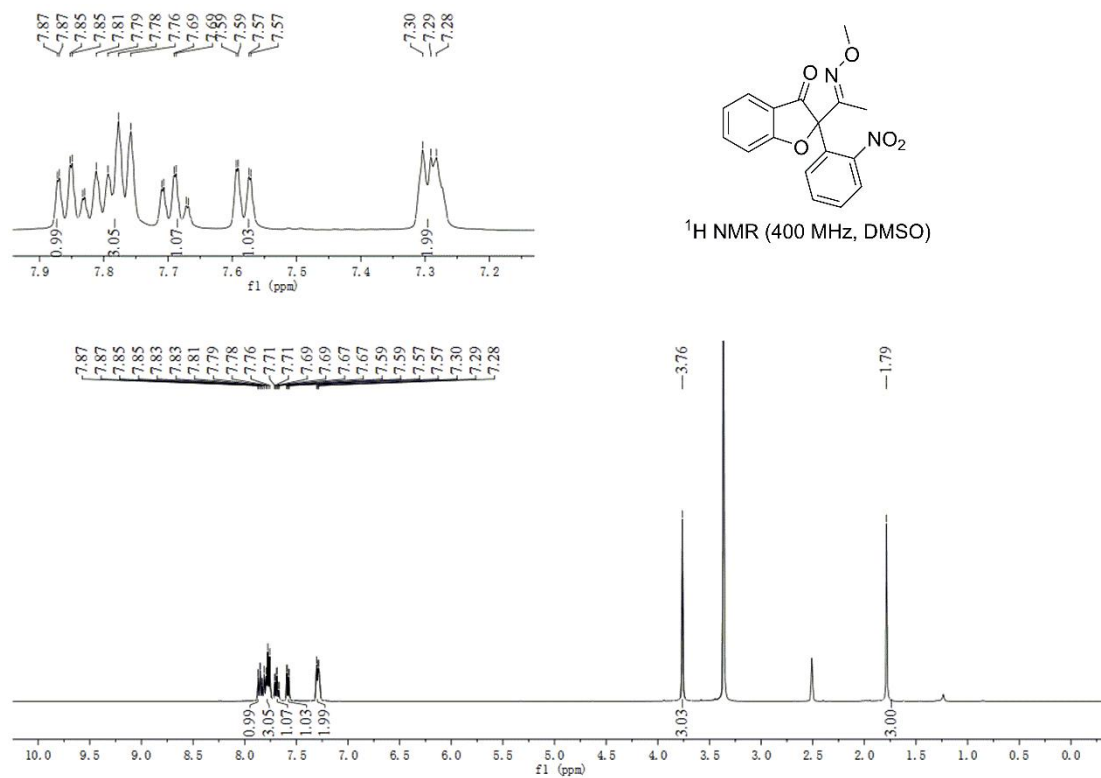
**(E)-2-(2-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3f): <sup>13</sup>C NMR**



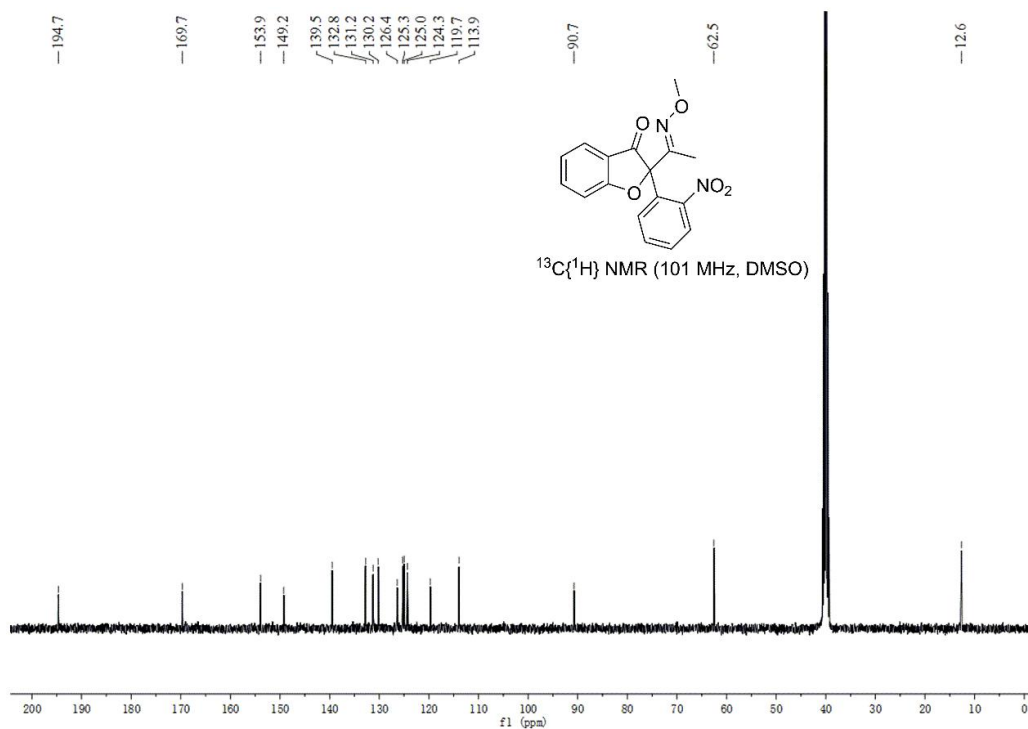
**(E)-2-(2-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3f): MS**



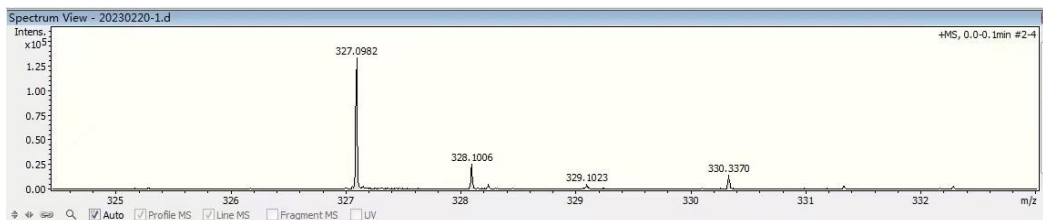
**(E)-2-(1-(methoxyimino)ethyl)-2-(2-nitrophenyl)benzofuran-3(2H)-one (3g): <sup>1</sup>H NMR**



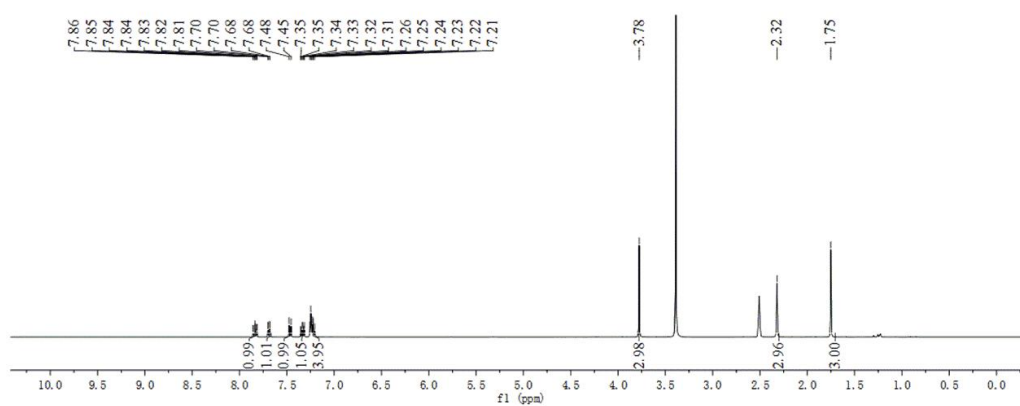
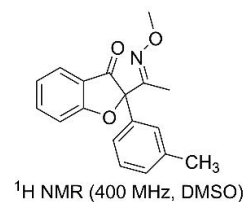
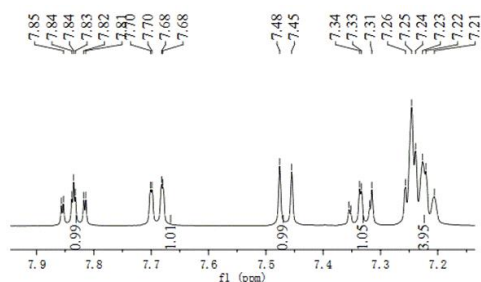
**(E)-2-(1-(methoxyimino)ethyl)-2-(2-nitrophenyl)benzofuran-3(2H)-one (3g):  $^{13}\text{C}$  NMR**



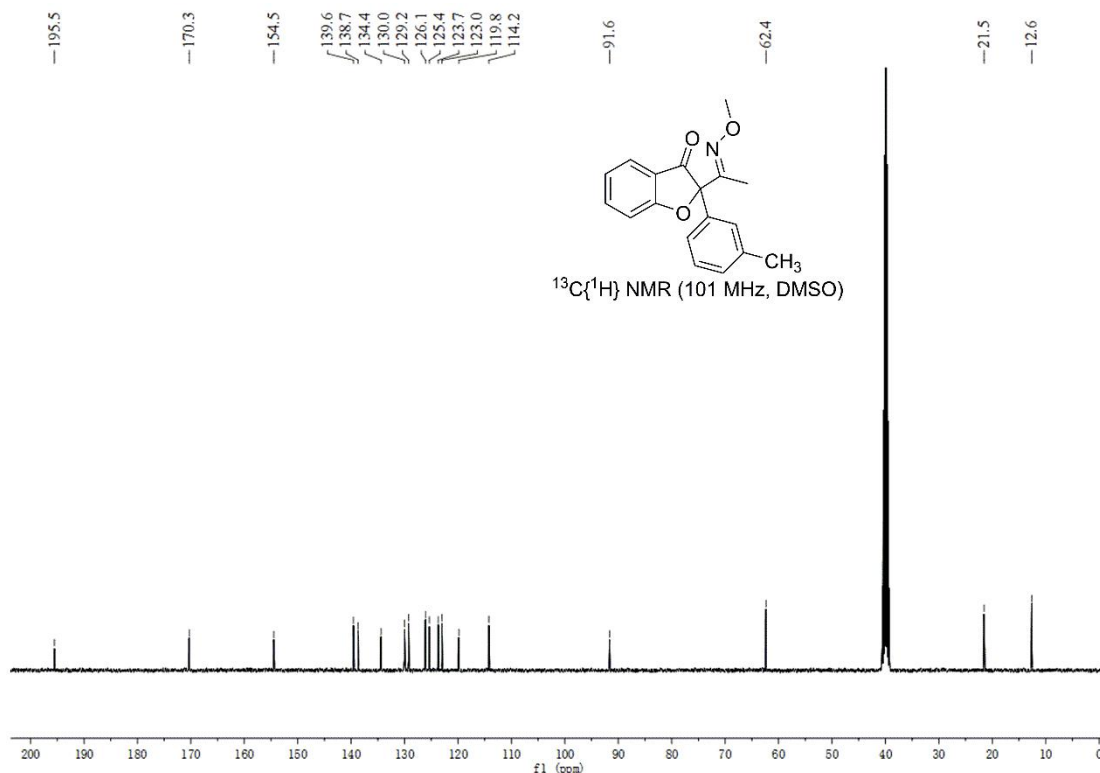
**(E)-2-(1-(methoxyimino)ethyl)-2-(2-nitrophenyl)benzofuran-3(2H)-one (3g): MS**



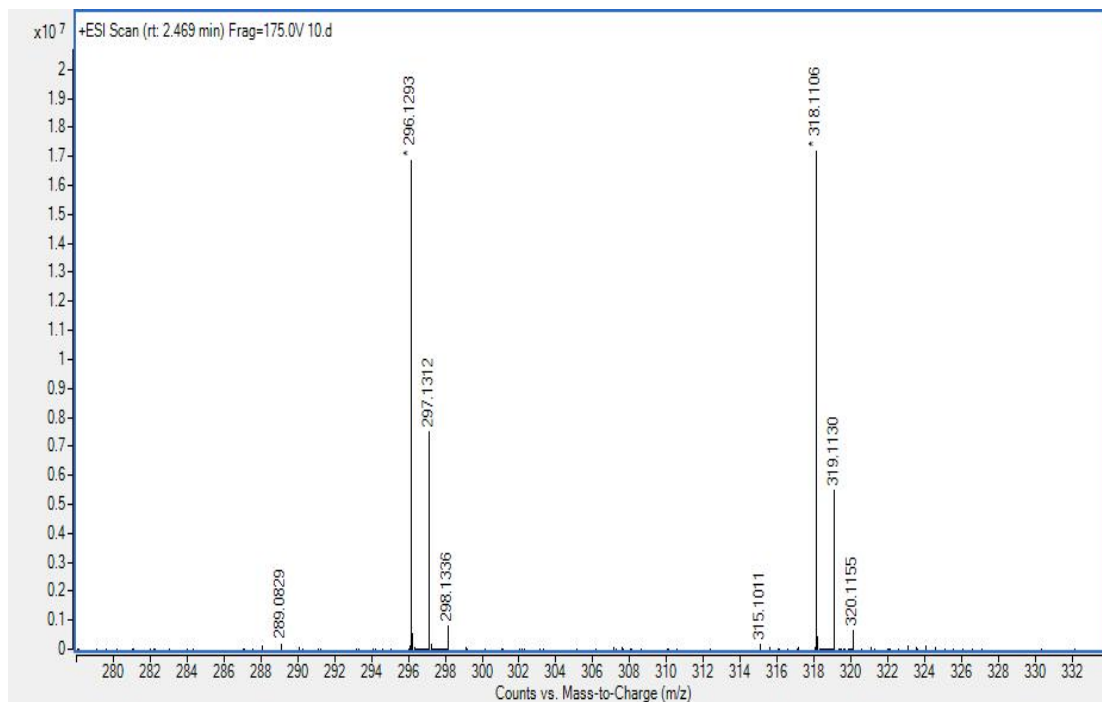
**(E)-2-(1-(methoxyimino)ethyl)-2-(m-tolyl)benzofuran-3(2H)-one (3h): <sup>1</sup>H NMR**



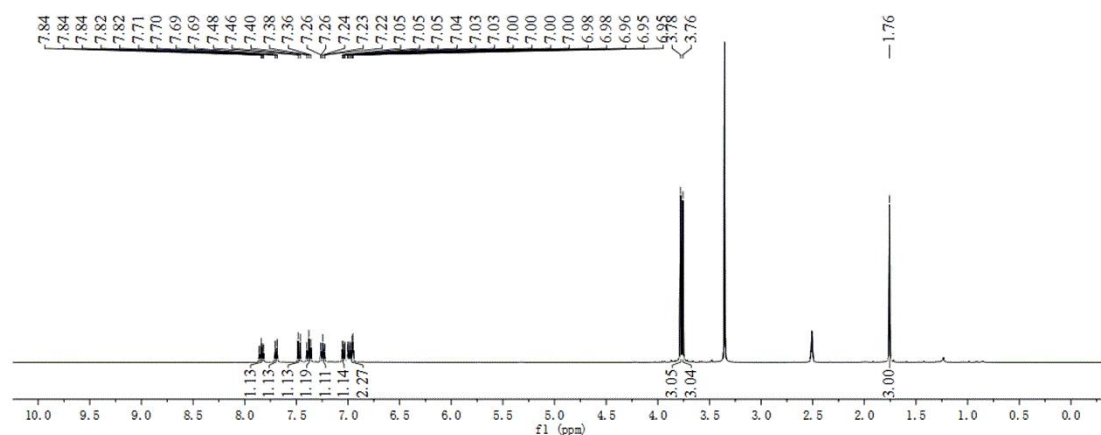
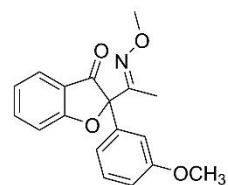
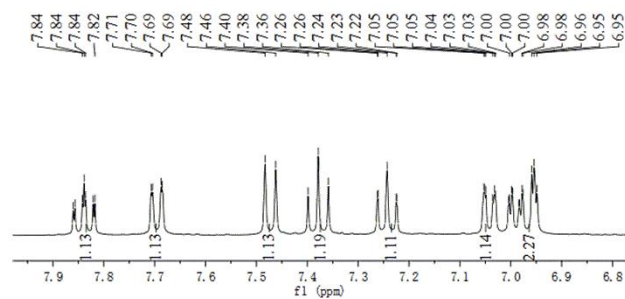
**(E)-2-(1-(methoxyimino)ethyl)-2-(m-tolyl)benzofuran-3(2H)-one (3h): <sup>13</sup>C NMR**



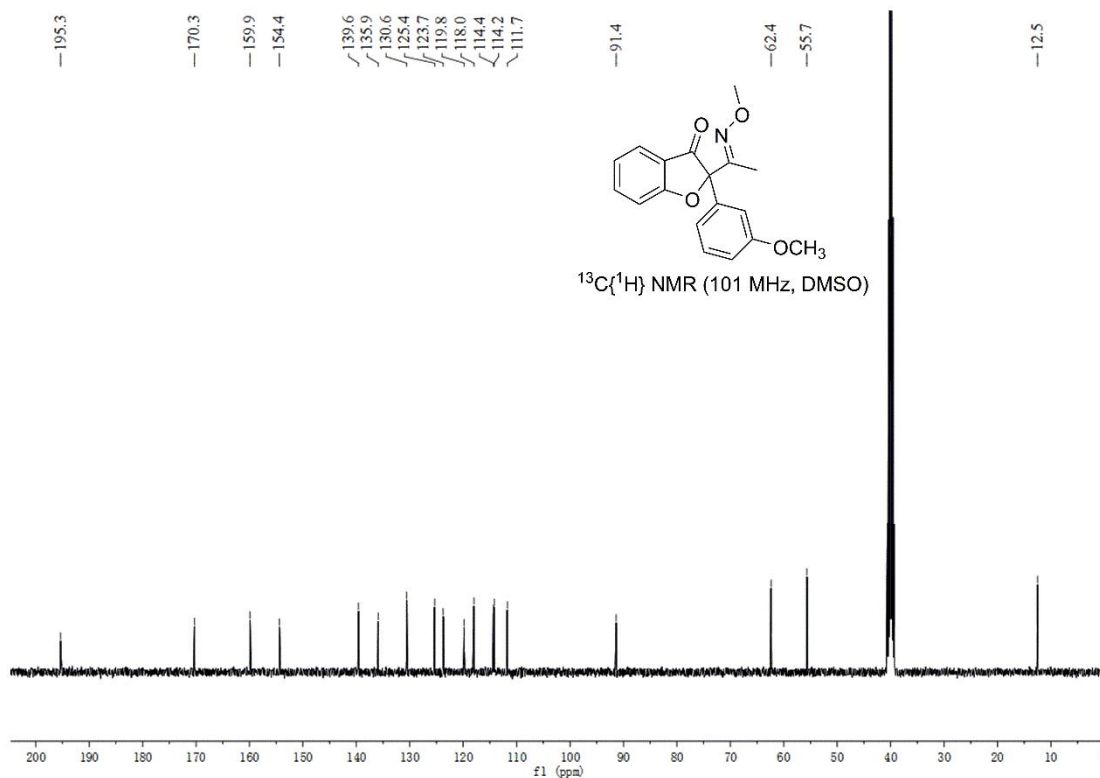
**(E)-2-(1-(methoxyimino)ethyl)-2-(m-tolyl)benzofuran-3(2H)-one (3h): MS**



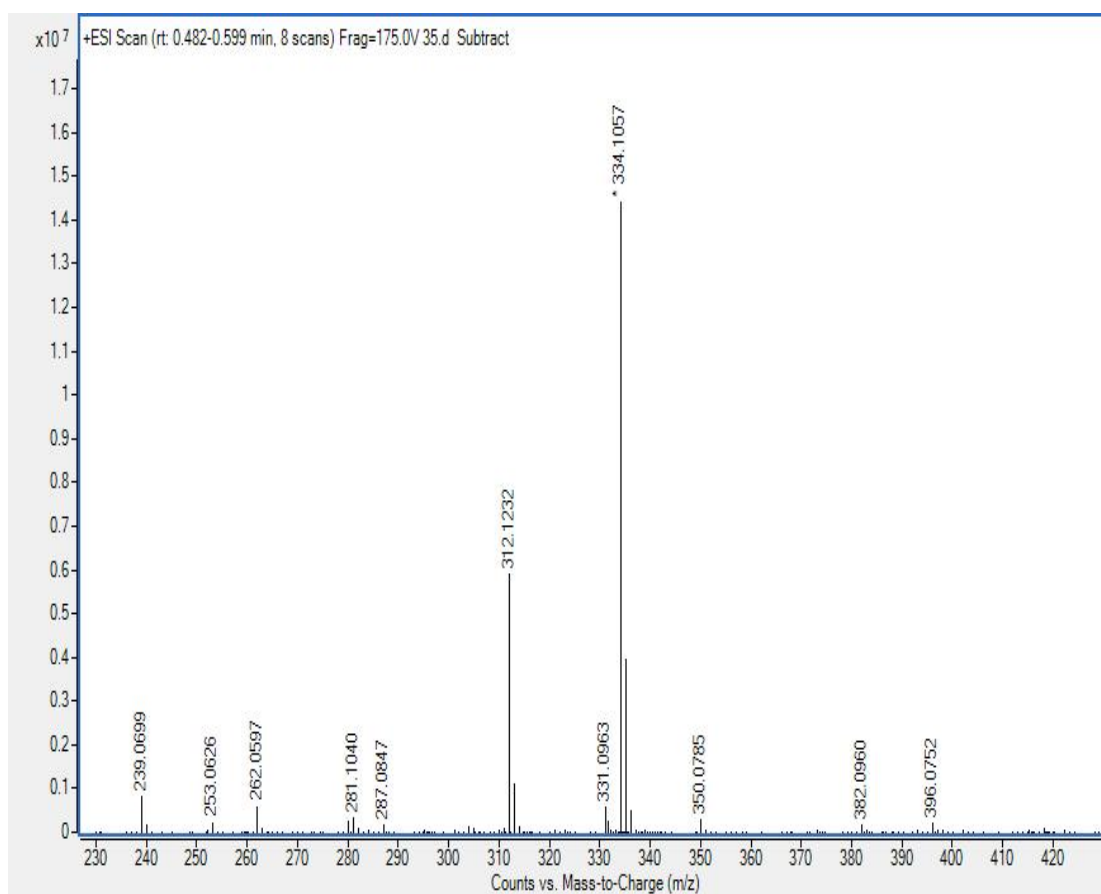
**(E)-2-(1-(methoxyimino)ethyl)-2-(3-methoxyphenyl)benzofuran-3(2H)-one (3i): <sup>1</sup>H NMR**



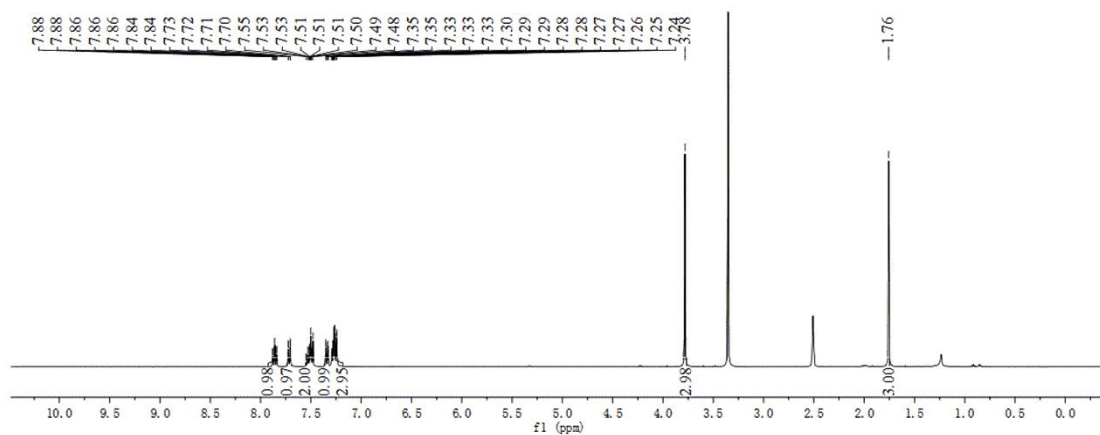
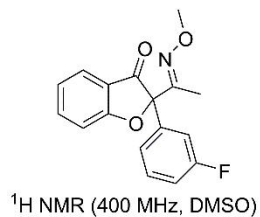
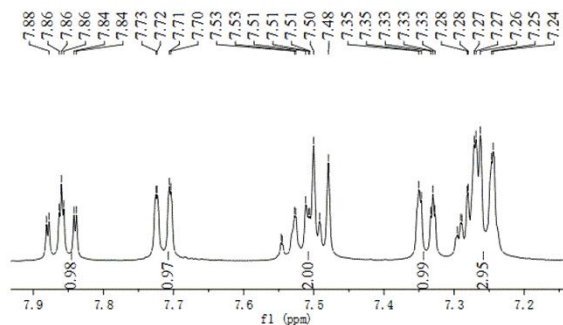
**(E)-2-(1-(methoxyimino)ethyl)-2-(3-methoxyphenyl)benzofuran-3(2H)-one (3i):  $^{13}\text{C}$  NMR**



