

## Supporting Information

### Copper-catalyzed synthesis of 2-aminopyridylbenzoxazoles *via* domino reactions of intermolecular *N*-arylation and intramolecular *O*-arylation

Ju-You Lu <sup>\*a</sup>

<sup>a</sup>Laboratory of Green Catalysis and Reaction Engineering of Haikou, Hainan Provincial Fine Chemical Engineering Research Center, School of Chemical Engineering and Technology, Hainan University, Haikou 570228, China. E-mail: [lujy@hainanu.edu.cn](mailto:lujy@hainanu.edu.cn)

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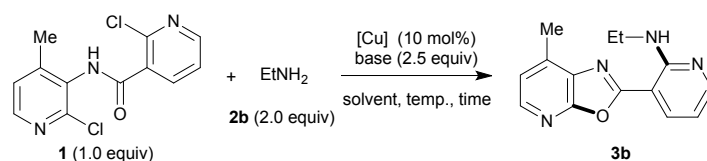
## 1. General Procedures

All reactions were carried out under a nitrogen atmosphere using oven dried glassware and standard Schlenk techniques. All organic solvents were freshly dried and distilled over sodium.  $^1\text{H}$  NMR spectra at 300 MHz, and  $^{13}\text{C}$  NMR spectra at 75 MHz or 150 MHz were obtained on JEOL-ECA300 or ECA600 spectrometers.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR were recorded using tetramethylsilane (TMS) in the solvent of  $\text{CDCl}_3$  as the internal standard ( $^1\text{H}$  NMR: TMS at 0.00 ppm,  $\text{CDCl}_3$  at 7.26 ppm.  $^{13}\text{C}$  NMR:  $\text{CDCl}_3$  at 77.0 ppm). Mass spectra were recorded on a ThermoFisher Q Exactive GC spectrometer.

## 2. Experimental Section

### Optimization of the domino reaction conditions

**Table S1.** Optimization of conditions<sup>a</sup>

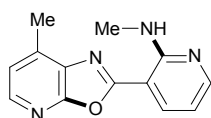


Entry	Cat.	Base	Solvent	Temperature [°C]	Time [h]	Yield [%] <sup>[a, b]</sup>
1	Cu	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	40
2	CuCl	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	72
3	CuBr	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	75
4	<b>CuI</b>	<b>K<sub>2</sub>CO<sub>3</sub></b>	<b>DMSO</b>	<b>80</b>	<b>16</b>	<b>82</b>
5	Cu <sub>2</sub> O	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	65 <sup>[c]</sup>
6	CuCl <sub>2</sub>	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	63
7	CuO	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	60
8	CuSO <sub>4</sub>	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	54
9	Cu(OAc) <sub>2</sub>	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	65
10	-	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	0 <sup>[d]</sup>
11	CuI	Na <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	54
12	CuI	CS <sub>2</sub> CO <sub>3</sub>	DMSO	80	16	38
13	CuI	K <sub>3</sub> PO <sub>4</sub>	DMSO	80	16	46
14	CuI	K <sub>2</sub> CO <sub>3</sub>	DMSO	60	16	68
15	CuI	K <sub>2</sub> CO <sub>3</sub>	DMSO	70	16	74
16	CuI	K <sub>2</sub> CO <sub>3</sub>	DMSO	90	16	80
17	CuI	K <sub>2</sub> CO <sub>3</sub>	DMSO	100	16	78
18	CuI	K <sub>2</sub> CO <sub>3</sub>	DMF	80	16	35
19	CuI	K <sub>2</sub> CO <sub>3</sub>	DMA	80	16	30
20	CuI	K <sub>2</sub> CO <sub>3</sub>	1,4-Dioxane	80	16	44
21	CuI	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	12	65
22	CuI	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	14	74
23	CuI	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	18	82
24	CuI	K <sub>2</sub> CO <sub>3</sub>	DMSO	80	20	83

<sup>a</sup> Reaction condition: **1** (0.5 mmol), **2b** (1 mmol), catalyst (0.05 mmol), base (1.25 mmol), solvent (2 mL) in a Schlenk tube under nitrogen atmosphere. <sup>b</sup> Isolated yield. <sup>c</sup> Cu<sub>2</sub>O (0.025 mmol). <sup>d</sup> In the absence of catalyst. DMSO = dimethyl sulfoxide, DMF = N,N-Dimethylformamide, DMA = N,N-

Dimethylacetamide.

**General procedure for synthesis of 2-aminopyridylbenzoxazoles:** A 10 mL Schlenk tube equipped with a magnetic stirring bar was charged with CuI (0.05 mmol), K<sub>2</sub>CO<sub>3</sub> (1.25 mmol for free amine or 1.75 mmol for amine hydrogen chloride), and 2-halo-*N*-(2-haloaryl)nicotinamides (0.5 mmol). The tube was evacuated twice and back-filled with nitrogen. Amine (1 mmol) and DMSO (2 mL) were added to the tube at room temperature under a stream of nitrogen, and the tube was sealed and put into a pre-heated oil bath at 80 °C for 16 h under a positive pressure of nitrogen. After the resulting solution was cooled to room temperature, the solvent was concentrated, and the residue was purified by column chromatography on silica gel to provide the desired product.

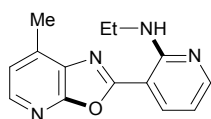


**3a:** Yield 78%. Colorless crystal, mp 151-153 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm) δ 8.20 (s, br, 1H), 8.14-8.12 (m, 1H), 8.06-8.02 (m, 1H), 7.98-7.95 (m, 1H), 6.89 (t, 1H, *J* = 5.5 Hz), 6.49-6.43 (m, 1H), 3.02 (t, 3H, *J* = 4.8 Hz), 2.43 (d, 3H, *J* = 6.2 Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm) δ 160.8, 158.2, 156.8, 152.0, 143.8, 139.5, 136.9, 132.4, 121.9, 111.1, 103.4, 28.1, 16.2.

HRMS: *m/z* calcd for C<sub>13</sub>H<sub>12</sub>N<sub>4</sub>O [M]<sup>+</sup>: 240.1011. Found: 240.1013.

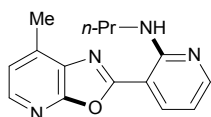


**3b:** Yield 82%. Colorless crystal, mp 147-148 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm) δ 8.32 (t, 1H, *J* = 5.1 Hz), 8.12 (dd, 1H, *J* = 11.3 Hz, *J* = 2.0 Hz), 8.10 (dd, 1H, *J* = 14.4 Hz, *J* = 1.7 Hz), 7.99 (d, 1H, *J* = 5.1 Hz), 6.93 (d, 1H, *J* = 5.1 Hz), 6.48 (dd, 1H, *J* = 7.5 Hz, *J* = 4.8 Hz), 3.55-3.46 (m, 2H), 2.45 (s, 3H), 1.25 (t, 3H, *J* = 7.2 Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm) δ 160.9, 158.3, 156.3, 152.1, 143.8, 139.5, 137.0, 132.5, 121.9, 111.1, 103.2, 36.0, 16.1, 14.8.

HRMS: *m/z* calcd for C<sub>14</sub>H<sub>14</sub>N<sub>4</sub>O [M]<sup>+</sup>: 254.1168. Found: 254.1165.

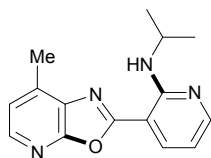


**3c:** Yield 80%. Colorless crystal, mp 140-141 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm) δ 8.52 (t, 1H, *J* = 5.1 Hz), 8.19 (dd, 1H, *J* = 8.0 Hz, *J* = 1.7 Hz), 8.17 (dd, 1H, *J* = 11.6 Hz, *J* = 2.0 Hz), 8.06 (d, 1H, *J* = 5.1 Hz), 7.00 (d, 1H, *J* = 5.1 Hz), 6.54 (dd, 1H, *J* = 7.5 Hz, *J* = 4.8 Hz), 3.51 (q, 2H, *J* = 6.8 Hz), 2.52 (s, 3H), 1.74-1.67 (m, 2H), 1.04 (t, 3H, *J* = 7.2 Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm) δ 161.0, 158.3, 156.5, 152.2, 143.8, 139.5, 137.0, 132.6, 121.9, 111.1, 103.2, 42.9, 22.7, 16.1, 11.7.

HRMS: *m/z* calcd for C<sub>15</sub>H<sub>16</sub>N<sub>4</sub>O [M]<sup>+</sup>: 268.1324. Found: 268.1322.

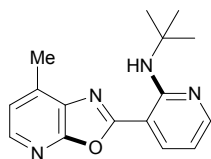


**3d:** Yield 69%. Colorless crystal, mp 121-122 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  8.43 (d, 1H,  $J$  = 6.8 Hz), 8.19 (dd, 1H,  $J$  = 10.3 Hz,  $J$  = 1.7 Hz), 8.13 (dd, 1H,  $J$  = 13.4 Hz,  $J$  = 2.0 Hz), 8.01 (d, 1H,  $J$  = 5.1 Hz), 6.95 (d, 1H,  $J$  = 5.1 Hz), 6.49 (dd, 1H,  $J$  = 7.5 Hz,  $J$  = 4.8 Hz), 4.37-4.26 (m, 1H), 2.49 (s, 3H), 1.28 (d, 6H,  $J$  = 6.2 Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm)  $\delta$  161.0, 158.3, 155.8, 152.2, 143.8, 139.3, 137.0, 132.6, 121.8, 110.9, 102.9, 42.5, 23.0, 15.9.

HRMS:  $m/z$  calcd for C<sub>15</sub>H<sub>16</sub>N<sub>4</sub>O [M]<sup>+</sup>: 268.1324. Found: 268.1323.

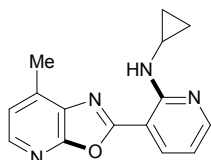


**3e:** Yield 62%. Colorless crystal, mp 161-163 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  8.79 (s, br, 1H), 8.29-8.27 (m, 2H), 8.16 (d, 1H,  $J$  = 5.1 Hz), 7.12 (d, 1H,  $J$  = 5.1 Hz), 6.61 (dd, 1H,  $J$  = 7.5 Hz,  $J$  = 5.1 Hz), 2.63 (s, 3H), 1.60 (s, 9H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm)  $\delta$  161.4, 158.5, 156.5, 151.7, 143.8, 139.5, 137.1, 132.7, 121.9, 110.8, 103.4, 51.8, 29.2, 16.0.

HRMS:  $m/z$  calcd for C<sub>16</sub>H<sub>18</sub>N<sub>4</sub>O [M]<sup>+</sup>: 282.1481. Found: 282.1484.

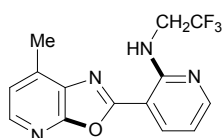


**3f:** Yield 78%. Colorless crystal, mp 138-139 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  8.62 (s, br, 1H), 8.31 (d, 1H,  $J$  = 4.8 Hz), 8.20 (d, 1H,  $J$  = 7.5 Hz), 8.08 (dd, 1H,  $J$  = 5.1 Hz,  $J$  = 1.3 Hz), 7.03 (d, 1H,  $J$  = 4.4 Hz), 6.63 (dd, 1H,  $J$  = 7.5 Hz,  $J$  = 5.0 Hz), 2.97-2.94 (m, 1H), 2.55 (s, 3H), 0.91-0.85 (m, 2H), 0.61-0.56 (m, 2H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm)  $\delta$  160.8, 158.4, 157.4, 152.3, 144.0, 139.6, 137.0, 132.5, 122.0, 112.0, 103.6, 24.0, 16.1, 7.3.

HRMS:  $m/z$  calcd for C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O [M]<sup>+</sup>: 266.1168. Found: 266.1169.

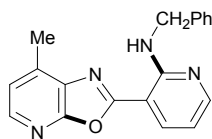


**3g:** Yield 86%. Colorless crystal, mp 146-147 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  8.97 (s, br, 1H), 8.32-8.27 (m, 2H), 8.16 (d, 1H,  $J$  = 4.8 Hz), 7.12 (d, 1H,  $J$  = 4.1 Hz), 6.79-6.75 (m, 1H), 4.49-4.38 (m, 2H), 2.62 (s, 3H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm)  $\delta$  160.4, 158.4, 155.6, 151.6, 144.4, 140.1, 137.3, 132.3, 125.0 ( $J$  = 279 Hz), 122.2, 113.3, 104.4, 41.9 ( $J$  = 34 Hz), 16.1.

HRMS:  $m/z$  calcd for  $C_{14}H_{11}F_3N_4O$   $[M]^+$ : 308.0885. Found: 308.0887.

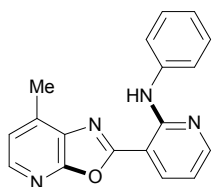


**3h:** Yield 85%. Colorless crystal, mp 175-176 °C.

$^1H$  NMR ( $CDCl_3$ , 300 MHz, ppm)  $\delta$  9.00 (t, 1H,  $J = 5.1$  Hz), 8.29-8.26 (m, 2H), 8.12 (d, 1H,  $J = 5.1$  Hz), 7.46 (d, 2H,  $J = 7.5$  Hz), 7.35 (t, 2H,  $J = 7.2$  Hz), 7.28 (d, 1H,  $J = 7.2$  Hz), 7.05 (d, 1H,  $J = 5.1$  Hz), 6.65 (dd, 1H,  $J = 7.5$  Hz,  $J = 4.8$  Hz), 4.86 (d, 2H,  $J = 5.5$  Hz), 2.51 (s, 3H).

$^{13}C$  NMR ( $CDCl_3$ , 75 MHz, ppm)  $\delta$  161.0, 158.4, 156.3, 152.2, 144.0, 139.7, 139.5, 137.2, 132.6, 128.6, 127.4, 127.1, 122.1, 111.8, 103.6, 45.2, 16.1.

HRMS:  $m/z$  calcd for  $C_{19}H_{16}N_4O$   $[M]^+$ : 316.1324. Found: 316.1325.

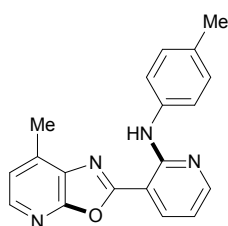


**3i:** Yield 93%. Colorless crystal, mp 190-191 °C.

$^1H$  NMR ( $CDCl_3$ , 300 MHz, ppm)  $\delta$  10.79 (s, br, 1H), 8.29-8.25 (m, 2H), 8.11 (d, 1H,  $J = 5.1$  Hz), 7.76 (s, 1H), 7.73 (s, 1H), 7.33 (t, 2H,  $J = 7.2$  Hz), 7.06-7.01 (m, 2H), 6.75-6.71 (m, 1H), 2.58 (s, 3H).

$^{13}C$  NMR ( $CDCl_3$ , 75 MHz, ppm)  $\delta$  160.4, 158.3, 153.7, 151.5, 144.4, 140.2, 140.0, 137.3, 132.3, 128.9, 122.7, 122.2, 120.4, 113.7, 104.6, 16.2.

HRMS:  $m/z$  calcd for  $C_{18}H_{14}N_4O$   $[M]^+$ : 302.1168. Found: 302.1167.

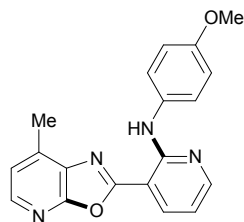


**3j:** Yield 91%. Colorless crystal, mp 188-189 °C.

$^1H$  NMR ( $CDCl_3$ , 300 MHz, ppm)  $\delta$  10.71 (s, br, 1H), 8.31-8.29 (m, 2H), 8.14 (d, 1H,  $J = 4.8$  Hz), 7.61 (d, 2H,  $J = 8.2$  Hz), 7.15 (d, 2H,  $J = 7.9$  Hz), 7.08 (d, 1H,  $J = 4.8$  Hz), 6.74 (t, 1H,  $J = 6.2$  Hz), 2.61 (s, 3H), 2.33 (s, 3H).

$^{13}C$  NMR ( $CDCl_3$ , 75 MHz, ppm)  $\delta$  160.5, 158.4, 154.0, 151.7, 144.4, 139.9, 137.4, 137.3, 132.4, 129.5, 122.2, 121.0, 113.4, 104.3, 21.0, 16.3.

HRMS:  $m/z$  calcd for  $C_{19}H_{16}N_4O$   $[M]^+$ : 316.1324. Found: 316.1321.

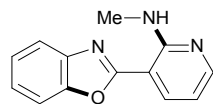


**3k:** Yield 88%. Colorless crystal, mp 156-157 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  10.61 (s, br, 1H), 8.34-8.29 (m, 2H), 8.16 (dd, 1H,  $J = 5.1$  Hz,  $J = 2.0$  Hz), 7.63 (d, 2H,  $J = 7.2$  Hz), 7.11 (d, 1H,  $J = 5.1$  Hz), 6.92 (d, 2H,  $J = 7.2$  Hz), 6.77-6.73 (m, 1H), 3.81 (s, 3H), 2.63 (d, 3H,  $J = 1.7$  Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm)  $\delta$  160.6, 158.4, 155.8, 154.2, 151.8, 144.4, 139.9, 137.4, 133.1, 132.4, 122.9, 122.2, 114.2, 113.2, 104.1, 55.6, 16.3.

HRMS:  $m/z$  calcd for C<sub>19</sub>H<sub>16</sub>N<sub>4</sub>O<sub>2</sub> [M]<sup>+</sup>: 332.1273. Found: 332.1270.

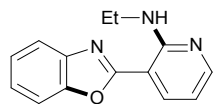


**5a:** Yield 73%. Colorless crystal, mp 100-101 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  8.54 (s, br, 1H), 8.28 (dd, 1H,  $J = 4.8$  Hz,  $J = 1.7$  Hz), 8.19 (dd, 1H,  $J = 7.6$  Hz,  $J = 1.7$  Hz), 7.69-7.66 (m, 1H), 7.50-7.47 (m, 1H), 7.31-7.28 (m, 2H), 6.59 (dd, 1H,  $J = 7.6$  Hz,  $J = 4.8$  Hz), 3.17 (d, 3H,  $J = 4.8$  Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm)  $\delta$  161.8, 156.9, 151.6, 149.5, 141.4, 136.6, 125.0, 124.5, 119.5, 111.0, 110.3, 104.3, 28.1.

HRMS:  $m/z$  calcd for C<sub>13</sub>H<sub>11</sub>N<sub>3</sub>O [M]<sup>+</sup>: 225.0902. Found: 225.0905.

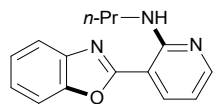


**5b:** Yield 75%. Colorless crystal, mp 65-67 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  8.59 (s, br, 1H), 8.26 (dd, 1H,  $J = 4.8$  Hz,  $J = 1.7$  Hz), 8.19 (dd, 1H,  $J = 7.6$  Hz,  $J = 1.7$  Hz), 7.70-7.67 (m, 1H), 7.50-7.47 (m, 1H), 7.31-7.27 (m, 2H), 6.58 (dd, 1H,  $J = 7.6$  Hz,  $J = 4.8$  Hz), 3.70-3.62 (m, 2H), 1.37 (t, 3H,  $J = 7.2$  Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm)  $\delta$  161.8, 156.3, 151.7, 149.5, 141.5, 136.7, 125.0, 124.5, 119.5, 111.0, 110.3, 104.0, 36.0, 15.1.

HRMS:  $m/z$  calcd for C<sub>14</sub>H<sub>13</sub>N<sub>3</sub>O [M]<sup>+</sup>: 239.1059. Found: 239.1060.

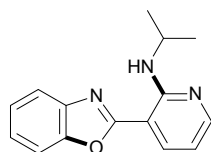


**5c:** Yield 82%. Colorless crystal, mp 49-50 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  8.67 (s, br, 1H), 8.26 (dd, 1H,  $J = 4.8$  Hz,  $J = 2.0$  Hz), 8.21 (dd, 1H,  $J = 7.6$  Hz,  $J = 1.7$  Hz), 7.70-7.67 (m, 1H), 7.51-7.48 (m, 1H), 7.31-7.28 (m, 2H), 6.58 (dd, 1H,  $J = 7.6$  Hz,  $J = 4.8$  Hz), 3.61-3.57 (m, 2H), 1.79-1.74 (m, 2H), 1.07 (t, 3H,  $J = 7.2$  Hz).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, ppm)  $\delta$  161.8, 156.5, 151.7, 149.5, 141.5, 136.7, 125.0, 124.5, 119.5, 110.9, 110.3, 104.0, 43.1, 22.9, 11.8.

HRMS:  $m/z$  calcd for  $\text{C}_{15}\text{H}_{15}\text{N}_3\text{O}$   $[\text{M}]^+$ : 253.1215. Found: 253.1213.

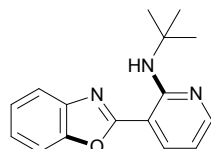


**5d:** Yield 70%. Colorless crystal, mp 91-92 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  8.57 (d, 1H,  $J = 6.2$  Hz), 8.27 (dd, 1H,  $J = 4.8$  Hz,  $J = 2.0$  Hz), 8.23 (dd, 1H,  $J = 7.6$  Hz,  $J = 2.0$  Hz), 7.72-7.69 (m, 1H), 7.52-7.49 (m, 1H), 7.32-7.28 (m, 2H), 6.58 (dd, 1H,  $J = 7.9$  Hz,  $J = 4.8$  Hz), 4.49-4.43 (m, 1H), 1.38 (m, 6H,  $J = 6.5$  Hz).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, ppm)  $\delta$  161.9, 155.8, 151.7, 149.5, 141.5, 136.8, 125.0, 124.5, 119.6, 110.9, 110.3, 103.9, 42.5, 23.2.

HRMS:  $m/z$  calcd for  $\text{C}_{15}\text{H}_{15}\text{N}_3\text{O}$   $[\text{M}]^+$ : 253.1215. Found: 253.1217.

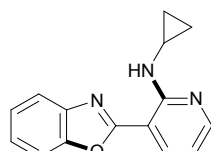


**5e:** Yield 68%. Colorless crystal, mp 100-101 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  8.75 (s, br, 1H), 8.25-8.22 (m, 2H), 7.71-7.68 (m, 1H), 7.53-7.50 (m, 1H), 7.32-7.29 (m, 2H), 6.59-6.55 (m, 1H), 1.60 (s, 9H).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, ppm)  $\delta$  162.2, 156.3, 151.1, 149.5, 141.5, 136.7, 124.9, 124.5, 119.6, 110.6, 110.2, 104.1, 51.8, 29.3.

HRMS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{17}\text{N}_3\text{O}$   $[\text{M}]^+$ : 267.1372. Found: 267.1374.

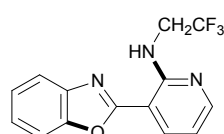


**5f:** Yield 76%. Colorless crystal, mp 105-106 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  8.76 (s, br, 1H), 8.37 (dd, 1H,  $J = 4.8$  Hz,  $J = 1.7$  Hz), 8.23 (dd, 1H,  $J = 7.9$  Hz,  $J = 1.7$  Hz), 7.71-7.68 (m, 1H), 7.53-7.50 (m, 1H), 7.33-7.30 (m, 2H), 6.67 (dd, 1H,  $J = 7.9$  Hz,  $J = 5.1$  Hz), 3.03-2.98 (m, 1H), 0.96-0.90 (m, 2H), 0.71-0.66 (m, 2H).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, ppm)  $\delta$  161.3, 157.3, 151.8, 149.5, 141.4, 136.6, 125.1, 124.5, 119.6, 111.8, 110.3, 104.4, 24.0, 7.3.

HRMS:  $m/z$  calcd for  $\text{C}_{15}\text{H}_{13}\text{N}_3\text{O}$   $[\text{M}]^+$ : 251.1059. Found: 251.1058.

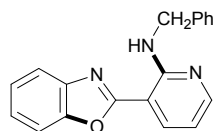


**5g:** Yield 65%. Colorless crystal, mp 113-114 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  9.03 (s, br, 1H), 8.27-8.24 (m, 2H), 7.71-7.68 (m, 1H), 7.52-7.49 (m, 1H), 7.33-7.28 (m, 2H), 6.73 (dd, 1H,  $J = 7.2$  Hz,  $J = 5.1$  Hz), 4.49-4.37 (m, 2H).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, ppm)  $\delta$  161.2, 155.5, 151.1, 149.5, 141.1, 136.8, 125.4, 125.1 ( $J = 279$  Hz), 124.7, 119.8, 113.1, 110.4, 105.2, 41.9 ( $J = 34$  Hz).

HRMS:  $m/z$  calcd for  $\text{C}_{14}\text{H}_{10}\text{F}_3\text{N}_3\text{O}$   $[\text{M}]^+$ : 293.0776. Found: 293.0774.

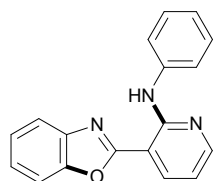


**5h**: Yield 69%. Colorless crystal, mp 106-107 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  9.09 (s, br, 1H), 8.26-8.23 (m, 2H), 7.64-7.62 (m, 1H), 7.49-7.42 (m, 3H), 7.35-7.24 (m, 5H), 6.65-6.60 (m, 1H), 4.91 (d, 2H,  $J = 5.5$  Hz).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, ppm)  $\delta$  161.7, 156.3, 151.7, 149.6, 141.5, 140.0, 136.7, 128.6, 127.4, 127.0, 125.1, 124.6, 119.7, 111.6, 110.3, 104.3, 44.9.

HRMS:  $m/z$  calcd for  $\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}$   $[\text{M}]^+$ : 301.1215. Found: 301.1216.

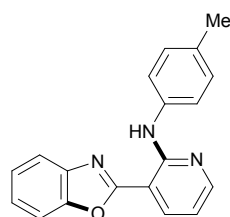


**5i**: Yield 80%. Colorless crystal, mp 122-123 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  10.91 (s, br, 1H), 8.37-8.35 (m, 2H), 7.83 (s, 1H), 7.81 (s, 1H), 7.77-7.74 (m, 1H), 7.57-7.54 (m, 1H), 7.40-7.34 (m, 4H), 7.07 (t, 1H,  $J = 7.5$  Hz), 6.80 (dd, 1H,  $J = 7.5$  Hz,  $J = 5.1$  Hz).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, ppm)  $\delta$  161.3, 153.9, 151.1, 149.6, 141.2, 140.2, 137.0, 128.9, 125.5, 124.9, 122.9, 121.1, 119.8, 113.5, 110.5, 105.4.

HRMS:  $m/z$  calcd for  $\text{C}_{18}\text{H}_{13}\text{N}_3\text{O}$   $[\text{M}]^+$ : 287.1059. Found: 287.1055.



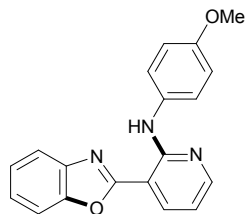
**5j**: Yield 81%. Colorless crystal, mp 131-132 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  10.78 (s, br, 1H), 8.37-8.33 (m, 2H), 7.77-7.74 (m, 1H), 7.68 (s, 1H), 7.65 (s, 1H), 7.58-7.55 (m, 1H), 7.37-7.34 (m, 2H), 7.20 (s, 1H), 7.17 (s, 1H), 6.78 (dd, 1H,  $J = 7.5$  Hz,  $J = 4.8$  Hz), 2.35 (s, 3H).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, ppm)  $\delta$  161.4, 154.1, 151.3, 149.6, 141.2, 137.4, 136.9, 132.6, 129.4, 125.4, 124.8, 121.6, 119.8, 113.2, 110.5, 105.2, 21.0.

