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# Supporting Information

## Facile Synthesis of Benzofurans via Copper-Catalyzed Aerobic Oxidative Cyclization of Phenols and Alkynes

**Wei Zeng, Wanqing Wu, Huanfeng Jiang, * Liangbin Huang, Yadong Sun, Zhengwang Chen and Xianwei Li**

School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China

*E-mail: jianghf@scut.edu.cn; Fax and Tel.: (+86) 20-87112906*

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## General Information

$^{1}H$ and $^{13}C$ NMR spectra were recorded on a Brüker Advance 400 spectrometer ($^{1}H$: 400 MHz, $^{13}C$: 100 MHz). The chemical shifts were referenced to signals at 7.26 and 77.0 ppm, respectively. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Mass spectra were recorded on a Shimadzu GCMS-QP5050A spectrometer at an ionization voltage of 70 eV equipped with a DB-WAX capillary column (internal diameter: 0.25 mm, length: 30 m). Elemental analyses were performed with a Vario EL elemental analyzer. GC-MS was obtained using electron ionization. Melting point was recorded with Buchi Melting Point B-545.

## Typical procedure for the copper-catalyzed reaction of 2,3-Diphenylbenzofuran

In a 20 mL Schlenk tube was charged with phenol (1.5 mmol), 1,2-diphenylethyne (1.0 mmol), $ZnCl_2$ (1.5 eq), $Cu(OTf)_2$ (10% mol) and $PhNO_2$ (2 mL) under $O_2$ (filled with a balloon) atmosphere. The resulting mixture was heated at 120 °C, and the reaction was allowed to stir for the time specified (24 h). After reaction completion, as monitored by TLC and GC-MS analysis. the mixture was washed with brine and extracted with ethyl acetate. The organic layer was dried ($MgSO_4$), concentrated in vacuum and purified by flash silica gel chromatography using pure *n*-hexane to give the desired products.

## Analytical Data

### 2,3-Diphenylbenzofuran (3a)

Yellow oil, $^{1}H$ NMR (400 MHz, $CDCl_3$) $\delta$ = 7.65-7.67 (m, 2H), 7.55 (d, $J$ = 8.0Hz, 1H), 7.44-7.51(m, 5H), 7.38-7.41 (m, 1H), 7.28-7.34 (m, 4H), 7.23 (t, $J$ = 8.0Hz, 1H). $^{13}C$ NMR (100 MHz, $CDCl_3$) $\delta$ = 154.0, 150.6, 132.9, 130.7, 130.3, 129.8, 129.0, 128.4, 128.4, 127.7, 127.1, 124.7, 122.9, 120.1, 117.5, 111.1. MS (EI) m/z: 270, 239, 215, 189, 165, 134. Anal. Calcd for $C_{20}H_{14}O$: C, 88.86; H, 5.22. Found: C, 88.79; H, 5.24.

### 5-Methyl-2,3-diphenylbenzofuran (3b)

Yellow oil, $^{1}H$ NMR (400 MHz, $CDCl_3$) $\delta$ = 7.63-7.64 (m, 2H), 7.36-7.48 (m, 6H), 7.24-7.26 (m, 4H), 7.09-7.11 (m, 1H), 2.38 (s, 3H). $^{13}C$ NMR (100 MHz, $CDCl_3$) $\delta$ = 152.6, 150.8, 133.2, 132.5, 130.9, 130.5, 129.9, 129.1, 128.5, 128.3, 127.7, 127.1, 126.1, 119.9, 117.5, 110.7, 21.5. MS (EI) m/z: 284, 269, 255, 239, 226. Anal. Calcd for $C_{21}H_{16}O$: C, 88.70; H, 5.67. Found: C, 88.66; H, 5.69.

### 5-Methoxy-2,3-diphenylbenzofuran (3c)

Yellow solid, mp: 80-81$^{o}$C, $^{1}H$ NMR (400 MHz, $CDCl_3$) $\delta$ = 7.61 (d, $J$ = 8.0Hz, 2H), 7.39-7.49 (m, 6H), 7.26-7.28 (m, 3H), 6.91-6.93 (m, 2H), 3.78 (s, 3H). $^{13}C$ NMR (100 MHz, $CDCl_3$) $\delta$ = 156.3, 151.4, 149.1, 133.0, 130.8, 130.8, 129.8, 129.1, 128.4, 128.3, 127.7, 127.0, 117.8, 113.6, 111.7,

102.3, 56.0. MS (EI) m/z: 300, 257, 239, 228, 202. Anal. Calcd for $C_{21}H_{16}O_2$: C, 83.98; H, 5.37. Found: C, 83.94; H, 5.39.

**5-Isopropyl-2,3-diphenylbenzofuran (3d)**

Yellow oil, $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.62-7.64 (m, 2H), 7.43-7.51 (m, 5H), 7.37-7.39 (m, 1H), 7.24-7.32 (m, 4H), 7.18-7.20 (m, 1H), 2.93-3.01 (m, 1H), 1.27 (d, $J$ = 7.2Hz, 3H), 1.25 (d, $J$ = 7.2Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 152.8, 150.9, 144.0, 133.2, 131.0, 130.3, 130.0, 129.1, 128.5, 128.3, 127.7, 127.1, 123.6, 117.7, 117.2, 110.9, 34.4, 24.7. MS (EI) m/z: 312, 297, 269, 239, 226. Anal. Calcd for $C_{23}H_{20}O$: C, 88.43; H, 6.45. Found: C, 88.40; H, 6.46.

**5-Fluoro-2,3-diphenylbenzofuran (3e)**

White solid, mp: 117-118$^o$C, $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.62-7.64 (m, 2H), 7.38-7.46 (m, 6H), 7.28-7.31 (m, 3H), 7.12-7.14 (m, 1H), 6.99-7.04 (m, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 159.6 (d, $J_{C,F}$ = 237.1Hz), 151.3 (d, $J_{C,F}$ = 237.1Hz), 132.4, 131.2 (d, $J_{C,F}$ = 10.3Hz), 130.4, 129.6, 129.1, 128.7, 128.5, 127.9, 127.1, 116.2 (d, $J_{C,F}$ = 23.0Hz), 117 (d, $J_{C,F}$ = 4.0Hz), 112.3 (d, $J_{C,F}$ = 26.3Hz), 111.7 (d, $J_{C,F}$ = 9.4Hz), 105.6 (d, $J_{C,F}$ = 25.2Hz). MS (EI) m/z: 288, 273, 259, 239. Anal. Calcd for $C_{20}H_{13}FO$: C, 83.32; H, 4.54. Found: C, 83.30; H, 4.55.

**5-Chloro-2,3-diphenylbenzofuran (3f)**

Orange solid, mp: 113-114$^o$C, $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.61-7.64 (m, 2H), 7.40-7.46 (m, 7H), 7.24-7.29 (m, 4H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 152.4, 152.0, 132.2, 131.7, 130.2, 129.7, 129.2, 128.5, 128.0, 127.1, 124.9, 119.7, 117.2, 112.1. MS (EI) m/z: 304, 289, 268, 239, 226. Anal. Calcd for $C_{20}H_{13}ClO$: C, 78.82; H, 4.30. Found: C, 78.79; H, 4.31.

**5-Bromo-2,3-diphenylbenzofuran (3g)**

Yellow solid, mp: 134-135$^o$C, $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.58-7.63 (m, 3H), 7.42-7.45 (m, 4H), 7.38-7.41 (m, 3H), 7.28-7.29 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 152.8, 151.8, 132.3, 132.2, 130.2, 129.7, 129.2, 128.8, 128.5, 128.0, 127.6, 127.1, 122.7, 117.0, 116.2, 112.6. MS (EI) m/z: 348, 268, 239, 213, 189. Anal. Calcd for $C_{20}H_{13}BrO$: C, 68.79; H, 3.75. Found: C, 68.76; H, 3.76.

**5-Iodo-2,3-diphenylbenzofuran (3h)**

White solid, mp: 166-167$^o$C, $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.79 (m, 3H), 7.58-7.64 (m, 3H), 7.42-7.48 (m, 5H), 7.30-7.33 (m, 4H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 153.4, 151.4, 133.2, 133.0, 132.1, 130.1, 129.7, 129.2, 128.8, 128.8, 128.5, 128.0, 127.1, 116.7, 113.2, 86.5. MS (EI) m/z: 396, 268, 239, 226, 213. Anal. Calcd for $C_{20}H_{13}IO$: C, 60.63; H, 3.31. Found: C, 60.61; H, 3.32.

**5-Chloro-4,6-dimethyl-2,3-diphenylbenzofuran (3i)**

Light orange solid, mp: 130-131$^o$C, $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.40-7.44 (m, 5H), 7.34-7.36 (m, 2H), 7.22 (m, 1H), 7.17-7.18 (m, 1H), 2.45 (s, 3H), 2.03 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 152.0, 150.7, 134.4, 133.0, 130.9, 130.7, 130.0, 130.0, 129.0, 128.4, 128.1, 128.1, 127.8, 126.5, 118.4, 110.5, 21.9, 16.2. MS (EI) m/z: 332, 297, 281, 252, 239. Anal. Calcd for $C_{22}H_{17}ClO$: C, 79.39; H, 5.15. Found: C, 79.35; H, 5.16.

**7-Chloro-2,3-diphenylbenzofuran (3j)**

Brown oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.72-7.75 (m, 2H), 7.47-7.53 (m, 5H), 7.41-7.43 (m, 1H), 7.36-7.37 (m, 4H), 7.20 (t, *J* = 8.0Hz, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 151.5, 149.8, 132.3, 131.9, 130.1, 129.7, 129.1, 128.8, 128.5, 127.9, 127.2, 124.8, 123.8, 118.6, 118.0, 116.7. MS (EI) m/z: 304, 289, 268, 239, 226. Anal. Calcd for $C_{20}H_{13}ClO$: C, 78.82; H, 4.30. Found: C, 78.80; H, 4.31.

**7-Bromo-2,3-diphenylbenzofuran (3k)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.67-7.70 (m, 2H), 7.46-7.48 (m, 5H), 7.40-7.42 (m, 2H), 7.30-7.32 (m, 3H), 7.10 (t, *J* = 8.0Hz, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 151.4, 151.2, 132.4, 131.6, 130.1, 129.7, 129.1, 128.8, 128.5, 127.9, 127.6, 127.2, 124.2, 119.2, 118.1, 104.0. MS (EI) m/z: 348, 268, 239, 213, 189. Anal. Calcd for $C_{20}H_{13}BrO$: C, 68.79; H, 3.75. Found: C, 68.77; H, 3.75.

**7-Methyl-2,3-diphenylbenzofuran (3l)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.66-7.67 (m, 2H), 7.48-7.49 (m, 2H), 7.43 (t, *J* = 8.0Hz, 2H), 7.37-7.38 (m, 1H), 7.25-7.32 (m, 4H), 7.11-7.13 (m, 2H), 2.60 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 153.1, 150.3, 133.2, 131.0, 129.9, 129.8, 129.0, 128.5, 128.3, 127.6, 127.1, 125.7, 123.1, 121.4, 117.9, 117.6, 15.1. MS (EI) m/z: 284, 269, 255, 239, 226. Anal. Calcd for $C_{21}H_{16}O$: C, 88.70; H, 5.67. Found: C, 88.68; H, 5.68.

**4-Isopropyl-7-methyl-2,3-diphenylbenzofuran (3m)**

Light yellow solid, mp: 98-99$^{o}$C, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.44-7.48 (m, 7H), 7.20-7.24 (m, 3H), 7.43 (t, *J* = 8.0Hz, 2H), 7.10 (d, *J* = 8.0Hz, 1H), 7.06 (t, *J* = 8.0Hz, 1H), 2.82-2.89 (m, 1H), 2.59 (s, 3H), 1.03 (s, 3H), 1.01 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 152.6, 150.1, 141.3, 135.2, 131.1, 130.6, 129.5, 128.8, 128.3, 127.9, 127.8, 126.5, 125.7, 119.2, 118.6, 118.4, 27.5, 23.9, 14.8. MS (EI) m/z: 326, 311, 296, 281, 252. Anal. Calcd for $C_{24}H_{22}O$: C, 88.31; H, 6.79. Found: C, 88.27; H, 6.80.

**5-(Methylthio)-2,3-diphenylbenzofuran (3n)**

Yellow solid, mp: 105-106$^{o}$C, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.62-7.64 (m, 2H), 7.46-7.48 (m, 5H), 7.42-7.44 (m, 2H), 7.29-7.32 (m, 4H), 2.48 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 152.7, 151.3, 132.6, 132.1, 131.1, 130.5, 129.8, 129.1, 128.5, 128.5, 127.8, 127.0, 125.7, 119.8, 117.1, 111.6, 18.1. MS (EI) m/z: 316, 301, 283, 268, 239. Anal. Calcd for $C_{21}H_{16}OS$: C, 79.71; H, 5.10. Found: C, 79.69; H, 5.12.

**2,3-Diphenylnaphtho[1,2-*b*]furan (3o)**

Yellow solid, mp: 94-95$^{o}$C, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 8.42 (d, *J* = 8.0Hz, 1H), 7.93 (d, *J* = 8.0Hz, 1H), 7.74 (d, *J* = 8.0Hz, 2H), 7.61-7.66 (m, 2H), 7.54-7.56 (m, 3H), 7.47-7.51 (m, 3H), 7.42-7.44 (m, 1H), 7.29-7.36 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 150.1, 149.5, 133.0, 131.8, 131.0, 129.9, 129.0, 128.5, 128.4, 128.1, 127.7, 126.8, 126.4, 125.6, 125.3, 123.6, 121.3, 120.2, 118.6, 118.5. MS (EI) m/z: 320, 291, 289, 276. Anal. Calcd for $C_{24}H_{16}O$: C, 89.97; H, 5.03. Found: C, 89.94; H, 5.04.

**2,3,7-Triphenylbenzofuran (3p)**

Brown solid, mp: 92-93°C, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.96-7.98 (m, 2H), 7.65-7.67 (m, 2H), 7.46-7.56 (m, 8H), 7.42-7.45 (m, 2H), 7.28-7.33 (m, 4H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 151.2, 150.7, 136.6, 132.9, 131.2, 130.6, 129.9, 128.7, 128.5, 128.4, 127.7, 127.7, 127.0, 125.3, 124.3, 123.6, 119.2, 117.7. MS (EI) m/z: 346, 331, 317, 302, 289. Anal. Calcd for $C_{24}H_{18}O$: C, 90.14; H, 5.24. Found: C, 90.13; H, 5.25.

**2,3-Di-*m*-tolylbenzofuran (4a)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.48-7.56 (m, 3H), 7.40-7.41 (m, 1H), 7.29-7.33 (m, 4H), 7.13-7.23 (m, 3H), 7.07-7.09 (m, 1H), 2.37 (s, 3H), 2.30 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 154.0, 150.7, 138.6, 138.1, 132.9, 130.7, 130.5, 130.4, 129.2, 128.9, 128.4, 128.3, 127.6, 127.0, 124.6, 124.3, 122.9, 120.1, 117.6, 111.1, 21.5. MS (EI) m/z: 298, 282, 268, 255, 239. Anal. Calcd for $C_{22}H_{18}O$: C, 88.56; H, 6.08. Found: C, 88.53; H, 6.10.

**2,3-*Bis*(2-chlorophenyl)benzofuran (4b)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.58 (d, $J$ = 8.0Hz, 1H), 7.46 (d, $J$ = 8.0Hz, 2H), 7.34-7.41 (m, 3H), 7.25-7.28 (m, 4H), 7.18-7.22 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 154.5, 150.4, 134.3, 134.1, 132.3, 132.2, 131.5, 130.4, 130.3, 130.0, 129.9, 129.2, 128.7, 126.8, 126.6, 124.9, 122.9, 121.0, 118.1, 111.5. MS (EI) m/z: 340, 302, 268, 239, 213. Anal. Calcd for $C_{20}H_{12}Cl_2O$: C, 70.81; H, 3.57. Found: C, 70.78; H, 3.58.

**2,3-Bis(4-butylphenyl)benzofuran (4c)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.56 (d, $J$ = 8.0Hz, 2H), 7.52 (d, $J$ = 8.0Hz, 1H), 7.48 (d, $J$ = 8.0Hz, 1H), 7.39-7.41 (m, 2H), 7.19-7.31 (m, 4H), 7.11 (d, $J$ = 8.0Hz, 2H), 2.68 (t, $J$ = 8.0Hz, 2H), 2.59 (t, $J$ = 8.0Hz, 2H), 1.64-1.72 (m, 2H), 1.55-1.63 (m, 2H), 1.40-1.47 (m, 2H), 1.31-1.38 (m, 2H), 0.97 (t, $J$ = 7.6Hz, 3H), 0.92 (t, $J$ = 7.6Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 153.9, 150.7, 143.3, 142.2, 130.6, 130.1, 129.6, 128.9, 128.5, 128.2, 126.9, 124.4, 122.7, 120.0, 116.9, 111.0, 35.5, 35.5, 33.6, 33.4, 22.5, 22.4, 14.0, 14.0. MS (EI) m/z: 382, 339, 297, 281, 252. Anal. Calcd for $C_{28}H_{30}O$: C, 87.91; H, 7.90. Found: C, 87.78; H, 7.92.

**2,3-Bis(4-fluorophenyl)benzofuran (4d)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.58-7.62 (m, 2H), 7.53 (d, $J$ = 8.0Hz, 1H), 7.42-7.45 (m, 3H), 7.31-7.35 (m, 1H), 7.22-7.26 (m, 1H), 7.14-7.18 (m, 2H), 6.99-7.03 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 162.7 (d, $J_{C,F}$ = 247.8Hz), 162.4 (d, $J_{C,F}$ = 245.7Hz), 153.9, 149.8, 131.4 (d, $J_{C,F}$ = 7.9Hz), 130.1, 128.9 (d, $J_{C,F}$ = 8.1Hz), 128.6 (d, $J_{C,F}$ = 3.4Hz), 126.7 (d, $J_{C,F}$ = 3.4Hz), 124.9, 123.1, 119.8, 116.3, 116.2 (d, $J_{C,F}$ = 21.3Hz), 115.6 (d, $J_{C,F}$ = 21.7Hz), 111.2. MS (EI) m/z: 306, 277, 274, 257, 251. Anal. Calcd for $C_{20}H_{12}F_2O$: C, 78.42; H, 3.95. Found: C, 78.40; H, 3.96.

**2,3-Bis(3-chlorophenyl)benzofuran (4e)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.69 (m, 1H), 7.52-7.54 (m, 1H), 7.38-7.49 (m, 5H), 7.32-7.36 (m, 2H), 7.18-7.26 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 154.0, 149.3, 135.0, 134.7, 134.3, 132.0, 130.4, 129.8, 129.7, 129.6, 128.6, 128.2, 128.0, 126.9, 125.4, 125.0, 123.4, 120.0, 117.3, 111.3. MS (EI) m/z: 340, 302, 268, 239, 213. Anal. Calcd for $C_{20}H_{12}Cl_2O$: C, 70.81; H, 3.57. Found: C, 70.79; H, 3.58.

**2,3-Di-*p*-tolylbenzofuran (4f)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.55 (d, *J* = 8.0Hz, 2H), 7.51-7.53 (m, 1H), 7.47-7.48 (m, 1H), 7.38 (d, *J* = 8.0Hz, 2H), 7.24-7.30 (m, 3H), 7.18-7.22 (m, 1H), 7.11 (d, *J* = 8.0Hz, 2H), 2.41 (s, 3H), 2.33 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 154.0, 150.7, 138.3, 137.2, 130.5, 130.0, 129.7, 129.7, 129.2, 128.1, 127.0, 124.4, 122.8, 120.0, 116.8, 111.0, 21.4. MS (EI) m/z: 298, 282, 268, 255, 239. Anal. Calcd for $C_{22}H_{18}O$: C, 88.56; H, 6.08. Found: C, 88.54; H, 6.09.

**2-Hexyl-3-phenylbenzofuran (4g)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.54 (d, *J* = 8.0Hz, 1H), 7.45-7.48 (m, 5H), 7.35-7.38 (m, 1H), 7.19-7.27 (m, 2H), 2.85 (t, *J* = 7.6Hz, 2H), 1.73-1.81 (m, 2H), 1.27-1.37 (m, 6H), 0.84-0.87 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 155.4, 154.0, 132.9, 129.1, 128.9, 128.7, 127.0, 123.5, 122.5, 119.4, 116.8, 110.8, 31.5, 29.0, 28.4, 26.8, 22.6, 14.1. MS (EI) m/z: 278, 207, 179, 152. Anal. Calcd for $C_{20}H_{22}O$: C, 86.29; H, 7.97. Found: C, 86.25; H, 7.98.

