

## Supporting Information

### An Easy Arylation of 2-Substituted 1,2,3-Triazole

Suping Shi,<sup>a</sup> Wei Liu,<sup>a</sup> Ping He<sup>a</sup> and Chunxiang Kuang<sup>ab\*</sup>.

<sup>1</sup> Department of Chemistry, Tongji University, Siping Road 1239, Shanghai 200092, China

<sup>2</sup> Key Laboratory of Yangtze River Water Environment, Ministry of Education, Shanghai 200092, China

Fax: +86-21-65983191; E-mail: kuangcx@tongji.edu.cn.

### Contents

1) General considerations.....	1
2) Experimental details and characterization data for 1,2,3-triazoles <b>1</b> ..	1
3) Experimental details and characterization data for products <b>3</b> .....	2
4) References.....	12
5) <sup>1</sup> H NMR and <sup>13</sup> C NMR spectra for all compounds .....	12

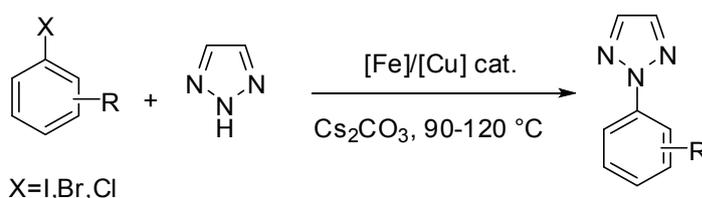
### ● Experimental procedures

#### 1. General considerations

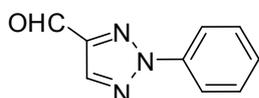
All commercially available reagents and solvent were obtained from the commercial providers and used without further purification. Melting points were recorded using a WRS-2A melting point apparatus and were uncorrected. IR spectra were obtained on a Nexus FT-IR spectrophotometer. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded using a Bruker Avance 400 MHz spectrometer. Chemical shifts were reported relative to internal tetramethylsilane (0.00 ppm) for <sup>1</sup>H and CDCl<sub>3</sub> (77.0 ppm) for <sup>13</sup>C. High resolution mass spectra were determined using a Finnigan-NAT GC/MS/DS 8430 spectrometer. Flash column chromatography was performed on 300-400 mesh silica gel. 2-Substituted 1,2,3-Triazoles **1** (except **1h**) were prepared according to literature procedures<sup>[1,2]</sup>.

#### 2. Experimental details and characterization data for 1,2,3-Triazoles **1**

##### 1) Experimental details and characterization data for 1a-1i



##### Spectral data of Starting Materials **1** (1a-1g, 1i)<sup>[2]</sup>



**2-phenyl-2H-1,2,3-triazole-4-carbaldehyde(1h)**<sup>[3]</sup>: pale yellow solid, mp: 83.5-84.2 °C.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.24 (s, 1H), 8.29 (s, 1H), 8.16 (d, *J* = 7.8 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 2H), 7.47 (t, *J* = 7.1 Hz, 1H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 184.23, 147.77, 139.26, 135.46, 129.54, 128.93, 119.51

HR-MS: *m/z* calcd for C<sub>9</sub>H<sub>7</sub>N<sub>3</sub>O: 173.0589; found: 173.0585.

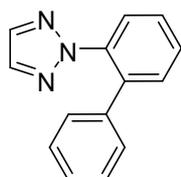
IR:<sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3543, 3465, 3402, 3237, 3025, 1698, 1604, 1470, 1427, 1316, 1104

### 3. Experimental details and characterization data for products 3

#### 3.1 General Procedure for Palladium-catalyzed Arylation of 2-Substituted 1,2,3-Triazoles:

A mixture of 2-Substituted 1,2,3-Triazole **1** (0.3mmol), ArI **2** (0.33mmol), Pd(OAc)<sub>2</sub> (0.015mmol) and AgOAc (0.6 mmol) in CF<sub>3</sub>COOH (4 ml) was stirred at 120 °C for 12h in sealed tube. The mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (15 ml) and washed with water (10 ml x 3). The organic phase was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated under reduced pressure. The resulting residue was purified on silica gel chromatography to give the products **3**.

#### 3.2 characterization data for products 3



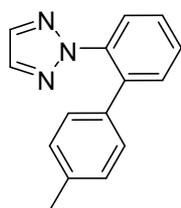
**2-(biphenyl-2-yl)-2H-1,2,3-triazole (3a)** : According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 20/1) to give **3a** (55.0 mg, 83 %) as a yellow liquid.

<sup>1</sup>H NMR (400 MHz, DMSO) δ 7.93 (s, 2H), 7.69–7.56 (m, 4H), 7.30 – 7.23 (m, 3H), 7.03 – 6.94 (m, 2H)

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 138.59, 138.55, 137.96, 135.08, 131.28, 129.52, 128.27, 128.25, 128.12, 127.34, 126.59

HR-MS: *m/z* calcd for C<sub>14</sub>H<sub>11</sub>N<sub>3</sub>: 221.0953; found: 221.0957.

IR:<sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3505, 3468, 3401, 3112, 3025, 2996, 2921, 1614, 1488, 953, 1149, 954



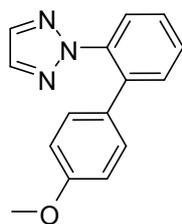
**2-(4'-methylbiphenyl-2-yl)-2H-1,2,3-triazole(3b)**: According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 20/1) to give **3b** (56.4 mg, 80 %) as a pale yellow liquid.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (s, 2H), 7.63 – 7.44 (m, 4H), 7.07 (d, *J* = 7.9 Hz, 2H), 6.94 (d, *J* = 8.1 Hz, 2H), 2.33 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 138.49, 137.94, 137.06, 135.57, 135.02, 131.23, 129.50, 129.02, 128.06, 127.84, 126.63, 21.16

HR-MS:  $m/z$  calcd for  $C_{15}H_{13}N_3$ : 235.1109; found: 235.1113.

IR:  $\nu_{\max}$  (thin film) ( $cm^{-1}$ ) = 3562, 3401, 3401, 3382, 3215, 2921, 2897, 1648, 1601, 1491, 954, 819



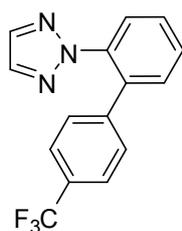
**2-(4'-methoxybiphenyl-2-yl)-2H-1,2,3-triazole (3c):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3c** (45.9 mg, 61 %) as a yellow liquid.

$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.69 (s, 2H), 7.60 – 7.43 (m, 4H), 6.97 (d,  $J$  = 8.6 Hz, 2H), 6.79 (d,  $J$  = 8.6 Hz, 2H), 3.78 (s, 3H).

$^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  158.90, 140.29, 135.08, 134.34, 131.52, 129.92, 129.58, 129.28, 128.72, 128.38, 126.03, 113.55, 55.14

HR-MS:  $m/z$  calcd for  $C_{15}H_{13}N_3O$ : 251.1059; found: 251.1057.

IR:  $\nu_{\max}$  (thin film) ( $cm^{-1}$ ) = 3471, 3414, 3405, 3112, 3025, 2990, 2924, 1691, 1481, 1384, 953, 828



**2-(4'-(trifluoromethyl)biphenyl-2-yl)-2H-1,2,3-triazole (3d):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 20/1) to give **3d** (79.9mg, 91 %) as a yellow liquid.

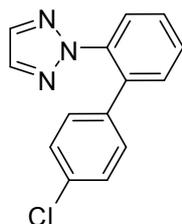
$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.72 – 7.65 (m, 3H), 7.60 – 7.54 (m, 2H), 7.54 – 7.49 (m, 3H), 7.16 (d,  $J$  = 8.0 Hz, 2H).

$^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  142.32, 138.45, 136.29, 135.34, 131.11, 129.58, 129.43 (q,  $J$  = 32.3 Hz), 128.93, 128.62, 126.55, 125.18 (q,  $J$  = 3.7 Hz), 124.13 (q,  $J$  = 270.3 Hz)

$^{19}F$  NMR (377 MHz,  $CDCl_3$ )  $\delta$  -62.53

HR-MS:  $m/z$  calcd for  $C_{15}H_{10}F_3N_3$ : 289.0827; found: 289.0825.

IR:  $\nu_{\max}$  (thin film) ( $cm^{-1}$ ) = 3467, 3438, 3406, 3120, 3025, 1618, 1493, 1408, 1326, 1126, 1070, 952, 843



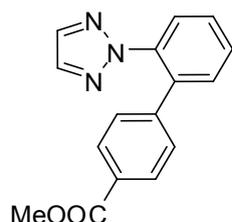
**2-(4'-chlorobiphenyl-2-yl)-2H-1,2,3-triazole (3e):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 25/1) to give **3e** (65.0 mg, 85%) as a yellow liquid.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (s, 2H), 7.65 – 7.61 (m, 1H), 7.57 – 7.46 (m, 3H), 7.23 (d,  $J = 8.5$  Hz, 2H), 6.98 (d,  $J = 8.5$  Hz, 2H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  138.44, 137.05, 136.65, 135.23, 133.51, 131.06, 129.58, 128.47, 126.62

HR-MS:  $m/z$  calcd for  $\text{C}_{14}\text{H}_{10}\text{ClN}_3$ : 255.0563; found: 255.0565

IR: $_{\text{max}}$ (thin film) ( $\text{cm}^{-1}$ ) = 3562, 3401, 3382, 3210, 1648, 1601, 1491, 1411, 1150, 953, 764



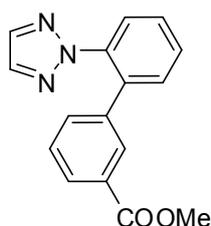
**methyl 2'-(2H-1,2,3-triazol-2-yl)biphenyl-4-carboxylate (3f):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 15/1) to give **3f** (72.0 mg, 86 %) as a yellow liquid.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 (d,  $J = 8.3$  Hz, 2H), 7.65 (d,  $J = 4.6$  Hz, 3H), 7.61 – 7.45 (m, 3H), 7.11 (d,  $J = 8.3$  Hz, 2H), 3.89 (s, 3H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.83, 143.34, 138.45, 136.69, 135.27, 131.06, 129.51, 129.00, 128.81, 128.31, 126.51, 52.09

HR-MS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{13}\text{N}_3\text{O}_2$ : 279.1008; found: 279.1013.

IR: $_{\text{max}}$ (thin film) ( $\text{cm}^{-1}$ ) = 3554, 3470, 3441, 3132, 3065, 2941, 2870, 1721, 1629, 1503, 1281, 1184, 1024, 953



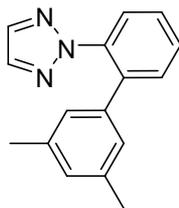
**methyl 2'-(2H-1,2,3-triazol-2-yl)biphenyl-3-carboxylate (3g):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 20/1) to give **3g** (67.0 mg, 82 %) as a yellow liquid.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 7.8$  Hz, 1H), 7.82 (s, 1H), 7.66 (s, 3H), 7.60 – 7.48 (m, 3H), 7.30 (t,  $J = 7.7$  Hz, 1H), 7.15 (d,  $J = 7.7$  Hz, 1H), 3.87 (s, 3H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.75, 138.89, 138.49, 136.69, 135.21, 132.65, 131.21, 130.33, 129.53, 128.59, 128.52, 128.20, 126.49, 52.08

HR-MS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{13}\text{N}_3\text{O}_2$ : 279.1008; found: 279.1012.

IR: $_{\text{max}}$ (thin film) ( $\text{cm}^{-1}$ ) = 3550, 3482, 3415, 3236, 3065, 2951, 2850, 2360, 2338, 1722, 1617, 1503, 1412, 1244, 953



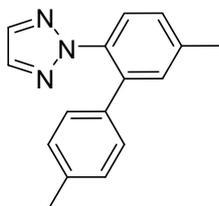
**2-(3',5'-dimethylbiphenyl-2-yl)-2H-1,2,3-triazole (3h):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 40/1) to give **3h** (39.6 mg, 53 %) as a yellow liquid.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69 (s, 2H), 7.62 – 7.44 (m, 4H), 6.89 (s, 1H), 6.65 (s, 2H), 2.22 (s, 6H)

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  138.48, 138.22, 138.18, 137.65, 134.90, 131.21, 129.48, 129.05, 127.85, 126.60, 125.98, 21.27

HR-MS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{15}\text{N}_3$ : 249.1266; found: 249.1263.

IR:  $_{\text{max}}$  (thin film) ( $\text{cm}^{-1}$ ) = 3484, 3453, 3418, 3234, 3065, 3027, 2920, 2858, 1630, 1615, 1500, 1411, 1080, 957, 764



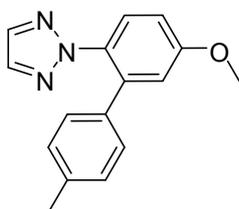
**2-(4',5-dimethylbiphenyl-2-yl)-2H-1,2,3-triazole (3i):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 20/1) to give **3i** (64.2 mg, 86 %) as a pale yellow solid, mp. 100.7-101.9 °C

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (s, 2H), 7.49 (d,  $J$  = 8.0 Hz, 1H), 7.34 (s, 1H), 7.28 (d,  $J$  = 8.0 Hz, 1H), 7.07 (d,  $J$  = 7.9 Hz, 2H), 6.95 (d,  $J$  = 8.1 Hz, 2H), 2.47 (s, 3H), 2.33 (s, 3H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  139.55, 137.70, 136.95, 136.27, 135.72, 134.88, 131.76, 128.99, 128.45, 128.07, 126.49, 21.28, 21.18

HR-MS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{15}\text{N}_3$ : 249.1266; found: 249.1262.

IR:  $_{\text{max}}$  (thin film) ( $\text{cm}^{-1}$ ) = 3554, 3500, 3484, 3441, 3118, 3024, 2996, 2921, 2860, 1638, 1614, 1451, 1410, 1149, 954, 822



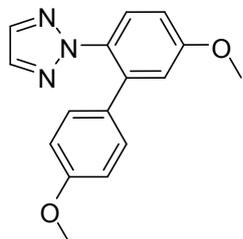
**2-(5-methoxy-4'-methylbiphenyl-2-yl)-2H-1,2,3-triazole (3j):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 20/1) to give **3j** (70.1 mg, 88 %) as a pale yellow solid, mp: 81.4-81.9 °C

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (s, 2H), 7.50 (d,  $J$  = 8.7 Hz, 1H), 7.06 (d,  $J$  = 7.9 Hz, 2H), 7.04 – 6.97 (m, 2H), 6.95 (d,  $J$  = 8.1 Hz, 2H), 3.89 (s, 3H), 2.32 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.08, 139.52, 137.23, 135.50, 134.77, 132.00, 129.01, 128.02, 127.98, 115.96, 113.10, 55.66, 21.16

HR-MS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{15}\text{N}_3$ : 265.1215; found: 265.1211.

IR: $_{\text{max}}$ (thin film) ( $\text{cm}^{-1}$ ) = 3562, 3401, 3382, 3219, 3121, 2921, 2897, 1646, 1601, 1491, 953, 819.



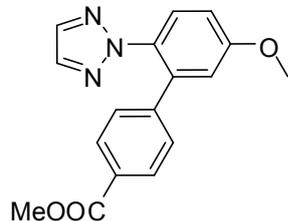
**2-(4',5'-dimethoxybiphenyl-2-yl)-2H-1,2,3-triazole (3k):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3k** (56.5 mg, 67 %) as a yellow solid, mp: 102.7-103.9 °C

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (s, 2H), 7.47 (d,  $J$  = 8.6 Hz, 1H), 7.02 – 6.92 (m, 4H), 6.77 (d,  $J$  = 8.6 Hz, 2H), 3.89 (s, 3H), 3.78 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.09, 159.03, 139.24, 134.77, 131.95, 130.73, 129.25, 128.05, 115.87, 113.73, 112.87, 55.66, 55.17

HR-MS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{15}\text{N}_3$ : 281.1164; found: 281.1158.

IR: $_{\text{max}}$ (thin film) ( $\text{cm}^{-1}$ ) = 3486, 3456, 3410, 3139, 3061, 2918, 2839, 1611, 1502, 1247, 1022, 860



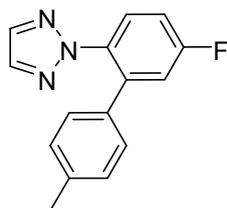
**methyl 5'-methoxy-2'-(2H-1,2,3-triazol-2-yl)biphenyl-4-carboxylate (3l):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 4/1) to give **3l** (68.6 mg, 74 %) as a black liquid.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 (d,  $J$  = 8.5 Hz, 2H), 7.63 (s, 2H), 7.55 (d,  $J$  = 8.6 Hz, 1H), 7.15 – 7.08 (m, 2H), 7.06 – 6.98 (m, 2H), 3.90 (d,  $J$  = 3.5 Hz, 6H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.80, 160.11, 143.16, 138.31, 134.96, 131.93, 130.13, 129.48, 129.13, 128.44, 128.23, 127.97, 115.96, 113.86, 55.73, 52.08.

HR-MS:  $m/z$  calcd for  $\text{C}_{17}\text{H}_{15}\text{N}_3\text{O}_3$ : 309.1113; found: 309.1117.

IR: $_{\text{max}}$ (thin film) ( $\text{cm}^{-1}$ ) = 3552, 3429, 3412, 3390, 3141, 2943, 2920, 1724, 1384, 1113, 958, 824



**2-(5-fluoro-4'-methylbiphenyl-2-yl)-2H-1,2,3-triazole (3m):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 20/1) to give **3m** (53.1 mg, 70 %) as a yellow liquid.

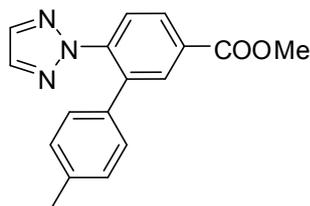
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.68 (s, 2H), 7.56 (dd, *J* = 8.7, 5.2 Hz, 1H), 7.23 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.20 – 7.12 (m, 1H), 7.07 (d, *J* = 7.9 Hz, 2H), 6.91 (d, *J* = 8.1 Hz, 2H), 2.32 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 162.64 (d, *J* = 249.9 Hz), 140.41 (d, *J* = 8.7 Hz), 137.72, 135.13, 134.69, (d, *J* = 3.1 Hz) 134.44, 129.14, 128.64 (d, *J* = 9.2 Hz), 127.87, 117.73 (d, *J* = 23.2 Hz), 114.63 (d, *J* = 22.9 Hz), 21.16

<sup>19</sup>F NMR (377 MHz, CDCl<sub>3</sub>) δ -111.25

HR-MS: *m/z* calcd for C<sub>15</sub>H<sub>12</sub>FN<sub>3</sub>: 253.1015; found: 253.1018.

