

## Supplementary Material

# Metal-free sequential reaction *via* a propargylation, annulation and isomerization sequence for the one-pot synthesis of 2,3-disubstituted benzofurans

Wen-Tao Li, Wen-Hui Nan and Qun-Li Luo<sup>\*</sup>

Key Laboratory of Applied Chemistry of Chongqing Municipality, College of Chemistry and Chemical Engineering, Southwest University, Chongqing, 400715, China. E-mail:  
[qlluo@swu.edu.cn](mailto:qlluo@swu.edu.cn)

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# Experimental Section

## General.

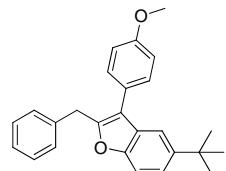
Commercially available reagents were used as received. *t*-BuOK (98%) was purchased from Aladdin® Reagent (Shanghai, China). Solvents for reactions were dried with standard procedures and stored with Schlenk flasks over molecular sieves if not noted otherwise. All solvents for chromatographic separations were distilled before use. Column chromatography was carried out with Haiyang 200–300 mesh silica gel (Qingdao, China). <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on a 300 MHz or 600 MHz spectrometer (Bruker) at 293 K and the chemical shifts ( $\delta$ ) were internally referenced by the residual solvent signals relative to tetramethylsilane (CDCl<sub>3</sub> at 7.26 ppm for <sup>1</sup>H, and at 77.00 ppm for <sup>13</sup>C). Data are reported as (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet; coupling constant(s) in Hz; integration). High resolution mass spectra (HRMS) of **4aa**, **4ee**, **4ga** and **4ia** were obtained on a APEXIII 7.0 TESLA FTMS (Bruker Daltonics) or Micromass GCT Premier (Waters) mass spectrometer at the Department of Analytical Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences (CAS), and those of the rest were on a LCMS TOF 6224 (Agilent) mass spectrometer at National Center for Drug Screening, Shanghai Institute of Materia Medica, CAS. All the known products were confirmed by comparison with spectroscopic analysis of the authentic samples. The yields in Tables 1–4 refer to isolated yields of compounds (average of two runs).

## General procedure for the one-pot sequential synthesis of benzofuran **4** from phenol **1** with propargyl alcohol **2** (Table 4).

In a typical run, a 25 mL reaction flask was charged with the solution of 4-toluenesulphonic acid monohydrate (TsOH·H<sub>2</sub>O, 19 mg, 0.1 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (4 mL). Then propargyl alcohol **2** (0.5 mmol) and phenol **1** (1 mmol) were added in sequential order, and the mixture was stirred at ambient temperature until **2** had disappeared as monitored by TLC (typically, for 2–5 h). For the reactions that need to be heated, the flask was equipped with a condenser and the mixture was stirred at the indicated temperature until **2** had disappeared as monitored by TLC (similarly hereinafter). Then potassium *tert*-butoxide (153 mg, 1.25 mmol) was recharged *in situ*. The reaction mixture was continually stirred at ambient temperature until the new component that generated at the first stage had fully transformed as monitored by TLC (typically, for 5–8 h), then diluted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL) and washed with brine (10 mL). The

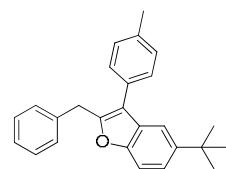
aqueous phase was extracted with  $\text{CH}_2\text{Cl}_2$  (two portions of 10 mL each). The combined organic phase was washed with deionized water and brine, dried over anhydrous  $\text{MgSO}_4$ , and then filtered and concentrated. The crude product was purified by column chromatography (silica, hexane or hexane/EtOAc mixture as eluent). Any deviations from this procedure are noted in Table 4.

**2-benzyl-5-(*tert*-butyl)-3-(4-methoxyphenyl)benzofuran (**4aa**).**



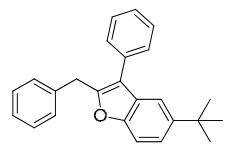
A white amorphous solid (166 mg, 90% yield). <sup>1</sup>H NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.46 (d,  $J$  = 1.2 Hz, 1H), 7.39–7.10 (m, 9H), 6.95 (d,  $J$  = 8.7 Hz, 2H), 4.08 (s, 2H), 3.78 (s, 3H), 1.27 (s, 9H). <sup>13</sup>C NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  158.8, 152.5, 152.4, 145.7, 138.1, 130.2, 128.5, 128.45, 128.42, 126.5, 124.9, 121.7, 118.0, 115.7, 114.3, 110.4, 55.3, 34.7, 32.8, 31.9. HRMS (ESI-FTMS) calcd for  $\text{C}_{26}\text{H}_{26}\text{NaO}_2$  ( $\text{M}^+ + \text{Na}$ ): 393.1825; found: 393.1814.

**2-benzyl-5-(*tert*-butyl)-3-(*p*-tolyl)benzofuran (**4ab**).**



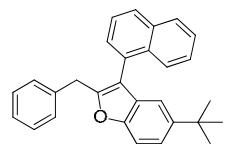
A white amorphous solid (132 mg, 74% yield). <sup>1</sup>H NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.56 (d,  $J$  = 1.2 Hz, 1H), 7.41 (d,  $J$  = 8.0 Hz, 2H), 7.37–7.18 (m, 9H), 4.18 (s, 2H), 2.43 (s, 3H), 1.35 (s, 9H). <sup>13</sup>C NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  152.54, 152.50, 145.8, 138.1, 136.9, 129.65, 129.58, 129.0, 128.54, 128.45, 128.3, 126.5, 121.7, 118.3, 115.8, 110.4, 34.8, 32.8, 31.9, 24.3. HRMS (ESI-TOF) calcd for  $\text{C}_{26}\text{H}_{27}\text{O}$  ( $\text{M}^+ + \text{H}$ ): 355.2056; found: 355.2053.

**2-benzyl-5-(*tert*-butyl)-3-phenylbenzofuran (**4ac**).<sup>1</sup>**



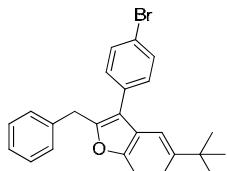
A white amorphous solid (134 mg, 79% yield). <sup>1</sup>H NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.60–7.45 (m, 5H), 7.41–7.16 (m, 8H), 4.18 (s, 2H), 1.35 (s, 9H). <sup>13</sup>C NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  152.7, 152.5, 145.8, 138.0, 132.7, 129.1, 128.9, 128.6, 128.4, 128.2, 127.2, 126.5, 121.8, 118.4, 115.7, 110.4, 34.8, 32.8, 31.9.

**2-benzyl-5-(*tert*-butyl)-3-(naphthalen-1-yl)benzofuran (**4ad**).**



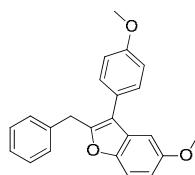
A white amorphous solid (167 mg, 86% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.94 (d,  $J = 8.5$  Hz, 2H), 7.81 (d,  $J = 8.4$  Hz, 1H), 7.60–7.48 (m, 3H), 7.46–7.31 (m, 3H), 7.25–7.12 (m, 6H), 4.07 (d,  $J = 15.7$  Hz, 1H), 3.96 (d,  $J = 15.7$  Hz, 1H), 1.25 (s, 9H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  155.1, 152.5, 145.8, 137.7, 133.7, 132.5, 130.07, 129.5, 128.6, 128.4, 128.34, 128.32, 128.2, 126.4, 126.3, 126.01, 125.98, 125.6, 121.7, 116.7, 116.5, 110.3, 34.7, 33.1, 31.8. HRMS (ESI-TOF) calcd for  $\text{C}_{29}\text{H}_{27}\text{O}$  ( $\text{M}^++\text{H}$ ): 391.2056; found: 391.2048.

**2-benzyl-3-(4-bromophenyl)-5-(*tert*-butyl)benzofuran (4ae).<sup>1</sup>**



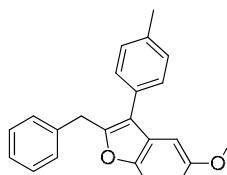
A white amorphous solid (132 mg, 63% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.61 (d,  $J = 8.3$  Hz, 2H), 7.50 (s, 1H), 7.41–7.32 (m, 4H), 7.31–7.17 (m, 5H), 4.15 (s, 2H), 1.35 (s, 9H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  152.9, 152.5, 146.0, 137.7, 132.0, 131.6, 130.7, 128.6, 128.4, 127.8, 126.6, 122.1, 121.2, 117.4, 115.4, 110.5, 34.8, 32.8, 31.8.

**2-benzyl-5-methoxy-3-(4-methoxyphenyl)benzofuran (4ba).**



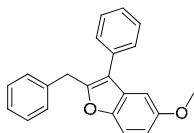
A white amorphous solid (137 mg, 80% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.42 (d,  $J = 8.7$  Hz, 2H), 7.35–7.18 (m, 6H), 7.05–6.98 (m, 3H), 6.86 (dd,  $J = 2.6$  Hz, 8.8 Hz, 1H), 4.15 (s, 2H), 3.85 (s, 3H), 3.80 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  158.9, 156.0, 153.1, 149.2, 138.0, 130.1, 129.4, 128.6, 128.4, 126.5, 124.7, 118.0, 114.3, 112.3, 111.5, 102.4, 56.0, 55.3, 32.9. HRMS (ESI-TOF) calcd for  $\text{C}_{23}\text{H}_{21}\text{O}_3$  ( $\text{M}^++\text{H}$ ): 345.1485; found: 345.1481.

**2-benzyl-5-methoxy-3-(*p*-tolyl)benzofuran (4bb).**



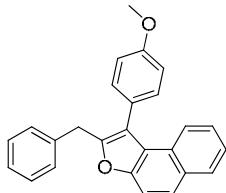
A white amorphous solid (123 mg, 75% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.40 (d,  $J = 8.0$  Hz, 2H), 7.36–7.18 (m, 8H), 7.02 (d,  $J = 2.5$  Hz, 1H), 6.86 (dd,  $J = 2.6$  Hz, 8.8 Hz, 1H), 4.17 (s, 2H), 3.80 (s, 3H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  156.0, 153.2, 149.2, 138.0, 137.0, 129.6, 129.5, 129.3, 128.8, 128.6, 128.5, 126.5, 118.3, 112.4, 111.5, 102.3, 56.0, 32.9, 21.3. HRMS (ESI-TOF) calcd for  $\text{C}_{23}\text{H}_{21}\text{O}_2$  ( $\text{M}^++\text{H}$ ): 329.1536; found: 329.1533.

**2-benzyl-5-methoxy-3-phenylbenzofuran (4bc).<sup>1</sup>**



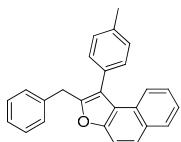
A white amorphous solid (116 mg, 74% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.53–7.45 (m, 4H), 7.43–7.19 (m, 7H), 7.03 (d,  $J$  = 2.4 Hz, 1H), 6.87 (dd,  $J$  = 2.5 Hz, 8.9 Hz, 1H), 4.18 (s, 2H), 3.81 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  155.9, 153.3, 149.1, 137.8, 132.4, 129.0, 128.9, 128.8, 128.5, 128.3, 127.2, 126.4, 118.3, 112.4, 111.4, 102.2, 55.9, 32.8.

#### **2-benzyl-1-(4-methoxyphenyl)naphtho[2,1-b]furan (4ca).**



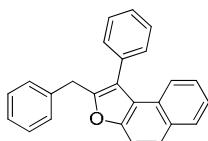
A white amorphous solid (127 mg, 70% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.90 (d,  $J$  = 8.0 Hz, 1H), 7.77 (d,  $J$  = 8.2 Hz, 1H), 7.68 (d,  $J$  = 8.9 Hz, 1H), 7.61 (d,  $J$  = 8.9 Hz, 1H), 7.43 (d,  $J$  = 8.6 Hz, 2H), 7.38 (t,  $J$  = 7.5 Hz, 1H), 7.33–7.18 (m, 6H), 7.06 (d,  $J$  = 8.6 Hz, 2H), 4.07 (s, 2H), 3.92 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  159.2, 152.7, 151.6, 138.2, 131.6, 130.7, 128.8, 128.53, 128.51, 128.1, 126.4, 126.4, 125.8, 125.7, 124.8, 124.0, 123.1, 122.4, 119.5, 114.1, 112.3, 55.3, 32.6. HRMS (ESI-TOF) calcd for  $\text{C}_{26}\text{H}_{21}\text{O}_2$  ( $\text{M}^++\text{H}$ ): 365.1536; found: 365.1519.

#### **2-benzyl-1-(*p*-tolyl)naphtho[2,1-b]furan (4cb).<sup>2</sup>**



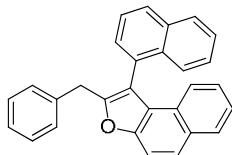
A white amorphous solid (139 mg, 80% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  7.86 (d,  $J$  = 8.1 Hz, 1H), 7.78 (d,  $J$  = 8.3 Hz, 1H), 7.64 (d,  $J$  = 8.9 Hz, 1H), 7.59 (d,  $J$  = 8.9 Hz, 1H), 7.39 (d,  $J$  = 8.0 Hz, 2H), 7.34 (dt,  $J$  = 1.1 Hz, 7.5 Hz, 4H), 7.30 (d,  $J$  = 8.0 Hz, 2H), 7.28–7.23 (m, 3H), 7.22–7.20 (m, 2H), 7.19–7.14 (m, 1H), 4.04 (s, 2H), 2.45 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  152.7, 151.7, 138.3, 137.5, 130.8, 130.4, 129.4, 128.8, 128.53, 128.51, 128.2, 126.4, 125.7, 124.8, 124.0, 123.2, 122.3, 112.3, 32.6, 21.3. HRMS (ESI-TOF) calcd for  $\text{C}_{26}\text{H}_{21}\text{O}$  ( $\text{M}^++\text{H}$ ): 349.1587; found: 349.1587.

#### **2-benzyl-1-phenylnaphtho[2,1-b]furan (4cc).<sup>1</sup>**



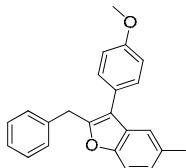
A white amorphous solid (136 mg, 81% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.87 (d,  $J$  = 8.1 Hz, 1H), 7.74 (d,  $J$  = 8.3 Hz, 1H), 7.66 (d,  $J$  = 9.0 Hz, 1H), 7.60 (d,  $J$  = 8.9 Hz, 1H), 7.54–7.42 (m, 5H), 7.35 (t,  $J$  = 7.2 Hz, 1H), 7.29–7.14 (m, 6H), 4.05 (s, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  152.7, 151.6, 138.1, 133.8, 130.7, 130.5, 128.8, 128.7, 128.52, 128.49, 128.0, 127.8, 126.5, 125.7, 124.5, 124.0, 123.1, 122.1, 119.9, 112.3, 32.6.

**2-benzyl-1-(naphthalen-1-yl)naphtho[2,1-*b*]furan (**4cd**).**



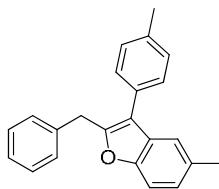
A white amorphous solid (140 mg, 73% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 8.04–7.95 (m, 2H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.75–7.57 (m, 5H), 7.50 (t, *J* = 7.1 Hz, 1H), 7.33–7.10 (m, 8H), 7.05–6.99 (m, 1H), 4.03 (d, *J* = 15.7 Hz, 1H), 3.92 (d, *J* = 15.7 Hz, 1H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz): δ 153.5, 151.8, 137.8, 133.8, 133.1, 131.2, 130.6, 128.67, 128.63, 128.56, 128.43, 128.3, 127.9, 126.5, 126.4, 126.21, 126.17, 125.8, 125.7, 125.0, 124.0, 123.23, 123.16, 117.4, 112.3, 32.9. HRMS (ESI-TOF) calcd for C<sub>29</sub>H<sub>21</sub>O (M<sup>+</sup>+H): 385.1587; found: 385.1581.

**2-benzyl-3-(4-methoxyphenyl)-5-methylbenzofuran (**4da**).**



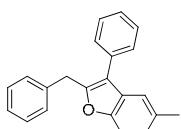
A white amorphous solid (118 mg, 72% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 7.42 (d, *J* = 8.7 Hz, 2H), 7.36–7.18 (m, 7H), 7.07 (dd, *J* = 1.0 Hz, 8.3 Hz, 1H), 7.01 (d, *J* = 8.7 Hz, 2H), 4.17 (s, 2H), 3.86 (s, 3H), 2.42 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz): δ 158.9, 152.7, 152.3, 138.1, 132.1, 130.2, 129.0, 128.6, 128.4, 126.5, 125.0, 124.9, 119.5, 117.6, 114.3, 55.3, 32.9, 21.3. HRMS (ESI-TOF) calcd for C<sub>23</sub>H<sub>21</sub>O<sub>2</sub> (M<sup>+</sup>+H): 329.1536; found: 329.1531.

**2-benzyl-5-methyl-3-(*p*-tolyl)benzofuran (**4db**).**



A white amorphous solid (117 mg, 75% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 7.50–7.43 (m, 3H), 7.41–7.24 (m, 8H), 7.13 (d, *J* = 8.2 Hz, 1H), 4.24 (s, 2H), 2.48 (s, 6H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz): δ 152.7, 152.4, 138.0, 136.9, 132.0, 129.6, 129.5, 128.9, 128.8, 128.5, 128.4, 126.5, 125.0, 119.6, 117.9, 110.6, 32.8, 21.3, 21.2. HRMS (ESI-TOF) calcd for C<sub>23</sub>H<sub>21</sub>O (M<sup>+</sup>+H): 313.1587; found: 313.1587.

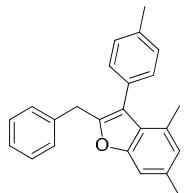
**2-benzyl-5-methyl-3-phenylbenzofuran (**4dc**).<sup>1</sup>**



A white amorphous solid (111 mg, 74% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ 7.49 (d, *J* = 7.1 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.38–7.14 (m, 8H), 7.04 (d, *J* = 8.2 Hz, 1H), 4.15 (s, 2H), 2.38 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>,

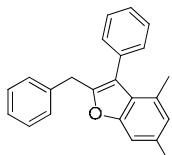
75 MHz):  $\delta$  152.7, 152.6, 137.9, 132.6, 132.1, 129.0, 128.8, 128.64, 128.55, 128.4, 127.2, 126.5, 125.1, 119.5, 118.0, 110.6, 32.8, 21.3.

**2-benzyl-4,6-dimethyl-3-(*p*-tolyl)benzofuran (**4eb**).**



A white amorphous solid (115 mg, 70% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz):  $\delta$  7.35–7.19 (m, 9H), 7.15 (s, 1H), 6.82 (s, 1H), 4.00 (s, 2H), 2.46 (s, 3H), 2.44 (s, 3H), 2.16 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz):  $\delta$  154.6, 152.2, 138.3, 137.0, 133.7, 130.9, 130.6, 128.8, 128.57, 128.47, 128.41, 126.3, 125.5, 125.0, 118.6, 109.0, 32.5, 21.4, 21.3, 19.3. HRMS (ESI-TOF) calcd for C<sub>24</sub>H<sub>23</sub>O (M<sup>+</sup>+H): 327.1743; found: 327.1741.

**2-benzyl-4,6-dimethyl-3-phenylbenzofuran (**4ec**).**



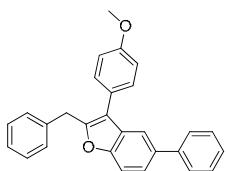
A white amorphous solid (110 mg, 70% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz):  $\delta$  7.42–7.30 (m, 5H), 7.26–7.12 (m, 5H), 7.09 (s, 1H), 6.76 (s, 1H), 3.93 (s, 2H), 2.37 (s, 3H), 2.07 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz):  $\delta$  154.6, 152.2, 138.1, 133.9, 133.7, 130.8, 130.7, 128.45, 128.42, 128.0, 127.3, 126.3, 125.6, 124.9, 118.7, 109.0, 32.5, 21.4, 19.3. HRMS (ESI-TOF) calcd for C<sub>23</sub>H<sub>21</sub>O (M<sup>+</sup>+H): 313.1587; found: 313.1585.

**2-benzyl-3-(4-bromophenyl)-4,6-dimethylbenzofuran (**4ee**).**



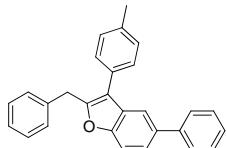
A white amorphous solid (117 mg, 60% yield). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz):  $\delta$  7.60 (d, *J* = 8.1 Hz, 2H), 7.36–7.19 (m, 7H), 7.17 (s, 1H), 6.84 (s, 1H), 3.99 (s, 2H), 2.46 (s, 3H), 2.14 (s, 3H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz):  $\delta$  154.6, 152.4, 137.9, 134.0, 132.9, 132.3, 131.2, 130.6, 128.5, 128.4, 126.5, 125.7, 124.6, 121.6, 117.5, 109.1, 32.5, 21.4, 19.4. HRMS (EI-TOF) calcd for C<sub>23</sub>H<sub>19</sub>BrO (M<sup>+</sup>): 390.0619; found: 390.0622.

**2-benzyl-3-(4-methoxyphenyl)-5-phenylbenzofuran (**4fa**).**



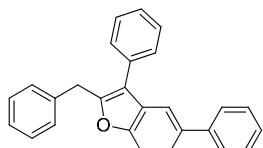
A white amorphous solid (151 mg, 77% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.74 (s, 1H), 7.59 (d,  $J = 7.4$  Hz, 2H), 7.51–7.38 (m, 6H), 7.35–7.20 (m, 6H), 7.03 (d,  $J = 8.6$  Hz, 2H), 4.21 (s, 2H), 3.86 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 75 MHz):  $\delta$  158.9, 153.9, 152.9, 141.8, 137.9, 136.4, 130.2, 129.4, 128.66, 128.62, 128.4, 127.5, 126.8, 126.6, 124.5, 123.5, 118.3, 118.1, 114.4, 111.2, 55.3, 32.9. HRMS (ESI-TOF) calcd for  $\text{C}_{28}\text{H}_{23}\text{O}_2$  ( $\text{M}^++\text{H}$ ): 391.1693; found: 391.1676.

**2-benzyl-5-phenyl-3-(*p*-tolyl)benzofuran (4fb).**



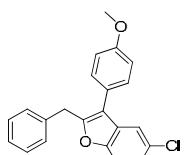
A white amorphous solid (132 mg, 70% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.82 (s, 1H), 7.64 (d,  $J = 7.4$  Hz, 2H), 7.56–7.41 (m, 6H), 7.39–7.22 (m, 8H), 4.26 (s, 2H), 2.47 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  153.9, 153.1, 141.8, 137.9, 137.1, 136.4, 129.6, 129.3, 128.9, 128.65, 128.61, 128.5, 127.44, 127.40, 126.8, 126.6, 123.5, 118.36, 118.32, 111.2, 32.9, 21.3. HRMS (ESI-TOF) calcd for  $\text{C}_{28}\text{H}_{23}\text{O}$  ( $\text{M}^++\text{H}$ ): 375.1743; found: 375.1741.

**2-benzyl-3,5-diphenylbenzofuran (4fc).**<sup>1</sup>



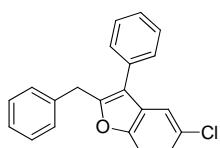
A white amorphous solid (122 mg, 68% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.76 (s, 1H), 7.50–7.08 (m, 17H), 4.22 (s, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  153.9, 153.3, 141.7, 137.8, 136.5, 132.3, 129.14, 129.08, 128.9, 128.67, 128.63, 128.5, 127.5, 127.4, 126.8, 126.6, 123.6, 118.5, 118.3, 111.2, 32.9.

**2-benzyl-5-chloro-3-(4-methoxyphenyl)benzofuran (4ga).**



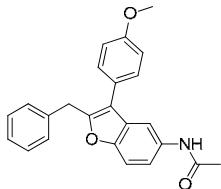
A white amorphous solid (78 mg, 45% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.51 (d,  $J = 1.9$  Hz, 1H), 7.42–7.18 (m, 9H), 7.02 (d,  $J = 8.7$  Hz, 2H), 4.17 (s, 2H), 3.86 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  159.1, 153.7, 152.6, 137.6, 130.3, 130.1, 128.6, 128.4, 128.3, 126.6, 124.0, 123.8, 119.4, 117.6, 114.4, 112.0, 55.3, 32.8. HRMS (EI-TOF) calcd for  $\text{C}_{22}\text{H}_{17}\text{ClO}_2$  ( $\text{M}^+$ ): 348.0917; found: 348.0913.

**2-benzyl-5-chloro-3-phenylbenzofuran (4gc).**<sup>1</sup>



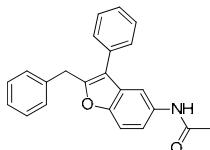
A white amorphous solid (87 mg, 55% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.62 (d,  $J = 1.7$  Hz, 1H), 7.55 (d,  $J = 4.4$  Hz, 4H), 7.49–7.24 (m, 8H), 4.26 (s, 2H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  154.0, 152.6, 137.4, 131.7, 130.3, 128.94, 128.91, 128.6, 128.42, 128.37, 127.6, 126.7, 124.1, 119.4, 118.0, 112.0, 32.8.

***N*-(2-benzyl-3-(4-methoxyphenyl)benzofuran-5-yl)acetamide (4ha).**



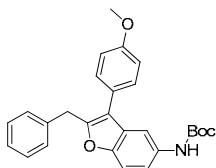
A brownish amorphous solid (90 mg, 49% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  7.73 (d,  $J = 2.0$  Hz, 1H), 7.40 (d,  $J = 8.7$  Hz, 2H), 7.35 (d,  $J = 8.6$  Hz, 2H), 7.32–7.26 (m, 3H), 7.25–7.21 (m, 3H), 6.99 (d,  $J = 8.6$  Hz, 2H), 4.17 (s, 2H), 3.85 (s, 3H), 2.15 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.3, 159.0, 153.2, 151.4, 137.9, 133.0, 130.1, 129.3, 128.6, 128.5, 126.6, 124.4, 118.1, 117.5, 114.4, 112.0, 111.1, 55.3, 32.9, 24.3. HRMS (ESI-TOF) calcd for  $\text{C}_{24}\text{H}_{22}\text{NO}_3$  ( $\text{M}^++\text{H}$ ): 372.1594; found: 372.1592.

***N*-(2-benzyl-3-phenylbenzofuran-5-yl)acetamide (4hc).**



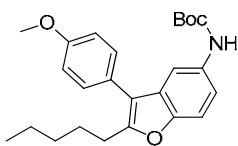
A brownish amorphous solid (86 mg, 50% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz):  $\delta$  7.73 (d,  $J = 1.9$  Hz, 1H), 7.47 (d,  $J = 7.0$  Hz, 2H), 7.44 (t,  $J = 7.6$  Hz, 2H), 7.39–7.33 (m, 3H), 7.31–7.27 (m, 3H), 7.25–7.21 (m, 3H), 4.18 (s, 2H), 2.13 (s, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 150 MHz):  $\delta$  168.3, 153.6, 151.5, 137.8, 133.1, 132.2, 129.1, 129.0, 128.9, 128.6, 128.5, 127.4, 126.6, 118.5, 117.7, 112.0, 111.1, 32.9, 24.3. HRMS (ESI-TOF) calcd for  $\text{C}_{23}\text{H}_{20}\text{NO}_2$  ( $\text{M}^++\text{H}$ ): 342.1489; found: 342.1488.

***tert*-butyl (2-benzyl-3-(4-methoxyphenyl)benzofuran-5-yl)carbamate (4ia).**



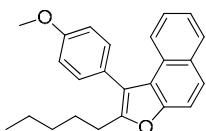
A light yellow amorphous solid (112 mg, 52% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.61 (s, 1H), 7.43 (dt,  $J = 8.8$  Hz, 2.1 Hz, 2H), 7.38–7.17 (m, 7H), 7.02 (dt,  $J = 8.8$  Hz, 2.5 Hz, 2H), 6.52 (s, 1H), 4.18 (s, 2H), 3.88 (s, 3H), 1.53 (s, 9H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  158.9, 153.2, 153.0, 150.8, 137.9, 133.5, 130.1, 129.3, 128.6, 128.4, 126.5, 124.5, 118.0, 116.3, 114.3, 111.0, 110.2, 80.2, 55.3, 32.9, 28.4. HRMS (ESI-FTMS) calcd for  $\text{C}_{27}\text{H}_{27}\text{NNaO}_4$  ( $\text{M}^++\text{Na}$ ): 452.1832; found: 452.1840.