HRMS:  $m/z$  calcd for  $\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}$   $[\text{M}]^+$ : 301.1215. Found: 301.1211.



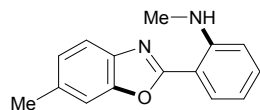


**5k:** Yield 85%. Colorless crystal, mp 141-142 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  10.66 (s, br, 1H), 8.36-8.31 (m, 2H), 7.76-7.73 (m, 1H), 7.66 (s, 1H), 7.63 (s, 1H), 7.57-7.54 (m, 1H), 7.36-7.34 (m, 2H), 6.96 (s, 1H), 6.93 (s, 1H), 6.77 (dd, 1H,  $J = 7.5$  Hz,  $J = 4.8$  Hz), 3.82 (s, 3H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, ppm)  $\delta$  161.4, 155.9, 154.4, 151.3, 149.6, 141.2, 136.9, 133.1, 125.4, 124.7, 123.6, 119.7, 114.3, 113.0, 110.5, 104.9, 55.6.

HRMS:  $m/z$  calcd for C<sub>19</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub> [M]<sup>+</sup>: 317.1164. Found: 317.1162.

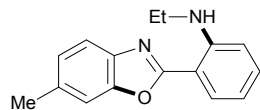


**7a:** Yield 80%. Colorless crystal, mp 140-141 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  8.22 (s, br, 1H), 8.06 (dd, 1H,  $J = 7.9$  Hz,  $J = 1.7$  Hz), 7.55 (d, 1H,  $J = 8.2$  Hz), 7.38-7.33 (m, 2H), 7.11 (d, 1H,  $J = 7.9$  Hz), 6.76-6.70 (m, 2H), 3.03 (d, 3H,  $J = 4.8$  Hz), 2.47 (s, 3H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz, ppm)  $\delta$  162.9, 149.5, 149.2, 139.6, 135.0, 132.6, 128.8, 125.4, 118.5, 115.0, 110.5, 110.4, 108.3, 29.8, 21.8.

HRMS:  $m/z$  calcd for C<sub>15</sub>H<sub>14</sub>N<sub>2</sub>O [M]<sup>+</sup>: 238.1106. Found: 238.1109.

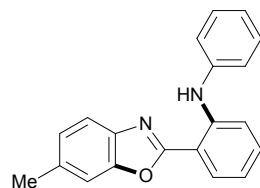


**7b:** Yield 73%. Colorless crystal, mp 107-108 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  8.23 (s, br, 1H), 8.06 (d, 1H,  $J = 7.9$  Hz), 7.56 (d, 1H,  $J = 8.2$  Hz), 7.36-7.31 (m, 2H), 7.11 (d, 1H,  $J = 8.2$  Hz), 6.76 (d, 1H,  $J = 8.6$  Hz), 6.70 (t, 1H,  $J = 7.9$  Hz), 3.39-3.34 (m, 2H), 2.48 (s, 3H), 1.40 (t, 3H,  $J = 7.2$  Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz, ppm)  $\delta$  162.9, 149.5, 148.3, 139.6, 135.0, 132.6, 128.9, 125.4, 118.6, 114.9, 110.9, 110.4, 108.1, 37.7, 21.8, 14.7.

HRMS:  $m/z$  calcd for C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O [M]<sup>+</sup>: 252.1263. Found: 252.1260.

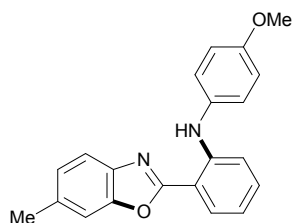


**7c:** Yield 82%. Colorless crystal, mp 122-123 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm)  $\delta$  10.22 (s, br, 1H), 8.17 (d, 1H,  $J = 7.9$  Hz), 7.60 (d, 1H,  $J = 8.2$  Hz), 7.41-7.29 (m, 7H), 7.18-7.15 (m, 2H), 6.88 (t, 1H,  $J = 7.9$  Hz), 2.52 (s, 3H).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, ppm)  $\delta$  162.4, 149.5, 145.2, 141.3, 139.4, 135.4, 132.1, 129.4, 129.0, 125.7, 123.5, 122.7, 118.8, 117.6, 113.8, 110.6, 110.2, 21.8.

HRMS:  $m/z$  calcd for  $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}$   $[\text{M}]^+$ : 300.1263. Found: 300.1261.

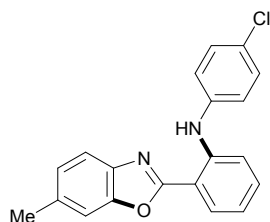


**7d**: Yield 78%. Colorless crystal, mp 164-165 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  9.94 (s, br, 1H), 8.09 (d, 1H,  $J = 7.9$  Hz), 7.54 (d, 1H,  $J = 7.9$  Hz), 7.33 (s, 1H), 7.27-7.20 (m, 3H), 7.12-7.05 (m, 2H), 6.93 (s, 1H), 6.90 (s, 1H), 6.77 (t, 1H,  $J = 7.9$  Hz), 3.80 (s, 3H), 2.46 (s, 3H).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, ppm)  $\delta$  162.6, 156.7, 149.5, 146.8, 139.4, 135.3, 133.9, 132.2, 128.9, 126.1, 125.6, 118.7, 116.8, 114.8, 113.1, 110.6, 109.2, 55.6, 21.9.

HRMS:  $m/z$  calcd for  $\text{C}_{21}\text{H}_{18}\text{N}_2\text{O}_2$   $[\text{M}]^+$ : 330.1368. Found: 330.1370.

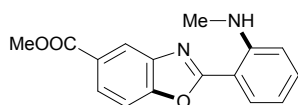


**7e**: Yield 70%. Colorless crystal, mp 156-157 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  10.15 (s, br, 1H), 8.11 (d, 1H,  $J = 7.9$  Hz), 7.55 (d, 1H,  $J = 8.2$  Hz), 7.34-7.24 (m, 7H), 7.12 (d, 1H,  $J = 7.9$  Hz), 6.87-6.87 (m, 1H), 2.47 (s, 3H).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, ppm)  $\delta$  162.2, 149.5, 144.7, 139.9, 139.2, 135.5, 132.1, 129.4, 129.1, 128.2, 125.7, 123.6, 118.8, 118.1, 113.8, 110.6, 110.5, 21.9.

HRMS:  $m/z$  calcd for  $\text{C}_{20}\text{H}_{15}\text{ClN}_2\text{O}$   $[\text{M}]^+$ : 334.0873. Found: 334.0876.

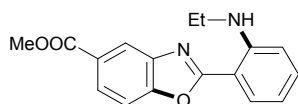


**7f**: Yield 78%. Colorless crystal, mp 139-140 °C.

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  8.38 (s, 1H), 8.18 (s, br, 1H), 8.07-8.04 (m, 2H), 7.55 (d, 1H,  $J = 8.6$  Hz), 7.40 (t, 1H,  $J = 8.6$  Hz), 6.79-6.71 (m, 2H), 3.95 (s, 3H), 3.05 (d, 3H,  $J = 4.8$  Hz).

$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz, ppm)  $\delta$  166.9, 164.6, 152.1, 149.6, 141.9, 133.4, 129.0, 126.7, 126.6, 121.0, 115.1, 110.6, 109.9, 107.3, 52.3, 29.8.

HRMS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{14}\text{N}_2\text{O}_3$   $[\text{M}]^+$ : 282.1004. Found: 282.1006.

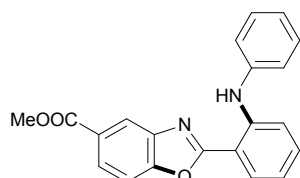


**7g:** Yield 75%. Colorless crystal, mp 103-104 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm) δ 8.36 (s, 1H), 8.17 (s, br, 1H), 8.05-8.02 (m, 2H), 7.51 (d, 1H, *J* = 8.6 Hz), 7.34 (t, 1H, *J* = 8.6 Hz), 6.77-6.67 (m, 2H), 3.94 (s, 3H), 3.37-3.33 (m, 2H), 1.41 (t, 3H, *J* = 7.2 Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz, ppm) δ 166.9, 164.6, 152.1, 148.7, 142.0, 133.3, 129.1, 126.7, 126.6, 121.1, 114.9, 111.0, 109.9, 107.1, 52.3, 37.7, 14.6.

HRMS: *m/z* calcd for C<sub>17</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub> [M]<sup>+</sup>: 296.1161. Found: 296.1165.

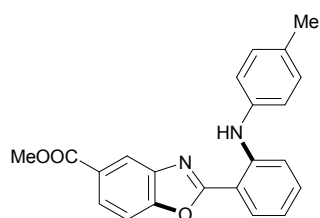


**7h:** Yield 80%. Colorless crystal, mp 153-154 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm) δ 10.08 (s, br, 1H), 8.38 (s, 1H), 8.11 (d, 1H, *J* = 7.5 Hz), 8.06 (d, 1H, *J* = 8.6 Hz), 7.55 (d, 1H, *J* = 8.6 Hz), 7.41-7.30 (m, 6H), 7.12 (t, 1H, *J* = 6.8 Hz), 6.84 (t, 1H, *J* = 7.9 Hz), 3.94 (s, 3H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz, ppm) δ 166.8, 164.1, 152.1, 145.7, 141.7, 140.9, 132.8, 129.5, 129.2, 126.9, 123.8, 122.8, 121.3, 117.7, 113.9, 110.1, 109.2, 52.3.

HRMS: *m/z* calcd for C<sub>21</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub> [M]<sup>+</sup>: 344.1161. Found: 344.1165.

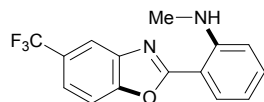


**7i:** Yield 81%. Colorless crystal, mp 168-169 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm) δ 9.98 (s, br, 1H), 8.38 (s, 1H), 8.11-8.05 (m, 2H), 7.56 (d, 1H, *J* = 8.2 Hz), 7.28-7.17 (m, 6H), 6.81 (t, 1H, *J* = 7.9 Hz), 3.94 (s, 3H), 2.36 (s, 3H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz, ppm) δ 166.8, 164.2, 152.2, 146.3, 141.7, 138.1, 133.7, 132.8, 130.1, 129.2, 126.9, 123.5, 121.2, 117.2, 113.6, 110.1, 108.7, 52.3, 21.0.

HRMS: *m/z* calcd for C<sub>22</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub> [M]<sup>+</sup>: 358.1317. Found: 358.1318.

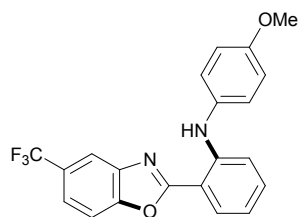


**7j:** Yield 70%. Colorless crystal, mp 98-99 °C.

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, ppm) δ 8.15 (s, br, 1H), 8.07 (d, 1H, *J* = 7.9 Hz), 7.96 (s, 1H), 7.63-7.59 (m, 2H), 7.41 (t, 1H, *J* = 7.9 Hz), 6.79-6.72 (m, 2H), 3.05 (d, 3H, *J* = 4.8 Hz).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz, ppm) δ 165.0, 150.9, 149.7, 142.0, 133.6, 129.1, 127.0 (*J* = 33 Hz), 124.4 (*J* = 272 Hz), 121.8, 116.7 (*J* = 4 Hz), 115.1, 110.7, 110.5, 107.1, 29.8.

HRMS: *m/z* calcd for C<sub>15</sub>H<sub>11</sub>F<sub>3</sub>N<sub>2</sub>O [M]<sup>+</sup>: 292.0823. Found: 292.0824.

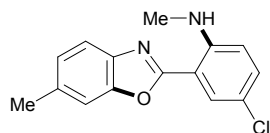


**7k:** Yield 72%. Colorless crystal, mp 127-128 °C.

$^1\text{H NMR}$  ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  9.82 (s, br, 1H), 8.11 (d, 1H,  $J = 7.9$  Hz), 7.97 (s, 1H), 7.62-7.60 (m, 2H), 7.27-7.25 (m, 3H), 7.07 (d, 1H,  $J = 8.6$  Hz), 6.96 (s, 1H), 6.93 (s, 1H), 6.79 (t, 1H,  $J = 7.9$  Hz), 3.83 (s, 3H).

$^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 150 MHz, ppm)  $\delta$  163.6, 155.9, 149.9, 146.3, 140.7, 132.3, 132.0, 128.0, 126.1 ( $J = 32$  Hz), 125.1, 123.2 ( $J = 272$  Hz), 120.9, 115.8 ( $J = 3$  Hz), 115.7, 113.7, 112.2, 109.5, 106.8, 54.5.

HRMS:  $m/z$  calcd for  $\text{C}_{21}\text{H}_{15}\text{F}_3\text{N}_2\text{O}_2$  [ $\text{M}$ ] $^+$ : 384.1086. Found: 384.1088.

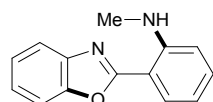


**7l:** Yield 75%. Colorless crystal, mp 148-149 °C.

$^1\text{H NMR}$  ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  8.21 (s, br, 1H), 8.02 (t, 1H,  $J = 2.7$  Hz), 7.55 (dd, 1H,  $J = 8.2$  Hz,  $J = 2.4$  Hz), 7.34 (s, 1H), 7.29 (d, 1H,  $J = 8.9$  Hz), 7.13 (d, 1H,  $J = 7.9$  Hz), 6.67 (dd, 1H,  $J = 8.9$  Hz,  $J = 2.4$  Hz), 3.02 (d, 3H,  $J = 4.8$  Hz), 2.49 (s, 3H).

$^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 150 MHz, ppm)  $\delta$  161.6, 149.4, 147.7, 139.4, 135.5, 132.3, 127.9, 125.7, 119.6, 118.7, 111.8, 110.5, 109.2, 29.9, 21.8.

HRMS:  $m/z$  calcd for  $\text{C}_{15}\text{H}_{13}\text{ClN}_2\text{O}$  [ $\text{M}$ ] $^+$ : 272.0716. Found: 272.0713.



**7m:** Yield 85%. Colorless crystal, mp 159-161 °C.

$^1\text{H NMR}$  ( $\text{CDCl}_3$ , 300 MHz, ppm)  $\delta$  8.22 (s, br, 1H), 8.08 (d, 1H,  $J = 7.9$  Hz), 7.68 (t, 1H,  $J = 4.6$  Hz), 7.52 (t, 1H,  $J = 4.6$  Hz), 7.36 (t, 1H,  $J = 7.4$  Hz), 7.30-7.27 (m, 2H), 6.76-6.69 (m, 2H), 3.02 (s, 3H).

$^{13}\text{C NMR}$  ( $\text{CDCl}_3$ , 150 MHz, ppm)  $\delta$  162.2, 148.2, 148.0, 140.6, 131.7, 127.8, 123.4, 123.1, 118.0, 113.9, 109.4, 109.0, 106.9, 28.6.

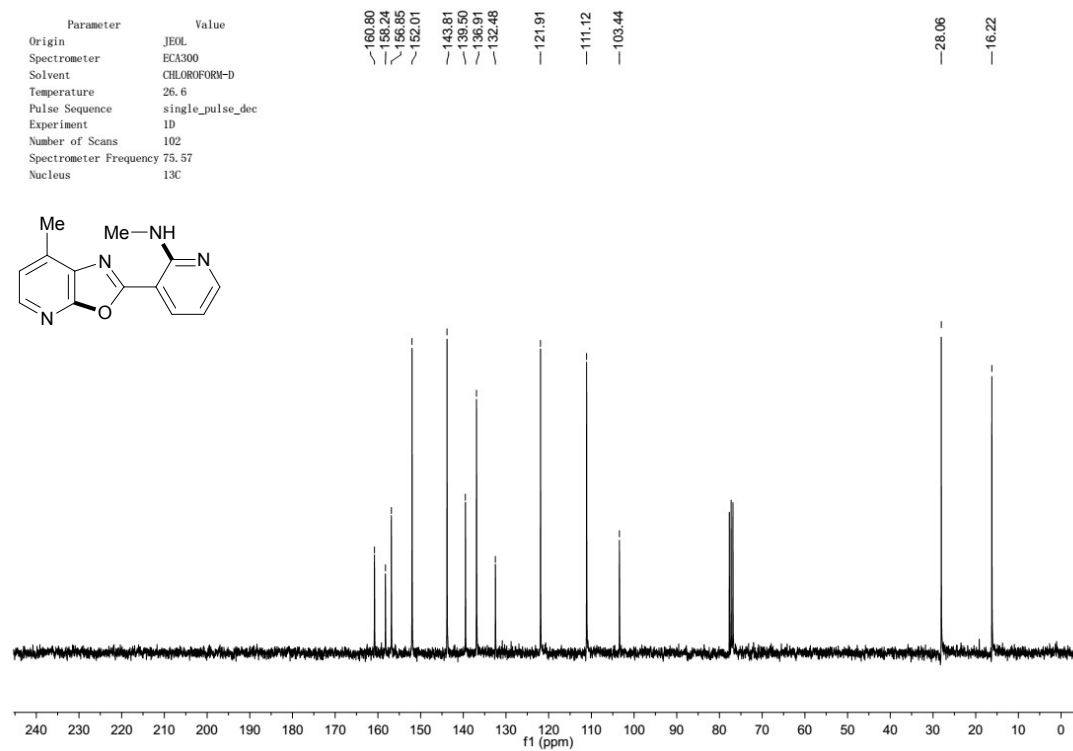
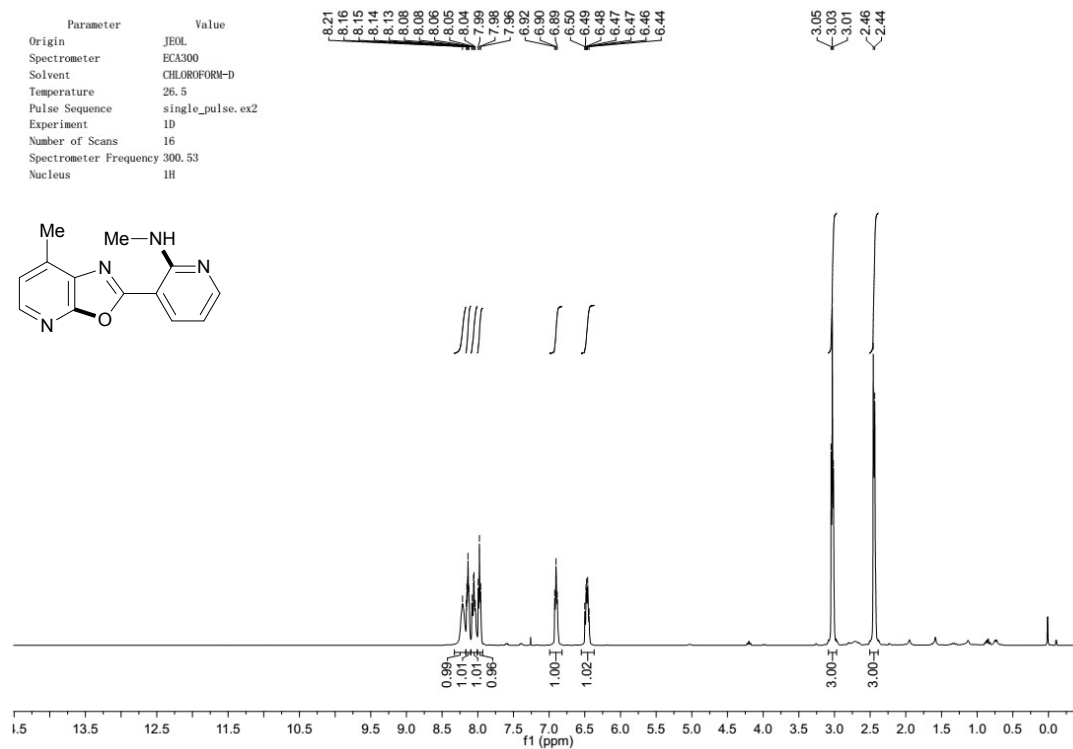
HRMS:  $m/z$  calcd for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}$  [ $\text{M}$ ] $^+$ : 224.0950. Found: 224.0953.

The NMR data are consistent with the reported ones.<sup>[1, 2]</sup>

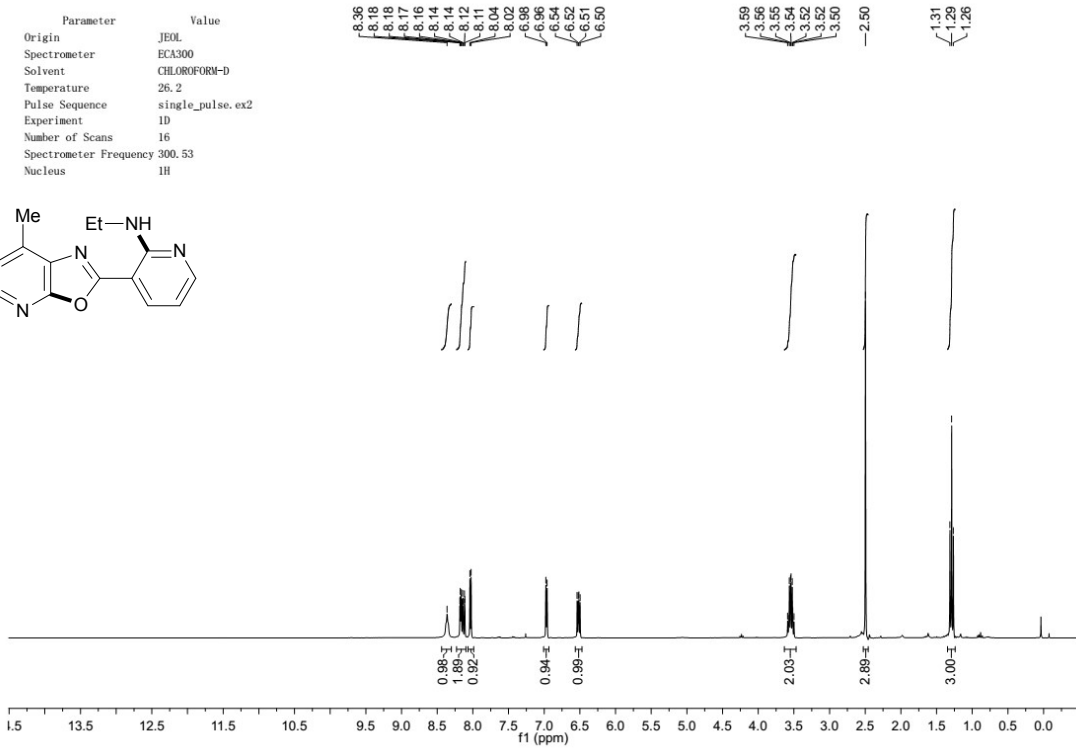
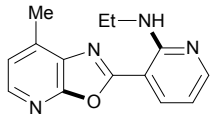
### 3. References

- [1] K. Wojciechowski, U. Siedlecka, H. Modrzejewska, S. Kosinski, *Tetrahedron*, 2002, **58**, 7583.
- [2] D. Miao, X. Shi, G. He, Y. Tong, Z. Jiang, S. Han, *Tetrahedron*, 2015, **71**, 431.

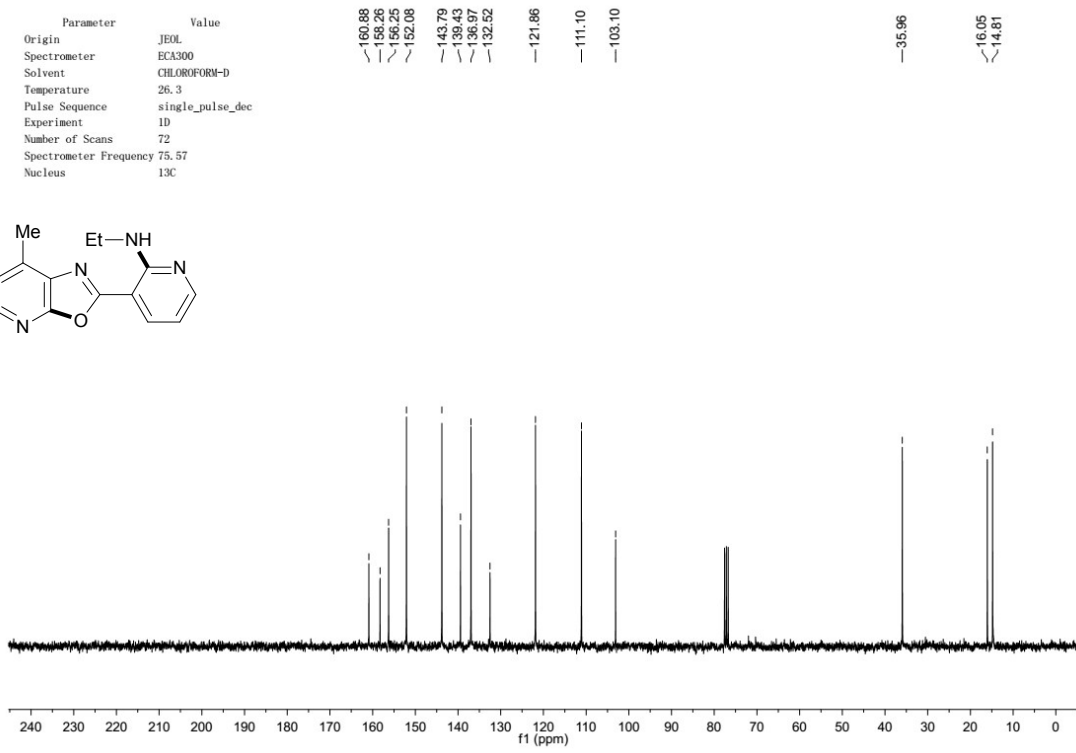
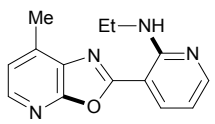
## 4. NMR Spectra



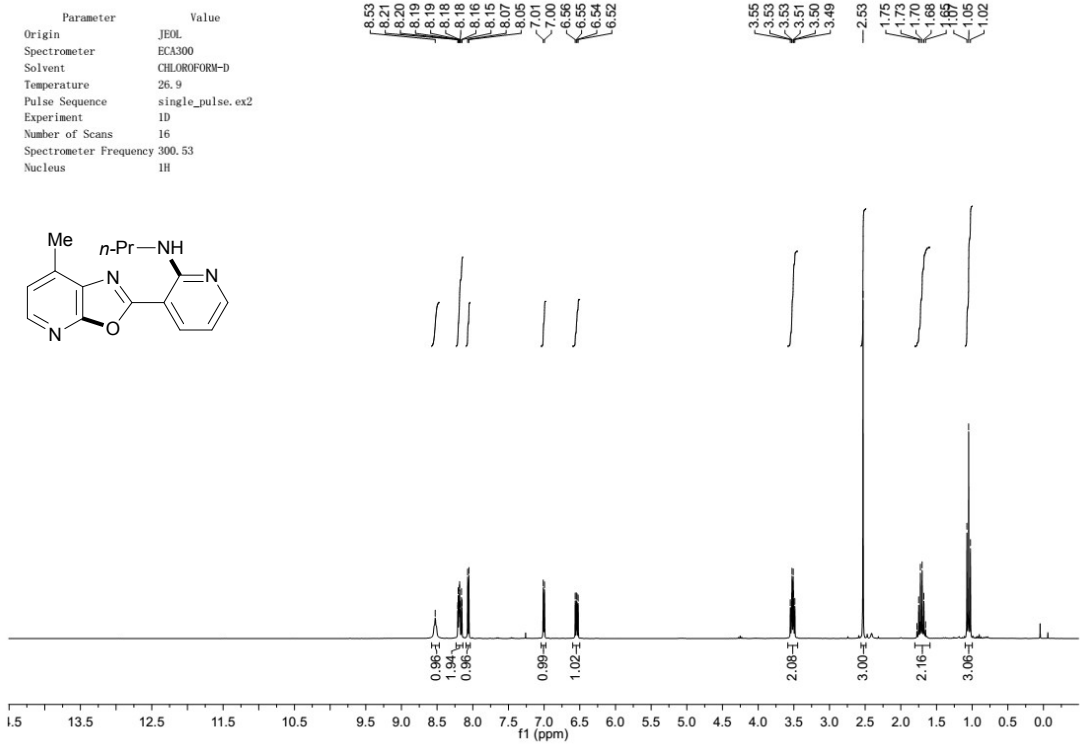
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Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	26.2
Pulse Sequence	single_pulse.ex2
Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	1H