IR: <sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3563, 3536, 3401, 3249, 3163, 2921, 2879, 1558, 1540, 1501, 1186, 954



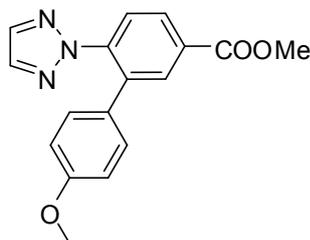
**methyl 4'-methyl-6-(2H-1,2,3-triazol-2-yl)biphenyl-3-carboxylate (3n):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3n** (74.7 mg, 85 %) as a yellow solid, mp: 102.9-103.6 °C

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.21 (d, *J* = 1.7 Hz, 1H), 8.13 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.71 (t, *J* = 4.0 Hz, 3H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.95 (d, *J* = 8.0 Hz, 2H), 3.96 (s, 3H), 2.33 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 166.10, 141.49, 137.67, 137.50, 135.56, 134.89, 132.90, 130.81, 129.14, 129.00, 128.08, 126.47, 52.45, 21.19

HR-MS: *m/z* calcd for C<sub>17</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>: 293.1164; found: 293.1162.

IR: <sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3551, 3474, 3412, 3236, 3121, 2952, 2924, 2853, 1726, 1616, 1311, 1251, 1111.



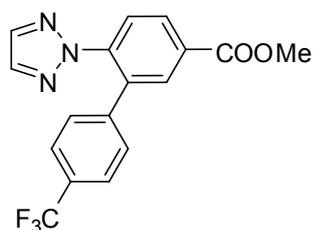
**methyl 4'-methoxy-6-(2H-1,2,3-triazol-2-yl)biphenyl-3-carboxylate (3o):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 8/1) to give **3o** (71.4 mg, 77 %) as a grey solid, mp: 97.0- 98.2 °C

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.19 (s, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 7.71-7.64 (m, 3H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.81 (d, *J* = 8.4 Hz, 2H), 3.96 (s, 3H), 3.79 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 166.12, 159.21, 141.46, 137.43, 135.56, 132.78, 130.84, 130.11, 129.40, 128.80, 126.56, 113.88, 55.21, 52.46

HR-MS: *m/z* calcd for C<sub>17</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub>: 309.1113; found: 309.1109.

IR:<sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3454, 3432, 3232, 2963, 2917, 2360, 2339, 1720, 1616, 1501,1309,1246.



**methyl 6-(2H-1,2,3-triazol-2-yl)-4'-(trifluoromethyl)biphenyl-3-carboxylate (3p):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 4/1) to give **3p** (87.4 mg, 84 %) as a yellow solid, mp:111.5- 112.3 °C

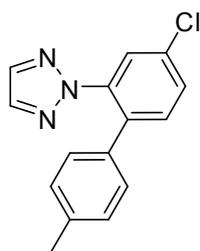
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.22-8.19 (m, 2H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.70 (s, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 3.97 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 165.78, 141.73, 141.39, 135.89, 135.86, 132.77, 130.85, 130.07, 129.79 (q, *J* = 32.6 Hz), 128.70, 126.24, 125.29 (q, *J* = 3.7 Hz), 124.05 (q, *J* = 270.4 Hz), 52.56

<sup>19</sup>F NMR (377 MHz, CDCl<sub>3</sub>) δ -62.60

HR-MS: *m/z* calcd for C<sub>17</sub>H<sub>12</sub>F<sub>3</sub>N<sub>3</sub>O<sub>2</sub>: 347.0882; found: 347.0885.

IR:<sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3499, 3468, 3404, 3025, 2921, 1638, 1617, 1491, 935, 819



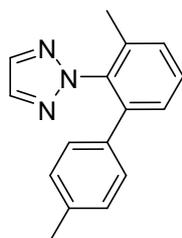
**2-(4-chloro-4'-methylbiphenyl-2-yl)-2H-1,2,3-triazole (3q):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3q** (65.4 mg, 81 %) as a brow solid, mp: 121.4-122.2 °C

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (s, 2H), 7.64 (d, *J* = 2.0 Hz, 1H), 7.51 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.45 (d, *J* = 8.3 Hz, 1H), 7.07 (d, *J* = 7.9 Hz, 2H), 6.90 (d, *J* = 8.1 Hz, 2H), 2.32 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 138.95, 137.44, 136.29, 135.40, 134.57, 133.35, 132.30, 129.55, 129.12, 127.98, 126.74, 21.16

HR-MS: *m/z* calcd for C<sub>15</sub>H<sub>12</sub>ClN<sub>3</sub>: 269.0720; found: 269.0715.

IR:<sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3552, 3451, 3420, 3237, 3066, 2948, 2921, 1638, 1617, 1481, 1429, 1410, 1101, 959, 817



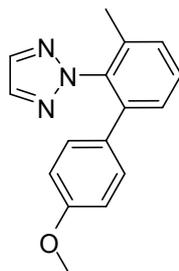
**2-(3,4'-dimethylbiphenyl-2-yl)-2H-1,2,3-triazole (3r):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3r**(58.3 mg, 78 %) as a grey solid, mp: 67.8-68.2 °C

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (s, 2H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.37 – 7.30 (m, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 2.29 (s, 3H), 2.06 (s, 3H)

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 140.12, 138.01, 136.94, 136.52, 135.58, 134.50, 129.84, 129.67, 128.80, 128.36, 128.00, 21.11, 17.53

HR-MS: *m/z* calcd for C<sub>16</sub>H<sub>15</sub>N<sub>3</sub>: 249.1266; found: 249.1269.

IR: <sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3560, 3471, 3408, 3387, 2933, 2911, 1614, 1470, 1412, 1149, 952, 810



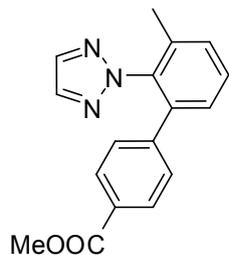
**2-(4'-methoxy-3-methylbiphenyl-2-yl)-2H-1,2,3-triazole (3s):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 20/1) to give **3s**(44.5 mg, 56 %) as a yellow liquid.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.70 (s, 2H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.35 – 7.27 (m, 2H), 6.99 (d, *J* = 8.6 Hz, 2H), 6.73 (d, *J* = 8.6 Hz, 2H), 3.75 (s, 3H), 2.04 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 158.84, 139.81, 138.00, 136.55, 134.52, 130.88, 129.83, 129.49, 129.28, 128.27, 113.53, 55.13, 17.50

HR-MS: *m/z* calcd for C<sub>16</sub>H<sub>15</sub>N<sub>3</sub>O: 265.1215; found: 265.1218.

IR: <sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3553, 3434, 3392, 3121, 2925, 1616, 1515, 1471, 1241, 1029, 794.



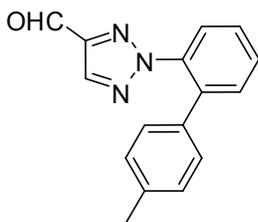
**methyl 3'-methyl-2'-(2H-1,2,3-triazol-2-yl)biphenyl-4-carboxylate (3t):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3t**(65.9 mg, 75 %) as a yellow solid, mp: 108.1- 108.9 °C

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.87 (d, *J* = 8.2 Hz, 2H), 7.67 (s, 2H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.43 – 7.30 (m, 2H), 7.13 (d, *J* = 8.3 Hz, 2H), 3.88 (s, 3H), 2.08 (s, 3H).

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 166.85, 143.21, 139.12, 137.93, 136.74, 134.73, 130.62, 129.97, 129.31, 128.91, 128.20, 128.12, 52.08, 17.54

HR-MS: *m/z* calcd for C<sub>17</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>: 293.1164; found: 293.1160.

IR: <sub>max</sub>(thin film) (cm<sup>-1</sup>) = 3482, 3413, 3383, 3230, 3121, 2942, 2913, 2839, 1723, 1279, 1108, 959



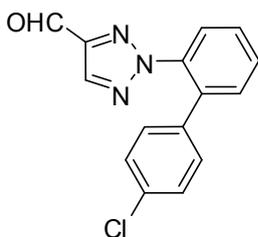
**2-(4'-methylbiphenyl-2-yl)-2H-1,2,3-triazole-4-carbaldehyde (3u):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3u** (55.2 mg, 70 %) as a yellow liquid.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  10.07 (s, 1H), 8.12 (s, 1H), 7.69 – 7.46 (m, 4H), 7.08 (d,  $J = 7.8$  Hz, 2H), 6.95 (d,  $J = 7.9$  Hz, 2H), 2.32 (s, 3H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  184.38, 147.63, 138.13, 137.86, 137.50, 134.95, 134.91, 131.44, 130.33, 129.20, 128.03, 126.45, 21.15

HR-MS:  $m/z$  calcd for  $\text{C}_{16}\text{H}_{13}\text{N}_3\text{O}$ : 263.1059; found: 263.1063.

IR:  $\text{max}$ (thin film) ( $\text{cm}^{-1}$ ) = 3551, 3485, 3414, 3237, 3131, 3025, 2921, 2853, 1703, 1617, 1485, 1451, 1309, 1213, 965



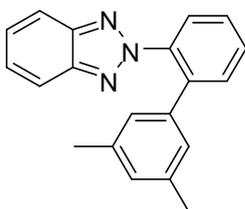
**2-(4-chlorobiphenyl-2-yl)-2H-1,2,3-triazole-4-carbaldehyde(3v):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3v** (46.7 mg, 55 %) as a pale yellow solid, mp: 110.1-111.2°C

$^1\text{H NMR}$  (400 MHz, DMSO)  $\delta$  10.06 (s, 1H), 8.51 (s, 1H), 7.79 – 7.72 (m, 2H), 7.67 (t,  $J = 8.3$  Hz, 2H), 7.37 (d,  $J = 8.5$  Hz, 2H), 7.05 (d,  $J = 8.5$  Hz, 2H).

$^{13}\text{C NMR}$  (101 MHz,  $\text{CDCl}_3$ )  $\delta$  184.15, 147.75, 137.79, 136.78, 136.40, 135.09, 133.92, 131.30, 130.39, 129.56, 128.66, 126.45

HR-MS:  $m/z$  calcd for  $\text{C}_{15}\text{H}_{10}\text{ClN}_3\text{O}$ : 283.0512; found: 283.0512.

IR:  $\text{max}$ (thin film) ( $\text{cm}^{-1}$ ) = 3569, 3467, 3408, 3109, 3121, 1699, 1616, 1489, 1315, 1031, 760.



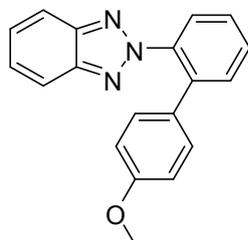
**2-(2',5'-dimethylbiphenyl-2-yl)-2H-benzo[d][1,2,3]triazole (3w):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3w** (52.9 mg, 59%) as a white solid, mp: 91.5°C

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 – 7.85 (m, 2H), 7.77 – 7.48 (m, 4H), 7.38 (dd,  $J = 7.0, 2.5$  Hz, 2H), 6.82 (s, 1H), 6.65 (s, 2H), 2.10 (s, 6H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  144.66, 139.13, 138.44, 137.83, 137.71, 131.25, 130.09, 129.14, 127.87, 127.05, 126.73, 125.91, 118.38, 21.15

HR-MS:  $m/z$  calcd for  $\text{C}_{20}\text{H}_{17}\text{N}_3$ : 299.1422; found: 299.1420.

IR: $_{\text{max}}$ (thin film) ( $\text{cm}^{-1}$ ) = 3409, 3238, 3104, 3045, 2934, 2854, 1615, 1488, 1440, 1376, 1227, 907, 869, 826, 778, 615.



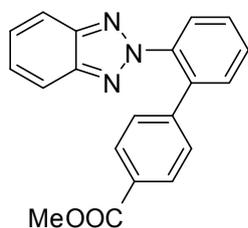
**2-(4'-methoxybiphenyl-2-yl)-2H-benzo[d][1,2,3]triazole (3x):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 20/1) to give **3x** (57.8 mg, 64%) as a white solid, mp: 95.4–96.5 °C

$^1\text{H}$  NMR (400 MHz, )  $\delta$  7.85 (dd,  $J$  = 6.6, 3.1 Hz, 2H), 7.72 – 7.46 (m, 4H), 7.38 (dd,  $J$  = 6.6, 3.0 Hz, 2H), 6.97 (d,  $J$  = 8.7 Hz, 2H), 6.70 (d,  $J$  = 8.7 Hz, 2H), 3.73 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz, )  $\delta$  159.08, 144.77, 139.05, 137.83, 131.32, 130.54, 130.18, 129.37, 127.72, 127.29, 126.82, 118.53, 113.91, 55.24

HR-MS:  $m/z$  calcd for  $\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}$ : 301.1215; found: 301.1220.

IR: $_{\text{max}}$ (thin film) ( $\text{cm}^{-1}$ ) = 3823, 3775, 3423, 3223, 2365, 1652, 1488, 1442, 1372, 1285, 1153, 1105, 1074, 950, 878, 668



**methyl 2'-(2H-benzo[d][1,2,3]triazol-2-yl)biphenyl-4-carboxylate (3y):** According to the General Procedure, a crude product was purified by using a preparative silica gel TLC (Hex/EA = 10/1) to give **3y** (78.0 mg, 79 %) as a white solid, mp: 138.0–138.5 °C

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 – 7.85 (m, 2H), 7.84 – 7.77 (m, 3H), 7.68 – 7.56 (m, 3H), 7.38 (dd,  $J$  = 6.6, 3.0 Hz, 2H), 7.18 (t,  $J$  = 7.7 Hz, 1H), 7.08 (d,  $J$  = 7.7 Hz, 1H), 3.81 (s, 3H).

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.69, 144.77, 139.06, 138.48, 136.94, 132.51, 131.32, 130.41, 130.20, 129.47, 128.65, 128.62, 128.25, 127.06, 126.93, 118.39, 100.00, 52.06

HR-MS:  $m/z$  calcd for  $\text{C}_{20}\text{H}_{15}\text{N}_3\text{O}_2$ : 329.1164; found: 329.1160.

IR: $_{\text{max}}$ (thin film) ( $\text{cm}^{-1}$ ) = 3525, 3446, 3227, 3114, 3097, 2947, 2876, 2356, 1652, 1560, 1433, 1138, 910, 878, 744

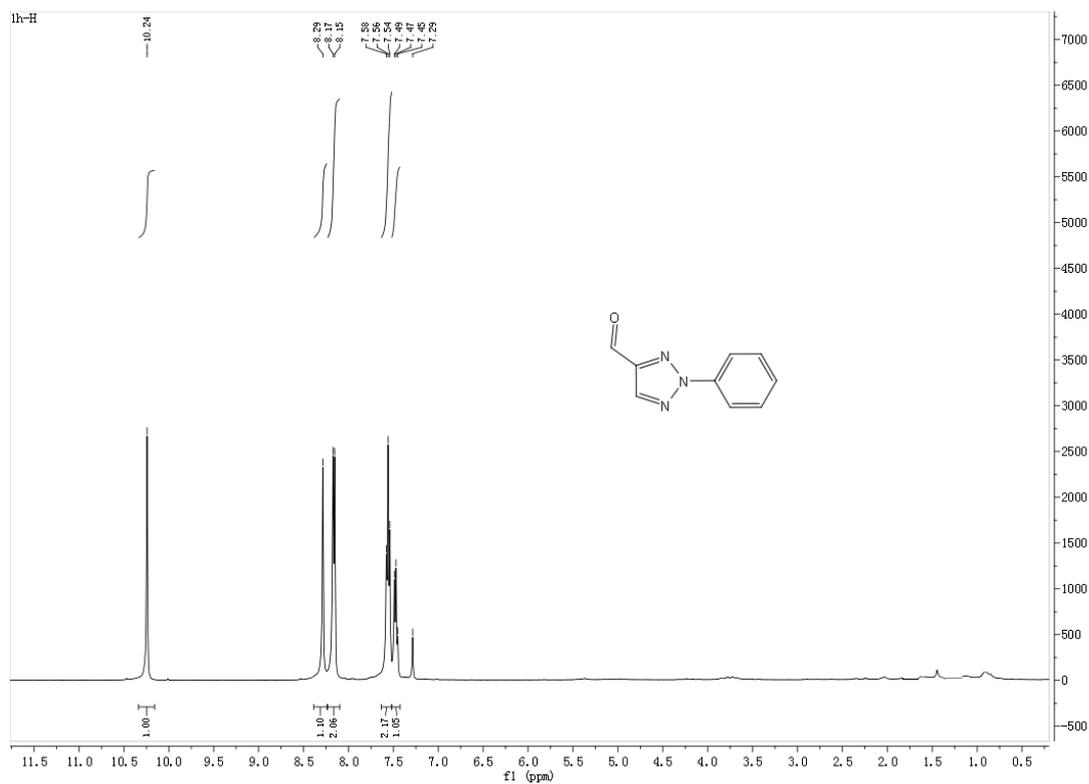
## 4. References

1. Taillefer, M.; Xia, N.; Ouali, A. *Angew. Chem. Int. Ed.* **2007**, *46*, 934–936
2. Tian, Q. S.; Kuang, C. X. *Org. Biomol. Chem.*, **2013**, *11*, 7830–7833

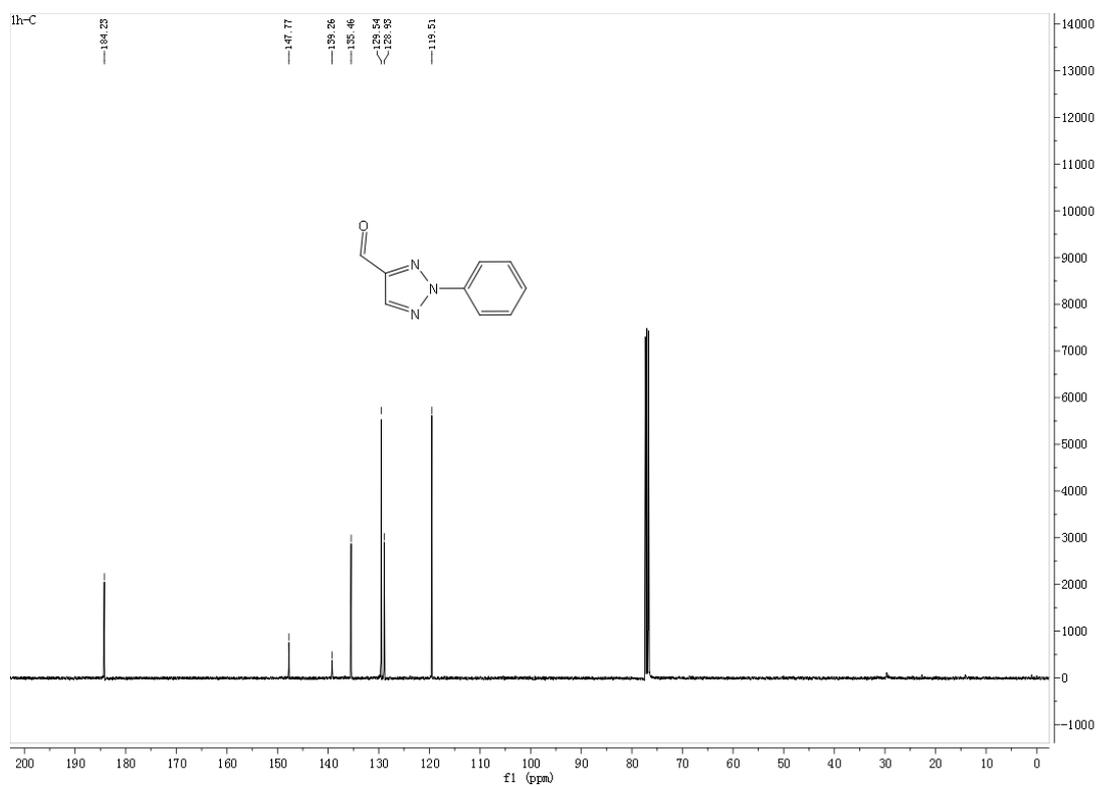
3. El Ashry, E. S. H.; Atta, K. F.; Aboul-Ela, S.; Beldi, R. *J. Carbohydr. Chem.* **2007**, 26, 429–437