**2-Methyl-3-phenylbenzofuran (4h)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.57 (d, *J* = 7.2Hz, 1H), 7.44-7.51 (m, 5H), 7.33-7.37 (m, 1H), 7.19-7.27 (m, 2H), 2.53 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 154.1, 151.3, 132.9, 129.0, 128.8, 127.0, 123.8, 123.6, 122.6, 119.4, 116.9, 110.8, 12.8. MS (EI) m/z: 208, 178, 165, 152, 131. Anal. Calcd for $C_{15}H_{12}O$: C, 86.51; H, 5.81. Found: C, 86.49; H, 5.82.

**2-Hexyl-3-*o*-tolylbenzofuran (4i)**

Yellow oil, $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ = 7.46 (d, *J* = 7.2Hz, 1H), 7.30-7.32 (m, 2H), 7.14-7.24 (m, 5H), 2.57-2.72 (m, 2H), 2.18 (s, 3H), 1.65-1.72 (m, 2H), 1.23-1.26 (m, 6H), 0.82-0.85 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 155.4, 153.9, 137.7, 131.9, 130.9, 130.2, 129.6, 127.8, 125.8, 123.3, 122.3, 119.8, 116.5, 110.8, 31.5, 28.9, 28.0, 26.8, 22.5, 20.1, 14.0. MS (EI) m/z: 292, 221, 205, 193, 178. Anal. Calcd for $C_{21}H_{24}O$: C, 86.26; H, 8.27. Found: C, 86.24; H, 8.28.