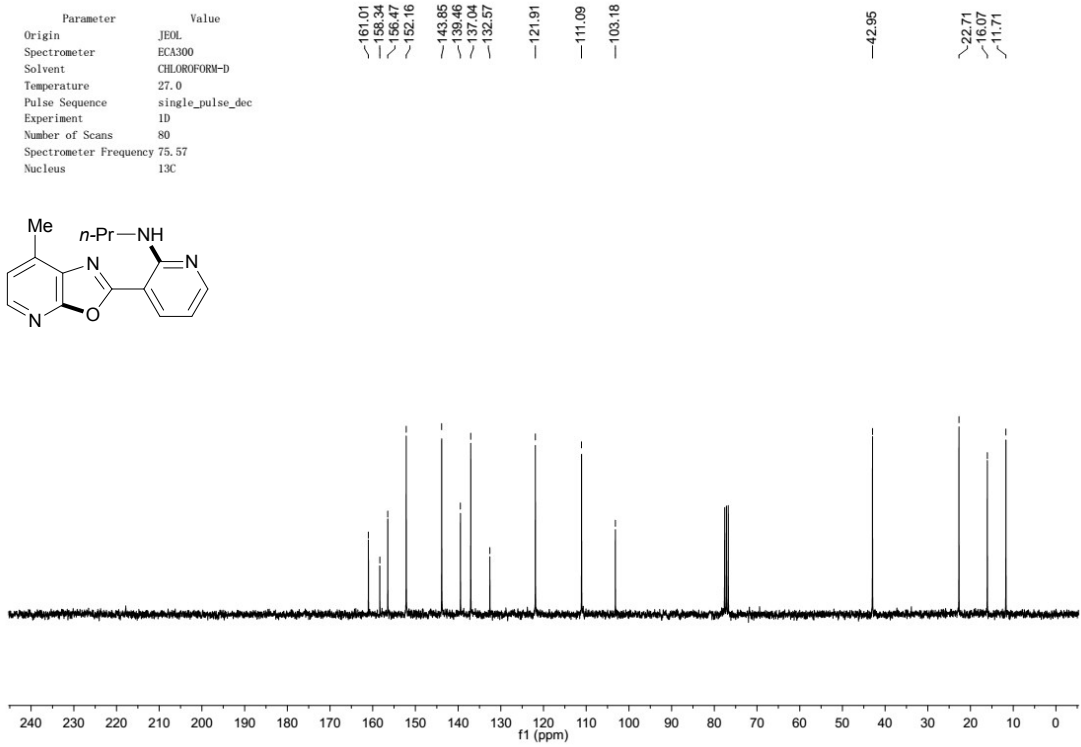
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Origin	JEOL
Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	26.3
Pulse Sequence	single_pulse_dec
Experiment	1D
Number of Scans	72
Spectrometer Frequency	75.57
Nucleus	13C



Parameter	Value
Origin	JEOL
Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	26.9
Pulse Sequence	single_pulse.ex2
Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	<sup>1</sup> H

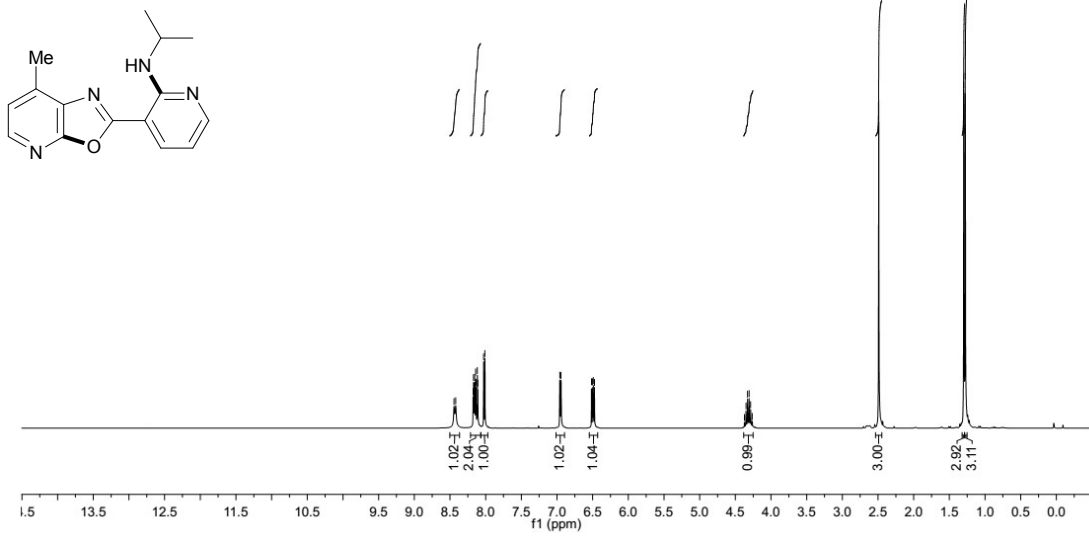


Parameter	Value
Origin	JEOL
Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	27.0
Pulse Sequence	single_pulse_dec
Experiment	1D
Number of Scans	80
Spectrometer Frequency	75.57
Nucleus	<sup>13</sup> C

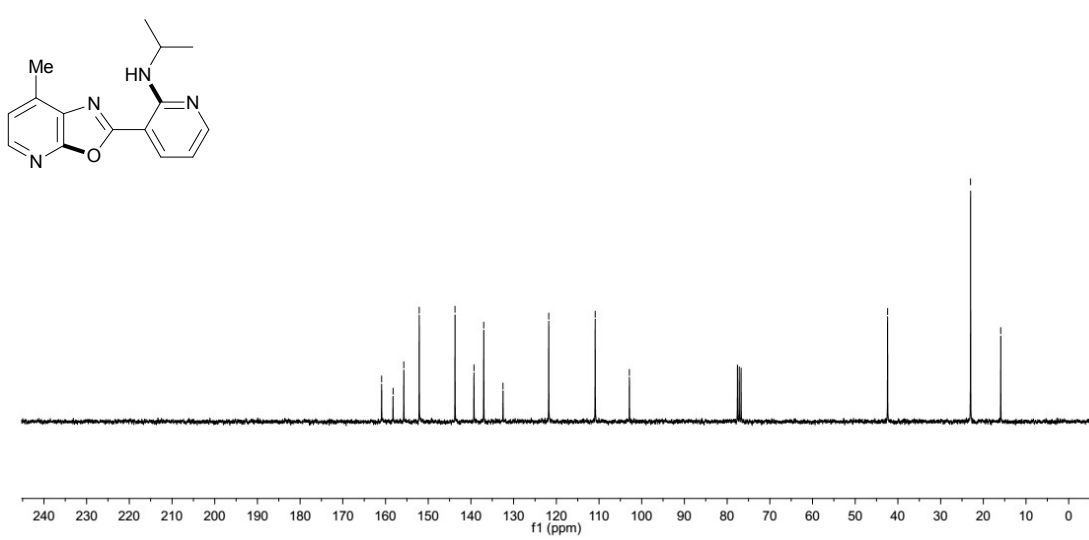




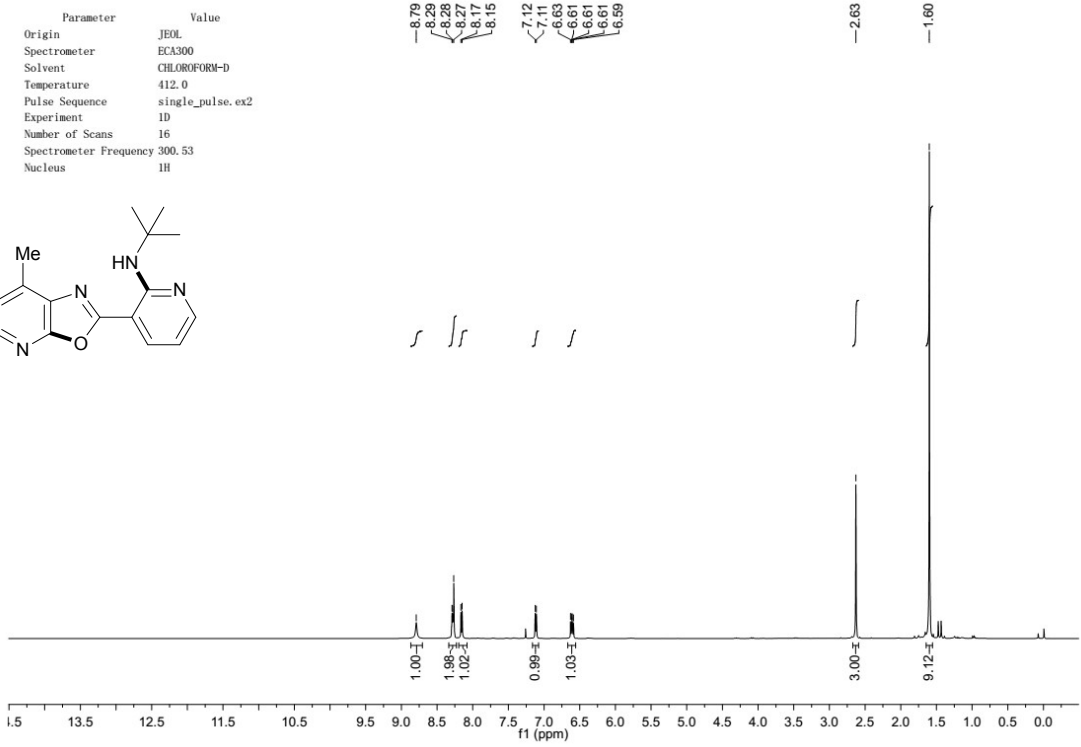
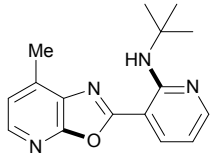
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Temperature	26.9
Pulse Sequence	single_pulse.ex2
Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	1H



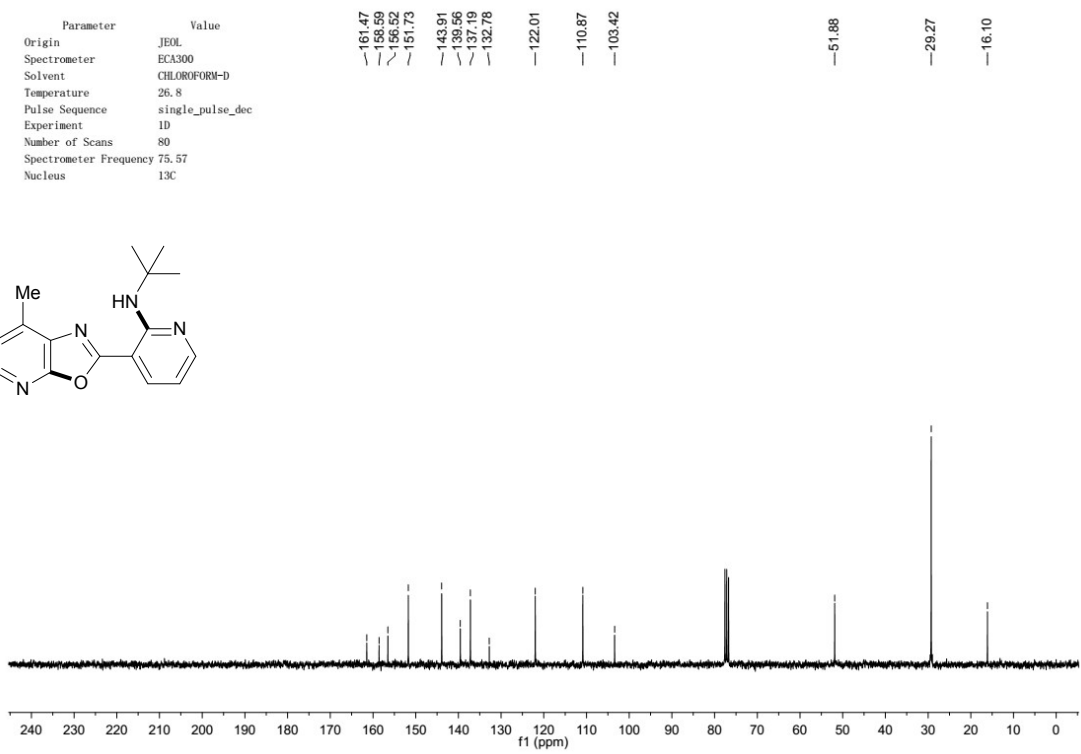
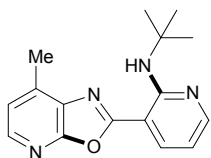
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Origin	JEOL
Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	27.0
Pulse Sequence	single_pulse_dec
Experiment	1D
Number of Scans	72
Spectrometer Frequency	75.57
Nucleus	13C



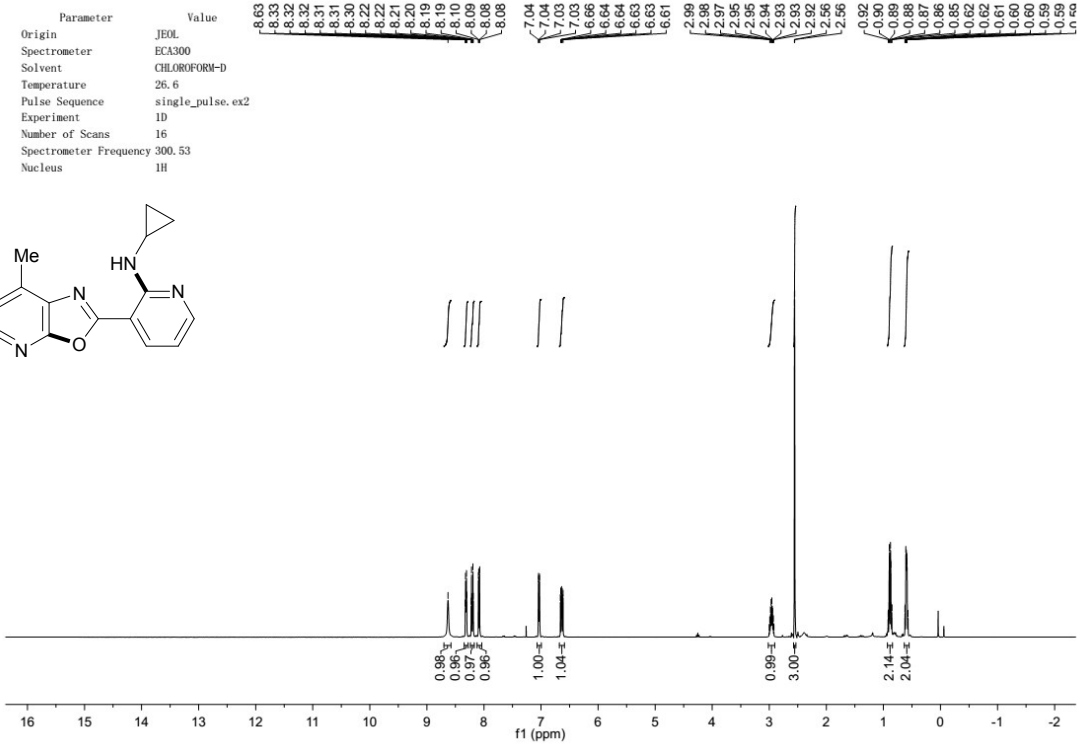
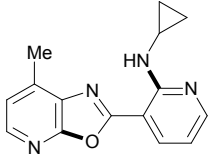
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Temperature	412.0
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Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	<sup>1</sup> H



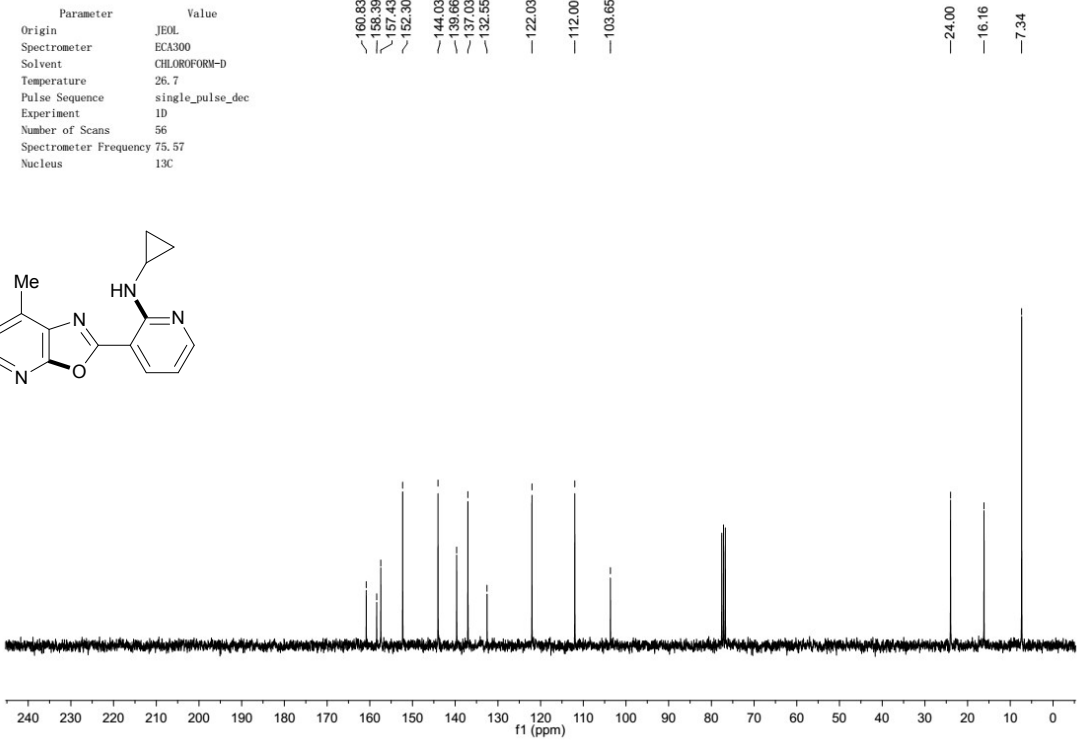
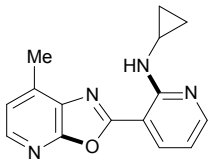
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Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	26.8
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Experiment	1D
Number of Scans	80
Spectrometer Frequency	75.57
Nucleus	<sup>13</sup> C



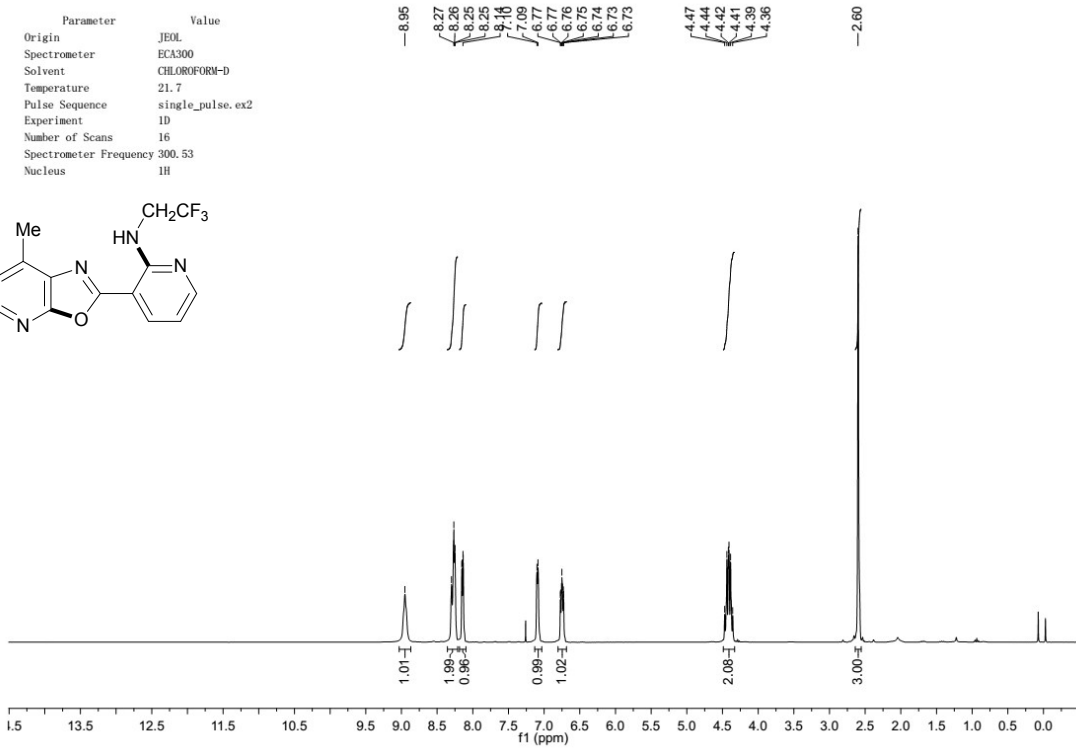
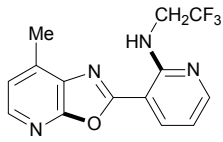
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 Spectrometer Frequency 300.53  
 Nucleus 1H



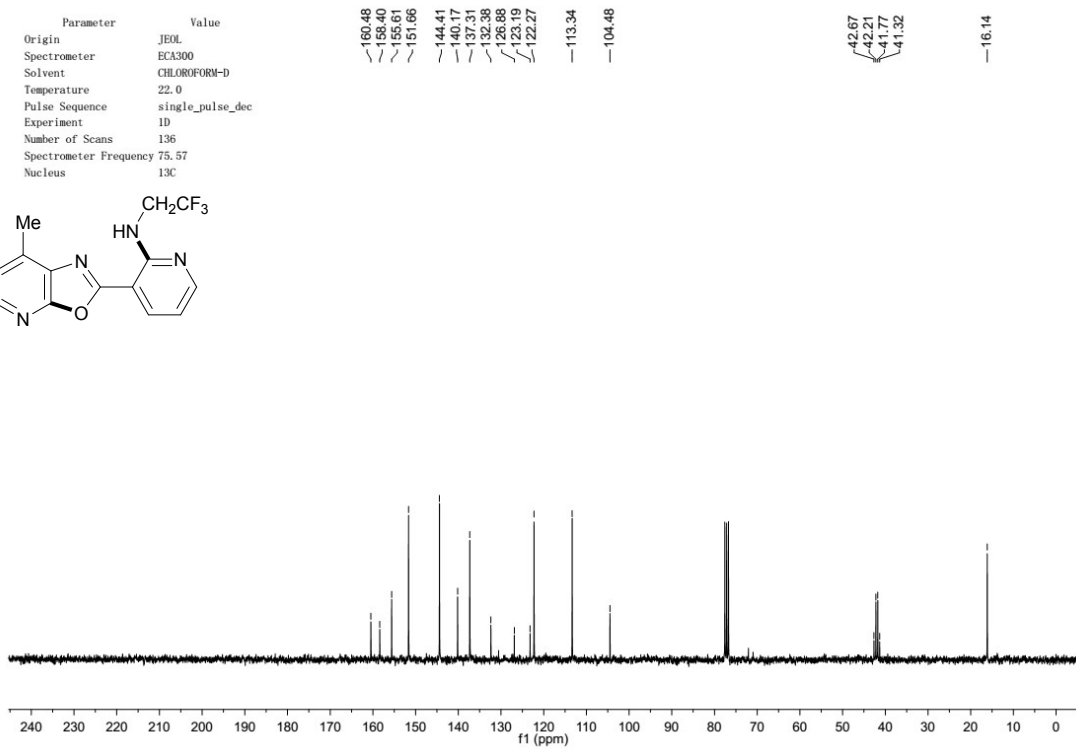
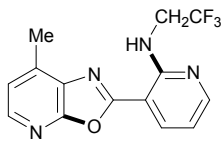
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 Spectrometer Frequency 75.57  
 Nucleus 13C



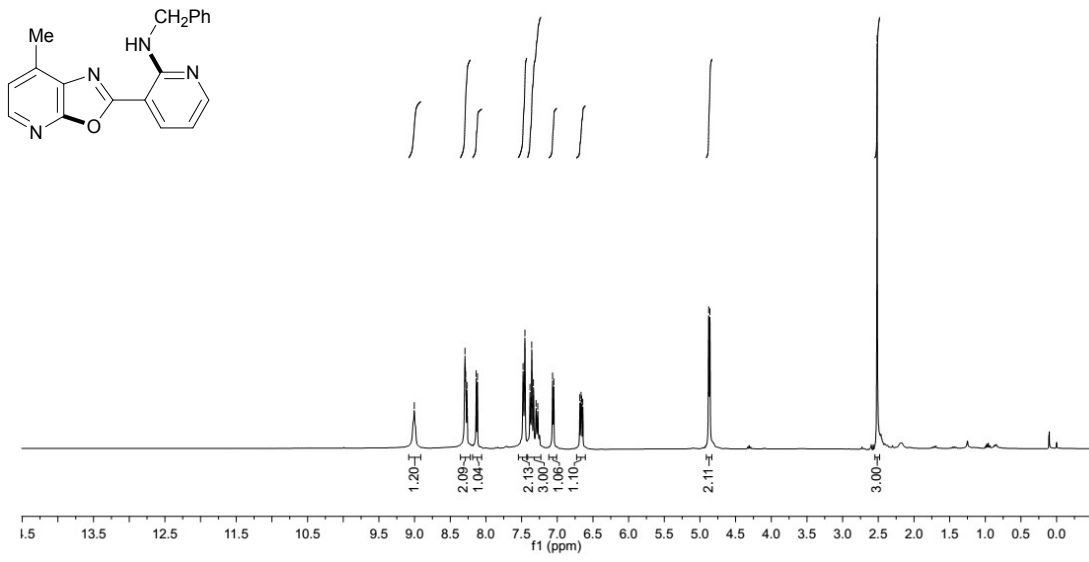
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Spectrometer	ECA300
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Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	1H