***tert*-butyl (3-(4-methoxyphenyl)-2-pentylbenzofuran-5-yl)carbamate (4if).**



Light yellow oil (114 mg, 56% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.56 (s, 1H), 7.37 (t,  $J$  = 8.4 Hz, 3H), 7.19 (d,  $J$  = 8.2 Hz, 1H), 7.01 (d,  $J$  = 8.6 Hz, 2H), 3.86 (s, 3H), 2.80 (t,  $J$  = 7.6 Hz, 4H), 1.82–1.68 (m, 2H), 1.37–1.27 (m, 4H), 0.89 (t,  $J$  = 6.7 Hz, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  158.8, 155.8, 153.2, 150.4, 133.4, 130.1, 129.5, 124.9, 116.4, 115.9, 114.2, 110.7, 109.9, 80.1, 55.2, 31.4, 28.3, 28.0, 26.7, 22.3, 13.9. HRMS (ESI-TOF) calcd for  $\text{C}_{25}\text{H}_{31}\text{NNaO}_4$  ( $\text{M}^+ + \text{Na}$ ): 432.2145; found: 432.2145.

### 1-(4-methoxyphenyl)-2-pentylnaphtho[2,1-*b*]furan (4cf).



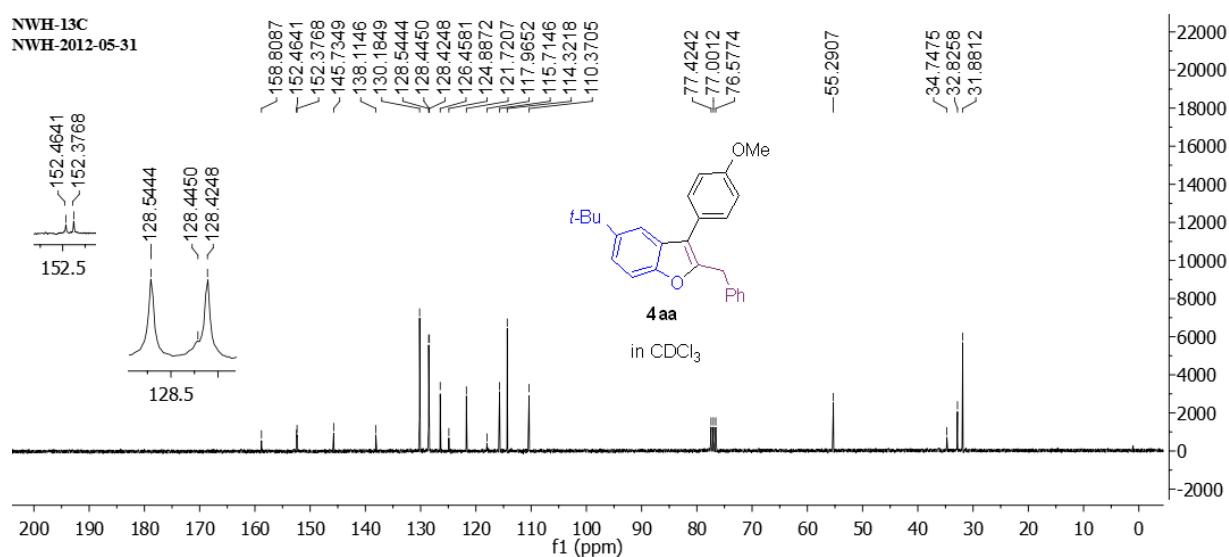
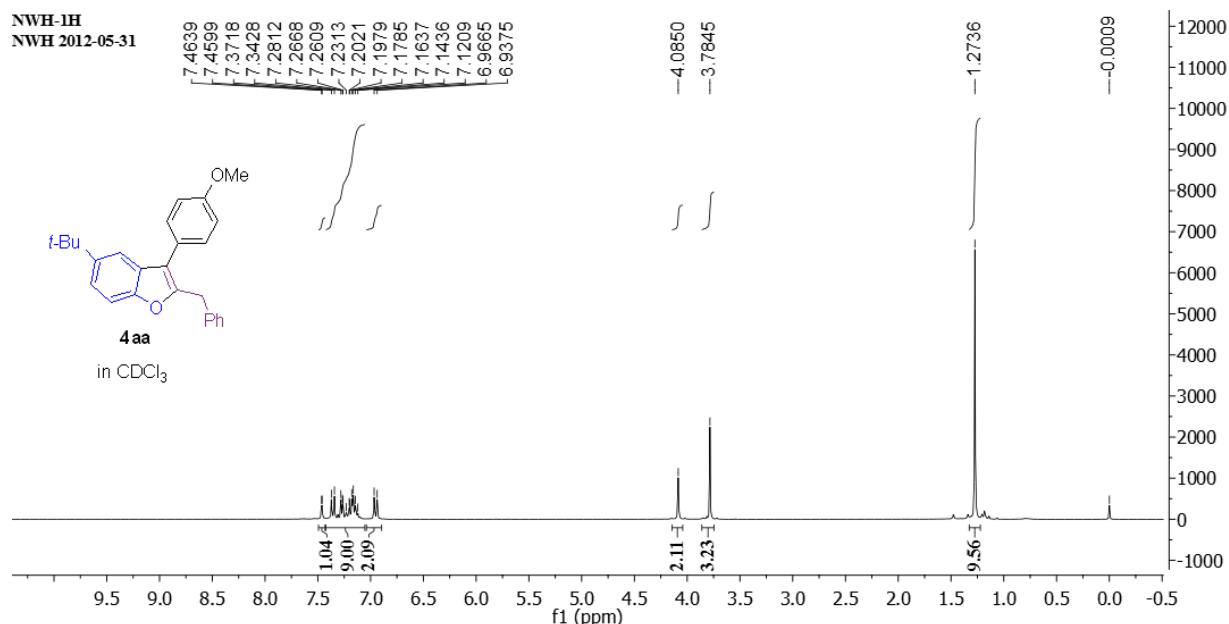
Light yellow oil (87 mg, 51% yield).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz):  $\delta$  7.87 (d,  $J$  = 8.0 Hz, 1H), 7.74 (d,  $J$  = 8.2 Hz, 1H), 7.65 (d,  $J$  = 9.0 Hz, 1H), 7.61 (d,  $J$  = 8.9 Hz, 1H), 7.40–7.10 (m, 4 H), 7.02 (d,  $J$  = 8.5 Hz, 2H), 3.88 (s, 3H), 2.69 (t,  $J$  = 7.5 Hz, 4H), 1.77–1.65 (m, 2H), 1.35–1.20 (m, 4H), 0.84 (t,  $J$  = 6.5 Hz, 3H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz):  $\delta$  159.0, 155.3, 151.1, 131.6, 130.7, 128.7, 128.0, 126.2, 125.5, 124.3, 123.9, 123.1, 122.6, 118.3, 114.0, 112.1, 55.2, 31.3, 28.3, 26.3, 22.3, 14.0. HRMS (ESI-TOF) calcd for  $\text{C}_{24}\text{H}_{25}\text{O}_2$  ( $\text{M}^+ + \text{H}$ ): 345.1849; found: 345.1844.

## Reference

1. F.-Q. Yuan and F.-S. Han, *Adv. Synth. Catal.*, 2013, **355**, 537–547.
2. J. Hu, L. Liu, X. Wang, Y. Hu, S. Yang, Y. Liang, *Green Sustain. Chem.*, 2011, **1**, 165–169.

## NMR and MS spectra

### 2-benzyl-5-(*tert*-butyl)-3-(4-methoxyphenyl)benzofuran (4aa).



Shanghai Mass Spectrometry Center  
Shanghai Institute of Organic Chemistry  
Chinese Academy of Sciences  
High Resolution MS Data Report



Instrument



Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

Card Serial Number E140742

Analysis Name D:\Data\zfj\2014\20140513\_000012.d

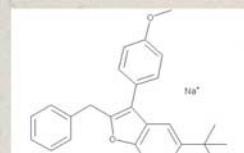
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Acquisition Date 5/11/2014 1:53:10 PM

Operator: zfj

Ionization Mode ESI-Positive

Ion Mass (Measured) 393.1814

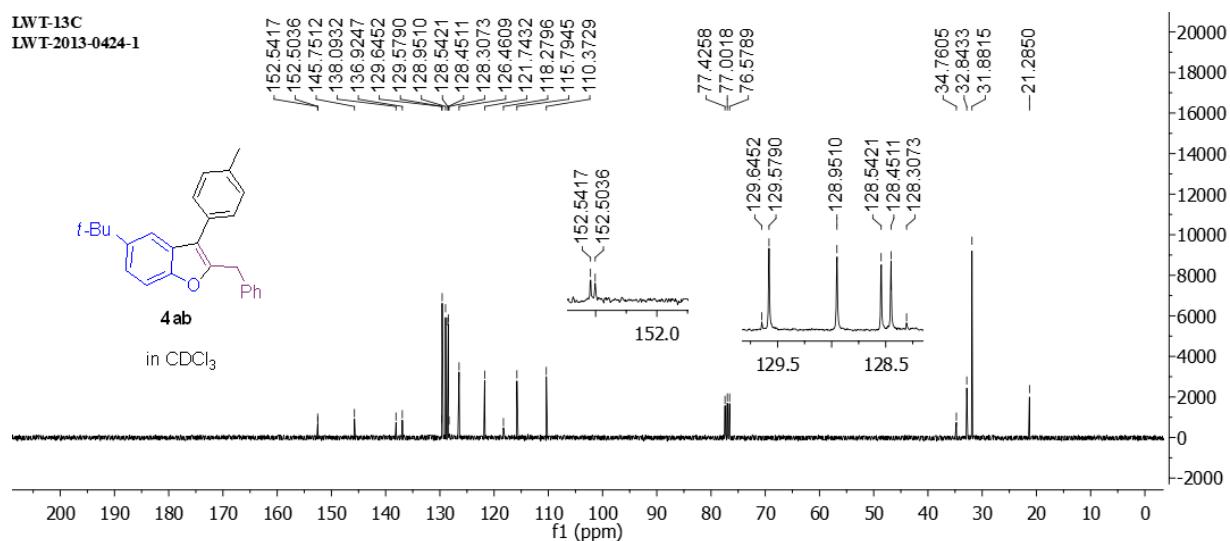
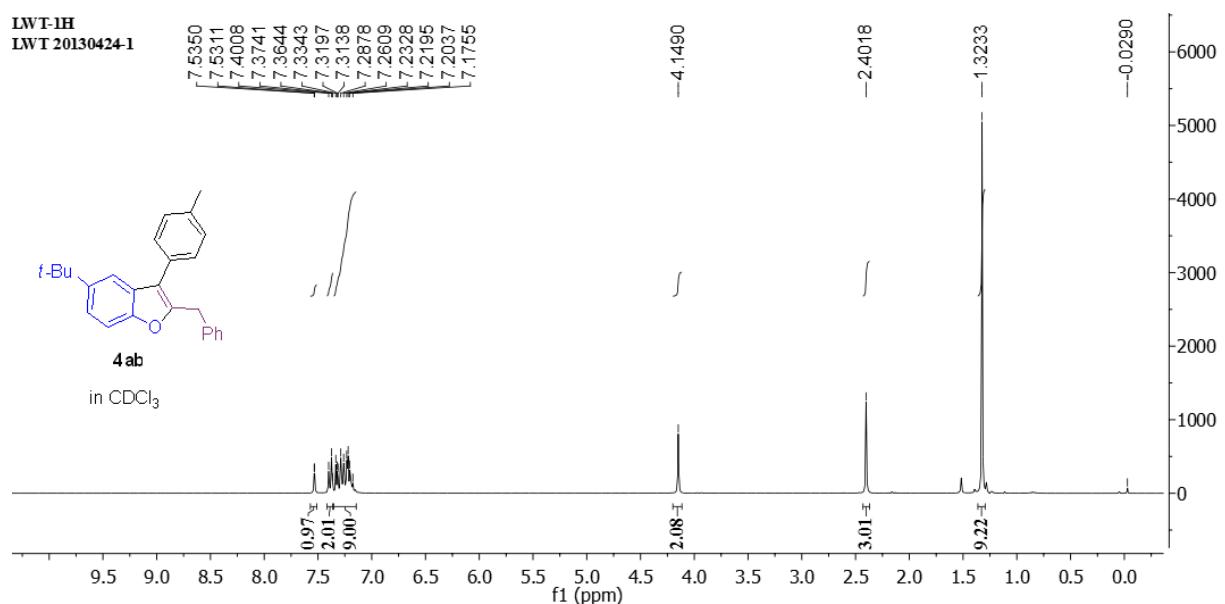


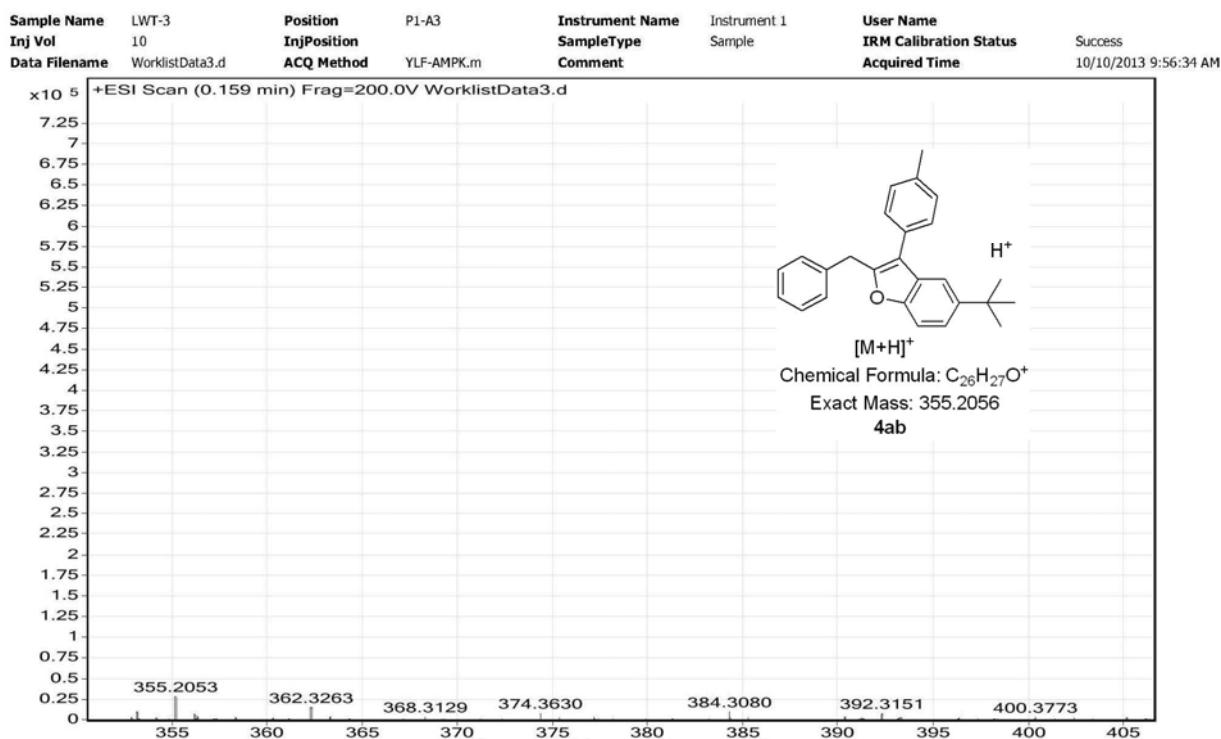
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4aa

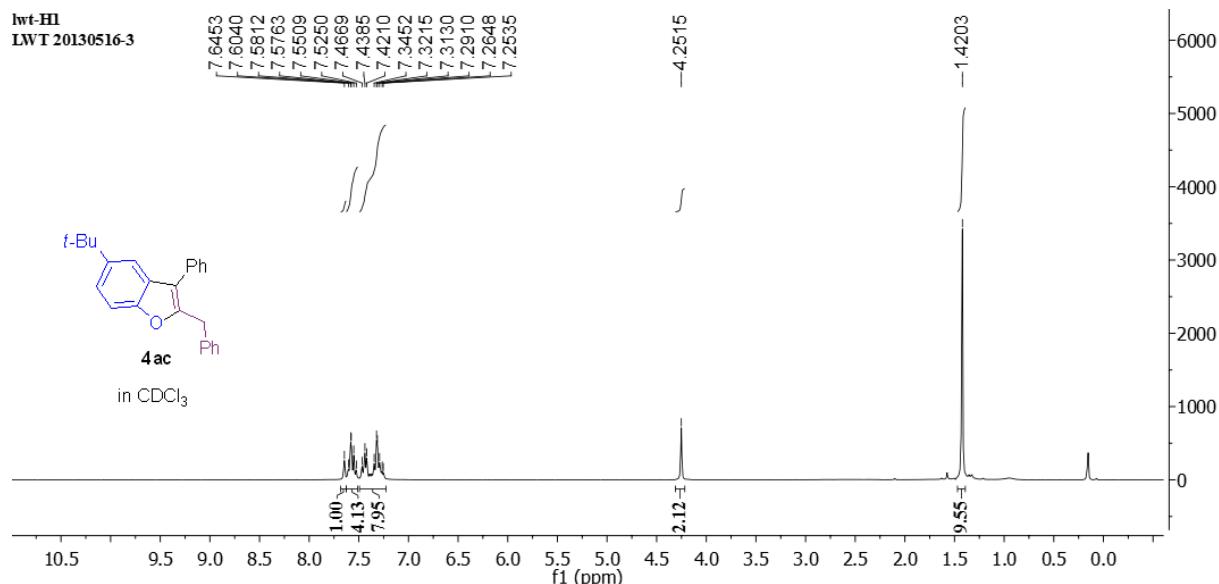
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C 24 H 24 N 3 Na 1 O 1	0.160	393.1812	-0.59	-0.59	-0.23	14.00	ok	odd
C 26 H 26 Na 1 O 2	0.166	393.1825	2.83	2.83	1.11	13.50	ok	even

**2-benzyl-5-(*tert*-butyl)-3-(*p*-tolyl)benzofuran (4ab).**

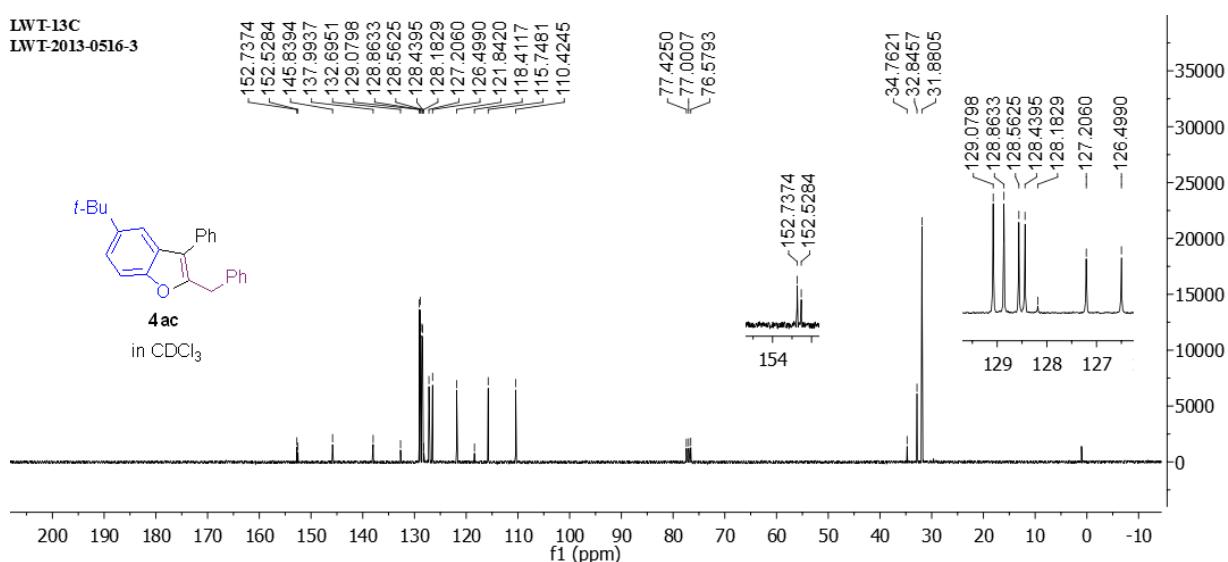




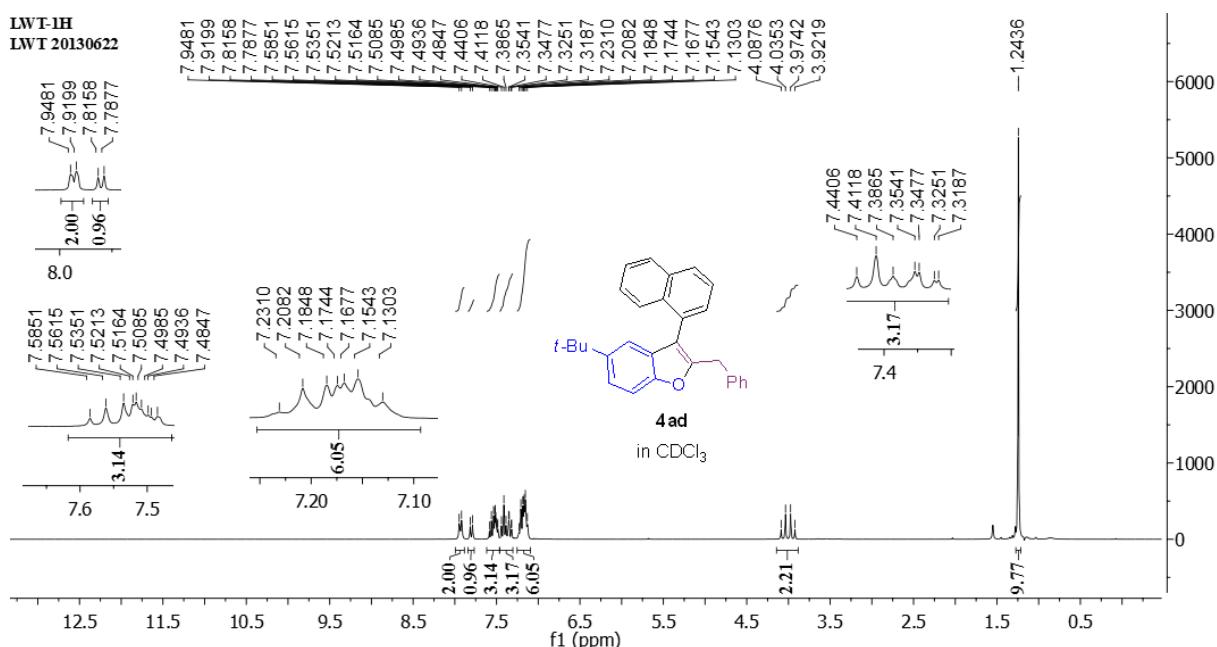
## 2-benzyl-5-(*tert*-butyl)-3-phenylbenzofuran (4ac)