**NMR Spectra**

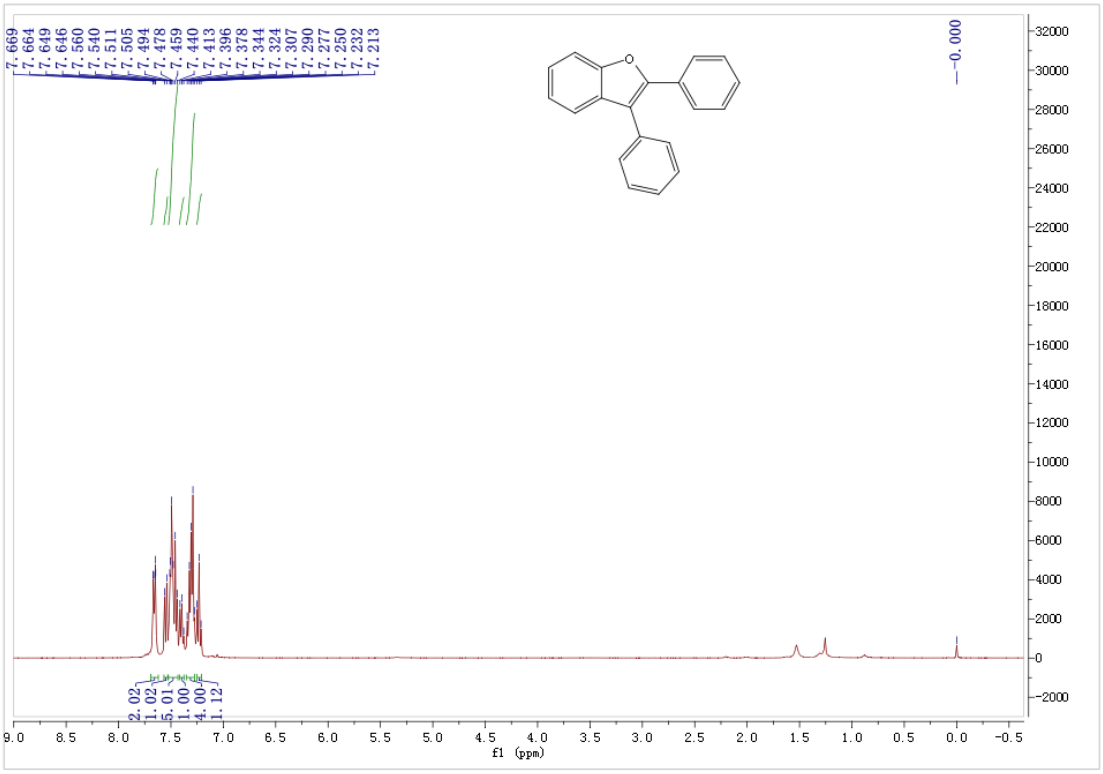


**Fig. S-1**. $^{1}$H-NMR spectrum of **3a**.

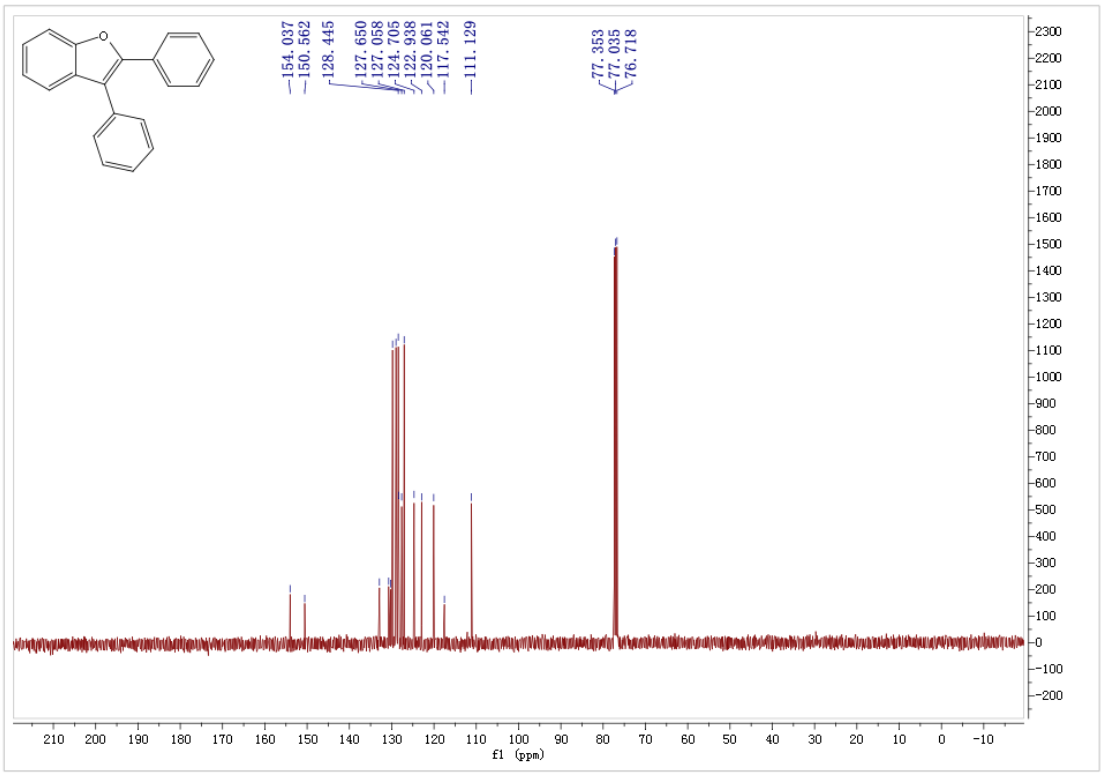


**Fig. S-2**. $^{13}$C-NMR spectrum of **3a**.

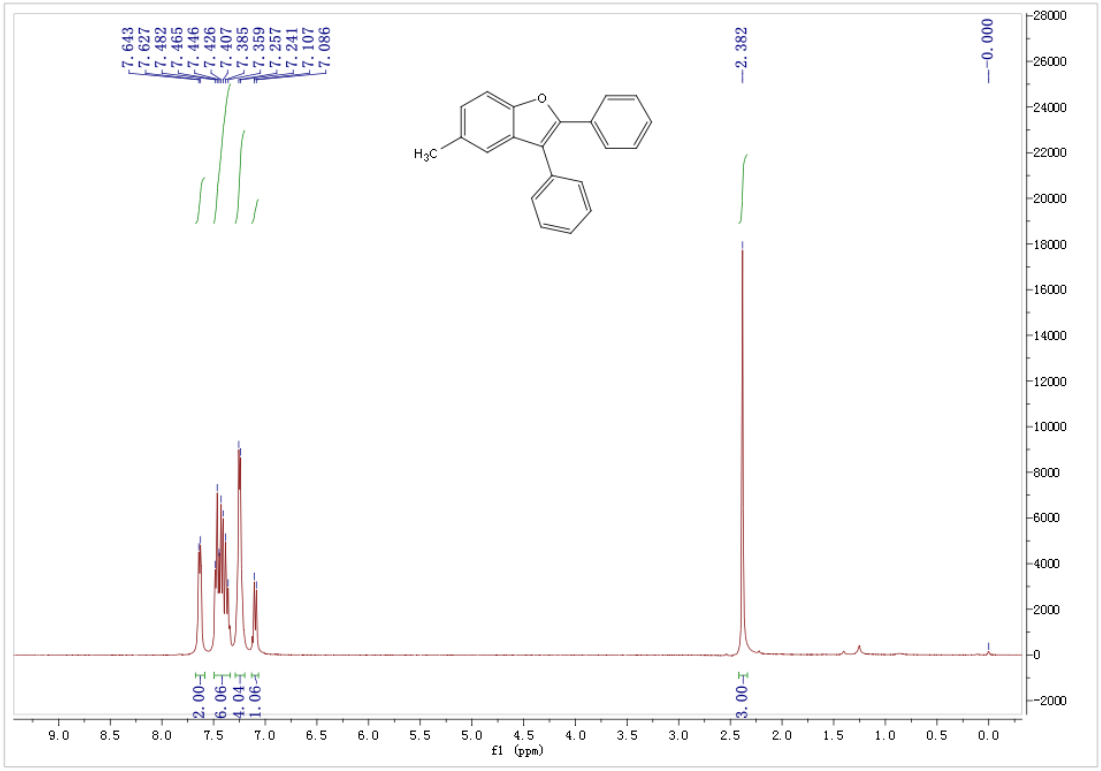


**Fig. S-3**. $^{1}$H-NMR spectrum of **3b**.

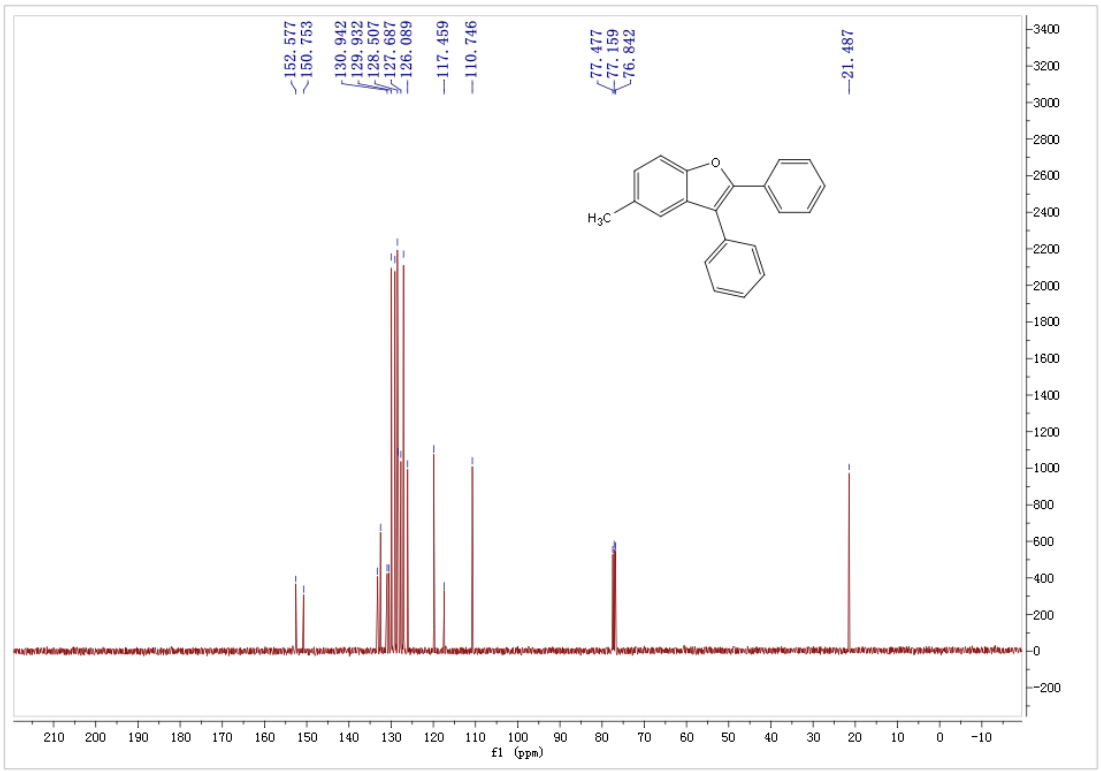


**Fig. S-4**. $^{13}$C-NMR spectrum of **3b**.

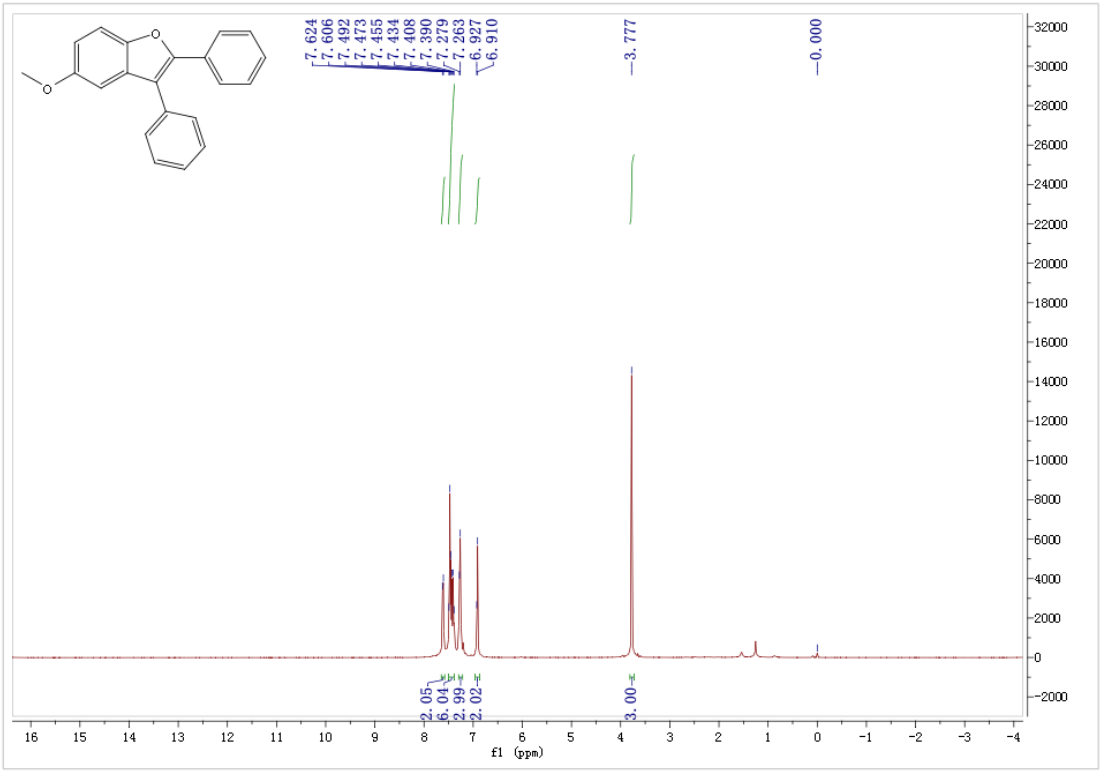


**Fig. S-5**. $^{1}$H-NMR spectrum of **3c**.

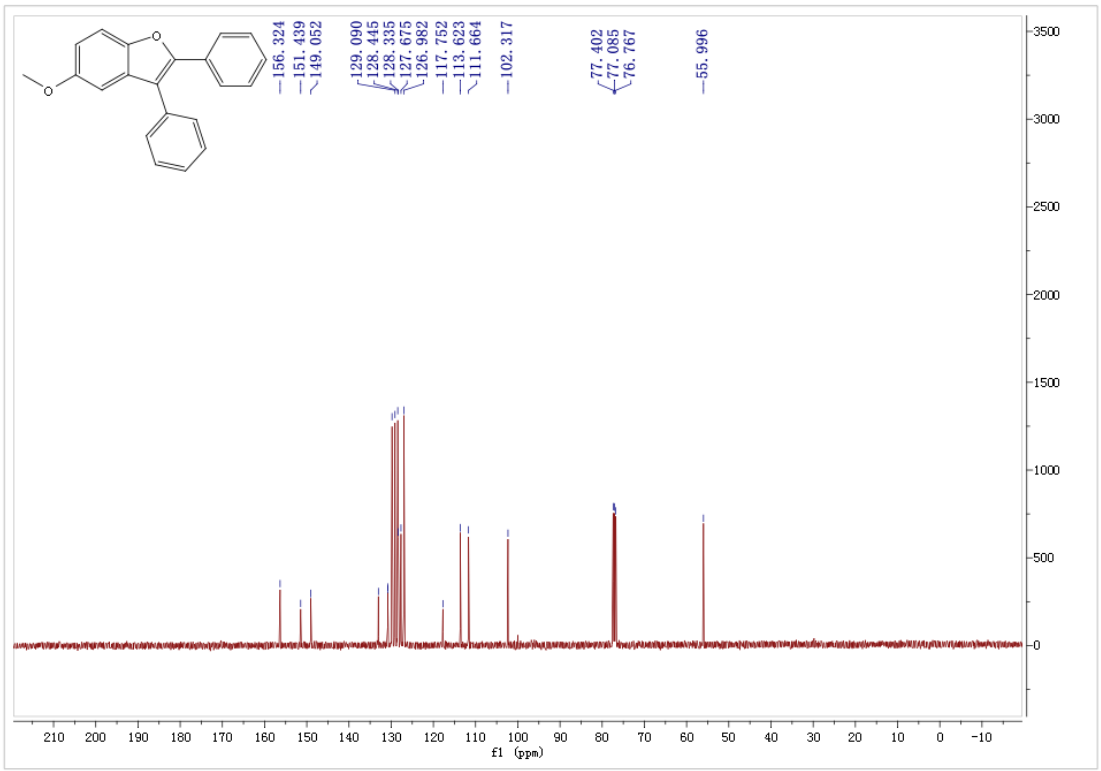


**Fig. S-6**. $^{13}$C-NMR spectrum of **3c**.

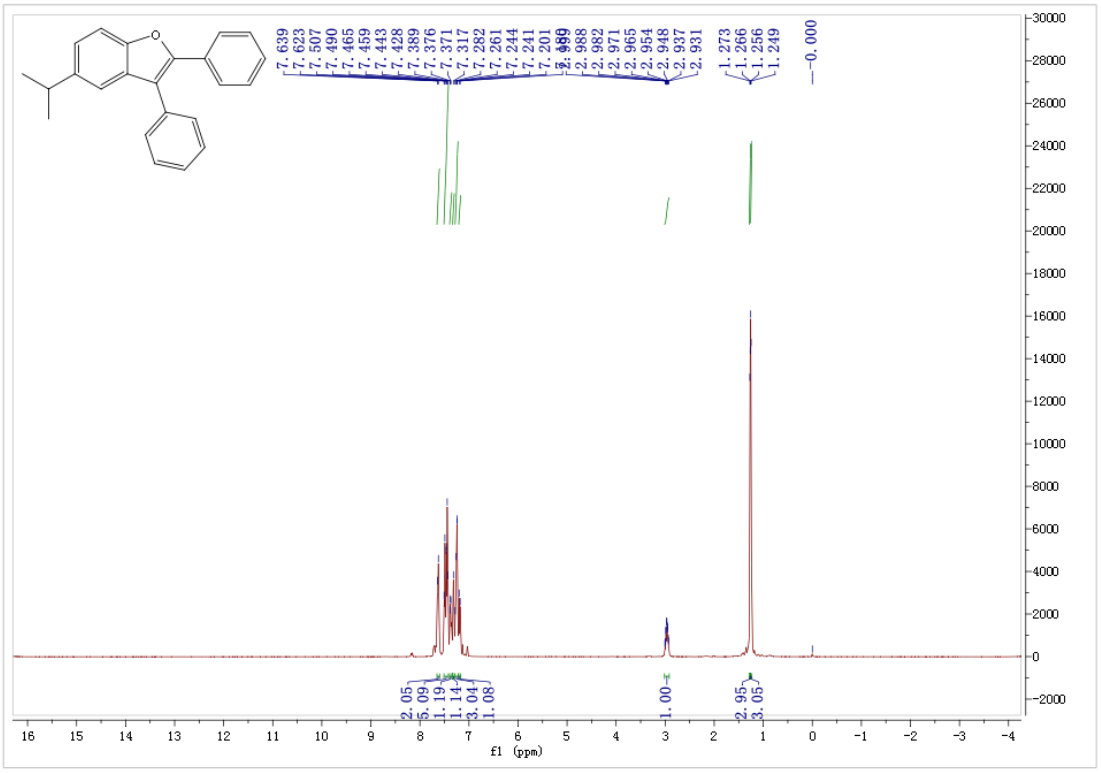


**Fig. S-7**. $^{1}$H-NMR spectrum of **3d**.

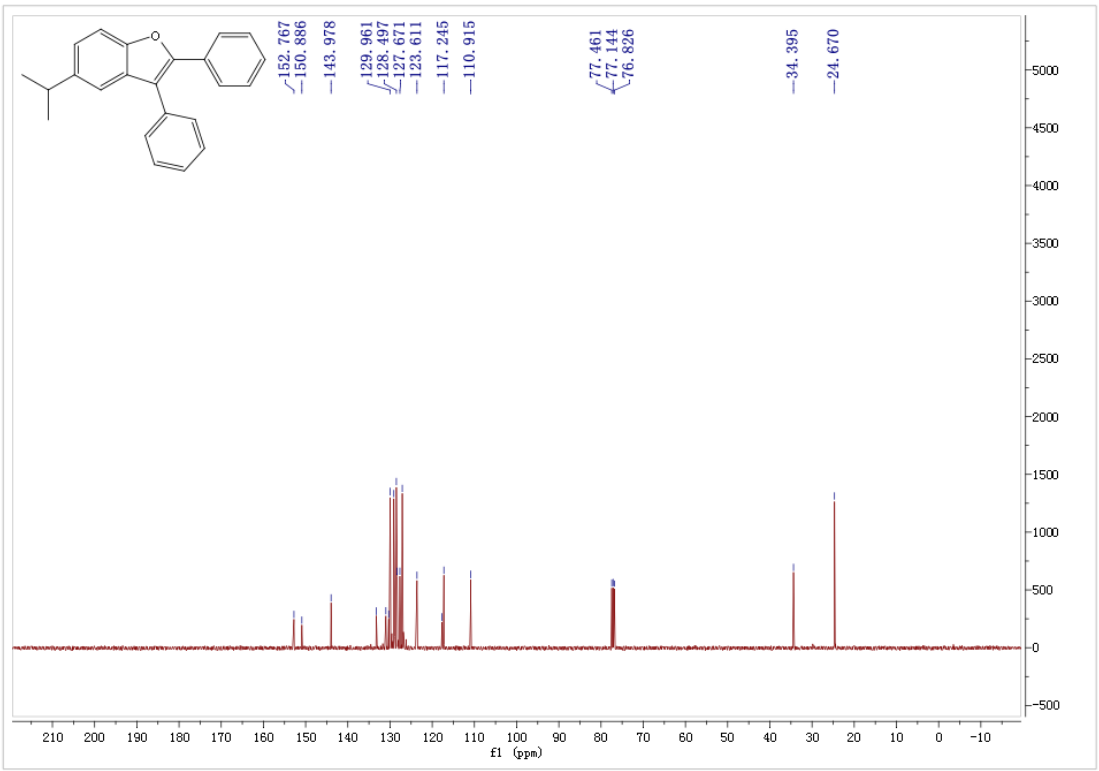


**Fig. S-8**. $^{13}$C-NMR spectrum of **3d**.

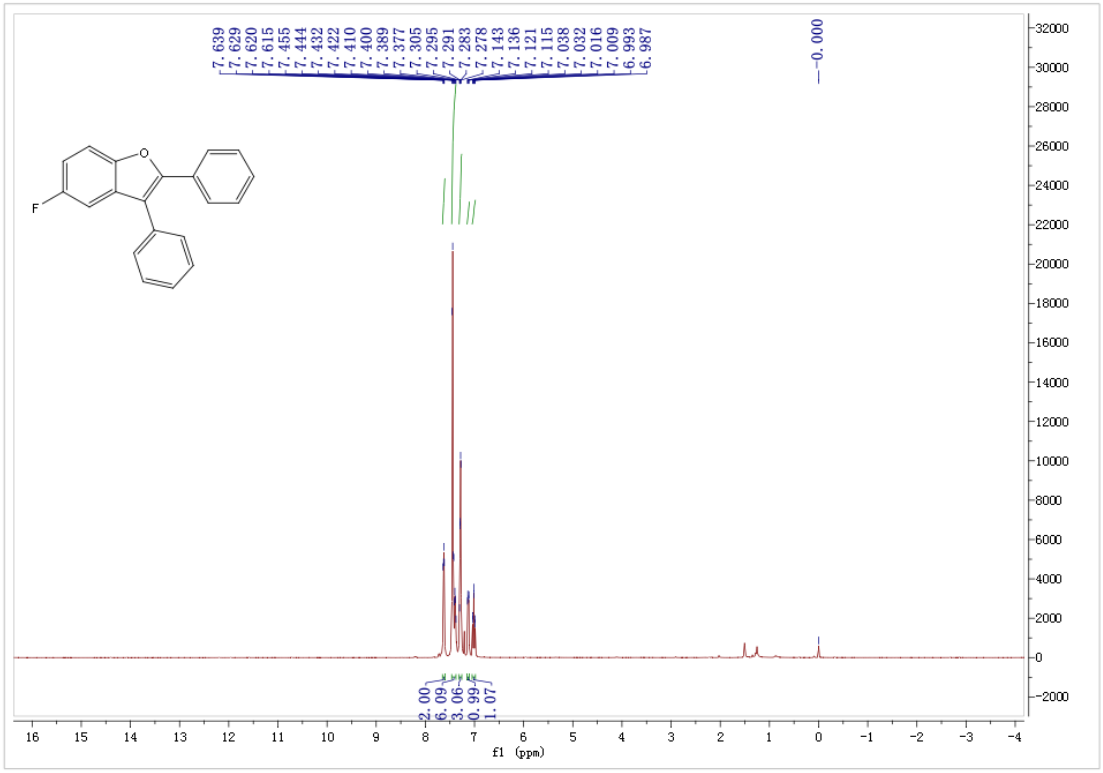