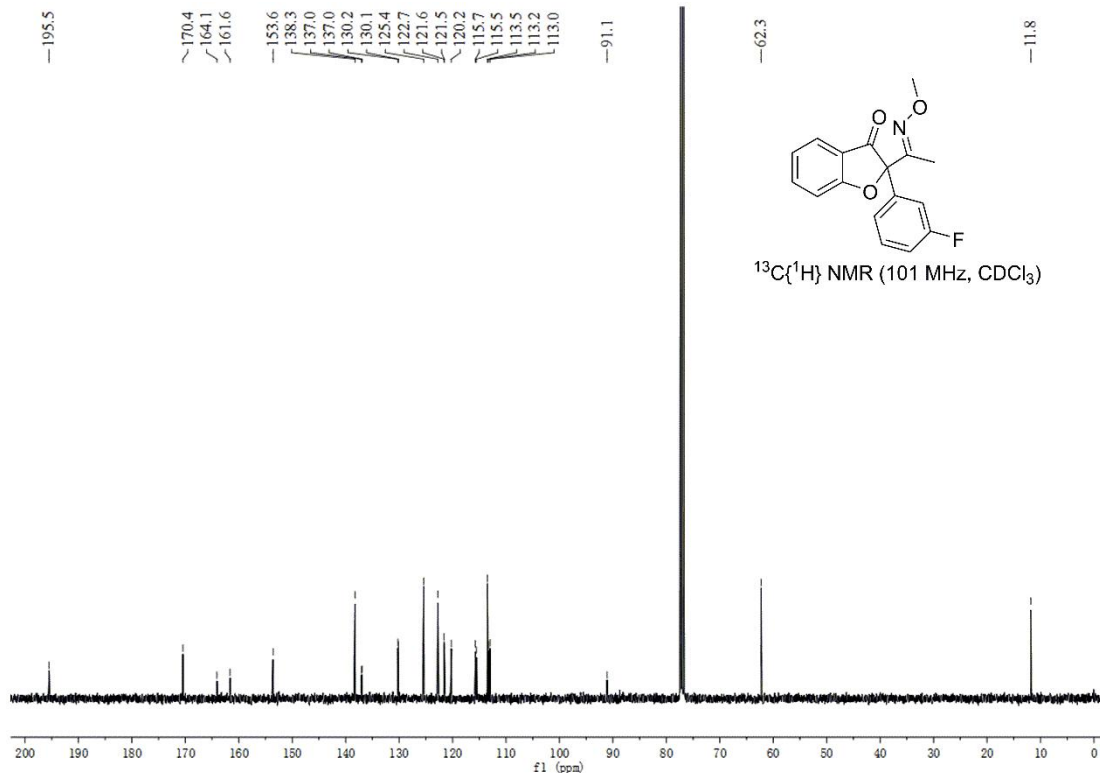
**(E)-2-(1-(methoxyimino)ethyl)-2-(3-methoxyphenyl)benzofuran-3(2H)-one (3i): MS**



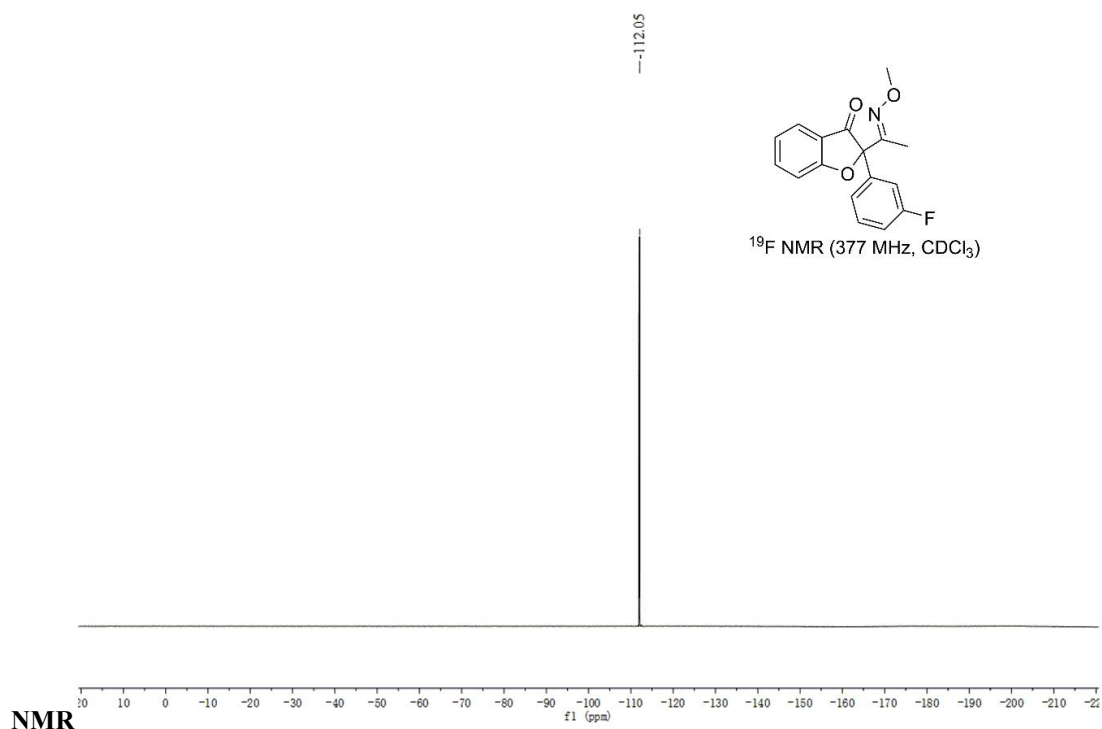
**(E)-2-(3-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3j): <sup>1</sup>H NMR**



**(E)-2-(3-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3j): <sup>13</sup>C NMR**

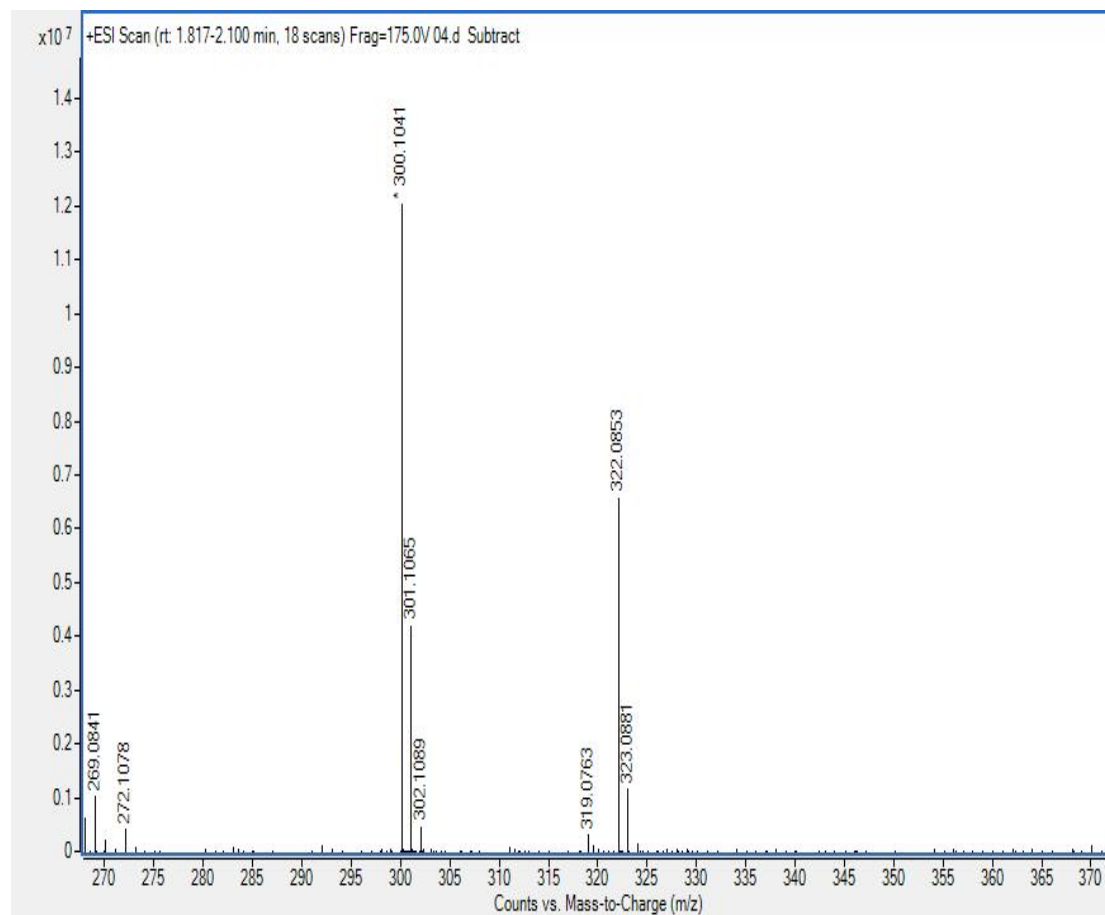


**(E)-2-(3-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3j): <sup>19</sup>F**



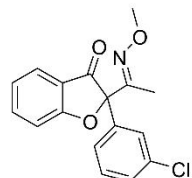
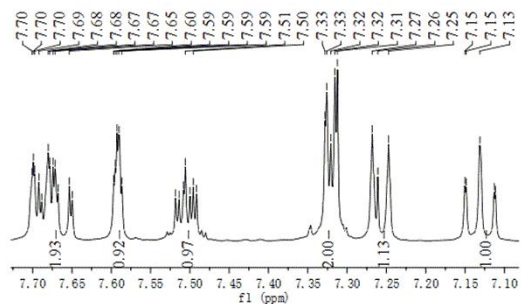
NMR

**(E)-2-(3-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3j): MS**

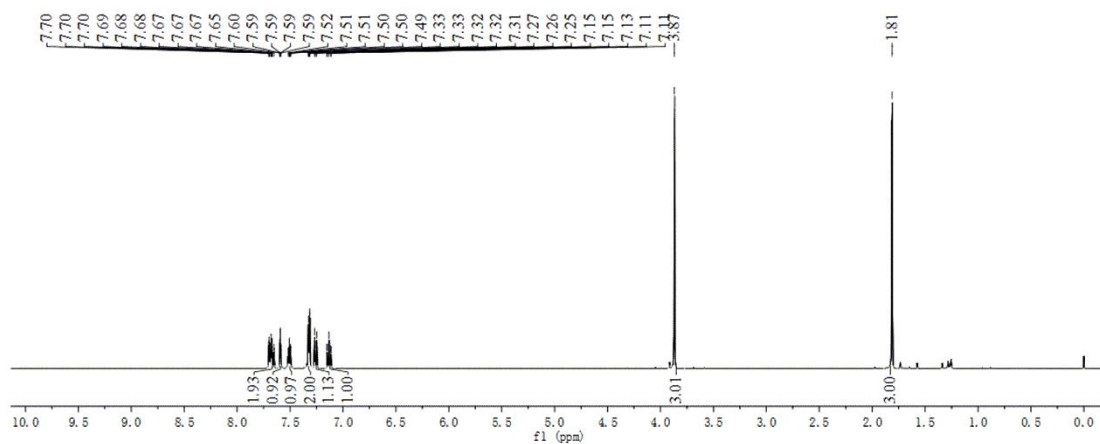




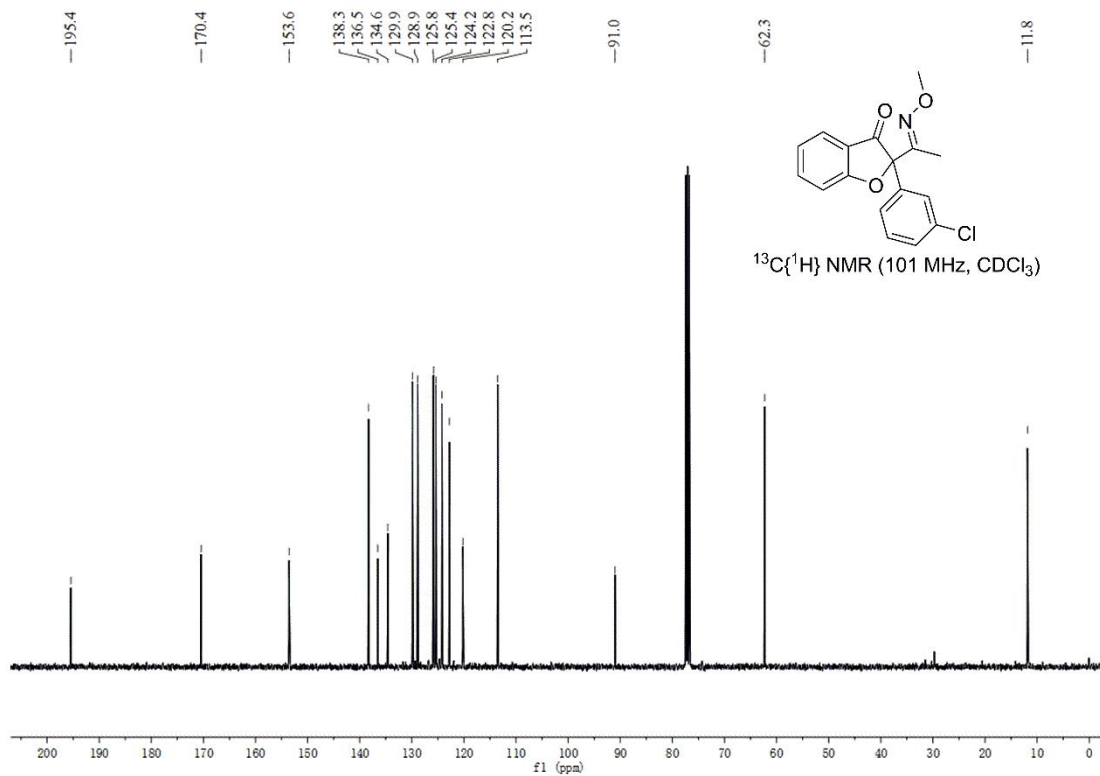
**(E)-2-(3-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3k): <sup>1</sup>H NMR**



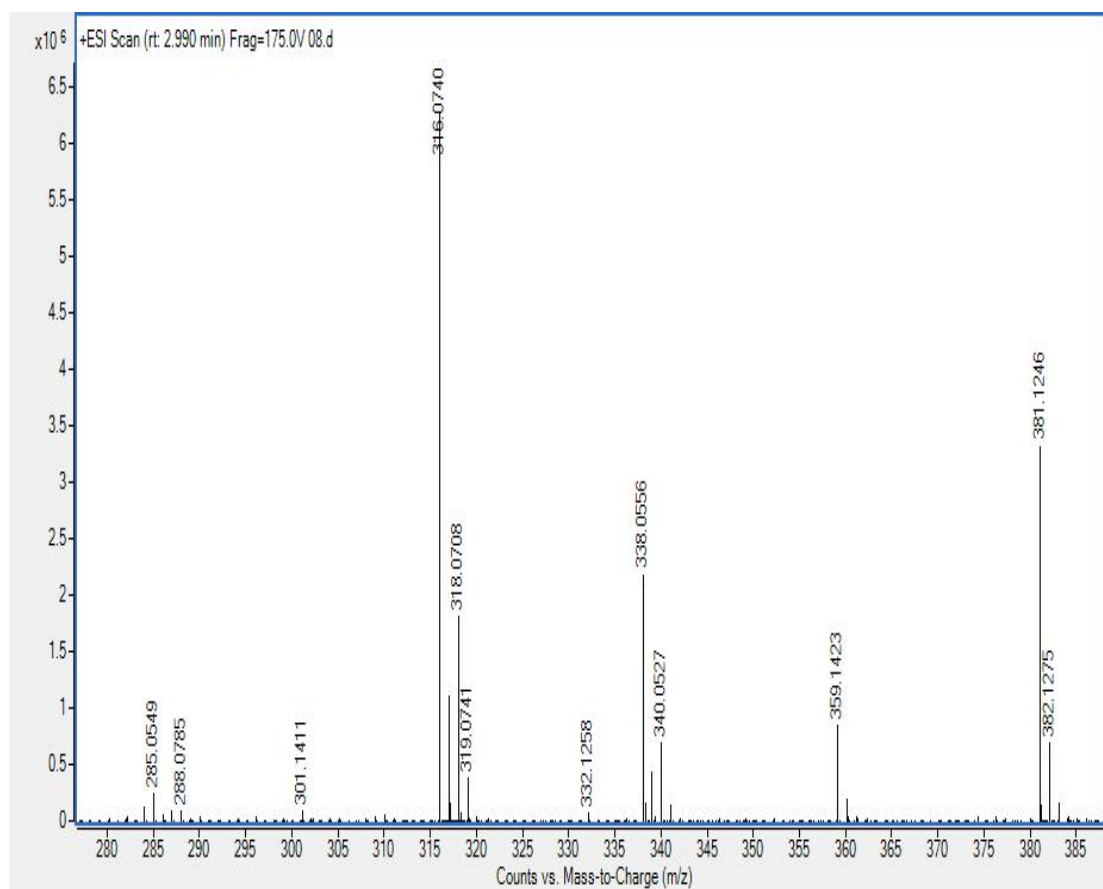
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)



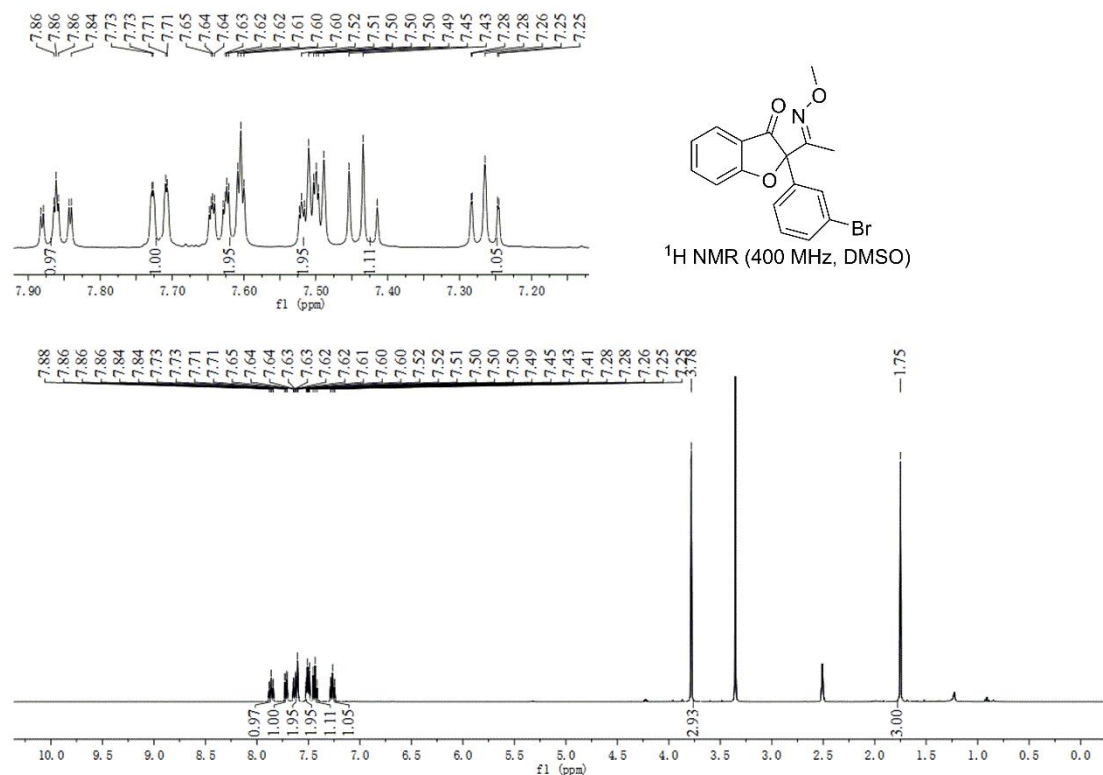
**(E)-2-(3-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3k): <sup>13</sup>C NMR**



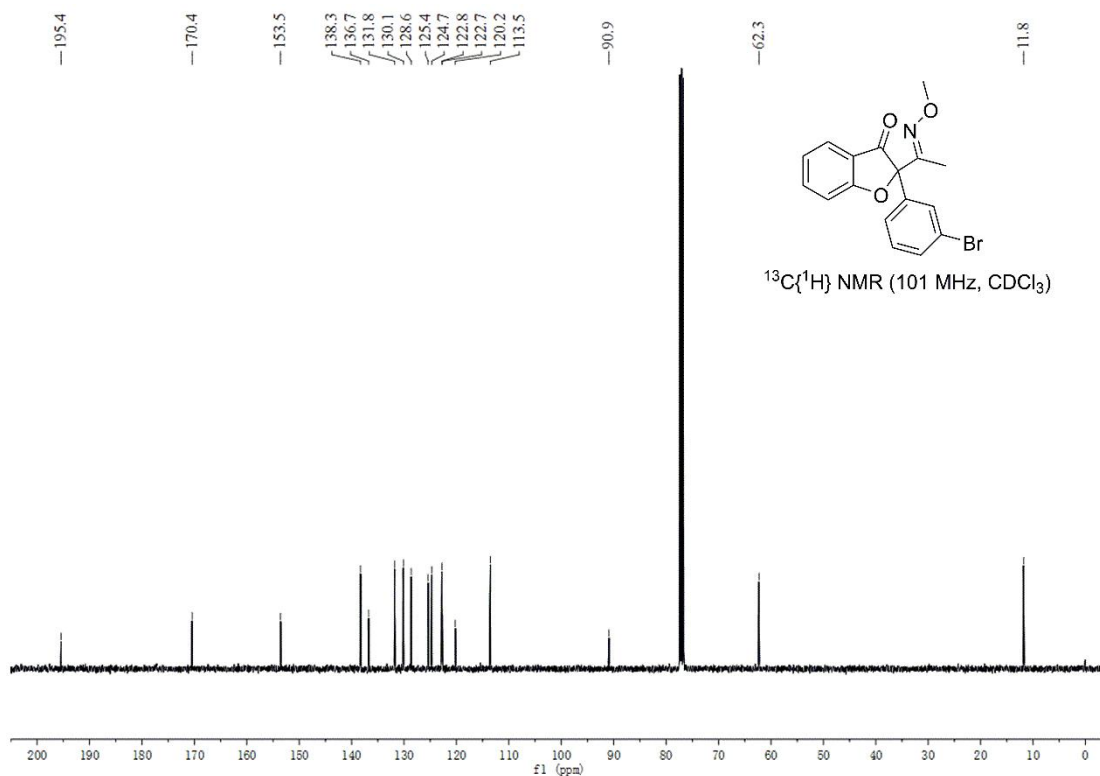
**(E)-2-(3-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3k): MS**



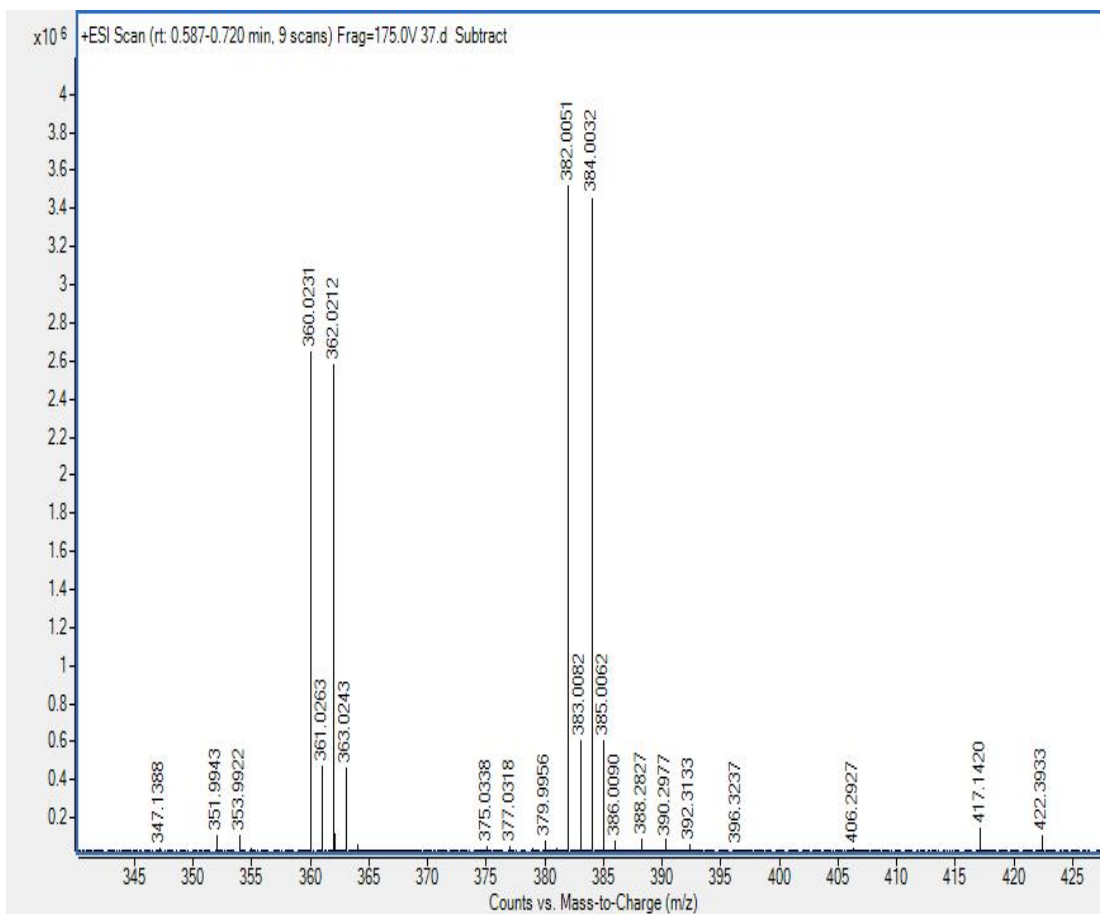
**(E)-2-(3-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3l): <sup>1</sup>H NMR**