## **5. NMR spectra data for all compounds**

### **<sup>1</sup>H NMR of 1h**

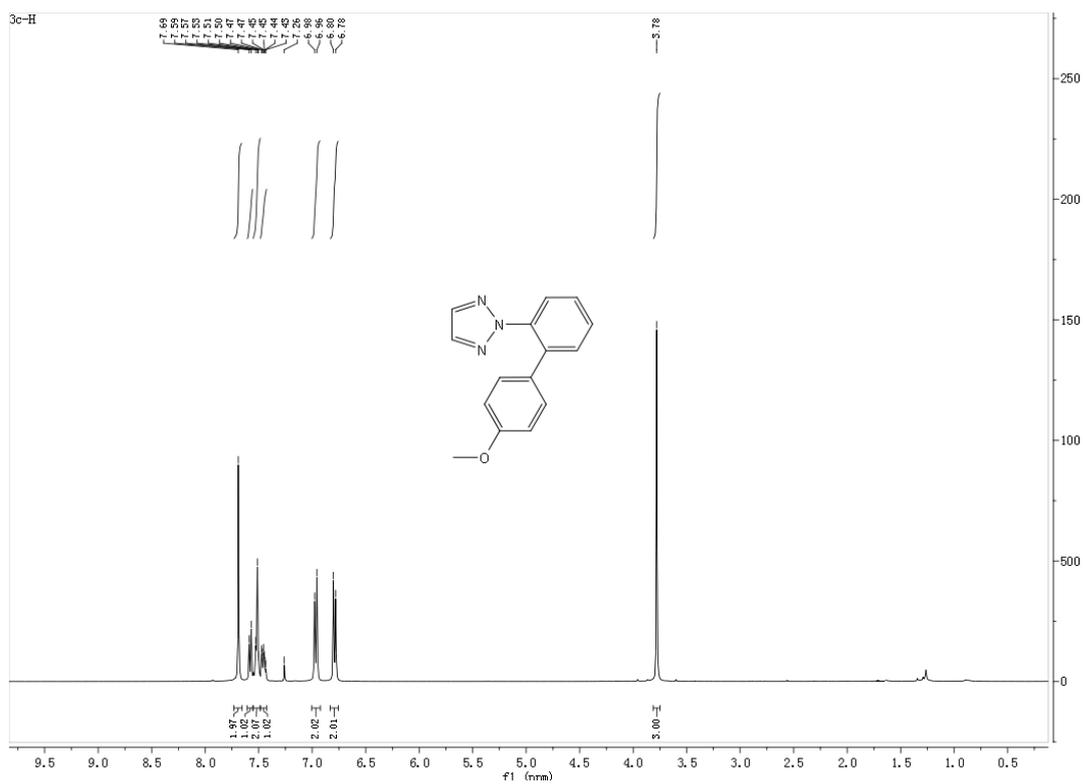


### <sup>13</sup>C NMR of 1h

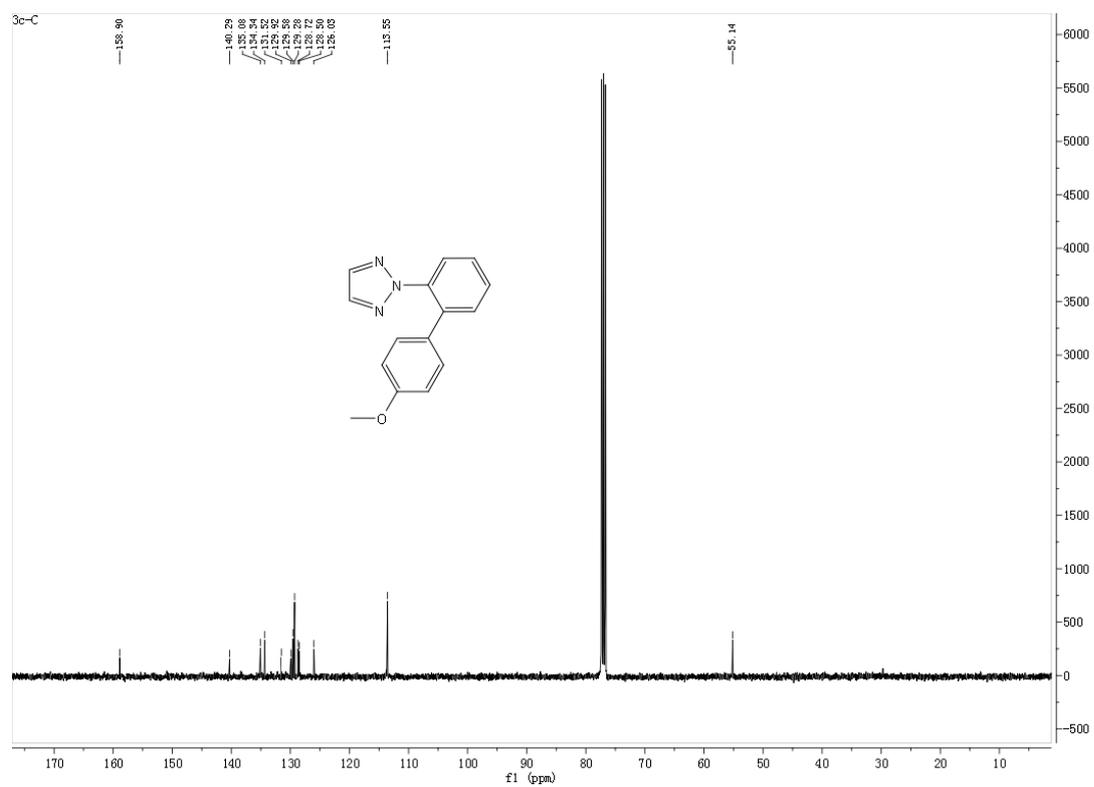








**<sup>13</sup>C NMR of 3c**

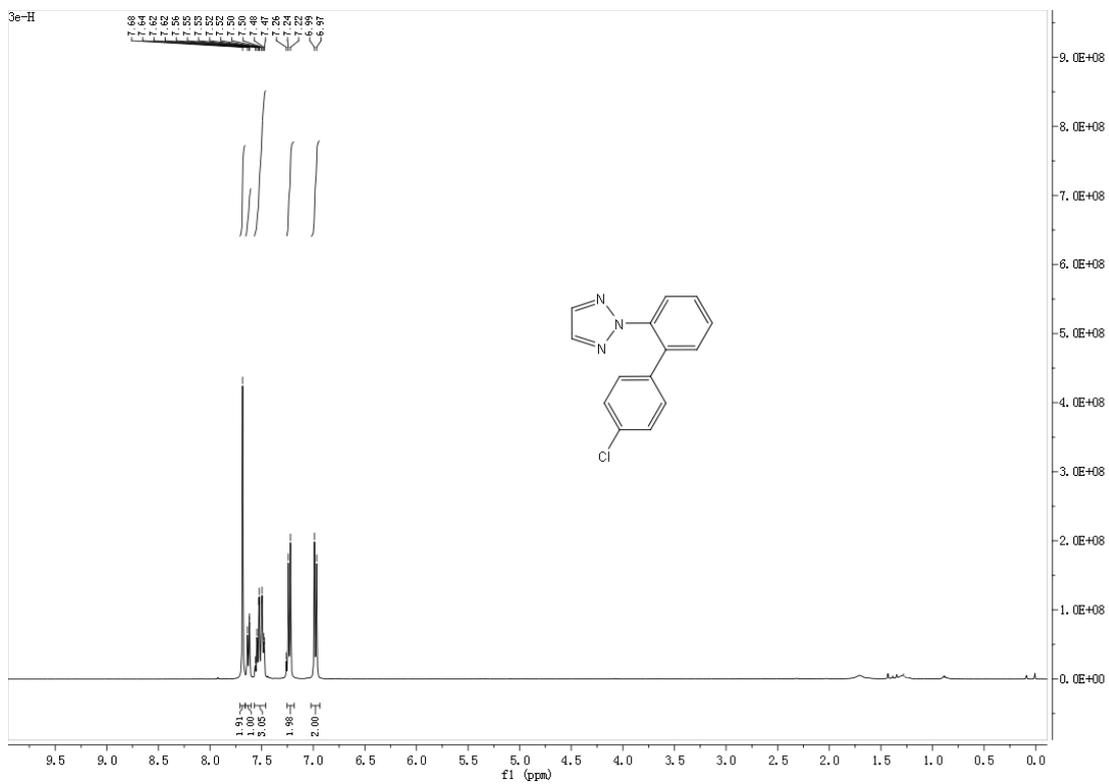


**<sup>1</sup>H NMR of 3d**

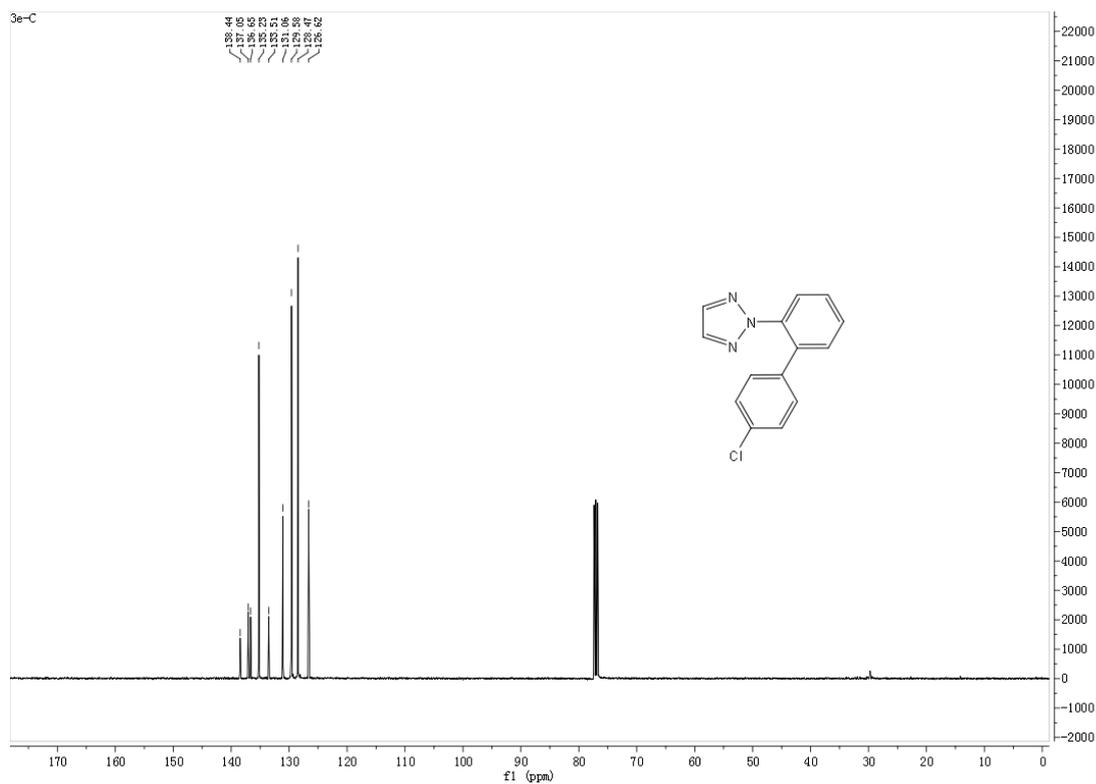




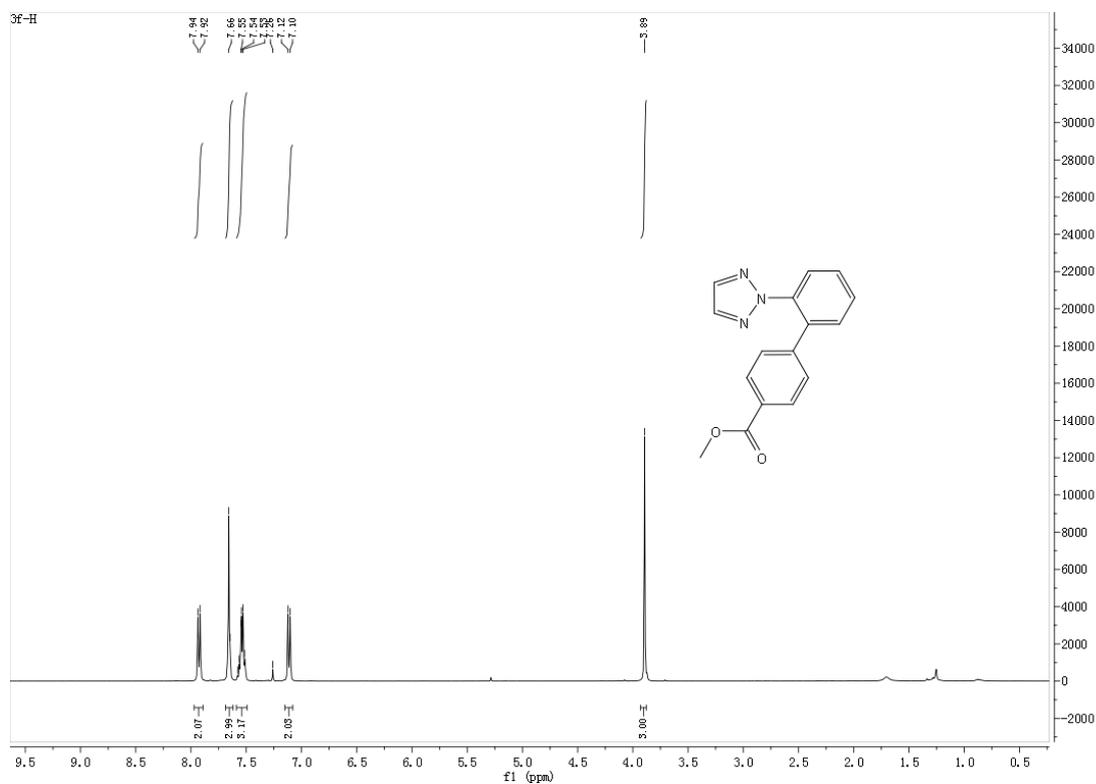
### <sup>1</sup>H NMR of 3e



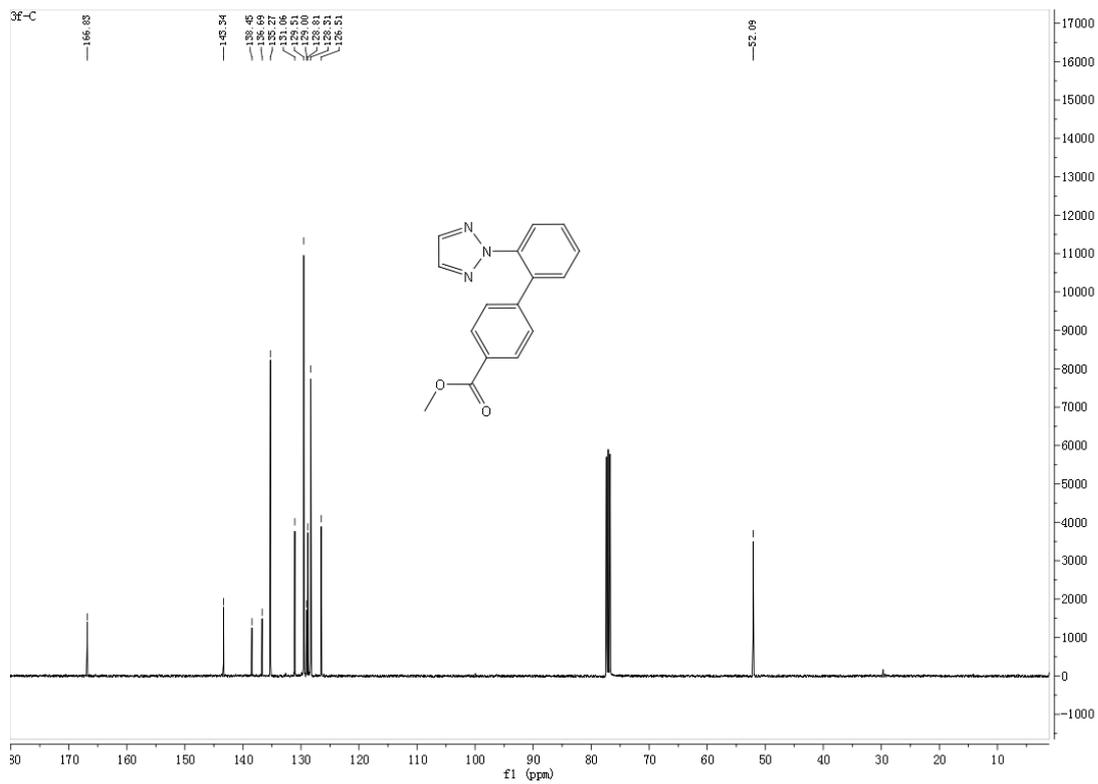
### <sup>13</sup>C NMR of 3e



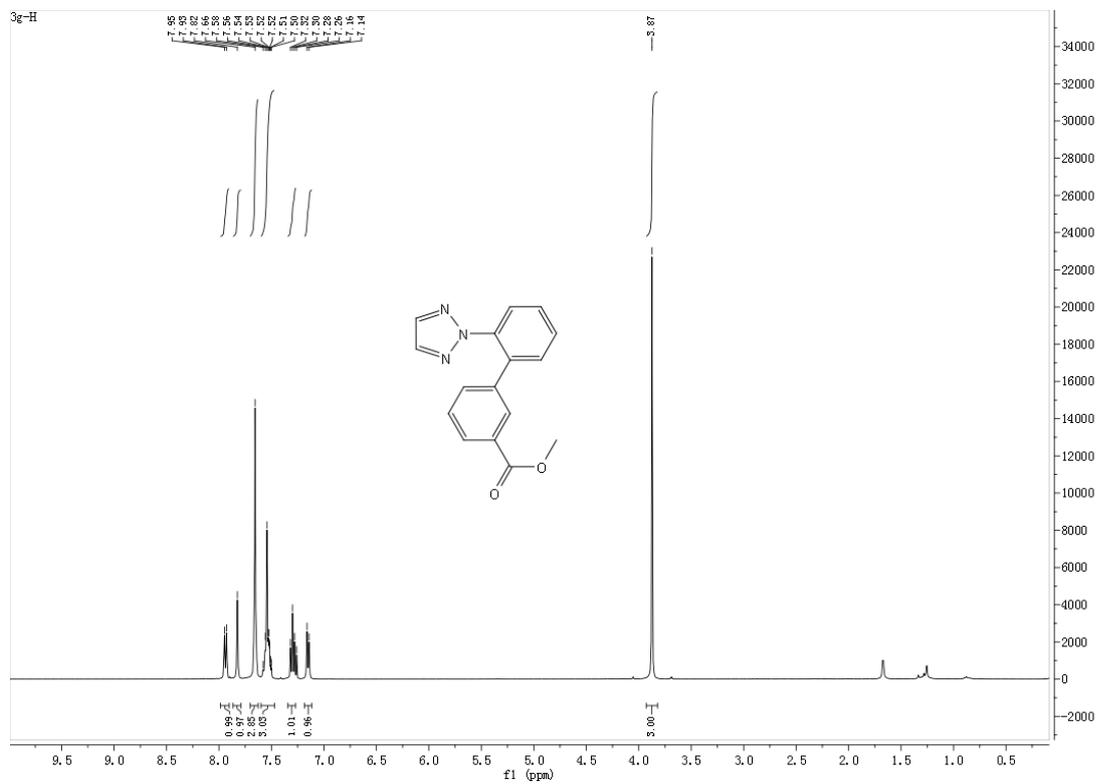