**Fig. S-9**. $^{1}$H-NMR spectrum of **3e**.

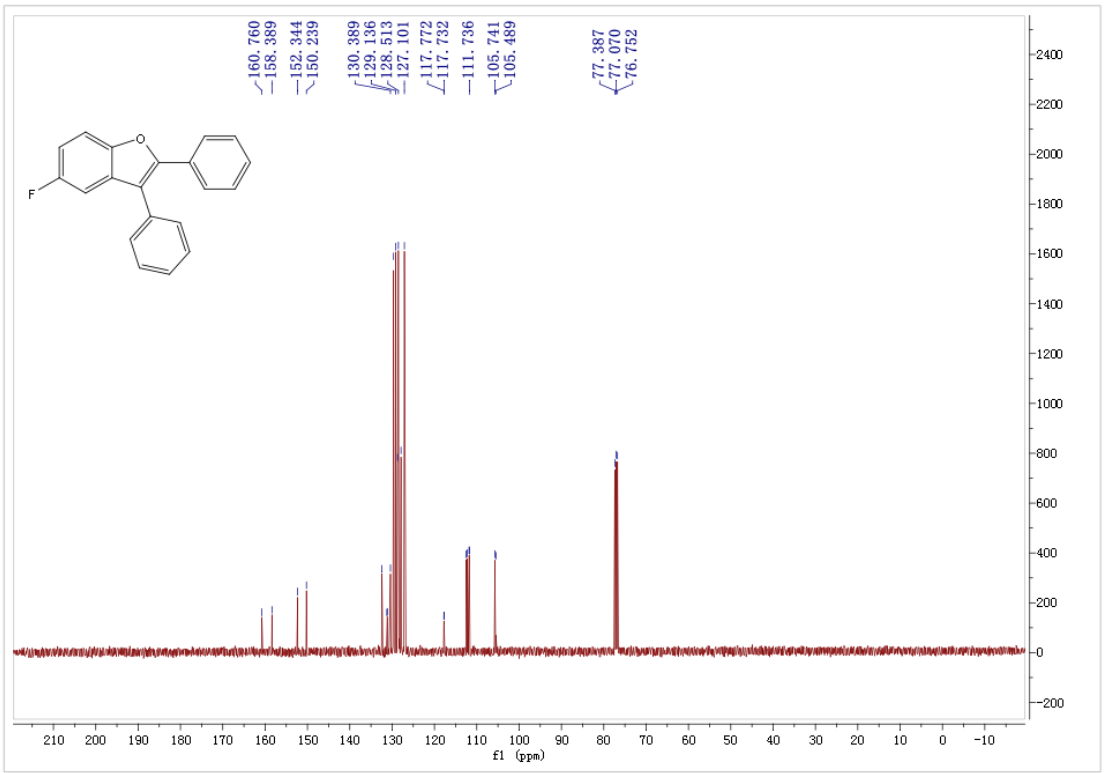


**Fig. S-10**. $^{13}$C-NMR spectrum of **3e**.

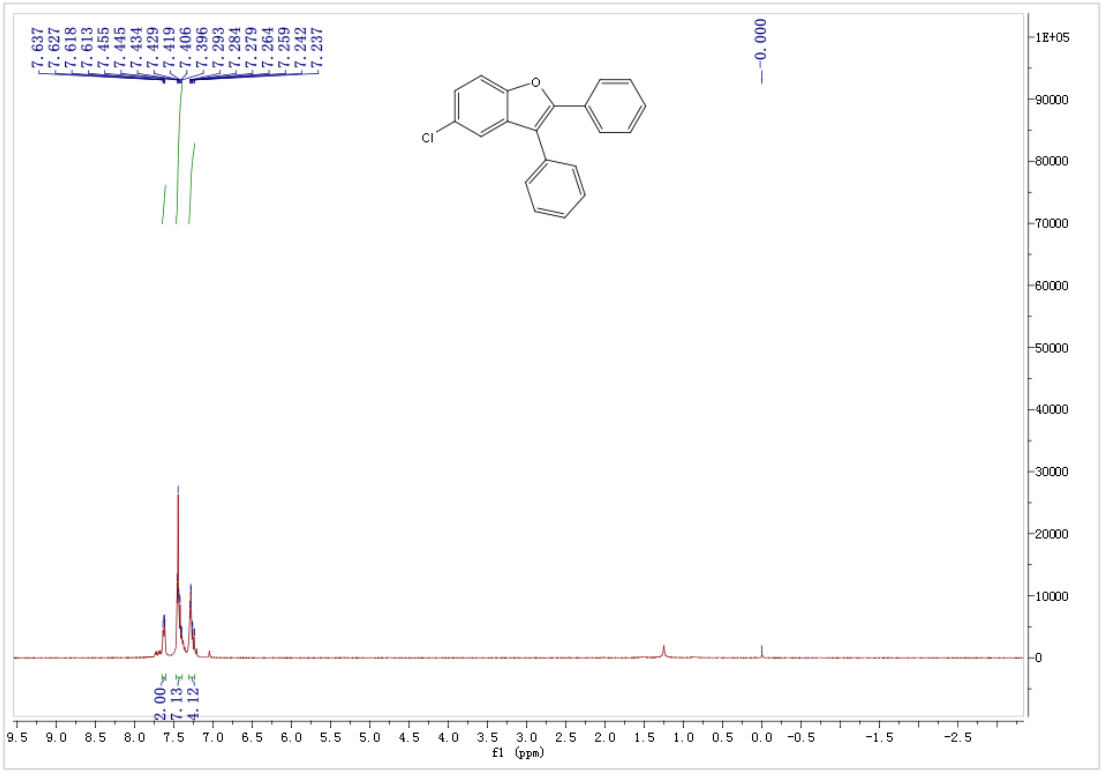


**Fig. S-11**. $^{1}$H-NMR spectrum of **3f**.

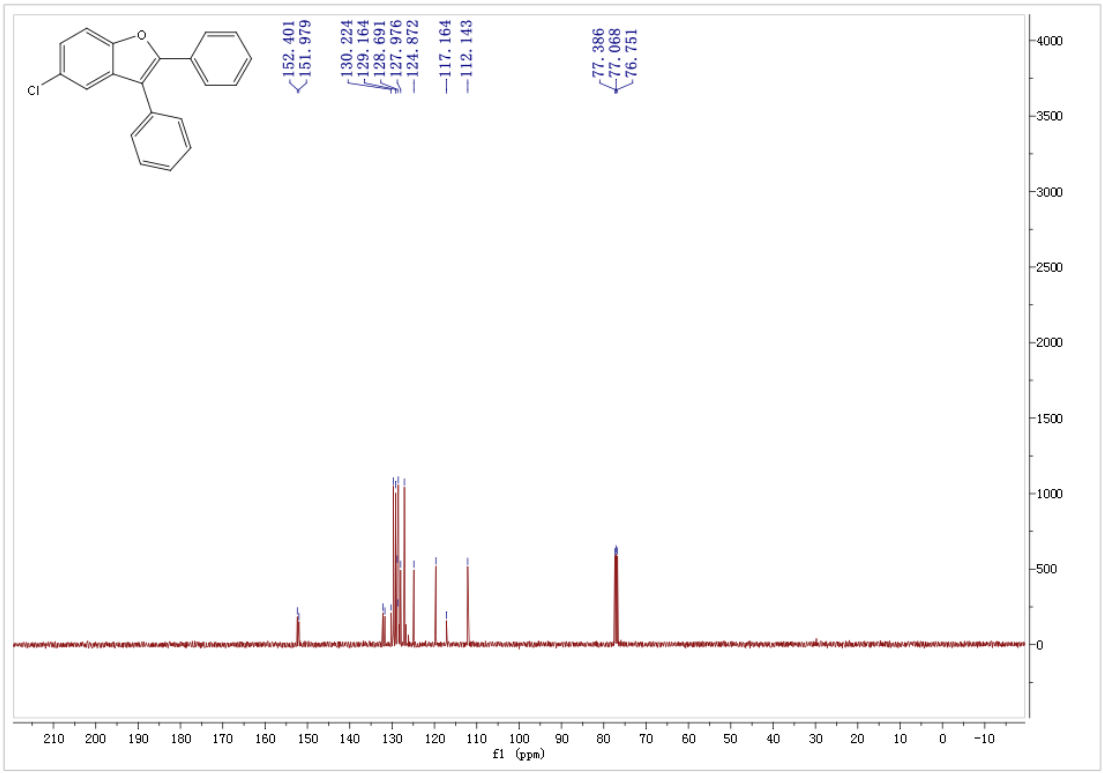


**Fig. S-12**. $^{13}$C-NMR spectrum of **3f**.

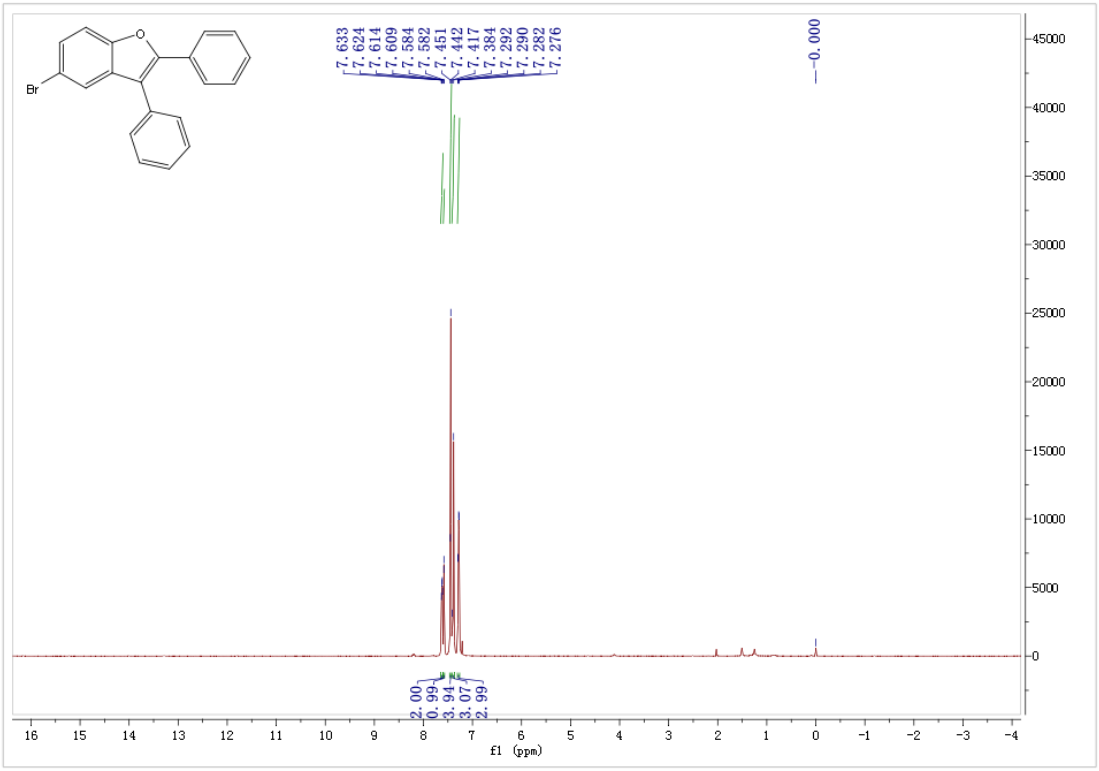


**Fig. S-13**. $^{1}$H-NMR spectrum of **3g**.

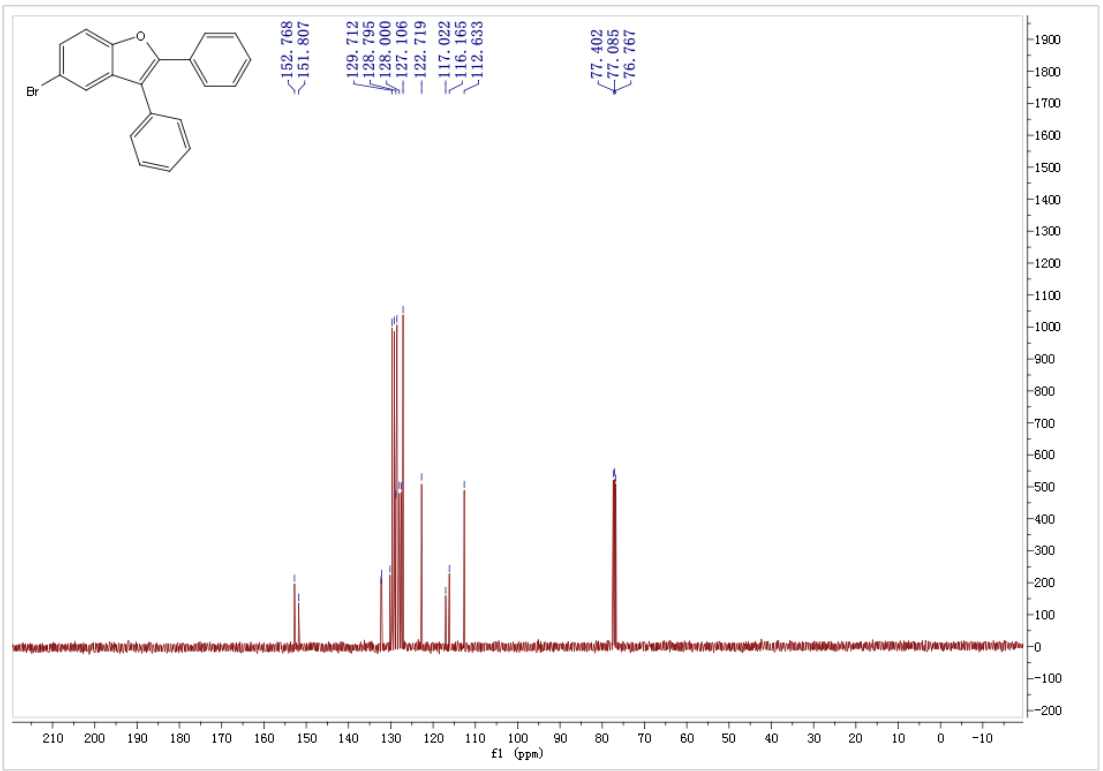


**Fig. S-14**. $^{13}$C-NMR spectrum of **3g**.

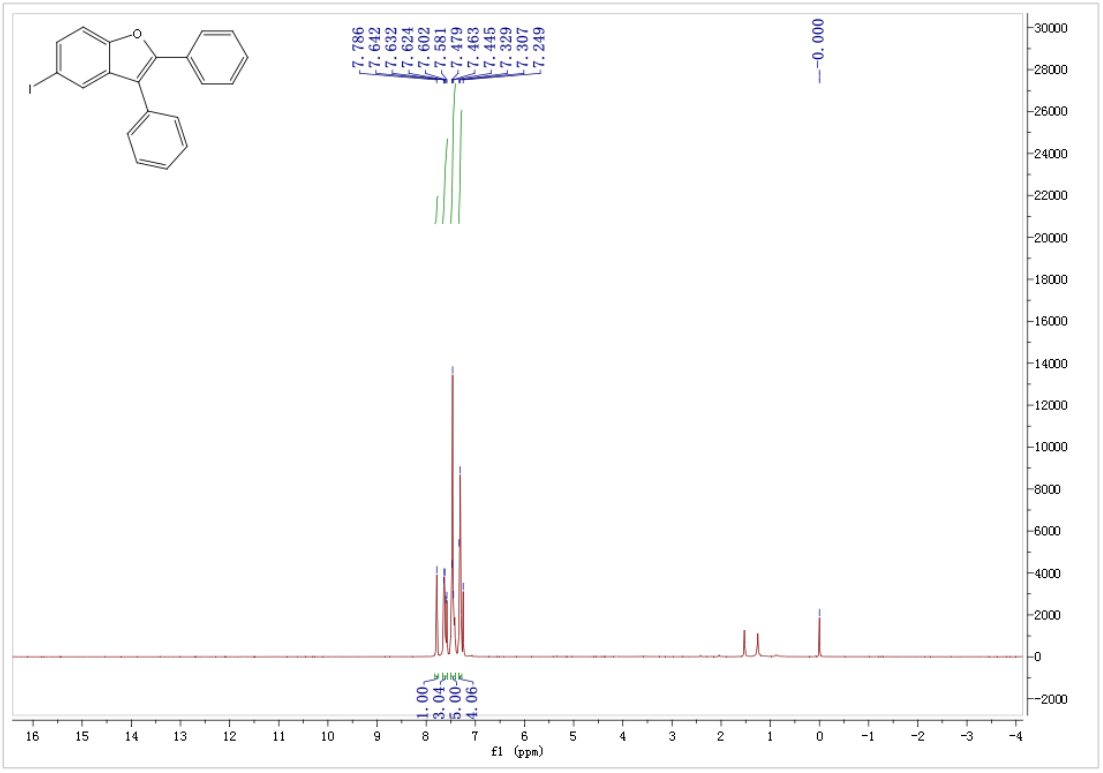


**Fig. S-15**. $^{1}$H-NMR spectrum of **3h**.

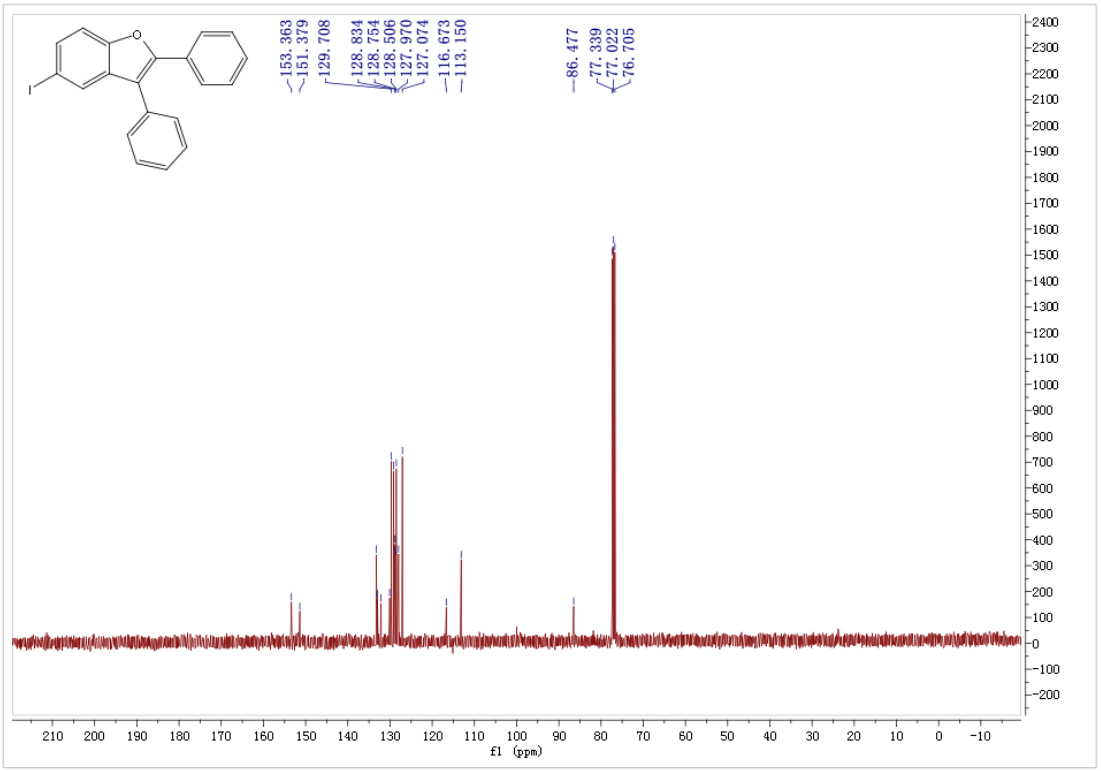


**Fig. S-16**. $^{13}$C-NMR spectrum of **3h**.

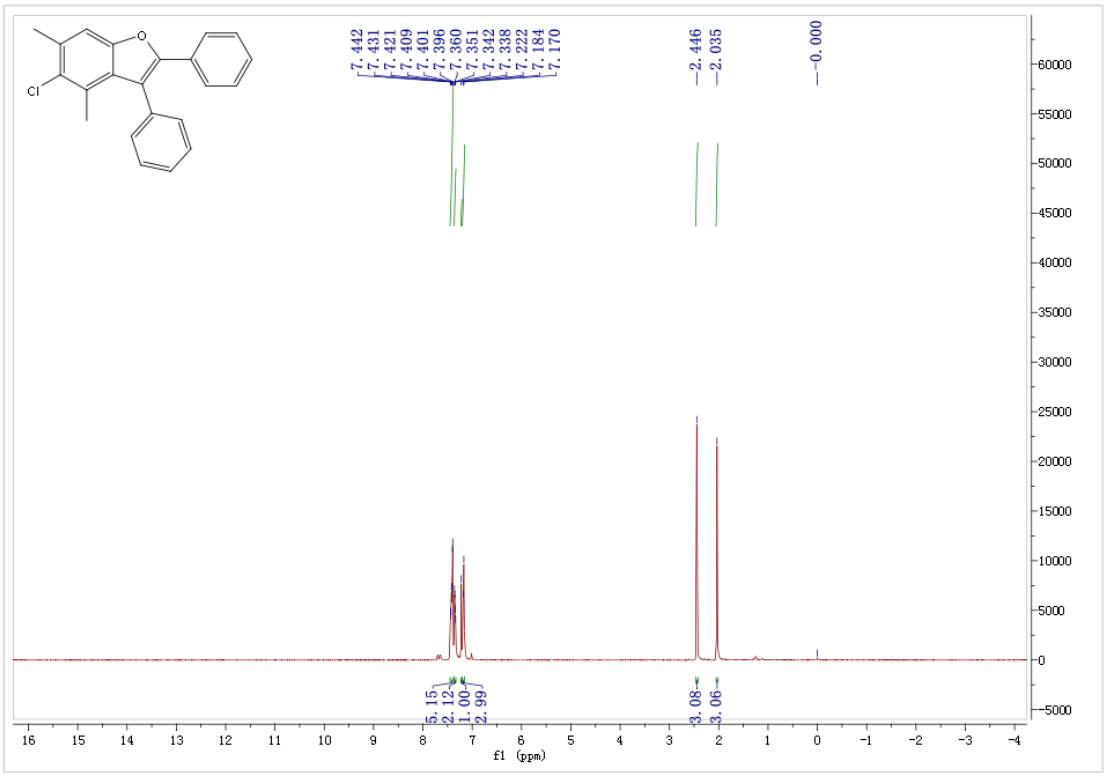