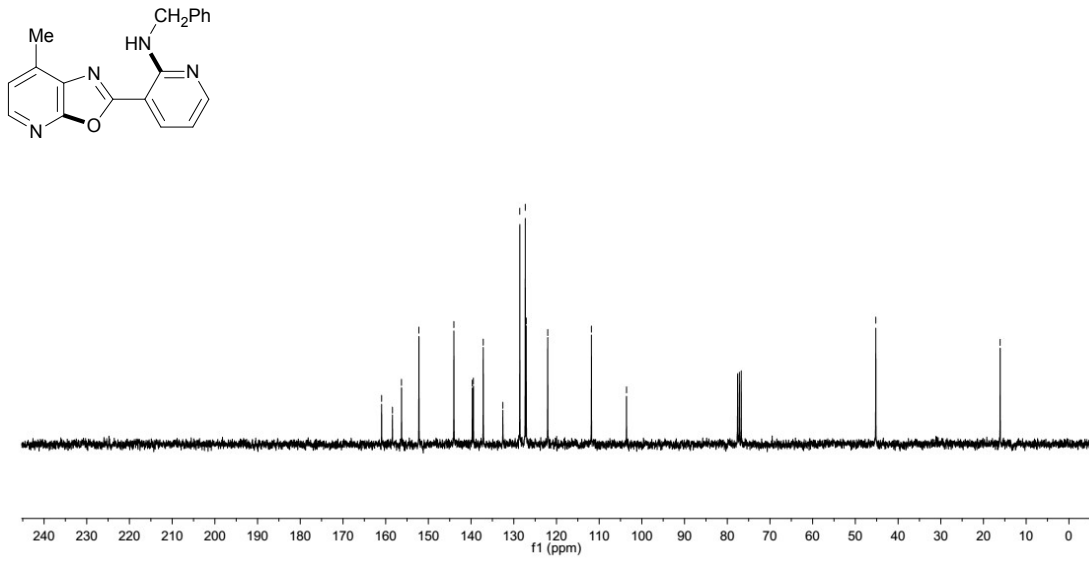
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Experiment	1D
Number of Scans	136
Spectrometer Frequency	75.57
Nucleus	13C

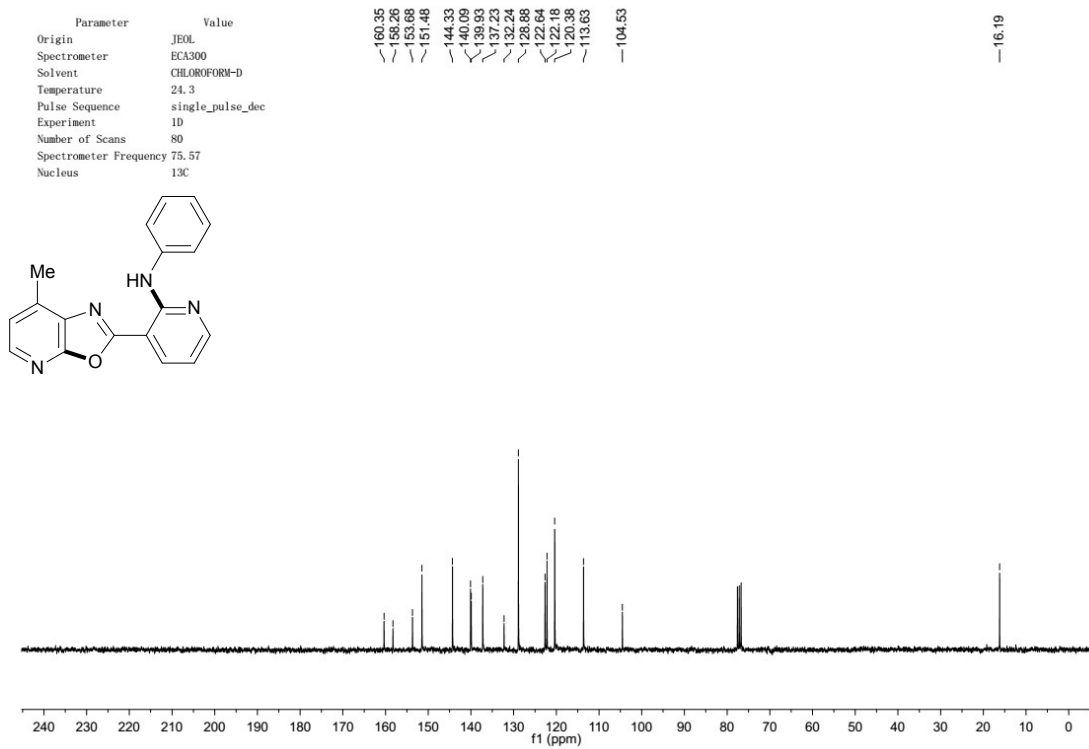
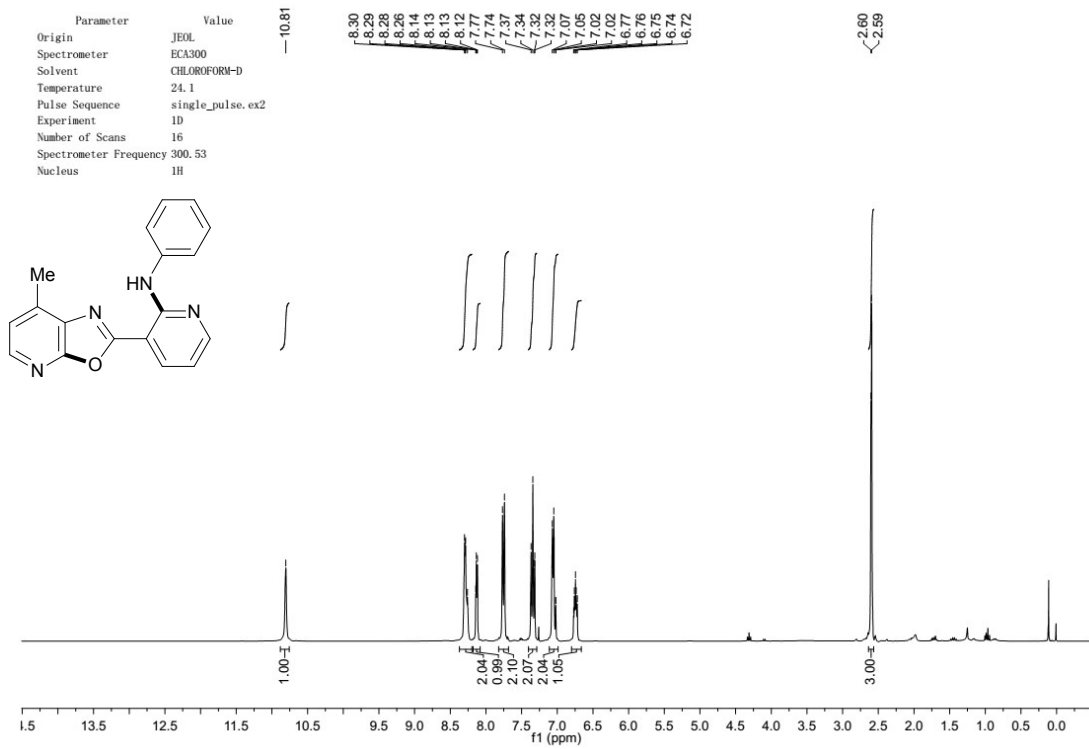


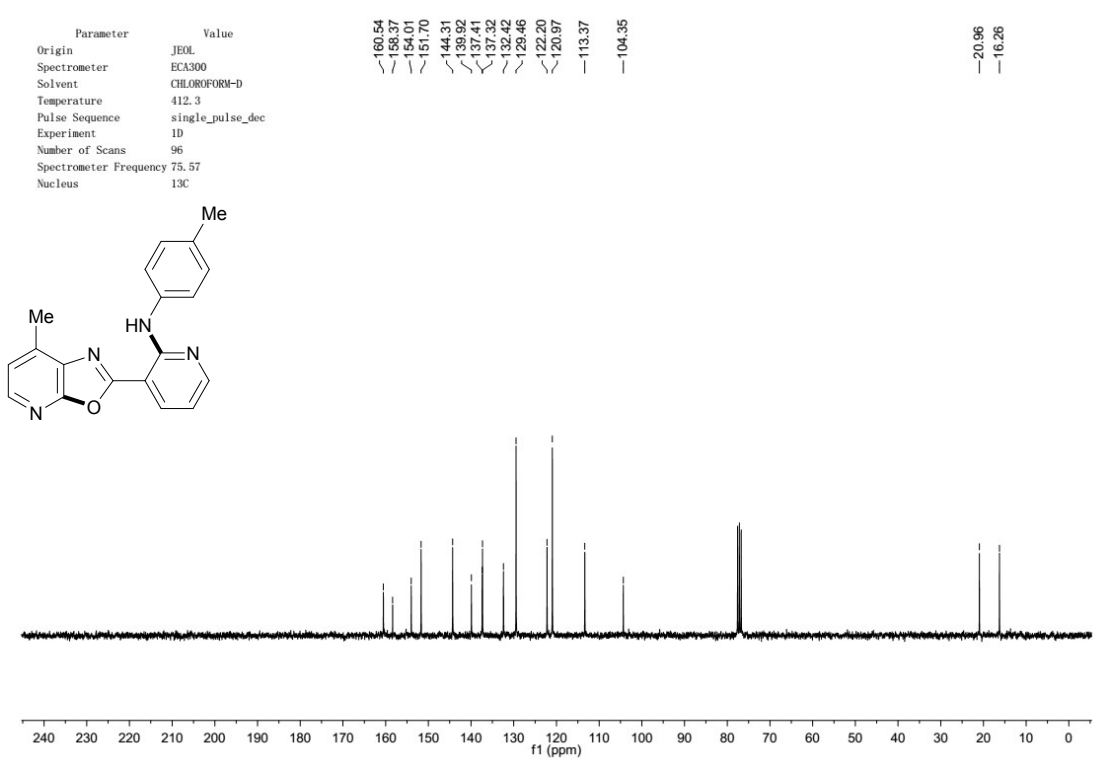
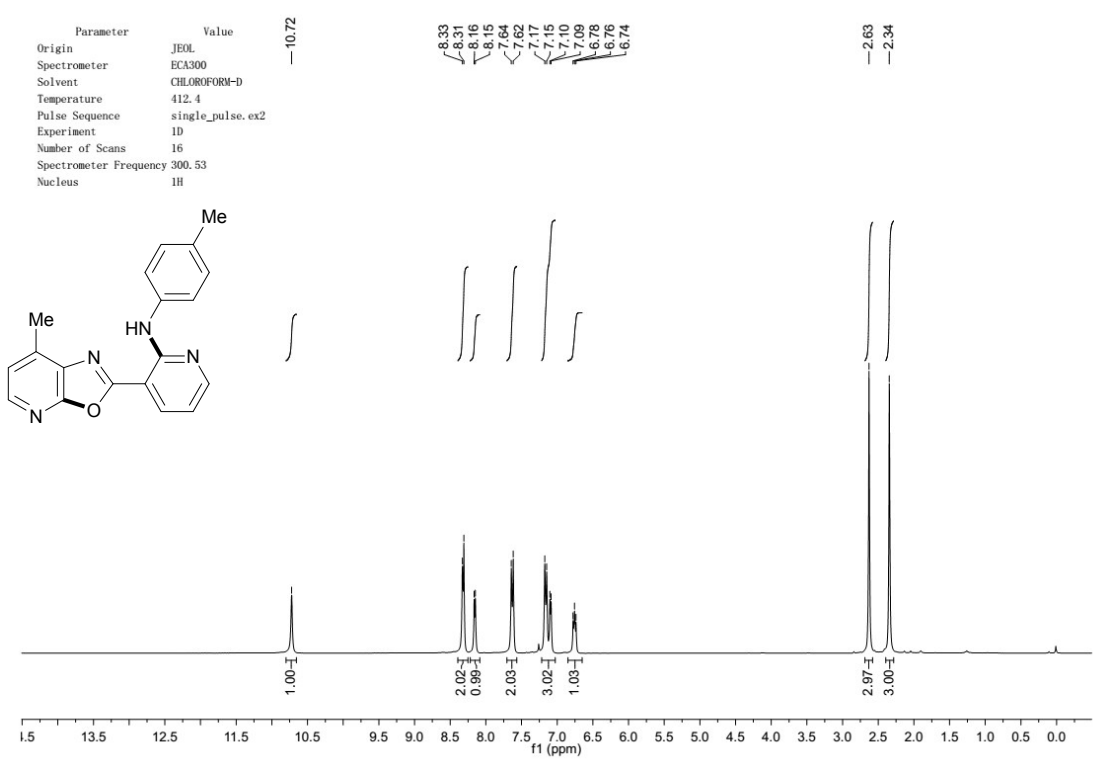
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Temperature	25.8
Pulse Sequence	single_pulse.ex2
Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	1H

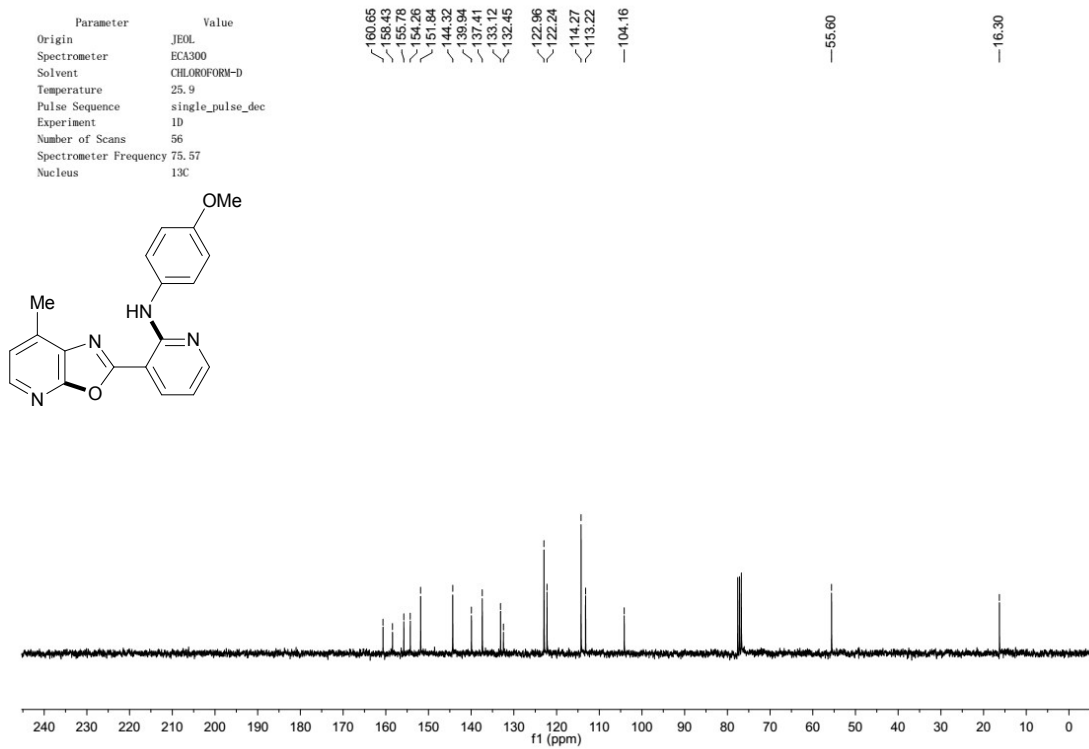
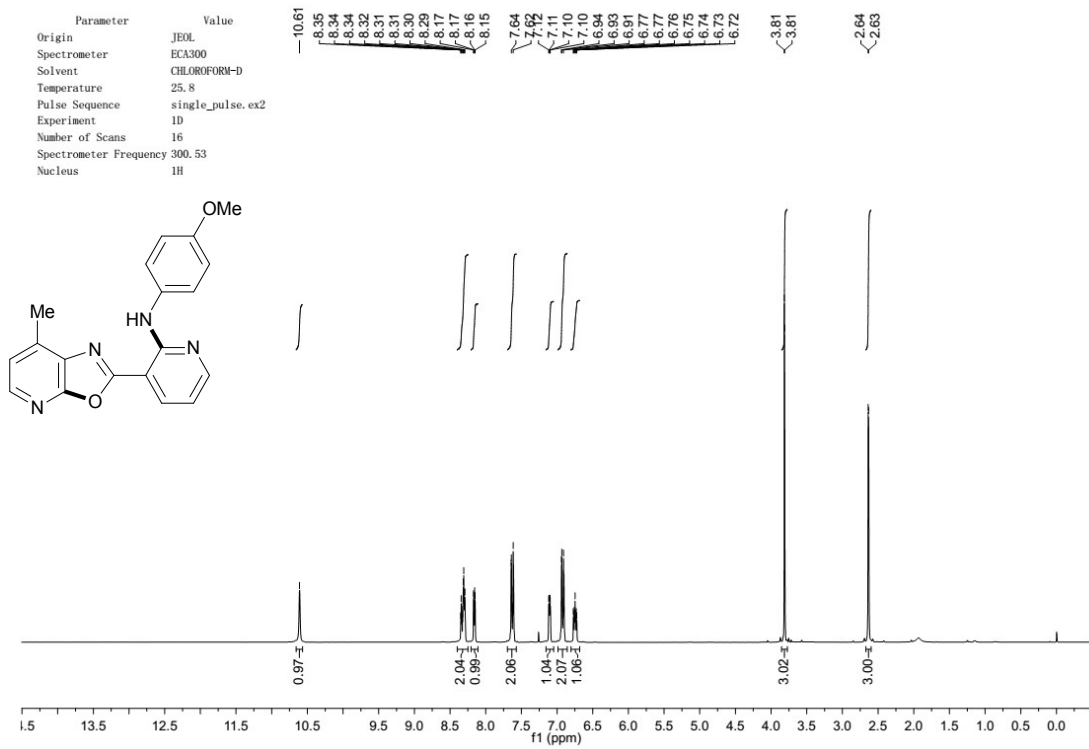


Parameter	Value
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Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	25.9
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Experiment	1D
Number of Scans	64
Spectrometer Frequency	75.57
Nucleus	13C



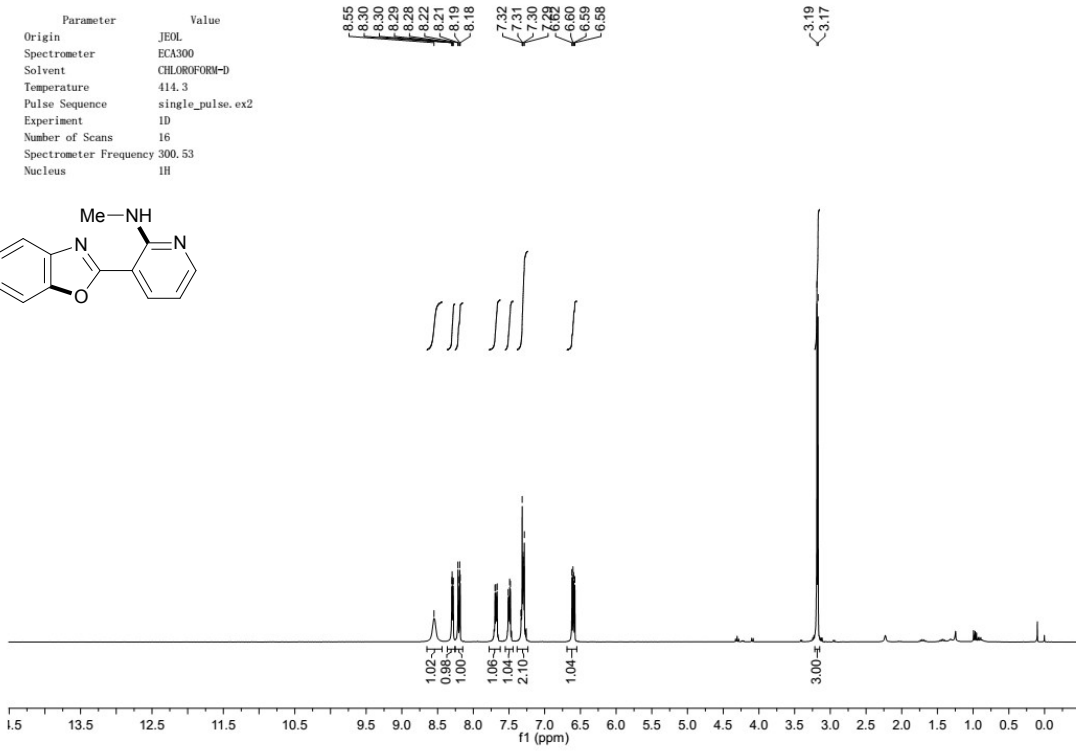
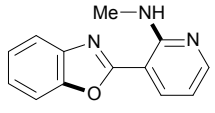




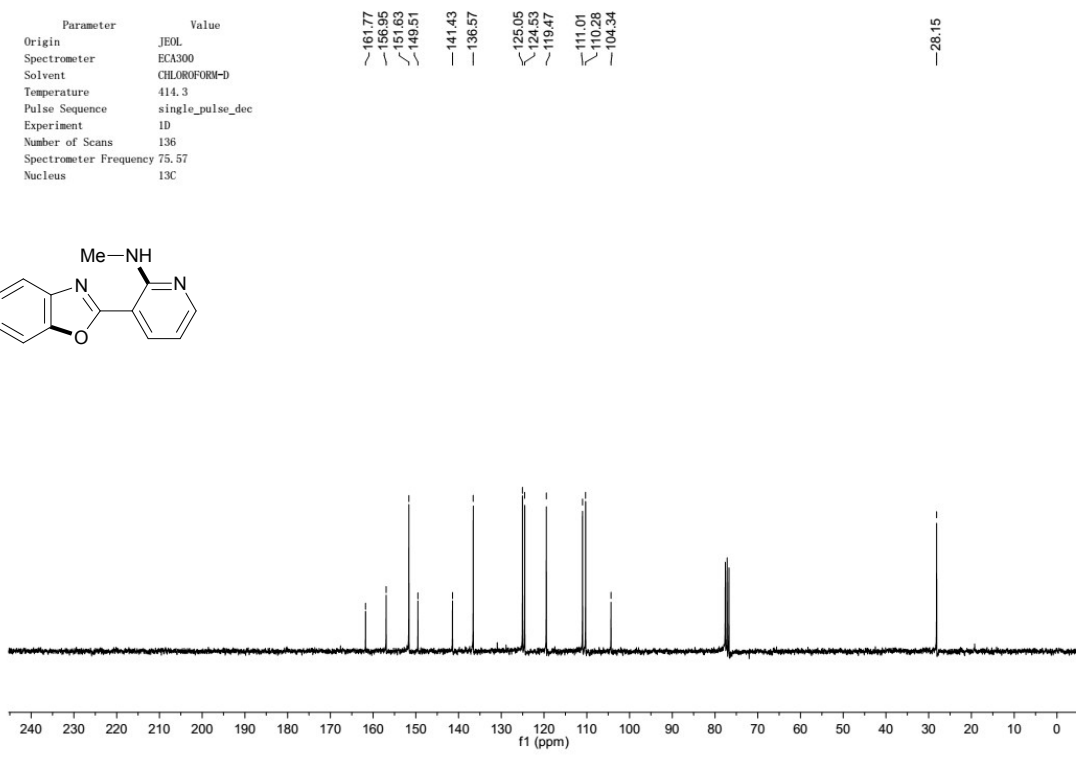
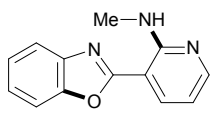




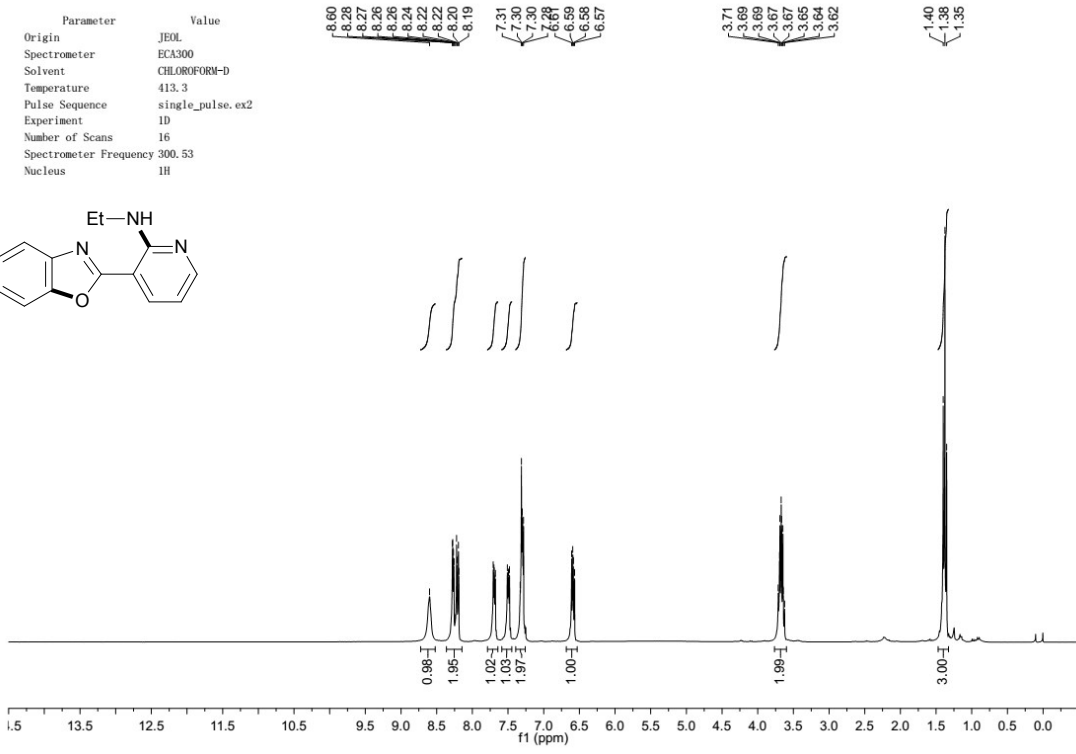
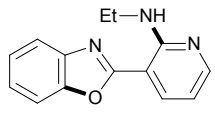
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Origin	JEOL
Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	414.3
Pulse Sequence	single_pulse_ex2
Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	1H



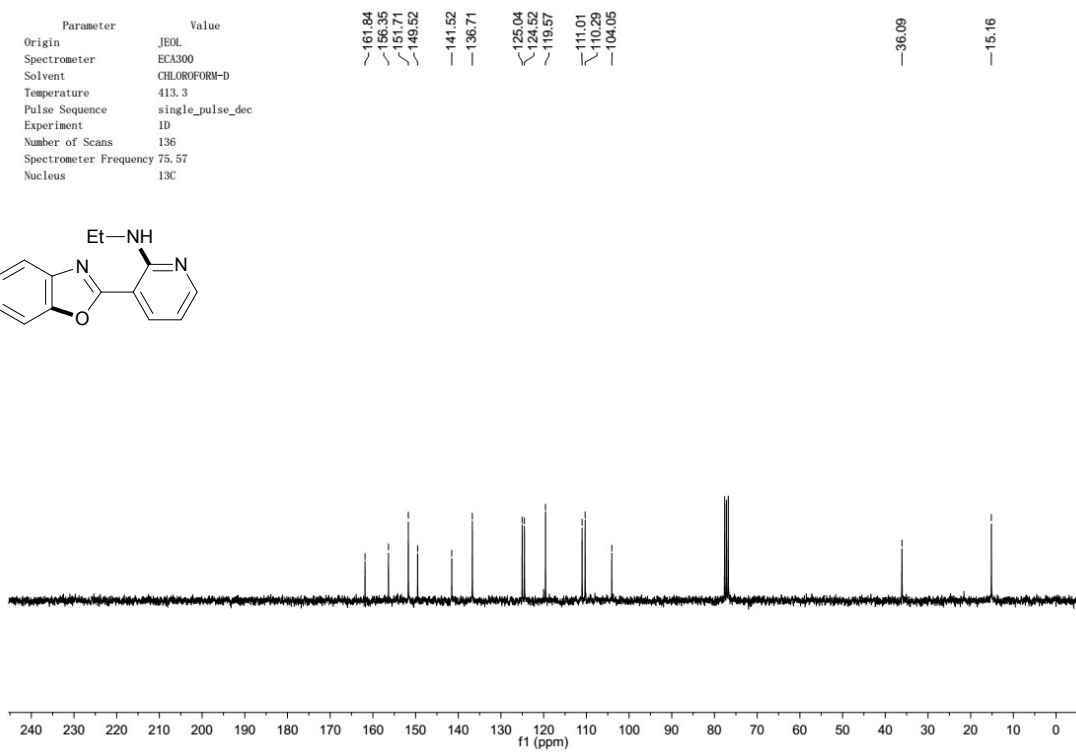
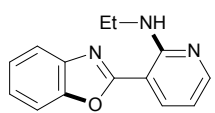
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Experiment	1D
Number of Scans	136
Spectrometer Frequency	75.57
Nucleus	13C