**<sup>1</sup>H NMR of 3f**



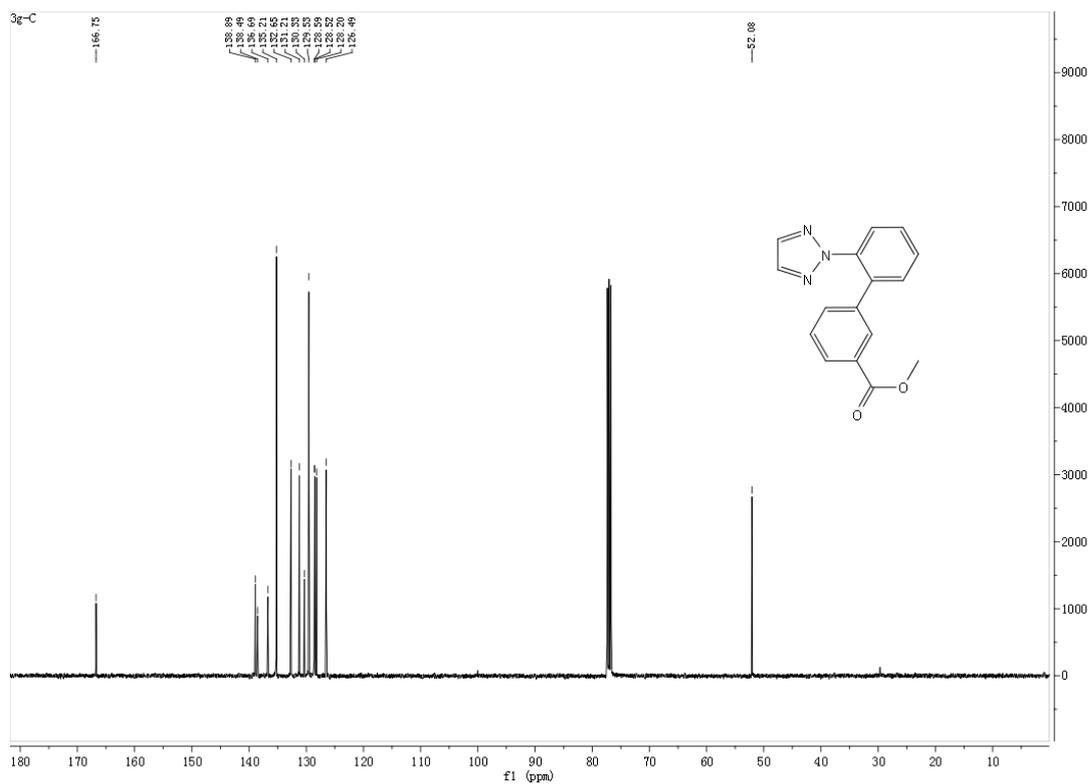
**<sup>13</sup>C NMR of 3f**



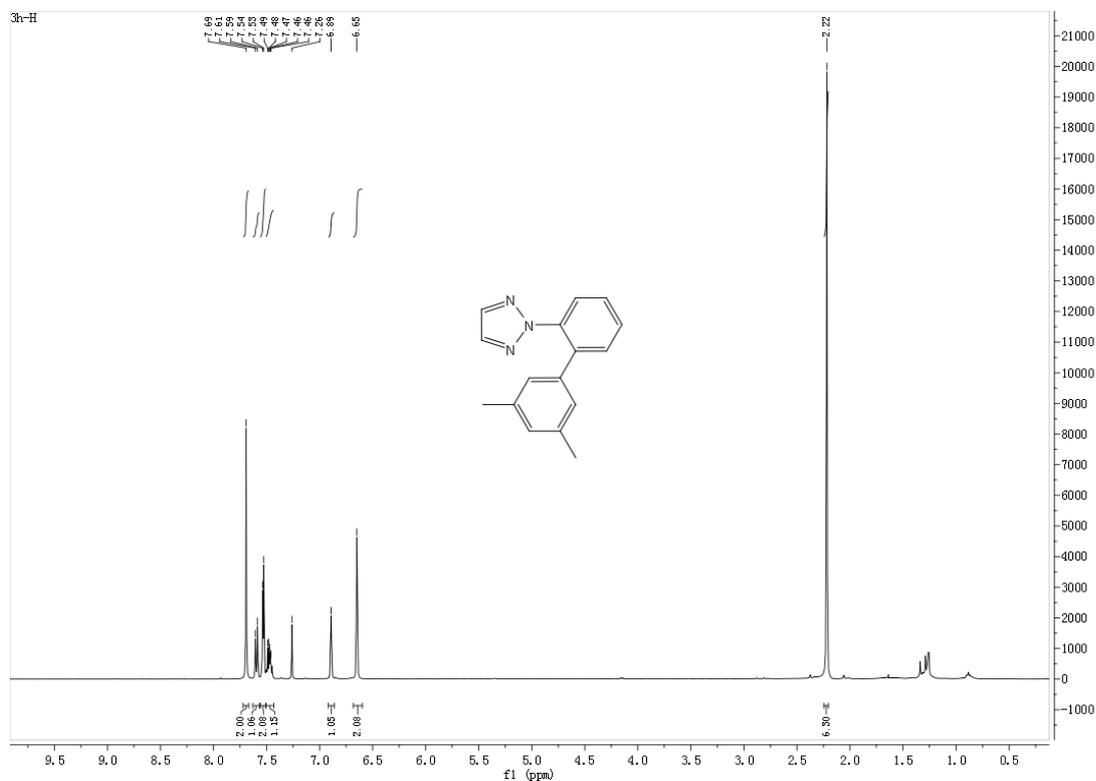
**<sup>1</sup>H NMR of 3g**



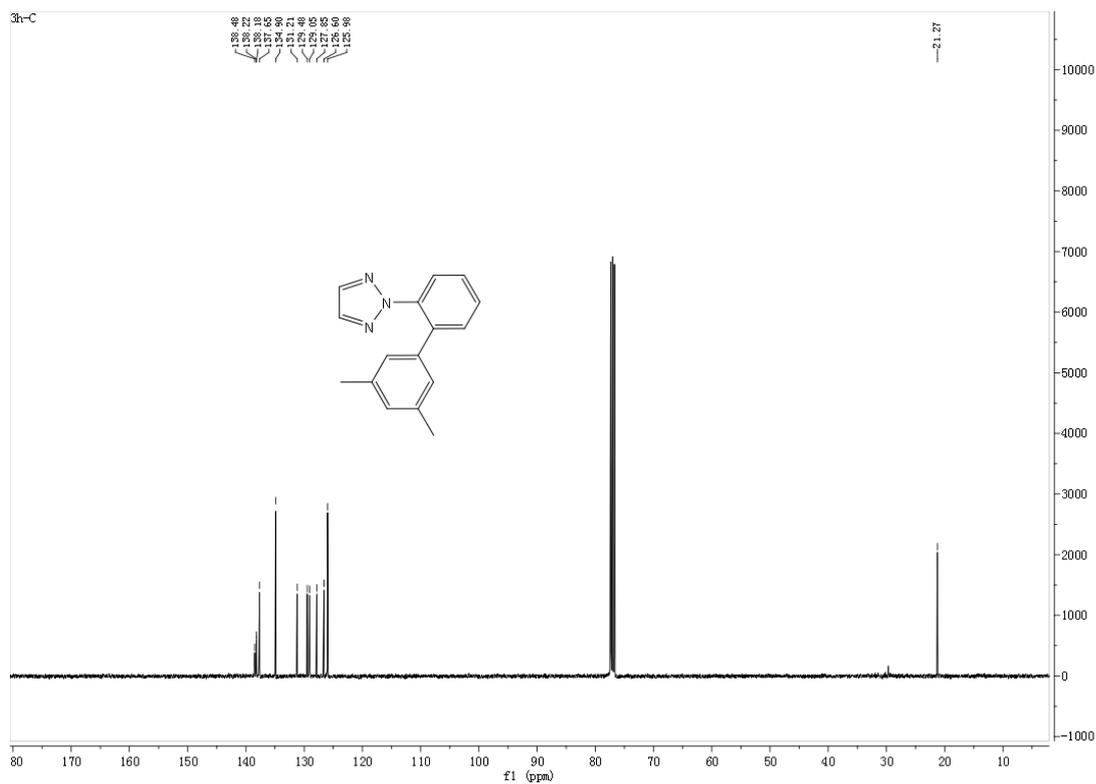
**<sup>13</sup>C NMR of 3g**



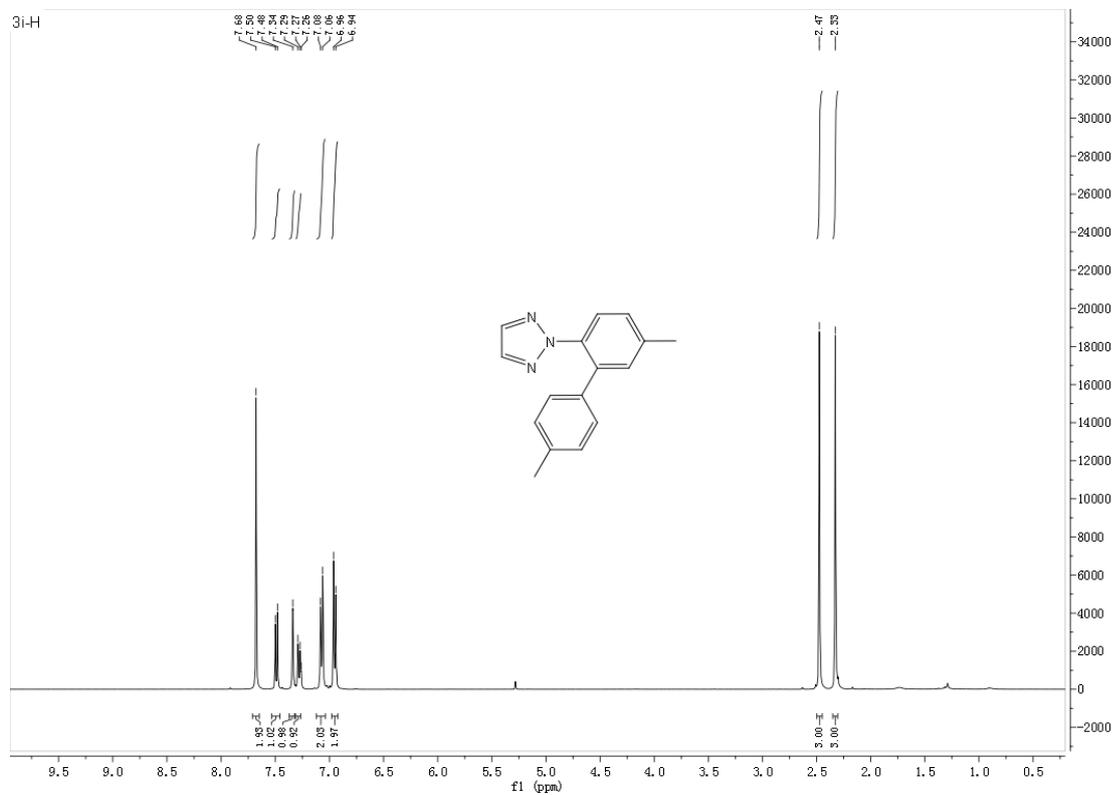
**<sup>1</sup>H NMR of 3h**



### <sup>13</sup>CNMR of 3h

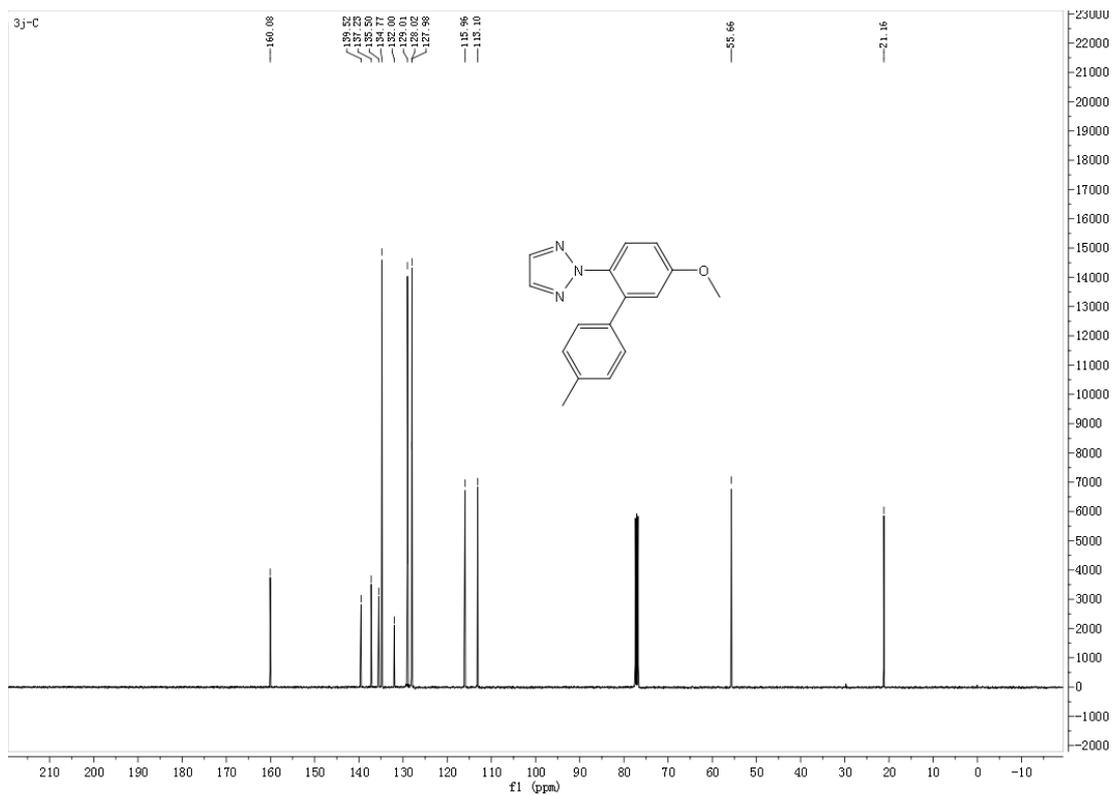


### <sup>1</sup>H NMR of 3i

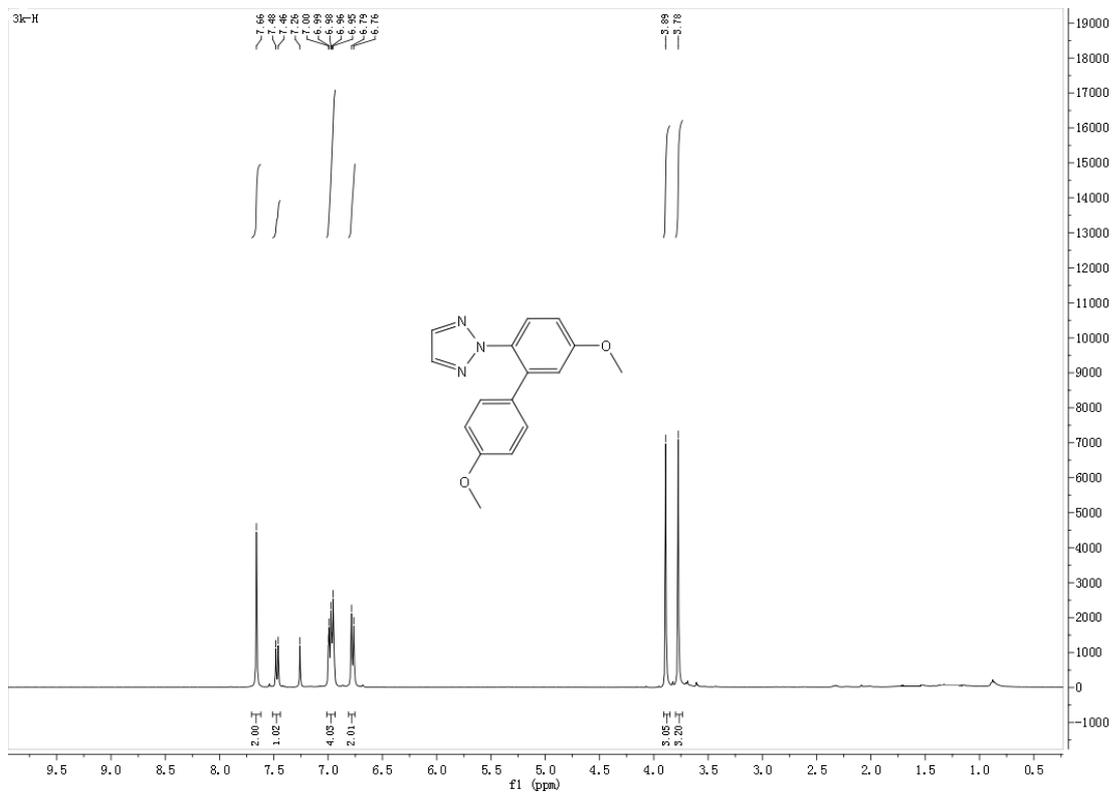