**Fig. S-17**. $^{1}$H-NMR spectrum of **3i**.

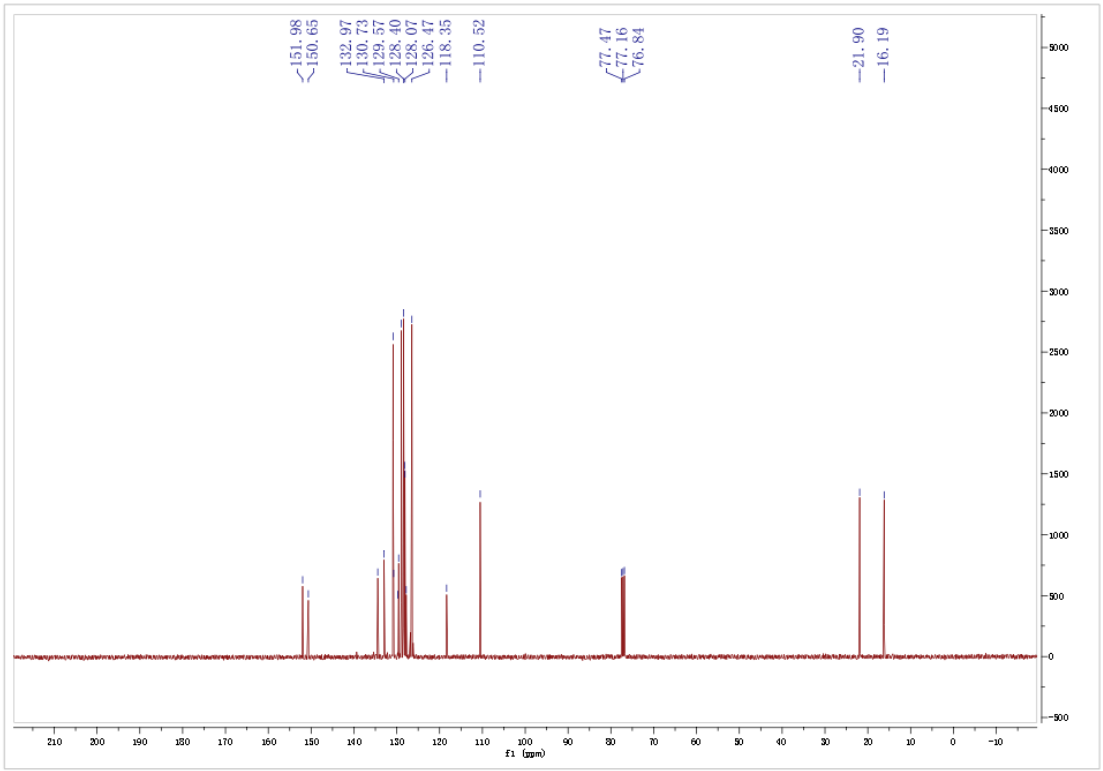


**Fig. S-18**. $^{13}$C-NMR spectrum of **3i**.

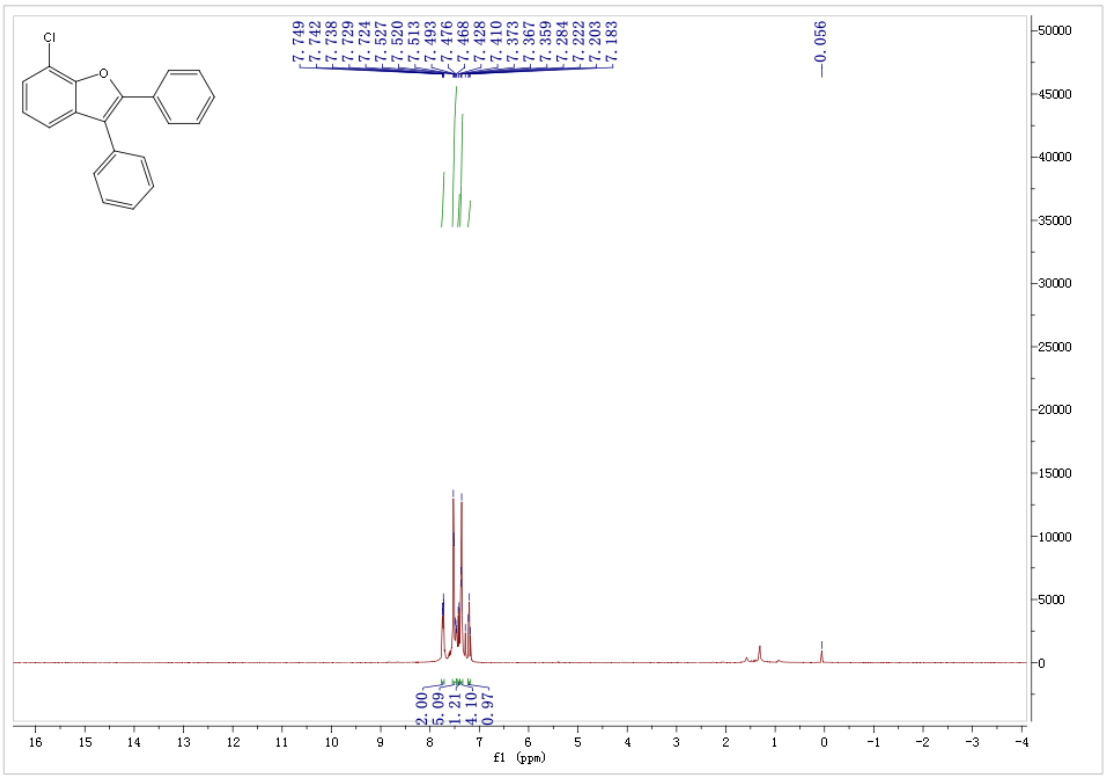


**Fig. S-19**. $^{1}$H-NMR spectrum of **3j**.

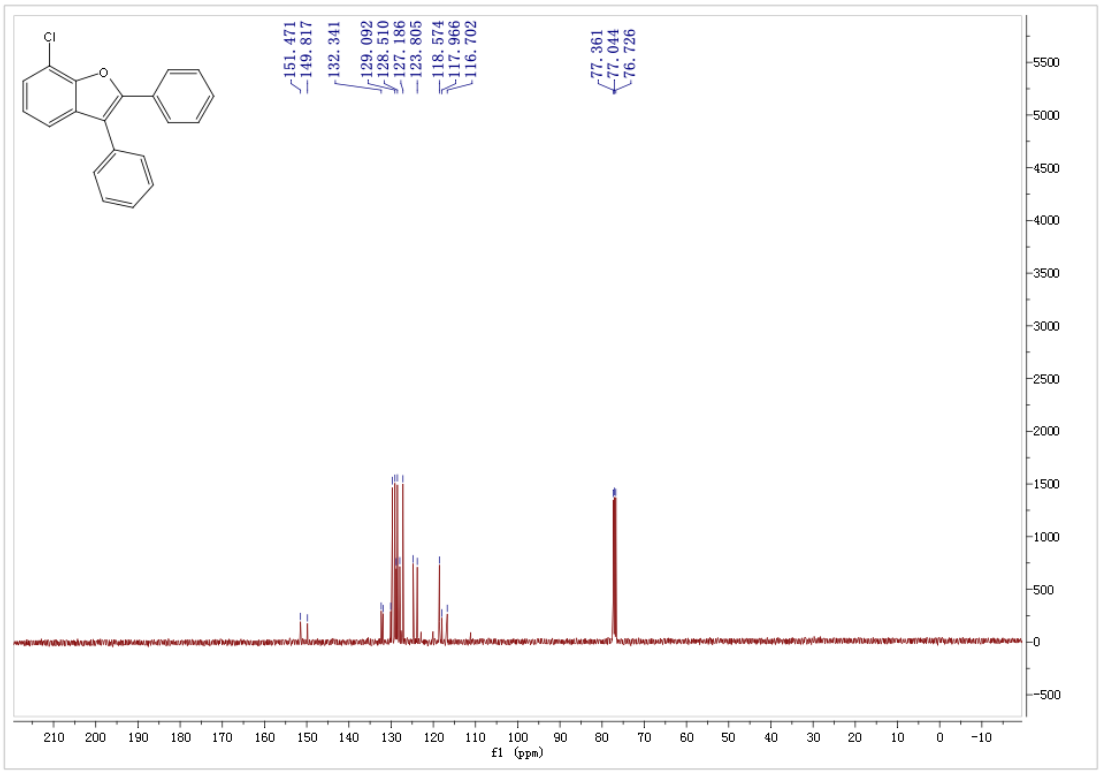


**Fig. S-20**. $^{13}$C-NMR spectrum of **3j**.

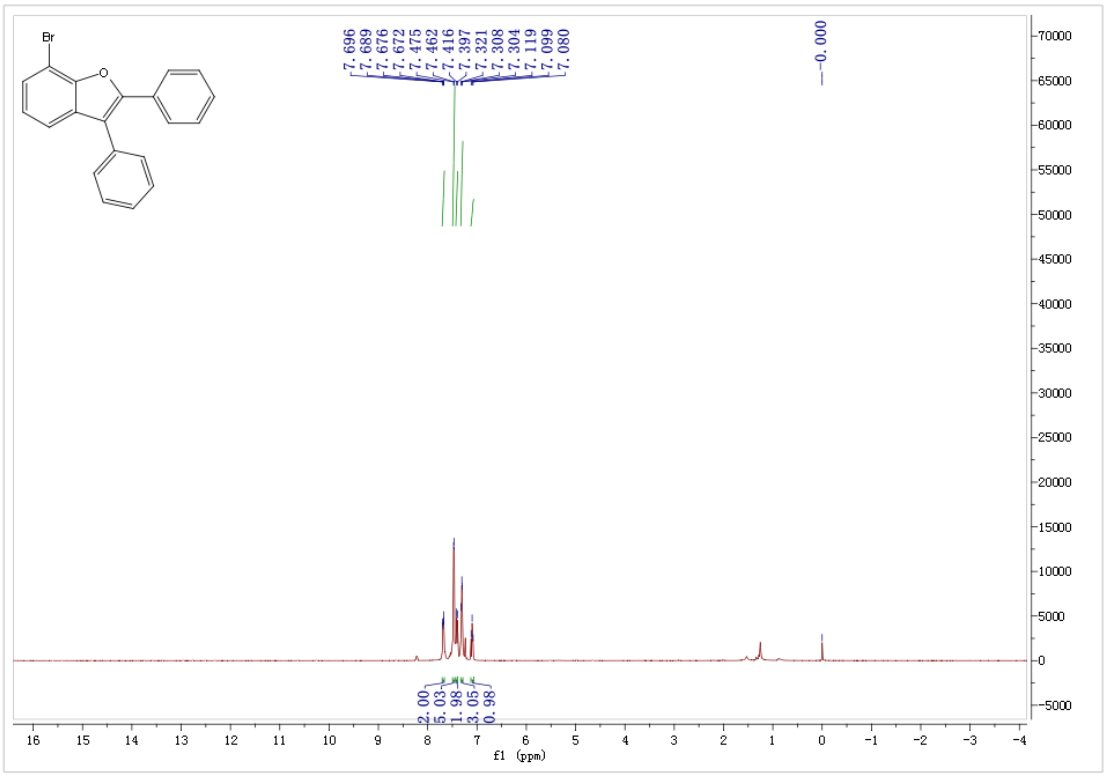


**Fig. S-21**. $^{1}$H-NMR spectrum of **3k**.

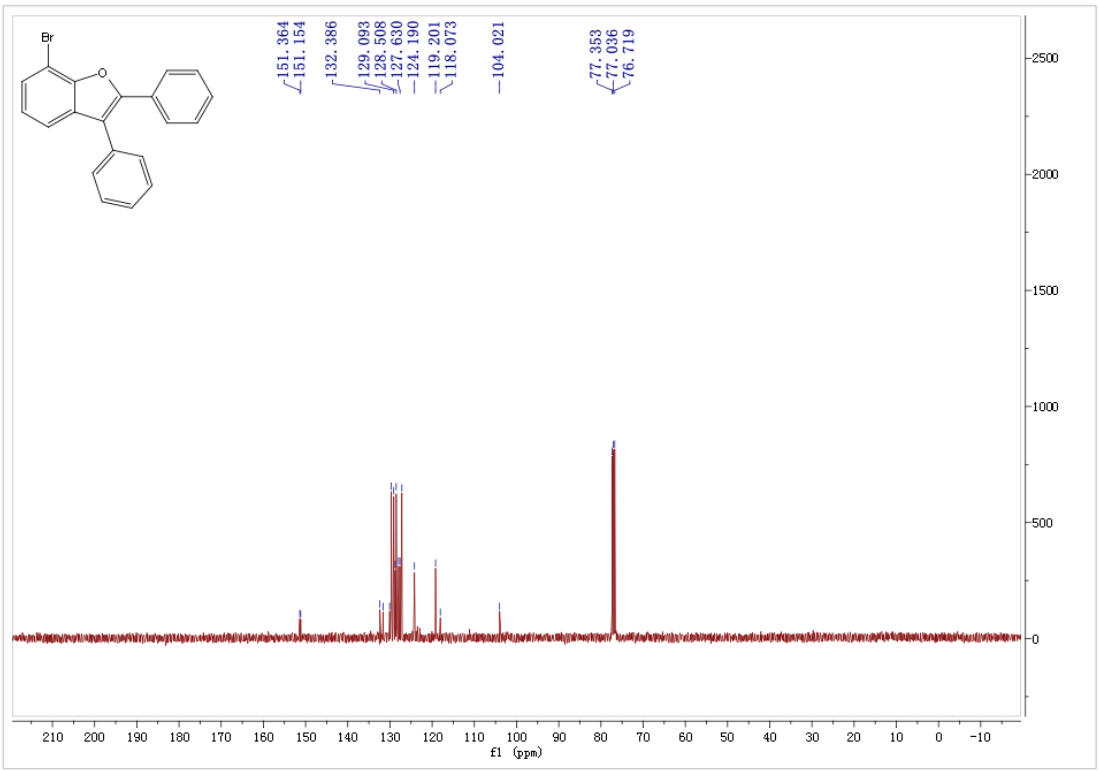


**Fig. S-22**. $^{13}$C-NMR spectrum of **3k**.

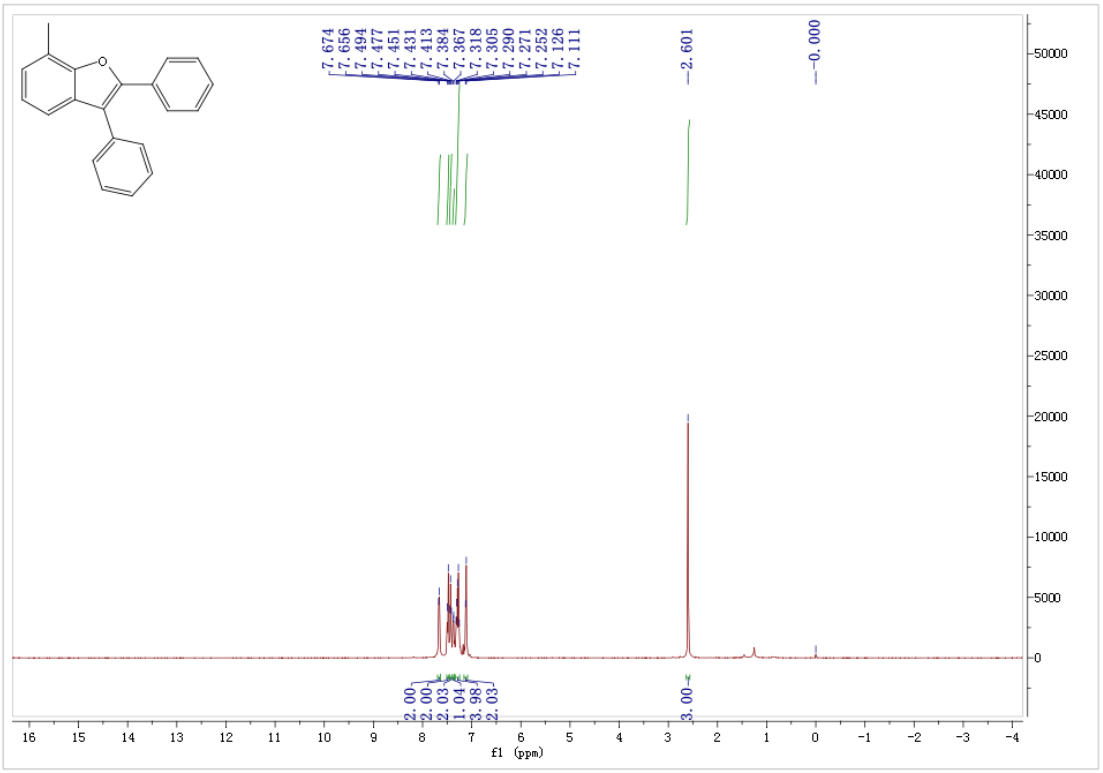


**Fig. S-23**. $^{1}$H-NMR spectrum of **3l**.

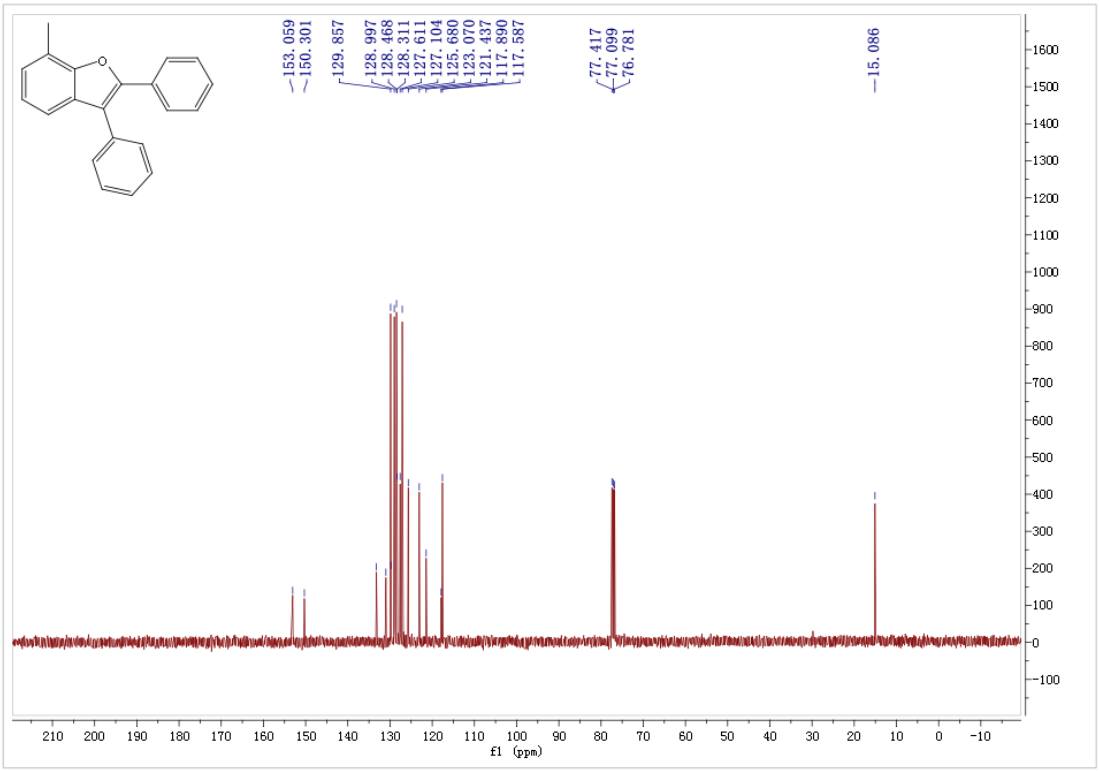


**Fig. S-24**. $^{13}$C-NMR spectrum of **3l**.

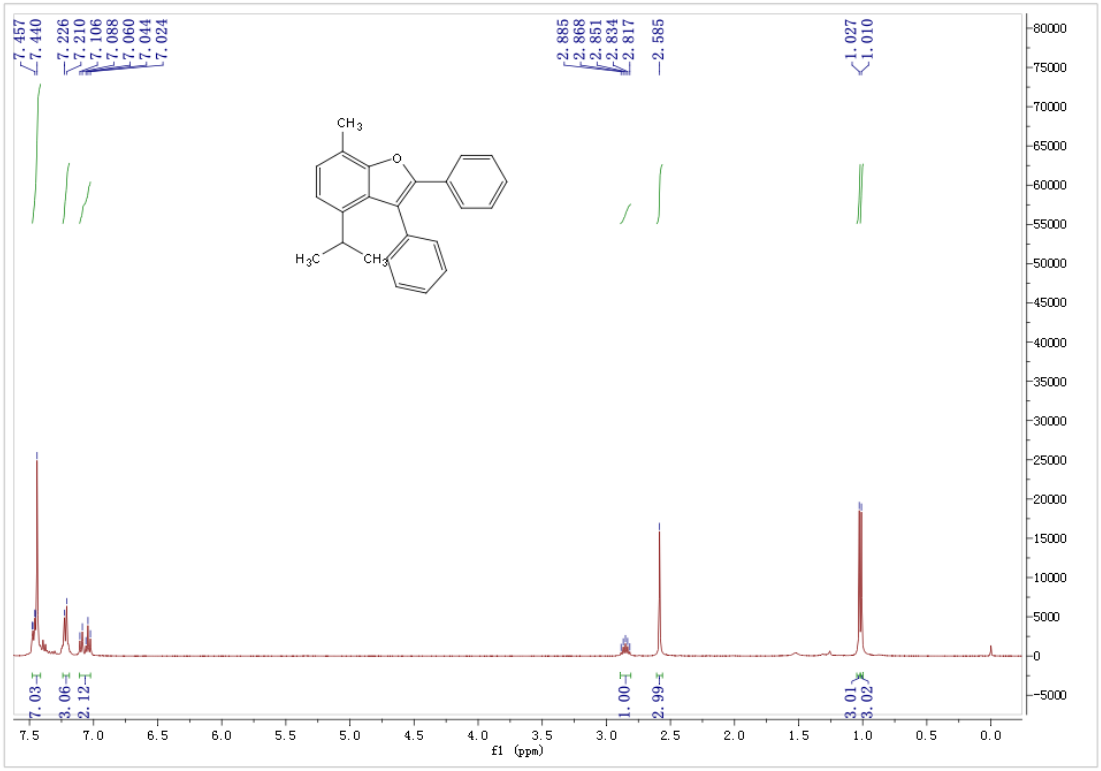


**Fig. S-25**. $^{1}$H-NMR spectrum of **3m**.

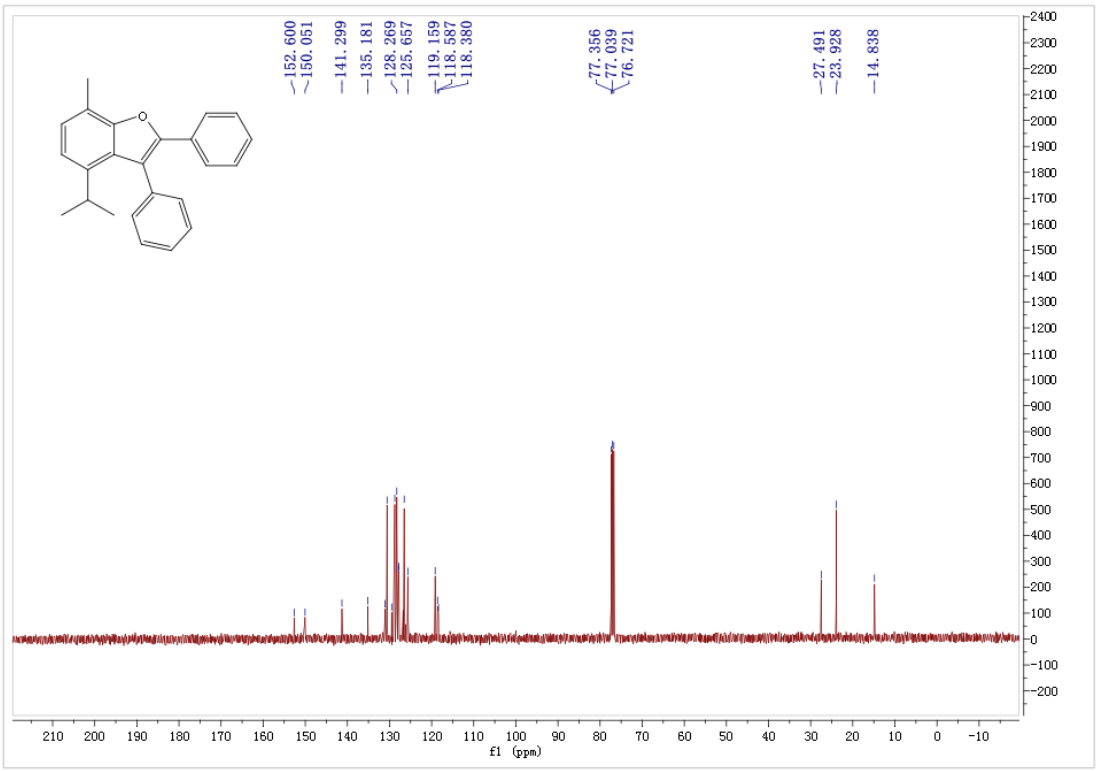