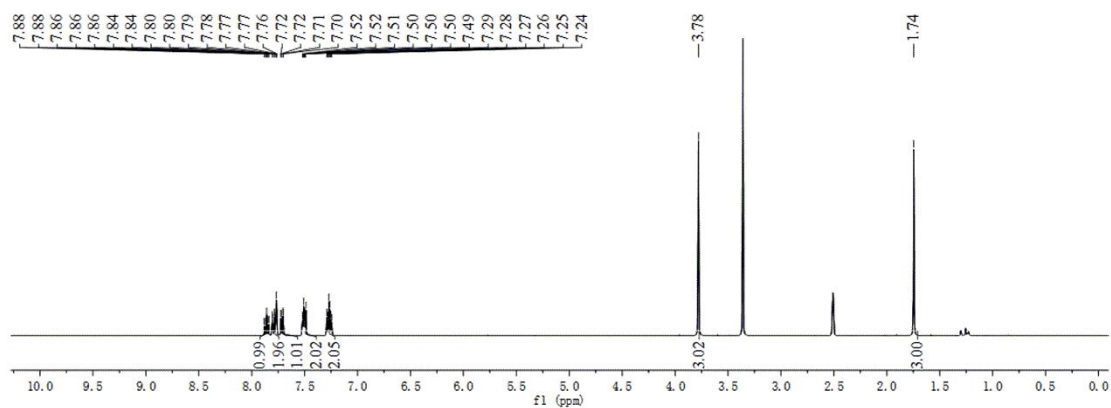
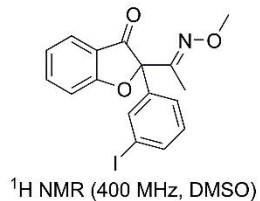
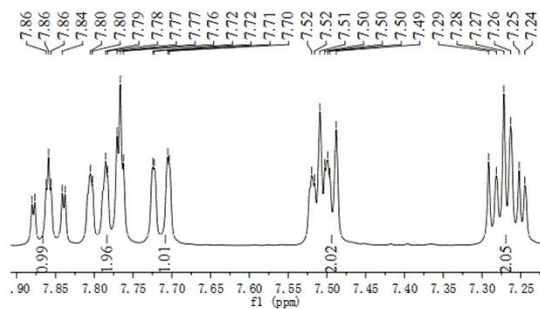
**(E)-2-(3-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (31):  $^{13}\text{C}$  NMR**



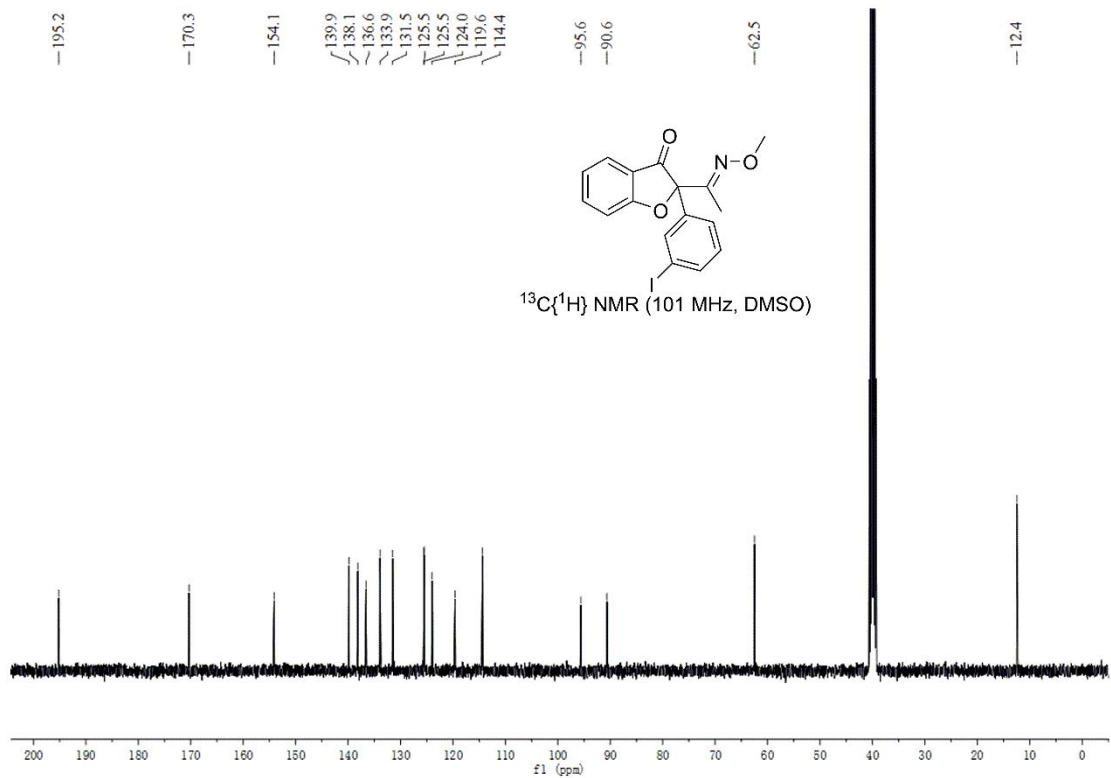
**(E)-2-(3-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (31): MS**



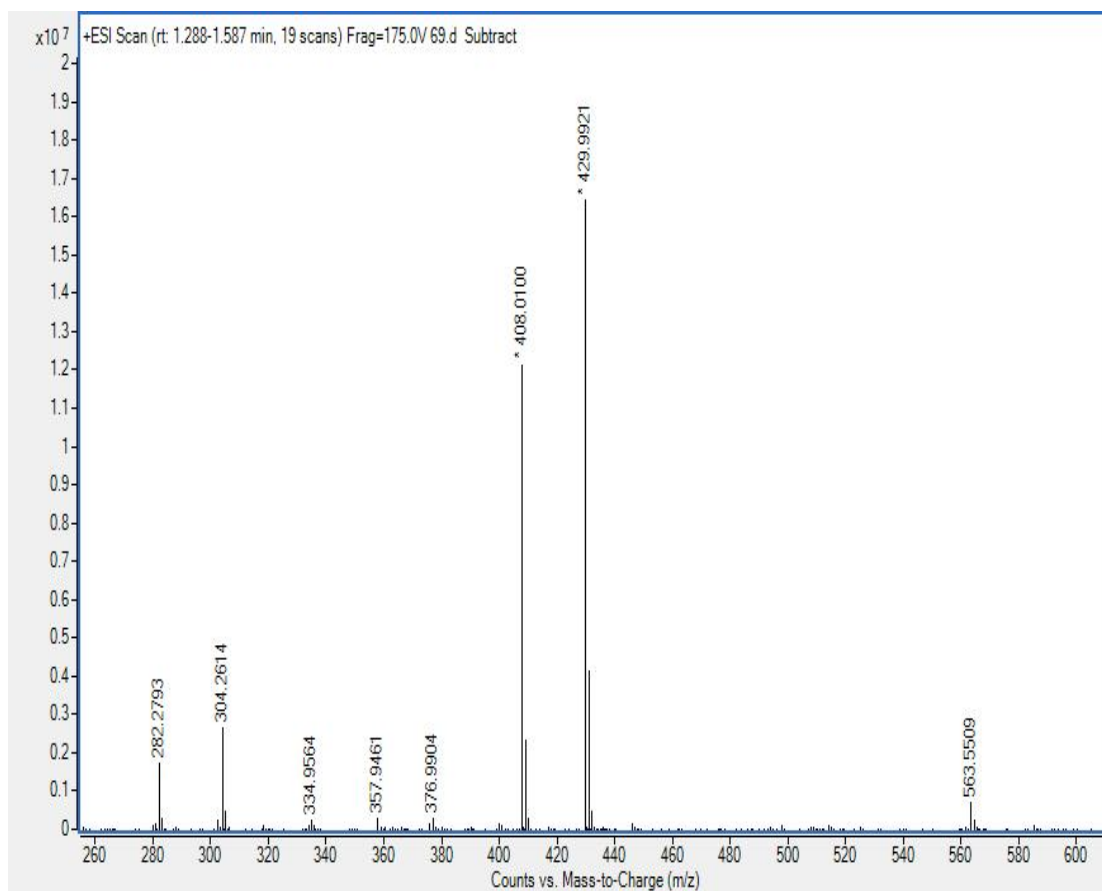
**(E)-2-(3-iodophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3m):  $^1\text{H}$  NMR**



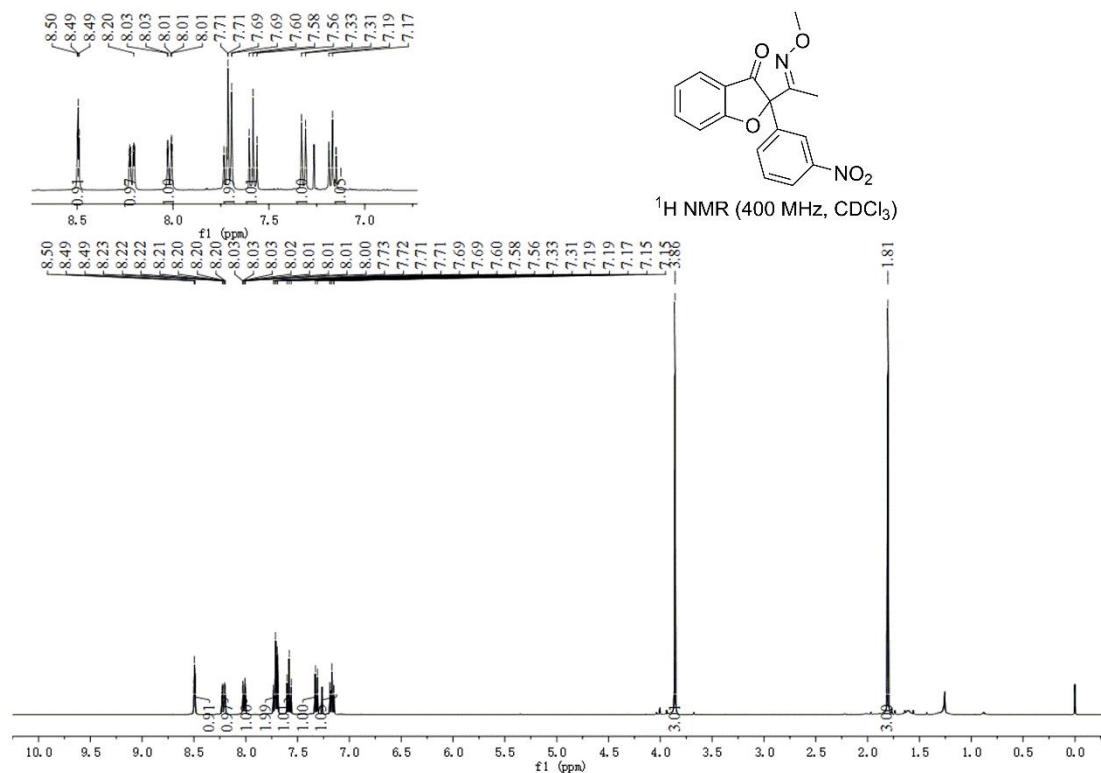
**(E)-2-(3-iodophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3m):  $^{13}\text{C}$  NMR**



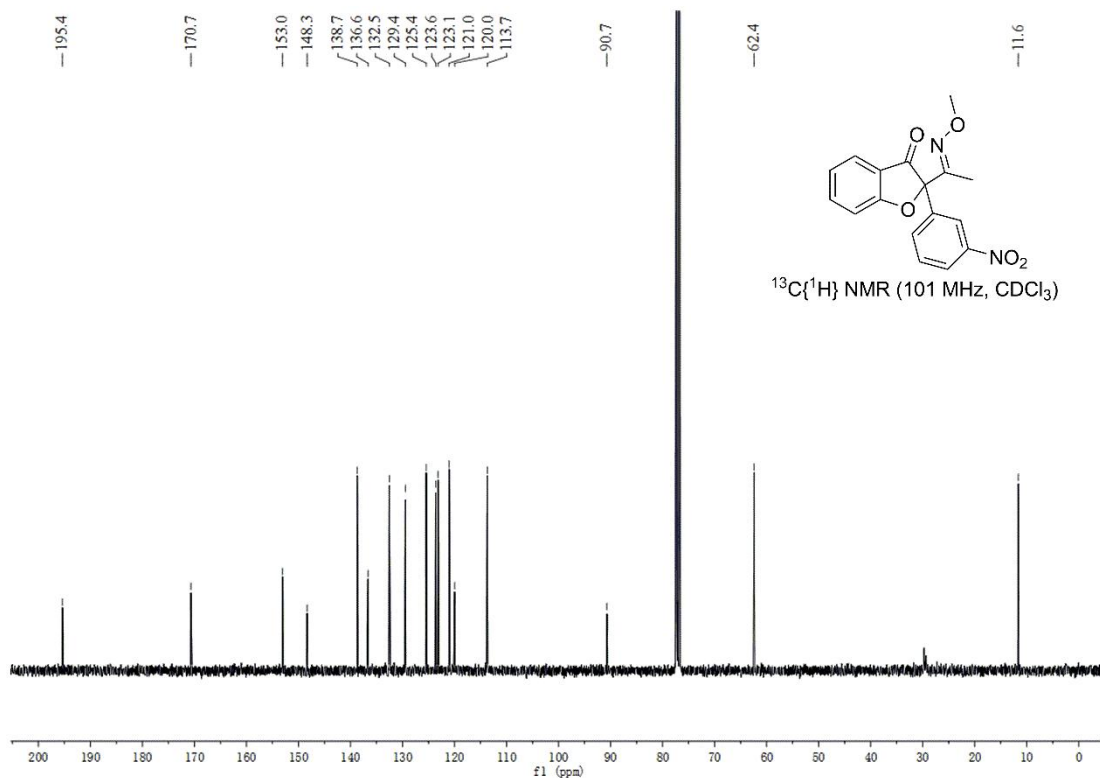
**(E)-2-(3-iodophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3m): MS**



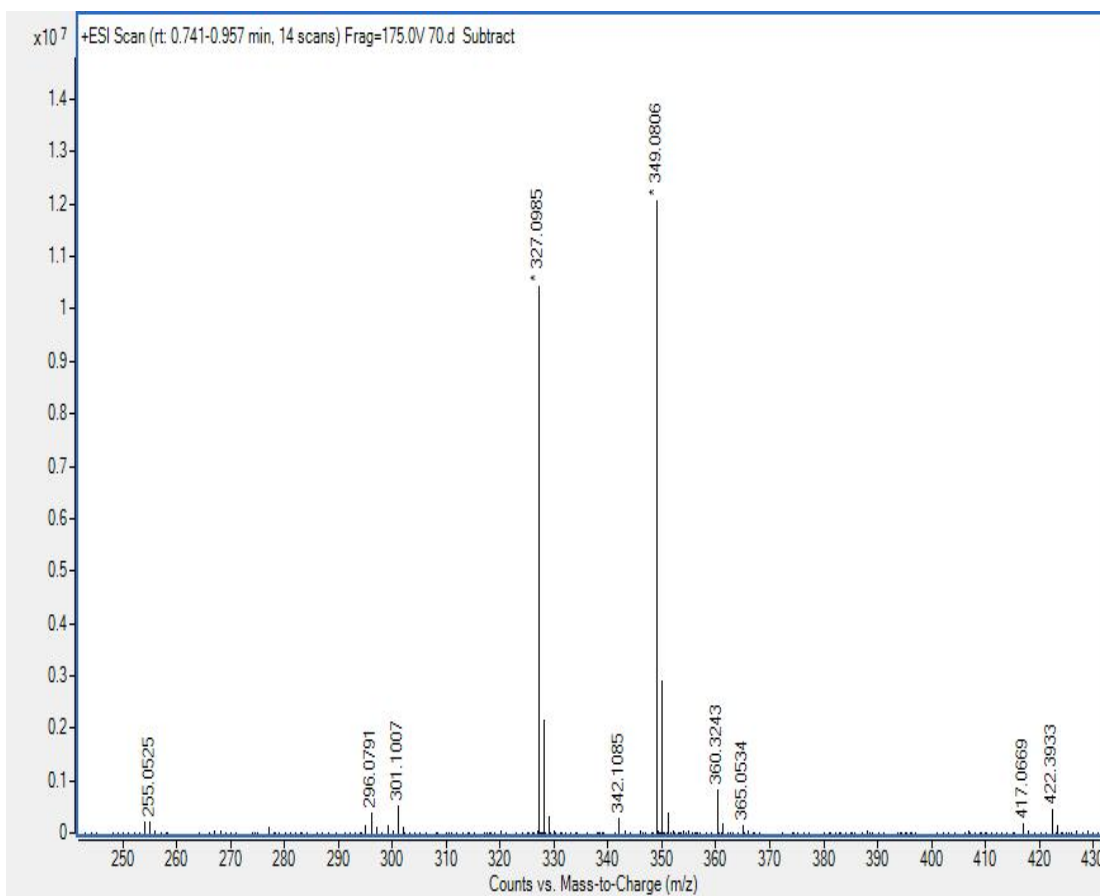
**(E)-2-(1-(methoxyimino)ethyl)-2-(3-nitrophenyl)benzofuran-3(2H)-one (3n): <sup>1</sup>H NMR**



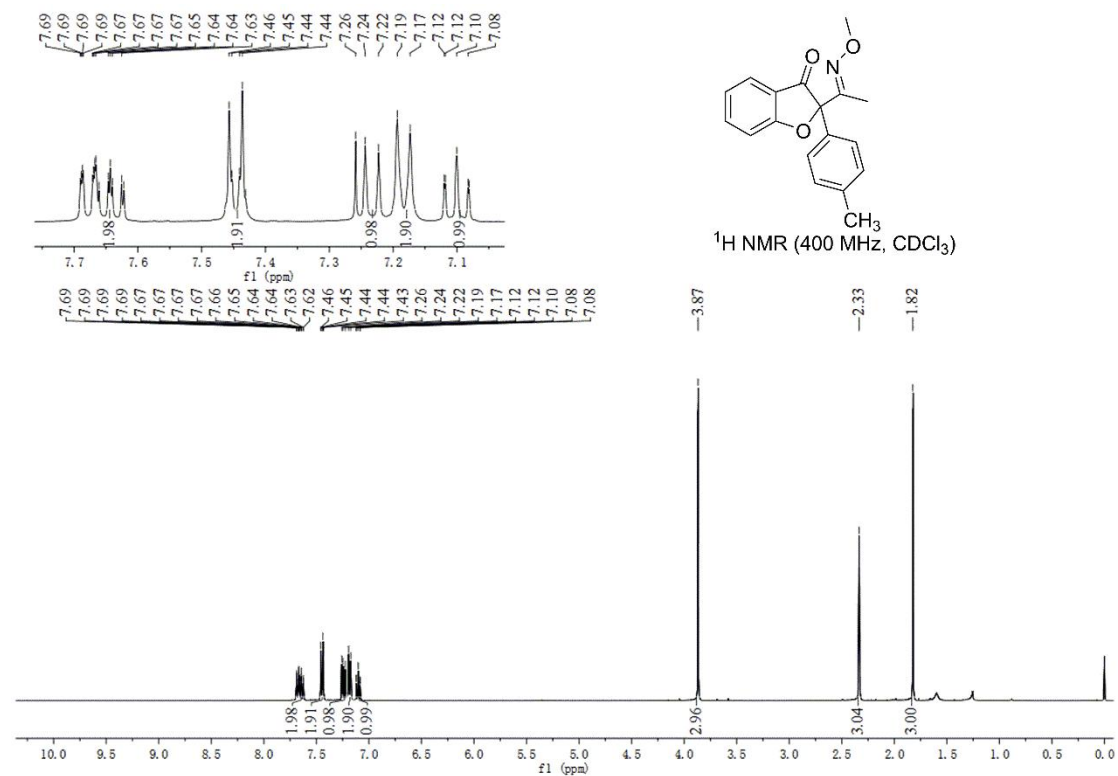
**(E)-2-(1-(methoxyimino)ethyl)-2-(3-nitrophenyl)benzofuran-3(2H)-one (3n): <sup>13</sup>C NMR**



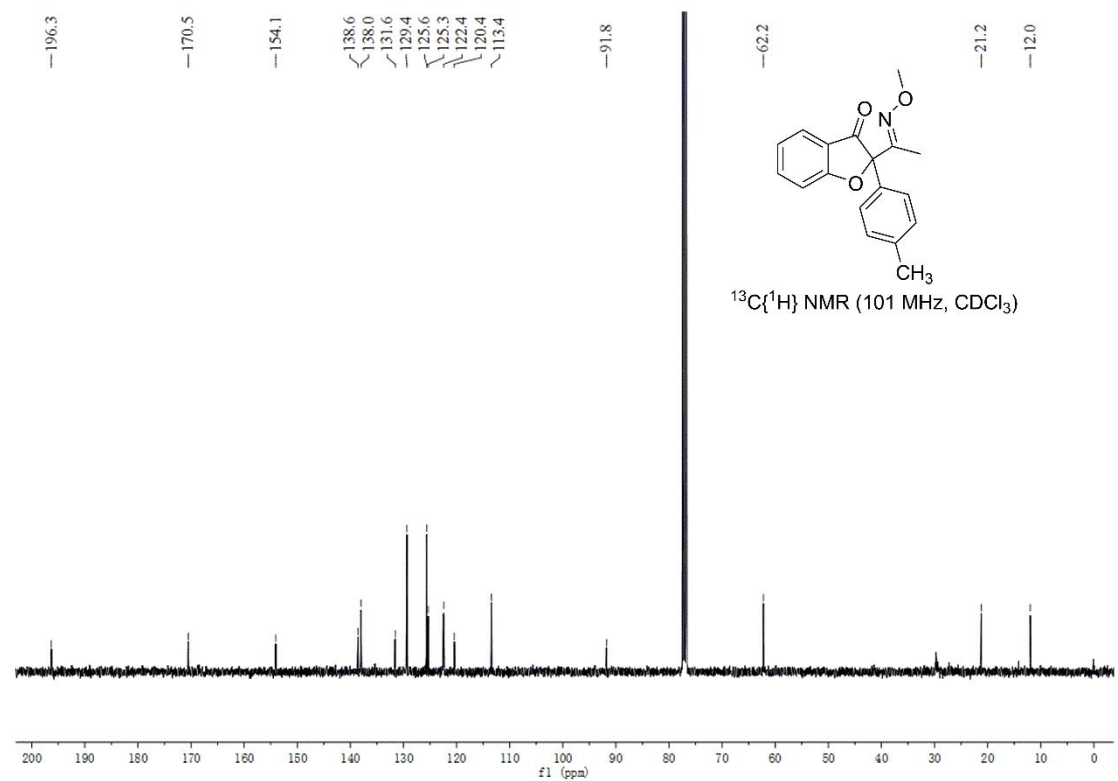
**(E)-2-(1-(methoxyimino)ethyl)-2-(3-nitrophenyl)benzofuran-3(2H)-one (3n): MS**



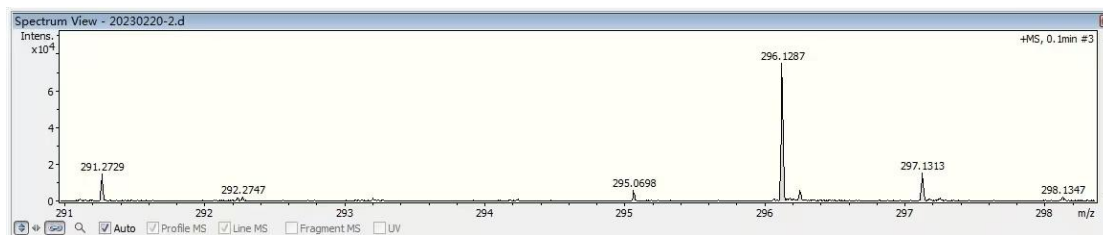
**(E)-2-(1-(methoxyimino)ethyl)-2-(p-tolyl)benzofuran-3(2H)-one (3o): <sup>1</sup>H NMR**