### <sup>13</sup>C NMR of 3i

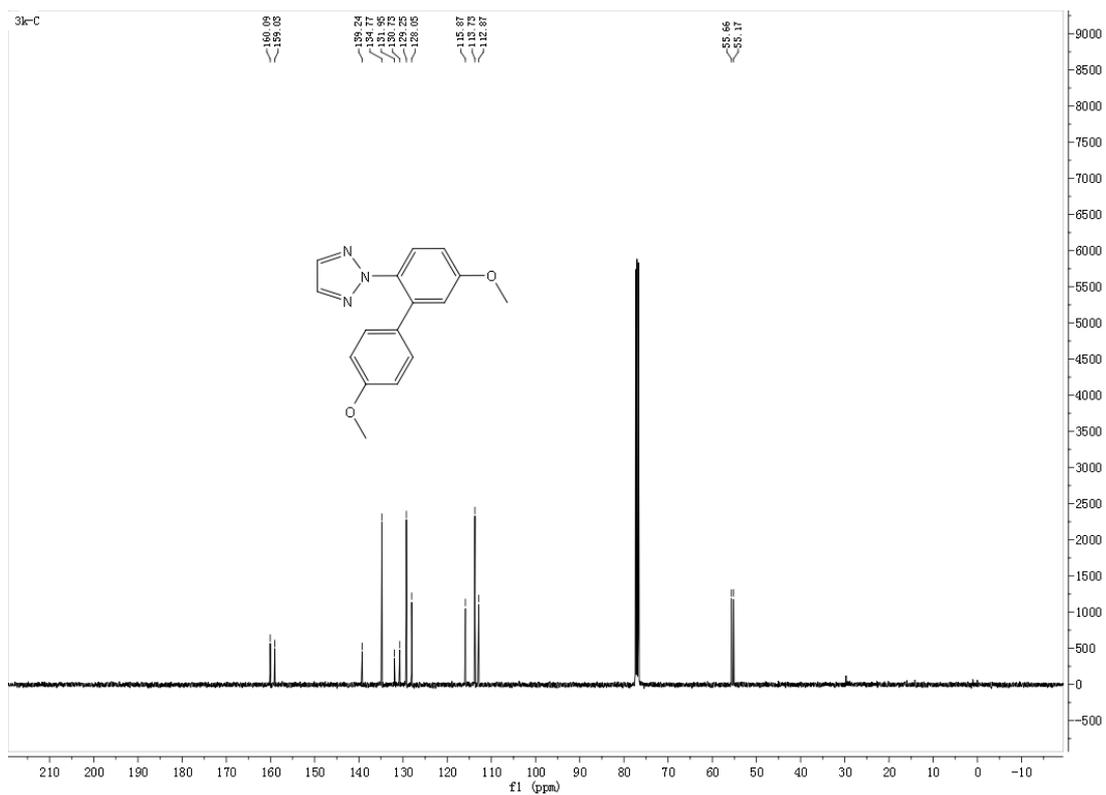




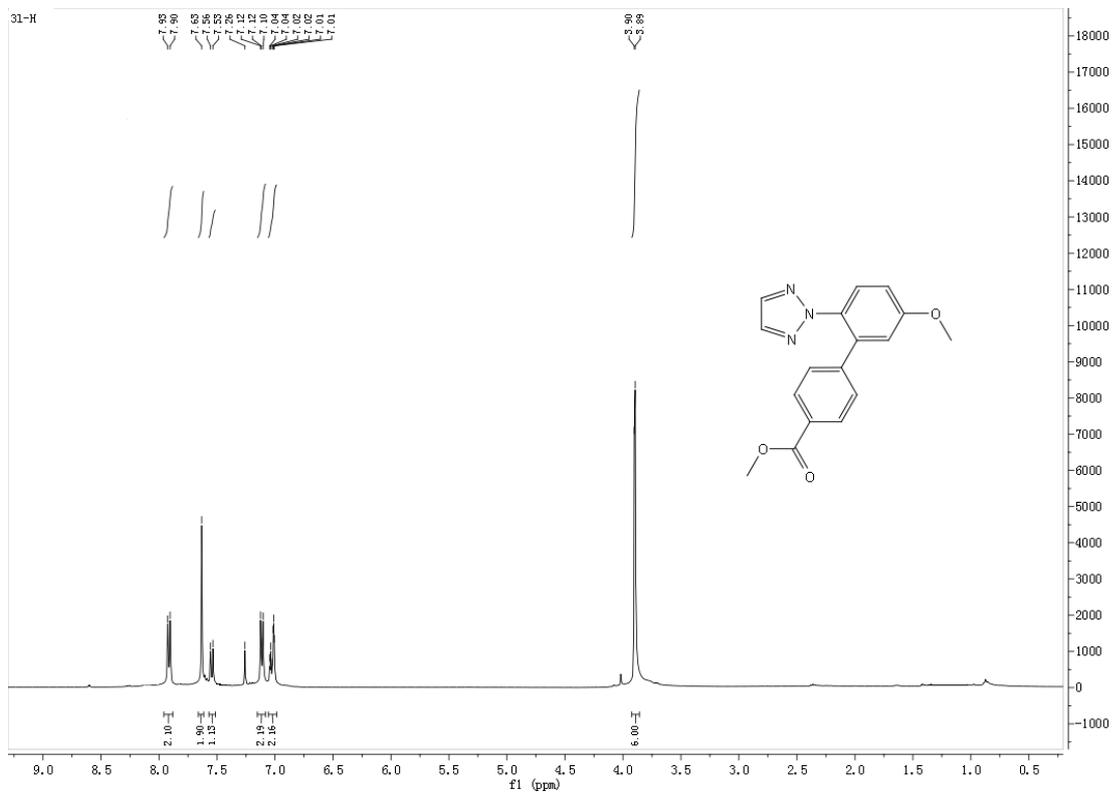
### <sup>1</sup>H NMR of 3k



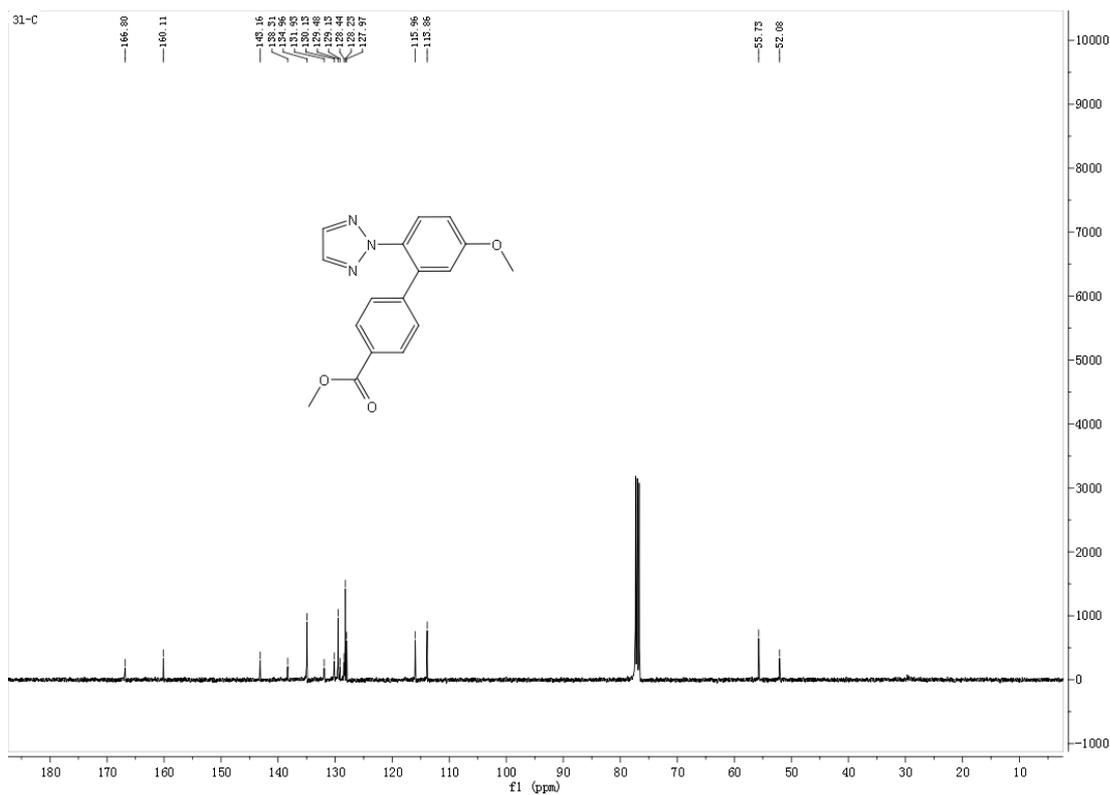
### <sup>13</sup>C NMR of 3k



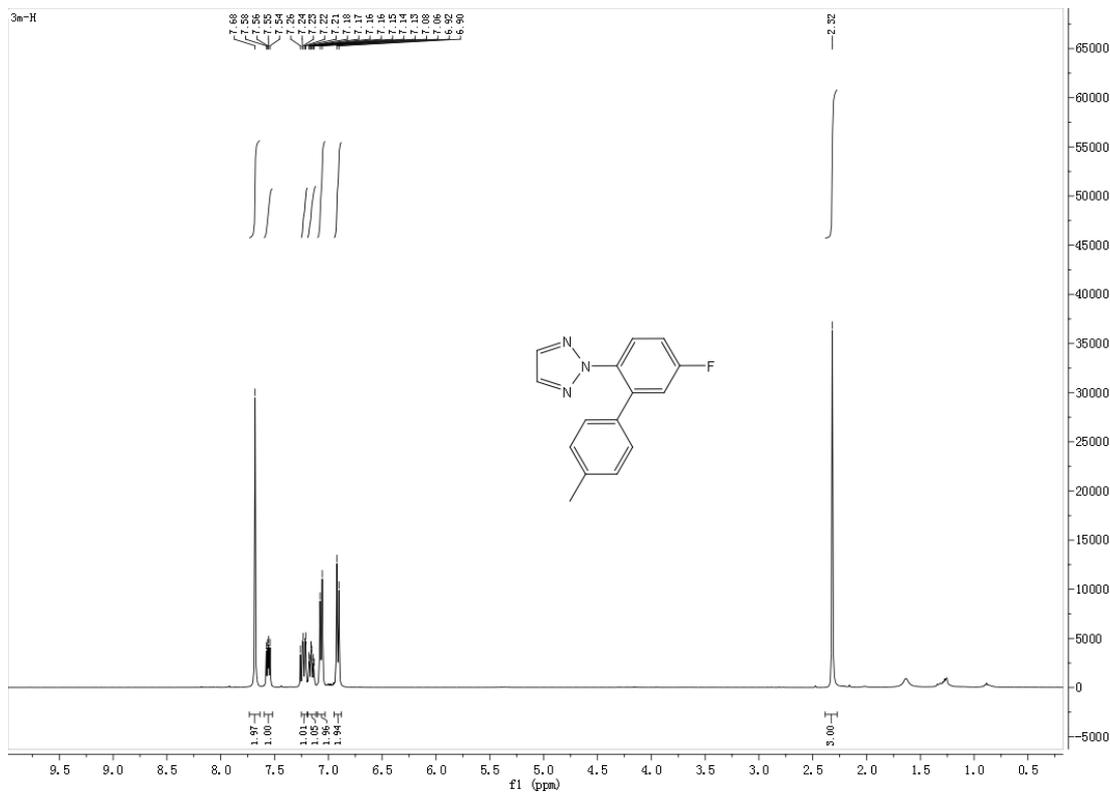
### <sup>1</sup>H NMR of 31



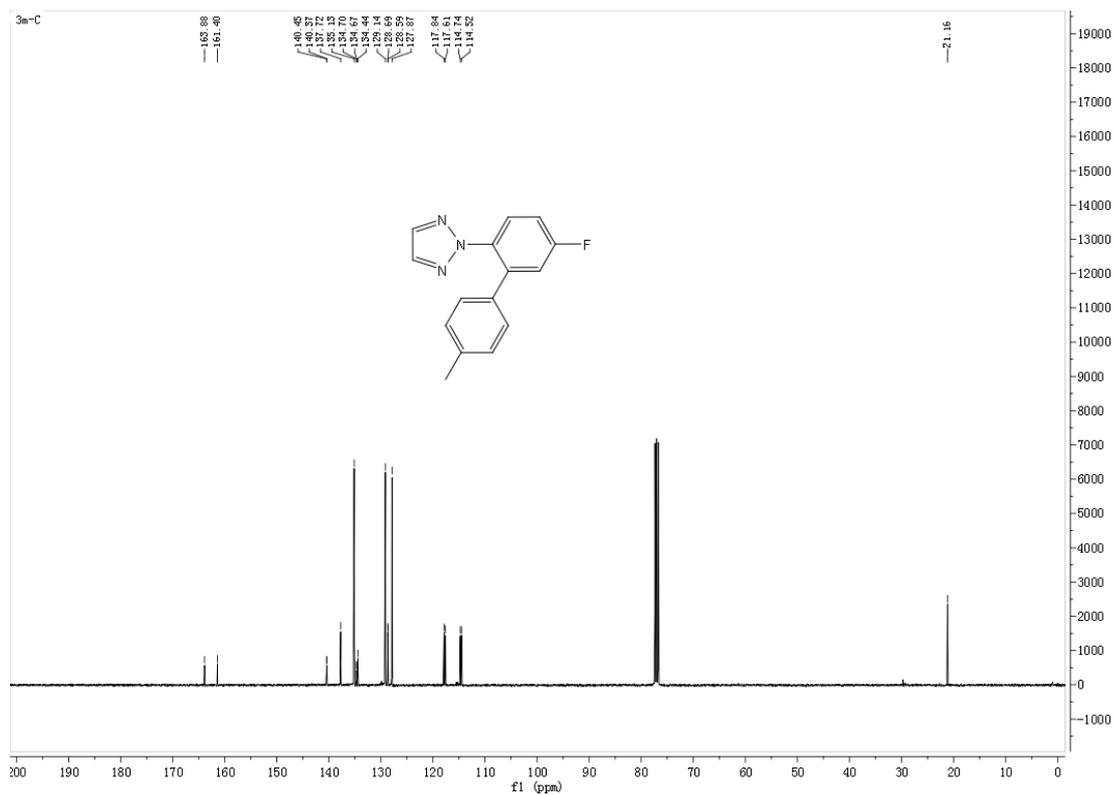
### <sup>13</sup>C NMR of 31



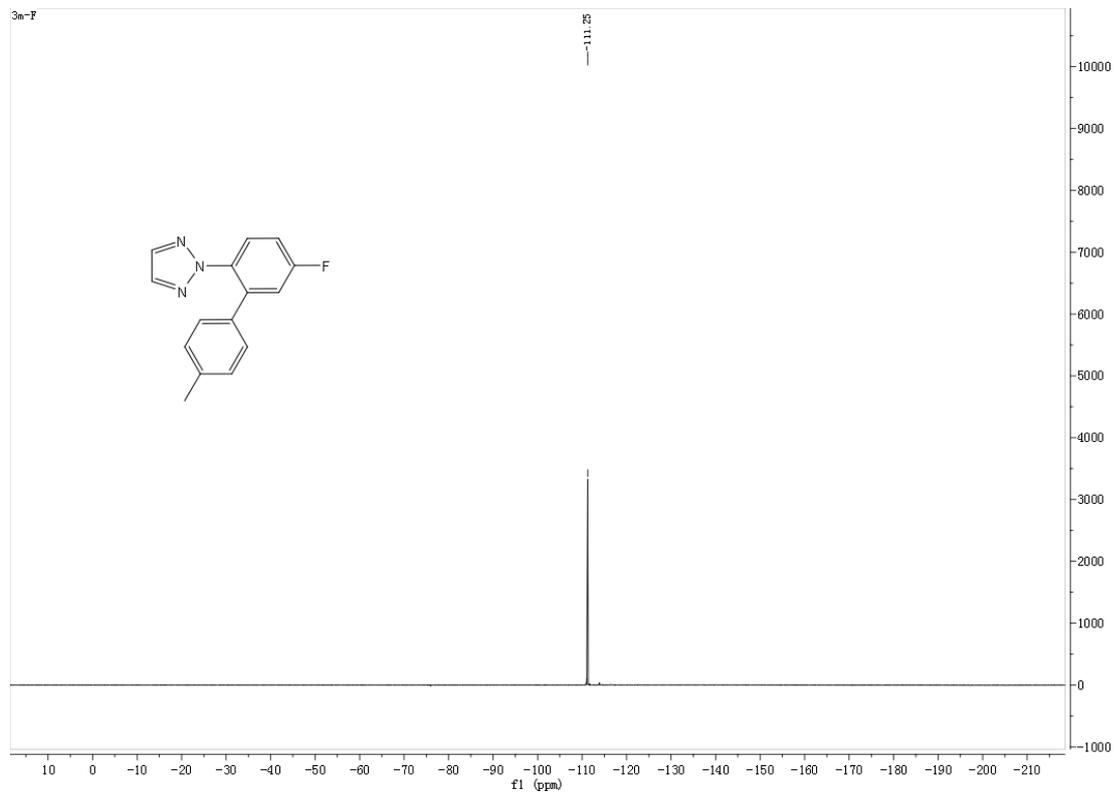
### <sup>1</sup>H NMR of 3m



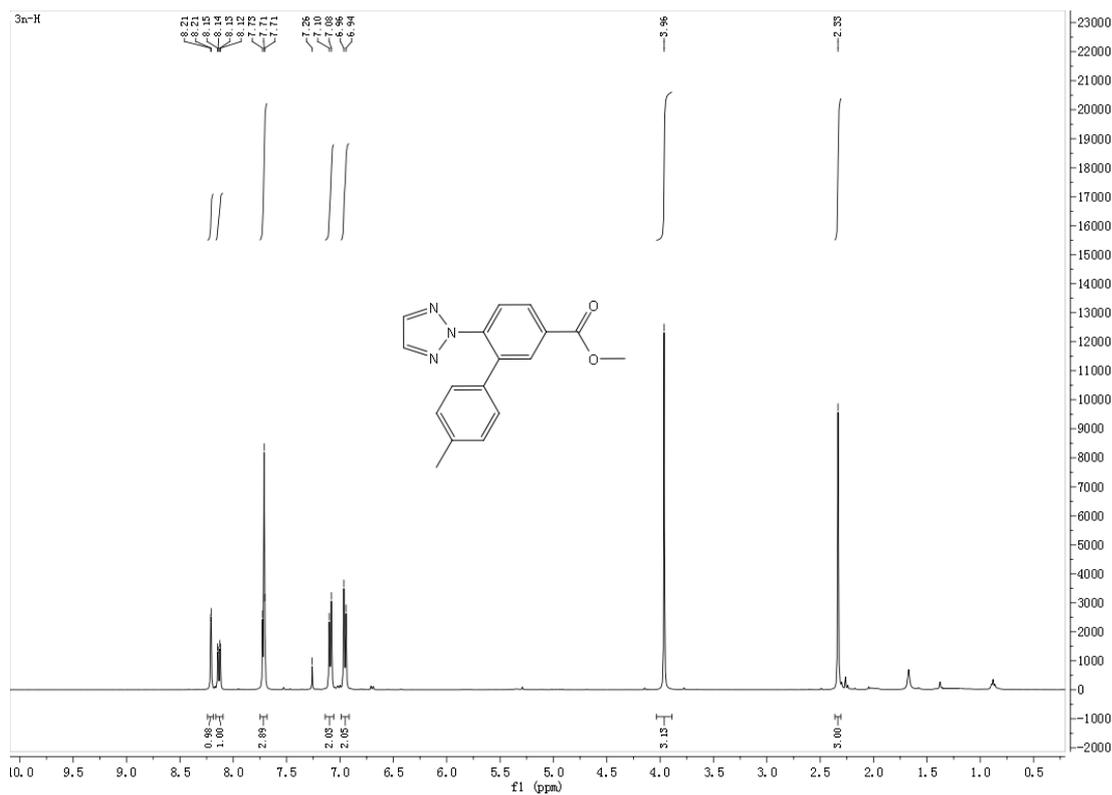