**Fig. S-26**. $^{13}$C-NMR spectrum of **3m**.

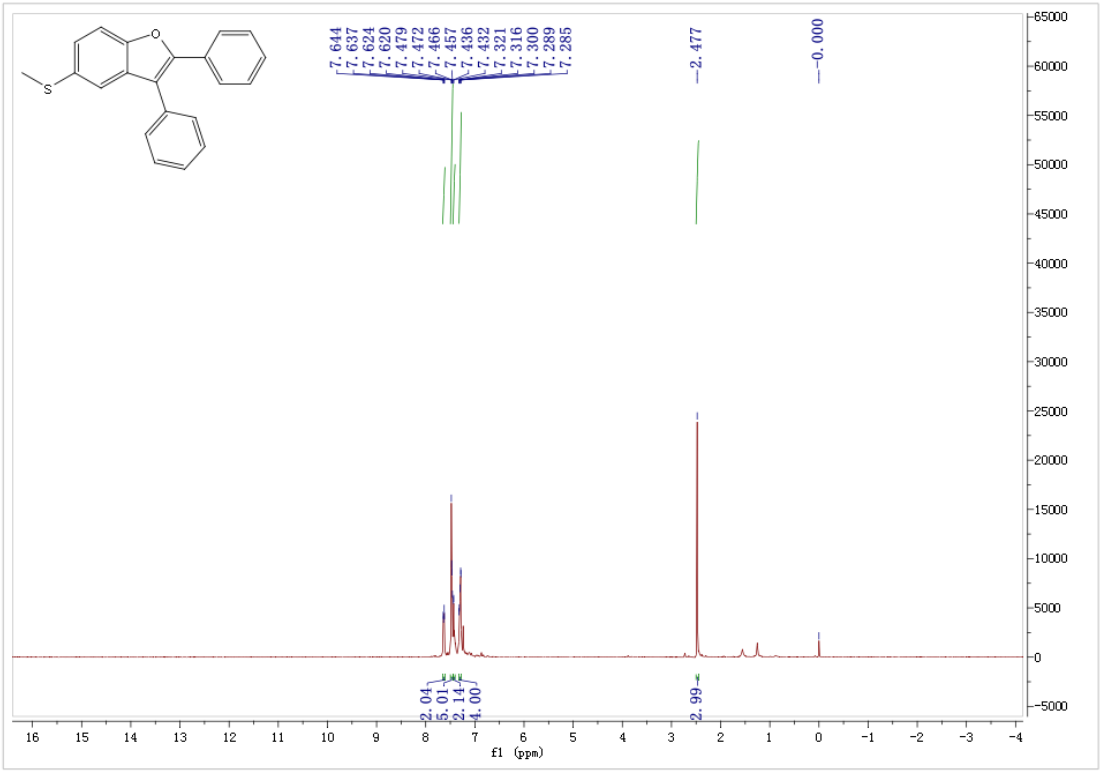


**Fig. S-27**. $^{1}$H-NMR spectrum of **3n**.

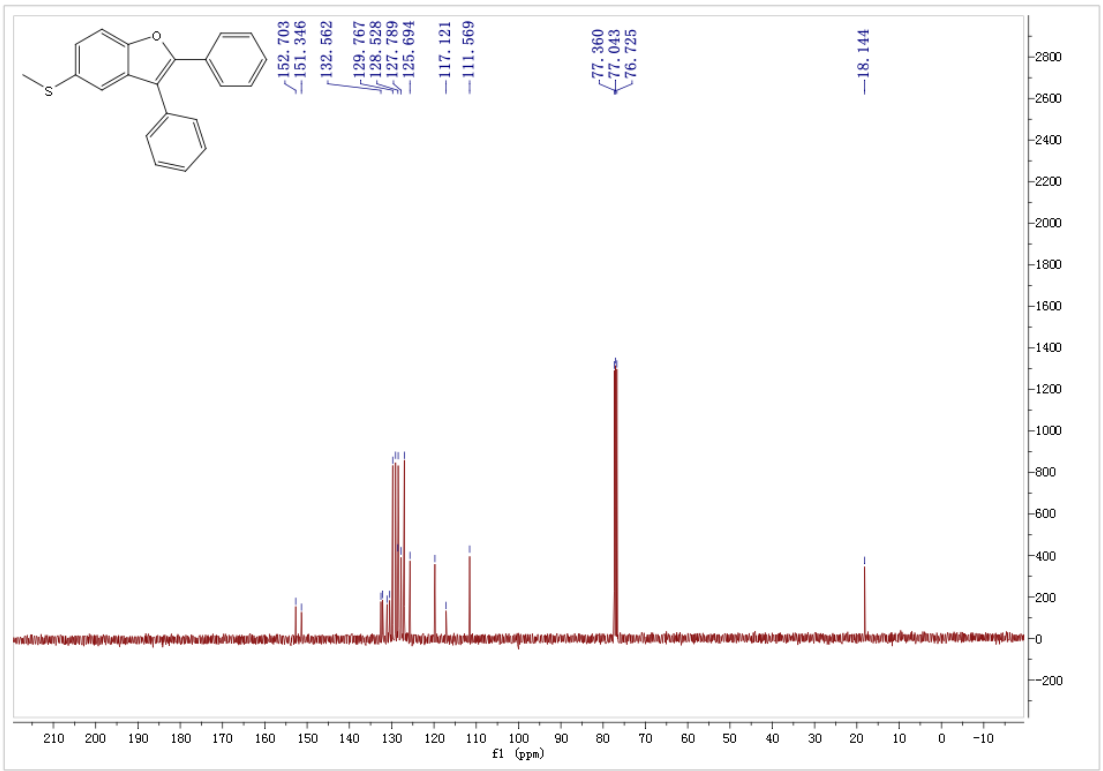


**Fig. S-28**. $^{13}$C-NMR spectrum of **3n**.

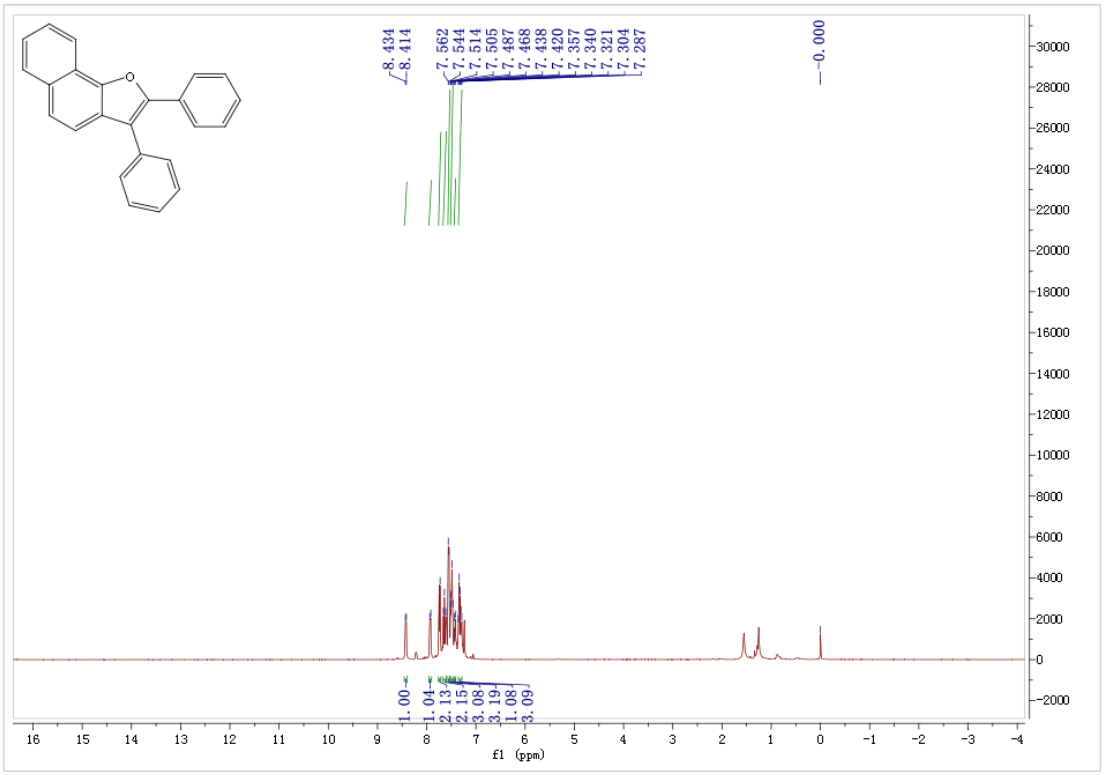


**Fig. S-29**. $^{1}$H-NMR spectrum of **3o**.

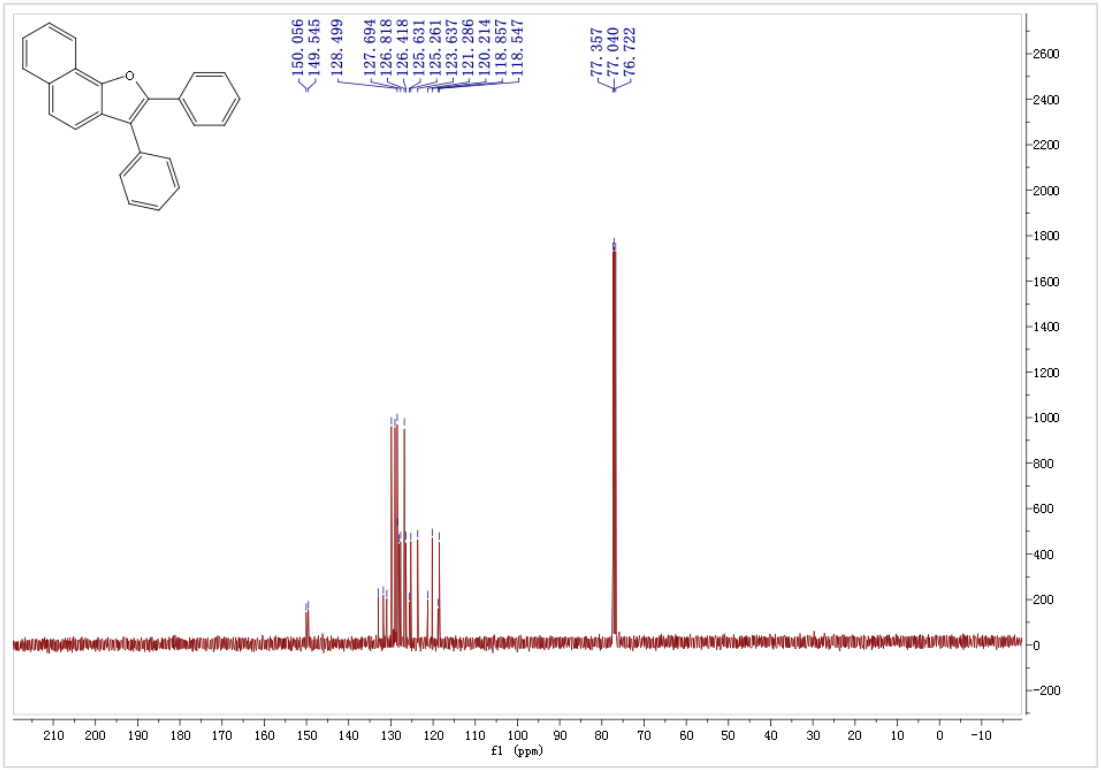


**Fig. S-30**. $^{13}$C-NMR spectrum of **3o**.

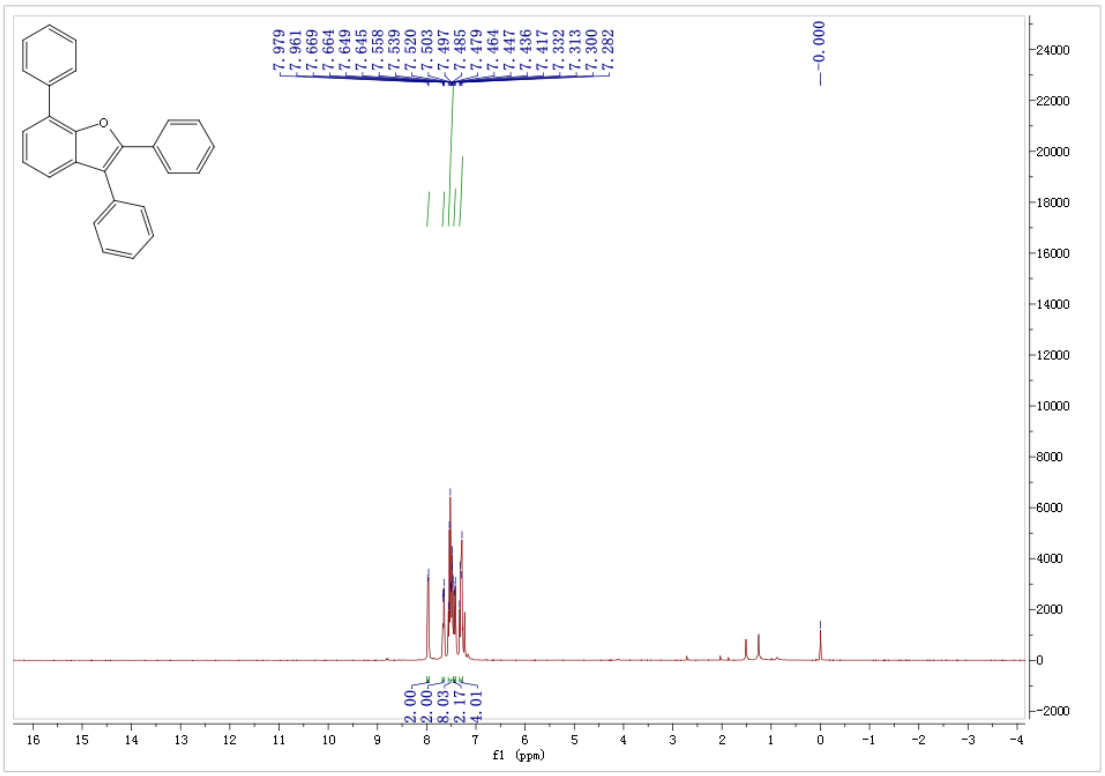


**Fig. S-31**. $^{1}$H-NMR spectrum of **3p**.

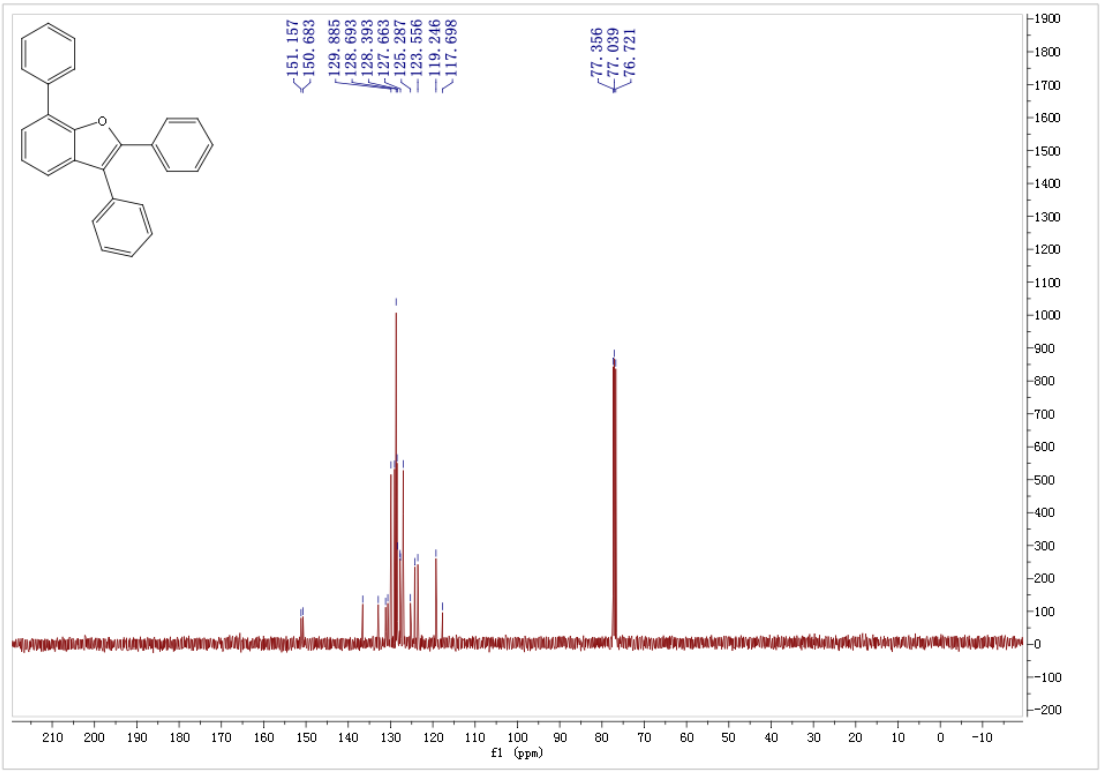


**Fig. S-32**. $^{13}$C-NMR spectrum of **3p**.

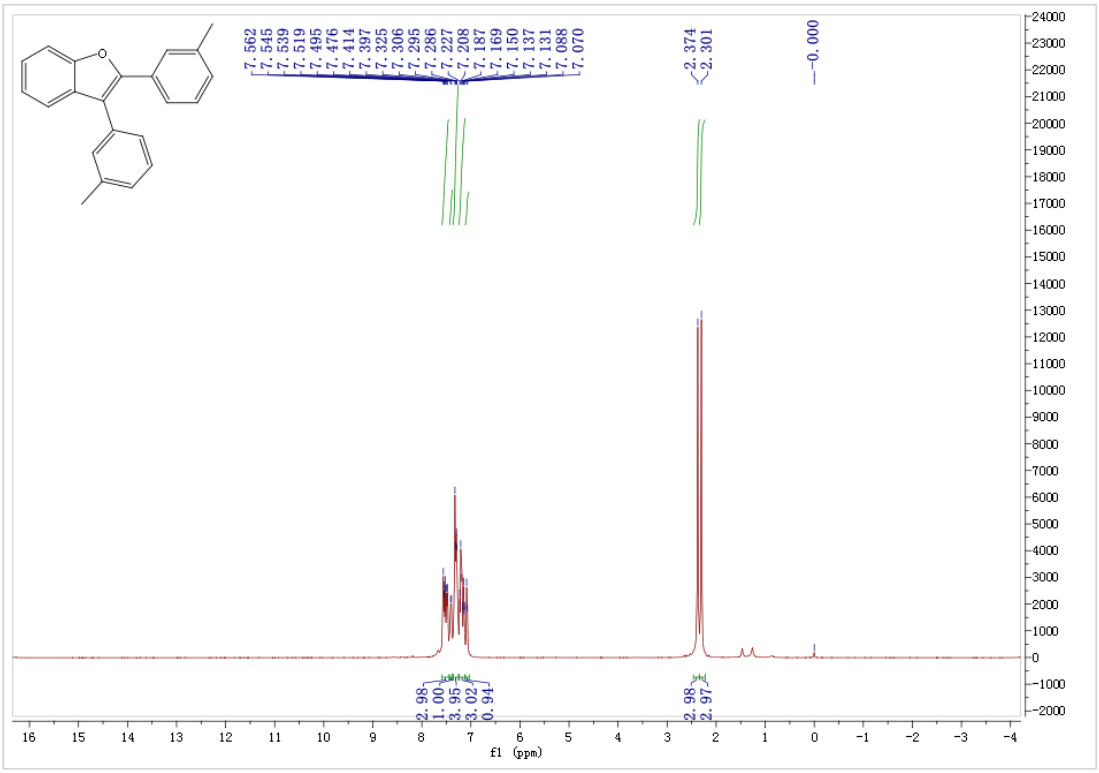


**Fig. S-33**. $^{1}$H-NMR spectrum of **4a**.

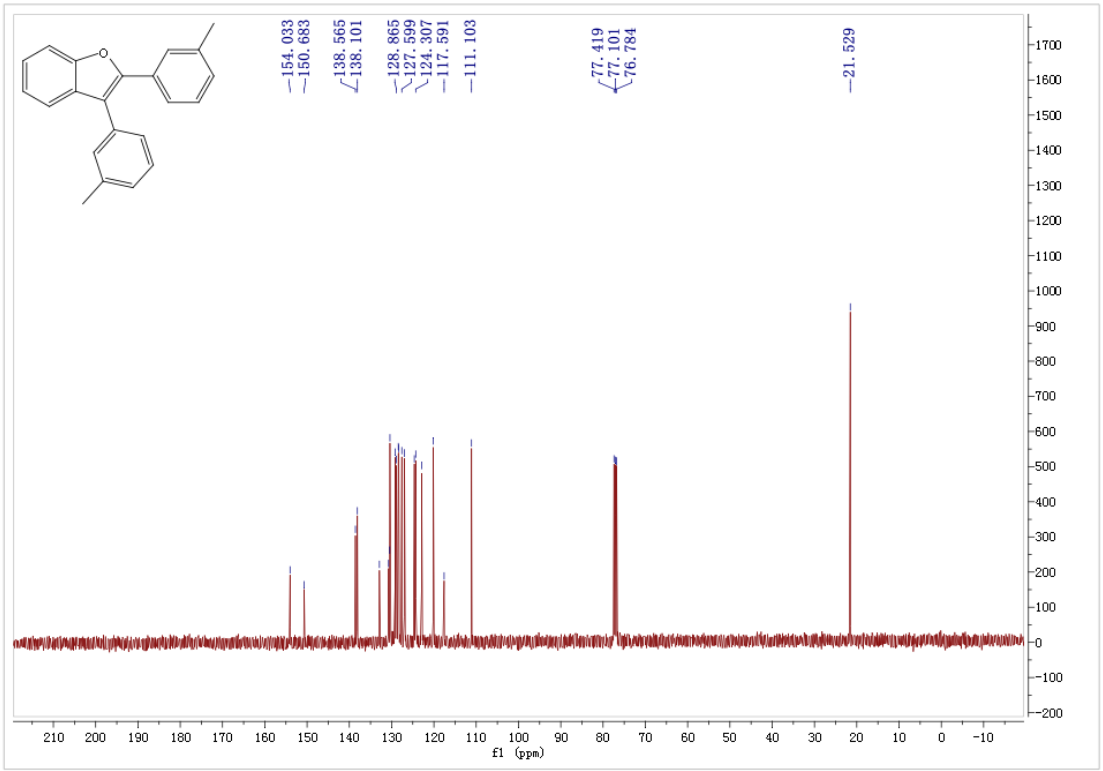


**Fig. S-34**. $^{13}$C-NMR spectrum of **4a**.

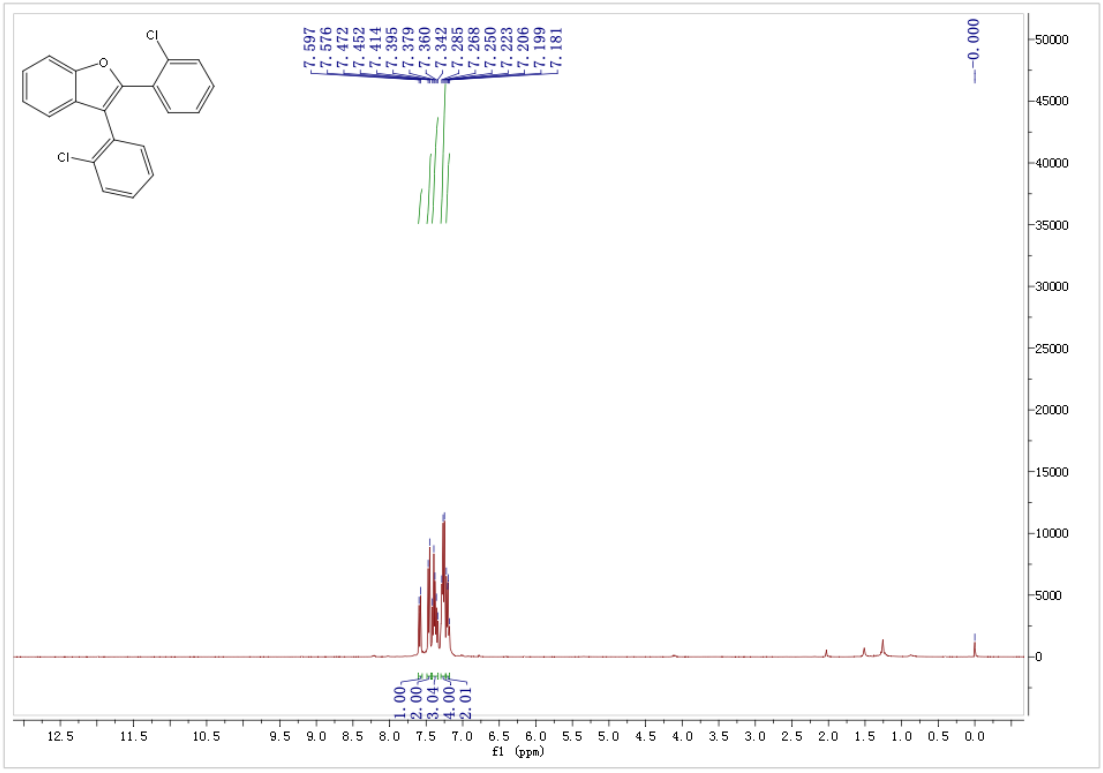