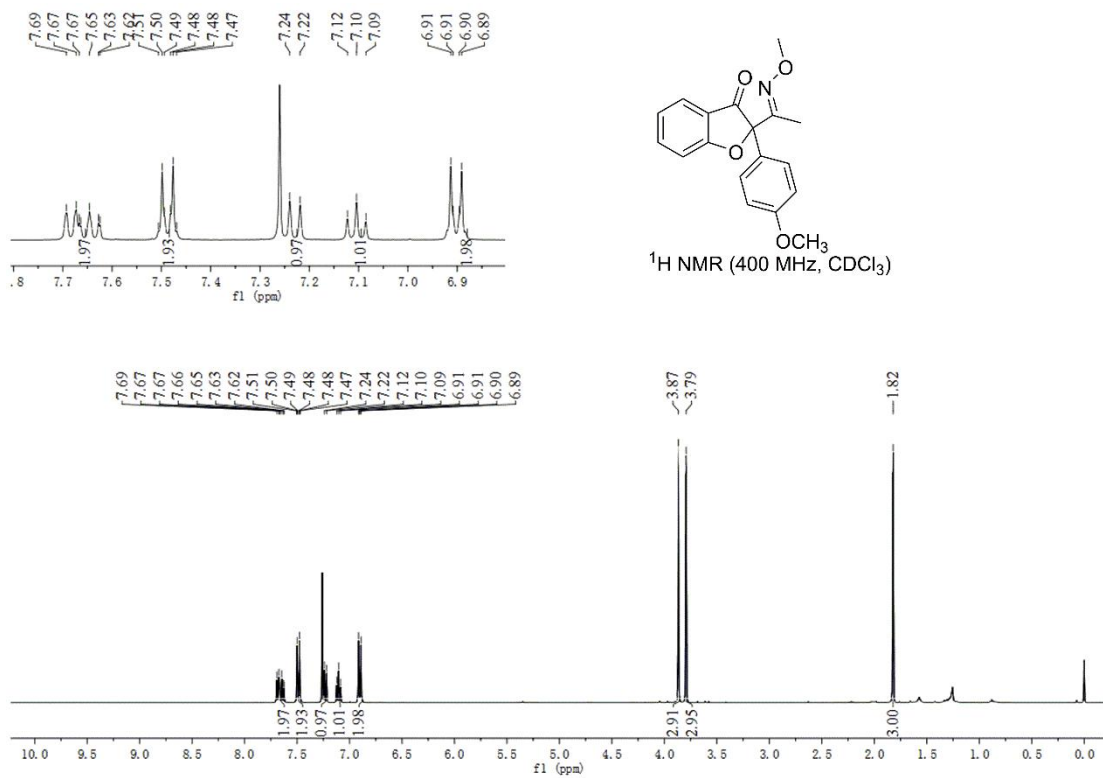
**(E)-2-(1-(methoxyimino)ethyl)-2-(p-tolyl)benzofuran-3(2H)-one (3o): <sup>13</sup>C NMR**



**(E)-2-(1-(methoxyimino)ethyl)-2-(p-tolyl)benzofuran-3(2H)-one (3o): MS**

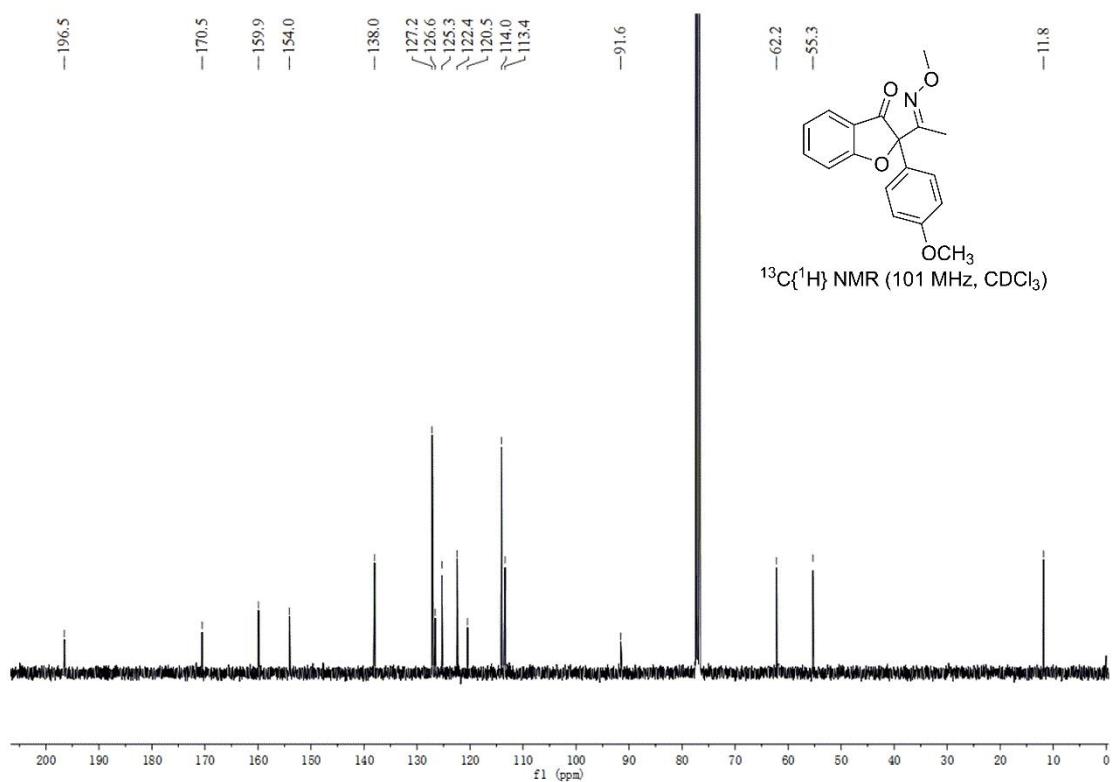


**(E)-2-(1-(methoxyimino)ethyl)-2-(4-methoxyphenyl)benzofuran-3(2H)-one (3p): <sup>1</sup>H NMR**



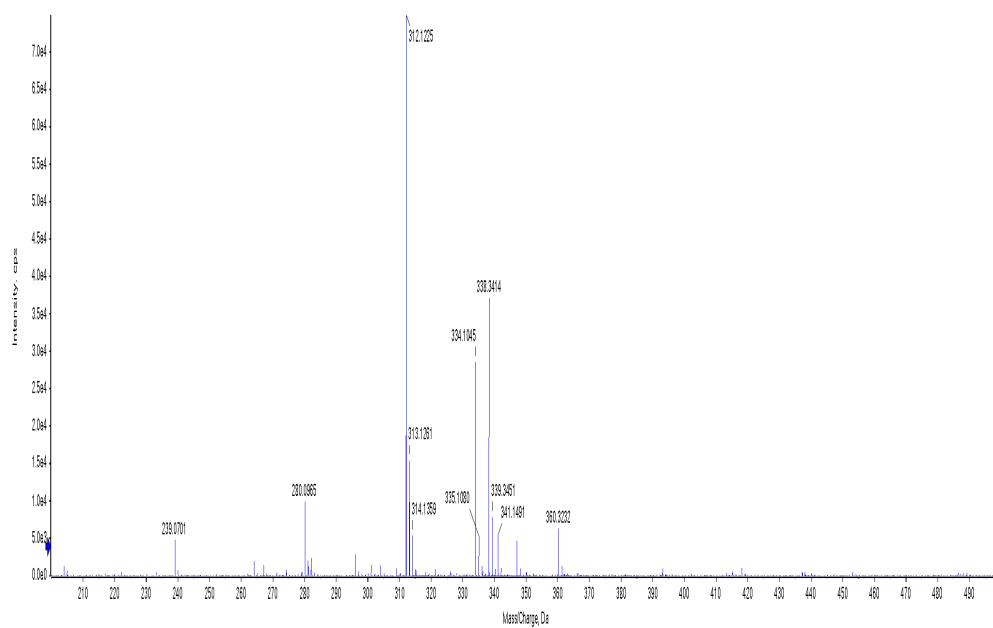


**(E)-2-(1-(methoxyimino)ethyl)-2-(4-methoxyphenyl)benzofuran-3(2H)-one (3p):  $^{13}\text{C}$  NMR**

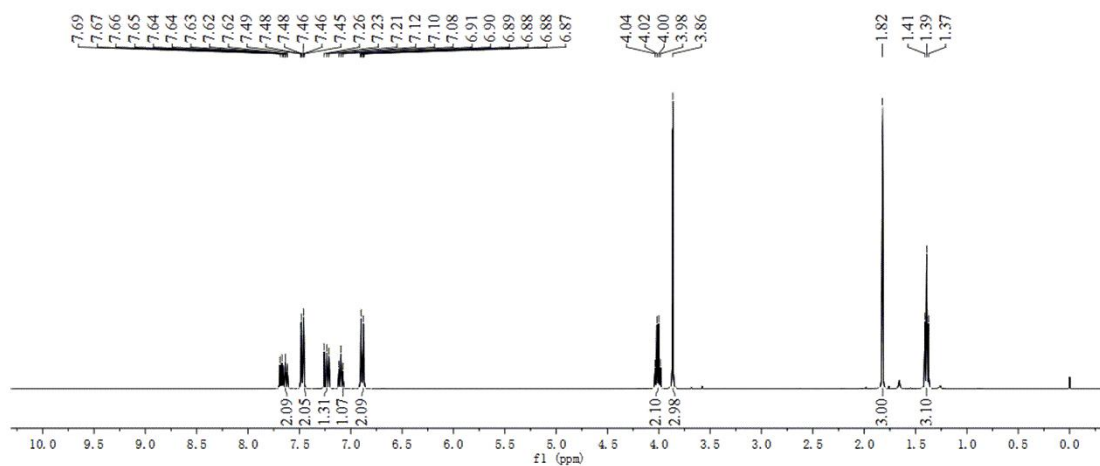
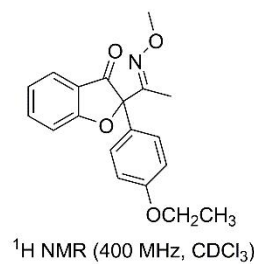
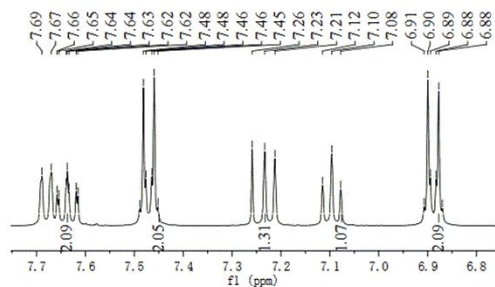


**(E)-2-(1-(methoxyimino)ethyl)-2-(4-methoxyphenyl)benzofuran-3(2H)-one (3p): MS**

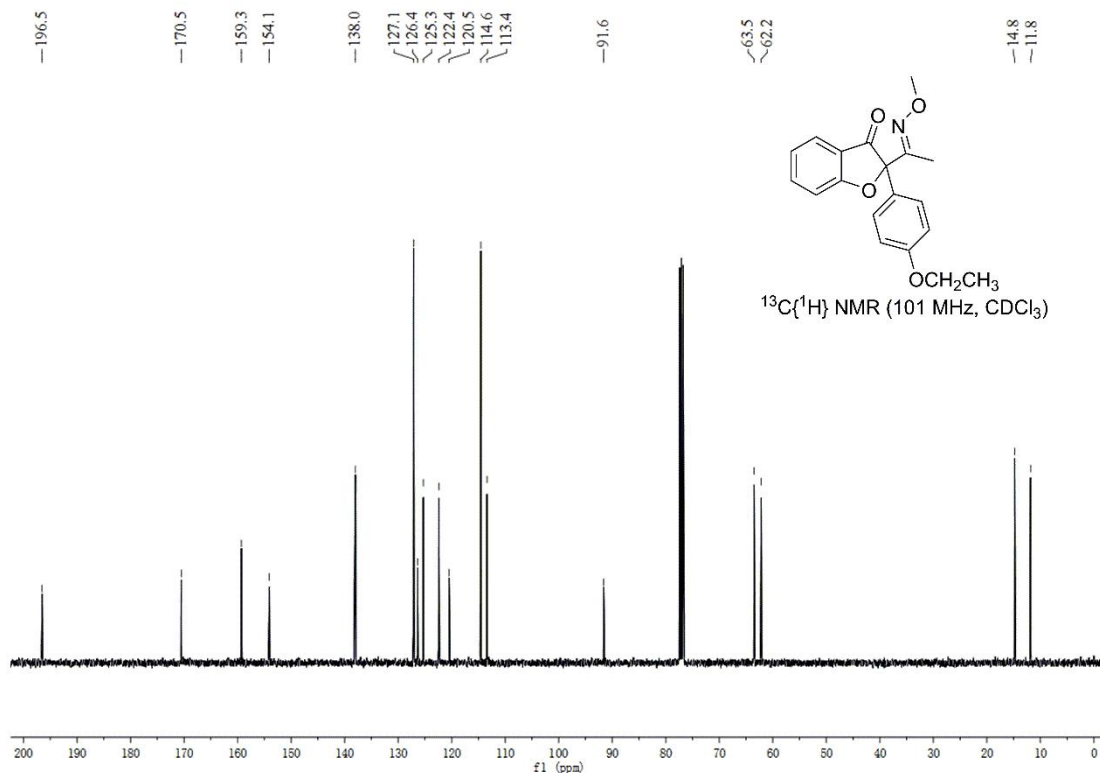
Spectrum from De6511-274-5.wf (sample 1) - 274-5, +TOF MS (200 - 500) from 0.042 to 0.377 min



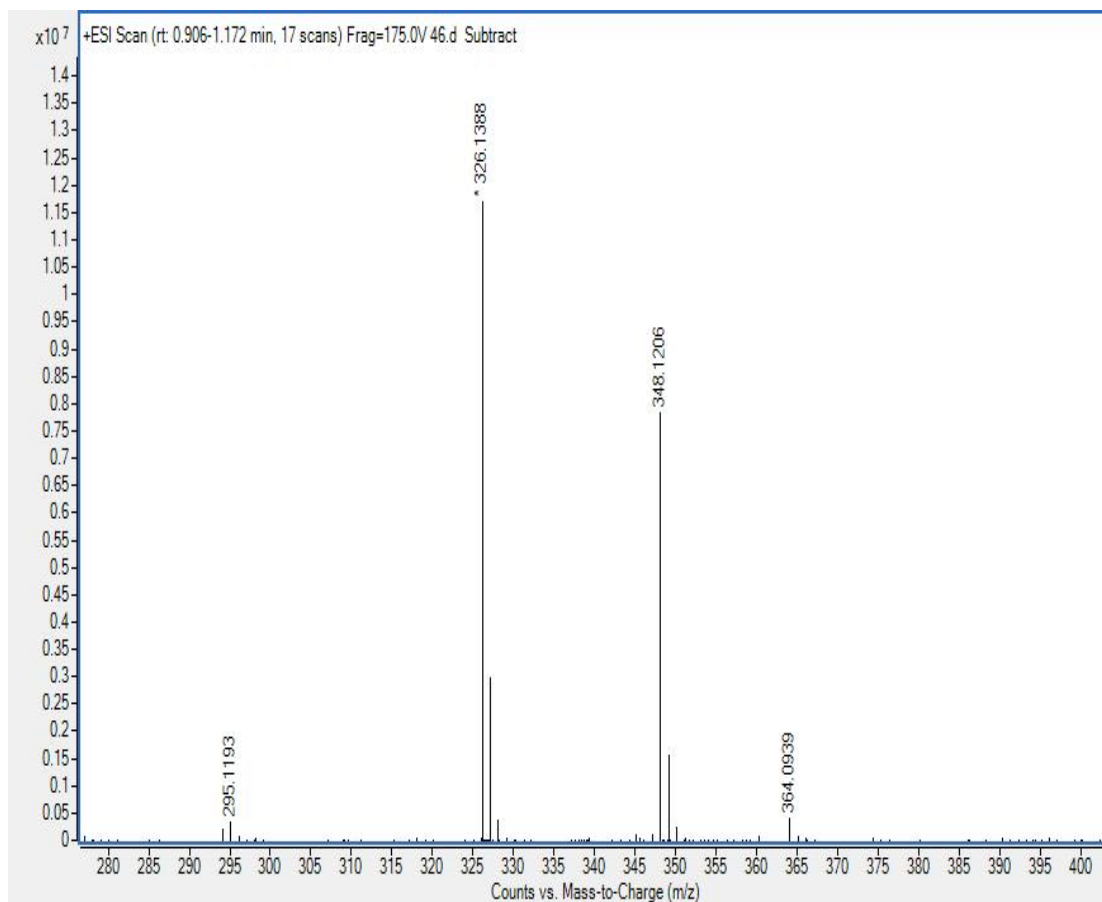
**(E)-2-(4-ethoxyphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3q): <sup>1</sup>H NMR**



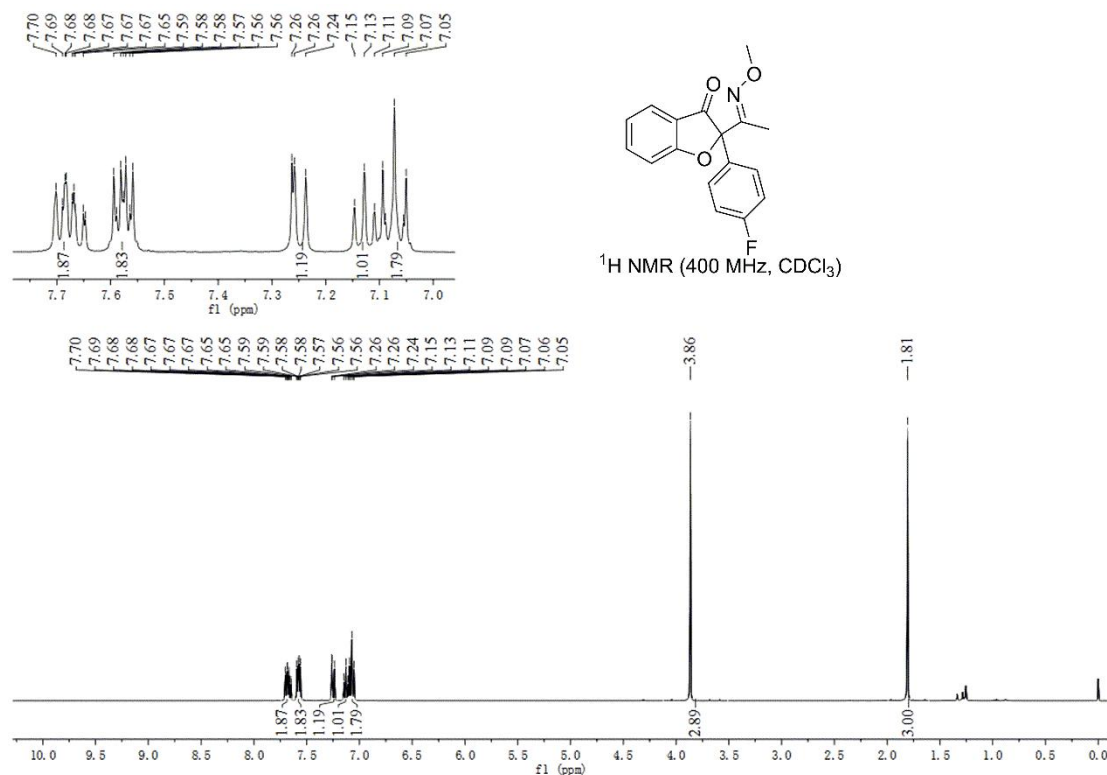
**(E)-2-(4-ethoxyphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3q): <sup>13</sup>C NMR**



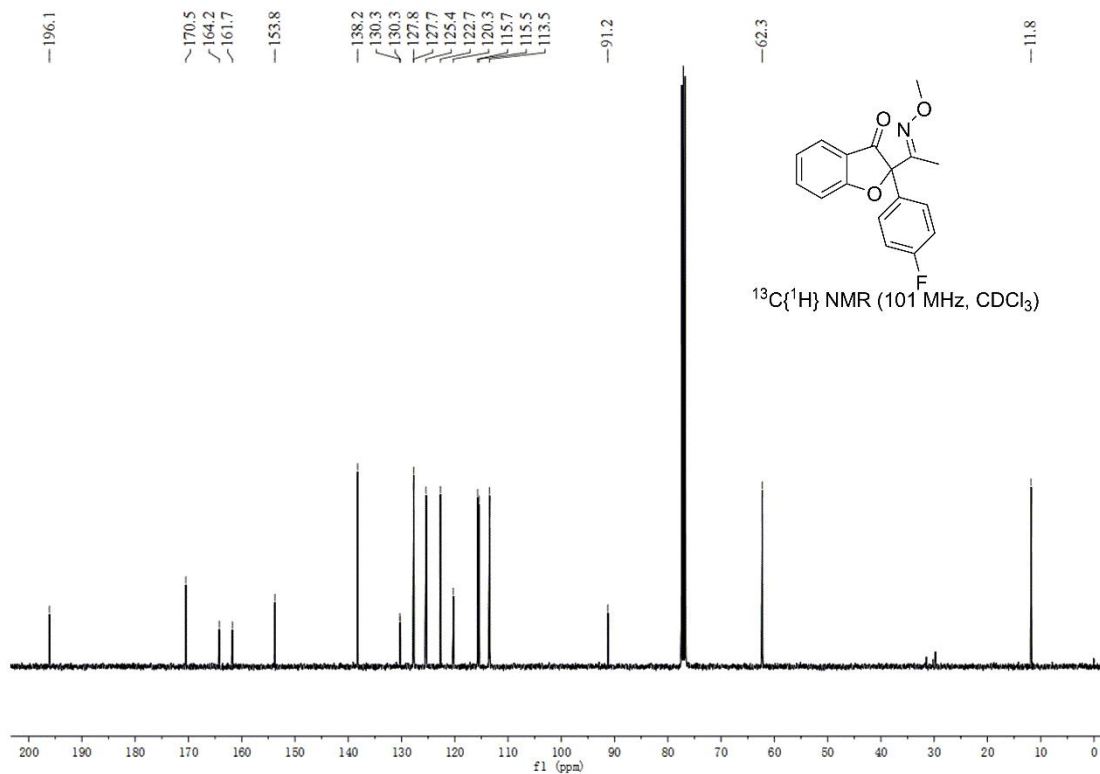
**(E)-2-(4-ethoxyphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3q): MS**



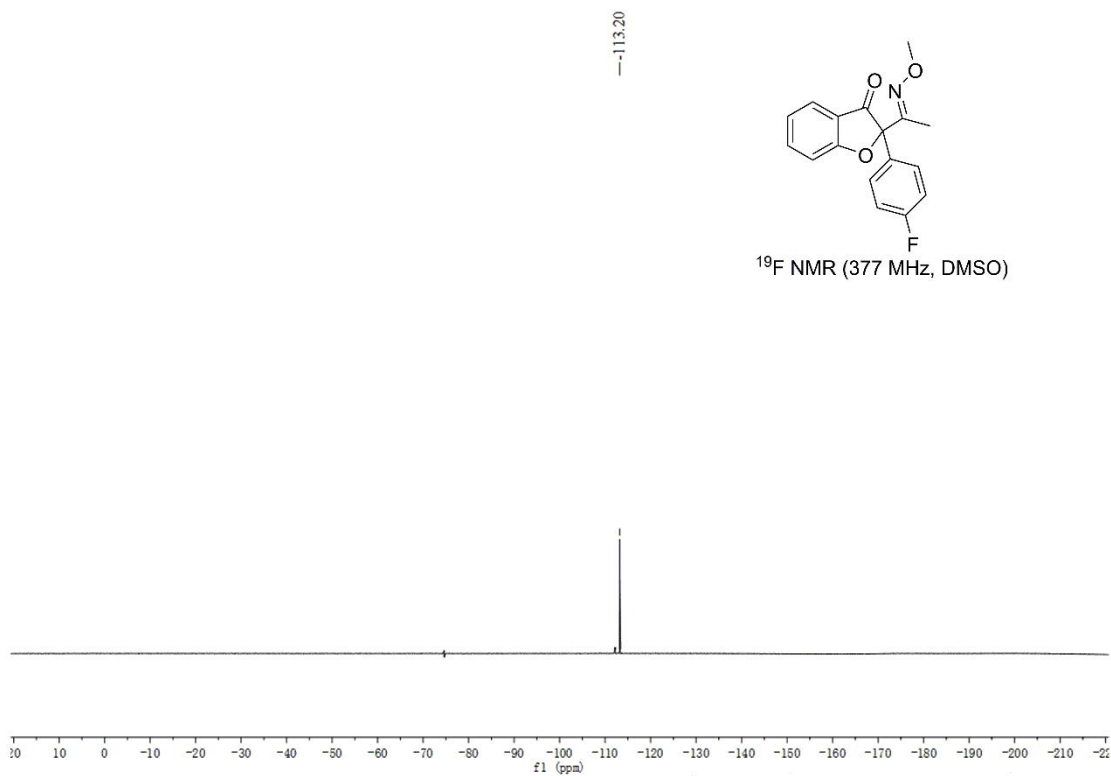
**(E)-2-(4-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3r): <sup>1</sup>H NMR**