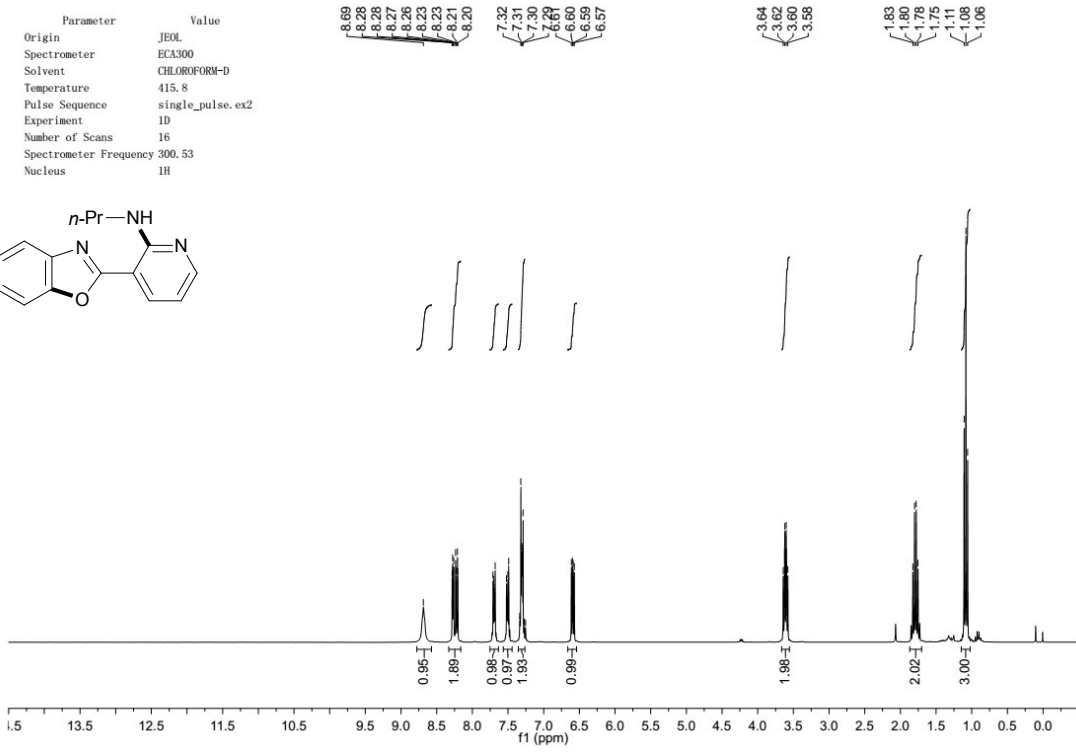
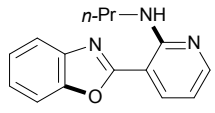
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 Nucleus 1H



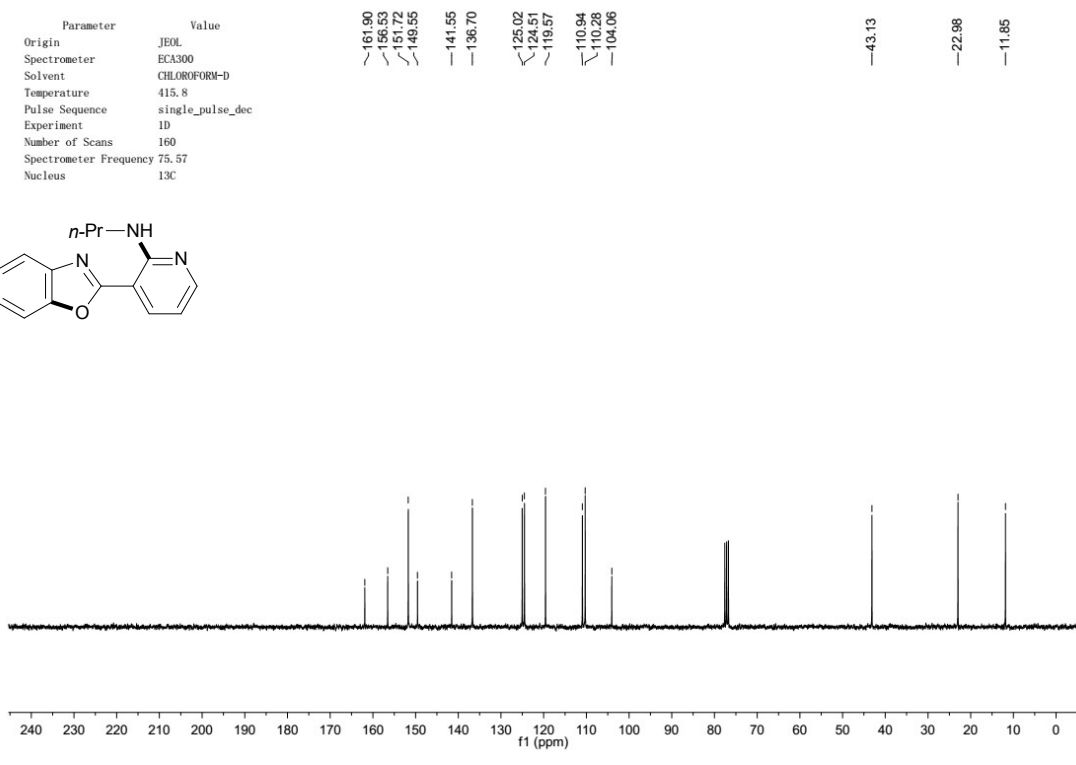
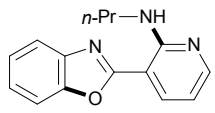
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 Spectrometer Frequency 75.57  
 Nucleus 13C



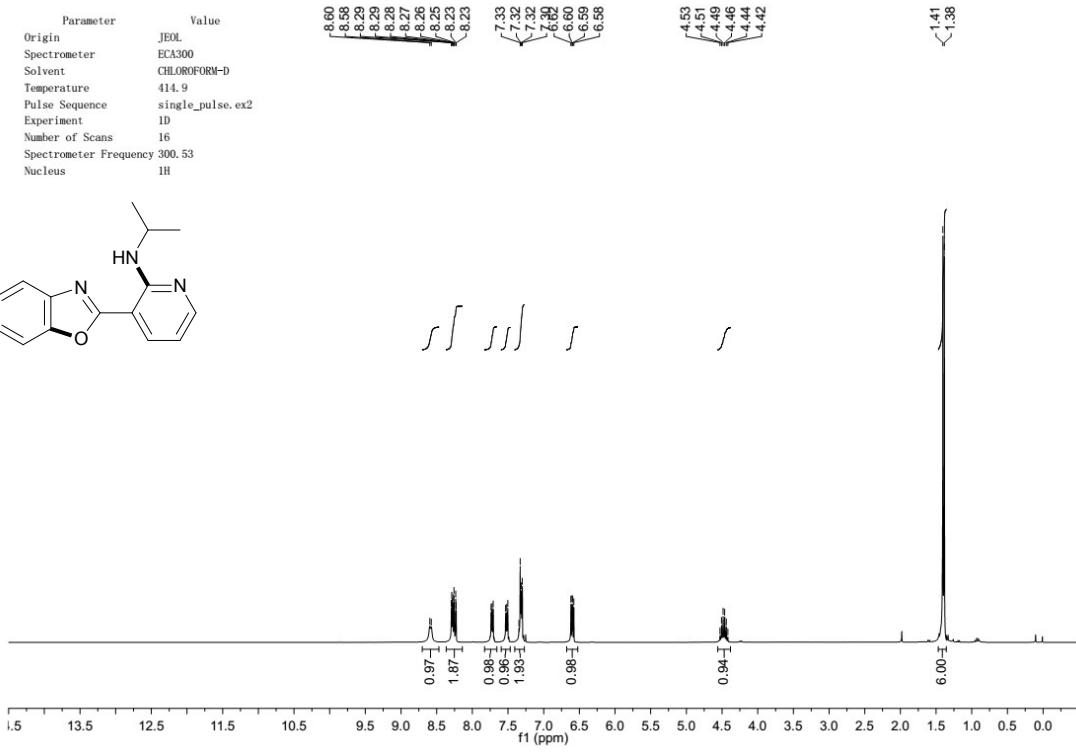
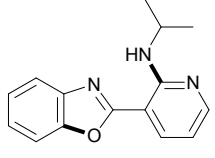
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Temperature	415.8
Pulse Sequence	single_pulse.ex2
Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	1H



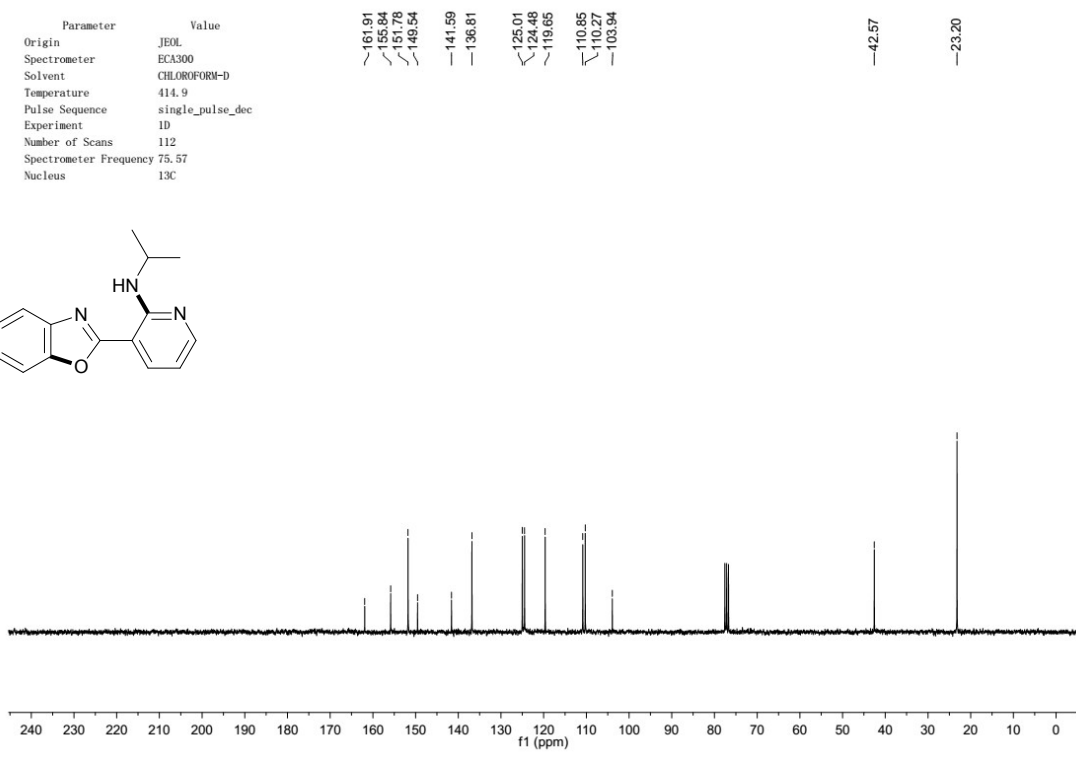
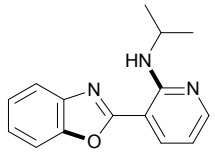
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Nucleus	13C



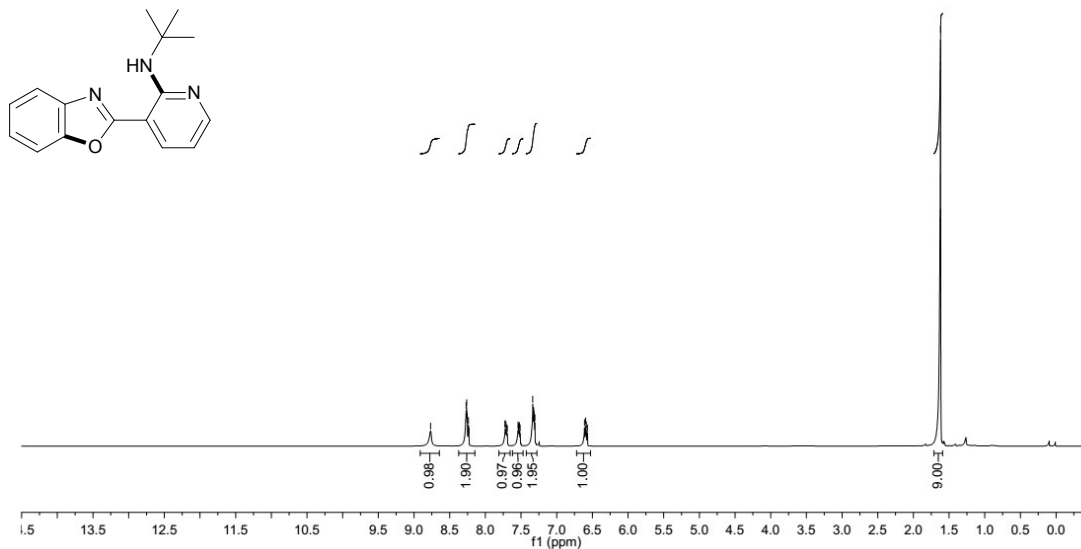
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 Nucleus 1H



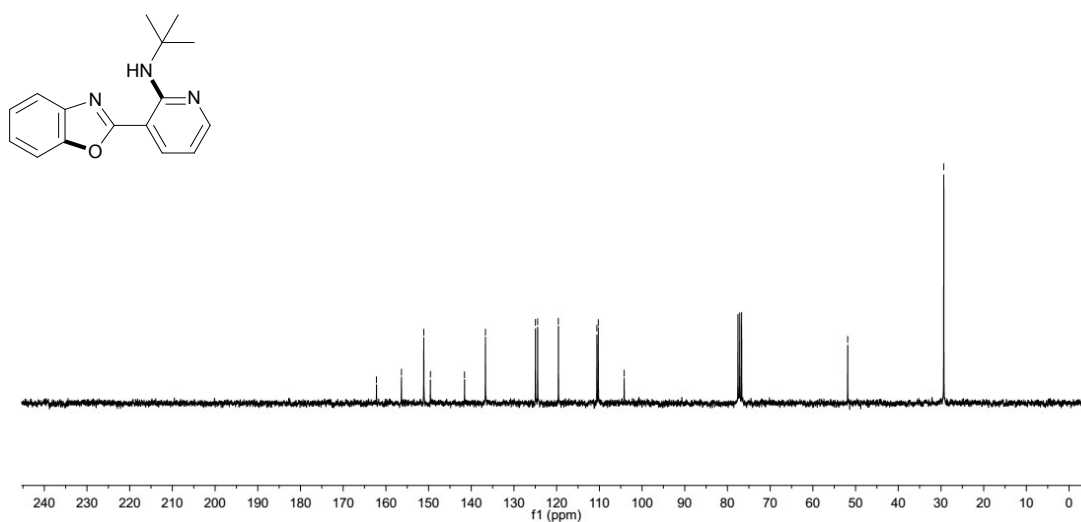
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 Nucleus 13C



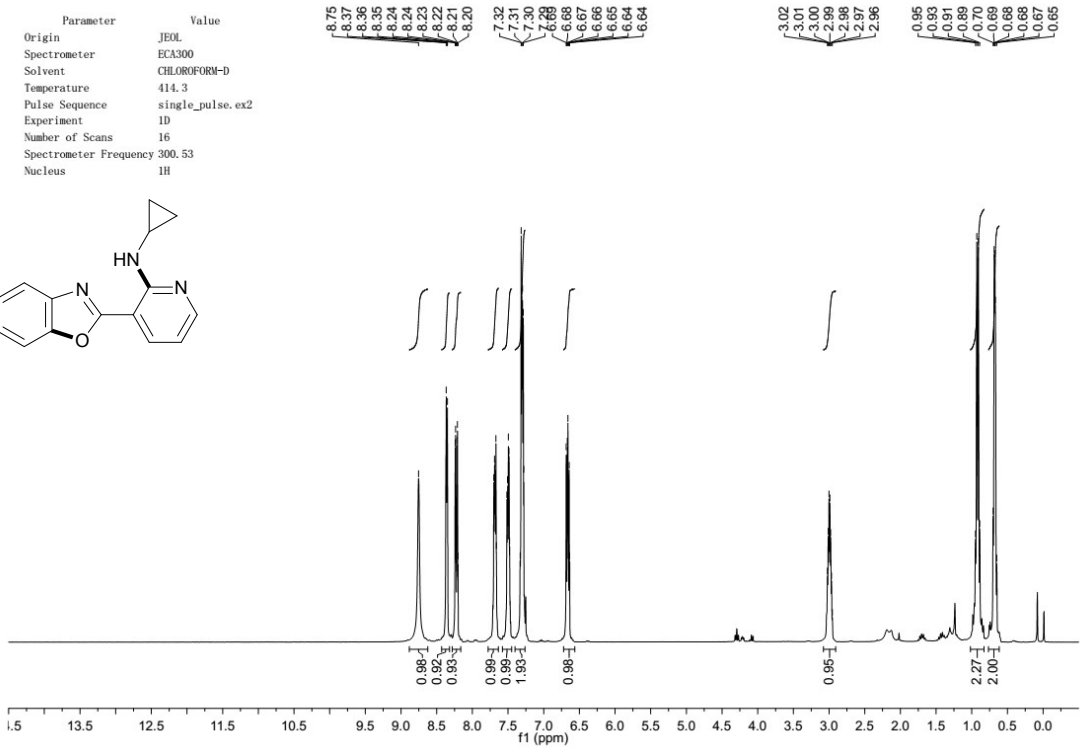
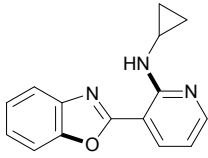
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Solvent	CHLOROFORM-D
Temperature	26.9
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Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	1H



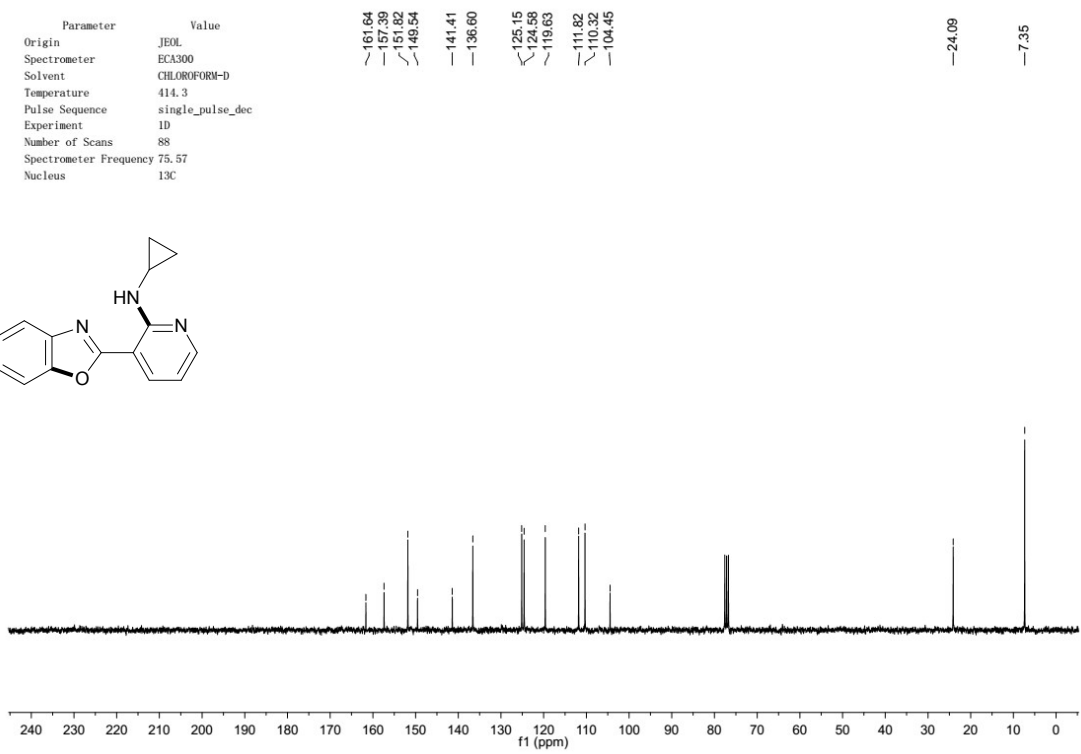
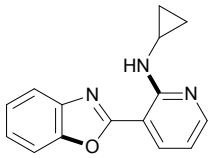
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Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	27.0
Pulse Sequence	single_pulse_dec
Experiment	1D
Number of Scans	128
Spectrometer Frequency	75.57
Nucleus	13C



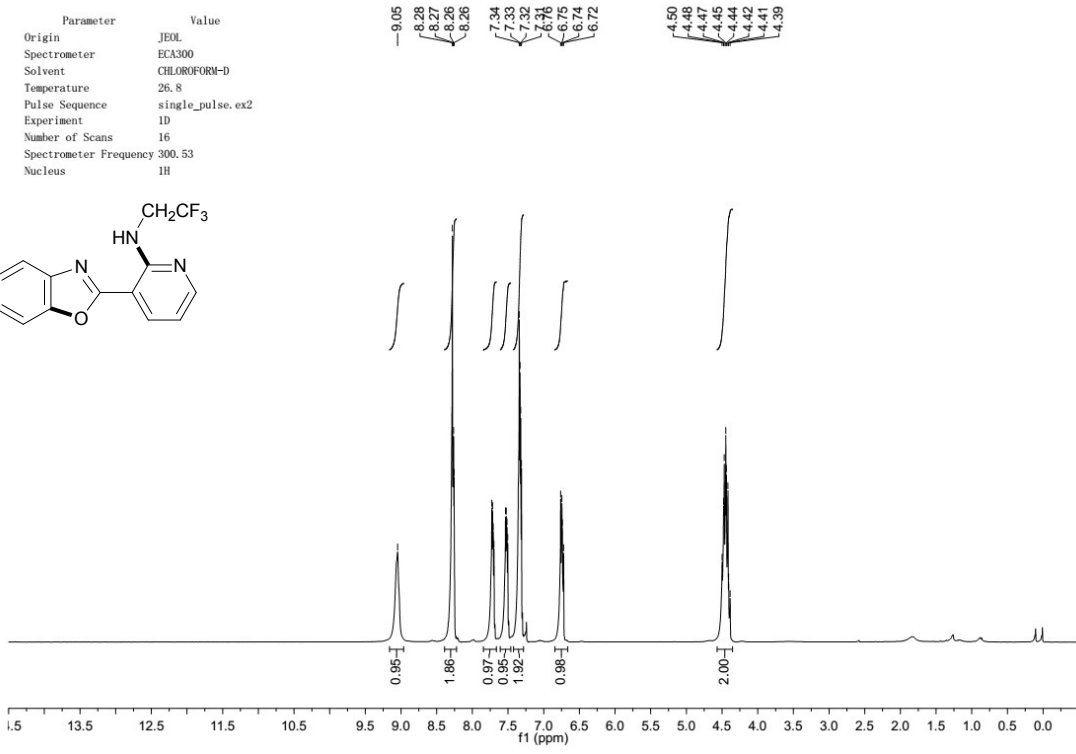
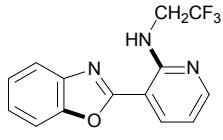
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 Spectrometer ECA300  
 Solvent CHLOROFORM-D  
 Temperature 414.3  
 Pulse Sequence single\_pulse.ex2  
 Experiment 1D  
 Number of Scans 16  
 Spectrometer Frequency 300.53  
 Nucleus 1H



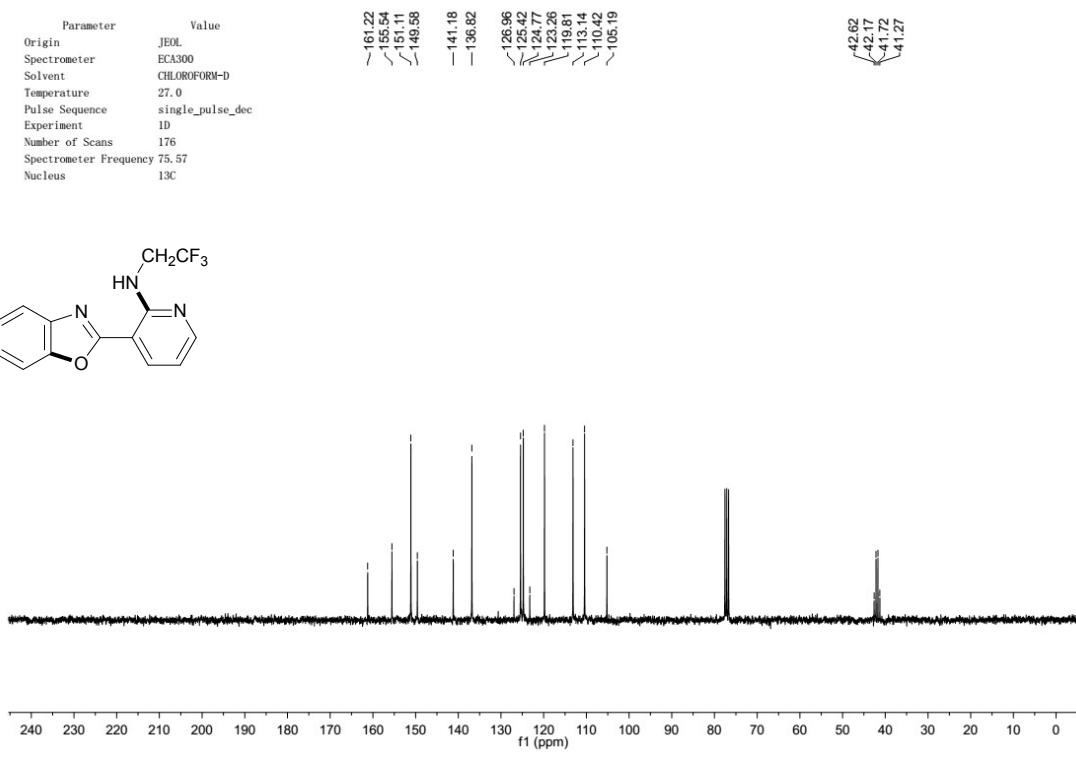
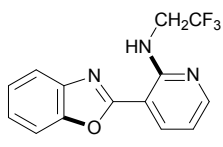
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 Solvent CHLOROFORM-D  
 Temperature 414.3  
 Pulse Sequence single\_pulse\_dec  
 Experiment 1D  
 Number of Scans 88  
 Spectrometer Frequency 75.57  
 Nucleus 13C



Parameter Value  
 Origin JEOL  
 Spectrometer ECA300  
 Solvent CHLOROFORM-D  
 Temperature 26.8  
 Pulse Sequence single\_pulse.ex2  
 Experiment 1D  
 Number of Scans 16  
 Spectrometer Frequency 300.53  
 Nucleus 1H