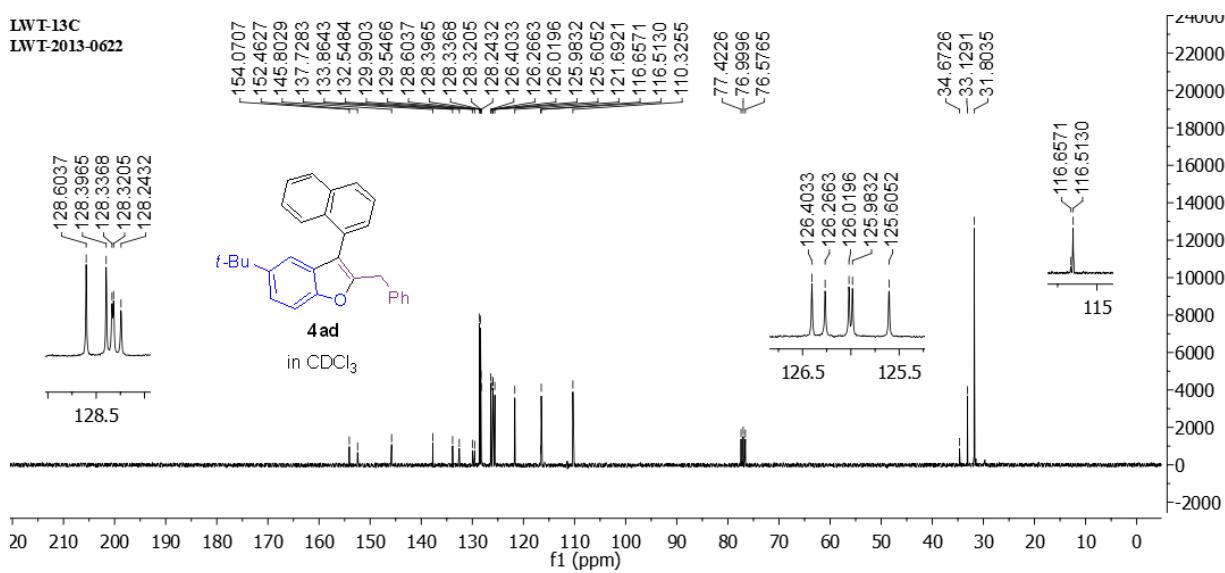
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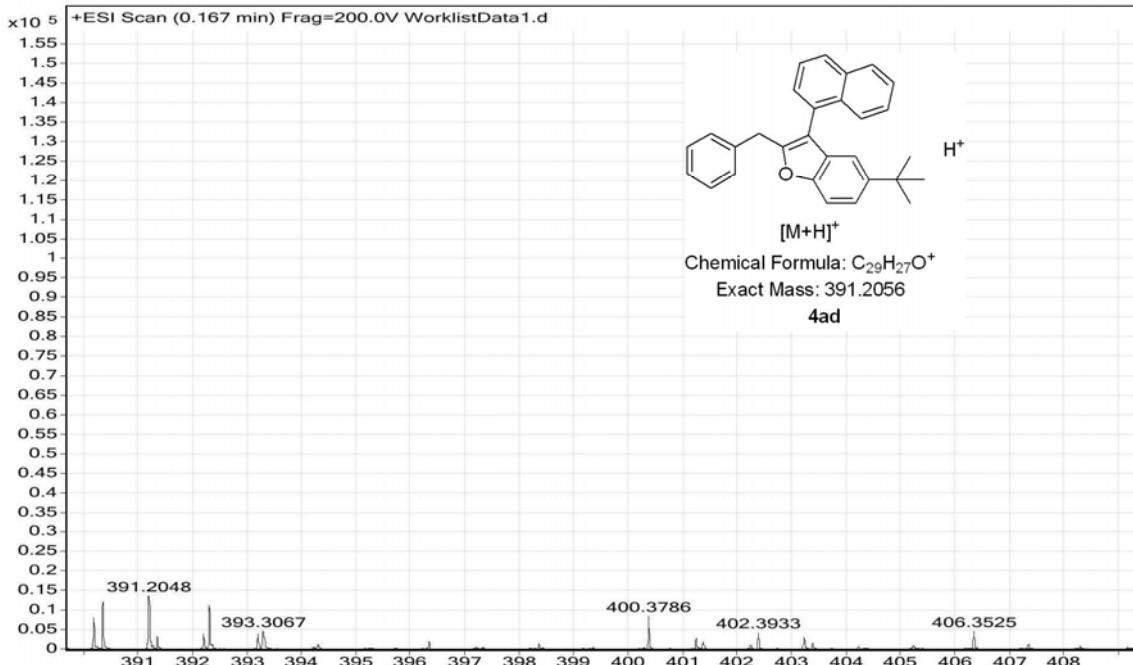
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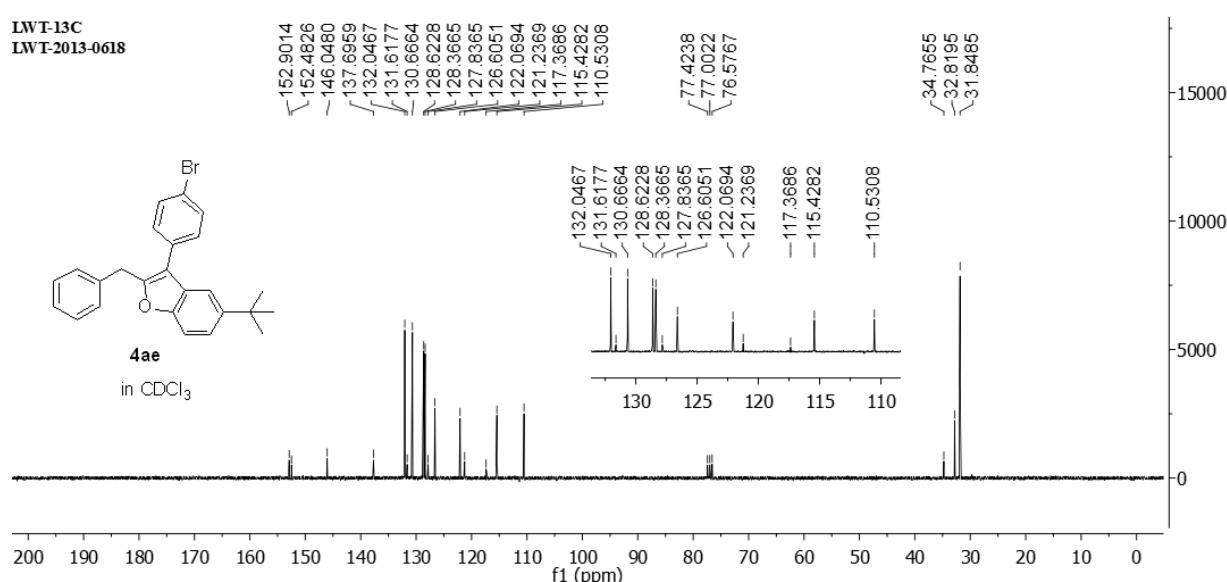
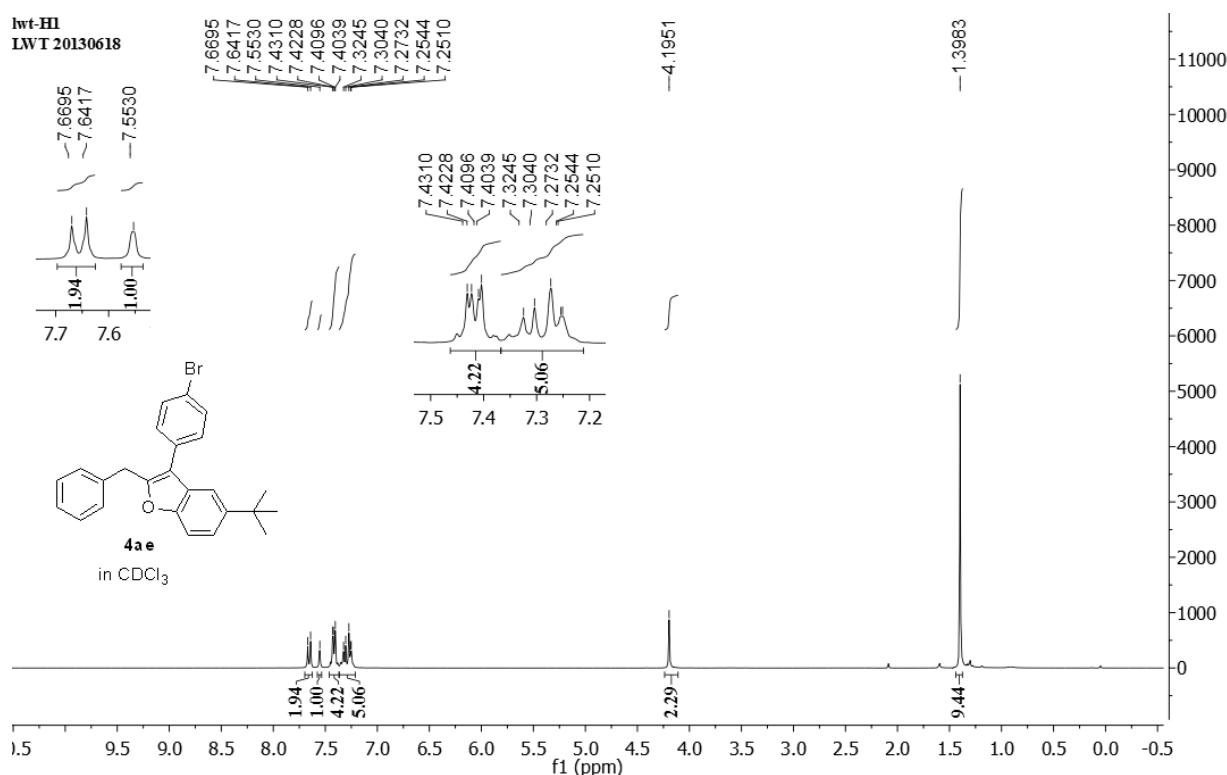
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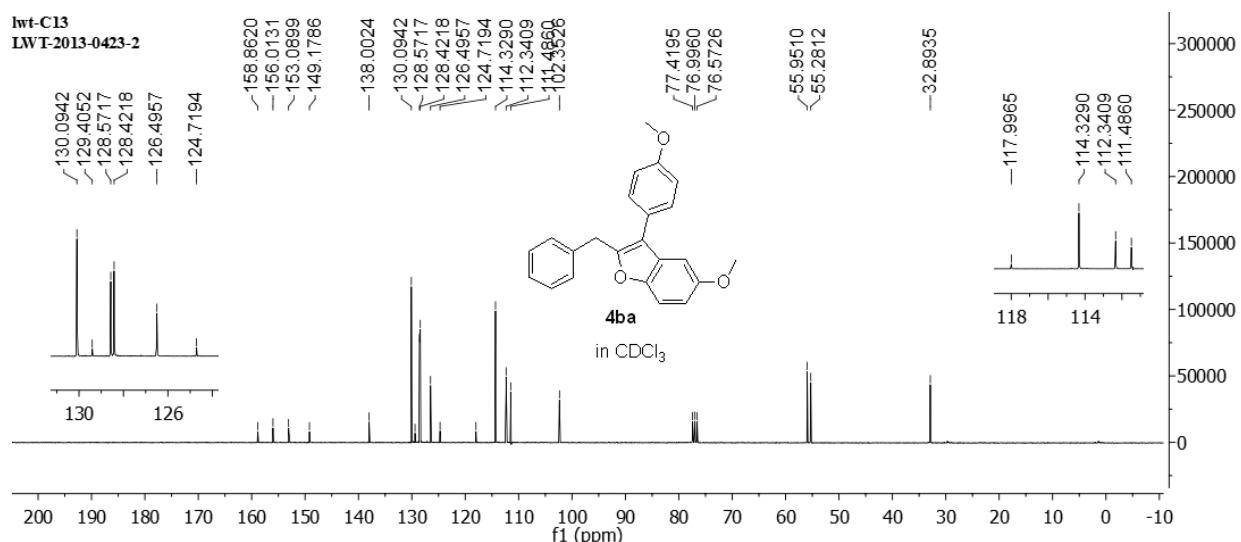
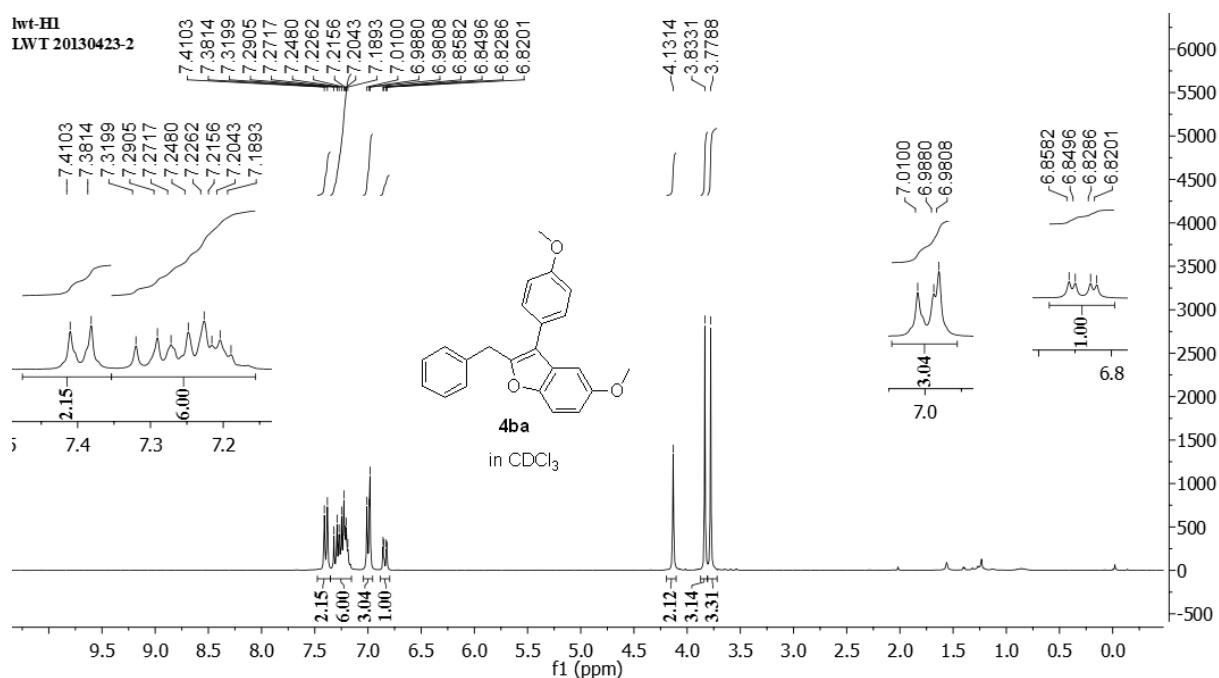
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Data Filename	WorklistData1.d	ACQ Method	YLF-AMPK.m	Comment		Acquired Time	10/10/2013 9:51:41 AM

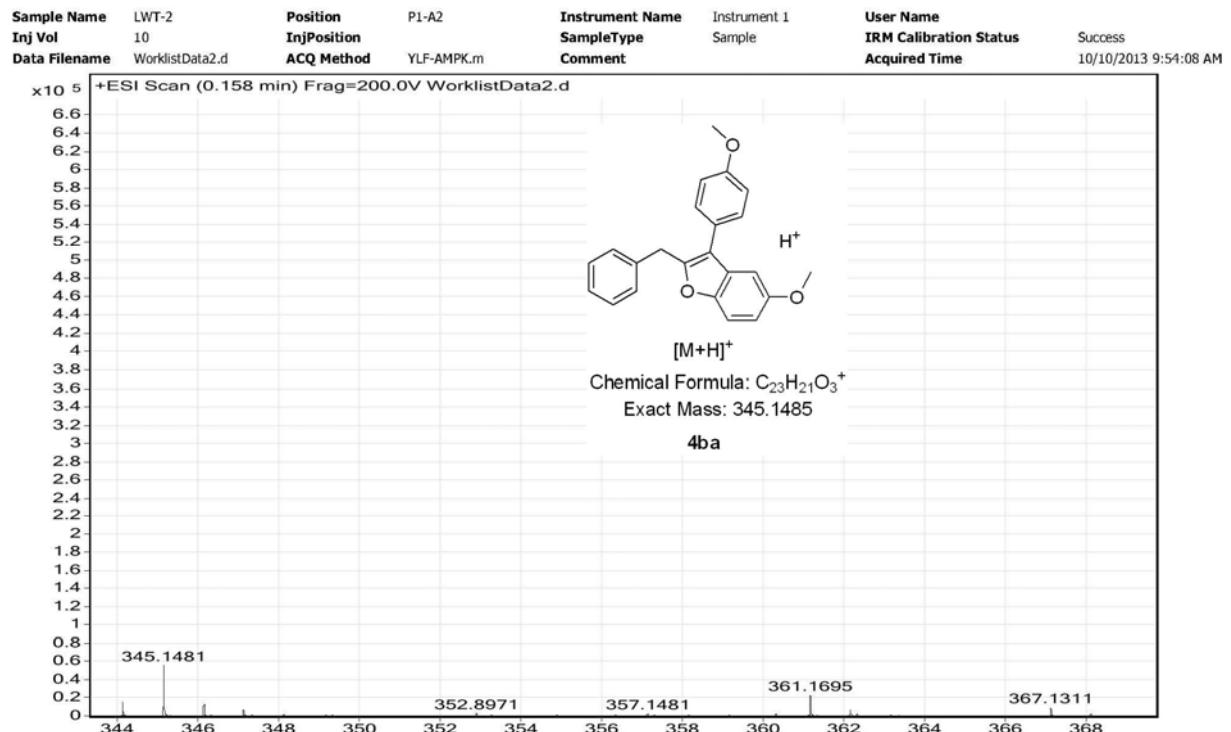


### 2-benzyl-3-(4-bromophenyl)-5-(*tert*-butyl)benzofuran (4ae)

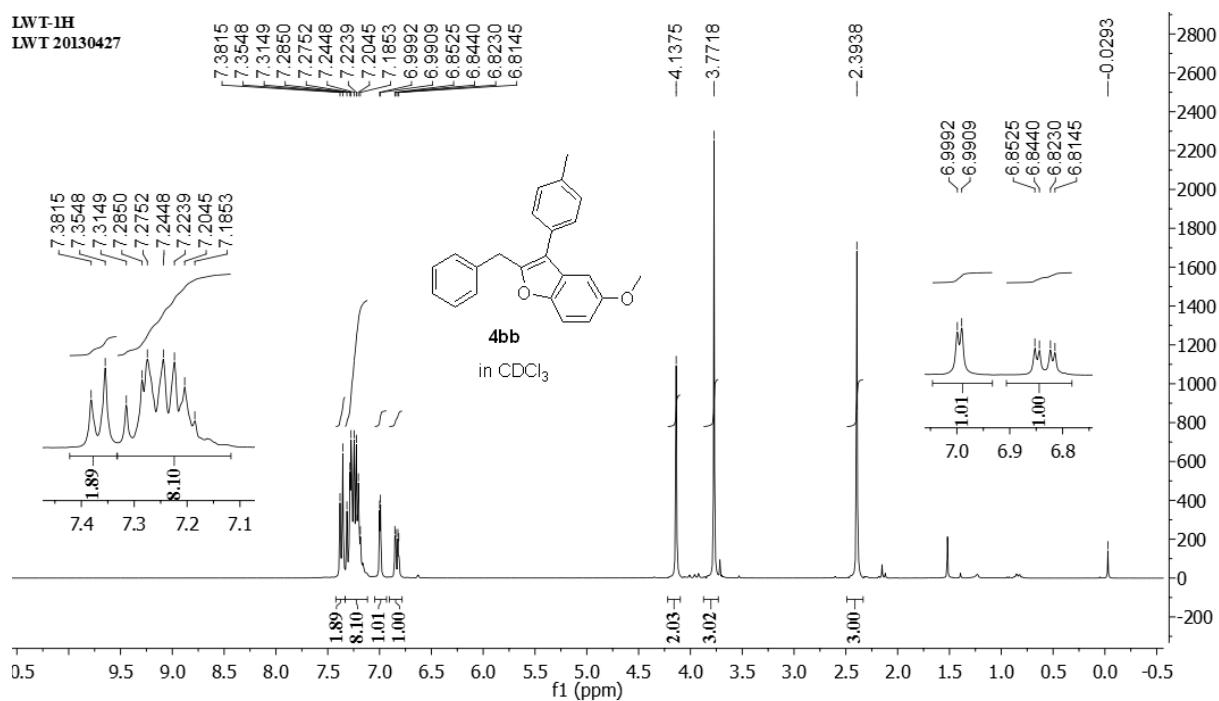


## 2-benzyl-5-methoxy-3-(4-methoxyphenyl)benzofuran (4ba)

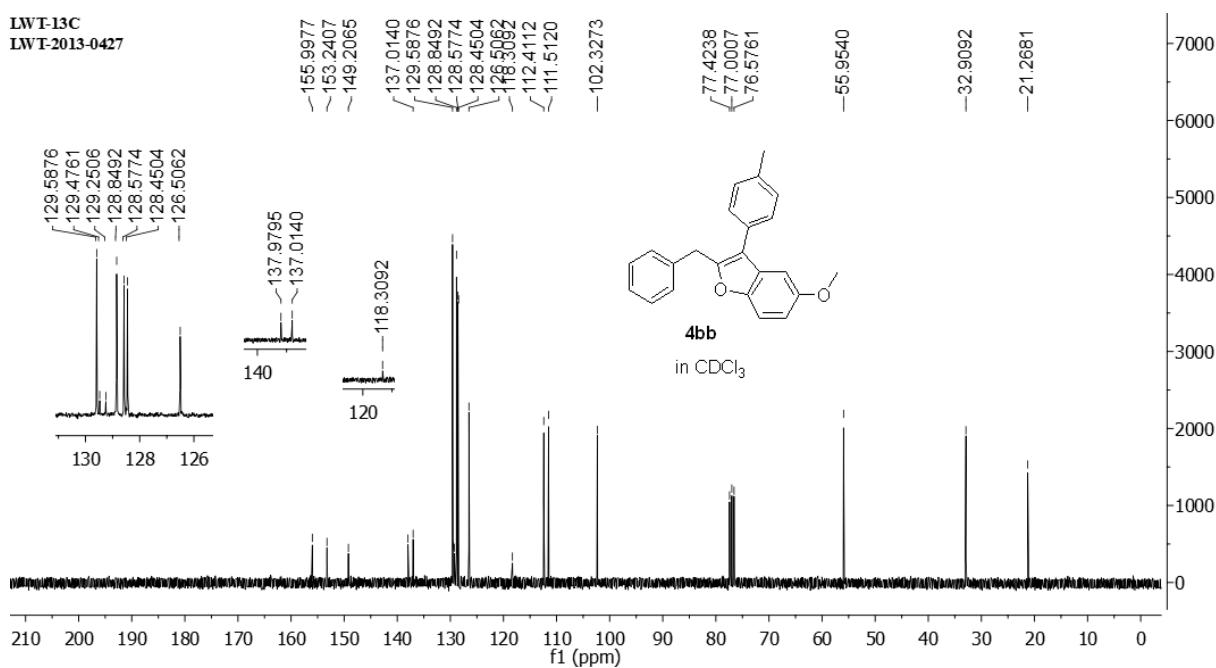




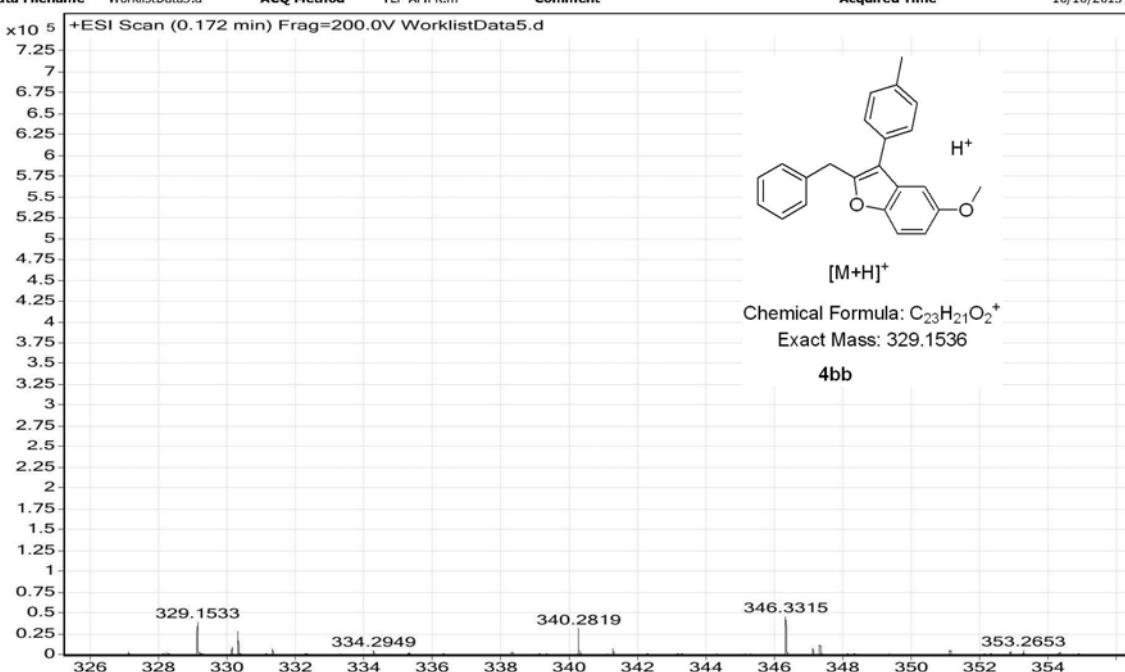
## 2-benzyl-5-methoxy-3-(*p*-tolyl)benzofuran (4bb)



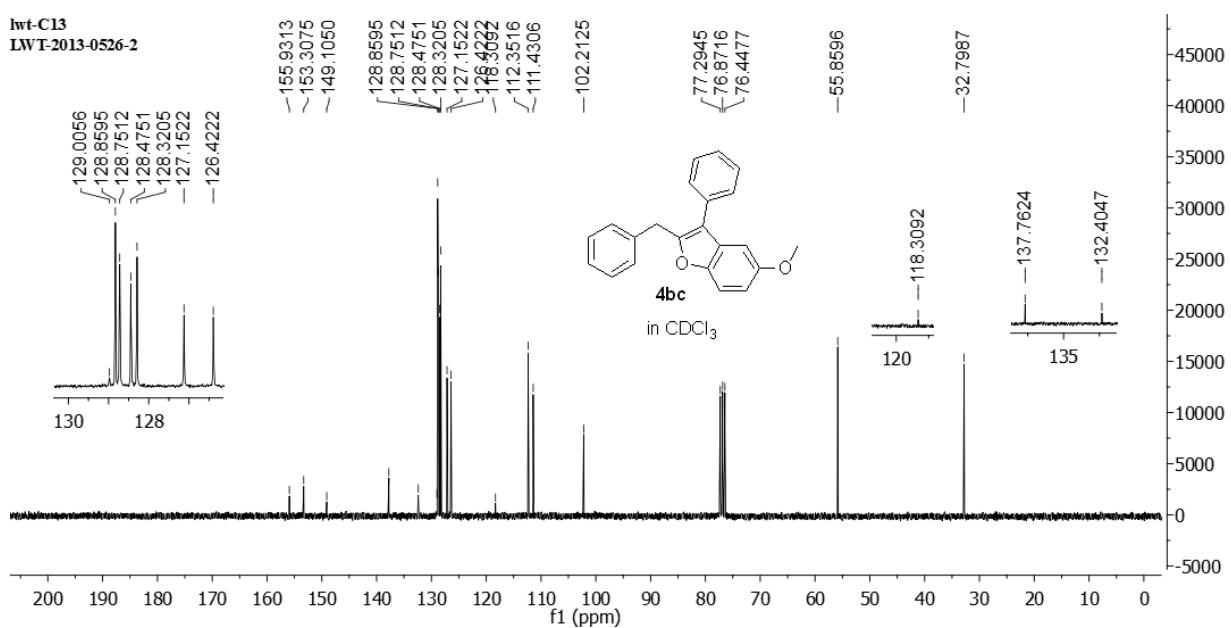
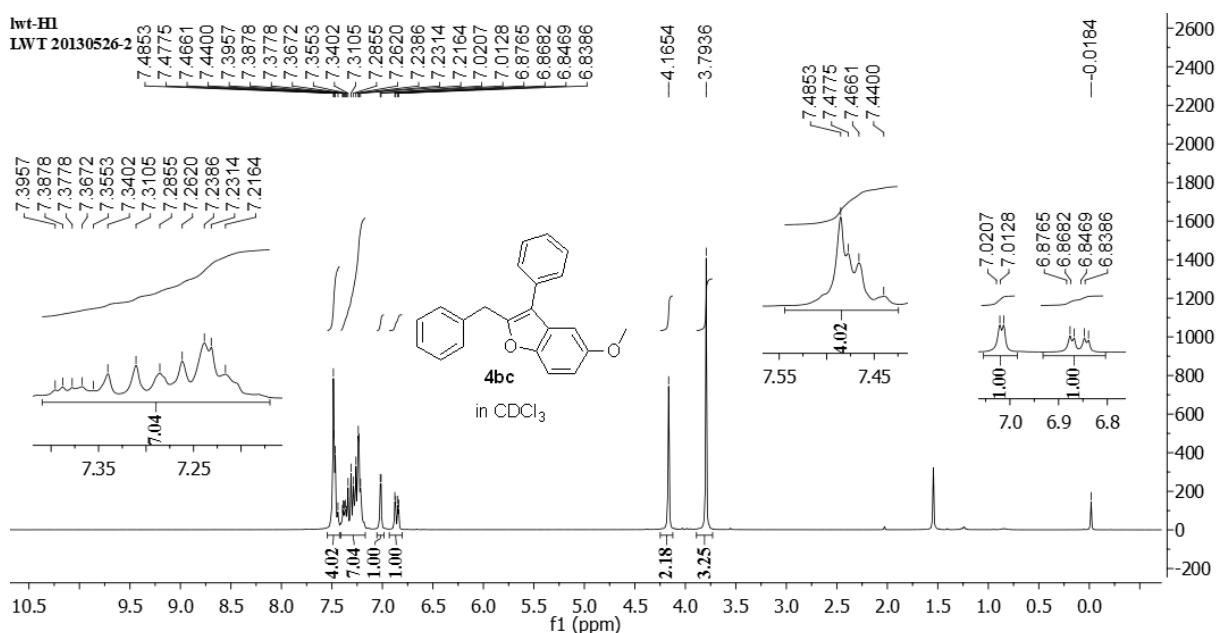
LWT-13C  
LWT-2013-0427