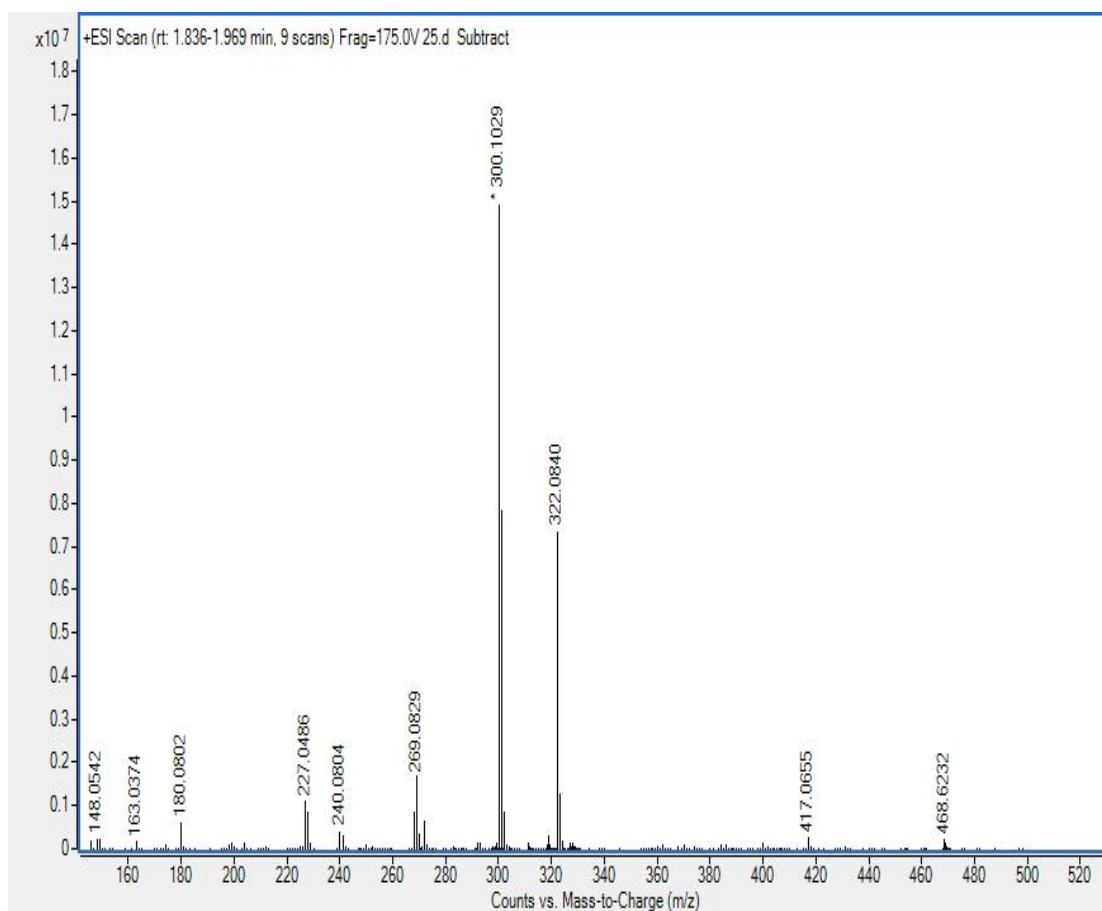
**(E)-2-(4-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3r):  $^{13}\text{C}$  NMR**



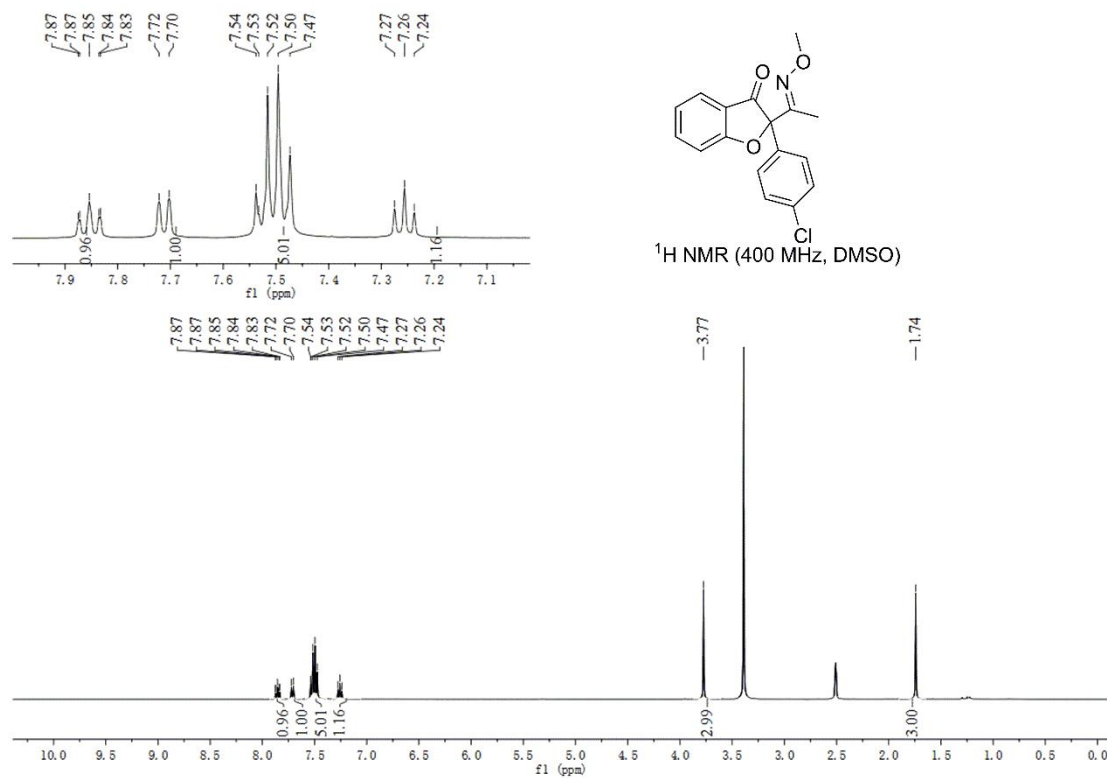
**(E)-2-(4-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3r):  $^{19}\text{F}$  NMR**



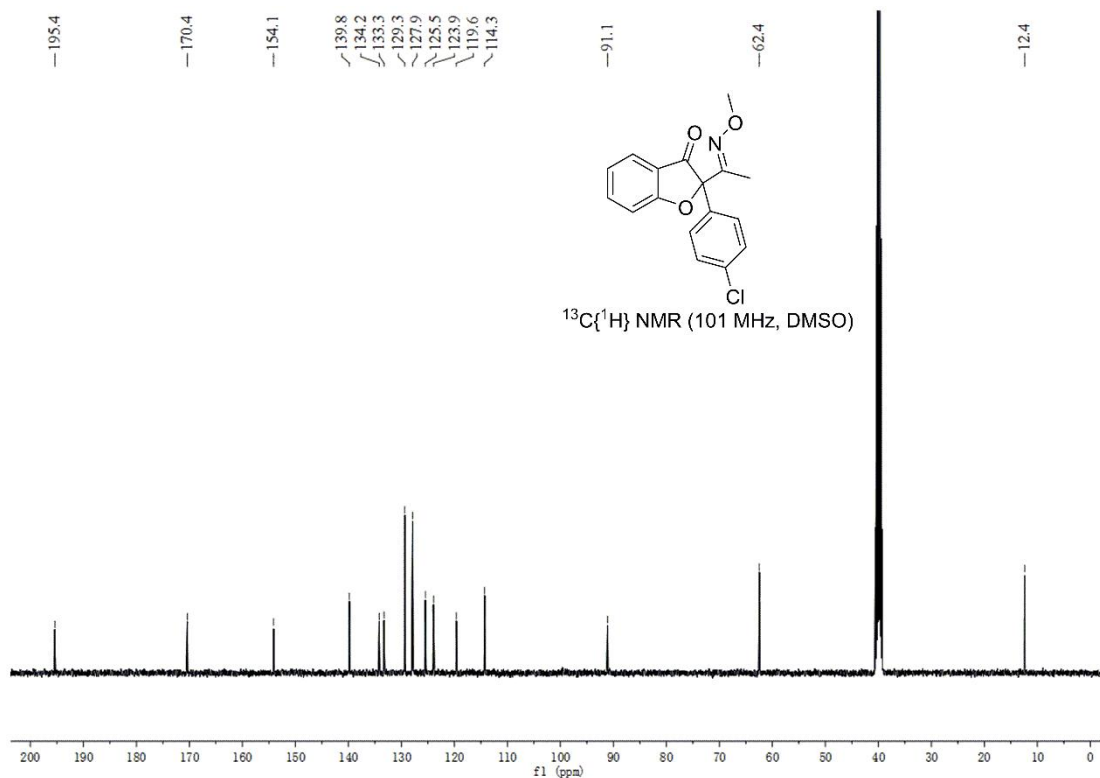
**(E)-2-(4-fluorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3r): MS**



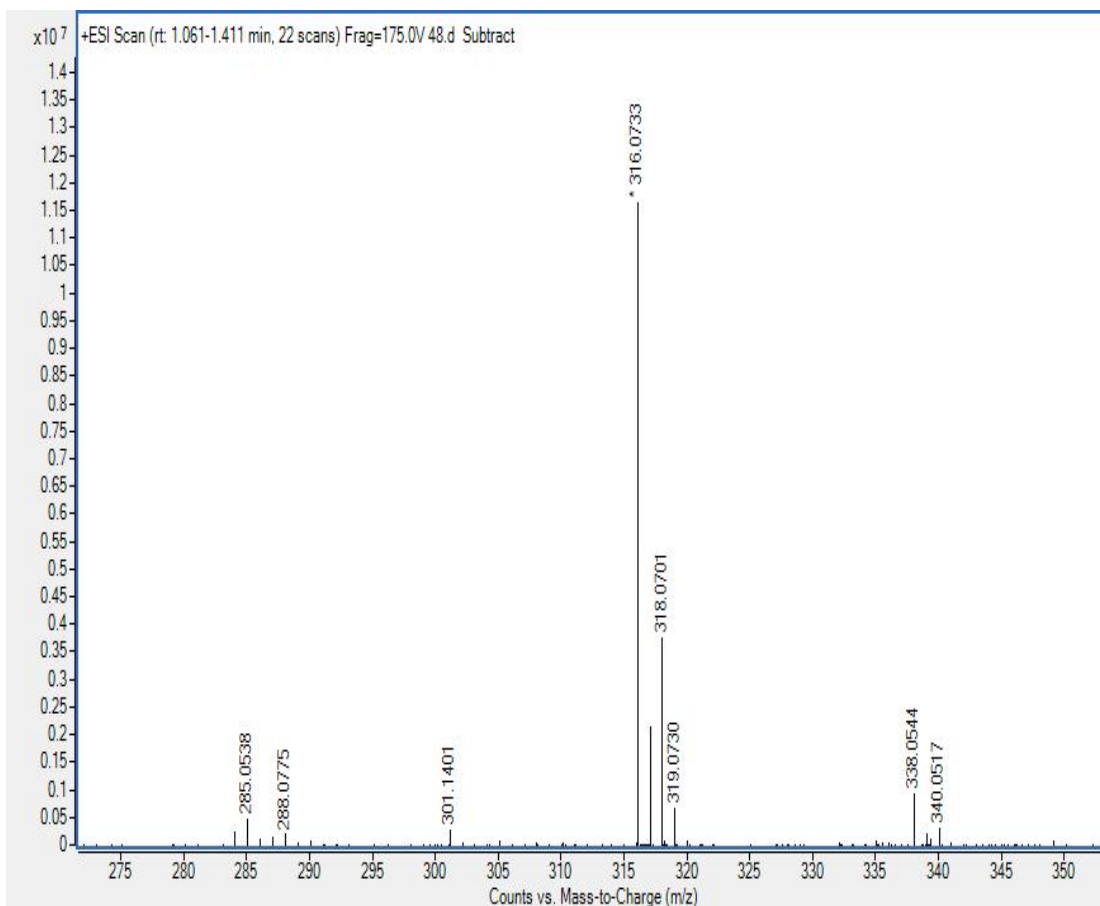
**(E)-2-(4-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3s): <sup>1</sup>H NMR**



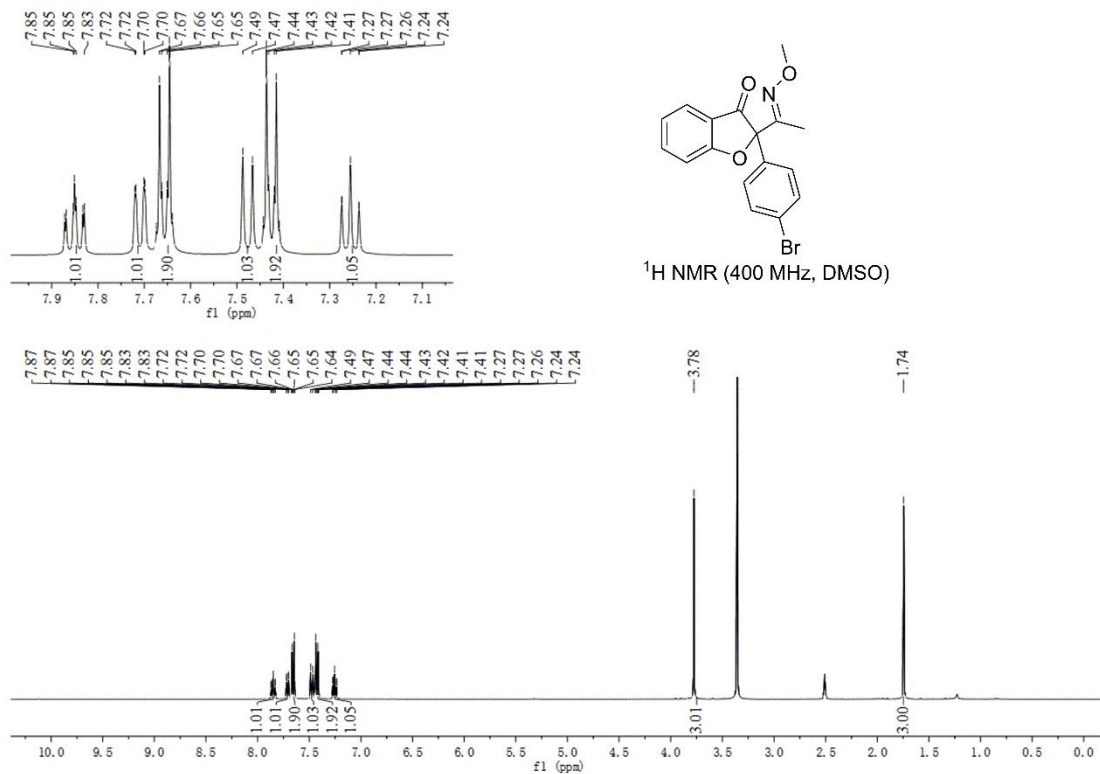
**(E)-2-(4-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3s):  $^{13}\text{C}$  NMR**



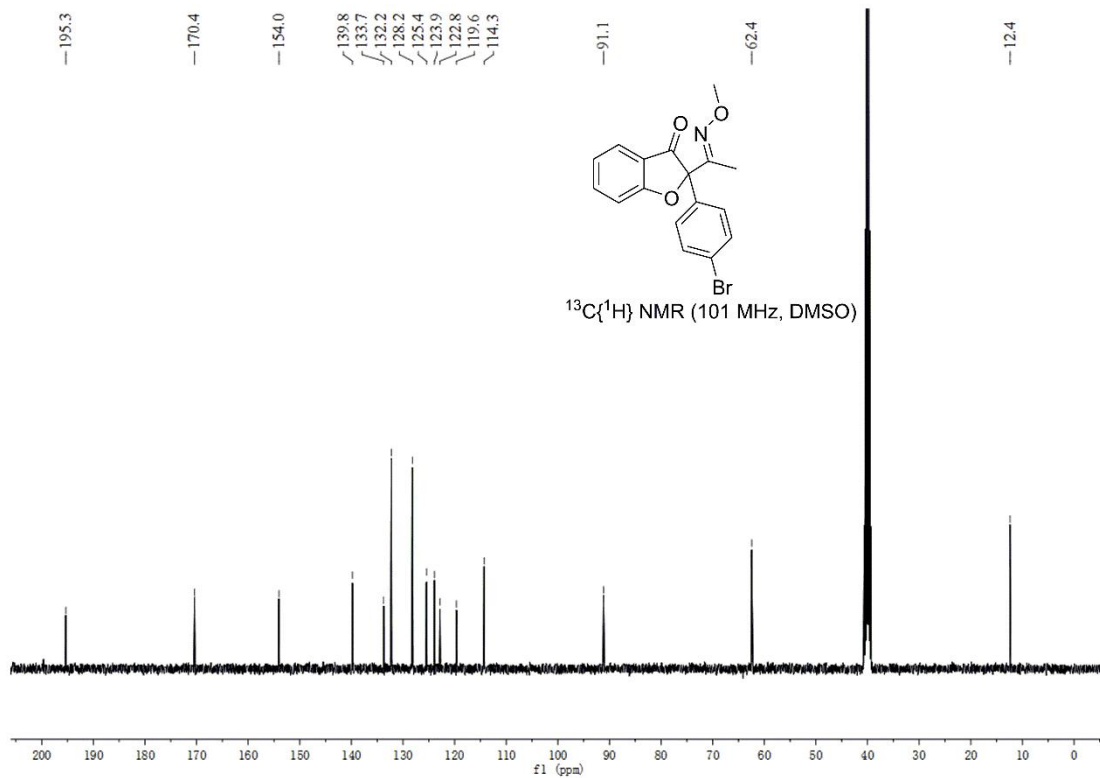
**(E)-2-(4-chlorophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3s): MS**



**(E)-2-(4-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3t): <sup>1</sup>H NMR**

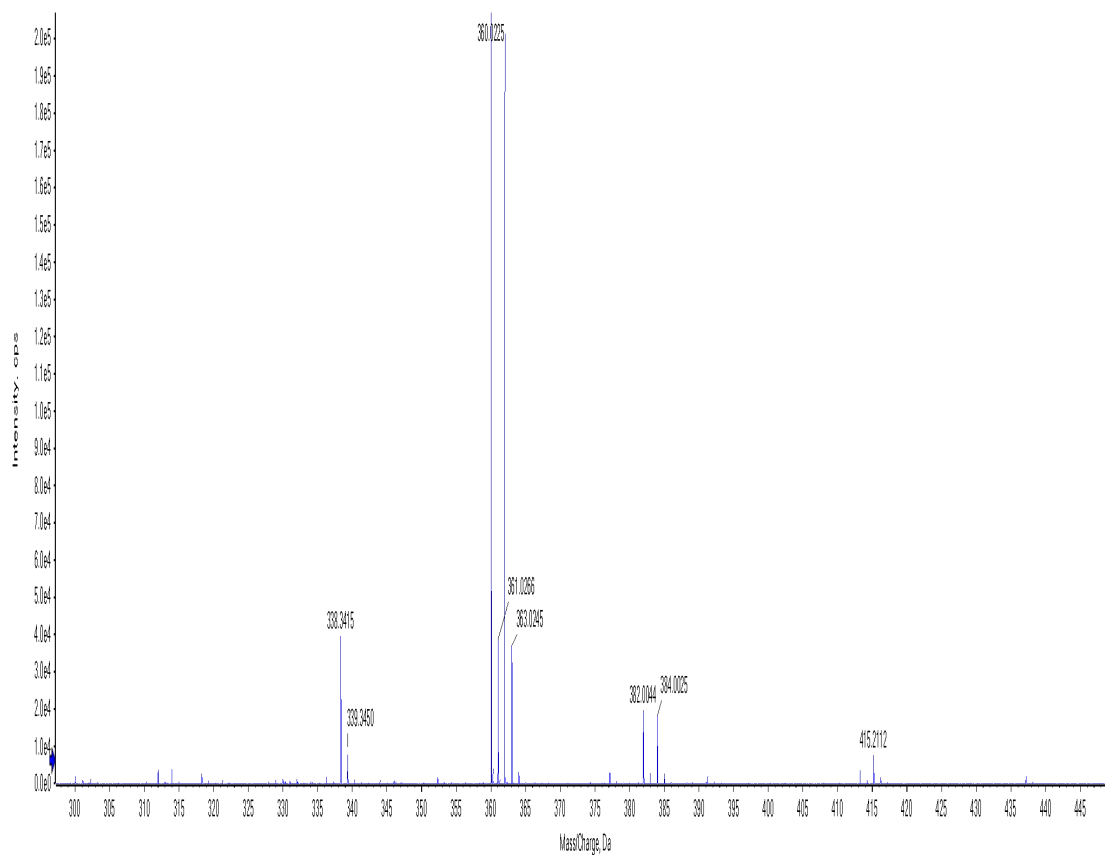


**(E)-2-(4-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3t): <sup>13</sup>C NMR**

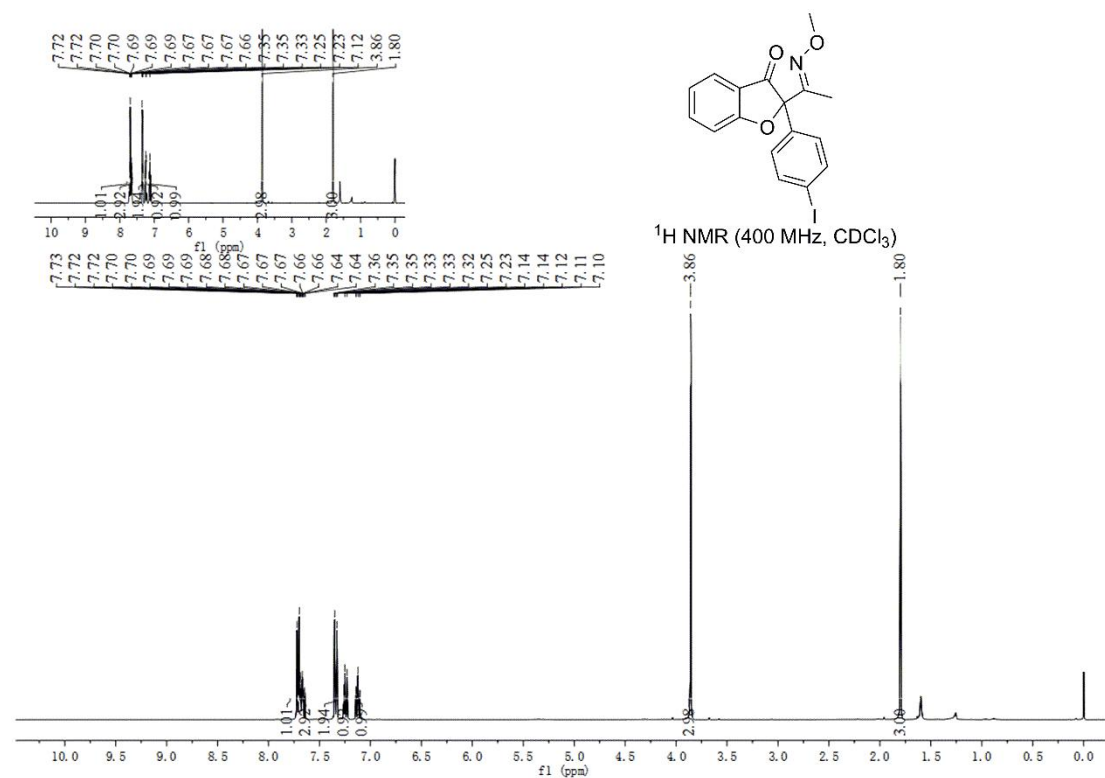


**(E)-2-(4-bromophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3t): MS**

Spectrum from DataS1\2\4U-2.wiff (sample 1) - 2N\2 - +TOF MS (200 - 500) from 0.037 to 0.414 min