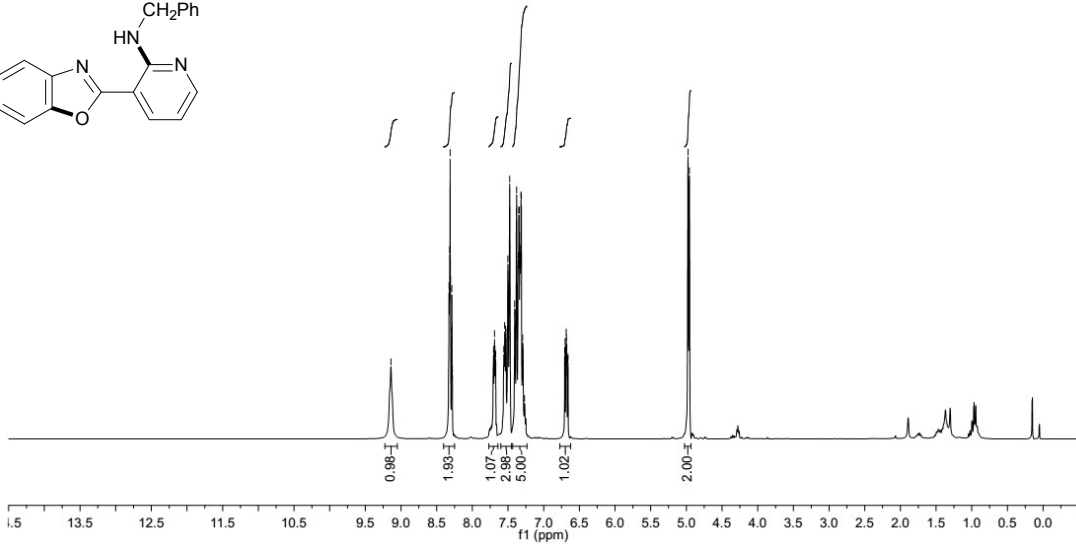
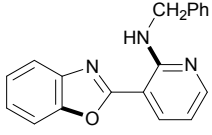


Parameter Value  
 Origin JEOL  
 Spectrometer ECA300  
 Solvent CHLOROFORM-D  
 Temperature 27.0  
 Pulse Sequence single\_pulse\_dec  
 Experiment 1D  
 Number of Scans 176  
 Spectrometer Frequency 75.57  
 Nucleus 13C



Parameter Value  
 Origin JEOL  
 Spectrometer ECA300  
 Solvent CHLOROFORM-D  
 Temperature 414.1  
 Pulse Sequence single\_pulse.ex2  
 Experiment 1D  
 Number of Scans 16  
 Spectrometer Frequency 300.53  
 Nucleus 1H

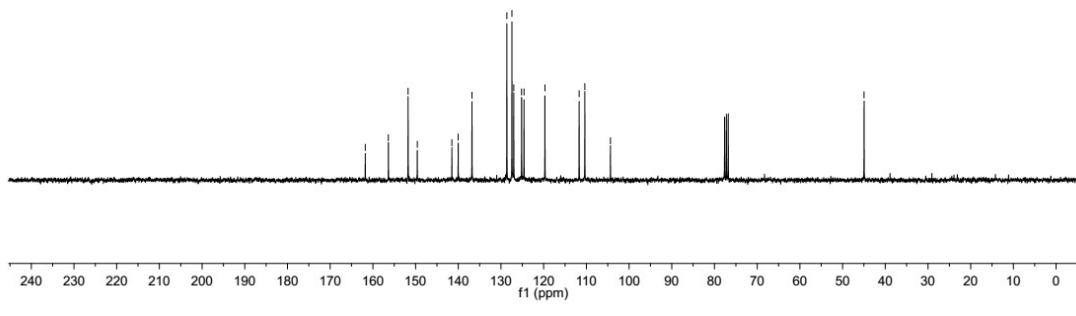
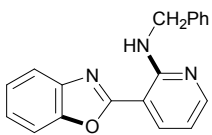
9.14  
 8.33  
 8.32  
 8.31  
 8.31  
 7.48  
 7.36  
 7.32  
 7.27  
 6.70  
 6.69  
 6.68  
 6.68  
 6.68  
 6.68  
 4.98  
 4.96



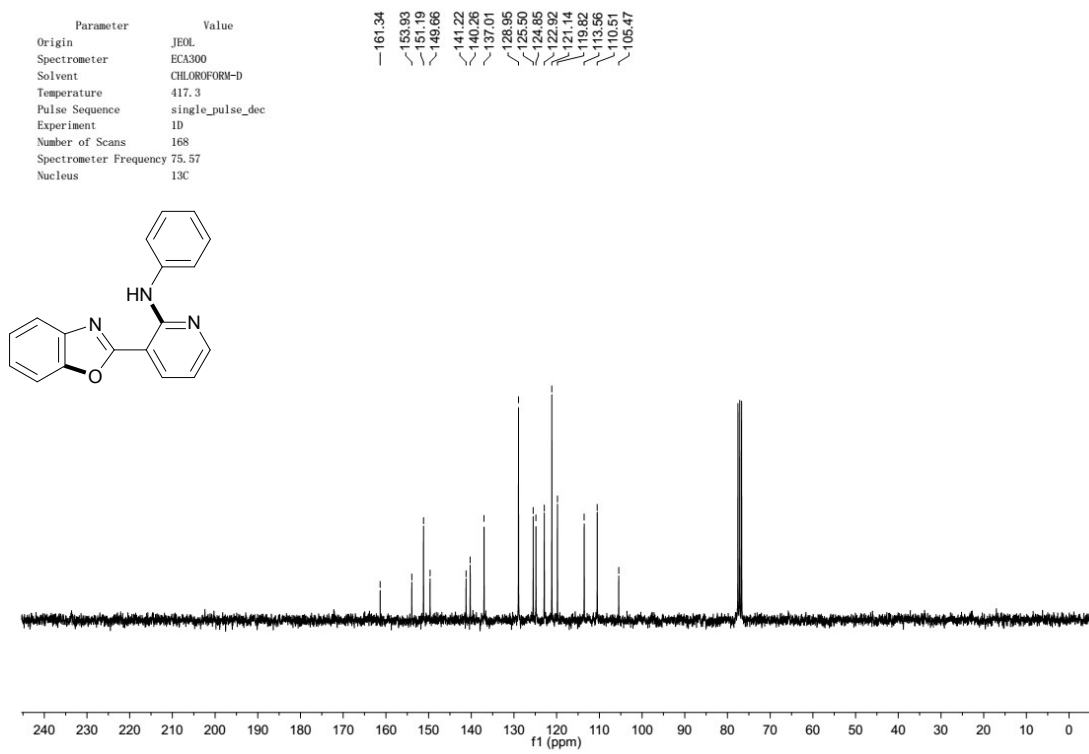
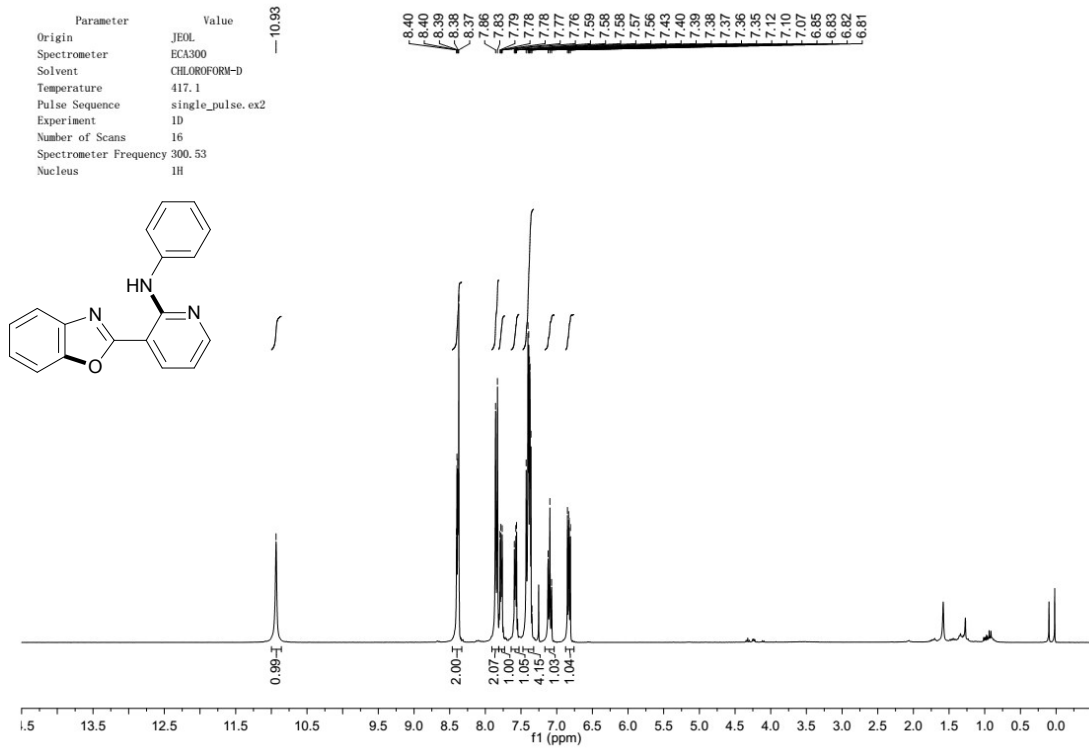
Parameter Value  
 Origin JEOL  
 Spectrometer ECA300  
 Solvent CHLOROFORM-D  
 Temperature 414.1  
 Pulse Sequence single\_pulse\_dec  
 Experiment 1D  
 Number of Scans 104  
 Spectrometer Frequency 75.57  
 Nucleus 13C

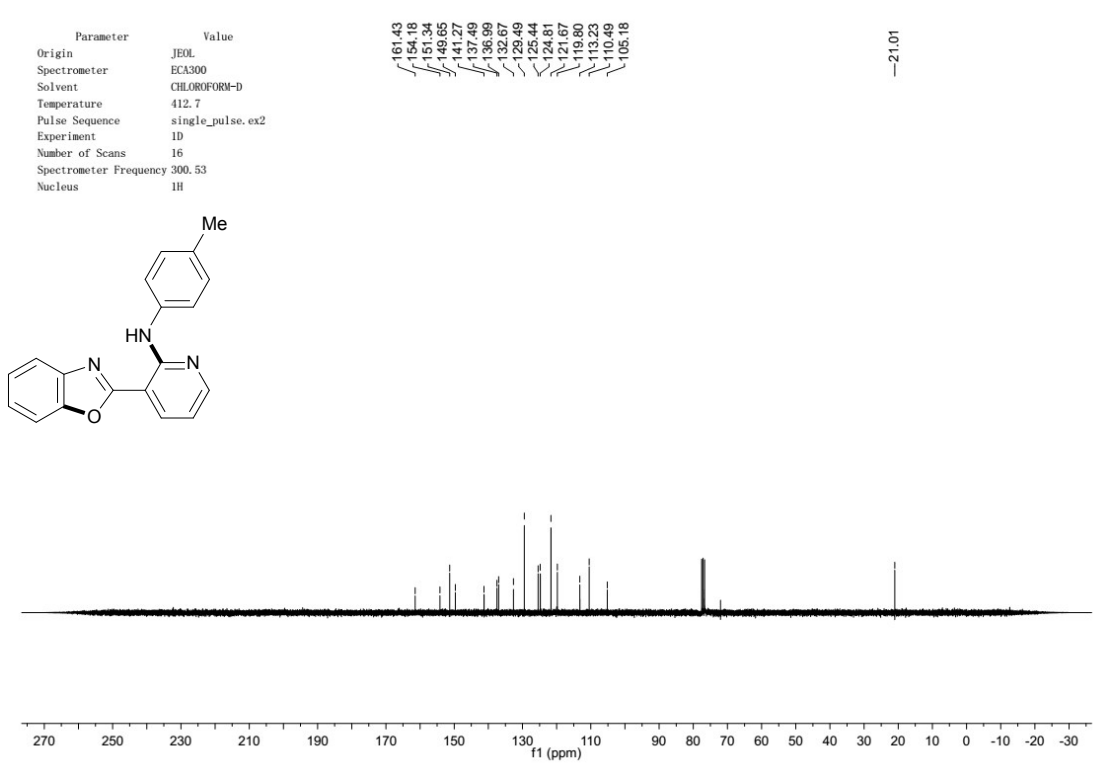
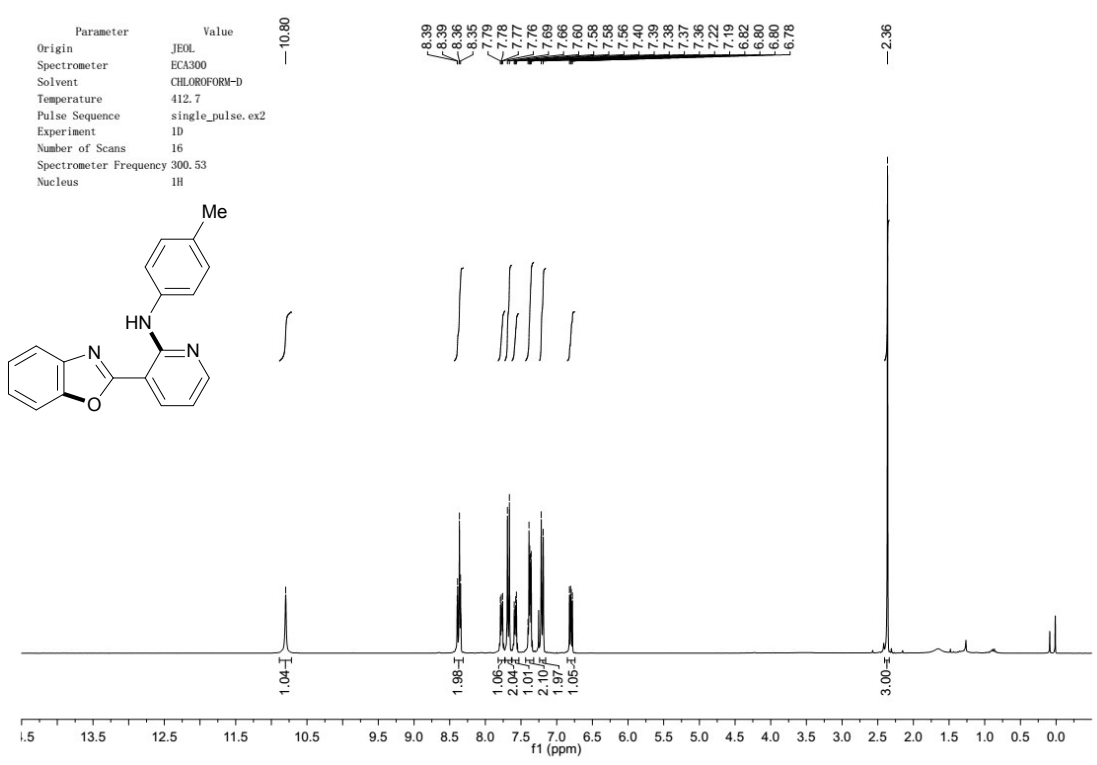
161.78  
 156.37  
 151.76  
 148.60  
 141.50  
 140.03  
 136.80  
 128.63  
 127.44  
 127.02  
 124.61  
 119.70  
 110.36  
 104.37

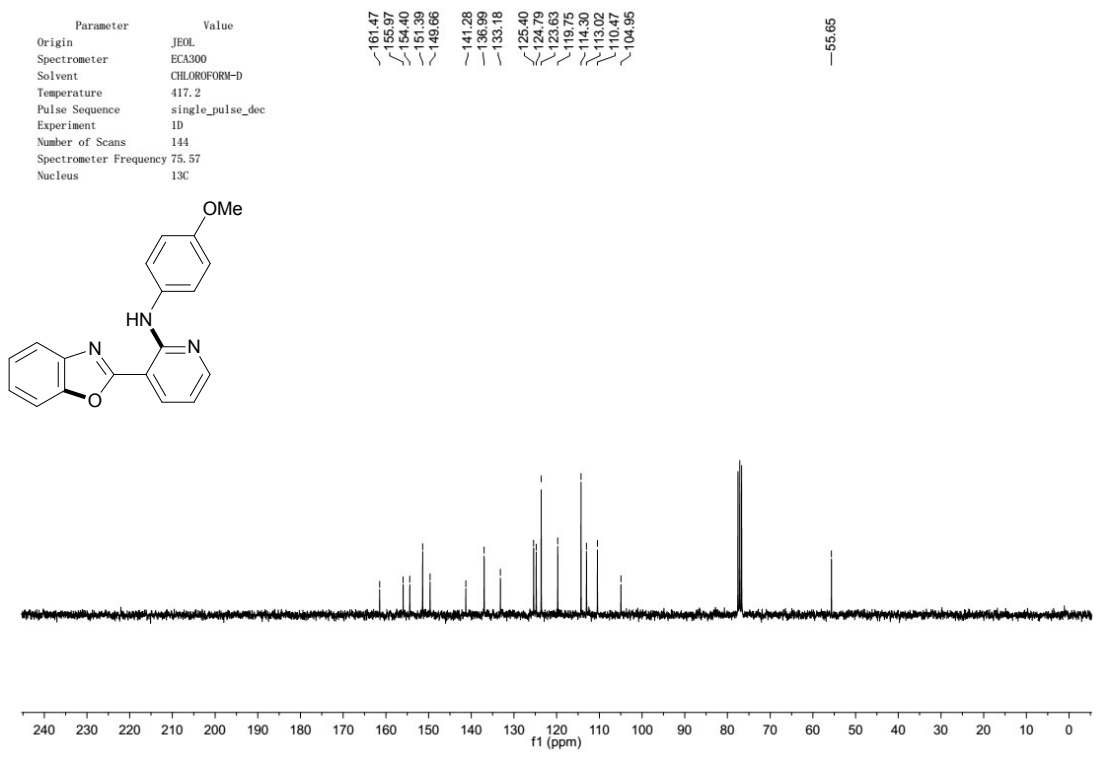
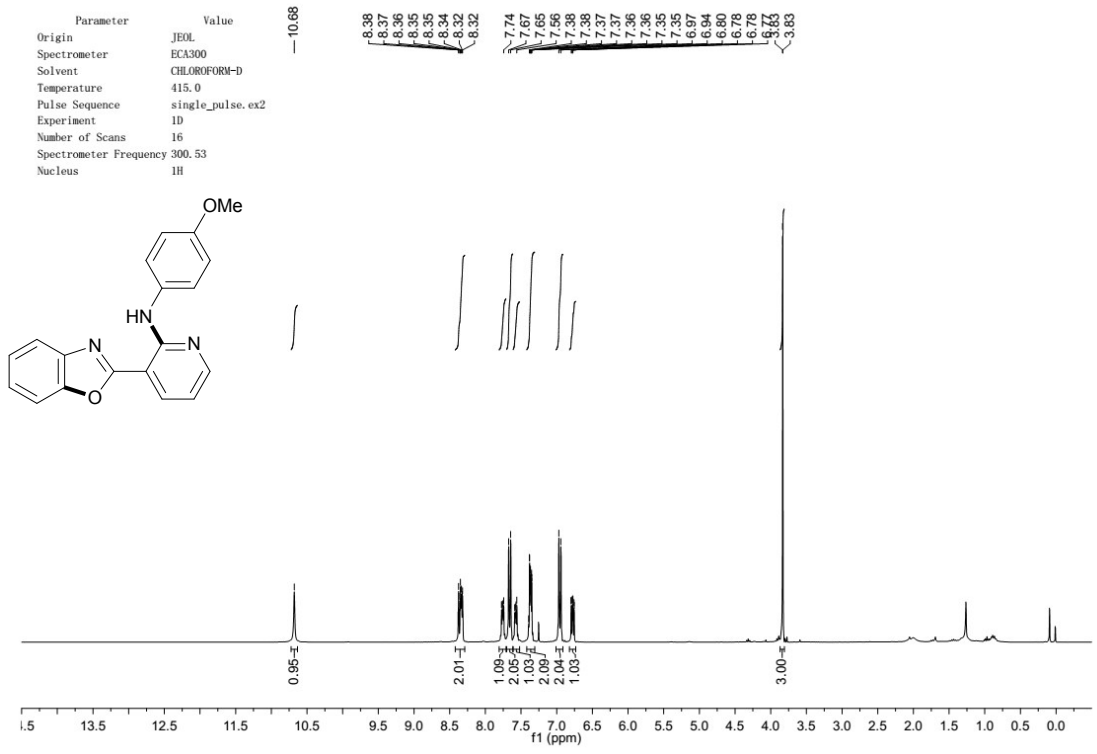
44.96



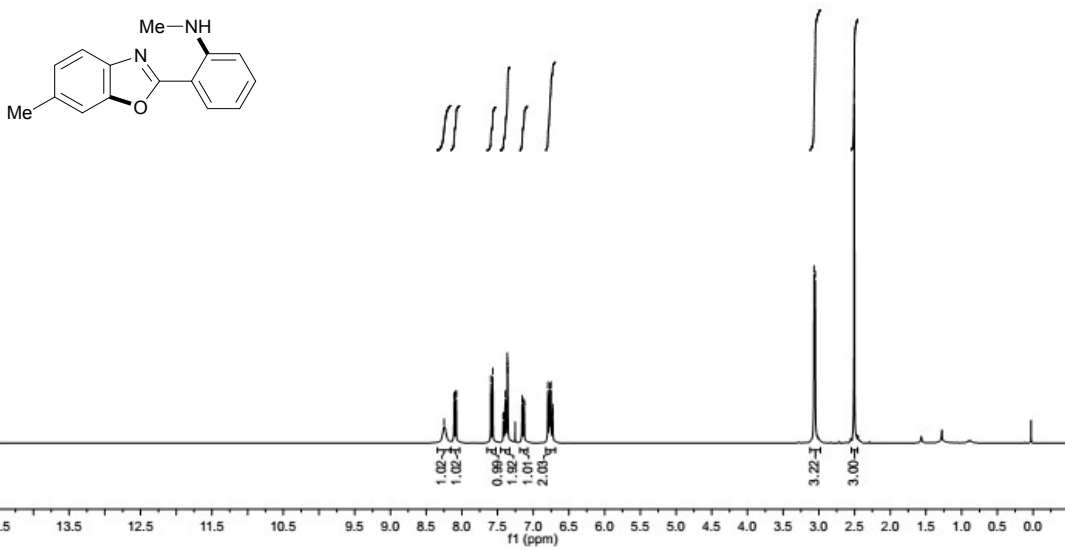




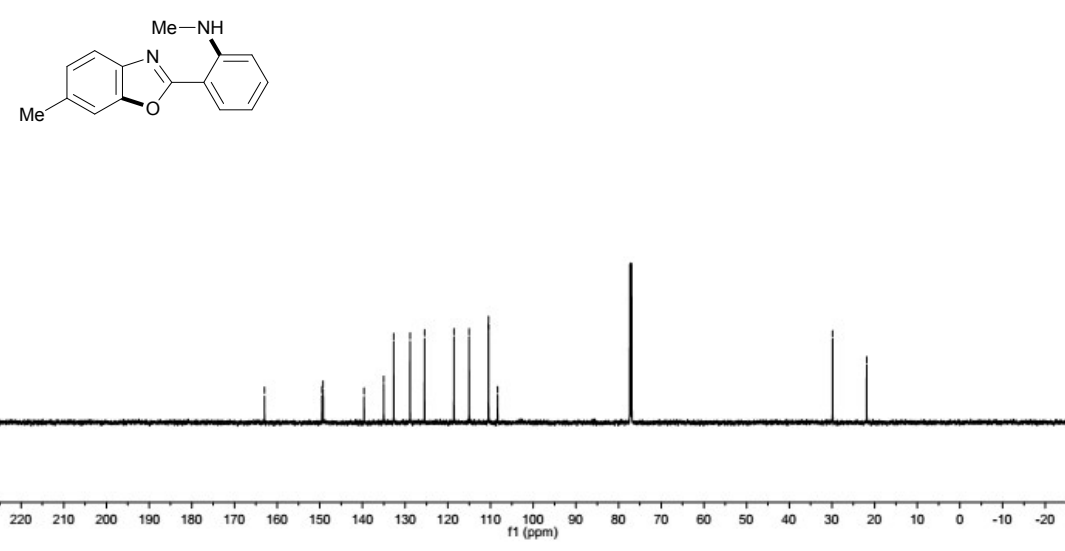




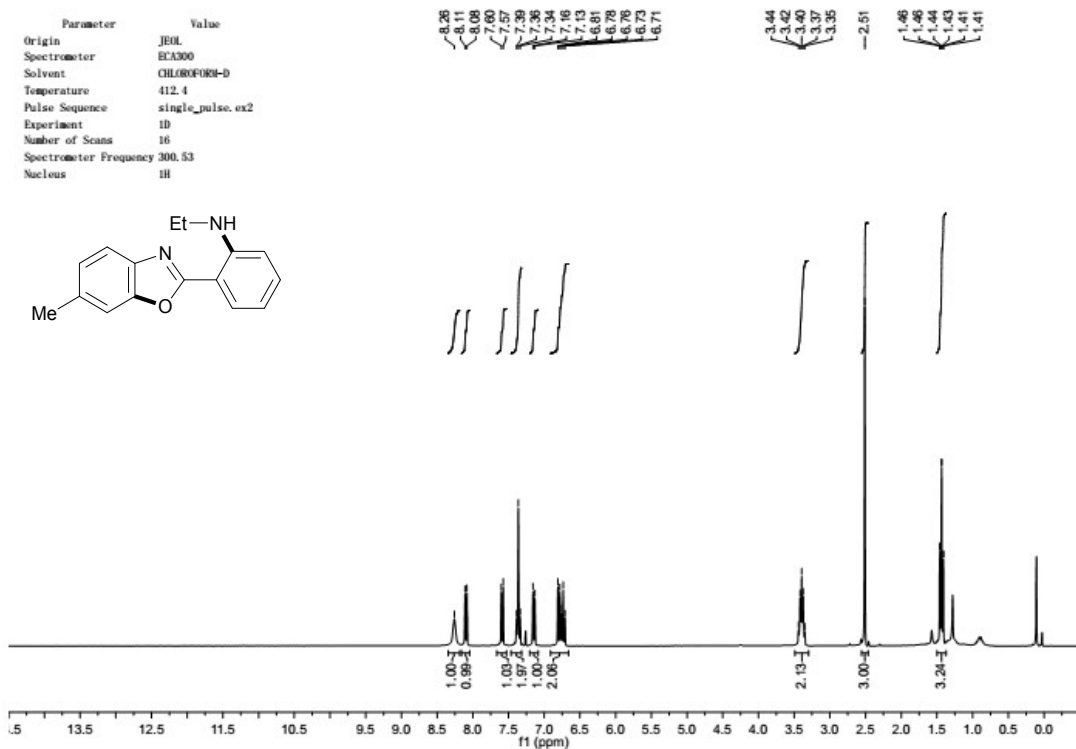
Parameter Value  
 Origin JEOL  
 Spectrometer ECA300  
 Solvent CHLOROFORM-D  
 Temperature 23.2  
 Pulse Sequence single\_pulse.ex2  
 Experiment 1D  
 Number of Scans 16  
 Spectrometer Frequency 300.53  
 Nucleus 1H