### <sup>13</sup>C NMR of 3m



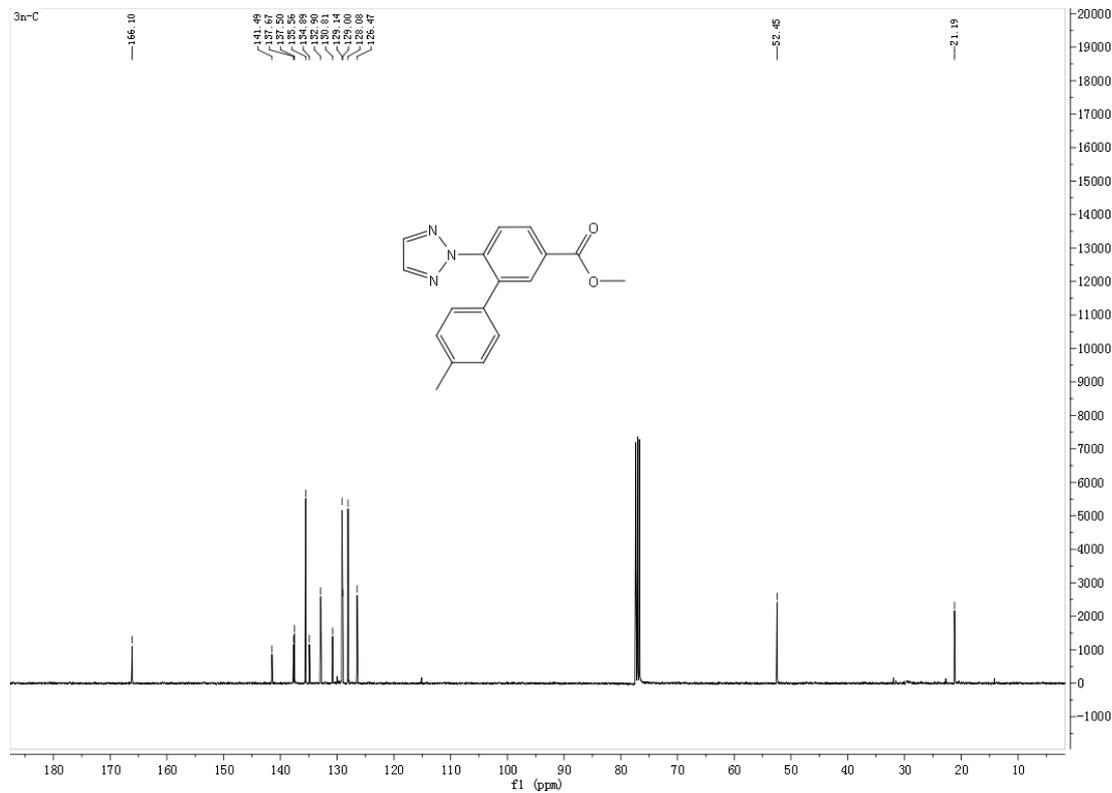
### <sup>19</sup>F NMR of 3m



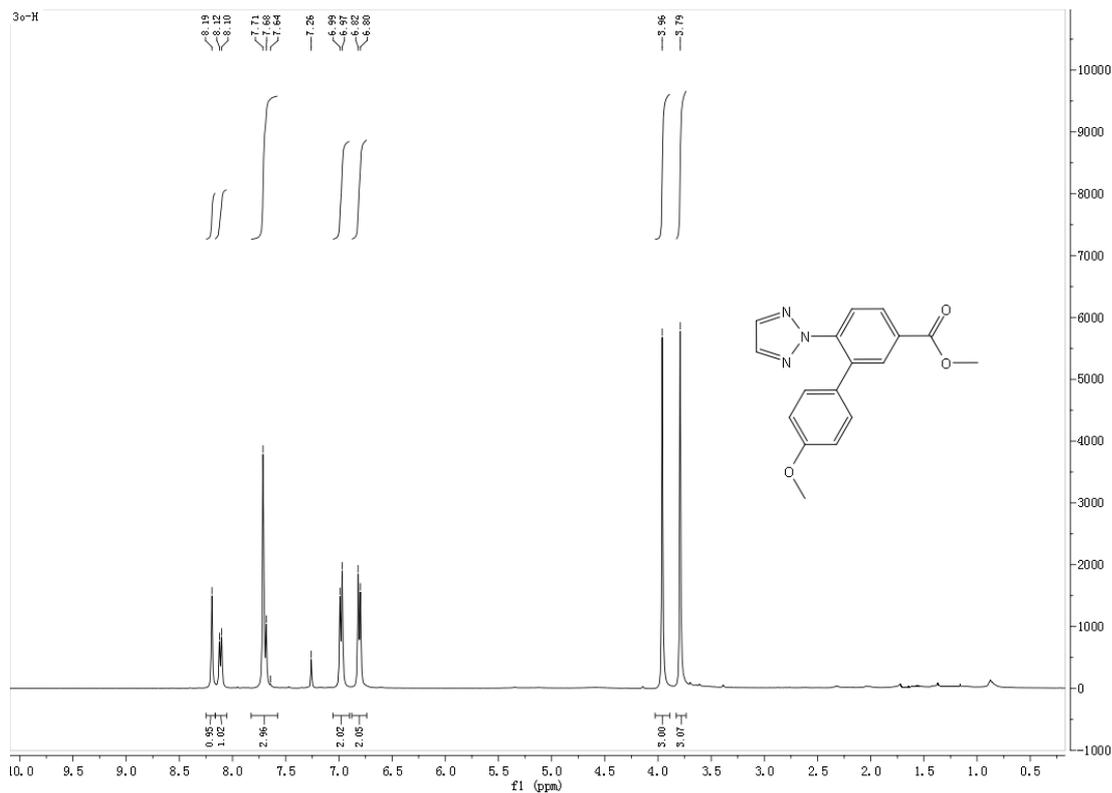
### <sup>1</sup>H NMR of 3n



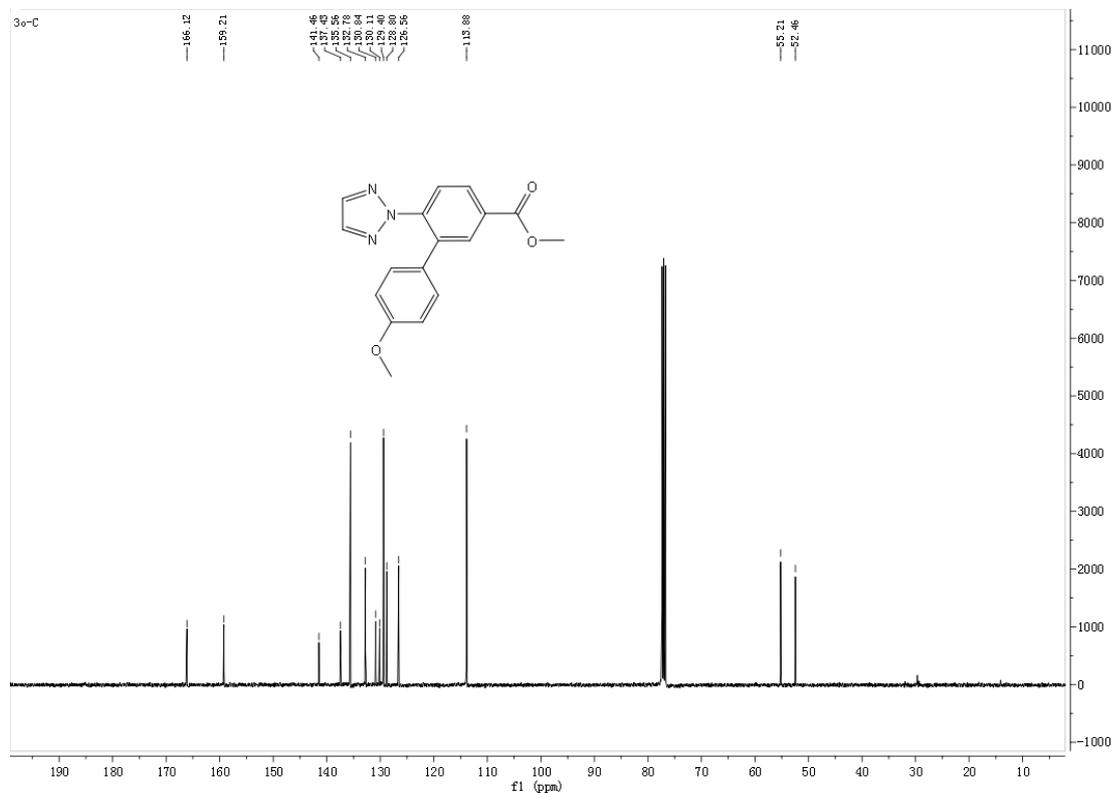
**<sup>13</sup>C NMR of 3n**



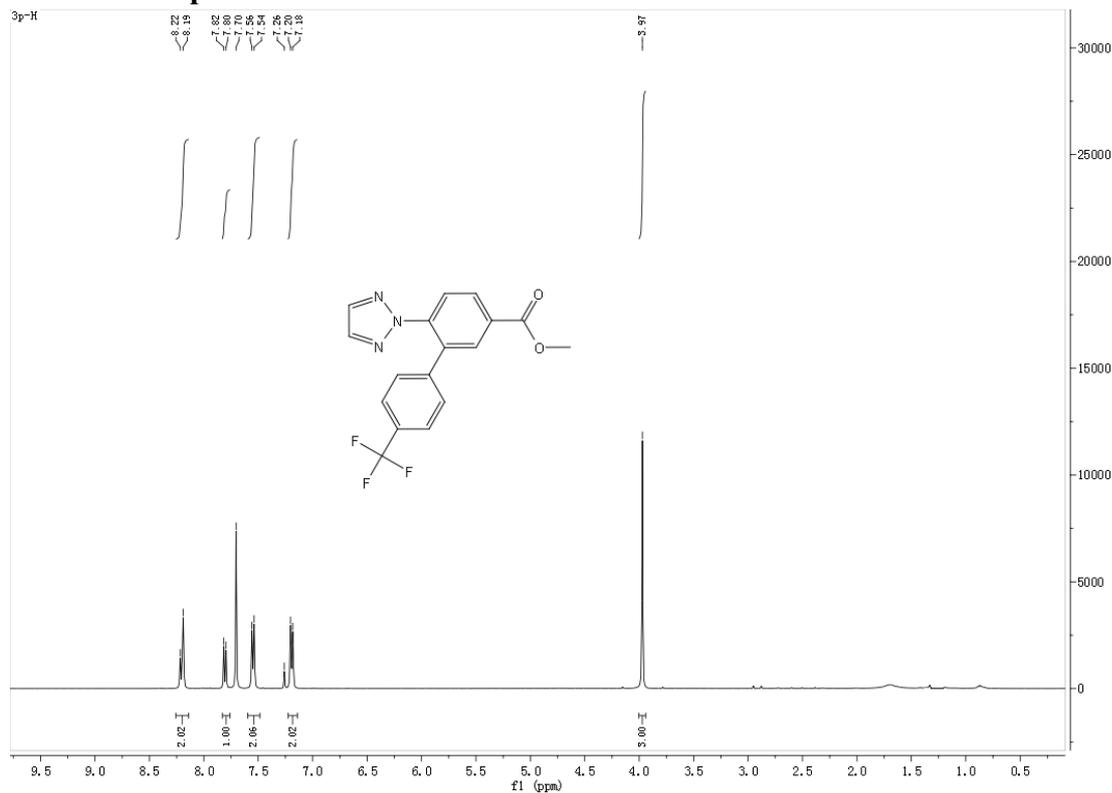
### <sup>1</sup>H NMR of 3o



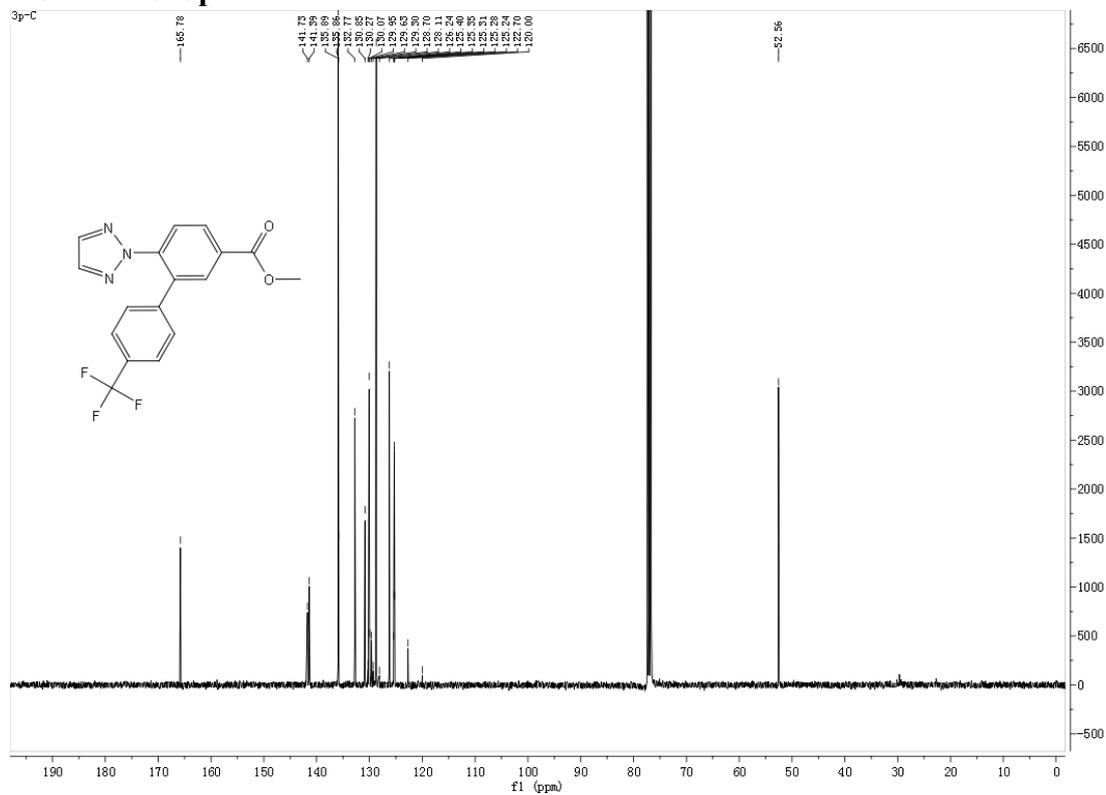
### <sup>13</sup>C NMR of 3o

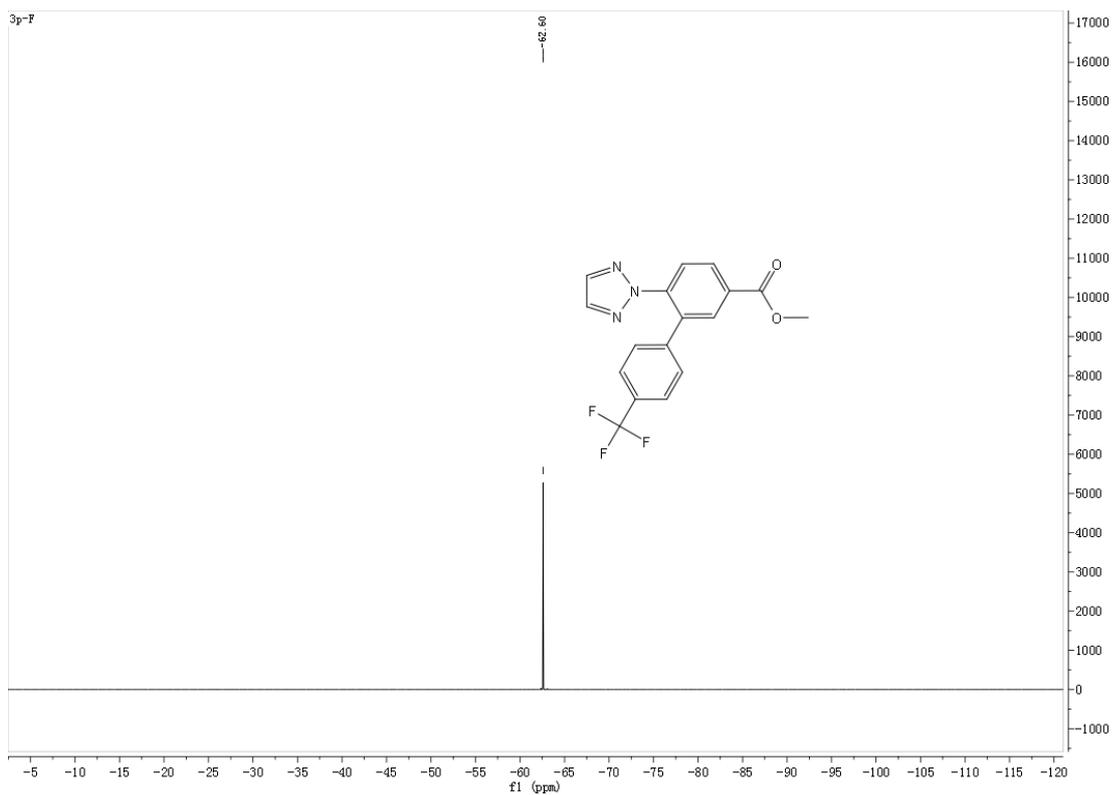


### <sup>1</sup>H NMR of 3p

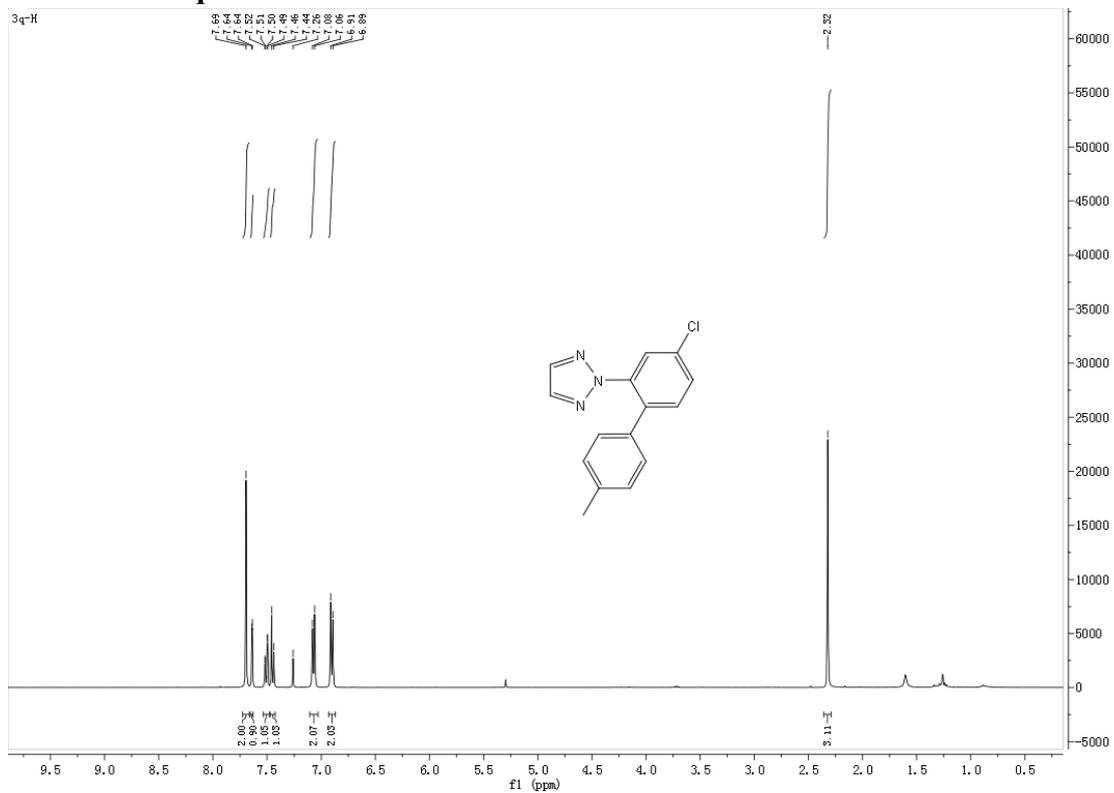