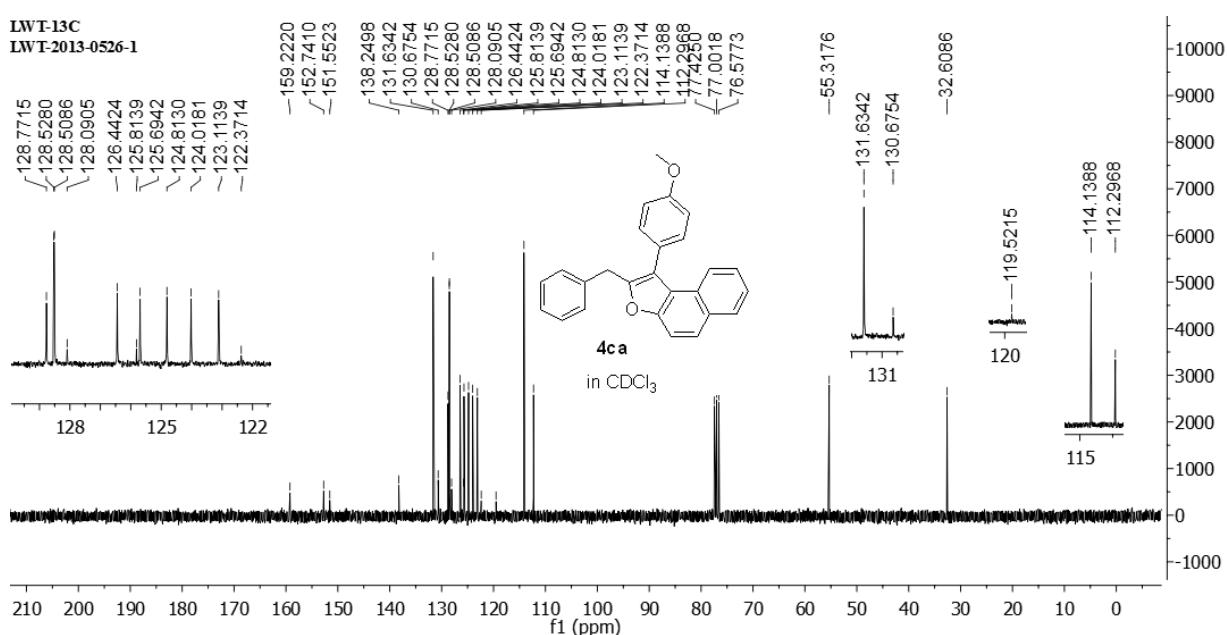
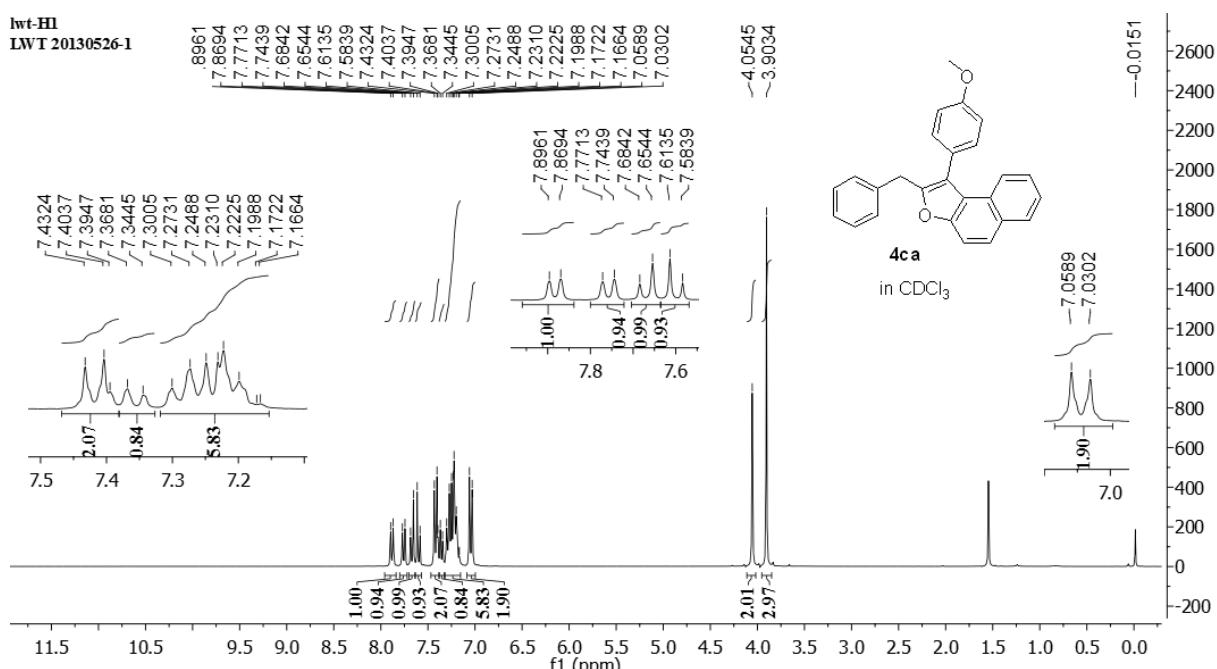
Sample Name	LWT-5	Position	P1-A5	Instrument Name	Instrument 1	User Name	
Inj Vol	10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	WorklistData5.d	ACQ Method	YLF-AMPK.m	Comment		Acquired Time	10/10/2013 10:01:26 AM



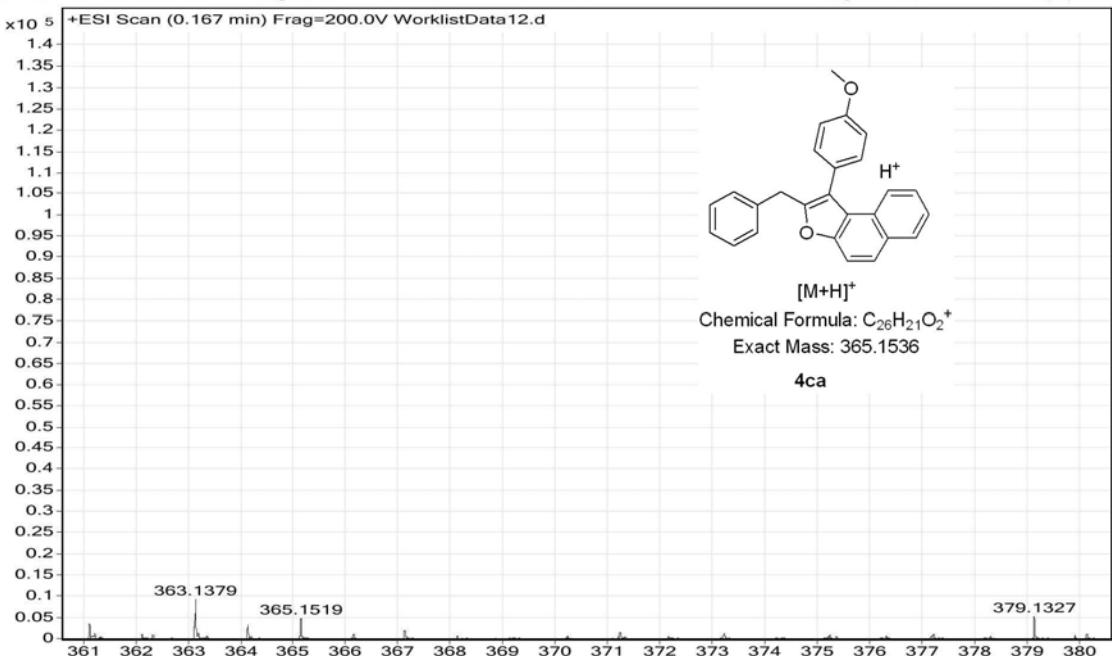
### **2-benzyl-5-methoxy-3-phenylbenzofuran (4bc)**



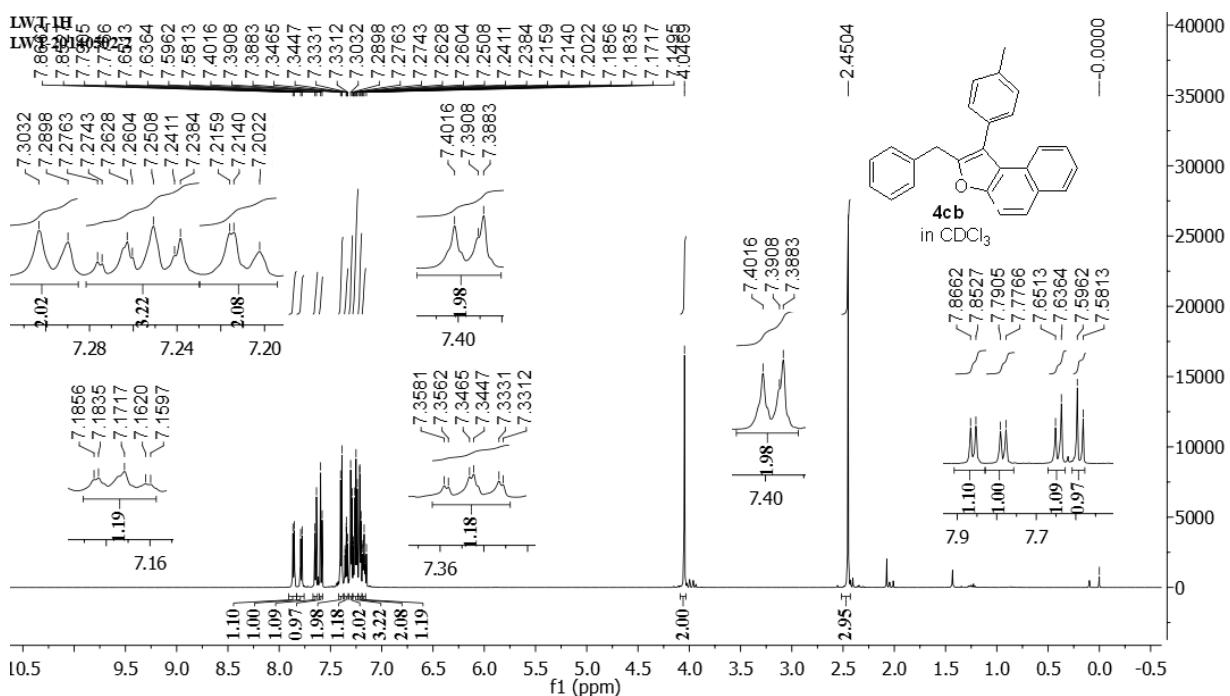
### 2-benzyl-1-(4-methoxyphenyl)naphtho[2,1-*b*]furan (4ca)

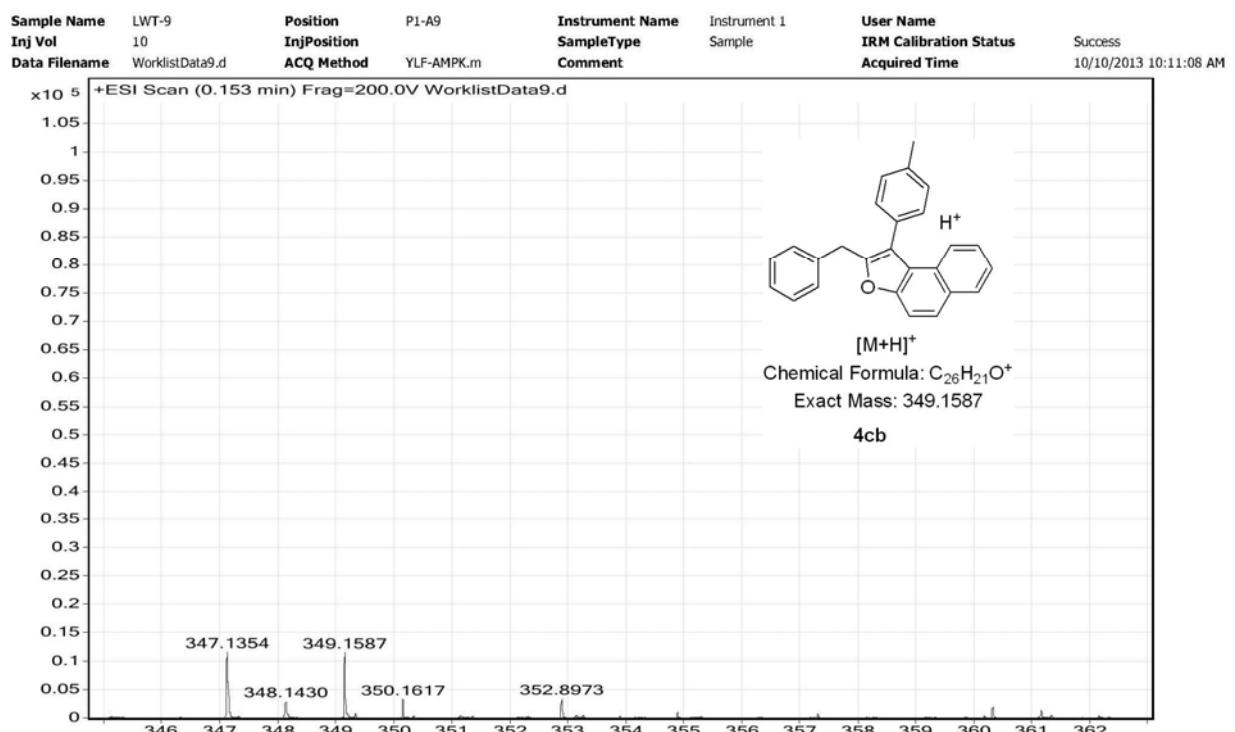
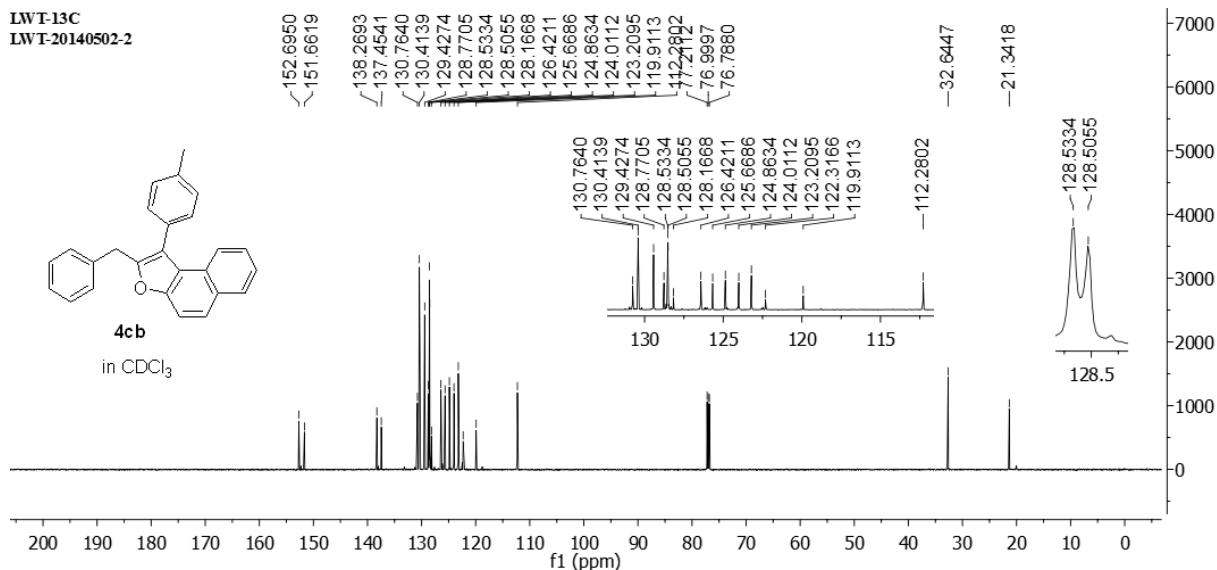


<b>Sample Name</b>	LWT-12	<b>Position</b>	P1-B3	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	WorklistData12.d	<b>ACQ Method</b>	YLF-AMPK.m	<b>Comment</b>		<b>Acquired Time</b>	10/10/2013 10:18:25 AM

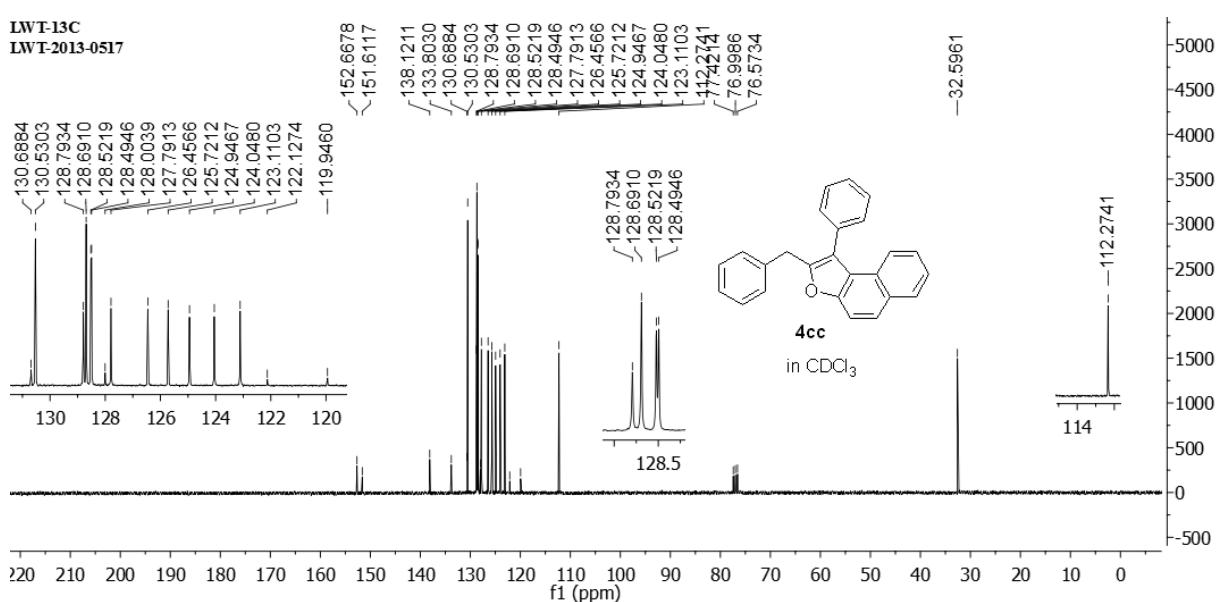
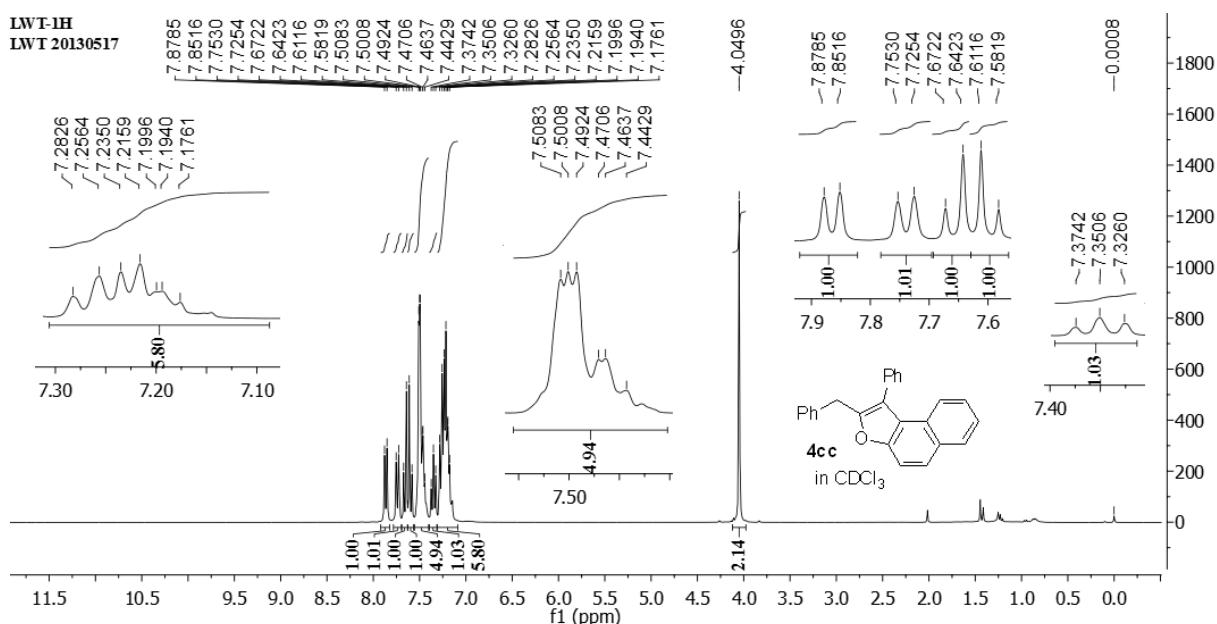


### 2-benzyl-1-(p-tolyl)naphtho[2,1-*b*]furan (4cb)

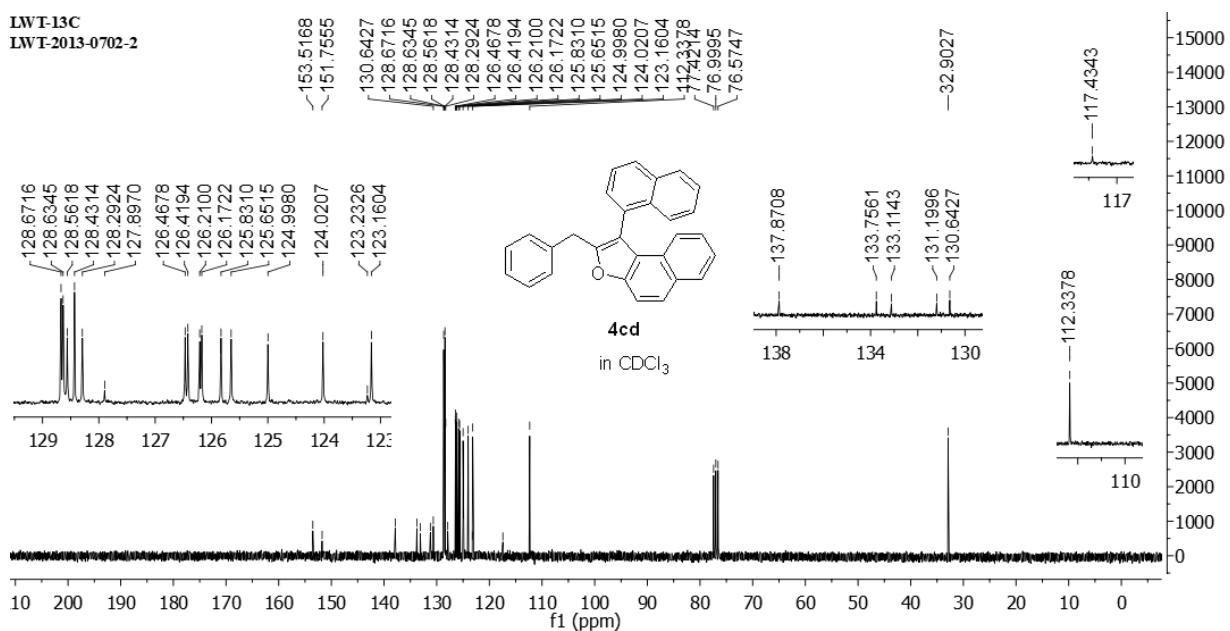
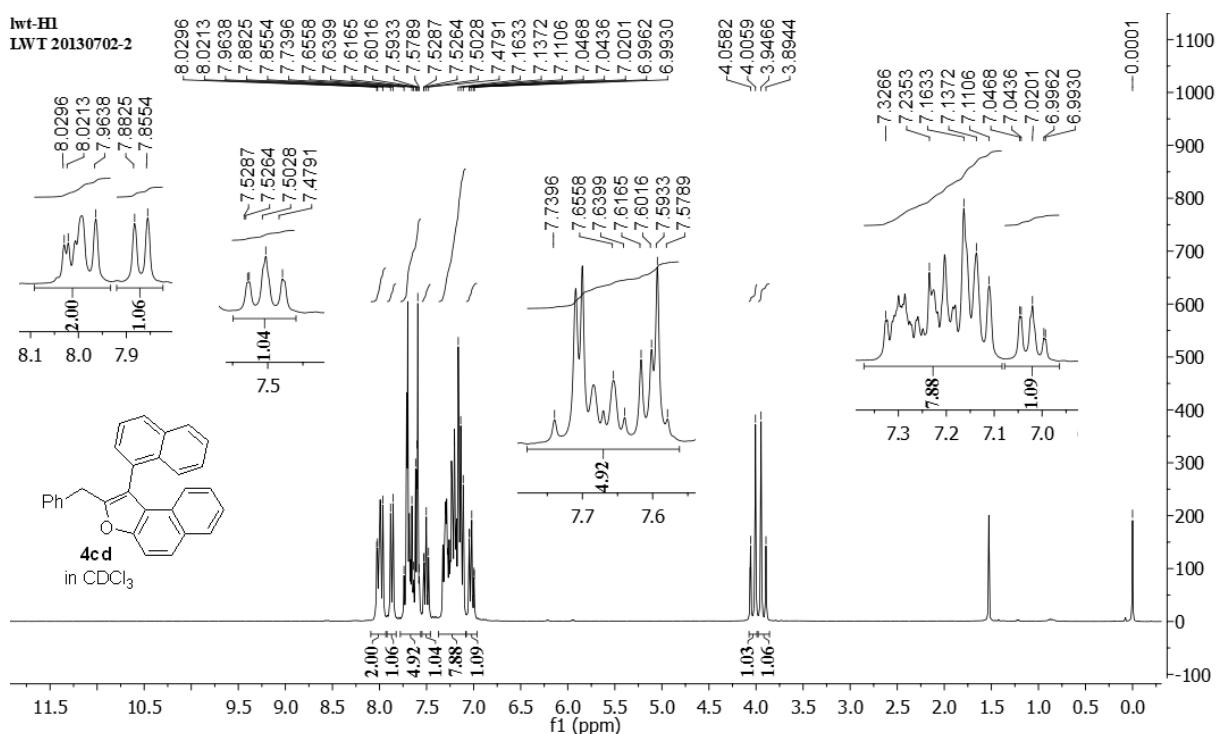




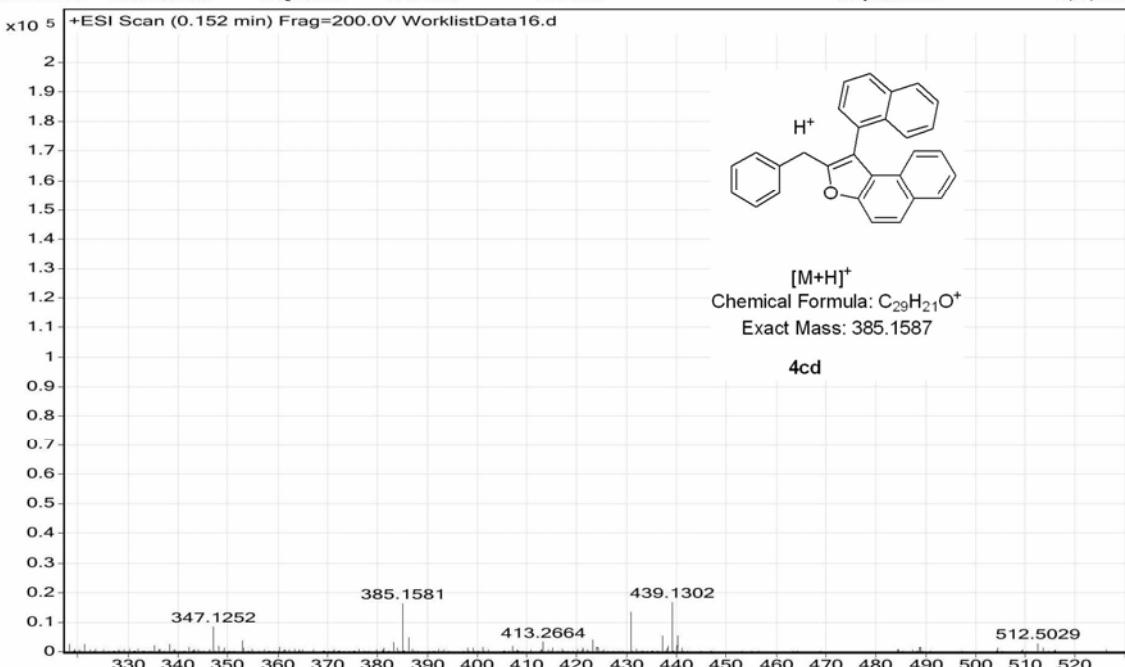
### **2-benzyl-1-phenylnaphtho[2,1-*b*]furan (4cc)**



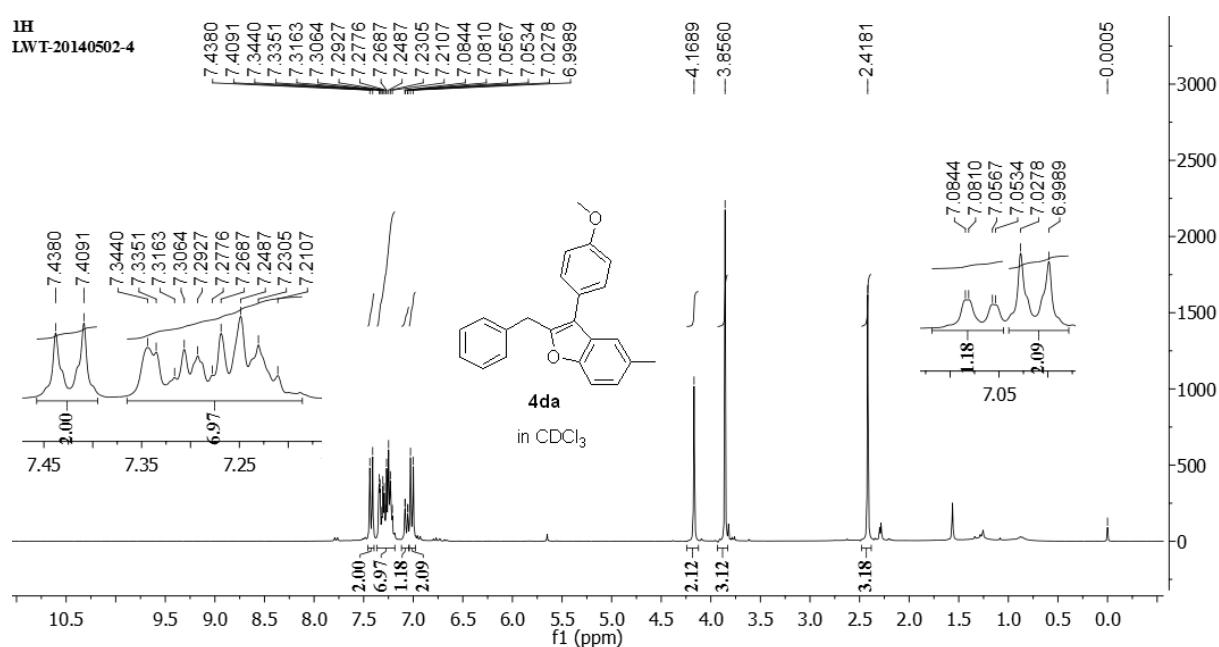
## 2-benzyl-1-(naphthalen-1-yl)naphtho[2,1-*b*]furan (4cd)