**Fig. S-35**. $^{1}$H-NMR spectrum of **4b**.

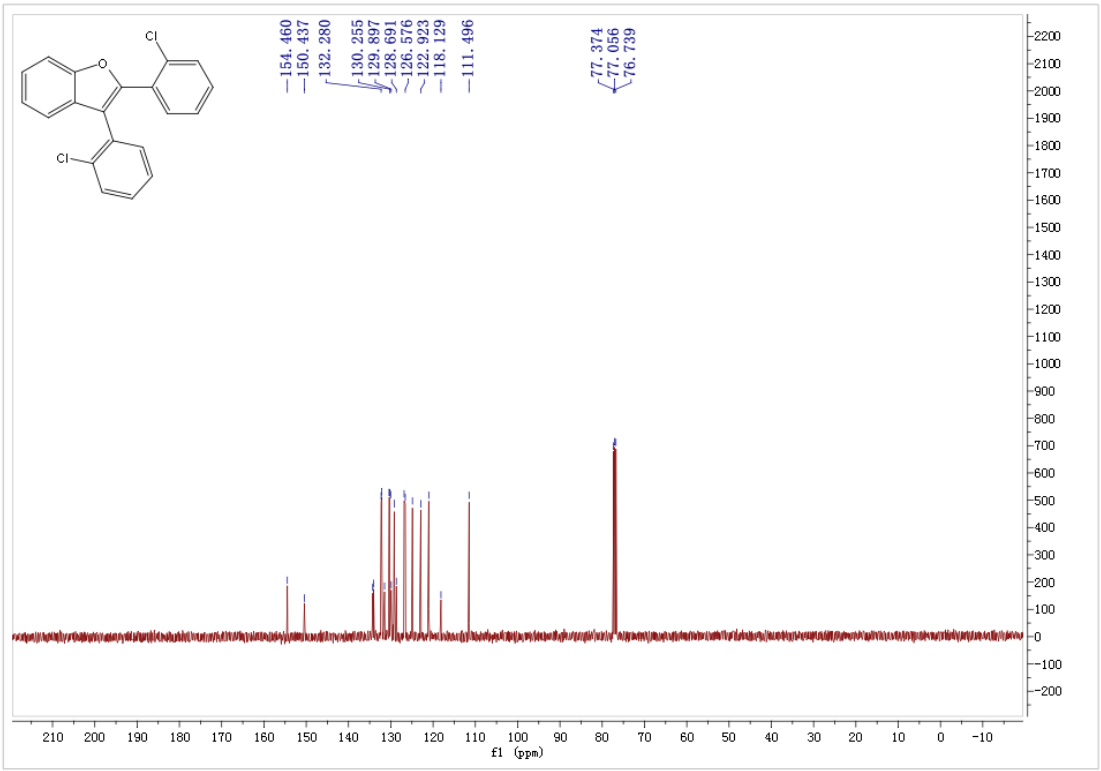


**Fig. S-36**. $^{13}$C-NMR spectrum of **4b**.

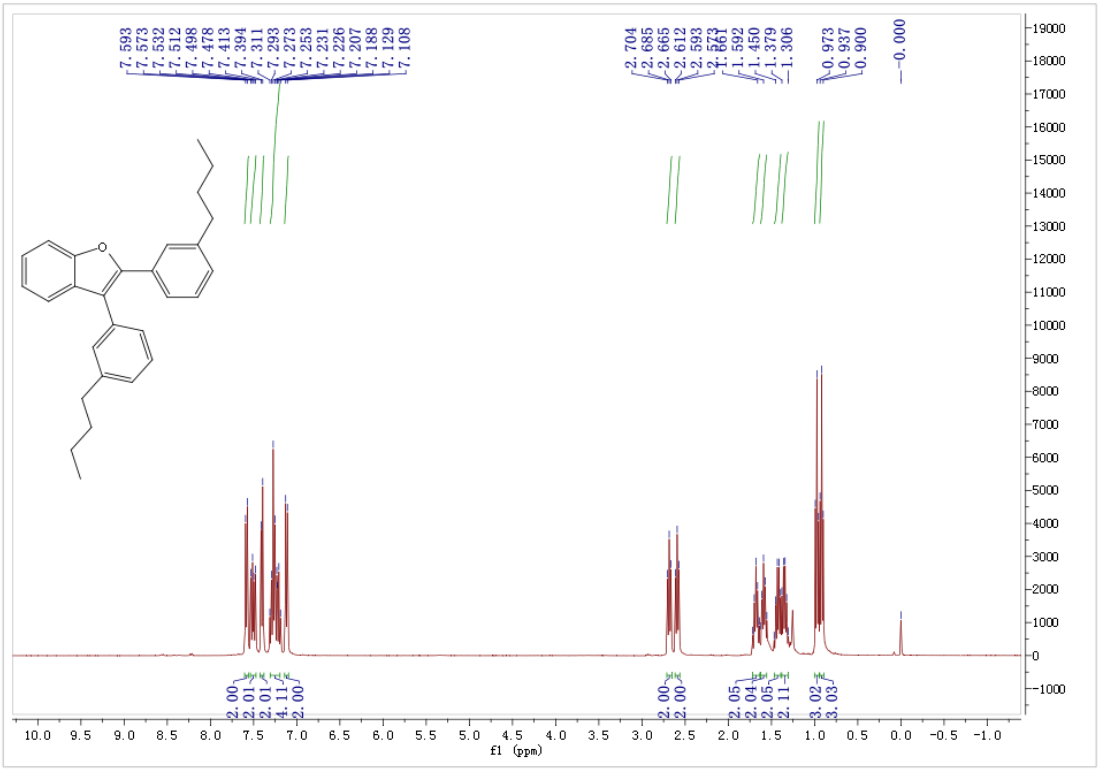


**Fig. S-37**. $^{1}$H-NMR spectrum of **4c**.

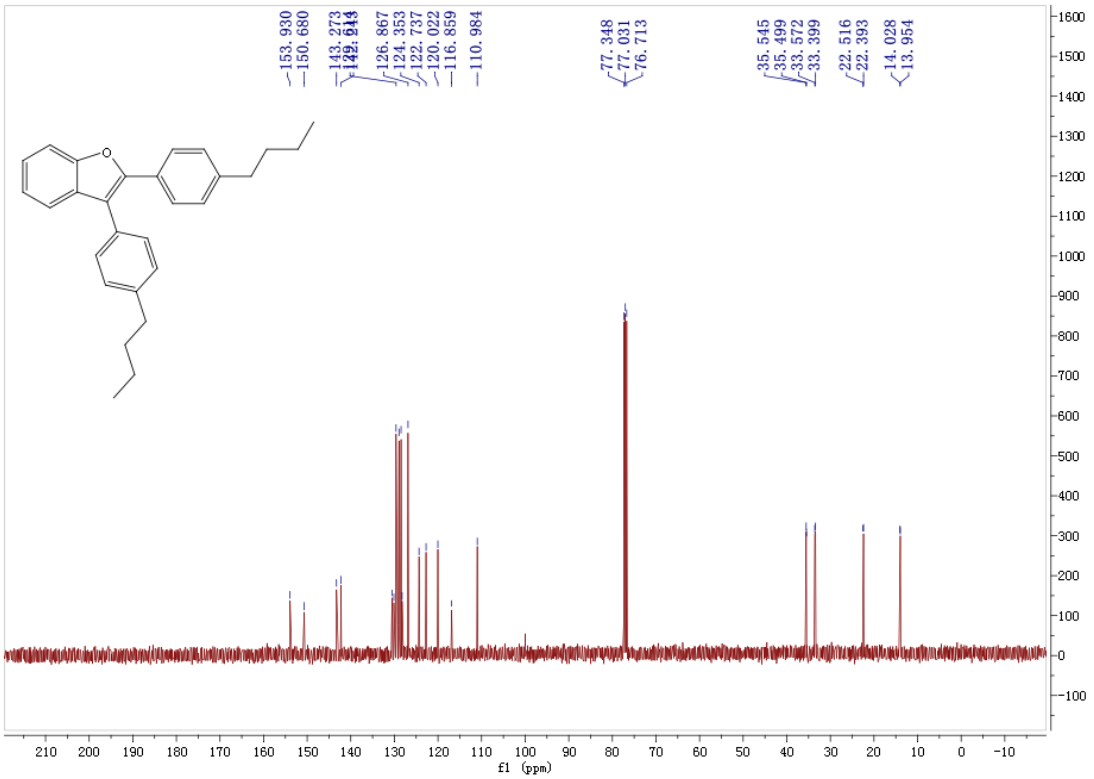


**Fig. S-38**. $^{13}$C-NMR spectrum of **4c**.

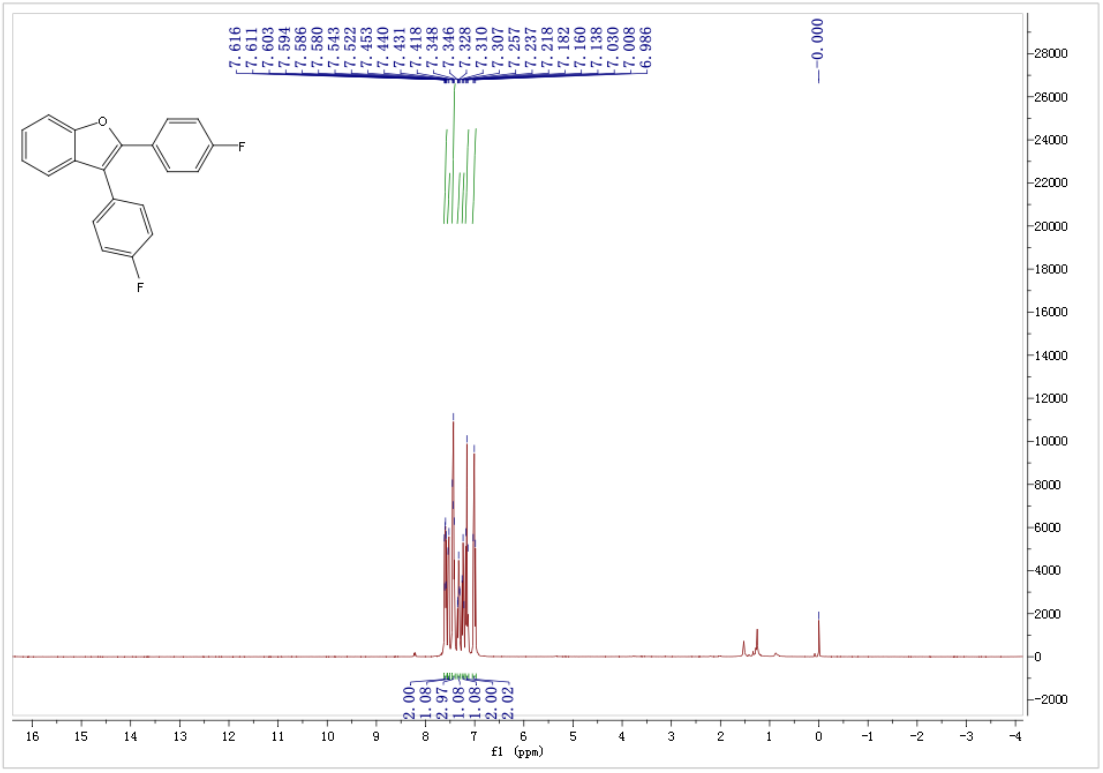


**Fig. S-39**. $^{1}$H-NMR spectrum of **4d**.

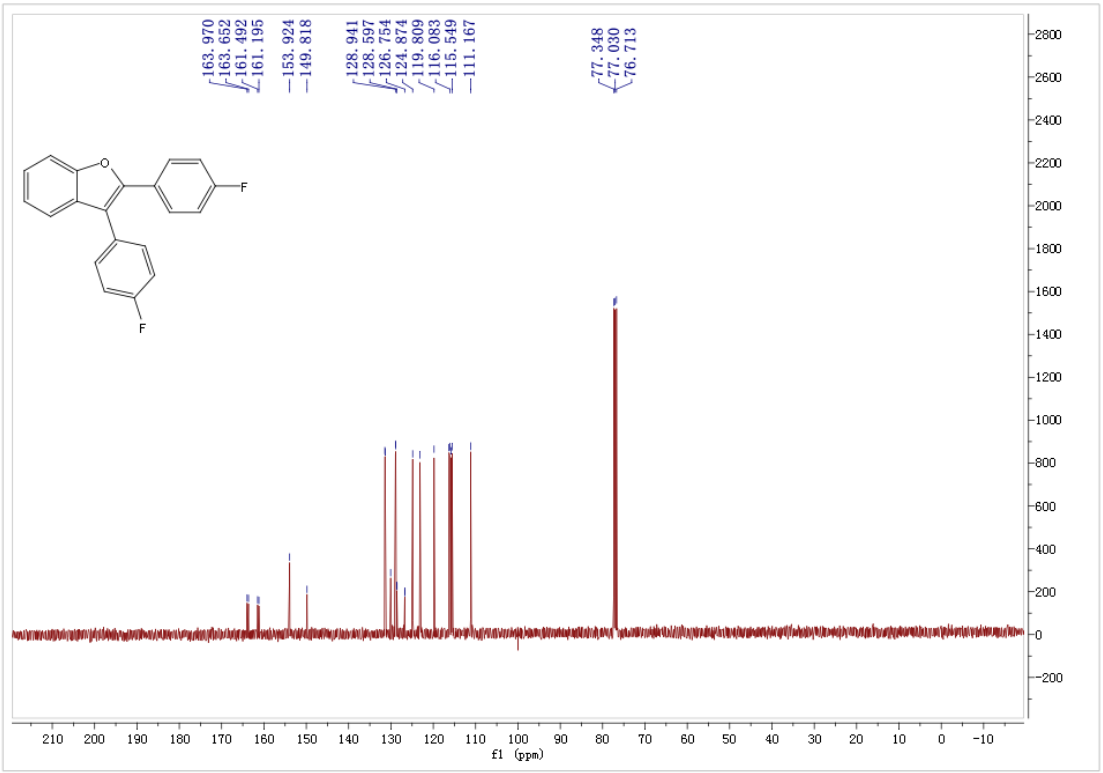


**Fig. S-40**. $^{13}$C-NMR spectrum of **4d**.

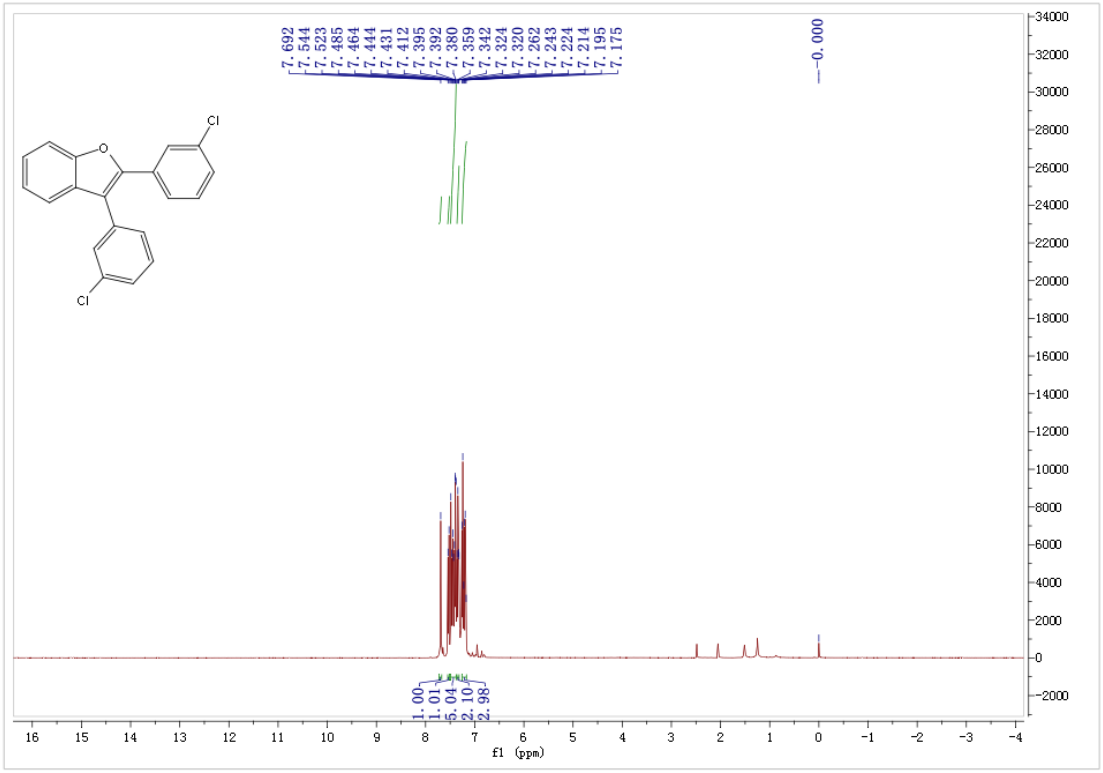


**Fig. S-41**. $^{1}$H-NMR spectrum of **4e**.

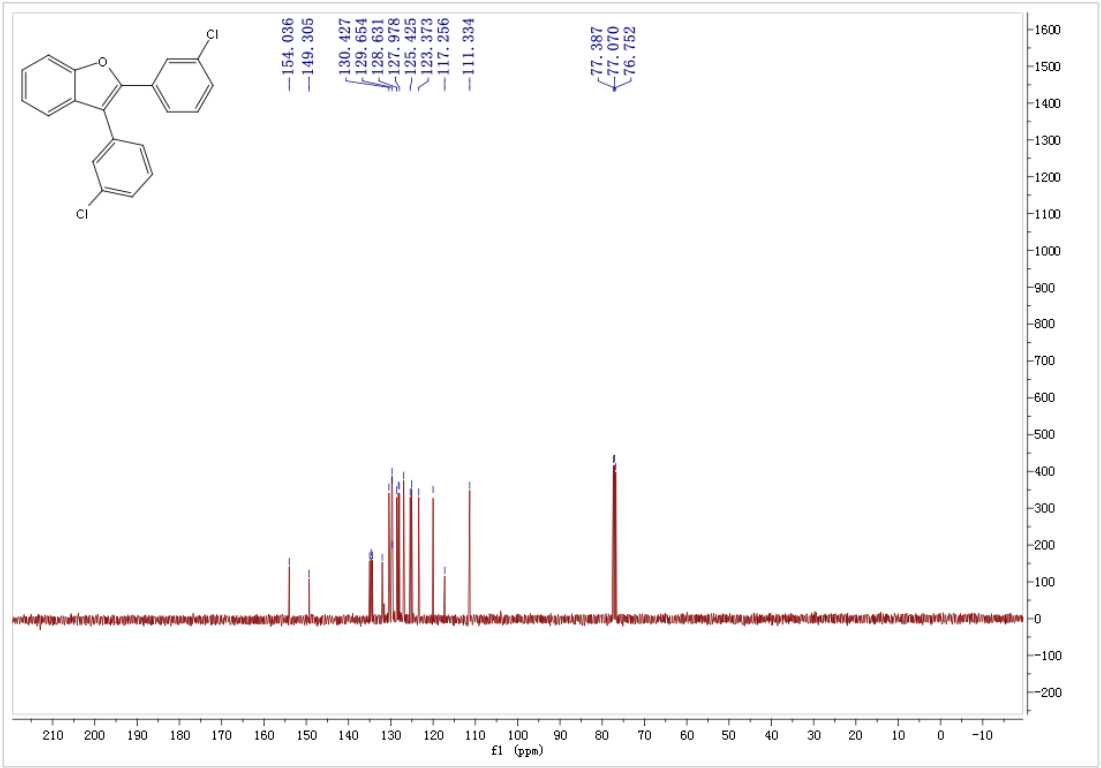


**Fig. S-42**. $^{13}$C-NMR spectrum of **4e**.

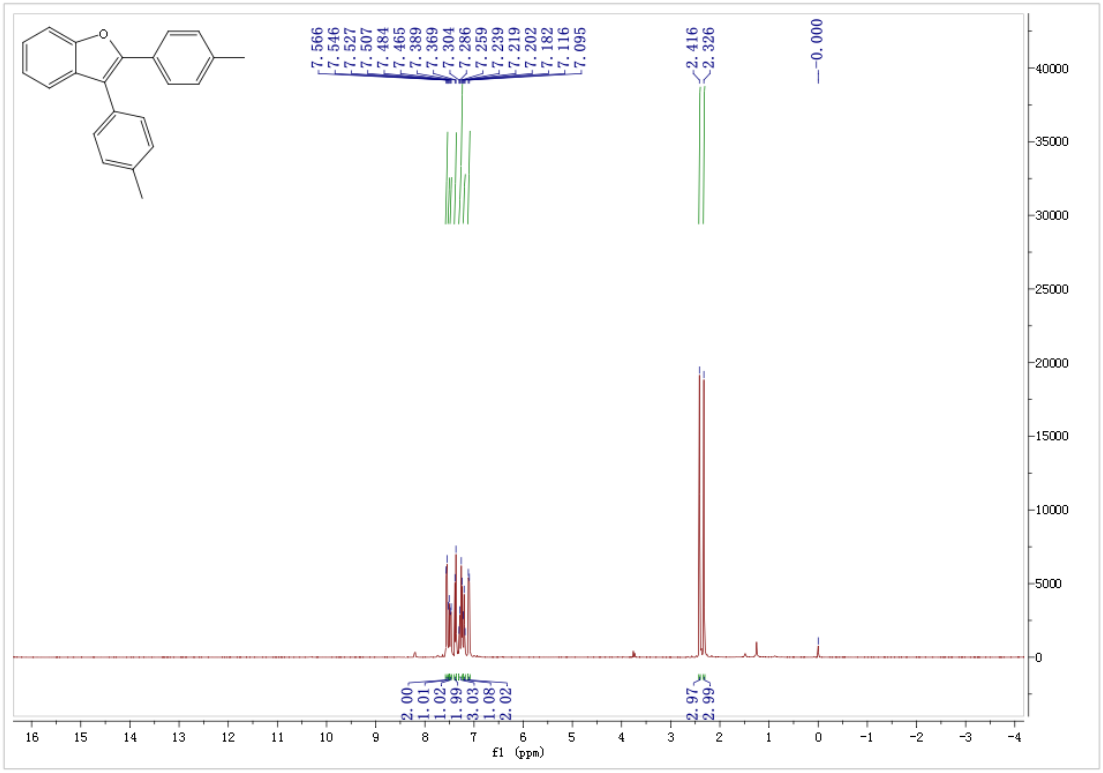