### <sup>13</sup>C NMR of 3p

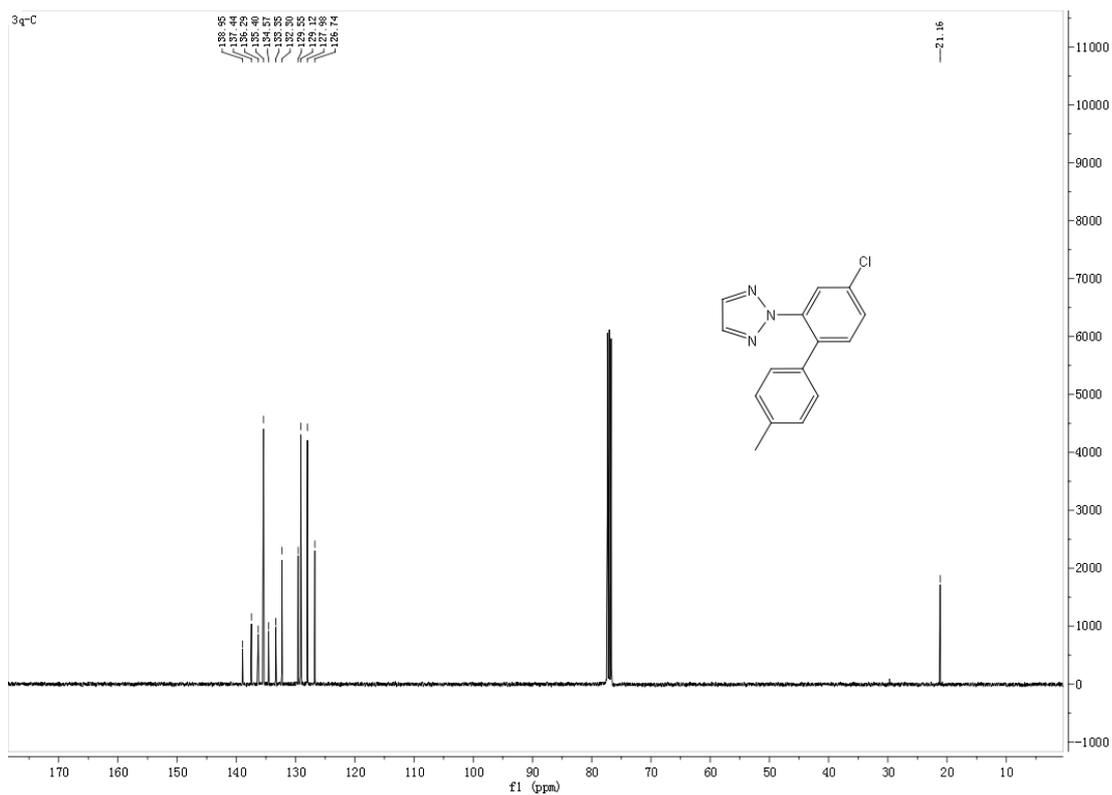




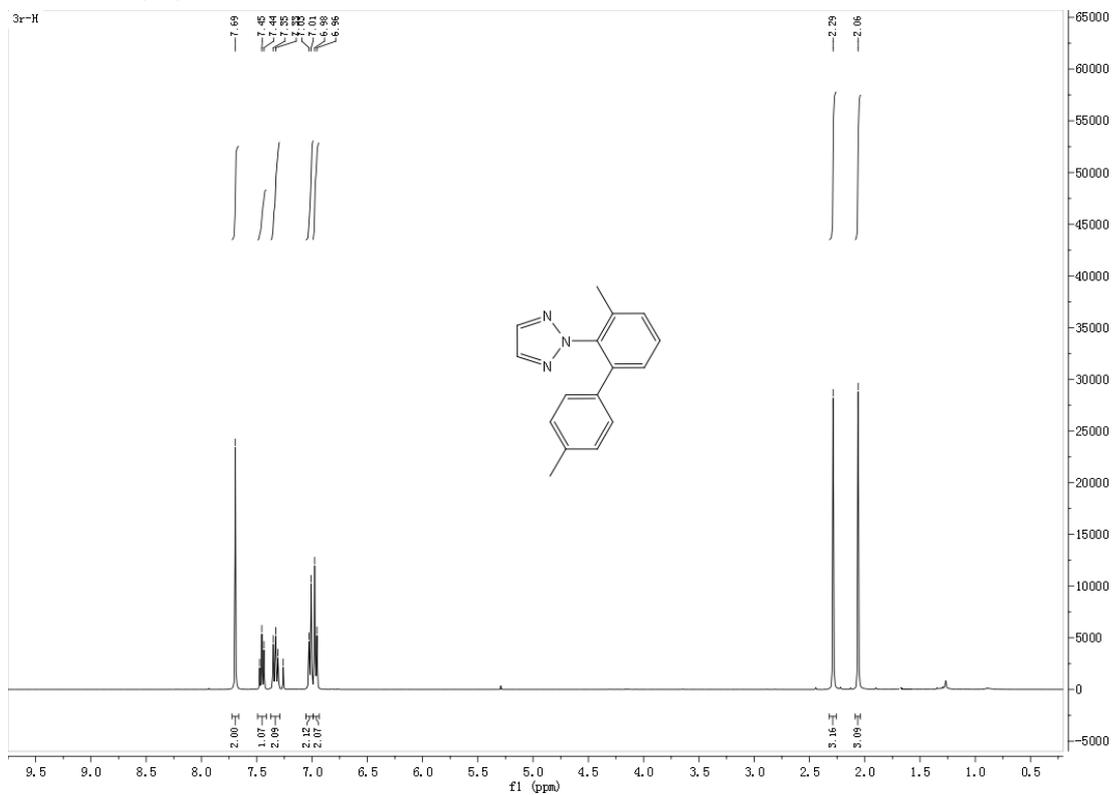
### <sup>1</sup>H NMR of 3q



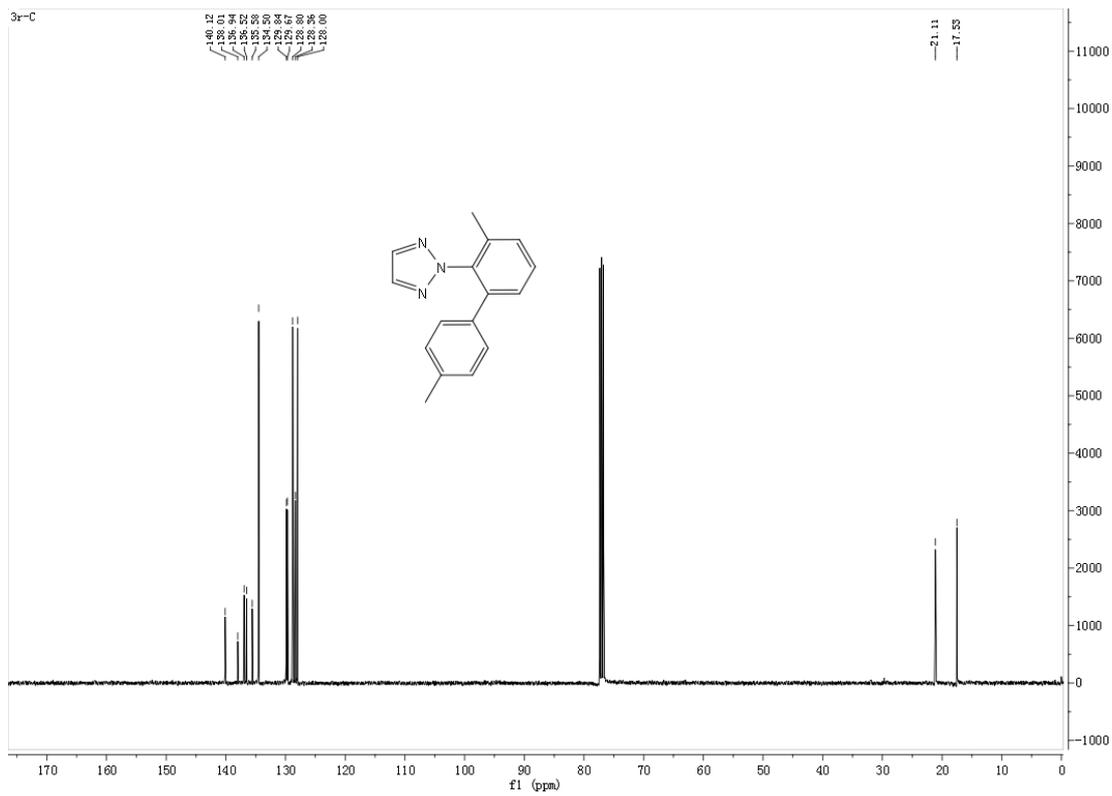
### <sup>13</sup>C NMR of 3q



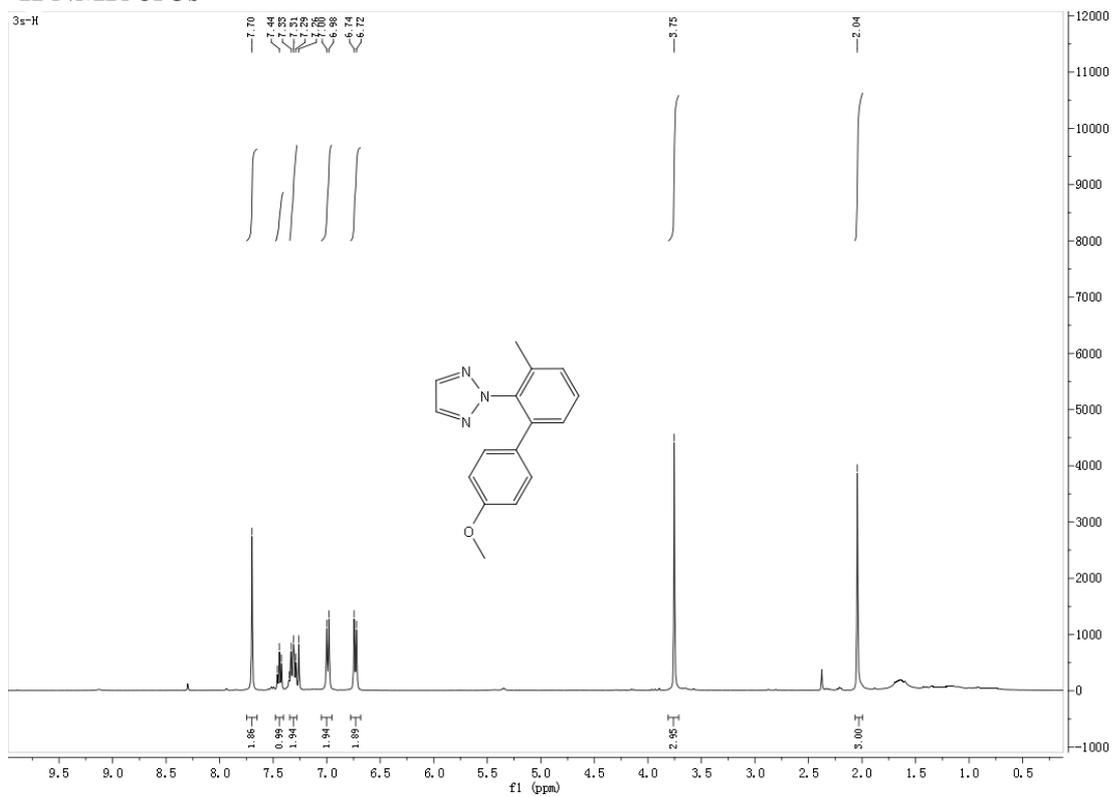
**<sup>1</sup>H NMR of 3r**



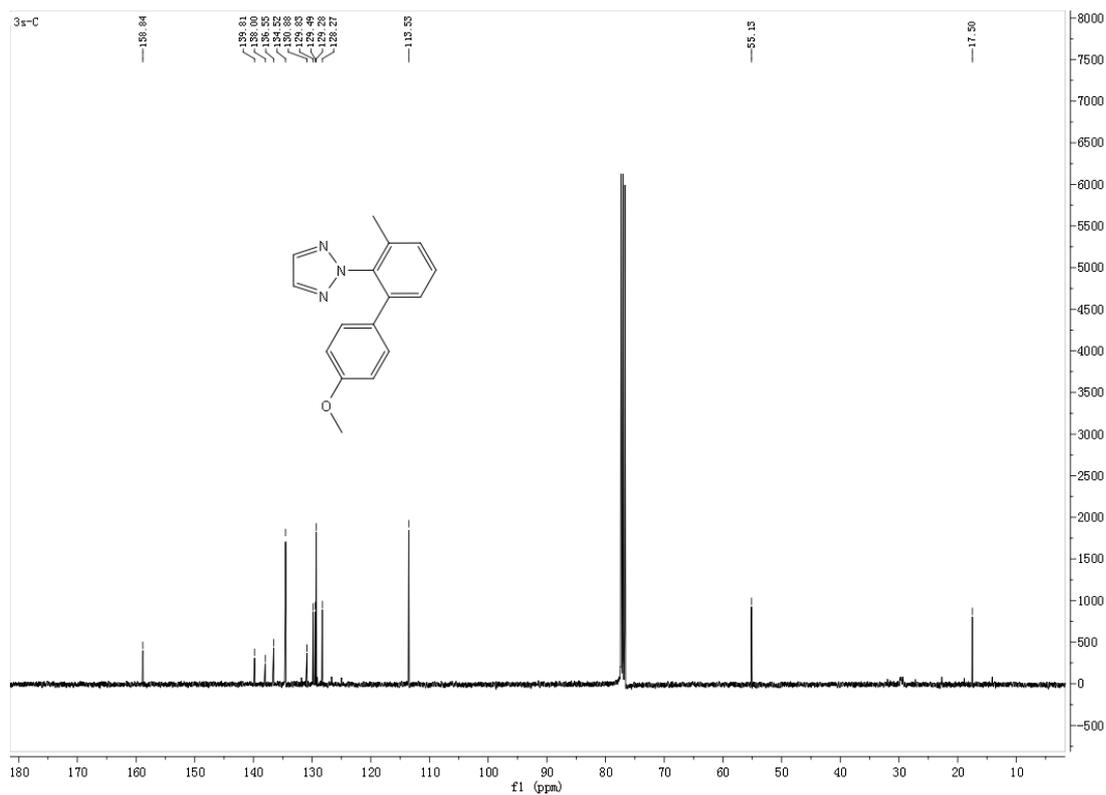
**<sup>13</sup>C NMR of 3r**



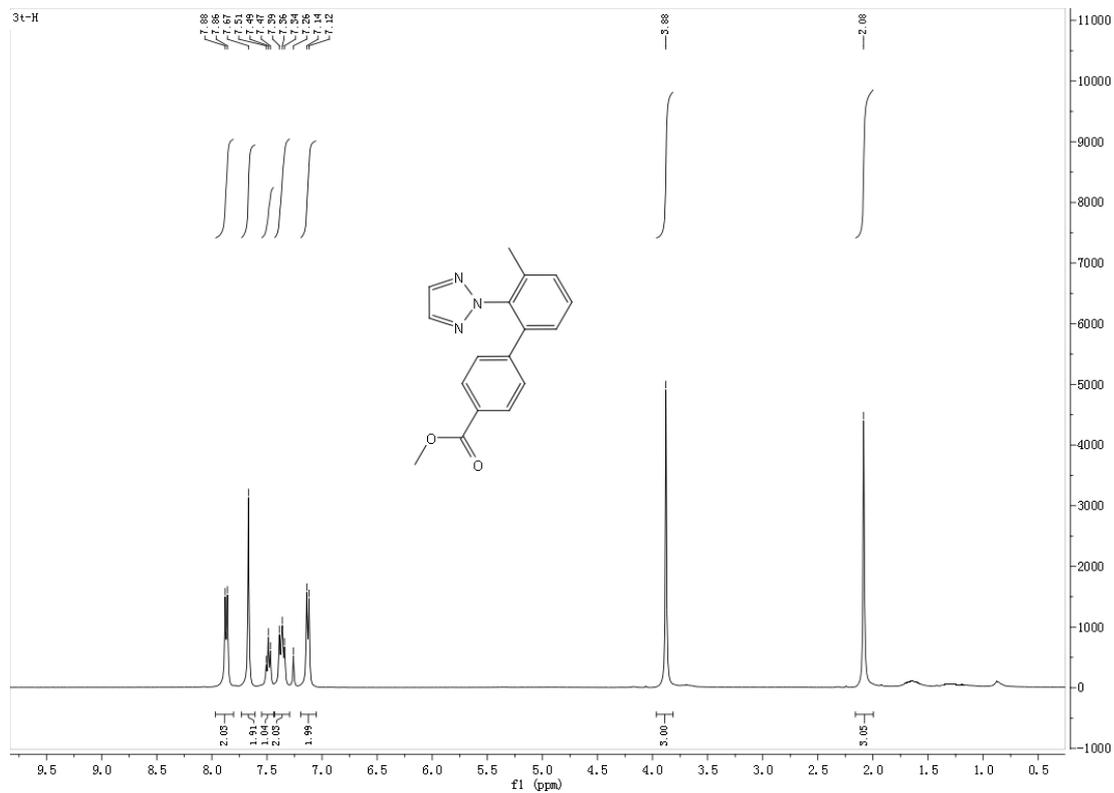
### <sup>1</sup>H NMR of 3s



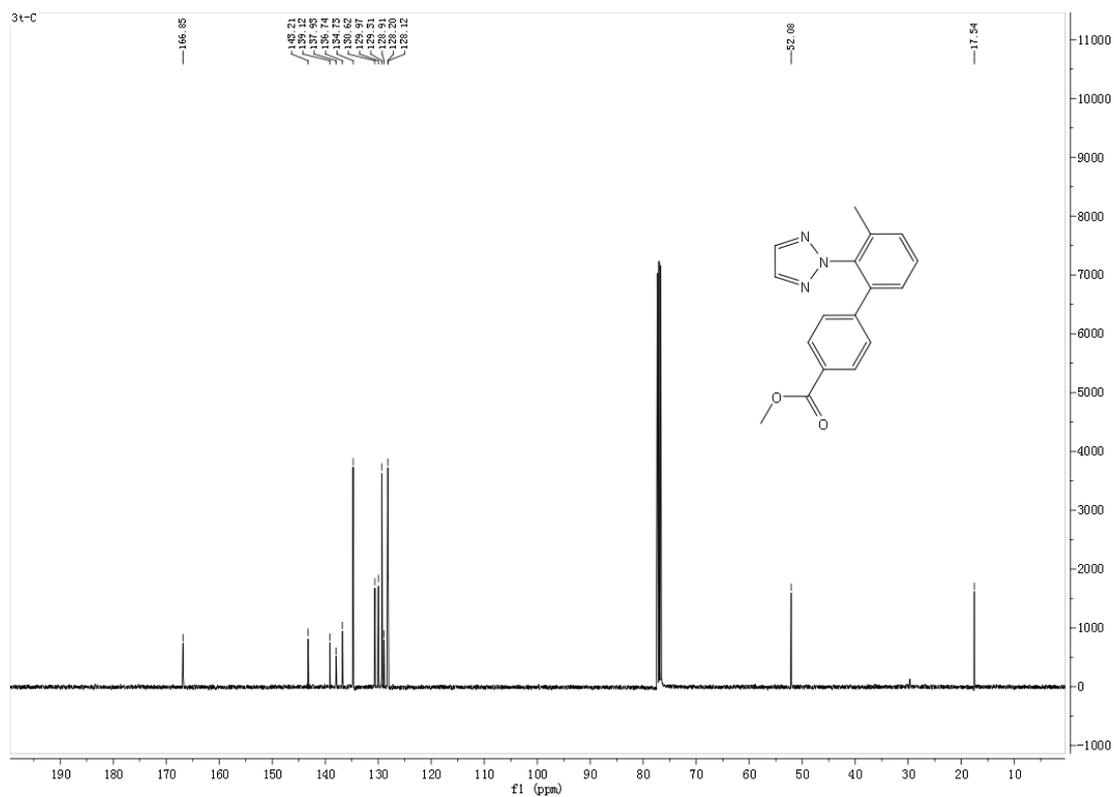