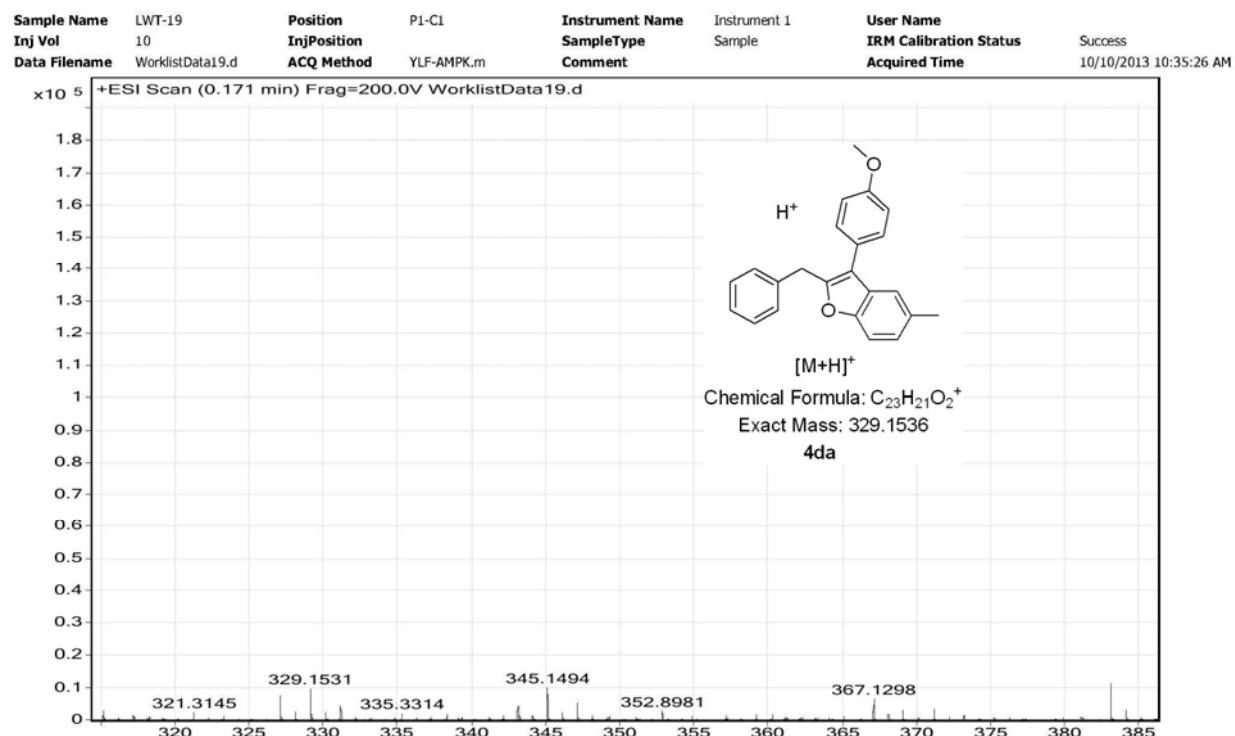
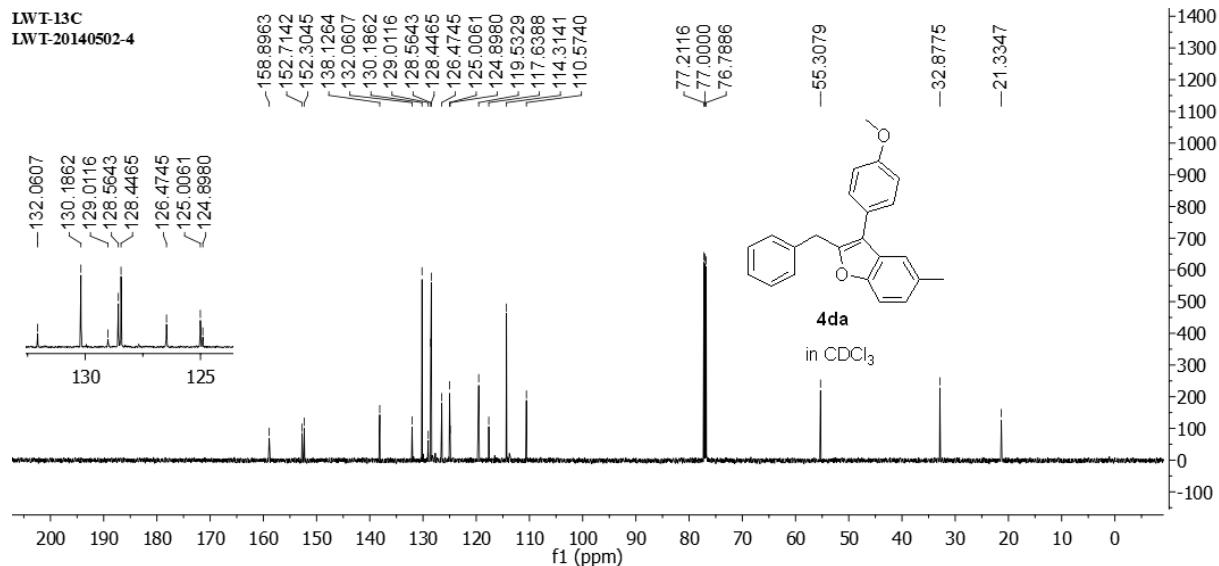


<b>Sample Name</b>	LWT-16	<b>Position</b>	P1-B7	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	WorklistData16.d	<b>ACQ Method</b>	YLF-AMPK.m	<b>Comment</b>		<b>Acquired Time</b>	10/10/2013 10:28:08 AM

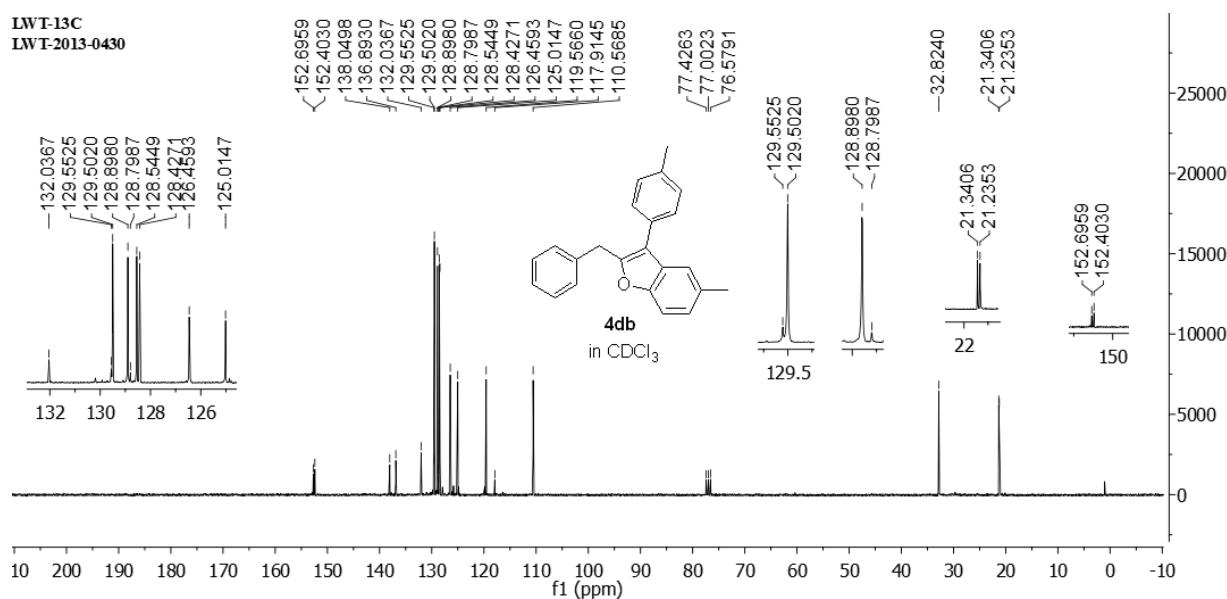
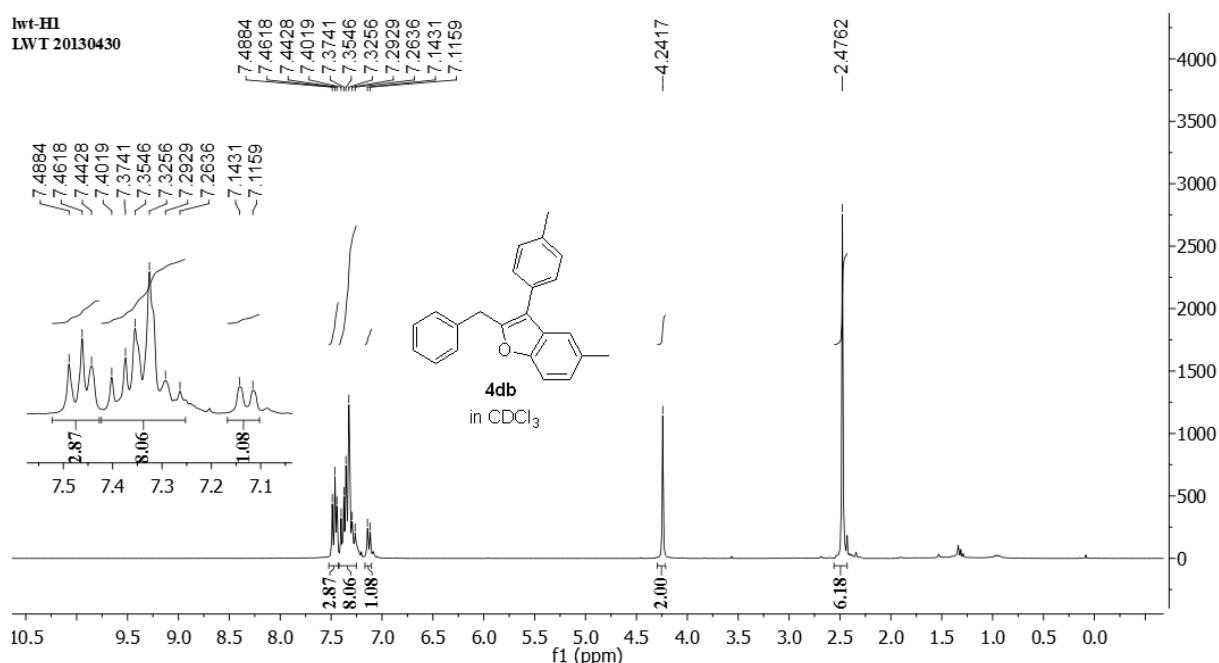


### 2-benzyl-3-(4-methoxyphenyl)-5-methylbenzofuran (4da)

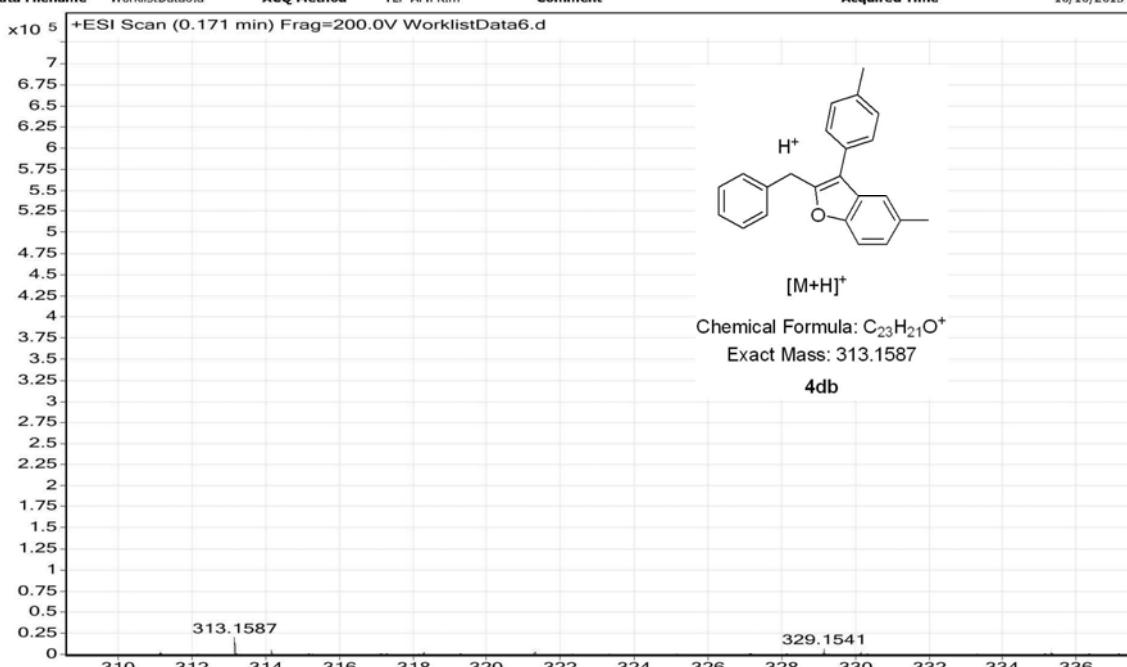




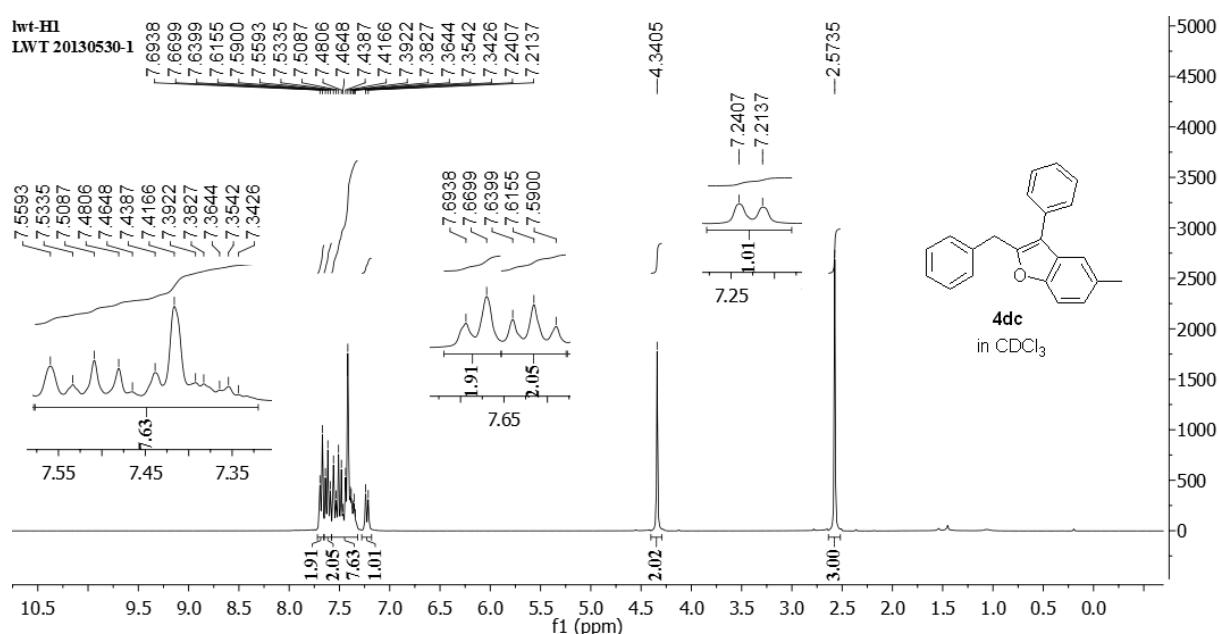
## 2-benzyl-5-methyl-3-(*p*-tolyl)benzofuran (4db)



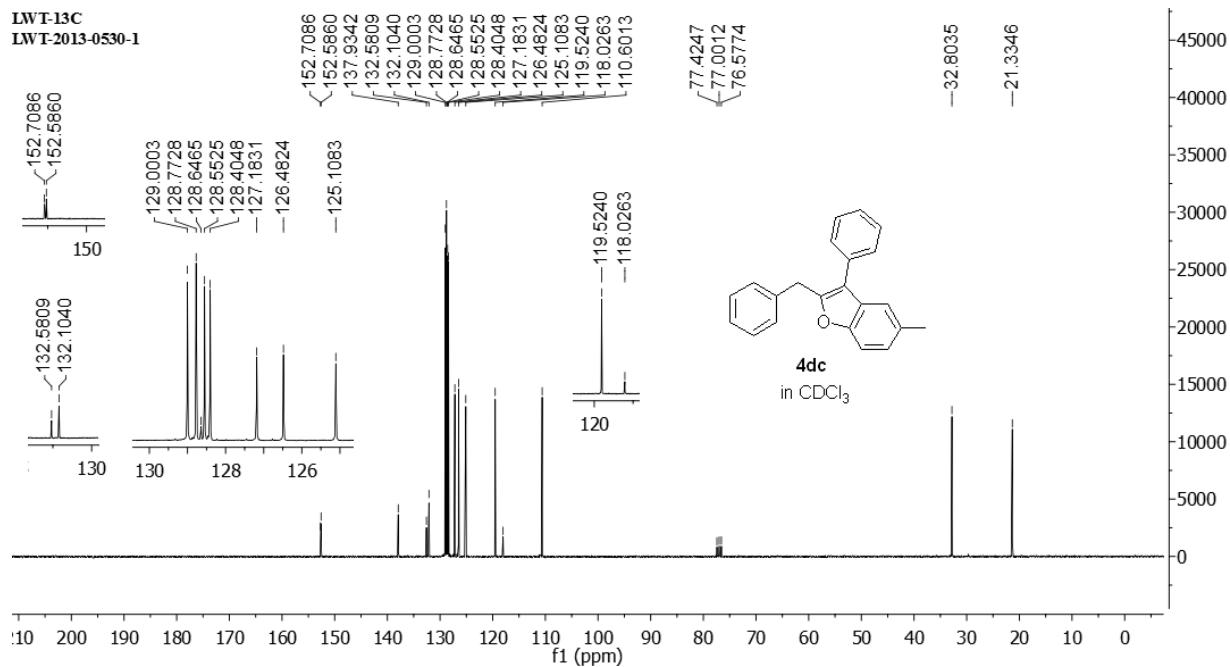
Sample Name	LWT-6	Position	P1-A6	Instrument Name	Instrument 1	User Name
Inj Vol	10	InjPosition		SampleType		IRM Calibration Status
Data Filename	WorklistData6.d	ACQ Method	YLF-AMPK.m	Comment	Sample	Acquired Time