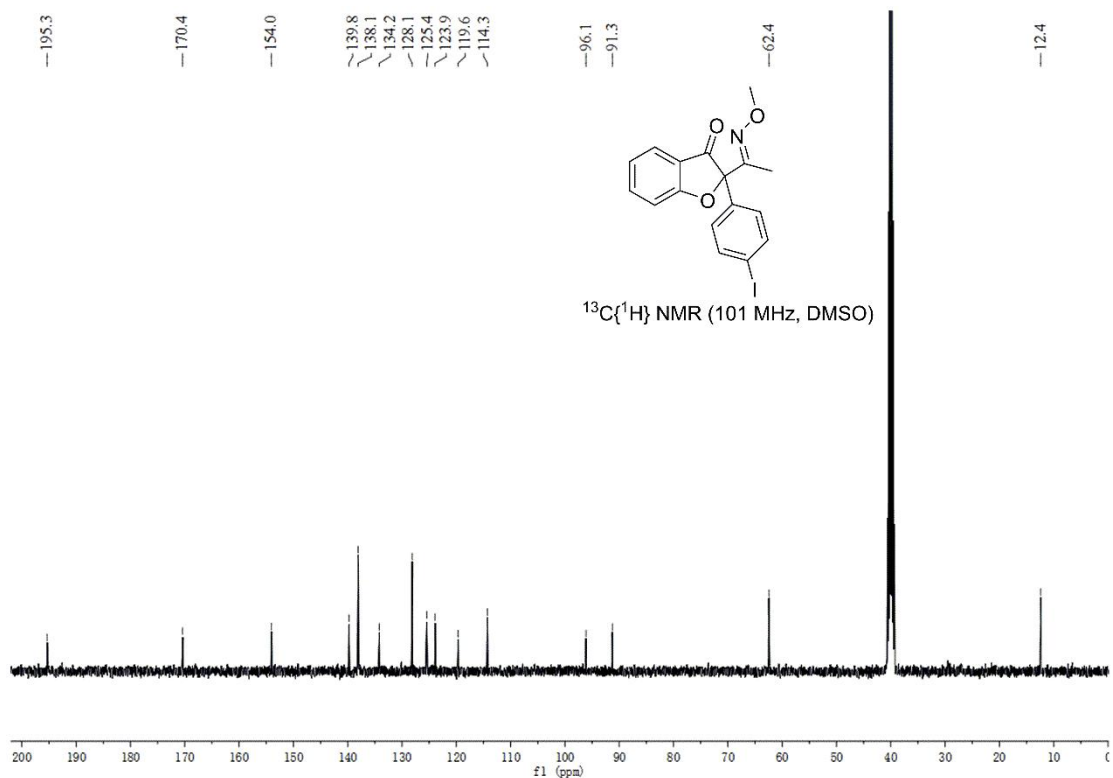


**(E)-2-(4-iodophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3u): <sup>1</sup>H NMR**

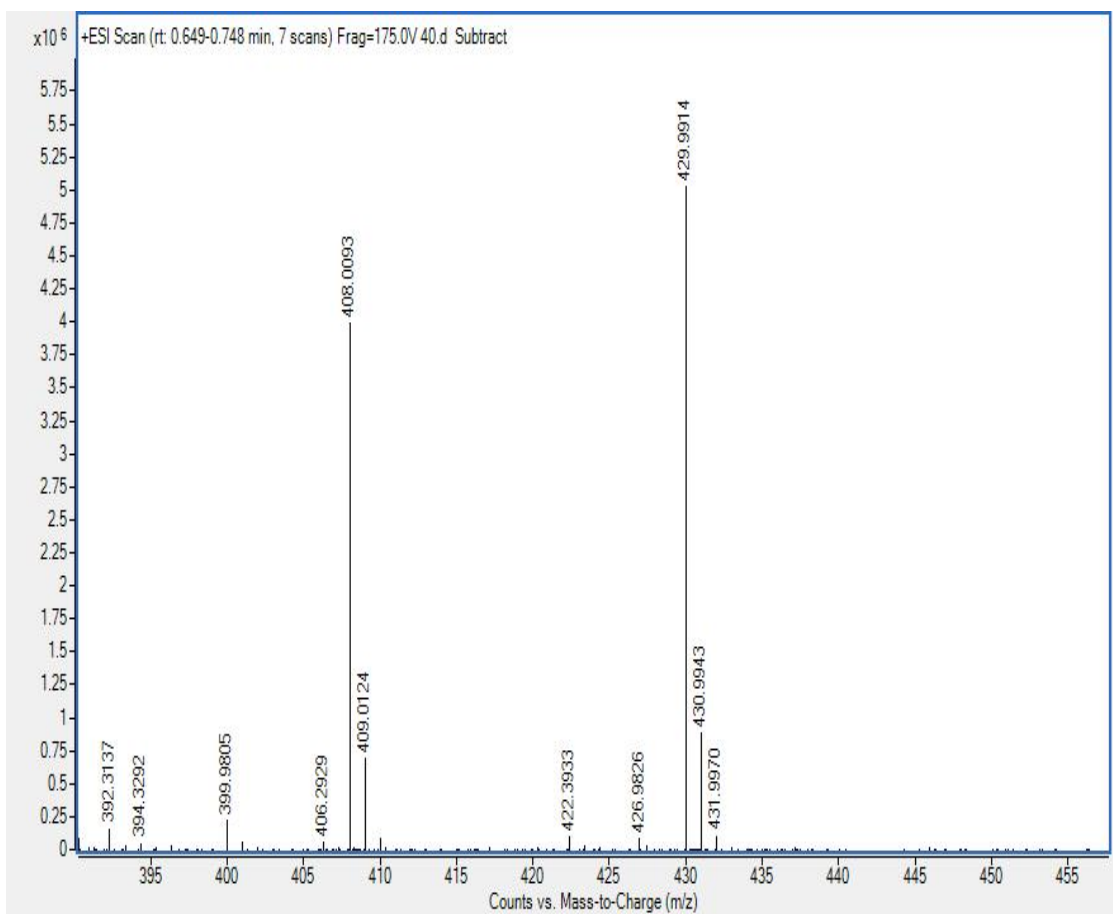




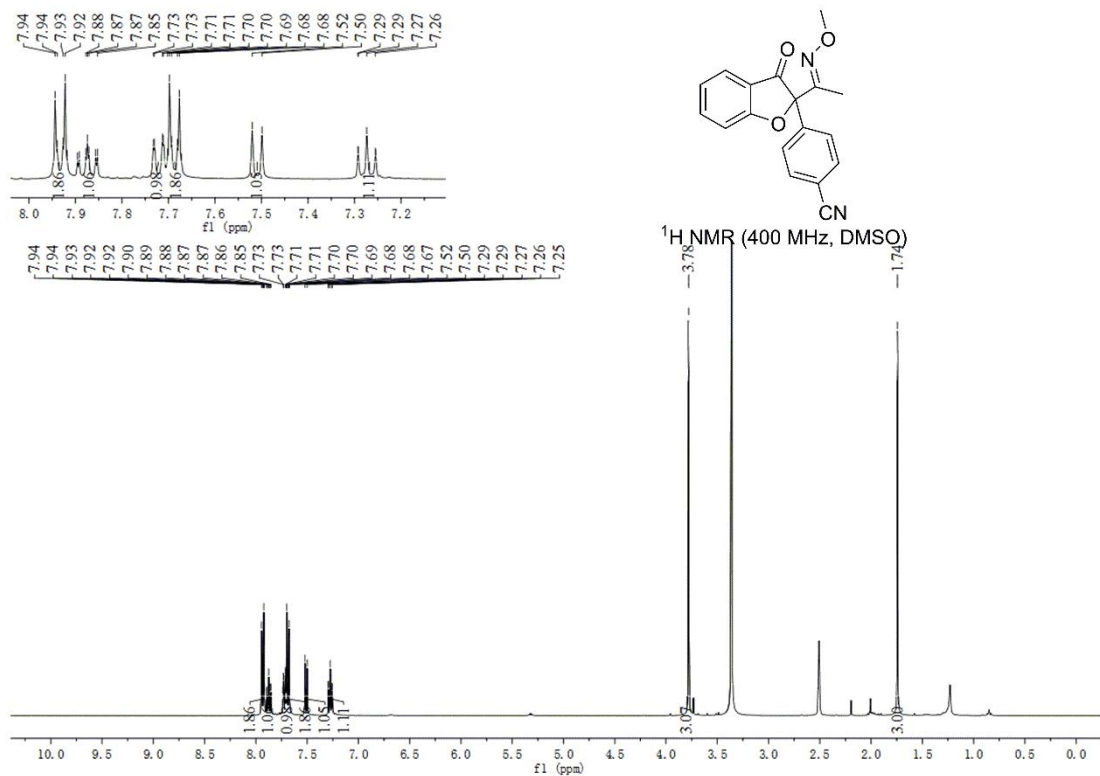
**(E)-2-(4-iodophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3u): <sup>13</sup>C NMR**



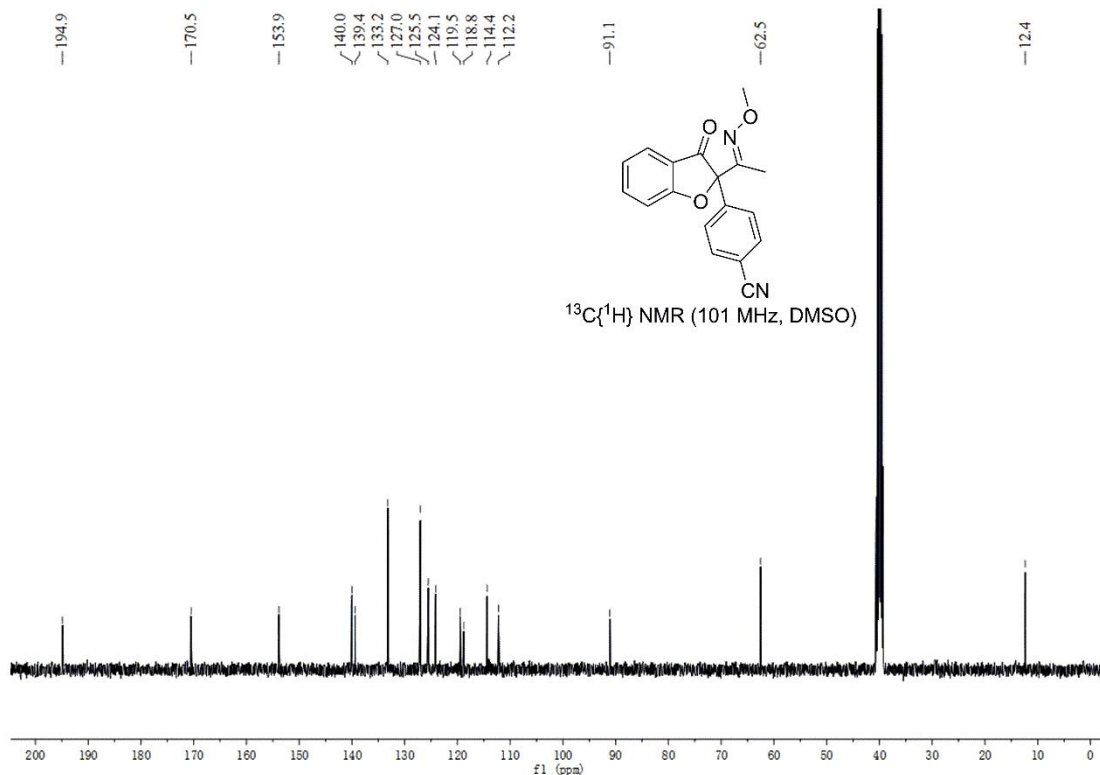
**(E)-2-(4-iodophenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3u): MS**



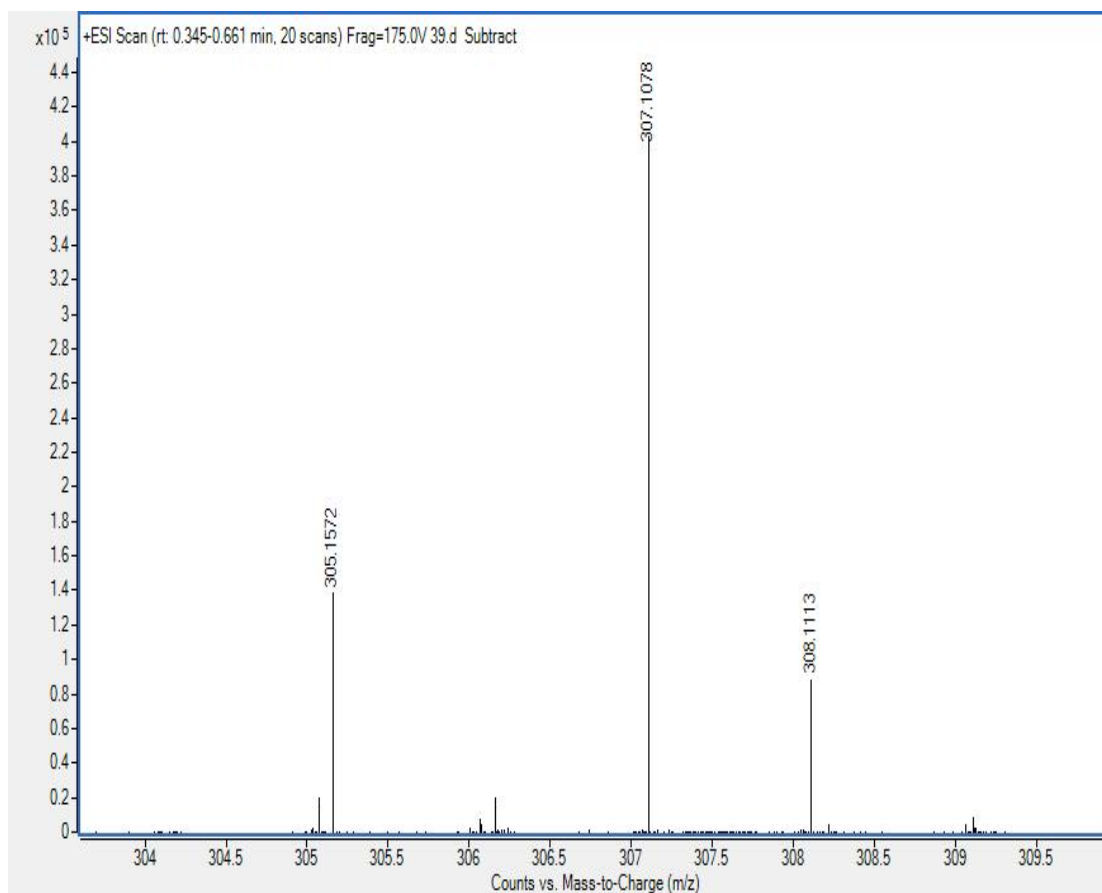
**(E)-4-(2-(1-(methoxyimino)ethyl)-3-oxo-2,3-dihydrobenzofuran-2-yl)benzonitrile (3v): <sup>1</sup>H NMR**



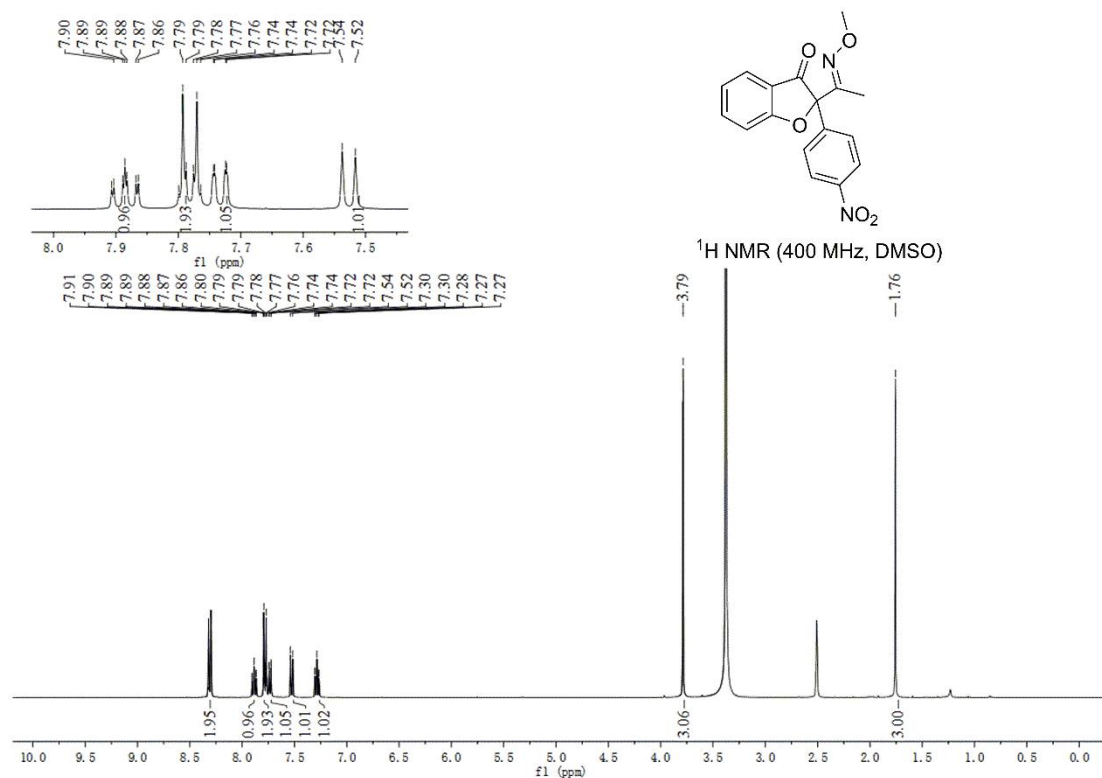
**(E)-4-(2-(1-(methoxyimino)ethyl)-3-oxo-2,3-dihydrobenzofuran-2-yl)benzonitrile (3v): <sup>13</sup>C NMR**



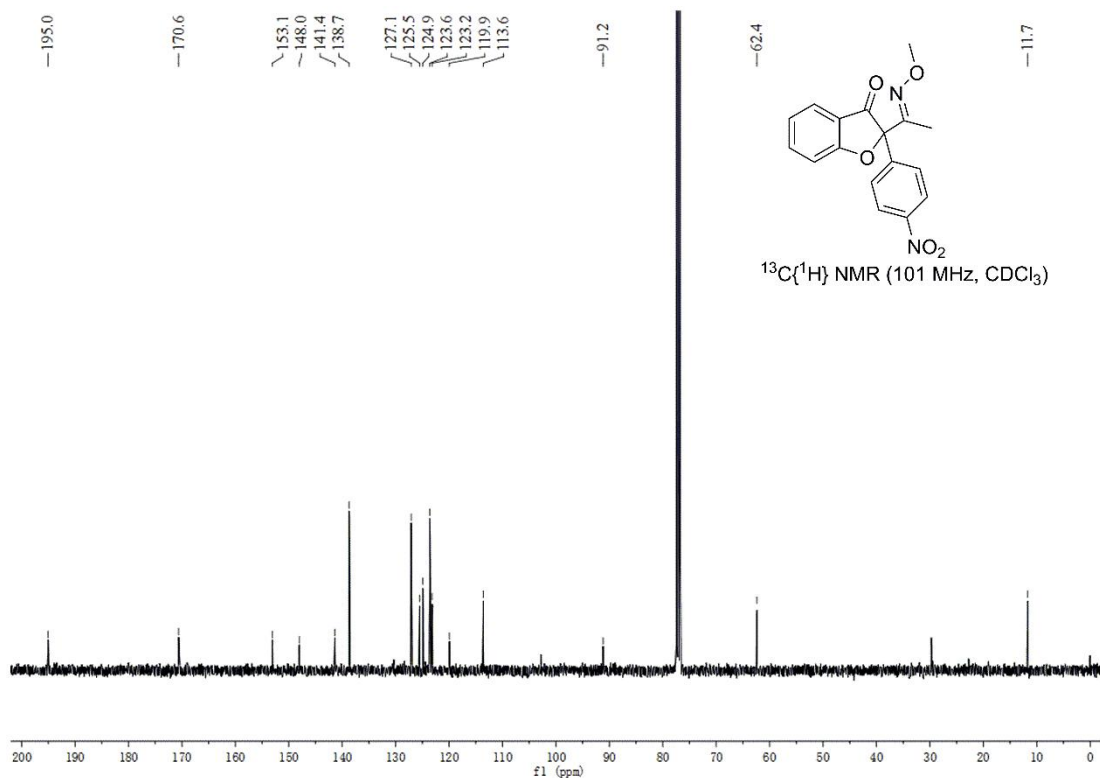
**(E)-4-(2-(1-(methoxyimino)ethyl)-3-oxo-2,3-dihydrobenzofuran-2-yl)benzonitrile (3v): MS**



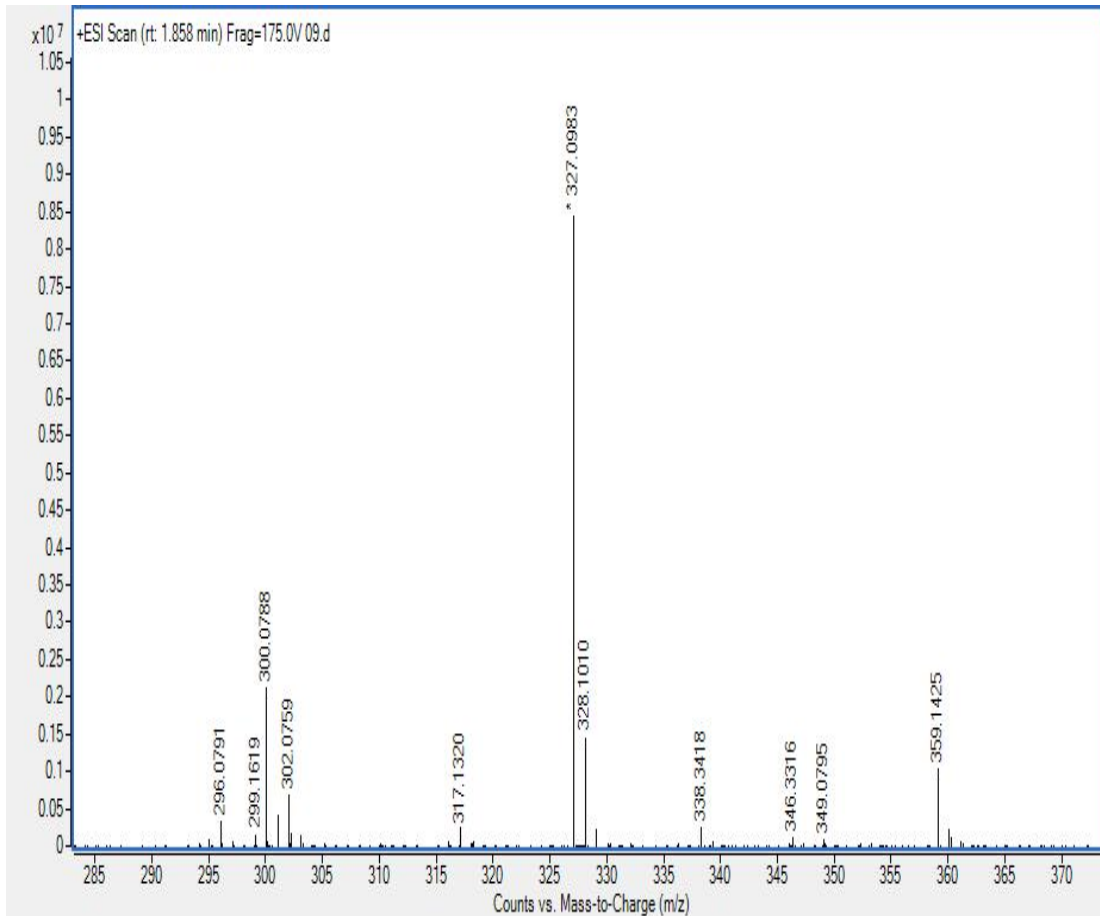
**(E)-2-(1-(methoxyimino)ethyl)-2-(4-nitrophenyl)benzofuran-3(2H)-one (3w): <sup>1</sup>H NMR**



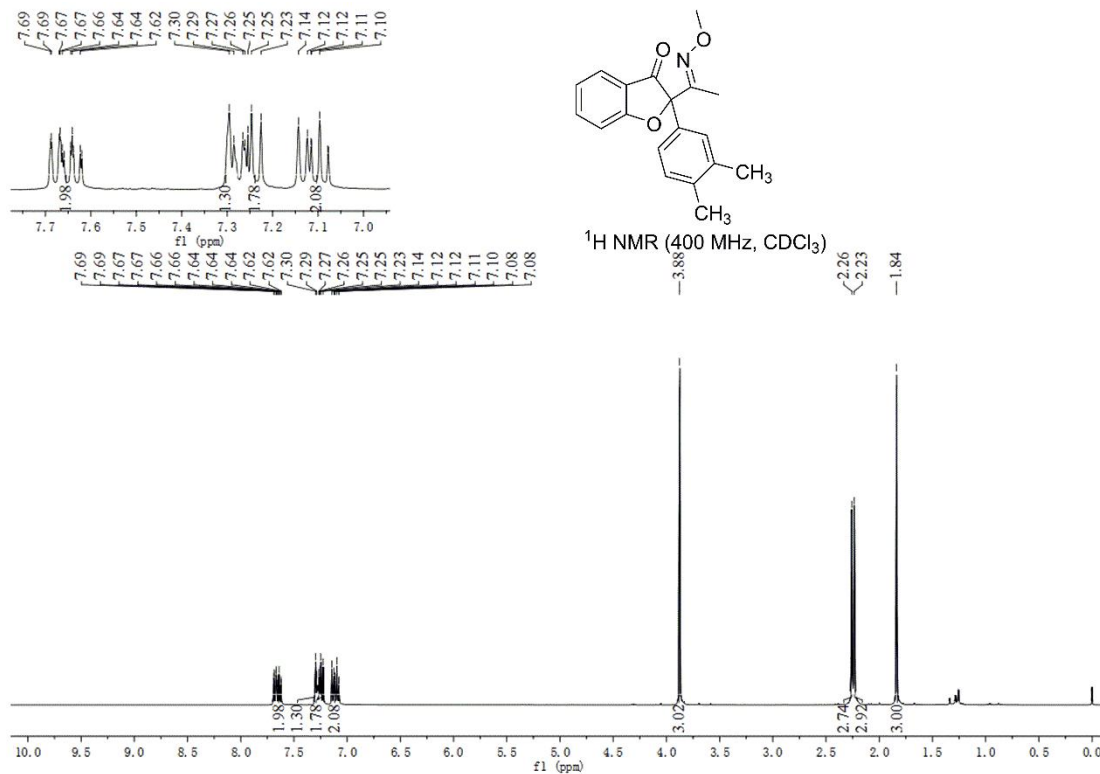
**(E)-2-(1-(methoxyimino)ethyl)-2-(4-nitrophenyl)benzofuran-3(2H)-one (3w):  $^{13}\text{C}$  NMR**