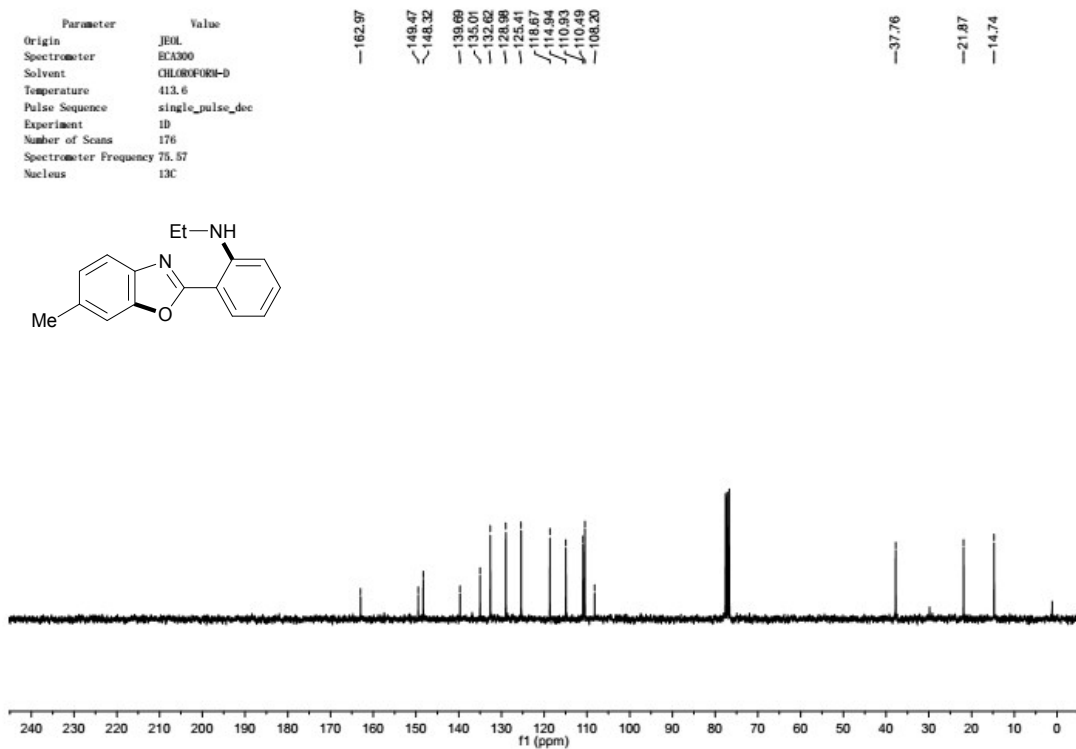
Parameter Value  
 Origin JEOL  
 Spectrometer ECA600  
 Solvent CHLOROFORM-D  
 Temperature 28.0  
 Pulse Sequence single\_pulse\_dec  
 Experiment 1D  
 Number of Scans 129  
 Spectrometer Frequency 150.91  
 Nucleus 13C



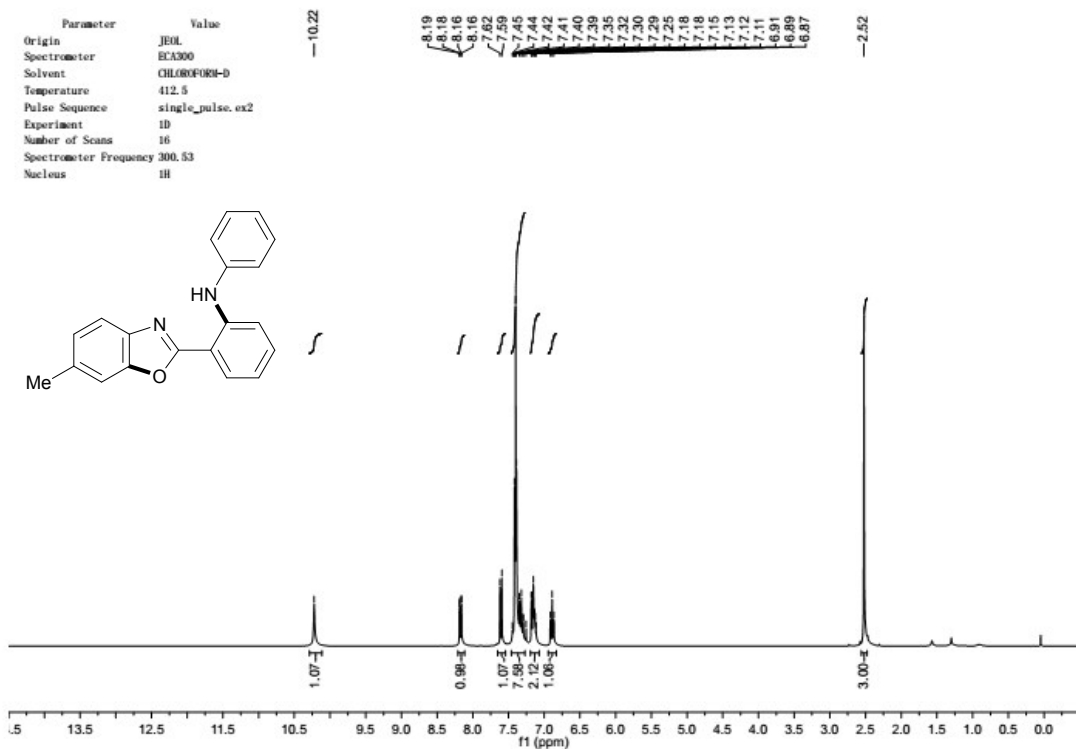
Parameter	Value
Origin	JEOL
Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	412.4
Pulse Sequence	single_pulse.ex2
Experiment	1D
Number of Scans	16
Spectrometer Frequency	300.53
Nucleus	<sup>1</sup> H



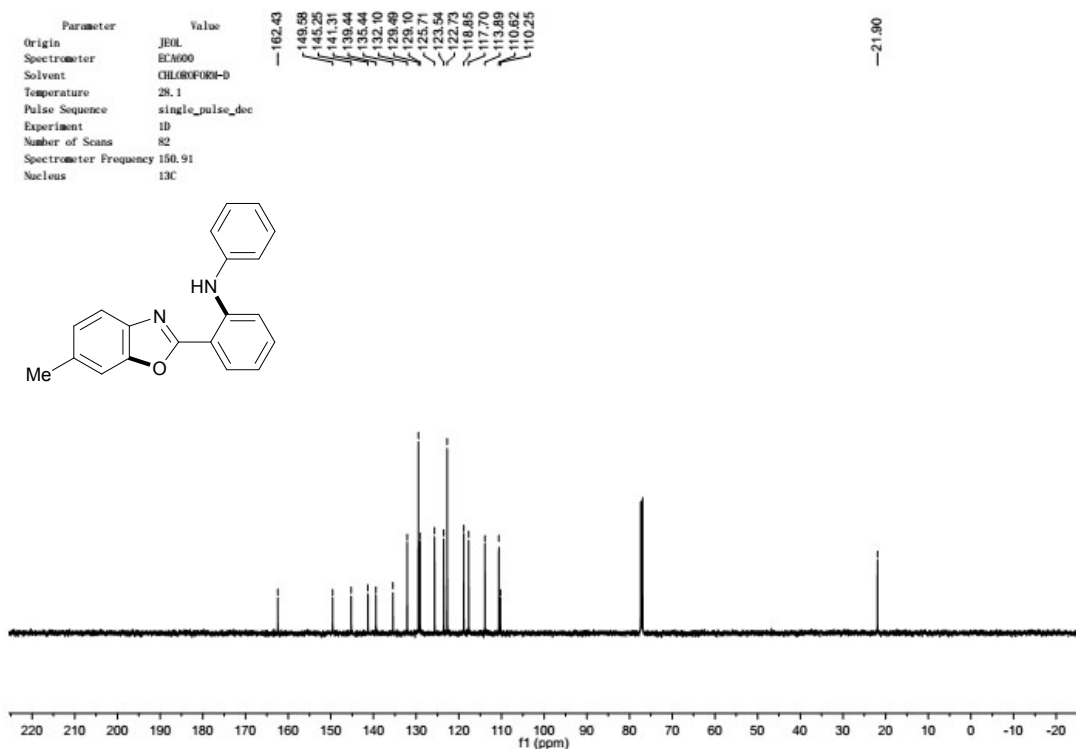
Parameter	Value
Origin	JEOL
Spectrometer	ECA300
Solvent	CHLOROFORM-D
Temperature	413.6
Pulse Sequence	single_pulse_dec
Experiment	1D
Number of Scans	176
Spectrometer Frequency	75.57
Nucleus	<sup>13</sup> C

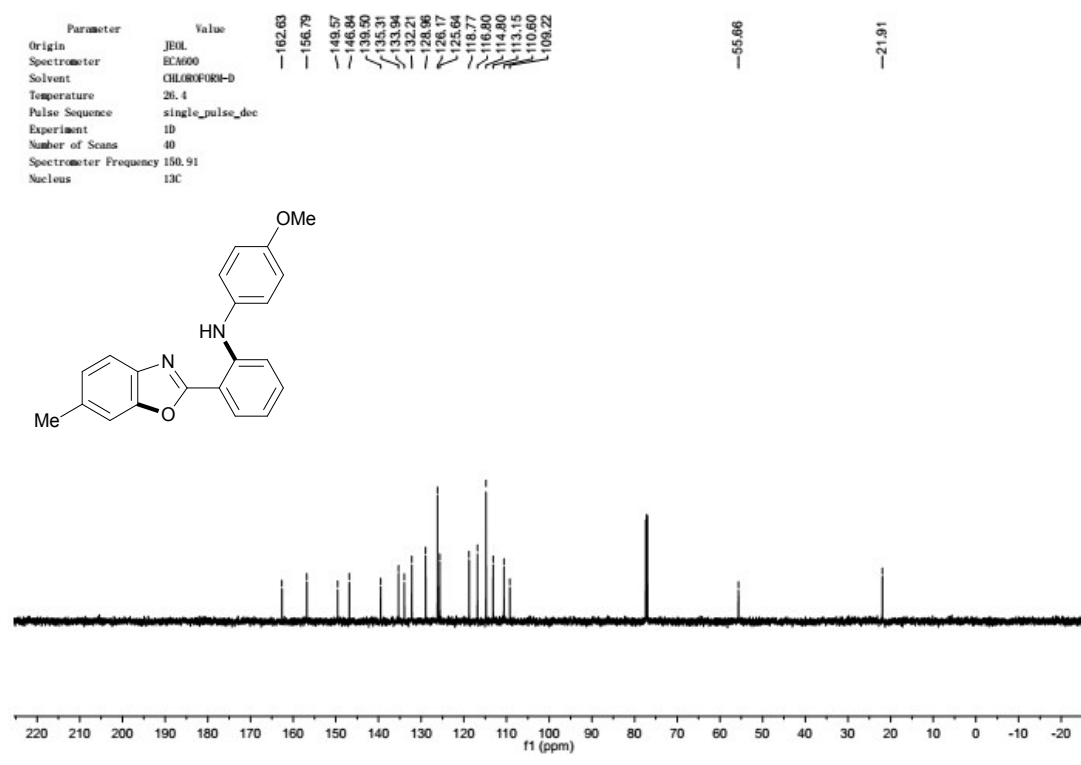
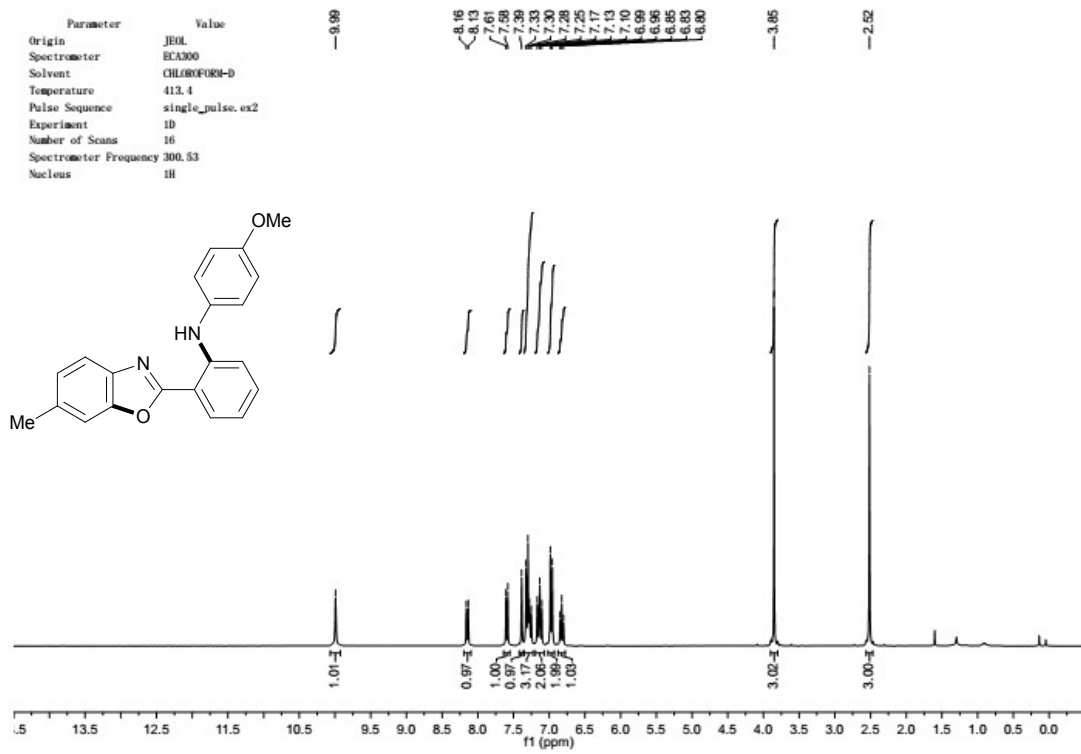


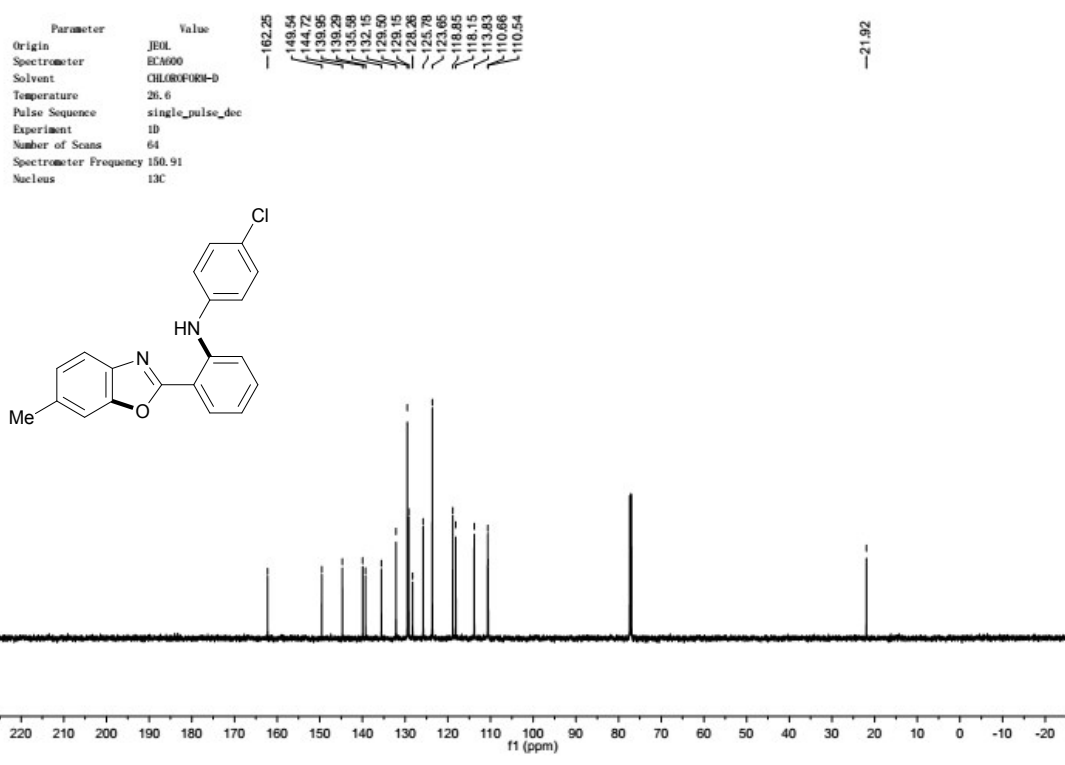
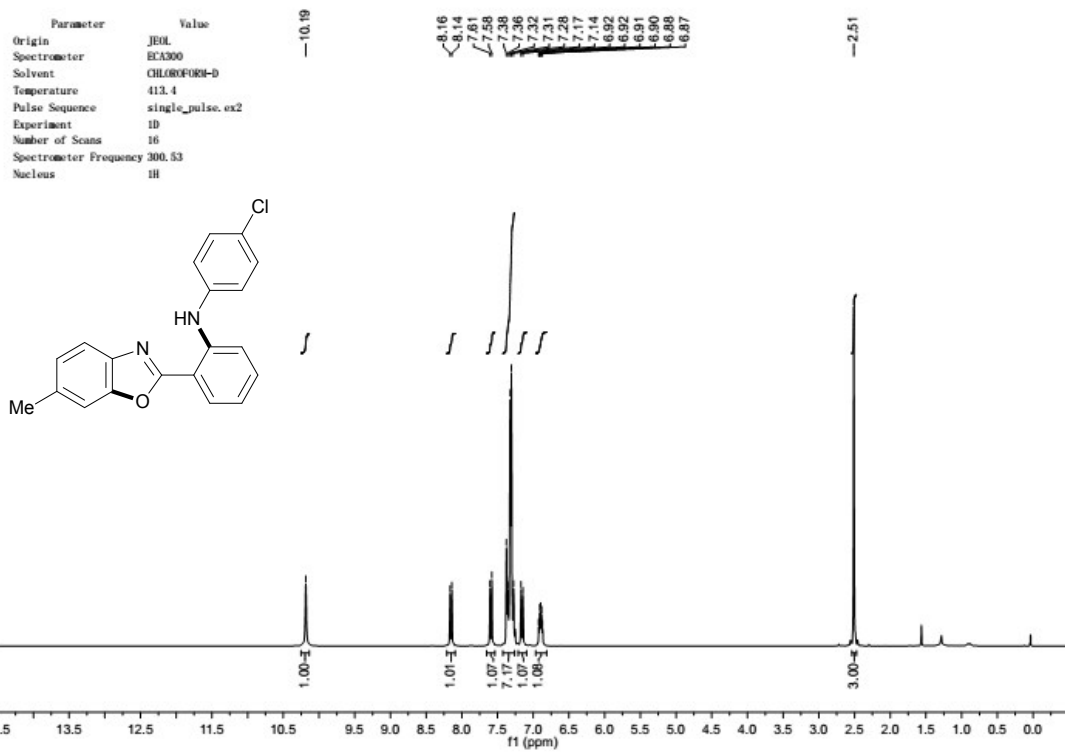
Parameter Value  
 Origin JEOL  
 Spectrometer EAM300  
 Solvent CHLOROFORM-D  
 Temperature 412.5  
 Pulse Sequence single\_pulse\_ex2  
 Experiment 1D  
 Number of Scans 16  
 Spectrometer Frequency 300.53  
 Nucleus 1H



Parameter Value  
 Origin JEOL  
 Spectrometer EAM600  
 Solvent CHLOROFORM-D  
 Temperature 28.1  
 Pulse Sequence single\_pulse\_dec  
 Experiment 1D  
 Number of Scans 82  
 Spectrometer Frequency 150.91  
 Nucleus 13C



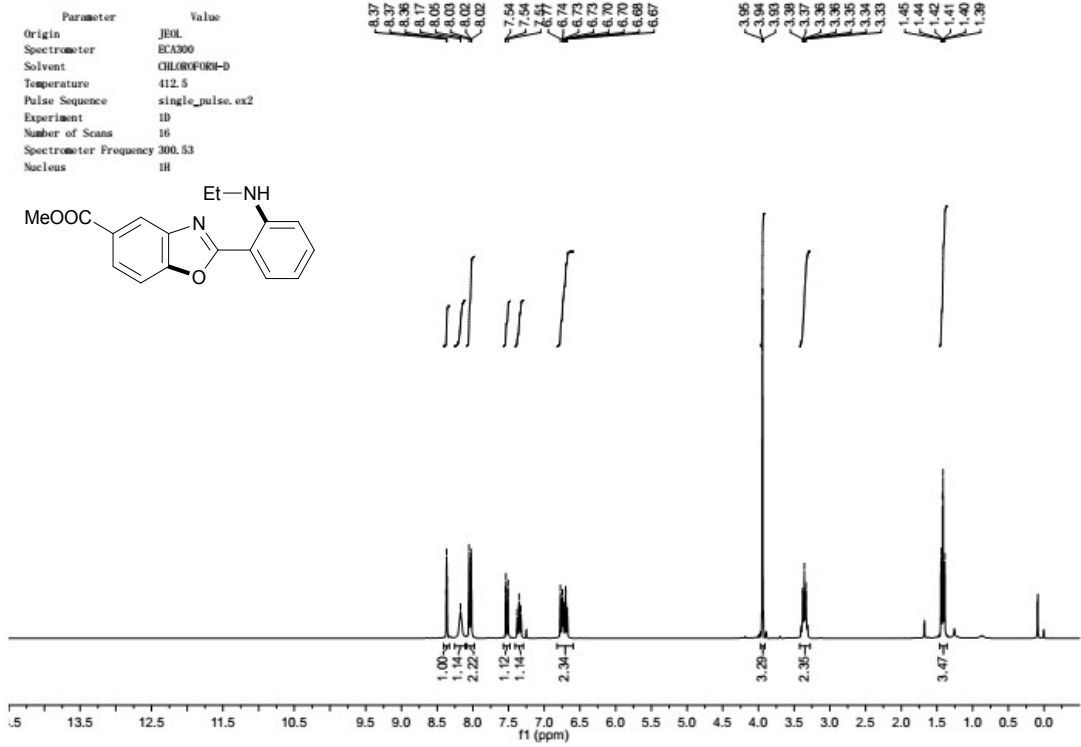
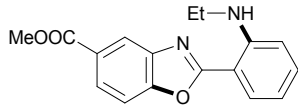




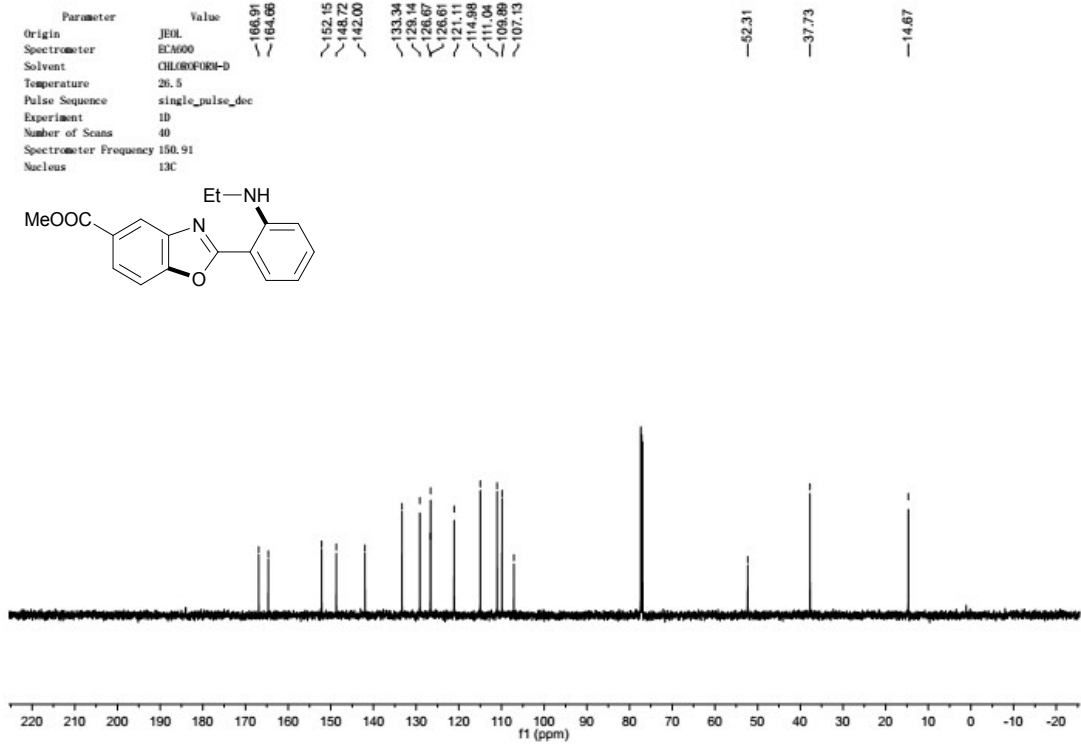
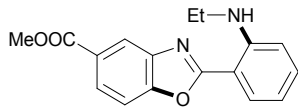


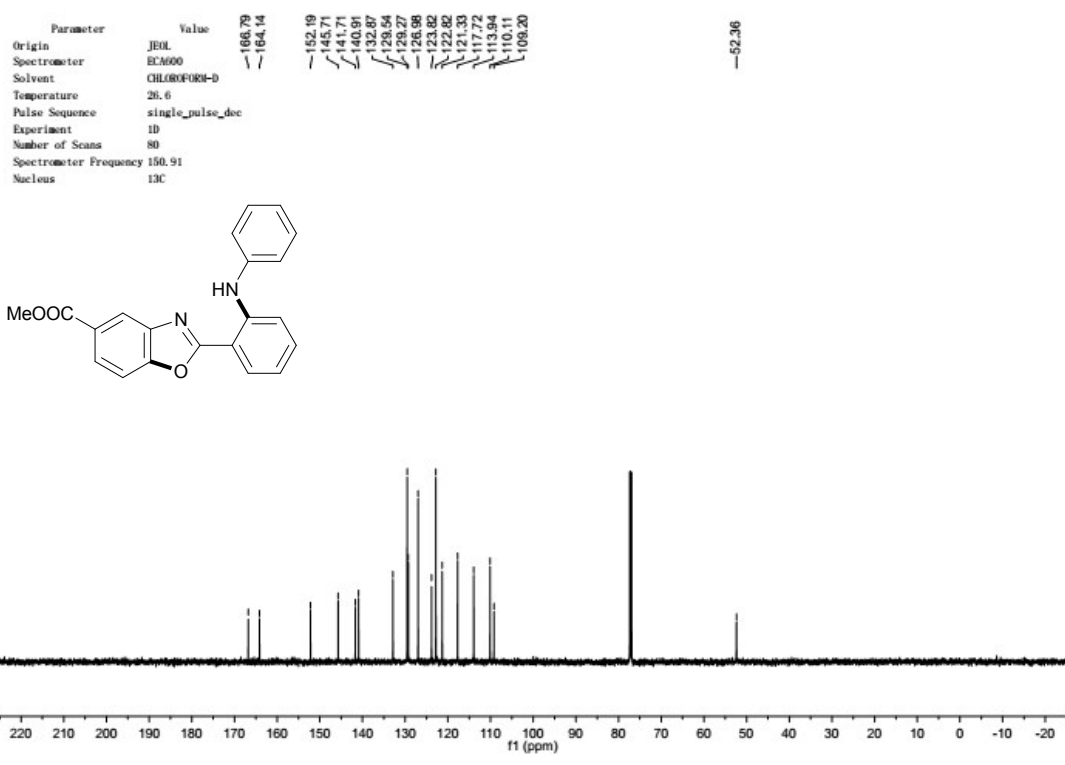
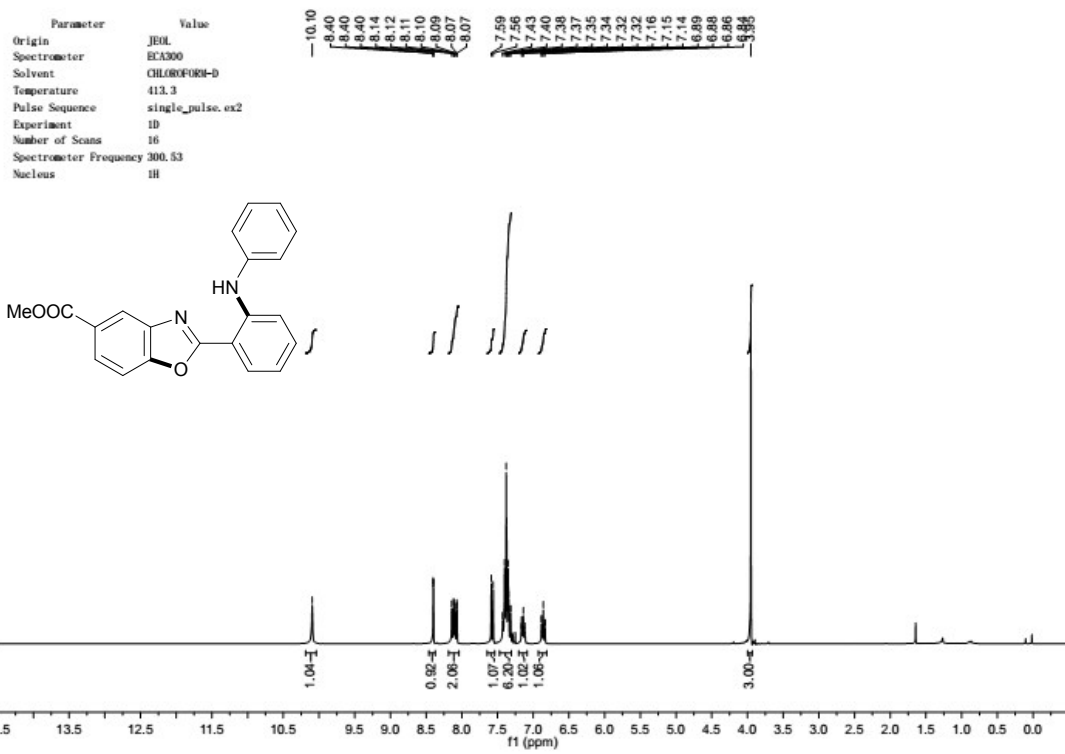