**Fig. S-43**. $^{1}$H-NMR spectrum of **4f**.

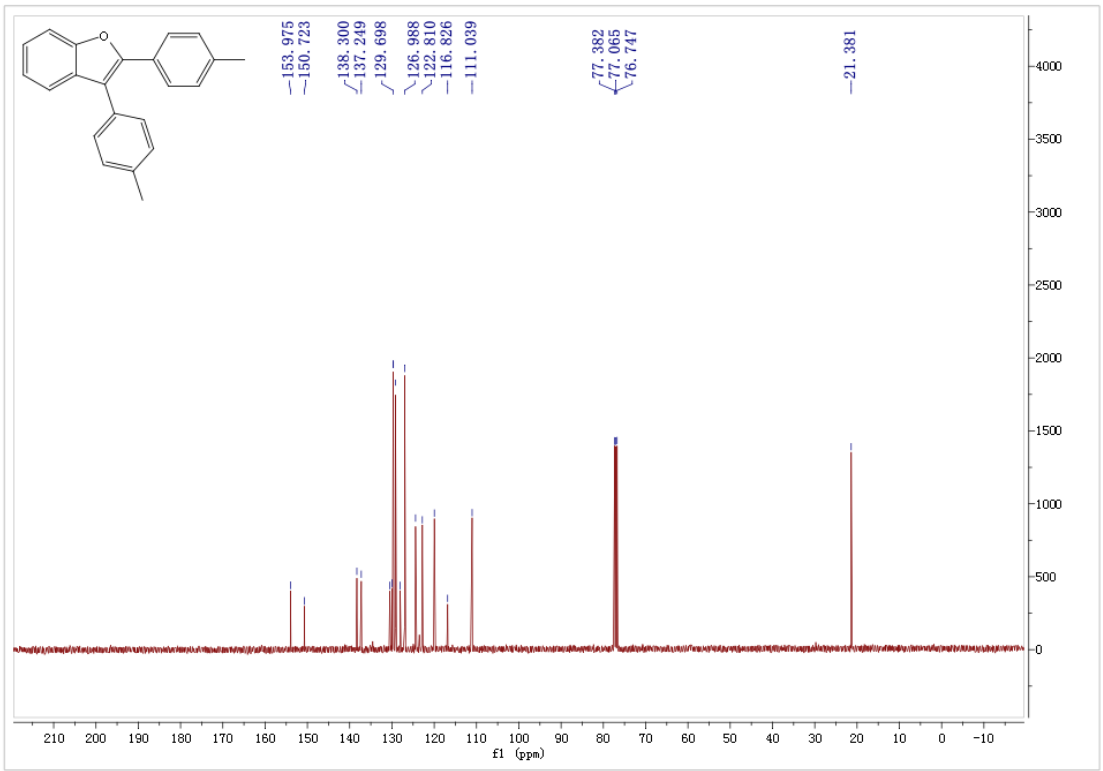


**Fig. S-44**. $^{13}$C-NMR spectrum of **4f**.

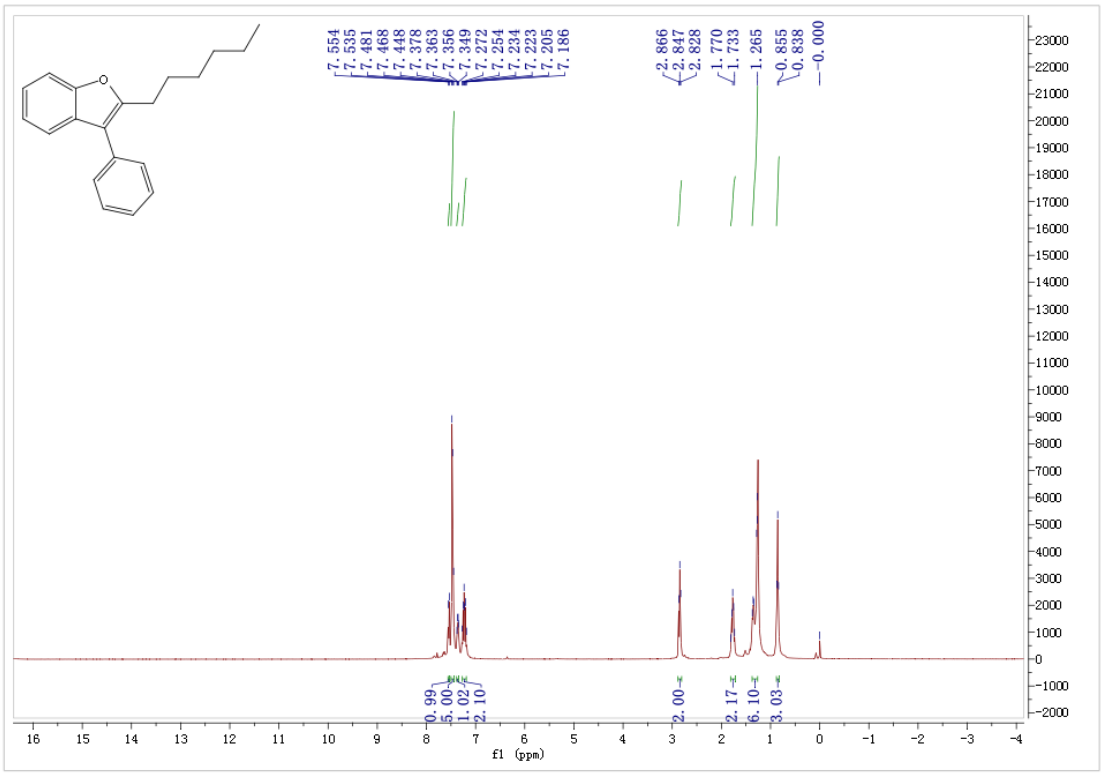


**Fig. S-45**. $^{1}$H-NMR spectrum of **4g**.

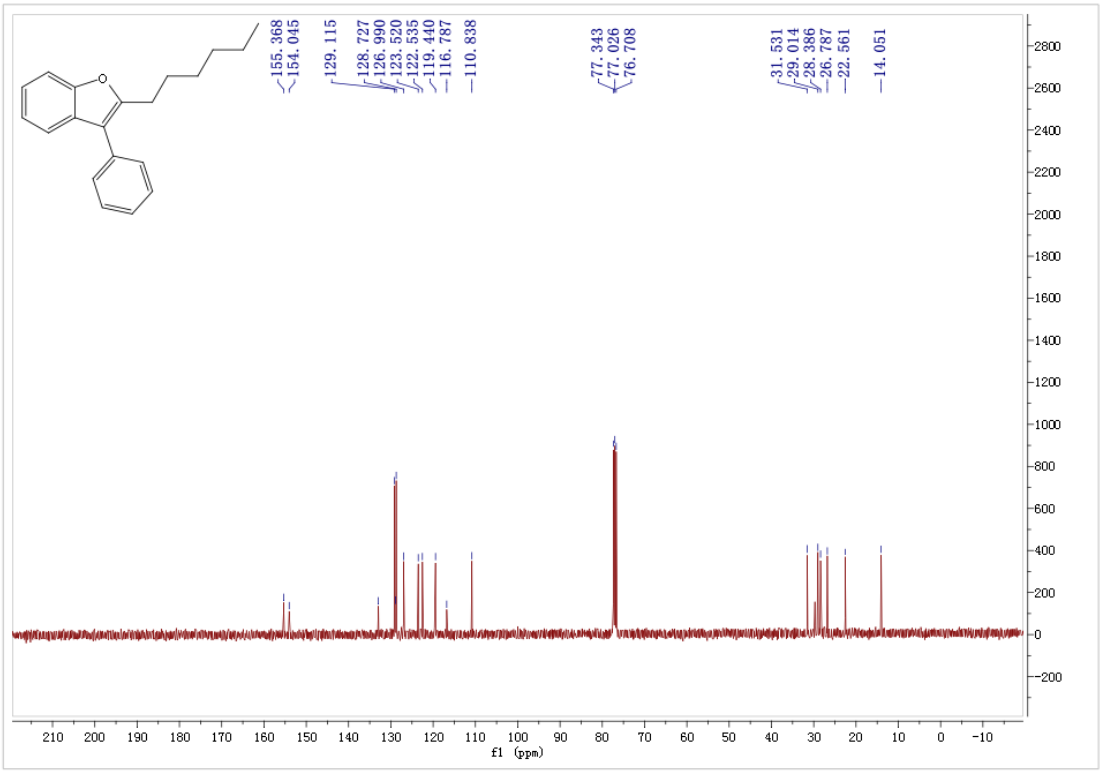


**Fig. S-46**. $^{13}$C-NMR spectrum of **4g**.

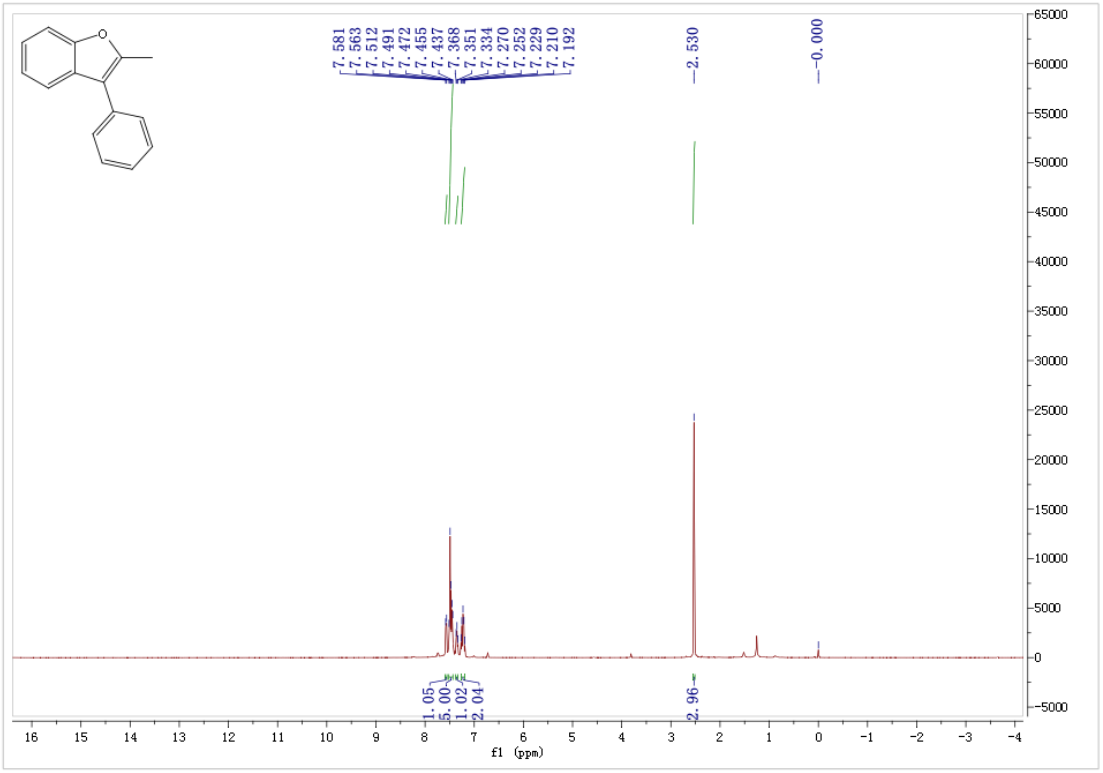


**Fig. S-47**. $^{1}$H-NMR spectrum of **4h**.

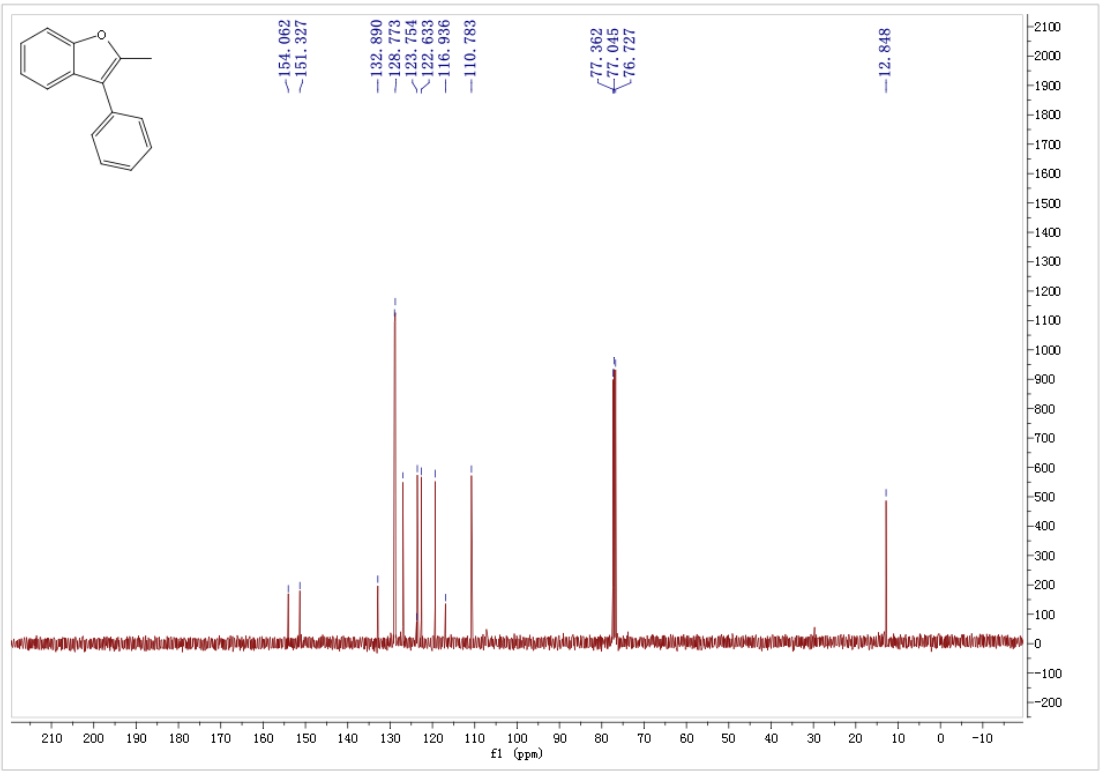


**Fig. S-48**. $^{13}$C-NMR spectrum of **4h**.

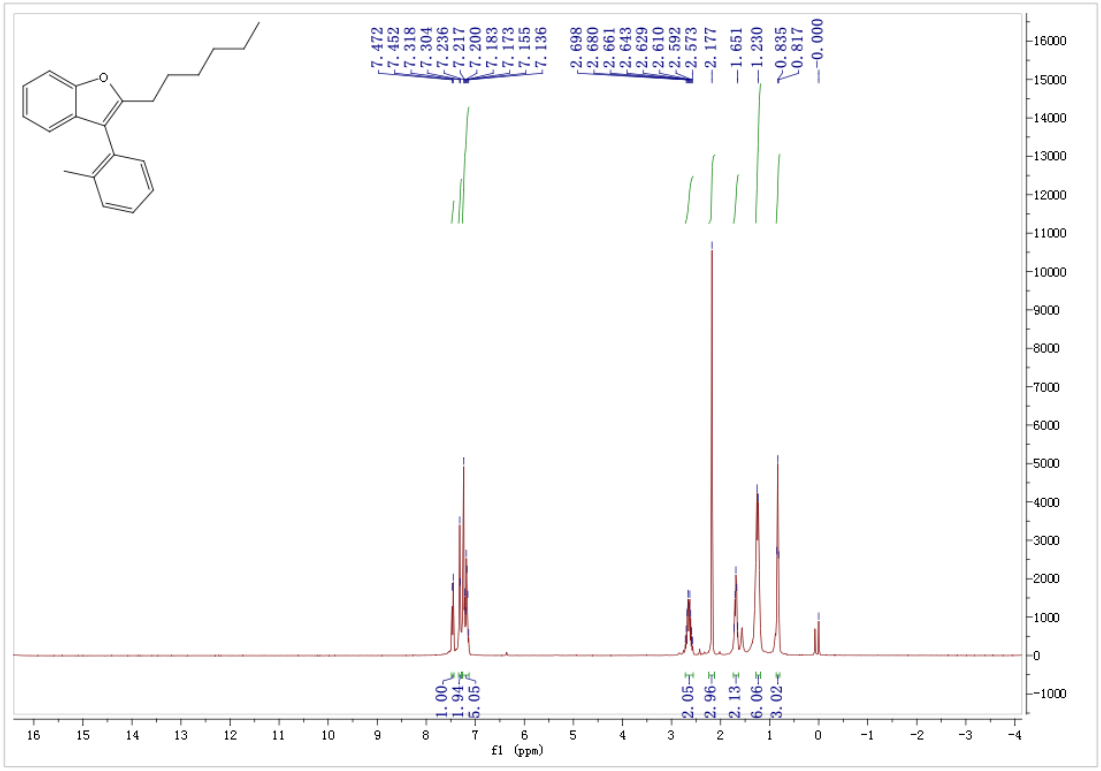


**Fig. S-49**. $^{1}$H-NMR spectrum of **4i**.

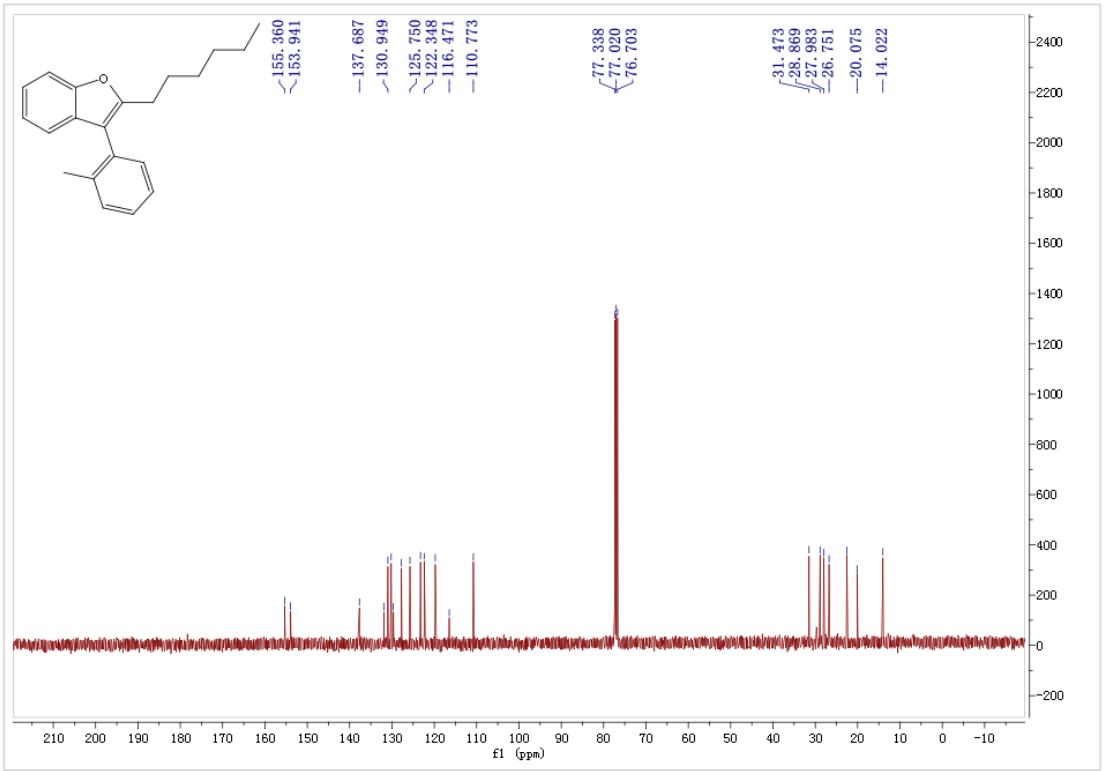


**Fig. S-50**. $^{13}$C-NMR spectrum of **4i**.

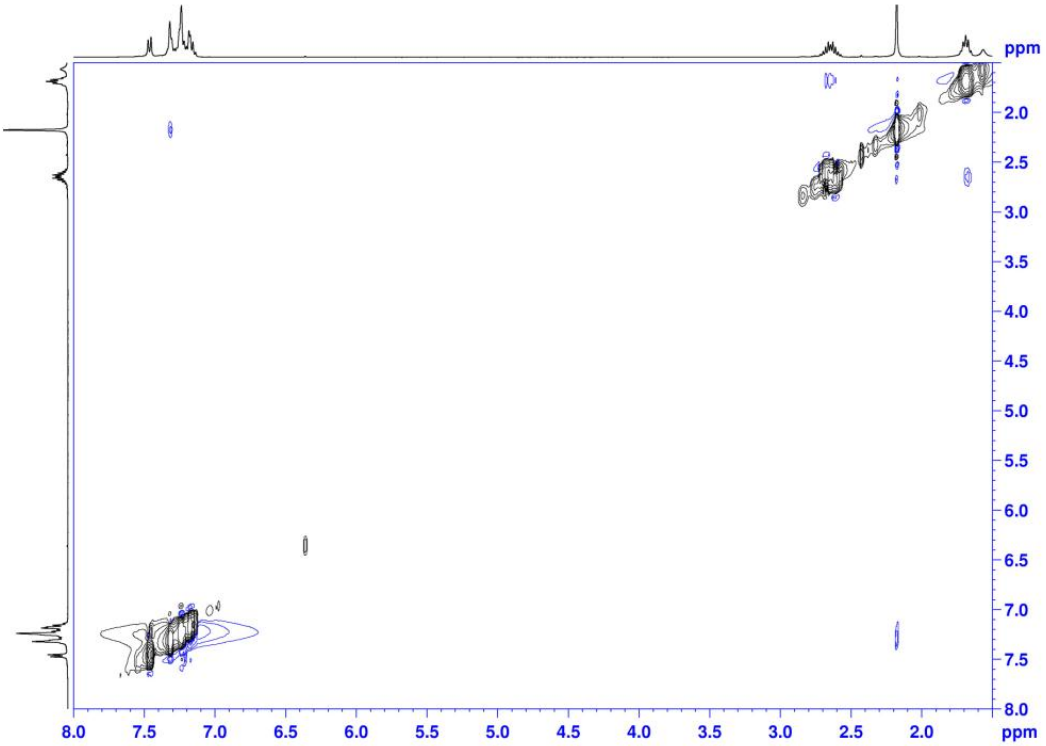


**Fig. S-51**. **NOESY** Spectrum for Compound **4i**