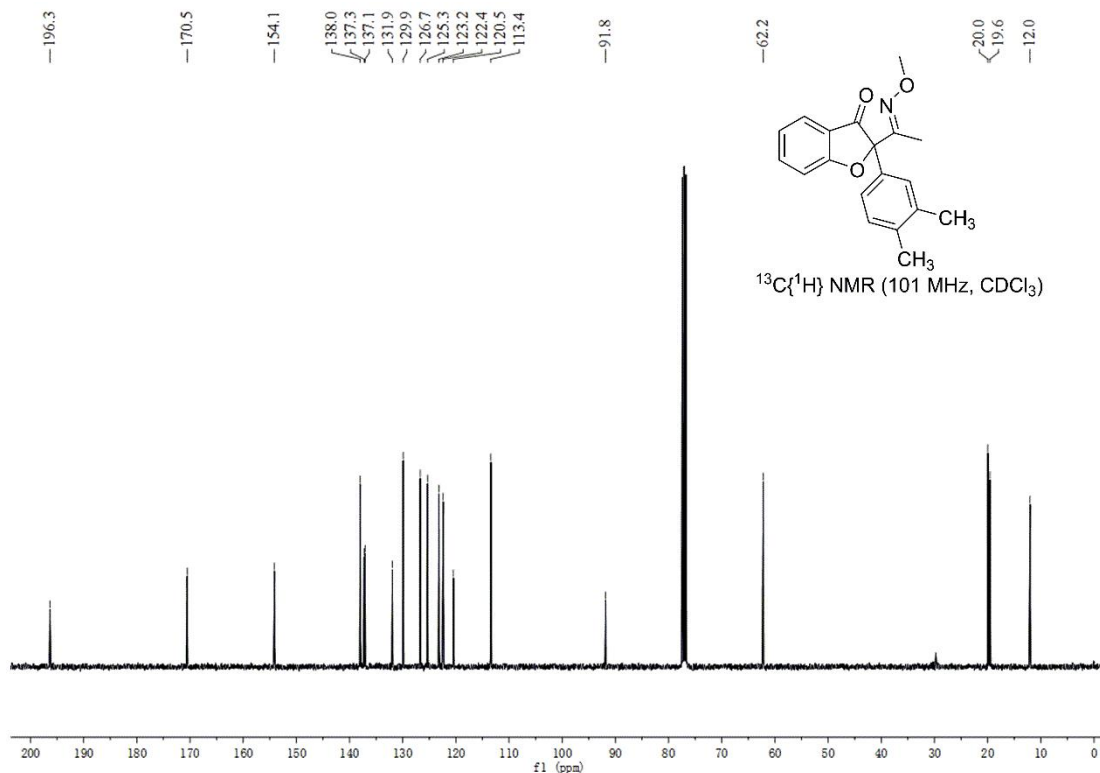
**(E)-2-(1-(methoxyimino)ethyl)-2-(4-nitrophenyl)benzofuran-3(2H)-one (3w): MS**



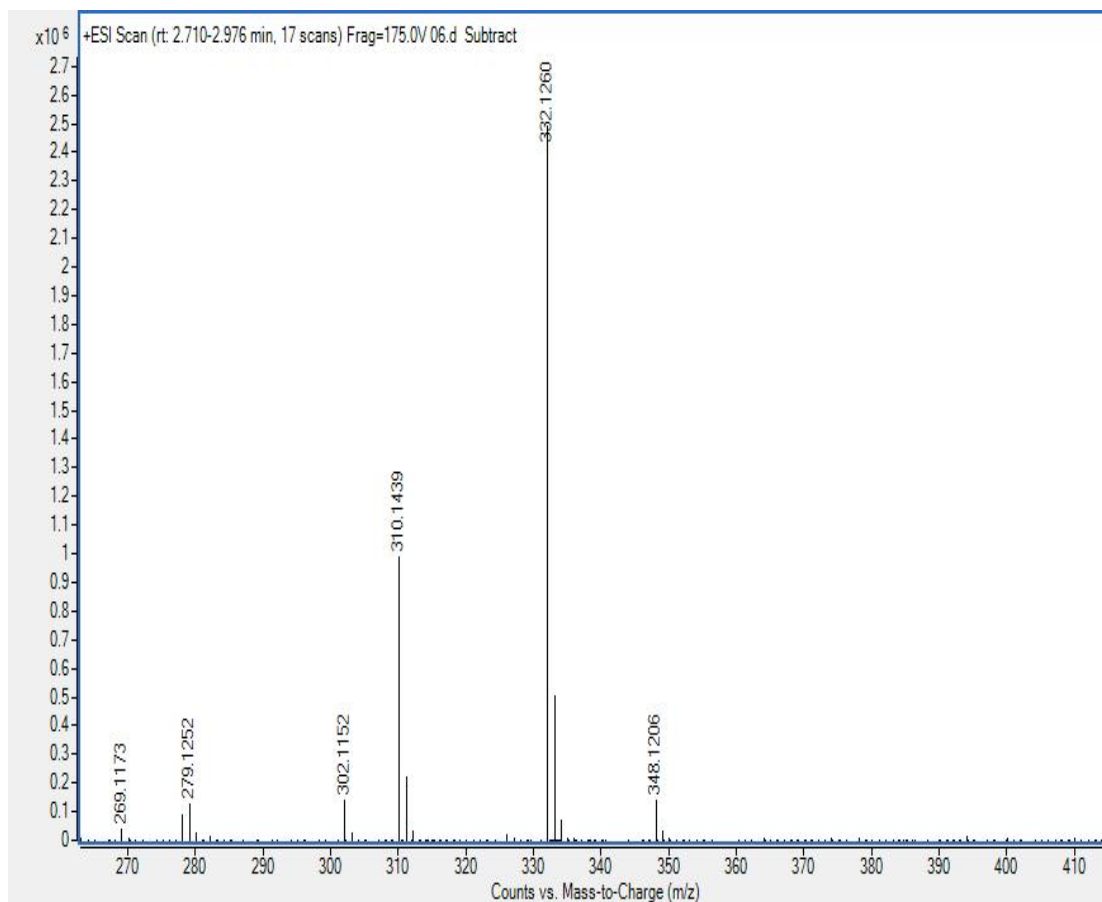
**(E)-2-(3,4-dimethylphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3x):  $^1\text{H}$  NMR**



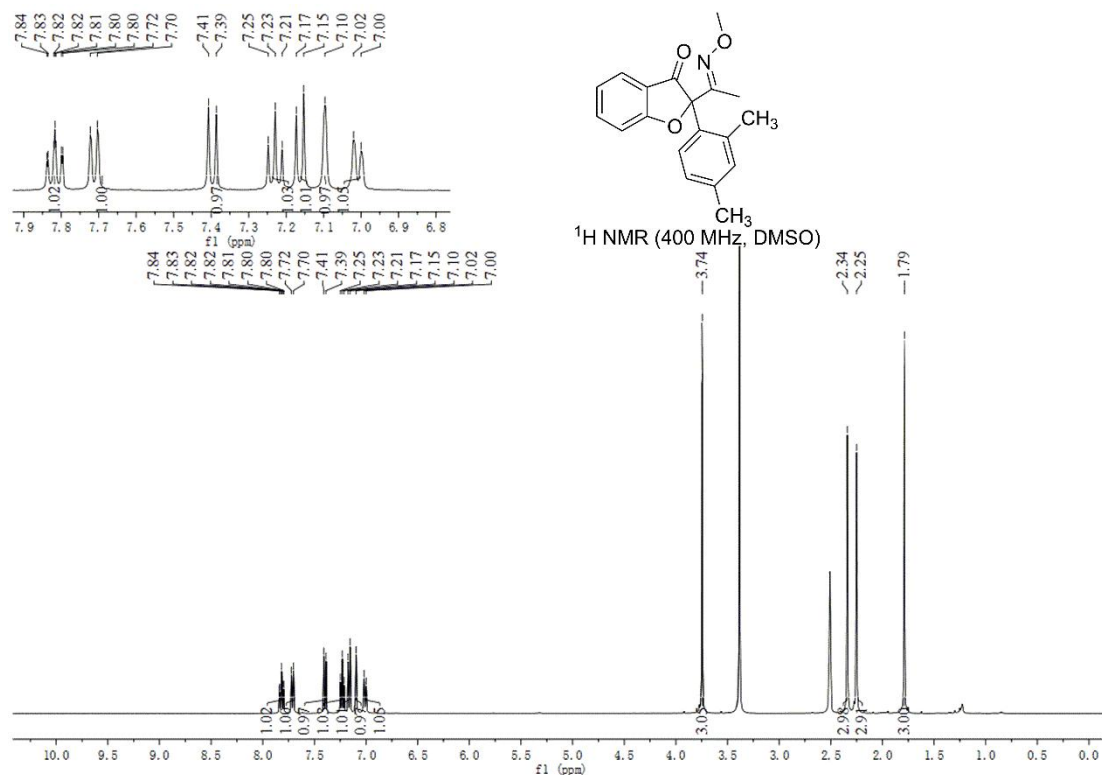
**(E)-2-(3,4-dimethylphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3x):  $^{13}\text{C}$  NMR**



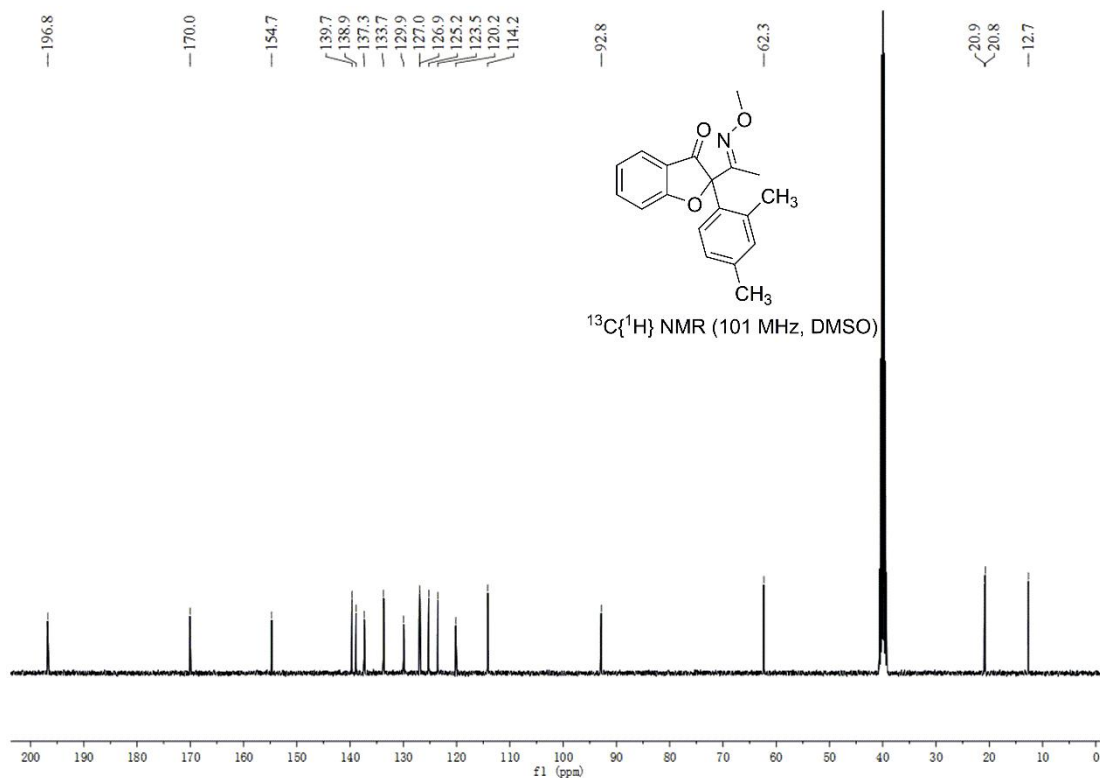
**(E)-2-(3,4-dimethylphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3x): MS**



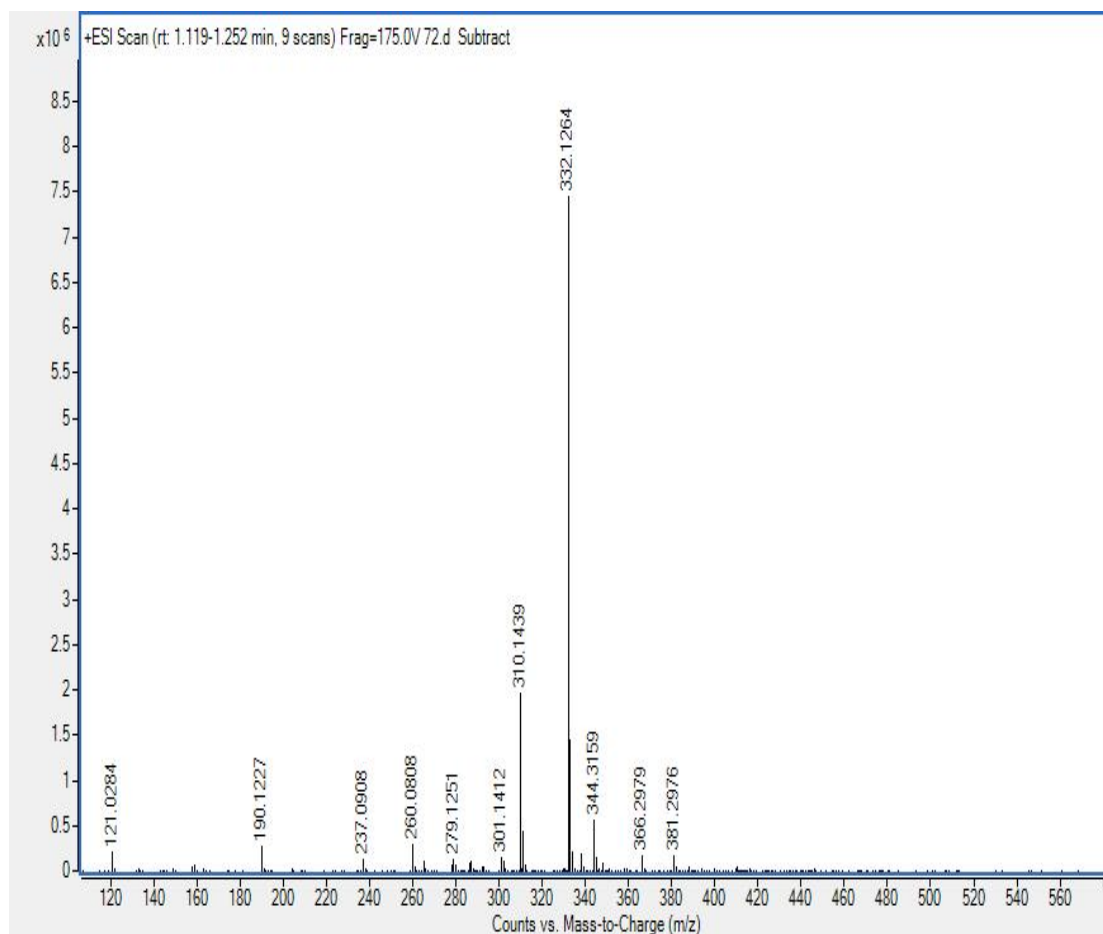
**(E)-2-(2,4-dimethylphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3y): <sup>1</sup>H NMR**



**(E)-2-(2,4-dimethylphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3y): <sup>13</sup>C NMR**

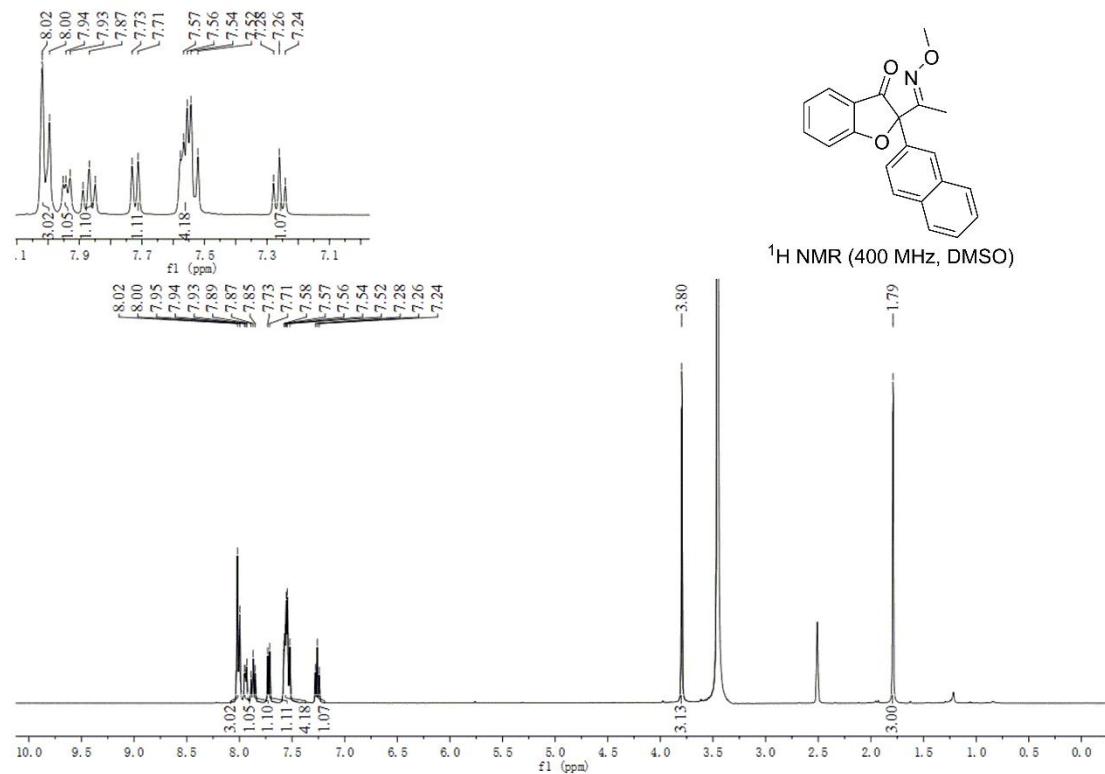


**(E)-2-(2,4-dimethylphenyl)-2-(1-(methoxyimino)ethyl)benzofuran-3(2H)-one (3y): MS**



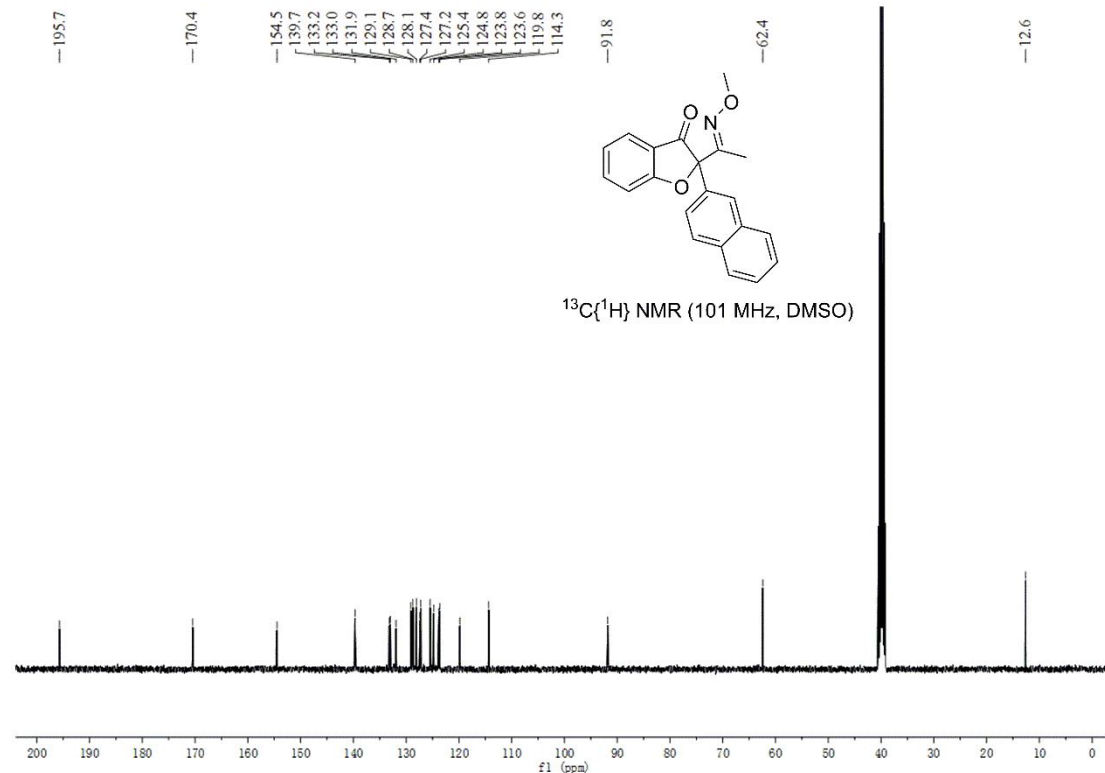
**(E)-7-methoxy-2-(1-(methoxyimino)ethyl)-2-(naphthalen-2-yl)benzofuran-3(2H)-one (3z) :  $^1\text{H}$**