## 2-benzyl-5-methyl-3-phenylbenzofuran (4dc)

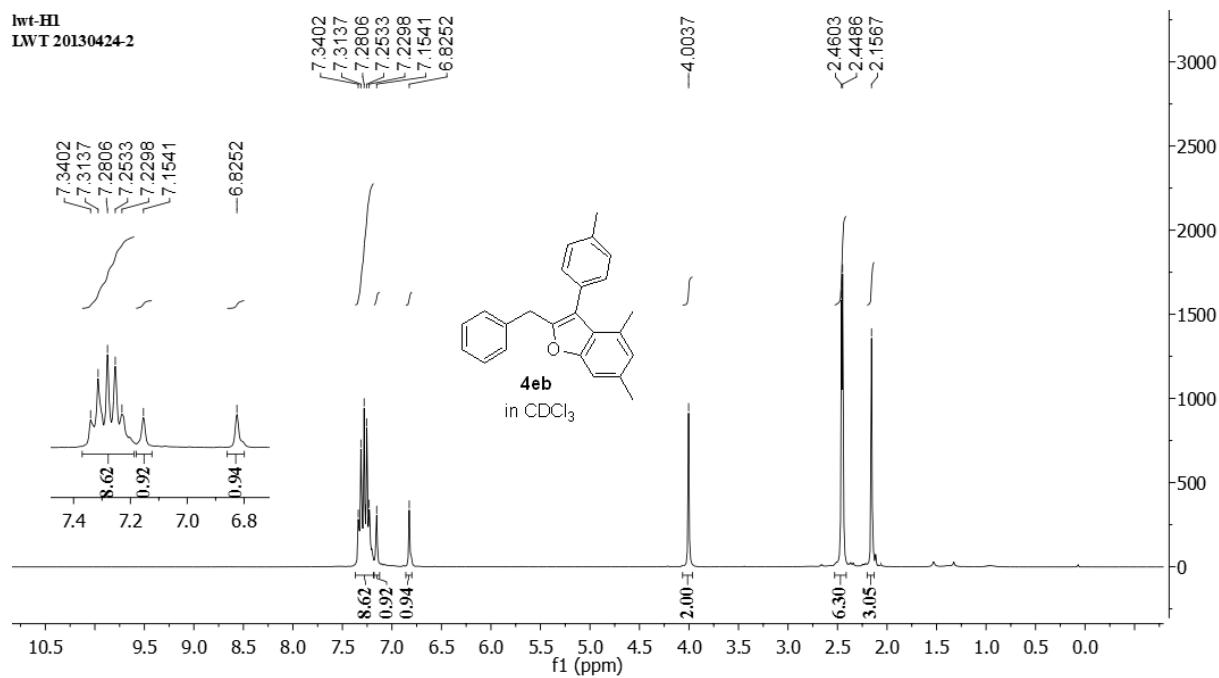


LWT-13C  
LWT-2013-0530-1

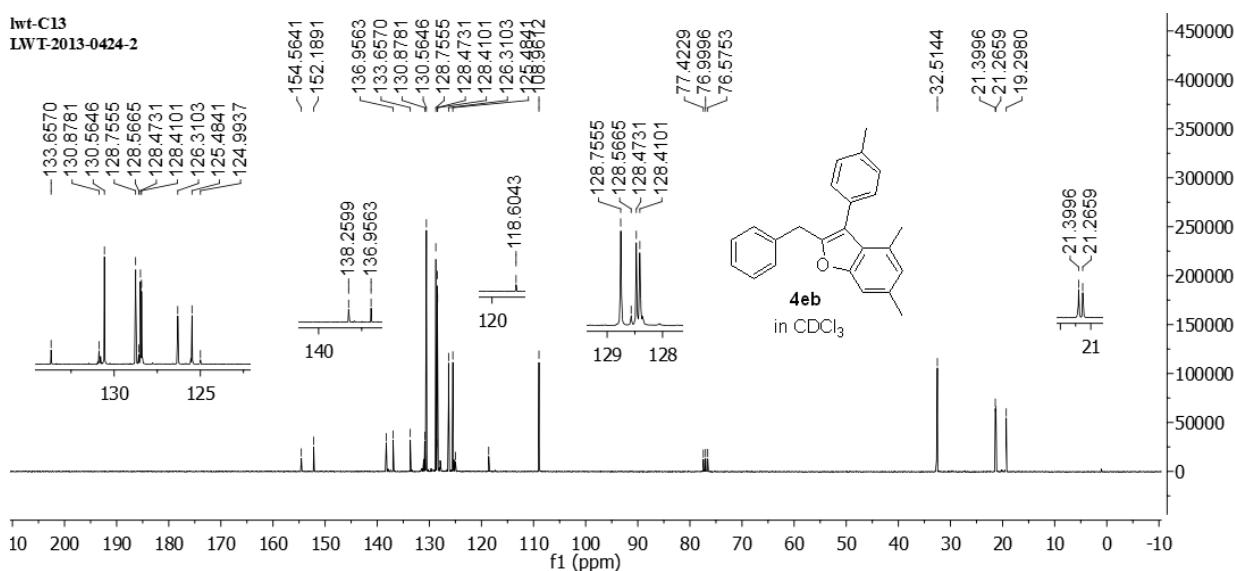


## 2-benzyl-4,6-dimethyl-3-(*p*-tolyl)benzofuran (**4eb**)

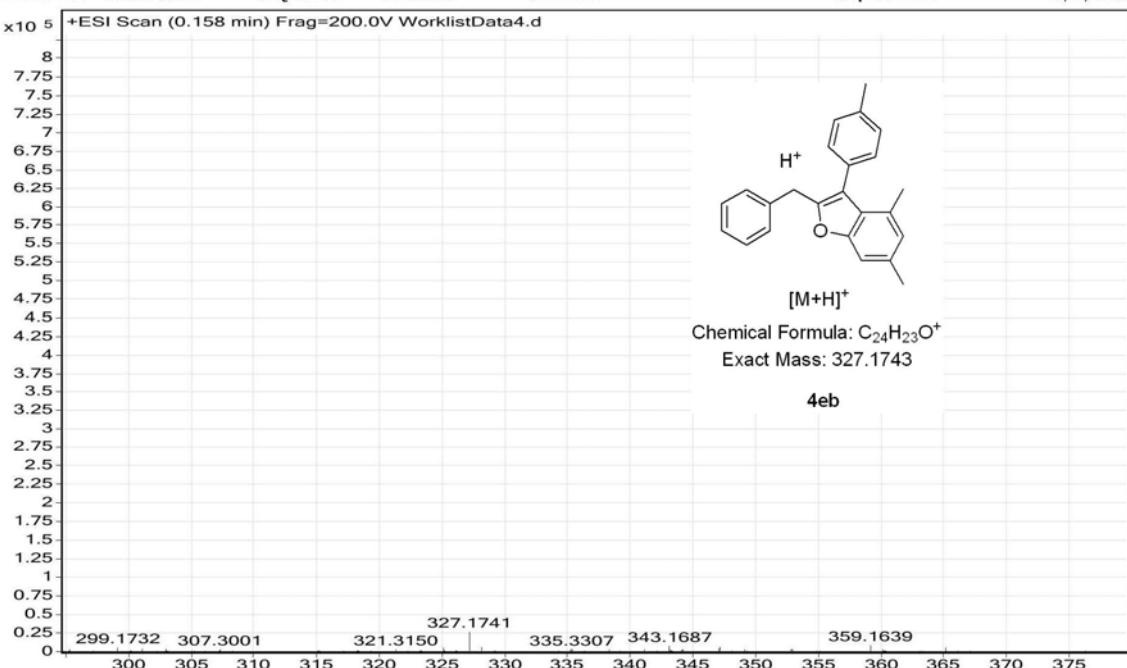
lwt-H1  
LWT 20130424-2



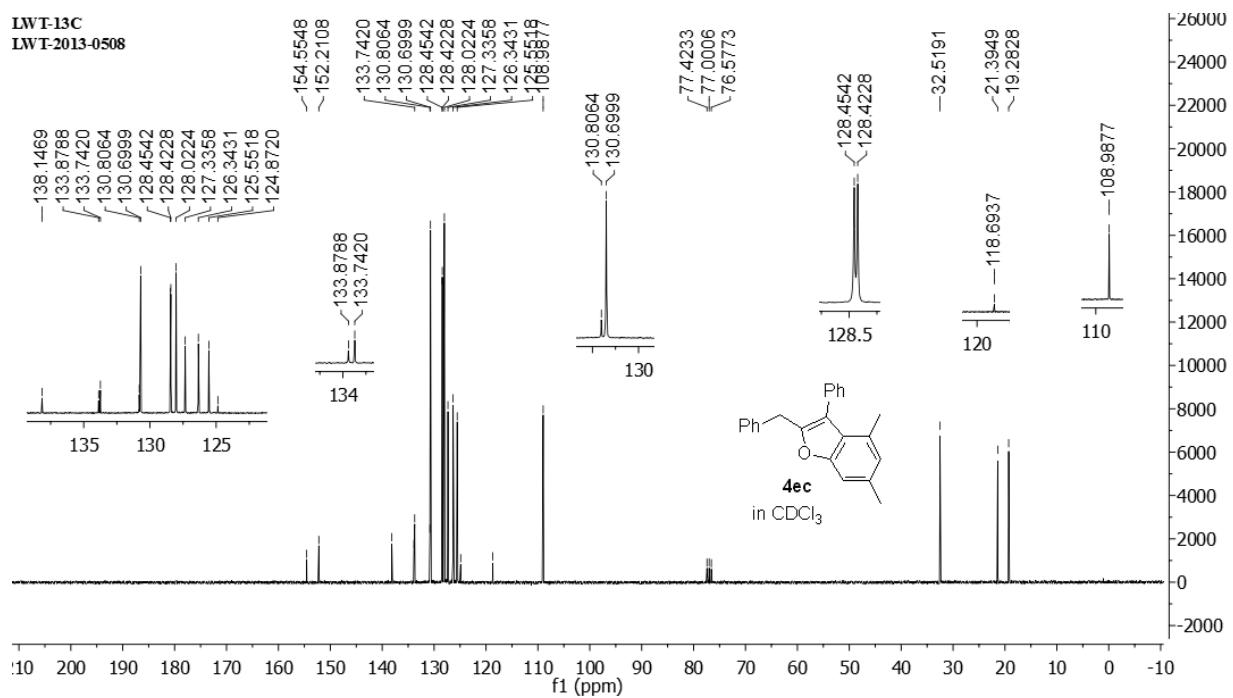
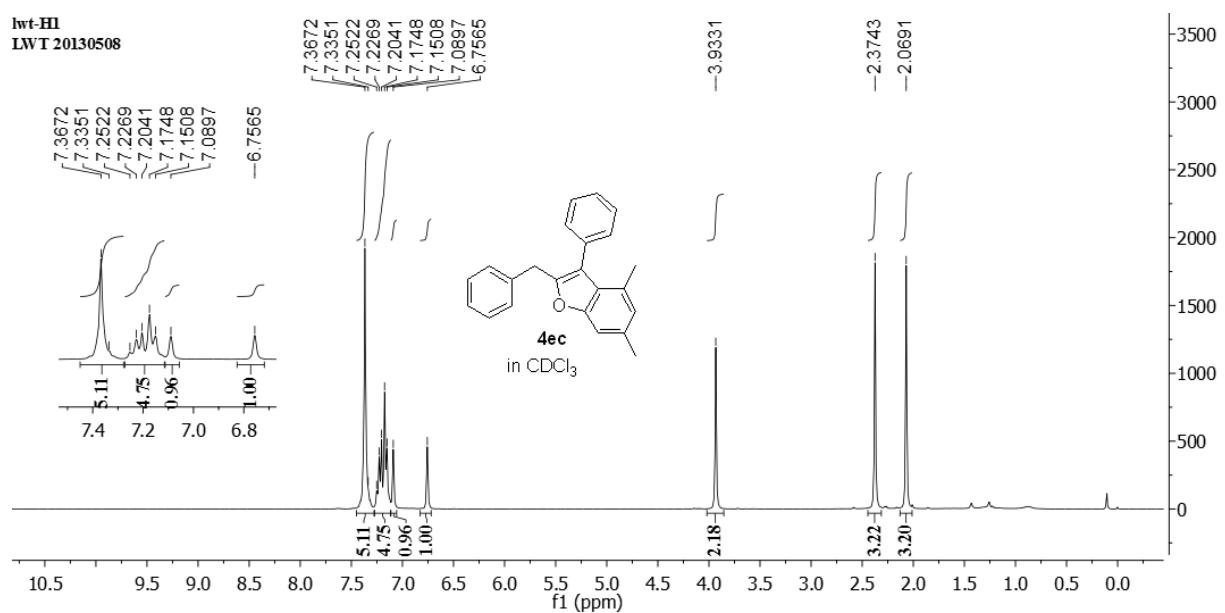
lwt-C13  
LWT-2013-0424-2

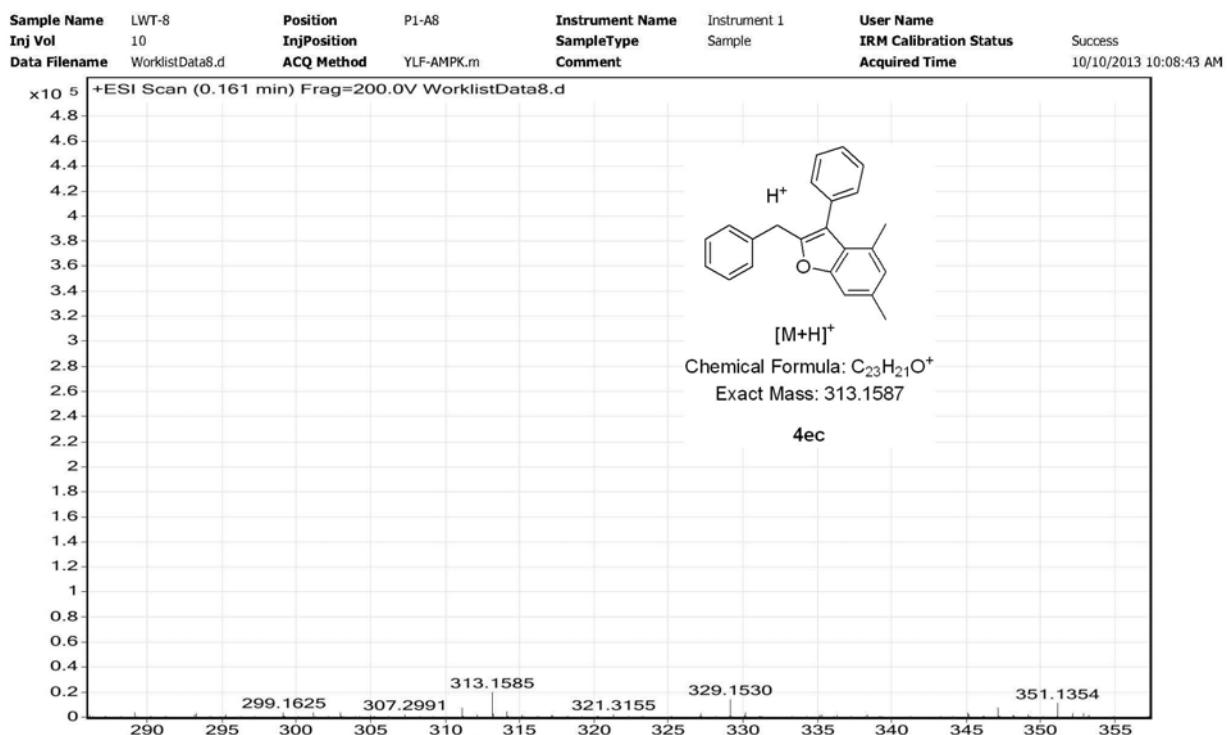


Sample Name	LWT-4	Position	P1-A4	Instrument Name	Instrument 1	User Name
Inj Vol	10	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename	WorklistData4.d	ACQ Method	YLF-AMPK.m	Comment		Acquired Time

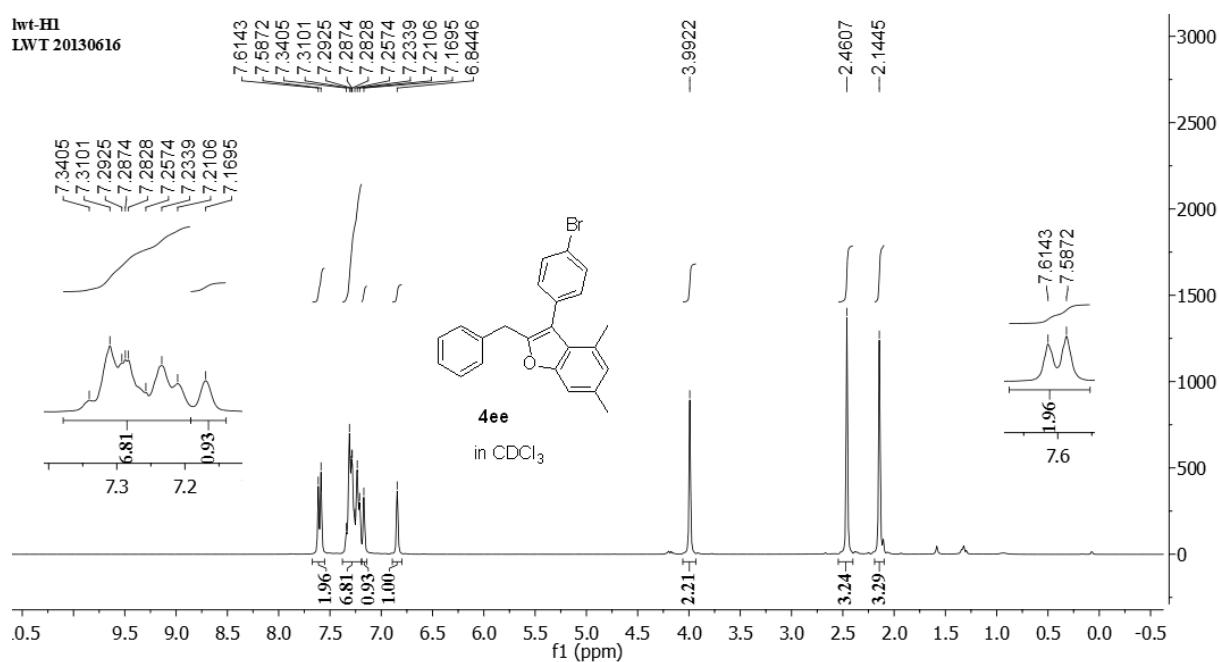


## 2-benzyl-4,6-dimethyl-3-phenylbenzofuran (4ec)

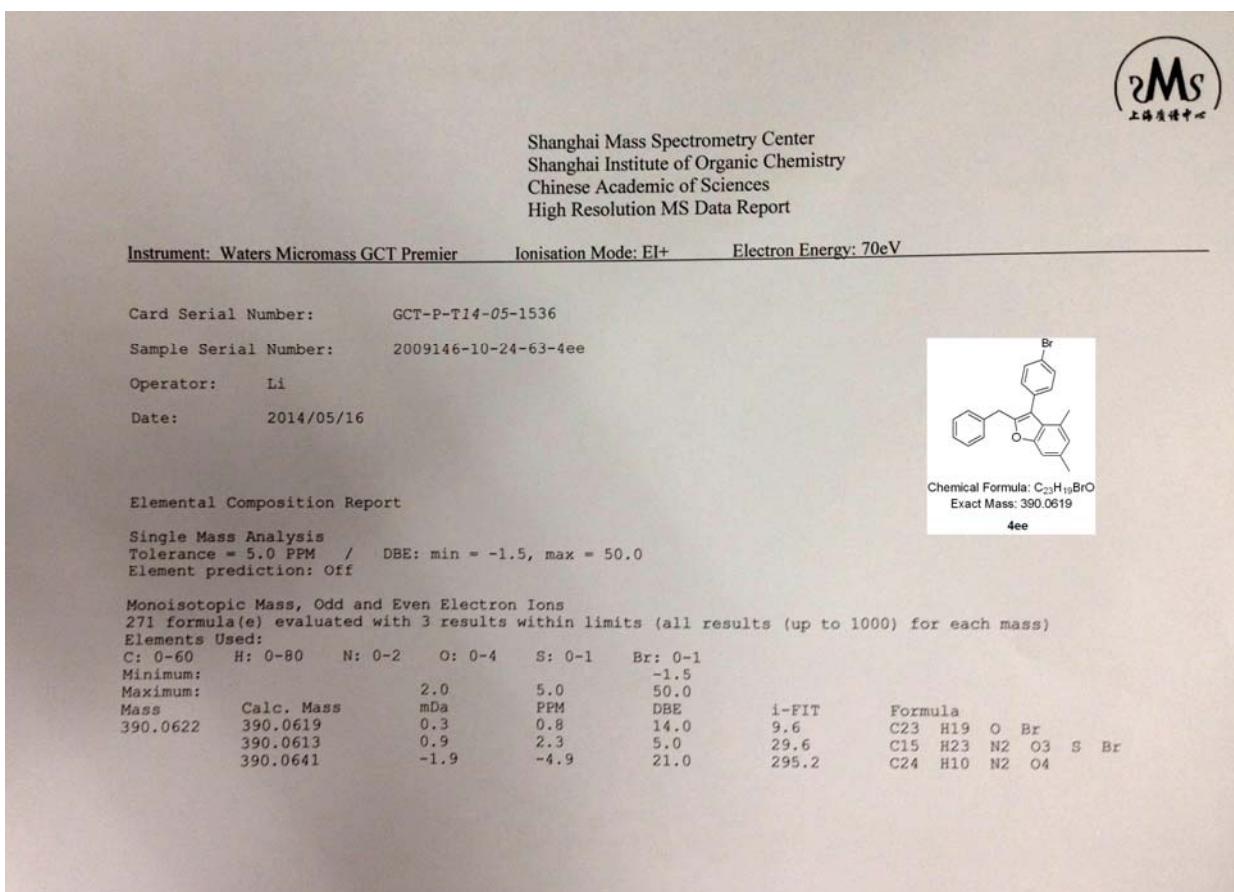
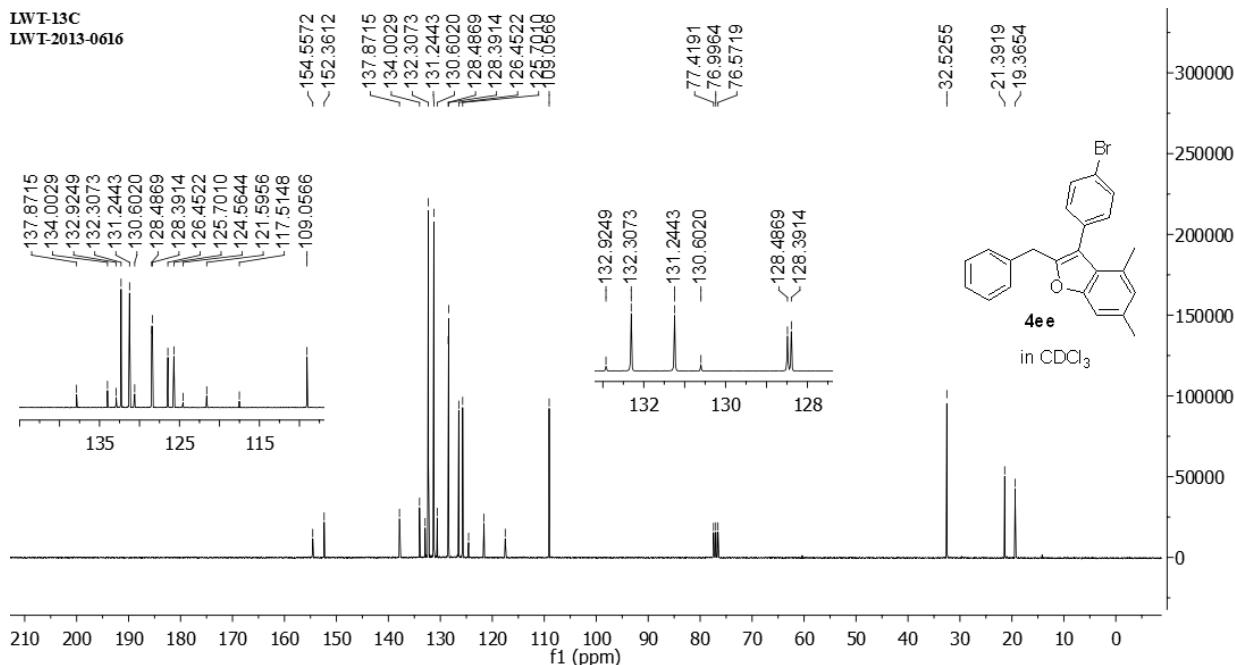




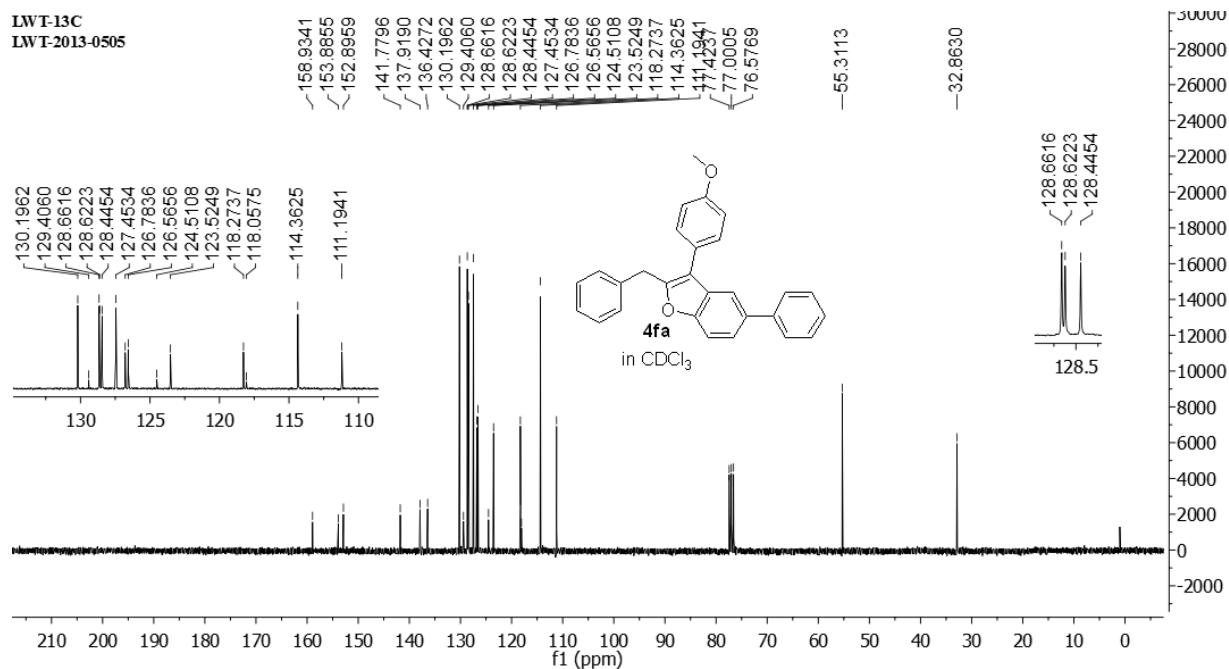
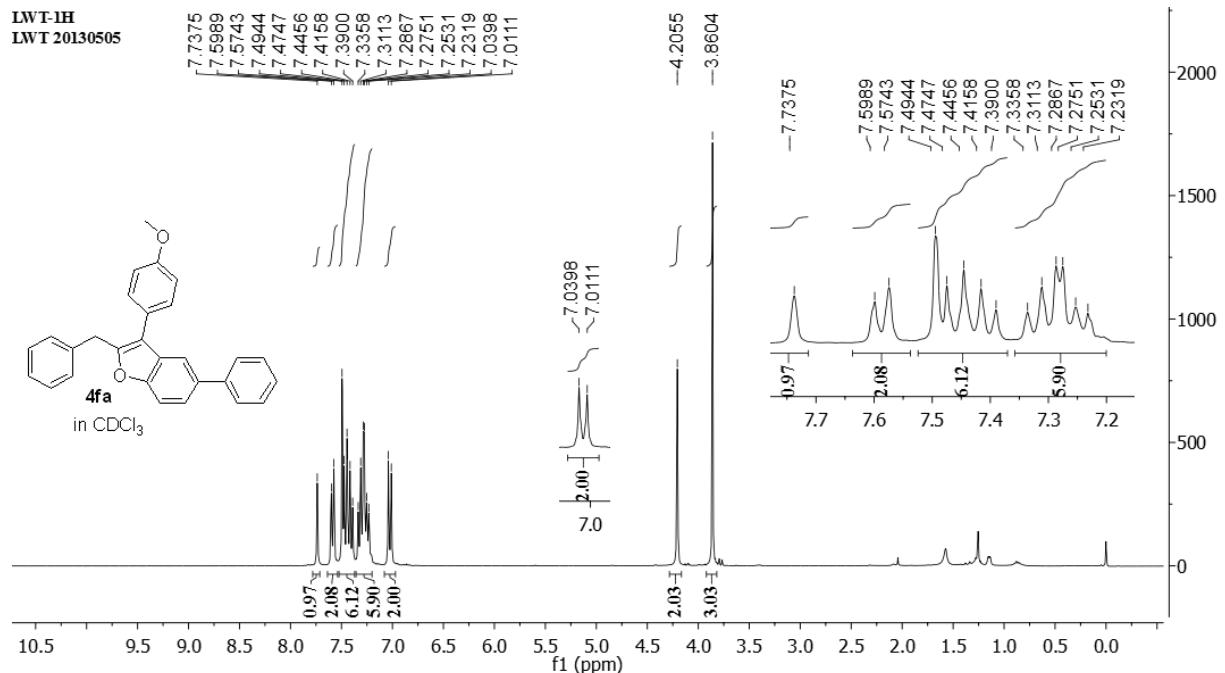
## 2-benzyl-3-(4-bromophenyl)-4,6-dimethylbenzofuran (4ee)