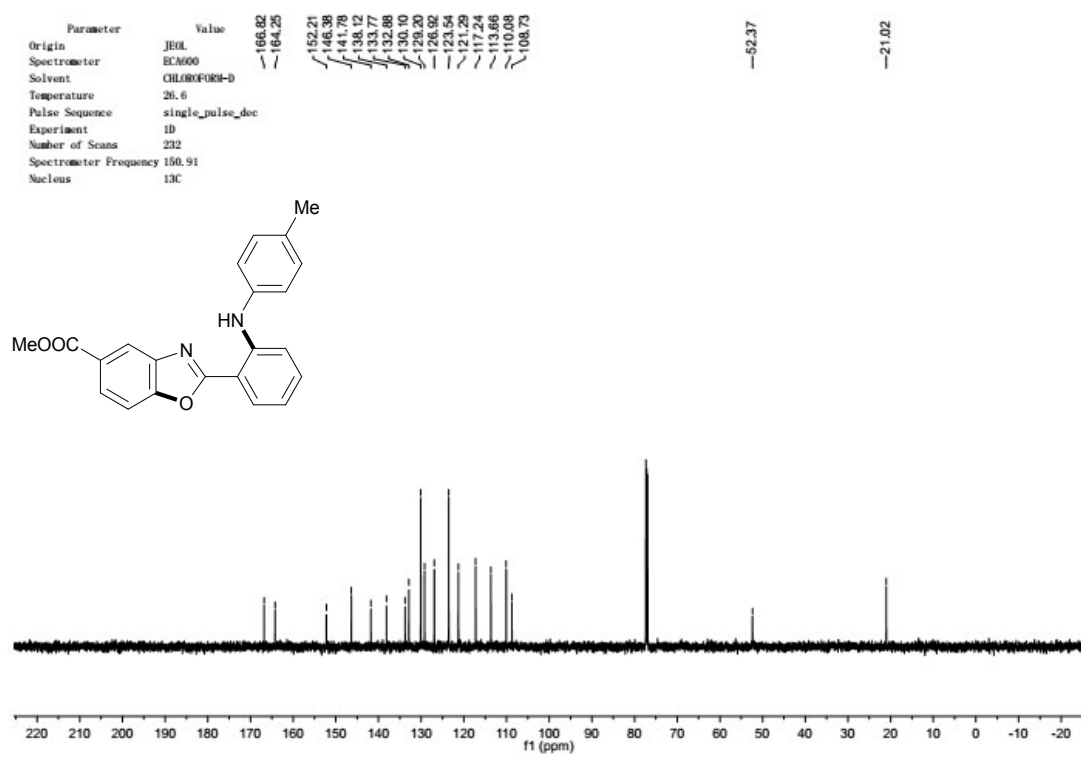
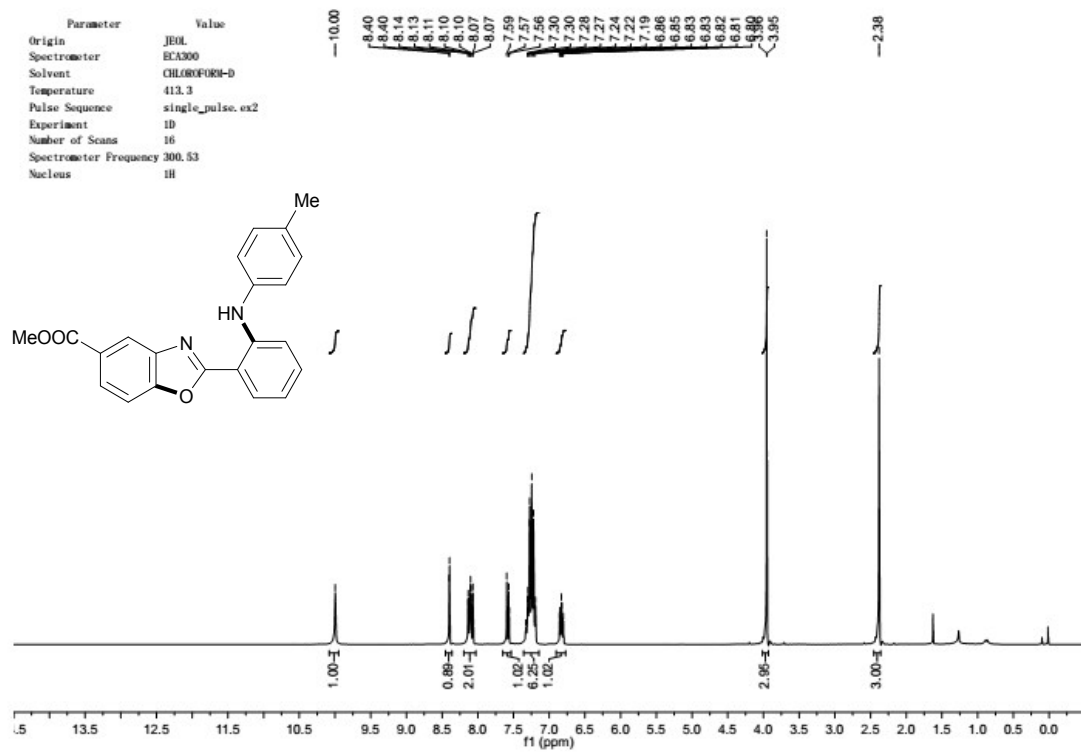
Parameter Value  
 Origin JEOL  
 Spectrometer ECA300  
 Solvent CHLOROFORM-D  
 Temperature 412.5  
 Pulse Sequence single\_pulse.ex2  
 Experiment 1D  
 Number of Scans 16  
 Spectrometer Frequency 300.53  
 Nucleus 1H

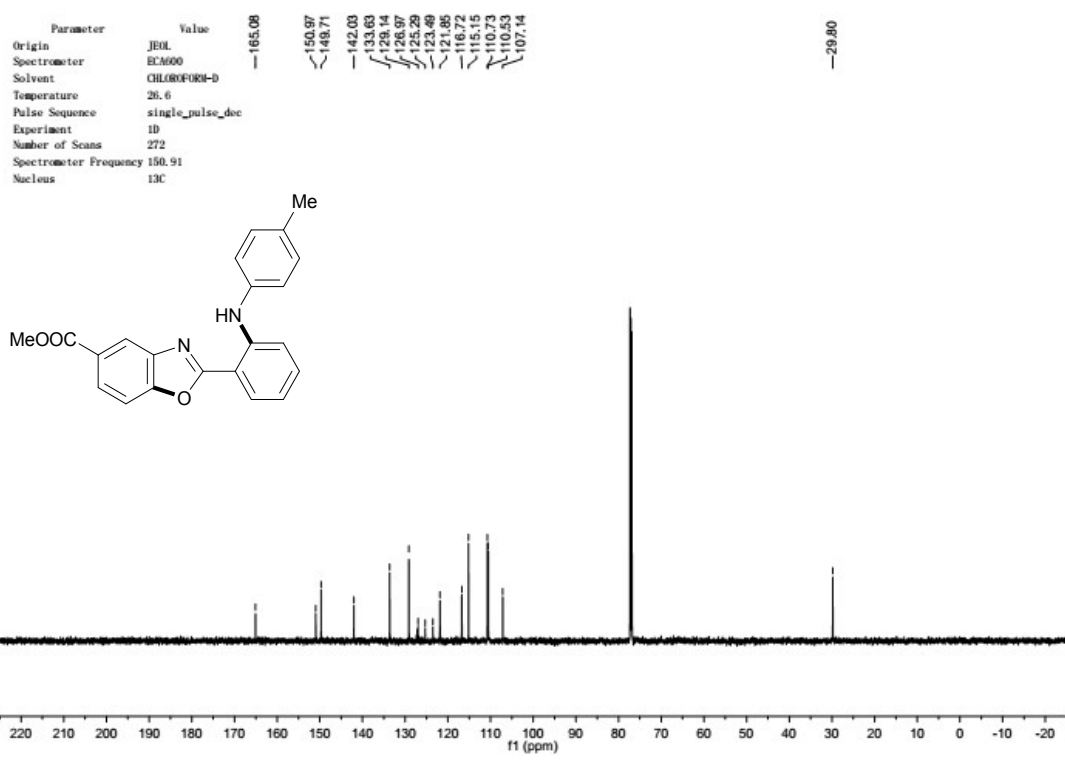
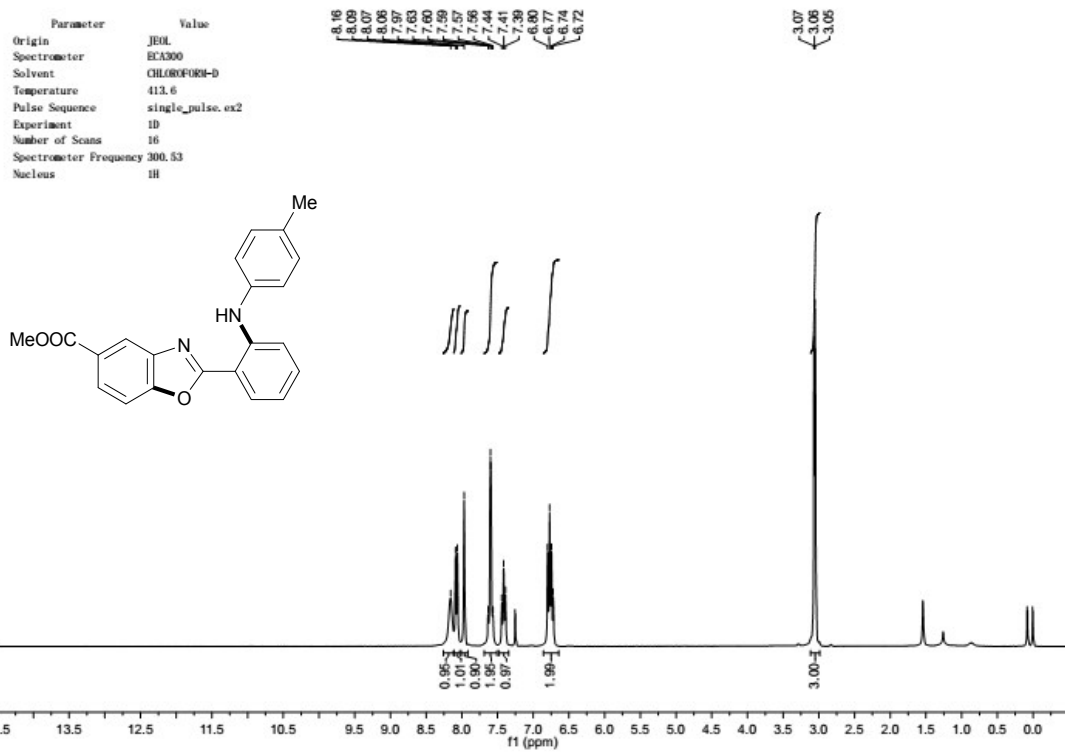


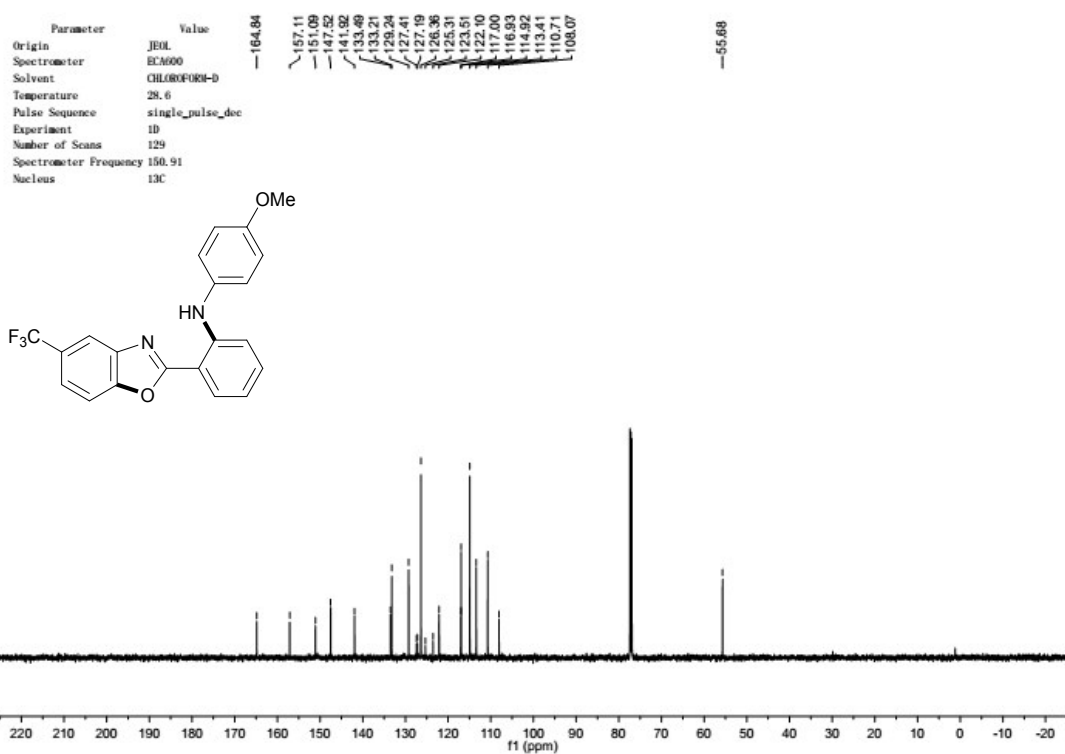
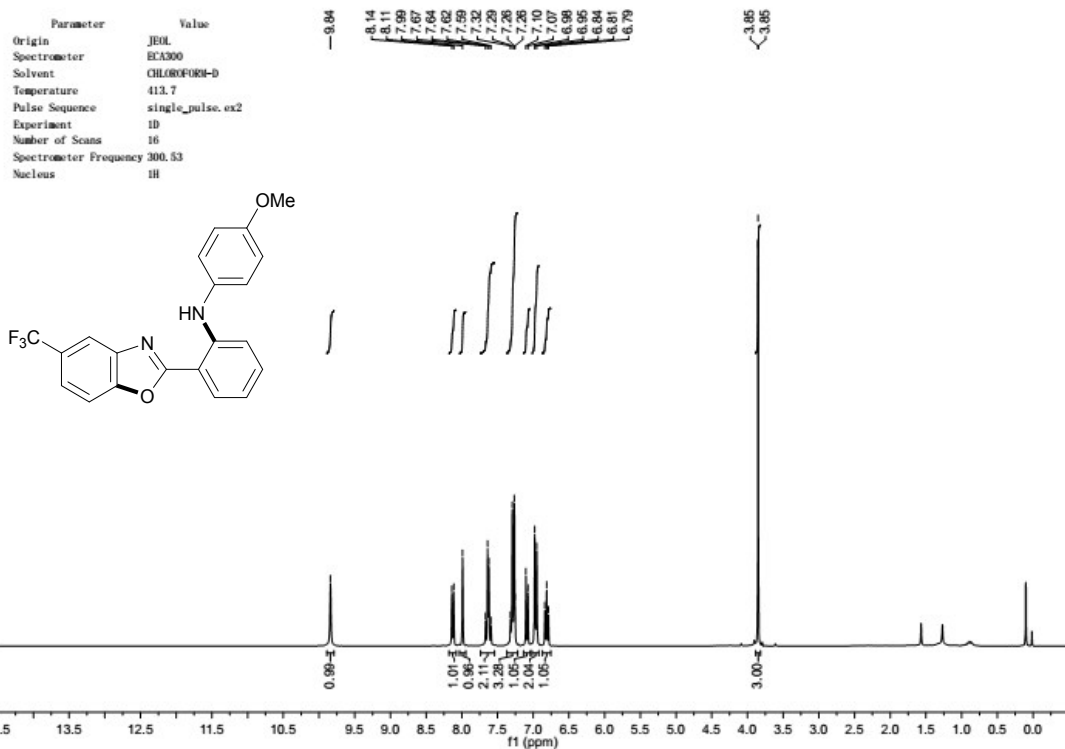
Parameter Value  
 Origin JEOL  
 Spectrometer ECA600  
 Solvent CHLOROFORM-D  
 Temperature 26.5  
 Pulse Sequence single\_pulse\_dec  
 Experiment 1D  
 Number of Scans 40  
 Spectrometer Frequency 150.91  
 Nucleus 13C



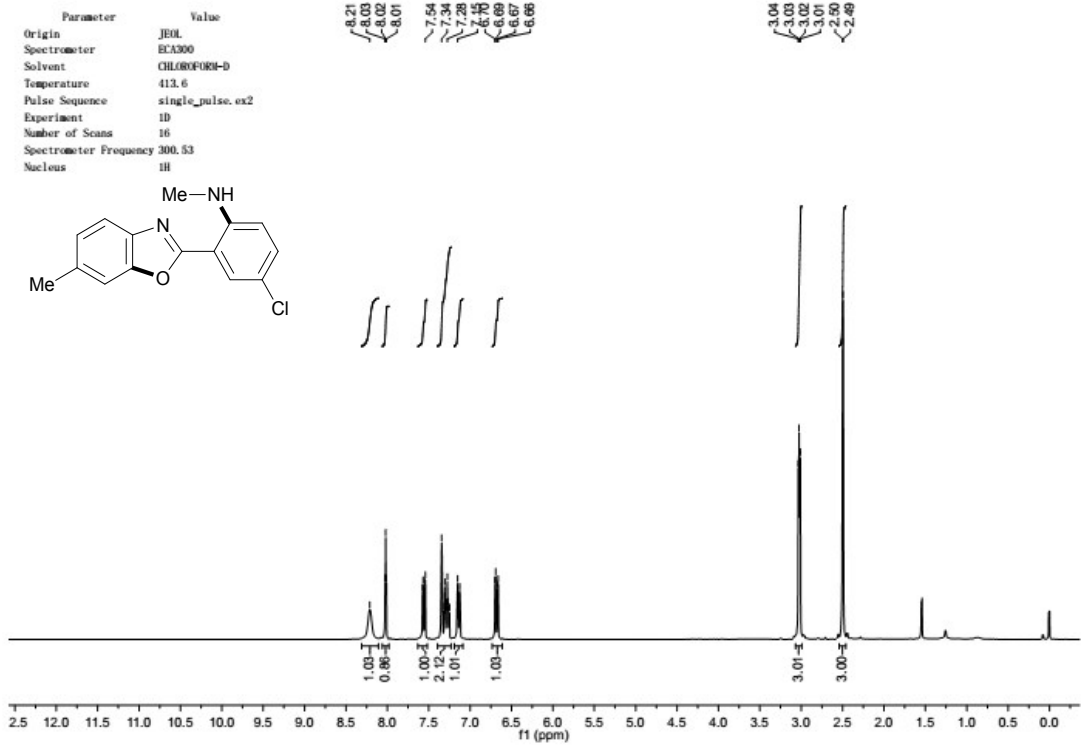
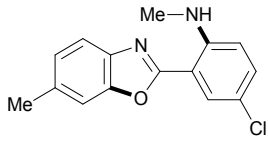




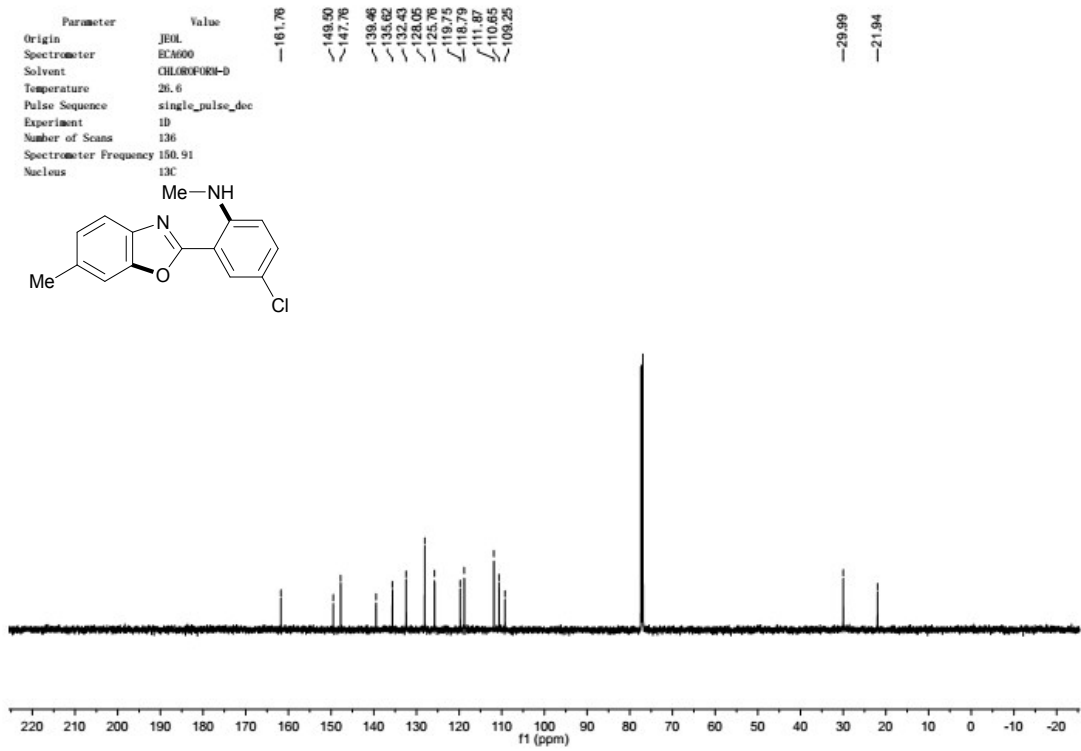
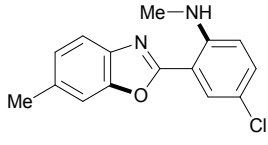




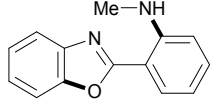
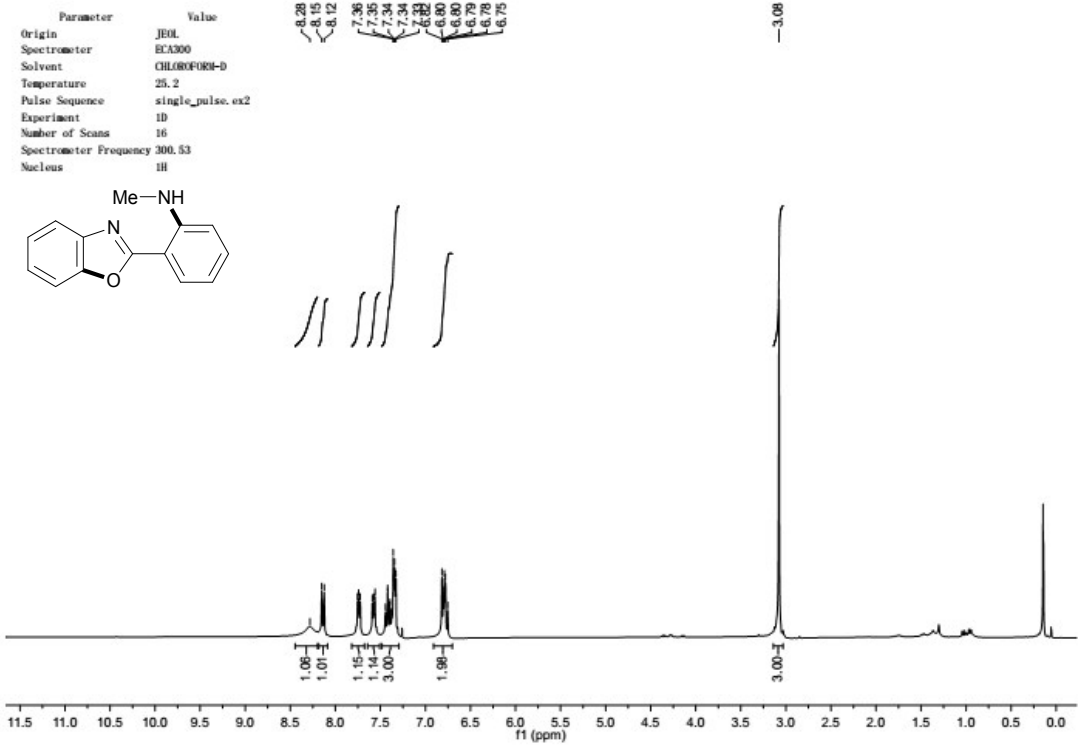
Parameter Value  
 Origin JEOL  
 Spectrometer ECA300  
 Solvent CHLOROFORM-D  
 Temperature 413.6  
 Pulse Sequence single\_pulse.ex2  
 Experiment 1D  
 Number of Scans 16  
 Spectrometer Frequency 300.53  
 Nucleus 1H



Parameter Value  
 Origin JEOL  
 Spectrometer ECA600  
 Solvent CHLOROFORM-D  
 Temperature 26.6  
 Pulse Sequence single\_pulse\_dec  
 Experiment 1D  
 Number of Scans 136  
 Spectrometer Frequency 150.91  
 Nucleus 13C



Parameter Value  
 Origin JEOL  
 Spectrometer ECA300  
 Solvent CHLOROFORM-D  
 Temperature 25.2  
 Pulse Sequence single\_pulse\_ex2  
 Experiment 1D  
 Number of Scans 16  
 Spectrometer Frequency 300.53  
 Nucleus 1H



Parameter Value  
 Origin JEOL  
 Spectrometer ECA600  
 Solvent CHLOROFORM-D  
 Temperature 26.4  
 Pulse Sequence single\_pulse\_dec  
 Experiment 1D  
 Number of Scans 172  
 Spectrometer Frequency 150.91  
 Nucleus 13C