**NMR**



**(E)-7-methoxy-2-(1-(methoxyimino)ethyl)-2-(naphthalen-2-yl)benzofuran-3(2H)-one (3z) :**

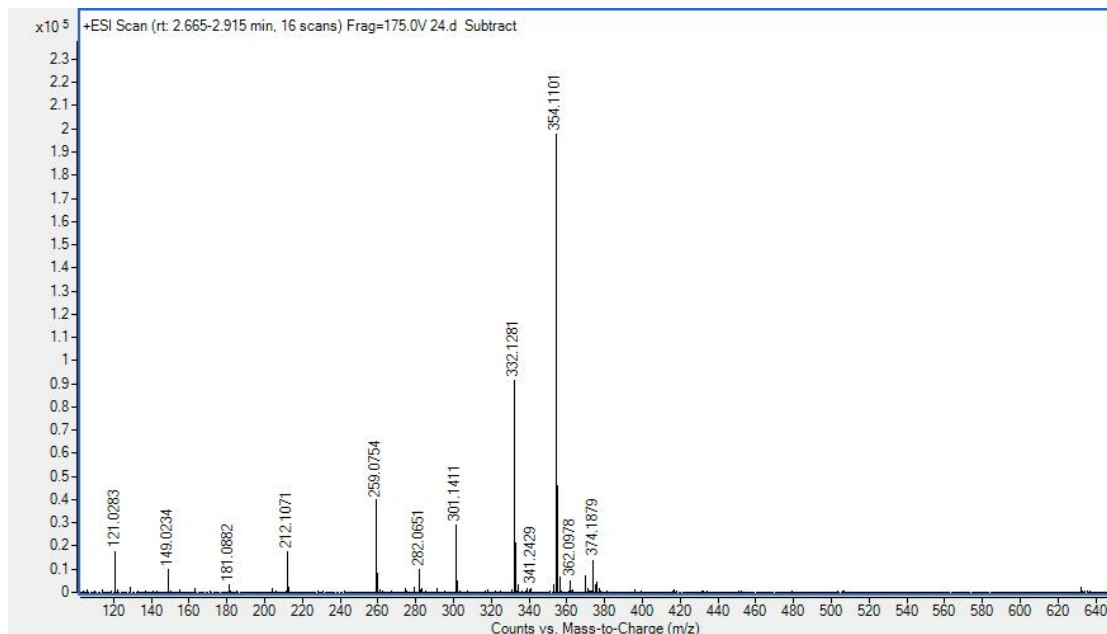
**$^{13}\text{C}$  NMR**



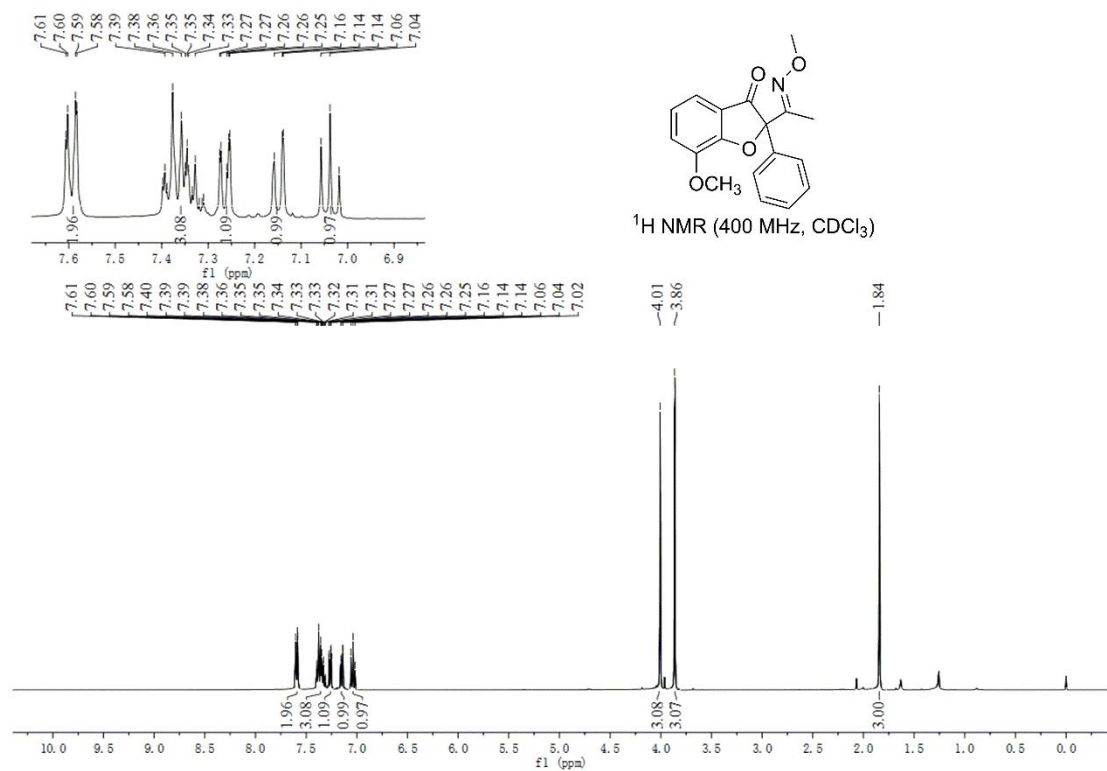


**(E)-7-methoxy-2-(1-(methoxyimino)ethyl)-2-(naphthalen-2-yl)benzofuran-3(2H)-one (3z) :**

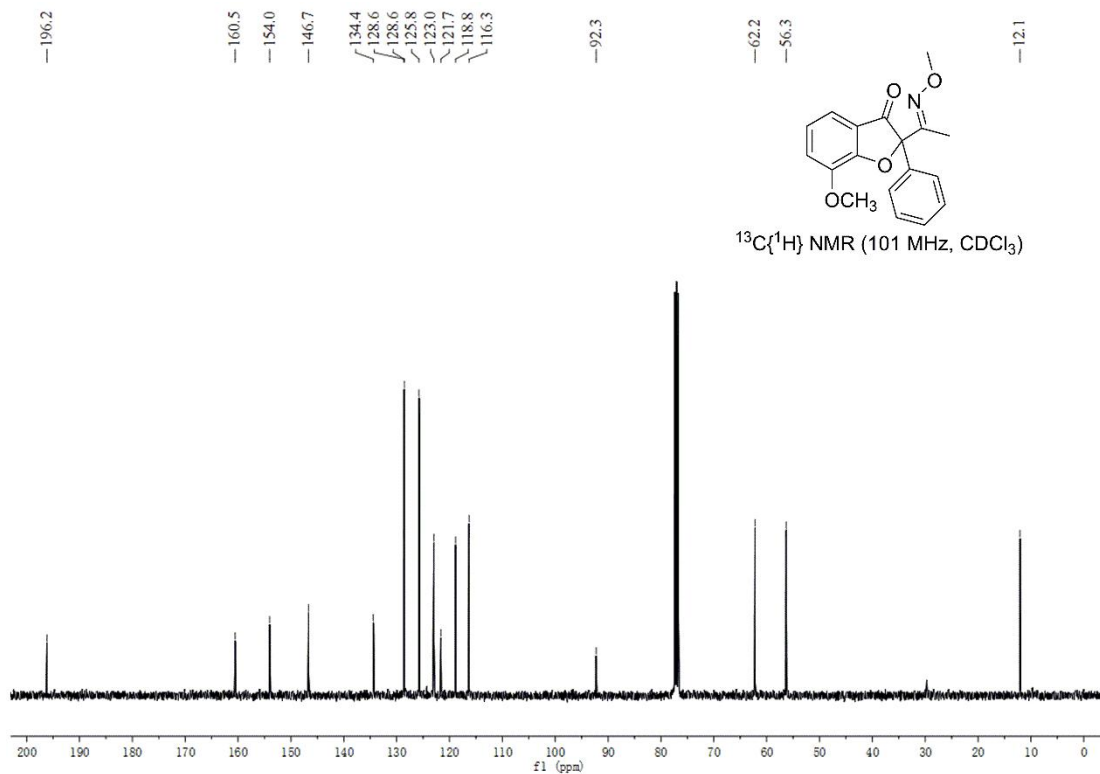
**MS**



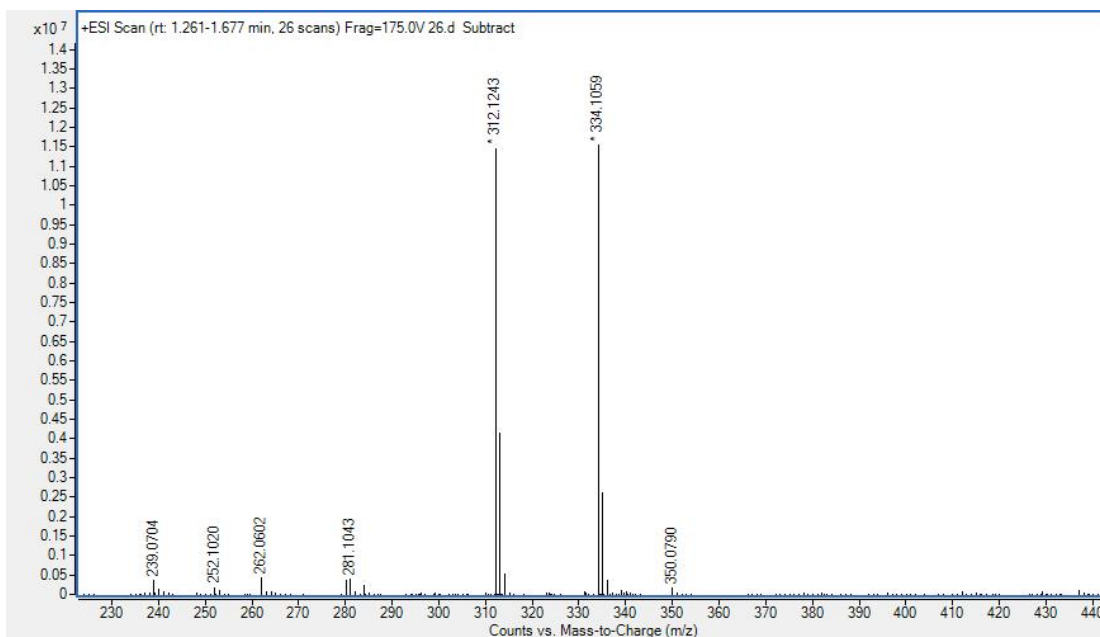
**(E)-7-methoxy-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one(3aa) : <sup>1</sup>H NMR**



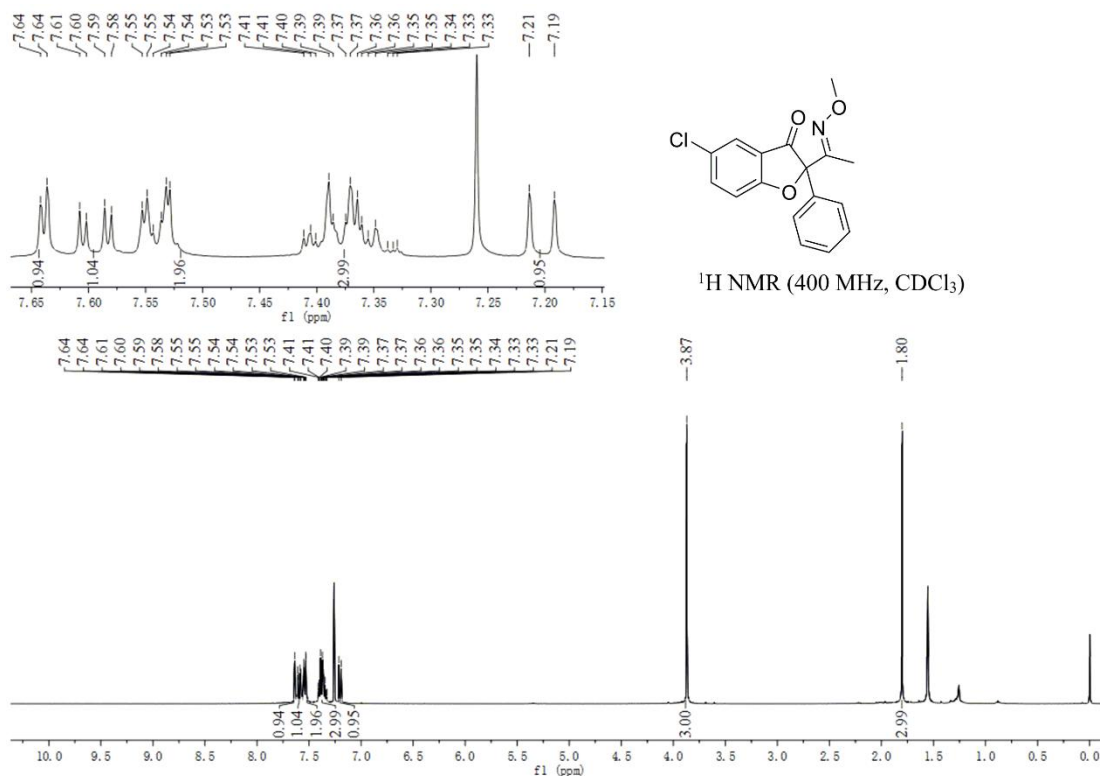
**(E)-7-methoxy-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one (3aa) :  $^{13}\text{C}$  NMR**



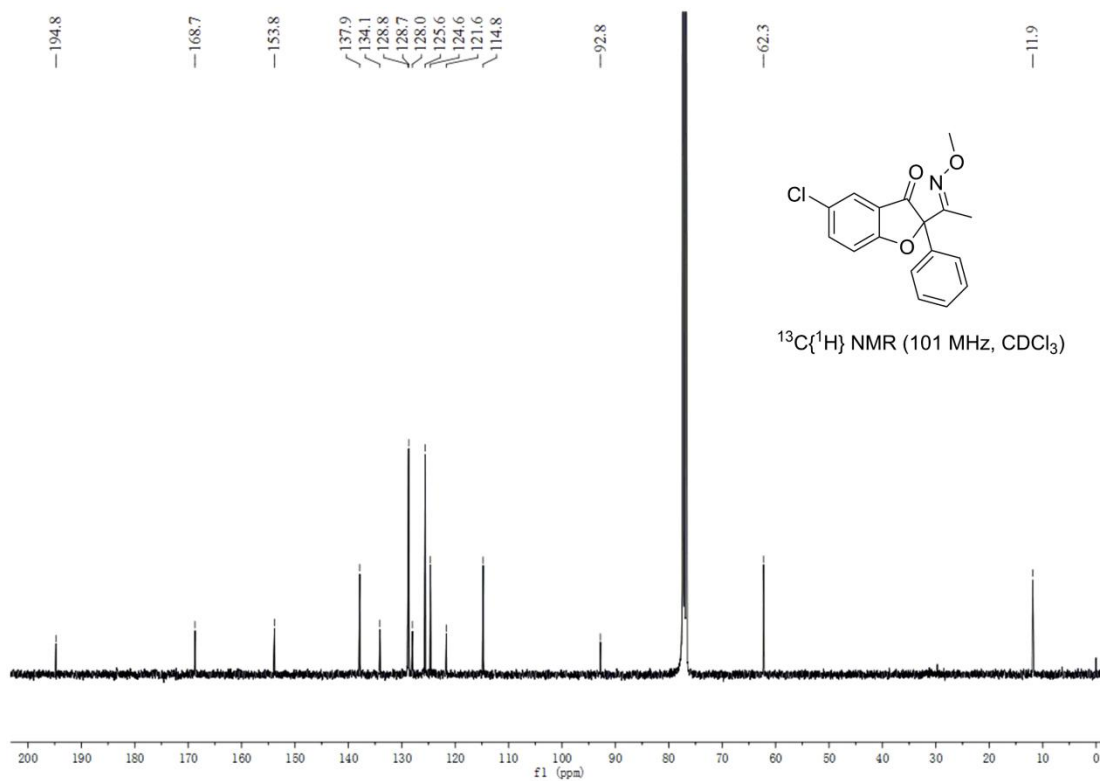
**(E)-7-methoxy-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one (3aa) : MS**



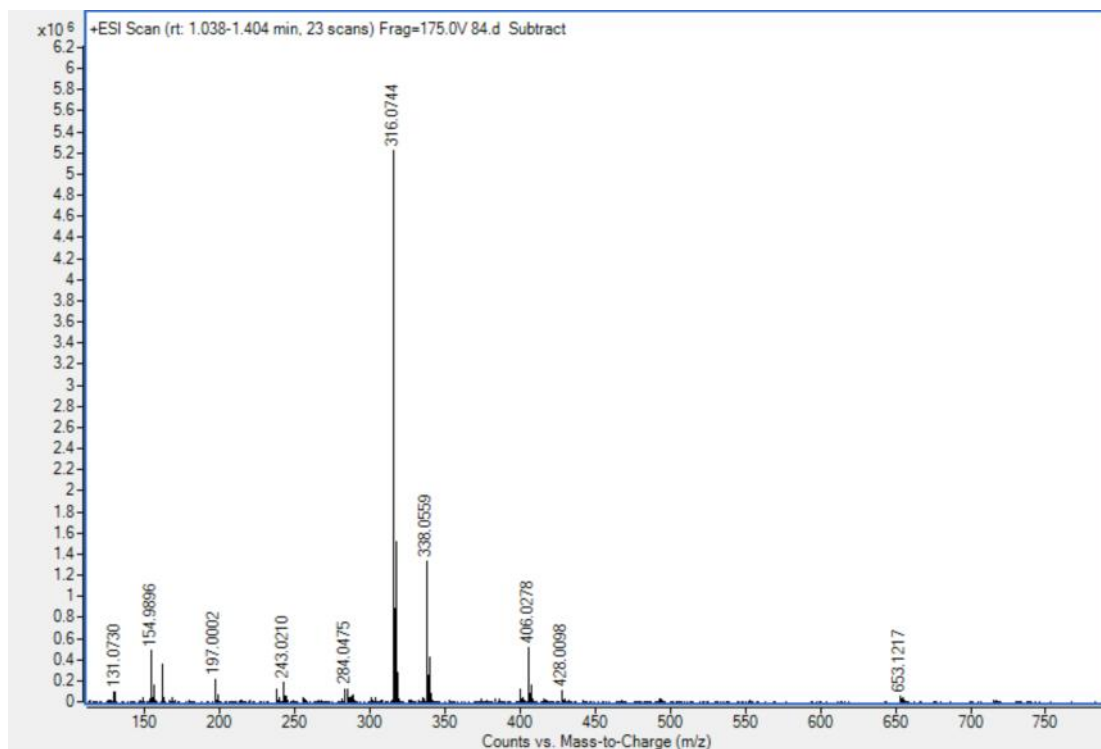
**(E)-5-chloro-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one (3ab) : <sup>1</sup>H NMR**



**(E)-5-chloro-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one (3ab) : <sup>13</sup>C NMR**

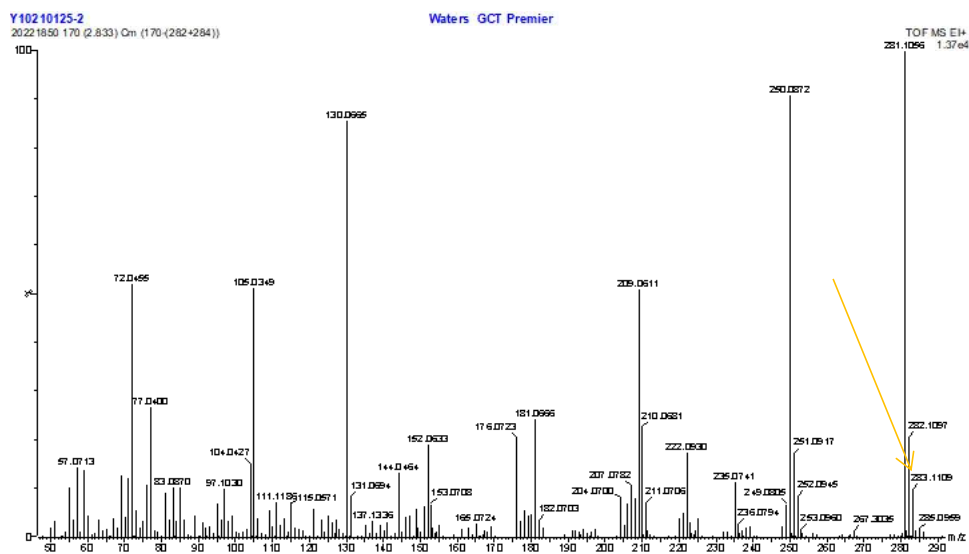


**(E)-5-chloro-2-(1-(methoxyimino)ethyl)-2-phenylbenzofuran-3(2H)-one (3ab) : MS**



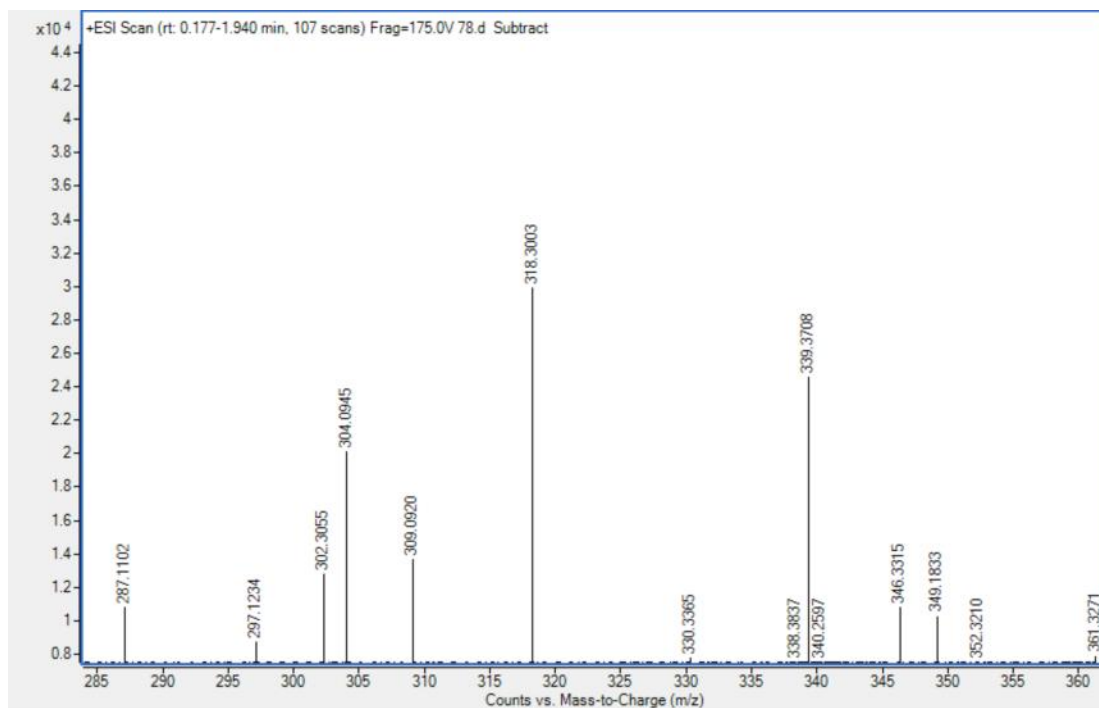
**Intermediate 3a'**

HRMS (ESI) m/z: [M+Na]<sup>+</sup> Calculated for C<sub>17</sub>H<sub>15</sub>NO<sub>2</sub>O<sup>18</sup> 283.1094; Found 283.1109.



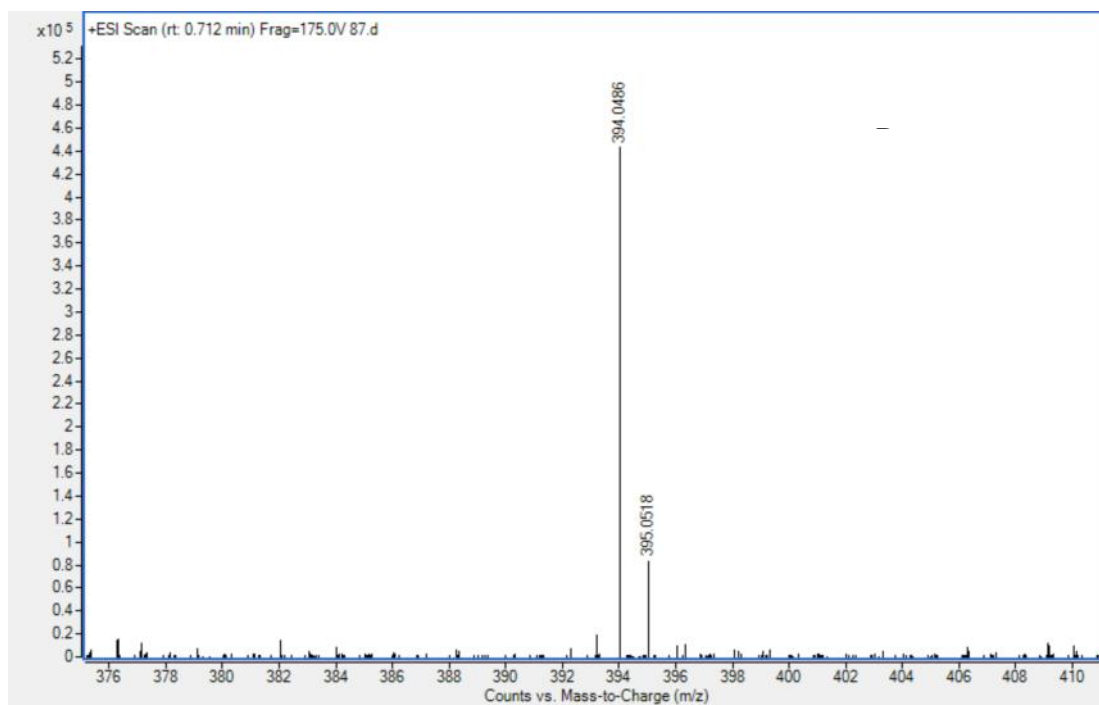
Intermediate A

HRMS (ESI) m/z:  $[M+Na]^+$  Calculated for  $C_{11}H_{11}NO_2PdNa$ , 318.4882; Found 318.3003.



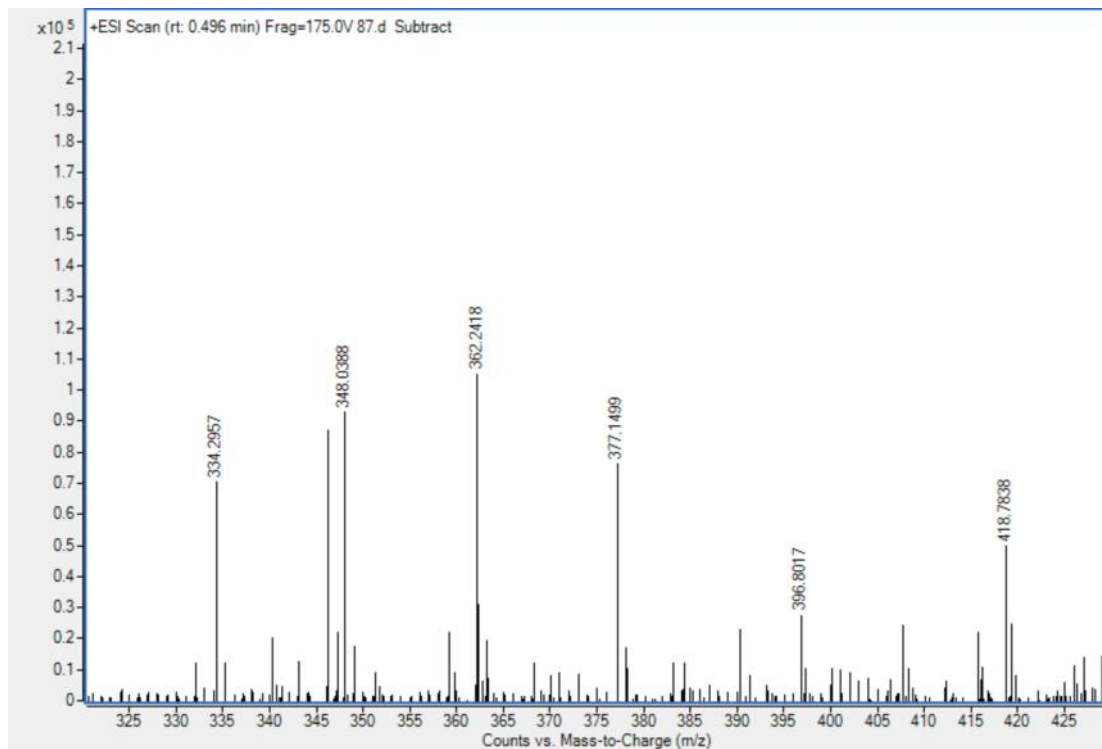
Intermediate D

HRMS (ESI) m/z:  $[M+Na]^+$  Calculated for  $C_{17}H_{16}INO_2Na$  394.0299; Found 394.0486.



Intermediate E

HRMS (ESI) m/z:  $[M+Na]^+$  Calculated for  $C_{19}H_{19}NO_4Na$  348.1206; Found 348.0388.



Intermediate F

HRMS (ESI) m/z:  $[M+Na]^+$  Calculated for  $C_{17}H_{16}NNaO_3^-$  305.1034; Found 305.0977.