### <sup>13</sup>C NMR of 3s



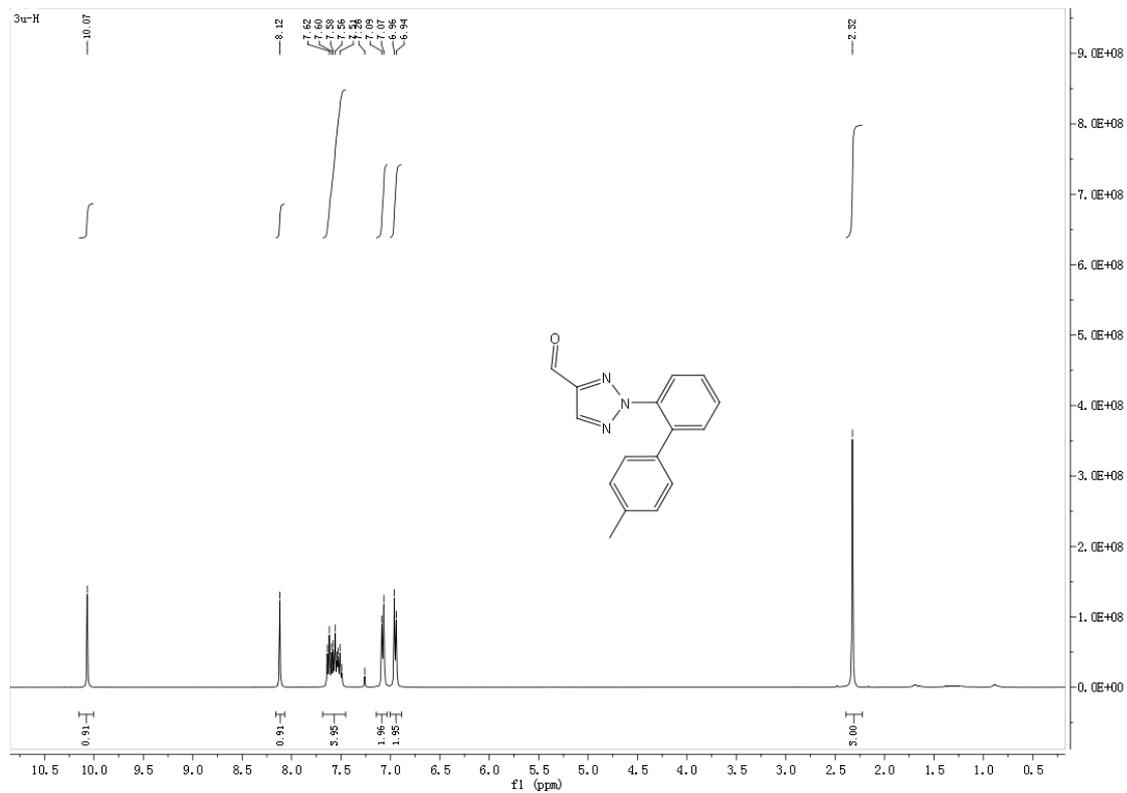
**<sup>1</sup>H NMR of 3t**



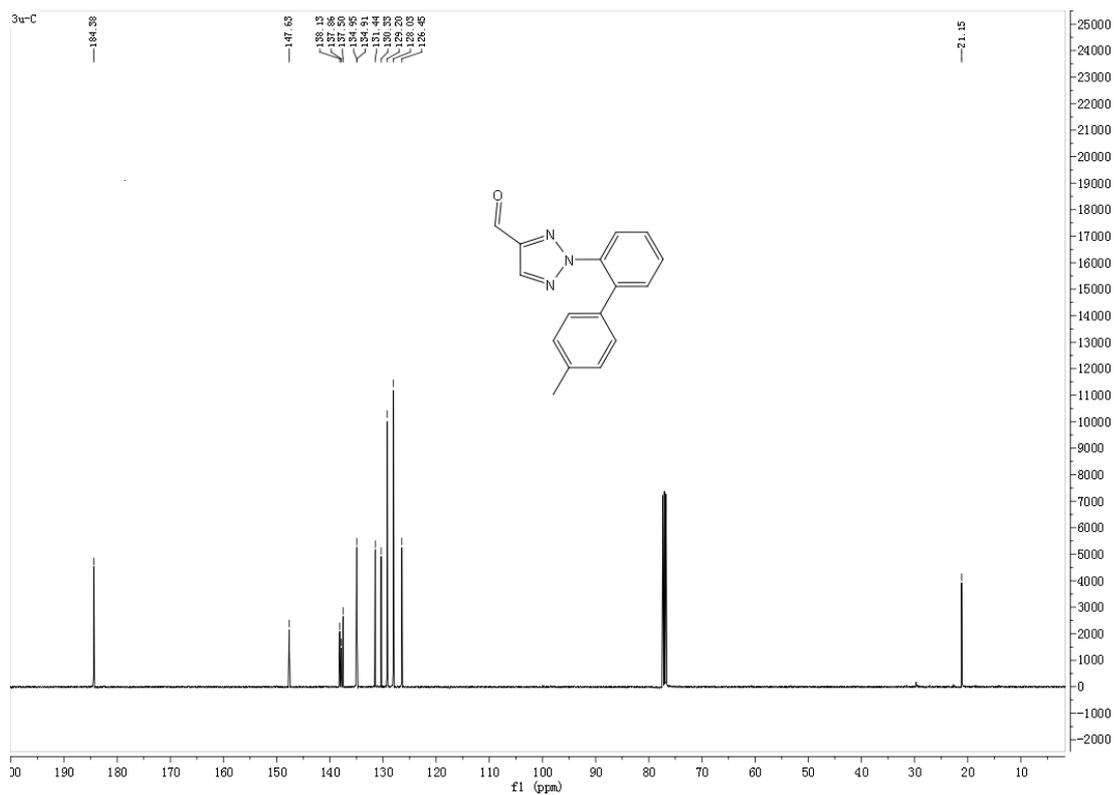
**<sup>13</sup>C NMR of 3t**



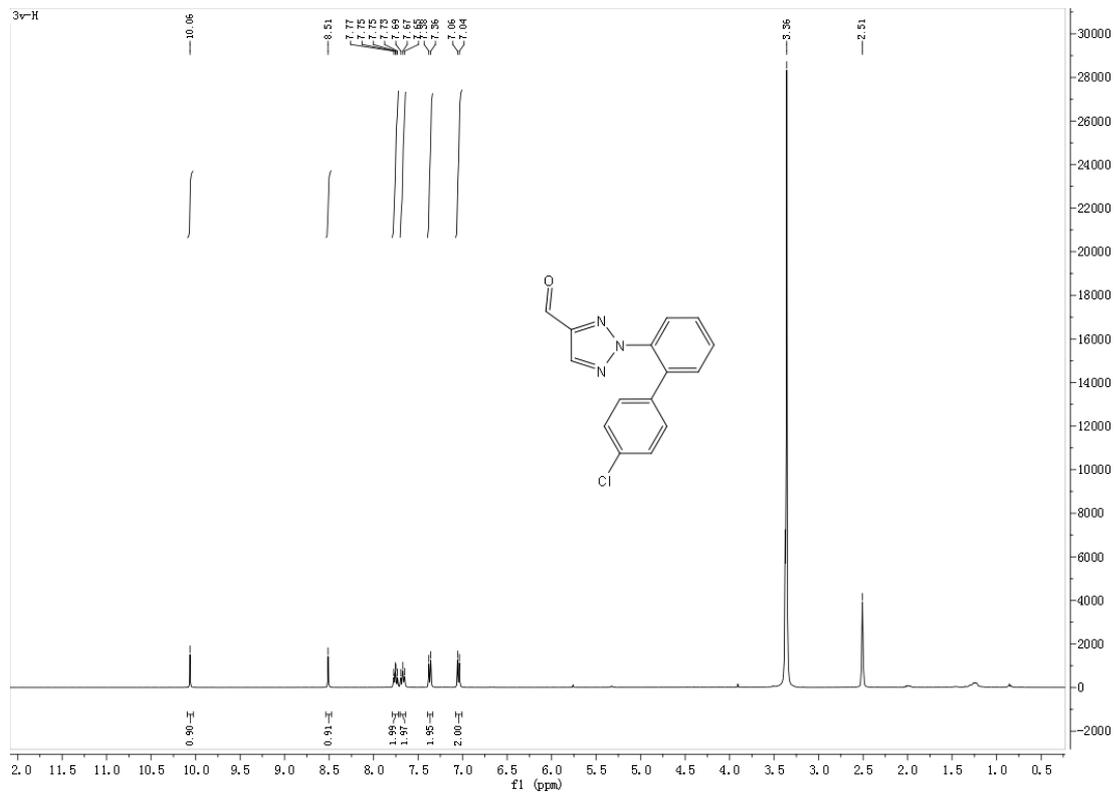
**<sup>1</sup>H NMR of 3u**



**<sup>13</sup>C NMR of 3u**

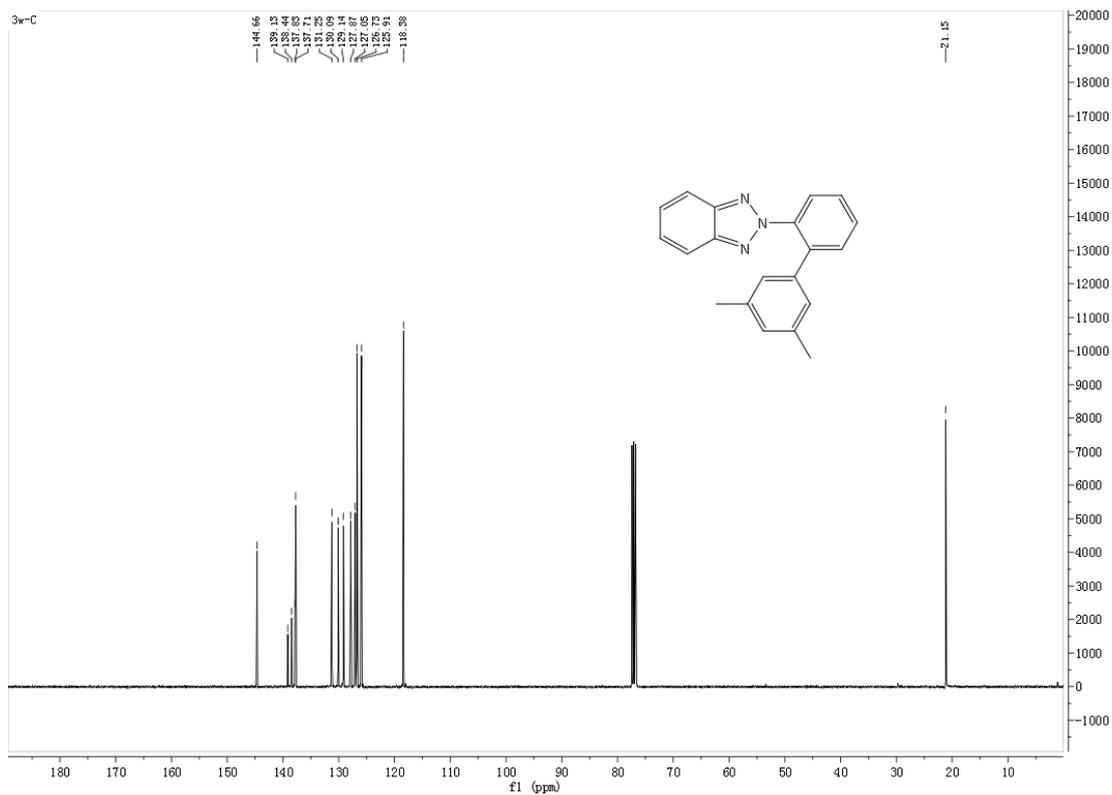


**<sup>1</sup>H NMR of 3v**

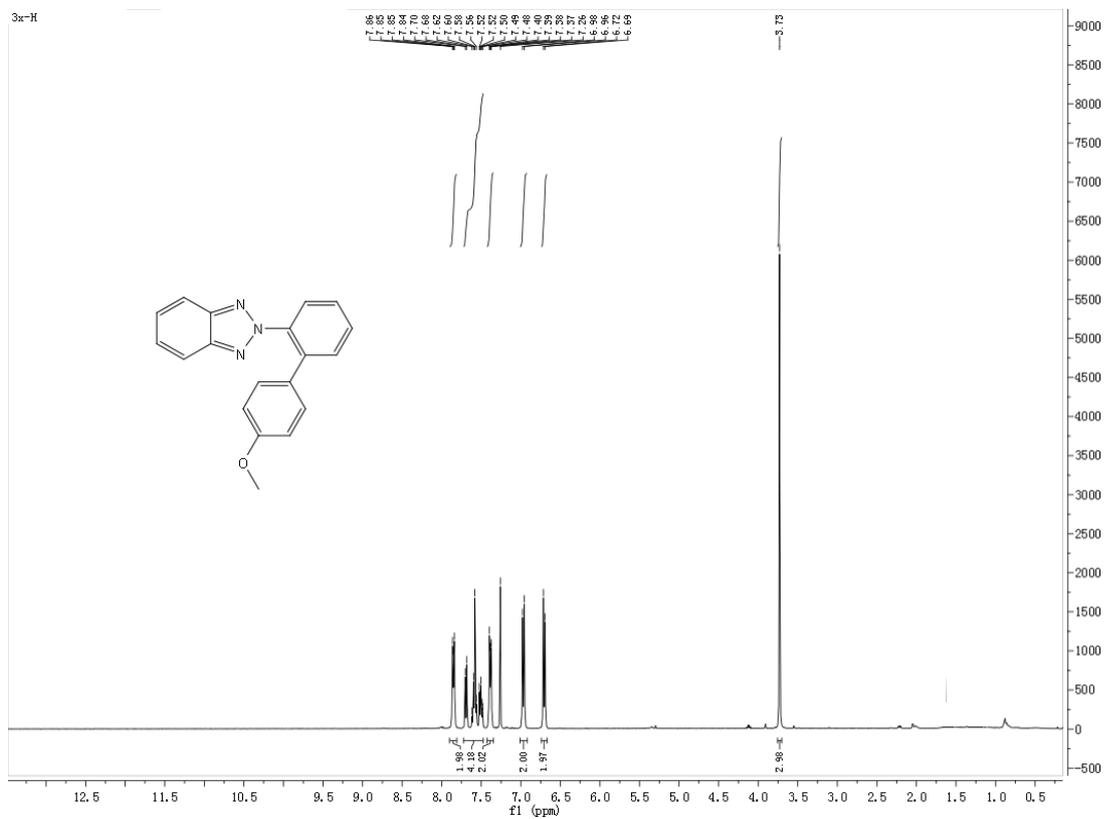


**<sup>13</sup>C NMR of 3v**





### **<sup>1</sup>H NMR of 3x**



### **<sup>13</sup>C NMR of 3x**



# <sup>13</sup>C NMR of 3y