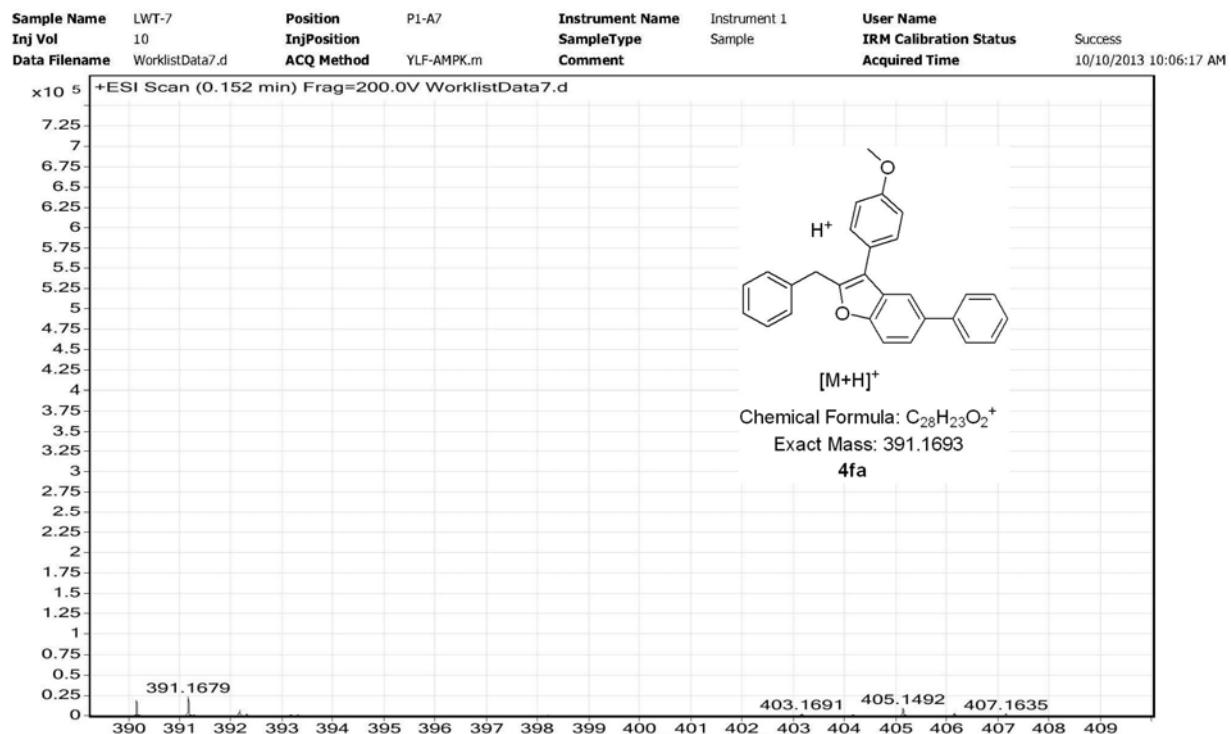


LWT-13C  
LWT-2013-0616

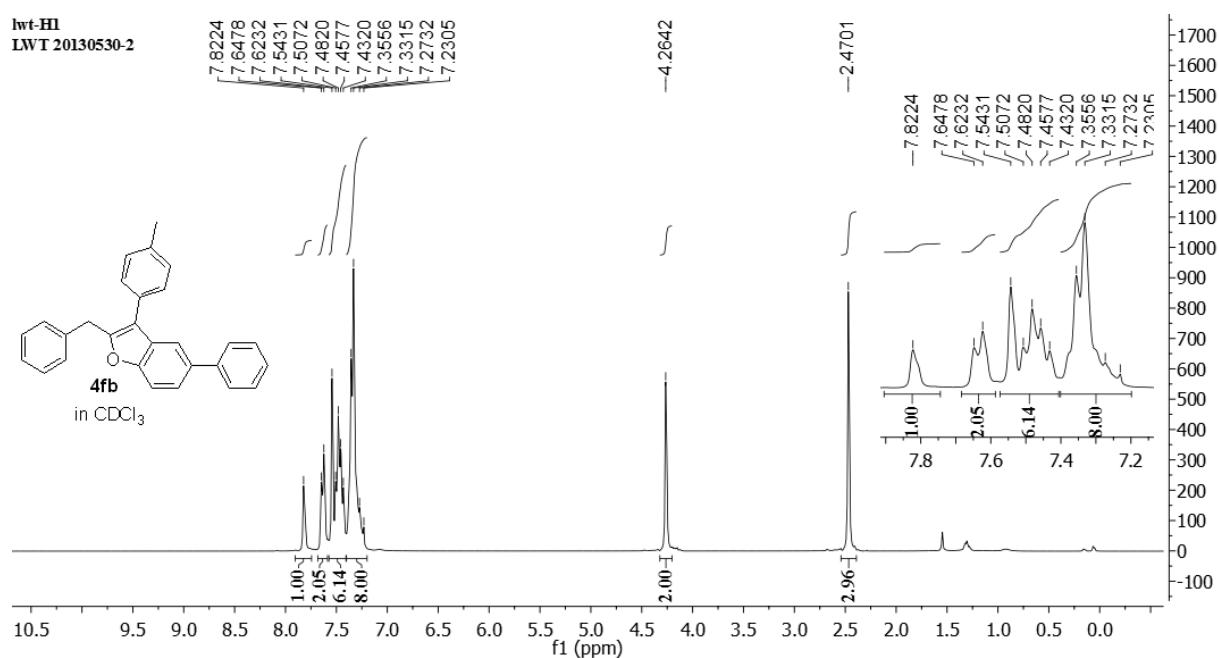


## 2-benzyl-3-(4-methoxyphenyl)-5-phenylbenzofuran (4fa)

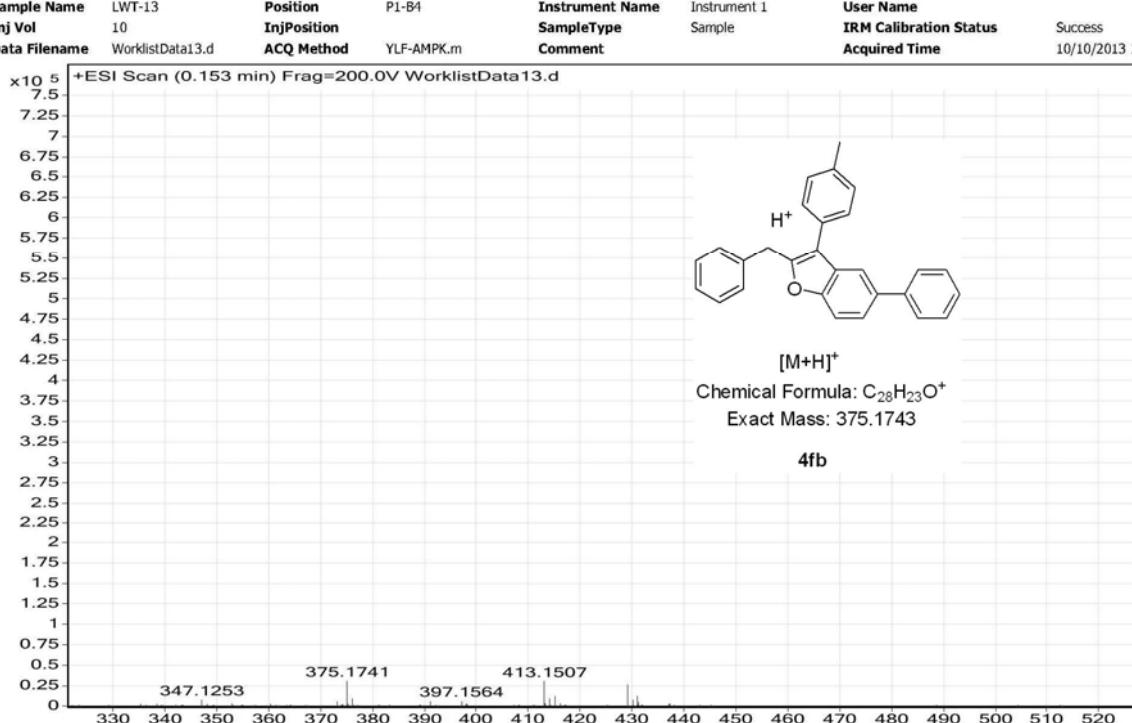
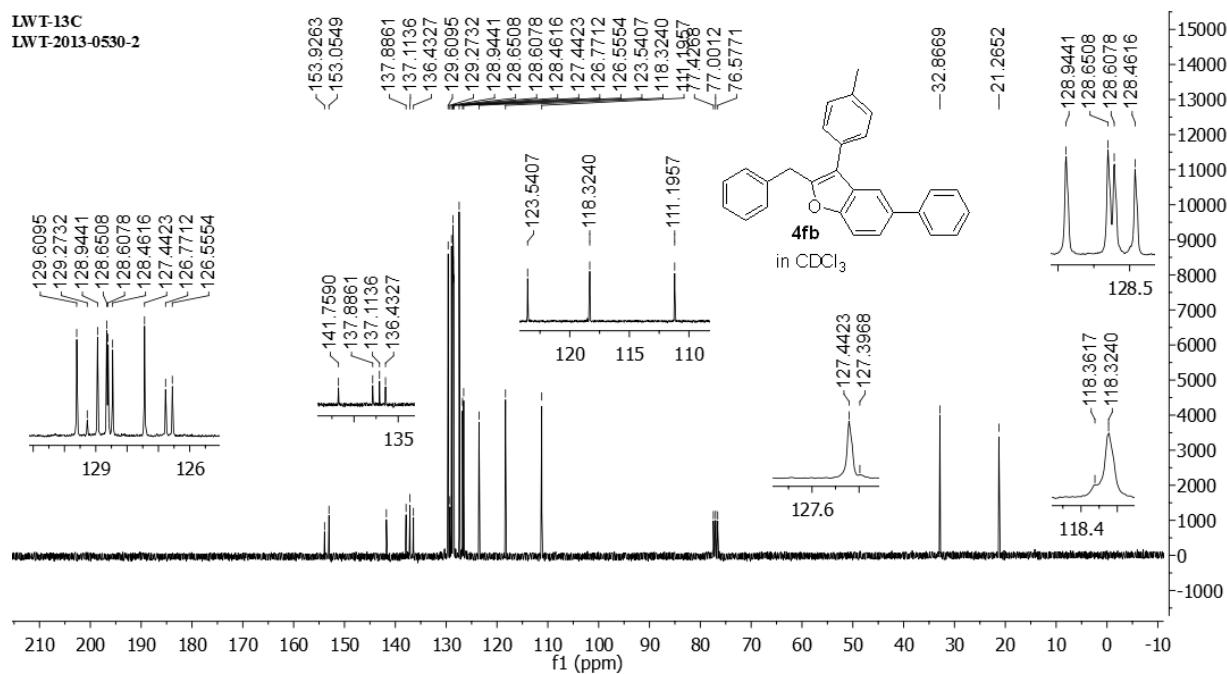




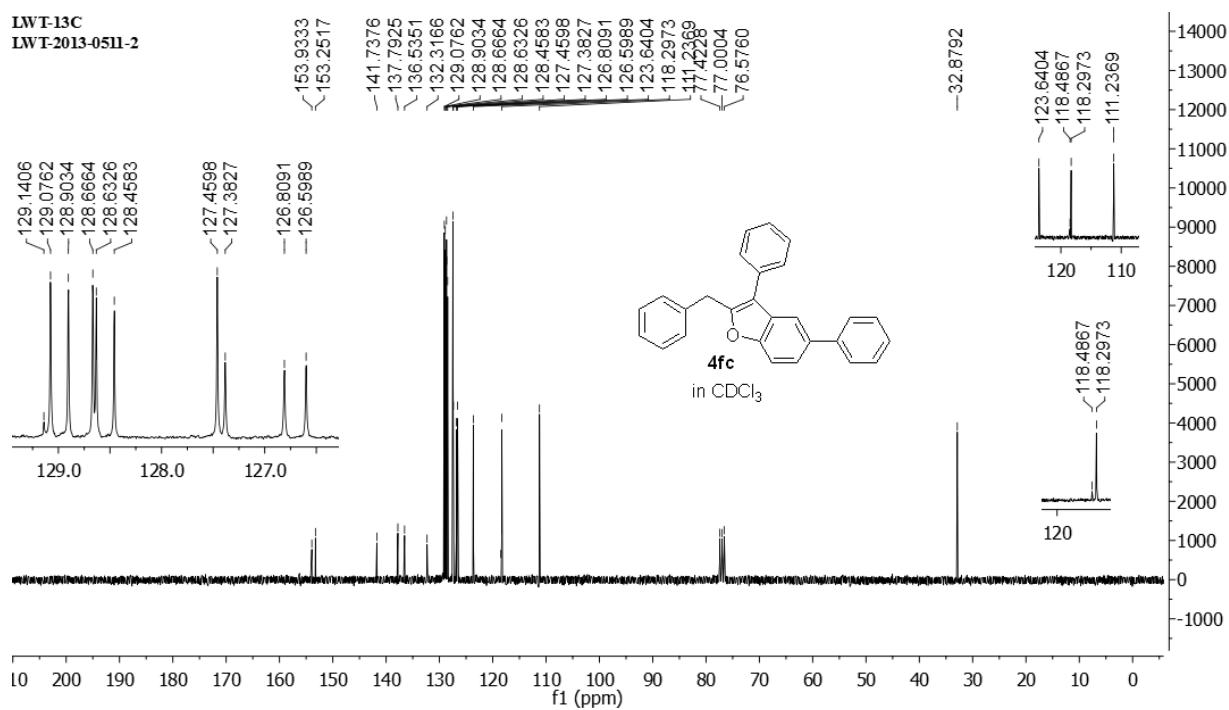
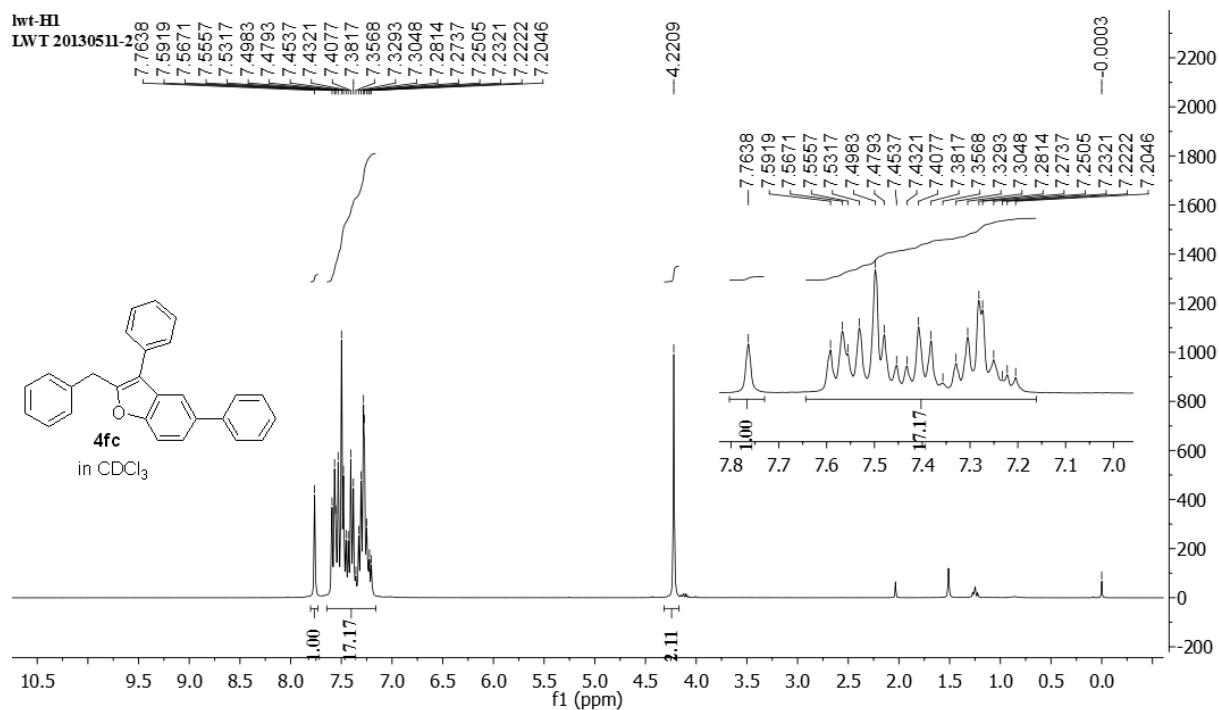
### 2-benzyl-5-phenyl-3-(*p*-tolyl)benzofuran (4fb)



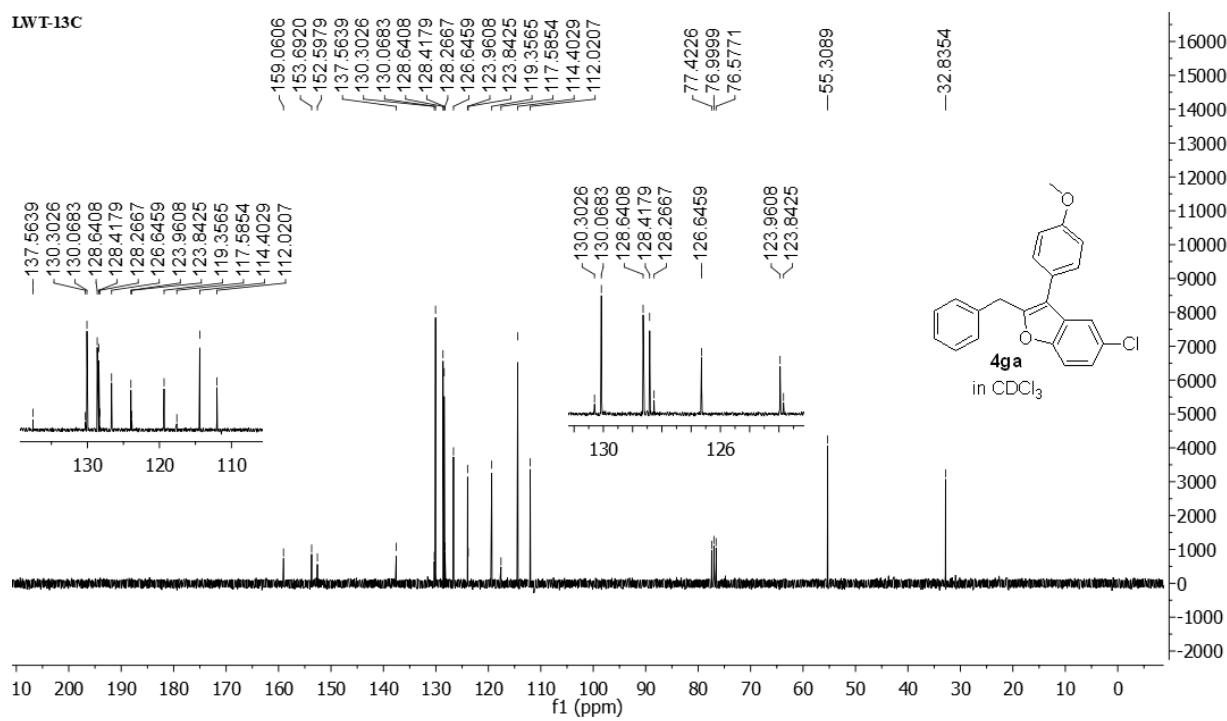
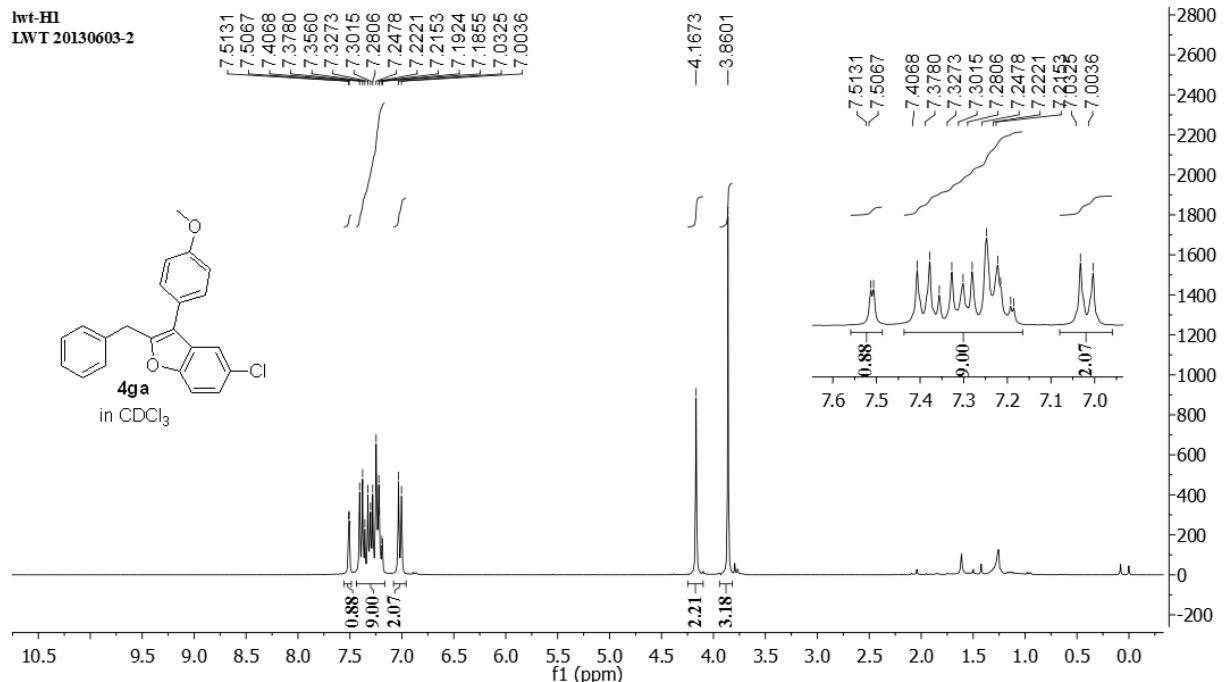
LWT-13C  
LWT-2013-0530-2



## 2-benzyl-3,5-diphenylbenzofuran (4fc)



## 2-benzyl-5-chloro-3-(4-methoxyphenyl)benzofuran (4ga)





Shanghai Mass Spectrometry Center  
Shanghai Institute of Organic Chemistry  
Chinese Academy of Sciences  
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier

Ionisation Mode: EI+

Electron Energy: 70eV

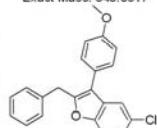
Card Serial Number: GCT-P-T14-05-1537

Sample Serial Number: 2009146-10-24-63-4ga

Operator: Li

Date: 2014/05/16

Chemical Formula: C<sub>22</sub>H<sub>17</sub>ClO<sub>2</sub>  
Exact Mass: 348.0917



Chemical Formula: C<sub>22</sub>H<sub>17</sub>ClO<sub>2</sub>  
Exact Mass: 348.0917  
4ga

#### Elemental Composition Report

##### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

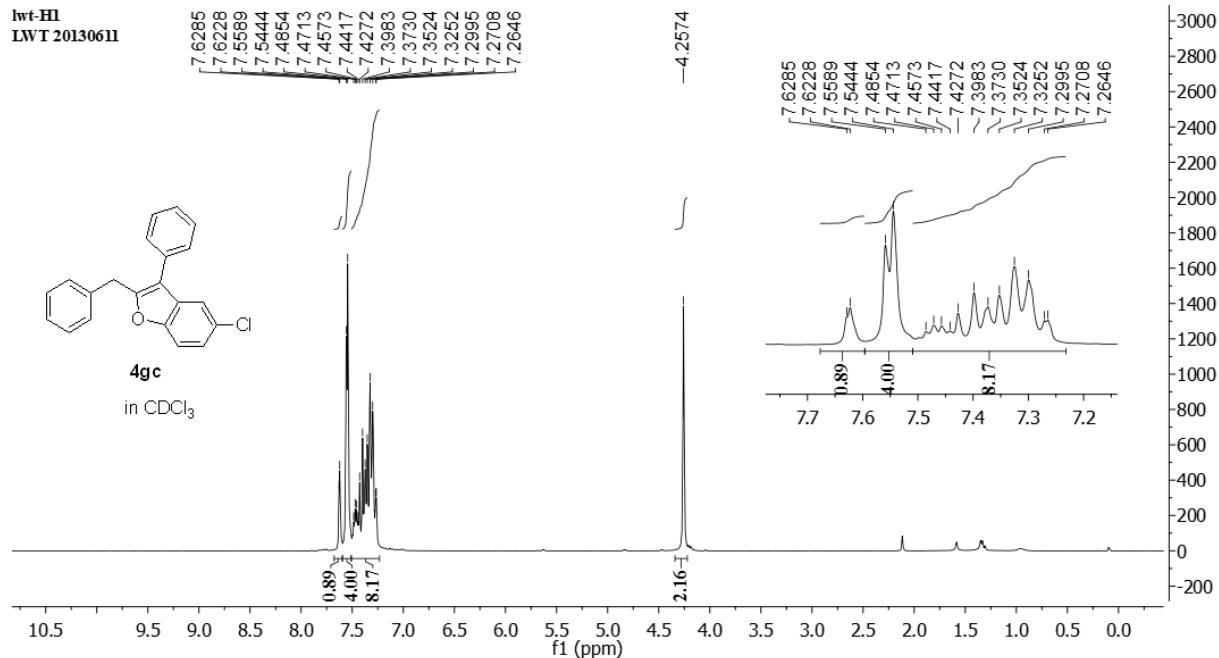
##### Monoisotopic Mass, Odd and Even Electron Ions

449 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

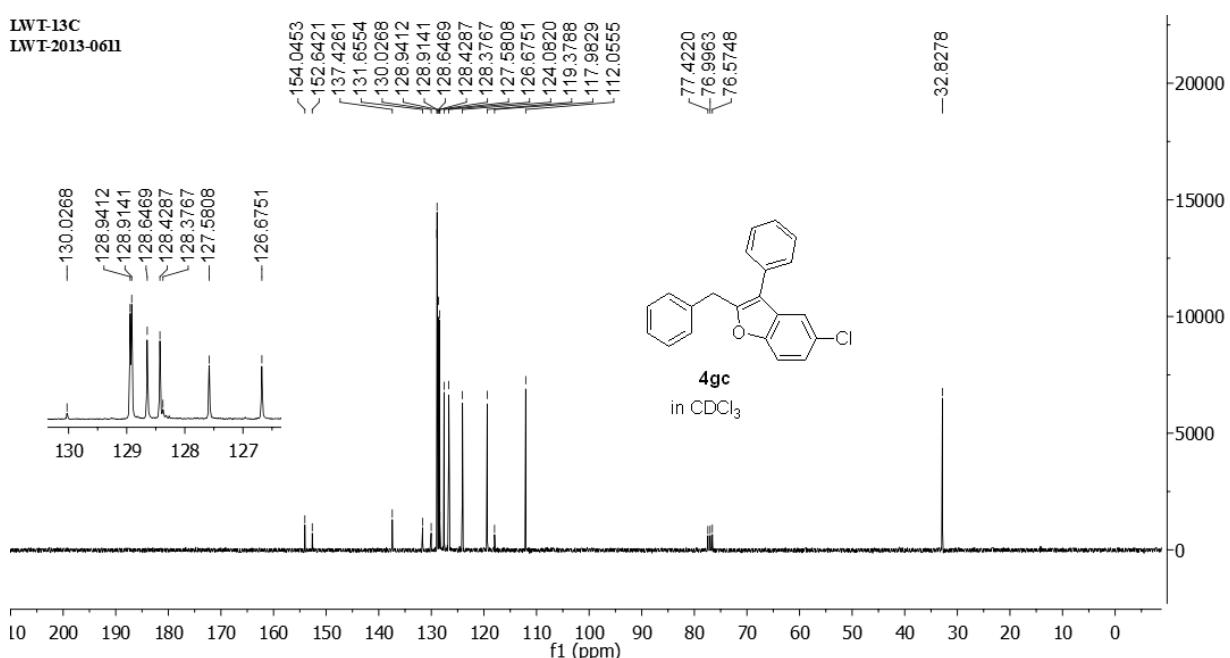
##### Elements Used:

C: 0-60	H: 0-80	N: 0-2	O: 0-4	S: 0-1	Cl: 0-1	Br: 0-1
Minimum:					-1.5	
Maximum:			2.0	5.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
348.0913	348.0911	0.2	0.6	5.0	5.8	C <sub>22</sub> H <sub>17</sub> ClO <sub>2</sub>
	348.0917	-0.4	-1.1	14.0	3.7	C <sub>22</sub> H <sub>17</sub> O <sub>2</sub> Cl
	348.0899	1.4	4.0	19.0	3.4	C <sub>23</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>

## 2-benzyl-5-chloro-3-phenylbenzofuran (4gc)

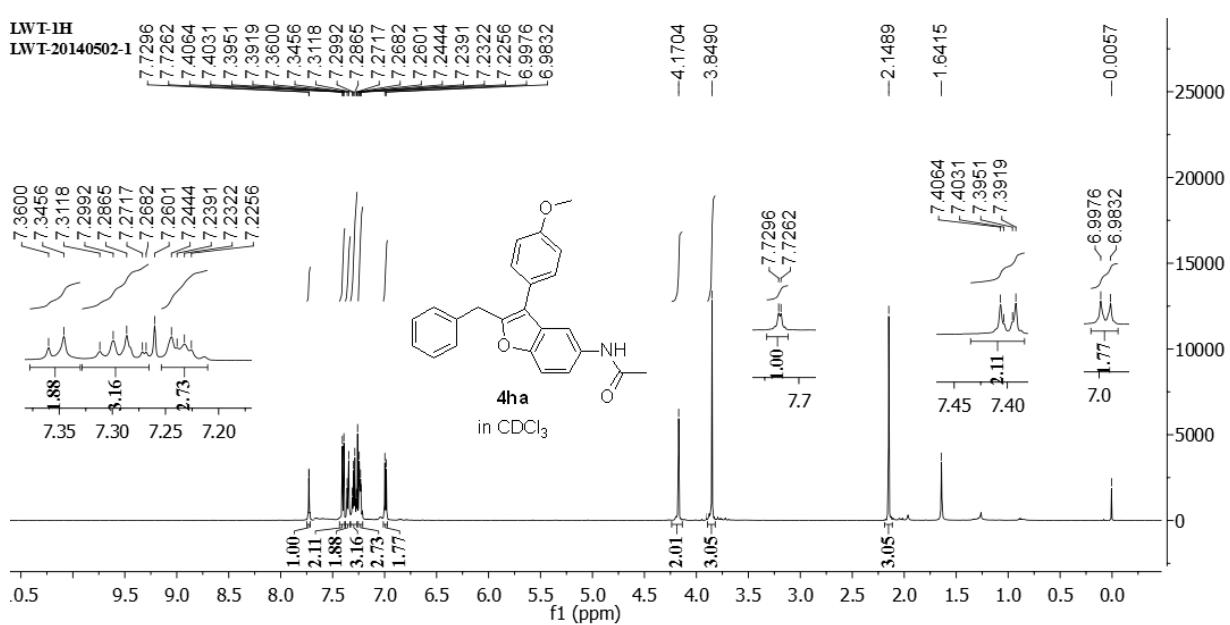


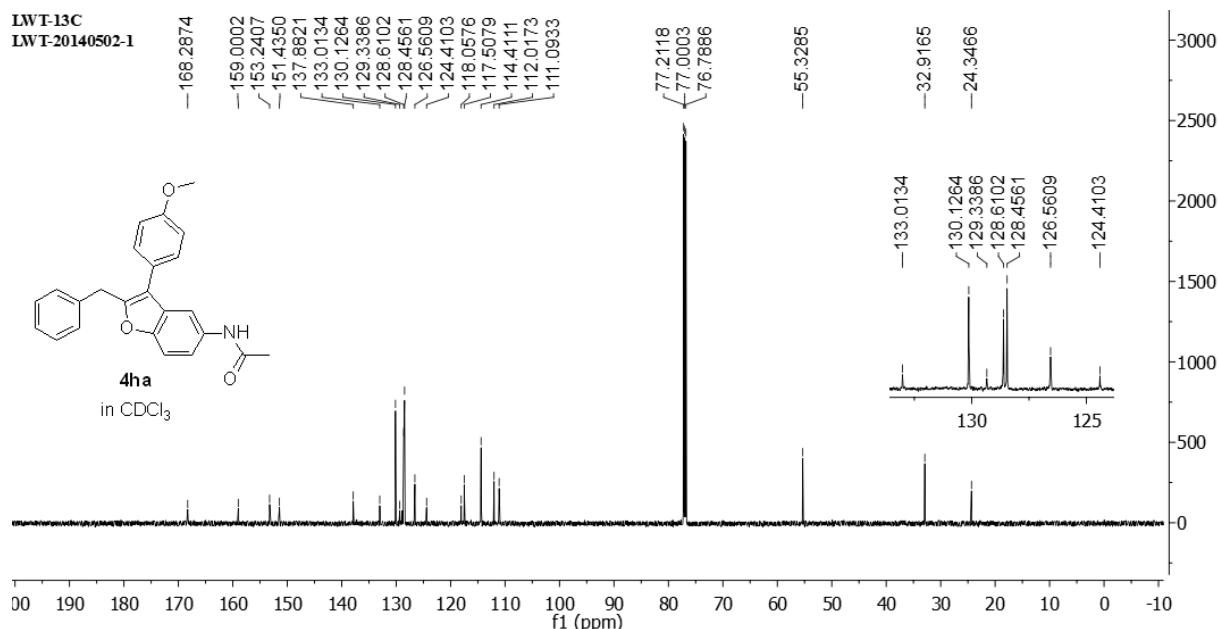
LWT-13C  
LWT-2013-0611



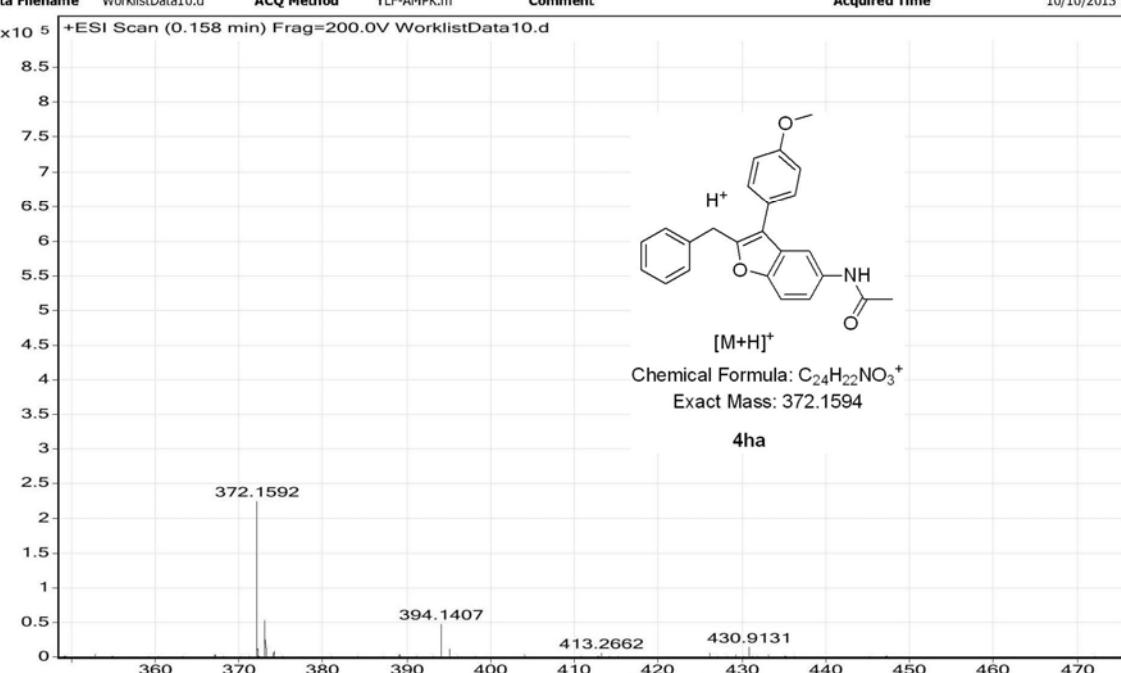
#### ***N*-(2-benzyl-3-(4-methoxyphenyl)benzofuran-5-yl)acetamide (4ha)**

LWT-1H  
LWT-201

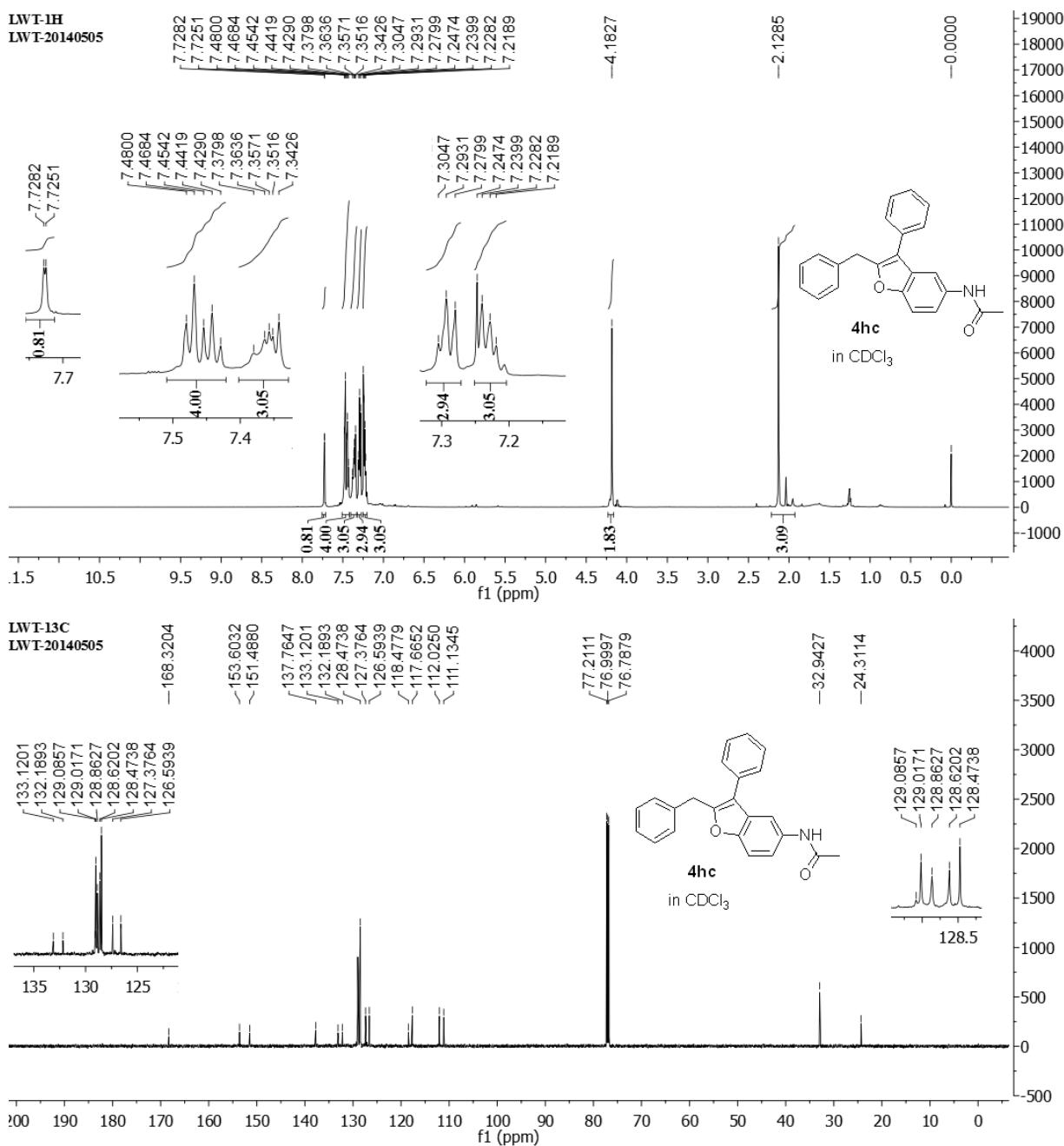


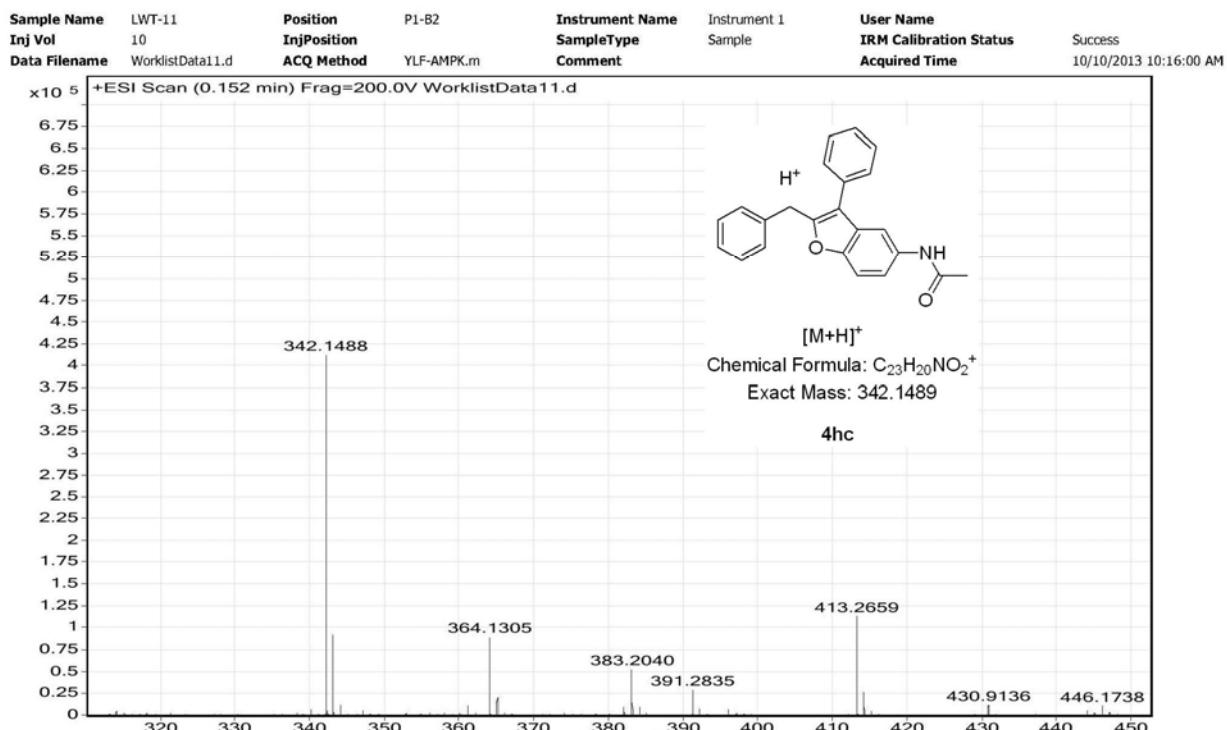


Sample Name	LWT-10	Position	P1-B1	Instrument Name	Instrument 1	User Name	
Inj Vol	10	InjPosition		SampleType	Sample	IRM Calibration Status	
Data Filename	WorklistData10.d	ACQ Method	YLF-AMPK.m	Comment		Acquired Time	Success
							10/10/2013 10:13:34 AM

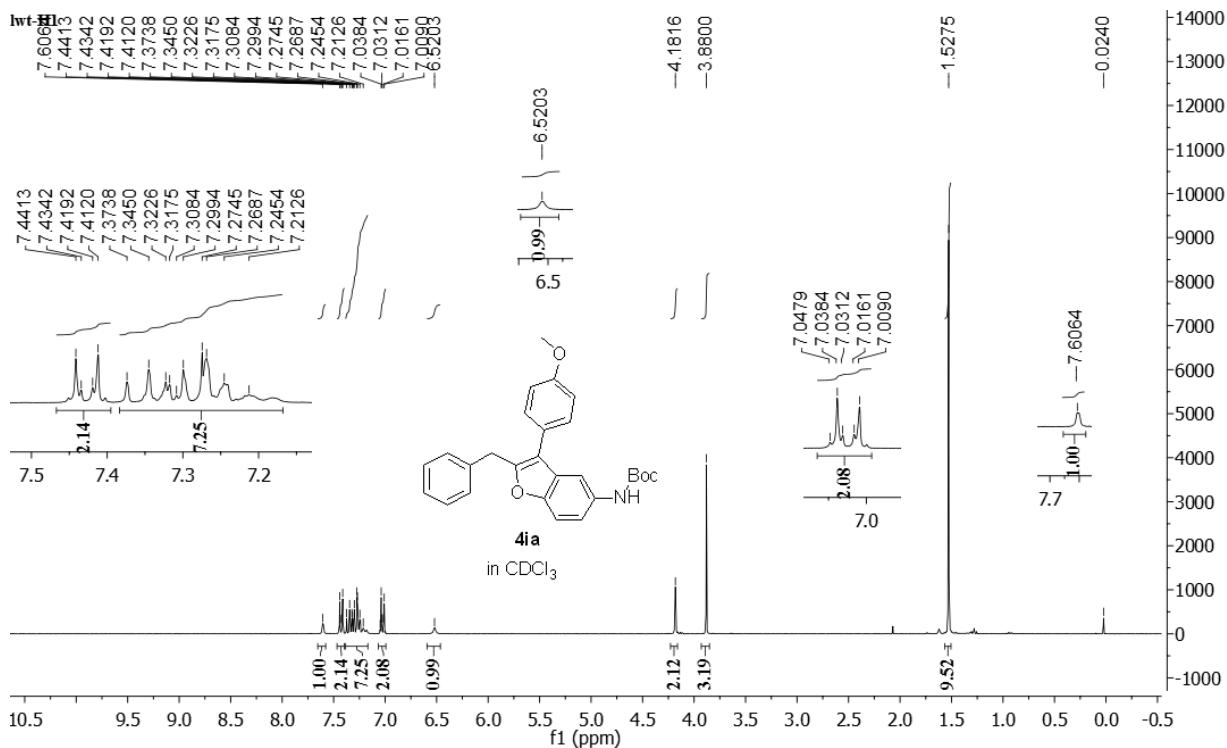


## N-(2-benzyl-3-phenylbenzofuran-5-yl)acetamide (4hc)

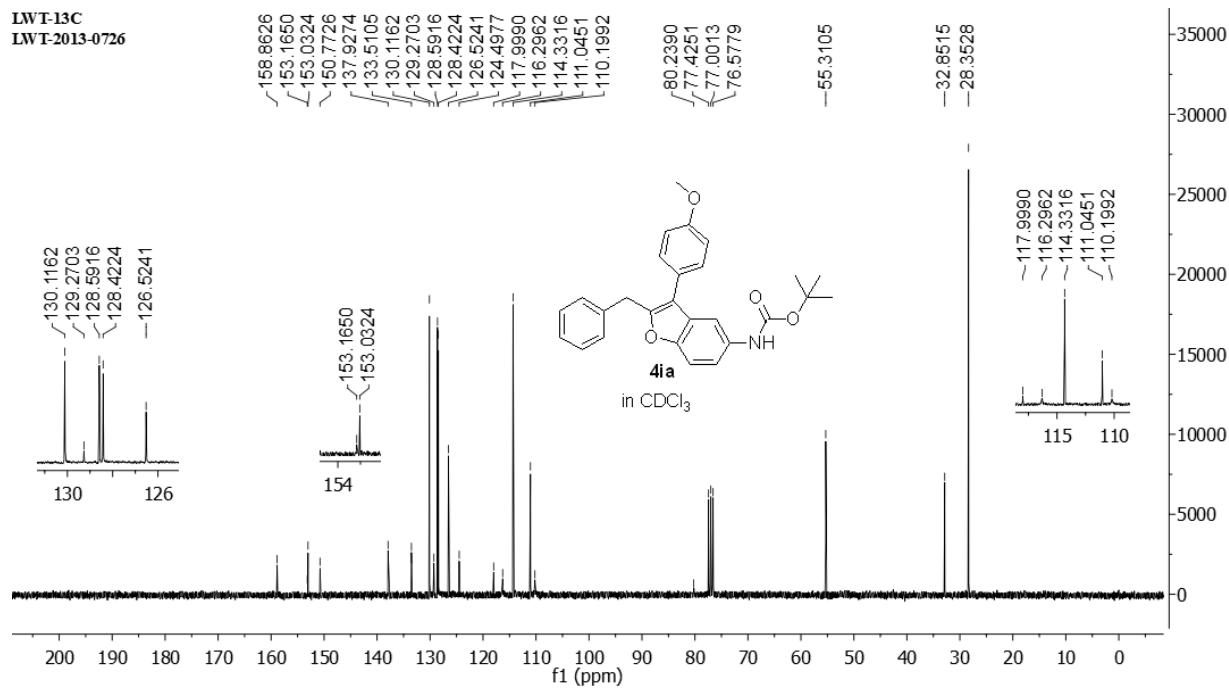




## **tert-butyl (2-benzyl-3-(4-methoxyphenyl)benzofuran-5-yl)carbamate (4ia)**



LWT-13C  
LWT-2013-0726



Shanghai Mass Spectrometry Center  
Shanghai Institute of Organic Chemistry  
Chinese Academy of Sciences  
High Resolution MS Data Report



Instrument



Bruker Daltonics, Inc. APEXIII 7.0 TESLA FTMS

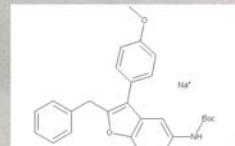
Card Serial Number E140741

Analysis Name D:\Data\zfj\2014\20140513\_000012.d

Sample Name 2009146-10-24-63-4IA

Acquisition Date 5/11/2014 1:53:10 PM

Operator: zfj



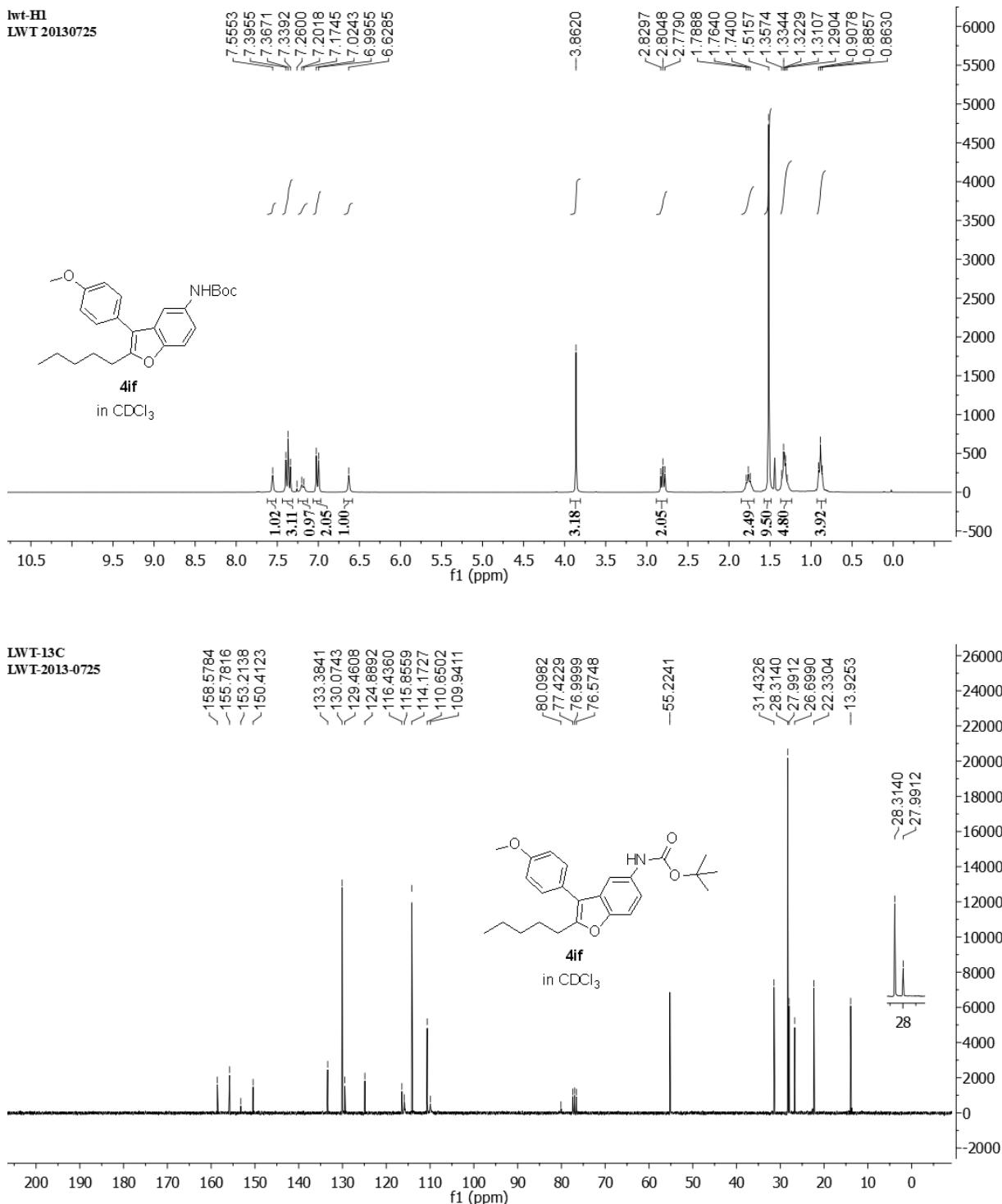
Ionization Mode ESI-Positive

4ia

Ion Mass (Measured) 452.1840

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e <sup>-</sup>
C 27 H 27 N 1 Na 1 O 4	0.006	452.1832	-1.64	-2.06	-0.74	14.50	ok	even
C 26 H 28 O 7	0.010	452.1830	-2.25	-2.63	-1.02	13.00	ok	odd
C 29 H 26 N 1 O 4	0.012	452.1856	3.67	3.22	1.66	17.50	ok	even
C 30 H 25 N 2 Na 1 O 1	0.019	452.1859	4.28	3.79	1.94	19.00	ok	odd
C 21 H 30 N 3 O 6 S 1	0.029	452.1850	2.23	1.10	1.01	8.50	ok	even
C 21 H 33 Na 1 O 7 S 1	0.034	452.1839	-0.12	-1.08	-0.05	5.00	ok	odd

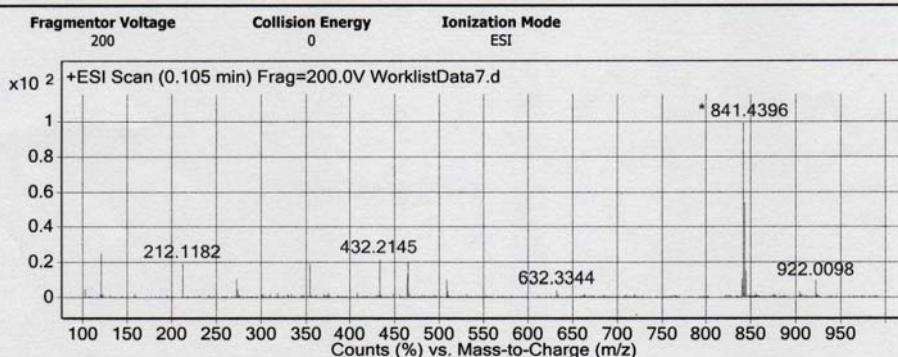
**tert-butyl (3-(4-methoxyphenyl)-2-pentylbenzofuran-5-yl)carbamate  
(4if)**



## Qualitative Analysis Report

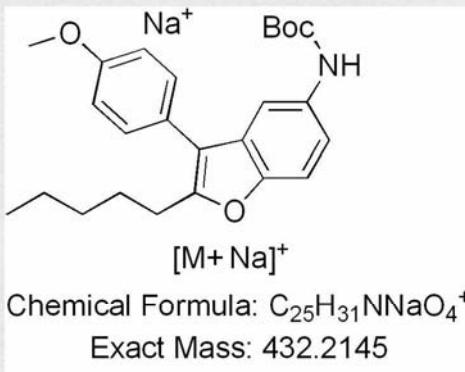
Data Filename	WorklistData7.d	Sample Name	NC
Sample Type	Sample	Position	P1-A7
Instrument Name	Instrument 1	User Name	
Acq Method		Acquired Time	1/29/2013 1:06:41 PM
IRM Calibration Status	Success	DA Method	test-1.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.00 (B5042.2)		

### User Spectra



### Peak List

m/z	z	Abund
121.0509	1	375985.77
212.1182	1	286070.17
273.0513	1	165855.94
354.1699	1	286933.21
432.2145	1	335504.08
464.204	1	301068.62
839.4236	1	154811.95
841.4396	1	1476907.22
842.4427	1	800336.08
843.445	1	225525.79



4if

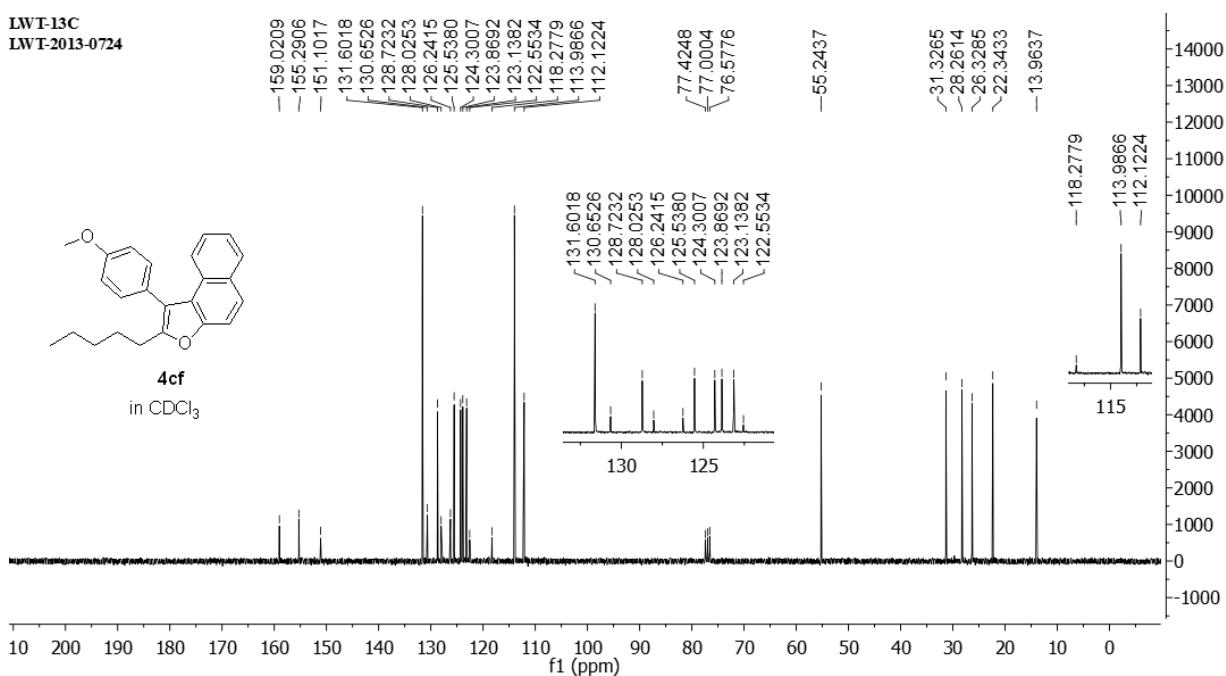
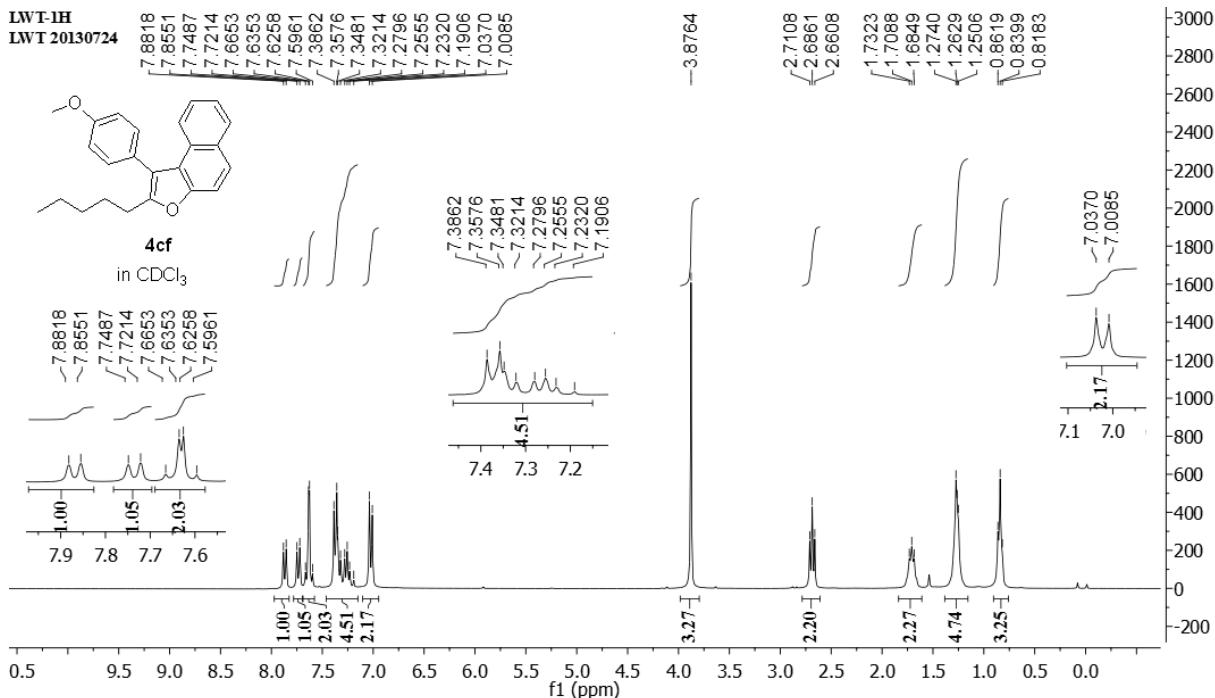


Agilent Technologies

Page 1 of 1

Printed at: 3:22 PM on: 1/29/2013

### 1-(4-methoxyphenyl)-2-pentylnaphtho[2,1-*b*]furan (4cf)



Sample Name	LWT-18	Position	P1-B9	Instrument Name	Instrument 1	User Name	
Inj Vol	10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	WorklistData18.d	ACQ Method	YLF-AMPK.m	Comment		Acquired Time	10/10/2013 10:33:00 AM

